

Metal-ions interactions with dodecapeptide fragments of Human Cationic Antimicrobial Protein hCAP (134-170)

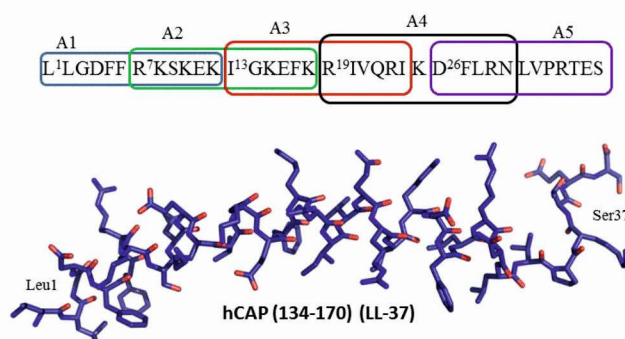
Joanna Makowska^a, Jakub Brzeski^a, Dariusz Wyrzykowski^a, Agnieszka Chylewska^a, Mariusz Makowski^a, Anna Maria Papini^b

^aFaculty of Chemistry, University of Gdańsk, Wita Stwosza 63, 80-308 Gdańsk, Poland

^bInterdepartmental Research Unit of Peptide and Protein Chemistry and Biology, Department of Chemistry "Ugo Schiff", University of Florence, Via della Lastruccia 13, 50019 Sesto Fiorentino, Italy

corresponding author e-mail address: joanna.makowska@ug.edu.pl

The interactions of hCAP (134-170) (LL-37) with selected metal ions, *i.e.*, Cu(II), Zn(II), Mn(II) and Ni(II), have previously been investigated.¹ It has been proven that hCAP (134-170) strongly interacts with Cu(II) and Zn(II) ions, and on this basis, it was found that an excess of both ions in the body may affect the biological activity of this peptide. In order to verify which fragments of the hCAP corresponding to overlapping dodecapeptide sequences, of hCAP(134-170) called LL-37, is involved in the interaction with Mn(II) and Zn(II) ions, ITC (isothermal titration calorimetry) studies on five peptide fragments of LL-37 were carried out. Stoichiometry of the peptide complexes with Mn(II) and Zn(II) ions was evaluated experimentally. It was found that only three sequences of the five peptides tested, form thermodynamically stable complexes with Mn(II) as well as Zn(II) cations. Additionally, based on the density functional theory (DFT) calculations, the most likely structures of the complexes of the peptides with Zn(II) and Mn(II) ions were proposed. This research gives a novel insight into the understanding of the influence of selected metal ions on the activity of the hCAP(134-170).



References

1. Makowska, J.; Wyrzykowski, D.; Kamysz, E.; Tesmar, A.; Kamysz, W.; Chmurzyński, L.; *J. Therm. Anal. Calorim.* **2019**, *138*, 4523.