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Synthesis, spectroscopic, NLO, HOMO-LUMO, antimicrobial analysis of (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl) prop-2-en-1-one

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Abstract

The title compound of (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl)prop-2-en-1-one have been synthesized and characterized by spectroscopic techniques. Density functional theory calculations at B3LYP/6-31+G(d) level of theory were performed for geometric parameters, NLO activity and frontier molecular orbital analyses of synthesized compounds. Frontier molecular orbitals (FMOs) investigation of synthesized molecule was performed for evaluation of kinetic stability. The dipole moment and first hyperpolarizabilities of the studied compounds indicate that the compound is a good candidate of nonlinear optical materials. 34FIPO compounds were screened in vitro for antimicrobial activity against three bacterial and three fungal strains and showed promising results.

Keywords: DFT, FT-IR, FT-Raman, NLO, antimicrobial

1. Introduction

Imidazole is a highly polar one of the five membered nitrogen containing heterocyclic ring. It is soluble in water. The nitrogen attached with the hydrogen has a lone pair of electrons bringing the required 6 π-electrons for aromatic city. The hydrogen atom can be located on either of the two nitrogen atoms due to resonance structures of imidazole [1]. Many researchers previously proved Imidazoles and Imidazoles substituent's compounds wide range biological applications. The biological activity of the compounds mainly depends upon the starting material and mechanism is well-studied at the molecular level [2]. Particularly, Imidazoles and Imidazoles derivatives of (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl)prop-2-en-1-one (34FIPO) extensive range of biological behaviors such as building blocks, anti-parasitic, anti-tumoral, antihistaminic, antihypertensive, anti-cancer [3-5], antibacterial, antifungal [6, 7]. Its molecular formula is $C_{12}H_9FN_2O$.

Based on above consideration and in continuation of our ongoing work on the development of imidazole analogues as antimicrobial agents, we report here the synthesis of (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl)prop-2-en-1-one with anticipated antimicrobial activities, by clubbing imidazole with fluorophenyl groups as spacers in one frame work. The title compound has been theoretically investigated by applying density functional theory (DFT) to understand the structure activity relationship.

2. Materials and methods

2.1 Synthesis

The equimolar quantity of 1-acetyl imidazole (0.01 mol) and 4-Fluorobenzaldehyde (0.01 mol) were dissolved in 20 ml of ethanol in a 150 mL round-bottomed flask. The reaction mixture was magnetically stirred for 3h in ice-cold condition, during stirring 10 ml of 10% sodium hydroxide solution was added dropwise. A flocculants precipitate was formed. The precipitate was filtered and washed with cold water. The solid obtained was purified by column chromatography using silica gel 60-120 mesh and n-hexane: acetone (7:3 v/v) as elevate. The reaction scheme is shown in Fig.1.

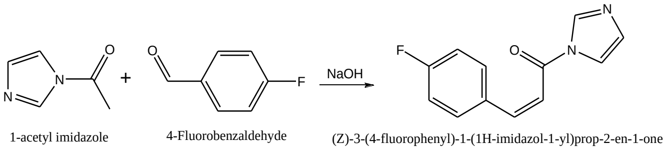

Fig 1: The scheme of the synthesis of 34FIPO

2.2 Experimental and Computational details

The experimental FT-Raman and FT-IR spectrum of the title compound were collected from Indian Institute of Technology Madras, Chennai, India. All the quantum chemical calculations are performed by Gaussian 09W [8] software with GaussView 5.0 [9] visualization program.

3. Results & Discussion

3.1 Molecular geometry

The geometrical parameters of bond lengths and bond angles are calculated using DFT/B3LYP method with 6-311++G (d,p) higher basis set and atom numbering of title molecule is shown in Fig 2. The theoretical results are compared with related molecule such as (Z)-3-(9-Anthryl)-1-(4-

chlorophenyl)-2-(4-nitro-1H-imidazol-1-yl) prop-2-en-1-one [10]. The four types of bond lengths (C-C, C-N, C-H and C-O) presented in title molecule and these values are listed in Table 1. From table 1 shows the calculated and experimental results are very good agreement. So the title molecule optimized successfully.

3.2 Vibrational analysis

Vibrational spectroscopy is very powerful tool for investigations of organic chemistry. It has been illustrious that the molecular functional groups of molecules. The Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl)prop-2-en-1-one (34FIPO) molecule consists of 25 atoms, which has 69 normal modes of vibration. The comparative observed and simulated FT-IR and FT-Raman spectra are shown in Fig. 3 and 4. IR intensity, Raman activity, Unscaled and Scaled frequencies are tabulated in Table 2.

