Commun. Comput. Chem.
doi: 10.4208/cicc.2013.v1.n3.5

Vol.**1**, No.**3**, pp.244-268
August 2013

REGULAR ARTICLE

Synthesis, Structure Investigation, Spectral Characteristics and Biological Activities of 4-benzyl-3-(2-hydroxyphenyl)-1H-1,2,4-triazole-5(4H)-thione

Metin Koparir [1*], Cahit Orek [1], Naci Ömer Alayunt [1], Akif Evren Parlak [1], Pelin Koparir [2], Kamiran Sarac [3], Sevgi Durna Dastan[4], Nevin Cankaya[5]

[1] *Firat University, Faculty of Science, Department of Chemistry, 23119, Elazig, Turkey*
[2] *Department of Chemistry, Forensic Medicine Institute, 44000, Malatya, Turkey*
[3] *Inönü University, Faculty of Science, Department of Chemistry, 44100, Malatya, Turkey*
[4] *Cumhuriyet University, Faculty of Science, Department of Biology, 58140, Sivas, Turkey*
[5] *Usak University, Faculty of Science and Arts, Department of Chemistry, 64100, Usak, Turkey*

Received 6 February 2013; Accepted (in revised version) 13 May 2013

Abstract: This work presents the characterization of 4-benzyl-3-(2-hydroxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (**III**) by quantum chemical calculations and spectral techniques. The molecular geometry, vibrational frequencies and gauge including atomic orbital (GIAO) ^{1}H and ^{13}C NMR chemical shift values of **III** in the ground state have been calculated using the density functional method (B3LYP) with the 6–31G(d,p) basis set. To determine conformational flexibility, the molecular energy profile of the title compound was obtained by using B3LYP/6–31G(d,p) method with respect to the selected torsion angle, which was varied from –180° to +180° in steps of 10°. The calculated results show that the optimized geometry can well reproduce the crystal structure, and the theoretical vibrational frequencies and chemical shift values show good agreement with experimental values. In addition, DFT calculations of molecular electrostatic potentials and frontier molecular orbitals of **III** were carried out at the

* Corresponding author. *E-mail address:* mkoparir@hotmail.com (M.Koparir).

B3LYP/6−31G(d,p) level of theory. The title compound was screened for antibacterial, antifungal and antioxidant activities.

AMS subject classifications: 81–08, 97M60

Key word: 4-Benzyl-3-(2-hydroxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione, Density-Functional Theory, Crystal-Structure, Ab-initio, Antimicrobial activity

1 Introduction

Triazole and its derivatives represent an important class of heterocycles. They are of biological important and are used in the synthesis of drugs [1,2]. A number of 1,3,4-thiadizoles showed antibacterial properties similar to those of well-known sulphonamide drugs [3]. Thus the thiadiazole nucleus, which incorporates an N-C-S linkage, exhibits a large number of biological activities [4]. Derivatives of 1,2,4-triazole have been reported to exhibit diverse biological activities [5–11]. Triazole derivatives are also used in the synthesis of antibiotics, fungicides, herbicides, plant growth hormone insulators [12] and potentially good corrosion inhibitions [13,14]. In addition there are some studies on electronic structures and thiol-thione tautomeric equilibrium of heterocyclic thione derivatives [15–16]. 1,2,4-Triazoles are very useful ligands in coordination chemistry. The utilization of the 1,2,4-Triazole moiety as a part of ligand system in metal complexes has gained considerable attention in recent years [17–19]. The application of triazole ligand lies in medical research-complex with Pt(II) [20] exhibit antitumor activity (human cancer) similar to *Cisplatin*.

Density functional theory (DFT) has been one of the widely used theories in theoretical modeling during recent years. By means of the development of better exchange-correlation functionals, it has become possible to calculate many molecular properties which have accuracies that can be comparable to traditionally correlated *ab initio* methods, all these could be done with more favorable computational costs [21]. It has been figured out during the literature survey that in reproducing the experimental values in geometry, dipole moment, vibrational frequency etc. DFT has a precise accuracy [22-26].

The aim of this study is to investigate the energetic and structural properties of the 4-benzyl-3-(2-hydroxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione (**Figure 1**), using density functional theory calculations. In this study, the optimized geometry, vibrational spectra and assignments, molecular electrostatic potential (MEP) and the statistical energetic parameters of **III** have been studied. These calculations are valuable for providing insight into molecular properties of 1,2,4-triazole compounds. Besides the characterization of the title compound, the biological activities of the **III**, such as antibacterial, antifungal and antioxidant activities were investigated.