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CONFORMATION AND SWEET TASTES OF L-ASP-D-XAA-OME DIPEPTIDES

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In order to investigate the conformational preferences to elicit the tastes, conformational free energy calculations using the empirical potential ECEPP/3 and the hydration shell model were carried out on the L-aspartyl dipeptide methyl esters, L-$^{+}$HAsp^{-}-D-Xaa-OMe, in the unhydrated state, where Xaa includes sweet (Ala, Abu, Ser, Thr, Val, and Ile), bitter (Phe, Trp, and Leu), and tasteless (Tyr and Met) residues. Irrespective of the Xaa and the taste, all the dipeptides have the same conformation for the Asp residue, which is attributable to the hydrogen bond between protonated amino hydrogen and carboxylate oxygen and the favored hydration of carboxylate group. This implies that the L-aspartyl residue is a necessary factor for the dipeptides to be sweet not a sufficient factor. The computed conformational preferences for sweet, bitter, and tasteless dipeptides in the unhydrated state indicate to us that the conformation about the N-C^{α} bond of the Xaa residue, i.e., the orientation of the hydrophobic moiety with respect to the AH/B functionalities in the aspartyl moiety, seems to be crucial to elicit the tastes. In addition, the hydrophobicity and the size of the Xaa residue are found to play an important role in determining the tastes. These results are similar to those of L-Asp-L-Xaa-OMe dipeptides studied previously.