Supporting Information

N-Phosphorylation labeling for analysis of twenty natural amino acids and small peptides using matrix-assisted laser desorption/ionization time-of-flight mass spectrometry

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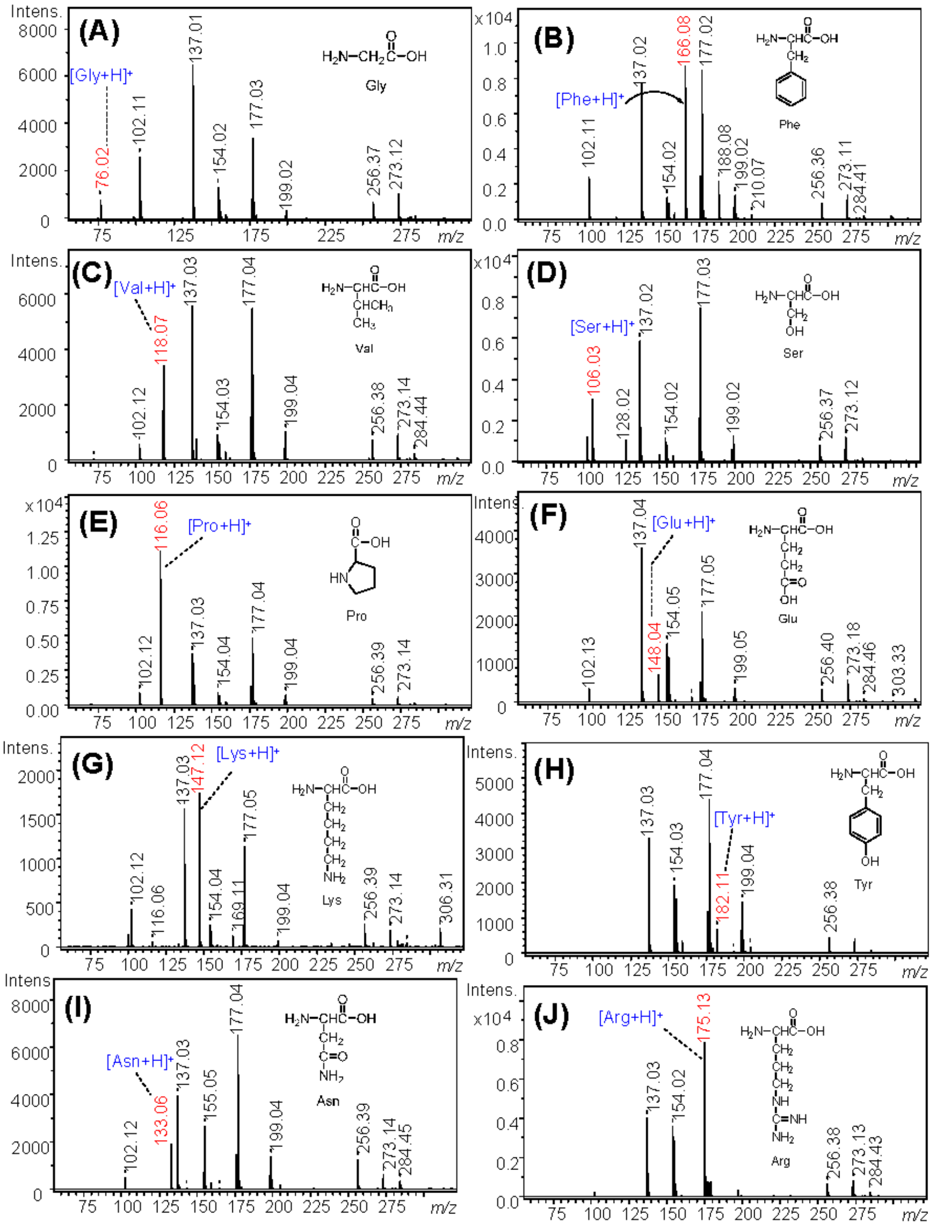
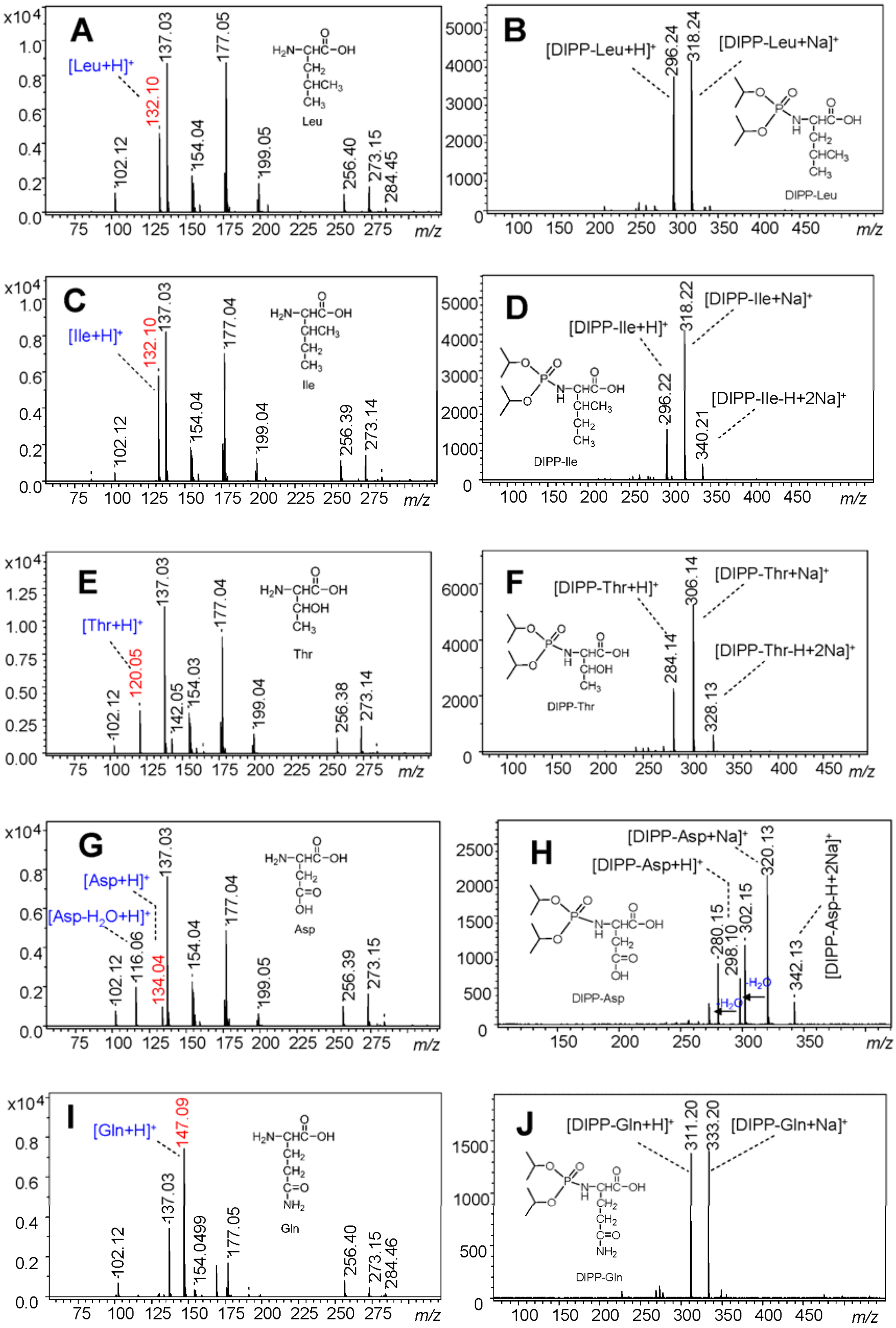


Fig. S1 MALDI-TOF MS spectra of amino acids without N-phosphorylation labeling with DHB as matrix in positive ion mode. (A) Gly (5 mM); (B) Phe (5 mM); (C) Val (5 mM); (D) Ser (5 mM); (E) Pro (5 mM); (F) Glu (5 mM); (G) Lys (5 mM); (H) Tyr (5 mM); (I) Asn (5 mM); (J) Arg (5 mM). The insets are the chemical structures of amino acids.