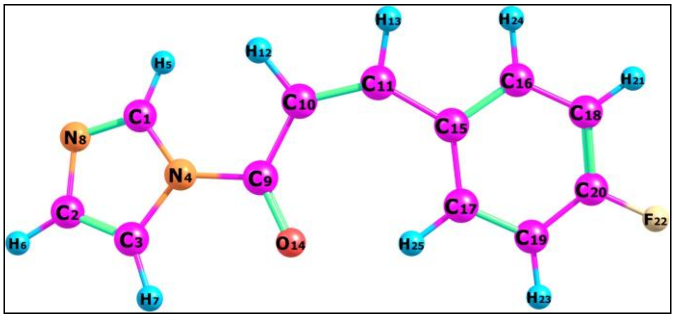

Fig 2: The theoretical optimized geometric structure with atoms numbering of 34FIPO

Table 1: Optimized geometrical parameters of (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl)prop-2-en-1-one (34FIPO) obtain by B3LYP/6-311++G (d,p) basis set.

Parameters	Experimental^a	B3LYP/ 6-311++G(d,p)	Parameter	Experimental^a	B3LYP/ 6-311++G(d,p)
Bond length(Å)			Bond angle(°)		
C1-N4	1.369	1.391	N4-C1-H5	127.9	122.8
C1-H5	0.930	1.077	N4-C1-N8	112.2	112.0
C1-N8	1.305	1.301	C1-N4-C3	106.9	105.8
C2-C3	1.357	1.361	C1-N4-C9	128.0	130.8
C2-H6	0.930	1.079	H5-C1-N8	123.9	125.1
C2-N8	1.369	1.387	C1-N8-C2	106.9	105.6
C3-N4	1.369	1.392	C3-C2-H6	127.9	128.1
C3-H7	0.930	1.075	C3-C2-N8	112.8	110.8
N4-C9	1.431	1.428	C2-C3-N4	104.2	105.8
C9-C10	1.477	1.466	C2-C3-H7	127.9	133.3
C9-O14	1.216	1.215	H6-C2-N8	123.9	121.2
C10-C11	1.355	1.357	N4-C3-H7	123.9	120.9
C10-H12	0.930	1.082	C3-N4-C9	125.0	123.4
C11-H13	0.930	1.088	N4-C9-C10	116.1	115.0
C11-C15	1.488	1.460	N4-C9-O14		118.1
C15-C16	1.415	1.412	C10-C9-O14	120.9	126.9
C15-C17	1.415	1.410	C9-C10-C11	129.3	130.4
C16-C18	1.389	1.387	C9-C10-H12	115.3	114.9
C16-H24	0.930	1.085	C11-C10-H12	115.3	114.7
C17-C19	1.389	1.389	C10-C11-H13	115.3	112.2
C17-H25	0.930	1.079	C10-C11-C15	129.3	136.7
C18-C20	1.385	1.387	H13-C11-C15	115.3	111.1
C18-H21	0.930	1.083	C11-C15-C16	117.7	115.9
C19-C20	1.385	1.387	C11-C15-C17	129.3	126.3
C19-H23	0.930	1.083	C16-C15-C17	117.7	117.8
C20-F22		1.350	C15-C16-C18	121.9	121.9
			C15-C16-H24	119.7	119.3
			C15-C17-C19	120.8	120.8
			C15-C17-H25	119.7	119.4
			C18-C16-H24	118.8	118.8
			C16-C18-C20	118.1	118.1
			C16-C18-H21	120.5	121.9
			C19-C17-H25	119.7	119.8
			C17-C19-C20	119.2	119.1
			C17-C19-H23	120.7	121.2
			C20-C18-H21	120.5	120.1
			C18-C20-C19	122.4	122.2
			C18-C20-F22		118.8
			C20-C19-H23	119.7	119.7
			C19-C20-F22		119.0

^{a}Taken from Ref [10]

3.2.1 C-H vibrations

In the heterocyclic compounds, the C-H stretching wavenumbers appear in the range 3000-3100 cm^{-1} [11]. In this present study, the C-H stretching vibrations are observed at 3168, 3138, 3080 and 3004 cm^{-1} by B3LYP/6-311++G(d,p) method show good agreements with experimental vibrations. The bands observed in the recorded FT-Raman spectrum 3185(w), 3118(w), 3097(m) and 3000(w) cm^{-1}. The PED corresponding to this pure mode of title molecule contributed 95, 97, 95 and 97 % is shown in Table 2.

