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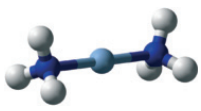
BOOK OF ABSTRACTS



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ZINC BINDING IN A MULTI-HISTIDINIC PEPTIDE FRAGMENT

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A multi-histidinic peptide and its minimal models have been investigated for metal binding. [M.A. Zoroddu et al., 2004, 2008, 2009]
We have used NMR spectroscopy to probe the binding of zinc to the three repeats $(T1R2S3R4S5H6T7S8E9G10)_3$ and to its mono-histidinic minimal models, the 9- and 10-aminoacid fragment. 1H-1H TOCSY, 1H-13C HSQC, 1H-1H NOESY and 1H-1H ROESY multidimensional NMR techniques were performed to understand the details of metal binding sites and the conformational behaviour of the peptides at different pH values and at different ligand to metal molar ratios. Zinc coordination involves imidazole Nδ of His6 and carboxyl γ-O of Glu9 residues; interaction with peptide oxygens of the His6-Thr7 or Thr7-Ser8 bonds in a tetrahedral arrangement with the minimal model peptides, cannot be excluded. Zinc coordination involves, at physiologic pH, all the three imidazole Nδ donors of His6, His16 and His26 as well as carboxyl γ -O of Glu residues in a tetra, penta or octahedral arrangement with the three repeats, the 30-aminoacid fragment. Zinc complexation induces important structural changes with the C-terminal portion of the ligand, constraining it to leave its disordered conformation. Our results give rise to a model of the induced structure of the peptides when bound to zinc. At high pH, amide deprotonation does not take place and hydroxo or high molecular weight polymeric species may be formed.

References

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