CID-Induced Formation of Deprotonated Cyclic Peptide Ions From Anionic Adducts

Autorzy

Maciej Modzel

Piotr Stefanowicz

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Streszczenie

MS analysis of cyclic peptides in negative ion mode has been a challenge, in particular if the peptide does not contain acidic functional groups. In this paper, we present a way to easily produce negative ions from anionic peptide adducts, utilising collision-induced dissociation (CID)-mediated elimination. Using two different mass spectrometers, we have generated series of adducts of three cyclic and one linear peptide with various anions. They were then isolated and subjected to CID with a range of collision energies. The deprotonation percentage was then calculated from the resultant spectrum, and compared between the spectrometers, as well as with an external reference—proton affinity values. The susceptibility to deprotonate by detaching a HX moiety is proportional to the proton affinity of the X^- species. Also, the linear peptide deprotonated more readily than the cyclic ones. On the other hand, lack of amino or acidic groups resulted in higher collision voltage (CV) necessary for the formation of deprotonated species. Moreover, the exact propensity for neutral loss depends on the ion temperature, which differs between mass spectrometers. We have developed a facile method for generating peptide anions for MS analysis of cyclic peptides, which works even if the peptide in question does not have easily ionisable groups. The deprotonated species generated in this way can be fragmented again in order to identify the peptide.

Słowa kluczowe

anionic adducts, cyclic peptides, deprotonated peptide ions

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