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Electronic Supplementary Information (ESI)

Visible-light-mediated synthesis of 3,4,5-trisubstituted furan-2-one derivative *via* bifunctional based Organo photocatalyst

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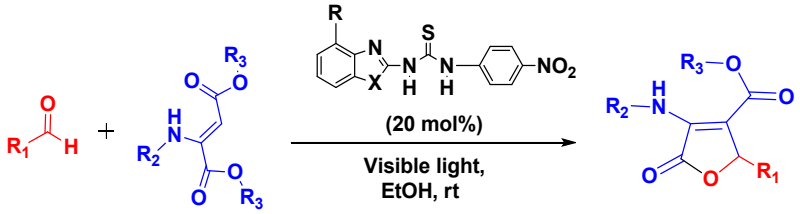
I. Experimental Section

All the chemicals were procured from Alfa Aesar, Sigma-Aldrich & Merck and were used without any further purification. The purity of the synthesized compounds was confirmed by FT-IR, ^{1}H-NMR, ^{13}C-NMR and Mass spectrometry. All reactions were monitored by thin-layer chromatography (TLC) using precoated aluminum sheets (silica gel 60 F 254 0.2 mm thickness) and developed in an iodine chamber. Melting points were recorded in the capillary using a Thermo Scientific 9300 apparatus. FT-IR spectra were recorded in KBr pellets on a BrukerAvance 400 (Model: ALPHA II). FT-IR instrument and the frequencies are expressed in cm^{-1}. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on a BrukerAvance II-400 spectrometer in $CDCl_3$ and DMSO-d_6 (chemical shifts in δ). Mass spectral data of the representative compounds were recorded with a Waters ZQ-4000 (ESI) mass spectrometer. For the UV–visible absorption studies, we have used spectroscopic grade ethanol solvents. All the electronic structure calculations were carried out using Gaussian 09 suite of program. The geometries of the compounds were optimized using the Density Functional Theory (DFT) based B3LYP method in conjugation with 6-31G (d,p) basis set.

I. 1. General procedure for the synthesis 3,4,5-trisubstituted furan-2-one derivatives



A mixture of diethyl 2-(phenylamino) fumarate (1 mmol), aldehydes (1mmol) and photocatalyst in 5 ml of ethanol was taken in a glass vial with screw cap and stirred at room temperature under the irradiation of white LEDs for 60-90 minutes. Upon completion of the reaction (monitored by TLC) the mixture was filtered and washed many times with de-ionized water. The solid product obtained was purified by recrystallization from hot ethanol or column chromatography.

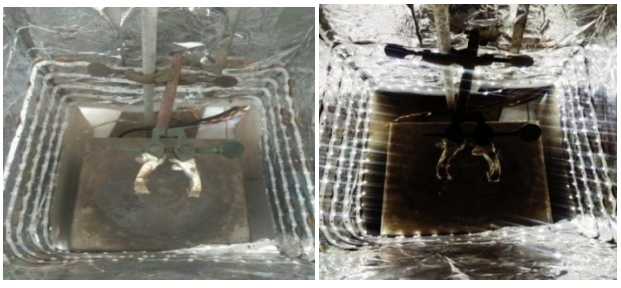
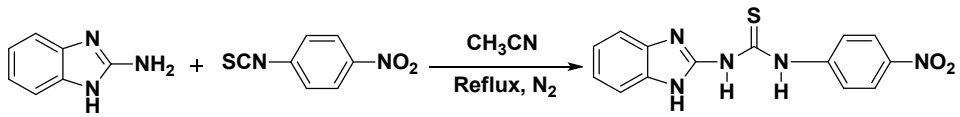


Figure S1. Homemade visible-light photo reactor

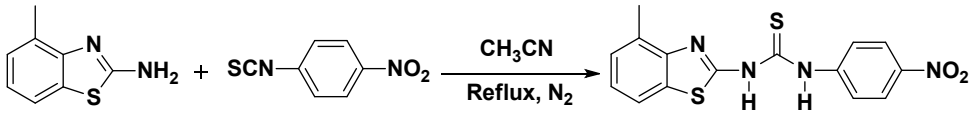
I. 2. General procedure for the synthesis of 1-(1H-benzo[d]imidazol-2-yl)-3-(4-nitrophenyl) thiourea (BINPT),[S1] 3a



Scheme S4A. Synthesis of **3a**

Synthesis of 2-(4-naphthalen-1-yl-phenyl)–2H-[1,2,3] triazole-4-carbaldehyde is shown in Scheme S4A. A mixture of 2-amino benzimidazole (2.00 mmol) and 4-nitrophenyl isothiocyanate (2.20 mmol) was refluxed in dry CH_3CN under N_2 for 3 h. A greenish yellow precipitate appeared after 30 mins and the reaction was continued to 3 hours to complete the conversion. The precipitate was collected by filtration, washed with CH_3CN and diethyl ether thoroughly and dried under vacuum.

I. 3. General procedure for the synthesis of 1-(4-methylbenzo[d]thiazol-2-yl)-3-(4-nitrophenyl) thiourea (MBNPT),[S1] 3b



Scheme S4B. Synthesis of **3b**

The synthetic route of 1-(4-methylbenzo[d]thiazol-2-yl)-3-(4-nitrophenyl) thiourea is shown in Scheme S4B. A mixture of 2-amino-4-methylbenzothiazole (2.00 mmol) and 4-nitrophenyl isothiocyanate (2.20 mmol) was dissolved in 15 ml of dry CH_3CN and refluxed for 3 hours under nitrogen atmosphere. An off-white precipitate appeared after 30 mins and the reaction was continued for 3 hours. The precipitate was collected by filtration and washed thoroughly with CH_3CN and diethyl ether and then dried under vacuum.

II. Mechanistic Investigation with UV-Vis Absorption Spectra:

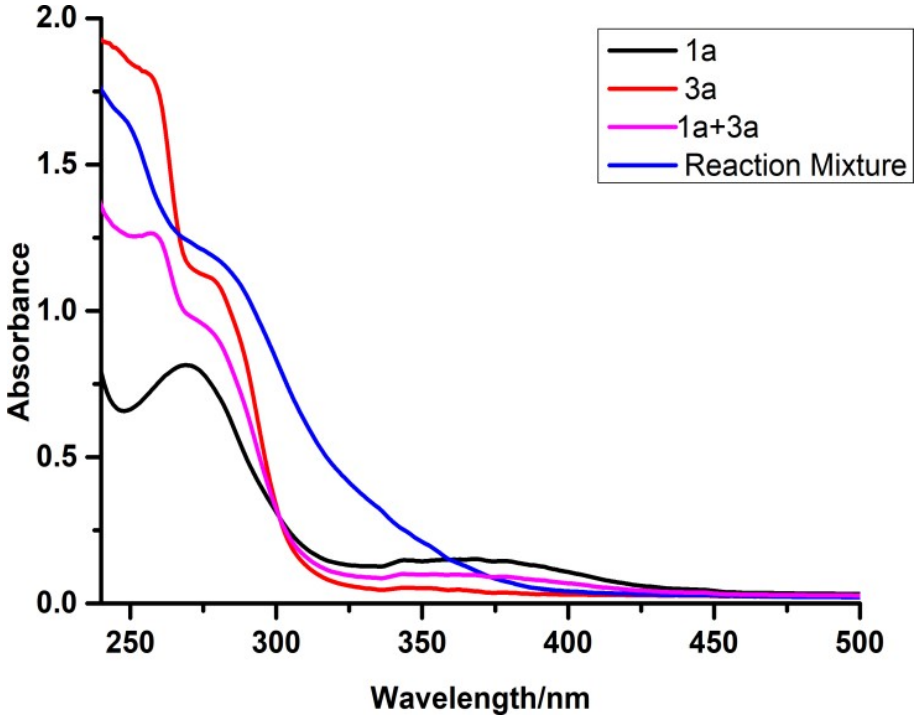


Figure S2: UV-Vis absorbance of benzaldehyde (**1a)** (1×10^{-5} M) in EtOH, benzaldehyde (1**a**) (1×10^{-5} M) and BINPT (**3a**) (1×10^{-5} M) in EtOH, and the reaction mixture (1×10^{-5} M) in EtOH

III. Light ON-OFF Experiments

In a glass vial with a screw cap containing benzaldehyde 1a (1mmol), diethyl 2-(phenylamino) fumarate 2a (1 mmol) and BINPT, **3a** (20 mol%) in 5 ml of ethanol. The mixture was stirred at room temperature for 5 min and then the visible light source was switched on. The mixture was stirred under visible light irradiation for 15 min and then one of the reaction vials were taken out, the mixture was filtered and washed many times with de-ionized water, and the solid product obtained was purified by recrystallization from hot ethanol and yield was calculated. The visible light was then switched off and the vials were stirred in the dark for 15 min followed by which one of the vials was removed and workup for the reaction mixture to isolate the desired product and yield was calculated. This process was repeated till the maximum yield was obtained.

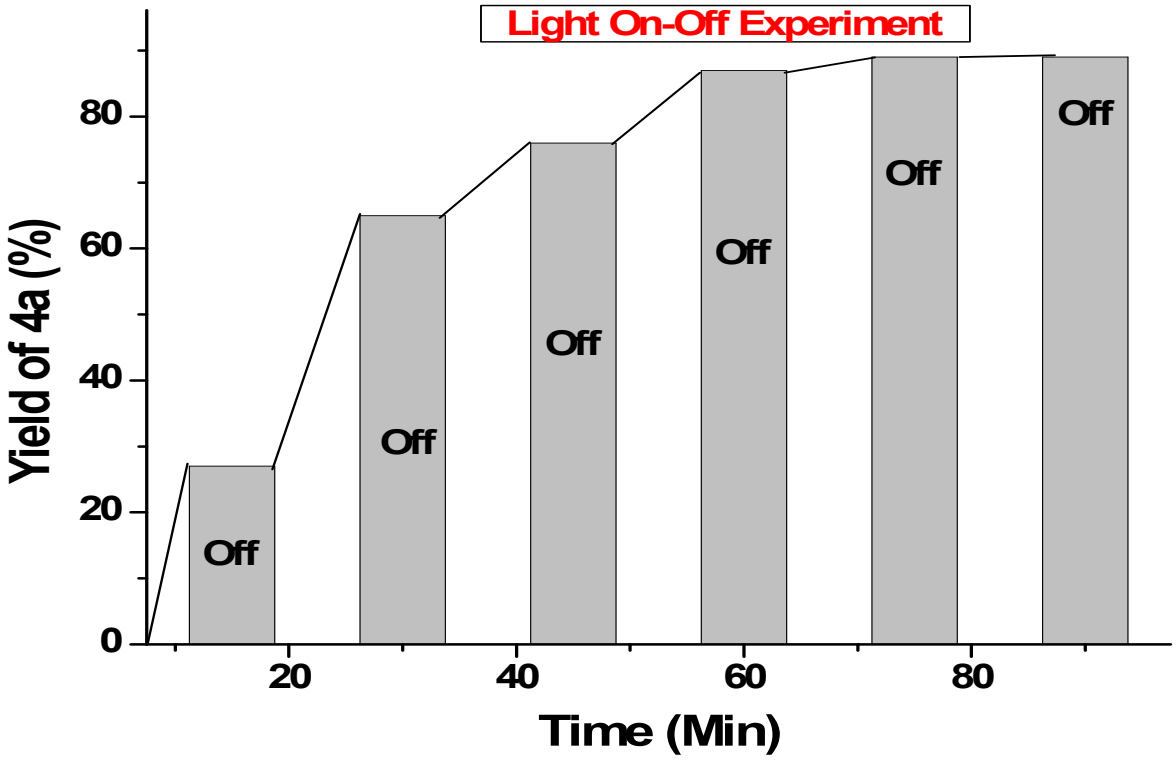


Figure S3. Light ON-OFF Experiment under the optimized condition

IV. Comparative study of Ecoscale

Table S1. comparative study of Ecoscale[S2] based for the synthesis of **4a** between **3a** (visible light) and sulfonic acid protocol.

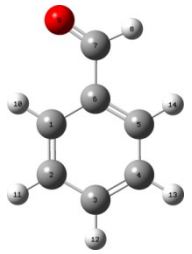
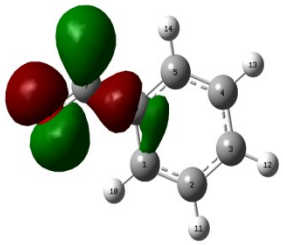
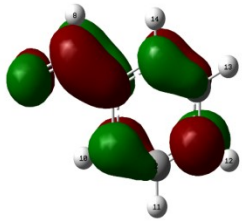
Parameter		**Penalty points**	
		3a (Visible light)	sulfonic acid
Yield		3	19.5
Price of reaction components Inexpensive (< $10)		0	0
Safety Safe for environment		0	5
Technical setup	Common setup	0	0
	Unconventional activation technique	-	-
Temperature/ time	R.T., < 1 h,	0	1
	Heating,< 1 h	-	-
Workup and purification Simple filtration		0	0
Eco scale score		100-3 = 97	100-25.5 = 74.5

V. Computational Details

Figure S4: Optimized geometries, FMO and the energies of molecule:

The geometry optimization was done without symmetry constrains using Density Functional Theory (DFT). It has been employed to clarify the structure-functional relationship of compounds using the Gaussian 09 program.[S3] The structures were optimized under a combination of the basis of the 6-31G basis set for H, C elements, and 6-31+G** with the B3LYP functional.[S4]

Benzaldehyde (1a)

Compound	HOMO	LUMO
		

HOMO = -0.37 a.u.; LUMO = -0.23 a.u.;

ΔE = HOMO-LUMO = 0.14 a.u.

SCF energy: -345.58 a. u.

Cartesian Coordinates:

C 31.615 -17.4372 0.

C 32.7832 -18.0995 0.

C 33.9426 -17.4237 0.

C 33.9364 -16.0817 0.

C 32.7726 -15.4119 0.

C 31.6123 -16.0923 0.

C 30.4326 -15.4188 0.

H 30.4917 -14.3057 0.

O 29.3306 -15.9168 0.

H 30.6788 -18.0224 0.

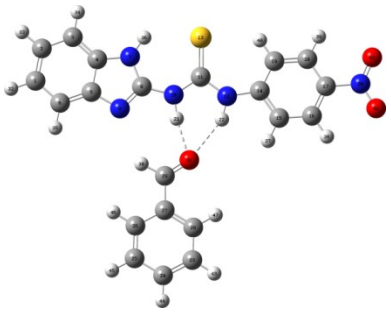
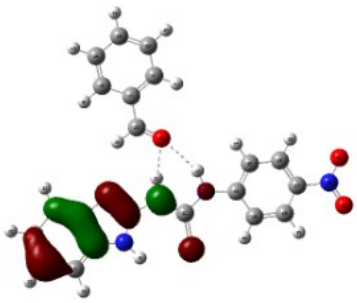
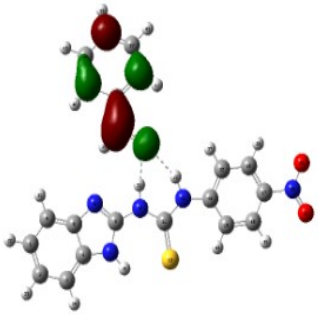
H 32.7915 -19.2035 0.

H 34.901 -17.9715 0.

H 34.8916 -15.5283 0.

H 32.7998 -14.3079 0.

Hydrogen bonding of BINPT (3a) and Benzaldehyde (1a)

Compound	HOMO	LUMO
		

HOMO = -0.21 a.u.; LUMO = -0.09 a.u.;

ΔE = HOMO-LUMO = 0.12 a.u.

SCF energy: -1707.62 a. u.

Cartesian Coordinates:

C 19.33249 -25.67813 2.50186

C 18.95939 -24.56543 1.84096

C 19.85679 -23.83453 1.15646

C 21.12039 -24.26793 1.16886

C 21.50569 -25.36813 1.81916

C 20.61159 -26.09523 2.50016

N 22.21529 -23.76653 0.59496

C 23.22759 -24.57473 0.92296

N 22.82629 -25.61053 1.69136

N	24.48009	-24.35993	0.49096
C	25.4808	-25.0964	0.9431
N	26.50846	-25.31916	0.09545
S	25.7327	-25.2313	2.6139
C	27.36736	-26.33446	0.31525
C	28.64946	-26.06516	0.61345
C	29.51136	-27.07006	0.83615
C	29.08706	-28.34116	0.75855
C	27.80736	-28.61356	0.45905
C	26.94606	-27.60806	0.23635
N	29.94976	-29.34826	0.98215
H	24.26878	-23.62316	-0.47148
H	26.72936	-24.90229	-0.87605
C	27.36971	-19.35066	-3.04128
C	27.19331	-19.21246	-4.36438
C	26.66381	-20.21776	-5.07828
C	26.30911	-21.36256	-4.47268
C	26.48691	-21.49856	-3.14608
C	27.01781	-20.49236	-2.42838
C	26.12901	-22.65546	-2.52688
H	25.69401	-23.43856	-3.19978
O	26.25151	-22.86276	-1.33748
H	18.57559	-26.25983	3.05596
H	17.90259	-24.24723	1.86016
H	19.56949	-22.92063	0.60956
H	20.91769	-27.00663	3.04136
H	22.28159	-22.93443	0.02956
H	28.99986	-25.02036	0.67975

H 30.56356 -26.84476 1.08255

H 27.45766 -29.65866 0.39405

H 25.89466 -27.83626 -0.01165

O 30.89996 -29.05746 1.20245

O 29.54976 -30.28096 0.90375

H 27.80541 -18.52196 -2.45628

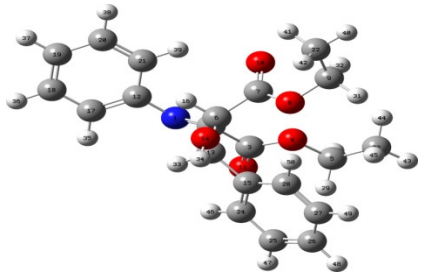
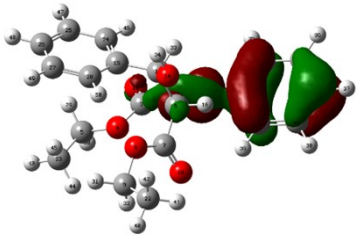
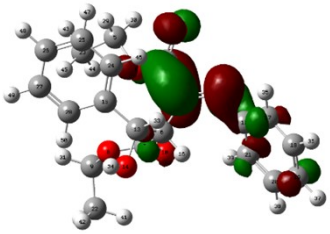
H 27.48361 -18.27236 -4.86518

H 26.51951 -20.10156 -6.16668

H 25.87591 -22.17026 -5.08858

H 27.17641 -20.57226 -1.33868

Intermediate (E)

Compound	HOMO	LUMO
		

HOMO = -0.22 a.u.; LUMO = -0.06 a.u.;

ΔE = HOMO-LUMO = 0.16 a.u.

SCF energy: -1244.89 A.U.

Cartesian Coordinates:

N 44.9725 -22.5839 -1.2167

C 44.6949 -23.7512 -0.5901

C 43.3745 -24.0747 -0.4461

O 42.9917 -25.3233 -0.1034

C 41.6178 -25.6308 -0.177

C 45.7926 -24.7124 -0.1258

C 45.6882 -26.0757 -0.7925

O 46.4837 -26.9663 -0.1812
C 46.5161 -28.2788 -0.6889
O 45.0097 -26.3009 -1.7671
O 42.5304 -23.2485 -0.7201
C 46.2443 -22.2483 -1.4971
C 45.9287 -24.6927 1.4162
O 47.1841 -25.2121 1.7738
C 44.84 -25.4122 2.1876
H 46.7773 -24.3636 -0.515
C 47.0803 -21.7928 -0.5502
C 48.3551 -21.5223 -0.8719
C 48.7835 -21.6868 -2.1337
C 47.9398 -22.1223 -3.0819
C 46.6697 -22.4129 -2.7603
C 47.4991 -28.3459 -1.8617
C 41.428 -27.1259 0.0976
C 43.7703 -24.7432 2.6565
C 42.7986 -25.3743 3.3355
C 42.8854 -26.6919 3.5697
C 43.9558 -27.3691 3.1318
C 44.921 -26.7281 2.4538
H 41.0896 -25.0298 0.6013
H 41.2358 -25.39 -1.1991
H 46.8543 -28.9249 0.1544
H 45.4886 -28.6106 -0.9722
H 45.987 -23.6335 1.7601
H 47.289 -25.0808 2.7012
H 46.7319 -21.6633 0.4887
H 49.0538 -21.1741 -0.0919
H 49.8337 -21.4704 -2.3964
H 48.2942 -22.2542 -4.119
H 45.9833 -22.7906 -3.5391
H 47.5602 -29.3817 -2.2675
H 47.191 -27.6714 -2.6934

H 48.523 -28.0429 -1.5409

H 40.3435 -27.3777 0.1576

H 41.88 -27.7433 -0.7123

H 41.8992 -27.429 1.0598

H 43.6773 -23.6579 2.4767

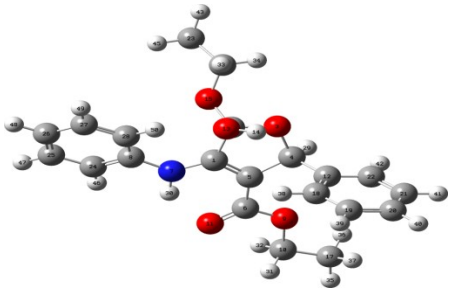
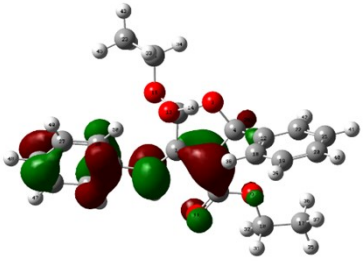
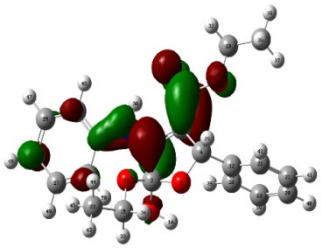
H 41.9222 -24.8117 3.7024

H 42.0871 -27.2161 4.1231

H 44.041 -28.4525 3.3301

H 45.7919 -27.3129 2.1194

Intermediate (G)

Compound	HOMO	LUMO
		

HOMO = -0.20 a.u.; LUMO = -0.04 a.u.;

ΔE = HOMO-LUMO = 0.20 a.u.

SCF energy: -1244.91 a. u.

Cartesian Coordinates:

C 48.1306 -34.6922 0.673

C 48.1615 -33.1926 0.5779

O 49.5077 -32.7907 0.6968

C 50.3231 -33.9455 0.6969

C 49.3957 -35.1284 0.7209

C 49.7861 -36.4277 0.7707

N 47.0261 -35.4667 0.6787

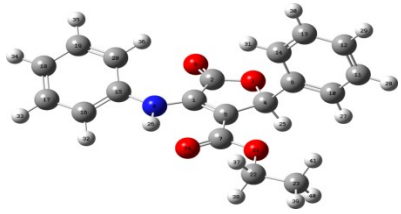
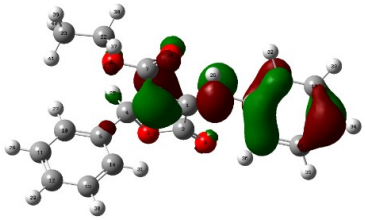
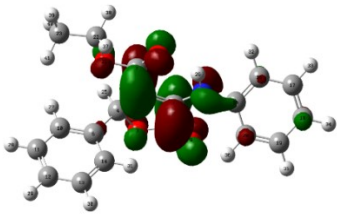
C 46.0938 -35.2409 -0.2702

O 51.1063 -36.6968 0.8284

C 51.5275 -38.0183 1.0688
O 48.9828 -37.3329 0.789
C 51.2482 -33.9368 1.8932
O 47.4998 -32.5673 1.6335
H 47.8949 -31.7251 1.7793
O 47.7448 -32.7408 -0.6849
C 47.5265 -31.3514 -0.7828
C 53.0276 -37.9756 1.3784
C 50.7572 -33.7551 3.1322
C 51.5644 -33.7597 4.2041
C 52.8828 -33.9529 4.0497
C 53.3854 -34.1394 2.8202
C 52.5719 -34.1289 1.7526
C 47.2092 -31.0383 -2.2482
C 45.9589 -36.1386 -1.2611
C 45.0499 -35.9449 -2.2296
C 44.2687 -34.8543 -2.2089
C 44.3939 -33.9609 -1.2161
C 45.3021 -34.1553 -0.247
H 50.8779 -33.9282 -0.2707
H 47.3266 -36.4401 0.6351
H 50.9706 -38.4346 1.9426
H 51.331 -38.6196 0.1492
H 46.6569 -31.0776 -0.1398
H 48.4452 -30.8088 -0.4577
H 53.4243 -38.9999 1.5667
H 53.601 -37.5371 0.529
H 53.2317 -37.3578 2.2836
H 49.6742 -33.6038 3.2784
H 51.144 -33.609 5.214
H 53.5492 -33.961 4.93
H 54.4692 -34.3048 2.6884
H 53.0041 -34.2905 0.7504
H 47.0226 -29.9492 -2.3931

H 48.0569 -31.3302 -2.9108
H 46.3021 -31.5904 -2.5892
H 46.6001 -37.0372 -1.2921
H 44.9469 -36.6814 -3.0457
H 43.5209 -34.6943 -3.006
H 43.7459 -33.0669 -1.1932
H 45.3755 -33.4181 0.5693

Product 4a

Compound	HOMO	LUMO
		

HOMO = -0.21 a.u.; LUMO = -0.07 a.u.;

ΔE = HOMO-LUMO = 0.14 a.u.

SCF energy: -1089.87 a. u.

Cartesian Coordinates:

C 51.0983 -26.5157 0.3022
C 52.4286 -26.7171 0.5079
O 53.1665 -25.5946 0.6476
C 52.2673 -24.5106 0.5414
C 50.9367 -25.1848 0.3476
C 52.6197 -23.6111 -0.6213
C 49.7442 -24.5419 0.25
N 50.1019 -27.4123 0.1994
O 52.982 -27.788 0.6074
C 52.671 -22.2755 -0.4675
C 52.9674 -21.4714 -1.5002

C 53.2177 -21.9965 -2.7089
C 53.1675 -23.3264 -2.8771
C 52.8687 -24.1239 -1.8399
C 50.2213 -28.7525 0.1957
C 49.3671 -29.4564 0.9577
C 49.4261 -30.7972 0.9802
C 50.3247 -31.4421 0.2204
C 51.1515 -30.7439 -0.5731
C 51.0923 -29.4028 -0.5949
O 49.7347 -23.1944 0.2786
C 48.5679 -22.5167 -0.1231
C 48.9268 -21.0369 -0.2915
O 48.7112 -25.153 0.0894
H 52.298 -23.9803 1.5225
H 49.2081 -27.0575 0.5346
H 52.4607 -21.8243 0.5171
H 53.0014 -20.3774 -1.3566
H 53.4597 -21.3378 -3.561
H 53.3679 -23.7639 -3.8706
H 52.8243 -25.2144 -2.
H 48.6173 -28.9376 1.5806
H 48.7316 -31.3702 1.619
H 50.3697 -32.545 0.2329
H 51.8704 -31.275 -1.2211
H 51.7531 -28.8525 -1.2863
H 48.2113 -22.934 -1.0954
H 47.796 -22.6484 0.6722
H 48.0355 -20.4437 -0.6013
H 49.3099 -20.6063 0.6626
H 49.7149 -20.9022 -1.0684

