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Combined Experimental and Computational Exploration of 4-(4-Bromophenyl)-6-(3,4-dimethoxyphenyl)-5,6-dihydropyrimidin-2(1H)-one

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ABSTRACT

This work deals with the synthesis of 4-(4-bromophenyl)-6-(3,4-dimethoxyphenyl)-5,6-dihydropyrimidin-2(1H)-one by condensation of 1-(4-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one with urea. The structure of the synthesized compound was established by FT-IR, ^{1}H NMR, ^{13}C NMR and HRMS spectral techniques. For the synthesized compound the density functional theory (DFT) calculations at the B3LYP level were performed using Gaussian 03(W) package. The optimized geometrical parameters, frontier molecular energies, electronic parameters and global chemical reactivity descriptors have been calculated by the DFT/B3LYP/6-311++G(d,p) level. The structure was characterized as a minimum in the potential energy surface using DFT. The molecular electrostatic potential (MEP) and thermodynamic properties were also investigated using the same level of theory. In addition, the vibrational wavenumbers of the title compound were calculated and the scaled values were compared with the experimental FT-IR spectrum. The result shows a good correlation between computed and experimental frequencies. The effect of different solvents on electronic parameters and global chemical reactivity descriptors were also examined. In solvents, no significant change was observed on the energy gap and global reactivity descriptors of the title molecule.

KEYWORDS: FT-IR, NMR, DFT, B3LYP, MEP.

INTRODUCTION

Heterocyclic compounds are abundant in nature and are important for survival because structural subunits of heterocycles can be found in many natural products including vitamins, proteins, and antibiotics. In synthetic organic chemistry, a feasible approach for the synthesis of such molecules is of great significance. Pyrimidine is a well-known heterocyclic compound possessing two nitrogen atoms in positions 1 and 3 of a six-member ring. Pyrimidine derivatives have a significant therapeutic noticeability as compared to other heterocycles and has far genetic and therapeutic implications. Pyrimidine derivatives have a wide spectrum of biological and pharmacological properties which include antimicrobial [1,2], antiviral [3], antihypertensive [4], anticancer [5-7], anti-inflammatory [8-10], antitubercular [11,12], and antihypertensive [13,14] activities. Due to their intriguing biological activity and medicinal potential, these compounds have received a lot of attention recently.

In recent years DFT-based theoretical computations have been used to determine several structural parameters of synthetically and pharmacologically significant organic compounds. The bond lengths, bond angles, dihedral angles, UV-visible spectra, IR and Raman frequencies, FMO energies, molecular electrostatic potential, and other properties of molecules can be predicted using DFT calculations [15-28].

In the current investigation, we report the synthesis as well as various structural and quantum chemical properties of the title compound i.e., 4-(4-bromophenyl)-6-(3,4-dimethoxyphenyl)-5,6-dihydropyrimidin-2(1H)-one.

EXPERIMENTAL

All the chemicals needed for synthesis were obtained from a commercial source (AR grade with purity >99%) and used without further purification. Melting points were determined in an open capillary tube and were uncorrected. FT-IR spectra were recorded on Shimadzu FT-IR spectrometer using potassium bromide pellets. ^{1}H NMR and ^{13}C NMR spectral analysis was carried on Bruker Avance II 500 MHz spectrometer using $CDCl_3$ as solvent and TMS as internal standard. The reaction was monitored by thin layer chromatography (TLC, Merck) using aluminium sheets coated with silica gel using n-hexane and ethyl acetate as an eluent.

Procedure for the synthesis of chalcone (3): An equimolar mixture of 4-bromo acetophenone (1, 0.01 mol) and 3,4-dimethoxy benzaldehyde (2, 0.01 mol) in ethanol catalysed by 10% NaOH (10 ml) was exposed to ultrasound irradiation at room temperature until the formation of desired chalcone derivative. The reaction was monitored by thin layer chromatography (eluent 20:80 ethyl acetate: n-hexane). After completion of the reaction (80 min), the reaction mixture was quenched by pouring on crushed ice and neutralized with dilute HCl. The resulting precipitate was filtered and dried to give the desired chalcone (3). The obtained chalcone was recrystallized from ethanol.

