



FT-IR, FT-Raman and NMR characterization of 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate and investigation of its reactive and optoelectronic properties by molecular dynamics simulations and DFT calculations

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ABSTRACT

The FT-IR and FT-Raman spectra of the synthesized compound, 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate is recorded and analyzed. Optimized molecular structure, wave numbers, corresponding assignments regarding 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate has become screened tentatively as well as hypothetically using Gaussian09 program package. Natural bonding orbital assessment has been completed with a reason to clarify charge transfer or conjugative interaction, the intra-molecular re-hybridization and delocalization of electron density within the molecule. The NMR spectral assessment had been made choosing structure property relationship by chemical shifts along with the magnetic shielding effects regarding the title compound. The first and second hyperpolarizabilities were calculated. The calculated first order hyperpolarizability is commensurate with the documented worth of very similar derivatives and could be an interesting object for more experiments on nonlinear optics. Local reactivity properties have been investigated using average local ionization energies and Fukui functions. Investigation of optoelectronic properties encompassed calculations of reorganization energies and hopping rates of charge carriers within the framework of Marcus semi-empiric approach. The docked ligand title compound forms a stable complex with CDK inhibitors and gives a binding affinity value of -9.7 kcal/mol and molecular docking results suggest that the compound might exhibit inhibitory activity against CDK inhibitors.

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1. Introduction

Quinoline is characterized by a double ring structure composed of a benzene and a pyridine ring fused at two adjacent carbon atoms [1]. Methylcyclohexane is a monosubstituted cyclohexane,

which has one branching via the attachment of one methyl group on one carbon atom of the cyclohexane ring and the lowest form of this monosubstituted methylcyclohexane occurs when the methyl group occupies an equatorial rather than an axial position [2]. Quinoline derivatives are well known for their nonlinear optical properties [3,4] and invite much interest due to their great potential application in the field of organic light emitting diodes (OLEDs) [5–8] and are used as dopants in the polymer LED materials [9]. Certain quinoline derivatives could generate a sharp green electroluminescence and a high quantum efficiency of emission in the

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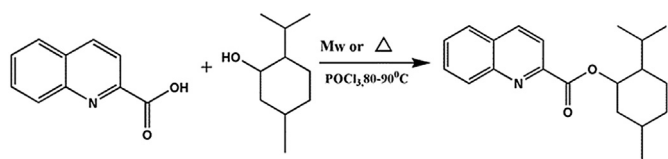
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blue and green region [10–13]. Quinoline derivatives are well known for anti-amoebic, antiviral, anti-parasitic, anti-microbial and anti-tubercular activities and possess anti-proliferative, anti-neoplastic, and cytotoxic properties [14–17]. Substituted quinoline derivatives possess a broad range of bioactivities such as anticancer, anti-malarial, antibiotic, antihypertensive, platelet-derived growth factor-receptors tyrosine kinase (PDGF-RTK) inhibition, DNA-intercalating carrier, anti-inflammatory, analgesic, anti-HIV, anti-tumour, DNA binding capability and many other functional material [18–21]. A series of tetracyclic indenoquinolines is used as potential anticancer agents. The compounds, which are obtained through the photo isomerization of Diels–Alder adducts formed between purpurogallin derivatives and nitrosobenzene, have in vitro anti-proliferative activities against breast (MCF-7), lung epithelial (A-549) and cervical (HeLa) adenocarcinoma cells [22]. Several novel functionalized quinolones, which exhibited potential antineoplastic activity against eukaryotic type II topoisomerases [23]. In addition to the antibacterial quinolones, specific members of this drug family display high activity against eukaryotic type II topoisomerases, as well as cultured mammalian cells and in vivo tumour models. These antineoplastic quinolones represent an exploitable source of new anticancer agents which might also help addressing undesirable-toxicity and resistance phenomena [23,24]. Jayashree et al. [25] reported the molecular docking experiments of 4-oxothieno [3,2-c]quinoline-2-carboxylates with DNA and their potential anticancer property. The author's group reported the vibrational spectroscopic studies of a number of quinoline derivatives [26–31]. The crystal structure of the title compound, $C_{20}H_{25}NO_2$ is reported Fazal et al. [32]. The present study carries out the vibrational spectral analysis of the title compound, 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate (EF3) to elucidate the correlation amongst the molecular structure and prediction of normal modes. The redistribution of electron density in various bonding and antibonding orbitals along with stabilization energies have been calculated by natural bond orbital analysis to give clear proof of stabilization originating from hyper-conjugation of a variety of intra-molecular interaction. NMR spectra were also reported both experimentally and theoretically. The nonlinear optical properties and global chemical descriptors are also reported. Average local ionization energy maps (ALIE), bond dissociation energies (BDE) and radial distribution functions (RDF) are also reported in the present work.