VI. UV-Visible Spectra of Catalyst

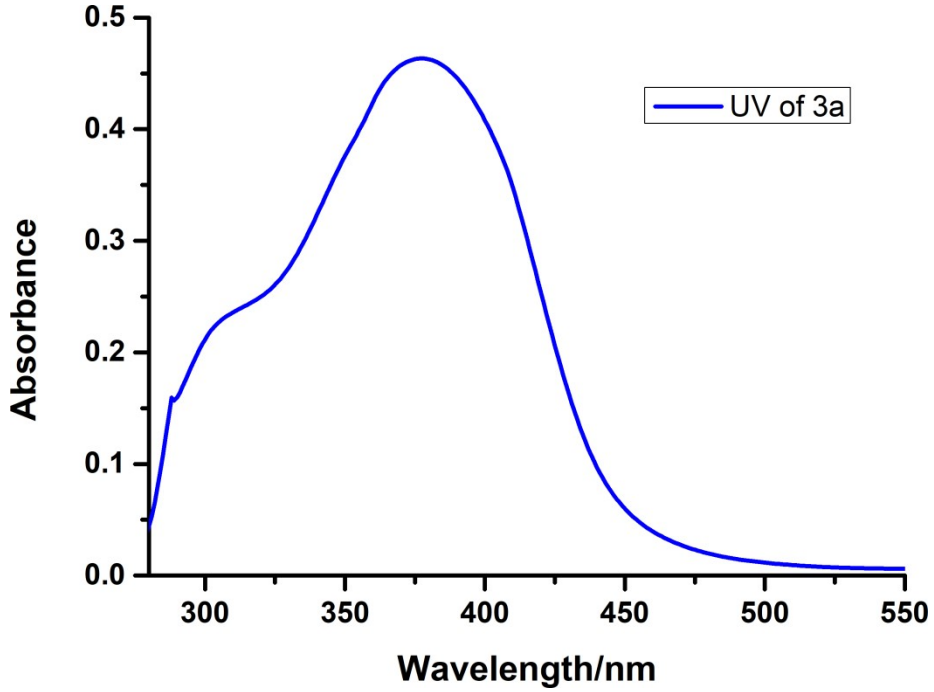


Figure S5. UV-visible spectra of the catalyst **3a**

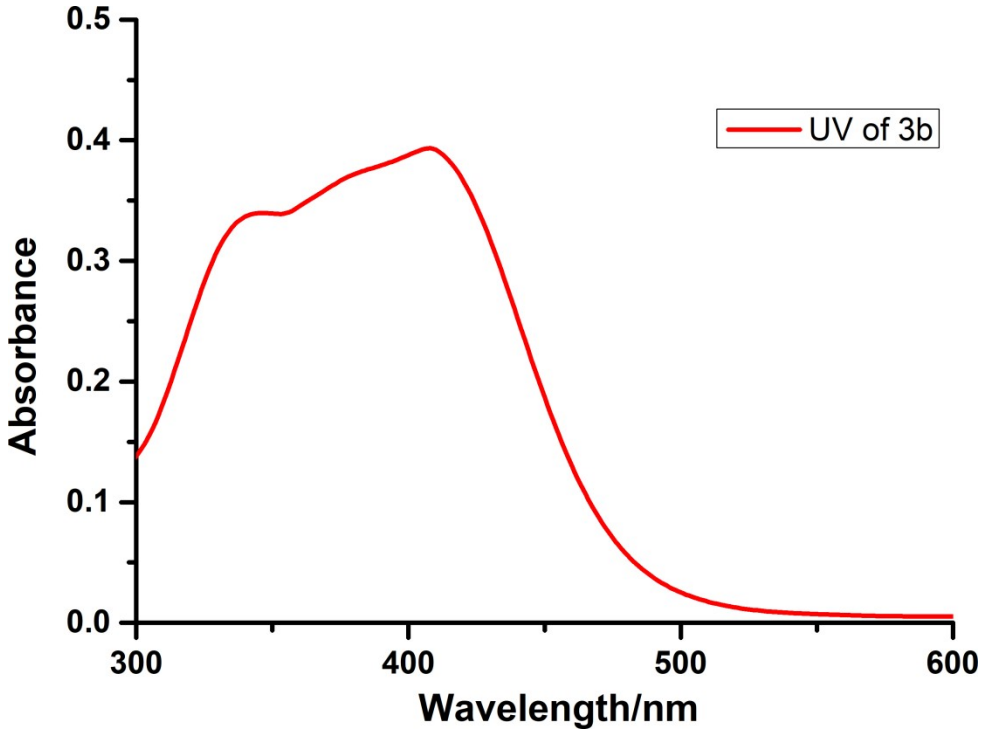


Figure S6. UV-visible spectra of the catalyst **3b**

VII. Photoluminescence (PL) spectra of catalyst

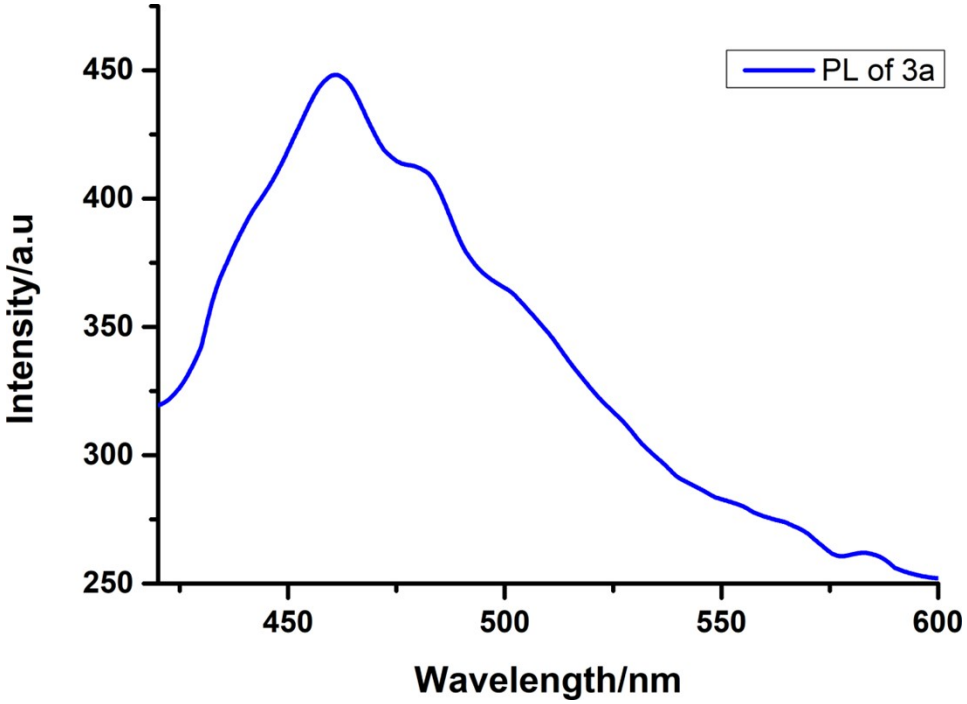


Figure S7. Photoluminescence (PL) spectra of catalyst **3a**

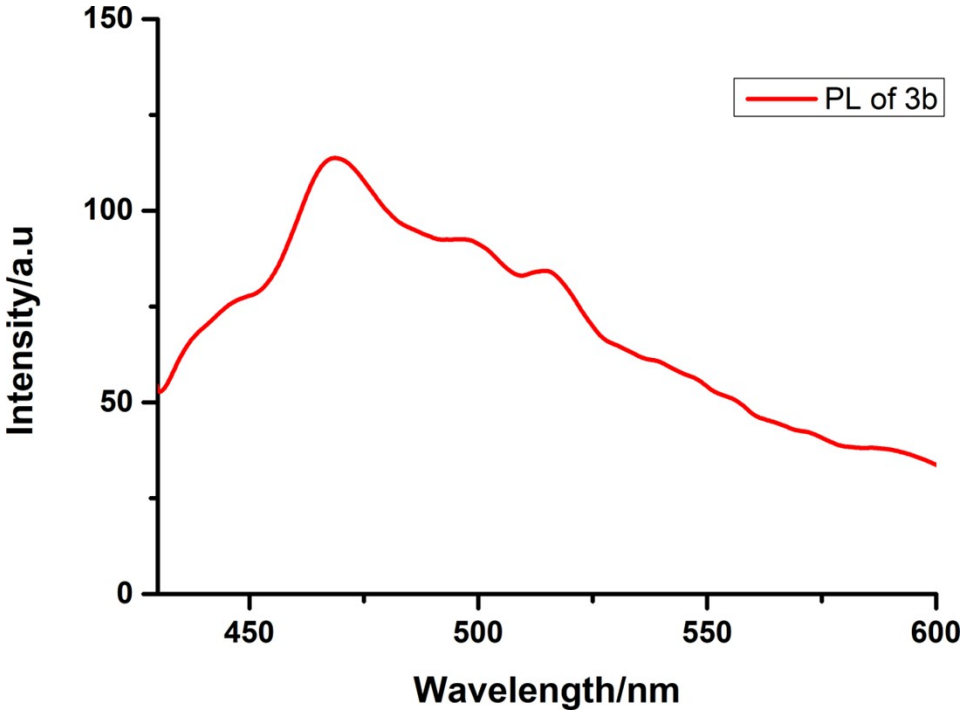
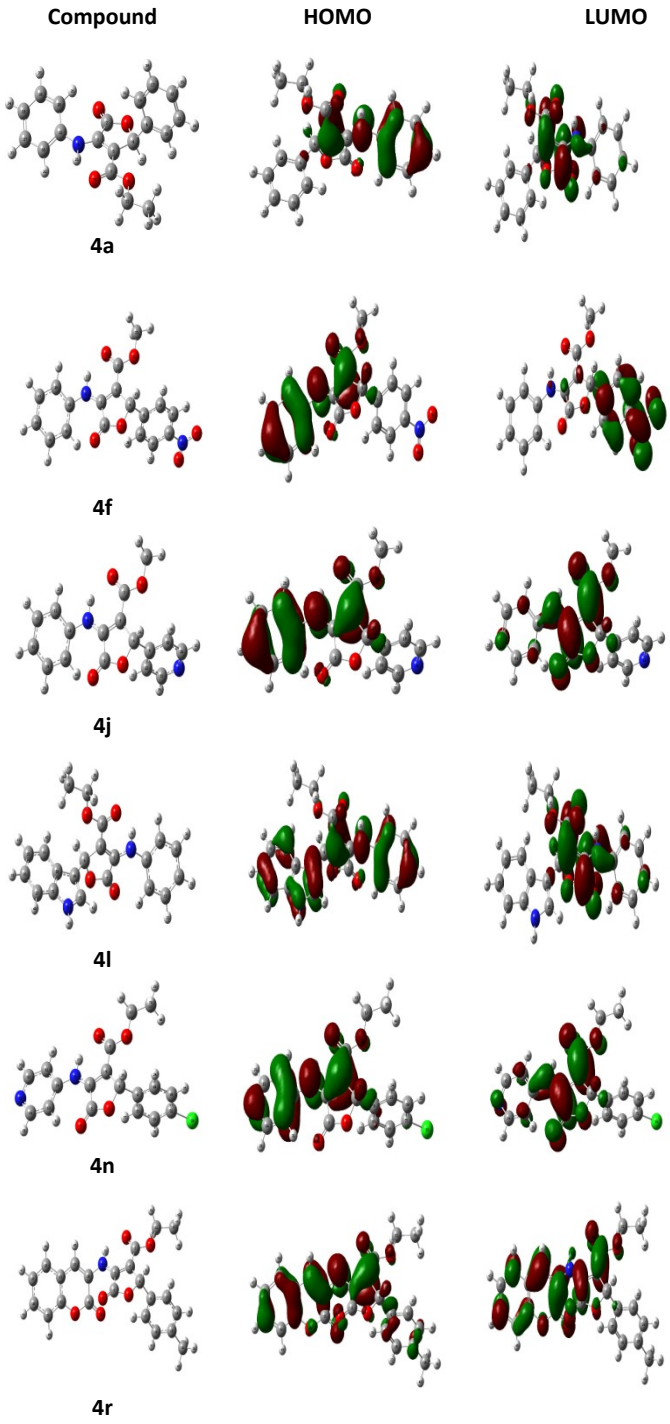


Figure S8. Photoluminescence (PL) spectra of catalyst **3a**

Figure S9. Calculated molecular orbital amplitude plot of HOMO and LUMO levels and optimized molecular structure of compounds



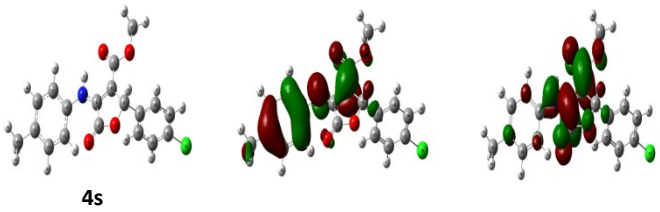
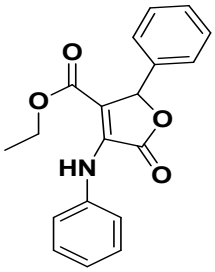


Table S2: Electrochemical data of compounds (Theoretical)

Compound	HOMO (a.u) (DFT)	LUMO (a.u) (DFT)	ΔE=HOMO-LUMO (a.u)
4a	-0.21	-0.07	0.14
4f	-0.22	-0.09	0.13
4j	-0.22	-0.08	0.17
4l	-0.20	-0.07	0.13
4n	-0.23	-0.09	0.14
4r	-0.22	-0.08	0.14
4s	-0.21	-0.07	0.14

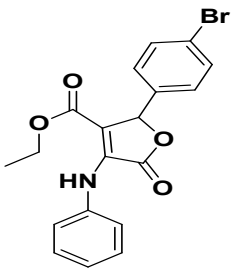
VIII. Analytical and spectroscopic data of the synthesized compounds

Ethyl 5-oxo-2-phenyl-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate*, *4a



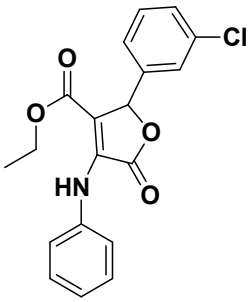
White solid (yield: 91%); mp: 179-180 °C. IR (KBr): ν 3215, 2941, 1709, 1496, 1091, cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 9.25 (s, 1H), 7.63 (d, 2H, *J* = 8.4 Hz), 7.44-7.35 (m, 6H), 7.25 (t, 1H, *J* = 7.6 Hz), 5.89 (s, 1H), 4.36 (q, 2H, *J* = 7.0 Hz), 1.34 (t, 3H, *J* = 7.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.7, 163.5, 157.1, 136.8, 136.6, 129.6, 129.2, 128.1, 126.4, 122.9, 113.8, 62.1, 61.9, 31.5, 14.5 ppm. HRMS (ESI) m/z: $[M + 1]^+$ calcd, 324.1236; found, 324.1237.

Ethyl 2-(4-bromophenyl)-5-oxo-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate*, *4b



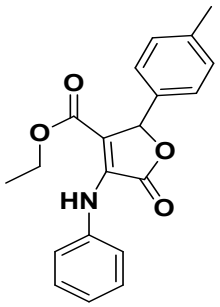
White solid (yield: 94%); mp:189-190 °C. IR (KBr): ν 3311, 2980, 1721, 1490, 1087 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 9.23 (s, 1H), 7.62 (d, 2H, *J* = 7.6 Hz), 7.56 (d, 2H, *J* = 7.4 Hz), 7.48 (d, 2H, *J* = 7.6 Hz), 7.32-7.27 (m, 3H), 5.89 (s, 1H), 4.39 (q, 2H, *J* = 7.2 Hz), 1.39 (t, 3H, *J* = 7.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.3, 163.1, 156.9, 136.3, 134.7, 132.2, 129.6, 129.5, 126.5, 122.9, 122.6, 113.1, 61.8, 61.3, 31.4, 14.4 ppm. ESI-MS: 401 $[M]^+$, 403 $[M+2]^+$

Ethyl 2-(3-chlorophenyl)-5-oxo-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate, 4c



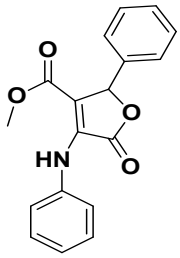
White solid (yield: 87%); mp:185-187 °C. IR (KBr): ν 3329, 2951, 1720, 1489, 1090, cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.90 (s, 1H), 7.28 (d, 2H, *J* = 7.6 Hz), 7.13-7.07 (m, 3H), 7.03-6.99 (m, 2H), 6.95 (d, 1H, *J* = 7.4 Hz), 6.92-6.89 (m, 1H), 5.52 (s, 1H), 4.02 (q, 2H, *J* = 7.0 Hz), 1.03 (t, 3H, *J* = 7.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.2, 162.9, 156.9, 137.6, 136.2, 134.6, 130.2, 129.4, 129.0, 128.1, 126.3, 125.7, 122.4, 112.9, 61.7, 61.1, 14.2 ppm. ESI-MS: *m/z* 358 $[M+1]^+$

Ethyl 5-oxo-4-(phenylamino)-2-(p-tolyl)-2,5-dihydrofuran-3-carboxylate, 4d



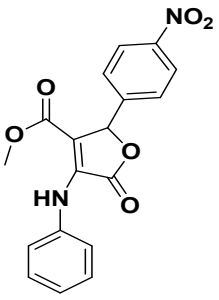
White solid (yield: 85%); mp:180-181 °C. IR (KBr): ν 3341, 2982, 1712, 1482, 1094, cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 9.21 (s, 1H), 7.66 (d, 2H, *J* = 7.6 Hz), 7.44 (t, 3H, *J* = 7.4 Hz), 7.28 (d, 3H, *J* = 7.6 Hz), 7.22 (d, 2H, *J* = 7.6 Hz), 5.88 (s, 1H), 4.37 (q, 2H, *J* = 7.0 Hz), 2.43 (s, 3H), 1.38 (t, 3H, *J* = 7.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.4, 163.1, 156.6, 138.5, 136.6, 132.1, 129.5, 129.2, 127.6, 126.0, 122.5, 113.5, 61.6, 61.5, 21.4, 14.2 ppm. ESI-MS: *m/z* 337 $[M]^+$

Methyl 5-oxo-2-phenyl-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate, 4e



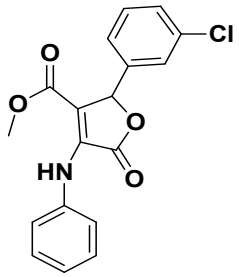
White solid (yield: 90%); mp: 185-187 °C. IR (KBr): ν 3462, 29459, 1712, 1486, 1091 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.90 (s, 1H), 7.50 (d, 2H, *J* = 7.6 Hz), 7.33-7.25 (m, 7H), 7.14 (m, 1H), 5.78 (s, 1H), 3.78 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.8, 162.5, 155.7, 135.7, 134.5, 128.6, 128.3, 128.2, 127.1, 125.6, 122.0, 112.5, 61.2, 51.7 ppm. ESI-MS: *m/z* 310 $[M+1]^+$

Methyl 2-(4-nitrophenyl)-5-oxo-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate, 4f



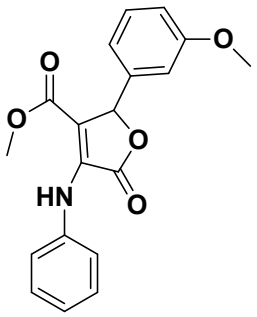
White solid (yield: 89%); mp:136-138 °C. IR (KBr): ν 3351, 2971, 1721, 1494, 1049, cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.90 (s, 1H), 7.97 (d, 2H, *J* = 7.6 Hz), 7.28 (d, 4H, *J* = 7.4 Hz), 7.14 (t, 2H, *J* = 7.6 Hz), 6.99 (s, 1H), 5.72 (s, 1H), 3.61 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.6, 163.1, 156.91, 148.2, 142.9, 135.7, 129.5, 128.8, 126.7, 124.2, 122.4, 112.4, 61.0, 52.5 ppm. HRMS (ESI) m/z: $[M + 1]^+$ calcd, 355.0922; found, 355.0926.

Methyl 2-(3-chlorophenyl)-5-oxo-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate, 4g



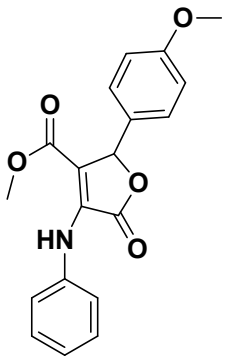
White solid (yield: 89%); mp: 170-172 °C. IR (KBr): ν 3442, 2951, 1727, 1494, 1079 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 9.06 (s, 1H), 7.50 (d, 2H, *J* = 8.0 Hz), 7.36 (t, 2H, *J* = 7.8 Hz), 7.32 (s, 1H), 7.25 (s, 1H), 7.22-7.16 (m, 3H), 5.77 (s, 1H), 3.83 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.1, 163.1, 156.3, 137.4, 136.0, 134.8, 130.2, 129.4, 129.4, 129.1, 127.8, 126.5, 125.9, 122.6, 112.7, 61.3, 52.4 ppm. ESI-MS: 343 $[M]^+$, 345 $[M+2]^+$

Methyl 2-(3-methoxyphenyl)-5-oxo-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate, 4h



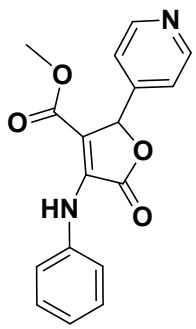
White solid (yield: 82%); mp: 169-170 °C. IR (KBr): ν 3450, 2953, 1710, 1491, 1033 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.95 (s, 1H), 7.46 (d, 2H, *J* = 7.4 Hz), 7.28 (t, 2H, *J* = 7.6 Hz), 7.17 (t, 1H, *J* = 7.6 Hz), 7.11 (t, 1H, *J* = 7.6 Hz), 6.83 (d, 1H, *J* = 7.6 Hz), 6.75 (t, 2H, *J* = 8.0 Hz), 5.71 (s, 1H), 3.76 (s, 3H), 3.73 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.9, 162.4, 159.3, 155.9, 136.2, 135.8, 129.3, 128.6, 125.6, 122.0, 119.6, 113.4, 112.7, 112.4, 61.1, 54.8, 51.7 ppm. ESI-MS: *m/z* 340 $[M+1]^+$

Methyl 2-(4-methoxyphenyl)-5-oxo-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate, 4i



White solid (yield : 84%); mp: 240-242 °C. IR (KBr): ν 3438, 3229, 2957, 1681, 1464, 1038 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.87 (s, 1H), 7.37 (d, 2H, *J* = 8.0 Hz), 7.19 (t, 2H, *J* = 7.8 Hz), 7.06-7.04 (m, 3H), 6.69 (d, 2H, *J* = 7.6 Hz), 5.62 (s, 1H), 3.67 (s, 3H), 3.66 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.5, 163.1, 159.8, 156.1, 136.4, 129.2, 128.9, 127.5, 126.9, 126.2, 126.1, 122.8, 114.3, 113.2, 61.4, 55.4, 52.3 ppm. HRMS (ESI) m/z: $[M + 1]^+$ calcd, 340.1185; found, 340.1183.

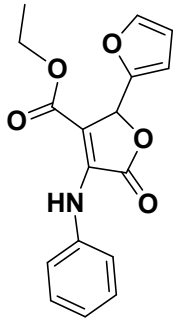
Methyl 5-oxo-4-(phenylamino)-2-(pyridin-4-yl)-2,5-dihydrofuran-3-carboxylate, 4j



White solid (yield: 77 %); mp: 136-137 °C. IR (KBr): ν 3441, 3226, 2922, 1670, 1464, 1093 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 12.29 (s, 1H), 8.27 (d, 2H, *J* = 8.4 Hz), 7.79 (t, 4H, *J* = 7.6 Hz), 7.49 (t, 2H, *J* = 8.0 Hz), 7.29 (t, 1H, *J* = 7.2 Hz), 6.49 (s, 1H), 3.78 (s, 3H) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 164.3, 162.8, 153.7, 147.6,

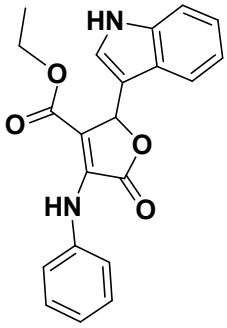
145.0, 136.3, 129.7, 129.3, 126.1, 123.9, 122.9, 111.5, 60.1, 56.5, 51.7, 31.1, 19.0 ppm. ESI-MS: *m/z* 311 $[M+1]^+$

Ethyl 5-oxo-4-(phenylamino)-2,5-dihydro-[2,2'-bifuran]-3-carboxylate, 4k



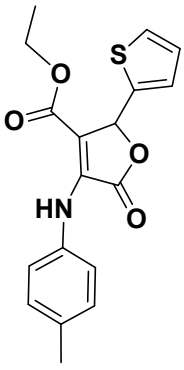
White solid (yield: 75 %); mp: 185-187 °C. IR (KBr): ν 3446, 3223, 2920, 1673, 1461, 1099 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 12.06 (s, 1H), 7.78 (d, 2H, *J* = 7.6 Hz), 7.60 (s, 1H), 7.50 (t, 2H, *J* = 8.0 Hz), 7.46-7.38 (m, 3H), 7.30 (t, 1H, *J* = 7.2 Hz), 6.31 (s, 1H), 4.30-4.15 (m, 2H). 1.29 (t, 3H, *J* = 6.8 Hz) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 164.4, 162.4, 153.5, 139.6, 136.5, 13.1, 130.6, 129.3, 128.7, 128.5, 126.6, 126.0, 122.9, 112.0, 60.3, 60.2, 14.5 ppm. ESI-MS: *m/z* 314 $[M+1]^+$

Ethyl 2-(1H-indol-3-yl)-5-oxo-4-(phenylamino)-2,5-dihydrofuran-3-carboxylate, 4l



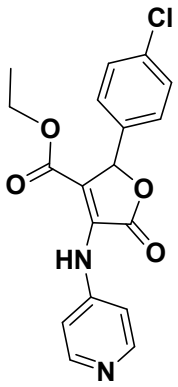
White solid (yield: 79 %); mp: 188-189 °C. IR (KBr): ν 3436, 3227, 2923, 1671, 1465, 1093 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 12.02 (s, 1H), 7.75 (d, 2H, *J* = 7.6 Hz), 7.60 (d, 2H, *J* = 8.4 Hz), 7.49 (t, 2H, *J* = 7.6 Hz), 7.43 (d, 2H, *J* = 8.4 Hz), 7.43 (d, 2H, *J* = 8.4 Hz), 7.29 (t, 1H, *J* = 7.6 Hz), 6.29 (s, 1H), 4.26-4.19 (m, 2H), 1.29 (t, 3H, *J* = 7.2 Hz) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 164.4, 162.4, 153.3, 136.7, 136.5, 131.6, 130.5, 129.2, 125.9, 123.0, 121.5, 112.1, 60.3, 60.2, 14.5 ppm. ESI-MS: *m/z* 363 $[M+1]^+$

Ethyl 5-oxo-2-(thiophen-2-yl)-4-(p-tolylamino)-2,5-dihydrofuran-3-carboxylate, 4m



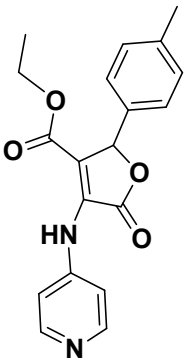
White solid (yield: 74 %); mp: 180-182 °C. IR (KBr): ν 3443, 3223, 2921, 1675, 1463, 1096 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 11.84 (s, 1H), 7.76 (d, 2H, *J* = 7.6 Hz), 7.47 (t, 2H, *J* = 7.6 Hz), 7.32 (d, 2H, *J* = 7.6 Hz), 7.27 (t, 1H, *J* = 7.2 Hz), 7.21 (d, 2H, *J* = 8.0 Hz), 6.21 (s, 1H), 4.29-4.17 (m, 2H), 2.37 (s, 3H), 1.29 (t, 3H, *J* = 6.8 Hz) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 164.0, 162.0, 152.5, 137.1, 136.3, 133.4, 128.9, 128.7, 127.6, 125.3, 122.5, 112.3, 60.4, 59.7, 20.7, 14.1 ppm. HRMS (ESI) m/z: $[M + 1]^+$ calcd, 344.0687; found, 344.0692.

Ethyl 2-(4-chlorophenyl)-5-oxo-4-(pyridin-4-ylamino)-2,5-dihydrofuran-3 carboxylate, 4n



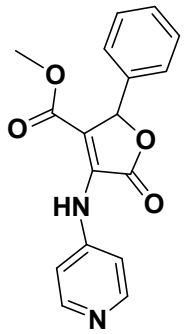
White solid (yield: 77 %); mp: 178-180 °C. IR (KBr): ν 3448, 3225, 2927, 1678, 1464, 1098 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 8.35 (d, 2H, *J* = 7.6 Hz), 8.11 (d, 2H, *J* = 7.4 Hz), 7.52 (d, 2H, *J* = 8.0 Hz), 7.44 (t, 2H, *J* = 7.6 Hz), 7.38 (t, 1H, *J* = 8.0 Hz), 6.39 (s, 1H), 4.28-4.18 (m, 2H), 1.28 (t, 3H, *J* = 6.8 Hz) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 164.9, 162.0, 152.0, 143.7, 142.2, 136.1, 128.6, 128.4, 127.9, 124.6, 121.8, 113.3, 60.5, 60.1, 14.1 ppm. HRMS (ESI) m/z: $[M + 1]^+$ calcd, 340.1185; found, 340.1183.

Ethyl 5-oxo-4-(pyridin-4-ylamino)-2-(p-tolyl)-2,5-dihydrofuran-3-carboxylate, 4o



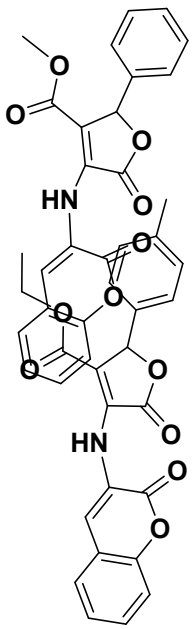
White solid (yield: 78 %); mp: 184-186 °C. IR (KBr): ν 3444, 3221, 2920, 1676, 1465, 1091 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 11.96 (s, 1H), 7.62 (d, 2H, *J* = 7.6 Hz), 7.42-7.40 (m, 3H), 7.36-7.33 (m, 1H), 7.27 (d, 2H, *J* = 7.4 Hz), 6.20 (s, 1H), 4.26-4.15 (m, 2H), 2.38 (s, 3H), 1.26 (t, 3H, *J* = 7.2 Hz) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 163.9, 162.1, 152.8, 136.7, 134.7, 133.8, 129.2, 128.3, 127.9, 127.8, 122.6, 112.1, 60.8, 59.7, 20.5, 14.1 ppm. ESI-MS: *m/z* 339 $[M+1]^+$

Methyl 5-oxo-2-phenyl-4-(pyridin-4-ylamino)-2,5-dihydrofuran-3-carboxylate, 4p



White solid (yield: 81 %); mp: 171-174 °C. IR (KBr): ν 3445, 3226, 2924, 1677, 1463, 1095 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 12.55 (s, 1H), 7.77 (d, 2H, *J* = 8.0 Hz), 7.58 (s, 1H), 7.50 (t, 2H, *J* = 7.6 Hz), 7.42 (s, 2H), 7.30 (t, 1H, *J* = 7.2 Hz), 6.32 (s, 1H), 3.80 (s, 3H) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 175.0, 171.7, 164.3, 162.9, 153.3, 139.7, 136.4, 133.1, 130.6, 129.2, 128.5, 1228.3, 126.6, 126.0, 122.9, 111.7, 72.9, 60.2, 51.6 ppm. ESI-MS: *m/z* 311 $[M+1]^+$

Methyl 5-oxo-4-((2-oxo-2H-chromen-3-yl)amino)-2-phenyl-2,5-dihydrofuran-3-carboxylate, 4q



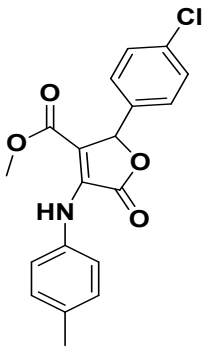
White solid (yield: 78 %); mp: 186-189 °C. IR (KBr): ν 3437, 3218, 2924, 1675, 1463, 1095 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 11.87 (s, 1H), 7.76 (d, 2H, *J* = 7.6 Hz), 7.49-7.33 (m, 8H), 7.27 (t, 1H, *J* = 7.6 Hz), 6.27 (s, 1H), 3.78 (s, 3H) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 164.7, 163.2, 153.3, 137.2, 137.0, 129.4, 129.0, 128.7, 128.4, 126.1, 123.3, 112.7, 61.3, 51.9 ppm. ESI-MS: *m/z* 378 $[M+1]^+$

Ethyl 5-oxo-4-((2-oxo-2H-chromen-3-yl)amino)-2-(p-tolyl)-2,5-dihydrofuran-3-carboxylate, 4r

White solid (yield: 78 %); mp: 177-180 °C. IR (KBr): ν 3437, 3218, 2924, 1675, 1463, 1095 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 11.92 (s, 1H), 7.76 (d, 2H, *J* = 7.6 Hz), 7.49-7.39 (m, 6H), 7.37-7.33 (m, 1H), 7.27 (t, 1H, *J* = 7.6 Hz), 6.26 (s, 1H), 4.27-4.16 (m, 2H), 1.27 (t, 3H, *J* = 6.8 Hz) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 164.4, 162.4, 153.0, 136.9, 136.7, 129.1, 128.6, 128.3, 128.1, 125.7, 122.9, 112.6, 61.0, 60.1, 14.4 ppm. ESI-MS: *m/z* 406 $[M+1]^+$

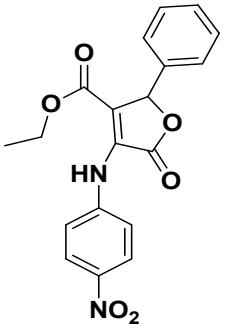
Methyl 2-(4-chlorophenyl)-5-oxo-4-(p-tolylamino)-2,5-dihydrofuran-3-carboxylate*, *4s

White solid (yield: 89%); mp: 180-182 °C. IR (KBr): ν 3442, 3229, 2926, 1672, 1468, 1090 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.88 (s, 1H), 7.21 (d, 2H, *J* = 8.4 Hz), 7.15 (d, 2H, *J* = 8.4 Hz), 7.07 (d, 2H, *J* = 8.0 Hz), 7.01(d, 2H, *J* = 8.0 Hz), 5.61 (s, 1H), 3.68 (s, 3H), 2.19 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.9, 162.6, 156.1, 136.0, 134.3, 133.6, 133.2, 129.6, 128.9, 128.8, 122.4, 112.3, 61.0, 52.0, 20.8 ppm. ESI-MS: *m/z* 357 $[M]^+$, 359 $[M+2]^+$



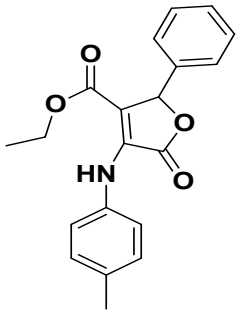
Ethyl 4-((4-nitrophenyl)amino)-5-oxo-2-phenyl-2,5-dihydrofuran-3-carboxylate*, *4t

White solid (yield: 90%); mp: 177-179 °C. IR (KBr): ν 3446, 2990, 1734, 1453, 1026 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 9.32 (s, 1H), 8.30 (d, 2H, *J* = 8.4 Hz), 7.96 (d, 2H, *J* = 8.0 Hz), 7.46-7.40 (m, 5H), 5.97 (s,1H), 4.37 (q, 2H, *J* = 7.2 Hz), 1.37 (t, 3H, *J* = 7.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.5, 162.9, 155.3, 143.7, 141.6, 133.8, 128.7, 128.6, 126.9, 124.3, 120.2, 113.7, 61.3, 60.7, 13.5 ppm. HRMS (ESI) m/z: $[M + 1]^+$ calcd, 369.1084; found, 369.1087.



