

The Role of the Unbinding Cycle on the Coordination Abilities of the Bi-Cyclopeptides toward Cu(II) Ions

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Streszczenie

Bicyclic peptides have attracted the interest of pharmaceutical companies because of their remarkable properties, putting them on a new path in medicine. Their conformational rigidity improves proteolytic stability and leads to rapid penetration into tissues via any possible route of administration. Moreover, elimination of renal metabolism is of great importance, for example, for people with a history of liver diseases. In addition, each ring can function independently, making bicyclic peptides extremely versatile molecules for further optimization. In this paper, we compared the potentiometric and spectroscopic properties studied by UV-vis, MCD, and EPR of four synthetic analogues of the bi-cyclic peptide c(PKKHP-c(CFWKTC)-PKKH) (BCL). In particular, we correlated the structural and spectral properties of complexes with coordinating abilities toward Cu(II) ions of MCL1 (Ac-PKKHPc(CFWKTC)PKKH-NH₂) that contains the unbinding cycle and N- and C-terminal linear parts with two histidine residues, one per part; two monocyclic ligands containing one histidine residue, both in the N-terminal position, i.e., MCL2 (Ac-PKKHPc(CFWKTC)PKKS-NH₂) and in the C-terminal position, i.e., MCL3 (Ac-PKKSPc(CFWKTC)PKKH-NH₂), respectively; and the linear structure LNL (Ac-PKKHPSFWKTSPKKH-NH₂). Potentiometric results have shown that the bicyclic structure promotes the involvement of the side chain imidazole donors in Cu(II) binding. On the other hand, the results obtained for the monocyclic analogues lead to the conclusion that the coordination of the histidine moiety as an anchoring group is promoted by its location in the peptide sequence further from the nonbinding cycle, strongly influencing the involvement of the amide donors in Cu(II) coordination.

Słowa kluczowe

bi-cyclopeptide, histidine, metal complex, copper ions, stability constant, spectroscopic studies

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