Procedure for the synthesis of title compound (4): The solution of chalcone (3, 0.002 mol), urea (0.002 mol), and sodium hydroxide (0.002 mol) in ethanol (15 ml) were refluxed for 6 hrs. Completion of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was poured into crushed ice and the product obtained was filtered, washed, dried, and recrystallized from ethanol to afford a pure compound (4). The reaction path is shown in scheme 1.

Computational details: The DFT calculations were performed on an Intel (R), Pentium (R) Dual-Core i7 computer using the Gaussian-03 (W) program package without any constraint on the geometry [29]. The geometry of the title molecule was optimized by DFT/B3LYP method using 6-31G(d,p) and 6-311++G(d,p) basis set [30,31]. The optimized structure of the compound was used for the frequency calculation. The electronic properties, thermochemical parameters, HOMO-LUMO energies, and MEP of the title compound were also explored. In addition, the effects of different solvents on electronic parameters and global chemical reactivity descriptors were examined by using the same level of theory.

RESULTS AND DISCUSSION

Spectral analysis of 4-(4-bromophenyl)-6-(3,4-dimethoxyphenyl)-5,6-dihydropyrimidin-2(1H)-one (4): Yellow solid; m.p. 115-117 ^{0}C; FT-IR ν_{max} (KBr; cm^{-1}): 3342.70, 2927.03, 1678.10, 1587.44, 1525.72, 1420.60, 1345.37, 1079.19, 687.63; ^{1}H NMR (500 MHz; $CDCl_3$, δ): 11.47 (s, 1H), 7.61 (dd, J = 8.3, 2.3 Hz, 2H), 7.49 (dd, J = 8.3, 2.3 Hz, 2H), 7.03-6.94 (m, 3H), 4.52 (dd, J = 7.1, 5.6 Hz, 1H), 4.02, (s, 3H), 3.96 (s, 3H); 3.27 (dd, J = 12.9, 5.6, 1H) 2.59 (dd, J = 12.9, 7.1, 1H); ^{13}C NMR (126 MHz; $CDCl_3$, δ): 166.21, 163.30, 147.80, 145.68, 137.45, 135.72, 131.59, 126.14, 122.41, 119.23, 112.34, 59.06, 58.87, 51.23, 37.89; HRMS: Calculated: 389.0501 [M+H], observed: 389.0479 [M+H].

Structural parameters and thermochemical study: The geometry optimized by DFT/B3LYP method with a 6-311++G(d,p) basis set shows that the title molecule has a non-planar shape with C1 point group symmetry. The optimized structure in the gas phase is shown in Figure 1 along with their atomic labelling. The bond lengths and bond angles are structural metrics that convey essential details about molecular conformation. Table 1 summarizes some selected optimized bond lengths and bond angles of the title compound computed at the B3LYP/6-311++G(d,p) level. The aromatic C=C bond lengths in the title compound range between 1.38 to 1.40 Å. The C18-Br41 bond has a length of 1.9135 Å, whereas the O30-C31 and O29-C35 bonds have lengths of 1.4370 and 1.4365 Å, respectively. The bonds N2-C1-N6, C16-C18-Br41, and C25-O30-C31 have bond angles of 117.48°, 119.51°, and 115.11°, respectively. All other bond lengths and angles are in the range of normal values.

The Mulliken atomic charges are an ordinarily utilized tool for assessing the properties of compounds based on their structure. The net charge on the studied molecule is zero. The Mulliken atomic charges of the title molecule calculated in the gaseous phase by DFT/B3LYP method with 6-31G(d,p) and 6-311++G(d,p) basis set are listed in Table 2. The charges depending on the basis set are likely to fluctuate due to polarizability. In comparison to the 6-31G(d,p) basis sets, Table 2 shows that the 6-311++G(d,p) basis set overstate the atomic charges. Figure 2 shows the graphical representation of the obtained results for a better understanding of the Mulliken charge of atoms.

The thermochemical parameters affecting the thermodynamic stability of a molecule, such as total thermal energy (E), total molar capacity at constant volume (Cv), entropy (S), zero-point vibrational energy, rotational constants, and total potential energy are computed at the B3LYP level with 6-311++G(d,p) basis set, at room temperature, 298.15 K, and 1 atm pressure. Table 3 lists the thermochemical parameters of the title molecule in the gas phase.

