



ANTIMICROBIAL, SPECTROSCOPIC, NBO AND NLO ANALYSIS OF (2E)-3-(2H-1,3-BENZODIOXOL-5-YL)-N-(4-CHLOROPHENYL) PROP-2-ENAMIDE

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ABSTRACT

The title compound, (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-(4-chlorophenyl)prop-2-enamide (3B5NCE) was synthesized and characterized by FT-IR and FT-Raman spectral analysis. The optimized molecular geometry, the vibrational wavenumbers, the infrared intensities and the Raman scattering activities were calculated by using density functional theory(DFT) B3LYP method with 6-311++G(d,p) basis set. The detailed interpretation of the vibrational spectra has been carried out by VEDA program. Stability of the molecule arising from hyperconjugative interactions, charge delocalization have been analyzed using natural bond orbital analysis (NBO). The first order hyperpolarizability was also performed. The title compound was screened in vitro for antimicrobial activity against three bacterial and two fungal strains.

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INTRODUCTION

The synthesis of enamide derivatives has generated vast interest to organics as well as for medicinal chemistry, agricultural and many other industrial processes [1]. Enamides or enecarbamates are well-known versatile motifs in organic synthesis [2,3]. The  $\pi$ -donating ability of their nitrogen atom renders enamines more electron-rich [4] than simple enols or enol ethers, thereby predisposing them to electrophilic activation. However, enamines are highly sensitive toward hydrolysis, thereby creating serious difficulties in their experimental handling [5,6]. Enamides and enecarbamates that carry an electron-withdrawing group on the nitrogen were found to be ideal candidates. Indeed, enamides are commonly present in natural products and active drugs [7,8] demonstrating their high stability. Several enamide derivatives have proved the efficiency and efficacy in combating various diseases. Particularly, enamide derivatives of (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-(4-chlorophenyl)prop-2-enamide (3B5NCE) wide variety of biological activities such as antifungal, antibacterial, antituberculosis, antitumor, hypoglycemic, anti-inflammatory, analgesic and antipyretic activities [1].

Therefore it is important to analyze the characterization of the title compound for future studies.

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Considering these biological importance of (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-(4-chlorophenyl)prop-2-enamide, this work is mainly focused to the detailed structural behavior of the molecule. FT-IR and FT-Raman spectra of 3B5NCE have been reported together with the assignments of the vibrational modes supported by PED. The linear polarizability ( $\alpha$ ) and the first order hyperpolarizability ( $\beta$ ) values investigated molecule have been computed using DFT calculations. In addition, 3B5NCE has been screened for antimicrobial activity against bacteria such as Staphylococcus Aureus, Moraxella and Enterobacter as well as fungi such as Candida albicans and A.niger at four different concentrations 25, 50, 75 and 100  $\mu$ m/ml. Docking analysis has been performed to find out the binding affinity and drug activity of the molecule.

Synthesis

A mixture of equimolar (0.01) concentrations of 1.35 g of finely powdered N-phenylacetamide and 1.5 g 2H-1,3-benzodioxole-4-carbaldehyde were dissolve in minimum amount of ethanol (30ml) taken in a round bottom flask. Sufficient 2N NaOH solution was added to the above solution and continuous stirring for 4 hrs in ice cold condition till yellow precipitate was formed. This was then neutralized with 2N HCl and dilutes with water and left overnight. The precipitate chalcones were filtered and washed with water and recrystallised from ethanol. The reaction scheme is shown in Fig.1.

**Experimental**

The FT-IR spectrum of the synthesis compound (2E)-3-(1H-indol-2-yl)-N-phenylprop-2-enamide (2INP) was recorded in the region 4000-450  $\text{cm}^{-1}$  in evacuation mode using a KBr pellet technique with 1.0  $\text{cm}^{-1}$  resolution on a PERKIN ELMER FT-IR spectrophotometer. The FT-Raman spectrum of the 3B5NCE compound was recorded in the region 4000-100  $\text{cm}^{-1}$  in a pure mode using Nd: YAG Laser of 100 mW with 2  $\text{cm}^{-1}$  resolution on a BRUCKER RFS 27 at SAIF, IIT, Chennai, India.

**Computational details**

The entire calculations (vibrational wavenumbers, geometric parameters, and other molecular properties) were implemented by using GaussView 5.0 program [9] and Gaussian 09W

program package on a computing system [10]. The molecular structure of 2INP the ground state (in the gas phase) was optimized by DFT/B3LYP methods with 6-311++G(d,p) basis set level, and the optimized structure was used in the vibrational frequency calculations. The calculated harmonic vibrational frequencies were scaled by 0.961 [11]. Molecular docking (ligand-protein) simulations have been performed by using autoDock 4.2.6 free software package.

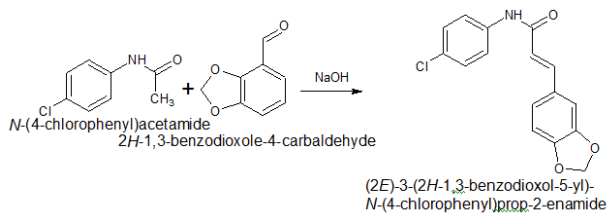
**RESULTS AND DISCUSSION****Molecular geometry**

The geometrical parameters (bond length and bond angles) of the synthesis 3B5NCE compound are listed in Table 1 using DFT/B3LYP method with 6-311++G(d,p) basis set.

