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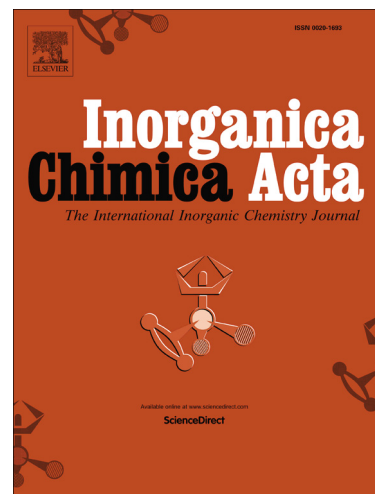
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Tetranuclear Cubane Cu₄O₄ complexes as prospective Anticancer Agents: Design, Synthesis, Structural Elucidation, Magnetism, Computational and Cytotoxicity Studies

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Abstract

Two new homometallic Cu₄O₄ cubane clusters **1** and **2** have been synthesized by self-assembly of copper(II) acetate and ligand, 2-[(2-Hydroxy-3-methoxy-benzylidene)-amino]-2-hydroxymethyl-propane-1,3-diol (**H₄L**) and characterized thoroughly by various spectroscopic techniques and single crystal X-ray diffraction analysis. Temperature-dependent magnetic susceptibility measurements have been performed to elucidate the antiferromagnetic and ferromagnetic nature in Cu₄O₄ clusters **1** and **2**, respectively. In vitro DNA binding studies of cubane clusters were carried out by employing optical spectroscopic techniques. Gel electrophoretic mobility assay performed to examine the nuclease activity of the complexes **1** and **2** with pBR322 DNA, and results revealed oxidative DNA cleavage via reactive oxygen species (ROS) species viz., O₂^{•-}, ¹O₂, etc. *In vitro* cell proliferation via MTT assay was studied to calculate the cytotoxicity of complexes **1** and **2**. The IC₅₀ evaluated were ~ 20 μM in MCF-7 (Breast) and ~ 30-35 μM in HepG2 (Liver) cancer cell lines. Additionally, in the presence of **1**

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