Electronic properties: The quantum chemical computations are crucial for predicting the electrochemical behaviour of organic compounds. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are called frontier molecular orbitals (FMO). The FMO analysis of the title compound was performed at the B3LYP/6-311++G(d,p) level. HOMO is an electron donor, while LUMO is an electron acceptor. The difference in energy between HOMO and LUMO is a key indicator of kinetic stability. High values of the HOMO-LUMO energy gap suggest that molecular structures have higher kinetic stability and lower chemical reactivity. In the gas phase, the HOMO-LUMO energy gap of the title compound is found to be 2.4234 eV which is not much deviated in solvents also (Table 4). Figure 3 shows a pictorial depiction of the frontier molecular orbitals of the title molecule in the gas phase.

The global reactivity descriptors such as electronegativity (χ), chemical hardness (η), chemical softness (σ), chemical potential (Pi), global electrophilicity index (ω) and a maximum number of electrons transferred (ΔNmax) are promising DFT descriptors to identify the chemical reactivity of molecules. Using Koopmans theorem [32,33], the global reactivity descriptors are calculated from the E_{HOMO} and E_{LUMO}.

To examine the effect of solvents on electronic parameters and reactivity descriptors of the title compound, the quantum chemical calculations are performed in ethanol, water, DMSO, and CCl_4 solvent by DFT/B3LYP method at 6-311++G(d,p) level. The data of electronic parameters of the title compound is given in Table 4 and the global reactivity descriptors calculated by using Koopmans theorem are given in Table 5.

The global reactivity descriptors evaluation result reveals that the title molecule is good electrophile because their global electrophilicity is more than 1.5 eV in all mediums. The maximum charge transfer is occurring in water solvent (6.2422 eV). The title molecule has the highest dipole moment in the water phase (8.8758 D), however, the lowest in the gaseous phase (6.3606 D).

The molecular electrostatic potential surface study provides information about the chemical reactivity of compounds. The existence of various colours implies the variation in the electron density distribution. The red and yellow colours denote high electron density, whereas blue and green denote positive and zero electrostatic potentials, respectively. The MEP plot of the title molecule is depicted in Figure 4. The carbonyl oxygen in the title molecule seems to have the most negative electrostatic potential, whereas C=N is a site for nucleophilic attack since it has the highest positive electrostatic potential.

Vibrational analysis: In the solid phase, the experimental FT-IR spectrum of the title molecule was recorded using a Shimadzu spectrometer in the range 4000-1000 cm^{-1}. The DFT/B3LYP method was used to perform a theoretical vibrational spectral analysis in the gas phase using a 6-311++G(d,p) basis set. Figures 5A and 5B represent the experimental and computed IR spectra of the title molecule, respectively. The title molecule has a total of 41 atoms with 117 fundamental modes of vibration. The empirical factor 0.9613 has been used to scale the theoretically calculated vibrational frequencies [34]. The results of the calculations were applied to the simulated IR spectrum of the title compound. Table 6 illustrates the results of the comparative analyses of the selected experimental and computed vibrational frequencies. The computed and experimental frequencies were found to be quite comparable (Table 6).

CONCLUSION

The title compound was synthesized from intermediate chalcone i.e. 1-(4-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one. The spectroscopic techniques and density functional theory with the B3LYP method and 6-311++G(d,p) basis set has been used to determine the detailed molecular structure of the title compound. The geometry optimization reveals the non-planar geometry of a studied molecule. The chemical reactivity of a molecule has been efficiently explored by using FMO and MEP analysis at the same level of theory. The FMO and global chemical reactivity descriptors analyses indicated no significant variation in energy gap and other reactivity descriptors values in gas, ethanol, water, DMSO, and CCl_4 phases. The vibrational analysis of the title molecule suggests that there is good agreement between the experimental and computed frequencies at 6311++G(d,p) level.

