

Metal coordination to solute binding proteins – exciting chemistry with potential biological meaning

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Streszczenie

Zn(II) is essential for bacterial survival and virulence. In host cells, its abundance is extremely limited, thus, bacteria have evolved transport mechanisms that enable them to take up this essential metal nutrient. *Paracoccus denitrificans* encodes two solute binding proteins (SBPs) – ZnuA and AztC, which are responsible for zinc acquisition from the host cells. We focus on understanding the interactions of Zn(II) and Ni(II) (zinc's potential competitor, which is a biologically relevant metal ion essential for various bacterial enzymes) with the extracellular ZnuA and AztC's loops from *P. denitrificans* that are expected to be possible Zn(II) binding sites. In the case of Zn(II) complexes with ZnuA outer cellular loop regions, the numerous histidines act as anchoring donors, forming complexes with up to four coordinated His residues, while in the AztC region, three imidazole nitrogens and one water molecule are involved in Zn(II) binding. In Zn(II) complexes with ZnuA His-rich loop regions, so-called polymorphic binding sites are observed. The large number of available imidazoles and carboxylic side chains also strongly affects the structure of Ni(II) complexes; the more histidines in the studied peptide, the higher the affinity to bind Ni(II) and the higher the pH value at which amide nitrogens start to participate in Ni(II) binding. Additionally, for Ni(II)-ZnuA complexes, a more rare octahedral geometry is observed and such complexes are more stable than the corresponding Zn(II) ones, in contrast to what was observed in the AztC region, suggesting that the numerous histidyl and glutamic acid side chains are more tempting for Ni(II) than for Zn(II). The general strong affinity of Zn(II)-zincophore complexes is also discussed.

Adres publiczny

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