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Insight into the coordination and the binding sites of Cu^{2+} by the histidyl-6-tag using experimental and computational tools.

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Streszczenie

His-tags are specific sequences containing six to nine subsequent histydyl residues, and they are used for purification of recombinant proteins by use of IMAC chromatography. Such polyhistydyl tags, often used in molecular biology, can be also found in nature. Proteins containing histidine-rich domains play a critical role in many life functions in both prokaryote and eukaryote organisms. Binding mode and the thermodynamic properties of the system depend on the specific metal ion and the histidine sequence. Despite the wide application of the His-tag for purification of proteins, little is known about the properties of metal-binding to such tag domains. This inspired us to undertake detailed studies on the coordination of Cu(2+) ion to hexa-His-tag. Experiments were performed using the potentiometric, UV-visible, CD, and EPR techniques. In addition, molecular dynamics (MD) simulations and density functional theory (DFT) calculations were applied. The experimental studies have shown that the Cu(2+) ion binds most likely to two imidazoles and one, two, or three amide nitrogens, depending on the pH. The structures and stabilities of the complexes for the Cu(2+)-Ac-(His)6-NH2 system using experimental and computational tools were established. Polymorphic binding states are suggested, with a possibility of the formation of α-helix structure induced by metal ion coordination. Metal ion is bound to various pairs of imidazole moieties derived from the tag with different efficiencies. The coordination sphere around the metal ion is completed by molecules of water. Finally, the Cu(2+) binding by Ac-(His)6-NH2 is much more efficient compared to other multihistidine protein domains.

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