SYNTHESIS, DFT, SPECTROSCOPIC CHARACTERISATION (FT-IR, FT-RAMAN, NMR AND UV-VISIBLE) AND MOLECULAR DOCKING INVESTIGATION OF 3-(4-BROMOPHENYL)-1-(THIOPHEN-2-YL) PROP-2-EN-1 ONE

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ABSTRACT

3-(4-bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 one (BPTP) was synthesized and characterized using FT-IR (3500-500 cm⁻¹), FT-Raman (3500-50 cm⁻¹) and UV-Visible spectrum (200-800 nm) to confirmed the synthesized molecule structure. Molecular geometry and vibrational wavenumbers of BPTP were studied by using B3LYP/6-311G (d,p) approach. The Total energy distribution (TED) utilized the VEDA 4 program for a complete vibrational analysis. The proton and carbon nuclear magnetic resonance (NMR) spectrum chemical shifts of the BPTP target compound were theoretically carried out by the gauge independent atomic orbital (GIAO) technique and were compared with the experimental solutions. The title molecule geometrical parameter was the best assent with the experimental one. NBO investigation, the conversion in the electron density of anti-bonding orbital and stabilization energies have been calculated to stretch clear proof of stabilization in the hyperconjugation of hydrogen-bonded interactions. NMR techniques of the target molecule are explained both experimentally and computational. The measured HOMO-LUMO band gap energies confirm that charge transfer occurs within the target compound. The computational technique using the Molecular Electrostatic Potential map (MEP) was also been calculated to stretch nucleophilic and electrophilic nature. The local reactivity of the molecule was studied using the Fukui indices. Molecular docking studies were also been followed to understand the BPTP compound biological activities.

Keywords: BPTP, UV-Vis, NMR, HOMO-LUMO, MEP.

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INTRODUCTION

The chalcone moiety has a π -conjugated system that gives an extreme charge-transfer axis. The moiety obeys the applications is used telecommunications, laser, optical computers, data storage, carrying the information optical sensing and optical systems. Chalcone moiety well switching behavior and optical limiting with a high-intensity laser pulse. Chalcone moiety has been used as pharmaceutical activities including antimicrobial (antifungal and antibacterial), anti-inflammatory, antileishmanial, antiviral, antitubercular, antioxidant, anticancer and antimalarial and etc., Recently, Shivaraj R et al have investigated the harmonic frequencies of (2E)-3-(4-fluorophenyl)-1-(4-[(1E)-(4-fluorophenyl)methylene]amino}phenyl)prop-2-en-1-one computed utilizing B3LYP/6-311G (d,p) method. Similarly, Nathiya A et. al, have reported the computed and experimental solutions on the synthesized compound (E)-N'(thiophene-2yl methylene) isonicotinohydrazide. A. Theresa et al and S. Bharanidhasan et al have reported that the theoretical and experimental comparison of the following compounds, (E)-1-(benzo[d][1,3]dioxol-6-yl)-3-(6-methoxynaphthalen-2-yl)prop-2-en-1-one, (E)-N'-(thiophene-2-ylmethylene) icotinohydrazide. Chemical compounds with chalcone derivative fascinate big research interest due to their presence in lots of organic activities.¹ Chalcone plays the most important role in biochemistry, so it has optical properties together with high extinction coefficients for absorption in the UV and notable nonlinear optical responses. Therefore, nonlinear optical (NLO) materials can be

stabilized, so that it does not make sense to understand the methods of the chalcone absorption spectrum and electronic transitions.² The best of authors knowledge there was no literature for theoretical investigation of the target compound. This research gap tempted the researchers to taken up the research for experimental and theoretical investigations.

In the present study, the target compound was synthesized and characterized by using analytical methods such as, FT-IR, FT-Raman, NMR, UV-Visible spectroscopy and compared the experimental one. Also, the studies were been carried out on NBO, MEP, Dipole moment, Homo-Lumo and Milliken analysis, etc. Furthermore, the docking analysis was also been carried out to recognize its biological application.

EXPERIMENTAL

Instruments

Fourier Transform Infrared range of BPTP transformed into a recorded on a Perkin Elmer FT-IR spectrophotometer using KBr pellet system as a piece of the area $3500\text{--}500\text{ cm}^{-1}$. Fourier Transform Raman range was recorded on a BRUKER RFS 27 spectrometer utilizing 1064 nm excitation wavelength from an Nd: YAG Laser inside the region $3500\text{--}50\text{ cm}^{-1}$. The laser yield for this strong example is around 300 mW . The ^1H and ^{13}C NMR range become recorded by means of using Bruker AVANCE III 500 MHz (AV 500) spectrometer with the guide of taking CDCl_3 as NMR dissolvable and TMS as reference. UV-Visible range of a fluid arrangement of the BPTP is recorded over a scope of $200\text{--}800\text{ nm}$ in the JASCO V-670 PC spectrophotometer, working at goals of 0.5 nm .

Synthesis of 3-(4-bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 One

A mixture of 4-Bromobenzaldehyde (0.01 mL) and 2-acetyl thiophene derivatives (0.01 mL) was dissolved in 10 mL rectified sprit in a 250 mL conical flask with a magnetic stirrer. Then 10 mL NaOH solution was added dropwise to the reaction mixture on stirring for 30 minutes when the solution became turbid. After vigorous stirring for $4\text{--}5\text{ hours}$, the reaction mixture was poured into cold water on filtering off crude chalcone were derived and recrystallized from ethanol.

