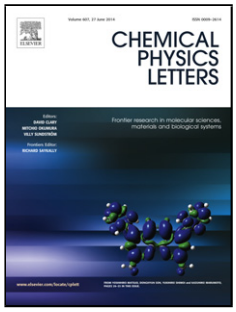

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Spectral Investigations, DFT Computations and molecular docking studies of the antimicrobial 5-Nitroisatin dimer

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Abstract

5-Nitroisatin is used for the treatment of fungal and bacterial strains exploring antimicrobial activity. Structural and vibrational spectroscopic studies were carried out by using FT-IR, FT Raman, UV and NMR spectral analysis together with DFT method using Gaussian'09 software. Assignments of vibrational spectra have been carried out with the aid of NCA. NBO analysis, Charge Analysis, HOMO LUMO, ESP, aromaticity and thermodynamic properties have been analyzed. Thermal stability has been analyzed by TG/DTA method. 5NI has been screened for its antimicrobial activity and found to exhibit antifungal and antibacterial effects. Docking simulation has been performed.

Keywords: 5-Nitroisatin, DFT, NBO, NCA, Molecular Docking, Antimicrobial.

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1. Introduction

5-Nitroisatin(5NI) has remarkable biological activities, such as anticonvulsant[1], anti-HIV[2], cytotoxic[3], tuberculostatic[4], anti-microbial[5,6], antiviral, anticancer, antimycobacterial and antimalarial which makes it considerable for pharmaceutical applications. Structural and bonding features reveal that this compound has several reactive groups which