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Supporting Information

Convenient one-pot synthesis of 1,2,4-oxadiazoles and 2,4,6-triarylpyridines using graphene oxide (GO) as a metal-free catalyst: Importance of dual catalytic activity

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Experimental section

1. General experimental procedure

All the chemicals and reagents were purchased from Sigma–Aldrich, Spectrochem, TCI and were used without further purification. The solvents were purchased from commercial suppliers and were used after proper distillation.The progress of the reaction was monitored by Merck TLC plates which are coated with silica gel (60 F_{254}) and UV light was used as visualizing agent. NMR spectra of all the synthesized compounds were carried out in $CDCl_3$/DMSO-d_6 solvent and TMS was used as an internal standard. All the NMR spectroscopic data are recorded in BrukerAvance FT-NMR operating for ^1H at 300/400 MHz. The ^1H NMR data are represented by chemical shift δ (ppm), multiplicity (s = singlet, d= doublet, t = triplet, m = multiplet), integration, coupling constants (*J*values) in Hertz (Hz). The ^{13}C NMR spectroscopic data are also reported in ppm as ^1H NMR spectra.

2. General procedure for the preparation of (GO) catalyst

There are several methods for the preparation of graphene oxide (GO). Herein, Graphene oxide (GO) was synthesized by the Tours method using graphite powder as starting material [1]. At first, 9:1 volume ratio of (180 mL) sulfuric acid (H_2SO_4) and (20 mL) phosphoric acid (H_3PO_4) were taken in a 500 ml conical flask, and then 1.5 g of graphite powder was added to it under stirring condition. The temperature of the whole mixture was kept below 10^oC using an ice bath and 9g of potassium permanganate ($KMnO_4$) was added very slowly into it as the addition of $KMnO_4$evolves heat. Then the reaction mixture was stirred for 12 hrs and after that hydrogen peroxide (H_2O_2) was added drops wise to eliminate excess $KMnO_4$. After that, 30-40 mL hydrochloric acid (HCl) (strength 30%) was added to this mixture followed by the addition of 200 mL of deionized water. Then the mixture was centrifuged at 5000 rpm for 20 minutes. After that, the supernatant liquid was decanted away and the residual was dried at 90 ^oC rotary evaporator to get dry graphene oxide (GO) with pH (4.2 at 0.1 mg/mL).

3. General procedure for the synthesis of 3,5-disubstituted 1,2,4 oxadiazoles

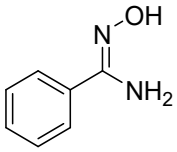
50-mL of RB was charged with benzonitrile (1.5 mmol), hydroxylamine hydrochloride (1.5 mmol), K_2CO_3 (1.5 mmol), and Ethanol-water (5 mL), and then the reaction mixture was stirred

at 80 °C for 8 hrs. After 8 hrs, benzaldehyde (1 mmol) and 25 mg of GO were added to it and the reaction was carried out for another 8 hrs. The progress of the reaction was governed by thin-layer chromatography (TLC). After completion of the reaction, the solvent was evaporated by a rotary evaporator. The reaction mixture was extracted by ethyl acetate and the catalyst was separated by a simple filtration procedure. After workup, ethyl acetate extract was concentrated in a water bath and further purified by column chromatography using silica gel 60-120 mesh.

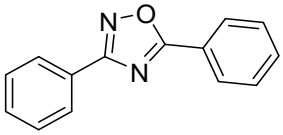
4. General procedure for the synthesis of 2,4,6-triarylpyridines

Amixture of acetophenone (1 mmol), aromatic aldehyde (1 mmol), ammonium acetate (1.5 mmol), and 30 mg of GO was stirred for 2h at 100°C temperature. The reaction was monitored by TLC and after completion of the reaction; the reaction mixture was extracted with ethyl acetate. The catalyst was recovered by centrifugation and washed with acetone and water and then dried. The ethyl acetate extractswere further purified by column chromatography using silica gel of 60-120 mesh and the desired product is obtained.

