Biological evaluation, molecular docking and DNA interaction studies of coordination compounds gleaned from a pyrazolone incorporated ligand

Alagarraj Arunadevi [1], Jeyaraman Porkodi [2], Lakshmanan Ramgeetha [1], Natarajan Raman [1]

Affiliations + expand

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Abstract

In this work, we have synthesized a few novel mononuclear complexes of Cu(II), Co(II), Ni(II) and Zn(II) using a pyrazolone-derived Schiff base ligand. They were characterized by spectroscopic and analytical methods. The elemental analyses, UV-Vis, magnetic moment values and molar conductance of the complexes reveal that the complexes adopt an octahedral arrangement around the central metal ions. The interaction of complexes with CT-DNA was studied by absorption spectral titration and viscosity measurements. The observed data show that the complexes bind with CT-DNA *via* an intercalation mode. Efficient pUC18 DNA cleavage ability of the synthesized compounds was explored by gel electrophoresis. The antimicrobial activity of these compounds against a set of bacterial and fungal strains reveals that the complexes exhibit better activity than the free ligand. Moreover, all the complexes were evaluated against two cancer (HeLa and HepG2) and one normal (NHDF) cell lines. The data were compared with cisplatin. Anti-inflammatory activity has been experimentally validated which proves that theoretical predictions concur with the experimental results. In addition, molecular docking studies have been performed to consider the nature of binding mode and binding affinity of these compounds with DNA (1BNA) and protein (3hb5). These studies reveal that the mode of binding is intercalation and the complexes have higher binding energy scores than the free ligand.

Keywords: Anti-inflammatory activity; DNA interaction; MTT assay; Molecular docking.