Scheme-1: Synthesis of 3-(4-Bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 one

Computational Details

The computational calculations, BPTP were calculated with the Gaussian 09W agendum.³ The same techniques are used to calculate the wavenumbers for vibrational modes. Estimated works based on TED has been made in a normal manner. TED were measured using the Vibrational Energy Distribution Analysis (VEDA) agendum of quantum chemical calculated vibration frequencies⁴ graphical interface, optimized molecular systems, vibration frequencies, nuclear systems and bipolar moment, NMR spectrum and UV-Visible spectrum. The proton and carbon nuclear magnetic resonance (NMR) chemical changes BPTP were calculated by the gauge-independent atomic orbital (GIAO) theory in amalgamation with B3LYP/6-311G (d,p) and related experimental data.⁵

RESULTS AND DISCUSSION

Molecular Geometry

The BPTP target compound was optimized by B3LYP/6-311G (d,p) level of basis set. This compound consists of bromophenyl and thiophene ring are fused by chalcone linkage. The calculated bond length of

C2-Br25→ 1.009 and C11-S15→1.771. Since the chalcone moiety is linked with 5C atom and their corresponding bond length are C5-C21 (1.005Å), C19-O22 (1.258Å), C19-C20 (1.005Å) and O22-C21 (1.355Å). The bond angles of C1-C2-Br25 (120), C3-C2-Br25 (120) equal value due to attached the bromine atom. C12-C11-S15 (110.5) is expected to be greater than the bond angles S15-C11-C19 (124.7). The dihedral angles of C6-C1-C2-Br25 (179.9), correspondingly. The optimized structure and geometrical parameters are given in Fig.-1 and Table-1.⁶

Table -1: Geometrical Parameters [Bond Length (Å), Bond Angle (°) and Dihedral Angle (°)] of the BPTP Target Compound.

Bond length	B3LYP/61 3-G (d, p)	Bond angle	B3LYP/61 3-G (d, p)	Dihedral angle	B3LYP/61 3-G (d, p)
C1-C2	1.401	C2-C1-C6	120	C6-C1-C2-C3	0.0
C1-C6	1.401	C2-C2-H7	120	C6-C1-C2-Br25	179.9
C1-H7	1.000	C6-C1-H7	120	H7-C1-C2-C3	-180.0
C2-C3	1.401	C1-C2-C3	120	H7-C1-C2-Br25	0.0
C2-Br25	1.009	C1-C2-Br25	120	C2-C1-C6-C5	0.0
C3-C4	1.401	C3-C2-Br25	120	C2-C1-C6-H10	180.0
C3-H8	1.000	C2-C3-C4	120	H7-C1-C6-C5	180.0
C4-C5	1.401	C2-C3-H8	120	H7-C1-C6-10	0.0
C4-H9	1.000	C2-C3-H8	120	C1-C2-C3-C4	0.0
C5-C6	1.401	C3-C4-C5	120	C1-C2-C3-H8	-180.0
C5-C21	1.005	C3-C4-H9	120	Br25-C2-C3-C4	-180.0
C6-C10	1.000	C5-C4-H9	120	Br25-C2-C3-H8	0.0
C11-C12	1.359	C4-C5-C6	120	C2-C3-C4-C5	0.0
C11-S15	1.771	C4-C5-C21	120	C2-C3-C4-H9	-179.9
C11-C19	1.005	C6-C5-C21	120	H8-C3-C4-C5	180.0
C12-C13	1.552	C1-C6-C5	120	H8-C3-C4-H9	0.0
C12-H16	1.000	C1-C6-H10	120	C3-C4-C5-C6	0.0
C13-C14	1.359	C5-C6-H10	120	C3-C4-C5-C21	179.9
C13-H17	1.000	C12-C11-S15	110.5	H9-C4-C5-C6	179.9
C14-S15	1.771	C12-C11-C19	124.7	H9-C4-C5-C21	0.0
C14-H18	1.000	S15-C11-C19	124.7	C4-C5-C6-C1	0.0
C19-C20	1.005	C11-C12-C13	112.1	C4-C5-C6-H10	-180
C19-O22	1.258	C11-C12-H16	123.9	C21-C5-C6-C1	-179.9
O22-C21	1.355	C13-C12-H16	123.9	C21-C5-C6-H10	0.0
C20-H23	1.000	C12-C13-C13	112.1	C4-C5-C21-C20	-179.9
C21-H24	1.000	C12-C13-H17	123.9	C4-C5-C21-H24	0.0
		C14-C13-H17	123.9	C6-C5-C21-C20	0.0
		C13-C14-S15	110.5	C6-C5-C21-H24	179.9
		C13-C14-H18	124.7	S15-C11-C12-C13	-7.5
		S15-C14-H18	124.7	S15-C11-C12-H16	173.1
		C11-S15-C14	93.3	C19-C11-C12-C13	172.1
		C11-C19-C20	120	C19-C11-C12-H16	-7.1
		C11-C19-O22	120	C12-C11-S15-C14	10.2
		C20-C19-O22	120	C19-C11-S15-C14	-169.5
		C19-C20-C21	120	C12-C11-C19-C20	0.1
		C19-C20-H23	120	C12-C11-C19-O22	-179.8
		C21-C20-H23	120	S15-C11-C19-C20	179.8
		C5-C21-C20	120	S15-C11-C19-O22	-0.1
		C5-C21-H24	120	C11-C12-C13-C14	0.0
		C20-C21-H24	120	C11-C12-C13-H17	-179.2

				H16-C12-C13-C14	179.2
				H16-C12-C13-H17	0.0
				C12-C13-C14-S15	7.5
				C12-C13-C14-H18	-172.1
				H17-C13-C14-S15	-173.1
				H17-C13-C14-H18	7.1
				C13-C14-S15-C11	-10.2
				H18-C14-S15-C11	169.4
				C11-C19-C20-C21	0.0
				C11-C19-C20-H23	-179.9
				O22-C19-C20-C21	-179.9
				O22-C19-C20-H23	0.0
				C19-C20-C21-C5	179.9
				C19-C20-C21-H24	0.0
				H23-C20-C21-C5	0.0
				H23-C20-C21-H24	179.9

Fig.-1: Optimized Structure of 3-(4-Bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one.

