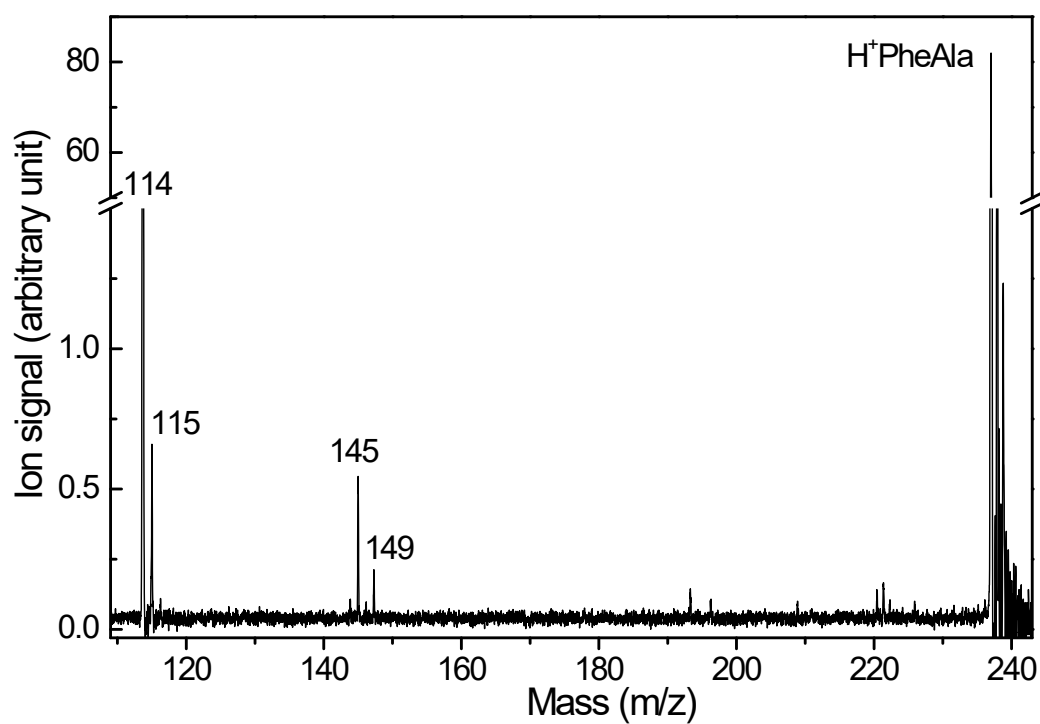


## **Supporting information**

# **Ultraviolet Photodissociation Circular Dichroism Spectroscopy of Protonated L-Phenylalanyl-L- Alanine in a Cryogenic Ion Trap**

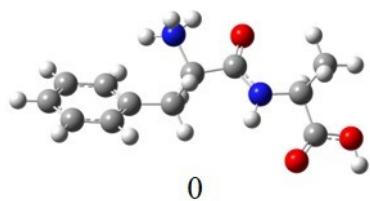
Il Tae Yoo,<sup>§</sup> Han Jun Eun,<sup>§</sup> Ahreum Min, Chang Wook Jeon, Jinho Jeong, Jiyoung Heo, and

Nam Joon Kim\*

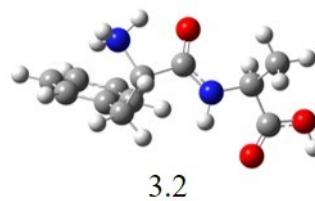


**Figure S1.** mass spectrum of L-H<sup>+</sup>PheAla obtained with irradiation of a UV laser pulse at 37 542 cm<sup>-1</sup>. The fragment ions at m/z 145 and 149 were produced by photo-induced dissociation, whereas the ions at m/z 114 and 115 were generated by collision-induced dissociation.

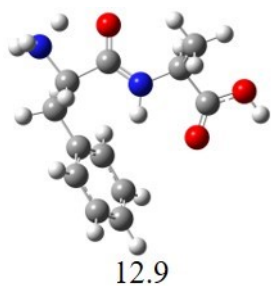
(a) TransA1



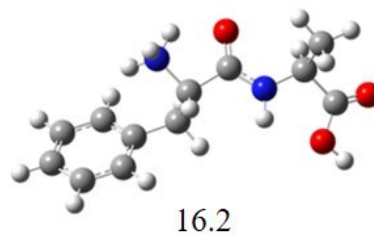
(b) TransA1'



