

Synthesis and Computational Insights on Molecular Structure, Frontier Molecular Orbital, Molecular electrostatic surface potential of (E)-3-(2,3-dihydrobenzofuran-5-yl)-1-(2-hydroxyphenyl)prop-2-en-1-one

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Abstract: In the current work, we described experimental and theoretical properties of chalcone, (E)-3-(2,3-dihydrobenzofuran-5-yl)-1-(2-hydroxyphenyl)prop-2-en-1-one (DHBFHP). The titled molecule were practically synthesized and characterized by FT-IR, ¹HNMR, and ¹³C NMR spectral techniques. The density functional theory approach (DFT) at the B3LYP/6-311G(d,p) basis set was used to inspect structural, spectroscopic, and chemical reactivity aspects of the synthesized molecule. To understand the geometrical architecture, a comprehensive investigation of bond lengths and bond angles is discussed. Mulliken atomic charges, molecule electrostatic potential surface, and electronic parameters are used to investigate its chemical behaviour. The time-dependent DFT (TD-DFT) method was used to determine the detailed examination of electronic properties such as HOMO and LUMO energies. The dipole moment of the titled molecule was found to be 4.8670 Debye with C₁ point group symmetry. The positive electrostatic potential is predicted to be near hydrogen atoms by the molecular electrostatic potential map. To evaluate the reactive electrophilic and nucleophilic sites, the electronic properties with consideration to the frontiers molecular orbitals, the quantum reactivity descriptors, and the molecule electrostatic potential were used.

Index Terms: Chalcone, benzofuran-5-carbaldehyde, DFT, FMO, Molecular electrostatic surface potential.

I. INTRODUCTION

In the View of the growing of bacterial resistance, which has become a medical problem today [1-3], the quest for novel

antibiotics is intensifying. Bacterial resistance is caused by a variety of reasons, include low plasma membrane permeability, drug adherence to the cell wall, efflux pump ejection, and the action of enzymes that reduce or prevent antibiotic effect [4, 5]. Natural biocides, chalcones are well-known intermediates in the synthesis of a wide range of heterocyclic chemicals [6]. The chalcone derivatives are possesses a wide range of biological activities including antimicrobial [7], anti-inflammatory [8] and anticancer [9], antimalarials [10], antiproliferative [11] etc. activities. Chalcones are flavonoids and isoflavonoids' precursors [12, 13], but they can also be obtained by synthesis [14]. The chemical scaffold for chalcone molecules is 1,3-diaryl-2-propen-1-one, also known as chalconoid, which comes in trans and cis isomers, with the trans isomer being more thermodynamically stable [15]. Several chalcone-based drugs have received clinical approval. Metochalcone, for example, was once sold as a choleric, whereas sofalcone was earlier marketed as an antiulcer and mucoprotective medication Figure 1. [16].

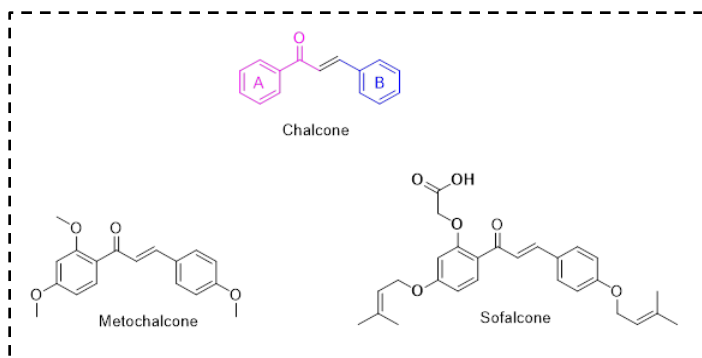


Figure 1: Chalcone and some medicinally approved chalcone-based compounds

Theoretical calculations based on DFT have been effectively investigated in the past several years to determine various structural characteristics of pharmacologically vital organic molecules like chalcones. For examining structural, chemical, and spectroscopic properties of molecules, DFT in combination with B3LYP method using different basis sets has been proven to be very important [16-21]. The electronic properties of the reactive electrophilic and nucleophilic sites in regards to the frontier molecular orbitals, the quantum reactivity descriptors, and the molecular electrostatic potential are also used to describe the reactive electrophilic and nucleophilic sites, which is extremely important [22]. Considering all mentioned properties, we have designed (E)-3-(2,3-dihydrobenzofuran-5-yl)-1-(2-hydroxyphenyl)prop-2-en-1-one chalcone derivative and explored it for the investigation of structural, chemical, electronic, and quantum chemical parameters.