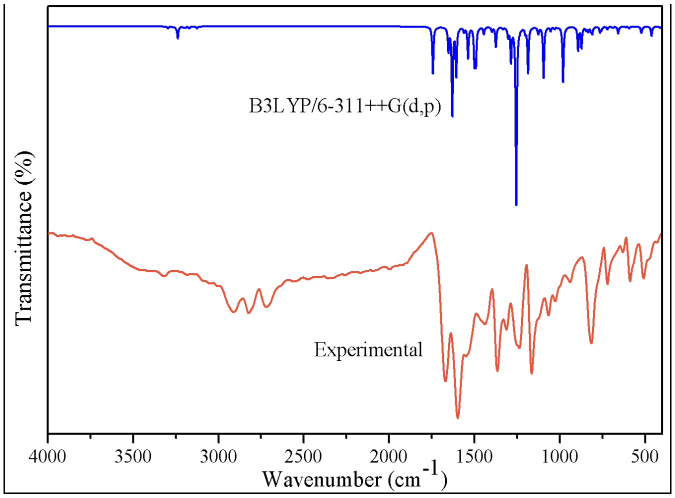

Fig 3: Experimental and theoretical FT-IR spectra of 34FIPO

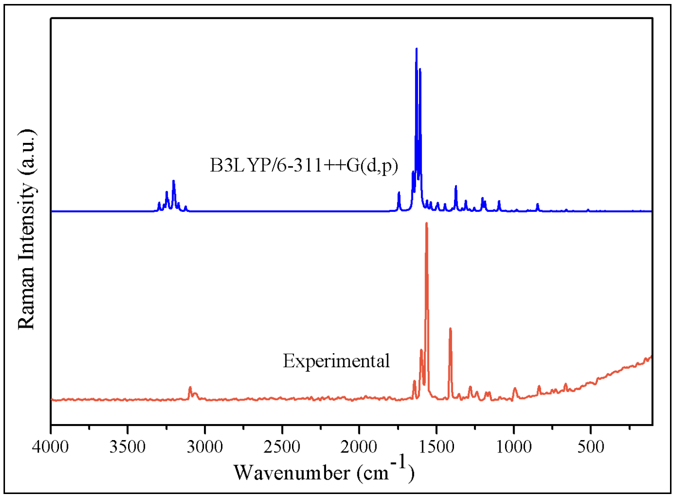

Fig 4: Experimental and theoretical FT-Raman spectra of 34FIPO

3.2.2 C-C ring vibrations

The C-C stretching vibrations are expected in the range from 1650 to 1100 cm^{-1} which are not significantly influenced by the nature of the substituents [12]. The C-C stretching vibrations of the 34FIPO compound were observed from1600 to 810 cm^{-1}. In this present study, the C-C stretching vibrations are found at 1598(vs), 1561(s), 1165(s), 1067(m), 816(s) cm^{-1} in FT-IR and 1599(s), 1564(vs), 1159(w), 1092(w), 993(w), 815(m) cm^{-1} in FT-Raman respectively. The theoretical wavenumbers at 1588, 1566, 1155, 1087, 991, 942 and 812 cm^{-1} are assigned as C-C stretching vibrations with PED contribution of 57, 59, 38, 14, 11, 29 and 51% respectively.

Table 2: Calculated vibrational frequencies (cm-1) assignments of 34FIPO based on B3LYP/6-311++G(d,p) basis set.

