

*Analyst*

**Ionization characteristics of amino acids in direct analysis in real time  
mass spectrometry**

Kanako Sekimoto<sup>1\*</sup>, Motoshi Sakakura<sup>2</sup>, Takatomo Kawamukai<sup>2</sup>, Hiroshi Hike<sup>2</sup>, Teruhisa

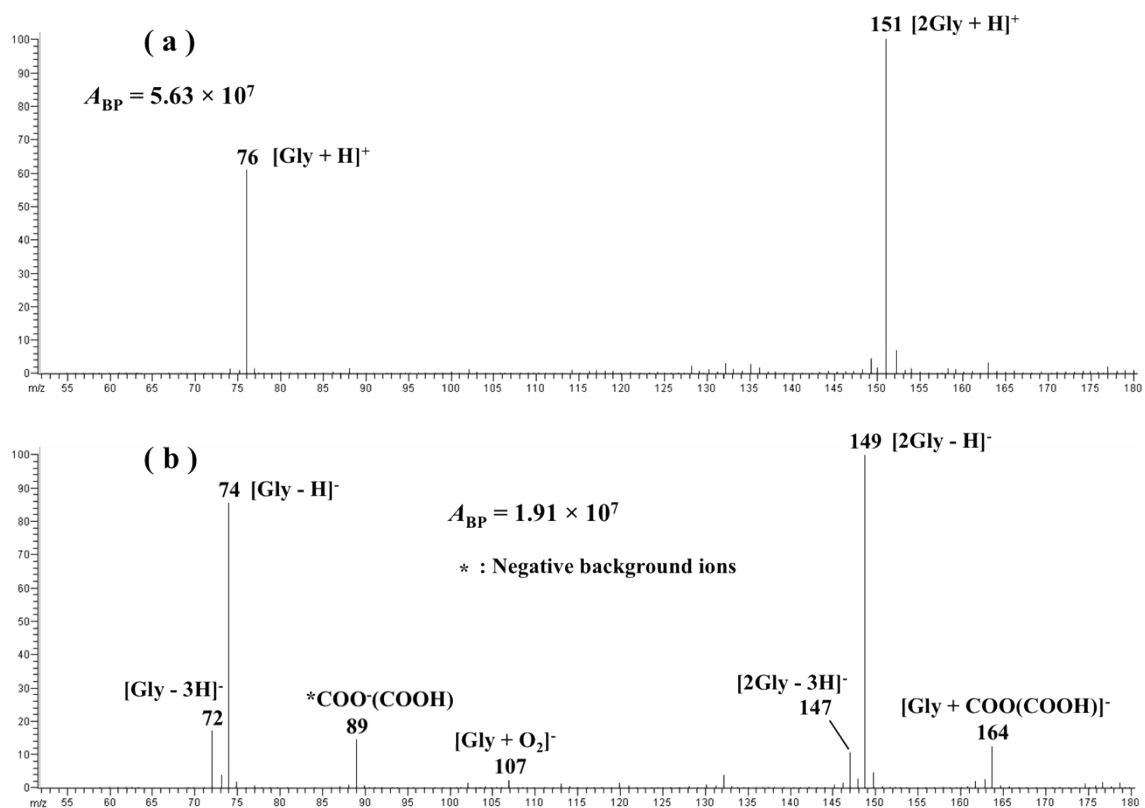
Shiota<sup>2</sup>, Fumihiko Usui<sup>2</sup>, Yasuhiko Bando<sup>2</sup> and Mitsuo Takayama<sup>1</sup>

<sup>1</sup>Graduate School of Nanobioscience, Yokohama City University, 22-2 Seto, Kanazawa-ku,

Yokohama, Kanagawa, 236-0027 Japan

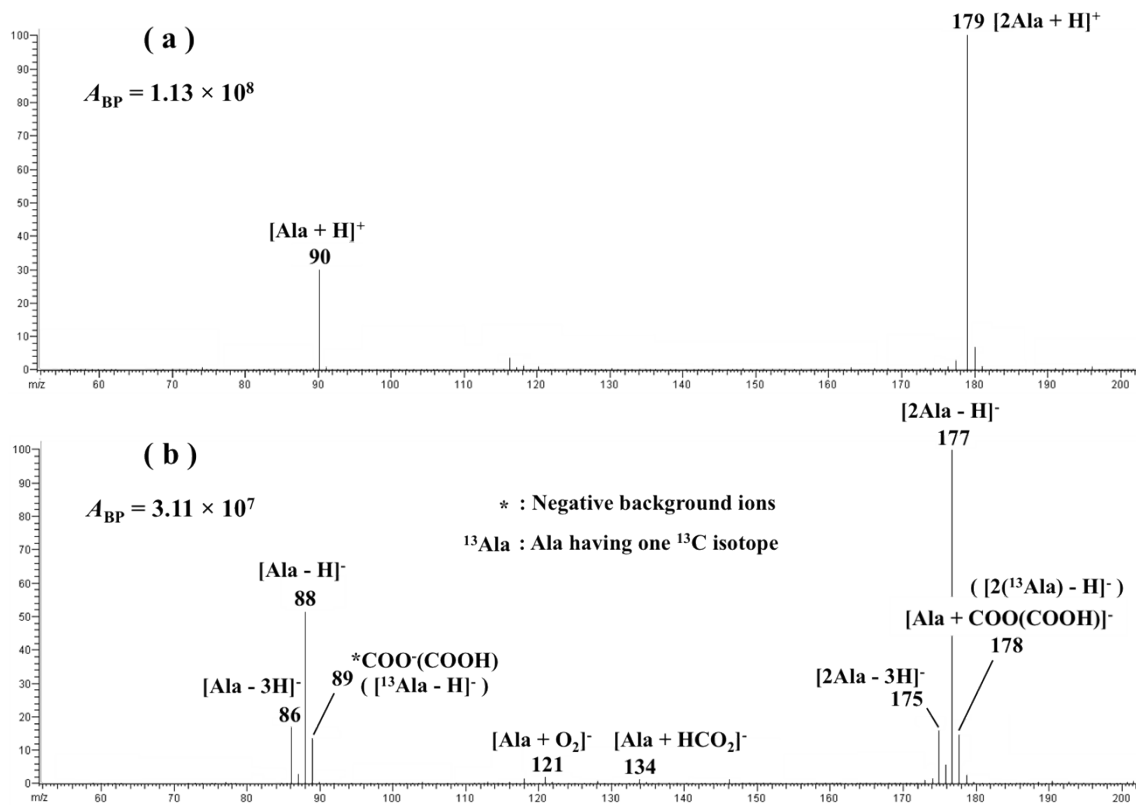
<sup>2</sup>AMR Inc., 13-18 Nakane-2, Meguro-ku, Tokyo, 152-0031 Japan

