New aspects of coordination chemistry and biological activity of NTMP-related diphosphonates containing a heterocyclic ring.

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Streszczenie

Two analogues of nitrilotris(methylene-phosphonic acid) (NTMP), namely **L^1** = N-(methylene-2-pyridine)-N,N,-di-(methylenephosphonate) and **L^2** = N-(methylene-1H-benzimidazol)-N,N,-di-(methylenephosphonate) in which one of the phosphonic arms was replaced by a heterocyclic moiety, pyridine and benzimidazole, were studied in terms of coordination chemistry towards transition (Cu^{2+}, Ni^{2+}, Zn^{2+}) and alkaline-earth metal ions (Ca^{2+} and Mg^{2+}) by means of potentiometry, UV-vis spectroscopy, mass spectrometry (ESI-MS), and isothermal titration calorimetry (ITC). The cytotoxicity of the ligands as well as their Zn^{2+}, Ca^{2+} and Mg^{2+} complexes was tested against various cell lines (human melanoma A375 and human colon adenocarcinoma HT29) revealing a selective antitumor effect in vivo. Both of the ligands exhibit a potent inhibitory effect on tumor cell migration and experimental metastasis. Potentiometric and ESI-MS measurements have shown the existence of monomeric species only, without the presence of biscomplexes or polynuclear species. The conditional stability constants ($logK_c$) of the Zn^{2+}, Ca^{2+}, and Mg^{2+} complexes were determined independently by two methods for both of the studied ligands and are a first example of comprehensive potentiometry/ITC studies made for phosphonic acid complexation. No significant differentiation in coordination models for the studied set of metal ions was noticed; however, as expected due to the different metal ion natures, the complexes revealed dissimilar thermodynamic stability and behavior, depending on the metal ion and pH used. The possible structures of the complexes formed are discussed on the basis of spectroscopic and spectrometric results.

Adres publiczny

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