area: FOT

Chalcones functionalized with methoxy groups ($-OCH_3$): Preparation, characterization and spectroscopic studies

Elizabeth Aparecida Alves (PG),[1] **Carla Cristina Schmitt Cavalheiro (PQ),**[1]

alvesselizabeth@usp.br; carla@iqsc.usp.br

[1]*Institute of Chemistry of São Carlos, USP, São Carlos, SP – Brasil.*

Key words: *Chalcone, methoxy, α,β-unsaturated, Claisen-Schmidt condensation.*

Highlights

Chalcones are directly affected by the insertion of substituent groups on their aromatic rings. Spectroscopy allows investigating how this highly conjugated system of π bonds is affected in the presence of methoxy substituents.

Abstract

Natural and synthetic chalcones are molecules known to have pharmacological and biological activity, widely exploited due to their antioxidant, anti-inflammatory, anticonvulsant, antitumor and bactericidal properties, among others. Its basic structure, Figure 1**,** consists of two aromatic rings that are connected by a carbonyl system α,β- unsaturated. The most used synthesis method for the preparation of these compounds is the Claisen-Schmidt condensation, which occurs between an acetophenone and a benzaldehyde by acid or base catalysis. Chalcones are directly affected by the insertion of different substituent groups on their aromatic rings, in which the carbonyl moiety of chalcones has its charge density altered due to the effect of substituents. In this work, it is reported how the methoxy group ($-OCH_3$), a strongly electron-donating substituent, affected the electronic properties of the α,β-unsaturated carbonyl system of chalcones. Disubstitution in ring B by methoxy groups was also investigated, evaluating its effect on the α,β-unsaturated carbonyl set. FTIR spectra showed characteristic bands, as the HC=CH (α-β) bond of the α,β-unsaturated system in the region close to 977 cm^{-1} for all compounds, indicating that they were obtained. By ^1H NMR, confirmation of obtaining α,β-unsaturated products could be observed in the region of 7.65 ppm for α hydrogen and in the region of 7.95 ppm for β hydrogen. The absorption spectra in the UV-Vis region showed that all compounds present an intense band in the region between 298 and 344 nm, characteristic of a $\pi \rightarrow \pi^*$ transition, with mixed character $\pi_{cinnamoyl} \rightarrow \pi^*$ and $n_{c=o} \rightarrow \pi^*$. Spectroscopic studies with solvents EtOAc; CH_3CN; EtOH; MeOH and PBS 7.4; showed a bathochromic shift, characteristic of positive solvatochromism for all compounds. The UV-Vis absorption spectrum of the $-OCH_3$ substituent at the para position showed great influence, shifting the absorption bands to the region of longer wavelength, confirming that electronic transitions $\pi_{cinnamoyl} \rightarrow \pi^*$ and $n_{c=o} \rightarrow \pi^*$ feel the effect of a donor group. These results are part of the photophysical study of the interaction of methoxylated chalcones with albumin proteins (BSA, HSA) in phosphate buffered saline (PBS).

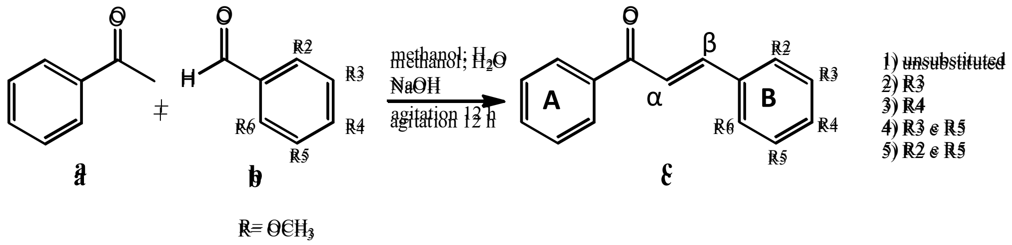

Figure 1. a) acetophenone; **b)** benzaldehyde; **c)** basic structure of chalcones [1,3-diphenyl-2-propen-1-one].

Acknowledgments

CNPQ, FAPESP, CAPES.