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The Structural Analysis of b5Type Mass Fragment Ions

NuranElmacı[a], **SılaKaraca**[a] and **SeckinBoz**[b]
a Department of Chemistry, Izmir Institute of Technology, Turkey
b Department of Molecular Biology, Izmir Institute of Technology, Turkey

Tandem mass spectrometry (MS/MS) coupled with collision-induced dissociation (CID) is commonly used method for proteomic studies. Upon low-energy CID, protonated or multiply-protonated peptides undergo fragmentation via cleavage of amide bonds to generate N-terminal b and a and/or C-terminal y ions. Understanding the gas-phase structures of these ions and their fragmentation reactions has played a vital role for correct and reliable peptide/protein identification. It has been shown that, bn (n=2-4) ions commonly have oxazolone structure. However, for some cases b_2 ions also adopt a six-membered ring; diketopiperazine structure. The formation of these two different structures entirely depends on the amino acid composition of the peptide sequence as well as peptide chain length.Themacrocyclic structure of b_5^+ and larger b ions has been predicted for aliphatic peptides in experimental and theoretical studies. The macrocyclic structure is a problem for determining the amino acid sequence of a peptide. The memory of original primary structure is lost if reopening of the macrocycle takes place at different sites on the cycle. In such cases, the databases of computer programs which are used with the MS/MS results will be insufficient to identify peptide/protein. These databases must be improved by the detailed and comprehensive studies of the gas phase fragmentations of protonated peptides. This will lead to get reliable results for the proteomic researches.In this work, the structures of b_5 ions; XA_4 composed of alanine and X= X; Asn, Asp, Leu, Phe, Tyr, Cys, amino acid residues have been investigated by using molecular dynamics simulation method and quantum chemical methods. The X-residues have different type of substituent groups; aliphatic (-CH2-), aromatic (C rings), alcohol (-OH), thiol (-SH), amides (-CONH2) and carboxyl (-COOH). To examine the position influence of X residue, three types of linear peptide sequences have been used in the computational calculations for b_5^+ fragment; XAAAA, AAXAA, AAAAX. It has been observed that the b_5 ions prefer to have a macrocyclic structure rather than linear oxazolone isomer. The macrocycle has some common features (backbone structure, proton location, H-bond etc.) for all b-ionsstudied in this research. The results of this work will be useful to understand the gas phase dissociation chemistry of peptides and will support and insight to the experimental studies.

nuranelmaci@iyte.edu.tr

Protein from edible bird's nest samples by mass spectrometry

Lee Suan Chua
UniversitiTeknologi Malaysia, Malaysia

Edible bird's nest (EBN) is a delicacy and nutritious salivary secretion of swiftlets. It contains mostly protein and carbohydrate, and fat as a minor component. The proteome of EBN is still intensively investigated, mainly due to the recent scientific findings on its medical benefits and rejuvenation of skin complexion. In the present study, proteins from EBN samples were extracted by ultrasonic and detergent assisted techniques, as well as buffer solublization. Aqueous extraction assisted by ultrasonic energy produced the highest protein content, followed by detergent assisted method and buffer solubilization. A wide range of protein sizes ranging from 17-150 kDa, mostly water soluble proteins were detected from EBN samples based on gel electrophoresis. EBN from different locations were found to have slight variance in their electrophoretic protein profile. This could be due to the difference in food sources for swiftlets. The use of detergents such as non-ionic Triton X-100 and ionic SDS produced additional protein bands which could be membrane or transmembrane proteins. The trypsinized proteins were subjected to LC-MS/MS analysis and the mass spectra were matched to the protein database. Acidic mammalian chitinase precursor is the most abundant protein in EBN. The protein was reported to have anti-inflammatory activity against allergy and airway diseases. There are also collagen, lysyl oxidase homolog 3 and co-enzyme Q-binding proteins which are important for skin complexion. The results could explain the remarkable findings of previous investigators on the benefits of EBN consumption. These proteins are first time reported to be presence in EBN.

chualeesuan@utm.my, lschua@ibd.utm.my