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Binding Interactions of Methoxy-Substituted Chalcones with Serum Albumin Proteins: Electronic Effects and Fluorescence Studies

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Highlights

The presence of methoxy (-OCH_3) substituents influences the electronic properties of chalcones by modifying the charge density of the carbonyl group. Spectroscopic techniques were used to analyze how the conjugated π-bond system of chalcones responds to methoxy substitution, including disubstitution on ring B. Fluorescence spectroscopy demonstrated that chalcones interact with serum albumins (BSA and HSA), leading to fluorescence quenching without significant changes in the polarity of the tryptophan microenvironment.

Abstract

Natural and synthetic chalcones are molecules with well-documented pharmacological and biological activities, widely explored for their antioxidant, anti-inflammatory, anticonvulsant, antitumor, and bactericidal properties, among others. Their fundamental structure, as illustrated in Figure 1, consists of two aromatic rings linked by an α,β-unsaturated carbonyl system. The most common synthesis method for these compounds is the Claisen-Schmidt condensation, which involves the reaction between an acetophenone and a benzaldehyde under acidic or basic catalysis.

The electronic properties of chalcones are directly influenced by the introduction of various substituent groups into their aromatic rings. In particular, the carbonyl moiety of chalcones changes charge density due to the effects of these substituents. This study investigates the impact of the methoxy group (-OCH_3), a strong electron-donating substituent, on the electronic characteristics of the α,β-unsaturated carbonyl system of chalcones. Additionally, the effect of disubstitution by methoxy groups on ring B was analyzed to evaluate its influence on the α,β-unsaturated carbonyl system and how these modifications could affect the properties and interaction parameters between chalcone derivatives and serum albumin proteins.

Fluorescence spectroscopy was used to determine the Stern-Volmer constant and the binding constant. Based on the Stern-Volmer equation and the modified Stern-Volmer equation, these binding parameters were calculated to obtain insights into the interactions between chalcones and serum albumin proteins, specifically bovine serum albumin (BSA) and human serum albumin (HSA).

Regarding the absorption and fluorescence properties of HSA, it is known that its primary fluorophore is tryptophan (Trp-214), which exhibits a maximum absorption wavelength (λ_{max}) at 280 nm and characteristic emission at 340 nm when excited at 280 nm. Similarly, BSA exhibits a maximum absorption wavelength at 280 nm and an emission at 340 nm. However, unlike HSA, it contains two fluorescence sites, Trp-134 and Trp-212. Therefore, the studies monitoring chalcone association with serum albumins (at a concentration of 1.0×10^{-6} mol L^{-1}) were performed with excitation at λ= 280 nm. In this study, the fluorescence emission of albumins was quenched by chalcones, resulting in a progressive decrease in emission intensity proportional to the addition of chalcone aliquots, up to a chalcone concentration of approximately 3.0×10^{-5} mol L^{-1}. Since no significant change was observed in the λ_{max} emission, this suggests that adding chalcones did not substantially alter the polarity of the hydrophobic microenvironment surrounding tryptophan in HSA and BSA but confirmed the presence of interactions.

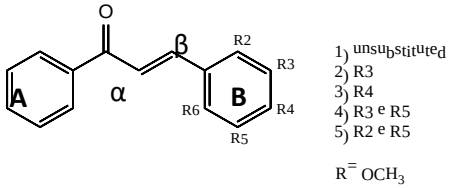

Figure 1. Basic structure of chalcones [1,3-diphenyl-2-propen-1-one].

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