Exploring zinc(II) ion binding and antimicrobial activity *via d*-amino acid substitution and *retro-inverso* modifications in MUC7 peptide from human saliva

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Streszczenie

Antimicrobial peptides are part of the host's innate immune response and have high therapeutic potential, especially in the complexes with Zn(II) ions. However, this potential is limited by poor proteolytic stability. To prevent this, their peptidomimetic modifications, such as D-amino acid substitution or *retro-inverso* strategy, are a worthy alternative. In this work, we investigate peptidomimetic modified fragments of MUC7, a protein present in human saliva, and their complexes with Zn(II) ions. A comprehensive analysis encompassing potentiometric titrations, far-UV circular dichroism and nuclear magnetic resonance spectroscopic techniques, mass spectrometry, density functional theory calculations, and biological assays revealed both similarities and distinctions compared to the native, non-modified peptide, offering valuable insights into the impact of sequence modifications on metal coordination, structural properties, and antimicrobial efficacy. This study is, to our knowledge, the first in-depth analysis of Zn(II) binding to *retro-inverso* peptides.

Adres publiczny

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