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Study of the binding interaction between bovine serum albumin and carbofuran insecticide: Multispectroscopic and molecular docking techniques

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Highlights

- Potent pesticide carbofuran binds to BSA at Site I.
- A strong static quenching of intrinsic florescence of BSA is observed with minor blue shifts.

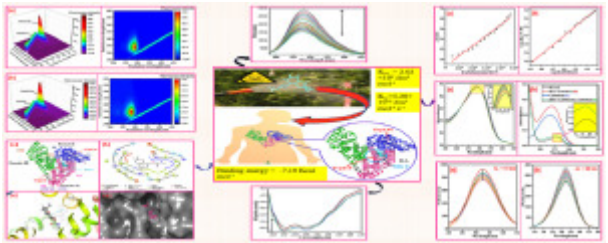
- As a result of binding α-helix percentage decreases.
- Docking study reveals the possible mode of binding.
- Hydrophobic interactions as well as hydrogen bonding, π-π bonding, π-cation interactions are predominant in the binding process.

Abstract

Carbofuran is an agricultural use nematicide, acaricide, and broad-spectrum systematic anticholinesterase carbamate insecticide. Carbofuran accumulates in foodstuffs and has many hazardous effects on animal and human health through ingestion and respiration. People with a cardiovascular condition, asthma, diabetes, mechanical obstruction of the gastrointestinal or urinary tract are more prone to these effects. Therefore, there is a need to develop a responsive and economical approach to understand the molecular interaction between carbofuran and serum protein. In this paper, carbofuran is examined for interaction with bovine serum albumin across several spectroscopic methods. The fluorescence quenching study of bovine serum albumin with

Carbofuran revealed the static nature of quenching. The Stern-Volmer constant (K_{sv}) for Carbofuran interaction with bovine serum albumin was found to be 2.02×10^4 dm^3 mol^{-1} at 298 K. Circular dichroism studies showed minor changes in the secondary structure of albumin on interaction with bovine serum albumin. The binding of carbofuran at Site I of bovine serum albumin was confirmed by competitive molecular docking studies. The present work may provide new insights into the mechanism of carbofuran toxicity and its health consequences.

Graphical abstract



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Keywords

Pesticide; Carbofuran; Highly toxic; BSA; Spectroscopic methods; Molecular docking

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