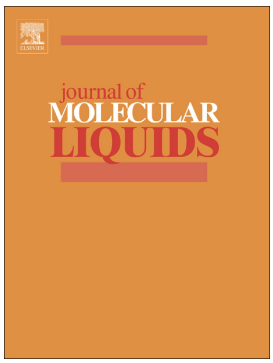

Synthesis, characterization and computational studies of semicarbazide derivative

M. Muthukkumar, T. Bhuvaneswari, G. Venkatesh, C. Kamal, P. Vennila, Stevan Armaković, Sanja J. Armaković, Y. Sheena Mary, C. Yohannan Panicker

PII: S0167-7322(18)31358-8
DOI: doi:10.1016/j.molliq.2018.09.123
Reference: MOLLIQ 9729

To appear in: *Journal of Molecular Liquids*

Received date: 15 March 2018
Revised date: 13 June 2018
Accepted date: 25 September 2018

Please cite this article as: M. Muthukkumar, T. Bhuvaneswari, G. Venkatesh, C. Kamal, P. Vennila, Stevan Armaković, Sanja J. Armaković, Y. Sheena Mary, C. Yohannan Panicker , Synthesis, characterization and computational studies of semicarbazide derivative. Molliq (2018), doi:10.1016/j.molliq.2018.09.123

Synthesis, characterization and computational studies of semicarbazide derivative

M. Muthukkumar[1], T. Bhuvaneswari[1], G.Venkatesh[2], C.Kamal[2], P. Vennila[3], Stevan Armaković[4], Sanja J. Armaković[5], Y. Sheena Mary[6], C. Yohannan Panicker[6]

[1]Department of Chemistry, Selvam Arts and Science College, Namakkal, Tamilnadu, India

[2]Department of Chemistry, VSA Group of Institutions, Salem, Tamilnadu, 636010, India

[3]Department of Chemistry, Thiruvalluvar Government Arts College, Rasipuram, 637 401, India

[4] University of Novi Sad, Faculty of Sciences, Department of Physics, Trg D. Obradovića 4, 21000 Novi Sad, Serbia

[5]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg D. Obradovića 3, 21000 Novi Sad, Serbia

[6] Department of Physics, Fatima Mata National College, Kollam, Kerala, 691001, India

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), ^{1}H and ^{13}C 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.