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Table 1: Selected optimized bond lengths and bond angles at B3LYP/6-311++G(d,p) level

Bond	Bond length (Å)	Bond	Bond angle (°)
C1-N2	1.3770	N2-C1-N6	117.48
C1-N6	1.1211	N2-C1-O28	122.07
C1-O28	1.2146	N6-C1-O28	120.44
N2-C3	1.4596	C1-N2-C3	122.60
C2-H8	1.0107	C1-N2-H8	114.46
C3-H9	1.1004	N2-C3-C20	111.4673
C3-C20	1.5172	C4-C3-C20	112.64
C5-N6	1.2855	C1-N6-C5	120.859
C5-C11	1.4857	N6-C5-C11	117.73
C18-Br41	1.9135	C16-C18-Br41	119.51
C25-O30	1.3746	C14-C18-Br41	119.40
C27-O29	1.3738	C23-C27-C25	119.25
O30-C31	1.4370	C25-O30-C31	115.11
O29-C35	1.4365	C27-O29-C35	115.34

Table 2: Mulliken atomic charges of title molecule calculated at 6-31G(d,p) and 6-311++G(d,p) basis set

Atom	Charge		Atom	Charge	
	6-31G(d,p)	6-311++G(d,p)		6-31G(d,p)	6-311++G(d,p)
C1	0.675294	0.262184	C22	-0.149850	-0.627588
N2	-0.538026	-0.299736	C23	-0.117373	-0.184888
C3	0.022669	0.144325	H24	0.086434	0.158892
C4	-0.225832	-1.080298	C25	0.308230	-0.269575
C5	0.290396	-0.116508	H26	0.107752	0.220136
N6	-0.517074	-0.034386	C27	0.310293	-0.223392
H7	0.145174	0.216471	O28	-0.484886	-0.289417
H8	0.268051	-0.344080	O29	-0.535961	-0.146711
H9	0.103486	0.238771	O30	-0.537162	-0.149077
H10	0.121969	0.143356	C31	-0.086868	-0.272001
C11	0.068730	0.992103	H32	0.128328	0.184532
C12	-0.126925	-0.270236	H33	0.121258	0.163379
C13	-0.088469	-0.221924	H34	0.108929	0.137170
C14	-0.097638	-0.719657	C35	-0.086656	-0.259072
H15	0.097432	0.144556	H36	0.129473	0.188129
C16	-0.093718	-0.411496	H37	0.120599	0.162963
H17	0.141256	0.230573	H38	0.106504	0.133140
C18	0.060420	0.146818	H39	0.100360	0.201314
H19	0.113485	0.234306	H40	0.117801	0.220981
C20	0.083100	0.970656	Br41	-0.114467	-0.171682
C21	-0.136518	-0.101190	-	-	-

Table 3: Thermochemical parameters calculated at the B3LYP/6-311++G(d,p) level

Parameters	Value
Total E Thermal kcal/mol	214.140
Translational	0.889
Rotational	0.889
Vibrational	212.362
Total Molar capacity at constant volume (Cv) Cal $mol^{-1}Kelvin^{-1}$	82.904
Translational	2.981
Rotational	2.981
Vibrational	76.942

Total entropy (S) Cal $mol^{-1}Kelvin^{-1}$	166.083
Translational	43.760
Rotational	36.785
Vibrational	85.538
Zero-point vibrational energy (kcal/mol)	200.121
Rotational Constant (GHz)	0.38306
	0.06018
	0.05478

Table 4: Electronic parameters of title compound calculated by B3LYP/6-311++ G(d,p) level in different solvents

Parameter	Medium				
	Gas	Ethanol	Water	DMSO	CCl_4
E (a.u.)	-3605.730	-3605.750	-3605.751	-3605.751	-3605.730
E_{HOMO} (eV)	-8.7705	-8.7680	-8.7647	-8.7677	-8.7691
E_{LUMO} (eV)	-6.3471	-6.3446	-6.3443	-6.3443	-6.3459
Eg (eV)	2.4234	2.4234	2.4204	2.4234	2.4231
I (eV)	8.7705	8.7680	8.7647	8.7677	8.7691
A (eV)	6.3470	6.3446	6.3443	6.3443	6.3459

Note: Abbreviations: I, ionization potential; A, electron affinity; (I = −EHOMO & A = −ELUMO)