**Table 1** Optimized geometrical parameters of (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-(4-chlorophenyl)prop-2-enamide (3B5NCE) obtain by B3LYP/6-311++G(d,p) basis set.

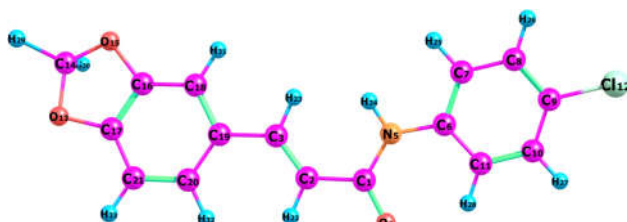
Parameters	Experimental <sup>a</sup>	B3LYP/ 6-311++G(d,p)	Parameters	Experimental <sup>a</sup>	B3LYP/ 6-311++G(d,p)
Bond length(Å)			Bond angle(°)		
C1-C2	1.493	1.486	C19-C3-H23	114.0	113.9
C1-O4	1.216	1.223	C3-C19-C18	117.7	117.8
C1-N5	1.363	1.382	C3-C19-C20	122.4	122.8
C2-C3	1.349	1.344	C6-N5-H24	116.0	115.0
C2-H22	0.960	1.084	N5-C6-C7	116.3	117.4
C3-C19	1.450	1.465	N5-C6-C11	124.7	123.6
C3-H23	0.960	1.089	C7-C6-C11	119.0	119.0
N5-C6	1.422	1.408	C6-C7-C8	120.5	121.0
N5-H24	0.860	1.008	C6-C7-H25	120.0	119.9
C6-C7	1.407	1.403	C6-C11-C10	119.9	119.8
C6-C11	1.407	1.402	C6-C11-H28	120.0	119.7
C7-C8	1.390	1.389	C8-C7-H25	119.0	119.1
C7-H25	0.960	1.086	C7-C8-C9	119.0	119.2
C8-C9	1.390	1.391	C7-C8-H26	120.0	120.4
C8-H26	0.960	1.082	C9-C8-H26	120.0	120.4
C9-C10	1.390	1.390	C8-C9-C10	120.6	120.5
C9-C112	1.493	1.760	C8-C9-C112	119.4	119.6
C10-C11	1.390	1.393	C10-C9-C112	119.9	119.8
C10-H27	0.960	1.083	C9-C10-C11	120.6	120.3
C11-H28	0.960	1.079	C9-C10-H27	120.0	120.0
O13-C14	1.296	1.436	C11-C10-H27	120.0	119.7
O13-C17	1.296	1.370	C10-C11-H28	120.0	120.4
C14-O15	1.216	1.433	C14-O13-C17	-	105.2
C14-H29	0.960	1.089	O13-C14-O15	-	107.2
C14-H30	0.960	1.097	O13-C14-H29	-	109.4
O15-C16	1.216	1.374	O13-C14-H30	-	109.2
C16-C17	1.393	1.390	O13-C17-C16	-	109.7
C16-C18	1.375	1.375	O13-C17-C21	121.2	128.7
C17-C21	1.385	1.381	O15-C14-H29	-	109.5
C18-C19	1.407	1.416	O15-C14-H30	-	109.4
C18-H31	0.960	1.083	C14-O15-C16	-	105.2
C19-C20	1.407	1.404	H29-C14-H30	110.0	111.9
C20-C21	1.397	1.398	O15-C16-C17	-	109.5
C20-H32	0.960	1.082	O15-C16-C18	121.2	128.5
C21-H33	0.960	1.082	C17-C16-C18	121.9	122.0
Bond angle(°)			C16-C17-C21	121.9	121.9
C2-C1-O4	121.2	120.6	C16-C18-C19	118.2	117.9
C2-C1-N5	116.3	115.9	C16-C18-H31	120.0	120.9
C1-C2-C3	125.7	126.2	C17-C21-C20	117.7	117.1
C1-C2-H22	114.0	112.1	C17-C21-H33	120.0	121.3
O4-C1-N5	124.0	123.5	C19-C18-H31	120.0	121.2
C1-N5-C6	128.4	128.9	C18-C19-C20	119.9	119.3
C1-N5-H24	116.3	115.8	C19-C20-C21	121.9	122.1
C3-C2-H22	120.0	121.5	C19-C20-H32	120.0	119.6
C2-C3-C19	125.7	127.6	C21-C20-H32	119.0	118.3
C2-C3-H23	119.0	118.5	C20-C21-H33	120.0	121.6

<sup>a</sup> Taken from Ref [16]



**Fig 1** The scheme of the synthesis of 3B5NCE

The optimized molecular structure of title compound is obtained from Gaussian 09W and GaussView 5.0 programs are shown in Fig. 2. To the best of our knowledge, exact experimental data on the geometrical parameters of 3B5NCE are not available in the literature. Therefore, the crystal data of a closely related molecule such as (E)-2-Cyano-3-[4-(dimethylamino)-phenyl]-N-phenylprop-2-enamide [12] is compared with that of the title compound.