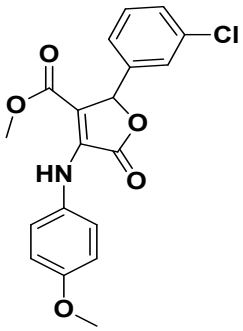
Ethyl 5-oxo-2-phenyl-4-(p-tolylamino)-2,5-dihydrofuran-3-carboxylate*, *4u

White solid (yield: 85%); mp: 185-187 °C. IR (KBr): ν 3307, 2984, 1690, 1494, 1098 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 9.12 (s, 1H), 7.38 (d, 2H, *J* = 8.4 Hz), 7.32-7.25 (m, 4H), 7.11 (d, 2H, *J* = 8.0 Hz), 5.74 (s, 1H), 4.23 (q, 2H, *J* = 7.2 Hz), 2.29 (s, 3H), 1.22 (t, 3H, *J* = 7.0 Hz) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.4, 163.0, 156.9, 136.0, 135.4, 133.9, 128.8, 127.8, 127.8, 122.6, 113.2, 61.9, 61.4, 31.2, 21.1, 14.2 ppm. ESI-MS: *m/z* 337 $[M]^+$

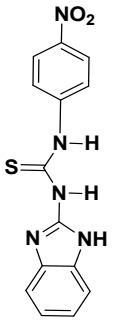


Methyl 2-(3-chlorophenyl)-4-((4-methoxyphenyl)amino)-5-oxo-2,5-dihydrofuran-3-carboxylate, 4v

White solid (yield: 85%); mp: 177-179 °C. IR (KBr): ν 3424, 3187, 2958, 1673, 1470, 1085 cm^{-1}. ^1H NMR ($CDCl_3$, 400 MHz): δ 8.95 (s, 1H), 7.20 (d, 3H, *J* = 9.2 Hz), 7.13-7.10 (m, 2H), 7.01 (d, 1H, *J* = 8.4 Hz), 6.74 (d, 2H, *J* = 8.6 Hz), 5.54 (s, 1H), 3.68 (s, 3H), 3.67 (s, 3H) ppm; ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.9, 162.6, 157.7, 156.3, 137.2, 134.4, 129.9, 128.8, 128.6, 127.5, 125.7, 124.4, 114.3, 112.1, 61.5, 55.3, 52.1 ppm. . HRMS (ESI) m/z: $[M + 1]^+$ calcd, 374.0793; found, 374.0795.

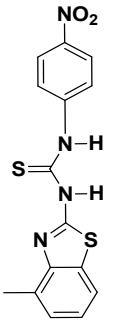


1-(1H-benzo[d]imidazol-2-yl)-3-(4-nitrophenyl) thiourea 3a (BINPT)



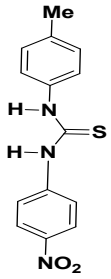
Greenish yellow solid (yield: 65%); mp: 219–221 °C. IR (KBr): ν 3259, 1621, 1582, 1547, 1452, 1323, 1295, 1246, 1112, 848, 746 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 13.02 (s, 2H), 10.46 (s, 1H), 8.22–8.17 (m, 4H), 7.61–7.58 (m, 2H), 7.34–7.31 (m, 2H) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 153.2, 147.0, 141.2, 129.2, 124.9, 123.5, 121.4, 120.2, 112.2, 111.8 ppm. ESI-MS: *m/z* 314 $[M+1]^+$

1-(4-methylbenzo[d]thiazol-2-yl)-3-(4-nitrophenyl) thiourea 3b (MBNPT)



Off-white solid (yield: 54%); mp: 227–230 °C. IR (KBr): ν 2956, 1574, 1515, 1335, 1264, 1193, 848, 740, 693 cm^{-1}. ^1H NMR (DMSO-d_6, 400 MHz): δ 13.20 (s, 1H), 10.95 (s, 1H), 8.20 (d, 2H, *J* = 8.8 Hz), 8.13 (d, 2H, *J* = 8.8 Hz), 7.72 (d, 1H, *J* = 7.2 Hz), 7.29–7.21 (m, 2H), 2.56 (S, 3H) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 145.6, 141.6, 127.9, 124.4, 123.8, 120.7, 119.9, 17.7 ppm. ESI-MS: *m/z* 345 $[M+1]^+$

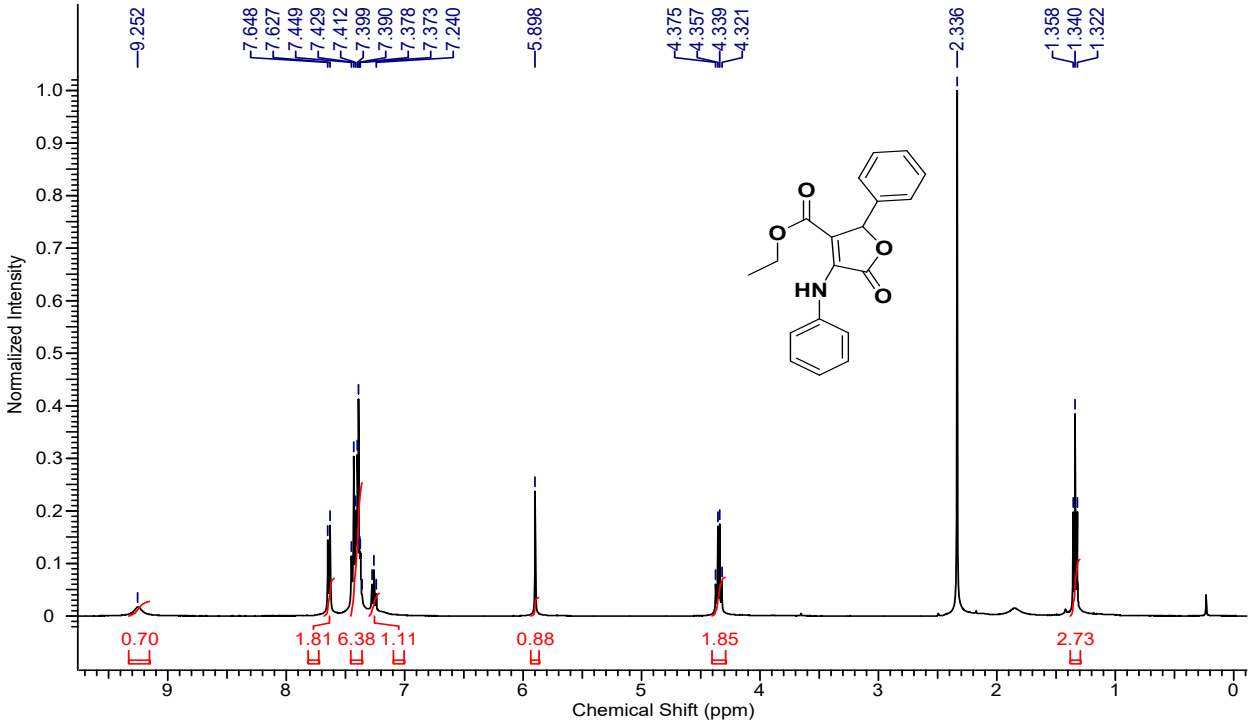
1-(4-nitrophenyl)-3-(p-tolyl)thiourea (NPTT)



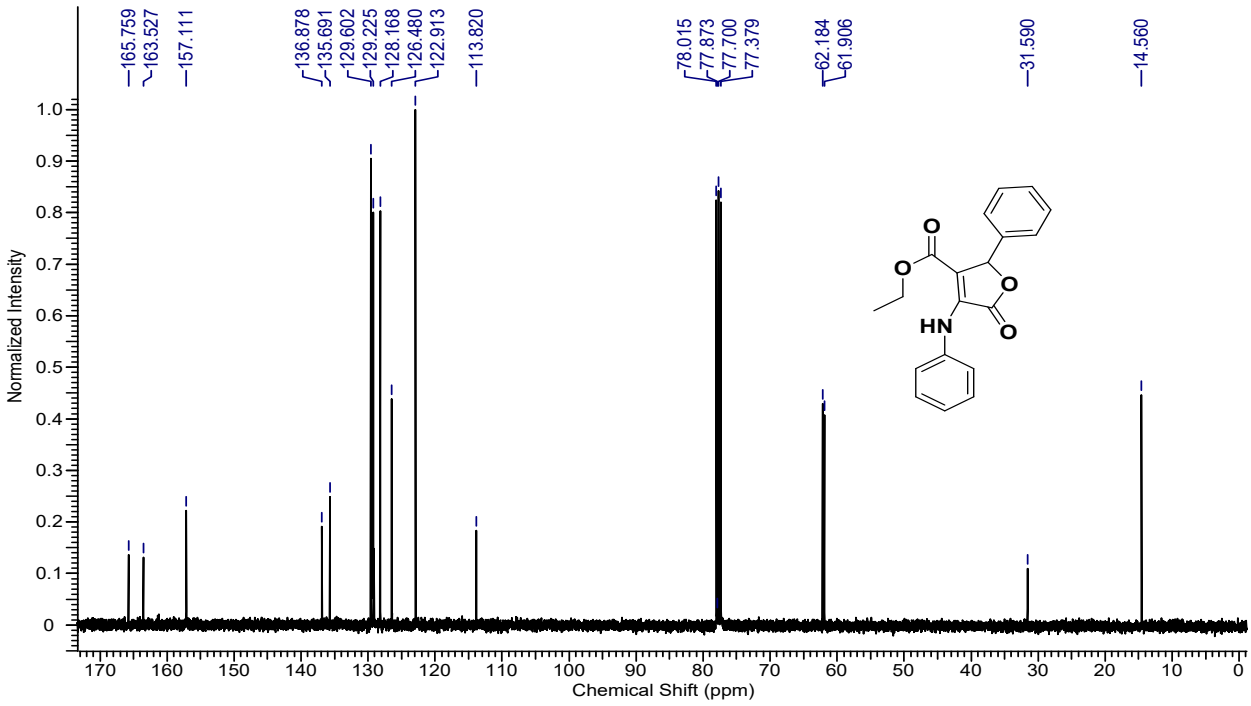
white solid (yield: 48%); mp: 212–213 °C. IR (KBr): ν 2952, 1573, 1517, 1339, 1260, 1191, 847, 742, 692 cm^{-1} . ^1H NMR (DMSO-d_6, 400 MHz): δ 13.20 (s, 1H), 10.95 (s, 1H), 8.20 (d, 2H, *J* = 8.8 Hz), 8.13 (d, 2H, *J* = 8.8 Hz), 7.72 (d, 1H, *J* = 7.2 Hz), 7.29–7.21 (m, 2H), 2.56 (S, 3H) ppm; ^{13}C NMR (DMSO-d_6, 100 MHz): δ 146.0,142.0, 128.4, 124.9, 124.3, 121.1, 120.4,18.1 ppm. ESI-MS: *m/z* 288 $[M+1]^+$