Table 5: Global reactivity parameters of title compound calculated by B3LYP/6-311++ G(d,p) level in different solvents

Parameter	Medium				
	Gas	Ethanol	Water	DMSO	CCl_4
χ (eV)	7.5588	7.5563	7.5545	7.5560	7.5575
η (eV)	1.2117	1.2117	1.2102	1.2117	1.2115
σ (eV^{-1})	0.8253	0.8253	0.8262	0.8252	0.8253
ω (eV)	23.5760	23.5607	23.5788	23.559	23.5710
Pi (eV)	-7.5588	-7.5563	-7.5545	-7.5560	-7.5575
ΔNmax (eV)	6.2380	6.2360	6.2422	6.2357	6.2377
Dipole moment (Debye)	6.3606	8.7349	8.8758	8.8317	7.3399

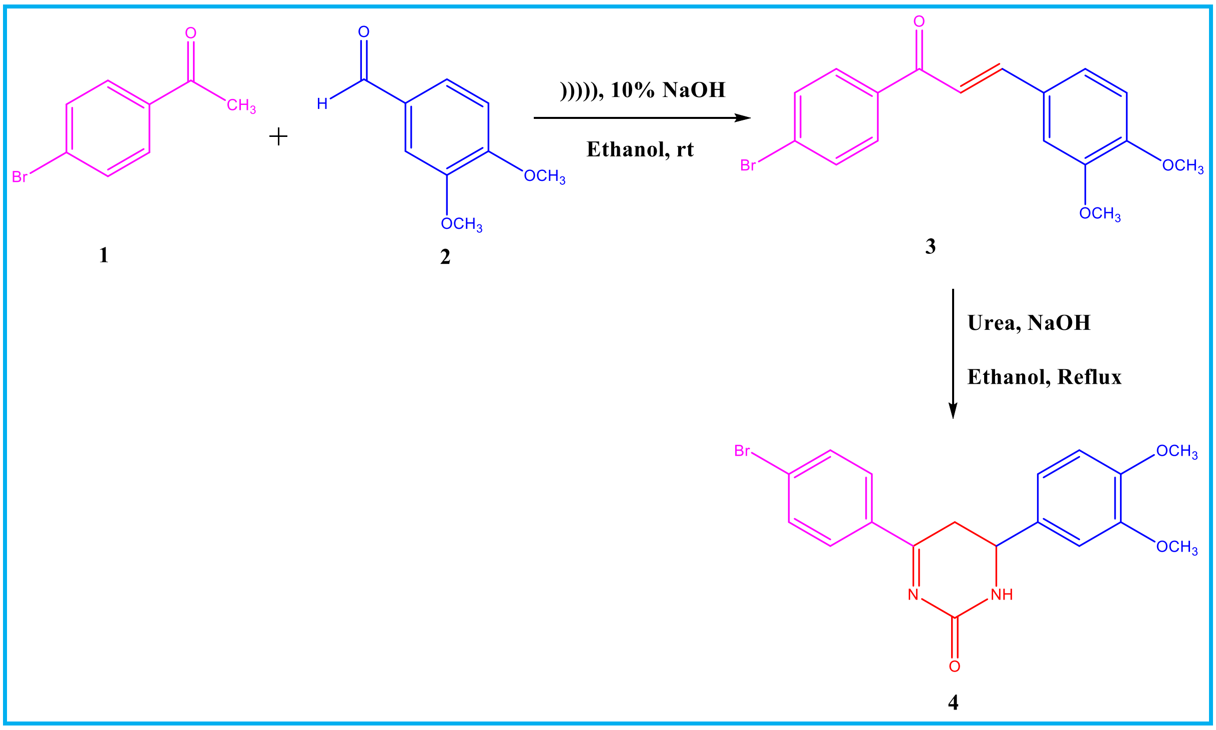
Note: $\chi = (I + A)/2$; $\eta = (I - A)/2$; $\sigma = 1/\eta$; $\omega = Pi^2/2\eta$; $Pi = -\chi$; $\Delta Nmax = -Pi/\eta$. (Abbreviations: χ, electronegativity; η, chemical hardness; σ, chemical softness; ω, global electrophilicity; Pi, chemical potential; ΔNmax, maximum no. of electron transferred).