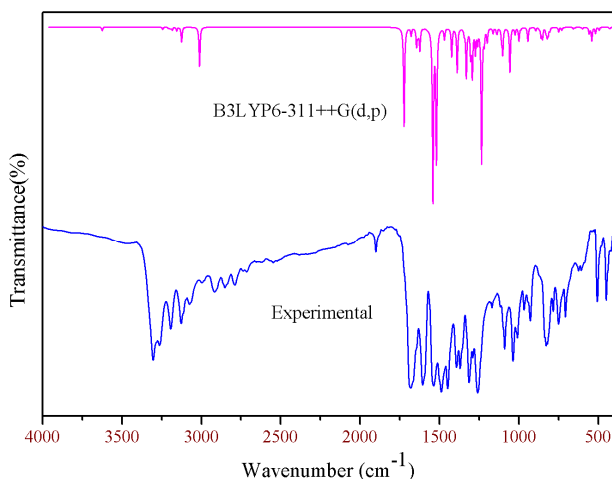


**Fig 2** Optimized geometric structure with atoms numbering of 3B5NCE

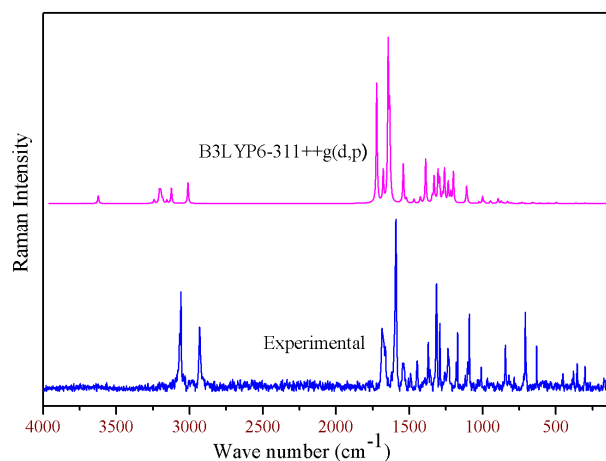
The theoretical calculations were carried out isolated molecule in the gaseous phase the experimental results are for a molecule in a solid state. This title molecule has sixteen C-C bond lengths, eleven C-H bond lengths, three O-C, two (C-O, N-C) bond lengths and one (N-H) bond lengths respectively. The highest bond length was calculated for C<sub>9</sub> – C<sub>12</sub>, C<sub>1</sub> – C<sub>2</sub> found to be 1.760 and 1.486 Å. The calculated bond length values for C-C and C-H in the benzene ring vary from 1.486-1.344 Å and 1.097-1.079 Å by B3LYP/6-311G(d,p) basis set. The C-C bond lengths are higher than the C-H bond lengths. The important reasons for the same charges are repulsive and opposite charges are attractive.

### Vibrational analysis

Vibrational spectroscopy is used extensively in organic chemistry for the identification of functional groups of organic compounds, the study of molecular confirmations, kinetics, reaction etc.



**Fig 3** FT- IR spectra of 3B5NCE (Experimental, B3LYP/6-311++G(d,p))



**Fig 4** FT-Raman spectra of 3B5NCE (Experimental, B3LYP/6-311++G(d,p))

The complete vibrational assignments of fundamental modes of 3B5NCE along with the PED are given in Table 2. The title molecule consists of 33 atoms, which has 93 normal modes of vibration. Potential energy distribution (PED) was computed for each normal mode among the symmetry coordinates of the molecule. Based on the computed PED values and FT-IR intensities and FT-Raman band activities a detailed assignment of the fundamentals was proposed. The calculated wavenumbers are scaled using the scaling factor 0.961. The comparative observed and simulated FT-IR and FT-Raman spectra are shown in Fig. 3 and 4. The calculated vibrational frequencies (Unscaled and Scaled), IR intensity, Raman activity are tabulated in Table 2.

### C-H vibrations

In the aromatic compounds, the C-H stretching wavenumbers appear in the range 3000-3100 cm<sup>-1</sup> which are the characteristic region for the ready identification of C-H stretching vibrations [13]. The C-H stretching and bending regions are of the most difficult regions to interpret in infrared spectra. The nature and position of the substituent cannot affect these vibrations. Most of the aromatic compounds have almost four infrared peaks in the region 3080-3010 cm<sup>-1</sup> due to ring C-H stretching bands [14]. In this present study, the C-H stretching vibrations are observed at 3117, 3076, 3069, 3067, 3059, 3032 and 3002 cm<sup>-1</sup> by B3LYP/6-311++G(d,P) method show good agreements with experimental vibrations. The bands observed in the recorded FT-IR spectrum 3127(s), 3074(m), 2998(m) cm<sup>-1</sup> and with the FT-Raman spectrum bands at 3118(s), 3069(vs), 3060(vs), 3045(s), 3031(s) cm<sup>-1</sup>. The PED corresponding to this pure mode of title molecule contributed 98, 96, 90, 96, 88, 97 and 99% is shown in Table 2.

### C-C ring vibrations

The C-C stretching vibrations are expected in the range from 1650 to 1100 cm<sup>-1</sup> which are not significantly influenced by the nature of the substituents [15]. The C-C stretching vibrations of the 3B5NCE compound were observed from 1625 to 910 cm<sup>-1</sup>. In this present study, the C-C stretching vibrations are found at 1606(vs), 1537(vs), 1489(vs), 1449(vs), 1393(vs), 1370(s), 1314(vs), 1260(vs), 1090(s), 928(s) cm<sup>-1</sup> in FT-IR and 1622(s), 1592(vs), 1540(s), 1493(s), 1448(s), 1393(m), 1360(s), 1257(s), 1237(s), 1180(s), 1119(s) cm<sup>-1</sup> in FT-Raman respectively.

**Table 2** Calculated vibrational frequencies (cm<sup>-1</sup>) assignments of 3B5NCE based on B3LYP/6-311++G(d,p) basis set.