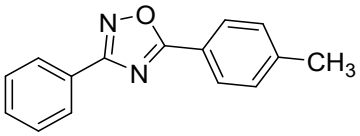
5. ^{1}H and ^{13}C NMR data of synthesized compounds



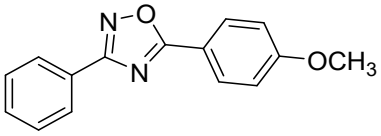
***N′*-Hydroxybenzenecarboximidamide** Yield 185 mg (91%), white solid; MP: 72-74 °C **^{1}H NMR (300 MHz, $CDCl_3$)** δ ppm: 5.07 (bs, 2H), 7.32-7.42 (m, 3H), 7.55-7.59 (m, 2H), 8.79 (bs, 1H); **^{13}C NMR** δ 126.00, 128.67, 130.01, 132.38, 158.88. [2]



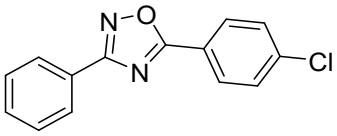
3,5-diphenyl-1,2,4-oxadiazole (3a): Yield 184 mg (83%), white solid; MP: 103-104 °C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.42-7.51 (m, 6H), 8.15-8.20 (m, 4H); **^{13}C NMR**δ 126.96, 127.52, 128.16, 128.84, 129.09, 131.17, 132.72, 133.90, 168.04, 173.96.[2]



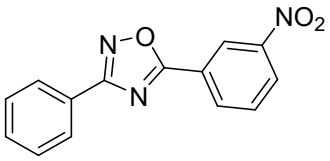
3-phenyl-5-(p-tolyl)-1,2,4-oxadiazole (3b): Yield 191 mg (81%), white solid; MP: 110-112 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 3.89 (s, 3H), 7.06-7.20 (m, 2H). 7.49-7.54 (m, 3H), 7.80-7.90 (m, 4H); **^{13}C NMR**δ 54.76, 126.98, 127.55, 128.19, 128.88, 129.13, 131.22, 132.77, 150.49, 168.76, 174.91.[2]



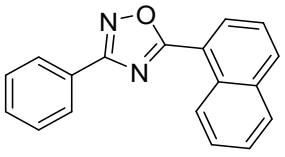
5-(4-methoxyphenyl)-3-phenyl-1,2,4-oxadiazole (3c): Yield 201 mg (80%), white solid: 100-101 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 3.89 (s, 3H), 7.04 (d, 2H, *J*= 8.7Hz), 7.50-7.52 (t, 3H), 8.15-8.18 (m, 4H); **^{13}C NMR**δ 55.07, 122.80, 126.71, 127.41, 128.09, 129.63, 130.62, 131.90, 133.93, 168.09, 174.91.[2]



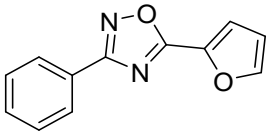
5-(4-chlorophenyl)-3-phenyl-1,2,4-oxadiazole (3d): Yield 199 mg (78%), white solid: 118-119 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.25 (d, 2H, *J*= 8.1 Hz), 7.52-7.57 (m, 3H), 8.21-8.47 (m, 4H); **^{13}C NMR**δ 120.80, 126.21, 127.10, 127.98, 128.77, 130.58, 130.74, 133.80, 169.05, 175.57.[2]



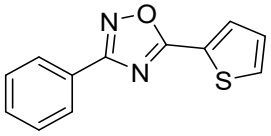
5-(3-nitrophenyl)-3-phenyl-1,2,4-oxadiazole (3e): Yield 200 mg (75%), white solid: 140-142 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.75-7.89 (m, 3H), 8.14-8.31 (m, 5H), 8.62 (s, 1H); **^{13}C NMR**δ 123.57, 126.25, 126.71, 127.41, 127.93, 129.34, 130.83, 131.93, 133.90, 149.04, 169.67, 173.91.[3]



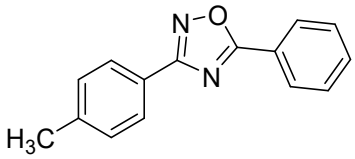
5-(naphthalen-1-yl)-3-phenyl-1,2,4-oxadiazole (3f): Yield 168 mg (62%), white solid: 99-101 ^{o}C; **^{1}H NMR (400 MHz, $CDCl_3$) δ ppm**: 7.63-7.73 (m, 5H), 8.02-8.14 (m, 5H), 8.60 (d, 1H, *J*= 8.4 Hz), 8.93 (d, 1H, *J*=8.4 Hz); **^{13}C NMR**δ 122.77, 126.77, 127.27, 127.53, 128.89, 129.15, 129.46, 129.53, 129.74, 130.89, 131.31, 131.79, 139.20, 169.06, 174.81.[2]



