

Exploring the specificity of rationally designed peptides reconstituted from the cell-free extract of *Deinococcus radiodurans* toward Mn(II) and Cu(II).

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Streszczenie

A series of five rationally designed decapeptides [DEHGTAVMLK (DP1), THMVLAKGED (DP2), GTAVMLKDEH (Term-DEH), TMVLDEHAKG (Mid-DEH), and DEHGGGGDEH (Bis-DEH)] have been studied for their interactions with Cu(II) and Mn(II) ions. The peptides, constructed including the most prevalent amino acid content found in the cell-free extract of *Deinococcus radiodurans* (DR), play a fundamental role in the antioxidant mechanism related to its exceptional radioresistance. Mn(II) ions, in complex with these peptides, are found to be an essential ingredient for the DR protection kit. In this work, a detailed characterization of Cu(II) systems was included, because Cu(II)–peptide complexes have also shown remarkable antioxidant properties. All peptides studied contain in their sequence coordinating residues that can bind effectively Mn(II) or Cu(II) ions with high affinity, such as Asp, Glu, and His. Using potentiometric techniques, NMR, EPR, UV–vis, and CD spectroscopies, ESI-MS spectrometry, and molecular model calculations, we explored the binding properties and coordination modes of all peptides toward the two metal ions, were able to make a metal affinity comparison for each metal system, and built a structural molecular model for the most stable Cu(II) and Mn(II) complexes in agreement with experimental evidence.

Słowa kluczowe

Amides, Peptides and proteins, Monomers, Ions, Electron paramagnetic resonance spectroscopy

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