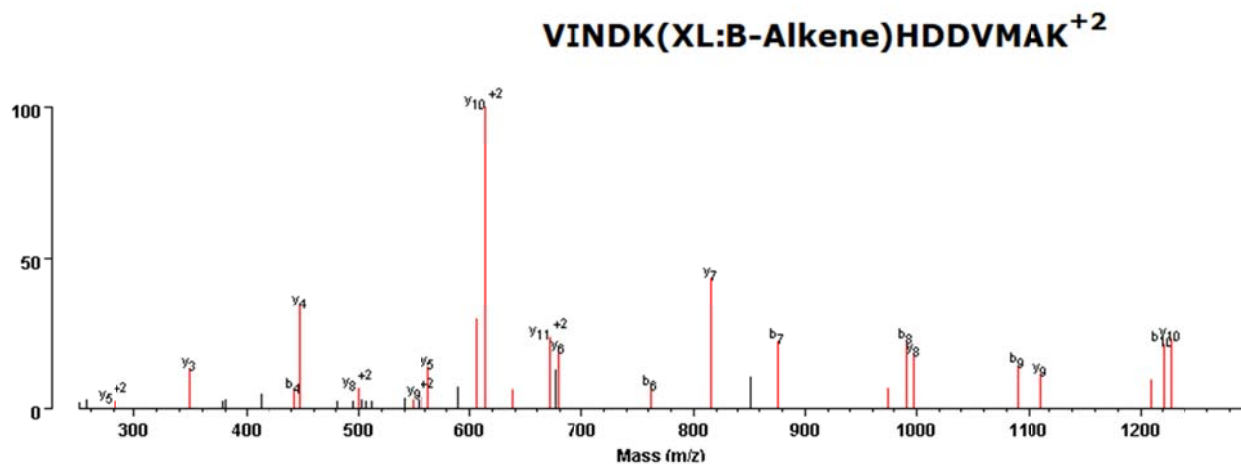


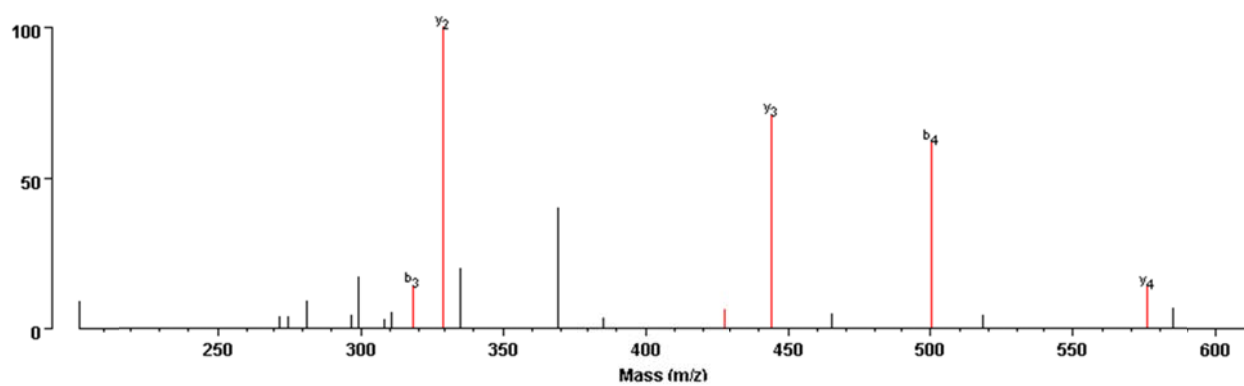
Supplemental Figure 8. MS3 Spectra of Identified Inter-linked Peptides Summarized in Supplemental Table 4.

m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
571.7661	4	719.858	2	VINDKHDDVMAK	646.323	1	AMDKK



m/z	Ion Type	Error
282.337	y,5,+2	0.19
349.232	y,3,+1	0.042
442.327	b,4,+1	0.097
448.292	y,4,+1	0.033
499.422	y,8,+2	0.18
547.494	y-H ₂ O,9,+2	-0.26
556.831	y,9,+2	0.075
563.125	y,5,+1	-0.16
605.848	b-H ₂ O,5,+1	-0.48
	y-NH ₃ ,10,+2	0.58
613.868	y,10,+2	0.091
637.768	b-H ₂ O,11,+2	-0.027
	b-NH ₃ ,11,+2	-0.52
670.469	y,11,+2	0.15
678.443	y,6,+1	0.13
761.402	b,6,+1	0.0079
815.266	y,7,+1	-0.11
876.468	b,7,+1	0.047
974.523	b-NH ₃ ,8,+1	0.1
991.548	b,8,+1	0.1
997.396	y,8,+1	-0.081
1090.87	b,9,+1	0.35
1112.16	y,9,+1	-0.34
1209.8	y-NH ₃ ,10,+1	0.28
1221.35	b,10,+1	-0.21
1226.71	y,10,+1	0.16

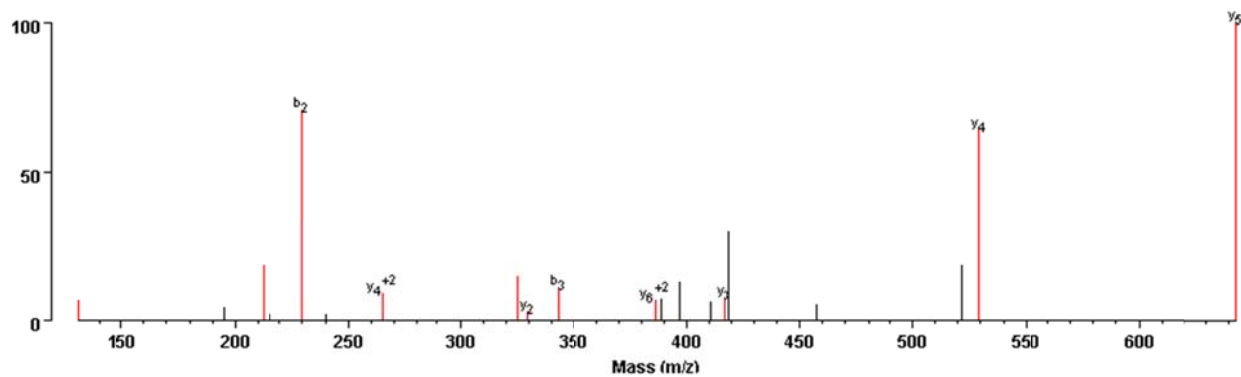
AMDK(XL:B-Alkene)K



m/z	Ion Type	Error
318.184	b ₃ ,+1	0.072
329.245	y ₂ ,+1	0.027
427.475	y-NH ₃ ,3,+1	0.26
444.221	y ₃ ,+1	-0.024
500.13	b ₄ ,+1	-0.087
575.362	y ₄ ,+1	0.076

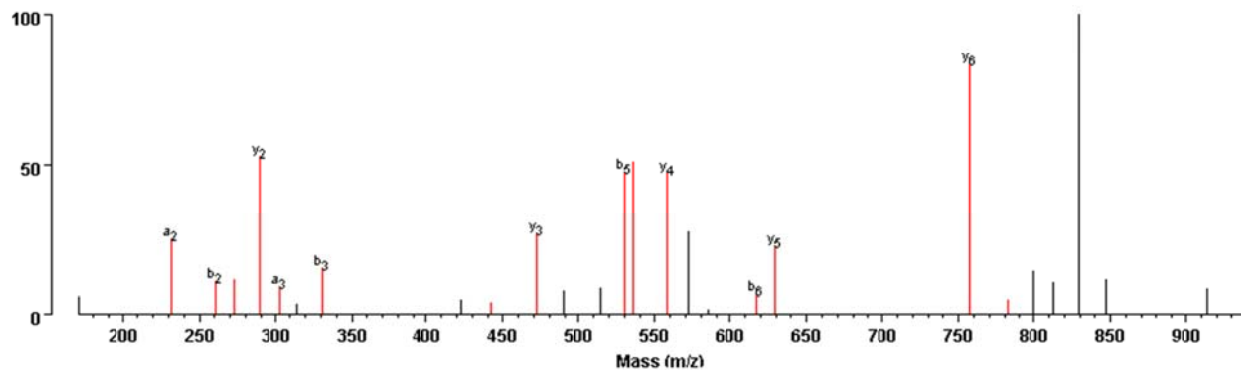
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
540.2740	4	436.266	2	TQIISK	544.271	2	CVAQASKNR

TQIISK(XL:B-Alkene)K⁺²



m/z	Ion Type	Error
130.418	y-NH3,1,+1	0.33
212.538	b-H2O,2,+1	0.44
	b-NH3,2,+1	-0.55
229.967	b,2,+1	-0.15
265.094	y,4,+2	-0.077
324.778	b-H2O,3,+1	-0.41
329.564	y,2,+1	0.35
343.052	b,3,+1	-0.15
386.121	y,6,+2	0.38
416.46	y,3,+1	0.21
529.338	y,4,+1	0.0036
642.615	y,5,+1	0.2

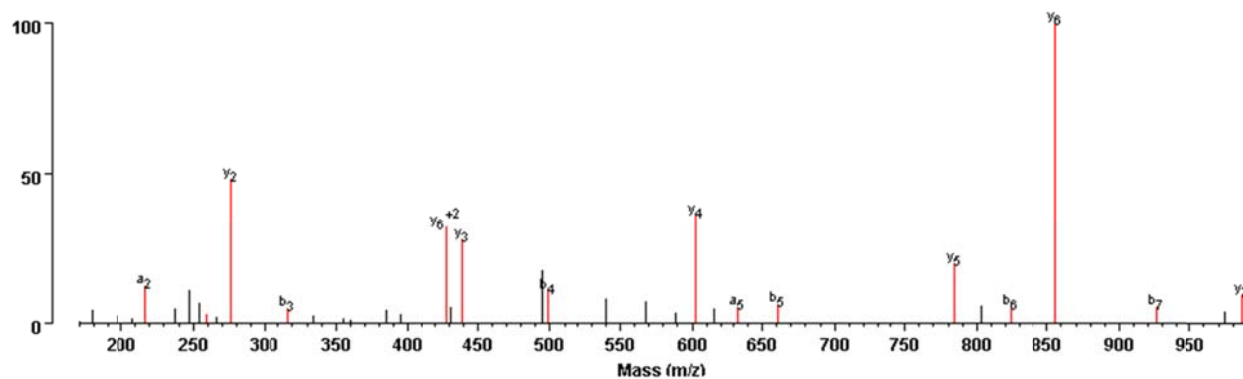
C(Carbamidomethyl)VAQASK(XL:B-Alkene)NR⁺²



m/z	Ion Type	Error
232.082	a ₂ ,+1	-0.029
260.184	b ₂ ,+1	0.078
272.173	y-NH ₃ ,2,+1	0.038
289.229	y ₂ ,+1	0.067
302.946	a ₃ ,+1	-0.2
330.685	b ₃ ,+1	-0.46
441.86	b-NH ₃ ,4,+1	-0.32
471.416	y ₃ ,+1	0.15
530.212	b ₅ ,+1	-0.027
535.554	MH-NH ₃ ,,+2	-0.2
	MH-H ₂ O,,+2	0.29
558.198	y ₄ ,+1	-0.1
616.862	b ₆ ,+1	-0.41
629.468	y ₅ ,+1	0.13
757.604	y ₆ ,+1	0.21
782.521	b-NH ₃ ,7,+1	0.17

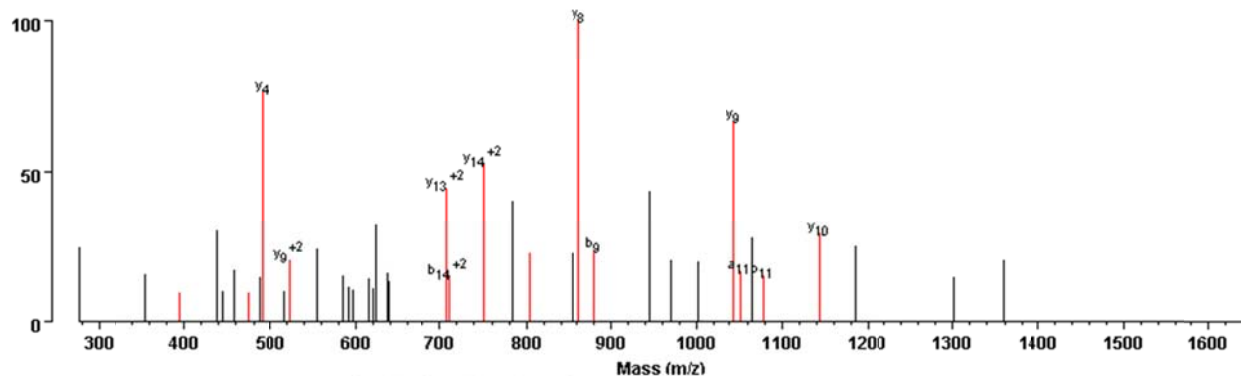
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
746.3817	4	550.286	2	IMAKYYTR	842.469	2	ALSVGLVKGSIDEVDK

IMAK(XL:B-Alkene)YYTR⁺²



m/z	Ion Type	Error
217.033	a,2,+1	-0.1
258.825	y-NH3,2,+1	-0.32
276.336	y,2,+1	0.17
316.162	b,3,+1	-0.0069
428.288	y,6,+2	0.066
439.251	y,3,+1	0.021
498.656	b,4,+1	0.38
602.246	y,4,+1	-0.047
633.413	a,5,+1	0.07
661.082	b,5,+1	-0.26
784.508	y,5,+1	0.11
824.457	b,6,+1	0.056
855.326	y,6,+1	-0.11
925.727	b,7,+1	0.28
986.494	y,7,+1	0.018

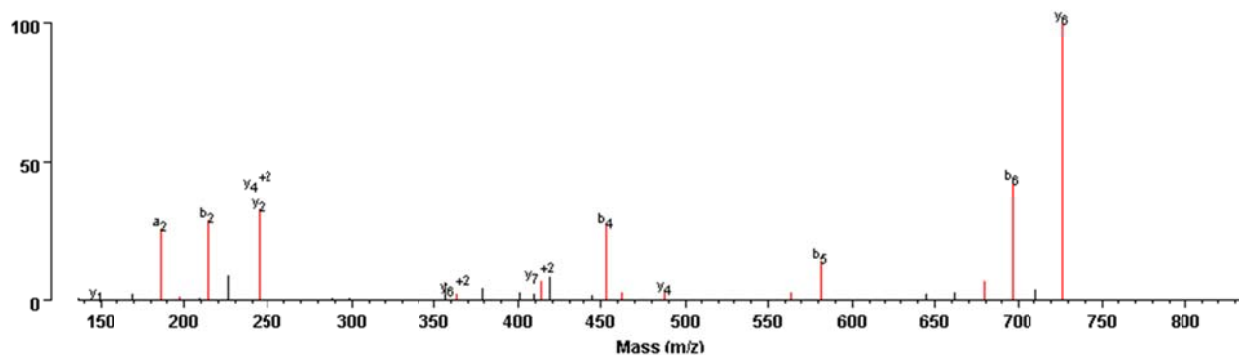
ALSVGLVK(XL:B-Alkene)GSIDEVDK⁺²



m/z	Ion Type	Error
395.203	y-NH3,7,+2	0.52
474.236	b-H2O,10,+2	-0.54
490.34	y,4,+1	0.089
523.148	b-H2O,6,+1	-0.18
	y,9,+2	0.38
707.222	y,13,+2	0.34
711.586	b,14,+2	-0.31
750.31	y,14,+2	-0.091
804.293	b-H2O,8,+1	-0.2
862.572	b-NH3,9,+1	0.069
	y,8,+1	0.16
879.568	b,9,+1	0.038
1044.48	y,9,+1	-0.041
1051.9	a,11,+1	0.25
1079.13	b,11,+1	-0.52
1143.51	y,10,+1	-0.079

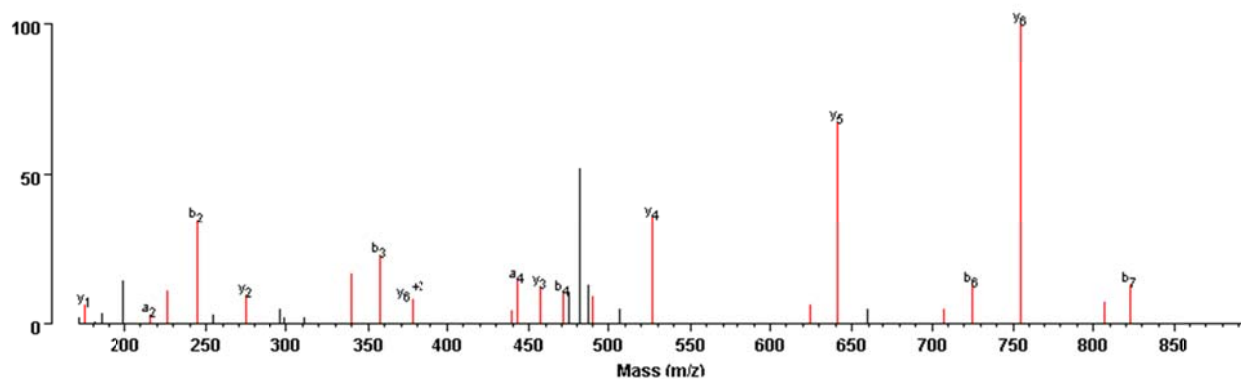
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
534.7686	4	470.249	2	NVGKQDPK	499.276	2	NELNAKVR

NVGK(XL:B-Alkene)QDPK⁺²



m/z	Ion Type	Error
146.987	y,1,+1	-0.13
186.227	a,2,+1	0.1
197.307	b-NH3,2,+1	0.21
214.181	b,2,+1	0.062
244.326	y,2,+1	0.16
	y,4,+2	0.2
363.664	y,6,+2	-0.029
413.512	y,7,+2	0.29
452.891	b,4,+1	-0.35
461.996	MH-NH3,,+2	0.26
487.489	y,4,+1	0.24
564.155	b-NH3,5,+1	-0.12
581.355	b,5,+1	0.051
679.224	b-NH3,6,+1	-0.081
696.23	b,6,+1	-0.1
726.457	y,6,+1	0.079

