

A new bis-3-hydroxy-4-pyrone as a potential therapeutic iron chelating agent. Effect of connecting and side chains on the complex structures and metal ion selectivity.

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Streszczenie

This work reports the synthesis, characterization and study of complex formation equilibria of the new ligand 6,6'-(2-(diethylamino)ethylazanediyl)bis(methylene)bis(5-hydroxy-2-hydroxymethyl-4H-pyran-4-one) with Fe(III), Al(III), Cu(II) and Zn(II). On the basis of previous encouraging results with tetradentate bis-kojic acid chelators, this ligand was designed to improve the pharmacokinetic properties: increase the solubility, neutral at physiological pH7.4, and enhancement of membrane crossing ability. Fe(III) and Al(III) complexation gave evidence of high metal-sequestering capacity of L9. Cellular assays showed that the ligand is capable of crossing cellular membranes and it does not present toxic effects. Complex formation equilibria with the essential metal ions Cu(II) and Zn(II) have been furthermore studied to evaluate disturbances of this chelator on the homeostatic equilibria of these essential metal ions. A variety of techniques (potentiometry, UV-visible spectrophotometry, 1D and 2D NMR spectroscopy, ESI-MS (electrospray ionization-mass spectrometry), quantum mechanical calculations and X-ray diffraction) have facilitated the characterization of the ligand, and the corresponding iron and zinc complexes, together with an exhaustive analysis of the protonation and complex equilibria.

Słowa kluczowe

Complex formation equilibria, Iron chelators, NMR, Speciation, X-ray structures

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