IX. ^1H & ^{13}C NMR spectra of the synthesized compounds

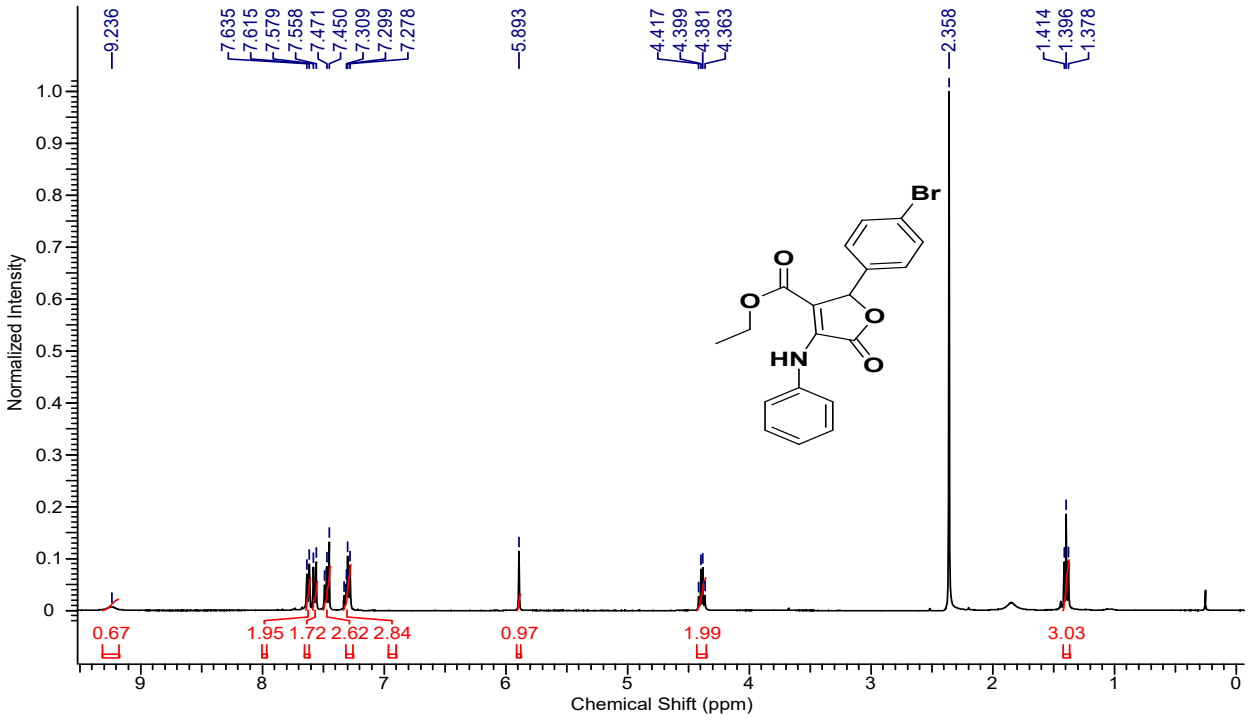
^1H NMR Spectrum of compound **4a**



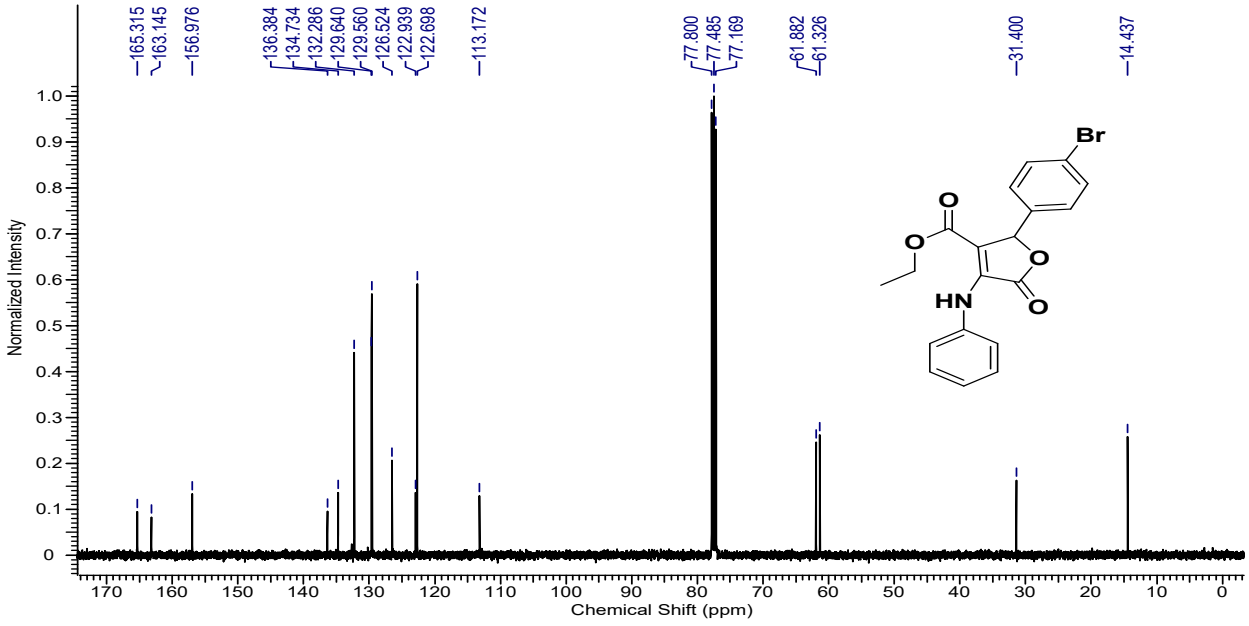
^{13}C NMR Spectrum of compound **4a**



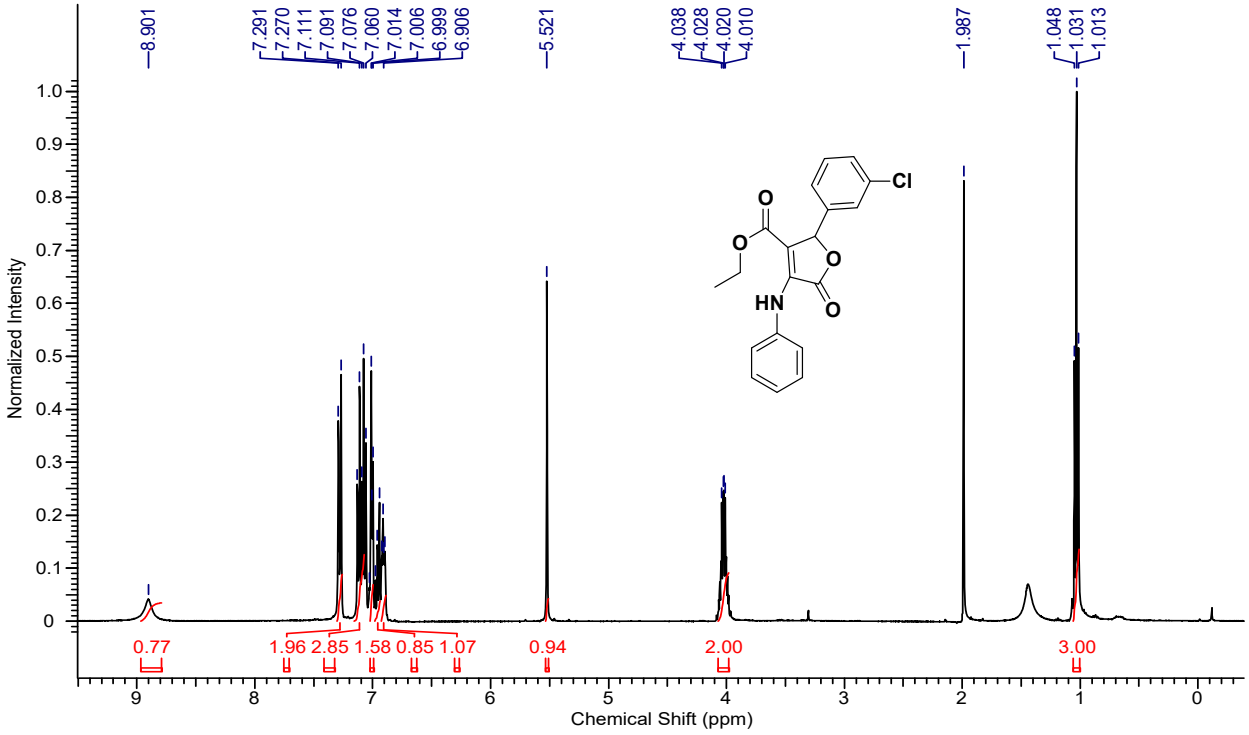
^{1}H NMR Spectrum of compound **4b**



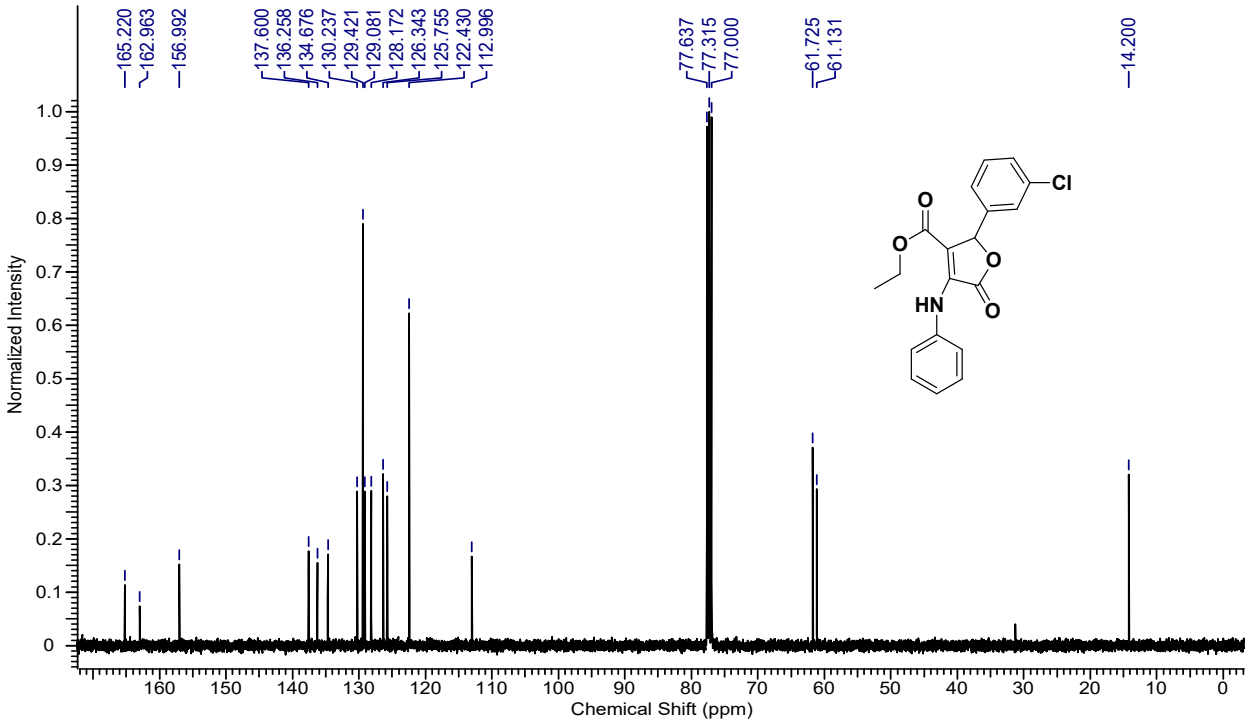
^{13}C NMR Spectrum of compound **4b**



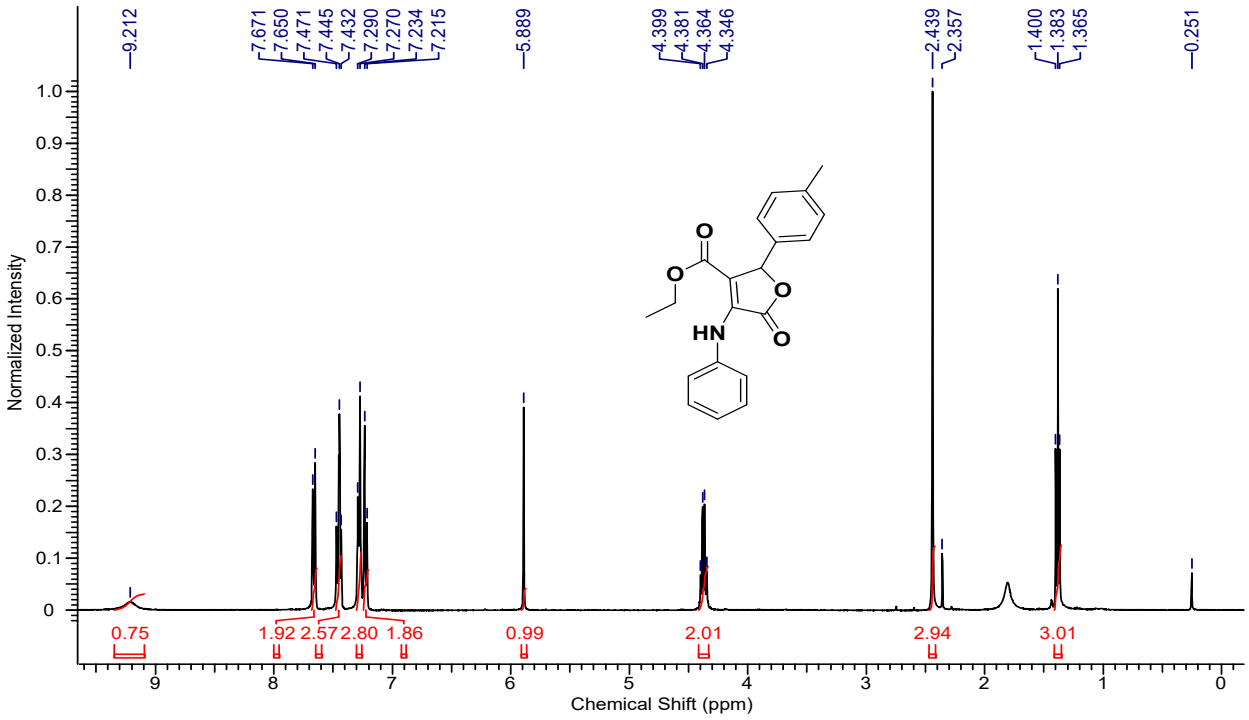
^{1}H NMR Spectrum of compound **4c**



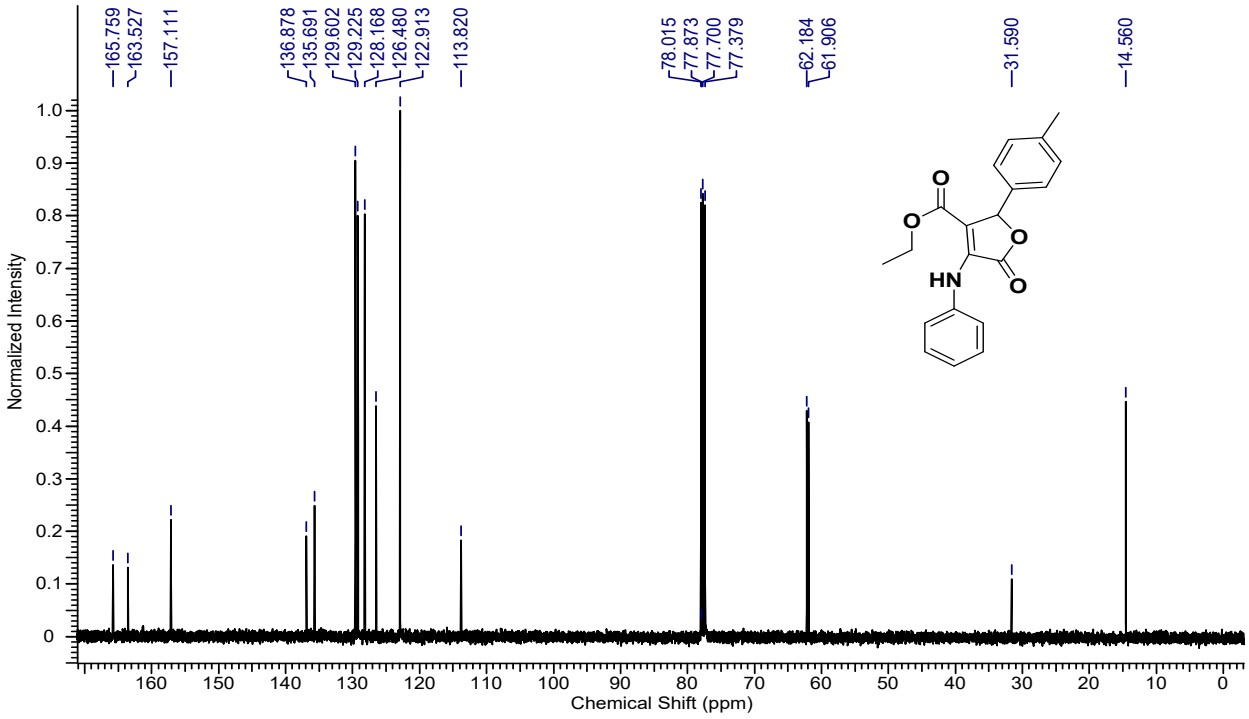
^{13}C NMR Spectrum of compound **4c**



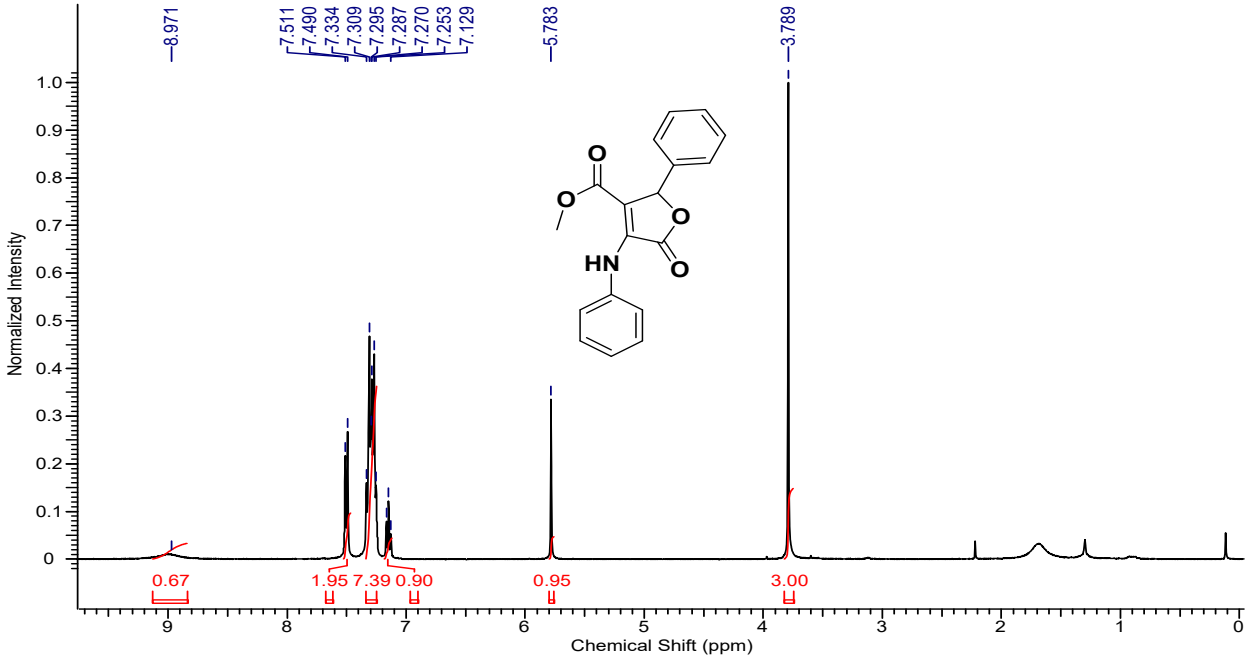
^{1}H NMR Spectrum of compound **4d**



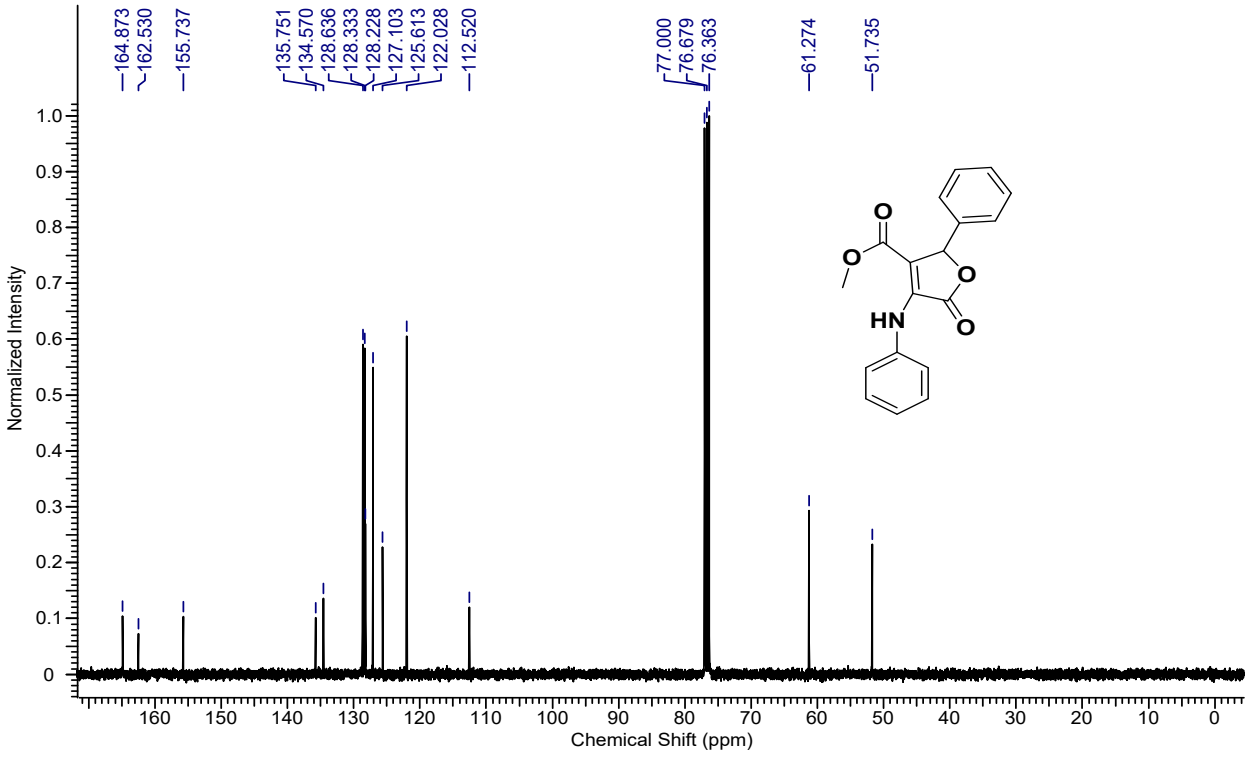
^{13}C NMR Spectrum of compound **4d**



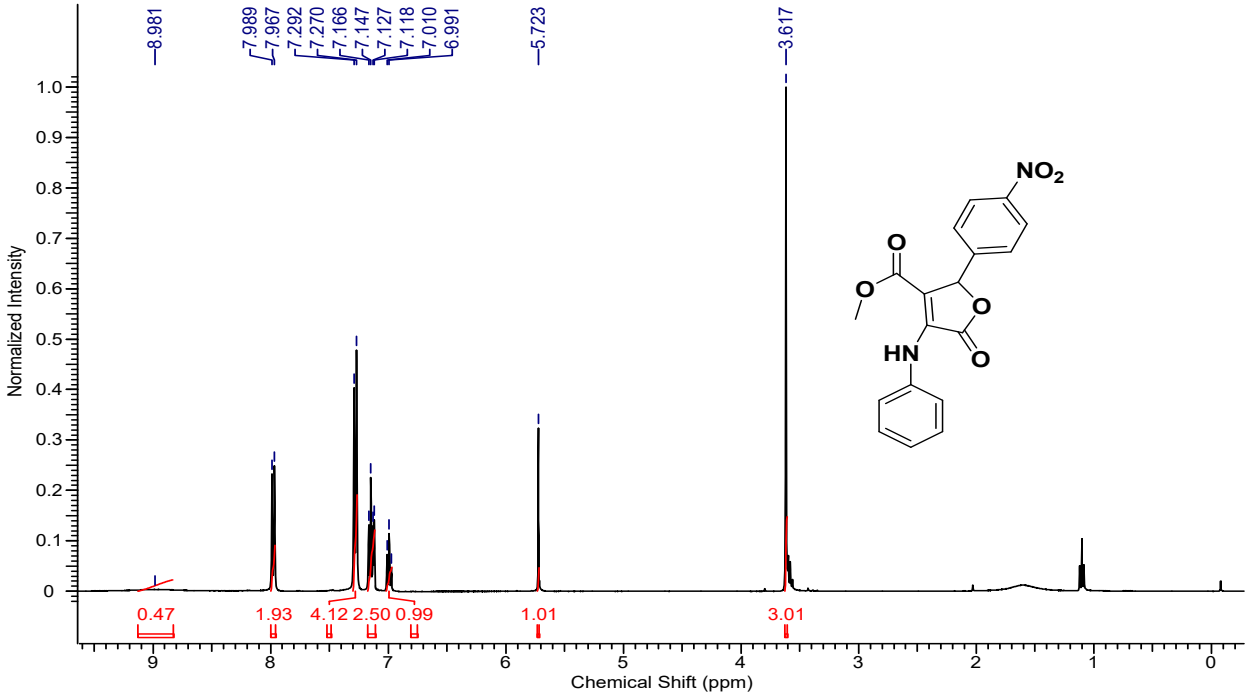
^{1}H NMR Spectrum of compound **4e**



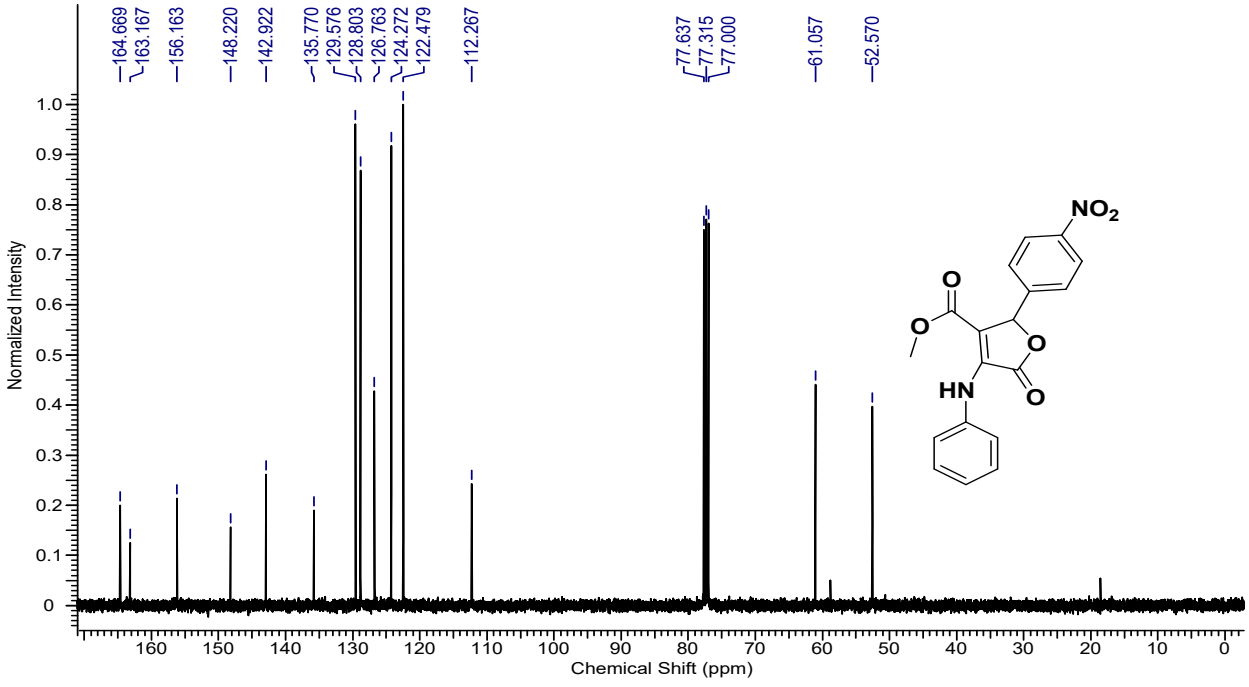
^{13}C NMR Spectrum of compound **4e**



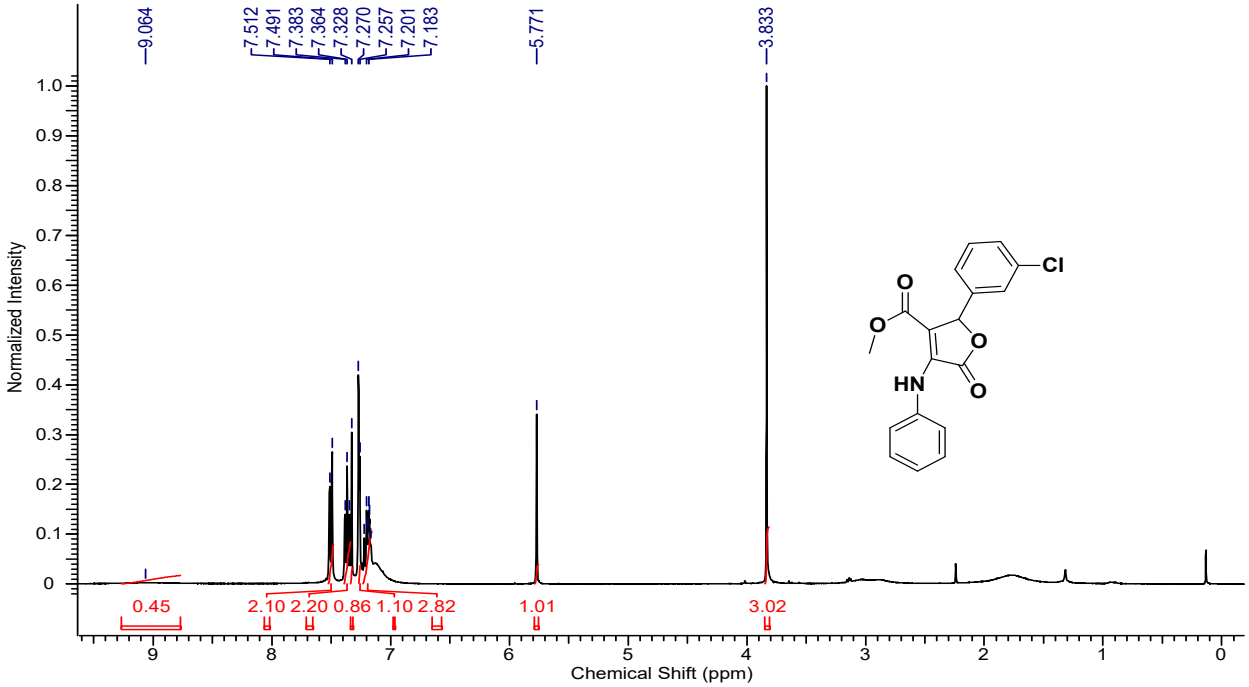
^{1}H NMR Spectrum of compound **4f**



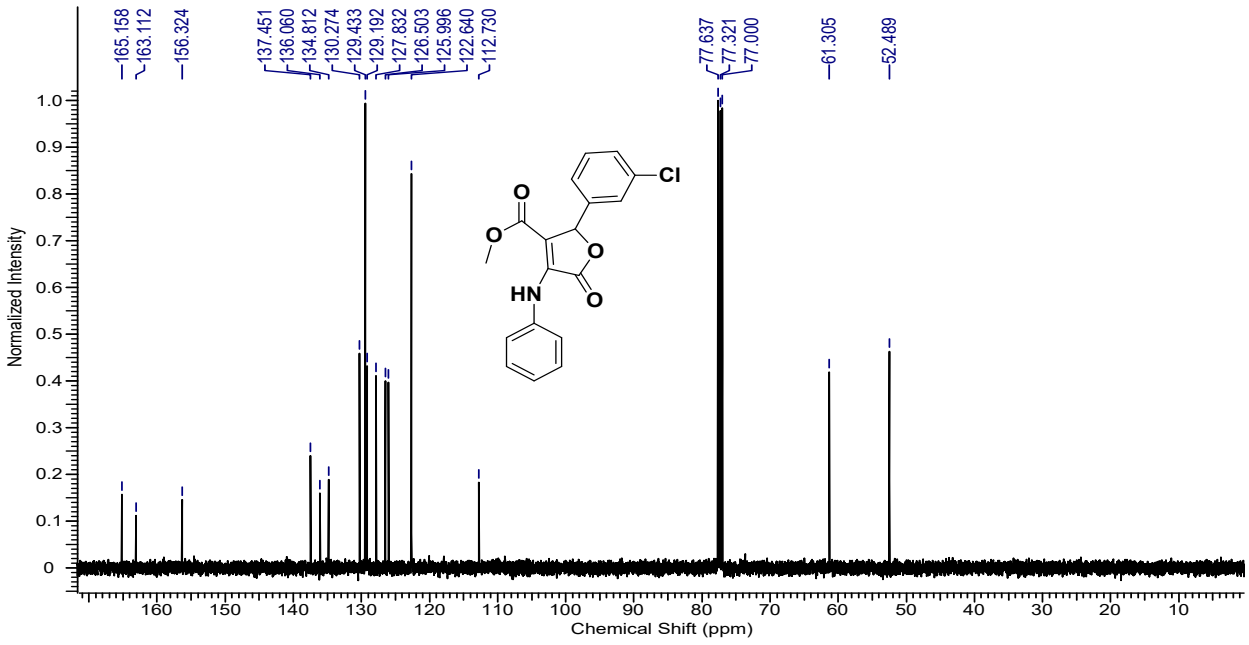