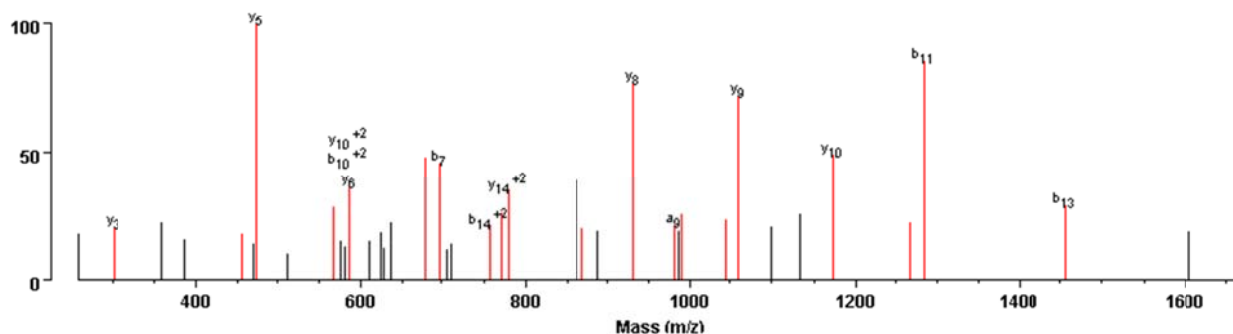
NELNAK(XL:B-Alkene)VR⁺²



m/z	Ion Type	Error
175.159	y,1,+1	0.04
215.993	a,2,+1	-0.1
226.208	b-H2O,2,+1	0.13
244.237	b,2,+1	0.14
274.298	y,2,+1	0.11
339.38	b-H2O,3,+1	0.21
357.189	b,3,+1	0.012
377.592	y,6,+2	-0.14
439.203	y-NH3,3,+1	-0.063
443.037	a,4,+1	-0.19
456.646	y,3,+1	0.35
471.188	b,4,+1	-0.032
489.707	MH-H2O,,+2	-0.56
527.069	y,4,+1	-0.26
624.561	y-NH3,5,+1	0.21
641.359	y,5,+1	-0.014
707.548	b-NH3,6,+1	0.21
724.467	b,6,+1	0.1
754.549	y,6,+1	0.092
806.536	b-NH3,7,+1	0.13
822.914	b,7,+1	-0.52

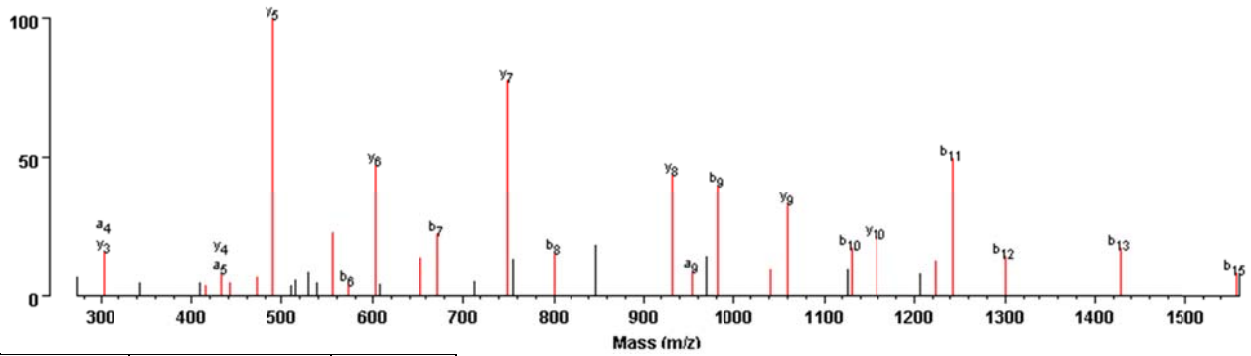
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
922.4770	4	878.969	2	VVGSELIQKYLGDGPK	865.958	2	VSGSELVQKFIGEGAR

VVGSELIQK(XL:B-Alkene)YLGDGPK⁺²



m/z	Ion Type	Error
301.243	y,3,+1	0.056
455.463	y-H2O,5,+1	0.24
473.305	y,5,+1	0.07
567.094	b-H2O,6,+1	-0.22
586.279	y,6,+1	-0.041
	b,10,+2	-0.043
	y,10,+2	-0.54
680.442	b-H2O,7,+1	0.044
698.343	b,7,+1	-0.065
	y-H2O,12,+2	-0.53
757.095	b,14,+2	-0.3
771.302	y-NH3,14,+2	-0.094
	y-H2O,14,+2	0.4
780.169	y,14,+2	0.26
869.868	MH-H2O,,+2	-0.1
	MH-NH3,,+2	-0.6
931.639	y,8,+1	0.15
980.373	a,9,+1	-0.2
990.182	b-H2O,9,+1	-0.38
1042.47	y-NH3,9,+1	-0.05
1059.35	y,9,+1	-0.2
1172.72	y,10,+1	0.089
1267.57	b-NH3,11,+1	-0.12
	y-H2O,11,+1	-0.13
1284.37	b,11,+1	-0.35
1456.6	b,13,+1	-0.17

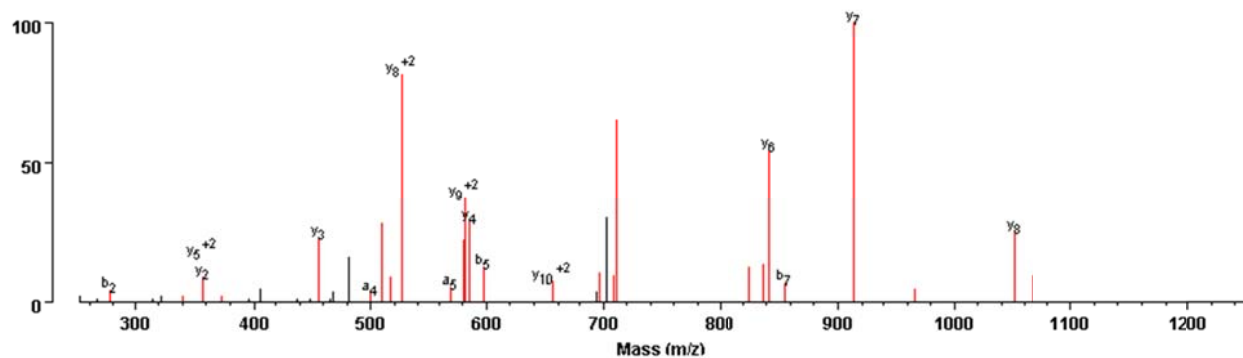
VSGSELVQK(XL:B-Alkene)FIGEGAR⁺²



m/z	Ion Type	Error
303.257	y,3,+1	0.079
	a,4,+1	0.091
415.533	y-NH3,4,+1	0.34
432.079	a,5,+1	-0.13
	y,4,+1	-0.14
442.27	b-H2O,5,+1	0.077
471.055	y-H2O,5,+1	-0.18
489.358	y,5,+1	0.12
555.207	b-H2O,6,+1	-0.07
573.181	b,6,+1	-0.11
602.361	y,6,+1	0.035
654.367	b-H2O,7,+1	0.021
672.195	b,7,+1	-0.16
749.617	y,7,+1	0.22
800.325	b,8,+1	-0.09
931.392	y,8,+1	-0.11
954.177	a,9,+1	-0.35
982.417	b,9,+1	-0.1
1041.48	y-H2O,9,+1	-0.068
1059.48	y,9,+1	-0.078
1129.69	b,10,+1	0.1
1158.68	y,10,+1	0.053
1224.3	b-H2O,11,+1	-0.36
1242.46	b,11,+1	-0.21
1299.72	b,12,+1	0.026
1428.73	b,13,+1	-0.0069
1556.49	b,15,+1	-0.31

m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
659.8259	4	720.366	2	EFLHAQEEVKR	499.274	2	NELNAKVR

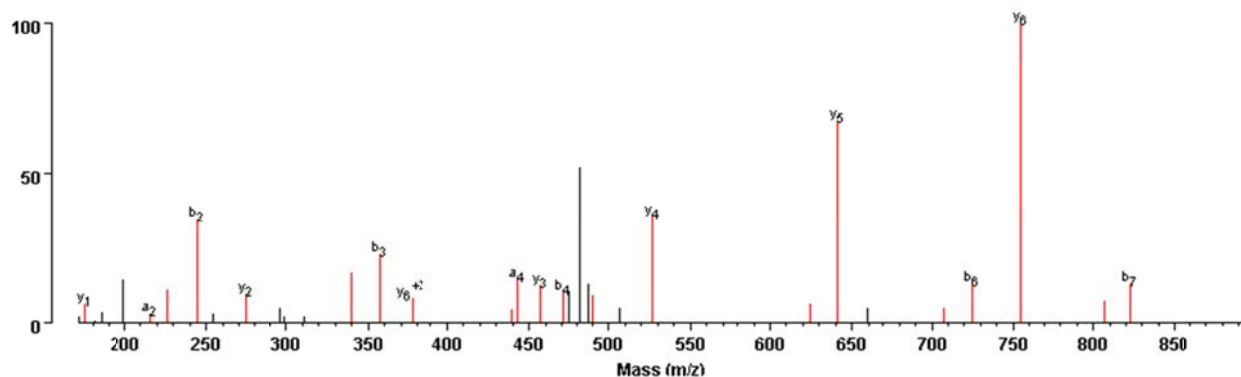
EFLHAQEEVK(XL:B-Alkene)R⁺²



m/z	Ion Type	Error
277.259	b,2,+1	0.14
339.775	y-NH3,2,+1	-0.42
357.394	y,2,+1	0.17
	y,5,+2	-0.3
372.395	b-H2O,3,+1	0.2
456.452	y,3,+1	0.16
499.525	a,4,+1	0.26
509.347	b-H2O,4,+1	0.096
516.857	y-H2O,8,+2	0.092
	y-NH3,8,+2	-0.4
525.88	y,8,+2	0.11
570.412	a,5,+1	0.11
580.315	b-H2O,5,+1	0.027
582.479	y,9,+2	0.17
585.567	y,4,+1	0.23
598.27	b,5,+1	-0.028
656.126	y,10,+2	0.28
696.269	y-H2O,5,+1	-0.099
708.408	b-H2O,6,+1	0.062
711.681	MH-NH3,,+2	-0.17
	MH-H2O,,+2	0.32
825.569	y-NH3,6,+1	0.16
837.647	b-H2O,7,+1	0.26
842.514	y,6,+1	0.077
855.308	b,7,+1	-0.092
913.615	y,7,+1	0.14

966.514	b-H ₂ O,8,+1	0.082
1050.68	y,8,+1	0.15
1066.55	b-NH ₃ ,9,+1	0.066
1247.72	b-H ₂ O,10,+1	0.11

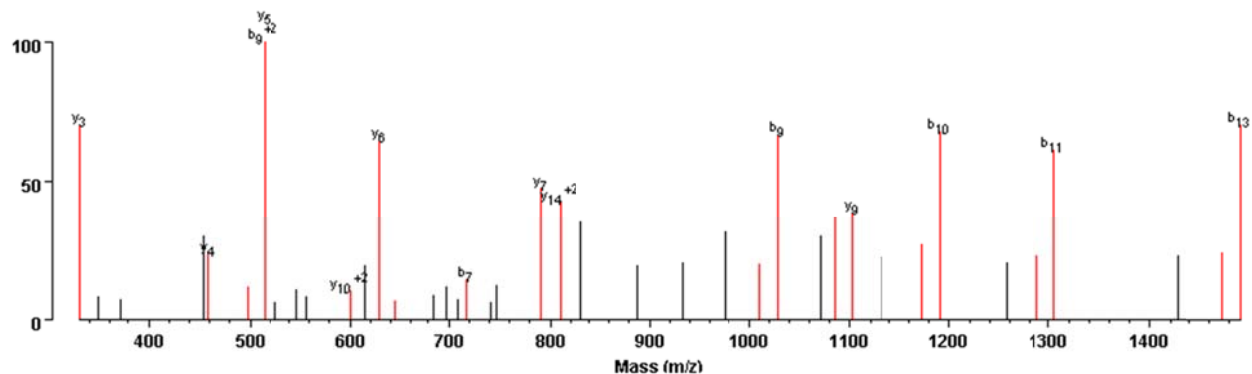
NELNAK(XL:B-Alkene)VR⁺²



m/z	Ion Type	Error
175.159	y,1,+1	0.04
215.993	a,2,+1	-0.1
226.208	b-H ₂ O,2,+1	0.13
244.237	b,2,+1	0.14
274.298	y,2,+1	0.11
339.38	b-H ₂ O,3,+1	0.21
357.189	b,3,+1	0.012
377.592	y,6,+2	-0.14
439.203	y-NH ₃ ,3,+1	-0.063
443.037	a,4,+1	-0.19
456.646	y,3,+1	0.35
471.188	b,4,+1	-0.032
489.707	MH-H ₂ O,,+2	-0.56
527.069	y,4,+1	-0.26
624.561	y-NH ₃ ,5,+1	0.21
641.359	y,5,+1	-0.014
707.548	b-NH ₃ ,6,+1	0.21
724.467	b,6,+1	0.1
754.549	y,6,+1	0.092
806.536	b-NH ₃ ,7,+1	0.13
822.914	b,7,+1	-0.52

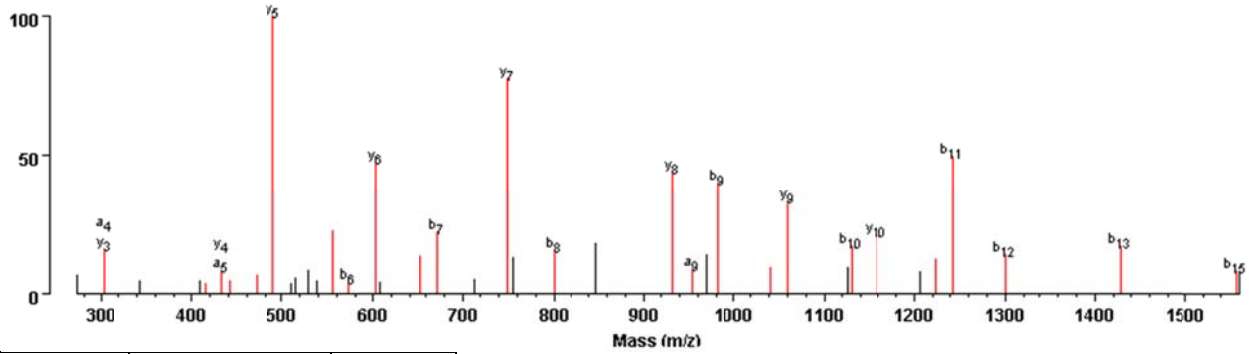
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
937.9707	4	909.974	2	VVGSEFVQKYLGEGR	865.959	2	VSGSELVQKFIGEGAR

VVGSEFVQK(XL:B-Alkene)YLGEGR⁺²



m/z	Ion Type	Error
1490.29	b,13,+1	-0.46
1173.21	b-H ₂ O,10,+1	-0.38
1191.23	b,10,+1	-0.37
	y,5,+1	-0.32
718.094	b,7,+1	-0.28
1472.46	b-H ₂ O,13,+1	-0.28
1304.54	b,11,+1	-0.15
1287.52	b-NH ₃ ,11,+1	-0.14
628.243	y,6,+1	-0.098
791.33	y,7,+1	-0.075
1101.51	y,9,+1	-0.059
601.262	b-H ₂ O,6,+1	-0.036
1028.54	b,9,+1	-0.0011
497.306	y-H ₂ O,5,+1	0.059
1084.65	y-NH ₃ ,9,+1	0.11
1010.68	b-H ₂ O,9,+1	0.15
329.349	y,3,+1	0.16
514.933	b,9,+2	0.16
811.177	y,14,+2	0.27
458.517	y,4,+1	0.28
644.659	b-NH ₃ ,11,+2	0.32
	y,10,+2	0.44

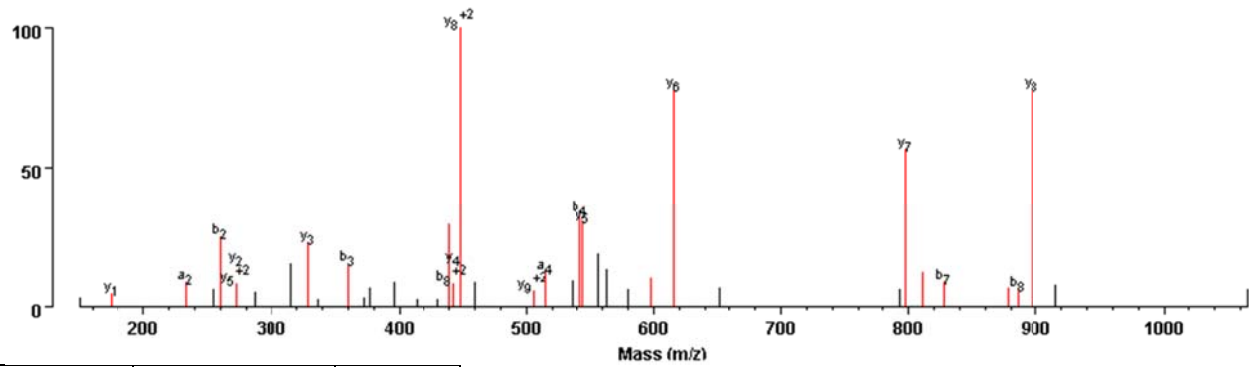
VSGSELVQK(XL:B-Alkene)FIGEGAR⁺²



m/z	Ion Type	Error
303.257	y,3,+1	0.079
	a,4,+1	0.091
415.533	y-NH3,4,+1	0.34
432.079	a,5,+1	-0.13
	y,4,+1	-0.14
442.27	b-H2O,5,+1	0.077
471.055	y-H2O,5,+1	-0.18
489.358	y,5,+1	0.12
555.207	b-H2O,6,+1	-0.07
573.181	b,6,+1	-0.11
602.361	y,6,+1	0.035
654.367	b-H2O,7,+1	0.021
672.195	b,7,+1	-0.16
749.617	y,7,+1	0.22
800.325	b,8,+1	-0.09
931.392	y,8,+1	-0.11
954.177	a,9,+1	-0.35
982.417	b,9,+1	-0.1
1041.48	y-H2O,9,+1	-0.068
1059.48	y,9,+1	-0.078
1129.69	b,10,+1	0.1
1158.68	y,10,+1	0.053
1224.3	b-H2O,11,+1	-0.36
1242.46	b,11,+1	-0.21
1299.72	b,12,+1	0.026
1428.73	b,13,+1	-0.0069
1556.49	b,15,+1	-0.31