Vibrational Analysis

The BPTP compound C1 symmetry system consists of 25 atoms and 69 normal vibrational modes. Vibration systems provide a systematic description of the FT-IR Fig.-2 and FT-Raman Fig. -2a and the TED analysis has been provided with basic criteria are shown in Table-2.

Fig.-2:[a]Experimental and [b]Theoretical FT-IR Spectrum of 3-(4-bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one

Fig.-2a: [a] Experimental and [b] Theoretical FT-Raman Spectrum of 3-(4-bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one.

Table -2: Vibrational Wave Numbers Obtained BPTP at 6-311G (d,p) Method [Harmonic Frequency (cm^{-1}), $\text{IR}_{\text{int}}(\text{kmmol}^{-1})$] Raman Intensity (Arb Units)].

Mode nos.	Experimental Wavenumber(cm^{-1})		Theoretical Wavenumber (cm^{-1})			TED ($\geq 10\%$) Assignments
	FT-IR	FT-Raman	B3LYP scaled	IR_{int}	Ram_{int}	
1	3154vw		3158	5.30	50.09	$\gamma\text{CH}(95)$
2			3118	21.88	159.21	$\gamma\text{CH}(97)$
3			3107	0.25	368.85	$\gamma\text{CH}(96)$
4		3105w	3105	3.30	111.48	$\gamma\text{CH}(80)$
5			3099	8.44	171.89	$\gamma\text{CH}(97)$
6	3074vw		3085	8.30	269.53	$\gamma\text{CH}(97)$
7		3067w	3068	0.89	53.91	$\gamma\text{CH}(91)$
8			3066	1.12	67.49	$\gamma\text{CH}(93)$
9	3009w	3012vw	3049	164.32	54.62	$\gamma\text{CH}(94)$
10	1638vs	1645w	1621	34.22	35.91	$\gamma\text{CC}(57)+\beta\text{HCC}(23)$
11	1582vs	1589vs	1573	153.04	233.80	$\gamma\text{CH}(30)$
12		1562m	1547	12.71	7.03	$\gamma\text{CC}(41)+\beta\text{CCC}(11)$
13			1536	19.41	5.79	$\gamma\text{OC}(41)+\gamma\text{CCC}(19)$
14	1511m	1515vw	1514	39.07	514.29	$\gamma\text{OC}(43)+\gamma\text{CC}(33)+\beta\text{HCC}(10)$
15	1481m		1486	9.87	16.65	$\beta\text{HCC}(68)$
16	1404vs	1414s	1427	107.48	526.31	$\gamma\text{CC}(42)+\beta\text{HCC}(13)$
17			1395	32.22	64.16	$\beta\text{HCC}(28)+\gamma\text{CC}(26)$
18	1350m	1352vw	1341	15.05	63.15	$\beta\text{HCC}(54)+\gamma\text{CC}(10)$
19	1322m		1332	24.89	7.24	$\beta\text{HCS}(25)+\beta\text{HCC}(21)+\gamma\text{CC}(12)$
20		1314vm	1310	84.33	103.96	$\beta\text{HCC}(70)$
21	1291w		1298	17.56	8.84	$\beta\text{HCC}(48)+\gamma\text{CC}(10)$
22			1279	28.66	4.11	$\gamma\text{CC}(30)$

