22nd Iranian Inorganic Chemistry Conference,
23-25 August, 2023
University of Kurdistan

Synthesis, crystal structure, DNA/BSA interaction, Molecular Docking, and catecholase activity of a new phenoxo-bridged dicopper Schiff base complex

Zahra Mohebbi Jahromi[a]*, Zahra Asadi[a] and Michal Dusek[b]

[a] *Department of Chemistry, School of Sciences, Shiraz University, Shiraz, 71454, Iran*

[b] *Institute of Physics ASCR, v.v.i, Na Slovance 2, 182 21, Prague, Czech Republic*

(* *zahra.mohebbi10@gmail.com*)

There have been enormous efforts towards synthesizing new compounds for cancer treatment. Since the interaction with DNA determines drug activity, designing new complexes with different DNA-binding modes is essential. The Cu(II) complexes could find better applications as pharmacological agents among various metals. Besides, a drug's distribution, metabolism, and efficacy depend on its effective interaction with proteins. BSA is the most practical protein in biochemical studies due to its diverse physiological functions [1]. Also, mimicking metalloenzymes' active sites is crucial in coordination chemistry studies. Considering the dicopper(II) moiety of catecholase structure, many dicopper(II) complexes have been used for this purpose [2].

In this study, the DNA/BSA interaction and catecholase activity of a new binuclear water-soluble Cu(II) complex $[Cu^{II}_2L(\mu_{1,1}\text{-}NO_3)(\mu\text{-}OH)(NO_3)(H_2O)]$, where L=[2,6-bis{N-(2-pyridylethyl)formidoyl}-4-methylphenol] involving μ-phenoxo N_2O_4 Schiff base ligand, have been studied. The complex interaction with FS-DNA/BSA was investigated by absorption and fluorescence titration, cyclic voltammetry, circular dichroism, and viscosity measurements. The complex is characterized by CHN, UV-vis, and FT-IR spectroscopy. X-ray analysis revealed the dinuclear Cu(II) ions in a six-coordinated distorted environment. Docking simulation analysis and competitive binding experiments with ethidium bromide showed the complex interaction with DNA mainly via intercalation mode with the K_b value of 2.78×10^4 M^{-1}. Furthermore, this binuclear system was employed to check the possibility of catecholase activity in acetonitrile and DMF, showing high activity in catalyzing the oxidation of 3,5-DTBC to 3,5-DTBQ in acetonitrile.

Keywords: Schiff base, Cu(II) complex; DNA/BSA interaction; Molecular docking; Catecholase activity.

References

[1] S. Gurusamy, M. Sankarganesh, N. Revathi, R. N. Asha, and A. Mathavan, "Synthesis and structural investigation of o-Vanillin scaffold Schiff base metal complexes: Biomolecular interaction and molecular docking studies," *J. Mol. Liq.*, vol. 369, p. 120941, 2023.

[2] R. Maity, M. Maity, K. Jana, T. Maity, N. Sepay, and B. C. Samanta, "Unveiling the catecholase activities and DNA binding of heterogeneous mono-, di-, and polymeric Schiff Base Cu (II) complexes," *New J. Chem.*, 2023.

22nd
Iranian
Inorganic
Chemistry Conference