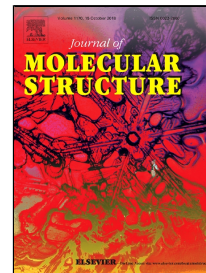


Accepted Manuscript

Antiradical, Antimicrobial and Enzyme Inhibition Evaluation of Sulfonamide
Derived Esters; Synthesis, X-Ray Analysis and DFT Studies



Muhammad Danish, Ayesha Bibi, Khola Gilani, Muhammad Asam Raza,
Muhammad Ashfaq, Muhammad Nadeem Arshad, Abdullah Mohamed Asiri, Khurshid Ayub

PII: S0022-2860(18)30943-8
DOI: 10.1016/j.molstruc.2018.07.116
Reference: MOLSTR 25521
To appear in: *Journal of Molecular Structure*
Received Date: 01 June 2018
Accepted Date: 31 July 2018

Please cite this article as: Muhammad Danish, Ayesha Bibi, Khola Gilani, Muhammad Asam Raza, Muhammad Ashfaq, Muhammad Nadeem Arshad, Abdullah Mohamed Asiri, Khurshid Ayub, Antiradical, Antimicrobial and Enzyme Inhibition Evaluation of Sulfonamide Derived Esters; Synthesis, X-Ray Analysis and DFT Studies, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.07.116

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Antiradical, Antimicrobial and Enzyme Inhibition Evaluation of Sulfonamide Derived Esters; Synthesis, X-Ray Analysis and DFT Studies

Muhammad Danish^{a*}, Ayesha Bibi^a, Khola Gilani^a, Muhammad Asam Raza^a, Muhammad Ashfaq^a, Muhammad Nadeem Arshad^b, Abdullah Mohamed Asiri^{b*}, Khurshid Ayub^c

^aDepartment of Chemistry, University of Gujrat, Gujrat 50700 Pakistan

^bChemistry Department, Faculty of Science, King Abdulaziz University, Jeddah 21589, Saudi Arabia

^cDepartment of Chemistry, COMSATS Institute of Information Technology, Abbottabad, KPK, Pakistan, 22060

Authors for correspondence: drdanish62@gmail.com, aasiri2@kau.edu.sa

Abstract

Two carboxylate esters (methyl: **(I)** and ethyl: **(II)**) of 4-((4-methylphenylsulfonamido)-methyl)cyclohexanecarboxylic acid (sulfonamide) were synthesized and characterized by FTIR and X-ray crystallography. DFT studies were conducted in order to optimize the structures using Gaussian software which confirmed the bond angles and bond lengths obtained from single crystal analysis. Both Compounds (**I** and **II**) were evaluated for their biological studies viz; antioxidant activity (DPPH), enzyme inhibition activity (esterase and proteases), antibacterial (*Halomonas halophila*, *Halomonas salina*, *Shigella sonnei*, *Bacillus subtilis*, *Chromohalobacter salexigens*, *Chromohalobacter israelensis*, *Staphylococcus aureus*, *Escherichia coli* and *Klebsiella pneumoniae*) and anti-fungal (*Aspergillus niger* and *Alternaria alternata*). Results depicted that **II** is more active as compared to **I** in antioxidant and esterases while **I** is more potent against protease while moderate results were shown by both.

Keywords: Antioxidant; DFT; Enzyme Inhibition; Ester; Sulfonamide.

1. Introduction

Sulfonamides have been found to show broad pharmacological profile. They are stable in human body and being used for the treatment of various diseases i.e. tumor, diabetes and other major

Download English Version:

<https://daneshyari.com/en/article/7806580>

Download Persian Version:

<https://daneshyari.com/article/7806580>

[Daneshyari.com](https://daneshyari.com)