II. MATERIALS AND METHODS

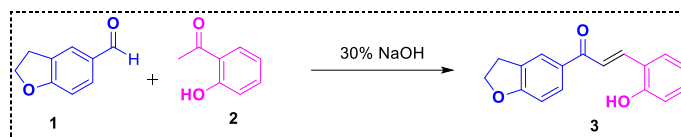
General remarks

The chemicals (Make- Sigma Aldrich and SD Fine) were purchased and used as received. The ¹H NMR and ¹³C NMR experiments were carried out on sophisticated multinuclear FT-NMR Spectrometer (500 MHz) model Advance-II (Bruker). The compound was dissolved in CDCl₃ and the chemical shifts were reported in ppm with reference to TMS. The FT-IR spectrum of the synthesized molecule was recorded on Shimadzu spectrometer and using a KBr disc technique, the sample was readied at room temperature. The reaction was monitored by using thin-layer chromatography on Merck Aluminium TLC plate, silica gel coated with fluorescent indicator F254. Before use, all of the glassware was washed, cleaned, and dried in the oven.

Experimental procedure for the synthesis of (E)-3-(2,3-dihydrobenzofuran-5-yl)-1-(2-hydroxyphenyl)prop-2-en-1-one (DHBFHP)

The DHBFHP molecule was synthesized using the well-known Claisen-Schmidt condensation reaction. In a typical synthesis scheme, benzofuran-5-carbaldehyde (1, 10 mmol) and 1-(2-hydroxyphenyl)ethan-1-one (2, 10 mmol) were dissolved in 10 mL ethyl alcohol. To this 5 mL of 30 % NaOH was added. The

alkaline mixture was then stirred at room temperature overnight until the product was formed. After the reaction was completed, it was quenched by pouring it upon crushed ice (as determined by TLC). To obtain a pure product, it was acidified with dilute HCl, filtered, dried, and recrystallized with hot ethanol (3). The reaction is presented in Scheme 1.



Scheme 1 Synthesis of the DHBFHP

Spectral data of the titled compound

(E)-3-(2,3-dihydrobenzofuran-5-yl)-1-(2-hydroxyphenyl) prop-2-en-1-one: yellow solid; m.p. 118 °C; FT-IR (KBr; cm⁻¹): 3309.85, 2970.38, 2926.01, 1645.28, 1597.06, 1558.48, 1490.97, 1436.97, 1340.53; δH (500 MHz; Chloroform-d): 12.98 (s, 1H), 7.95–7.87 (m, 2H), 7.56 (s, 1H), 7.52 (d, J = 15.4 Hz, 1H), 7.50–7.44 (m, 2H), 7.02 (d, J = 8.4 Hz, 1H), 6.94 (t, J = 7.6 Hz, 1H), 6.84 (d, J = 8.2 Hz, 1H), 4.67 (t, J = 8.7 Hz, 2H), 3.28 (t, J = 8.7 Hz, 2H). δC (126 MHz; Chloroform-d): 193.68, 163.56, 163.05, 145.89, 136.10, 130.59, 129.50, 128.36, 127.54, 125.26, 120.18, 118.73, 118.61, 116.91, 109.98, 72.05, 29.23. Computational details

density functional theory calculations were performed using the Gaussian-03 programme package on an Intel (R) Core (TM) i5 computer with no geometry constraints. The DFT/B3LYP method was used to optimise the geometry of the title molecules using the 6-311G (d,p) basis set. The Gauss View 4.1 molecular visualisation tool was used to create optimised geometry. The molecular electrostatic potential was computed using the same method to study the reactive sites of the title molecule. All of the computations were done in the gas phase for the optimised structure. The 6-311G (d,p) basis set was used to calculate Mulliken atomic charges.