23			1252	100.33	25.67	γ CC(16)+ β HCC(12)
24			1225	15.37	59.72	β HCC(38), γ CC(14)
25	1216vs	1202vw	1206	41.23	30.04	γ CC(44)+ β HCC(11)
26		1180w	1191	41.23	363.81	β HCC(68)
27	1109w		1111	57.38	15.40	β HCC(41)+ γ CC(27)
28			1096	63.80	32.54	β HCS(38)+ β HCC(33)+ γ CC(13)
29	1063vs	1067vw	1053	3.67	0.70	γ CC(53)
30			1047	1.99	18.11	γ CC(47)+ β HCC(15)+ β HCS(14)
31	1003w		1003	37.56	14.25	β CCC(81)
32			1000	1.46	2.98	τ HCCC(70)
33			980	34.34	7.76	β HCC(22)+ γ CC(14)
34		973w	978	15.94	37.07	τ HCCC(41)
35			968	5.87	169.38	τ CCCC(38)+ τ HCCC(31)
36			930	15.40	8.71	τ HCCS(43)+ τ HCCC(29)+CCCC(13)
37		882vw	906	17.37	5.17	τ HCCC(72)
38	854m	867w	867	55.46	156.47	τ HCCC(72)+ τ HCCS(20)+ τ HCSC(19)
39		867w	840	28.23	27.79	β CCC(19)
40			835	10.35	14.04	τ HCCC(98)
41			829	68.06	5.24	τ HCCC(45)
42	807vs		815	6.05	23.09	β CCC(53)
43	750s		739	58.81	59.03	β HCCC(25)+ τ OCCC(18)+ τ CCCC(12)
44			716	4.75	38.02	τ HCCSC(65)+ τ HCCS(25)
45			698	25.96	52.38	τ CCCC(10)+ δ OCCC(20)
46		667w	676	21.40	66.20	γ SC(29)+ β SCC(17)+ δ OCCC(12)
47		653vw	656	19.56	78.76	γ SC(30)
48			641	40.89	5.73	β CCC(51)
49			630	51.48	13.19	β SCC(28)+ β CCC(23)
50			605	23.56	29.82	β OCC(31)+ γ SC(18)
51			562	30.23	11.63	τ CCCC(66)+ τ HCCC(11)
52			519	38.37	19.35	τ CCCC(18)+ β SCC(10)
53			486	10.08	298.58	β SCC(18)+ β CCC(12)
54			438	10.48	20.47	τ SCCC(10)
55			414	0.00	245.46	τ CCCC(58)+ τ HCCC(10)
56			399	0.57	7.29	β CCC(26)+ γ CC(10)
57			373	11.43	49.53	β HCC(54)+ γ CC(20)+ γ BrCC(12)
58			337	1.84	85.06	δ BrCCC(22)+ δ CCCC(15)
59			282	0.45	5.61	γ BrC(29)+ γ BrCC(12)
60			224	10.30	81.90	β BrCC(56)
61		183vw	196	0.23	30.60	β CCC(26)+ τ CCCC(14)+ δ BrCCC(14)
62			174	1.27	4.28	τ CCCC(23)+ β CCC(18)
63			159	0.38	8.60	τ CCCC(65)
64			136	2.11	4.00	τ CCCC(45)+ δ OCCC(11)
65		89vw	103	0.66	8.67	β CCC(41)+ τ CCCC(20)
66			76	2.65	10.22	β CCC(10)+ τ CCCC(40)
67			36	172.68	39.40	γ CC(15)+ β CCC(13)
68			31	178.20	1485.23	τ CCCC(58)+ β BrCC(56)+ δ CCCC(13)
69			24	524.63	404.18	τ CCCC(55)+ δ OCCC(17)

Ram_{int} - Raman Intensity; IR_{int} - IR intensity; Kmmol⁻¹s-strong; vs-very strong; m-medium; w-weak; vw- very weak γ - stretching; δ - out-of-plane bending; β - in plane bending; τ - torsion.

C-H Vibration

The BPTP compound 9 CH stretching vibration and the C-H vibration commonly exhibits weak region at $3100-3000\text{cm}^{-1}$ ^{7,8} and they are not generally affected appreciably by the common substitutions. C-H stretching vibration normally pure mode contribution observed at $3049-3158\text{cm}^{-1}$. FT-IR bands observed at $3074(\text{w})$ - $3074(\text{w})$ and FT-Raman observed peaks at $3105(\text{w})$, $3067(\text{w})$ and $3012(\text{vw})$ are a good agreement with each other.

The HCC stretching vibrational in-plane bending region $1627-1087\text{cm}^{-1}$. FT-IR bands observed at $1638(\text{vs})$, $1511(\text{m})$, $1481(\text{m})$, $1404(\text{vs})$, $1350(\text{m})$, $1322(\text{m})$, $1291(\text{w})$, $1216(\text{vs})$ and $1109(\text{w})$ and Raman bands observed at $1645(\text{w})$, $1562(\text{m})$, $1515(\text{vw})$, $1414(\text{s})$, $1352(\text{vw})$, $1314(\text{vw})$, $1202(\text{vw})$ and $1180(\text{w})$ commonly. Torsion vibration of HCCC assessment at $1034-412\text{cm}^{-1}$. FT-IR observed bands at $854(\text{m})$ and in FT-Raman observed peaks at $973(\text{w})$, $882(\text{vw})$ and $867(\text{w})$ and the harmonic frequency with TED value 97%.

C=O Vibration

The C=O vibration pi-bonding between oxygen and carbon atoms. The C=O stretching vibration is observed in the region $1680-1715\text{cm}^{-1}$.⁹ This case calculated C=O stretching vibration present in the region $1514-1536\text{cm}^{-1}$. FT-IR bands observed at $1515(\text{vw})$ and FT-Raman observed bands at $1511(\text{m})$ and $1561(\text{w})$. TED contribution at 43%.

C=C and C-C vibrations.

The $\gamma(\text{C-C})$ stretching vibrations are expected bands range of $1590-1640$, $1560-1580$ and $1470-1510\text{cm}^{-1}$.¹⁰ The theoretical wavenumber for $\gamma(\text{C-C})$ mode lies at $36-1621\text{cm}^{-1}$ with TED value 57%. In this present study FT-IR bands observed $1638(\text{vs})$, $1582(\text{vs})$, $1404(\text{vs})$, $1350(\text{m})$, $1322(\text{m})$ and $1291(\text{w})$ and in FT-Raman observed at the bands $1645(\text{w})$, $1589(\text{vs})$, $1562(\text{m})$, $1515(\text{vw})$, $1414(\text{s})$, $1352(\text{vw})$, $1202(\text{vw})$ and $1167(\text{vw})$ are designated as $\gamma\text{C-C}$ vibrations. The βCCC in-plane bending region observed at $1583-37\text{cm}^{-1}$ at TED value 11%. FT-IR observed bands at 1003cm^{-1} (weak) and in Raman peaks observed at $1562(\text{m})$ and $89(\text{vw})$.

