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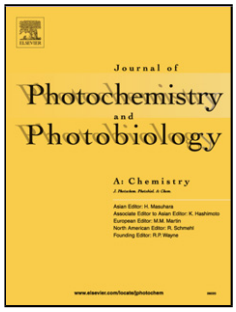

Title: Interaction of tetramethyl-substituted BODIPY dye with bovine serum albumin: spectroscopic study and molecular docking

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Interaction of tetramethyl-substituted BODIPY dye with bovine serum albumin: spectroscopic study and molecular docking

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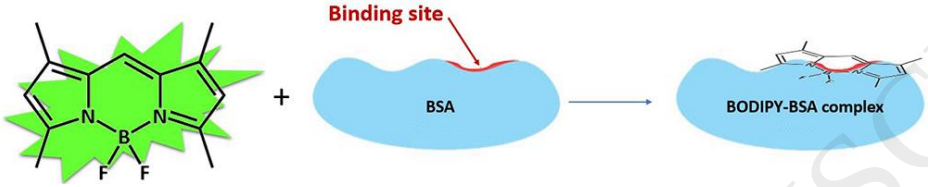
Graphical abstract



Highlights

- The interaction of **1** with BSA was studied *in vitro*.
- The formation of **1** – BSA complex was explained by means of spectral methods and molecular docking.
- The **1** – BSA complex is formed due to the prevailing specific interactions.

Abstract

In this paper the interaction between tetramethyl-substituted BODIPY and bovine serum albumin (BSA) was studied using a spectroscopic approach (UV/vis spectrophotometry, spectrofluorimetry) and molecular docking. The fluorescence of tetramethyl-substituted BODIPY was found to substantially quenched in the presence of BSA. It was observed that BODIPY interacts with the BSA in the sub-domain site IIA of BSA. The BODIPY-BSA complex is formed due to the prevailing specific interactions.

Keywords:
BODIPY; serum albumin; fluorescence; quenching; molecular docking

Introduction

Boron-dipyrromethenes (BODIPYs) are among the most multipurpose and frequently used luminescent dyes. BODIPYs wide range of applications are due to their high thermal and kinetic stability, high quantum yields and extinction coefficients, as well as tunable spectral-luminescent properties [1–3]. Recently, it has been shown [4,5] that BODIPYs can interact with various proteins and peptides acting as fluorescent sensors, markers. Furthermore, BODIPYs may be injected into the animals and humans