

Multiplex relative quantitation of peptides and proteins using amine-reactive metal element chelated tags coupled with mass spectrometry

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Electronic Supporting Information

Table S1 The synthetic peptides selected to verify the labeling efficiency in our paper.

No.	Sequence of peptides	m/z	PI	Value of hydrophobicity	m/z (DOTA-P)	m/z (Tb-DOTA-P)
1	AGYTAIVSHR	1074.57	8.8	0.14	1460.75	1616.65
2	LAELEAALQR	1113.63	4.53	0.18	1499.81	1655.71
3	VLDGAVSEDGR	1117.55	4.03	-0.236	1503.73	1659.63
4	GFYIYQEGSK	1191.57	6.00	-0.78	1963.93	2275.73
5	GNLGAGNGNLQGPR	1324.67	9.75	-0.907	1710.85	1866.75
6	NQNSWGTGEDVK	1334.60	4.37	-1.7	2106.96	2418.76
7	TATVDDIDNIYR	1395.68	3.93	-0.517	1781.85	1937.76
8	AFPAWADTSILSR	1434.74	5.88	0.285	1820.92	1976.82
9	TLTDEEVNEVHAR	1512.73	4.40	-0.969	1898.91	2054.81
10	SYVYGPIPTFDR	1551.76	6.46	-0.569	1937.94	2093.84