**Electronic Supplementary Material**



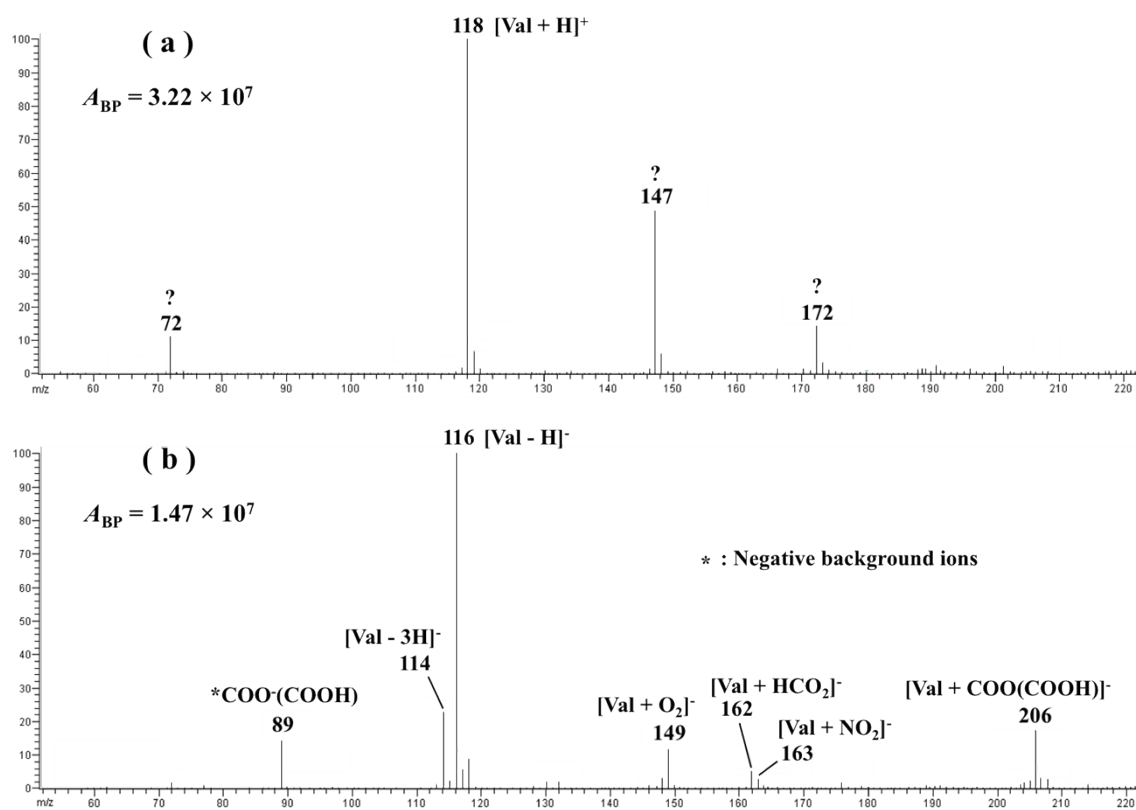
**Figure S1. (a) Positive- and (b) negative-ion DART mass spectra of glycine (Gly; Mr 75).**

$A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.



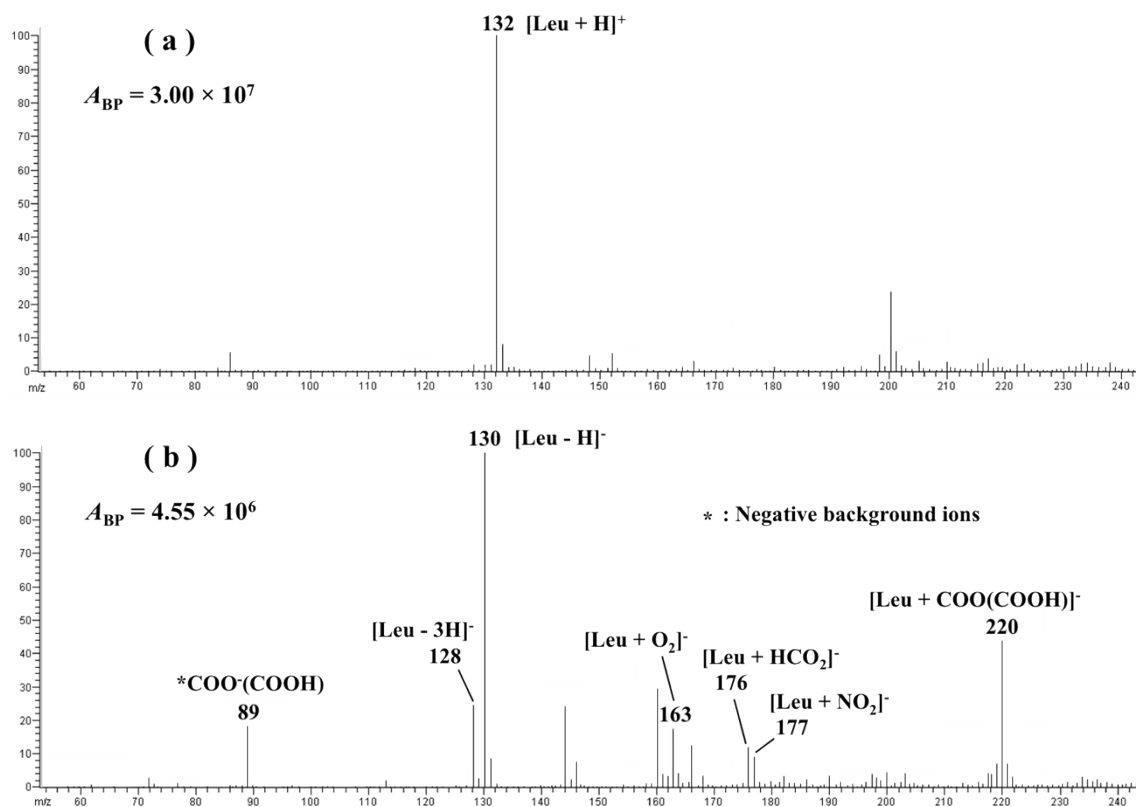
**Figure S2. (a) Positive- and (b) negative-ion DART mass spectra of L-alanine (Ala; Mr 89).**

$A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.

