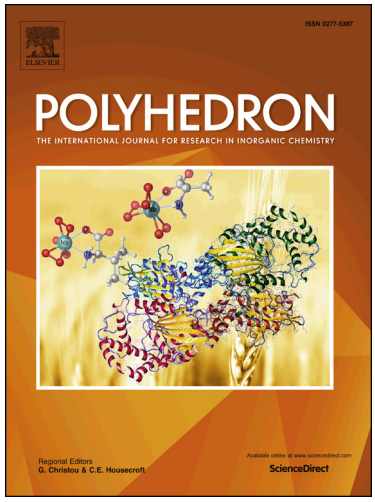

Copper(II) complexes of bidentate mixed ligands as artificial nucleases: Synthesis, crystal structure, characterization and evaluation of biological properties

Arumugam Jayamani, Rajesh Bellam, Gopalakrishnan Gopu, Stephen O. Ojwach, Nallathambi Sengottuvelan

PII: S0277-5387(18)30561-8
DOI: https://doi.org/10.1016/j.poly.2018.09.011
Reference: POLY 13409

To appear in: *Polyhedron*

Received Date: 1 June 2018
Revised Date: 27 August 2018
Accepted Date: 6 September 2018

Please cite this article as: A. Jayamani, R. Bellam, G. Gopu, S.O. Ojwach, N. Sengottuvelan, Copper(II) complexes of bidentate mixed ligands as artificial nucleases: Synthesis, crystal structure, characterization and evaluation of biological properties, *Polyhedron* (2018), doi: https://doi.org/10.1016/j.poly.2018.09.011

Copper(II) complexes of bidentate mixed ligands as artificial nucleases: Synthesis, crystal structure, characterization and evaluation of biological properties

Arumugam Jayamani[a,b], Rajesh Bellam[b], Gopalakrishnan Gopu[a], Stephen O. Ojwach[b], Nallathambi Sengottuvelan[a]*

[a]Department of Industrial Chemistry, School of Chemical Sciences, Alagappa University, Karaikudi – 630003, India

[b]Department of Chemistry, School of Chemistry and Physics, University of KwaZulu-Natal, Pietermaritzburg – 3209, South Africa

Abstract

Mixed ligand transition metal complexes play a significant role in biological processes by interacting with small molecules and activating the enzymes for nuclease activity. Four mixed ligand copper(II) complexes [Cu(5-nsal)(bipy)(ClO_4)] (**1**), [Cu(2-hnap)(bipy) (ClO_4)] (**2**), [Cu(5-nsal)(biim)(ClO_4)] (**3**) and [Cu(2-hnap)(biim)(ClO_4)] (**4**) (bipy = 2,2'-bipyridyl, biim = 2,2'-bi-1H-imidazole, 5-nsal = 5-nitrosalicylaldehyde and 2-hnap = 2-hydroxynaphthaldehyde) were successfully synthesized and physico-chemically characterized. The X-ray quality single crystals of copper(II) complexes **1** and **2** showed that the copper atom was penta-coordinated with square-pyramidal geometry. The physicochemical characterizations of the copper(II) complexes also confirmed the formation of anticipated structures. The redox potentials of the complexes assessed by cyclic voltammetry showed a quasi-reversible redox behavior consistent with Cu(II)/Cu(I) reduction in the cathodic region. The results of ctDNA binding studies using absorption, fluorescence and circular dichroism spectra exposed that the synthesized complexes interact via intercalation mode. The molecular docking studies (*in silico*) showed that complexes interact via major grooves which supported the results obtained from *in vitro* DNA binding studies. The