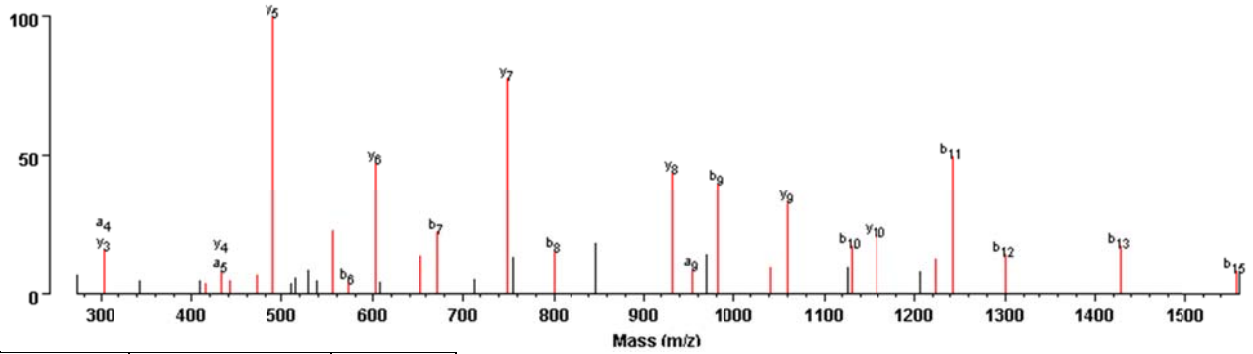
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
772.3973	4	578.828	2	FIVKATNGPR	865.956	2	VSGSELVQKFIGEGAR

FIVK(XL:B-Alkene)ATNGPR⁺²



m/z	Ion Type	Error
175.184	y ₁ ,+1	0.065
233.004	a ₂ ,+1	-0.16
260.698	b ₂ ,+1	-0.46
272.425	y ₅ ,+2	-0.22
	y ₂ ,+1	0.25
329.375	y ₃ ,+1	0.18
359.892	b ₃ ,+1	-0.34
440.1	y-NH ₃ ,8,+2	-0.14
	y-H ₂ O,8,+2	0.35
443.373	b ₈ ,+2	0.13
	y ₄ ,+1	0.14
448.939	y ₈ ,+2	0.19
505.886	y ₉ ,+2	0.59
514.258	a ₄ ,+1	-0.081
541.968	b ₄ ,+1	-0.37
544.158	y ₅ ,+1	-0.13
598.427	y-NH ₃ ,6,+1	0.13
615.526	y ₆ ,+1	0.21
797.455	y ₇ ,+1	0.029
811.47	b-NH ₃ ,7,+1	0.035
828.127	b ₇ ,+1	-0.33
878.353	y-H ₂ O,8,+1	-0.13
885.748	b ₈ ,+1	0.27
896.721	y ₈ ,+1	0.23

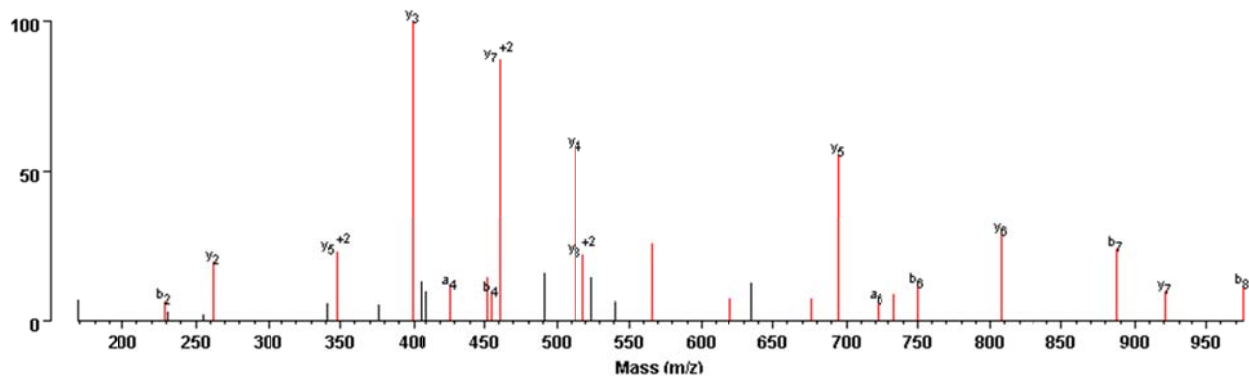
VSGSELVQK(XL:B-Alkene)FIGEGAR⁺²



m/z	Ion Type	Error
303.257	y,3,+1	0.079
	a,4,+1	0.091
415.533	y-NH3,4,+1	0.34
432.079	a,5,+1	-0.13
	y,4,+1	-0.14
442.27	b-H2O,5,+1	0.077
471.055	y-H2O,5,+1	-0.18
489.358	y,5,+1	0.12
555.207	b-H2O,6,+1	-0.07
573.181	b,6,+1	-0.11
602.361	y,6,+1	0.035
654.367	b-H2O,7,+1	0.021
672.195	b,7,+1	-0.16
749.617	y,7,+1	0.22
800.325	b,8,+1	-0.09
931.392	y,8,+1	-0.11
954.177	a,9,+1	-0.35
982.417	b,9,+1	-0.1
1041.48	y-H2O,9,+1	-0.068
1059.48	y,9,+1	-0.078
1129.69	b,10,+1	0.1
1158.68	y,10,+1	0.053
1224.3	b-H2O,11,+1	-0.36
1242.46	b,11,+1	-0.21
1299.72	b,12,+1	0.026
1428.73	b,13,+1	-0.0069
1556.49	b,15,+1	-0.31

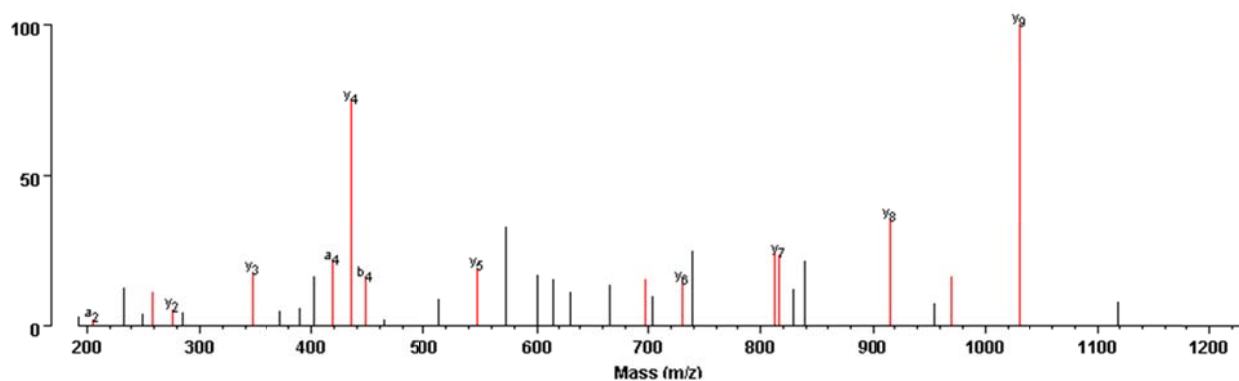
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
653.3353	4	574.845	2	LDILKIHSR	631.816	2	TMDVSKLSAEK

LDILK(XL:B-Alkene)IHSR⁺²



m/z	Ion Type	Error
228.984	b ₂ ,+1	-0.13
262.172	y ₂ ,+1	0.021
347.721	y ₅ ,+2	0.018
399.345	y ₃ ,+1	0.14
426.999	a ₄ ,+1	-0.29
452.057	y-NH ₃ ,7,+2	-0.22
	y-H ₂ O,7,+2	0.27
455.252	b ₄ ,+1	-0.034
460.853	y ₇ ,+2	0.066
512.429	y ₄ ,+1	0.14
518.27	y ₈ ,+2	-0.031
565.916	MH-H ₂ O,,+2	0.078
	MH-NH ₃ ,,+2	-0.41
620.234	b-NH ₃ ,5,+1	-0.13
676.234	y-H ₂ O,5,+1	-0.15
694.378	y ₅ ,+1	-0.021
722.086	a ₆ ,+1	-0.4
733.315	b-NH ₃ ,6,+1	-0.13
750.299	b ₆ ,+1	-0.18
807.44	y ₆ ,+1	-0.044
887.596	b ₇ ,+1	0.061
920.913	y ₇ ,+1	0.35
974.697	b ₈ ,+1	0.13

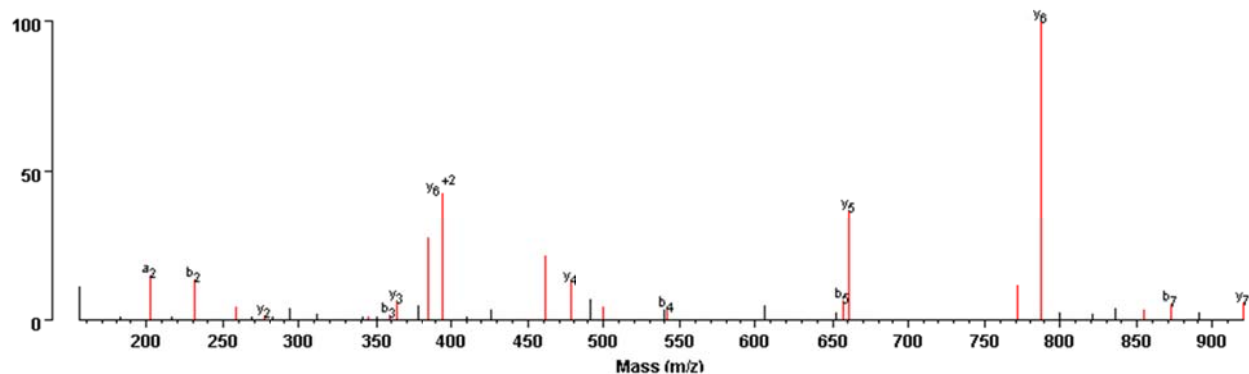
TMDVSK(XL:B-Alkene)LSAEK⁺²



m/z	Ion Type	Error
205.271	a ₂ ,+1	0.17
258.332	y-H ₂ O, ₂ ,+1	0.19
276.412	y ₂ ,+1	0.26
347.273	y ₃ ,+1	0.08
419.01	a ₄ ,+1	-0.19
434.159	y ₄ ,+1	-0.066
447.117	b ₄ ,+1	-0.074
547.467	y ₅ ,+1	0.16
697.834	b-H ₂ O, ₆ ,+1	-0.48
729.619	y ₆ ,+1	0.2
812.711	b-NH ₃ , ₇ ,+1	0.33
816.539	y ₇ ,+1	0.093
915.555	y ₈ ,+1	0.04
969.326	b-H ₂ O, ₉ ,+1	-0.14
1030.68	y ₉ ,+1	0.14

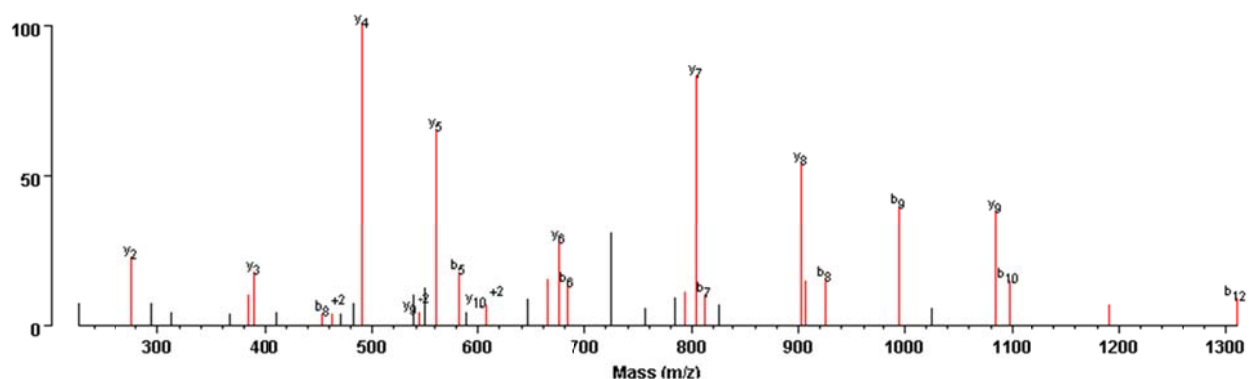
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
676.3400	4	509.748	2	VMQKDSEK	742.922	2	LSAEKVEIATLTR

VMQK(XL:B-Alkene)DSEK⁺²



m/z	Ion Type	Error
203.199	a ₂ ,+1	0.078
230.924	y-NH ₃ ,4,+2	-0.17
	b ₂ ,+1	-0.19
	y-H ₂ O,4,+2	0.32
258.182	y-H ₂ O,2,+1	0.037
276.18	y ₂ ,+1	0.025
345.313	y-H ₂ O,3,+1	0.14
358.795	b ₃ ,+1	-0.38
363.033	b-H ₂ O,6,+2	-0.13
	y ₃ ,+1	-0.15
385.892	y-H ₂ O,6,+2	0.2
	y-NH ₃ ,6,+2	-0.29
394.727	y ₆ ,+2	0.034
460.949	y-NH ₃ ,4,+1	-0.24
478.229	y ₄ ,+1	0.015
500.143	MH-H ₂ O,,+2	-0.6
541.51	b ₄ ,+1	0.23
656.593	b ₅ ,+1	0.29
660.29	y ₅ ,+1	-0.03
771.443	y-NH ₃ ,6,+1	0.091
788.243	y ₆ ,+1	-0.14
854.411	b-H ₂ O,7,+1	0.04
872.295	b ₇ ,+1	-0.087
919.503	y ₇ ,+1	0.084

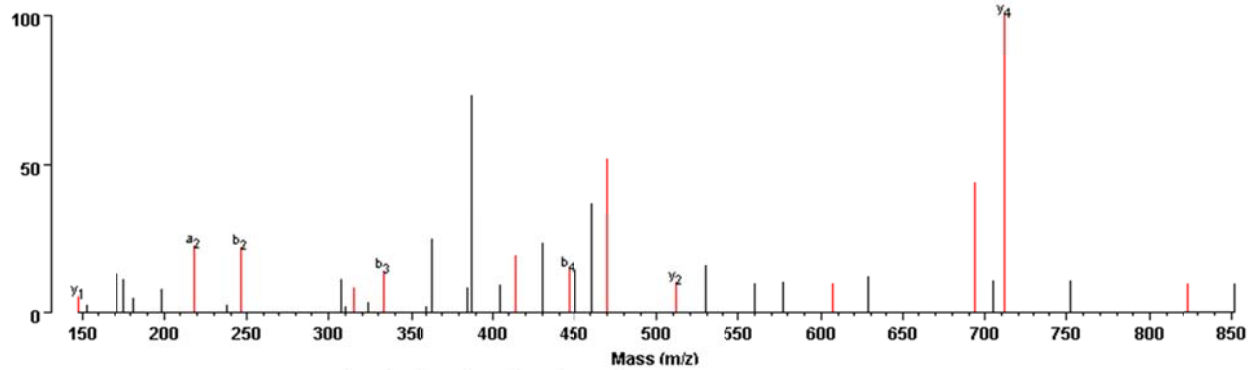
LSAEK(XL:B-Alkene)VEIATLTR⁺²



m/z	Ion Type	Error
276.235	y ₂ ,+1	0.068
383.295	b-H ₂ O, ₄ ,+1	0.1
389.584	y ₃ ,+1	0.33
453.475	b-H ₂ O, ₈ ,+2	-0.28
462.87	b, ₈ ,+2	0.11
490.259	y ₄ ,+1	-0.039
	b-NH ₃ , ₉ ,+2	0.5
542.95	y ₉ ,+2	0.13
	y-H ₂ O, ₅ ,+1	-0.37
561.344	y ₅ ,+1	0.0085
583.221	b, ₅ ,+1	-0.088
607.535	y ₁₀ ,+2	0.19
664.218	b-H ₂ O, ₆ ,+1	-0.15
674.322	y ₆ ,+1	-0.098
682.36	b, ₆ ,+1	-0.017
793.079	b-H ₂ O, ₇ ,+1	-0.33
803.344	y ₇ ,+1	-0.12
811.222	b, ₇ ,+1	-0.2
902.625	y ₈ ,+1	0.094
906.118	b-H ₂ O, ₈ ,+1	-0.38
924.537	b, ₈ ,+1	0.033
995.331	b, ₉ ,+1	-0.21
1084.63	y ₉ ,+1	-0.0061
1097.04	b, ₁₀ ,+1	0.45
1191.3	b-H ₂ O, ₁₁ ,+1	-0.36
1310.26	b, ₁₂ ,+1	-0.46

