

Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Coupling matrix-assisted ionization with high resolution mass spectrometry and electron transfer dissociation to characterize intact proteins and post-translational modifications

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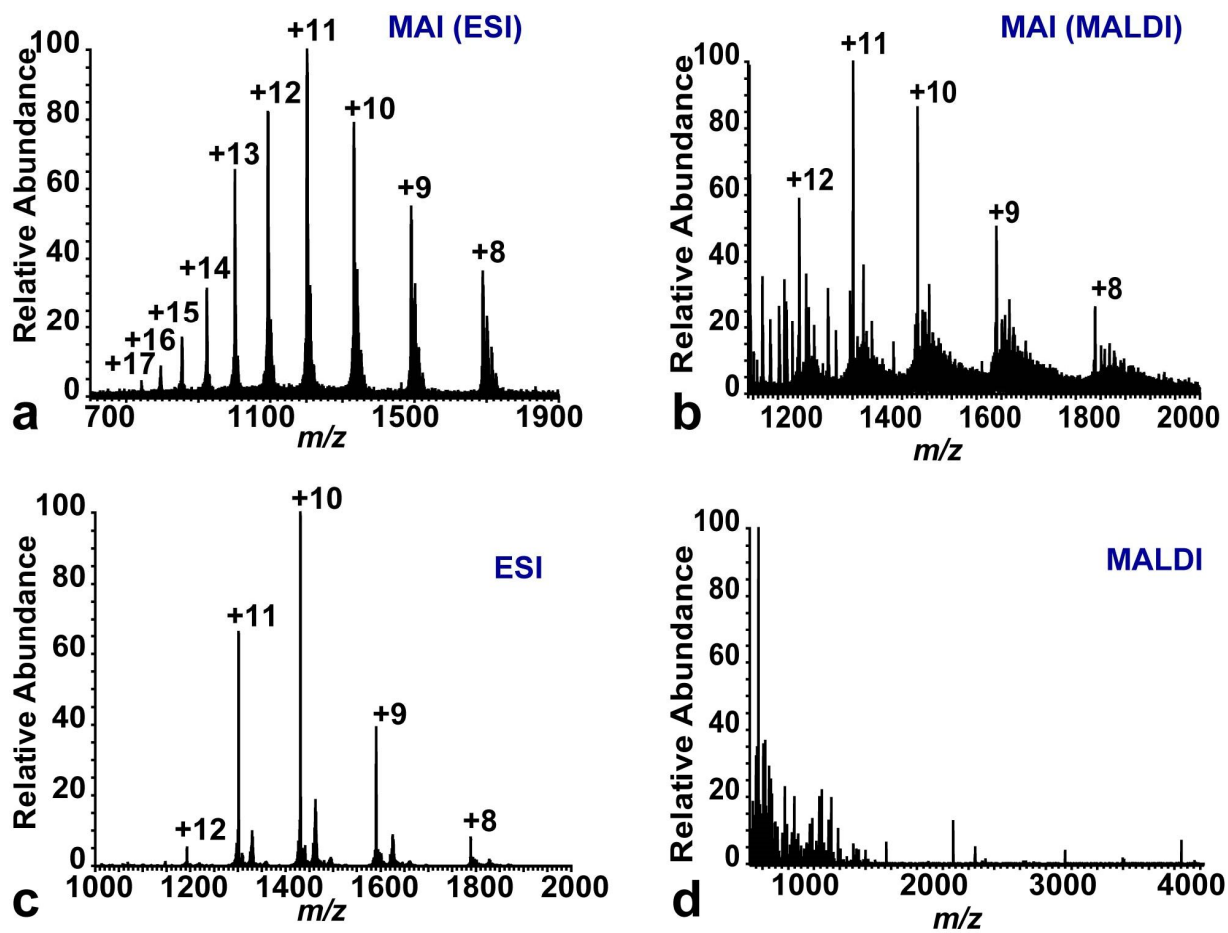


Fig. S1 Spectra comparison of lysozyme ionized by MAI (ESI) (a), MAI (MALDI) (b), ESI (c), and MALDI (d). The charge states were annotated on the spectra