Mode no	Experimental		Theoretical		I <sub>IR</sub> <sup>c</sup>	I <sub>RAMAN</sub> <sup>d</sup>	Assignments (PED) <sup>a,b</sup>
	wave number (cm <sup>-1</sup> )		wave number(cm <sup>-1</sup> )				
	FTIR	FT-RAMAN	Unscaled	scaled			
93	-	-	3624	3483	3	5	γNH(100)
92	3127(s)	3118(s)	3243	3117	2	3	γCH(98)
91	-	-	3207	3082	1	7	γCH(92)
90	3074(m)	-	3201	3076	0	5	γCH(96)
89	-	-	3197	3072	0	4	γCH(98)
88	-	3069(vs)	3193	3069	0	1	γCH(90)
87	-	3060(vs)	3191	3067	0	2	γCH(96)
86	-	3045(s)	3183	3059	2	2	γCH(-88)
85	-	3031(s)	3155	3032	3	2	γCH(97)
84	-	-	3125	3003	6	9	γCH(93)
83	2998(m)	-	3124	3002	4	2	γCH(99)
82	-	-	3012	2894	27	14	γCH(93)
81	1681(vs)	1663(vs)	1724	1656	68	79	γOC(72)
80	1606(vs)	1622(s)	1679	1614	6	21	γCC(59)
79	-	1592(vs)	1645	1581	12	100	γCC(64)
78	-	-	1639	1575	2	8	γCC(60)
77	-	-	1635	1571	4	54	γCC(-52)+βHCC(-17)
76	1537(vs)	1540(s)	1624	1561	15	3	γCC(58)+βHNC(-14)+βHCC(12)
75	1489(vs)	1493(s)	1542	1482	100	22	γCC(-11)+βHNC(-43)
74	-	-	1540	1480	22	5	βHCH(79)
73	-	-	1522	1463	28	2	βHCC(41)
72	1449(vs)	1448(s)	1520	1460	69	2	βHCC(-42)+γCC(13)
71	1393(vs)	1393(m)	1470	1412	8	2	βHCC(27)+γCC(29)
70	-	1372(s)	1427	1372	0	2	τHCO(77)
69	1370	1360(s)	1424	1368	20	3	βHCC(-32)+γCC(-45)
68	1314(vs)	-	1389	1335	30	29	γCC(-54)+βHCC(-12)
67	1291(vs)	1293(vs)	1345	1292	3	4	βHCC(57)+γCC(-10)
66	-	-	1332	1280	34	17	γCC(-42)+βHCC(24)
65	1260(vs)	-	1321	1270	2	2	γCC(28)+βHCC(49)
64	-	1257(s)	1305	1254	18	20	βHCC(25)+γCC(-13)
63	-	1237(s)	1294	1244	32	14	βHCC(-42)+γCC(-11)
62	-	-	1275	1225	16	5	γCC(30)+βHCC(15)
61	-	-	1261	1212	9	22	γCC(58)
60	-	1180(s)	1236	1187	93	14	γCC(-46)+βHCC(11)
59	1170(m)	1171(s)	1219	1172	9	7	βHCC(59)
58	-	-	1201	1155	0	2	βHCC(59)
57	-	-	1200	1153	9	19	βHCC(-33)
56	-	1119(s)	1163	1118	4	0	βHCC(38)+γCC(39)
55	-	1091(vs)	1142	1097	2	0	βHCO(90)
54	1090(s)	-	1138	1094	3	0	βHCC(-58)+γCC(27)
53	-	-	1110	1067	7	11	βHCC(-11)+γCC(21)
52	-	-	1103	1060	17	1	γCIC(-11)+βHCC(-13)+γCC(-56)
51	1038(vs)	1010(vs)	1057	1016	31	0	γOC(76)
50	-	-	1025	985	5	1	βHCC(69)+γCC(-18)
49	968(m)	968(m)	1001	962	9	5	τHCCO(-76)
48	-	-	988	950	1	1	γCC(52)
47	-	-	987	948	0	0	τHNCC(-77)
46	928(s)	-	948	911	0	1	γCC(-57)
45	-	-	944	907	9	1	γOC(69)+τHCCN(-89)
44	-	-	944	907	0	0	τHCCC(-84)
43	-	-	941	905	1	0	τHCCO(69)
42	-	-	895	860	2	3	βHNC(21)+τHCCO(-14)+γCC(28)
41	-	845(s)	873	839	1	2	τHCCO(62)
40	829(s)	821(s)	861	828	6	0	τHCCC(87)
39	-	-	852	819	7	0	βHCC(13)+γCC(56)
38	-	-	830	798	3	1	τHCCC(81)
37	-	-	823	791	6	0	τHCCN(-89)
36	784(m)	785(s)	816	784	5	0	βHCC(42)+γCC(15)
35	751(s)	-	806	774	2	0	βHCC(17)
34	-	719(s)	750	721	3	0	βHCC(55)
33	707(m)	709(vs)	731	702	2	1	τHCCC(58)
32	-	-	730	702	1	0	τHNCC(-80)
31	-	-	720	692	0	0	τHCCC(56)
30	-	-	708	680	0	0	βHCC(19)
29	625(m)	632(s)	658	632	1	1	βHCC(-79)
28	607(m)	-	647	622	1	0	τHCCC(-10)+βCCO(-50)
27	-	-	613	589	0	0	τHCCC(-56)
26	-	-	600	577	1	0	τHNCC(-10)
25	-	-	558	536	4	0	τHNCC(-58)
24	506(m)	-	542	521	9	0	τHNCC(78)

