

AdcA lipoprotein involved in Zn(II) transport in *Streptococcus mutans* – is it as metal-specific as expected?

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Rok wydania

2025

Czasopismo

Dalton Transactions

Numer woluminu

54

Strony

6795-6804

DOI

10.1039/d5dt00131e

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Streptococcus mutans, a Gram-positive pathogen, is a primary causative agent of dental caries. It modifies the oral biofilm architecture on tooth enamel and, like other bacteria, requires transition metal ions such as Zn(II), Cu(II), and Ni(II) for survival and virulence. Physiological salivary Zn(II) levels are insufficient for optimal bacterial growth, prompting *S. mutans* to develop a specialized ABC transport system comprising AdcA, AdcB, and AdcC. Among these, the lipoprotein AdcA plays a pivotal role in Zn(II) acquisition. In this study, we examined two probable Zn(II)-binding sites in AdcA—EGHGHKGGHHHA and HGIKSQKAEHFH—and their Zn(II), Cu(II), and Ni(II) complexes, keeping in mind that Cu(II) and Ni(II) are essential nutrients for bacterial enzymes and can compete with Zn(II) for its binding sites. At physiological pH, in the Zn(II)–Ac–EGHGHKGGHHHA–NH₂ species, Zn(II) binds to histidine residues, forming complexes with up to four coordinated imidazole nitrogens, while in the Zn(II)–Ac–HGIKSQKAEHFH–NH₂ complex, we found three coordinated histidine side chains. The same regions of the AdcA lipoprotein are able to bind Cu(II) with even higher affinity. The stability of Zn(II) and Ni(II) complexes, on the other hand, is more comparable, with a slight advantage for Ni(II). In this case, at pH 7.4, the coordination spheres of both Zn(II) and Ni(II) consist of the same set of donor atoms. The metal binding preferences align with the Irving–Williams series; however, given the significantly higher Zn(II) concentrations in saliva and dental plaques, Zn(II) occupies the AdcA binding sites *in vivo*, highlighting its critical role in *S. mutans* virulence and metal ion homeostasis.

Adres publiczny

<http://dx.doi.org/10.1039/D5DT00131E>

<https://www.rsc.org/>

Plik został wygenerowany dnia 2026-10-31 02:16:35

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/V98oWKu>.