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Quantitative structure-activity relationship studies of series of chalcones derivatives as inhibitors of tumor necrosis factor-alpha

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ABSTRACT

Quantitative structure-activity relationship (QSAR) teqnique was used to predict the biological activity of a series of chalcones compounds as anti-inflammatory. 26 physicochemical descriptors are tested in QSAR equations configuration to predict biological effectiveness of compounds under study. The geometries of the compounds under investigation were initially optimized at level (PM3) in accordance to the semi-empirical theory, and subsequently through the B3LYP procedure at the 6-31G(d) basis set in accordance to the DFT theory. The values of correlation coefficients (R^2) in Eqs (1–3) ranged from 0.794–0.873, the Fisher ratios (F) values ranged from 14.161–26.206 and the standard errors (S) values ranged from 0.262–0.334. The results demonstrated good models based on Eq.3, along with high of R^2, F and minimum S by employing three parameters *r*(C3-C5), (LUMO+1) and (LUMO+2). This signifies that these parameters play a significant role in determining anti-inflammatory characteristics.

MSC: 30C45, 30C50

1. Introduction

Chalcone is regarded as a key class of natural product that is broadly distributed in vegetables, fruits, soya-based foodstuff, spices and tea. Its pharmacological activities have recently garnered much interest [1]. Chalcones, or 1,3- diaryl-2-propen-1-ones, fall under the flavonoid family. Chemically, they are made up from open-chain flavonoids, in which a three-carbon α, β-unsaturated carbonyl system joins the two aromatic rings. The most commonly occurring chalcones in nature are usually polyhydroxylated in the aryl rings. Many chalcones' phenolic groups possess radical quenching properties and have gained popularity in using the chalcones rich plant extract or the compounds as food preservatives or drugs [2].

Quantitative structure-activity relationship (QSAR) defines how a difference can occur in a known biological activity in terms of a function of molecular descriptors that have been derived

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