23	-	-	518	498	4	0	$\gamma$ CIC(-14)+ $\beta$ HCC(-43)
22	-	-	495	476	2	1	$\tau$ HCCC(48)+ $\beta$ HCC(19)
21	-	-	431	414	1	0	$\tau$ HCCC(25)+ $\beta$ HCC(-30)
20	-	-	426	410	1	0	$\tau$ HCCC(97)
19	-	-	421	405	0	0	$\beta$ HNC(55)
18	-	381(s)	394	379	2	0	$\tau$ HCCC(-71)
17	-	355(s)	363	349	1	0	$\tau$ HNCC(-26)+ $\beta$ HCC(12)
16	-	-	348	335	3	0	$\tau$ HNCC(54)
15	-	-	332	319	1	0	$\beta$ CCC(46)
14	-	301(s)	299	288	1	0	$\beta$ CNC(-49)+ $\tau$ HCCN(-14)+ $\beta$ HCC(-10)
13	-	-	269	259	0	0	$\tau$ HCCN(63)
12	-	-	251	241	0	0	$\tau$ HCCN(-66)
11	-	173(s)	202	194	0	0	$\tau$ CNCC(43)
10	-	-	165	159	0	0	$\beta$ HNC(43)+ $\tau$ HCCO(-16)
9	-	-	142	136	2	0	$\beta$ HCC(-14)
8	-	-	135	129	0	0	$\beta$ HNC(11)+ $\tau$ CNCC(-27)
7	-	-	126	122	2	0	$\tau$ HCOC(-79)
6	-	-	107	103	1	0	$\tau$ HCCO(39)
5	-	-	68	65	0	0	$\tau$ HCCO(-48)+ $\beta$ HCC(12)
4	-	-	47	45	0	0	$\tau$ HCCC(-48)+ $\tau$ HNCC(10)
3	-	-	31	30	0	0	$\tau$ HCCO(10)+ $\tau$ HNCC(20)+ $\beta$ HCC(25)
2	-	-	22	21	0	0	$\tau$ HNCC(-47)
1	-	-	15	14	0	0	$\tau$ CCCC(57)

<sup>a</sup> $\gamma$ -stretching,  $\beta$ - inplane bending,  $\omega$ - outplane bending,  $\tau$ -torsion, vs-very strong, s- strong, m-medium, w-weak.

<sup>b</sup>scaling factor : 0.961 for B3LYP/6-311+G(d,p)

<sup>c</sup>Relative absorption intensities normalized with highest peak absorption equal to 100.

<sup>d</sup>Relative Raman intensities normalized to 100.

The theoretical wavenumbers at 1614, 1581, 1561, 1482, 1460, 1412, 1368, 1335, 1270, 1254, 1244, 1187, 1118, 1094 and 911  $\text{cm}^{-1}$  are assigned as C-C stretching vibrations with PED contribution of 59, 64, 58, 22, 23, 29, 45, 54, 28, 23, 25, 46, 39, 27 and 57% respectively.

#### C-O vibration

The C-O stretching vibration occurs at 1627 (vs)  $\text{cm}^{-1}$  in FT-IR and 1626  $\text{cm}^{-1}$  in solid FT-Raman [16]. Normally, the C-O stretching vibrations occur in the region 1260-1000  $\text{cm}^{-1}$  [17]. The C-C stretching vibrations of the 3B5NCE compound were observed from 1660 to 1010  $\text{cm}^{-1}$ . In this present study, the C-C stretching vibrations are found at 1681(vs), 1038(vs)  $\text{cm}^{-1}$  in FT-IR and 1663(vs), 1010(vs)  $\text{cm}^{-1}$  in FT-Raman. The theoretical wavenumbers at 1656, 1016  $\text{cm}^{-1}$  are assigned as C-C stretching vibrations with PED contributions of 72, 76%.

#### Hyperpolarizability calculation

NLO is at the future of current research because it provides the key functions of frequency shifting, optical modulation, optical switching, optical logic, and optical memory for the emerging technologies in areas such as telecommunications, signal processing, and optical interconnections [18,19].

In discussing NLO properties, the polarization of the molecule by an external radiation field is often approximated as the creation of an induced dipole moment by an external electric field. The first hyperpolarizability ( $\beta_0$ ) of this molecular system is calculated using B3LYP/6-311++G (d,p) method, based on the finite field approach.

Urea is the prototypical molecule utilized in investigating of the NLO properties of the compound. For this reason, urea was used often as a threshold value for comparative purpose. The calculated dipole moment and hyperpolarizability values obtained from B3LYP/6-311++G(d,p) methods are collected in Table 3. The first order hyperpolarizability of 3B5NCE with B3LYP/6-311++G(d,p) basis set is  $16.4610 \times 10^{-30}$  twenty six times greater than the value of urea ( $\beta_0 = 0.6230 \times 10^{-30}$  esu).

