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TD-DFT and Molecular Docking Studies of 4- hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid

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Abstract

Quinoline derivatives are extensively studied due to their great potential to use as organic light emitting diode materials. They are used as antimicrobials too. TD-DFT studies on 4- hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid in the excited state were reported. The molecular docking studies were performed to analyze the antimicrobial properties.

Keywords: **TD-DFT, OLED, Molecular docking**

1. Introduction

Quinoline derivatives are reported to have good electron mobility, high photoluminescence efficiency, good film forming properties, good thermal and oxidative stabilities, thus used in OLEDs (Chen & Shi, 1998; Kulkarni et.al, 2004). Certain derivatives exhibit anticancer activity against a wide spectrum of human malignancies, including, lung, prostrate, breast, colon, stomach, ovaries, carcinomas, melanoma, lymphomas and sarcomas (Dancey & Elsenhauer,1996). The FT-IR, FT-Raman and NLO properties of 4- hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid were reported. In this work the TD-DFT calculations are reported and compared with that of the experimental UV-Vis spectra and thus analyse its potential to be used as an OLED material. The molecular docking studies are also reported.

2. Computational details

TD-DFT calculations of the title compound are carried out with Gaussian09 program (Takimoto et.al, 1998) using B3LYP/6-31G method. The GAUSSVIEW program, gives a visual presentation of the molecule (Dennington et.al, 2009). The molecular docking studies were performed using Autodock vina software available in Mgltool package.

3. Results and Discussions

3.1 Electronic absorption spectra

TD-DFT calculation on electron absorption spectrum in vacuum was performed. The chemically interested electronic transitions in organic compounds are π-π*, n–π* and π*(acceptor)-π(donor).The UV–visible bands in 4- hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid are observed at 326, 299, 284, 275, 238, 233 nm theoretically and at 361, 276, 288, 258, 236, 224nm. The second-order perturbation theory analysis of Fock matrix in NBO basis shows that the hyperconjugative interactions from the lone pairs of O and N to the

antibonding orbitals of CO, CC, CN are with large stabilization energies. The absorption spectra of organic compounds are due to the ground-to-excited state vibrational transition of electrons. The presence of C=O being a chromophore, COOH and OH being auxochromes are responsible for the above said strong absorption bands in the UV-Vis spectrum. The calculated six transitions of the molecule from TD-DFT method and the observed electron transitions are listed in Table 1.

Table1. Calculated electronic absorption spectrum of 4- hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid using TD-DFT/6-31G

Excitation	CI expansion coefficient	Energy (eV)	Wavelength calc. (nm)	Wavelength Exp. (nm)	Oscillator Strength (f)
Excited State 1 52 -> 54 52 -> 55 53 -> 54	0.12410 -0.13285 0.64248	3.8029 eV	326	361	0.0886
Excited State 2 51 -> 54 51 -> 55	0.10231 0.68335	4.1428 eV	299	276	0.0003
Excited State 3 49 -> 54 50 -> 54 52 -> 54 53 -> 55	0.23904 0.30245 0.52803 -0.10569	4.3699 eV	284	288	0.0621
Excited State 4 50 -> 54 52 -> 54 53 -> 55	0.57805 -0.26809 -0.19018	4.5095 eV	275	258	0.0123
Excited State 5 51 -> 54 51 -> 55 51 -> 56 51 -> 57	0.11882 0.65158 -0.13534 0.15692	5.2106 eV	238	236	0.0004
Excited state 6 49 -> 54 52 -> 54 52 -> 55 52 -> 56 53 -> 55 53 -> 56 53 -> 57	0.21248 -0.19622 -0.18056 0.15177 0.48368 -0.19793 -0.10260	5.3254 eV	233	224	0.2178

The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbitals were visualised(Fig.1) and the energy gap is observed to be 3.18 eV. The simplest structure of an OLED consists of a thin film of organic material attached between two electrodes. In π –conjugated molecules, light is produced by recombination of holes and electrons which have to be injected at the electrodes. The colour of the emitted light is a function of energy difference between HOMO and LUMO levels of the electroluminescent molecule. The wavelength of the light emission can thus be controlled by the extend of conjugation in the molecule (Geffroy et.al, 2006). From the electronic absorption spectra and HOMO-LUMO energies, we assume the title compound has a great potential to be used in OLEDs.

