OBTAINING A NEW PROTOCOL FOR STRUCTURAL DETERMINATION OF POLYPHENOLS BY CALCULATIONS OF ^{13}C NMR CHEMICAL SHIFT

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Abstract

Structure Elucidation, is based on the analysis of available spectral data. Nuclear Magnetic Resonance (NMR) spectroscopy is certainly one of the main analytical methods applied to these challenges and is a powerful technique for acquiring highly informative spectra associated with a structure [1]. Chalcones, a group of naturally occurring compounds, have attracted increasingly widespread attention in present-day society, since they possess a wide range of pharmacological properties possess a variety of bioactivities [2]. In this work it was desired to create a ^{13}C NMR chemical shift protocol for polyphenois based on the application of scaling factor with chalcone molecules. This factor was obtained from a linear regression between experimental chemical shift versus those calculated for a set of selected chalcones. This protocol consists of GIAO-DFT calculations of chemical shifts (mPW1PW91/6-31G*//mPW1PW91/6-31G*). Thus, by calculating the ^{13}C chemical shifts of all molecules, a linear regression was performed, using all chemical shifts obtained theoretically and experimentally [3]. The equation was used as the scaling factor. It was possible to observe that the level of applied theory led to a good reproduction of experimental chemical shift. This is translated into satisfactory the Mean Absolute Deviation and the Root Mean Square values for most of the molecules used in the parametrization of the calculation protocol. For the set of chalcone , the Mean Absolute Deviation and the Root Mean Square, in ppm, before and after (in parenthesis) are: Mean Absolute Deviation = 5.84 (2.71) and Root Mean Square = 6.61 (3.86).The obtained r^2 value, 0.9755, indicates a good correlation between experimental and theoretical chemical shifts. With the above, it can be concluded that the level of GIAO-mPW1PW91/6-31G theory applied, together with the use of the scaling factor, represented by the linear equation, is an efficient and low cost tool for the calculation of ^{13}C NMR chemical shifts of polyphenols.

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