Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

CH vs. HC—Promiscuous Metal Sponges in Antimicrobial Peptides and Metallophores

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Rok wydania

2023

Czasopismo

Molecules

Numer woluminu

28

Strony

3985/1-3985/14

DOI

10.3390/molecules28103985

Kolekcja

Naukowa

Język

Angielski

Streszczenie

Histidine and cysteine residues, with their imidazole and thiol moieties that deprotonate at approximately physiological pH values, are primary binding sites for Zn(II), Ni(II) and Fe(II) ions and are thus ubiquitous both in peptidic metallophores and in antimicrobial peptides that may use nutritional immunity as a way to limit pathogenicity during infection. We focus on metal complex solution equilibria of model sequences encompassing Cys–His and His–Cys motifs, showing that the position of histidine and cysteine residues in the sequence has a crucial impact on its coordination properties. CH and HC motifs occur as many as 411 times in the antimicrobial peptide database, while similar CC and HH regions are found 348 and 94 times, respectively. Complex stabilities increase in the series Fe(II) < Ni(II) < Zn(II), with Zn(II) complexes dominating at physiological pH, and Ni(II) ones—above pH 9. The stabilities of Zn(II) complexes with Ac-ACHA-NH_2 and Ac-AHCA-NH_2 are comparable, and a similar tendency is observed for Fe(II), while in the case of Ni(II), the order of Cys and His does matter—complexes in which the metal is anchored on the third Cys (Ac-AHCA-NH_2) are thermodynamically stronger than those where Cys is in position two (Ac-ACHA-NH_2) at basic pH, at which point amides start to take part in the binding. Cysteine residues are much better Zn(II)-anchoring sites than histidines; Zn(II) clearly prefers the Cys–Cys type of ligands to Cys–His and His–Cys ones. In the case of His- and Cys-containing peptides, non-binding residues may have an impact on the stability of Ni(II) complexes, most likely protecting the central Ni(II) atom from interacting with solvent molecules.

Słowa kluczowe

bioinorganic chemistry, antimicrobial peptides, metallophores, thermodynamics, potentiometry, metal coordination

Typ publikacji

Artykuł

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Adres publiczny

http://dx.doi.org/10.3390/molecules28103985

Strona internetowa wydawcy

http://www.mdpi.com/journal/metals

Plik został wygenerowany dnia 2026-10-30 07:07:00

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/hl3BxyW.