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MOLECULAR INSIGHTS INTO (*E*)-2-(4-CHLOROBENZYLIDENE)-5,6-DIMETHOXY-2,3-DIHYDRO-1*H*-INDEN-1-ONE: SYNTHESIS, STRUCTURE, FMO ANALYSIS, SPECTROSCOPY, AND ANTIMICROBIAL ACTIVITY – AN EXPERIMENTAL AND COMPUTATIONAL STUDY

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Abstract
This study looks into the structure, electronics and microbial activity of (E)-2-(4-chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one by using both experimental and computer-based methods. The compound is made by performing the Claisen-Schmidt reaction and the structure of the molecule is analyzed by the use of FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy. To find out how a molecule reacts and interacts with electrons, DFT is utilized to examine frontier molecular orbitals (FMOs). Its ability to kill different microbial types is measured by testing the compound against several types of strains. It links research from both laboratories and theories to give a complete explanation of the compound's behavior. This implies that it could play a role in medicinal chemistry and medicine development. Mixing experimental and computer-based techniques, this research adds useful knowledge about the compound and how it helps the development of antimicrobial agents.
Keywords- DFT, 5,6-dimethoxy-2,3-dihydro-1*H*-inden-1-one, FMO, antimicrobial.

Introduction

As α,β-unsaturated ketones, chalcones are vital members of the group of organic compounds. Biogenesis shows that they are commonly found as precursors to flavonoids and isoflavonoids; moreover, they prove to be important intermediates in making various heterocyclic systems[i-iv]. What stands out is that these derivatives have various uses in medicine, serving as antioxidants[v,vi], anticancer agents[vii], antivirals[viii] , antimalarials[ix,x] and anti-inflammatory compounds[xi,xii]. Due to their strong pharmacology, chalcones now occupy a top position in ongoing efforts to create new medicines.

Indanone chalcones are among the chalcones whose structures are built by combining chalcone rings with indanones and they have attracted much interest from researchers[xiii] . Prior scientific research has pointed out that they show beneficial properties against viruses, bacteria and cancer [xiv-xviii] . Furthermore, 5,6-dimethoxy-1-indanone plays a vital role in organic synthesis because it is important both chemically and biologically and is often a key intermediary in making donepezil used for Alzheimer's disease and thiosemicarbazone derivatives that are good at fighting viruses[xvii, xix].

While the various properties and functions of chalcones have been studied a lot and the same is true for 5,6-dimethoxy-1-indanone, there is not much written about specific chalcones derived from 5,6-dimethoxy-1-indanone, especially about their detailed molecular features and the connections between their properties and activities. Several reports about biologically active molecules have been published, but research on their electronic structure, stability and potential for drug design is usually missing.

The study is centered on synthesizing, carefully investigating the structure and characterizing (*E*)-2-(4-Chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one. Experiments that analyze absorption and emission spectra and calculations with Density Functional Theory (DFT) are both parts of our study. This strategy enables us to learn about the electronic structure of the molecule through Frontier Molecular Orbital (FMO) analysis, find out – without performing experiments, how it will behave chemically and physically and check its effectiveness against bacteria. With this study, we hope to gain better knowledge of this indanone chalcone derivative, which can help guide the development of better biologically based compounds in the future.

2. Materials and Methods

All chemicals used in the synthesis were of analytical grade and employed without further purification. The following reagents were specifically sourced:

p-Chlorobenzaldehyde: Purchased from [Loba Chemie, India] with ≥[Purity 98 %]% purity.

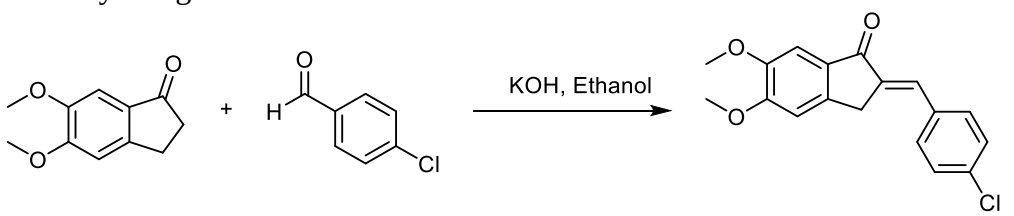
5,6-Dimethoxy-1-indanone: Purchased from [Loba Chemie, India] with ≥[99%] purity.