C-Br Vibration

The BPTP title compound C- Br, vibrational in the region $650-395\text{cm}^{-1}$.¹¹ This absorbs the stretching vibration. The stretching vibrations present in the part of $373-282\text{cm}^{-1}$. In-plane bending observed mode $224-31\text{cm}^{-1}$ and out of bending mode $337-196\text{cm}^{-1}$. The computational vibrational frequency appears in $373-196\text{cm}^{-1}$. FT-Raman bands at $183(\text{vw})$ with TED 56%.

Fig.-4: NMR Spectrum of [a] ^1H and [b] ^{13}C 3-(4-bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 one

Thiophene Ring Vibration

In common, the assignment of vibration in the alternate compound is arduous in the infrared. The adsorption of this group is of unstable intensity and may be found over a broad part $1035-245\text{cm}^{-1}$ both aromatic and aliphatic sulphide.¹² FT-Raman bands at $667(\text{w})$ and $653(\text{vw})$ and the C-S stretching mode TED contribution 30%.

NMR Spectral Analysis

The proton and carbon nuclear magnetic resonance spectra were calculated to confirm the target compound structure. Both ^1H and ^{13}C NMR spectra (Experimental and theoretical) have seen in Fig-3. The proton NMR, a multiplet peak presented in the constituent 7.11-7.80 ppm with 9 proton entire value barely arrangement to the aromatic ring protons. The ^1H signals were theoretically calculated and it is received between the constituent 6.75-8.57 ppm values are good agreement shown in Table-3. The carbon signals at 122.14-145.35 are due to the presence in the aromatic ring carbons. The signal at 181.75 ppm is due to the C=O carbon present in the compound. All the theoretical values are a good agreement with the experimental one.

Table -3: The Predicted and Observed ^1H and ^{13}C Isotopic Chemical Shifts for BPTP

Atom Number	B3LYP/6-311G(d,p.)		Experimental
	Gas Phase	Solvent Phase	
2C	178.62	178.88	176.34
3C	162.71	163.97	-
4C	147.15	149.09	-
5C	145.88	145.51	145.35
6C	140.05	141.27	142.58
8C	139.64	140.24	134.16
10C	139.43	139.37	133.63
12C	137.29	138.95	132.24
13C	136.78	136.13	131.96
14C	134.34	134.27	129.85
15C	126.23	127.27	128.32
16C	125.30	126.15	124.89
17C	118.52	119.64	122.14
11H	8.37	8.57	7.80
9H	7.69	7.99	7.75
19H	7.65	7.87	7.71
20H	7.71	7.64	7.52
21H	7.58	7.70	7.50
22H	7.26	7.48	7.32
23H	6.92	7.14	7.31
24H	6.90	7.13	7.19
25H	6.53	6.75	7.13

UV-VIS Spectral Analysis

The TD-DFT calculation has been carried out using B3LYP/6-311G (d,p) basis set and concluded the low-lying excited states of BPTP were present. In this calculation both solvent phase and gas and employing ethanol environment. Obtained computed values are given in Table-4 and the spectrum was shown in Fig.-4.¹³ The theoretical data at 496.97, 319.27 and 305.60 nm in the gas phase, 494.95 318.65 and 304.70 nm. The measured oscillator strength of BPTP found to be 0.0039(496.96), 0.2180(319.27nm) and 0.0079(305.60) nm in the gas phase, and 0.0039(494.95), 0.220(318.65nm) and 0.0078(304.70nm) in ethanol medium.

The predicted $\pi \rightarrow \pi^*$ transitions was responsible for HOMO $\rightarrow$ LUMO (95%), H-12 $\rightarrow$ LUMO (3%), H-1 $\rightarrow$ LUMO (82%), H-4 $\rightarrow$ LUMO (7%), H-3 $\rightarrow$ LUMO (5%) and H-4 $\rightarrow$ LUMO (14%), H-2 $\rightarrow$ LUMO (77%), H-3 $\rightarrow$ LUMO (2%), H-1 $\rightarrow$ LUMO (3%) ethanol solvent also transition under Gas-phase mode, It is there HOMO $\rightarrow$ LUMO (95%), H-12 $\rightarrow$ LUMO (3%), H-1 $\rightarrow$ LUMO (83%), H-4 $\rightarrow$ LUMO (7%), H- $\rightarrow$ LUMO 5%) and H-4 $\rightarrow$ LUMO (14%), H-2 $\rightarrow$ LUMO (77%), H-1 $\rightarrow$ LUMO (3%).¹³

Fukui Function

The Fukui functions in between a simpler and normal-enabled reaction indicator the replacement of the Fukui function of the molecular density function $\rho N(r)$. The Fukui function indices are the calculation of chemical reactivity, an indicator of reactive place and the electrophilic and nucleophilic reaction of the molecules it is to identify the electron acceptor center and donor centers. If f^+ is real value then the imaginary value of f^- implies electrophilic attract.

The Fukui indices for summation of electron to a BPTP are given by:

$$f^+(r) = \rho_{N+1}(r) - \rho_N(r) \quad (1)$$

Fig.-4: Optical Absorption Spectrum of 3-(4-Bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one [a] Experimental, [b] Simulated in Ethanol and [c] Gas Phase Using TD-DFT method.

Table-4: Experimental and Calculated Absorption Wavelength, Energies and Oscillator Strengths of 3-(4-bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 one using the TD-DFT Method of B3LYP/6-311G (d,p) Method.

