Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Key role of histidine residues orientation in affinity binding of model pentapeptides with Ni^{2+} ions : a theoretical supported experimental study.

Autorzy

Krzysztof Żamojć

Dariusz Wyrzykowski

Giuseppina Sabatino

Anna Maria Papini

Robert Wieczorek

Lech Chmurzyński

Joanna Makowska

Rok wydania

2021

Czasopismo

Journal of Molecular Liquids

Numer woluminu

341

Strony

117414

DOI

10.1016/j.molliq.2021.117414

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Understanding the metal ion-protein interactions is crucial in transport, accumulation, and excretion of metals. Furthermore, it seems to be highly important to investigate the role of such complexes in many diseases, such as cancer and neurodegenerative disorders. Unexpectedly, such studies in the systems comprising peptides and Ni^{2+} ions are still scarce and should be given more importance – particularly considering the toxicity and carcinogenicity of nickel compounds on the living organisms.

We report herein the results of a study on the interactions of Ni^{2+} ions and four pentapeptide analogs: EYHHQ (**p1**), EHYHQ (**p2**), HEYHQ (**p3**), and HEYQH (**p4**). Potentiometric titration was used to study acid-base properties as well as binding properties of the investigated peptides. Furthermore, stoichiometry of the peptide complexes with Ni^{2+} ions was evaluated by steady-state fluorescence spectroscopy and potentiometric titration method. Additionally, based on the density functional theory (DFT) calculations, we propose the most likely structures of the complexes of the peptides **p1-p4** with Ni^{2+} ions. It was found that all the peptides form 1:1 and 1:2 thermodynamically stable complexes with Ni^{2+} cation. In particular, we observed that the interaction between the metal ion and histidine-containing peptide sequences does not depend only on histidines splicing, but also on their orientation in respect to other amino acids in the sequence. Also, the closer proximity of His residue in these short peptides does not increase complex stability, due to stacking interaction between the neighboring imidazole rings.

Słowa kluczowe

Ni2+ complexes, Fluorescent peptides, Coordination properties, Steady-state fluorescence spectroscopy, Potentiometric titration method, DFT

Adres publiczny

http://dx.doi.org/10.1016/j.molliq.2021.117414

Strona internetowa wydawcy

http://www.elsevier.com

Plik został wygenerowany dnia 2026-11-09 13:22:25

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/F3DO9-p.