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# Calculation of the Caulerpenynol NMR $^{13}C$ chemical shifts using hybrid functionals

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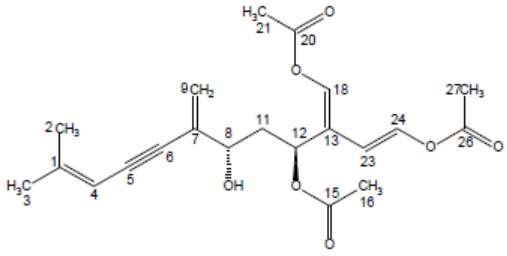
## Abstract

Currently, there is a great need to analyze and value organic compounds in the scope of scientific research to obtain reliable results about them. A powerful technique used to ascertain the three-dimensional structure, organization, and configuration is nuclear magnetic resonance [1-2]. The molecule of interest in this research is Caulerpenynol. This molecule is a terpene into the class of sesquiterpenes, which are organic compounds found in plants as secondary metabolites which are molecules about the adaptation of the plant. These compounds have great scientific value for obtaining new drugs which can fight infectious diseases[3]. The purpose of this study is to do a computational analysis taking place in the GIAO-HDFT (B3PW91, X3LYP and BhandHLYP) with 6-31G(d) basis set in order to determine Caulerpenynol NMR$^{13}C$ chemical shifts. To evaluate which has the closest result to the experimental data and then analyze which technique is more reliable using statistical methods such as MAD and RMSD. The functional BhandHLYP was positioned as the best result when comparing the values of MAD and RMSD in relation to the others hybrid functionals used in the present work. Its results of the statistical parameters were MAD: 3.97ppm and RMSD: 5.3ppm. This demonstrates that the level of theory BhandHLYP/6-31G(d) had the best performance. Therefore, this level of theory could be an effective and low cost tool for the determination of NMR $^{13}C$ chemical shifts of non-aromatic sesquiterpenes.




Caulerpenynol molecule

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