Validation of a natural product structure by quantum-mechanical GIAO calculations of *^{13}C* NMR chemical shifts

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Abstract

Computational chemistry can revolutionized the way that we practice chemistry.[1] A question which arises is how can computational chemistry be used to address real world problems? Computational chemistry can provide experimental data at a reduced cost without the need to perform difficult, expensive, and potentially dangerous experiments.[2] In this work we used computational calculations to validation of a natural product structure by quantum-mechanical GIAO calculations of ^{13}C NMR chemical shifts. The calculated NMR theoretical values obtained at GIAO-B3PW91/cc-pVDZ//B3PW91/cc-pVDZ scaling factor protocols show good correlations and high predictive power, which was confirmed by the statistical analysis of their calculated chemical shifts. Thus the present studies confirm the conclusion that the GIAO approach can reach high accuracy for the relative chemical shifts of natural products at a low cost. This is a promising fact for the use of calculated carbon and proton chemical shifts as a tool of conformational analysis for protein structure determination.

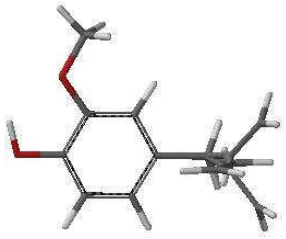

Figure 1. Superimposed minimum energy structures of eugenol according to MC with MMFF force field calculations.

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1 Martin, Y and Shoichet, B, Nature Reviews/Drugs Discovery, 6. 251, **2007**.

2 Jones, R. O, Rev. Mod. Phys, 87, 897, **2015**.

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