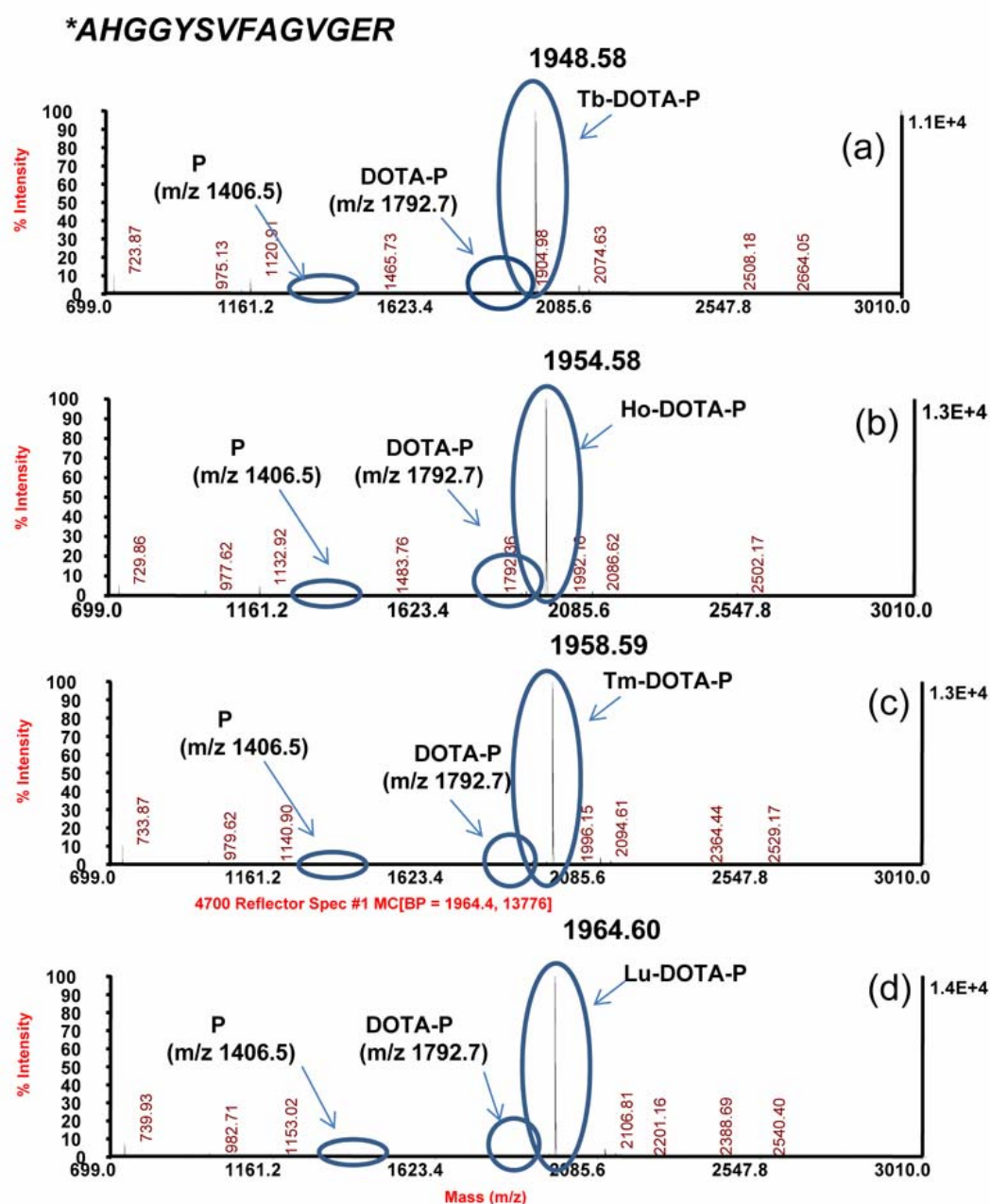


Figure S1 MALDI-TOF MS spectra of M-DOTA-AHGGYSVFAGVGER (Tb(a), Ho (b), Tm (c) and Lu (d) respectively) dissolving in 0.1% TFA at 4°C for 24h. The metal tag is indicated by an asterisk incorporating at the N-terminus.