	Excitation	CI Expansion Coefficient	Wavelength λ (nm)	Oscillator Strength (f)	Expt.	Assign.	In Solvent a Major contribution ($\geq 10\%$)
Cal. DMSO phase	Excited State 1						
	69 $\rightarrow$ 74 73 $\rightarrow$ 74	-0.12995 0.68878	496.97	0.0039		$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$	HOMO $\rightarrow$ LUMO (95%)
	Excited State 2						
	69 $\rightarrow$ 74 70 $\rightarrow$ 74 72 $\rightarrow$ 74	0.19164 0.16069 0.64185	319.27	0.2180	325	$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$	H-1 $\rightarrow$ LUMO (82%)
Cal. Gas-	Excited State 3						
	69 $\rightarrow$ 74 70 $\rightarrow$ 74 71 $\rightarrow$ 74 72 $\rightarrow$ 74	-0.26435 -0.10078 0.61979 0.12112	305.60	0.0079		$\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$ $\pi \rightarrow \pi^*$	H-2 $\rightarrow$ LUMO (77%)
	Excited State 1						
	69 $\rightarrow$ 74	-0.26832	304.70	0.0078		$\pi \rightarrow \pi^*$	HOMO $\rightarrow$ LUMO (95%)

phase	71 -> 74	0.61970				$\pi \rightarrow \pi^*$	
	72 -> 74	0.11737					
	Excited State 2						
	69 -> 74	-0.13065	494.95	0.0039		$\pi \rightarrow \pi^*$	H-1 $\rightarrow$ LUMO (83%)
	73 -> 74	0.68885				$\pi \rightarrow \pi^*$	
						$\pi \rightarrow \pi^*$	
	Excited State 3						
	69 -> 74	0.19004	318.65	0.2220		$\pi \rightarrow \pi^*$	H-2 $\rightarrow$ LUMO (77%)
	70 -> 74	0.15753				$\pi \rightarrow \pi^*$	
	72 -> 74	0.64327				$\pi \rightarrow \pi^*$	

The Fukui indices for removal of an electron from a BPTP are given by:

$$f^-(r) = \rho N(r) - \rho N-1(r) \quad (2)$$

The first part of an f^+ function represents a nucleophilic reaction. On the other hand, the first part of an f^- function represents electrophilic reaction. The Fukui indices (f), global and local electrophilicity index (ω) and global-local softness (S) of the molecule under study are presented in Table-5. It is seen that the atoms 7C, 8C, 9H, 10C, 11H, 12C, 15C, 16C, 18Br, 19H, 23H, and 24H are good nucleophiles having negative local electrophilic index $\Delta\omega$ and they are ready to donate an electron pair to form a bond and which is capable to electrophilic attack. The atoms 1C, 2C, 3C, 4C, 6C, 13C, 14C, 17C, 20H, 22H, and 25H are good electrophiles having positive local electrophilic index $\Delta\omega$ and they are ready to accept electron pair to form a bond and which is capable to nucleophilic attack.¹⁴

Table-5: Fukui Function and Global and Local Softness, and Electrophilicity Index of Fig.-1 Optimized Structure of 3-(4-Bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one.

$f^+ = (q+1) - q$	$f^- = q - (q+1)$	$\Delta f = (f^+) - (f^-)$	$\Delta f = \Delta f S_{gs}$	$\Delta\omega = \Delta f \omega_{ei}$
-0.12867	0.53157	-0.66024	0.17261	-0.90545
-3.68903	0.06673	-3.75576	0.98194	-5.15060
-0.13039	0.10698	-0.23737	0.06206	-0.32553
-0.13912	0.07310	-0.21222	0.05548	-0.29104
-0.07270	-0.16882	0.09612	-0.02513	0.13182
-0.04728	0.36938	-0.41667	0.10893	-0.57142
-0.47124	0.66172	-1.13296	0.03476	-1.55374
0.52241	-0.70769	-0.18528	0.04844	-0.25409
-0.10245	0.13498	-0.23743	0.06207	-0.32562
-0.43625	0.00000	-0.43625	0.11405	-0.64031
-0.38942	-0.44039	-0.82981	-0.21695	1.13800
0.30243	0.16446	0.46690	0.04585	0.64031
-0.18787	0.33202	-0.51989	0.13592	-0.71298
-0.08408	0.09130	-0.17538	-0.12207	-0.24052
-0.36476	0.50124	-0.86600	0.22641	-0.18764
-0.411302	-0.07547	-0.33582	0.88780	-0.46055

Dipole Moment

The target compound obtained dipole moment is 4.2457. The three axes represent the three directions and these are XYZ Cartesian coordinates. X-axis 4-bromophenyl direction, however, refers to the Y-axis chalcone moieties direction Dipole moment match with the water the dipole moment value is higher than the water value. This BPTP is a white color compound and has medicinal properties is shown in Fig-5 and Table- 6.¹⁶

Table -6: Dipole Moment Components of 3-(4-Bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one

Dipole vector components	Dipole moment, μ (Debye)
μ_x	1.0174
μ_y	-4.1220
μ_z	0.0183
μ_{total}	4.2457

Fig-5: Dipole Moment of 3-(4-Bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 one

