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MDPI

Supplementary Materials

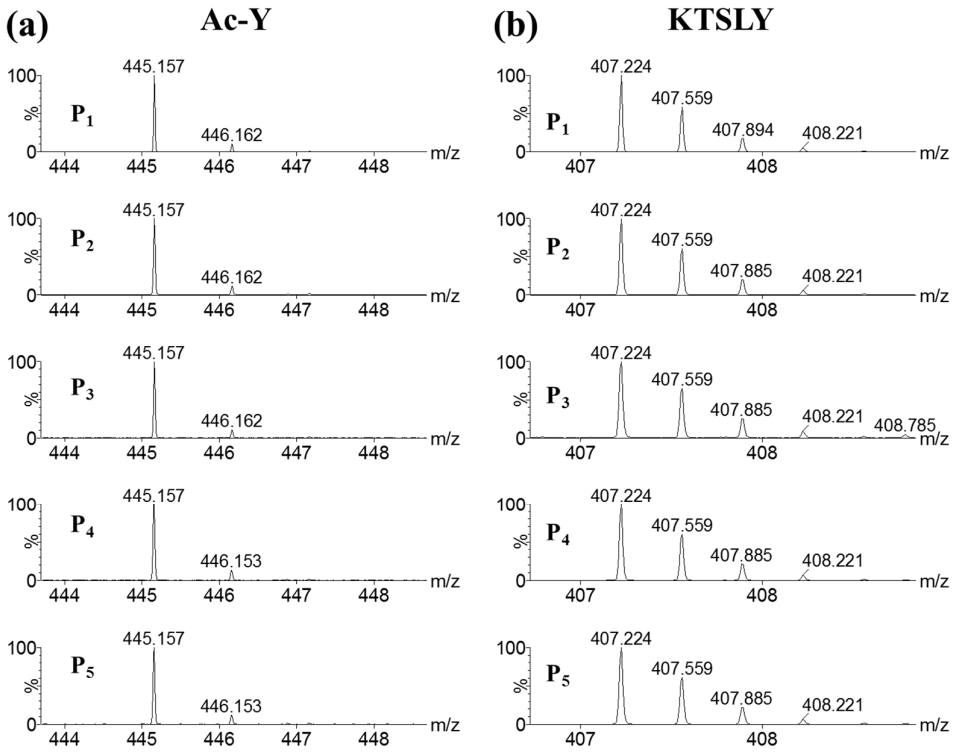

Figure S1: Oxidation of Ac-Y (a) and KTSLY peptide (b) in H_2O. Full scan MS spectra extracted at RT of dimers.

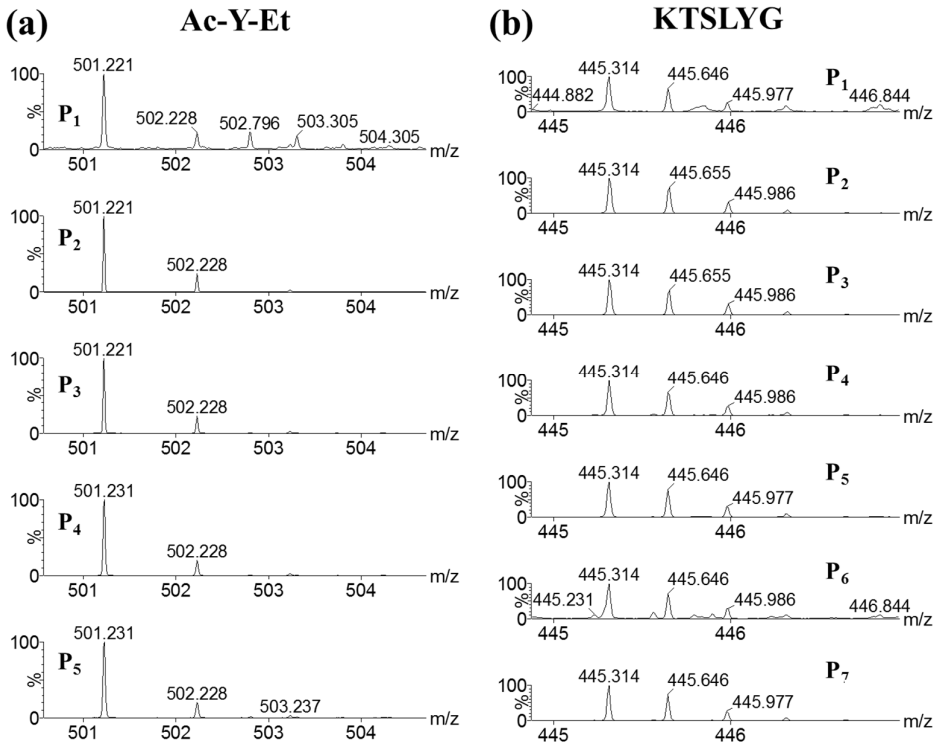

Figure S2: Oxidation of Ac-Y-Et (a) and KTSLYG peptide (b) in H_2O. Full scan MS spectra extracted at RT of dimers.

Species \ Monoisotopic *m/z*	**Monomer** *(theoretical)*	**Dimer** $[M+xH]^{x+}_{dimer} = \frac{2 * M_{monomer} - 2 * M(H) + x * M(H)}{x}$		
		$[M+H]^+$ *(theoretical)*	**Selected $[M+xH]^{x+}$** *(theoretical)*	**Detected $[M+xH]^{x+}$** (*experimental*)
Ac-Y	223.085	445.161^+	445.161^+	445.157^+
Ac-Y-Et	251.116	501.224^+	501.224^+	501.223^+
KTSLY peptide	611.341	1219.657^+	407.224^{3+}	407.235^{3+}
KTSLYG peptide	668.362	1333.700^+	445.238^{3+}	445.314^{3+}
^{168}KTSLY^{172} in CEN2	611.341	1219.657^+	610.332^{2+} [M+2H+1] 610.836^{2+}	610.336^{2+} [M+2H+1] 610.832^{2+}
^{92}V-R^{107} in CaM	1753.864	3506.719^+	702.150^{5+}	702.144^{5+}
^{92}V-R^{107} in CaM **^{128}E-K^{149} in CaM**	1753.864 2489.073	4241.928^+	849.191^{5+}	849.178^{5+}

Table S1: Theoretical and experimental *m*/*z* of considered species.

		P_1	P_2	P_3	P_4	P_5	P_6	P_7
Ac-Y	T0	0.03	0.70	0.94	-0.01	ND	-	-
	T48	-0.01	ND	ND	-0.02	**2.24**	-	-
KTSLY	T0	0.09	0.87	0.75	0.09	1.35	-	-
	T5	0.05	1.59	1.64	0.07	**3.26**	-	-
	T48	0.10	ND	ND	0.07	**3.85**	-	-
Ac-Y-Et	T0	0.86	0.39	1.56	0.01	-0.04	-	-
	T48	ND	-0.03	**2.70**	0.01	**2.66**	-	-
KTSLYG	T0	0.06	0.70	1.83	0.14	1.44	ND	ND
	T72	0.01	ND	**3.49**	0.01	**3.53**	**3.44**	**2.93**

Table S2: Average deuterium incorporation after H/D exchange for the different chromatographic peaks.