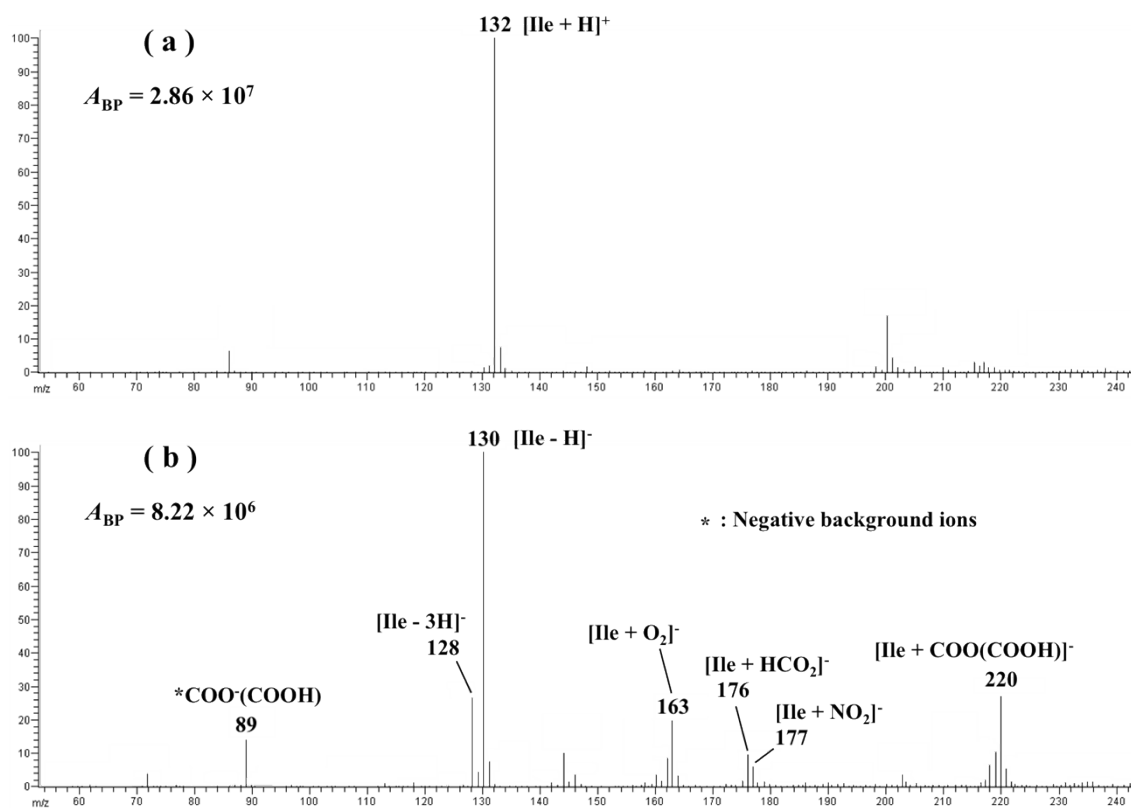


**Figure S3. (a) Positive- and (b) negative-ion DART mass spectra of L-valine (Val; Mr 117).**

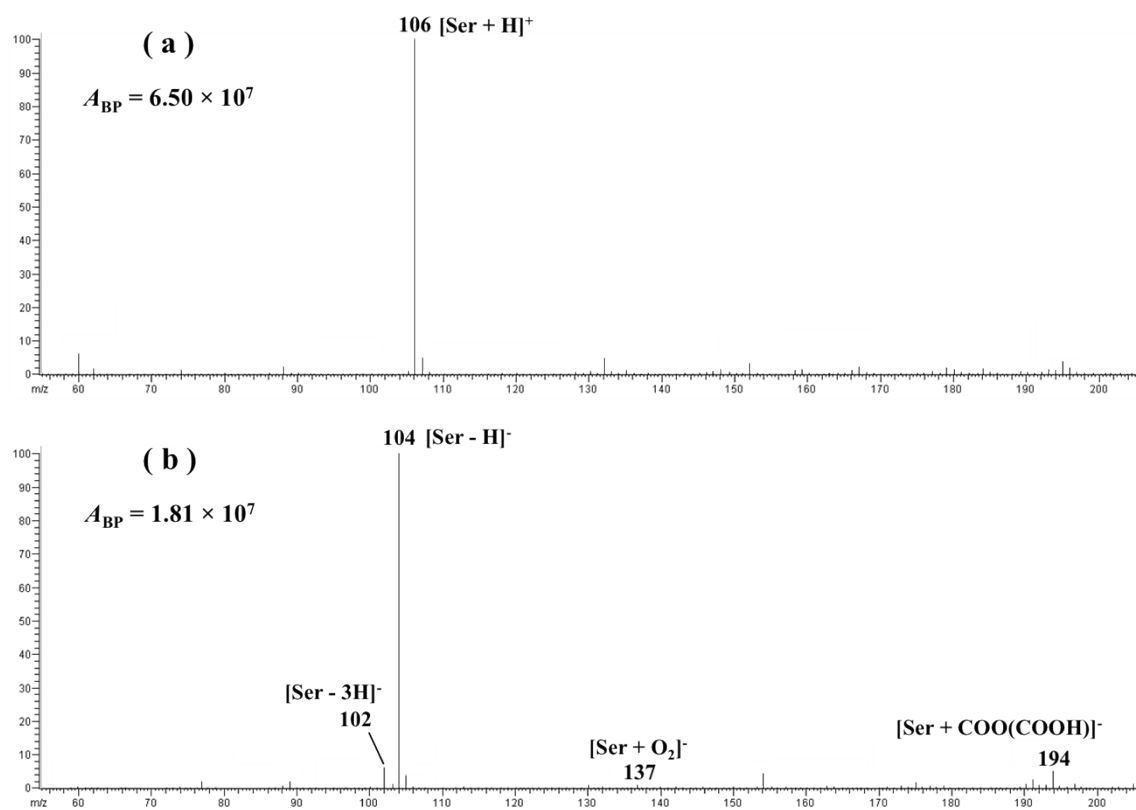
$A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.