Potassium Hydroxide (KOH): Purchased from [Loba Chemie, India] with ≥[Purity 95 %] purity, as pellets.

The synthesized compound was comprehensively characterized using a suite of analytical techniques: The melting point was determined using the open capillary method in a Thiele's tube with paraffin oil as the heating medium. All reported melting points are uncorrected. The IR spectra were recorded on a Shimadzu spectrometer using KBr pellets. The ^{1}H NMR and ^{13}C NMR spectra were obtained on a Bruker Avance NEO 500 MHz NMR Spectrometer (Bruker Corporation, Germany). Deuterated chloroform ($CDCl_3$) was used as the solvent, and tetramethylsilane (TMS) served as an internal standard. All chemical shifts (δ) are expressed in parts per million (ppm). Thin-Layer Chromatography (TLC): Reaction progress was monitored by thin-layer chromatography using pre-coated silica gel [Merck, Germany]. Compounds were visualized under UV light (254 nm).

2.1. Procedure

To a conical flask containing p-chlorobenzaldehyde (0.01 mol) in ethanol (15-20 mL), potassium hydroxide 5 mL (20%) solution was added dropwise. 5,6-Dimethoxy indanone (0.01 mol) was added, and the stirring at room temperature, the progress of the reaction was monitored by thin layer chromatography. After the completion of the reaction mixture, poured into ice cold water, the product was filtered and dried. The crude product obtained was recrystallized by using a suitable solvent.



Scheme 1 Synthesis of (E)-2-(4-chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one

2.2. Spectral data of the synthesized compounds

(*E*)-2-(4-chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1*H*-inden-1-one

Chemical formula: $C_{18}H_{15}ClO_3$; FT-IR (KBr, cm^{-1}): 3064.89, 3005.10, 2968.45, 1695.43, 1685.79, 1635.64, 1585.49, 1489.05, 1456.26, 1307.74, 1300.02, 1255.66, 1226.73, 1128.36, 1091.71, 1006.84,798.53; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, J = 8.5 Hz, 2H), 7.45 – 7.34 (m, 3H), 7.28 (s, 1H), 6.82 (s, 1H), 3.94 (s, 3H), 3.92 (s, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 192.59, 155.12, 149.96, 142.5, 139.82, 139.4 136.35, 130.97, 129.55, 127.13, 122.77, 107.27, 105.01, 56.25, 56.13, 33.07.

2.3 Computational details

On an Intel (R) Core (TM) Intel Core i7 personal computer, density functional theory calculations were carried out using the Gaussian-03 software package[xxx] without regard to geometry. The geometry was optimized by using Becke's hybrid three-parameter method together with the Lee-Yang-Parr correlation function and the DFT theory using the B3LYP function. With the help of the DFT method and the proper basis set, molecular geometry, bond length, atomic charges, bond angle and harmonic vibrational frequencies were examined. The geometry shape was examined with the Gauss View 4.1 molecular visualization program. When optimizing the structure, all the calculations were done in the gas phase.

2.4 Results and Discussion

Molecular geometry

The optimized molecular structure of **(**E)-2-(4-chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one (CBDDI), obtained from DFT calculations, is presented in Figure 1. The comprehensive set of optimized geometrical parameters, including all bond lengths and bond angles, is detailed in Table 1. Structurally, CBDDI features an indanone core, which consists of a five-membered ring fused to a six-membered benzene ring. Analysis of the calculated bond lengths within this core reveals that the C4-C5 double bond exhibits the longest length at 1.419 Å, while the C1-C2 double bond has the shortest length at 1.386 Å. Additionally, the carbonyl double bond (C=O) was determined to be 1.258 Å, and the olefinic carbon-carbon double bond (C8-C14) is 1.355 Å. The C–Cl bond length in the 4-chlorobenzylidene moiety was calculated as 1.760 Å. Significantly, all calculated bond lengths and angles are found to be consistent with those reported for analogous chalcone derivatives and related organic compounds in the existing literature. This agreement serves to validate our computational methodology and reinforces the reliability of the optimized structure of CBDDI [xxxi].

