

–HH and –HAAAH motifs act as fishing nets for biologically relevant metal ions in metallopeptides

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Streszczenie

Histidine are one of the most common residues involved in transition metal ion binding in the active sites of metalloenzymes. In order to mimic enzymatic metal binding sites, it is crucial to understand the basic coordination modes of histidine residues, distributed at different positions in the peptide sequence. We show that: (i) the separation of two histidines has a large effect on complex stability – a sequence with adjusting histidine residues forms more stable complexes with Zn(II) than the one in which the residues are separated, while the contrary is observed for Cu(II) complexes, in which amide nitrogens participate in metal binding. No pronounced effect is observed for Ni(II) complexes, where the amides participate in binding at higher pH; (ii) non-coordinating amino acid residues (basic, acidic and aromatic ones) have a significant impact on complex stability; charged and aromatic residues may enhance Zn(II) binding, while the contrary is observed for the amide-binding Cu(II); (iii) cysteine containing sequences are much more effective Zn(II) and Ni(II) binding motifs at pH above 8, while histidine containing ligands are more suitable for effective Zn(II) and Ni(II) binding at lower pH.

Słowa kluczowe

Zn(II), Cu(II) and Ni(II)-binding peptides, Complex stability, Histidine residue, Model peptides

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