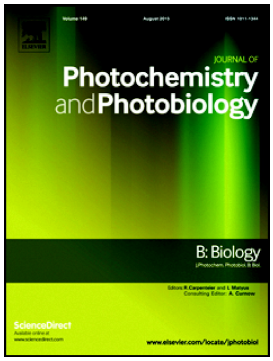

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Fereshteh Shiri, Somaye Shahraki, Amin Shahriyar, Mostafa Heidari Majd

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Exploring isoxsuprine hydrochloride binding with human serum albumin in the presence of folic acid and ascorbic acid using multispectroscopic and molecular modeling methods

Fereshteh Shiri,*[,a] Somaye Shahraki[a], Amin Shahriyar[a] and Mostafa Heidari Majd[b]

[a]*Department of Chemistry, University of Zabol, P.O. Box 98615-538, Zabol, Iran.*
[b]*Faculty of Pharmacy, Zabol University of Medical Sciences, Zabol, Iran*

Abstract

Isoxsuprine hydrochloride (vasodilator drug), folic acid and ascorbic acid are medicines which can be utilized alone or simultaneously by pregnant women. In the present work the competitive binding of isoxsuprine hydrochloride (ISO) with human serum albumin (HSA) in the absence and presence of folic acid (FOL) and ascorbic acid (AS) was investigated using different spectroscopic probes and molecular docking studies. The results of fluorescence suggested that isoxsuprine alone or in the presence of ascorbic acid can bind to HSA and quench the fluorescence of HSA with static mechanism but For HSA–folic acid–isoxsuprine system, dynamic type of quenching mechanisms is involved. The values of binding constants ($K_{HSA\text{-}ISO}$ ~ 1.2 $\times 10^3$ M^{-1}, $K_{HSA\text{-}AS\text{-}ISO}$ ~ 2.1 $\times 10^3$ $M^{-1}$and $K_{HSA\text{-}FOL\text{-}ISO}$ ~ 0.7 $\times 10^3$ M^{-1}) suggested that affinity of HSA to isoxsuprine increased in the presence of ascorbic acid while the presence of folic acid reduced the affinity of protein to isoxsuprine. The results of FT-IR and circular dichroism measurements indicated that the binding of isoxsuprine to HSA in the absence and the presence of folic acid and ascorbic acid may induce conformational and microenvironmental changes of protein. Not only do these types of spectroscopy techniques provide all the information about the systems, molecular docking, also emphasizes the results and is employed for the identification of the active site residues, bioactive conformer of Isoxsuprine and their critical interactions.

Key words: Isoxsuprine hydrochloride, ascorbic acid, folic acid, Human serum albumin, Interaction, spectroscopic studies, molecular docking

*Corresponding author:
E-mail address: fereshteh.shiri@gmail.com and Fereshteh.shiri@uoz.ac.ir ,
Department of Chemistry, University of Zabol, P.O. Box 98615-538, Zabol, Iran.
Tel: 0985424822186, Fax: 0985424822180