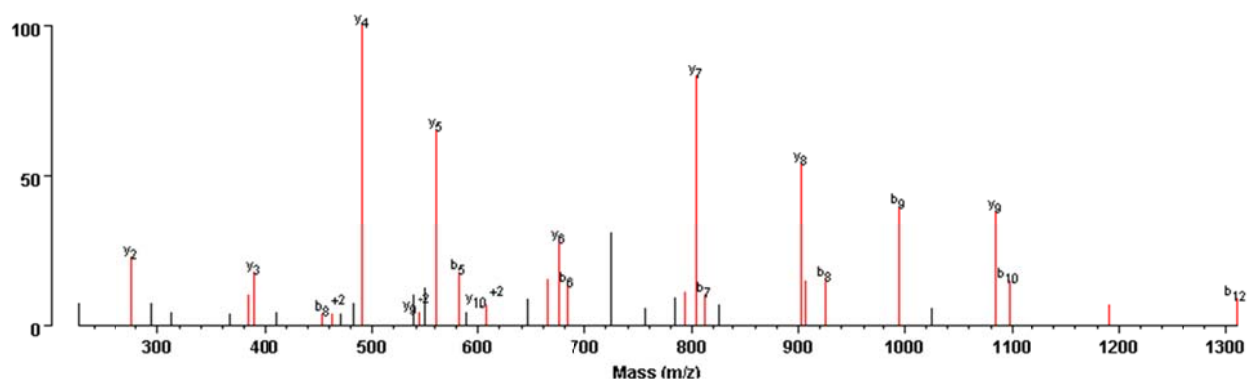
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
615.3207	4	478.715	2	NMSIKK	742.921	2	LSAEKVEIATLTR

NMSIK(XL:B-Thiol(Unsaturated))K⁺²



m/z	Ion Type	Error
147.271	y,1,+1	0.16
218.24	a,2,+1	0.14
246.006	b,2,+1	-0.085
314.971	b-H2O,3,+1	-0.14
333.053	b,3,+1	-0.07
413.7	y-NH3,5,+2	0.52
446.178	b,4,+1	-0.029
469.921	MH-H2O,,+2	0.21
	MH-NH3,,+2	-0.28
511.382	y,2,+1	0.16
607.039	y-NH3,3,+1	-0.24
693.286	y-H2O,4,+1	-0.045
711.414	y,4,+1	0.072
824.078	y-H2O,5,+1	-0.29

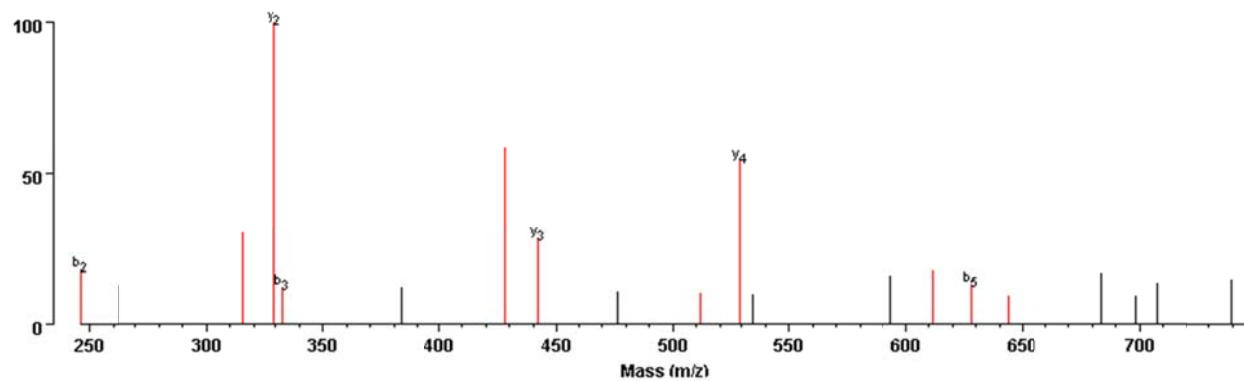
LSAEK(XL:B-Alkene)VEIATLTR⁺²



m/z	Ion Type	Error
276.235	y,2,+1	0.068
383.295	b-H2O,4,+1	0.1
389.584	y,3,+1	0.33
453.475	b-H2O,8,+2	-0.28
462.87	b,8,+2	0.11
490.259	y,4,+1	-0.039
	b-NH3,9,+2	0.5
542.95	y,9,+2	0.13
	y-H2O,5,+1	-0.37
561.344	y,5,+1	0.0085
583.221	b,5,+1	-0.088
607.535	y,10,+2	0.19
664.218	b-H2O,6,+1	-0.15
674.322	y,6,+1	-0.098
682.36	b,6,+1	-0.017
793.079	b-H2O,7,+1	-0.33
803.344	y,7,+1	-0.12
811.222	b,7,+1	-0.2
902.625	y,8,+1	0.094
906.118	b-H2O,8,+1	-0.38
924.537	b,8,+1	0.033
995.331	b,9,+1	-0.21
1084.63	y,9,+1	-0.0061
1097.04	b,10,+1	0.45
1191.3	b-H2O,11,+1	-0.36
1310.26	b,12,+1	-0.46

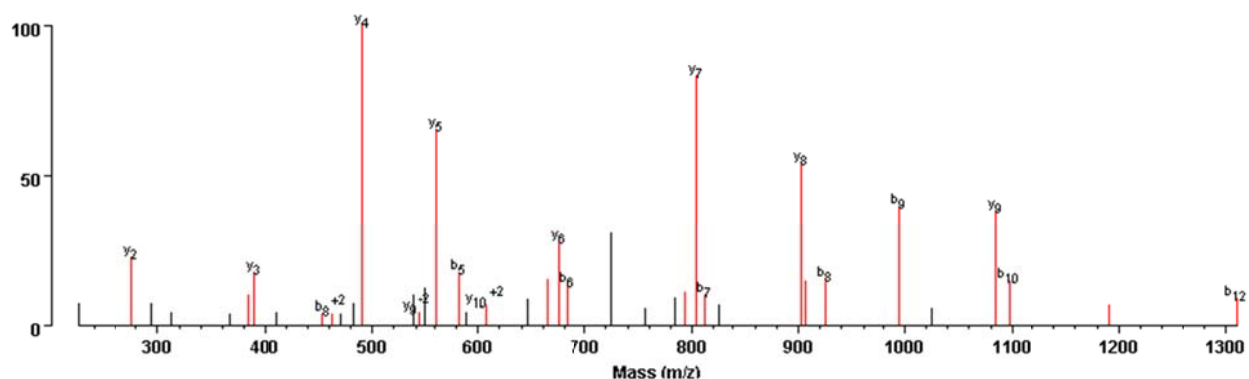
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
820.0922	3	774.417	1	NMSIKK	742.92	2	LSAEKVEIATLTR

NMSIK(XL:B-Alkene)K



m/z	Ion Type	Error
245.821	b,2,+1	-0.27
315.06	b-H ₂ O,3,+1	-0.052
329.258	y,2,+1	0.04
332.834	b,3,+1	-0.29
427.991	b-H ₂ O,4,+1	-0.21
442.135	y,3,+1	-0.17
511.653	y-H ₂ O,4,+1	0.33
529.31	y,4,+1	-0.024
611.367	b-NH ₃ ,5,+1	0.081
627.955	b,5,+1	-0.36
643.547	y-NH ₃ ,5,+1	0.2

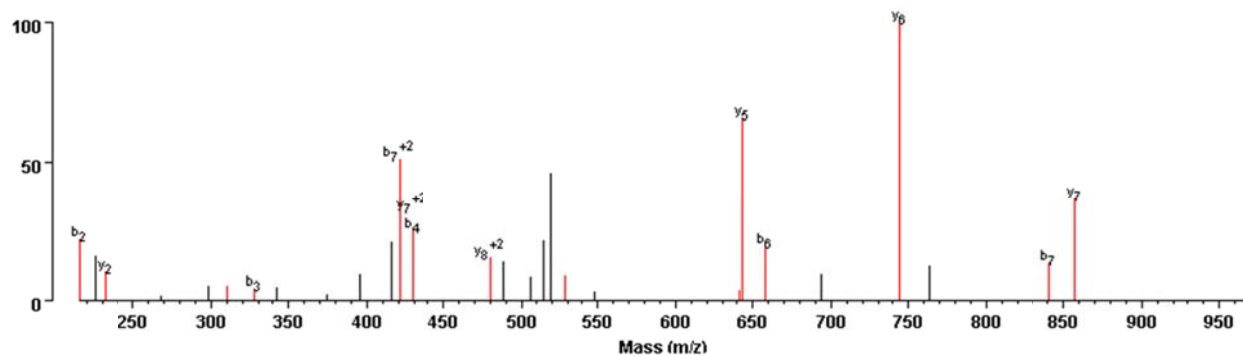
LSAEK(XL:B-Alkene)VEIATLTR⁺²



m/z	Ion Type	Error
276.235	y ₂ ,+1	0.068
383.295	b-H ₂ O, ₄ ,+1	0.1
389.584	y ₃ ,+1	0.33
453.475	b-H ₂ O, ₈ ,+2	-0.28
462.87	b, ₈ ,+2	0.11
490.259	y ₄ ,+1	-0.039
	b-NH ₃ , ₉ ,+2	0.5
542.95	y ₉ ,+2	0.13
	y-H ₂ O, ₅ ,+1	-0.37
561.344	y ₅ ,+1	0.0085
583.221	b, ₅ ,+1	-0.088
607.535	y, ₁₀ ,+2	0.19
664.218	b-H ₂ O, ₆ ,+1	-0.15
674.322	y, ₆ ,+1	-0.098
682.36	b, ₆ ,+1	-0.017
793.079	b-H ₂ O, ₇ ,+1	-0.33
803.344	y, ₇ ,+1	-0.12
811.222	b, ₇ ,+1	-0.2
902.625	y, ₈ ,+1	0.094
906.118	b-H ₂ O, ₈ ,+1	-0.38
924.537	b, ₈ ,+1	0.033
995.331	b, ₉ ,+1	-0.21
1084.63	y, ₉ ,+1	-0.0061
1097.04	b, ₁₀ ,+1	0.45
1191.3	b-H ₂ O, ₁₁ ,+1	-0.36
1310.26	b, ₁₂ ,+1	-0.46

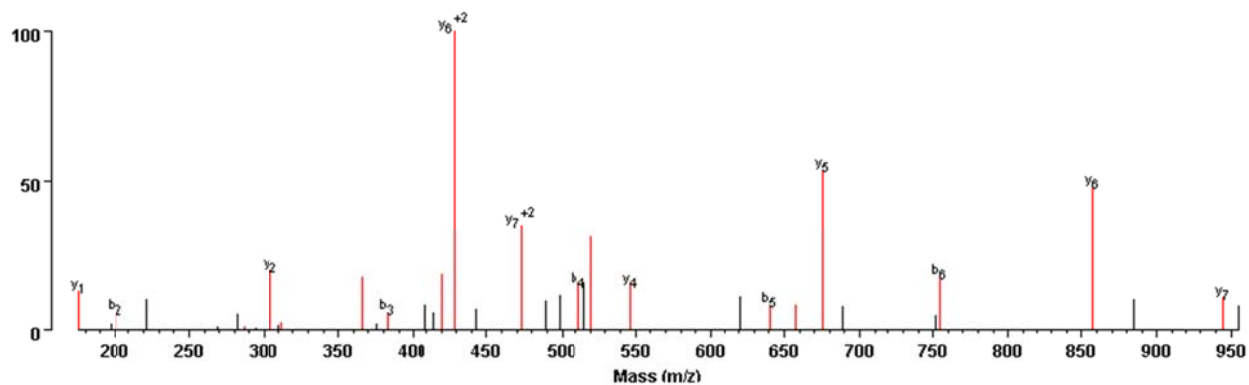
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
582.7930	4	536.290	2	ITITNDKGR	529.282	2	LSKEEIER

ITITNDK(XL:B-Alkene)GR⁺²



m/z	Ion Type	Error
215.136	b ₂ ,+1	-0.003
	y-NH ₃ ,2,+1	0.022
232.29	y ₂ ,+1	0.15
309.997	b-H ₂ O,3,+1	-0.22
327.918	b ₃ ,+1	-0.31
420.989	b ₇ ,+2	0.26
	y-NH ₃ ,7,+2	0.27
429.783	b ₄ ,+1	0.51
	y ₇ ,+2	0.56
480.286	y ₈ ,+2	0.53
527.344	MH-H ₂ O,,+2	0.056
	MH-NH ₃ ,,+2	-0.44
641.316	b-NH ₃ ,6,+1	0.0019
643.464	y ₅ ,+1	0.15
657.823	b ₆ ,+1	-0.52
744.449	y ₆ ,+1	0.086
840.767	b ₇ ,+1	0.32
	y-NH ₃ ,7,+1	0.35
857.498	y ₇ ,+1	0.05

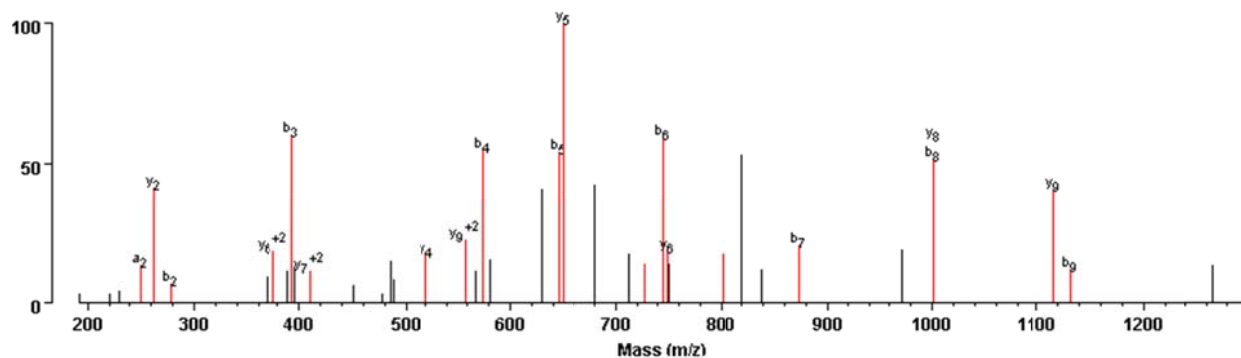
LSK(XL:B-Alkene)EEIER⁺²



m/z	Ion Type	Error
175.178	y,1,+1	0.059
200.943	b,2,+1	-0.18
	y-NH3,3,+2	0.33
286.268	y-H2O,2,+1	0.12
304.281	y,2,+1	0.12
312.46	b-NH3,5,+2	-0.19
	b-H2O,5,+2	0.3
365.384	b-H2O,3,+1	0.17
383.045	b,3,+1	-0.18
419.987	y-H2O,6,+2	-0.23
429.308	y,6,+2	0.086
472.691	y,7,+2	-0.047
511.733	b,4,+1	-0.54
520.295	MH-H2O,,+2	0.02
	MH-NH3,,+2	-0.47
546.307	y,4,+1	0.019
641.097	b,5,+1	-0.22
657.545	y-H2O,5,+1	0.22
675.345	y,5,+1	0.014
754.194	b,6,+1	-0.2
857.508	y,6,+1	0.072
944.918	y,7,+1	0.45

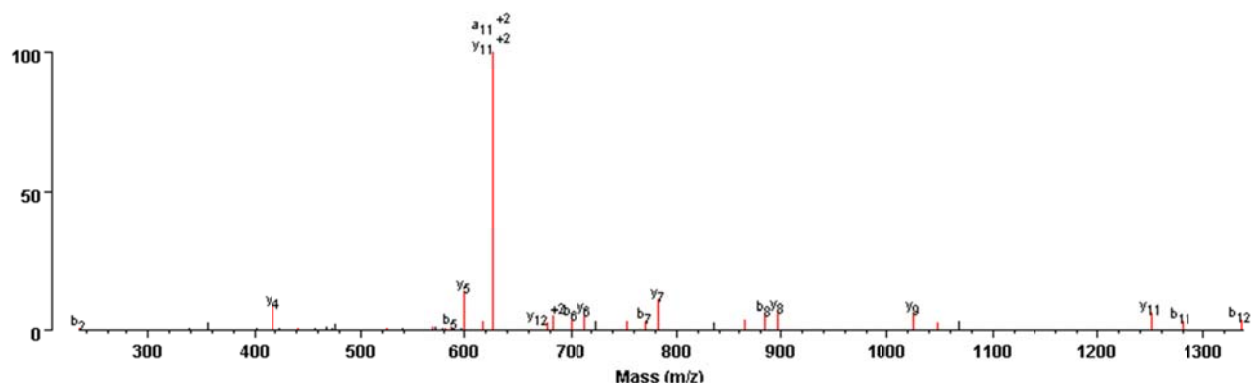
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
769.3677	4	696.824	2	NYNKAVEEEDK	741.91	2	MTPEQLAIKNVGK

NYNK(XL:B-Alkene)AVEEEDK⁺²



m/z	Ion Type	Error
250.087	a ₂ ,+1	-0.032
262.357	y ₂ ,+1	0.22
278.296	b ₂ ,+1	0.18
374.913	b-NH ₃ ,3,+1	-0.22
	y ₆ ,+2	0.24
392.427	b ₃ ,+1	0.27
410.136	y ₇ ,+2	-0.054
520.454	y ₄ ,+1	0.23
558.638	y ₉ ,+2	0.37
574.14	b ₄ ,+1	-0.12
645.21	b ₅ ,+1	-0.089
649.333	y ₅ ,+1	0.065
727.205	b-NH ₃ ,6,+1	-0.14
744.347	b ₆ ,+1	-0.021
748.25	y ₆ ,+1	-0.086
801.315	y-H ₂ O,7,+1	-0.047
873.555	b ₇ ,+1	0.14
1001.98	b ₈ ,+1	-0.47
	y ₈ ,+1	0.5
1115.51	y ₉ ,+1	-0.012
1132.06	b ₉ ,+1	0.56

