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Synthesis, antimicrobial activity and DFT studies of 4,5-dihydro-9-methoxy-4-(5-methylisoxazol-3-yl)benzo[*f*][1,4]oxazepin-3(2*H*)-one

Gaddam Ramesh [a], Ramu Kakkerla [b], Srinivas Marri [c], R. Haripriya [d], Byru Venkatram Reddy [e,*]

[a] Department of Physics, University P.G. College, Satavahana University, Godavarikhani 505209,Telangana, India
[b] Department of Chemistry, Satavahana University, Karimnagar 505001, Telangana, India
[c] Department of Chemistry, Siddhartha Degree & P.G. College, Narsampet 506132, Warangal, Telangana, India
[d] Department of Chemistry, Chaitanya Postgraduate College (Autonomous), Hanamkonda 506001, Warangal, Telangana, India
[e] Department of Physics, Kakatiya University, Warangal 506009, Telangana, India

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ABSTRACT

A new 4,5-dihydro-9-Methoxy-4-(5-Methylisoxazol-3-yl)Benzo[*f*][1,4]Oxazepin-3(2*H*)-One **(5)** was prepared by taking a facile and simple methodology. The reaction of 3-amino-5-methylisoxazole (1) with 3-methoxy salicylaldehyde **(2)**, pursued by reduction with $NaBH_4$, and *in situ* chloroacetylation and cyclization with chloroacetyl chloride and triethyl amine affords isoxazolyl benzo[*f*][1,4]oxazepin-3-(2*H*)-one **(5)**. The structures of the synthesized molecules **(3–5)** were established with the help of ^1H NMR and ^{13}C NMR data. Title compound **5** has been evaluated for their *in vitro* antibacterial and antifungal activity against different bacterial and fungal strains, results revealed tested compound show good antimicrobial activity, when compared to the respective standard drugs. The theoretical studies such as optimized structural parameters, Frontier molecular orbitals (FMO's), polarizability (α), first order hyperpolarizability (β), dipole moment, NLO properties, thermodynamic parameters and Molecular electrostatic potential (MEP) were calculated by using DFT/B3LYP/6–311++G(d,p) method for compound 5. Theoretical NMR chemical shifts of the molecule were computed using GIAO method.

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1. Introduction

The multi-drug defiant microbial pathogens have been explored with widespread use of antibiotics. This focuses the persistent need for the growth of new modules of antimicrobial agents and modification of known drugs so as to permit them to preserve physiological action at the cost of lowering their resistance to the pathogen. The design of new chemotherapeutic agents is favorable because of their disparate style of action which can evade cross resistance to known drugs. Structure property correlations are among the most widely used computational technology for analogue-based drug design. Besides biological reactivity against a target which is primary requirement, there are so many essential properties and characteristics that are mandatory to be possessed by a molecule to be considered as a drug. The use of computational methods for designing of molecules with desired activity, reactivity or property has been a growing area in chemistry and medicine. The 1,4-oxazepine structural design has achieved potential significance in medicinal chemistry, as its derivatives exhibited various biological activities, such as effective protease inhibitors [1], non-peptidergic GPCR inhibitors [2], integrin antagonists [3], squalene synthase [4] and reverse transcriptase inhibitors [5]. For example, *N*-pyrrolidinyl derivatives of benzo-1,4-oxazepins-3-ones **(1)** emerge to comprise tranquilizer and analgesic activity [6]. Benzo-1,4-oxazepin-5-ones **(2)** exhibit antihistaminic activity [7], whereas benzo-1,4-oxazepin-3,5-diones **(3)** were found to be suitable for use as psychotropics [8]. Some novel benzo-1,4-oxazepin-5-ones **(4)** were found to act as 5-HT_1A receptor agonists, and show anti-ischemic effects [9] (Fig. 1). Further, its derivatives are demonstrated as progesterone receptor agonists [10] and telomerase inhibitors [11]. In the recent past, Peng-Cheng LV et al. [12] reported that the oxazepine derivatives also perform as choosy inhibitors of PI3Kα for cancer curing. Isoxazole derivatives are found to possess a wide variety of biological activities [13–17]. Recently 7-substituted-3,4-dihydrobenzo[*f*][1,4]oxazepin-5(2*H*)-ones shows

* Corresponding author.
E-mail address: bvreddy67@yahoo.com (B. Venkatram Reddy).

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