Abstract

Today, the synthesis of new chemical compounds that have medicinal properties has received much attention. In this study, two binuclear complexes [(N-N)Zn(μ-pr-dtc)Zn(N-N)]$(NO_3)_2$ (μ-pr-dtc = propylenebis-dithiocarbamate; N-N = 2,2′-bipyridine, complex **a**, and 1,10-phenanthroline, complex **b**) were synthesized. The antioxidant properties of the two complexes were evaluated using DPPH free radical (2,2-diphenyl-1-picrylhydrazyl). The interaction between the above complexes and the β-lactoglobulin (β-LG) was investigated by spectroscopic and molecular docking methods. Fluorescence spectroscopic results showed that the interaction between palladium complexes and β-LG leads to the quenching of the β-LG fluorescence emission by dynamic quenching mechanism. The binding constant values were 1.6×10^3 M^{-1} for the complex **a** and 1.94×10^4 M^{-1} for the complex **b**, at 300 K. Thermodynamic parameters showed that hydrogen bonds and Van der Waals interactions play a major role in the interaction between the two complexes and β-LG. Experiments performed by FT-IR, UV-Vis, and CD spectroscopy confirmed that the interaction between two complexes and β-LG leads to change in the structure and decrease in α-helix of protein. The Molecular docking studies indicate the Zn(II) complexes bind to amino acid residues located in site II of β-LG.

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Keywords: Beta-lactoglobulin; Zinc Complexes; Anticancer Properties, Molecular Docking

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