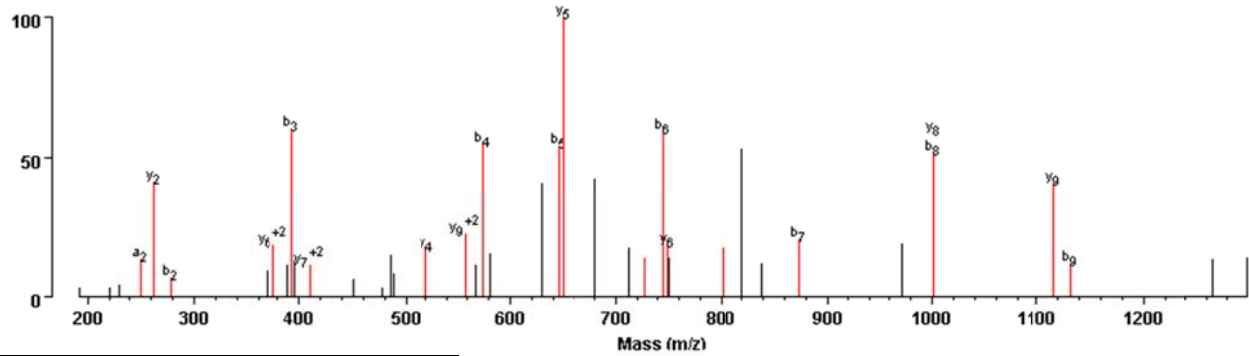
MTPEQLAIK(XL:B-Alkene)NVGK⁺²



m/z	Ion Type	Error
233.163	b,2,+1	0.068
417.244	y,4,+1	-0.0016
441.309	b-H ₂ O,4,+1	0.13
524.196	b-H ₂ O,9,+2	-0.58
569.57	b-H ₂ O,5,+1	0.33
582.255	b-NH ₃ ,10,+2	-0.037
	y-NH ₃ ,5,+1	-0.07
	b-H ₂ O,10,+2	0.46
586.977	b,5,+1	-0.27
599.365	y,5,+1	0.014
617.072	y-H ₂ O,11,+2	0.22
	y-NH ₃ ,11,+2	-0.27
626.1	y,11,+2	0.24
	a,11,+2	-0.24
676.439	y,12,+2	0.056
682.483	b-H ₂ O,6,+1	0.16
700.363	b,6,+1	0.03
712.645	y,6,+1	0.21
753.521	b-H ₂ O,7,+1	0.16
771.185	b,7,+1	-0.19
783.526	y,7,+1	0.054
866.226	b-H ₂ O,8,+1	-0.22
884.453	b,8,+1	-0.0016
896.307	y,8,+1	-0.25
1024.67	y,9,+1	0.055
1048	b-H ₂ O,9,+1	-0.55
1250.38	y,11,+1	-0.33
1279.71	b,11,+1	0.039
1336.61	b,12,+1	-0.083

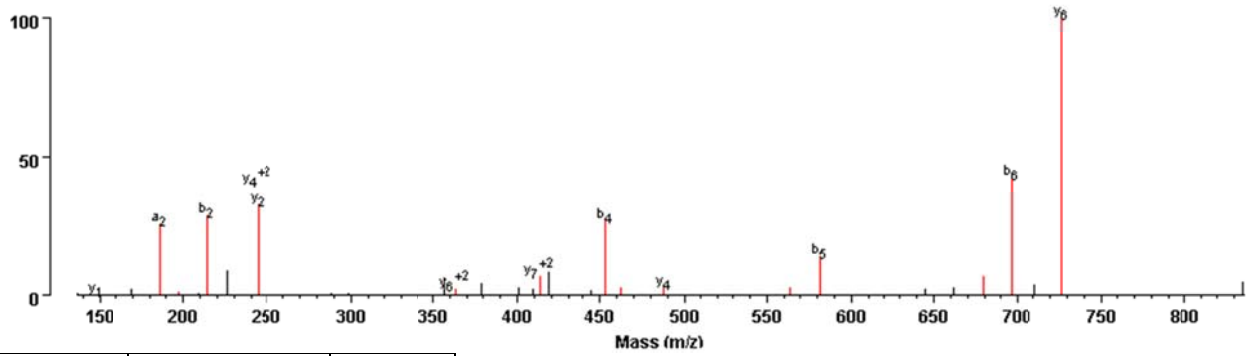
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
633.5399	4	696.819	2	NYNKAVEEEDK	470.25	2	NVGKQDPK

NYNK(XL:B-Alkene)AVEEEDK⁺²



m/z	Ion Type	Error
250.087	a ₂ ,+1	-0.032
262.357	y ₂ ,+1	0.22
278.296	b ₂ ,+1	0.18
374.913	b-NH ₃ ,3,+1	-0.22
	y ₆ ,+2	0.24
392.427	b ₃ ,+1	0.27
410.136	y ₇ ,+2	-0.054
520.454	y ₄ ,+1	0.23
558.638	y ₉ ,+2	0.37
574.14	b ₄ ,+1	-0.12
645.21	b ₅ ,+1	-0.089
649.333	y ₅ ,+1	0.065
727.205	b-NH ₃ ,6,+1	-0.14
744.347	b ₆ ,+1	-0.021
748.25	y ₆ ,+1	-0.086
801.315	y-H ₂ O,7,+1	-0.047
873.555	b ₇ ,+1	0.14
1001.98	b ₈ ,+1	-0.47
	y ₈ ,+1	0.5
1115.51	y ₉ ,+1	-0.012
1132.06	b ₉ ,+1	0.56

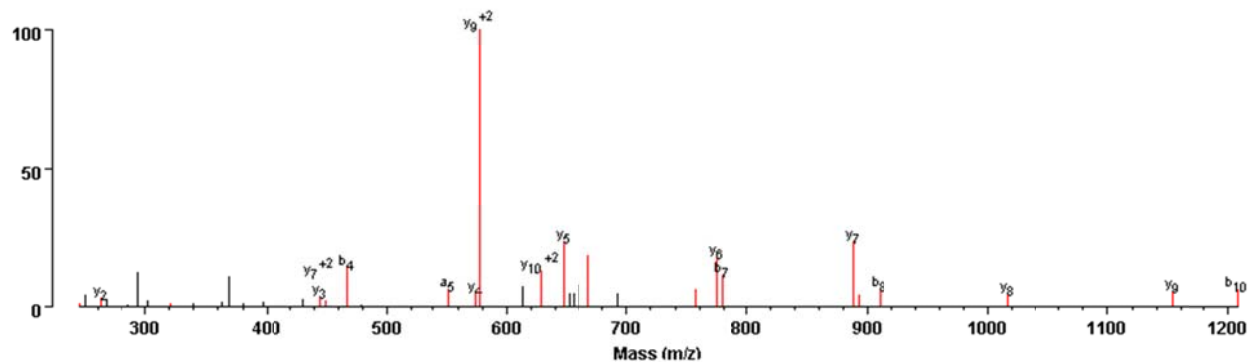
NVGK(XL:B-Alkene)QDPK⁺²



m/z	Ion Type	Error
146.987	y,1,+1	-0.13
186.227	a,2,+1	0.1
197.307	b-NH3,2,+1	0.21
214.181	b,2,+1	0.062
244.326	y,2,+1	0.16
	y,4,+2	0.2
363.664	y,6,+2	-0.029
413.512	y,7,+2	0.29
452.891	b,4,+1	-0.35
461.996	MH-NH3,,+2	0.26
487.489	y,4,+1	0.24
564.155	b-NH3,5,+1	-0.12
581.355	b,5,+1	0.051
679.224	b-NH3,6,+1	-0.081
696.23	b,6,+1	-0.1
726.457	y,6,+1	0.079

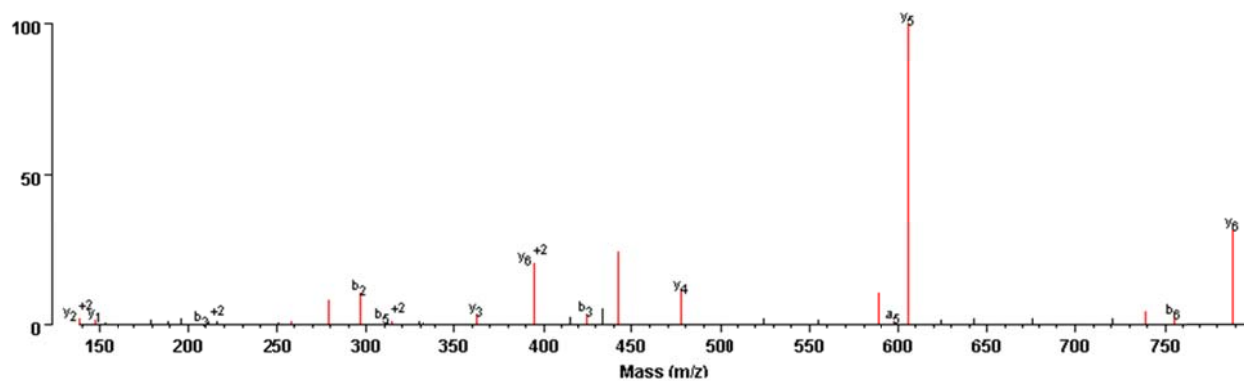
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
614.2955	4	677.346	2	VTHELQAMKDK	451.235	2	IKENSEK

VTHELQAMK(XL:A-Alkene)DK⁺²



m/z	Ion Type	Error
244.271	y-H ₂ O, ₂ ,+ ₁	0.14
262.16	y, ₂ ,+ ₁	0.02
320.566	b-H ₂ O, ₃ ,+ ₁	0.39
444.583	y, ₃ ,+ ₁	0.34
	y, ₇ ,+ ₂	0.35
449.237	b-H ₂ O, ₄ ,+ ₁	0.023
467.353	b, ₄ ,+ ₁	0.13
552.274	a, ₅ ,+ ₁	-0.04
575.097	y, ₄ ,+ ₁	-0.19
577.511	y, ₉ ,+ ₂	0.22
628.194	y-H ₂ O, ₅ ,+ ₁	-0.12
	y, ₁₀ ,+ ₂	0.38
646.475	y, ₅ ,+ ₁	0.15
668.534	MH-H ₂ O, _, + ₂	0.19
	MH-NH ₃ , _, + ₂	-0.3
757.194	y-NH ₃ , ₆ ,+ ₁	-0.16
774.338	y, ₆ ,+ ₁	-0.043
779.658	b, ₇ ,+ ₁	0.25
887.598	y, ₇ ,+ ₁	0.13
892.491	b-H ₂ O, ₈ ,+ ₁	0.056
910.344	b, ₈ ,+ ₁	-0.1
1016.66	y, ₈ ,+ ₁	0.15
1153.2	y, ₉ ,+ ₁	-0.37
1207.56	b, ₁₀ ,+ ₁	-0.018

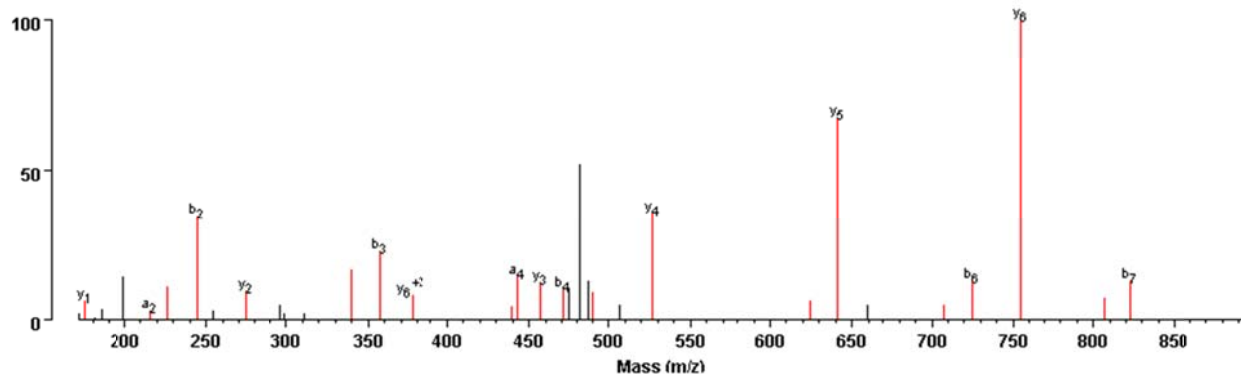
IK(XL:A-Alkene)ENSEK⁺²



m/z	Ion Type	Error
138.278	y,2,+2	-0.3
147.292	y,1,+1	0.18
213.204	b,3,+2	0.081
258.384	y-H ₂ O,2,+1	0.24
279.197	b-NH ₃ ,2,+1	0.027
296.163	b,2,+1	-0.034
314.227	b,5,+2	0.57
362.994	y,3,+1	-0.19
394.889	y,6,+2	0.2
425.263	b,3,+1	0.024
442.077	MH-H ₂ O,,+2	-0.15
477.373	y,4,+1	0.14
588.348	y-H ₂ O,5,+1	0.086
598.136	a,5,+1	-0.18
606.186	y,5,+1	-0.087
738.682	b-NH ₃ ,6,+1	0.35
755.389	b,6,+1	0.032
788.382	y,6,+1	0.0035

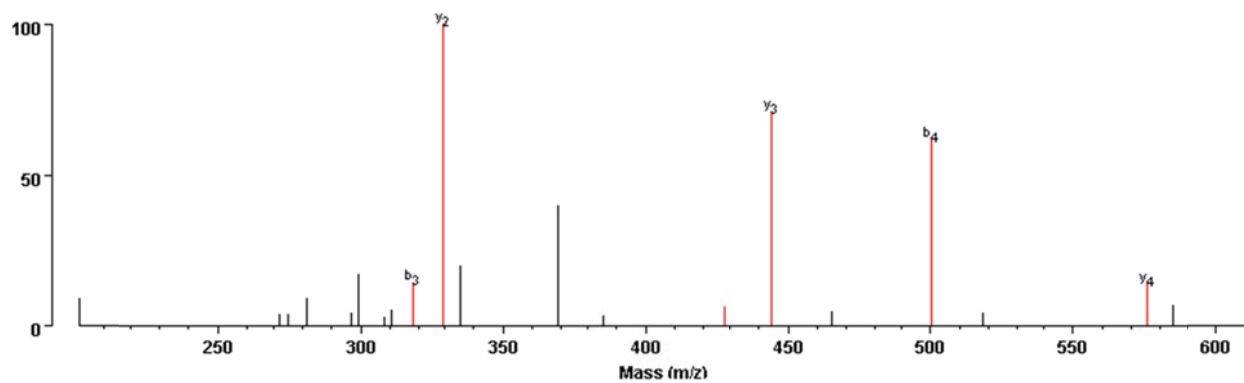
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
461.4756	4	499.276	2	NELNAKVR	646.324	1	AMDKK

NELNAK(XL:B-Alkene)VR⁺²



m/z	Ion Type	Error
175.159	y ₁ ,+1	0.04
215.993	a ₂ ,+1	-0.1
226.208	b-H ₂ O, ₂ ,+1	0.13
244.237	b, ₂ ,+1	0.14
274.298	y, ₂ ,+1	0.11
339.38	b-H ₂ O, ₃ ,+1	0.21
357.189	b, ₃ ,+1	0.012
377.592	y, ₆ ,+2	-0.14
439.203	y-NH ₃ , ₃ ,+1	-0.063
443.037	a, ₄ ,+1	-0.19
456.646	y, ₃ ,+1	0.35
471.188	b, ₄ ,+1	-0.032
489.707	MH-H ₂ O,,+2	-0.56
527.069	y, ₄ ,+1	-0.26
624.561	y-NH ₃ , ₅ ,+1	0.21
641.359	y, ₅ ,+1	-0.014
707.548	b-NH ₃ , ₆ ,+1	0.21
724.467	b, ₆ ,+1	0.1
754.549	y, ₆ ,+1	0.092
806.536	b-NH ₃ , ₇ ,+1	0.13
822.914	b, ₇ ,+1	-0.52

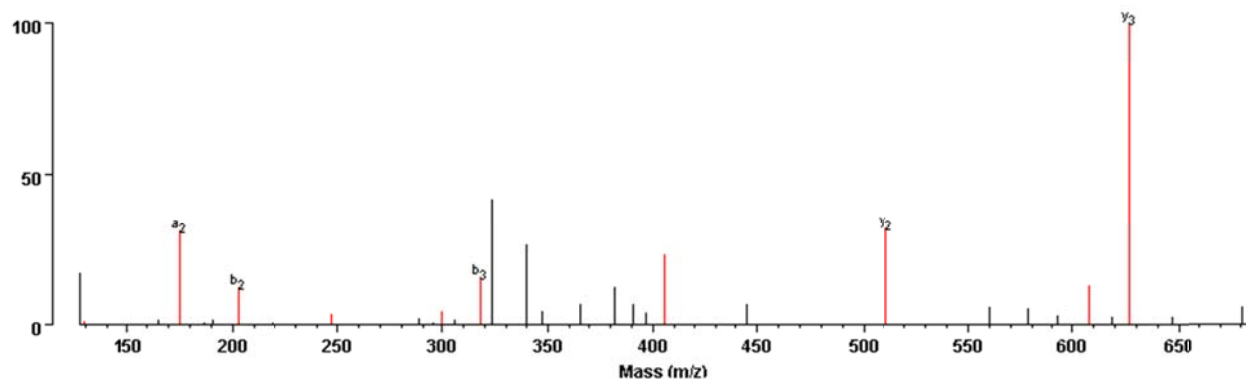
AMDK(XL:B-Alkene)K



m/z	Ion Type	Error
318.184	b ₃ ,+1	0.072
329.245	y ₂ ,+1	0.027
427.475	γ-NH ₃ ,3,+1	0.26
444.221	y ₃ ,+1	-0.024
500.13	b ₄ ,+1	-0.087
575.362	y ₄ ,+1	0.076