**Table 3** The values of calculated dipole moment  $\mu$  (D), polarizability ( $\alpha_0$ ), first order hyperpolarizability ( $\beta_{\text{tot}}$ ) components of 3B5NCE

Parameters	B3LYP/6-311++G(d,p)	Parameters	B3LYP/6-311++G(d,p)
$\mu_x$	-2.1850	$\beta_{xxx}$	1652.1517
$\mu_y$	-1.1096	$\beta_{xxy}$	1089.3198
$\mu_z$	-0.2932	$\beta_{xyy}$	-136.6774
$\mu$ (D)	2.4681	$\beta_{yyy}$	84.7987
$\alpha_{xx}$	417.1405	$\beta_{zxx}$	166.0636
$\alpha_{xy}$	7.6179	$\beta_{xyz}$	-19.8863
$\alpha_{yy}$	208.9670	$\beta_{zyy}$	-5.6903
$\alpha_{xz}$	4.6006	$\beta_{nzz}$	-25.7611
$\alpha_{yz}$	3.8657	$\beta_{yzz}$	-2.4566
$\alpha_{zz}$	124.3771	$\beta_{zzz}$	35.5808
$\alpha_0$ (e.s.u)	$3.7074 \times 10^{-23}$	$\beta_{\text{tot}}$ (e.s.u)	$16.4610 \times 10^{-30}$
$\Delta\alpha$ (e.s.u)	$11.3850 \times 10^{-23}$		

From the computation, the high values of the hyperpolarizabilities of 3B5NCE are probably attributed to the charge transfer existing amid the benzene rings within the molecular skeleton. This is evidence for the nonlinear optical (NLO) property of the molecule.

#### Donor- acceptor interactions

The second order fock matrix was carried out to investigate the donor-acceptor interactions in the NBO analysis [20]. NBO analysis has been carried out on the (2E)-3-(2H-1,3-benzodioxol-5-yl)-N-(4-chlorophenyl)prop-2-enamide at the B3LYP/6-311++G(d,p) level in order to elucidate the intra molecular, rehybridization and delocalization of electron density within the molecule. The higher the E(2) value, the molecular interaction between electron donors and electron acceptors is more intensive and the greater the extent of conjugation of the entire system. Delocalization of electron density amid occupied Lewis-type (bond or lone pair) NBO orbitals and properly unoccupied (antibond or Rydberg) non-Lewis NBO orbitals resemble to a stabilizing donor-acceptor interaction.