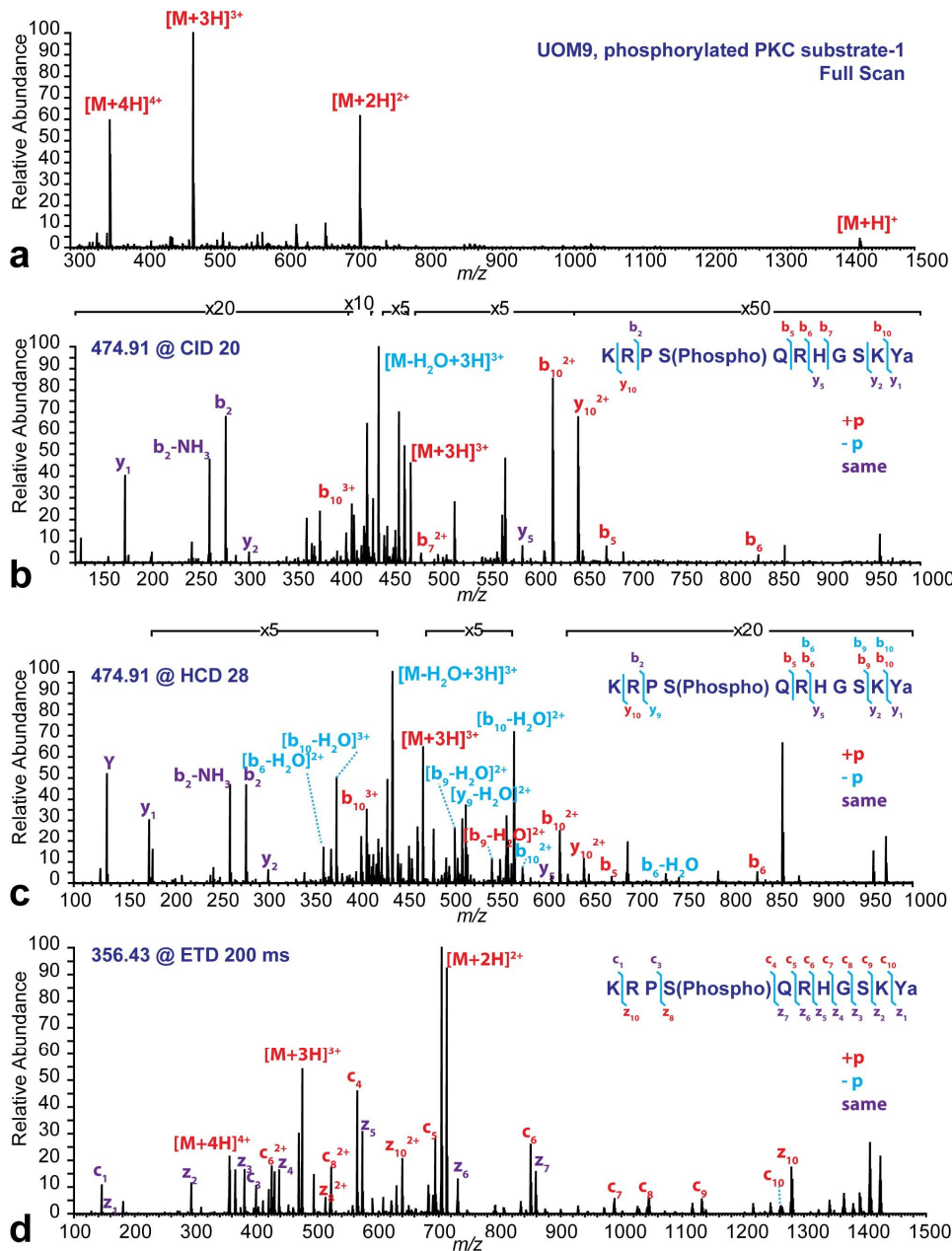


Fig. S2 MAI full MS (a), CID (b), HCD (c) and ETD (d) spectra of the phosphopeptide UOM9 (phosphorylated PKC substrate). The detected ion species on the full scan were annotated on the spectrum. NCEs or activation time were labeled on the figure. The detected fragments under each condition were annotated on the spectra and listed on the peptide sequence. The red letters represent the fragments with phosphate group preserved, the blue letters represent the fragments with phosphate group detached and the purple letters represent the fragments before phosphate group