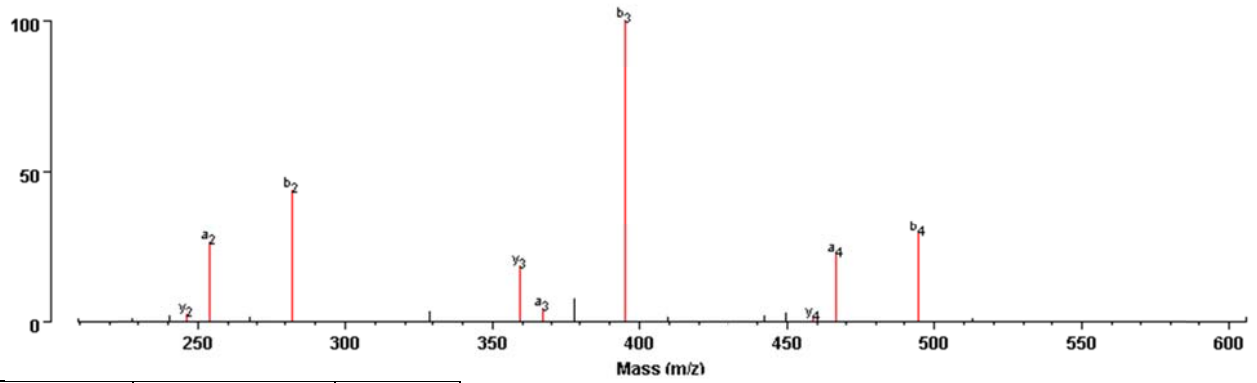
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
495.9291	3	414.669	2	AMDKK	640.44	1	KVLVK

AMDK(XL:B-Thiol(Unsaturated))K⁺²



m/z	Ion Type	Error
129.68	γ -NH3,1,+1	-0.41
175.19	a,2,+1	0.1
202.908	b,2,+1	-0.18
247.344	γ -NH3,2,+2	-0.26
299.886	b-H2O,3,+1	-0.22
318.085	b,3,+1	-0.027
405.733	MH-H2O,,+2	0.07
	MH-NH3,,+2	-0.42
511.232	γ ,2,+1	0.0065
607.869	γ -H2O,3,+1	-0.37
626.361	γ ,3,+1	0.11

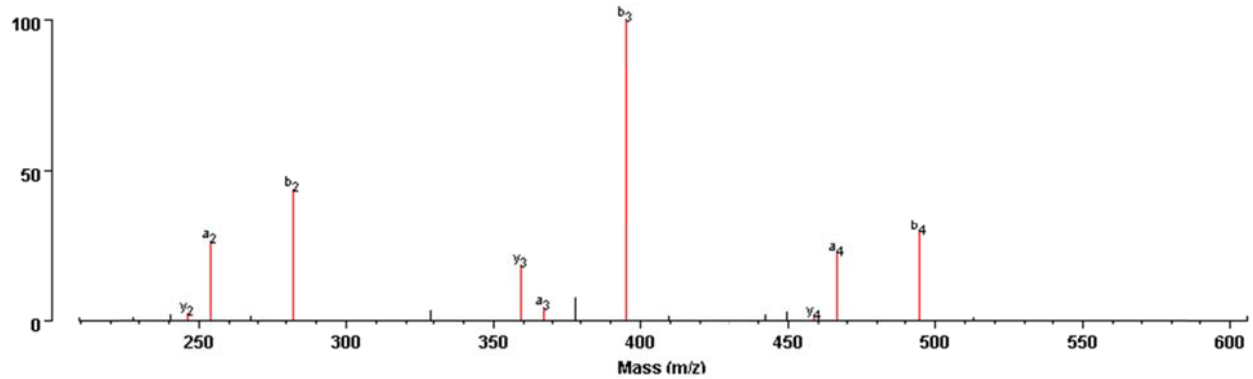
K(XL:B-Alkene)VLVK



m/z	Ion Type	Error
246.368	y _{2,+1}	0.19
254.231	a _{2,+1}	0.045
282.249	b _{2,+1}	0.068
359.197	y _{3,+1}	-0.068
367.133	a _{3,+1}	-0.14
395.182	b _{3,+1}	-0.083
458.802	y _{4,+1}	0.47
466.241	a _{4,+1}	-0.098
494.46	b _{4,+1}	0.13

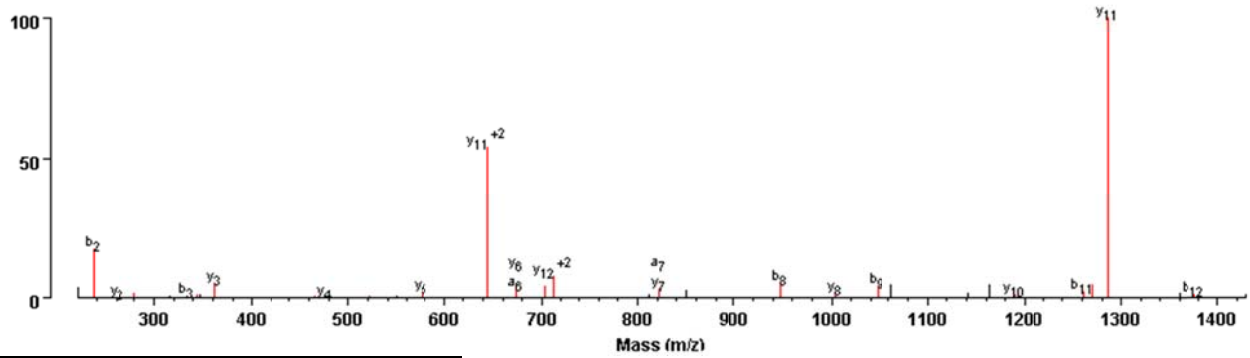
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
591.3166	4	640.440	1	KVLVK	761.9	2	VHPEGKFVVDVDK

K(XL:B-Alkene)VLVK



m/z	Ion Type	Error
246.368	y ₂ ,+1	0.19
254.231	a ₂ ,+1	0.045
282.249	b ₂ ,+1	0.068
359.197	y ₃ ,+1	-0.068
367.133	a ₃ ,+1	-0.14
395.182	b ₃ ,+1	-0.083
458.802	y ₄ ,+1	0.47
466.241	a ₄ ,+1	-0.098
494.46	b ₄ ,+1	0.13

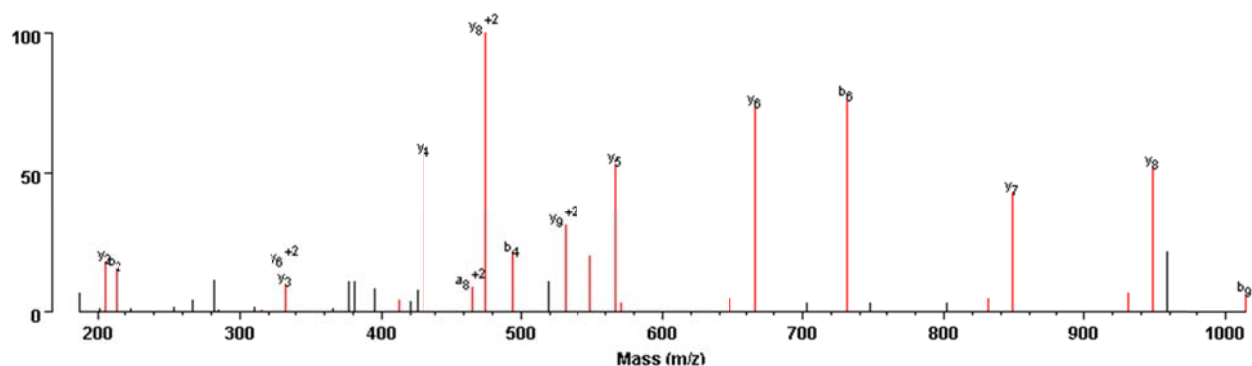
VHPEGK(XL:A-Alkene)FVVDVDK⁺²



m/z	Ion Type	Error
237.271	b,2,+1	0.14
262.084	y,2,+1	-0.056
279.243	y-H2O,5,+2	0.093
	y-NH3,5,+2	-0.4
334.417	b,3,+1	0.23
344.207	y-NH3,3,+1	0.025
361.204	y,3,+1	-0.0042
466.33	b-NH3,8,+2	0.093
	b-H2O,8,+2	0.58
476.268	y,4,+1	0.033
521.686	y-H2O,9,+2	-0.096
	y-NH3,9,+2	-0.59
575.267	y,5,+1	-0.037
644.109	y,11,+2	0.27
674.241	a,6,+1	-0.12
	y,6,+1	-0.13
703.245	y-H2O,12,+2	-0.11
712.309	y,12,+2	-0.055
821.474	y,7,+1	0.034
	a,7,+1	0.044
948.291	b,8,+1	-0.2
1003.44	y,8,+1	-0.11
1047.4	b,9,+1	-0.16
1189.91	y,10,+1	0.3
1261.64	b,11,+1	-0.018
1269.75	y-NH3,11,+1	0.11
1286.54	y,11,+1	-0.12
1376.62	b,12,+1	-0.064

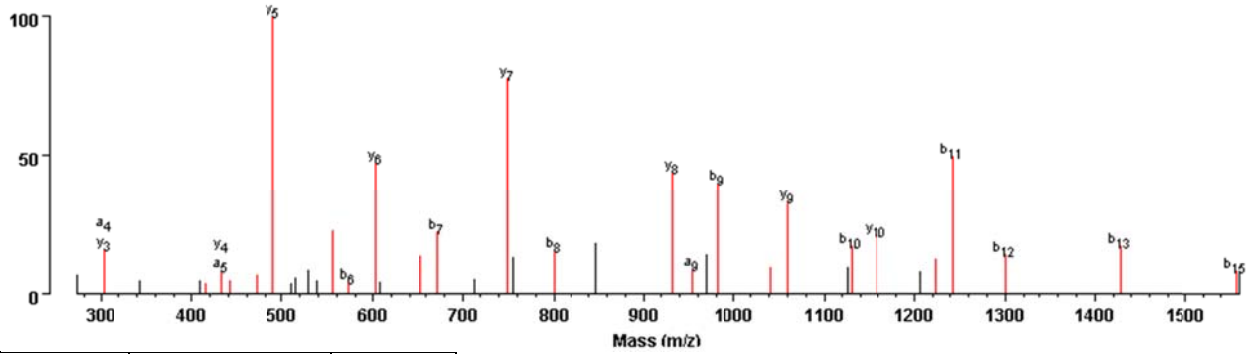
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
773.1585	4	580.346	2	VLVKVHPEGK	865.958	2	VSGSELVQKFIGEGAR

VLVK(XL:B-Alkene)VHPEGK⁺²



m/z	Ion Type	Error
204.293	y ₂ ⁺¹	0.16
213.069	b ₂ ⁺¹	-0.091
315.48	y-H ₂ O ₃ ⁺¹	0.31
333.19	y ₃ ⁺¹	0.013
	y ₆ ⁺²	-0.49
412.474	y-H ₂ O ₄ ⁺¹	0.25
430.356	y ₄ ⁺¹	0.13
465.38	y-H ₂ O ₈ ⁺²	0.12
	y-NH ₃ ₈ ⁺²	-0.38
	a ₈ ⁺²	0.6
474.441	y ₈ ⁺²	0.17
494.28	b ₄ ⁺¹	-0.054
530.708	y ₉ ⁺²	-0.1
549.027	y-H ₂ O ₅ ⁺¹	-0.25
567.403	y ₅ ⁺¹	0.11
571.233	MH-H ₂ O ₈ ⁺²	-0.11
	MH-NH ₃ ₈ ⁺²	-0.6
648.404	y-H ₂ O ₆ ⁺¹	0.058
666.217	y ₆ ⁺¹	-0.14
730.517	b ₆ ⁺¹	0.056
831.506	y-NH ₃ ₇ ⁺¹	0.07
848.535	y ₇ ⁺¹	0.073
930.654	y-NH ₃ ₈ ⁺¹	0.15
947.607	y ₈ ⁺¹	0.076
1013.52	b ₉ ⁺¹	-0.058

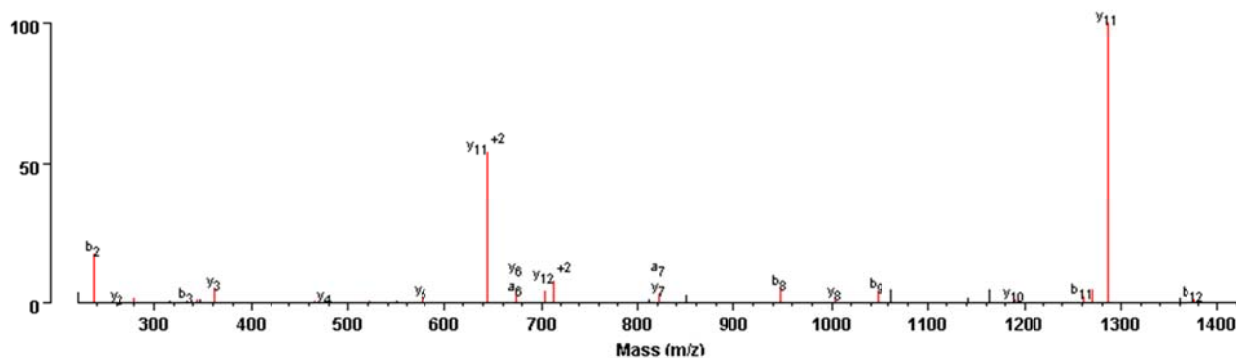
VSGSELVQK(XL:B-Alkene)FIGEGAR⁺²



m/z	Ion Type	Error
303.257	y,3,+1	0.079
	a,4,+1	0.091
415.533	y-NH3,4,+1	0.34
432.079	a,5,+1	-0.13
	y,4,+1	-0.14
442.27	b-H2O,5,+1	0.077
471.055	y-H2O,5,+1	-0.18
489.358	y,5,+1	0.12
555.207	b-H2O,6,+1	-0.07
573.181	b,6,+1	-0.11
602.361	y,6,+1	0.035
654.367	b-H2O,7,+1	0.021
672.195	b,7,+1	-0.16
749.617	y,7,+1	0.22
800.325	b,8,+1	-0.09
931.392	y,8,+1	-0.11
954.177	a,9,+1	-0.35
982.417	b,9,+1	-0.1
1041.48	y-H2O,9,+1	-0.068
1059.48	y,9,+1	-0.078
1129.69	b,10,+1	0.1
1158.68	y,10,+1	0.053
1224.3	b-H2O,11,+1	-0.36
1242.46	b,11,+1	-0.21
1299.72	b,12,+1	0.026
1428.73	b,13,+1	-0.0069
1556.49	b,15,+1	-0.31

m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
863.9333	4	761.901	2	VHPEGK FVVDV DK	956.957	2	VSGSELVQK F I G E G A R

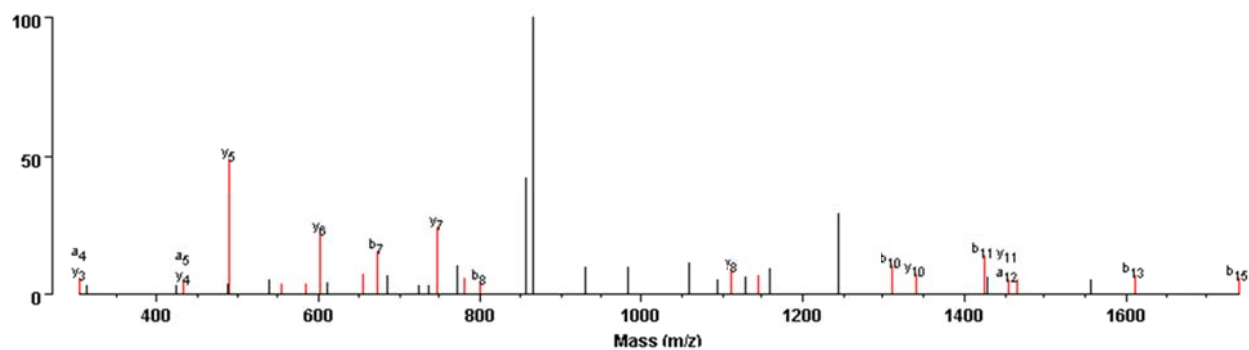
VHPEGK(XL:A-Alkene)FVVDV DK⁺²



m/z	Ion Type	Error
237.271	b ₂ ,+1	0.14
262.084	y ₂ ,+1	-0.056
279.243	y-H ₂ O, ₅ ,+2	0.093
	y-NH ₃ , ₅ ,+2	-0.4
334.417	b ₃ ,+1	0.23
344.207	y-NH ₃ , ₃ ,+1	0.025
361.204	y ₃ ,+1	-0.0042
466.33	b-NH ₃ , ₈ ,+2	0.093
	b-H ₂ O, ₈ ,+2	0.58
476.268	y ₄ ,+1	0.033
521.686	y-H ₂ O, ₉ ,+2	-0.096
	y-NH ₃ , ₉ ,+2	-0.59
575.267	y ₅ ,+1	-0.037
644.109	y ₁₁ ,+2	0.27
674.241	a ₆ ,+1	-0.12
	y ₆ ,+1	-0.13
703.245	y-H ₂ O, ₁₂ ,+2	-0.11
712.309	y ₁₂ ,+2	-0.055
821.474	y ₇ ,+1	0.034
	a ₇ ,+1	0.044
948.291	b ₈ ,+1	-0.2
1003.44	y ₈ ,+1	-0.11
1047.4	b ₉ ,+1	-0.16
1189.91	y ₁₀ ,+1	0.3
1261.64	b ₁₁ ,+1	-0.018
1269.75	y-NH ₃ , ₁₁ ,+1	0.11

