

Metal interactions with the transmembrane region of HupE Ni²⁺ transporter explain its efficiency.

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Efficient nickel transport is crucial for the survival and virulence of various bacteria and fungi, with Ni²⁺ being required for the activity of nine enzymes such as [NiFe] hydrogenase, which catalyzes the reversible oxidation of molecular hydrogen for energy production.

This work focuses on a region of transmembrane domain I from the HupE nickel transporter, highly conserved in the HupE/UreJ and NiCoT permease families, analyzing its interactions with native Ni²⁺ and two other metal ions (Cu²⁺ and Zn²⁺), which might interfere with nickel binding. Metal coordination sites are pointed out and thermodynamic parameters are discussed in detail. Their comparison to the previously studied periplasmic metal binding region satisfies our chemical curiosity and allows to draw conclusions about HupE metal specificity. The results of this study explain one of the reasons why HupE is a medium-affinity and low-capacity transporter – its periplasmic region, ₂₂HVGLHADGTLAGLN₃₅, binds Ni²⁺ with much higher affinity than the transmembrane ₃₆HPFSGLDH₄₃ one, which should transport the metal inside the cell. Moreover, the specificity of the transmembrane region is similar to that of the periplasmic one and to that of the full-length HupE – Cu²⁺ ions are able to outcompete Ni²⁺.

Słowa kluczowe

Metal-peptide complexes, thermodynamic stability, HupE nickel transporter

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