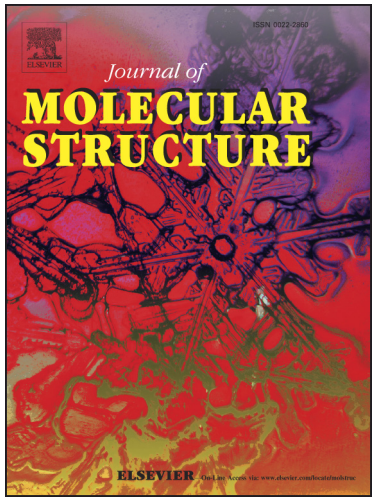

Novel synthetic ester of Brassicasterol, DFT investigation including NBO, NLO response, reactivity descriptor and its intramolecular interactions analyzed by AIM theory

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Novel synthetic ester of Brassicasterol, DFT investigation including NBO, NLO response, reactivity descriptor and its intramolecular interactions analyzed by AIM theory

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Abstract

In the present work, Brassicasterol (compound **1**) isolated from *Allamanda Violacea* reacted with the well known NSAID ibuprofen by Steglich esterification yielding a novel steroidal ester, 3β-(2-(4-isobutyl phenyl) propionoxy) 24 methyl cholest-5, 22-dien (compound **2**). Identity of synthetic derivative (compound **2**) was done with the help of modern spectroscopic techniques like, ^{1}H NMR, IR and UV as well as mass spectrometry. Molecular geometry and vibrational frequencies of compound **2** were calculated using density functional method (DFT/B3LYP) and 6-31(d,p) basis set. NMR chemical shifts of the compound were calculated with GIAO method. Electronic properties such as HOMO-LUMO energies were measured with the help of time dependent DFT method. Natural bond orbital (NBO) analysis was carried out to study hyperconjugative interactions. Non linear optical (NLO) response of compound **2** was also evaluated. Molecular electrostatic potential (MEP) surface has been used to indicate nucleophilic and electrophilic sites. Global reactivity descriptors of compound **1** and **2** were also calculated. Intramolecular interactions were analyzed using Atoms in molecule (AIM) theory.

Keywords *Allamanda violacea*, Brassicasterol, DFT, NBO, NLO, AIM.

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1. Introduction

Phytosterols are one of the most important classes of steroid which are structurally and physiologically related to cholesterol, but they cannot be synthesized by humans and as a result they are always obtained from diet [1]. In plants they contribute to the regulation of the fluidity and permeability of cell membranes. They act as the substrates for the synthesis of various