A THEORICAL INVESTIGATION OF THE STRUCTURE OF CHALCONES

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Abstract

Secondary metabolites in plants produce the majority of flavonoids; in the biosynthesis of this appears as intermediates the chalcones[1]. Due to its biological activities, more and more attention has been devoted[2]. For the elucidation of structures, NMR spectroscopy is one of the most valuable tools. Not infrequently, in experimental NMR appear incomplete or incorrect structural assignment. To support structural analyzes of experimental organic compounds, much effort was devoted to the development of quantum calculations[3]. ^{13}C Computational NMR spectroscopy is a good parameter to identify two compounds and accurate prediction of chemical shift could be a good compatibility test between a proposed structure and the observed NMR data[4]. Due to its reliability and applicability at different levels of theory, the GIAO method is often approved for shielding constant calculation. One of the choices of researchers that investigate NMR parameters in recent years is the DFT due to its low computational effort and the good agreement of the results obtained with experiment[5]. In this work we intend to test the robustness of a scaling factor based on GIAO-DFT calculations of chemical shift (mPW1PW91/6-31G*//mPW1PW91/6-31G*) and applying of a scaling factor based on a linear regression equation was generated: $\delta scal = 1.06.\delta calc - 2.56$. The robustness of the new protocol to polyphenols was evaluated to difference between scall and experimental chemical shifts ^{13}C NMR for 2 natural compounds with synthesis, biological and therapeutic interest: chalcone (I) and 4-Hydroxyderricin (II), figure 1. The average $|\Delta\delta|$ was (I) 1.92 ppm and (II) 0.96, and the maximum was (I) 5.26 ppm and (II) 4.66 ppm. The average chemical shift for each compound are all under 2 ppm, and the maximum deviations are less than 6 ppm. The prediction of ^{13}C chemical shifts by calculation using DFT mPW1PW91/6-31G* is a very powerful tool for screening proposed structures and be used more widely.

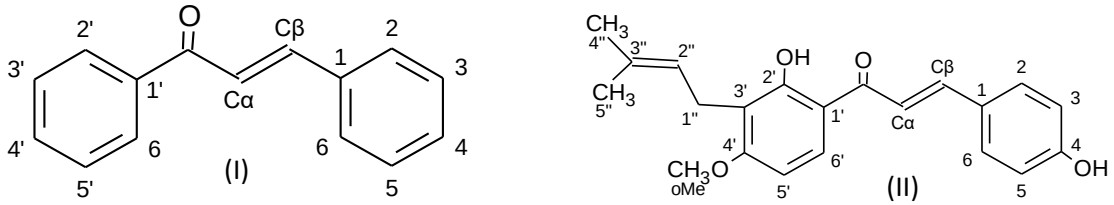

Figure 1: chalcone (I) and 4-Hydroxyderricin (II) molecules.

[1] Hwang et al., "Synthesis and complete assignment of NMR data of 20 chalcones".
[2] Orlikova et al., "Dietary chalcones with chemopreventive and chemotherapeutic potential".
[3] Sarotti e Pellegrinet, "A multi-standard approach for GIAO 13C NMR calculations".
[4] Rychnovsky, "Predicting NMR spectra by computational methods: Structure revision of hexacyclinol".
[5] Migda e Rys, "GIAO/DFT evaluation of 13C NMR chemical shifts of selected acetals based on DFT optimized geometries".