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Calculation of the Ekipodine NMR ^{13}C chemical shifts using hybrid functionals

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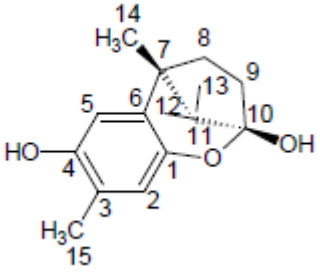
Abstract

Ekipodine is a compound derived from sesquiterpenes. When it comes to discuss about its functionality, it is important to mention that this molecule has been studied in science field because of its high degree of combat against infectious agents such as bacteria. The compound comes from the mushroom Flammulina velutipes [1]. Since its discovery, approximately a decade ago, compounds are synthesized and tested for the production and development of new drugs[1]. Currently, the use of computational chemistry to obtain comparative organic structures with their respective experimental calculations is used to streamline the study involving several molecules[2].The purpose of this study is to do a computational analysis taking place in the GIAO-HDFT (B3PW91, X3LYP and ωB97X-D) with 6-31G(d) basis set in order to determine Ekipodine NMR^{13}C chemical shifts. For the analysis to be better interpreted, we will use the statistical parameters MAD and RMSD, which must have a low number to approximate the value calculated with the experimental ones. B3PW91 functional it obtained an MAD of 5.6 ppm and RMSD of 6.87 ppm. X3LYP obtained an MAD of 6.1ppm and an RMSD of 6.8ppm. ωB97X-D got a result of MAD 5.4ppm and RMSD of 6.25ppm. Therefore, ωB97X-D obtained the most satisfactory result of the bases analyzed. ωB97X-D is a range-separated functional, which is capable of capturing both short-rangr and long-range interactions. In conclusion, further studies using the ωB97X-D functional seem to be necessary in order to confirm its applicability in NMR calculations.



Enokipodine molecule

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