STRUCTURAL DETERMINATION OF BY CALCULATIONS OF 2',6'-DIHYDROXY-4,4'-DIMETHOXY-DIHYDROCHALCONE AND 2-[3-(1,3-BENZODIOXOL-5-YL)PROPYL]-5-METHOXYPHENOL ^{13}C NMR CHEMICAL SHIFT

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Abstract

Polyphenols are one of the most important and certainly the most numerous among the groups of phytochemicals present in the plant kingdom [1]. Herein, we use a protocol designed for determination of polyphenols structures [2]. Thus, in the present work, we aim to calculation of the δ for 2 naturals compounds with synthesis, biological and therapeutic interest: 2',6'-dihydroxy-4,4'-dimethoxy-dihydrochalcone (dihydrochalcone) **(I)** and 2-[3-(1,3-benzodioxol-5-yl)propyl]-5-methoxyphenol (diarylpropane) **(II)**, figure 1a e 1b, respectively. This protocol consists of GIAO-DFT calculations of chemical shifts at the mPW1PW91/6-31G*//mPW1PW91/6-31G* level of theory and application of a scaling factor based on a linear regression equation [2]. Thus, for the molecules **I** and **II**, the Mean Absolute Deviation and the Root Mean Square, in ppm, before and after (in parenthesis) the application of the equation generated: **(I)** Mean Absolute Deviation= 4.66 (1.14); Root Mean Square = 5.21 (1.81) and **(II)** Mean Absolute Deviation **=** 4.94 (1.65); Root Mean Square = 5.44 (2.38). Therefore, based on ours outcome, the protocol recently developed could be a very attractive tool as an alternative to more computationally demanding approaches for the calculation of polyphenols, such as dihydrochalcones and diarylpropanoids.

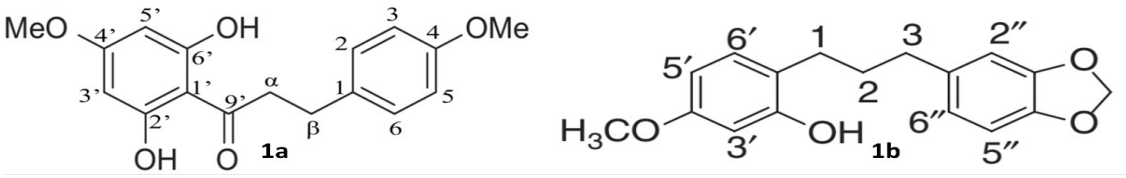

Figure 1. 2',6'-dihydroxy-4,4'-dimethoxy-dihydrochalcone (1a) and 2-[3-(1,3-benzodioxol-5-yl)propyl]-5-methoxyphenol (1b) molecules.

1. N. R. Perron, J. L.et all. “A review of the antioxidant mechanisms of polyphenol compounds related to iron binding,” Cell Biochem. Biophys., vol. 53, no. 2, pp. 75–100, 2009.
2. R. Kachadourian et al., “A Synthetic Chalcone as a Potent Inducer of Glutathione Biosynthesis,” J. Med. Chem., vol. 55, no. 3, pp. 1382–1388, Feb. 2012.