A
x10⁴
[Leu+H]⁺
102.12
132.10
137.03
154.04
177.05
199.05
256.40
273.15
284.45
Leu
m/z
B
[DIPP-Leu+H]⁺
296.24
318.24
[DIPP-Leu+Na]⁺
DIPP-Leu
m/z
C
[Ile+H]⁺
102.12
132.10
137.03
154.04
177.04
199.04
256.39
273.14
Ile
m/z
D
[DIPP-Ile+H]⁺
296.22
318.22
[DIPP-Ile+Na]⁺
[DIPP-Ile-H+2Na]⁺
340.21
DIPP-Ile
m/z
E
[Thr+H]⁺
102.12
120.05
137.03
142.05
154.03
177.04
199.04
256.38
273.14
Thr
m/z
F
[DIPP-Thr+H]⁺
284.14
306.14
[DIPP-Thr+Na]⁺
[DIPP-Thr-H+2Na]⁺
328.13
DIPP-Thr
m/z
G
[Asp+H]⁺
[Asp-H2O+H]⁺
102.12
116.06
134.04
137.03
154.04
177.04
199.05
256.39
273.15
Asp
m/z
H
[DIPP-Asp+Na]⁺
[DIPP-Asp+H]⁺
280.15
298.10
302.15
320.13
342.13
[DIPP-Asp-H+2Na]⁺
-H2O
-H2O
DIPP-Asp
m/z
I
[Gln+H]⁺
102.12
137.03
147.09
154.0499
177.05
256.40
273.15
284.46
Gln
m/z
J
[DIPP-Gln+H]⁺
311.20
333.20
[DIPP-Gln+Na]⁺
DIPP-Gln
m/z

