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Molecular and Electronic Structure Elucidation of a New Class of Cannabisin. An Experimental and Theoretical study

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Abstract: The *Xylopia* genus belonging to the *Annonaceae* family is composed for approximately 160 species. The *Xylopia aromatica* (Lam.) Mart species aromatic is a typical plant of the savannah, known popularly as monkey pepper or monkey banana. After the application of several experimental techniques, cannabisin-b was isolated for the first time along plants found in Cerrado Bioma. This organic molecule is unpublished in the species *Xylopia aromatica*. Because of the potential medicinal properties [1], as well as the novel architectures, the total synthesis of several members of the lignanamide family has received considerable interest [2]. In this sense, theoretical calculation is used in order to probe the experimental data and obtain a molecular structure agreement. In the present work, we choose molecular dynamics (MD) [3] simulation and DFT [4,5] to compare the experimental data with PCM and explicit solvent at the structure, initially were performed geometry optimizations using GROMACS [6] with solvent methanol, soon after, we performed geometry optimizations and spectroscopies properties computations using Gaussian 09 [7] software suite. The computations were carried out using B3LYP [8,9] and 6-311++G (d,p) [10] basis set.

The MD simulations were carried out using the Optimized Potentials for Liquid Simulations (OPLS-AA) force field [11] along with organic parameter set extension within the GROMACS 5.1.4 program, as presented in Figure 1. The simple point charge (SPC) model was used to describe the methanol molecules.

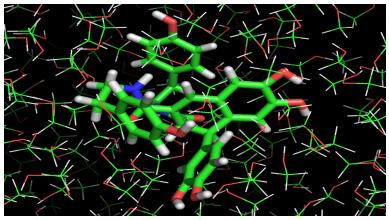

Figure 1. Snapshot presentation of periodic boundary condition simulation of cannabisin-b in methanol solvent.

After MD optimization, the cannabisin-b internal coordinates was submitted to infrared (IR) and nuclear magnetic resonance (NMR) computations, in order to compare to experimental data, as observed in Figure 2.

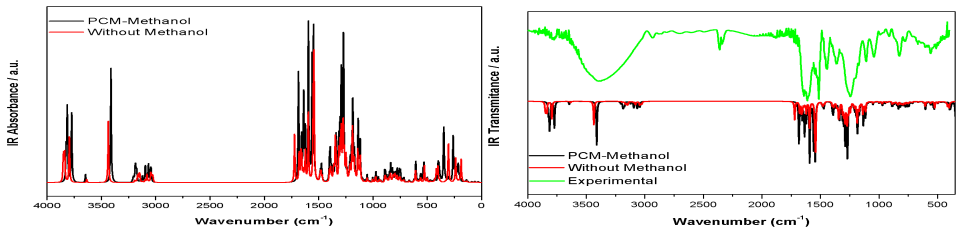

Figure 2. Theoretical IR spectra of cannabisin-b structure in PCM – methanol, without methanol and experimental IR data.

The values obtained using DFT display good agreement when compared for experimental, because the bands at theoretical computations are generally closer wavenumber and intensity to the experimental data.

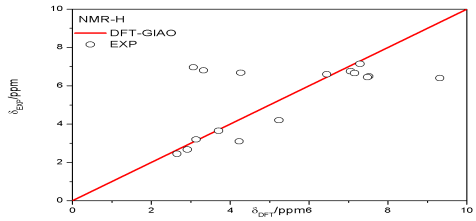

Figure 3. Correlation graphic between experimental and theoretical NMR ^{1}H.

As can be seen from Figure 3, the theoretical ^{1}H are in agreement to the experimental data. It is seen from the theoretical results, there is no remarkable difference between the results of the level of theory used in evaluating vibrational frequencies and experimental characterization.

Key-words: Cannabisin-b, MD, DFT
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References:

[1] Xia, Yamu, et al. J. of Chemical Research 39.10 (2015).
[2] F. Bailly et al,.*Med*. Chem. Lett., ,**23**, 574 (2013).
[3] J. McCammon et al, Nature 267.5612(1977).
[4] Pierre Hohenberg and Walter Kohn. Physical Review 136.3B(1964).
[5] Walter Kohn and Lu Jeu Sham, Physical Review 140.4A(1965).
[6] Herman J. C. Berendsen et al, Computer Physics Communications 91.1-3 (1995)
[7] M. J. Frisch et al., Gaussian Inc., Wallingford CT, G09, Revision D.01(2009).
[8] A. D. Becke, J. Chem. Phys. 98, 5648 (1993).
[9] C. Lee, W. Yang, and R. G. Parr, Phys. Rev. B 37, 785 (1988).
[10] M. J. Frisch, J. A. Pople and J. S. Binkley, J. Chem. Phys. 80, 3265 (1984)
[11] W. L. Jorgensen et al, J. of the American Chemical Society 110.6 (1988).