

African viper poly-his tag peptide fragment efficiently binds metal ions and is folded into an α -helical structure.

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Snake venoms are complex mixtures of toxic and often spectacularly biologically active components. Some African vipers contain polyhistidine and polyglycine peptides, which play a crucial role in the interaction with metal ions during the inhibition of snake metalloproteases. Polyhistidine peptide fragments, known as poly-His tags, play many important functions, e.g., in metal ion transport in bacterial chaperon proteins. In this paper, we report a detailed characterization of $\text{Cu}(2+)$, $\text{Ni}(2+)$, and $\text{Zn}(2+)$ complexes with the EDDHHHHHHHHHG peptide fragment (pHG) derived from the venom of the rough scale bush viper (*Atheris squamigera*). In order to determine the thermodynamic properties, stoichiometry, binding sites, and structures of the metal-pHG complexes, we used a combination of experimental techniques (potentiometric titrations, electrospray ionization mass spectrometry, UV-vis spectroscopy, circular dichroism spectroscopy, and electron paramagnetic resonance spectroscopy) and extensive computational tools (molecular dynamics simulations and density functional theory calculations). The results showed that pHG has a high affinity toward metal ions. The numerous histidine residues located along this sequence are efficient metal ion chelators with high affinities toward $\text{Cu}(2+)$, $\text{Ni}(2+)$, and $\text{Zn}(2+)$ ions. The formation of an α -helical structure induced by metal ion coordination and the occurrence of polymorphic binding states were observed. It is proposed that metal ions can "move along" the poly-His tag, which serves as a metal ion transport pathway. The coordination of $\text{Cu}(2+)$, $\text{Ni}(2+)$, and $\text{Zn}(2+)$ ions to the histidine tag is very effective in comparison with other histidine-rich peptides. The stabilities of the metal-pHG complexes increase in the order $\text{Zn}(2+) < \text{Ni}(2+) \ll \text{Cu}(2+)$.

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