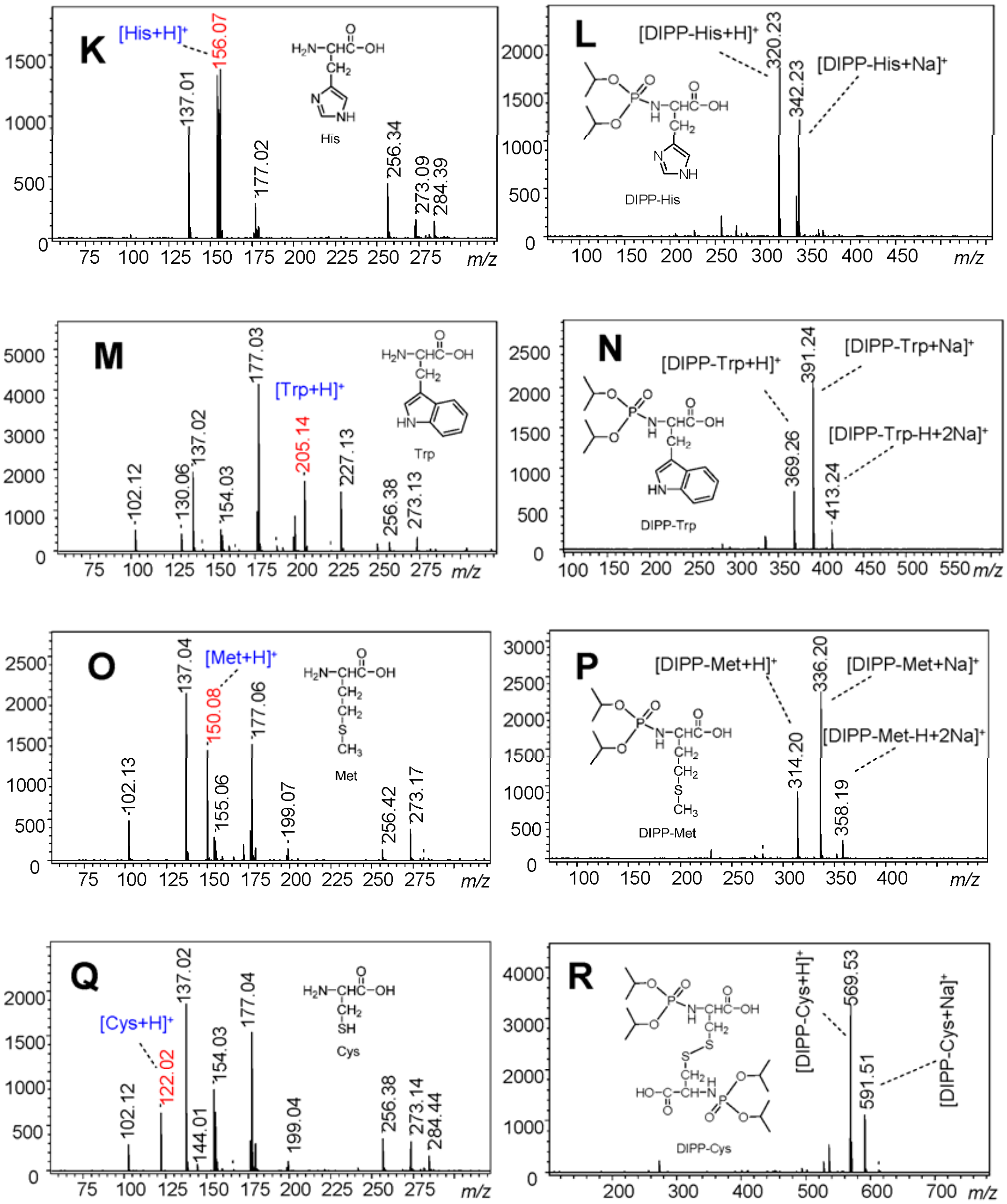


Fig. S2 Comparison of MALDI-TOF MS spectra of amino acids and N-phosphoryl amino acids (DIPP-AAs) with DHB as matrix in positive ion mode. (A) Leu (5 mM); (B) DIPP-Leu (1 mM); (C) Ile (5 mM); (D) DIPP-Ile (1 mM); (E) Thr (5 mM); (F) DIPP-Thr (1 mM); (G) Asp (5 mM); (H) DIPP-Asp (1 mM); (I) Gln (5 mM); (J) DIPP-Gln (1 mM); (K) His (5 mM); (L) DIPP-His (1 mM); (M) Trp (5 mM); (N) DIPP-Trp (1 mM); (O) Met (5 mM); (P) DIPP-Met (1 mM); (Q) Cys (5 mM); (R) di-DIPP-Cys (1 mM). The insets are the chemical structures of amino acids and DIPP-AAs.

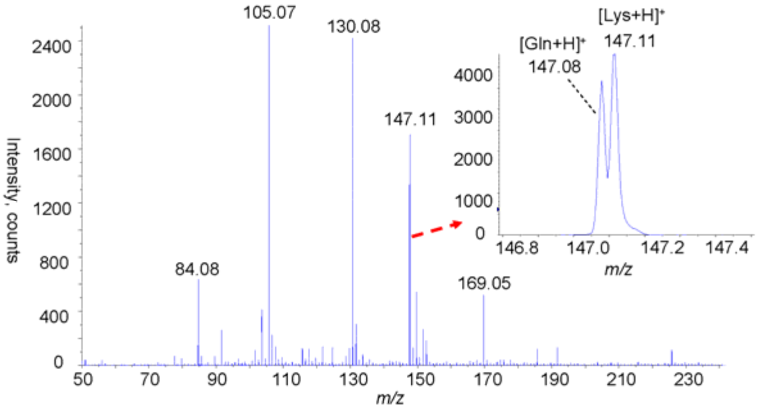


Fig. S3 Nano ESI-TOF MS spectrum of amino acid mixture of Lys and Gln in positive ion mode.