Abstract

Isoxsuprine hydrochloride (vasodilator drug), folic acid and ascorbic acid are medicines that pregnant women may utilize alone or simultaneously. In the present work, the competitive binding of isoxsuprine hydrochloride with human serum albumin (HSA) in the absence and presence of folic acid and ascorbic acid was investigated using different spectroscopic methods and molecular docking studies. The results of fluorescence suggested that isoxsuprine alone or in the presence of ascorbic acid can bind to HSA and quencher 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 suggested that affinity of HSA to isoxsuprine increase in the presence of ascorbic acid while the presence of folic acid reduced the affinity of protein to isoxsuprine. The distance between the bound isoxsuprine and protein (r) was determined based on the Forster resonance energy transfer mechanism and showed that isoxsuprine has the shortest distance in HSA–isoxsuprine system. 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. Finally, molecular docking for identification of the active site residues, keys interactions involved and to confirm the experimental results was employed.

Keywords: Human Serum Albumin, Folic acid, Ascorbic acid, Isoxsuprine, molecular docking.

University of Zabol
Graduate School
Faculty of Science
Department of Chemistry

The Thesis Submitted for the Degree of Master of Science
(In the field of Analytical Chemistry)

The combination of spectroscopic and molecular modeling methods for investigation of folic acid and ascorbic acid effects on tendency of isoxsuprine to human serum albumin

Supervisors:
Dr. Fereshteh Shiri
Dr. Somaye Shahraki

Advisor:
Dr. Mostafa Heidari Majd

By:
Amin shahriar

Winter 2017