**Figure S4. (a) Positive- and (b) negative-ion DART mass spectra of L-leucine (Leu; Mr 131).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**

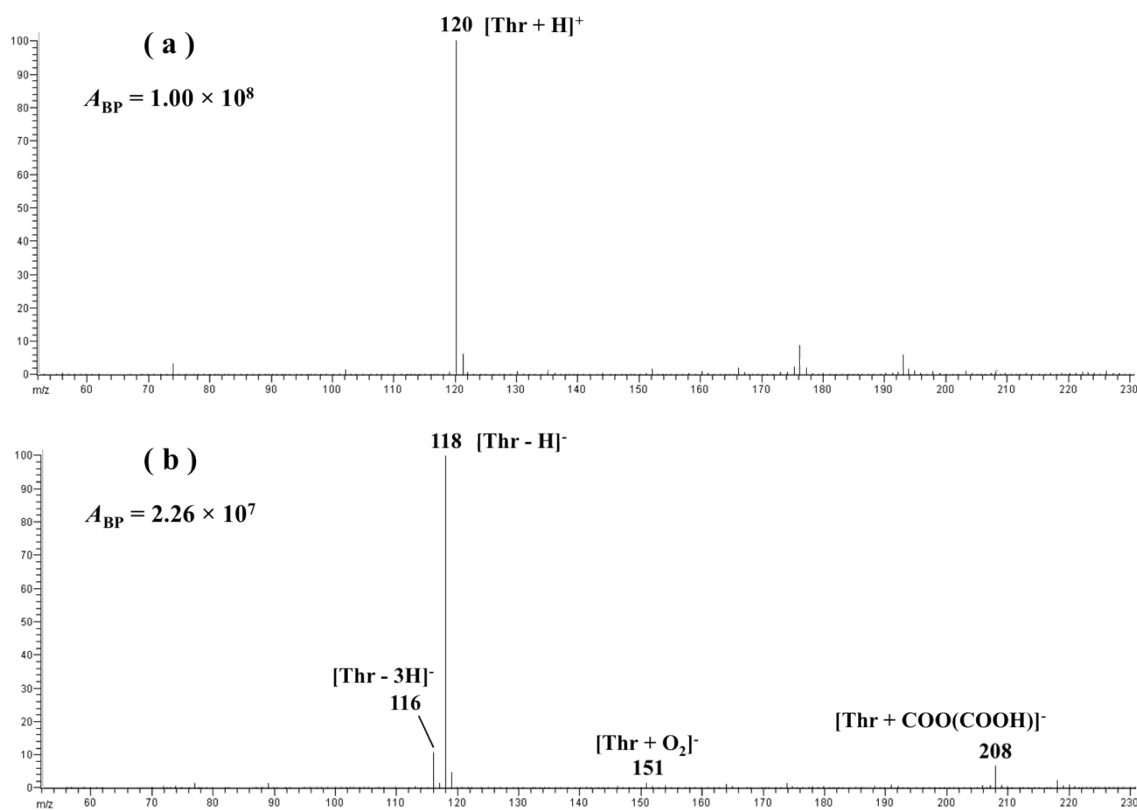


**Figure S5. (a) Positive- and (b) negative-ion DART mass spectra of L-isoleucine (Ile; Mr 131).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**



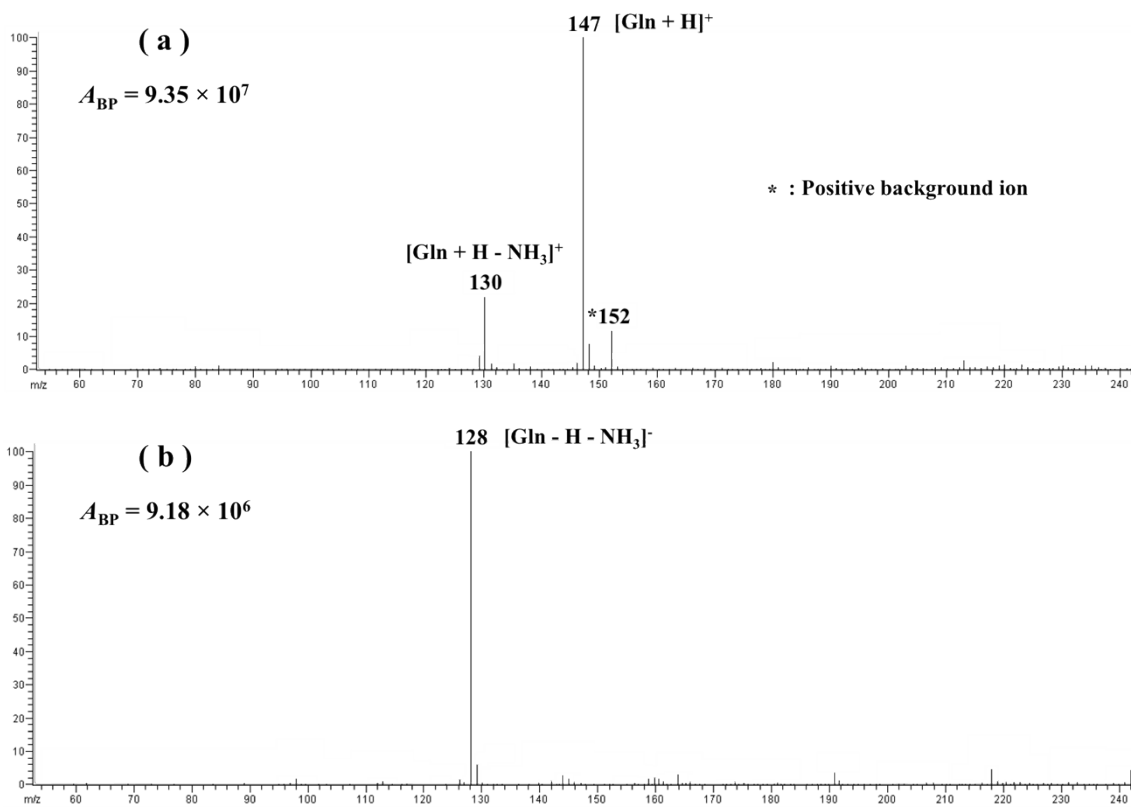
**Figure S6. (a) Positive- and (b) negative-ion DART mass spectra of L-serine (Ser; Mr 105).**

$A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.

