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Zahra Asadi, Maryam Golchin, Vaclav Eigner, Michal Dusek, Zahra Amirghofran

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A detailed study on the interaction of a novel water-soluble glycine bridged zinc(II) Schiff base coordination polymer with BSA: synthesis, crystal structure, molecular docking and cytotoxicity effect against A549, Jurkat and Raji cell lines

Zahra Asadi^{*a}, Maryam Golchin^a, Vaclav Eigner^b, Michal Dusek^b, Zahra Amirghofran^c

a) Department of Chemistry, College of Sciences, Shiraz University, Shiraz 71454, Iran

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

c) Department of Immunology and Medicinal and Natural Products Chemistry Research Center, Shiraz University of Medical Sciences, Shiraz 71454, Iran

Abstract

A novel water-soluble glycine bridged zinc(II) Schiff base coordination polymer was synthesized by the condensation of 2,6-diformyl-4-methylphenol, glycine, and zinc(II) chloride. The complex was characterized by ¹HNMR, FT-IR, elemental analyses and X-ray crystallography. The polymeric complex was built up of two glycine-bridged Zn/L moieties, where L denotes the Schiff base containing 2,6-diformyl-4-methylphenol and glycine in 1:1 molar ratio. The carboxylic group of L was coordinated to the Zn atoms of the neighboring moieties; thus each Zn center was five-coordinated. The interaction between polymeric Zn(II) complex and bovine serum albumin (BSA) was studied by UV-Vis, fluorescence, and synchronous fluorescence spectroscopic techniques. By considering the sign and values of the thermodynamic parameters (ΔH and ΔS), it is clear that the binding between BSA and complex was exothermic and entropy-driven and electrostatic interactions between the complex and BSA was supposed. Site-selective binding studies revealed that the complex were mainly located in the region of site II (subdomain IIIA) in BSA. From the synchronous fluorescence spectroscopic studies, it is concluded that complex could bind to tyrosine and tryptophan residues simultaneously. The K_b values indicated a high binding affinity of the complex to BSA. In vitro anticancer activity of the polymeric Zn(II) complex was evaluated against A549, Jurkat, and Raji cell lines by MTT assay. The complex was remarkably active against the cell lines and can be a good candidate for an

* Corresponding author. E-mail address: zasadi@shirazu.ac.ir

Tel: +98 713 6137118; Fax: +98 713 646 0788

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