Abstract

A new dithiocarbamate ligand, 5- dithiocarbamato -1,3,4-thiadiazole-2-thiol (thia-dtc) and its Zn(II) complex ([Zn(bpy)(thia-dtc)]Cl) have been synthesised and characterized by spectroscopic methods (^{1}HNMR, FT-IR, UV–Vis). The biological properties of ligand and Zn complex were investigated *in vitro* conditions using MCF-7 breast cancer cell line. The values of IC_{50} for these compunds showed significant cytotoxic activity against human breast cancer cells. The interaction of above compounds with human serum albumin (HSA) was investigated in Tris–HCl buffer solution at pH 7.4 by various spectroscopic techniques; fluorescence, UV-Vis, FT-IR and circular dicorism. The fluorescence data depicted that thia-dtc and Zn complex had ability to quench the intrinsic fluorescence of HSA through a static quenching procedure. Binding constants (K_b) and the number of binding sites (n ~ 1) were calculated. Thermodynamic analysis displayed that both hydrophobic interaction and hydrogen bonding played major roles in the binding of thia-dtc and Zn complex to HSA. The distance r between donor (HSA) and acceptor (thia-dtc and Zn complex) was obtained according to fluorescence resonance energy transfer. The alterations of HSA secondary structure induced by above compounds were confirmed using FT-IR and CD spectroscopy. Finally, molecular docking for identification of the active site residues, critical interactions involved and to confirm the experimental results was employed.

Keywords: Dithiocarbamate, Zn Complex, Human Serum Albumin, Spectroscopic Methods, Molecular Docking

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The Thesis Submitted for the Degree of Master of Science (In the field of Analytical Chemistry)

Interaction of new water soluble zinc(II) dithiocarbamate complex as anti-cancer agent with human serum albumin: spectroscopic and molecular docking studies

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November 2015