1286.54	y,11,+1	-0.12
1376.62	b,12,+1	-0.064

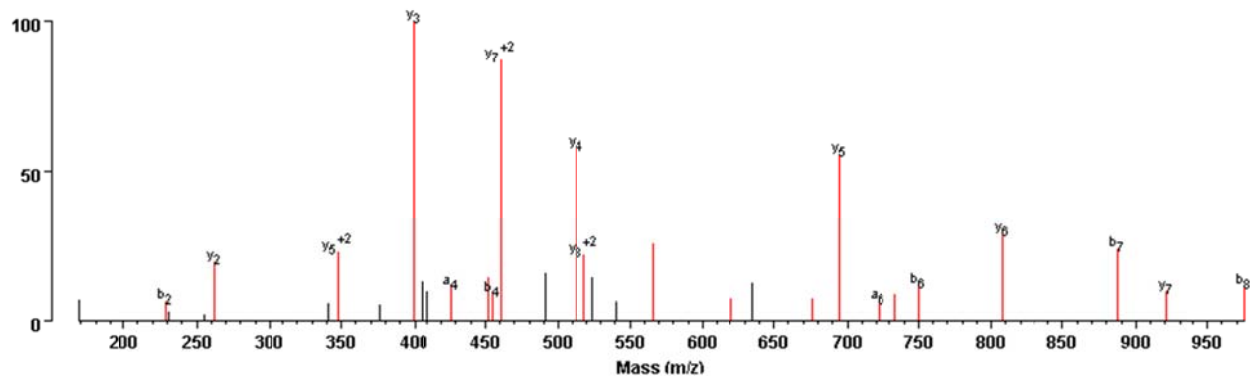
VSGSELVQK(XL:B-Thiol(Unsaturated))FIGEGAR⁺²



m/z	Ion Type	Error
303.296	y,3,+1	0.12
	a,4,+1	0.13
432.271	y,4,+1	0.051
	a,5,+1	0.062
489.417	y,5,+1	0.18
555.443	b-H2O,6,+1	0.17
584.427	y-H2O,6,+1	0.11
602.326	y,6,+1	3.50E-04
654.581	b-H2O,7,+1	0.24
672.288	b,7,+1	-0.068
749.401	y,7,+1	0.0069
782.263	b-H2O,8,+1	-0.14
800.195	b,8,+1	-0.22
1113.44	y,8,+1	-0.067
1146.37	b-H2O,9,+1	-0.15
1311.62	b,10,+1	0.024
1340.82	y,10,+1	0.19
1424.32	b,11,+1	-0.36
1453.66	a,12,+1	-0.047
	y,11,+1	-0.058
1464.06	b-H2O,12,+1	0.37
1611.02	b,13,+1	0.28
1739.24	b,15,+1	0.44

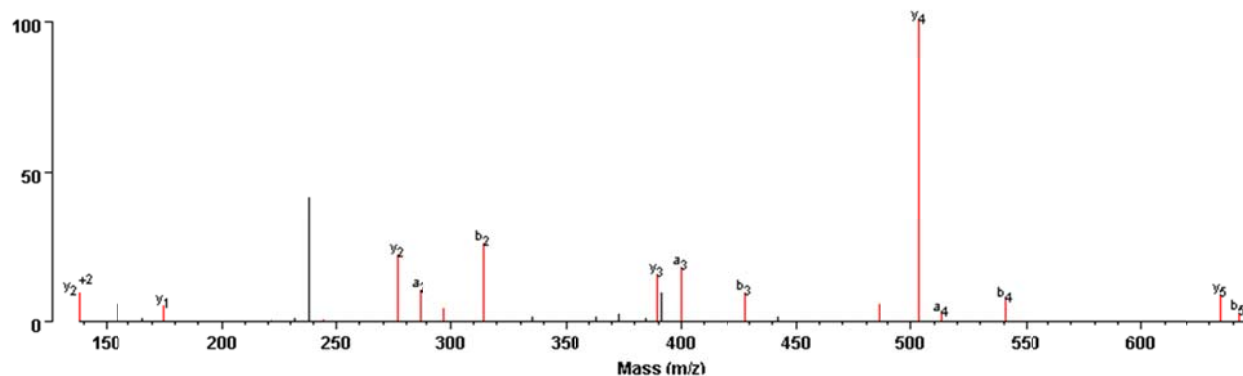
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
541.7886	4	574.843	2	LDILKIHSR	408.724	2	KMNLTR

LDILK(XL:B-Alkene)IHSR⁺²



m/z	Ion Type	Error
228.984	b ₂ ,+1	-0.13
262.172	y ₂ ,+1	0.021
347.721	y ₅ ,+2	0.018
399.345	y ₃ ,+1	0.14
426.999	a ₄ ,+1	-0.29
452.057	y-NH ₃ ,7,+2	-0.22
	y-H ₂ O,7,+2	0.27
455.252	b ₄ ,+1	-0.034
460.853	y ₇ ,+2	0.066
512.429	y ₄ ,+1	0.14
518.27	y ₈ ,+2	-0.031
565.916	MH-H ₂ O,,+2	0.078
	MH-NH ₃ ,,+2	-0.41
620.234	b-NH ₃ ,5,+1	-0.13
676.234	y-H ₂ O,5,+1	-0.15
694.378	y ₅ ,+1	-0.021
722.086	a ₆ ,+1	-0.4
733.315	b-NH ₃ ,6,+1	-0.13
750.299	b ₆ ,+1	-0.18
807.44	y ₆ ,+1	-0.044
887.596	b ₇ ,+1	0.061
920.913	y ₇ ,+1	0.35
974.697	b ₈ ,+1	0.13

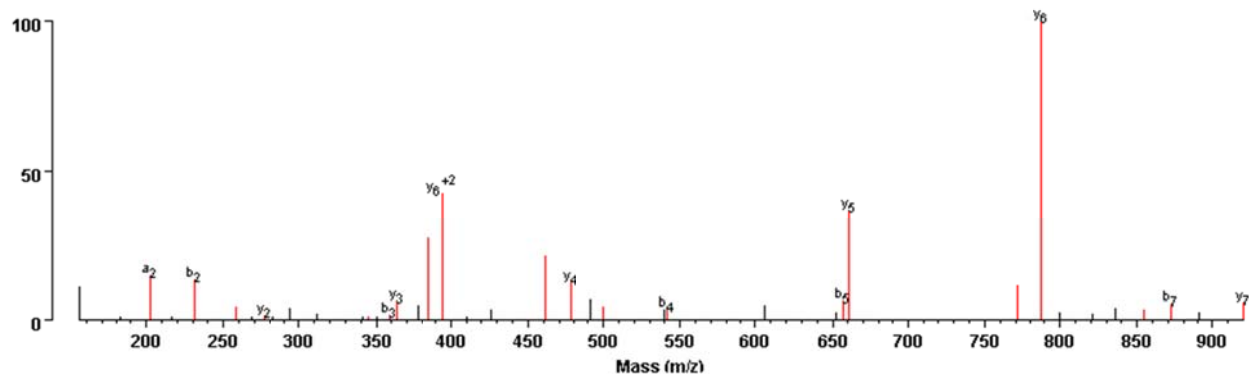
K(XL:B-Alkene)MNLTR⁺²



m/z	Ion Type	Error
138.091	y ₂ ,+2	-0.5
175.06	y ₁ ,+1	-0.059
244.185	γ-NH ₃ ,4,+2	0.55
276.302	y ₂ ,+1	0.14
286.06	a ₂ ,+1	-0.098
297.246	b-NH ₃ ,2,+1	0.12
314.138	b ₂ ,+1	-0.015
389.42	y ₃ ,+1	0.17
400.08	a ₃ ,+1	-0.12
	MH-NH ₃ ,,+2	-0.13
	MH-H ₂ O,,+2	0.36
428.259	b ₃ ,+1	0.063
485.995	γ-NH ₃ ,4,+1	-0.27
503.326	y ₄ ,+1	0.032
513.457	a ₄ ,+1	0.17
541.023	b ₄ ,+1	-0.26
634.719	y ₅ ,+1	0.38
642.507	b ₅ ,+1	0.18

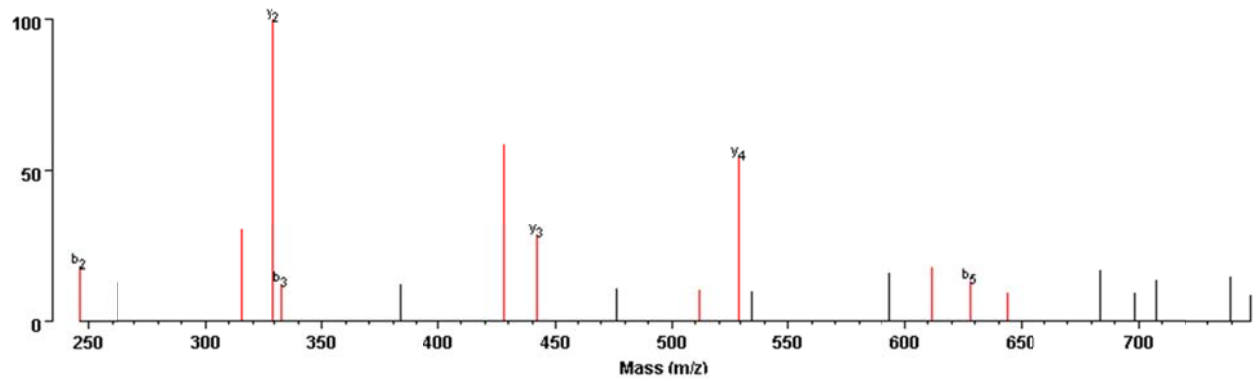
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
664.6444	3	509.748	2	VMQKDSEK	774.419	1	NMSIKK

VMQK(XL:B-Alkene)DSEK⁺²



m/z	Ion Type	Error
203.199	a ₂ ,+1	0.078
230.924	y-NH ₃ ,4,+2	-0.17
	b ₂ ,+1	-0.19
	y-H ₂ O,4,+2	0.32
258.182	y-H ₂ O,2,+1	0.037
276.18	y ₂ ,+1	0.025
345.313	y-H ₂ O,3,+1	0.14
358.795	b ₃ ,+1	-0.38
363.033	b-H ₂ O,6,+2	-0.13
	y ₃ ,+1	-0.15
385.892	y-H ₂ O,6,+2	0.2
	y-NH ₃ ,6,+2	-0.29
394.727	y ₆ ,+2	0.034
460.949	y-NH ₃ ,4,+1	-0.24
478.229	y ₄ ,+1	0.015
500.143	MH-H ₂ O,,+2	-0.6
541.51	b ₄ ,+1	0.23
656.593	b ₅ ,+1	0.29
660.29	y ₅ ,+1	-0.03
771.443	y-NH ₃ ,6,+1	0.091
788.243	y ₆ ,+1	-0.14
854.411	b-H ₂ O,7,+1	0.04
872.295	b ₇ ,+1	-0.087
919.503	y ₇ ,+1	0.084

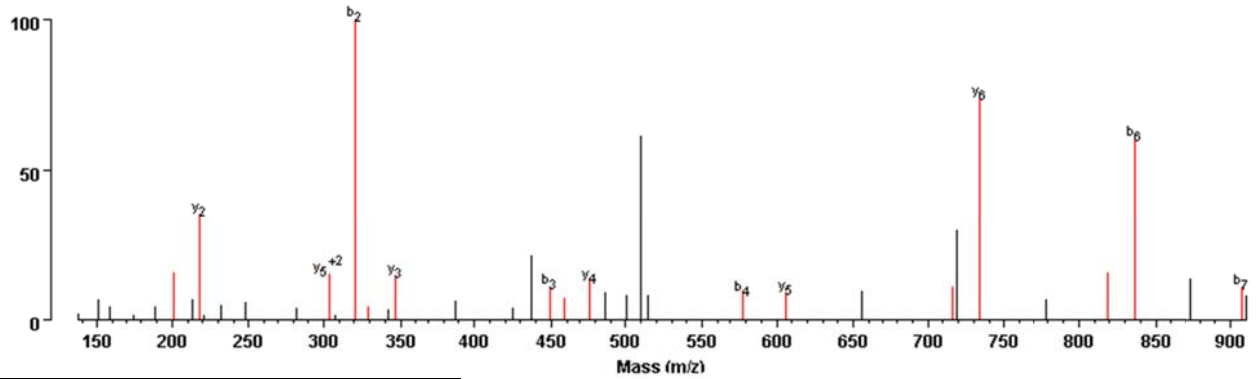
NMSIK(XL:B-Alkene)K



m/z	Ion Type	Error
245.821	b ₂ ,+1	-0.27
315.06	b-H ₂ O, ₃ ,+1	-0.052
329.258	y ₂ ,+1	0.04
332.834	b ₃ ,+1	-0.29
427.991	b-H ₂ O, ₄ ,+1	-0.21
442.135	y ₃ ,+1	-0.17
511.653	y-H ₂ O, ₄ ,+1	0.33
529.31	y ₄ ,+1	-0.024
611.367	b-NH ₃ , ₅ ,+1	0.081
627.955	b ₅ ,+1	-0.36
643.547	y-NH ₃ , ₅ ,+1	0.2

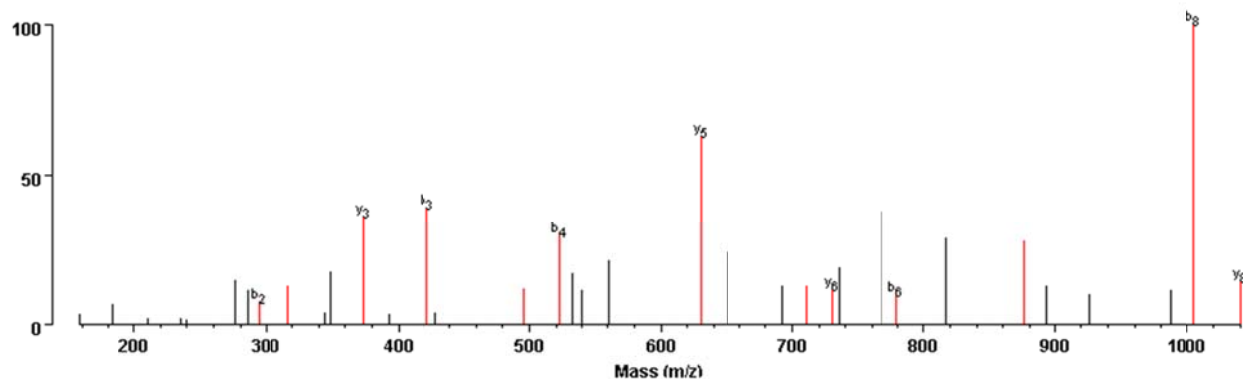
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
601.7863	4	527.246	2	KHEEEEAQ	576.323	2	QKEVEQLIK

K(XL:B-Alkene)HEEEEAQ⁺²



m/z	Ion Type	Error
201.21	y-NH ₃ ,2,+1	0.087
218.316	y ₂ ,+1	0.17
303.281	b-NH ₃ ,2,+1	0.14
	y ₅ ,+2	0.14
320.175	b ₂ ,+1	0.0033
329.162	y-H ₂ O,3,+1	-0.02
347.007	y ₃ ,+1	-0.19
449.345	b ₃ ,+1	0.13
458.488	y-H ₂ O,4,+1	0.26
476.288	y ₄ ,+1	0.053
578.202	b ₄ ,+1	-0.055
605.874	y ₅ ,+1	0.6
716.064	y-H ₂ O,6,+1	-0.25
734.116	y ₆ ,+1	-0.2
818.542	b-H ₂ O,6,+1	0.21
836.447	b ₆ ,+1	0.1
907.25	b ₇ ,+1	-0.13

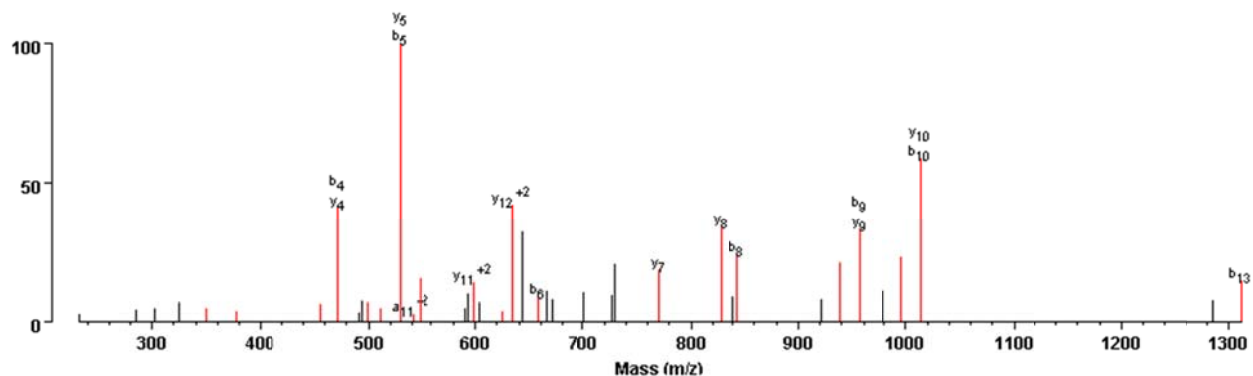
Q(Gln->pyro-Glu)K(XL:B-Alkene)EVEQLIK⁺²



m/z	Ion Type	Error
294.097	b ₂ ,+1	-0.048
317.282	b-H ₂ O, ₅ ,+2	0.13
	b-NH ₃ , ₅ ,+2	-0.36
373.274	y ₃ ,+1	-0.0069
423.119	b ₃ ,+1	-0.068
495.086	b-NH ₃ , ₈ ,+2	0.33
522.396	b ₄ ,+1	0.14
630.359	y ₅ ,+1	-0.023
711.01	y-H ₂ O, ₆ ,+1	-0.43
729.639	y ₆ ,+1	0.19
779.333	b ₆ ,+1	-0.024
875.272	b-NH ₃ , ₇ ,+1	-0.14
1005.43	b ₈ ,+1	-0.095
1040	y ₈ ,+1	-0.6

m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
678.1033	4	742.878	2	FAAKGEGQLGPAER	513.315	2	LIEKLDIK

