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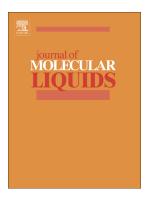
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Synthesis, characterization and computational studies of semicarbazide derivative M. Muthukkumar¹, T. Bhuvaneswari¹, G.Venkatesh², C.Kamal², P. Vennila³, Stevan Armaković⁴, Sanja J. Armaković⁵, Y. Sheena Mary⁶, C. Yohannan Panicker⁶

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Abstract

The ((E)-1-(3, 5 dibromo benzylidene) semicarbazide (35DBBS) has been synthesized and characterized using Fourier-transform infrared (FT-IR), Fourier transform Raman (FT-Raman), ¹H and ¹³C Nuclear magnetic resonance (NMR) spectral analyzes. Fukui functions, molecular electrostatic potential (MEP), bond dissociation energies (BDE) and average local ionization energy (ALIE) values have been studied with help of Density Functional Theory (DFT). Further, the stability of 35DBBS in water has been analyzed using molecular dynamics (MD) simulations. The optimized molecular geometrical parameters such as bond length, bond angle and dihedral angle were calculated in different phases viz., gaseous and aqueous and were compared with experimental values. The title compound's binding energy and antifungal ability of the title compound were evaluated using molecular docking studies. Further, Nonlinear Optical Properties (NLO) of 35DBBS have been examined by first order hyperpolarizability studies.

Keyword: Molecular dynamics simulations; Bond dissociation energies; Molecular docking; Geometrical parameters; Fukui functions.

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