Mode no	Experimental wave number (cm^{-1})		Theoretical wave number(cm^{-1})		I_{IR} ^{c}	I_{RAMAN}^{d}	Assignments (PED)^{a,b}
	FTIR	FT-RAMAN	Unscaled	scaled			
69	-	3185(w)	3296	3168	1	5	γ CH (95)
68	-	-	3266	3138	0	4	γ CH (97)
67	-	3118(w)	3248	3121	1	12	γ CH (95)
66	-	-	3238	3111	7	5	γ CH (98)
65	-	3097(m)	3205	3080	0	15	γ CH (95)
64	-	-	3200	3075	0	9	γ CH (98)
63	-	-	3194	3070	1	6	γ CH (95)
62	-	-	3171	3048	1	5	γ CH (94)
61	-	3000(w)	3125	3004	1	3	γ CH (97)
60	1671(vs)	1644(m)	1743	1675	27	12	γ OC (78)
59	1598(vs)	1599(s)	1652	1588	14	22	γ CC (57)
58	1561(s)	1564(vs)	1630	1566	51	100	γ CC (59)+ β HCC(-13)
57	-	-	1606	1544	28	87	γ CC (69)
56	-	-	1562	1501	3	6	γ CC (72)+ β HCC(15)
55	-	-	1537	1477	18	6	β HCC(42)+ γ CC(19)
54	1440(s)	-	1500	1441	21	3	β HCN(11)+ β HCC(11)
53	-	1410(s)	1491	1433	20	5	β HCC(51)
52	-	-	1445	1389	4	5	γ CC(40)+ β HCC(28)
51	-	-	1398	1344	3	2	γ CC(45)
50	1312(s)	-	1374	1321	12	16	β HCC(28)+ γ CC (12)
49	-	1282(m)	1334	1282	1	2	β HCC(49)+ γ CC (27)
48	-	-	1310	1259	0	7	γ NC (41)
47	-	-	1303	1252	5	0	γ CC(40)
46	1238(s)	1240(m)	1286	1236	20	1	β HCN(64)
45	-	-	1256	1207	4	2	γ CC(31)
44	-		1255	1206	100	1	γ NC (29)+ β HCN(12)

43	1165(s)	1159(w)	1202	1155	3	8	β HCC (22)+ γ CC(38)
42	-		1186	1140	27	6	β HCC(54)
41	1067(m)	1092(w)	1131	1087	1	0	γ CC(14)+ β HCC(53)
40	-		1125	1082	4	1	γ NC (61)
39	1027(m)	1061(w)	1095	1052	30	7	β HCC(24)+ β HCN (14)
38	-	1025(w)	1054	1013	2	1	β HCN (04)+ β HCC(5)
37	-	993(w)	1031	991	1	0	β HCC(68)+ γ CC(11)
36	-	-	1013	974	0	0	τ HCCH(10)+ τ HCCN (31)
35	-	-	1012	972	0	0	τ HCCH(83)
34	940(m)	-	981	942	32	1	γ CC(29)+ β HCN(34)
33	-	900(w)	961	924	0	0	τ HCCH (82)
32	-	-	909	873	0	1	γ NC(10)+ β HCN (70)
31	-	-	893	858	13	0	β HCC(36)+ β HCN (11)
30	-	-	891	856	0	0	τ HCCH(82)
29	-	836(m)	873	839	12	0	τ HCCC(81)
28	816(s)	815(m)	845	812	2	5	γ CC(51)+ β HCC(10)
27	-	-	833	801	3	0	τ HCCN(81)
26	-	786(m)	817	785	2	0	τ HCNC(56)
25	-	-	809	778	4	0	τ HCNC(69)
24	-	751(m)	765	735	3	0	τ HCCH(13)+ τ HCNC(81)
23	721(m)	730(m)	757	727	2	0	τ HCCN(73)
22	-	-	722	694	2	0	β HCC(16)+ γ CC(34)
21	-	664(m)	690	663	1	0	τ HCCN(63)
20	-	-	659	634	1	1	β HCC(62)
19	631(w)	637(m)	658	632	3	0	τ HCCN(10)+ τ HCNC(55)
18	589(m)	595(m)	615	591	0	0	τ HCNC(53)
17	-	-	594	571	1	0	γ CC(14)
16	510(m)	505(s)	523	503	3	0	τ HCCO(42)
15	-	-	519	499	1	1	γ NC(11)+ β CNC(26)
14	-	451(s)	463	445	5	0	β HCC(49)
13	-	-	439	422	0	0	τ HCNC(10)+ τ HCCO(52)
12	-	-	413	397	1	0	β CCF(75)
11	-	391(s)	409	393	0	0	τ HCCO(54)
10	-	290(s)	321	309	3	0	β HCC(15)+ β CNC(6)
9	-	-	290	279	0	0	τ HCCN(15)+ τ HCNC(13)
8	-	200(s)	229	220	1	0	β HCNC(23)+ β CNC(10)
7	-	-	178	171	0	0	β HCC(19)+ τ HCNC(21)
6	-	145(s)	156	150	0	0	τ HCNC(47)
5	-	-	121	116	0	0	β HCC(26)+ τ HCNC(23)+ τ HCCC(10)
4	-	-	94	91	0	0	β HCC(31)+ β CNC(16)
3	-	-	66	64	0	0	β HCC(10)+ τ HCCC(32)
2	-	-	37	36	0	0	τ HCCC(71)
1	-	-	15	14	0	0	τ HCCC(11)+ τ HCCN(44)

[a]γ-stretching, β- bending, τ-torsion, vs-very strong, s- strong, m-medium, w-weak, vw-very weak.

