

Supplementary table: Mass and charge states observed for the ETD fragment ions from the [NCX+4H]⁴⁺(Figure 1C), [NCX+5H]⁵⁺(Figure 2C), and [NCX+6H]⁶⁺(Figure 2D).

AP= Acidic peptide SAQEpSQGNT, BP= Basic peptide RRRRKRVTNKRSSR

Fragment ion	Notation on figure	ETD NCX ⁴⁺ (Figure1C)			ETD NCX ⁵⁺ (Figure2C)			ETD NCX ⁶⁺ (Figure2D)		
		+	2+	3+	+	2+	3+	+	2+	3+
[AP+Z'14]	z*14		1420.737	947.493		1420.73	947.496		1420.74	947.495
[AP+Z'13]	z*13		1342.701	895.47		1342.703	895.478		1342.701	895.47
[AP+Z'12]	z*12		1264.621				843.425			843.429
[AP+C13]	c*13		1350.201			1350.207	900.473		1350.206	900.474
[AP+C12]	c*12		1306.684			1306.689	871.459		1306.689	871.458
[AP+C11]	c*11		1263.168			1263.169	842.449		1263.171	842.446
[AP+C10]	c*10		1185.119			1185.117	790.417		1185.122	790.418
[AP+C9]	c*9		1121.07			1121.074			1121.072	
[AP+C8]	c*8		1070.547			1070.551			1070.549	
[AP+C7]	c*7		1013.524			1013.525			1013.528	
[AP+C6]	c*6	1926.975	963.993			963.984		1926.976	963.99	
[AP+C5]	c*5	1770.877	885.942		1770.882	885.945		1770.88	885.944	
[AP+C4]	c*4	1642.783	821.894		1642.789	821.897		1642.79	821.897	
[AP+C3]	c*3					743.852		1486.693	743.847	
[Z'9+BP]	z*9		1420.737	947.493		1420.73	947.496		1420.74	947.495
[Z'8+BP]	z*8		1377.217	918.482		1377.22	918.486		1377.219	918.487
[Z'7+BP]	z*7		1341.691	894.806		1341.69			1341.707	
[Z'6+BP]	z*6		1277.675	852.116		1277.666			1277.674	
[Z'5+BP]	z*5		1213.15	809.104						
[C8+BP]	c*8		1377.722	918.817		1377.722	918.82		1377.721	918.822
[C7+BP]	c*7		1320.706	880.805				1320.689	880.797	
[C6+BP]	c*6		1292.196	861.798						
[C5+BP]	c*5		1228.167	819.112						
Z'11	z'11				1371.812			1371.812	686.406	
Z'10	z'10				1215.719	608.361		1215.71	608.361	
Z'9	z'9	1087.622			1087.623	544.313		1087.623	544.313	
Z'8	z'8	931.518			931.52			931.518	466.263	
Z'7	z'7	832.447			832.45	416.729		832.45	416.729	
Z'6	z'6	718.404			718.407	359.705		718.408	359.708	
Z'5	z'5	617.359			617.36			617.359		
Z'4	z'4	489.264			489.265			489.265		
Z'3	z'3				333.164			333.164		
Z'2	z'2				246.132			246.132		
Z'1	z'1				159.1					
C3	c3	486.336						486.344		
C2	c2	330.235			330.236			330.236		
C1	c1				174.135					