Experimental data and ^{13}C NMR chemical shifts calculation of the: α-amyrin, β-amyrin, α-amyrin acetate and β-amyrin acetate from natural sources

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Abstract

The genus Dorstenia (Moraceae) is a large genus occurring in the tropics around the World that encompasses 170 herbaceous perennials species with succulent rhizomes. This genus is recognized as a rich source of prenyl and geranyl-substituted coumarins, chalcones, flavanones, flavones, flavonol and terpenoids. In this work, we present an application of a GIAO-HDFT universal scaling factor to predict the 30 ^{13}C NMR chemical shifts of 4 triterpenes isolated from genus Dorstenia (Moraceae): α-amyrin (1), β-amyrin (2) α-amyrin acetate (3) β-amyrin acetate. Both the geometry optimizations and the vibrational frequencies were obtained using PM7 level of theory. Magnetics properties were obtained using GIAO-mPW1PW91/3-21G level of theory. For the 4 triterpenes root-mean-square errors were smaller than 2% after the application of the scale factor . In conclusion, GIAO-mPW1PW91/3-21G//PM7 linear regression obtained by using the experimental and the calculated data, is a very attractive tool as an alternative to more computationally demanding approaches, which are usually applied in order to achieve ^{13}C NMR chemical shifts calculations.

Keywords: mPW1PW91/3-21G, PM7, GIAO-NMR, triterpenes