III. RESULTS AND DISCUSSION

Chemistry

The DHBFHP molecule was synthesized via the Claisen–Smith condensation reaction and the best yield (92%) was gotten. The synthesized DHBFHP molecule was characterized by FT-IR, ¹³C NMR, and ¹H-NMR spectroscopy, and the findings were correlated with literature data. In the FT-IR spectra of synthesized chalcone the appearance of the broad peak at 3309.85 cm⁻¹ indicate the presence of hydroxyl (–OH) group, and peaks in the range of 2971-2926 cm⁻¹ due to Ar-CH stretching vibrations. The intense peaks at 1645.28 cm⁻¹ due to νCO stretching. The carbonyl peak was observed at a lower wavenumber than a normal ketone carbonyl peak in the infrared spectra due to the existence of a ketonic carbonyl group conjugated with the olefinic carbon–carbon bond. The ¹H NMR coupling constant analyses indicated that hydrogen atoms of the olefinic carbon–carbon bond were in a trans configuration (J approximately 15 Hz). The broad peak at 12.98 ppm affirms

presence of hydroxyl (-OH) in the synthesized molecule. The two methylene (CH₂) groups of benzofuran part of synthesized chalcone appeared at 4.67 ppm and 3.28 ppm and one of methylene with at downfield clearly indicate its attachment with oxygen. The signals for these two methylene (CH₂) groups can also be observed in the ¹³C NMR spectrum at 72.05 and 29.23 ppm. Additionally, multiplets in the aromatic region (6.80-8.00 ppm) indicate the presence of aromatic protons in the compound. The ¹³C NMR signal at approximately 193.68 ppm in the synthesized compound concerns to α,β-unsaturated carbonyl carbon. Despite the fact that the ketone absorbs approximately 200 ppm, the existence of unsaturation leads an slight uprooting to the high field, and the reasonable cause is charge delocalization by the benzene ring or by the double bond, which makes the carbonyl carbon less electron deficient.

Computational Study

Molecular structure study

The DHBFHP molecule was analysed in the current examination using the density functional theory method with a B3LYP/6-311G(d,p) basis set to build up different structural and chemical parameters. DHBFHP is a non-planer molecule with C₁ point group symmetry, as predicted by the DFT analysis. Figure 2 depicts the optimized molecular structures. The DHBFHP compound has appreciable polarity with dipole moment ($\mu = 4.8670$ Debye). The phenomenon of polarity is extremely crucial to foresee which compounds would enter through the lipophilic membrane of the microorganisms. The bond length and bond angle data of DHBFHP are given in Table 1 and Table 2 respectively. In DHBFHP compound, the carbonyl bond (C21-O22) length is 1.2336 Å and olefinic bond length (C17-C19) is 1.3531 Å. The C10-C13 bond is the longest while O33-H34 (0.96) is the shortest of all bonds present in DHBFHP molecule. The presence of intramolecular hydrogen bonding between carbonyl group and hydroxyl group of DHBFHP molecule is confirmed by observing O33-H34 bond with bond length 1.678 Å (Table 1). All other bond length values are showing good agreement with the structure of the titled molecule. The bond angle between C19-C21-C23 bonds is 118.9912°. Similarly, other bond angle data are rightly matching with the various bond angles of titled molecule.

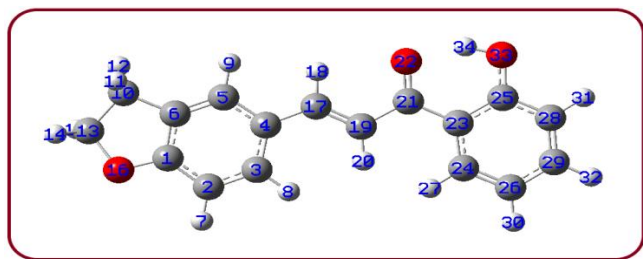


Figure 2: The optimized molecular structures of DHBFHP at DFT B3LYP/6-311G(d,p) basis set

Table 1: Optimized geometrical parameters of DHBFHP by DFT/ B3LYP with 6-311G (d,p) basis set

Bond lengths (Å)

C1-C2	1.3954	C17-C19	1.3531
C1-C6	1.3987	C19-H20	1.0842
C1-O16	1.3607	C19-C21	1.4787
C2-C3	1.393	C21-O22	1.2336
C2-H7	1.0845	C21-C23	1.5034
C3-C4	1.4133	O22-H34	1.678
C3-H8	1.0853	C23-C24	1.4051
C4-C5	1.4156	C23-C25	1.4063
C4-C17	1.4574	C24-C26	1.3959
C5-C6	1.3854	C24-H27	1.0842
C5-H9	1.0872	C25-C28	1.3919
C6-C10	1.5134	C25-O33	1.43
C1-H11	1.0972	C26-C29	1.3892
C10-H12	1.0941	C26-H30	1.0845
C10-C13	1.5476	C28-C29	1.3917
C13-H14	1.0911	C28-H31	1.0847
C13-H15	1.0957	C29-H32	1.07
C13-O16	1.4588	O33-H34	0.96
C17-H18	1.0894	-	-

