α-helical peptides are not protonated at the N-terminus in the gas phase.

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Rok wydania

2004

Czasopismo

Journal of the American Chemical Society

Numer woluminu

126

Strony

12278-12279

DOI

10.1021/ja048033s

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

DFT/AM1 ONIOM calculations using B3LY/D95** indicate that protonations of α-helical ala_N (N = 14, 17) occur preferentially at the COOH and CO groups near the COOH terminus of the peptides. Protonations at the N-termini lead to local helical unraveling. The preference for protonation at or near the COOH terminus increases with N. Hydration should relatively favor the N-protonated structures, but at the expense of further unraveling. Since α-helices in proteins often form “bundles” that are not well-hydrated, the CO groups at the ends of these helices might be readily protonated.

Słowa kluczowe

Carboxyls, Chemical structure, Peptides and proteins, Protein structure

Adres publiczny

https://doi.org/10.1021/ja048033s

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html