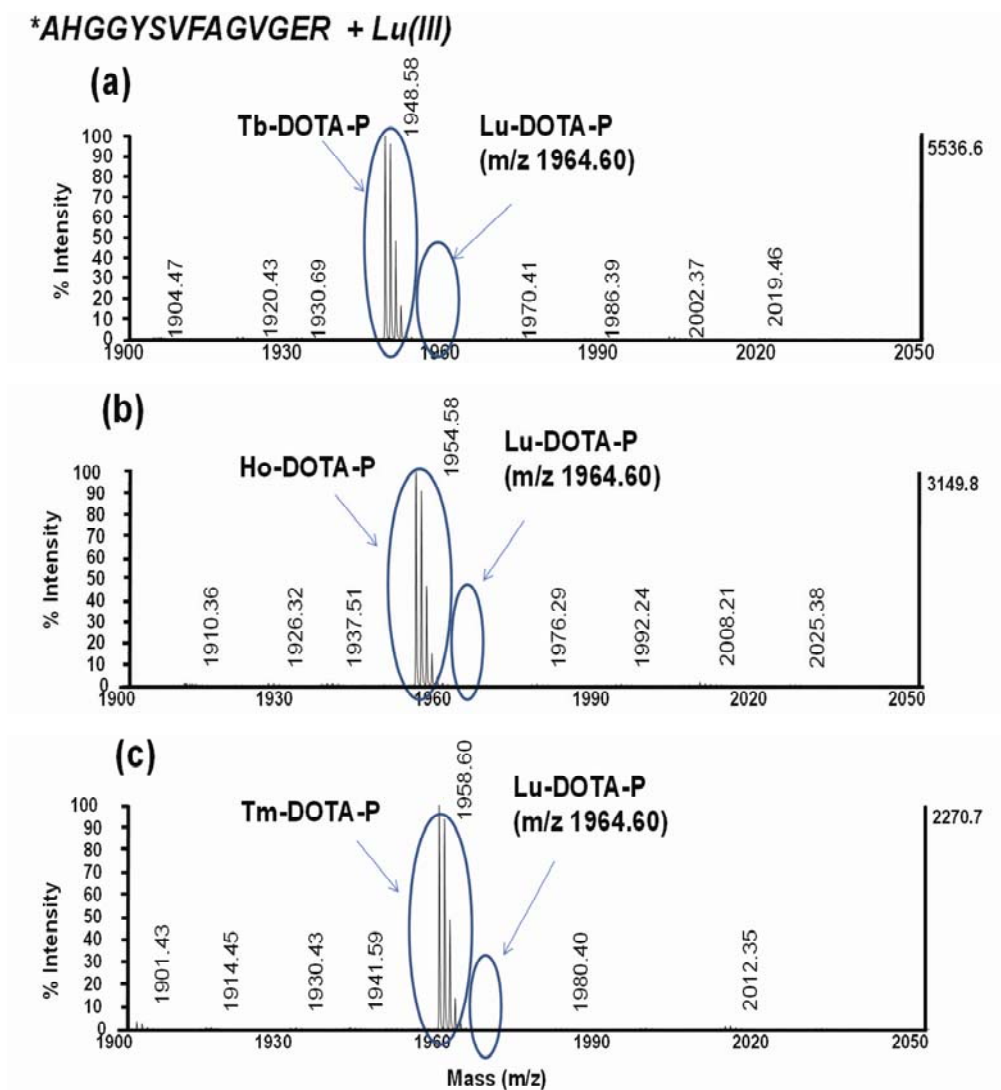


Figure S2 MS analysis of the reaction solutions of Tb-DOTA-AHGGYSVFAGVGER (a), Ho-DOTA-AHGGYSVFAGVGER(b) and Tm-DOTA-AHGGYSVFAGVGER (c) incubating with 2 equivalents LuCl₃ solution at 37 °C for 1h. The metal tag is indicated by an asterisk incorporating at the N-terminus of the peptide AHGGYSVFAGER.

