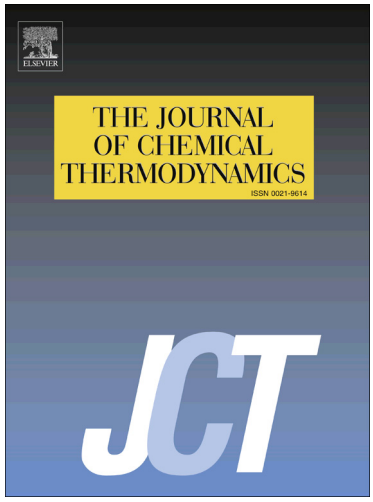

Probing of the binding profile of anti-hypertensive drug, captopril with bovine serum albumin: A detailed calorimetric, spectroscopic and molecular docking studies

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Probing of the binding profile of anti-hypertensive drug, captopril with bovine serum albumin: A detailed calorimetric, spectroscopic and molecular docking studies

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Abstract:

Captopril (CAP), an angiotensin-converting enzyme inhibitor, widely used for the treatment of hypertension. The current study was undertaken to explore the interaction between CAP and the primary plasma protein, bovine serum albumin (BSA) by fluorescence, isothermal titration calorimetric, Förster's resonance energy transfer, circular dichroism, fourier transform infrared and molecular docking studies. The fluorescence result indicated that the fluorescence intensity of native BSA quenched on increasing concentration of CAP in a static manner with blue shift in wavelength maxima. Thermodynamic analysis from ITC suggested that hydrogen bonding and van der Waals forces play major role in the association process and enthalpically driven process. The distance between donor (BSA) and acceptor (CAP) has been calculated according to FRET theory. The ITC based displacement experiments concluded that CAP primarily bound to near sub-domain IIA (Sudlow's site I) of BSA. Alteration in the secondary structure of BSA in the presence of CAP revealed by CD was further substantiated by synchronous, 3D fluorescence and FTIR spectroscopy. In addition, molecular docking was performed to further confirm the biophysical methods. This study provides an insight into the molecular basis of interaction between CAP and BSA helping to understand the activity and mechanism of drug binding.

Keywords: Bovine serum albumin; Captopril; Isothermal titration calorimetry; Spectroscopy; Conformational change; Molecular docking.

1. Introduction