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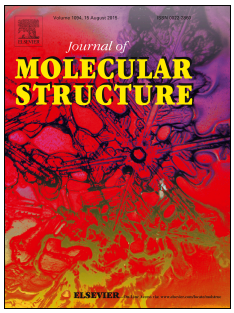

Interactions between epinastine and human serum albumin: Investigation by fluorescence, UV–vis, FT–IR, CD, lifetime measurement and molecular docking

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PII: S0022-2860(16)31386-2

DOI: 10.1016/j.molstruc.2016.12.066

Reference: MOLSTR 23264

To appear in: *Journal of Molecular Structure*

Received Date: 24 July 2016

Revised Date: 21 December 2016

Accepted Date: 22 December 2016

Please cite this article as: G.G. Ariga, P.N. Naik, S.A. Chimatadar, S.T. Nandibewoor, Interactions between epinastine and human serum albumin: Investigation by fluorescence, UV–vis, FT–IR, CD, lifetime measurement and molecular docking, *Journal of Molecular Structure* (2017), doi: 10.1016/j.molstruc.2016.12.066.

Interactions between epinastine and human serum albumin: investigation by fluorescence, UV–vis, FT–IR, CD, lifetime measurement and molecular docking

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ABSTRACT

The fluorescence quenching of human serum albumin (HSA) by epinastine hydrochloride (EPN) at pH 7.4 buffer was studied using absorption, fluorescence quenching, time–resolved, circular–dichroism, synchronous and molecular docking studies have been employed in the system. The fluorescence quenching study revealed that the static quenching mechanism was involved in the interaction of EPN with human serum albumin. The value number of binding sites, *n*, is close to unity, EPN–HSA, indicated the presence of a single class of binding site for the drug in protein. The binding constant value of EPN–HSA was observed to be 2.72×10^4 M^{-1} at 298K. The spectral results attest that the binding of EPN–HSA induced conformational changes in the HSA. The metal ions *viz*., Ca^{2+}, Co^{2+}, Cu^{2+}, Ni^{2+} and Zn^{2+} were found to influence the binding of the EPN to HSA. Based on the Forster's theory of non–radiation energy transfer, the binding average distance, *r*, between the donor (HSA) and acceptor (EPN) was found to be 4.33 nm. The circular dichroism data revealed that the presence of EPN decreased the α–helix content of serum albumin, which indicated conformation changes in HSA upon interaction with EPN.

KEYWORDS Epinastine hydrochloride; Human serum albumin; Fluorescence quenching; Thermodynamic parameters; Circular dichroism; Molecular docking

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