HOMO and LUMO Analysis

HOMO and LUMO are very important roles of electron transfer are known as frontier molecular orbitals (FMOs). HOMO and LUMO (π -acceptor) the energy gap was calculated. The HOMO and LUMO analysis have been measured by B3LYP/6-311G (d,p) basis set. The HOMO and LUMO of BPTP are given in Table-7 and Fig-6. The HOMO is presented at the thiophene ring and LUMO is presented at the chalcone moiety and the energy values are -7.06370 eV and -0.58585 eV, correspondingly. BPTP molecule calculated energy gap is -6.47785 eV.¹⁷ The physicochemical properties of conclusive charge transfer explain. The BPTP title compound using Koopmans theory and given in table; results of Koopmans theorem HOMO-LUMO and energy gap, the ionization potential (I)-ELUMO, electron affinity (A) = -ELUMO, softness (ν) is $\nu = 1/\eta$, the global hardness (η) is $\eta = (I-A)/2$, Chemical potential (μ) is $\mu = -(I+A)/2$, global electrophilicity (ω) is $\omega = \mu^2 / 2\eta$ and Electronegativity (χ) is $\chi = (I+A)/2$.¹⁸

Fig -6: Density Functional Theory HOMO-LUMO of 3-(4-Bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one

Table -7: HOMO and LUMO Calculated Values of 3-(4-Bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 one by B3LYP/6-311G (d,p) Method.

BASIS SET	B3LYP/6-311G(d,p)
E_{Homo} (a.u)	-7.0637
E_{Lumo} (a.u)	-0.5858
Energy gap(a.u)	-6.4778
Ionization energy(I)	7.0637
Electron affinity(A)	0.5858
Global hardness(η)	-3.8247
Chemical potential(μ)	-3.2389
Electro philicity index(ω)	1.3714
Chemical softness(s)	-0.2614

Molecular Electrostatic Potential

The molecular electrostatic potential (MEP) was mostly used. Its potential diagram is found in areas where it is possible. The simplest method was used to calculate the different connections on the MEP diagram. The reactive sites for nucleophiles and electrophilic attract of the MEP was measured B3LYP/6-311G (d,p) basis set. The negative sites were presented in the carbonyl group and positive sites were presented in thiophene moiety is given in Fig-7.

Fig-7: Molecular Electrostatic Potential (MEP) of 3-(4-Bromophenyl)-1-(thiophene-2-yl) prop-2-en-1 one

Mulliken Atomic Charges

The charge evaluates the electronic structure charges under the atomic movement. It is connected straightforwardly to the chemical bonds shown in the title compound, its position, polarizability, electronic structure, dipole moment, and more effects of molecular systems, The Mulliken and natural charge sharing of the compound calculated on B3LYP /6-311G(d,p) technique are given in Table-8 and Fig-8. The Mulliken charge distribution in the BPTP is found to be atoms C1, C6, C11, C12, S15, C19, C20, C21, and Br25 positive Natural charge and Mulliken charge possess definite charge in Mulliken C1, C2, C3, C4, C5, C6, C11, C13, C14, C21, C22 and S15 possess negative natural charge and Mulliken charge.¹⁹

NBO Analysis

The E (2) value displays are more related to the donor and acceptor BPTP molecular. The most definitive structure of the C=C ring consists of electrons hyperconjugation connections with σ and π . In the current debate π -character and σ character play an important role. The hyperconjugation interactions π (C12-

$C13 \rightarrow \pi^*(C12-C17)$, $\pi(C13-C14) \rightarrow \pi^*(C13-C14)$, transfer stabilization energy: 24.66 and 22.32 KJ/mol to the molecular arrangement. The lone pair of sulphur, bromine, and oxygen atom plays a good role in BPTP. The S1, O7, and Br18 atoms relocate the energy 24.78, 15.42 and 1.76KJ/ mol to (C2-C3), (C2-C6) and C15 bonds, correspondingly. The extreme hyperconjugation E (2) energy of chalcone compare moiety during the inter-molecular interaction leads the molecular biological and medicinal applications. The bond σ (S1-C2) 3.97KJ/mol to $\sigma^*(S1-C2)$ bond on comparing with energy transfer 3.97 KJ/mol from $\pi(C4-C5) \rightarrow \pi^*(C4-C5)$ 15.31KJ/mol $\pi(C6-O7) \rightarrow \pi^*(C6-O7)$ 7.79KJ/ mol given in Table- 9.

Molecular Docking Analysis

Autodock 4.2 tools are used by molecular docking calculating binding mode and competence connector. The molecular analysis section of cancel cell (PDI: 8F8G) is used as a receptor and Autodock 4.2 package simulation. Autodock 4.2 tools are created using a protein system. Therefore, polar hydrogen bonds are provided. PDB is constructed $80\text{\AA} \times 80\text{\AA} \times 80\text{\AA}$ using a structural analysis bonding and make use of the size of the grid to create energy. Cancer cell-related blocking 8F8G protein had good binding energy (-7.68 stone/mol), which clearly illustrates the formation of hydrogen bonding protein is given Fig-9a. The pyMol package utilized for the visualizations of proton and target compound interactions. Discovery studio package 4.0 is used to detect the best bond in 2D is shown in Fig.-9b.

