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A comprehensive multispectroscopic and molecular docking studies on the interaction of bioactive coumarins with bovine serum albumin

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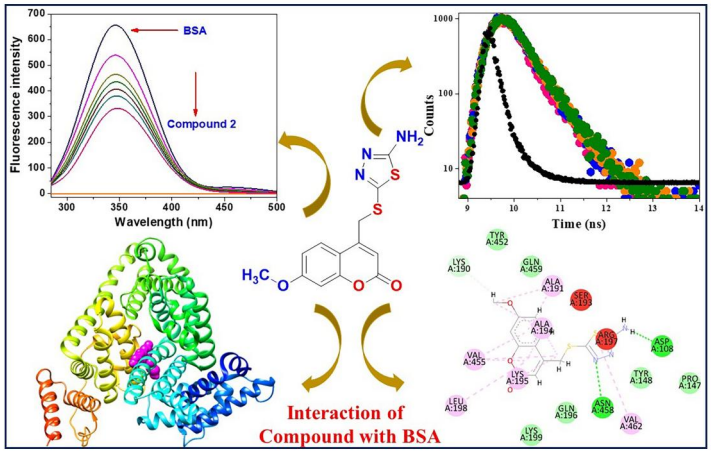
ABSTRACT

The investigation focused on the interaction between bovine serum albumin (BSA) and the biologically active coumarin derivatives 4-(5-amino-[1,3,4]thiadiazol-2-ylsulfanylmethyl)-7-methoxy-chrome-2-one (1) and 4-(5-amino-[1,3,4]thiadiazol-2-ylsulfanyl methyl)-7-methyl-chrome-2-one (2). Molecular docking approaches, synchronous fluorescence spectroscopy, UV–Vis spectroscopy, circular dichroism (CD) spectra and fluorescence spectroscopy were among the multispectroscopic methods used to study the interaction between BSA and coumarin derivatives. The examined coumarin compounds' interaction with BSA yielded a static quenching mechanism for fluorescence. Values for the binding constant (K_b) and quenching constant (K_q) for BSA–coumarin derivatives have been calculated using the Stern–Volmer equation. A change in the tryptophan residue of BSA was seen in its surroundings using synchronous fluorescence quenching investigations. The potential of the compounds under investigation to bind BSA was examined, and it was found that each compound had around one binding site. According to the free energy estimate, there is a spontaneous and very favorable binding interaction between BSA and test compounds. Using the Forster energy transfer theory, the binding average distance between BSA and the chemicals under investigation was found. In conjunction with the findings of CD spectral and fluorescence investigations, it shown that compound 2 has a higher affinity for BSA than compound 1. Molecular docking studies and spectroscopic experimental data are found to be in good agreement. The binding pocket for the development of the ligand–protein complex through hydrophobic and hydrogen bonding interactions was identified by the molecular docking investigation. Furthermore, the results of the Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) prediction and drug-likeness analysis demonstrated the medicinal chemistry characteristics and drug-likeness of these compounds.



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Introduction

As a functional perspective, proteins are the most plentiful and varied of all the chemicals found in living creatures. This class of compounds is essential to almost all biological processes. One kind of protein that is commonly present in the blood of vertebrates is serum albumin (Topală et al., 2014). Serum albumin's primary role in the human body is to move and eliminate chemicals found in the blood. Thus, there has been increased

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