A multi-technique approach to enlighten the role of metal coordination in calcitermin antiviral properties

Autorzy

Anna Caproni

Silvia Leveraro

Klaudia Szarszoń

Chiara Nordi

Riccardo Fontana

Mattia Buratto

Peggy Marconi

Maurizio Remelli

Mariaconcetta Sicurella

Denise Bellotti

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In this work we presented how the use of suitable electroanalytical, thermodynamic and spectroscopic methods combined with proper experimental conditions can provide comprehensive information on the interaction between metal ions and peptides in solution, as a successful strategy for studying biological systems. Our candidate peptide is calcitermin, an effective metal chelator with significant anti-*Candida* and antibacterial activity in the presence of divalent metals. While the bioinorganic chemistry of calcitermin with zinc and copper is quite well described in the literature, no data about nickel complexes are available; we therefore deepened calcitermin ability to form nickel complexes by different analytical techniques, including potentiometry, ultraviolet–visible absorption spectrophotometry, circular dichroism and high-resolution mass spectrometry. Moreover, for the first time we have investigated the antiviral activity of calcitermin and its metal complexes towards *Herpes simplex* type 1. Despite the nickel-associated slow kinetics, which requires specific experimental precautions, calcitermin forms stable complexes with this cation at different pH conditions. Both the apopeptide and its metal complexes show a random coil secondary structure, which is often characteristic of viral cellular adhesion inhibition. This research highlights that calcitermin and its metal complexes can interfere with viral infections, particularly HSV-1, most likely by altering cell membrane permeability.

Słowa kluczowe

Potentiometry, Spectroscopic methods, Solution equilibria, Antiviral peptides, Herpes simplex, Calcitermin