^{13}C NMR Spectrum of compound **4f**



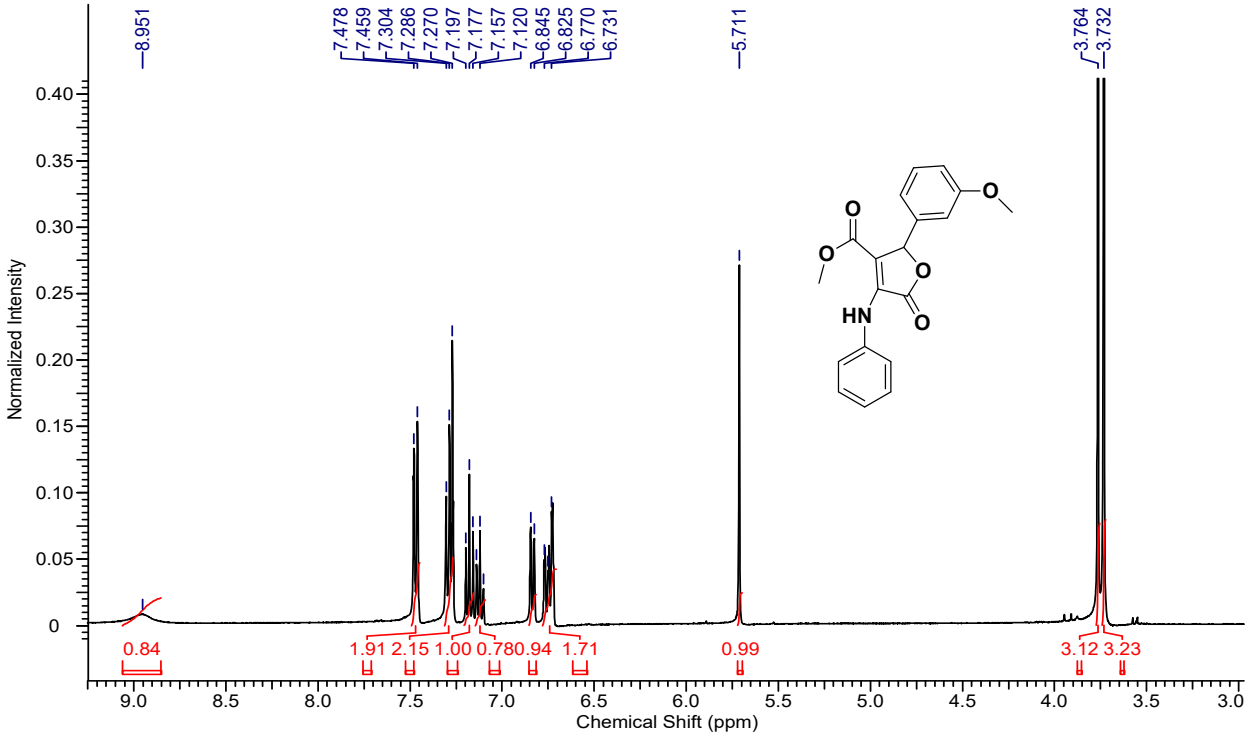
^{1}H NMR Spectrum of compound **4g**



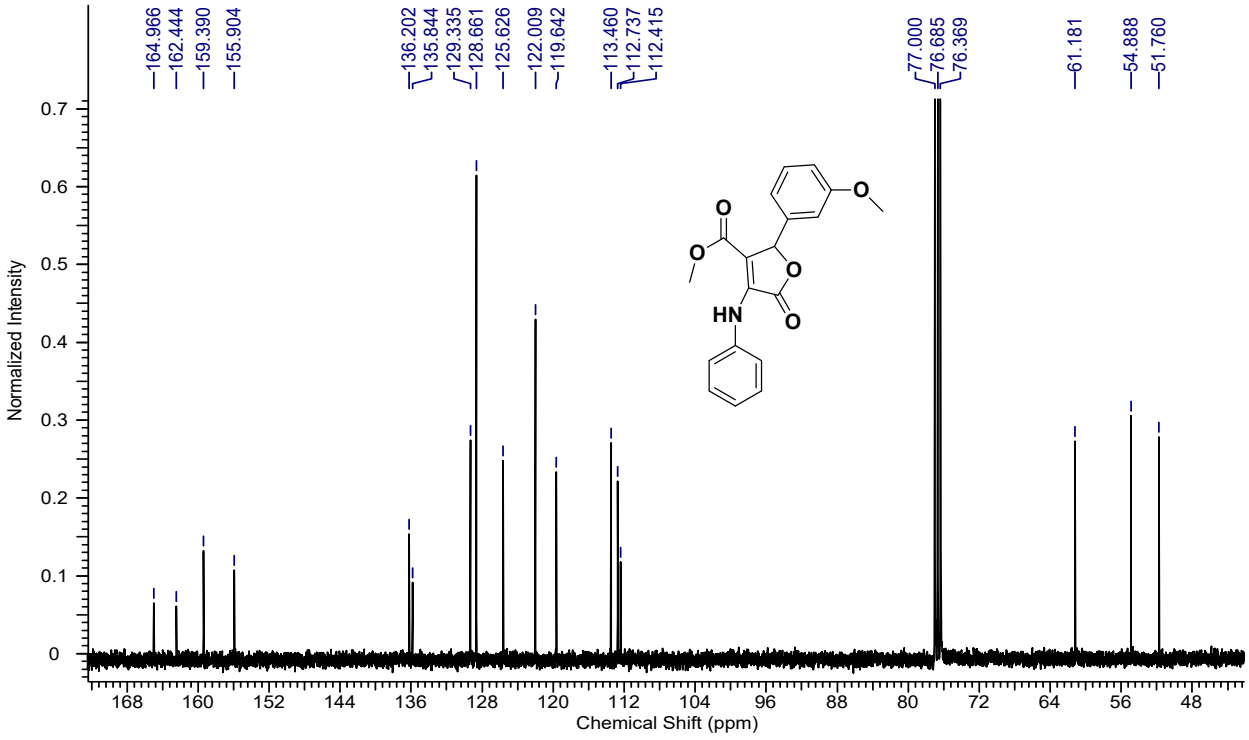
^{13}C NMR Spectrum of compound **4g**



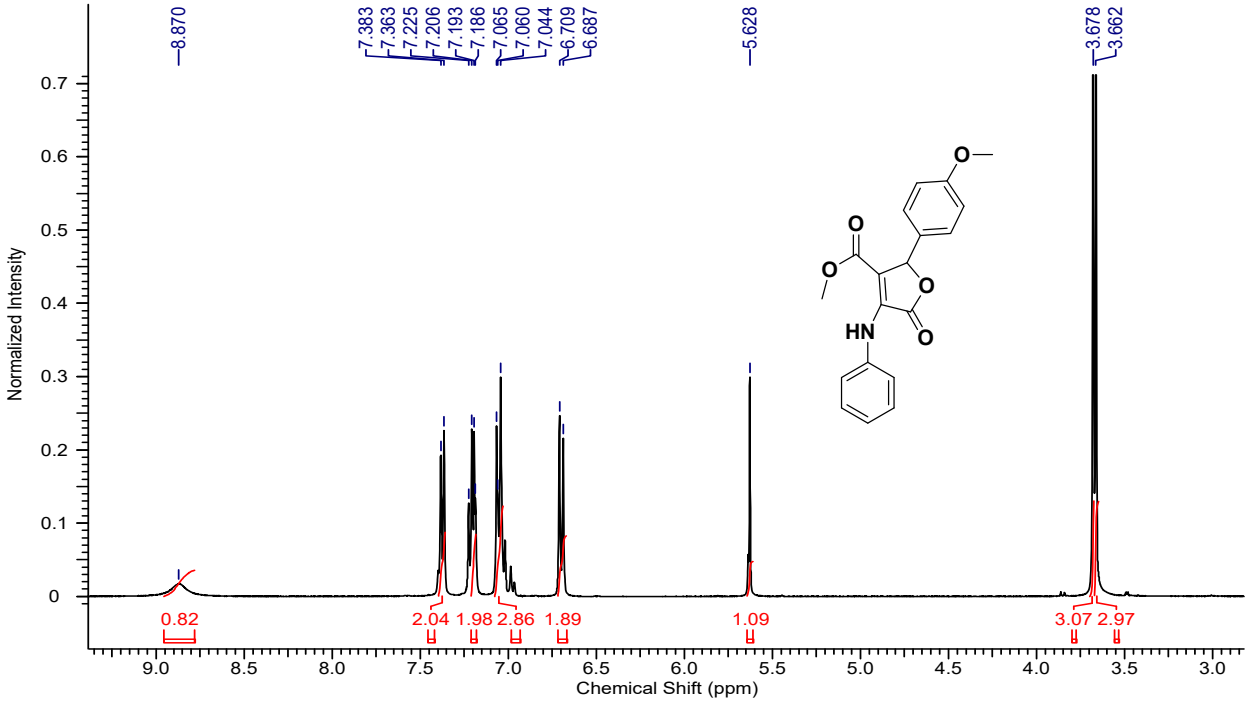
^{1}H NMR Spectrum of compound **4h**



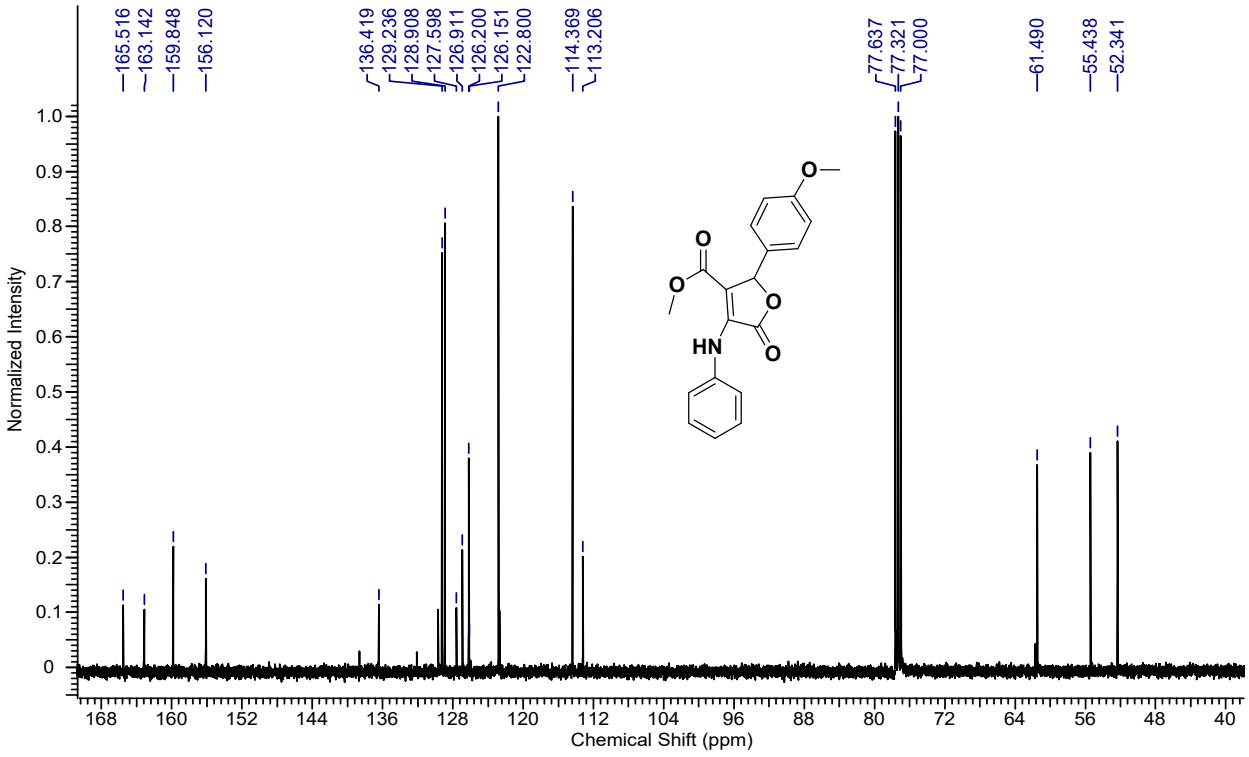
^{13}C NMR Spectrum of compound **4h**



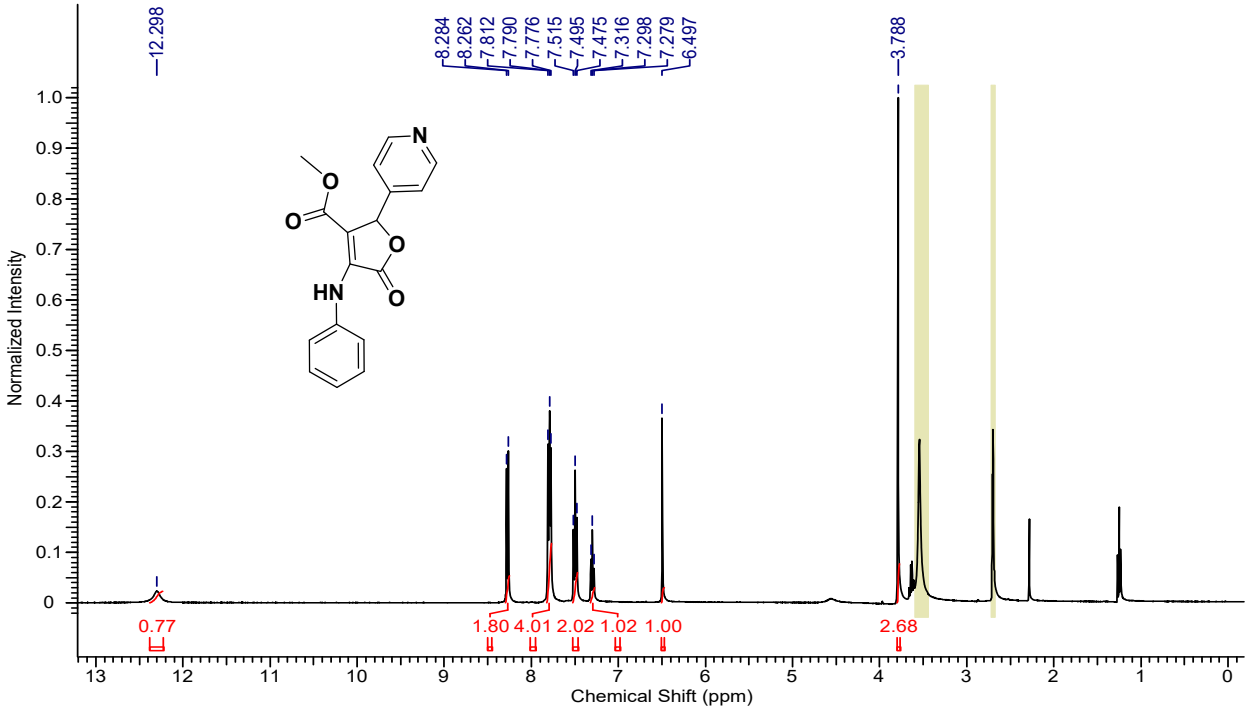
^{1}H NMR Spectrum of compound **4i**



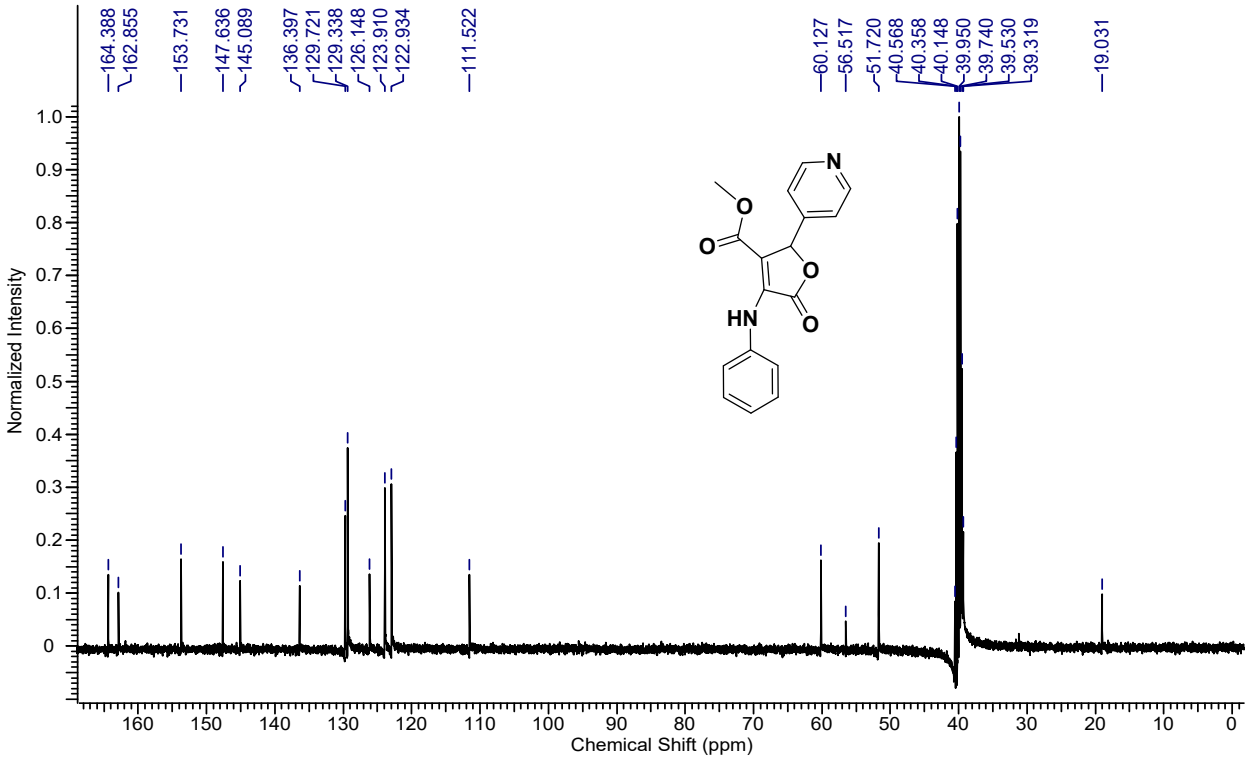
^{13}C NMR Spectrum of compound **4i**



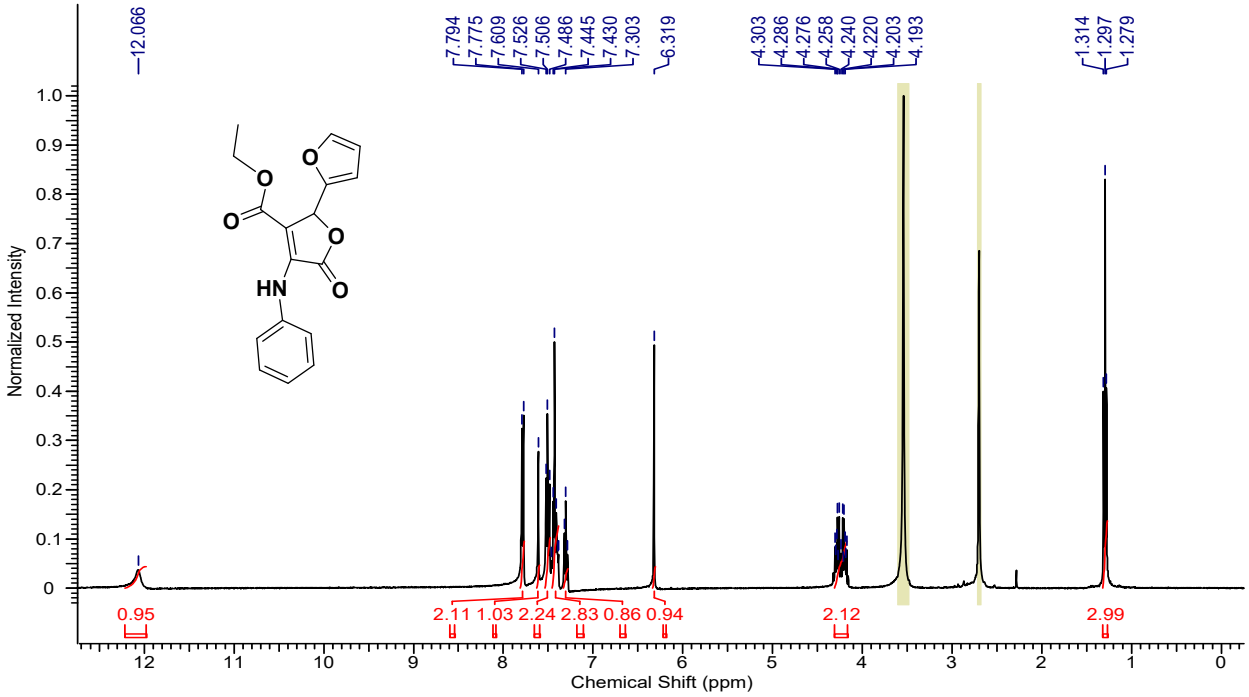
^{1}H NMR Spectrum of compound **4j**



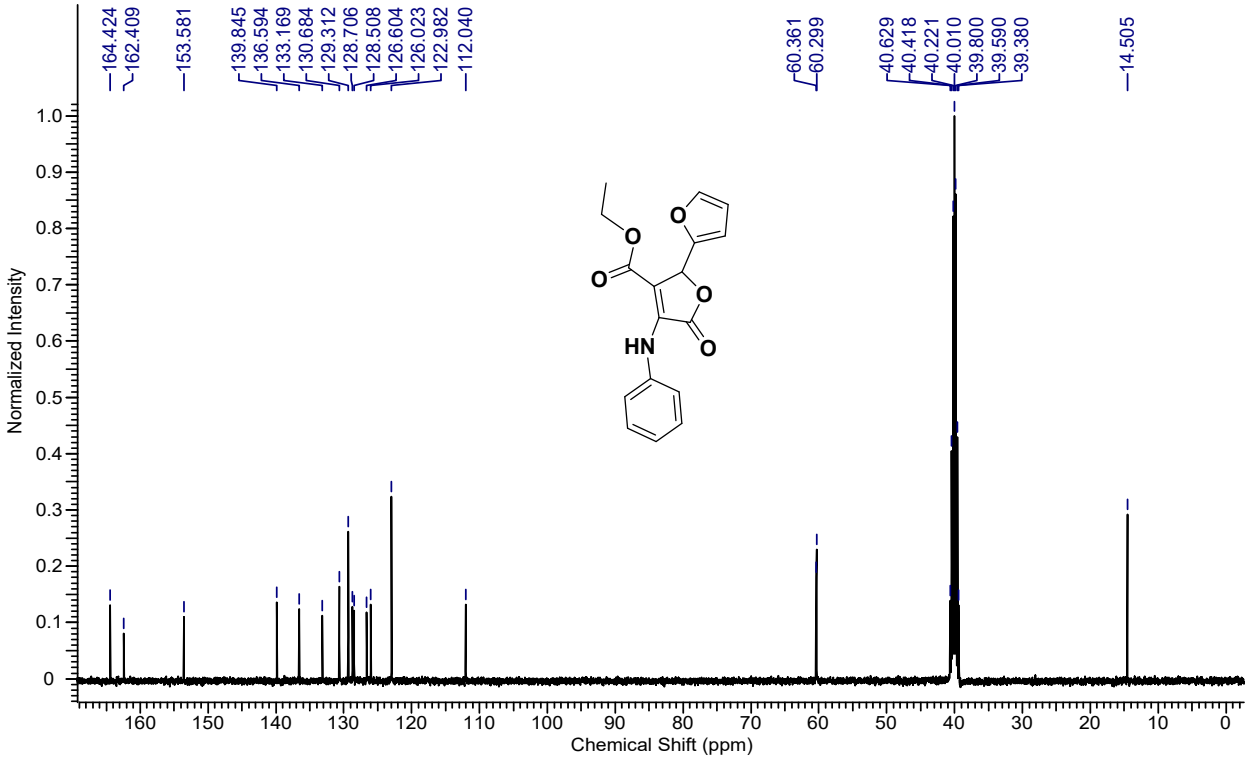
^{13}C NMR Spectrum of compound **4j**



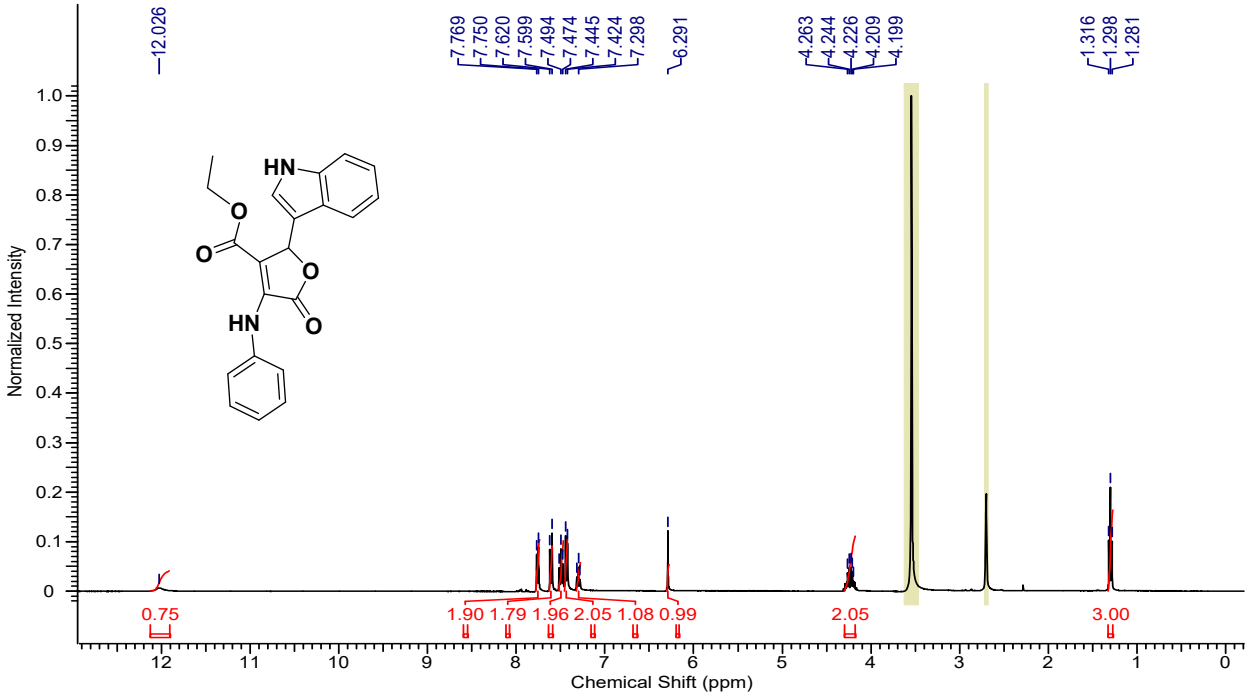
^{1}H NMR Spectrum of compound **4k**



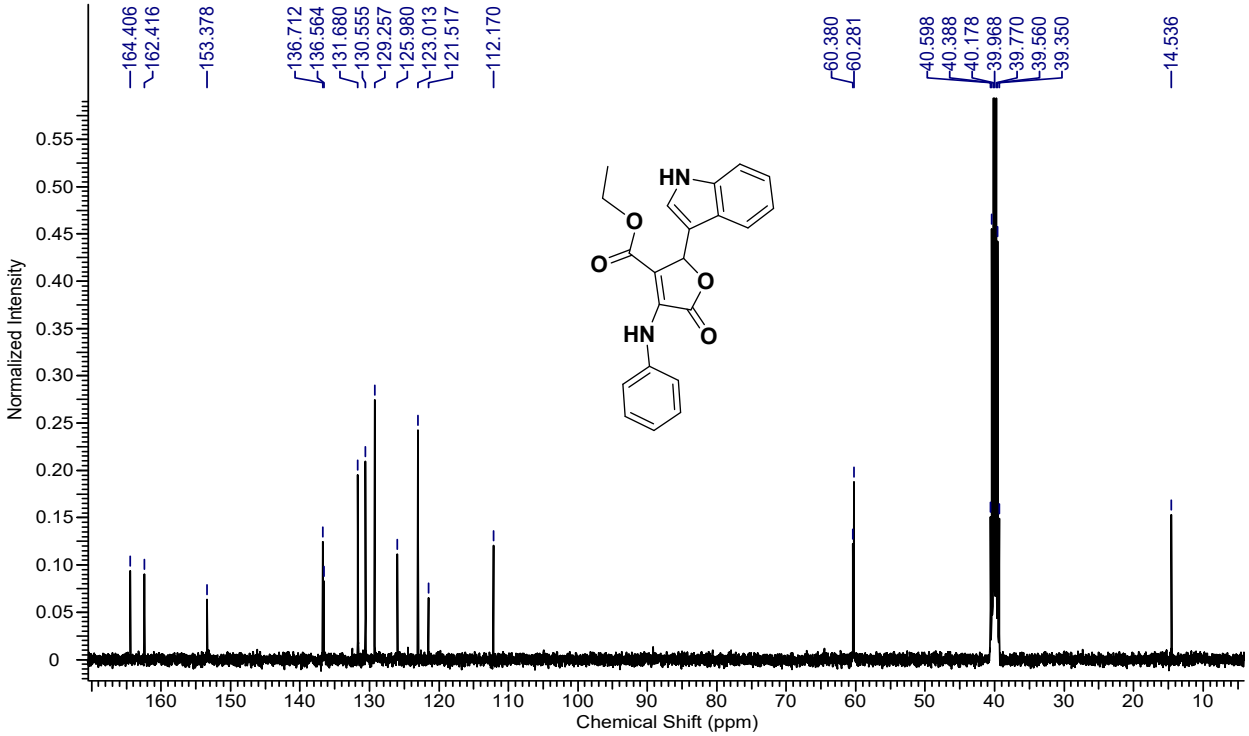
^{13}C NMR Spectrum of compound **4k**



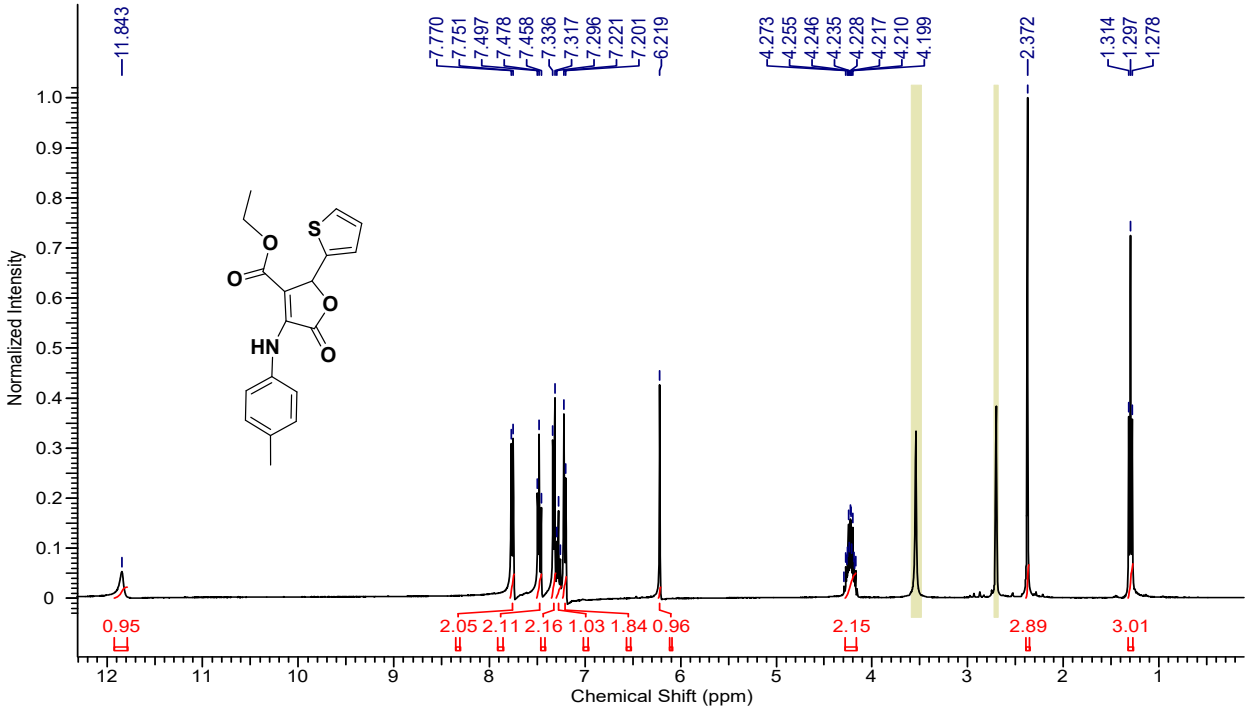
^{1}H NMR Spectrum of compound **4l**



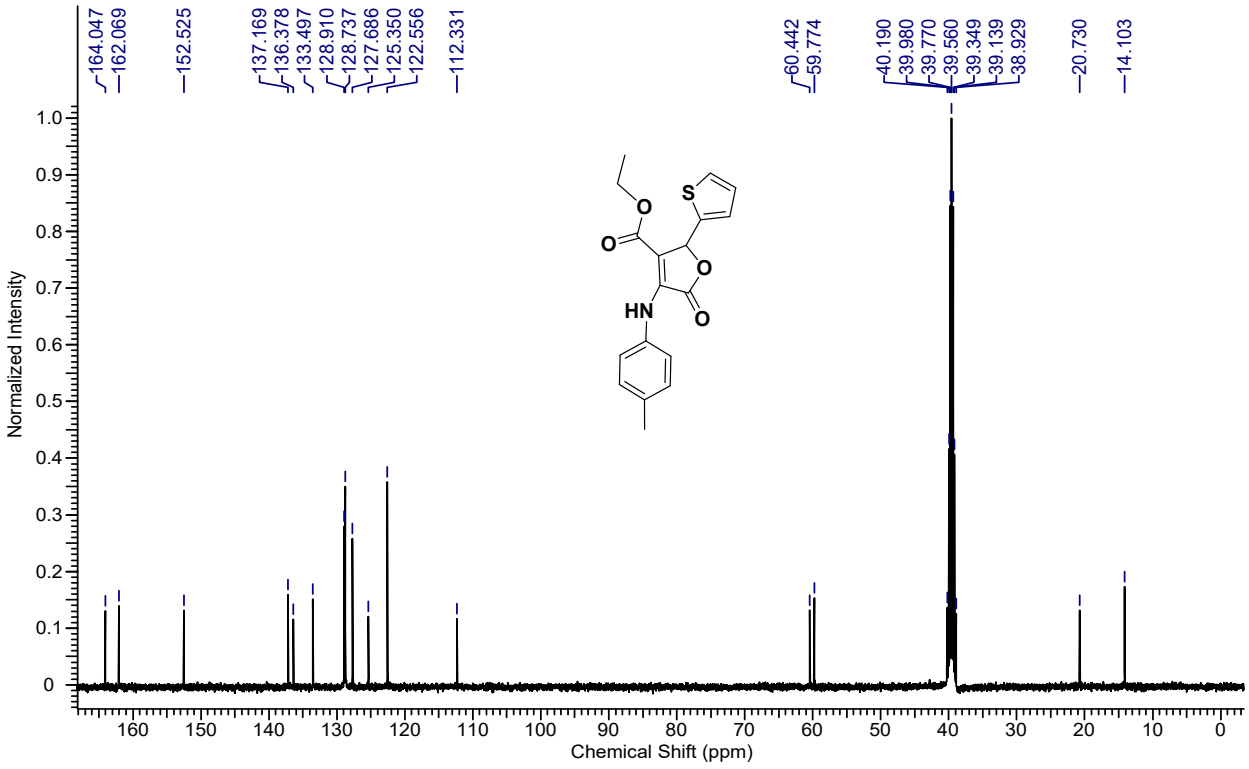