**Table 4** Second order perturbation theory analysis of Fock matrix in NBO basis for 3B5NCE

Donor(i)	Type	ED/e	Acceptor(i)	Type	ED/e	<sup>a</sup> E(2) (KJ mol <sup>-1</sup> )	<sup>b</sup> E(J)-E(i) (a.u.)	<sup>c</sup> F(I,j) (a.u.)			
C1-C2	$\sigma$	1.97224	C1-O4	$\sigma^*$	0.021	4.050	1.380	0.067			
			C1-N5	$\sigma^*$	0.067	4.550	1.350	0.071			
			C2-C3	$\sigma^*$	0.021	4.850	1.370	0.073			
C1-O4	$\sigma$	1.98732	C1-C2	$\sigma^*$	0.041	4.280	1.660	0.076			
C1-O4	$\pi$	1.95749	C2-C3	$\pi^*$	0.169	7.910	0.410	0.052			
			C11-H28	$\sigma^*$	0.060	3.930	0.480	0.039			
			O15-C16	$\sigma^*$	0.025	2.360	0.610	0.034			
			C16-C18	$\pi^*$	0.395	3.950	0.200	0.028			
C1-N5	$\sigma$	1.98004	C9-C10	$\sigma^*$	0.035	12.660	2.550	0.161			
C2-C3	$\pi$	1.82051	C1-O4	$\pi^*$	0.413	29.530	0.300	0.090			
C3-H23	$\sigma$	1.96754	C2-H22	$\sigma^*$	0.020	5.030	1.010	0.064			
N5-H24	$\sigma$	1.97771	C1-O4	$\sigma^*$	0.021	5.190	1.310	0.074			
			C20-C21	$\sigma^*$	0.015	9.260	1.390	0.101			
			C21-H33	$\sigma^*$	0.018	7.030	1.020	0.076			
C6-C7	$\sigma$	1.96274	C6-C11	$\sigma^*$	0.034	10.390	1.780	0.122			
			C7-C8	$\sigma^*$	0.020	6.890	1.760	0.099			
			C9-C10	$\sigma^*$	0.035	8.620	1.740	0.110			
C6-C7	$\pi$	1.64127	C8-C9	$\pi^*$	0.419	28.620	0.300	0.084			
			C10-C11	$\pi^*$	0.309	19.910	0.340	0.074			
			N5-C6	$\sigma^*$	0.035	5.400	1.340	0.076			
C6-C11	$\sigma$	1.95236	N5-H24	$\sigma^*$	0.041	5.390	1.010	0.066			
			C6-C7	$\sigma^*$	0.030	8.540	1.370	0.097			
			C8-C9	$\sigma^*$	0.033	6.470	1.370	0.084			
C7-C8	$\sigma$	1.96397	C11-H28	$\sigma^*$	0.060	54.820	0.690	0.175			
C7-H25	$\sigma$	1.97561	O15-C16	$\sigma^*$	0.025	32.630	0.820	0.146			
			C16-C18	$\pi^*$	0.395	32.070	0.410	0.113			
			C6-C7	$\pi^*$	0.432	18.840	0.300	0.070			
C8-C9	$\pi$	1.68466	C10-C11	$\pi^*$	0.309	21.010	0.340	0.075			
			C6-C7	$\pi^*$	0.432	27.220	0.270	0.079			
			C8-C9	$\pi^*$	0.419	23.570	0.270	0.073			
O13-C14	$\sigma$	1.98671	C20-C21	$\sigma^*$	0.015	12.780	1.670	0.130			
C14-H29	$\sigma$	1.99096	C21-H33	$\sigma^*$	0.018	12.550	1.300	0.114			
			C9-C10	$\sigma^*$	0.035	10.890	2.070	0.135			
			C20-C21	$\sigma^*$	0.015	14.360	1.280	0.121			
C14-H30	$\sigma$	1.99127	C21-H33	$\sigma^*$	0.018	8.900	0.920	0.081			
			O15-C16	$\sigma^*$	0.025	20.940	1.050	0.133			
			C17-C21	$\sigma^*$	0.030	14.330	1.360	0.125			
C16-C17	$\sigma$	1.96337	C20-C21	$\sigma^*$	0.015	8.750	1.020	0.091			
			C21-H33	$\sigma^*$	0.018	6.790	0.650	0.064			
			C18-C19	$\sigma^*$	0.029	11.870	0.770	0.085			
C16-C18	$\pi$	1.68488	C20-C21	$\sigma^*$	0.015	13.010	1.250	0.114			
			C21-H33	$\sigma^*$	0.018	17.310	0.870	0.110			
			C18-C19	$\sigma^*$	0.029	11.870	0.770	0.085			
C18-H31	$\sigma$	1.97589	C20-C21	$\sigma^*$	0.015	13.010	1.250	0.114			
			C9-C10	$\sigma^*$	0.035	17.310	0.870	0.110			
			C1-N5	$\sigma^*$	0.067	4.590	1.240	0.068			
C21-H33	$\sigma$	1.9754	C11-H28	$\sigma^*$	0.060	22.920	0.730	0.116			
			O4	LP(1)	1.95265	C1-C2	$\sigma^*$	0.041	14.750	0.900	0.105
			O4	LP(2)	1.88183	C1-N5	$\sigma^*$	0.067	16.070	0.910	0.109
O4	LP(1)	1.61559	C11-H28	$\sigma^*$	0.060	43.120	0.400	0.119			
			C1-O4	$\pi^*$	0.413	86.120	0.300	0.144			
			C2-C3	$\pi^*$	0.169	0.630	0.310	0.013			
C112	LP(1)	1.99199	C6-C7	$\pi^*$	0.432	54.610	0.310	0.118			
			C20-C21	$\sigma^*$	0.015	16.720	1.630	0.148			
			C21-H33	$\sigma^*$	0.018	8.710	1.270	0.094			
C112	LP(2)	1.97339	C8-C9	$\sigma^*$	0.033	4.370	0.950	0.058			
			C9-C10	$\sigma^*$	0.035	4.460	0.940	0.058			
			C8-C9	$\pi^*$	0.419	13.020	0.340	0.066			
C112	LP(3)	1.93307	C11-H28	$\sigma^*$	0.060	11.550	0.690	0.080			
			O13	LP(1)	1.94583	O15-C16	$\sigma^*$	0.025	8.200	0.830	0.074
			O13	LP(2)	1.80261	C14-H29	$\sigma^*$	0.033	5.400	0.690	0.057
O13	LP(1)	1.94583	C17-C21	$\pi^*$	0.417	46.200	0.340	0.119			
			O15	LP(2)	1.81525	C16-C18	$\pi^*$	0.395	91.190	0.190	0.125
			O15	LP(2)	1.81525	C16-C18	$\pi^*$	0.395	91.190	0.190	0.125

The strong intramolecular hyper conjugative interaction of the  $\sigma$  and  $\pi$  electrons of C-C to the anti C - C bond of the ring leads to stabilization and evidence of some part of ring values are listed in Table 4. The strong intramolecular hyperconjugative interaction of  $\sigma$  (C<sub>6</sub>-C<sub>7</sub>) distributes to  $\sigma^*$  (C<sub>6</sub> - C<sub>11</sub>, C<sub>7</sub> - C<sub>8</sub> and C<sub>9</sub> - C<sub>10</sub>) of the ring. On the other hand, side the  $\pi$  C<sub>6</sub>- C<sub>7</sub> in the ring conjugate to the anti-bonding orbital of  $\pi^*$ (C<sub>8</sub> - C<sub>9</sub>) and  $\pi^*$ (C<sub>10</sub> - C<sub>11</sub>) which leads to strong delocalization of 28.620 and 19.91 kJ/mol respectively. Some important second order perturbation energies and molecular orbital interactions investigated from the NBO calculation are

between Lewis and non-Lewis orbital with Oxygen and nitrogen lone pairs. The very significant interaction between them was the electron donation of LP(2) O<sub>4</sub>, LP(1) N<sub>5</sub>, LP(1) Cl<sub>12</sub>, LP (2) O<sub>13</sub> and O<sub>15</sub> to the neighbouring antibonding acceptor  $\sigma^*$ (C<sub>1</sub>-C<sub>2</sub>),  $\sigma^*$ (C<sub>1</sub>-N<sub>5</sub>),  $\sigma^*$ (C<sub>11</sub>-H<sub>28</sub>),  $\pi^*$ (C<sub>1</sub>-O<sub>4</sub>),  $\pi^*$ (C<sub>20</sub>-C<sub>21</sub>),  $\sigma^*$ (N<sub>1</sub>-C<sub>3</sub>),  $\pi^*$ (C<sub>17</sub>-C<sub>21</sub>) and  $\pi^*$ (C<sub>16</sub>-C<sub>18</sub>) of the 3B5NCE energy by 14.75, 16.07, 43.12, 86.12, 16.71, 46.20 and 91.19 kJ/mol.