3.4 Molecular docking

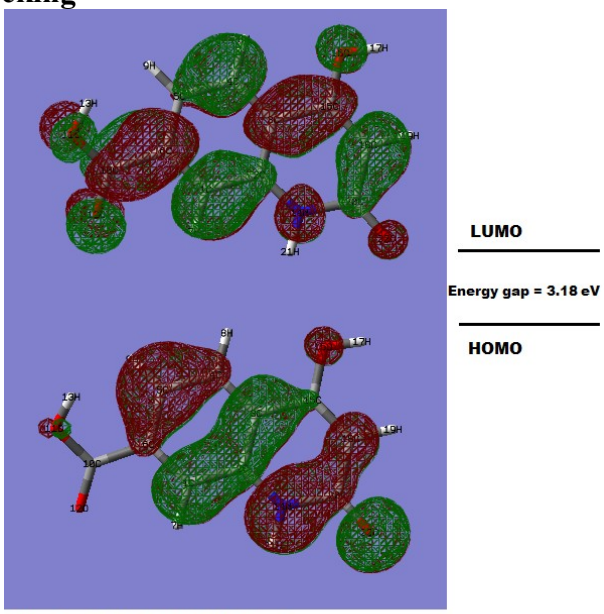

Fig. 1. HOMO-LUMO plot

Molecular docking simulations were performed on AutoDock-Vina software (Trott & Olson, 2010). The 3D crystal structure of *Hepatitis C virus* was obtained from Protein Data Bank (PDB ID: 5FGB) (Keck et.al, 2016). For docking it was prepared by removing the co-crystallized ligands, water molecules etc.and the ligand was prepared for docking by minimizing its energy at B3LYP/6-31G level of theory. Active site of the protein was defined and the Lamarckian Genetic Algorithm (LGA) available in Autodock was employed for docking. The ligand-protein interactions were visualised in Discover Studio Visualizer 4.0. The ligand binds at the catalytic site of substrate (Fig.2) with H bond (green) at a distance of 2.49631, 2.24003Å,Electrostatic pi-Anion interaction (orange) with a distance 4.11348Å, Hydrophobic, pi-Sigma interaction (violet) 3.92674Å. Though the computational results suggest 4- hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid to be anti-hepatitis, experimental results are required to validate it.

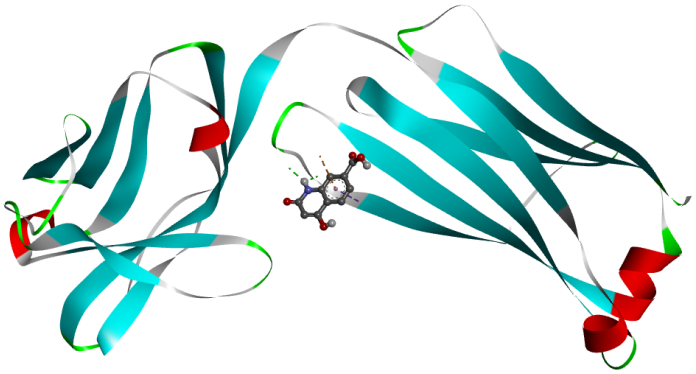

Fig.2. Molecular docking

4. Conclusion

The Electron absorption spectral studies of 4- hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid was made experimentally using the UV-Vis spectrum and computationally with TD-DFT calculations. The theoretical data agree well with that of the experimental. This suggest the compound has the potential to be used as OLED material. The molecular docking studies prove that the compound can be used as a drug against Hepatitis C virus.

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