Table 6: Selected experimental and computed vibrational assignments of title molecule

Mode	Computed scaled frequencies (cm^{-1})	IR Intensity (km) mol^{-1}	Experimental frequencies (cm^{-1})	Assignment
117	3402	34.95	3342	N-H str
115	3005	2.81	2927	C12-H15, C14-H19 str
102	2899	77.25	-	C35-H38, C15-H37, C15-H36 str
101	2853	30.32	2846	C3-H9 str
100	1691	599.05	1678	C=O str
99	1588	188.28	1587	C=N str
98	1579	3.51	1525	Ring B aro C=C str
95	1530	104.90	-	Ring A aro C=C str
87	1410	21.69	1420	C31-H32, C31-H33, C31-H34 ip bend
83	1367	50.18	1345	Ring A Ar-H ip bend

82	1325	18.83	-	C3-H9 ip bend
77	1260	42.18	1264	Ring B Ar-H ip bend
75	1235	404.85	-	C1-N2 str
59	1006	83.46	1017	C31-O38 str
39	677	9.02	687	C18-Br41 str

(str: stretching; ip bend: in plane bending; aro: aromatic; Ar: aryl; Ring A: 4-bromoophenyl ring attached to C5; Ring B: 3,4-dimethoxyphenyl ring attached to C3).



