COVER LETTER

Dear Dr. Branislav Ž. Nikolić

We would like to submit our research manuscript, entitled “**Theoretical study via DFT for prediction of 13C and 1H NMR data of two diterpenoids derived from the root of Salvia grandifolia**”for possible publication in the Journal of the Serbian Chemical Society.

The DFT method has become a promising alternative in support of traditional NMR experimental techniques, comparing experimental data with theoretical data, achieving accurate and satisfactory results. In the present study, the experimental data of two diterpenes are compared to the theoretical data obtained by the GIAO method, applying the DFT levels B3LYP/cc-pVDZ and B3PW91/DGDZVP to verify the degree of correlation, significance and predictability of the models obtained with theobjective of proving which of the computational methods is the most efficient for this class of substances. We use the best theoretical method for defining Hα and Hβ 1, 2, 3, 6 and 7 for the diterpene 1 and 1, 2, 3 and 6 to diterpene 2, which have not been elucidated experimentally showing that the quantum method can help in the structural elucidation of natural products.

The authors guarantee that the manuscript submitted to the Journal for review is original, was written by the stated authors and has not been published elsewhere; is currently not being considered for publication by any other journal and will not be submitted for such a review while under review by the Journal; the manuscript contains no libellous or other unlawful statements and does not contain any materials that violate any personal or proprietary rights of any other person or entity. We declare that there are no conflicts of interest. Moreover, we are aware that, if the manuscript is accepted for publication, copyright now belong to the Journal of the Serbian Chemical Society.

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Belém-PA, July 19, 2018, Brazil.

Yours faithfully,

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