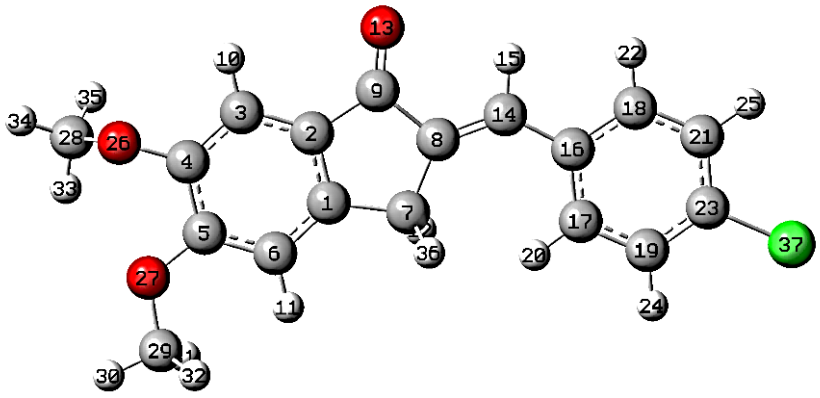


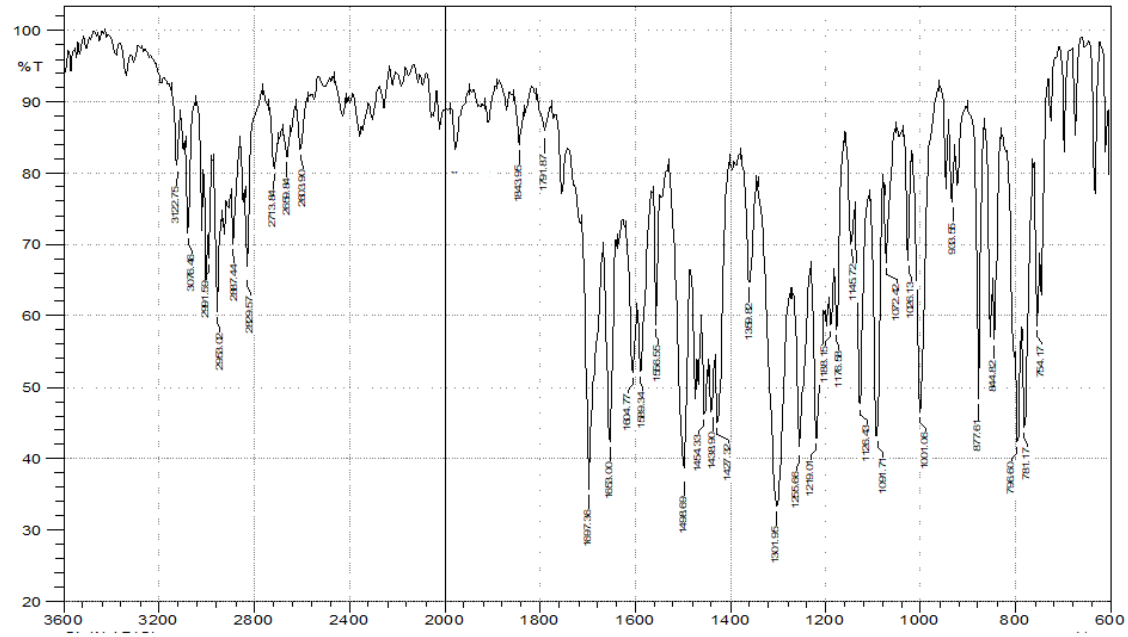
Figure 1. Optimized structure of CBDDI Molecule

Table 1. Selected Geometrical Parameters of the CBDDI Molecule Calculated at B3LYP/6-31+G(d,p) Level