Table 2: Optimized geometrical parameters of DHBFHP by DFT/ B3LYP with 6-311G(d,p) basis set

Bond angles (°)			
C2-C1-C6	122.1305	C1-O16-C13	107.5155
C2-C1-O16	124.4481	C4-C17-H18	115.7827
C6-C1-O16	113.4175	C4-C17-C19	128.52
C1-C2-C3	117.5671	H18-C17-C19	115.6973
C1-C2-H7	120.8089	C17-C19-H20	121.0387
C3-C2-H7	121.6238	C17-C19-C21	120.305
C2-C3-C4	122.0613	H20-C19-C21	118.6471
C2-C3-H8	118.4518	C19-C21-O22	121.6059
C4-C3-H8	119.4868	C19-C21-C23	118.9912
C3-C4-C5	118.4002	O22-C21-C23	119.3981
C3-C4-C17	123.3076	C21-C23-C24	123.569
C5-C4-C17	118.2922	C21-C23-C25	117.7382
C4-C5-C6	120.1653	C24-C23-C25	118.6792
C4-C5-H9	119.2165	C23-C24-C26	120.9937
C6-C5-H9	120.6181	C23-C24-H27	120.6859

C1-C6-C5	119.6726	C26-C24-H27	118.3062
C1-C6-C10	107.8949	C23-C25-C28	121.1597
C5-C6-C10	132.3727	C23-C25-O33	118.1849
C6-C10-H11	111.0031	C28-C25-O33	120.6553
C6-C10-H12	113.4716	C24-C26-C29	118.3345
C6-C10-C13	101.3868	C24-C26-H30	121.7581
H11-C10-H12	107.6279	C29-C26-H30	119.907
H11-C10-C13	111.6321	C25-C28-C29	118.2722
H12-C10-C13	111.7331	C25-C28-H31	121.8693
C10-C13-H14	114.1835	C29-C28-H31	119.8585
C10-C13-H15	111.7939	C26-C29-C28	122.5561
C10-C13-O16	106.6997	C26-C29-H32	118.6911
H14-C13-H15	109.2856	C28-C29-H32	118.7527
H14-C13-O16	107.2453	C25-O33-H34	120.0
H15-C13-O16	107.2741	-	-

Frontier molecular orbitals' and global descriptors' study

The frontier molecular orbitals (FMOs) of the synthesized molecule are presented in Figure 3. The FMO are highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The electronic parameters and global reactivity descriptor data of DHBFP are shown in Table 3 and Table 4 respectively. The Koopmans theorem was used to resolve the insights of global descriptors [23]. The Frontier molecular orbitals calculations showed that the energy gap between highest occupied molecular orbital and lowest unoccupied molecular orbital was ($E_g = 3.66$ eV). The concept of hard and soft nature of molecules is a significant tool for analysing chemical reactivity, according to the HSAB principle. The global softness (σ) and absolute hardness (η), values for DHBFP molecule were found 0.55 eV⁻¹ and 1.83 eV respectively. The chemical potential (μ) of an electron determines the ease with which it can be ejected, and it is also associated to its electronegativity. The global electrophilicity index has a higher value for a good electrophile, and a lower value for a good nucleophile. Because the value of global electrophilicity is more than 1.5 eV, the global descriptor study reveals that the DHBFP molecule is a good electrophile. A greater value of the global electrophilicity index implies a good electrophile, while a lower value indicates a good nucleophile. Our studies revealed that DHBFP molecule has a higher global electrophilicity index (4.73 eV), signifying that it is more likely to accept electrons and nucleophilic attack.

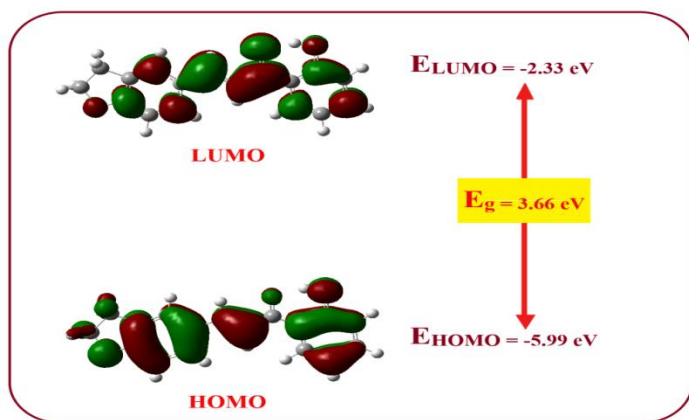


Figure 3: Frontier molecular orbitals (FMO) of DHBFP

Table 3: Electronic parameters

Electronic parameters	DHBFP
Total thermal energy (E_{total})	-882.13 (a.u)
HOMO energy (E_{HOMO})	-5.99 eV
LUMO energy (E_{LUMO})	-2.33 eV
Ionization enthalpy (I)	5.99 eV
Electron affinity (A)	2.33 eV
HOMO-LUMO energy gap (E_g)	3.66 eV

