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Data Article

Structural data of DNA binding and molecular docking studies of dihydropyrimidinone transition metal complexes

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ABSTRACT

A series of some novel copper complexes derived from Biginelli condensation of DHPHS. The ligand and its transition metal complexes show more antimicrobial activities which was substantiated by molecular docking studies. Transition metal complexes four possess antioxidant properties supported by the DNA-binding, cleavage, and viscosity measurement (Prasad et al., 2011) [1]. The in Silicon DNA binding reveals copper complex is bound to be Minor groove and other manganese, cobalt, nickel complexes are bound to the Major groove portion of DNA through hydrogen bonds and hence copper (II), manganese (II), cobalt (II), nickel (II) complexes are called Minor groove and Major groove binder respectively. The DNA cleavage studies of metal complexes presented more protruding activity in the attendance of H_2O_2 associated to that in the absence of H_2O_2. In continuance of our ongoing research on DNA binding and cleavage happenings of transition metal complexes, in this paper we obtainable the synthesis, characterization and DNA cleavage activities.

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Specifications Table

Subject area	Chemistry, Biology,
More specific subject area	DNA Binding, Antioxidant, Molecular Docking
Type of data	Table, text file, graph, figure
How data was acquired	JASCO UV spectra (200–800 nm),Ubbelohde viscometer, Gel electrophoresis, superoxide dismutase, Schrodinger Maestro 9.9 OPLS-2005
Data format	Analyzed
Experimental factors	DNA binding experiments were performed in Tris–HCl/NaCl buffer (5 mmol L^{-1} Tris–HCl/50 mmol L^{-1} NaCl buffer pH) using DMSO (10%) solution of metal complexes. Absorption titration experiments were made using different concentration of CT-DNA, while keeping the complex concentration constant. Correction was made for the absorbance of CT-DNA. Viscosity experiments were conducted on the Ubbelohde viscometer, immersed in a water bath maintained at 25 ± 0.1 °C. Titrations were performed for the compound (10–90 μl) and each compound was introduced into CT-DNA solution (50 μl) in the viscometer. DNA cleavage experiment was conducted using CT DNA by gel electrophoresis with the corresponding metal complex in the presence of H_2O_2 as an oxidant The superoxide dismutase activity (SOD) of the Mn(II), Co(II), Ni(II), Cu(II) complexes were evaluated using alkaline DMSO as source of superoxide radicals ($O_2^{\cdot-}$) generating system in association with nitro blue tetrazolium (NBT) as a scavenger of superoxide, mixture were kept in ice for 15 min and then 1.5 mL of alkaline DMSO solution was added while stirring. The absorbance was monitored at 540 nm against a sample prepared under similar condition except NaOH in DMSO synthesized CuL_2 and Cocrystal ligands (08B, NDP, 9AR, GWH, RLT) are constructed using fragment dictionary of Maestro 9.9, Totally all the docking calculation results are performed by “Extra precision” (XP) mode of Glide program
Experimental features	DNA binding studies of metal complexes (Mn (II), Co (II), Ni (II), Cu (II)) to DNA helix has been characterized through absorption spectral titrations, significant hypochromism with a red shift of 10 nm (bathochromism) of absorption band implicates intercalative mode of binding and is likely that the all complexes with aromatic chromophore stabilizes the DNA duplex. The lower electropositive character of the metal which increases the binding mode with DNA. The electropositive character of the metal decreases as the following order: Cu (II) < Ni(II). Increase in viscosity of DNA as much for all M(II) complexes is observed, this increase in separation of base pairs at intercalation sites and hence an increase in DNA contour length, results from the viscosity experiments confirm the mode of these compounds intercalating into DNA base pairs. The double-stranded DNA tends to gradually dissociate to single strands on increase in the solution temperature and generates a hyperchromic effect on the absorption spectra of DNA bases, insertion of planar aromatic ligand in between the DNA base pairs via intercalation cause stabilization of base stack and hence raises the melting temperature of the double-stranded DNA. Introduction of metal group (Mn, Co, Ni, Cu) in the ligand system markedly increases the antioxidant efficient due to decreased electropositive character of metals. The activity was found in the following order $MnL_2 < CoL_2 < NiL_2 < CuL_2$. Redox behaviour of the complexes responsible for its antioxidant activity, difference in reactivity of the synthesized complexes

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