MODIFCATION OF THE PROLYL RING OF VAL-PRO-ALA AND THE IMPACT OF THIS MODIFICATION ON B2 ION STRUCTURE

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Here we present b2 ion studies on one tripeptide (VPA) and show how the addition of a fluorine or a hydroxyl group on the 3rd position of the proline ring can affect the b2 ion formation. Action IRMPD results of ValHyp (Hyp=hydroxyproline), ValFlp (Flp=trans-fluoroproline), and Valflp (flp=cis-fluoroproline) all show the presence of a strong oxazolone band in the CO region at 1900 cm-1. The presence of peaks in the diketopiperazine region between 1700 and 1800 cm-1 varies depending on which substituent is placed on the prolyl ring. Recently published data from our group showed a pair of medium sized diketopiperazine bands at 1760 and 1701 cm-1 for ValPro and we observed similarly intense bands for Valflp at 1752 and 1689 cm-1. ValHyp and ValFlp fail to show any significant diketopiperazine bands, but if zoomed in x10 a small band can be observed at 1756 cm-1 for ValHyp. From this data it is apparent that substitution of the second position prolyl ring can alter the formation of the b2 diketopiperazine ion.