Abstract

The synthesis of new drugs by means of transition metals is a wide range of pharmaceutical studies. In this study, two binuclear complexes $[(N\text{-}N)Pd(\mu\text{-}pr\text{-}dtc)Pd(N\text{-}N)](NO_3)_2$ (μ-pr-dtc= propylene bis-dithiocarbamate; N-N = 2,2′-bipyridine, complex **a**, and 1,10-phenanthroline, complex **b**) were synthesized. The interaction between the above complexes and the human serum albumin (HSA) was investigated by spectroscopic and molecular docking methods. Fluorescence spectroscopic results showed that the interaction between the palladium complexes and HSA leads to the quenching of the HSA fluorescence emission by dynamic quenching mechanism. The binding constant values were 7.6×10^2 M^{-1} for the complex **a** and 3.4×10^3 M^{-1} for the complex **b** at 300 K. Thermodynamic parameters showed that hydrophobic interactions play a major role in the interaction between the two complexes and HSA. Experiments performed by FT-IR, UV-Vis, and CD spectroscopy confirmed that the interaction between two complexes and HSA resulted in limited changes in protein structure. The Molecular docking studies indicate the Pd(II) complexes bind to residues located at site I and in the subdomain IIA of HSA.

Keywords: Human Serum Albumin; Palladium Complexes; Anticancer Properties**,** Molecular Docking

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