Fig-8: Milliken Charge Distribution of 3-(4-Bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one

Table-8: Mulliken Charges of 3-(4-bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one

Atom	Mulliken charge	Natural charge
C1	-0.128443	0.338669
C2	-0.368945	-0.275715
C3	-0.130388	-0.040173
C4	-0.139122	-0.084954
C5	-0.072702	-0.275627
C6	-0.049014	0.27606
H7	0.175943	-0.330222
H8	0.175004	-0.121738
H9	0.165105	0.09335
H10	0.178777	0.002848

C11	-0.486188	0.11868
C12	0.04107	-0.167293
C13	-0.092632	-0.000628
C14	-0.436983	-0.024634
S15	0.398703	-0.179176
H16	0.139821	-0.025176
H17	0.17606	-0.001525
H18	0.208638	-0.029418
C19	0.302433	0.110706
C20	-0.18797	0.105283
C21	-0.084085	0.135985
O22	-0.365313	0.081979
H23	0.179434	0.104858
H24	0.187959	0.104851
Br25	0.212837	0.083009

Fig. -9a: The docked pose of the 3-(4-bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one

Fig.-9b: 2D the 3-(4-bromophenyl)-1-(thiophen-2-yl) prop-2-en-1 one

The length of the binding obtained at the end of the test is hydrogen bonding with THR A: 6.8 (threonine) interactive at 3.4 and LEUA:134 (teucine) interactive at 3.8 releases both Amino acids.²⁰ The final result is confirmed that the target compound is one of the best solutions for cancer treatment the results are shown in Table -10.²¹

Table-9: Second-Order Perturbation Theory Analysis of Fock Matrix in NBO Basis Corresponding to the Intermolecular Bonds of the BPTP Compound

Donar	Type	ED/e	Acceptor	Type	ED/e	Kcal /mol	Ej-Ei a.u	F(I,j) a.u
S1-C2	σ	1.9701	S1-C2	σ^*	0.3422	03.97	1.10	0.059
S1-C5	σ	1.9812	S1-C5	σ^*	0.0177	04.16	1.10	0.060
C2-C3	π	1.7846	C2-C3	σ^*	0.3593	24.05	0.32	0.079
C2-C6	σ	1.9729	C2-C6	σ^*	0.0542	06.10	1.33	0.00
C3-C4	σ	1.9766	C3-C4	σ^*	0.01455	04.31	1.29	0.007
C4-C5	π	1.8368	C4-C5	π	0.3116	15.31	0.30	0.064
C6-O7	π	1.9426	C6-O7	π	0.2684	07.79	0.41	0.051
C8-C10	σ	1.8409	C6-C10	π	0.0687	30.36	0.31	0.090
C10-C12	σ	1.9657	C10-C12	σ	0.0276	5.45	1.40	0.078
C12-C13	σ	1.9527	C12-C13	σ	0.0340	5.31	1.26	0.073
C12-C17	π	1.6318	C12-C17	π	0.3638	24.66	0.21	0.073
C13-C14	π	1.6728	C13-C14	π	0.3208	22.32	0.29	0.072
C15- Br18	σ	1.9832	C15- Br18	σ	0.0331	02.90	1.25	0.054
Lp(2)	S1			π	1.5755			
Lp(2)	O7			π	1.8913			
Lp(2)	Br18			π	1.9753			

Table -10: Estimated Free Energy, Electrostatic Energy, Inhibition Constant, and Total Molecular Energy Obtained From Ligand-Protein Interactions Between the Target Receptor 8F8G and BPTP.

S.No.	Binding Energy (Kcal/ Mol)	Ligand Efficiency	Inhibition Constant Ki (μ M)	Intermolecular Energy (Kcal/Mol)	Vdw + H- Bonding + Desolv. Energy (Kcal/Mol)	Electrostat ic Energy (Kcal/Mol)	Total Internal Energy	Torsion Energy (Kcal/ Mol)
1	-7.68	-0.48	2.33	8.58	-8.48	-0.1	-0.35	0.89
2	-7.09	-0.44	6.41	-7.98	-7.90	-0.08	-0.36	0.89
3	-7.08	-0.44	6.42	-7.98	-7.89	0.08	-3.36	0.89
4	-7.06	-0.44	6.66	-7.96	-7.89	-0.07	-3.39	0.89
5	-6.88	-0.43	9.07	-7.77	-7.64	-0.13	-0.36	0.89
6	-6.79	-0.42	10.55	-7.68	-7.52	-0.17	-0.38	0.89
7	-6.53	-0.41	16.22	-7.43	-7.22	-0.21	-0.43	0.89
8	-6.47	-0.40	18.24	-7.36	-7.36	0.0	-0.41	0.89
9	-6.38	-0.4	21.1	-7.27	-7.15	-0.13	0.38	0.89
10	-6.31	-0.39	23.72	-7.20	-7.06	-0.14	0.45	0.89

CONCLUSION

The synthesized molecule 3-(4-bromophenyl)-1-(thiophene-2-yl) prop-2-en-1-one (BPTP) was characterized by using several analytical methods such as FT-IR, and NMR. The B3LYP/6-311G basis

set was adopted for target compound optimization. The experimentally recorded FT-IR and FT-Raman spectrum was remarkable in the agreement with theoretical one. Nuclear magnetic resonance spectroscopy was confirmed the structure of the BPTP; proton and carbon NMR chemical shifts were determined and compared with the experimental values. Natural bond orbital study stabilizes that the intermolecular charge relocates formed between $\pi(\text{C6-O7}) \rightarrow \pi^*(\text{C6-O7})$. The experimental UV-Visible absorption spectrum was good agreement within the BPTP theoretical one. The FMOs energy gap given in the compound exhibit the charge transfer in takes place in the compound. The molecular electrostatic potential map utilized to identify the nucleophilic and electrophilic attacks nature. The synthesized compound atomic theory was also been made with NBO and Milliken, MEP results and Fukui indices.

ACKNOWLEDGMENT

The authors are thankful to SAIF, IIT, and Madras for providing Spectral measurements.

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[RJC-5436/2019]