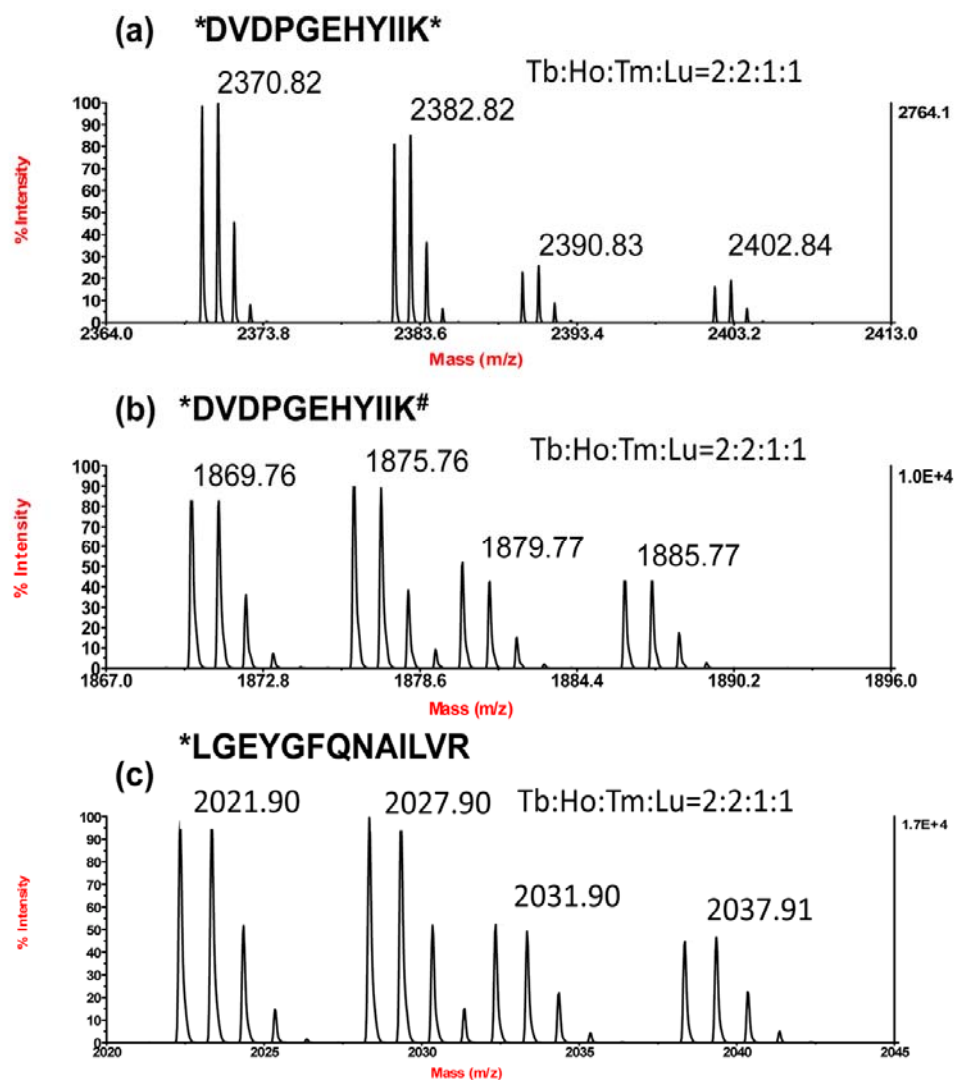


Figure S3 MALDI-MS spectra of the Tb-, Ho-, Tm- and Lu-plex MECT labeled peptides at molar ratio of 2:2:1:1. The panel(a), (b) and (c) are the spectra of peptide DVDPGEHYIIK, its K-guanidinated counterpart and the control peptide LGEYGFQNAILVR, respectively. “#” indicates the guanidination of ϵ - amino group of lysine; “*” indicates the MECT tag.

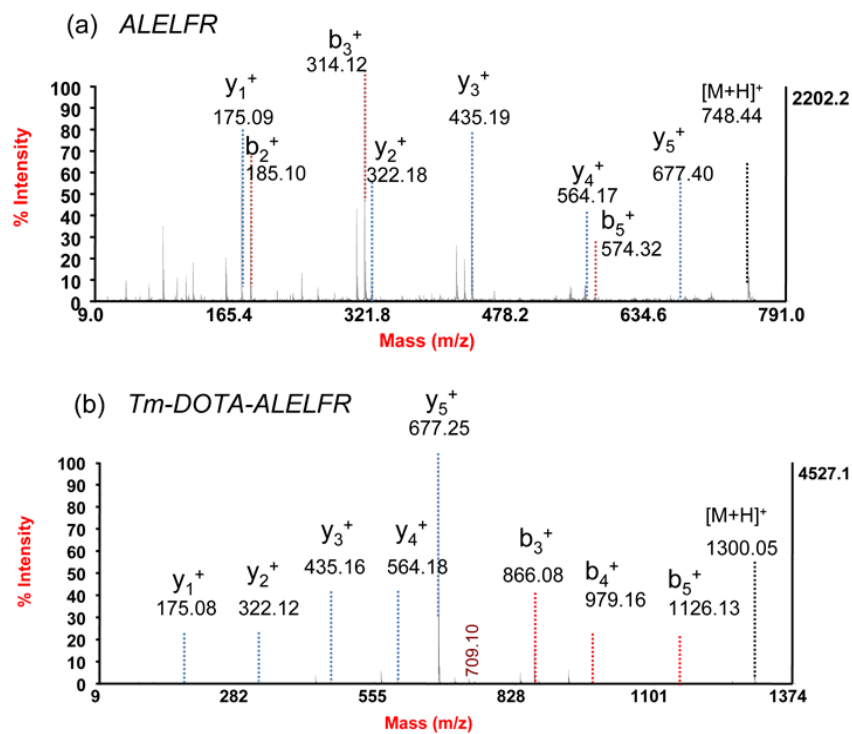


Figure S4 The CID fragments of the peptide ALELFR (a) and its Tm-MECT labeled peptide (b) in MALDI-MS/MS.

