Modeling of copper(II) sites in proteins based on histidyl and glycyl residues.

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Rok wydania

2003

Czasopismo

Journal of Inorganic Biochemistry

Numer woluminu

97

Strony

299-307

DOI

10.1016/S0162-0134(03)00283-6

Kolekcja

Naukowa

Język

Angielski

Streszczenie

The complexes between copper(II) and four synthetic tetrapeptides bearing a single histidine residue within the sequence (AcHGGG, AcGHGG, AcGGHG and AcGGGH, respectively), have been investigated by potentiometric and spectroscopic methods (UV–Vis, circular dichroism and electron paramagnetic resonance). Potentiometric studies in the pH range 4–12 allowed identification and quantitative determination of the species present in solution for each copper–peptide complex. In all cases, upon raising pH, copper(II) coordination starts from the imidazole nitrogen of the His; afterwards three deprotonated amide nitrogens are progressively involved in copper coordination, except in the case of AcGHGG. Based on the potentiometric and spectroscopic results, detailed molecular structures are proposed for the dominant copper(II) tetrapeptide species existing in solution, either at neutral or alkaline pH. The structural consequences of the presence and of the location of a unique histidine residue within the tetrameric sequence are specifically analyzed. Results are discussed in relation to the modeling of copper(II) binding sites in proteins, particular emphasis being devoted to the copper complexes of the prion protein.

Słowa kluczowe

Circular dichroism, Copper(II) complexes, EPR spectroscopy, Histidine-containing tetrapeptides, Protein models

Adres publiczny

https://doi.org/10.1016/S0162-0134(03)00283-6

Strona internetowa wydawcy

http://www.elsevier.com

Typ publikacji

Artykuł