Kojic acid derivatives as powerful chelators for iron(III) and aluminium(III).

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Streszczenie

Proceeding from a ligand constituted by two units of kojic acid linked by a methylene group, which proved a very promising chelator for excess iron(III) and aluminium(III) pathologies, two new ligands have been designed and synthesized: one by adding a vanillin molecule in the linker and the second by adding an o-vanillin molecule. Both these ligands, on the basis of complex formation studies presented here, show significant potential as therapeutic agents for iron and aluminium overload. Protonation constants of the pure ligands have been determined by potentiometry, and standard reaction heats by calorimetry. Hydrogen bonding plays an important role in the protonation reactions. The crystal structures of both ligands have furthermore been resolved. Complex formation equilibria for the iron complexes have been studied by combined potentiometry-spectrophotometry and those of aluminium by potentiometry alone. All complexes were found to contain two metal ions. NMR diffusion measurements hardly applied to complex formation equilibria and the results of density functional theory (DFT) calculations were powerful tools in confirming the proposed reaction model and in evaluating the relative stabilities of the products. Further support was given by NMR chemical shift measurements and electrospray mass spectrometry.

Adres publiczny

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