Connectivity	Bond length (Å)	Connectivity	Bond length (Å)	Connectivity	Bond Angle (°)
C1-C2	1.388	C9-O13	1.258	C1-C7-C8	102.77
C1-C6	1.393	C14-H15	1.070	C2-C9-C8	105.83
C1-C7	1.552	C14-C16	1.540	C7-C8-C9	107.44
C2-C3	1.391	C16-C17	1.401	H12-C7-H36	108.52
C2-C9	1.531	C16-C18	1.401	C1-C7-H36	109.67
C3-C4	1.410	C17-C19	1.401	C2-C1-C7	111.47
C3-H10	1.070	C17-H20	1.070	C1-C7-H12	113.04
C4-C5	1.419	C18-C21	1.401	C2-C3-C4	117.77
C4-O26	1.430	C18-H22	1.070	C1-C6-C5	118.04
C5-C6	1.411	C19-C23	1.401	C6-C5-O27	119.76
C5-O27	1.430	C19-H24	1.070	C8-C14-H15	120.00
C6-H11	1.070	C21-C23	1.401	C1-C6-H11	120.98
C7-C8	1.543	C21-H25	1.070	C2-C1-C6	121.04
C7-H12	1.070	C23-Cl37	1.760	C9-C8-C14	126.27
C7-H36	1.070	O26-C28	1.430	C8-C9-O13	127.10
C8-C9	1.531	O27-C29	1.430	C6-C1-C7	127.49
C8-C14	1.355	C28-H33	1.070	C3-C2-C9	128.52

Vibrational assignments

The structure of CBDDI with ring naming is presented in Figure 1. Figure 2 depicts the experimental and theoretical IR spectrum. The total number of atoms in the CBDDI molecule is 37 and therefore it will have 105 fundamental modes of vibrations. The DFT computed IR spectrum often overestimates the vibrational frequencies and therefore a scaling factor of 0.96 has been used to correct the vibrational assignments[xxiv] . The theoretical vibrational data have shown good agreement with the experimental findings. Table 2 shows the selected observed FT-IR and scaled vibrational frequency. Carbonyl stretching frequency was Experimentally observed at 1697.36 cm^{-1} and scaled wavenumbers at 1691.67 cm^{-1}. C-H stretching frequency was experimentally observed in the range of 3122.75 to 2887.44 cm^{-1} and scaled wavenumbers in the range of 3118.36 to 2901.65 cm^{-1}



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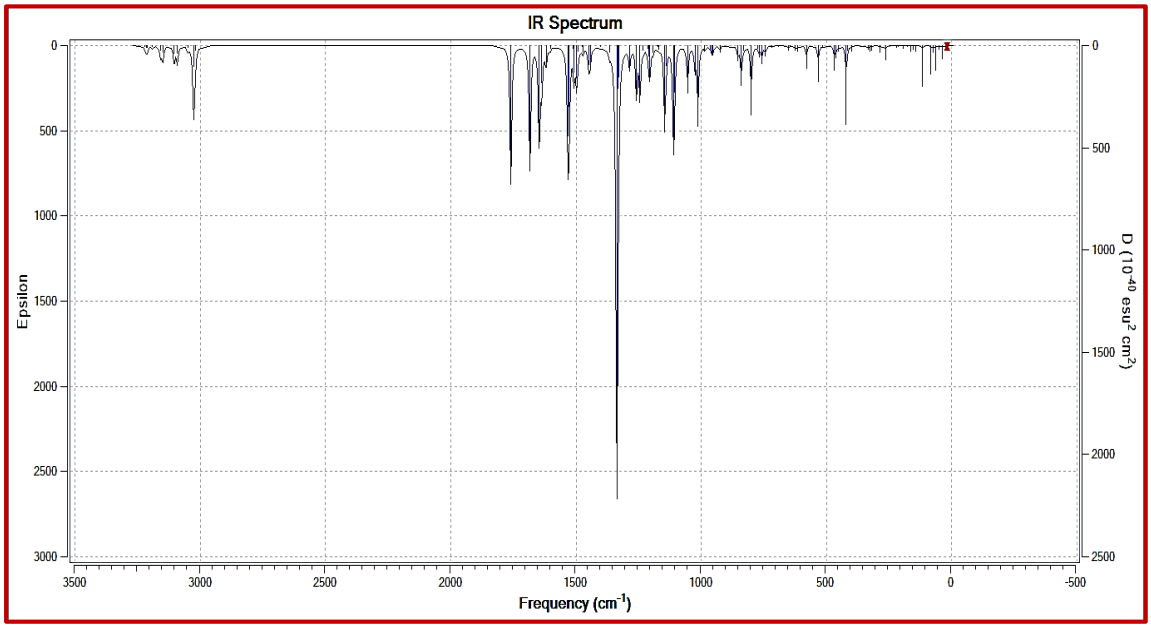

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Figure 2. a Experimental and b Theoretical IR spectrum.

