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Comparative between hybrid functionals of the molecule artemisinin

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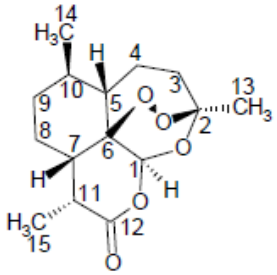
Abstract

Artemisin is an organic compound which has the impact in the elimination of malaria causing death of the vector *Plasmodium falciparum*. The mechanism of action of this drug has not yet been well elucidated, but it is believed to act in the protein synthesis of the vector, damaging it [1.] Currently, magnetic nuclear resonance techniques have been used to obtain structures, dynamics and isomeries of organic compounds for scientific studies and also to mention its importance to chemistry development studies. The necessity of this technique allows the use of molecular modeling through the calculation of the chemical shifts provided by computer software used in this research[1]. The purpose of this study is to do a computational analysis taking place in the GIAO-HDFT (B3PW91, B3LYP and CAM-B3LYP) with 6-31G(d) basis set in order to determine Artemisine NMR ^{13}C chemical shifts. After running the calculations, the results were evaluated with statistical parameters MAD and RSMD, whose lowest value per ppm shows the lowest error ratio between the calculated by the program and the experimental, previously researched in scientific articles. The B3PW91 functional achieved an MAD of 2.1ppm and a RMSD of 3.67ppm. The B3LYP obtained a MAD of 2.0ppm and a RMSD of 3.72ppm. The CAM-3LYP obtained a result of MAD 2.1ppm and RMSD of 3.34ppm. Therefore, the famous B3LYP functional obtained the best result in this research because its outcome is close to the experimental one.



Artemisin molecule

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