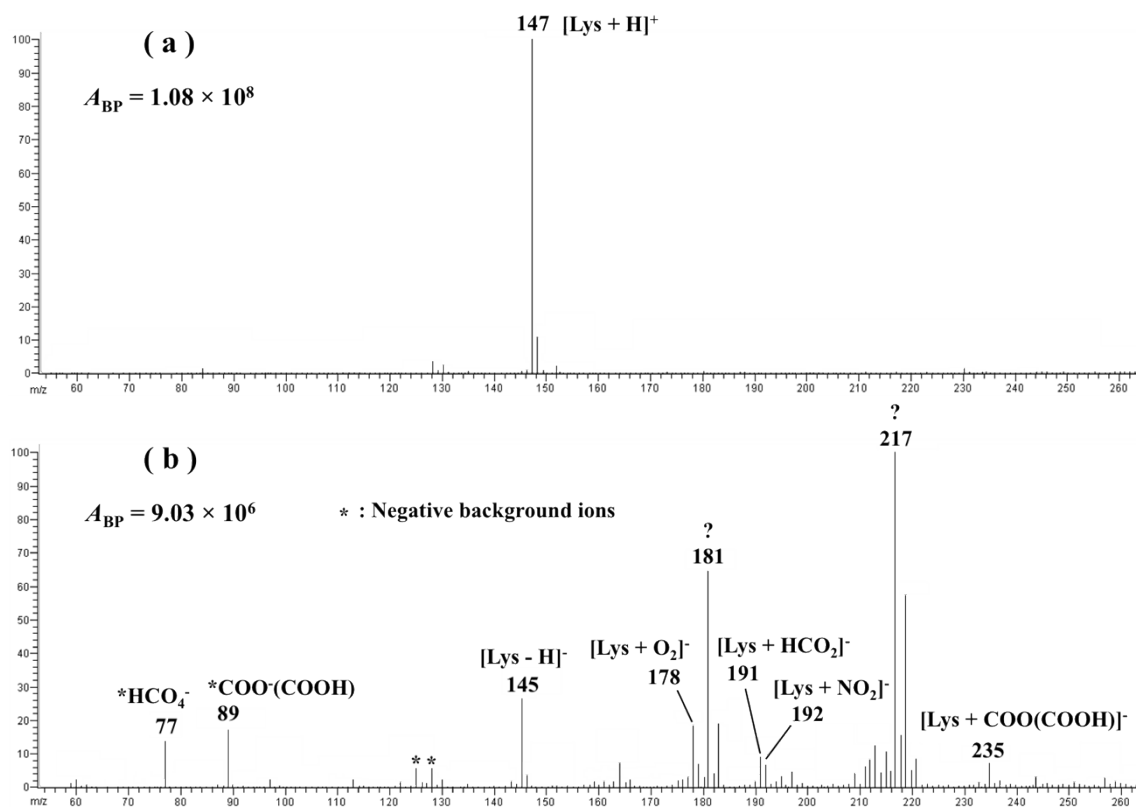


**Figure S7. (a) Positive- and (b) negative-ion DART mass spectra of L-threonine (Thr; Mr 119).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**



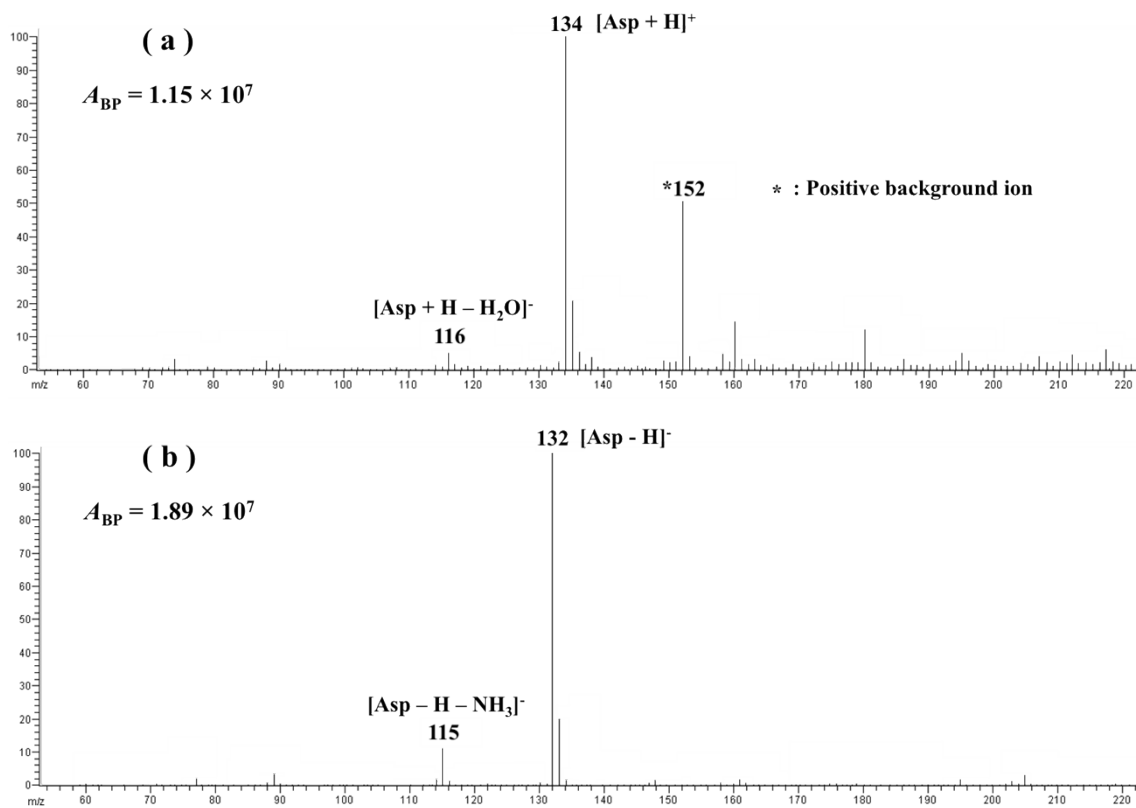


**Figure S8. (a) Positive- and (b) negative-ion DART mass spectra of L-glutamine (Gln; Mr 146).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**

