

## The unusual metal ion binding ability of histidyl tags and their mutated derivatives.

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### Rok wydania

2016

### Czasopismo

Dalton Transactions

### Numer woluminu

45

### Strony

5629-5639

### DOI

10.1039/C5DT04747A

### Kolekcja

Naukowa

### Język

Angielski

### Streszczenie

Polyhistidine-tags are often used for the affinity purification of polyhistidine-tagged recombinant proteins. These sequences are also found in nature and are often highly conserved across different species. However, their exact role in the biological systems is not clear. The purpose of this work is to shed light on the behavior of poly-His sequences in their interactions with metal ions. This work illustrates the first study of novel poly-(His-Ala) peptides that bind Cu(II) applying both experimental techniques and extensive computational tools. The studied novel peptides are analogues of the short protected fragment of the pHPG (EDDH<sub>9</sub>GVG<sub>10</sub>) peptide, which was found in the venom of *Atheris squamigera*. Our study presents the properties of metal ion binding-histidine tag complexes and their mutated derivatives. The Cu(II) binding ability in pHG (Ac-EDDH<sub>9</sub>G-NH<sub>2</sub>) is more efficient than in the mutated derivatives, although the number of imidazoles that bind to Cu(II) ions are similar. Finally, the formation of an  $\alpha$ -helical structure is observed in pHG and in one of the mutated derivatives, indicating the importance of the sequence in the poly-(His-Ala) tags.

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### Adres publiczny

<http://dx.doi.org/10.1039/C5DT04747A>

Artykuł

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

Plik został wygenerowany dnia 2026-04-27 14:14:47

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