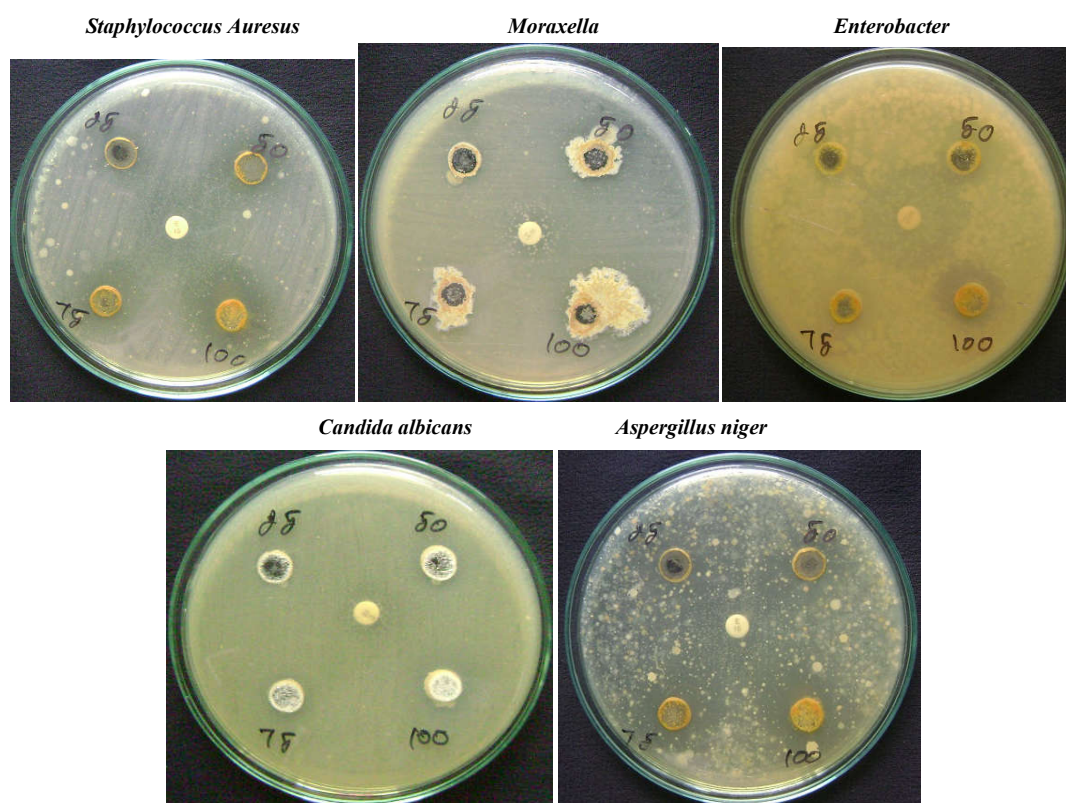


Fig 5 Antibacterial activity and antifungal activity of title molecule

#### Antimicrobial activity

The title compound was screened for its antimicrobial activity against bacterial and fungal strains by Kirby–Bauer agar well diffusion method [21]. The activity was determined by measuring the inhibition zone diameter values (mm) of the investigated compound and antimicrobial activity of 3B5NCE against bacterial and fungal pathogens are shown in Fig. 5. The antimicrobial and solvent sensitivity tests for both bacterial and fungal strains were observed and listed in Table 5 respectively.

Table 5 Antimicrobial activity of 3B5NCE

S. No.	Organisms	Zone of inhibition (mm/ $\mu$ L)				Control
		25 $\mu$ L	50 $\mu$ L	75 $\mu$ L	100 $\mu$ L	
1	Bacterial Strain <i>Staphylococcus Aureus</i>	16	20	25	32	25
2	<i>Moraxella</i>	14	18	24	29	30
3	<i>Enterobacter</i>	17	21	23	26	17
4	Fungi <i>Candida albicans</i>	15	19	21	25	24
5	Strain <i>A.niger</i>	13	17	21	24	12

It is noted that the DMSO solvent, it has no activity on the microbes. 3B5NCE dissolved at four concentrations ( 25, 50, 75 and 100  $\mu$ L) were screened for their antibacterial activity against three bacterial strains such as, *Staphylococcus Aureus*, *Moraxella* and *Enterobacter* and two fungal strains such as, *Candida albicans* and *A.niger* which were selected for the present investigation by the agar well diffusion method. From Tables 5 shows a good activity of 3B5NCE against the three bacterial strains *Staphylococcus Aureus*, *Moraxella* and *Enterobacter* and the two fungal strains *Candida albicans* and *A.niger*.

#### CONCLUSION

In the present work, we have thoroughly analyzed spectroscopic (FT-IR, FT-Raman), NLO and NBO analysis of 3B5NCE molecule with B3LYP/6-311++G(d,p) methods. The structural parameters, vibrational frequencies, infrared intensities and Raman activities calculated by B3LYP/6-311++G(d,p) method agree very well with experimental results. The complete vibrational assignments of wave numbers are made on the basis of potential energy distribution (PED). The nonlinear optical properties are also addressed theoretically. The first order hyperpolarizability of the title compound is twenty six times greater than the value of urea. Furthermore, antimicrobial studies of the title molecule show that a molecule is an attractive object for the future studies of biological activity.

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