^{13}C NMR Spectrum of compound **4l**



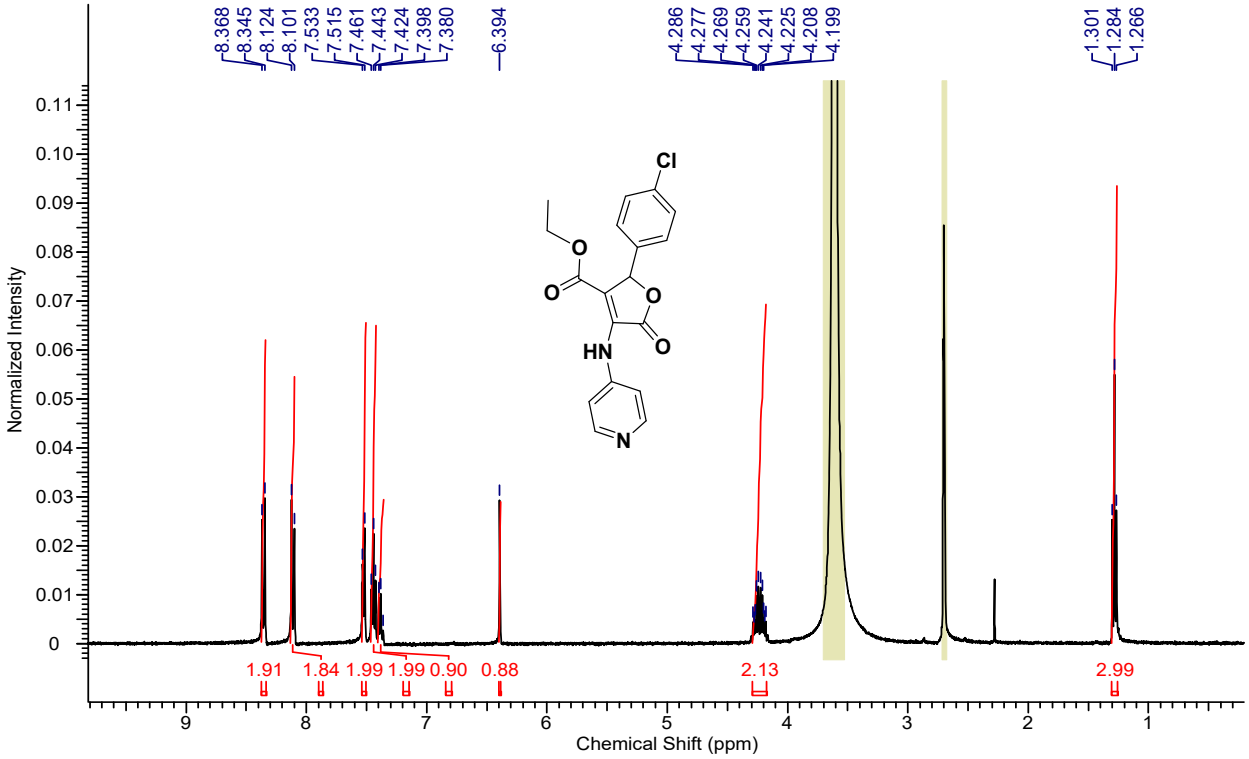
^{1}H NMR Spectrum of compound **4m**



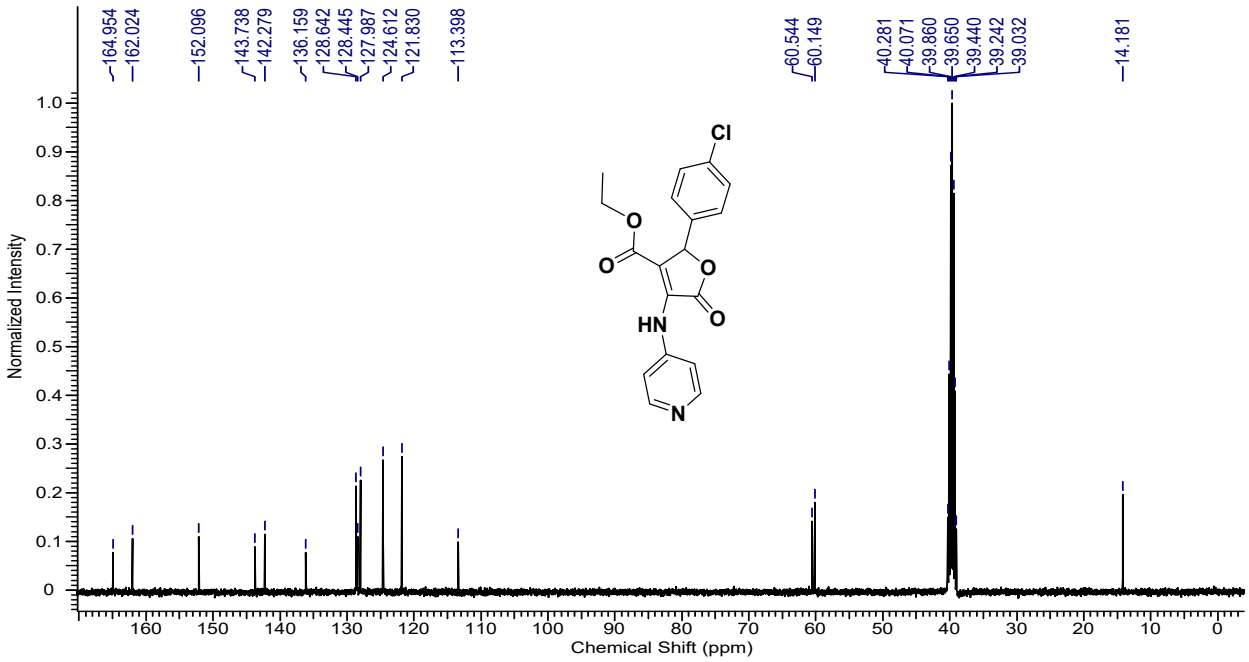
^{13}C NMR Spectrum of compound **4m**



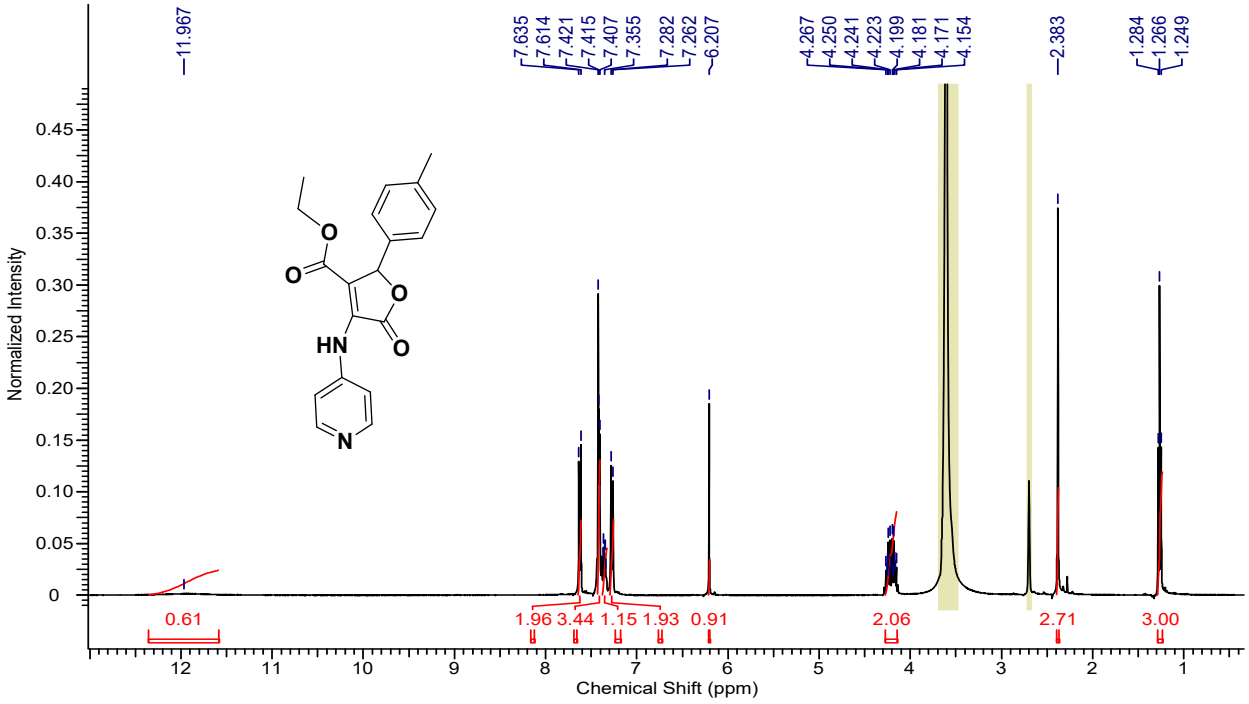
^{1}H NMR Spectrum of compound **4n**



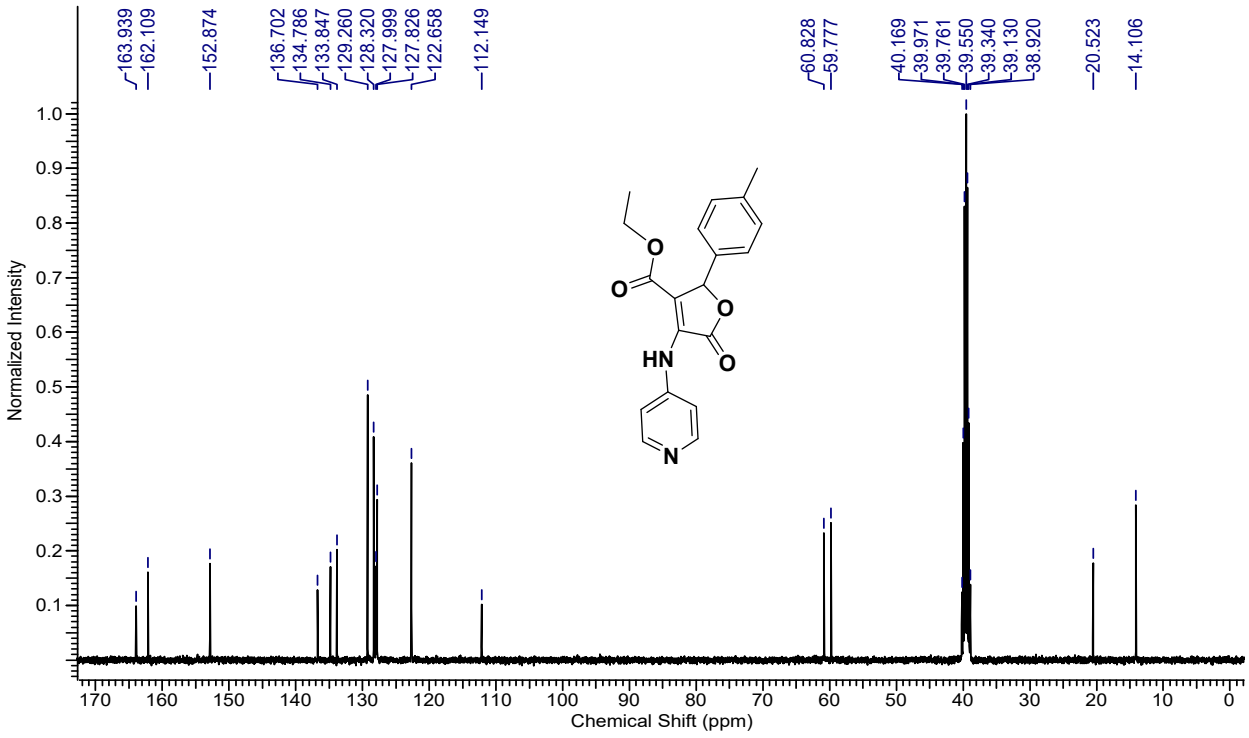
^{13}C NMR Spectrum of compound **4n**



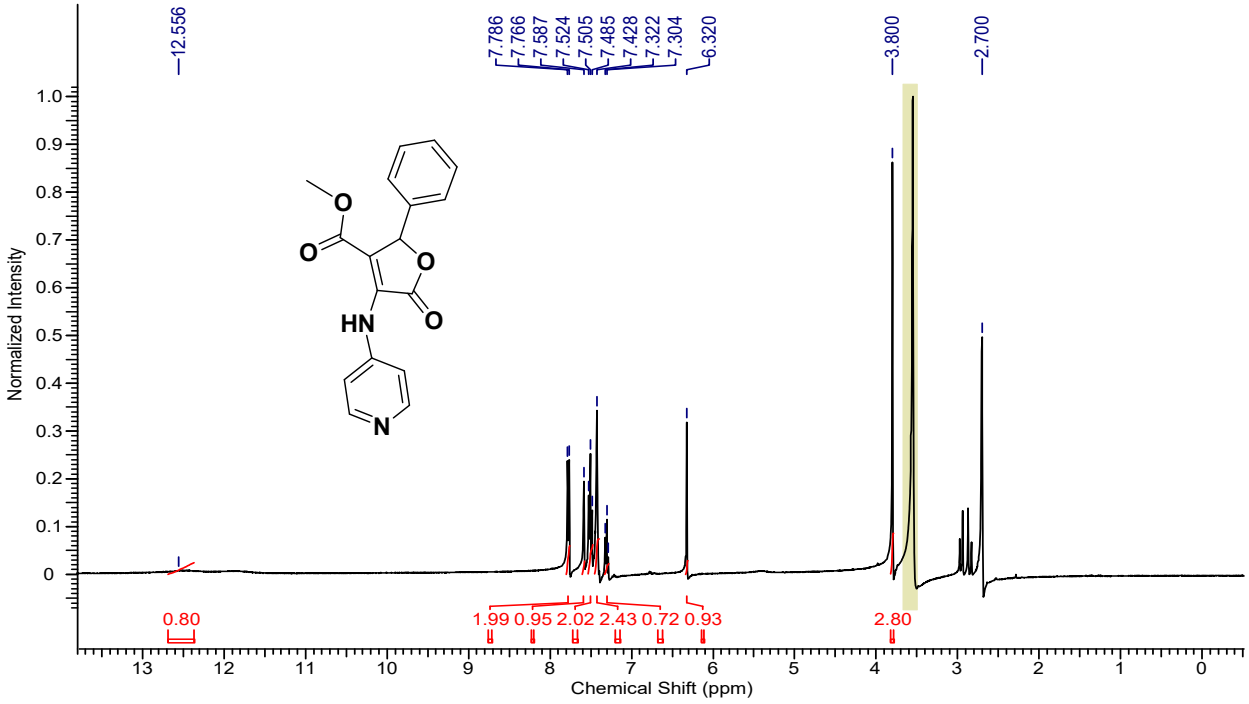
^{1}H NMR Spectrum of compound **4o**



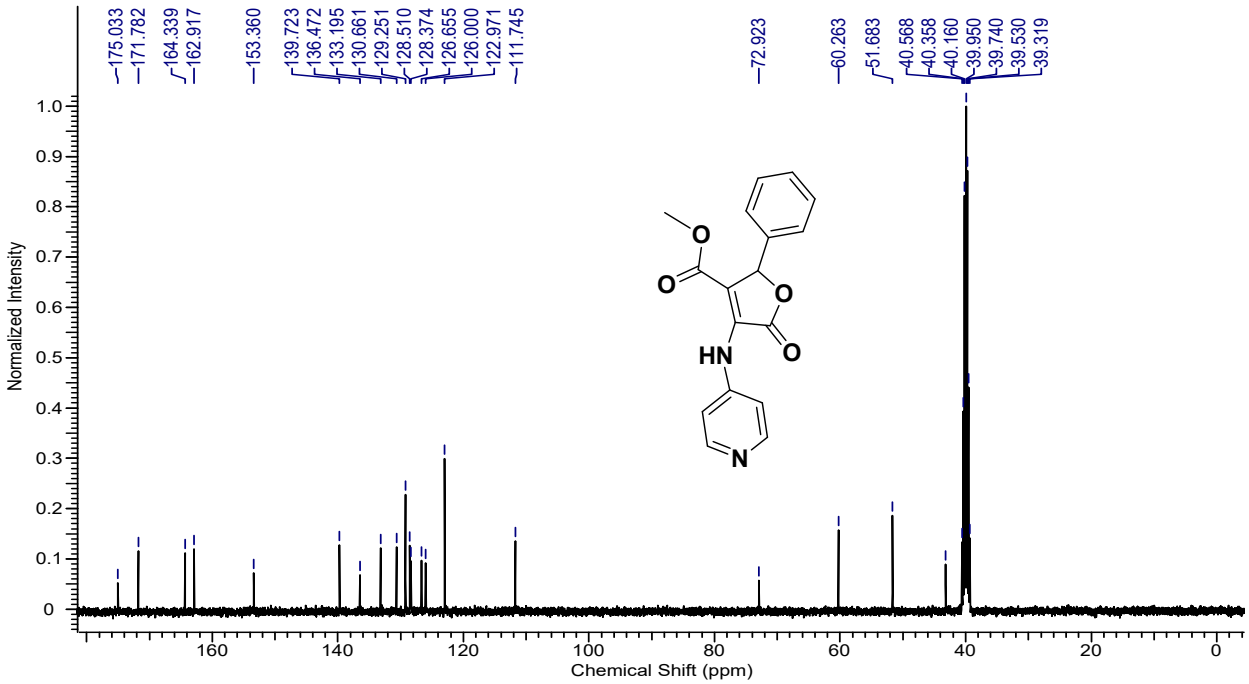
^{13}C NMR Spectrum of compound **4o**



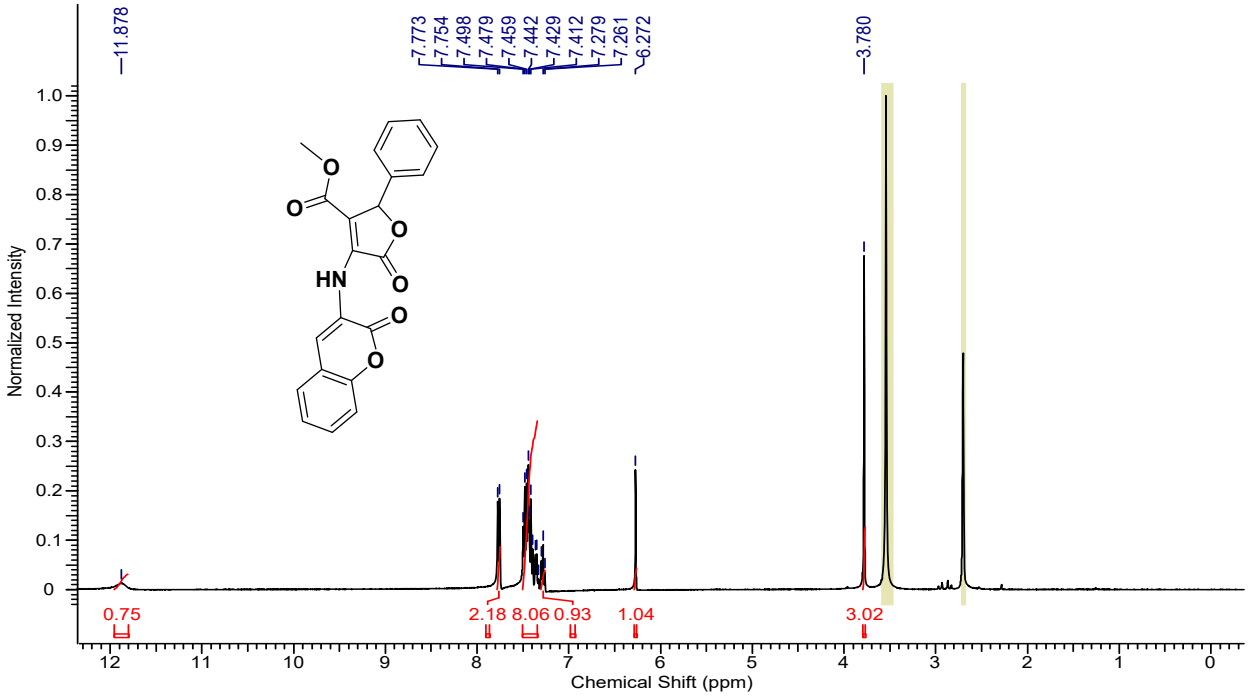
^{1}H NMR Spectrum of compound **4p**



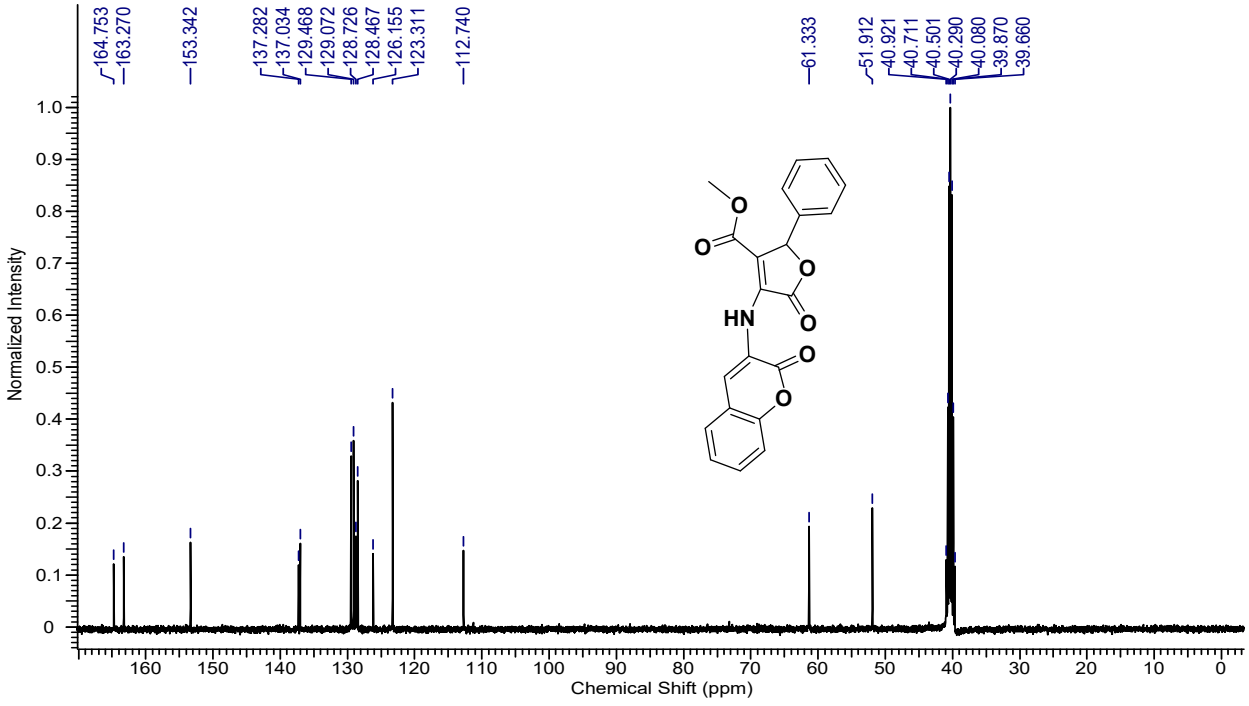
^{13}C NMR Spectrum of compound **4p**



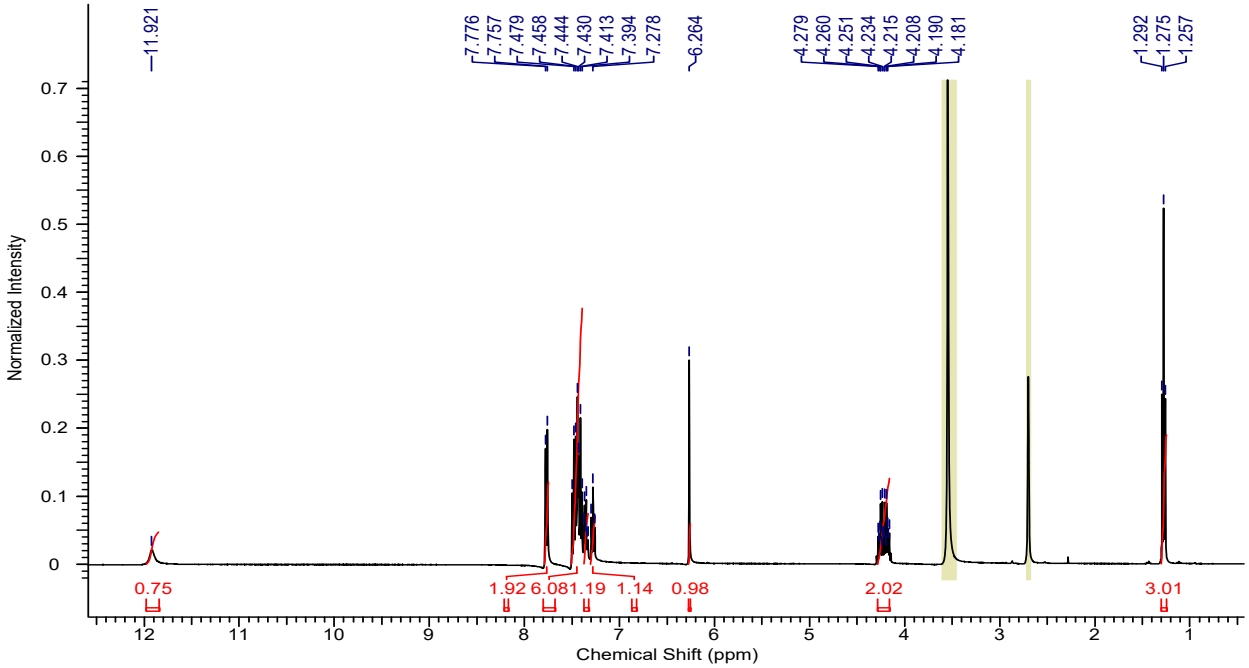
^{1}H NMR Spectrum of compound **4q**



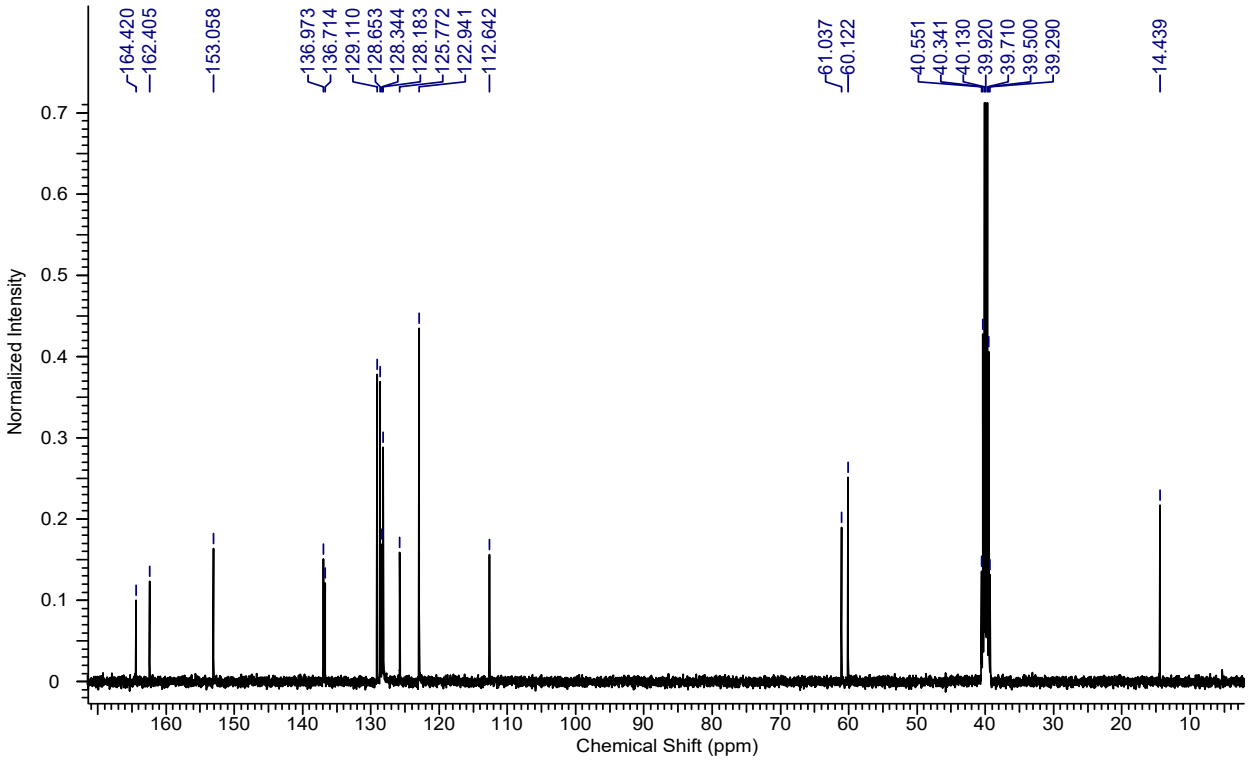
^{13}C NMR Spectrum of compound **4q**



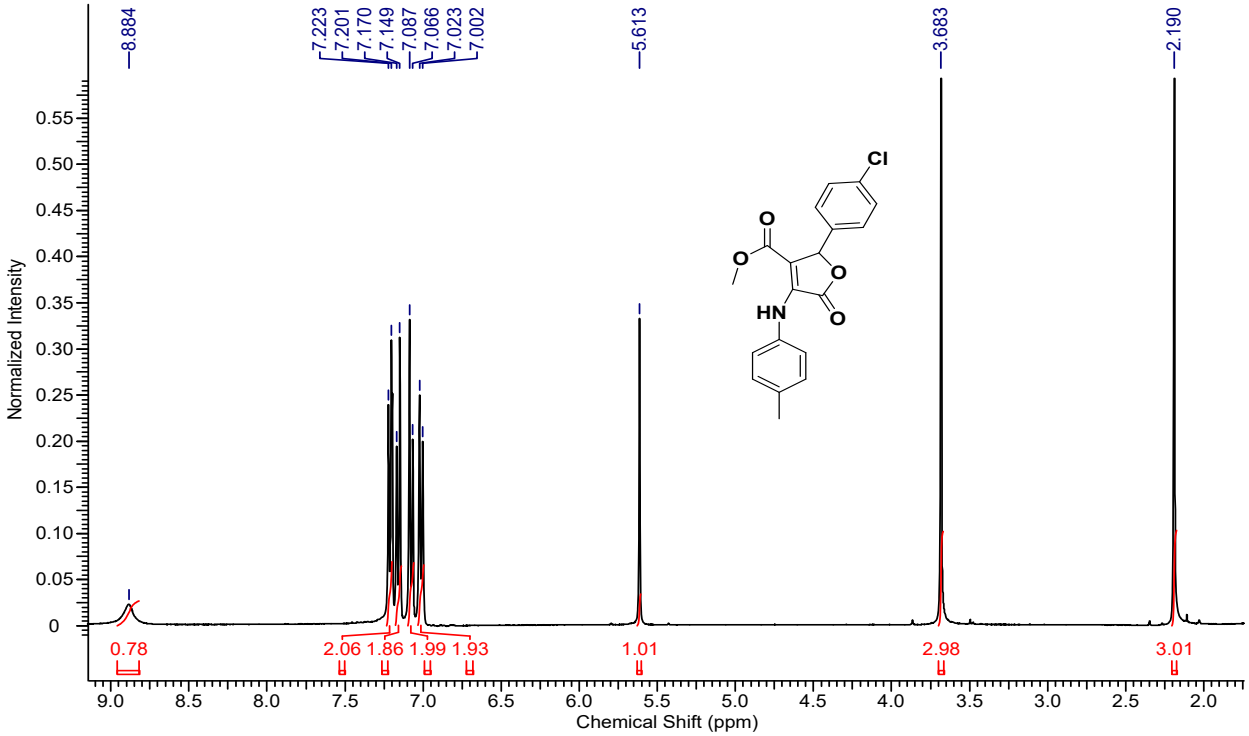
^{1}H NMR Spectrum of compound **4r**