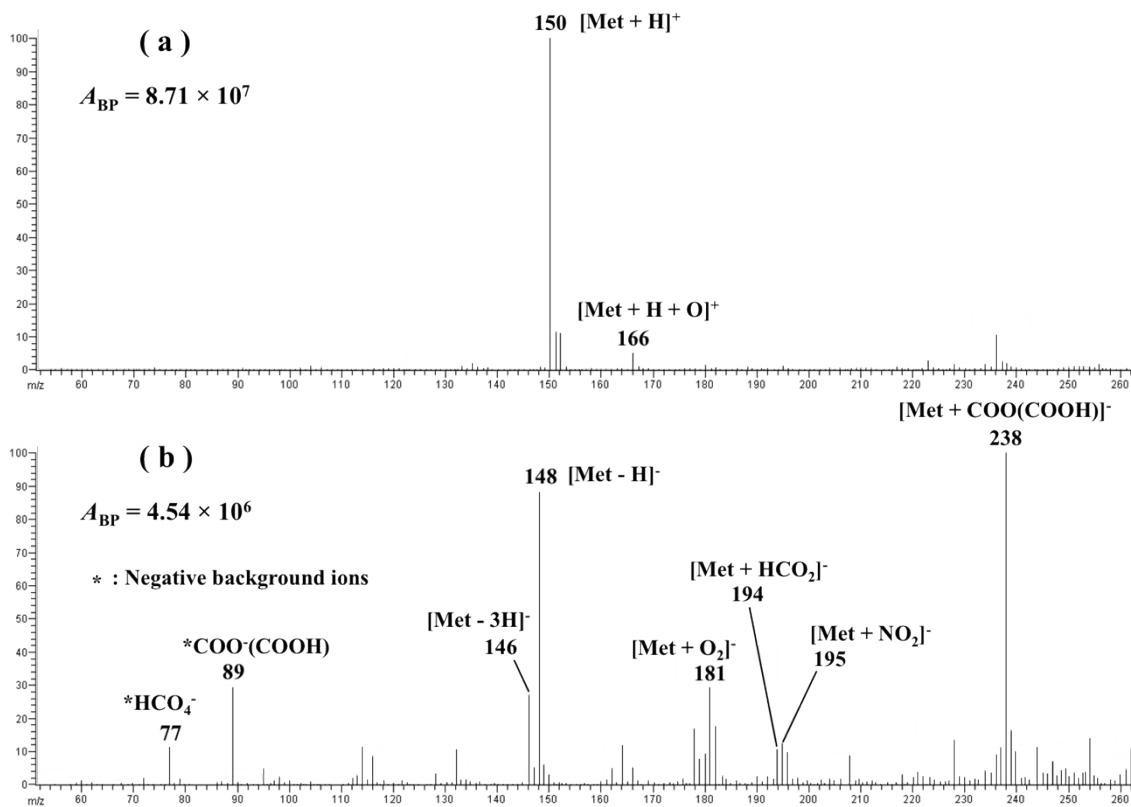


**Figure S9. (a) Positive- and (b) negative-ion DART mass spectra of L-lysine (Lys; Mr 146).**

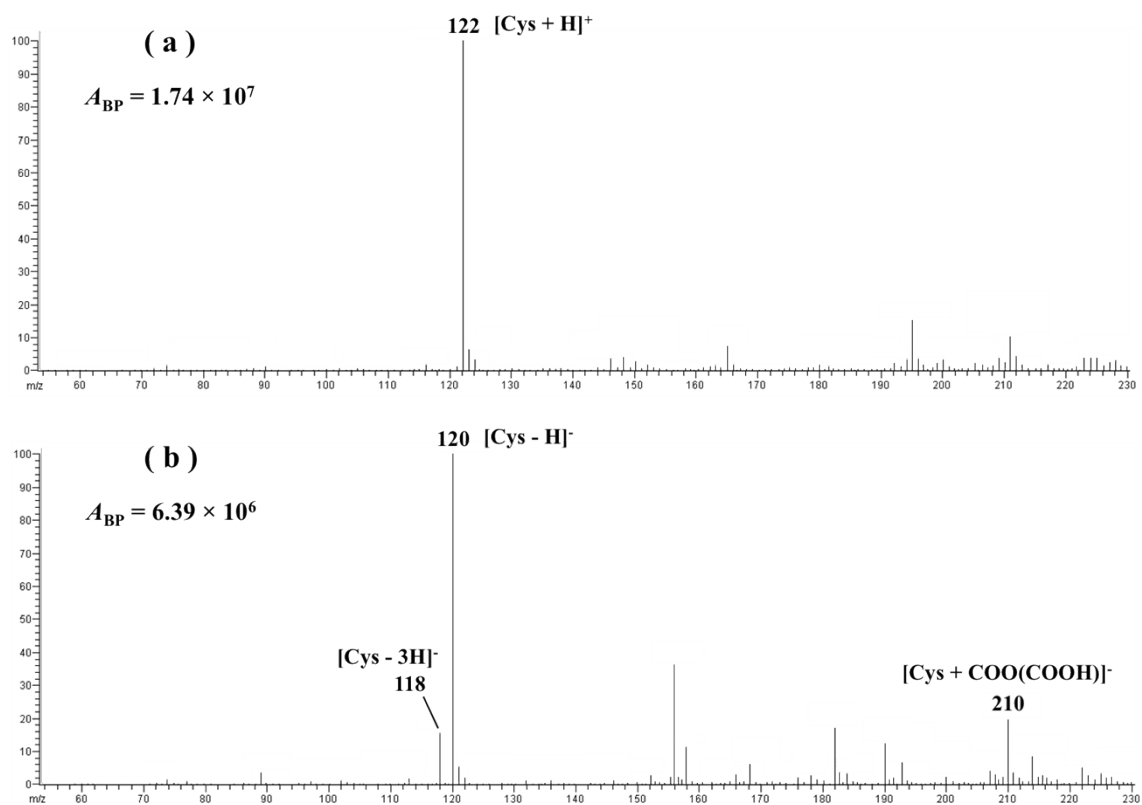
$A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.