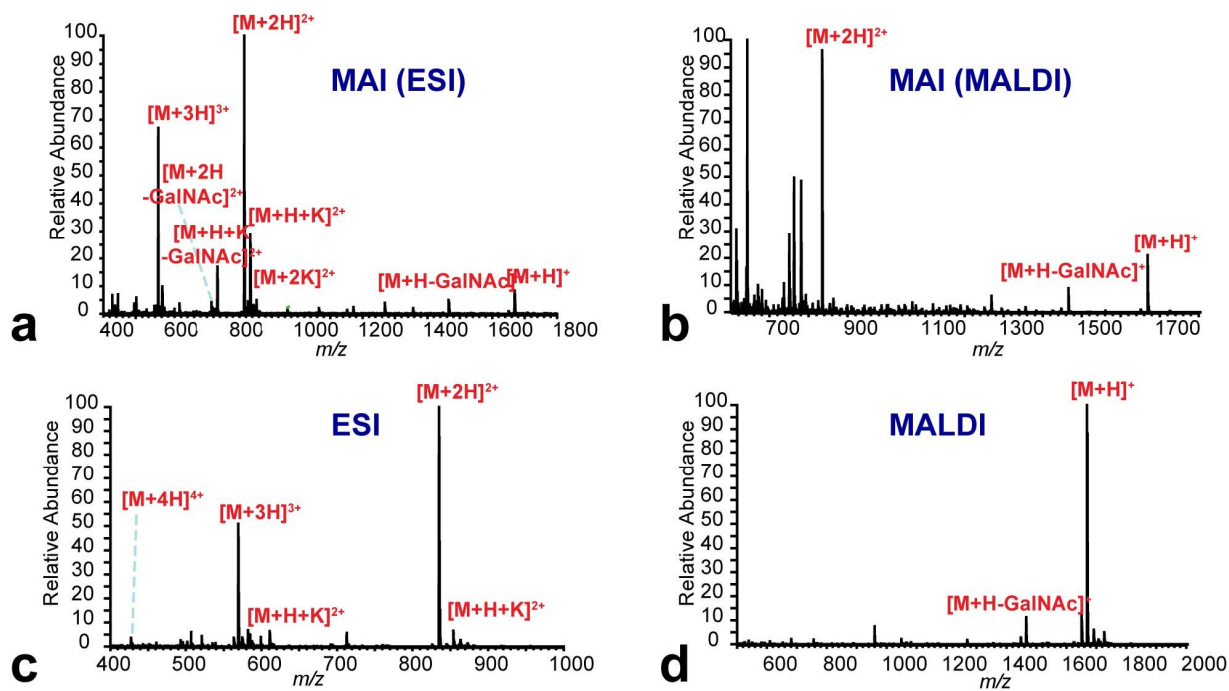


Fig. S3 Spectra comparison of glycopeptide EPO ionized by MAI (ESI) (a), MAI (MALDI) (b), ESI (c) and MALDI (d). The detected ion species were annotated on the spectra

Table S1 Proteins identified on MAI (MALDI) MS platform from rat brain protein extraction. Protein's theoretical mass, experimental mass and mass error were listed

Protein Name	Theoretical Mass (Da)	Experimental Mass (Da)	Mass Error (ppm)
Acyl-CoA-binding protein	9932.12	9932.19	7.05
ATP synthase-coupling factor 6	8921.55	8921.57	2.24
Cytochrome c oxidase subunit 6b	9971.80	9971.75	-5.01
Mitochondria import inner membrane translocase	10276.08	10276.05	-2.92
Superoxidase dismutase [Cu-Zn]	15810.82	15810.91	5.69
Thymosin beta 4	4960.48	4960.57	18.14
Ubiquitin	8560.63	8560.47	-18.69

Table S2 Phospho-depleted and phosphorylated peptides detected from alpha-casein digest (both phospho-depleted and IMAC enriched fractions). The theoretical mass, experimental mass and mass error for tryptic digest peptides were listed

	Alpha-Casein Digest	Theoretical Mass [M+H]⁺	Experimental Mass [M+H]⁺	Mass Error (ppm)
Phospho-depleted	23-37	1759.9450	1759.9476	1.49
	38-49	1384.7300	1384.7320	1.47
	106-115	1267.7045	1267.7060	1.18
	140-166	3207.5932	3207.5971	1.20
	148-166	2316.1369	2316.1394	1.08
	209-214	748.3698	748.3707	1.16
Phosphorylated	52-73 (P56, 61, 63)	2678.0229	2678.0251	0.84
	58-73 (P61,63)	1927.6916	1927.6925	0.45
	58-94 (P61,63,79,81,82,83,90)	4629.5867	4629.6024	3.40
	119-134 (P130)	1951.9525	1951.9511	0.71
	121-134 (P130)	1660.7942	1660.7937	0.28
	121-139 (P130)	2257.1046	2257.1027	0.86