



Computational and Experimental Study on the Interaction of Terbium(III), Dysprosium(III) Complexes Containing 2, 2'-bipyridine with Human Serum Albumin

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ABSTRACT

In this paper, terbium(III), dysprosium(III) complexes containing 2, 2'-bipyridine (bpy) ligand, were successfully synthesized and characterized by means of elemental analysis (CHN), infrared spectroscopy (FT-IR), UV-vis absorption spectroscopy and ¹HNMR. To explore the potential medicinal value of these complexes, their binding interactions with Human Serum Albumin (HSA) were investigated through UV-vis and fluorescence spectroscopies and also molecular docking examinations. The thermodynamic parameters, binding forces, and Förster resonance distance between these complexes and Trp-214 of HSA were estimated from the analysis of fluorescence measurements. Furthermore, the results of molecular docking calculation and competitive binding experiments represent the binding of these complexes to site 3 of HSA located in subdomain IB, containing both polar and apolar residues. The consistency of computational and experimental results, according to the binding sites and the order of binding affinities (Tb-complex > Dy-complex) supports the accuracy of docking calculation.

Keywords: Terbium(III) complex, Dysprosium(III) complex, Human Serum Albumin, Binding affinity, Molecular docking