



## Biophysical Studies on the Interactions of Nitrofurantoin with Bovine Serum Albumin by Spectroscopic and Molecular Modeling Methods

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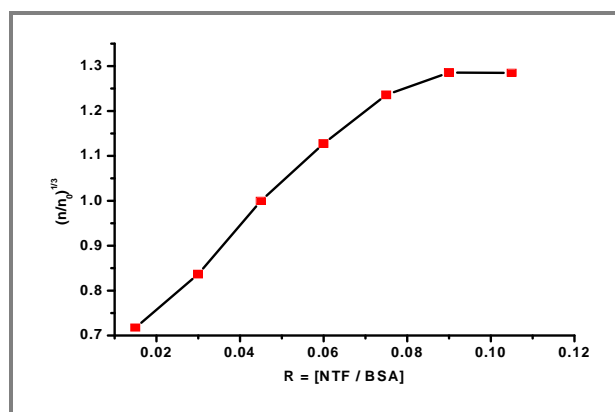
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Accepted on 9<sup>th</sup> August, 2020

### ABSTRACT

The interaction between nitrofurantoin (NTF) and bovine serum albumin (BSA) has been studied. The studies were carried out in a buffer medium of pH 7.4 using fluorescence spectroscopy, UV-Vis spectroscopy, Viscometry and molecular modeling methods. The results of fluorescence quenching and UV-Vis absorption spectra experiments indicated the formation of the complex of BSA-NTF. Binding parameters were determined using the Stern-Volmer equation. From fluorescence and UV-Vis spectroscopic data, the binding constant between NTF and BSA was calculated to be  $4.275 \times 10^3 \text{ L mol}^{-1}$  and  $8.173 \times 10^3 \text{ L mol}^{-1}$  respectively. The results of thermodynamic parameters  $\Delta G^\circ$ ,  $\Delta H^\circ$  and  $\Delta S^\circ$  at different temperature indicate that the electrostatic interactions and also hydrogen bonds play a major role for NTF-BSA association. Molecular modeling calculation demonstrated that NTF is mainly located within the hydrophobic pocket of the subdomain IIIA of BSA.

### Graphical Abstract



Effect of increasing the concentration of BSA on the relative viscosity of NTF.

**Keywords:** Nitrofurantoin macrocrystals, BSA, Spectroscopic, Molecular modelling.