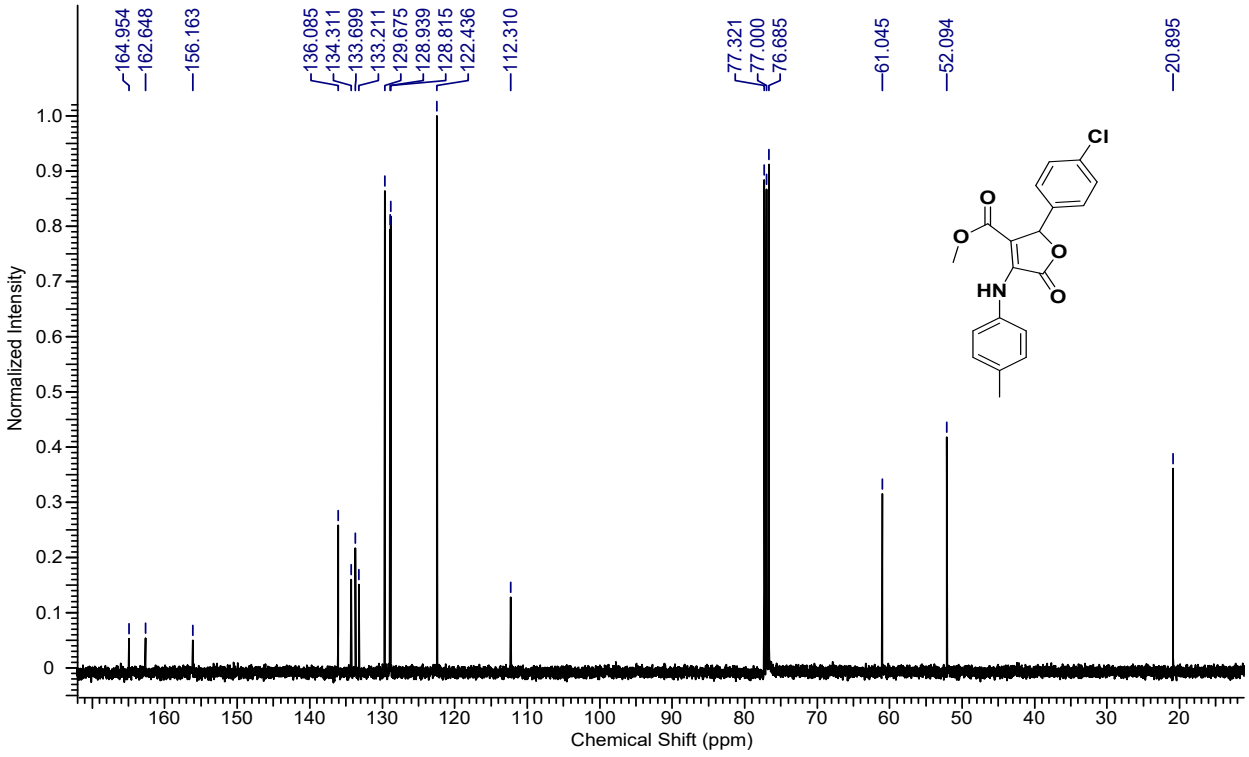
^{13}C NMR Spectrum of compound **4r**



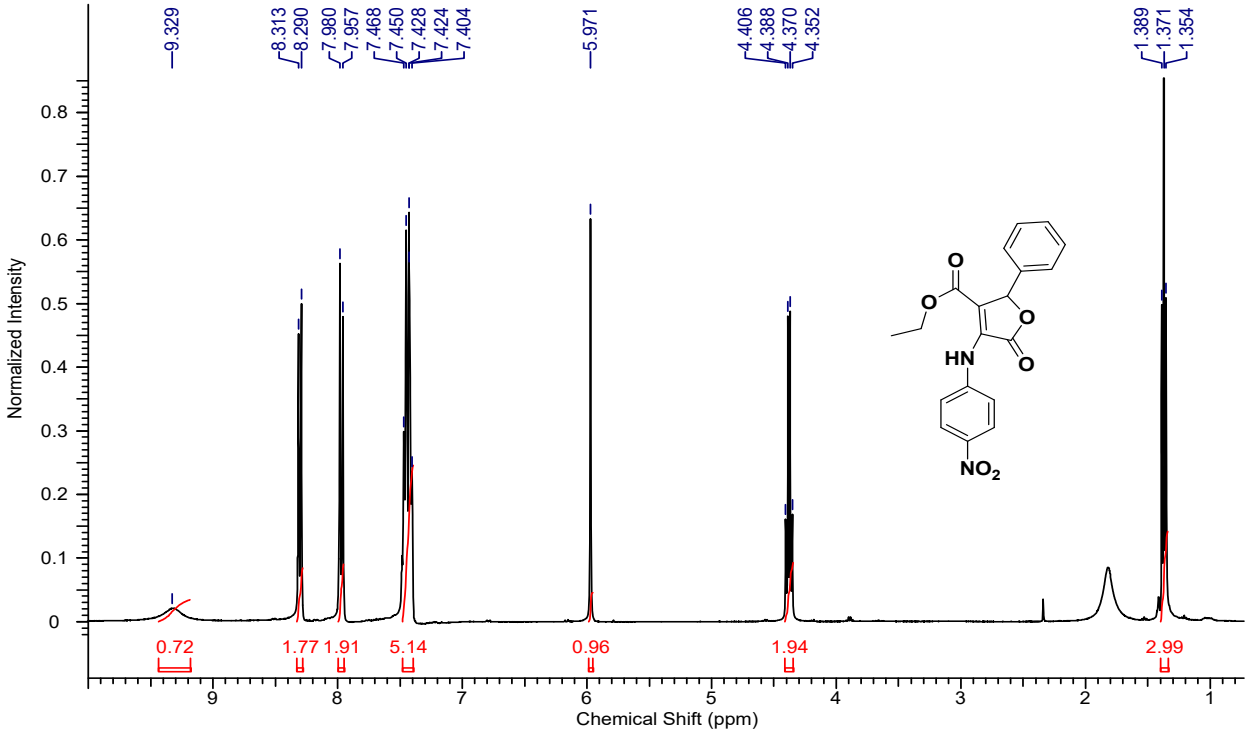
^{1}H NMR Spectrum of compound **4s**



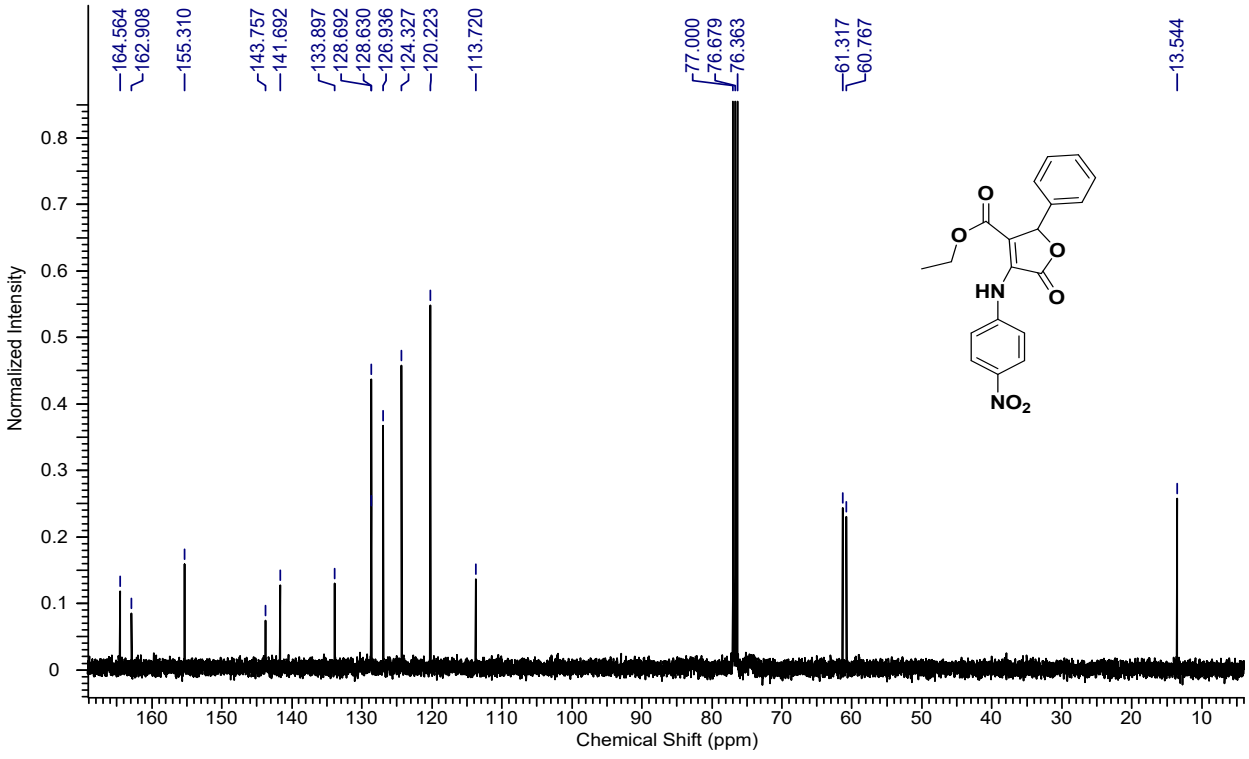
^{13}C NMR Spectrum of compound **4s**



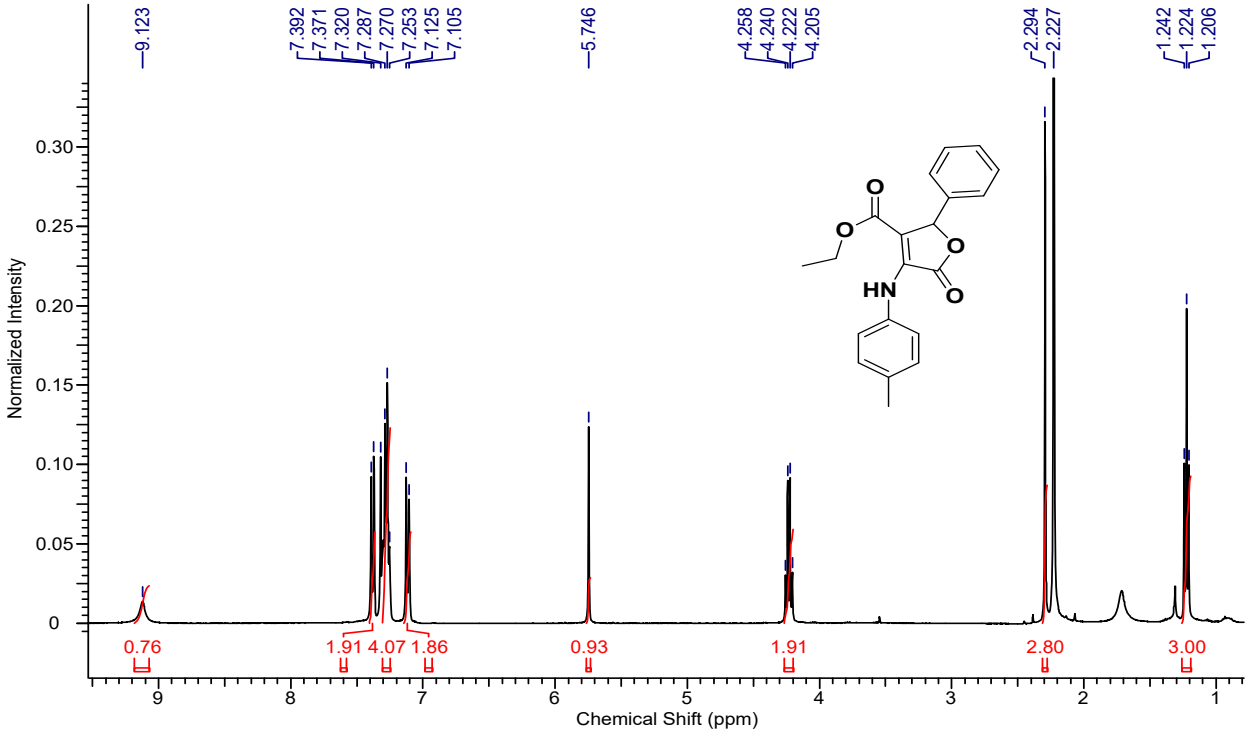
^{1}H NMR Spectrum of compound **4t**



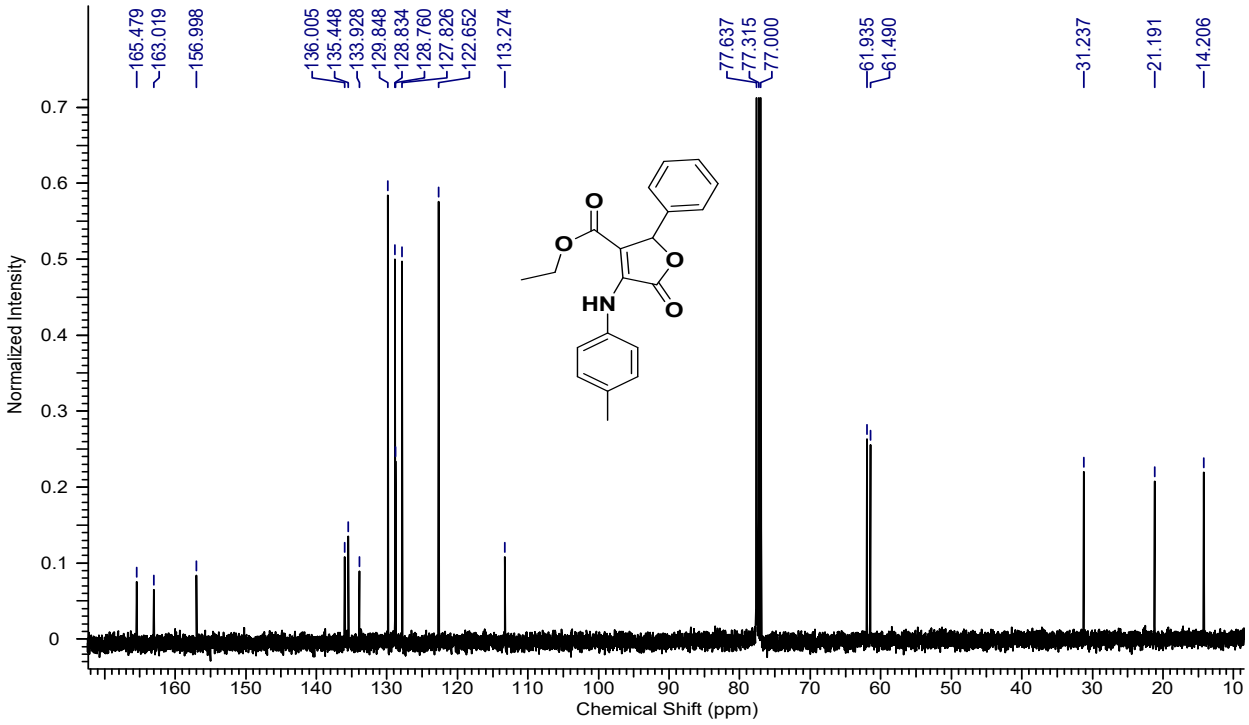
^{13}C NMR Spectrum of compound **4t**



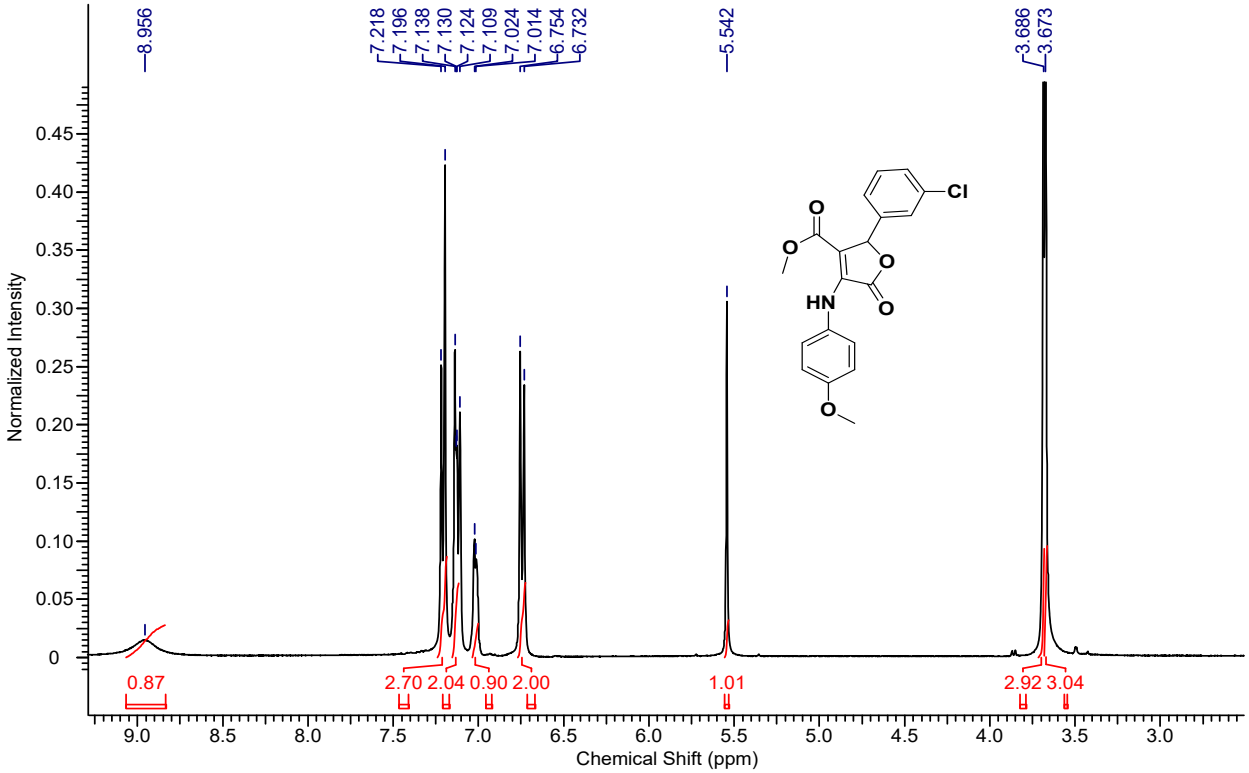
^{1}H NMR Spectrum of compound **4u**



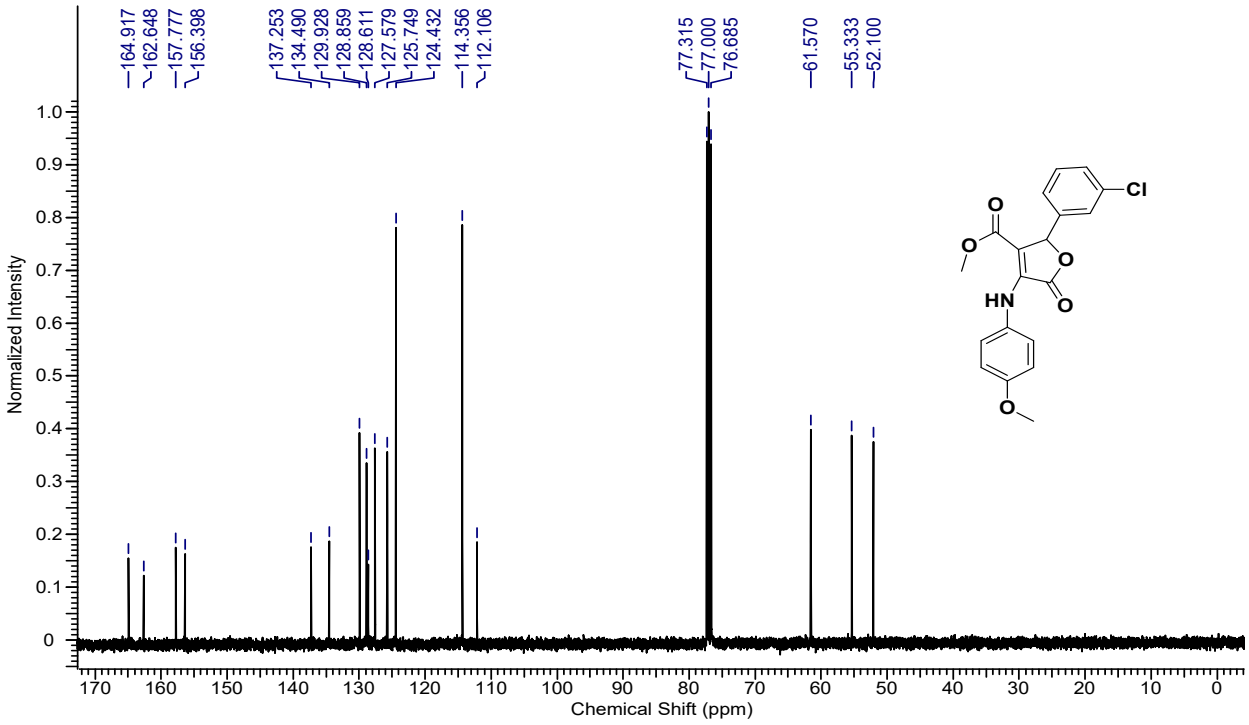
^{13}C NMR Spectrum of compound **4u**



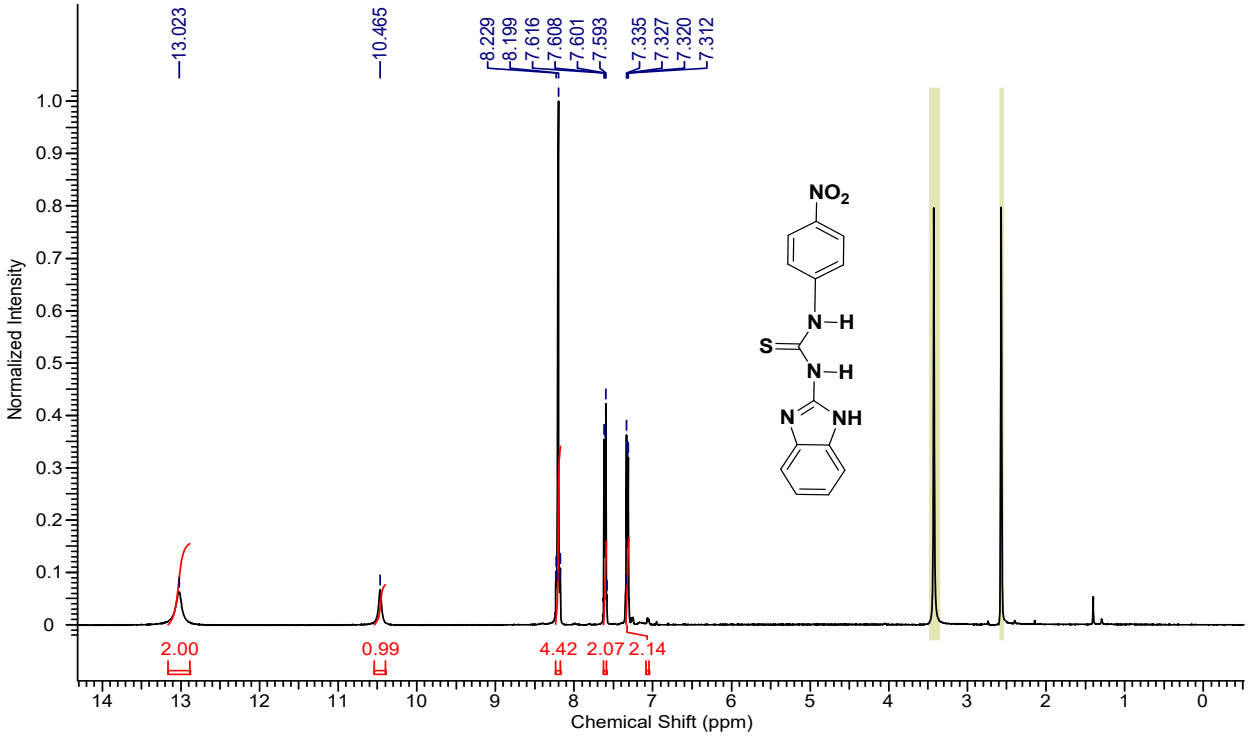
^{1}H NMR Spectrum of compound **4v**



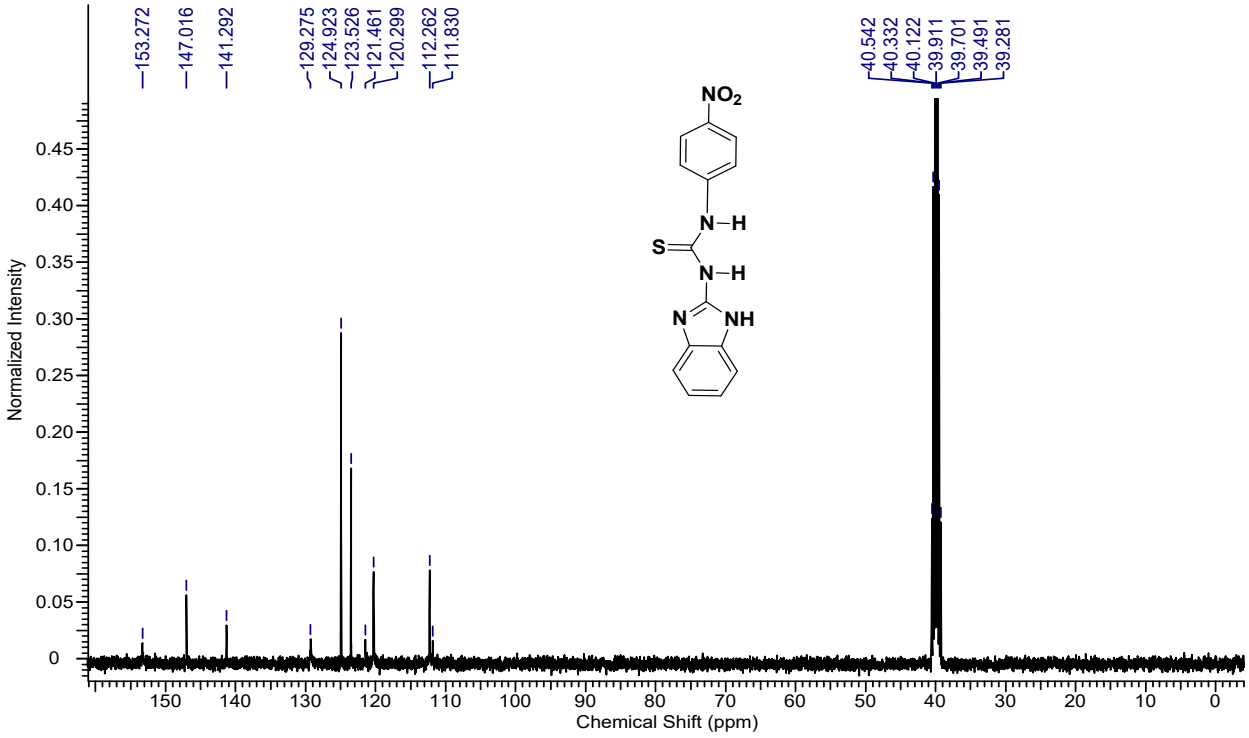
^{13}C NMR Spectrum of compound **4v**



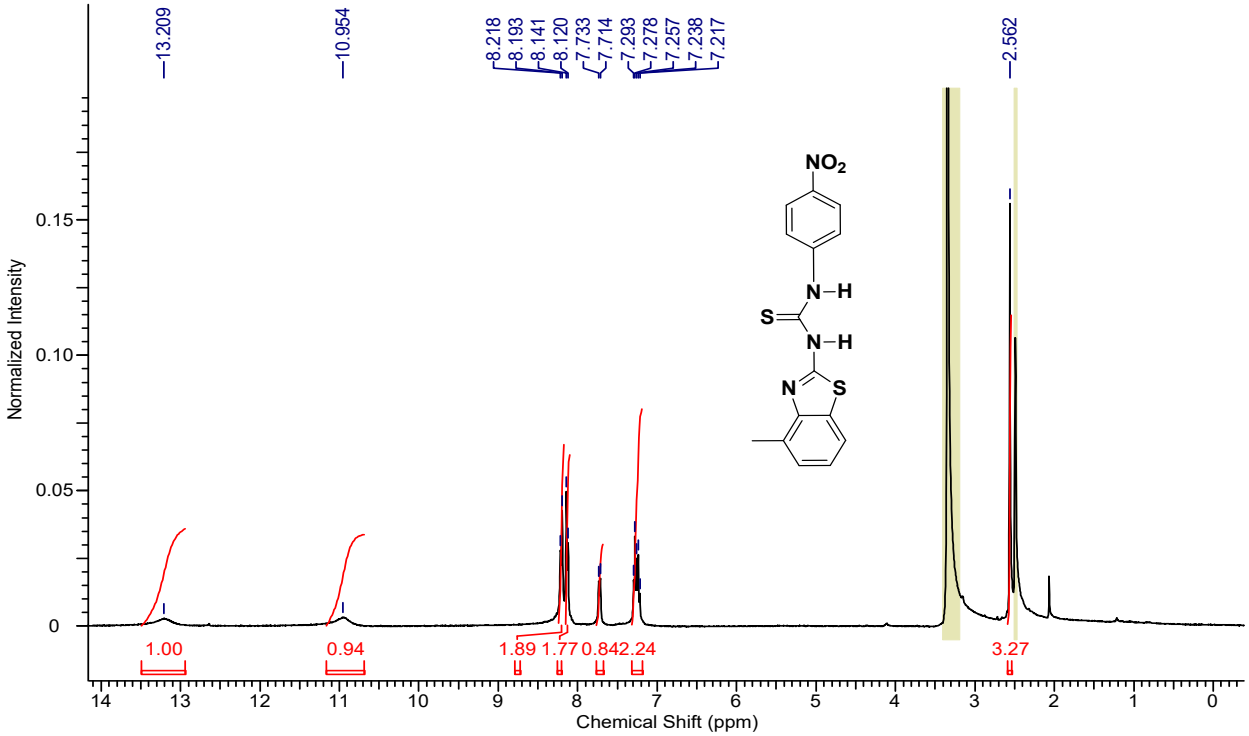
^{1}H NMR Spectrum of compound **3a BINPT**



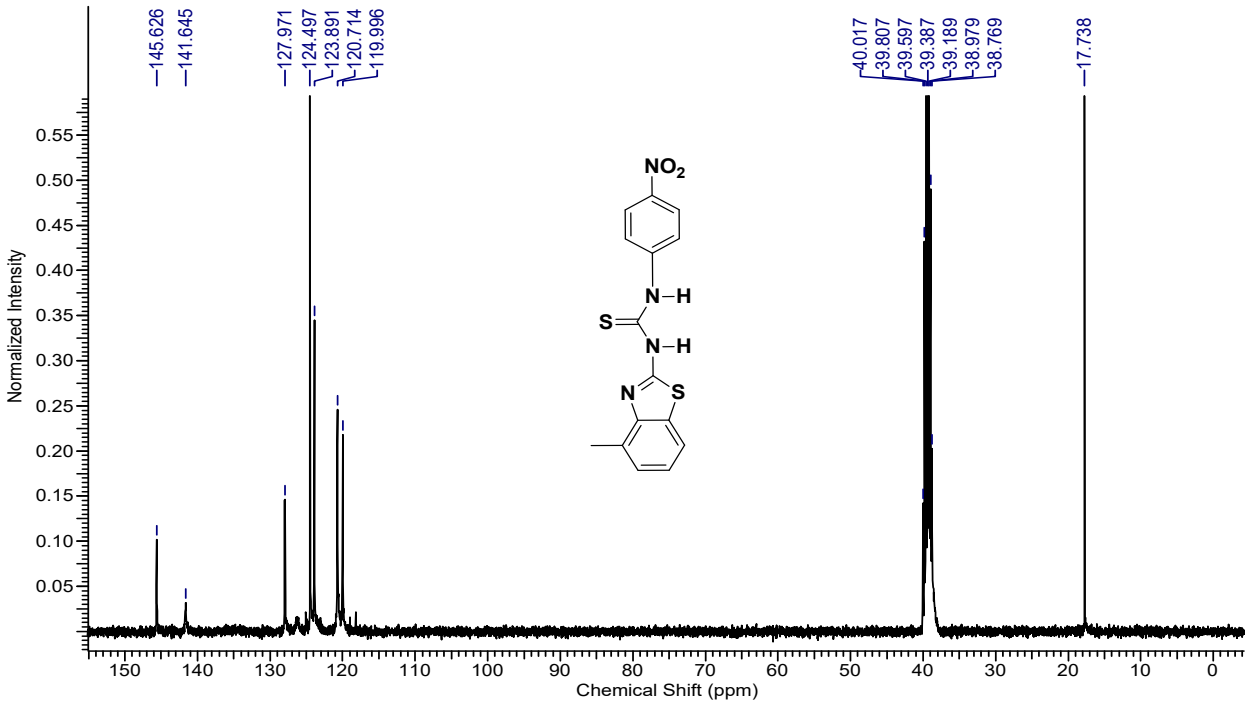
^{13}C NMR Spectrum of compound **3a BINPT**



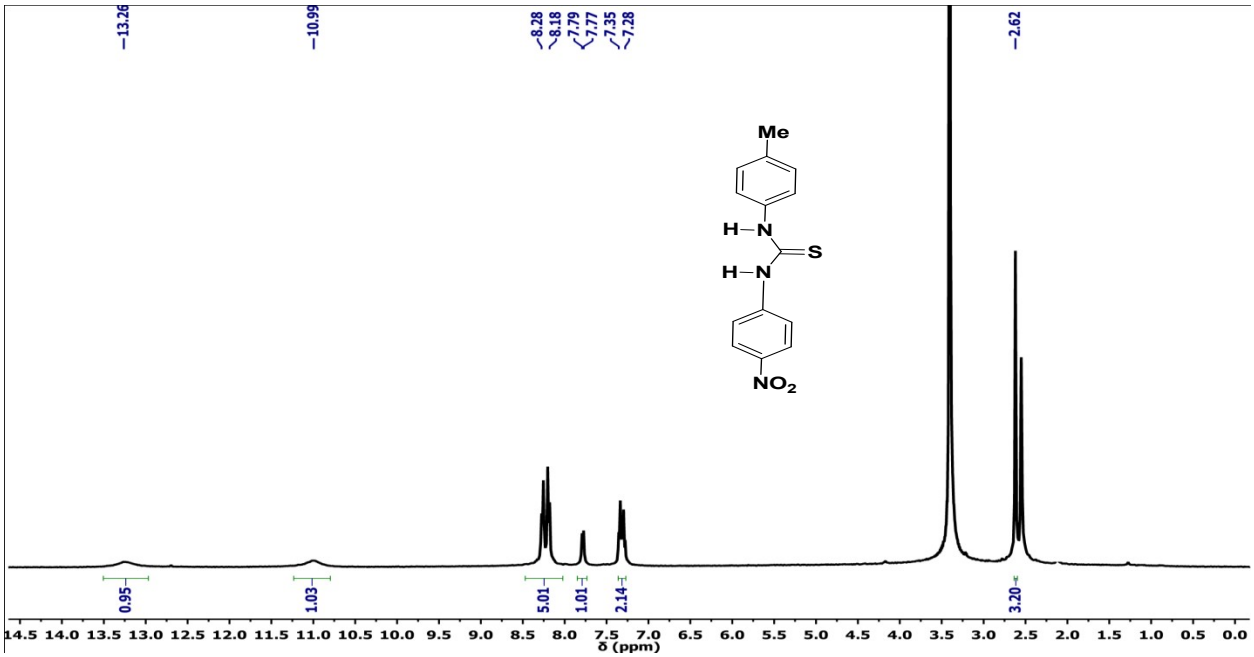
^{1}H NMR Spectrum of compound **3b MBNPT**