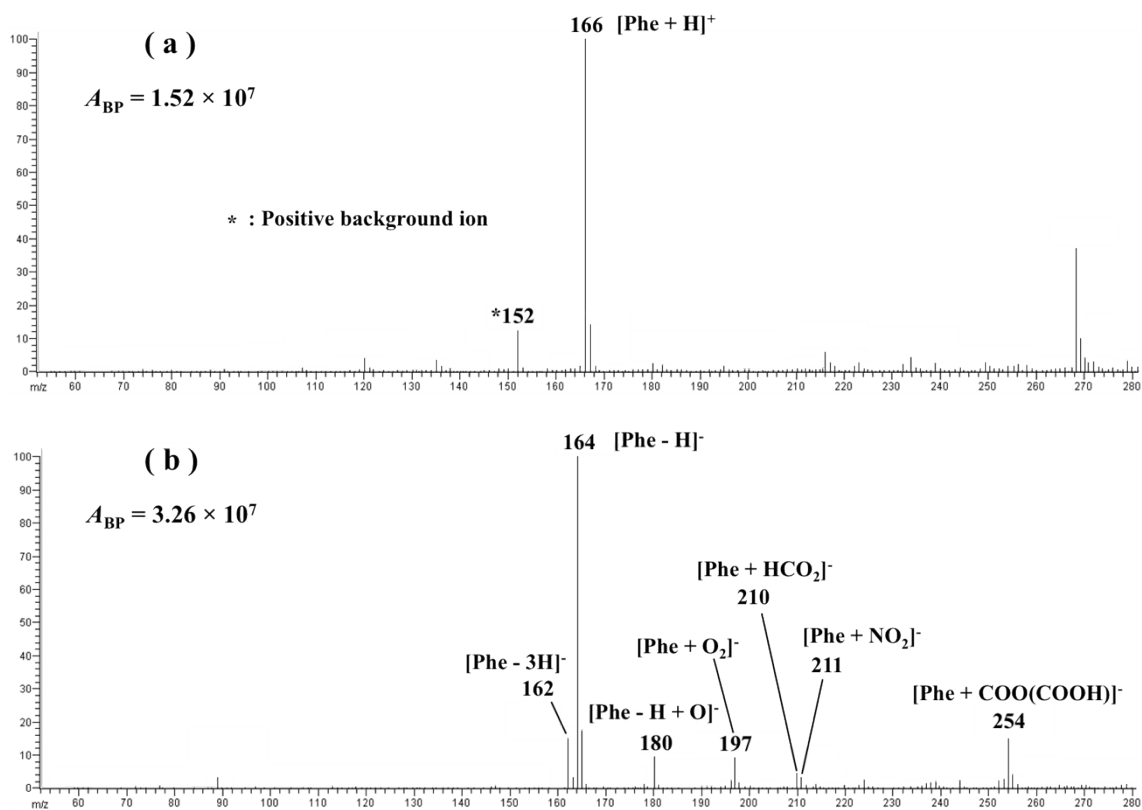
**Figure S10. (a) Positive- and (b) negative-ion DART mass spectra of L-aspartic acid (Asp; Mr 133).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**



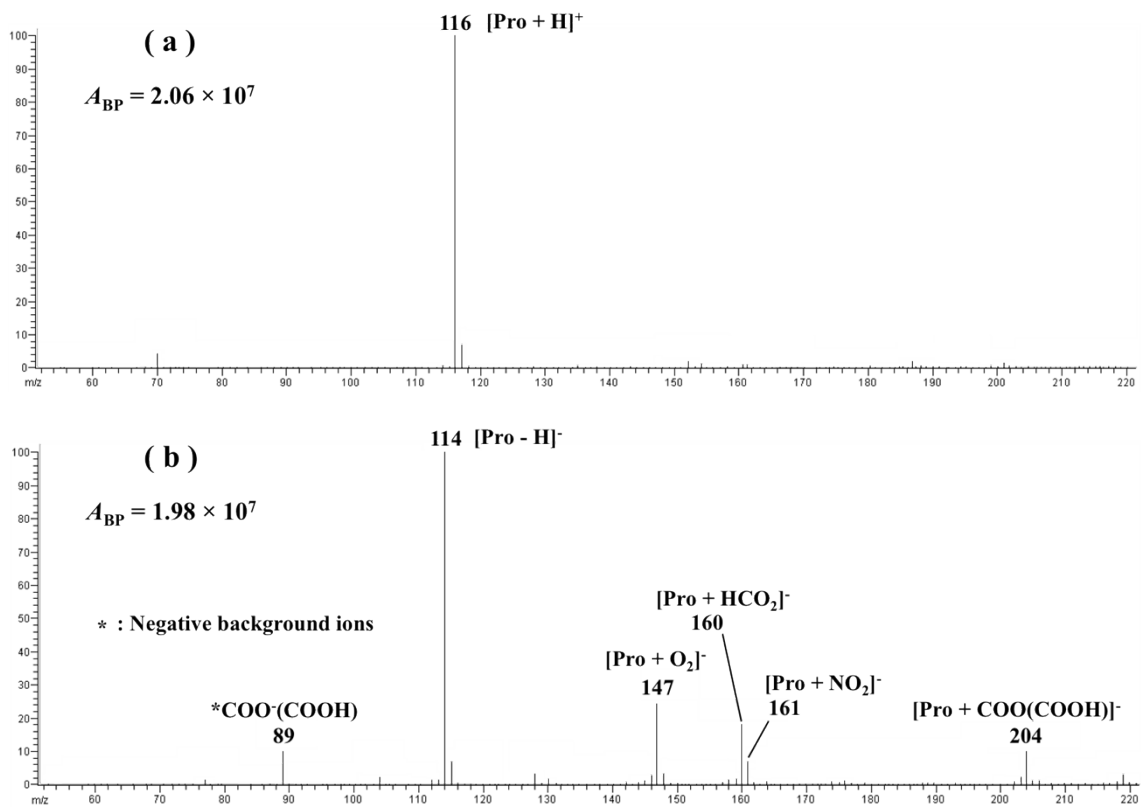
**Figure S11. (a) Positive- and (b) negative-ion DART mass spectra of L-methionine (Met; Mr 149).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**



