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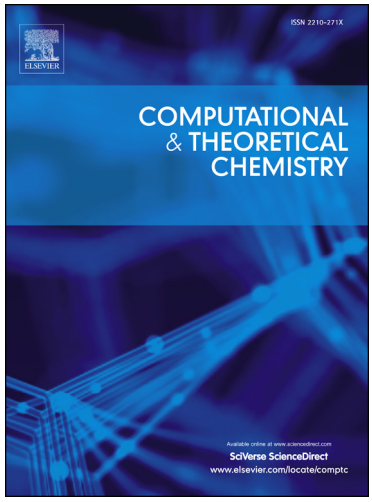

Structure of flavones and flavonols. Part I: Role of substituents on the planarity of the system

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Structure of flavones and flavonols. Part I: Role of substituents on the planarity of the system

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Abstract

In this first part of our investigation the effect of -OH, $-NH_2$, $-NO_2$ and other substituents on the planarity (and the level of delocalization) of a series of flavones and flavonols is assessed. This feature is particularly important with respect to the biological activity of flavonoids. The values of the dihedral angles were obtained from the optimized in gas phase and in water geometries at the density functional theory B3LYP/6-31G(d,p) level.

Keywords: flavones; flavonols; structure; substituents; DFT; PCM

1 Introduction

Being potent radical scavengers, the flavonoids have attracted generous interest in the last years [1]. Kinetics analyses of the protein tyrosine kinases inhibition indicated that flavonoids are competitive inhibitors of the nucleotide adenosine triphosphate [2-4]. There is now substantial evidence indicating that the inappropriate or enhanced expression of these enzymes may also contribute to the transformed state of cells in many human malignancies [5-7]. Some flavones as primuletin, chrysin, and luteolin show vasorelaxing, antioxidative, and chemopreventive effects, respectively [8-10]. A number of studies suggest that flavonoids manifest anti-inflammatory action via their ability to modulate free radical production by phagocytic leukocytes [11-13]. Flavonoids have been identified as good aldose reductase inhibitors, an enzyme of the polyol pathway which regulates glucose blood levels in the body and has been linked with numerous detrimental complications [14].

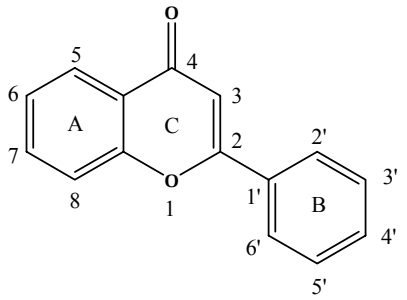

Figure 1: Basic structure of flavones [2-*(2'-phenyl)-chromen-4-one*].

Kador et al. [15-17] have shown that the structural requirements for the inhibitory activity are generally the planar structure with two aromatic hydrophobic regions, and a common region susceptible to charge-transfer interactions. Flavonoids were found to be more potent than other inhibitors [18].

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