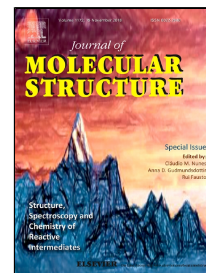


Accepted Manuscript

Structure Elucidation, Biological Evaluation and Molecular Docking Studies on a new organic salt: 2-aminobenzimidazolium 5-nitro-2-hydroxybenzoate



K. Saiadali Fathima, M. Sathiyendran, K. Anitha

PII: S0022-2860(18)31137-2
DOI: 10.1016/j.molstruc.2018.09.059
Reference: MOLSTR 25693
To appear in: *Journal of Molecular Structure*
Received Date: 16 July 2018
Accepted Date: 21 September 2018

Please cite this article as: K. Saiadali Fathima, M. Sathiyendran, K. Anitha, Structure Elucidation, Biological Evaluation and Molecular Docking Studies on a new organic salt: 2-aminobenzimidazolium 5-nitro-2-hydroxybenzoate, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.09.059

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.

Structure Elucidation, Biological Evaluation and Molecular Docking Studies on a new organic salt: 2-aminobenzimidazolium 5-nitro-2-hydroxybenzoate

K. Saiadali Fathima^a, M. Sathiyendran^b, K. Anitha^{a,*}

^a CAD4 Laboratory, Department of Physics, School of Physics, Madurai Kamaraj University, Madurai-625021, Tamilnadu, India

^b Chemistry Research Centre, National Engineering College, Kovilpatti-628503, Tamilnadu, India

*E-mail address: singlecrystalxrd@gmail.com

Abstract

An organic salt, 2-aminobenzimidazolium 5-nitro-2-hydroxybenzoate was synthesized and crystals were successfully grown from methanol using slow evaporation solution growth technique and recrystallization was done further to increase the purity of the crystal. The density of the grown crystals was evaluated by flotation method using carbon tetrachloride and xylene as solvents. Single crystal X-ray diffraction showed that the crystal is monoclinic system with $P2_1/n$ space group and molecular structure was stabilized *via* three dimensional hydrogen bonding interactions. For the present crystal structure, Hirshfeld surface and fingerprint plots were drawn and analysed for the intermolecular interactions. The title compound AB5N2HB was characterized by ¹H and ¹³C NMR spectroscopy to predict hydrogen and carbon bonded network. FT-IR and Raman spectral studies confirmed the presence of functional groups and their modes of vibrations. In the UV-Vis absorption spectrum the band at 313nm confirmed that the proton was transferred from cation to anion. Simultaneous thermogravimetric and differential thermal analyses revealed the thermal stability and decomposition point of compound and it was stable up to 289°C. The synthesized compound exhibited significant anti-bacterial and anti-fungal activity against different pathogens. Among them it showed good antibacterial and anti-fungal activity against *Escherichia Coli* and *Candida albicans* when compared to standard drug *Pencilin G* and *Ketaconazole* respectively. A molecular docking interaction of compound was also studied.

Introduction

In the past 30 years, the occurrence of microbial infections has increased on dreadful level as of result of microbial implications for mortality, morbidity and costs of health care have become a serious panic [1]. Moreover, for medical and agricultural field, due to the rise in discrete pathogenic fungi and advent of resistance fungal strain, demand for novel antifungal drugs has increase. In addition, some fungal infections are simple to treat but others are associated with

Download English Version:

<https://daneshyari.com/en/article/11027146>

Download Persian Version:

<https://daneshyari.com/article/11027146>

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