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Zinc(II) and Copper(II) Binding of a MUC7 Peptide Fragment: Coordination, Thermodynamic Stability, and Antimicrobial Potency

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Streszczenie

Metal ions play a key role in regulating antimicrobial peptides (AMPs), either inducing or enhancing their effects against pathogens. In human saliva, AMPs, including fragments of the glycoprotein MUC7, form a natural defense against oral and systemic infections. This study investigates a 20-residue MUC7-derived peptide containing three histidine residues as potential coordination sites for divalent metal ions. Complexes are analyzed using electrospray ionization mass spectrometry, potentiometry, and spectroscopic methods: ultraviolet–visible spectroscopy, circular dichroism, and electron paramagnetic resonance, together with antimicrobial assays. Cu(II) coordination did not significantly alter secondary structure or improve antimicrobial properties. In contrast, Zn(II) induced conformational changes under alkaline conditions, correlating with slightly enhanced antimicrobial performance. Proline, tyrosine, and phenylalanine residues likely modulate metal coordination through steric hindrance and conformational effects. These findings highlight the role of metal coordination in modulating AMP function. Although this particular MUC7-derived fragment exhibits only modest antimicrobial activity compared to other known fragments of this protein, its distinct metal-binding behavior suggests that it may serve an alternative biological role in the oral environment beyond direct pathogen inhibition.

Słowa kluczowe

antimicrobial peptides, bioinorganic chemistry, copper(II), metal–peptide interactions, zinc(II)

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