Supporting information

Ultraviolet Photodissociation Circular Dichroism Spectroscopy of Protonated \textit{L}-Phenylalanyl-\textit{L}-Alanine in a Cryogenic Ion Trap

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Figure S1. Mass spectrum of L-H’PheAla obtained with irradiation of a UV laser pulse at 37 542 cm\(^{-1}\). 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.
Figure S2. Structures of the low-lying conformers of L-H\textsuperscript{+}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\textsuperscript{1}. 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\(^+\)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