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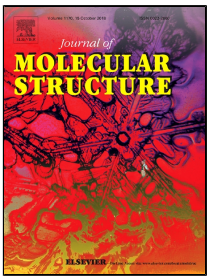

Antiradical, Antimicrobial and Enzyme Inhibition Evaluation of Sulfonamide Derived Esters; Synthesis, X-Ray Analysis and DFT Studies

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

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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 angels 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