Mulliken atomic charges and molecular electrostatic potential surface analysis

Mulliken charges are useful for characterizing the electronic structure and bonding in molecules[xxv-xxviii]. The Mulliken atomic charges of CBDDI are calculated using the 6-31+G(d,p) basis set shown in **Table 2**. It is observed that the C2 atom in the compound holds the greatest positive charge of all carbon atoms, so it is the most likely point of attack by a nucleophile. On the other hand, C7 has a negative charge that is the largest of all the carbons in the ring, -0.978. The Molecular Electrostatic Potential clearly shows where the charges are located in a molecule and how it reacts with other substances. Markings say that CBDDI exhibits polarity with a Dipole Moment of 5.66 Debye. You can see the MESP plot in Figure 3

Table 2. Mulliken atomic charges Calculated (B3LYP/6-31+G(d,p) Level)

Atom	Charge	Atom	Charge	Atom	Charge
1C	0.066	14C	0.217	26O	-0.321
2C	0.567	15H	0.152	27O	-0.321
3C	0.183	16C	0.118	28C	-0.159
4C	-0.364	17C	-0.500	29C	-0.139
5C	-0.209	18C	-0.071	30H	0.151
6C	0.425	19C	-0.121	31H	0.124
7C	-0.978	20H	0.090	32H	0.156
8C	0.429	21C	-0.163	33H	0.148
9C	-0.766	22H	0.135	34H	0.145
10H	0.165	23C	0.168	35H	0.140
11H	0.111	24H	0.138	36H	0.202
12H	0.159	25H	0.145	37Cl	0.275
13O	-0.494				

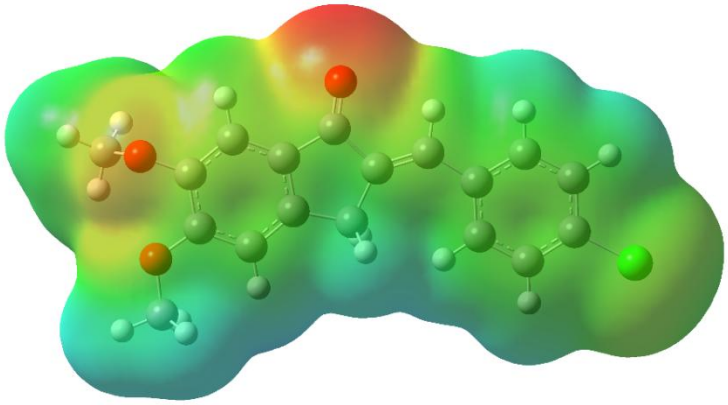

Figure 3. MESP Plot of CBDDI

Global Chemical Reactivity Descriptors

Frontier Molecular Orbital (FMO) analysis, comprising the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), provides critical insights into a molecule's reactivity and selectivity. For the (E)-2-(4-chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one (CBDDI) molecule, the HOMO-LUMO energy values and their corresponding energy gap were calculated using the TD-DFT method at the B3LYP/6-31+G(d,p) basis set in the gas phase. The HOMO-LUMO plot for CBDDI in the gas phase is displayed in Figure 4. The calculated energies of the HOMO and LUMO are -6.374 eV and -2.415 eV, respectively, resulting in an energy gap of 3.959 eV for the title compound. From these HOMO-LUMO energies, various chemical reactivity parameters, including Ionisation potential (I), Electron Affinity (A), Chemical hardness (η), Chemical softness (S), Electronic chemical potential (μ), and Global Electrophilicity index (ω), were determined using Koopmans' theorem[xxix] . These computed parameters are presented in Tables 3 and 4.

