

Fe(II), Mn(II), and Zn(II) Binding to the C-Terminal Region of FeoB Protein: An Insight into the Coordination Chemistry and Specificity of the *Escherichia coli* Fe(II) Transporter

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Rok wydania

2023

Czasopismo

Inorganic Chemistry

Numer woluminu

62

Strony

18607-18624

DOI

10.1021/acs.inorgchem.3c02910

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The interactions between two peptide ligands [Ac₇₆₃CCAATTGDCH₇₇₃ (**P1**) and Ac₇₄₃RRARSRVDIELLATRKSVSSCCAATTGDCH₇₇₃ (**P2**)] derived from the cytoplasmic C-terminal region of *Escherichia coli* FeoB protein and Fe(II), Mn(II), and Zn(II) ions were investigated. The Feo system is regarded as the most important bacterial Fe(II) acquisition system, being one of the key virulence factors, especially in anaerobic conditions. Located in the inner membrane of Gram-negative bacteria, FeoB protein transports Fe(II) from the periplasm to the cytoplasm. Despite its crucial role in bacterial pathogenicity, the mechanism in which the metal ion is trafficked through the membrane is not yet elucidated. In the gammaproteobacteria class, the cytoplasmic C-terminal part of FeoB contains conserved cysteine, histidine, and glutamic and aspartic acid residues, which could play a vital role in Fe(II) binding in the cytoplasm, receiving the metal ion from the transmembrane helices. In this work, we characterized the complexes formed between the whole cytosolic C-terminal sequence of *E. coli* FeoB (**P2**) and its key polycysteine region (**P1**) with Fe(II), Mn(II), and Zn(II) ions, exploring the specificity of the C-terminal region of FeoB. With the help of a variety of potentiometric, spectroscopic (electron paramagnetic resonance and NMR), and spectrometric (electrospray ionization mass spectrometry) techniques and molecular dynamics, we propose the metal-binding modes of the ligands, compare their affinities toward the metal ions, and discuss the possible physiological role of the C-terminal region of *E. coli* FeoB.

Słowa kluczowe

Bacteria, Ions, Ligands, Monomers, Peptides and proteins

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Adres publiczny

<http://dx.doi.org/10.1021/acs.inorgchem.3c02910>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>