Table 4: Global reactivity parameters

Global reactivity parameters	DHBFP
Absolute hardness (η)	1.83 eV
Global softness (σ)	0.55 eV ⁻¹
Global electrophilicity index (ω)	4.73 eV
Electronegativity (X)	4.16 eV
Chemical potential (μ)	-4.16 eV
Charge transferred (ΔN_{max})	2.27 eV

Mulliken atomic charges and MESP analysis

Mulliken atomic charges rise out of the Mulliken population analysis [24]. It explains to use computational simulations to calculate partial atomic charges. Mulliken charges are those that are based on charge density. Table 5 shows the Mulliken atomic charges of DHBFP. The Mulliken atomic charges analysis revealed that all of the hydrogen atoms in DHBFP have a positive charge. The most negative and positive carbon atoms in DHBFP, according to Mulliken population analysis, are C23 (-0.213279) and C21 (0.315949), respectively. Figure 4 depicts the Molecular electrostatic surface potential plot of the DHBFP molecule. MESP correlates a molecule's total charge distribution to its dipole moment, electronegativity, and partial charges, as well as the site of chemical reactivity. It provides a visual technique for understanding a molecule's relative polarity

and can be used to explain hydrogen bonding, reactivity, and the structure-activity relationship. It's a proton's potential energy at a specific position near a molecule. Different colours correspond to different values of the electrostatic potential at a molecule's surface. In general, locations with attracting potential look red, whereas those with repulsive potential appear blue

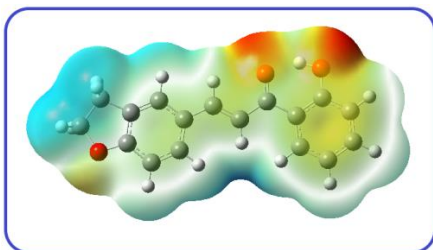


Figure 4: Molecular electrostatic surface potential plot of DHBFP

Table 5: Mulliken atomic charges of DHBFP

Atom	Charge	Atom	Charge
1 C	0.235773	18 H	0.114087
2 C	-0.079123	19 C	-0.182848
3 C	-0.046044	20 H	0.107198
4 C	-0.089827	21 C	0.315949
5 C	-0.029972	22 O	-0.420248
6 C	-0.175465	23 C	-0.213279
7 H	0.104359	24 C	-0.040693
8 H	0.092187	25 C	0.213505
9 H	0.090891	26 C	-0.109697
10 C	-0.194699	27 H	0.089989
11 H	0.141647	28 C	-0.090005
12 H	0.136356	29 C	-0.067304
13 C	-0.012918	30 H	0.089433
14 H	0.127227	31 H	0.105184
15 H	0.127061	32 H	0.098305
16 O	-0.343930	33 O	-0.352009
17 C	-0.007551	34 H	0.266463

IV. CONCLUSIONS

In this work, the chalcone (E)-3-(2,3-dihydrobenzofuran-5-yl)-1-(2-hydroxyphenyl)prop-2-en-1-one (DHBFP) was synthesized by Claisen-Schmidt condensation reaction. Spectroscopy methods were used to characterise the molecular structure, and Density Functional Theory was used to determine the electronic

and reactivity properties. To analyze the reactive electrophilic and nucleophilic sites, the electronic properties with respect to the frontier molecular orbitals, the quantum reactivity descriptors, and the molecular electrostatic potential were used. The presence of intramolecular hydrogen bonding between carbonyl group and hydroxyl group of DHBFP molecule is confirmed by observing O33-H34 bond with bond length 1.678 Å. The Mulliken atomic charges analysis revealed that all of the hydrogen atoms in DHBFP have a positive charge. The most negative and positive carbon atoms in DHBFP, according to Mulliken population analysis, were C23 (-0.213279) and C21 (0.315949), respectively.

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Conflict of Interest

Authors declared that he do not have any conflict of interest regarding this research article

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