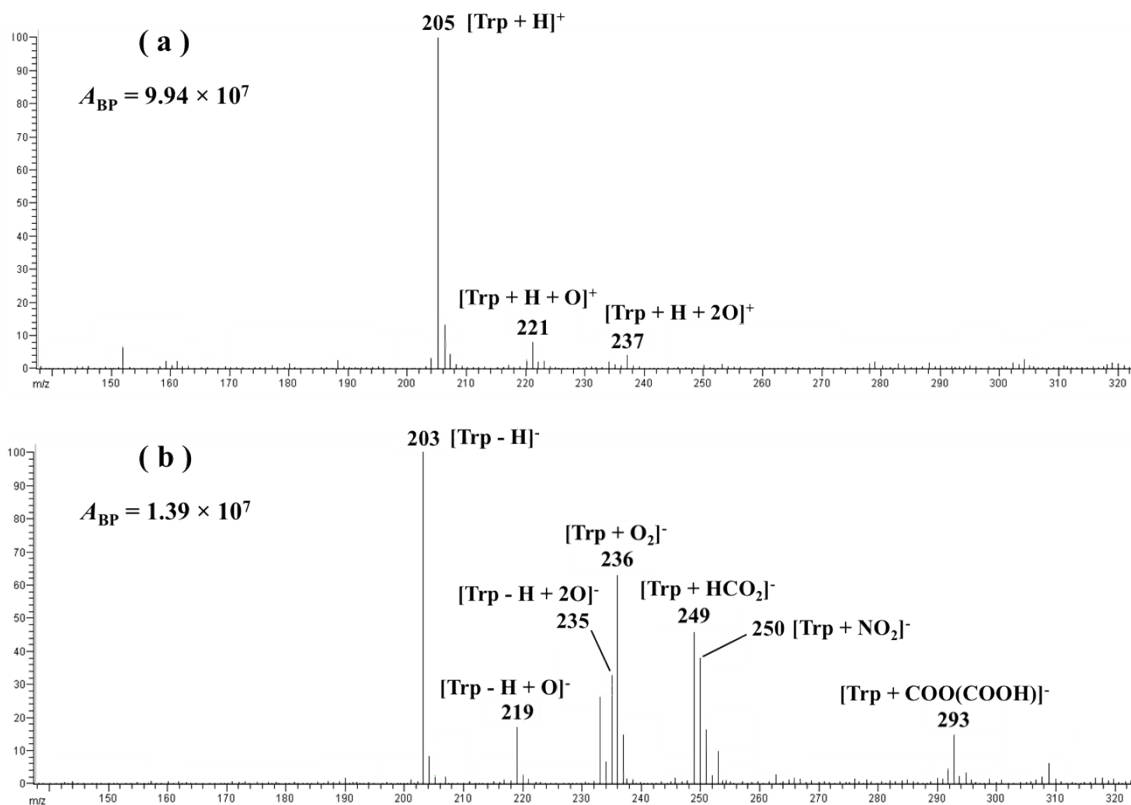
**Figure S12. (a) Positive- and (b) negative-ion DART mass spectra of L-cysteine (Cys; Mr 121).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**



**Figure S13. (a) Positive- and (b) negative-ion DART mass spectra of L-phenylalanine (Phe; Mr 165).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**

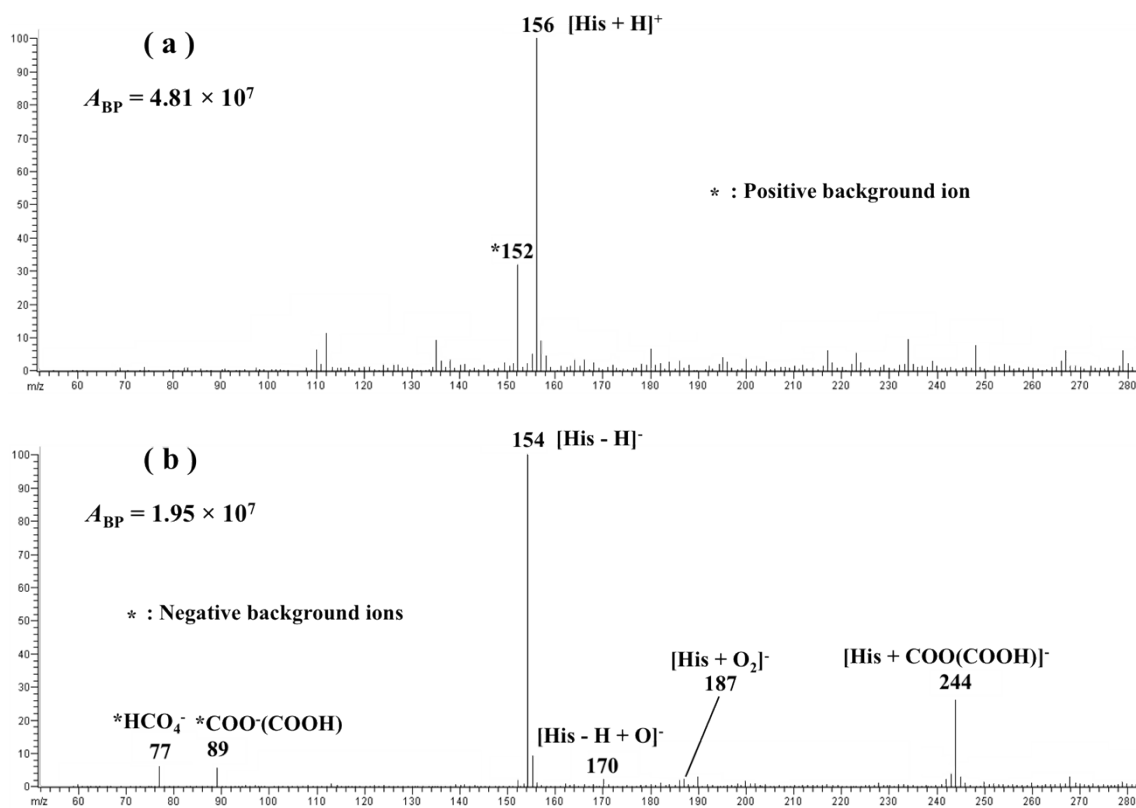


**Figure S14. (a) Positive- and (b) negative-ion DART mass spectra of L-proline (Pro; Mr 115).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**



**Figure S15. (a) Positive- and (b) negative-ion DART mass spectra of L-tryptophane (Trp; Mr 204).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**





**Figure S16. (a) Positive- and (b) negative-ion DART mass spectra of L-histidine (His; Mr 155).  $A_{BP}$  represents the absolute abundance (arbitrary units) of the base peak in each mass spectrum.**

**Table S1. Absolute abundances of deprotonated analytes [M – H]<sup>-</sup> (M: Gly, Val, Asp and Phe) obtained under ambient air condition and N<sub>2</sub> atmosphere condition in the closed analyte ionization area.**

Analyte (M)	Absolute abundances of [M - H] <sup>-</sup> [arb.]	
	Ambient air condition	N <sub>2</sub> atmosphere condition
Gly	$1.54 \times 10^4$	$1.61 \times 10^3$
Val	$1.99 \times 10^5$	$4.43 \times 10^4$
Asp	$2.12 \times 10^4$	$2.05 \times 10^4$
Phe	$1.31 \times 10^5$	$2.98 \times 10^4$