2. Materials and methods

2.1. Experimental details

All the solvents and reagents used for the synthesis were of analytical grade and procured from Sigma Chemical Co. (St. Louis, MO, USA) and quinaldic acid and menthol from Hi Media Ltd., Mumbai, India. The title compound was synthesized (Scheme 1) as reported Fazal et al. [33]. Elemental analyses were recorded on Varioel elemental analyzer (Elementar Americas, Inc. NJ, USA). NMR spectra (1H and ^{13}C) for the compound were recorded on a



Scheme 1. Synthetic pathway of 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate.

500 MHz NMR Spectrometer (Bruker advance, Reinstetten, Germany) using deuteriated DMSO and methanol as the solvent. The chemical shift values (ppm) and coupling constants (J) are given in δ and Hz respectively. Mass spectral analysis were carried out in the ESI positive mode using MS mass spectrometer (Waters Q-ToF-Utima, Manchester UK). Infrared spectrum (Fig. 1) was recorded on a Shimadzu IR prestige-21 FT spectrophotometer with KBr pellets ($4000\text{--}400\text{ cm}^{-1}$). The FT-Raman spectrum (Fig. 2) was obtained on a Bruker RFS 100/s, Germany. For excitation of the spectrum, the emission of Nd:YAG laser was used with an excitation wavelength of 1064 nm, maximal power 150 mW; measurement on solid sample. One thousand scans were accumulated with a total registration time of about 30 min. The spectral resolution after apodization was 2 cm^{-1} . MP: 414–416 K. Elemental analysis. Calculated: (C, 77.14; H, 8.09; N, 4.50; O, 10.28) Found: (C, 77.12; H, 8.07; N, 4.52; O, 10.30) and MS: Mass (ESI): $[M + 1]$ for $C_{20}H_{25}NO_2$, Calculated: 311.19; Found: 311.84.

2.2. Computational details

In the present work, the density functional theory (B3LYP) at 6-31G(d) (6D, 7F) basis set was adopted to calculate the vibrational wave numbers of the title compound and the theoretical calculations were performed using the Gaussian09 program [34]. Vibrational wave numbers were computed at DFT level which has reliable one to one correspondence to experimental values and in the present study we have used the scaling factor 0.9613 for the DFT method [35]. At the optimized structure (Fig. 3) of the title compound, no imaginary wave number modes were obtained. The calculated geometrical parameters with experimental data are given in Table S1 (supporting information). The vibrational assignments are done with the help of potential energy distribution analysis [36] and GaussView software [37].

Jaguar 9.0 program as implemented in Schrödinger Materials Science Suite 2015 [38,39] has been employed for DFT calculations of average local ionization energy (ALIE) surfaces, Fukui functions and bond dissociation energies (BDE). In order to obtain ALIE

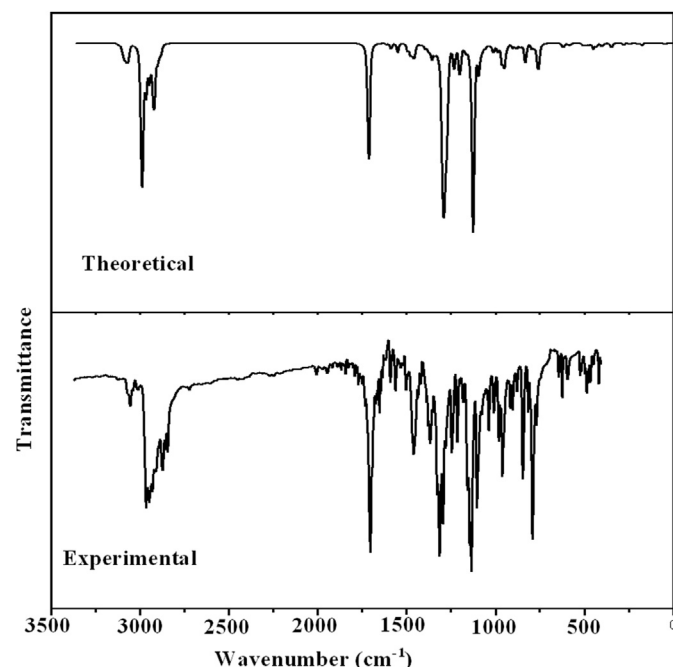


Fig. 1. FT-IR spectrum of 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate.

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