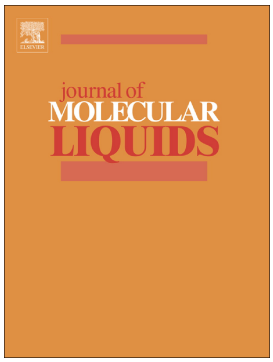

Insights in to the mechanism of interaction of a thrombin inhibitor, dabigatran etexilate with human serum albumin and influence of β-cyclodextrin on binding: Spectroscopic and computational approach

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Insights in to the mechanism of interaction of a thrombin inhibitor, dabigatran etexilate with human serum albumin and influence of *β*-cyclodextrin on binding: Spectroscopic and computational approach

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A B S T R A C T

The present work investigates the characteristics of interaction of a thrombin inhibitor, dabigatran etexilate (DAB) with a model transport protein, human serum albumin (HSA). *In vitro* studies on DAB-HSA interactions were carried out by spectroscopic, molecular docking and simulation approaches in phosphate buffer solution of pH 7.4. Fluorescence results revealed that the intrinsic fluorescence intensity of HSA was quenched by DAB *via* static quenching mechanism. Further, these results suggested the decreased binding affinity (K) and increased Stern-Volmer quenching constant (K_{sv}) with increase in temperature. Spontaneity of DAB-HSA interaction was evident from negative free energy change values. The measurement of change in entropy and change in enthalpy unfolded the signature of hydrogen bonding and hydrophobic forces in DAB-HSA interaction. Circular dichroism, absorption and 3D-fluorescence studies indicated the changes in secondary structure of protein. Docking simulation unravels the possible binding position of DAB on site I of HSA and dynamic facets of DAB-protein interaction process. The effect of Cu^{2+} and Zn^{2+} on the binding of DAB to HSA was investigated.

Keywords:

Dabigatran etexilate, Human serum albumin, *β*-cyclodextrin, Fluorescence quenching, Computational approach