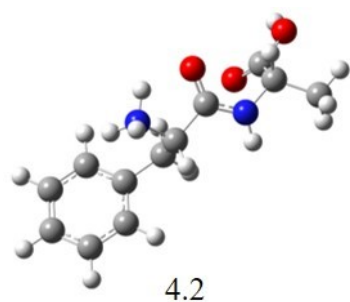
(c) TransA1''



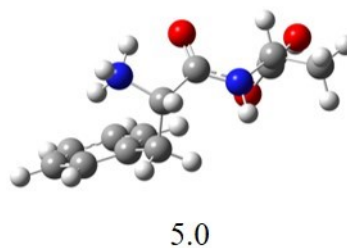
(d) TransA1R



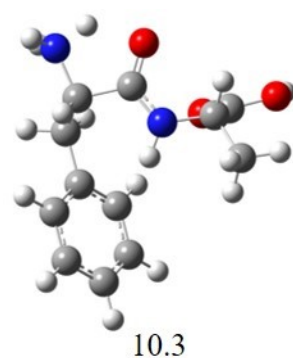
(e) TransA2



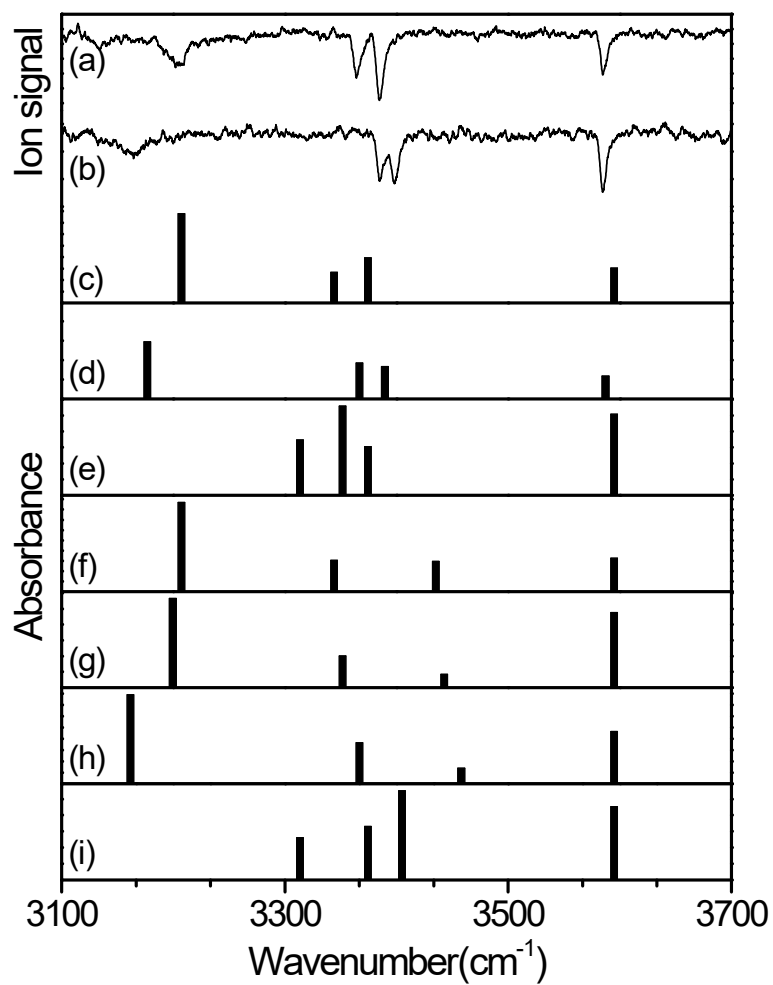
(f) TransA2'



(g) TransA2''



**Figure S2.** Structures of the low-lying conformers of L-H<sup>+</sup>PheAla optimized at the CAM-B3LYP/6-311++G(d,p) level. The names of the low-lying conformers were adopted from the previous report.<sup>1</sup> The numbers in parenthesis indicate relative energies in kJ/mol.



**Figure S3.** IR ion-dip spectra of conformers (a) I and (b) II of L-H<sup>+</sup>PheAla, and theoretical IR spectra of conformers (c) TransA1, (d) TransA1', (e) TransA1'', (f) TransA1R, (g) TransA2, (h) TransA2', and (i) TransA2''. The theoretical spectra were predicted at the CAM-B3LYP/6-311++G(d,p) level with a scale factor of 0.95.

## References

1. R. C. Dunbar, J. D. Steill, N. C. Polfer and J. Oomens, *Int. J. Mass Spectrom.*, 2009, **283**, 77-84.