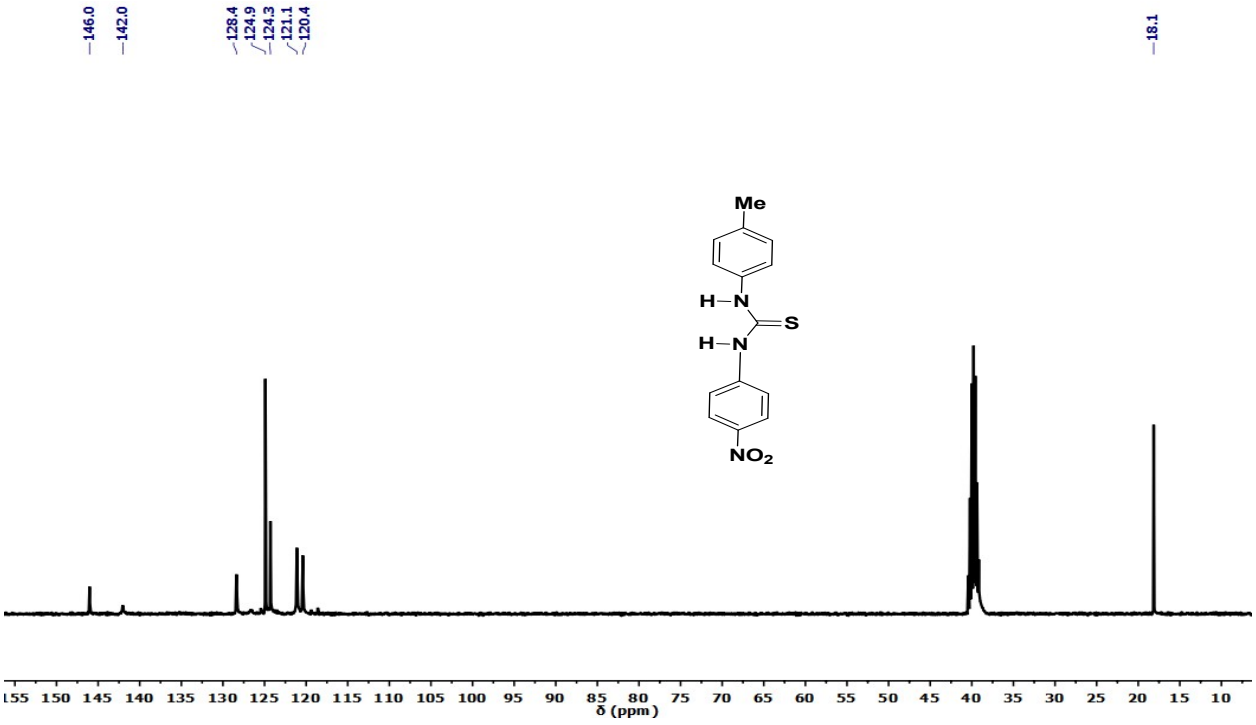
^{13}C NMR Spectrum of compound **3b MBNPT**



^{1}H NMR Spectrum of compound (***NPTT***)

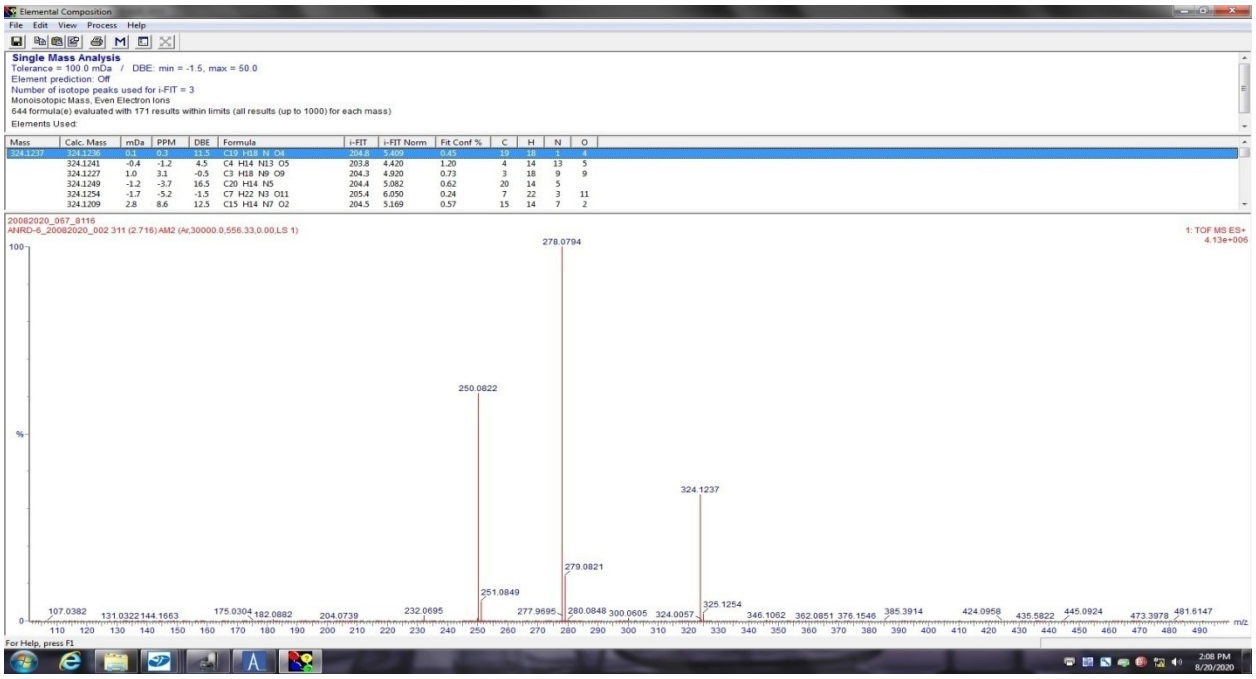


^{13}C NMR Spectrum of compound (***NPTT***)

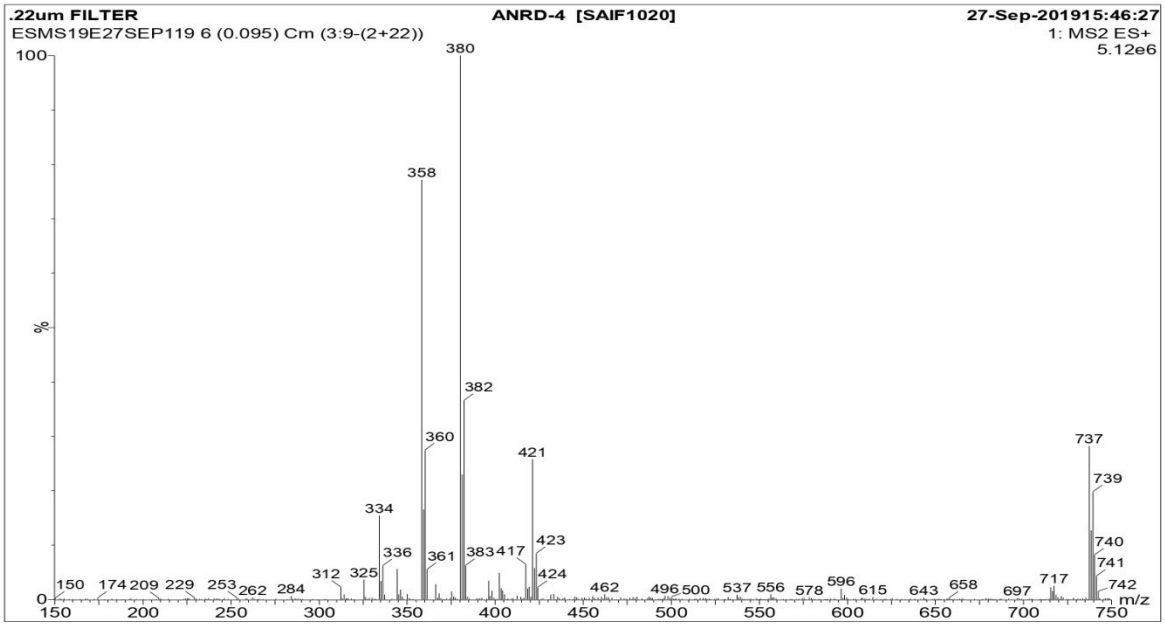


X. Mass spectra of the synthesized compounds

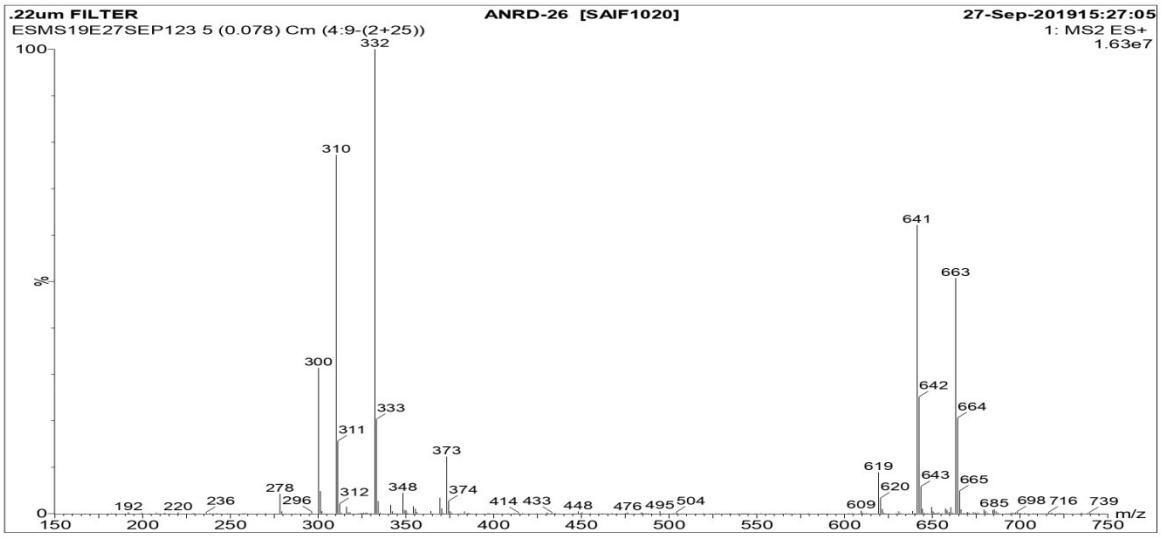
High resolution mass spectrum of compound **4a**



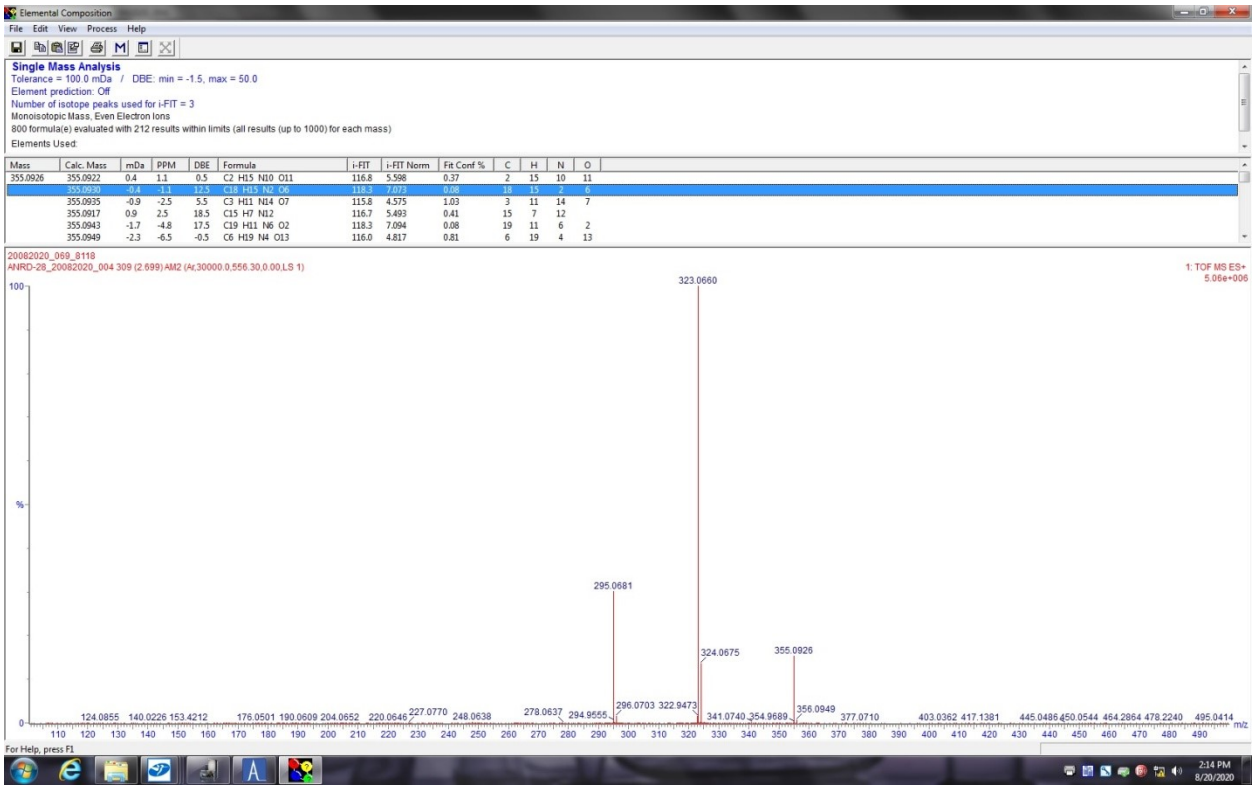
Mass spectrum of compound **4c**



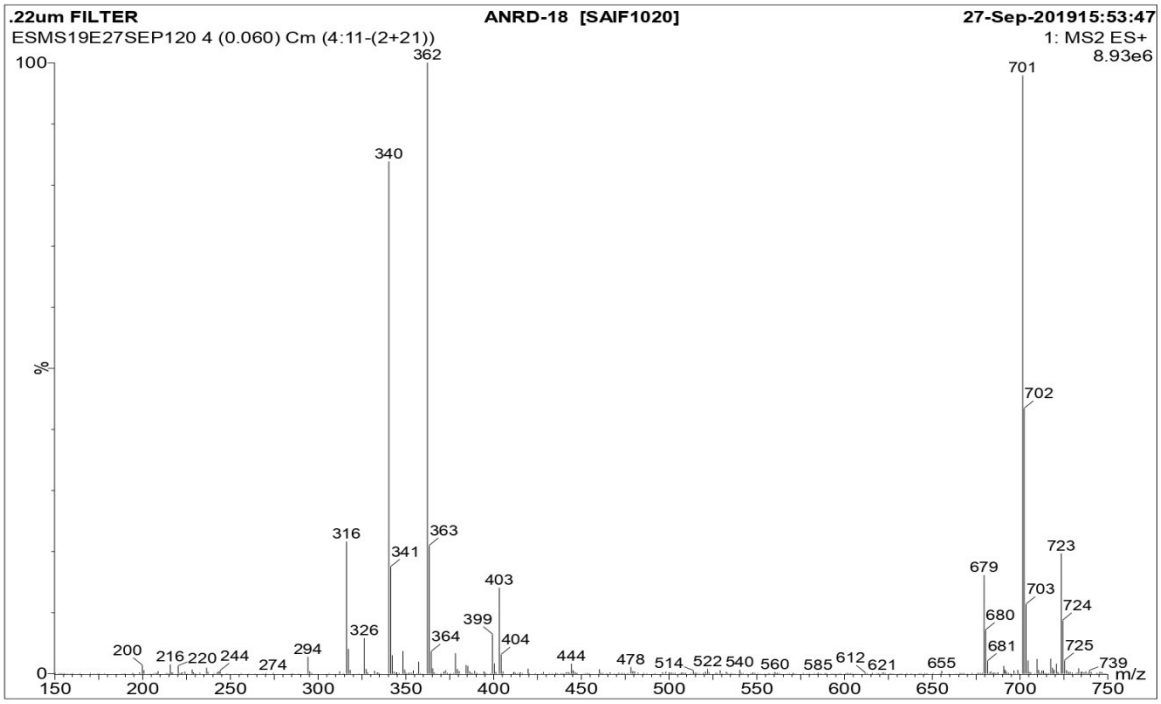
Mass spectrum of compound **4e**



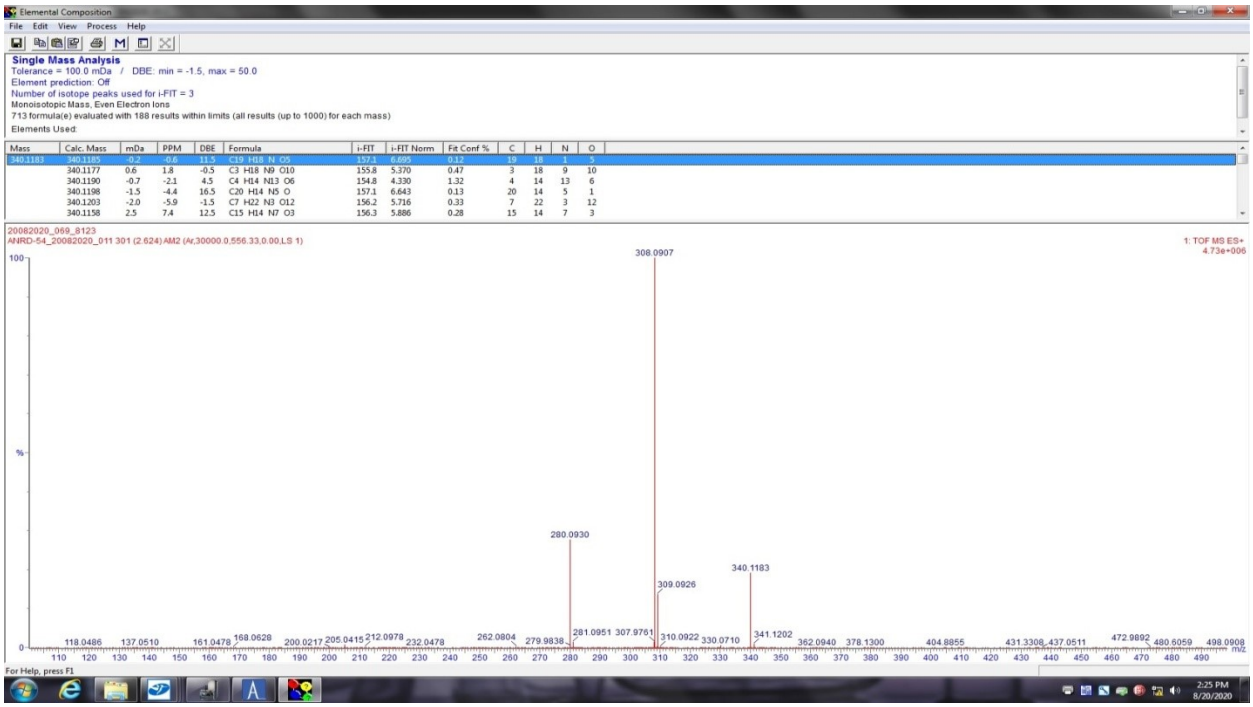
High resolution mass spectrum of compound **4f**



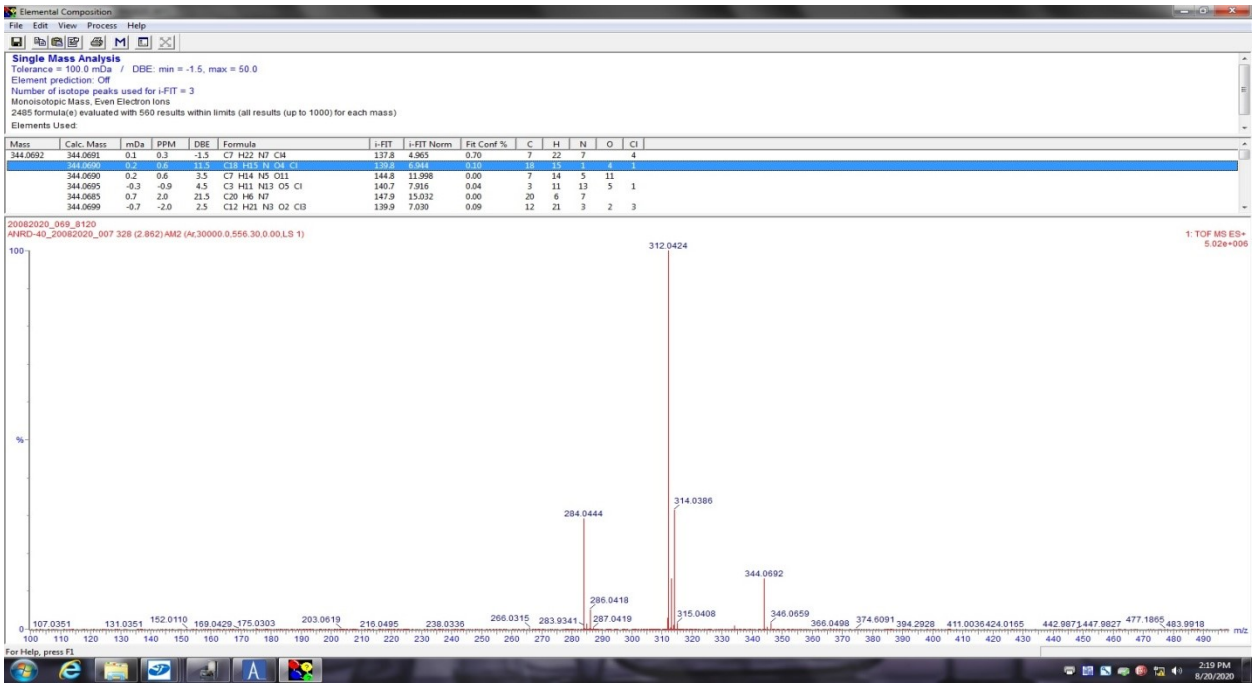
Mass spectrum of compound **4h**



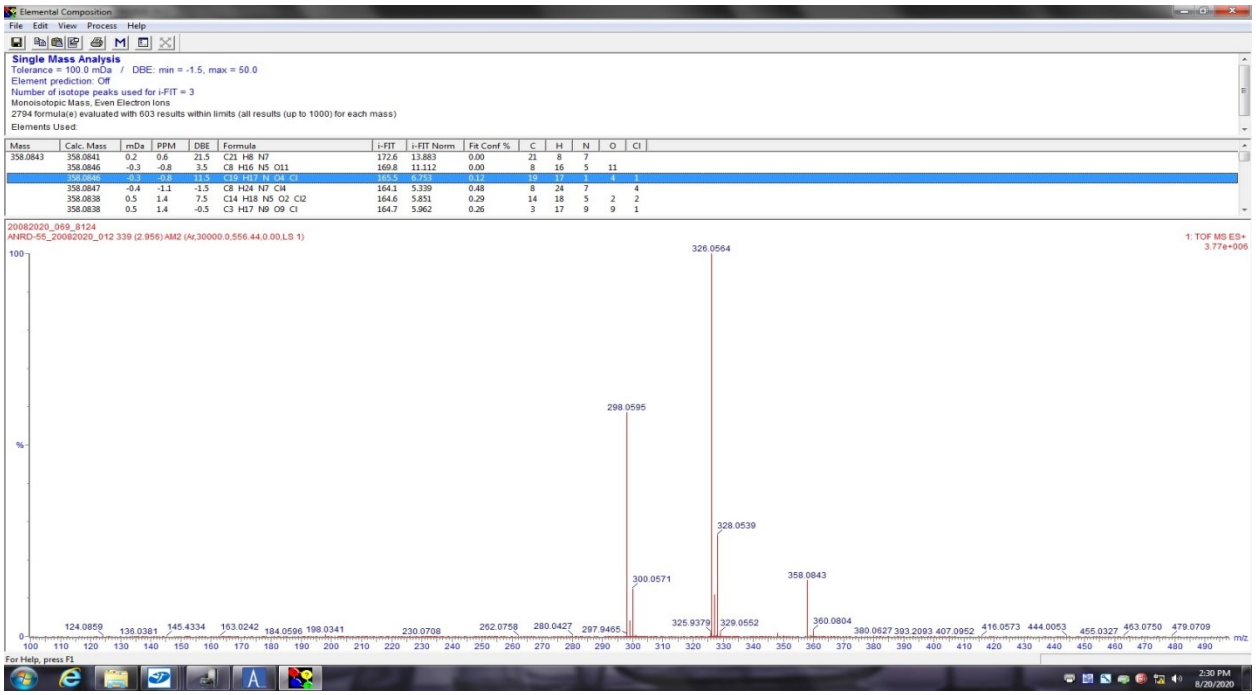
High resolution mass spectrum of compound **4i**



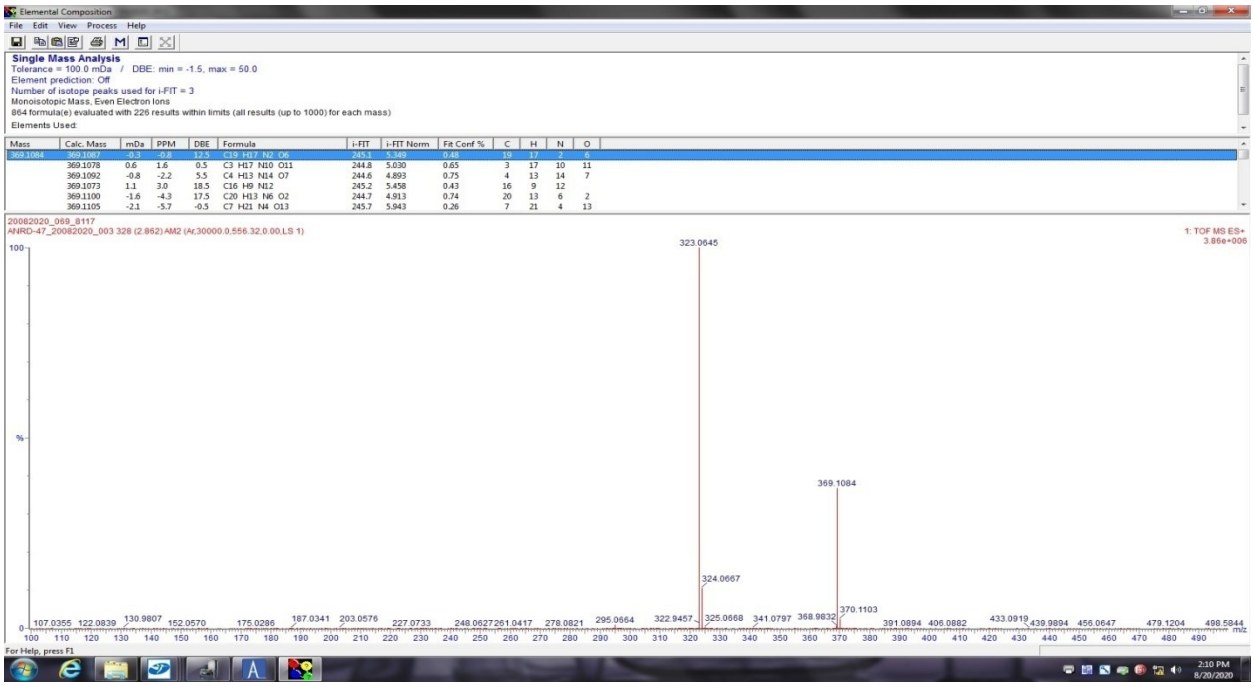
High resolution mass spectrum of compound **4m**



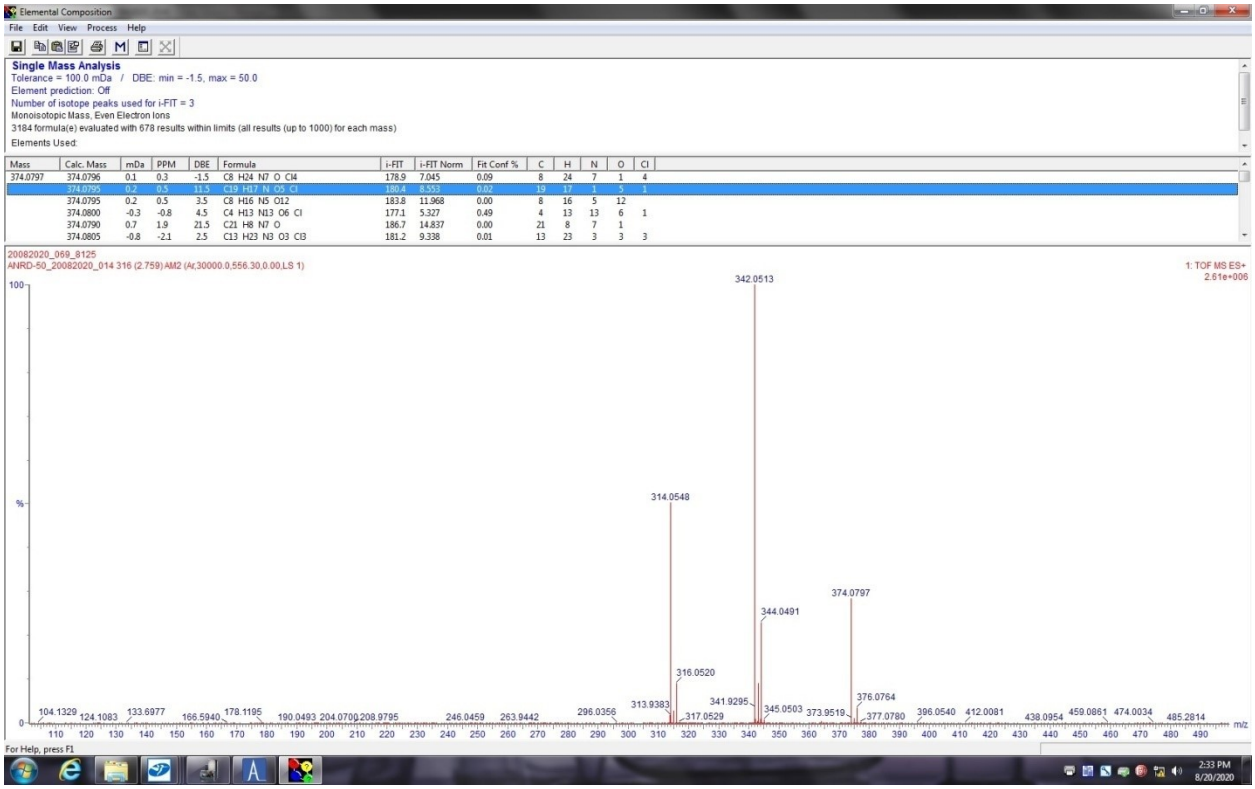
High resolution mass spectrum of compound **4n**



High resolution mass spectrum of compound **4t**



High resolution mass spectrum of compound **4v**



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