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Investigating the conformation of alkalized leucine-enkephalin complex by H/D exchange and theoretical calculations

Chuan-Fan Ding Fudan University, China

The gas-phase conformation of the complexes of leucine-enkephalin (YGGFL) with Li⁺, Na⁺, and K⁺ were investigated by gas phase hydrogen/deuterium exchange-mass spectrometry (HDX-MS) combined with theoretical calculations. Different HDX performance were observed of enkephalin complexed with proton and Li⁺, Na⁺, and K⁺ ions. It was observed that [YGGFL⁺H]⁺ reacts continuously while the quenched reaction was found in the complexes of YGGFL with metal ions. For example, at the same HDX conditions, hydrogen exchanged in [YGGFL⁺H]⁺ and [YGGFL⁺Na]⁺ is 8 and 4, respectively. It is indicated that the two ions are of different conformation through various HDX performance. To further clarify the experimental results, the conformations were calculated by using density functional theory. It shows that the terminal amino group is the most thermodynamically stable protonation site, while the sodium ion coordinated four carbonyl oxygen atoms forms the most favorable sodium adduct. It is found that the difference in HDX might be attributed to less acidic hydrogen atoms in [YGGFL⁺Na]⁺ according to the charge and proton affinity calculated. The different conformations of leucine-enkephalin with Li⁺, and K⁺ complexes were further investigated for comparison. The results of this work is significant in physiology.

Biography

Chuan-Fan Ding has completed his PhD from Fudan University (China). He has published more than 50 papers in reputed journals and serving as an editorial board member of repute.

makhapam@mintek.co.za

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