عنوان مقاله:

Preparation, Characterization And Study Of Biological Potency In Binuclear Zinc(II) Complex Of Dithiocarbamate Derivatives

محل انتشار:

بیستمین سمینار شیمی معدنی ایران (سال: 1397)

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خلاصه مقاله:

It is, essential to investigate the interactions between drugs and carrier proteins in order to specify the pharmacology and pharmacodynamics of drugs (1). A binuclear dithiocarbamate Zn(II) complex [(phen)Zn(μ-pr-dtc)Zn(phen)](NO3)2 (where phen = 1,10-phenanthroline, pr-dtc = propylenebisdithiocarbamate, Fig. 1) was synthesized and characterized in the present study. The formulated complex was evaluated for in vitro antioxidant activity as radical scavengers against 1,1-diphenyl-2-picrylhydrazyl radicals (DPPH.). According to the results, antioxidant activity of Zn complex (IC50 = 21 mg L-1) was effective. Biophysical techniques along with computational modeling were employed to examine the binding of this complex with bovine β-lactoglobulin (βLG) as the model protein. The trial findings revealed an interaction between binuclear complex and βLG with a modest binding affinity (Kb = 6.01 × 104 M−1. An intense fluorescence quenching of protein through a static quenching mechanism was occurred due to the binding of complex to βLG. Hydrogen bonds and Van der Waals forces was the main stabilizing forces in the development of drug-protein complex. Analysis of protein-ligand docking demonstrated binding of complex to residues placed in the site B of βLG

کلمات کلیدی:

Carrier protein; Antioxidant agent; Molecular docking