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Study of the interaction between a new Schiff-base ligand and human serum albumin by voltammetry and spectroscopy methods and molecular docking

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Abstract

Human serum albumin, the most abundant plasma carrier protein, has long been the center of attention of pharmaceutical industry due to its ability to bind a diverse range of metabolites and drugs. This astonishing binding capacity often seriously impacts pharmacokinetic properties of drugs [1]. In this work new Schiff-base ligand, 1,1'-((1E,1'E)-(naphthalene-1,5-diylbis(azanylylidene))bis(methanylylidene))bis(naphthalen-2-ol) (SNL), was synthesized and the interaction between this ligand and human serum albumin (HSA) was investigated by fluorescence and absorption spectroscopies. A marked decrease in the fluorescence intensity of this compound was observed at 475 nm upon addition of HSA when excitation wavelength was set at 370 nm in pH 7.4 Tris–HCl buffer solution. Reversely, the intrinsic fluorescence of HSA could be quenched by Schiff-base ligand. The quenching mechanism was suggested as static quenching according to the Stern–Volmer equation and the UV–vis absorption spectral change upon addition of HSA[2]. The binding constants Kb and the number of binding sites (n=1) were calculated. Molecular docking results revealed that the primary HSA-SNL binding sites are in the subdomain IA of the HSA structure.

Key words: Schiff-base, human serum albumin, anticancer potential, molecular properties, molecular docking,

References

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