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Thermodynamic and spectroscopic analysis of peptide-based enzyme mimics containing the ATCUN site

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Enzyme mimics (EMs) are molecular entities that typically replicate the binding and catalytic function of natural enzymes [1]. In this work we focus on peptide-based EMs with an ATCUN (Amino-Terminal Copper and Nickel) binding site, in order to promote a multitarget antimicrobial mechanism. Our approach in designing novel EMs relies on synthetic branched peptides to generate a previously unexplored category of EMs. A biocompatible central scaffold serves as the core of the EM structure, to which various oligopeptides can be attached [2,3]. The presented work consists of a preliminary study of two selected oligopeptides: AAHAWG-NH_2 and AAHAWGELLKKLLEELKG-NH_2. The peptide ability to form stable Cu(II) complexes has been investigated, together with the ability to generate reactive oxygen species. Indeed, the presence of an ATCUN motif can lead to an increased antimicrobial power, due to copper catalytic action. Potentiometric titrations, mass spectrometry and different spectroscopic techniques (e.g. UV-Vis absorption, circular dichroism) have been employed to thoroughly study the metal interaction with the selected peptides (Figure 1).

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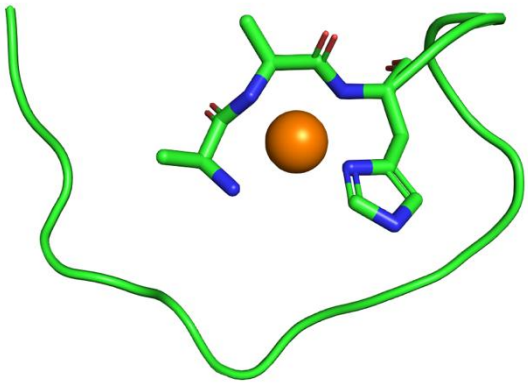

Figure 1. Coordination hypothesis for the Cu(II)/AAHAWGELLKKLLEELKG-NH_2 complex.

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