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FULL PAPER

Probing of effective pyrazolone based metallonucleases: Molecular docking and *in vitro* biological critiques

Alagarraj Arunadevi, Rajakkani Paulpandiyan, Natarajan Raman

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Abstract

Four novel tryptophan based metal (II) complexes of the type [ML $(Try)_2$] were prepared by using pyrazolone derived Schiff base ligand. The proposed structure was confirmed by physicochemical methods which reveal octahedral coordination environment around the metal center. Intercalative binding mode of the complexes with CT DNA was confirmed by electronic absorption titration, viscosity measurements and fluorescence spectroscopy. Efficiency of DNA cleavage ability of the metal complexes was explored by the gel electrophoresis technique. The antimicrobial activities of the metal complexes showed potent biocidal activity. The percentage of free radical scavenging activity shows that the complexes are very reactive towards DPPH. Moreover, their cytotoxicity was tested against the two cancer cell lines (MCF-7 and HepG2) and one normal cell line (NHDF) respectively. The MTT assay shows that the complexes have the anticancer efficacy. Moreover, the complexes exhibit a limited cytotoxicity effect on normal cell line NHDF. The morphological changes of apoptosis cell death were investigated by using Hoechst 33258 staining method. In addition, the Molecular docking studies was executed to consider the nature of binding and binding affinity of the synthesized compounds with DNA (PDB: 1BNA) and protein (PDB: 3hb5).