[b]scaling factor: 0.961 for B3LYP/6-311+G(d,p)

[c]Relative absorption intensities normalized with highest peak absorption equal to 100.

[d]Relative Raman intensities normalized to 100.

3.2.2 C-O vibrations

The C-O stretching vibration occurs at 1627 (vs) cm^{-1} in FT-IR and 1626 cm^{-1} in solid FT-Raman [13]. The C-C stretching vibrations of the 34FIPO compound were observed from1675 to 1640 cm^{-1}. In this present study, the C-C stretching vibration is found at 1671(vs) cm^{-1} in FT-IR and 1644(m) cm^{-1} in FT-Raman. The theoretical wavenumber at 1675 cm^{-1} are assigned as C-C stretching vibration with PED contribution of 78%.

3.3 Electronic property

The ground state (HOMO) and first order exited state energy (LUMO) is calculated using same basis set. The HOMO-LUMO energies are clearly explained in molecular structural activity. So, many researchers interest to investigate structural activities in recent years. The electronic properties are precisely reported in many researchers in various organic compounds [14, 15]. The HOMO-LUMO energies and other related properties of energy gap, ionization potential (I), the electron affinity (A), the absolute electronegativity (χ), the absolute hardness (η) and softness (S) for the 34FIPO molecule have been calculated and values are given in table 3. The molecular energy transfer of 34FIPO compound is shown in Fig 5. HOMO and LUMO energy values for a molecule, electronegativity and chemical hardness can be calculated as follow:

$\chi = (I+A)/2$ (Electronegativity) (1)

$\mu = -((I+A))/2$ (Chemical potential) (2)

$\eta = (I-A)/2$ (Chemical hardness) (3)

$s=1/2\eta$ (chemical softness) (4)

$\omega=\mu2/2\eta$ (Electrophilicity index) (5)

Where I and A are ionization potential and electron affinity; I= - EHOMO and A= - ELUMO respectively. The ground state (LUMO) energy is -2.2014 eV and the first exited state (HOMO) energy is -5.9351eV. The ground state and first exited state energy gap of 34FIPO is found to be 3.7337 eV. Hence, the energy gap of title compound 34FIPO is low. This energy gap is elucidate the eventual charge transfer occur within the molecule.

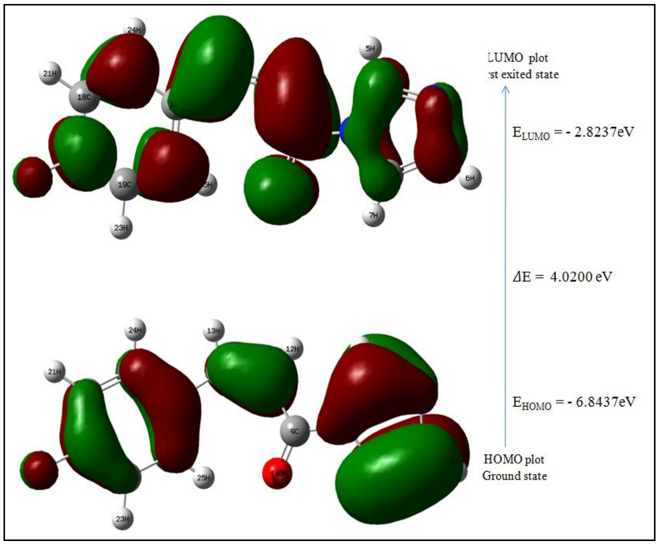

Fig 5: Highest occupied and lowest unoccupied molecular orbital of 34FIPO obtain with B3LYP/6-311++G(d,p) method

Table 3: Calculated energy values of title compound by B3LYP/6-311++G(d,p) method.