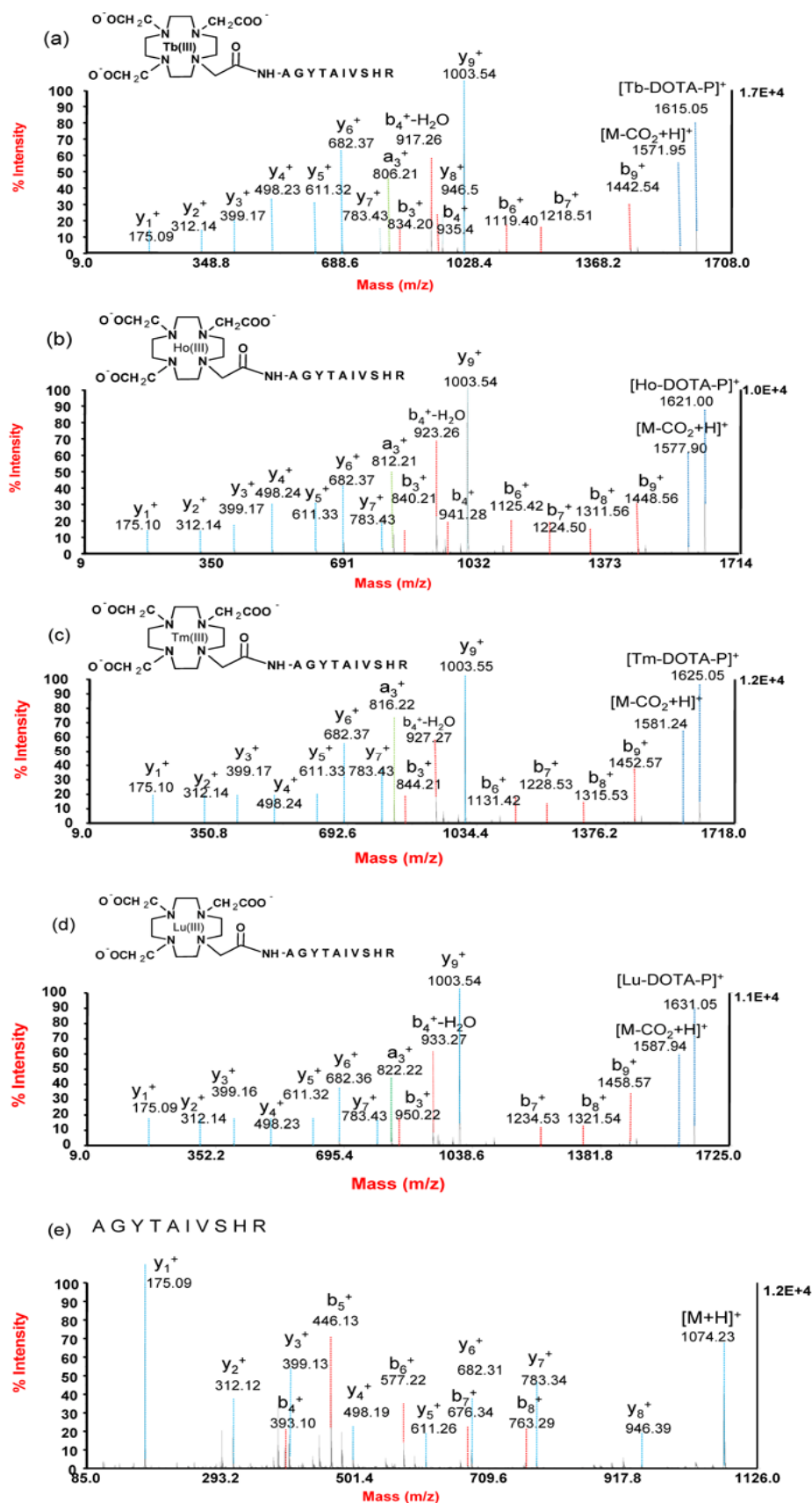


Figure S5 The CID fragments of the Tb, Ho-, Tm-, Lu-labeled peptides AGYTAIVSHR and its counterpart-in MALDI-MS/MS.