



Evaluation of DNA, BSA binding, DNA cleavage and antimicrobial activity of ytterbium(III) complex containing 2,2'-bipyridine ligand

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ABSTRACT

In order to estimate biological potential of a synthesized complex $[Yb(bpy)_2Cl_3.OH_2]$ where bpy is 2,2'-bipyridine, its binding behavior with fish salmon-DNA (FS-DNA) and bovine serum albumin (BSA) were studied by different kinds of spectroscopic and molecular modeling methods. Also, this complex was selected for its antibacterial and antifungal activities, while, the DNA cleavage activities were examined by agarose gel electrophoresis. The analysis of fluorescence data at four temperatures were done in order to evaluation the binding parameters and the thermodynamics parameters of interactions between Yb(III) complex with DNA and BSA. In addition, iodide quenching studies, ethidium bromide (EB) exclusion assay, ionic strength effect, circular dichroism and viscosity study reflects binding of explicit to the FS-DNA mainly in a groove binding mode. Moreover, molecular docking study indicated that this complex bind to the minor groove of DNA and to polar and apolar residues located in the subdomain IB of BSA (site 3). Also, the results of competitive experiments assessed site 3 of BSA as the most probable binding site for this complex. From both experimental and docking results, the value of binding constant existing the remarkably high affinity of ytterbium complex to DNA as well as BSA. The molecular docking results kept in good agreement with experimental results.



Keywords: Ytterbium (III) complex, Fish salmon-DNA, Bovine serum albumin, Binding interaction, Molecular docking