Scheme 1: Synthesis of title molecule

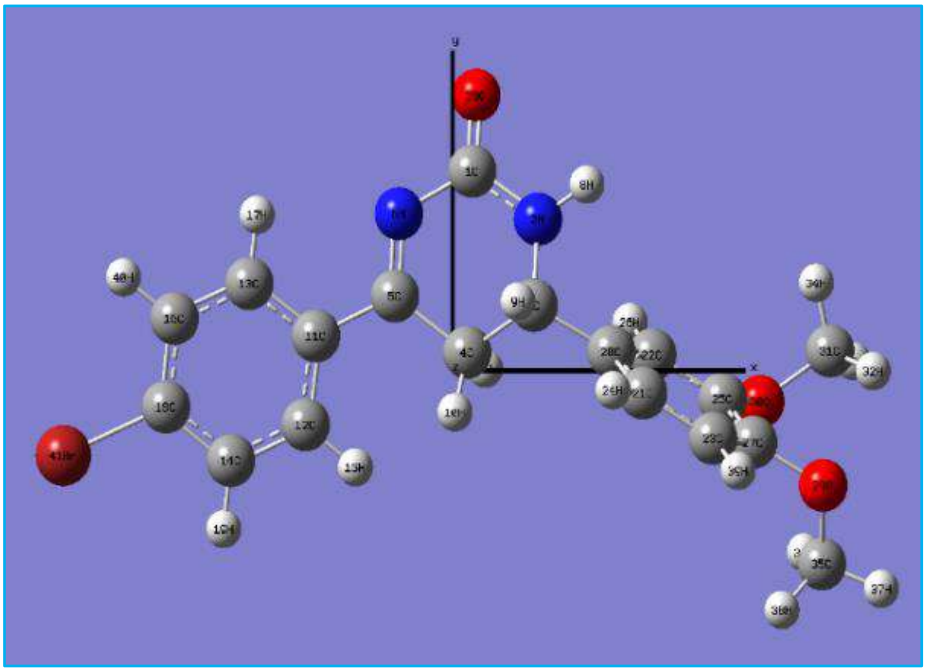


Fig. 1: Optimized structure of the title molecule with atomic labeling

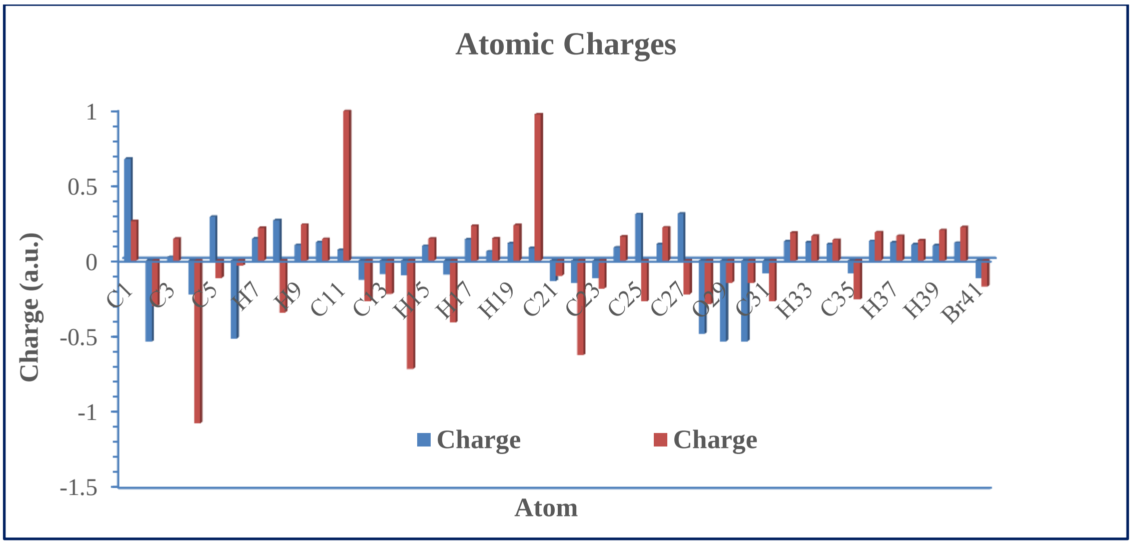
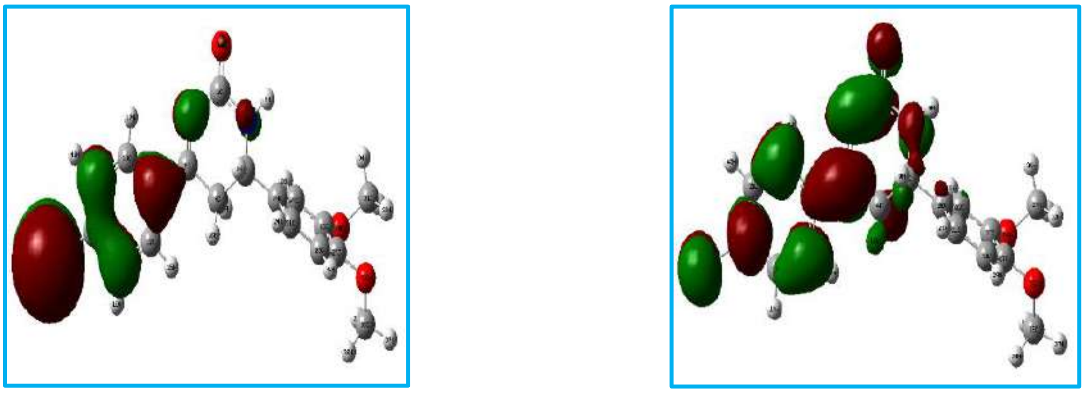