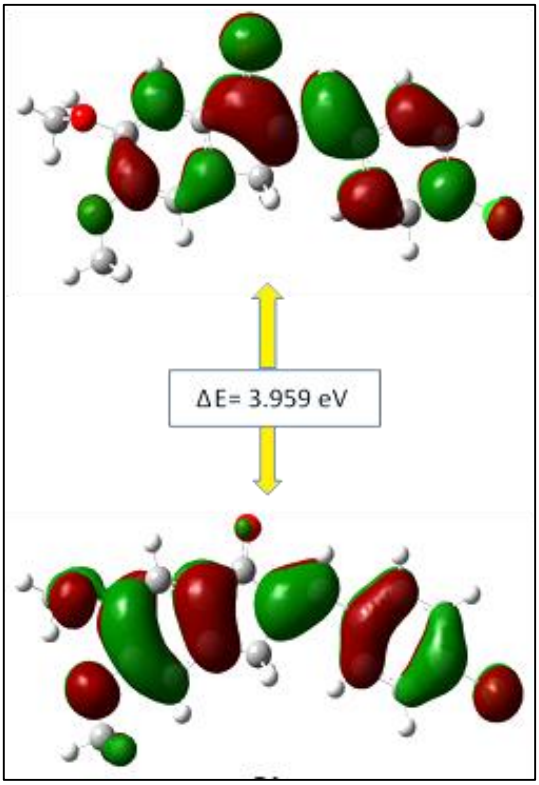

Figure 4. HOMO- LUMO plot of CBDDI Molecule

Table 3 Electronic parameters of the CBDDI Molecule

Entry	**E_{HOMO} energy (eV)**	**E_{LUMO} energy (eV)**	**I (eV)**	**A (eV)**	**Eg (eV)**
CBDDI	-6.374	-2.415	6.374	2.415	3.959

Table 4 Global chemical reactivity parameters of CBDDI Molecule

Entry	**χ (eV)**	**η (eV)**	**S $(eV)^{-1}$**	**μ (eV)**	**ω (eV)**	**Δ Nmax (eV)**	**Dipole Moment (Debye)**
CBDDI	4.395	1.979	0.505	-4.395	4.878	2.220	5.601

3.2. Antimicrobial activity.

The antibacterial and antifungal activity was ascertained by our earlier report [xxx-xxi]. The MICs of synthesized compounds were evaluated using the broth microdilution procedures using DMSO as diluents to establish the appropriate doses for screening on standard bacterial strains. The broth dilution method was utilized to investigate the antibacterial properties of the synthesized CBDDI. For in vitro antibacterial activity against *E. Coli*, *P. aerogenosa*, *S. aureus*, and *S. pyogenus*, all synthesized compounds were tested. Using the highest dilution that exhibits at least 99% inhibition, the MIC is obtained. Table 5 shows the MIC values determined from the antibacterial screening of synthesized drugs. The CBDDI compound shows good antibacterial activity against *E.coli*, *S. pyogenus* compared to the standard drug chloramphenicol and Ampicillin.

Table 5 Minimum inhibitory concentration of synthesized CBDDI against some bacterial strains.

Entry	***E.coli***	***P. aeruginosa***	***S. aureus***	***S .pyogenus***

	MTCC 443	MTCC 1688	MTCC 96	MTCC 442
CBDDI	62.5	125	100	62.5
Ampicillin	40	NA	32	25
Chloramphenicol	50	50	50	50
Ciprofloxacin	25	25	50	50

Conclusion

This study shows the synthesis of (*E*)-2-(4-chlorobenzylidene)-5,6-dimethoxy-2,3-dihydro-1H-inden-1-one (CBDDI). Its structure was experimentally verified using ^{1}H and ^{13}C NMR spectroscopy. Furthermore, a comprehensive structural investigation of CBDDI was conducted using Density Functional Theory (DFT) at the B3LYP/6-31+G(d,p) level of theory. The geometry of the molecule was optimized at this theoretical level, and key geometrical parameters, including bond lengths and bond angles, were subsequently calculated. Our analysis of the Molecular Electrostatic Potential (MESP) indicates that the carbonyl group is the primary site of negative electrostatic potential regions, suggesting it as a potential target for electrophilic attack. Finally, global reactivity parameters and other electronic parameters, derived from HOMO-LUMO energy analysis, were thoroughly examined to understand the compound's chemical behavior and stability.

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Compliance with ethical standards

The authors declare that they have no conflict of interest.

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