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Title:	Design of a mononuclear copper(II)-phenanthroline complex: Catechol oxidation, DNA cleavage and antitumor properties
Authors:	Yadav, H.R. (/jspui/browse?type=author&value=Yadav%2C+H.R.) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
Keywords:	Copper(II) Crystal structure Catecholase activity DNA cleavage Antitumor activity
Issue Date:	2016
Publisher:	Elsevier Ltd
Citation:	Polyhedron, 106, pp. 106-114
Abstract:	<p>A mononuclear copper(II) complex [Cu(phen)(OH<sub>2</sub>)<sub>2</sub>(NO<sub>3</sub>)](NO<sub>3</sub>) (1) [phen = 1,10-phenanthroline] has been synthesized and structurally characterized by different spectroscopic characterization methods including single crystal X-ray diffraction study. X-ray crystal structure analysis shows that 1 adopts square pyramidal geometry with CuN<sub>2</sub>O<sub>3</sub> chromophore and the molecule crystallises in P2<sub>1</sub>/n space group. 1 has been evaluated as model system for the catechol oxidase enzyme by using 3,5-di-tert-butylcatechol (DTBC) as the substrate in methanol medium, revealing that 1 exhibits greater catalytic activity with K<sub>cat</sub> value 3.91 × 10<sup>3</sup> h<sup>-1</sup> compared to a few copper(II) complexes of the same class. Electrochemical analysis suggests that the mononuclear Cu(II) complex mimics the catechol oxidase enzyme in methanolic medium through radical pathway. The complex cleaves the double strand of pBR 322 plasmid DNA in a concentration-dependent manner so as for the DNA to change from super coiled form to both nicked circular and linear forms. The complex is cytotoxic to the human hepatocarcinoma cell HepG2, as revealed in MTT assay. AO/EB and Hoechst 33528 fluorescent staining techniques were used to find the mode of cell death. Interestingly, AO/EB and Hoechst stained cells observed at IC<sub>50</sub> concentration shows that 1 brings about conformational change on DNA to induce apoptosis which would be the basis underlying its cytotoxic property.</p>
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