Fig. 2: The atomic charge plot of the title compound



HOMO **LUMO**

Fig. 3: Frontier molecular orbitals of title compound

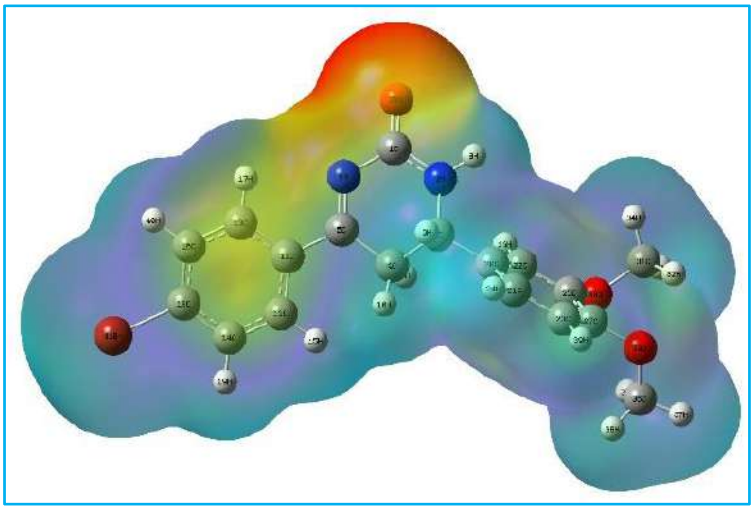


Fig. 4: MEP surface diagram of title molecule

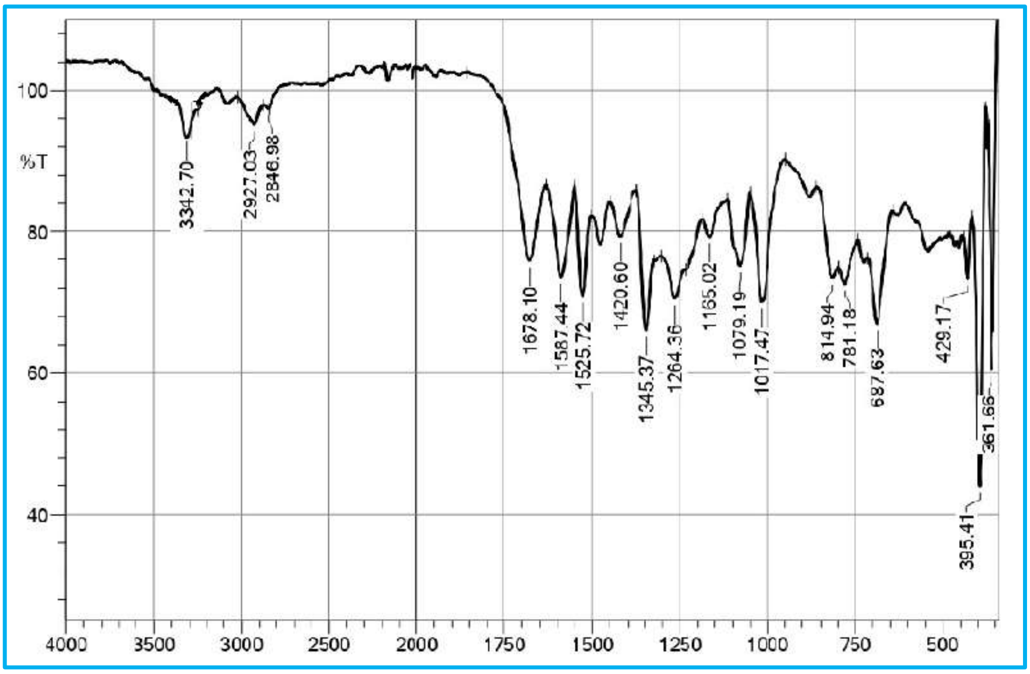


Fig. 5A: Experimental FT-IR spectrum

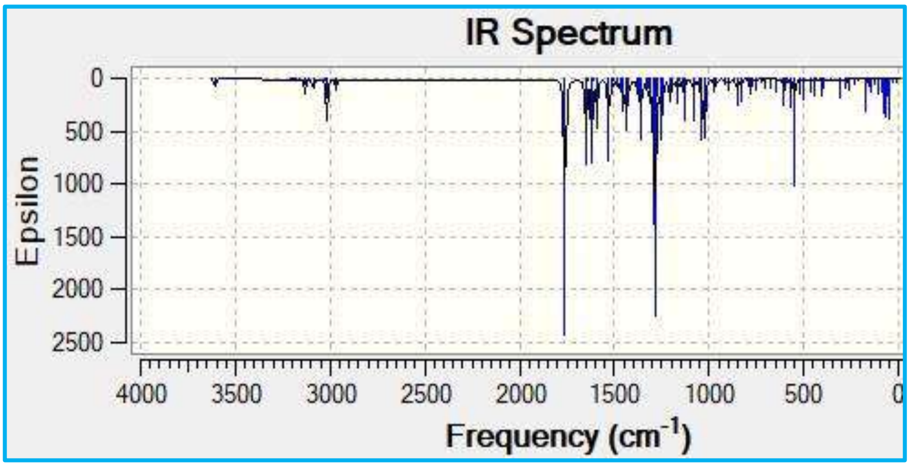


Fig. 5B: Computed FT-IR spectrum