Combining Monte Carlo Simulations and GIAO-DFT Calculations to Determine the Chemical Structure of the 2',6'-dihydroxy-4',4-dimethoxydihydrochalcone

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Abstract

In this work, we present the robustness test of a new protocol combining Monte Carlo Simulations and GIAO-DFT calculations to determine the structure of the 2',6'-dihydroxy-4',4-dimethoxydihydrochalcone molecule.[1] In order to select the most stable conformer of flexible molecules, will be applied Monte Carlo simulations. Thus, a randomized conformational search of the 2',6'-dihydroxy-4',4-dimethoxydihydrochalcone molecule using the Monte Carlo method with a search limit of 200 structures, and employing the Merck molecular force field, by means of 10,000 simulations, as implemented in the Spartan'08 software package considering an initial energy cutoff of 10 kcal.mol^{-1} was performed. Figure 1 shows the 2 more significant conformations conformers of 2',6'-dihydroxy-4',4-dimethoxydihydrochalcone according to the geometry optimization calculations carried out at the mPW1PW91/6-31G(d) level of theory. The ^{13}C NMR chemical shifts were scaled accord to Giacomello *et al*.[2] The data comparison demonstrated a great agreement between experimental and calculated NMR chemical shifts. The root means square error, in ppm, before and after using the scale factor were, 11.02 and 1.67, respectively, it means that the . Thus, the new protocol combining Monte Carlo Simulations and GIAO-DFT calculations was evaluated for selecting the conformer to calculating the chemical shifts for flexible molecules was able to correctly reproduce the chemical shifts, despite the differences in the conditions of the experimental measurements and computational predictions.

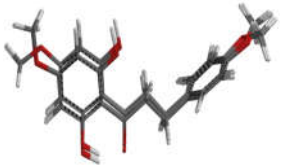

Figure1. The two more significant conformations conformers of 2',6'-dihydroxy-4',4-dimethoxydihydrochalcon.

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1. C. E. Fingolo; T. de S. Santos; M. D. M. Vianna Filho; M. A. C. Kaplan, Molecules, 18, 4248 **(2013)**.
2. F. L. P. Costa; T. F. Giacomello; R. A. de M. Rocha; A. M. de J. C. Neto; G. V. da S. Mota, Adv. Sci. Eng. Med. 9, 254, **(2017)**.