Basis set	B3LYP/6-311++G(d,p)
E_{Homo}(eV)	-6.8437
E_{Lumo}(eV)	-2.8237
Ionization potential	6.8437
Electron affinity	2.8237
Energy gap(eV)	4.0200
Electronegativity	4.8337
Chemical potential	-4.8337
Chemical hardness	2.0100
Chemical softness	0.2488
Electrophilicity index	5.8121

3.3 NLO activity

The non linear optical properties are calculated theoretically using same theoretical methodology. M. Raja *et al.* [16] reported first order hyperpolarizability, total dipole moments and polarizability of organic compound. P. Rajesh *et al.* [15] reported NLO activity compounds used to many communications systems. The title compound calculated NLO result compare to Urea compounds. Urea is one of the standard NLO activity molecules. It is used to comparative purpose only. The calculated dipole moment and hyperpolarizability values obtained from B3LYP/6-311++G (d,p) methods are listed in Table 4. The first order hyperpolarizability of 34FIPO with B3LYP/6-311++G (d,p) basis set is 5.7957 x 10-30 nine times greater than the value of urea (βo = 0.6230 x 10-30 esu).

Table 4: The values of calculated dipole moment μ(D), polarizability (α_0), first order hyperpolarizability (βtot) components of (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl)prop-2-en-1-one

Parameters	B3LYP/6 311++G(d,p)	Parameters	B3LYP/6-311++G(d,p)
μ_x	-1.9301	β_{xxx}	-753.9814
μ_y	0.3452	β_{xxy}	-3.5943
μ_z	0.1693	β_{xyy}	54.1434
μ(D)	1.9680	β_{yyy}	129.8911
α_{xx}	298.4767	β_{zxx}	-231.2178
α_{xy}	27.6237	β_{xyz}	66.0964
α_{yy}	109.8481	β_{zyy}	103.1867
α_{xz}	61.3858	β_{xzz}	76.5356
α_{yz}	19.7058	β_{yzz}	44.3379
α_{zz}	168.4653	β_{zzz}	308.0787
α_0 (e.s.u)	$2.8493x10^{-23}$	βtot (e.s.u)	$5.7957X10^{-30}$
Δα(e.s.u)	$8.0524\ x10^{-23}$		

3.4 Antimicrobial investigations

Antimicrobial (antibacterial and antifungal) activity of DMSO extracts with different concentration (25, 50, 75 and 100 μl) inhibition Zone (mm) in agar well diffusion method is tabulated in Tables 5. To further examine the invitro activity of (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl) prop-2-en-1-one (34FIPO) compound and results was compared to standard drug of Erythromycin. Title compound is more active Moraxella, Enterobacter, Pseudomonas aeruginosa, Candida albicans, A.niger and Trichophyton compared than standard drug. Together, these results indicate that 34FIPO shows broad-spectrum antimicrobial activity against. The activities of 34FIPO against bacterial and fungal pathogens are shown in Fig. 6.

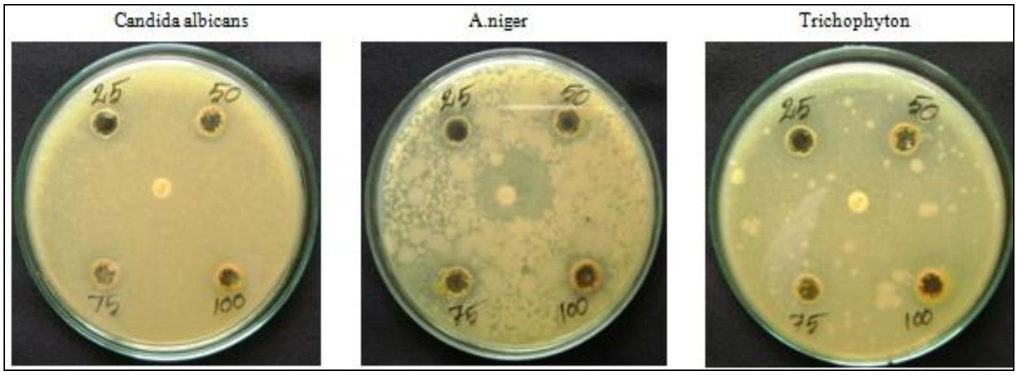

Fig 6: Antibacterial activity and antifungal activity of title molecule

4. Conclusions

In this present work, we have reported on complete structural activity, vibrational and electronic properties of synthesized (Z)-3-(4-fluorophenyl)-1-(1H-imidazol-1-yl)prop-2-en-1-one compound using spectroscopic and computational technique. The vibrational frequencies of the fundamental modes of the compound have been accurately assigned and investigated. Theoretical results were compared with the experimental vibrations. Moreover, HOMO and LUMO orbitals have been visualized. The nonlinear optical properties were calculated theoretically. The title compound may be a potential applicant in the development of NLO materials. The synthesized compound was tested against three different bacterial and three different fungal strains are exhibited moderate to good activity.

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