



Chelating ability and biological activity of hesperetin Schiff base.

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Streszczenie

Hydrazone hesperetin Schiff base (HHSB) — N-[(±)-[5,7-dihydroxy-2-(3-hydroxy-4-methoxy-phenyl)chroman-4-ylidene]amino]benzamide has been synthesized and its crystal structure was determined. This compound was used for the formation of Cu(II) complexes in solid state and in solution which were characterized using different spectroscopic methods. The analyses of potentiometric titration curves revealed that monomeric and dimeric complexes of Cu(II) are formed above pH 7. The ESI–MS (electrospray ionization–mass spectrometry) spectra confirmed their formation. The EPR and UV–visible spectra evidenced the involvement of oxygen and nitrogen atoms in Cu(II) coordination. Hydrazone hesperetin Schiff base can show keto-enol tautomerism and coordinate Cu(II) in the keto (O^- , N, O_{ket}) and in the enolate form (O^- , N, O^-enol). The semi-empirical molecular orbital method PM6 and DFT (density functional theory) calculations have revealed that the more stable form of the dimeric complex is that one in which the ligand is present in the enol form. The CuHHSB complex has shown high efficiency in the cleavage of plasmid DNA in aqueous solution, indicating its potential as chemical nuclease. Studies on DNA interactions, antimicrobial and cytotoxic activities have been undertaken to gain more information on the biological significance of HHSB and copper(II)–HHSB chelate species.

Słowa kluczowe

Flavonoids, hesperetin, Schiff bases, Copper complexes, Metal–ionophore complexes

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