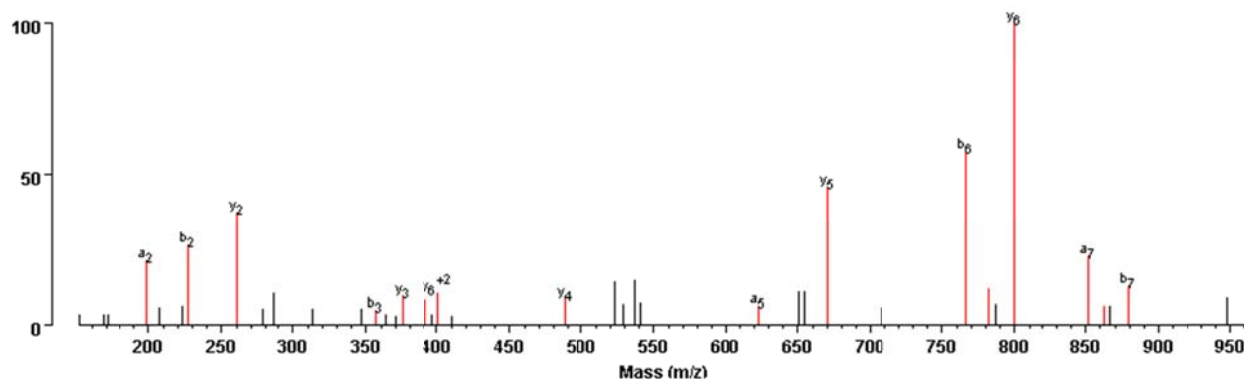
FAAK(XL:B-Alkene)GEGQLGPAER⁺²



m/z	Ion Type	Error
349.512	b-NH3,7,+2	-0.15
	b-H2O,7,+2	0.34
377.326	y-NH3,7,+2	0.13
455.3	b-NH3,4,+1	0.071
	y-NH3,4,+1	0.075
472.237	y,4,+1	-0.014
	b,4,+1	-0.018
498.819	b-NH3,10,+2	0.076
	y-NH3,10,+2	0.078
	b-H2O,10,+2	0.57
	y-H2O,10,+2	0.57
511.351	y-H2O,5,+1	0.089
529.388	b,5,+1	0.11
	y,5,+1	0.12
541.366	a,11,+2	-0.42
547.432	b-NH3,11,+2	0.16
598.662	y,11,+2	0.36
625.262	y-NH3,12,+2	-0.05
	y-NH3,6,+1	-0.068
	y-H2O,12,+2	0.44
634.143	y,12,+2	0.32
658.286	b,6,+1	-0.034
770.496	y,7,+1	0.08
827.615	y,8,+1	0.18
843.55	b,8,+1	0.15
938.393	y-H2O,9,+1	-0.076

	b-H2O,9,+1	-0.08
956.387	y,9,+1	-0.093
	b,9,+1	-0.097
996.126	y-NH3,10,+1	-0.35
	b-NH3,10,+1	-0.35
1013.64	b,10,+1	0.13
	y,10,+1	0.14
1310.79	b,13,+1	0.15

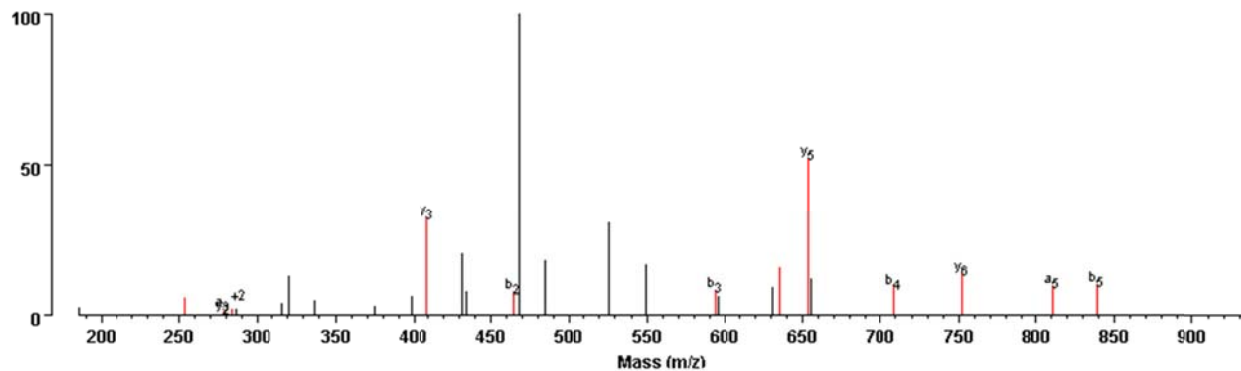
LIEK(XL:B-Alkene)LDIK⁺²



m/z	Ion Type	Error
198.954	a,2,+1	-0.23
227.03	b,2,+1	-0.15
260.26	y,2,+1	0.063
	b-H2O,4,+2	-0.4
356.202	b,3,+1	-0.016
375.278	y,3,+1	0.054
	b-NH3,6,+2	0.07
	b-H2O,6,+2	0.56
391.332	y-H2O,6,+2	0.11
	y-NH3,6,+2	-0.39
400.622	y,6,+2	0.39
487.86	y,4,+1	-0.45
622.942	a,5,+1	-0.47
670.709	y,5,+1	0.3
766.441	b,6,+1	0.0065
782.433	y-NH3,6,+1	0.0036
799.487	y,6,+1	0.031
851.426	a,7,+1	-0.098
862.711	b-NH3,7,+1	0.22
879.36	b,7,+1	-0.16

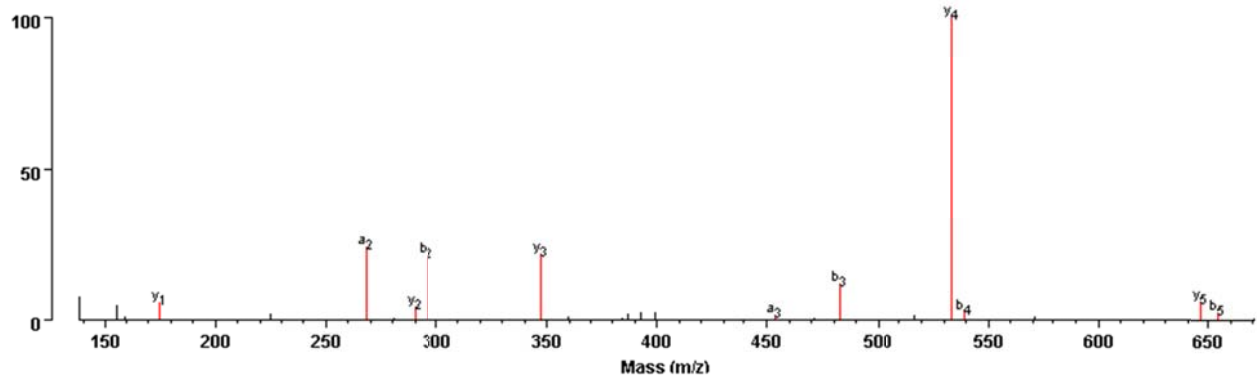
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
491.2270	4	558.724	2	KVEDMMK	414.723	2	KLWGDR

K(XL:B-Thiol(Unsaturated))VEDMMK⁺²



m/z	Ion Type	Error
253.972	y-NH3,4,+2	-0.13
	y-H2O,4,+2	0.36
278.277	y,2,+1	0.12
283.341	a,3,+2	0.22
409.405	y,3,+1	0.21
464.42	b,2,+1	0.23
593.347	b,3,+1	0.12
635.284	y-H2O,5,+1	0.031
653.308	y,5,+1	0.045
708.303	b,4,+1	0.045
752.388	y,6,+1	0.056
811.112	a,5,+1	-0.19
839.185	b,5,+1	-0.11

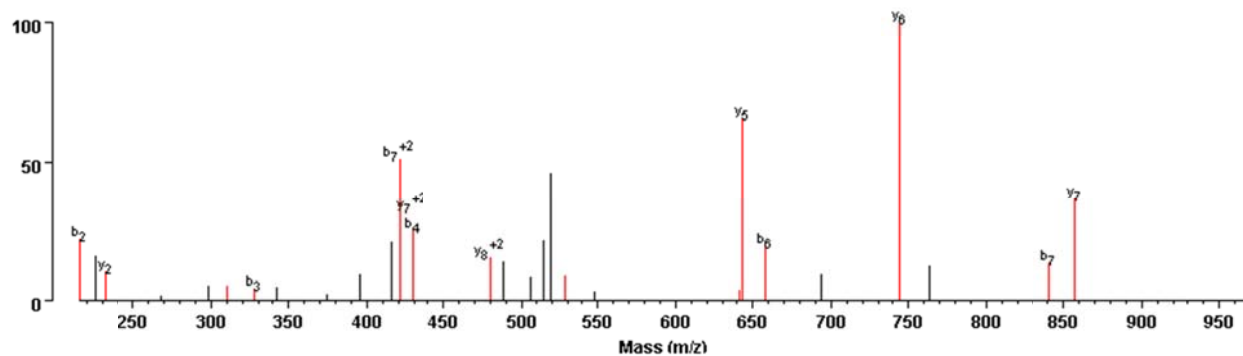
K(XL:B-Alkene)LWGDR⁺²



m/z	Ion Type	Error
175.037	y,1,+1	-0.082
268.085	a,2,+1	-0.12
290.269	y,2,+1	0.12
295.847	b,2,+1	-0.35
347.191	y,3,+1	0.024
454.122	a,3,+1	-0.16
482.729	b,3,+1	0.45
533.305	y,4,+1	0.058
539.523	b,4,+1	0.23
646.365	y,5,+1	0.034
654.285	b,5,+1	-0.04

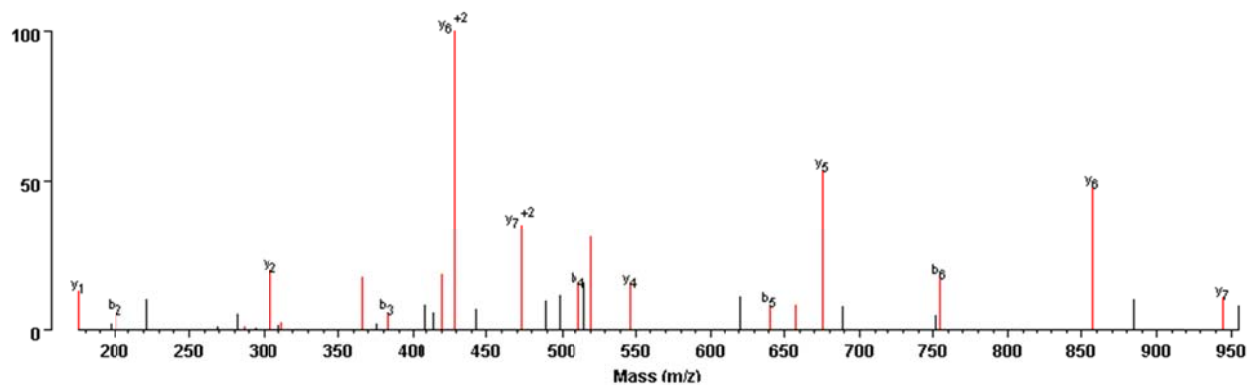
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
582.7930	4	536.290	2	ITITNDKGR	529.282	2	LSKEEIER

ITITNDK(XL:B-Alkene)GR⁺²



m/z	Ion Type	Error
215.136	b,2,+1	-0.003
	y-NH3,2,+1	0.022
232.29	y,2,+1	0.15
309.997	b-H2O,3,+1	-0.22
327.918	b,3,+1	-0.31
420.989	b,7,+2	0.26
	y-NH3,7,+2	0.27
429.783	b,4,+1	0.51
	y,7,+2	0.56
480.286	y,8,+2	0.53
527.344	MH-H2O,,+2	0.056
	MH-NH3,,+2	-0.44
641.316	b-NH3,6,+1	0.0019
643.464	y,5,+1	0.15
657.823	b,6,+1	-0.52
744.449	y,6,+1	0.086
840.767	b,7,+1	0.32
	y-NH3,7,+1	0.35
857.498	y,7,+1	0.05

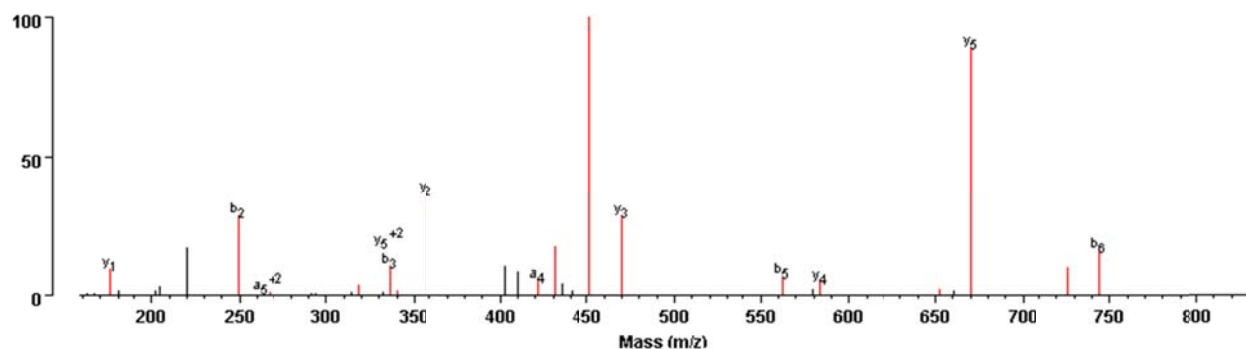
LSK(XL:B-Alkene)EEIER⁺²



m/z	Ion Type	Error
175.178	y,1,+1	0.059
200.943	b,2,+1	-0.18
	y-NH3,3,+2	0.33
286.268	y-H2O,2,+1	0.12
304.281	y,2,+1	0.12
312.46	b-NH3,5,+2	-0.19
	b-H2O,5,+2	0.3
365.384	b-H2O,3,+1	0.17
383.045	b,3,+1	-0.18
419.987	y-H2O,6,+2	-0.23
429.308	y,6,+2	0.086
472.691	y,7,+2	-0.047
511.733	b,4,+1	-0.54
520.295	MH-H2O,,+2	0.02
	MH-NH3,,+2	-0.47
546.307	y,4,+1	0.019
641.097	b,5,+1	-0.22
657.545	y-H2O,5,+1	0.22
675.345	y,5,+1	0.014
754.194	b,6,+1	-0.2
857.508	y,6,+1	0.072
944.918	y,7,+1	0.45

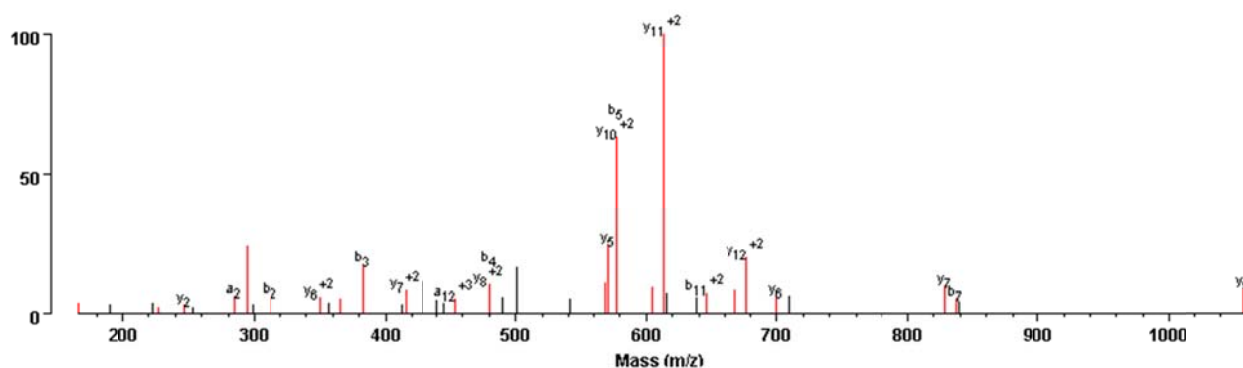
m/z	z	P1 m/z	P1 z	P1 peptide	P2 m/z	P2 z	P2 peptide
531.6768	5	459.763	2	QHSLLR	512.611	3	KEAPPMKPEVVK

Q(Gln->pyro-Glu)HSLRK(XL:B-Alkene)R⁺²



m/z	Ion Type	Error
158.076	y-NH3,1,+1	-0.016
175.187	y,1,+1	0.068
249.055	b,2,+1	-0.043
267.153	a,5,+2	-0.5
273.252	b-NH3,5,+2	0.11
318.244	b-H2O,3,+1	0.12
336.15	b,3,+1	0.02
	y,5,+2	0.43
340.319	y-NH3,2,+1	0.12
357.12	y,2,+1	-0.1
421.241	a,4,+1	0.022
430.929	b-H2O,4,+1	-0.27
450.99	MH-H2O,,+2	0.23
	MH-NH3,,+2	-0.26
470.267	y,3,+1	-0.042
562.478	b,5,+1	0.18
583.355	y,4,+1	-0.038
652.469	y-H2O,5,+1	0.055
670.421	y,5,+1	-0.0036
726.078	b-H2O,6,+1	-0.32
744.292	b,6,+1	-0.11

K(XL:B-Alkene)EAPPMEKPEVVK⁺³



m/z	Ion Type	Error
164.872	y-NH3,3,+2	0.26
227.289	y-H2O,6,+3	-0.53
246.36	y,2,+1	0.18
284.163	a,2,+1	0.0025
294.253	b-H2O,2,+1	0.11
312.034	b,2,+1	-0.12
350.22	y,6,+2	-0.0036
365.071	b-H2O,3,+1	-0.11
383.134	b,3,+1	-0.059
415.063	y,7,+2	0.32
454.242	a,12,+3	-0.33
480.274	y,8,+2	0.0088
	b,4,+1	0.029
568.633	y-NH3,10,+2	-0.17
	y-H2O,10,+2	0.32
571.594	y,5,+1	0.25
577.551	y,10,+2	0.23
	b,5,+1	0.25
604.295	y-NH3,11,+2	-0.028
	y-H2O,11,+2	0.46
613.046	y,11,+2	0.21
645.973	b,11,+2	0.15
668.972	y-NH3,12,+2	0.13
677.357	y,12,+2	-7.70E-04
699.608	y,6,+1	0.17
828.085	y,7,+1	-0.4
837.383	b,7,+1	0.0019
1056.31	y,9,+1	-0.27