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Bioinorganic chemistry of shepherin II complexes helps to fight *Candida albicans*?

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Streszczenie

The fungal cell wall and cell membrane are an important target for antifungal therapies, and a needle-like cell wall or membrane disruption may be an entirely novel antifungal mode of action. In this work, we show how the coordination of Zn(II) triggers the antifungal properties of shepherin II, a glycine- and histidine-rich antimicrobial peptide from the root of *Capsella bursa-pastoris*. We analyze Cu(II) and Zn(II) complexes of this peptide using experimental and theoretical methods, such as: mass spectrometry, potentiometry, UV–Vis and CD spectroscopies, AFM imaging, biological activity tests and DFT calculations in order to understand the correlation between their metal binding mode, structure, morphology and biological activity. We observe that Zn(II) coordinates to Shep II and causes a structural change, resulting in fibril formation, what has a pronounced biological consequence – a strong anticandidal activity. This phenomenon was observed neither for the peptide itself, nor for its copper(II) complex. The Zn(II) – shepherin II complex can be considered as a starting point for further anticandidal drug discovery, which is extremely important in the era of increasing antifungal drug resistance.

Słowa kluczowe

Antimicrobial peptides, Shepherin peptides, Antifungal activity, Fibril formation, Zn(II) and Cu(II) complexes of AMPs

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