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INCLUSION OF THE EFFECT OF THE SOLVENT USING THE PCM MODEL FOR THE STUDY OF MAGNETIC PROPERTIES OF POLYPHENOLS

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Abstract

Polyphenols exhibit a wide variety of beneficial biological activities, among them antioxidant, antimicrobial, antiviral, antimutagenic, anticarcinogenic, anti-inflammatory, antiproliferative and vasodilatory actions [1,2]. The correct structural determination of these compounds is crucial to understanding their properties [3]. Computational chemistry arises with the need to understand important aspects that can not be solved in a practical way. Therefore, the objective of this work is to develop a protocol for determination of chemical shifts using the PCM model, based on linear regression with ^{13}C nuclear magnetic resonance calculations with low computational cost and with accuracy to help elucidation of structures of polyphenols molecules. All quantum calculations were performed with the Gaussian software package 09 [4]. The optimization calculations of geometry and vibrational frequency were performed at the mPW1PW91 / 6-31G (d) level in the gas phase. Since the isotropic magnetic protection constants were obtained in liquid phase taking into account the effects of the solvent. For this purpose, the PCM (Polarizable Continuum Model) [5]. The scaling factors were generated using the Origin 8.0 program by plotting the chemical displacement values calculated by the experimental chemical shifts of the chalcone set. For the set of twenty chalcones, an equation was generated in the liquid phase $\delta_{scal} = 1{,}05.\ \delta_{cal} - 2{,}54$, $r^2 = 0{,}99342$. The Mean Absolute Deviation (MAD) and Root Mean Square Deviation (RMSD), in ppm, were calculated with calculated and stepped chemical displacement (in parentheses). There were obtained: MAD = 3,88 (1,50) and RMSD = 4,66 (2,39). The level of applied theory performed in PCM is capable of leading to a satisfactory reproduction of experimental chemical displacements, since the effects resulting from the interaction between solute and solvent are taken into account.

Keywords: Chalcones. Nuclear Magnetic Resonance. Chemical shift. Computational chemistry.

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