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Zn(II)-alloferon complexes - similar sequence, different coordination modes, no antibacterial activity.

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Streszczenie

Often, in the search for a highly defined scientific phenomenon, a different one becomes apparent. This was also the case of this work, in the scope of which we planned to search for metal-enhanced, novel antibacterial/antifungal compounds. Instead, we denied the existence of such and revealed the details of the bioinorganic chemistry of Zn(II)-alloferon complexes. Zinc(II) complexes of alloferon 1 and 2, ligands with a sequential difference of one amino acid only, show a substantially different coordination pattern at physiological pH. In the case of Zn(II)-alloferon 1 species, a histamine-like binding mode is observed (N-terminal amine and imidazole of His-1) and the coordination sphere is completed with the imidazole nitrogens of His-6 and His-9; His-12 is not involved in binding. In the case of Zn(II)-alloferon 2, the N-terminal amine and all the three imidazoles present in the sequence participate in the coordination, however, with the chemical shift of His-5 being less affected than those of other imidazoles. The histamine-like binding in Zn(II)-alloferon 1 complex strongly enhances its thermodynamic stability in comparison to the His-1 lacking alloferon 2 analogue. Despite previous reports on the antibacterial and antifungal activity of alloferon 1, no such activity was detected, neither for alloferon 1 and 2 nor for their Zn(II) complexes.

Słowa kluczowe

Alloferon, Zinc(II), Metal-antimicrobial peptide complex, Metal-peptide thermodynamics

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