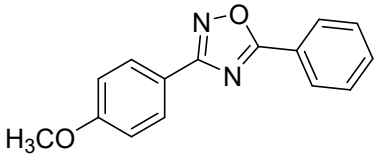
5-(furan-2-yl)-3-phenyl-1,2,4-oxadiazole (3g): Yield 152 mg (72%), yellow solid: 100-101 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.25-7.33 (t, 1H), 7.52-8.03 (m, 4H), 8.09 (d, 2H, *J*= 7.2 Hz), 8.18 (d, 2H, *J*= 6.9 Hz); **^{13}C NMR**δ 112.853, 116.69, 126.765, 127.916, 129.423, 131.689, 140.433, 147.055, 167.919, 168.997.[2]



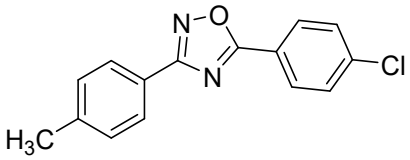
3-phenyl-5-(thiophen-2-yl)-1,2,4-oxadiazole (3h): Yield 159 mg (70%), white solid: 107-108 ^{o}C;**^{1}H NMR (400 MHz, $CDCl_3$)**δ ppm: 7.23-7.29 (m, 1H), 7.54-7.68 (m, 4H), 7.98 (s, 1H), 8.17-8.24 (m, 2H); **^{13}C NMR**δ 127.587, 128.178, 128.510, 129.114, 131.267, 131.748, 132.888, 168.857, 171.368.[2]



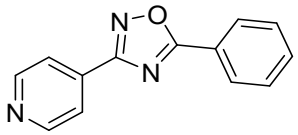
5-phenyl-3-(p-tolyl)-1,2,4-oxadiazole (3i): Yield 189 mg (80%), white solid: 100-102 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 2.43 (s, 3H), 7.53-7.61 (m, 3H), 8.00 (d, 2H, *J*= 6.9 Hz), 8.12 (d, 2H, *J*= 8.1 Hz), 8.59-8.78 (m, 2H); **^{13}C NMR**δ 21.61, 124.10, 127.95, 128.57, 128.92, 129.07, 129.39, 132.67, 141.50, 168.95, 174.10.[2]



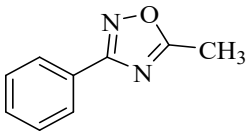
3-(4-methoxyphenyl)-5-phenyl-1,2,4-oxadiazole (3j): Yield 196 mg (78%), white solid: 101-102 °C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 3.88 (s, 3H), 7.02 (d, 2H, *J*= 8.7 Hz), 7.52-7.63 (m, 3H), 8.10-8.23 (m, 4H); **^{13}C NMR**δ 54.873, 113.759, 118.996, 123.972, 127.640, 128.544, 128.631, 132.091, 161.466, 168.180, 174.942.[2]



5-(4-chlorophenyl)-3-(*p*-tolyl)-1,2,4-oxadiazole (3k): Yield 234 mg (82%), white solid: 132-134 °C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 2.43 (s, 3H), 7.31 (d, 2H, *J*= 7.8 Hz), 7.51-7.54 (t, 2H), 8.04 (d, 2H, *J*= 8.1 Hz), 8.15 (d, 2H, *J*= 8.7 Hz); ^{13}C NMR δ 21.124, 122.329, 123.418, 126.418, 126.943, 128.945, 129.002, 129.105, 138.612, 141.162, 168.552, 174.135.[2]

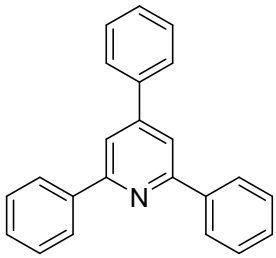


5-phenyl-3-(pyridin-4-yl)-1,2,4-oxadiazole (3l): Yield 151 mg (68%), white solid: 145-146 °C;**^{1}H NMR (300 MHz, $CDCl_3$) δ** ppm: 7.47-7.64 (m, 3H), 8.07-8.08 (t, 1H), 8.13-8.20 (m, 2H). 8.21-8.85 (m, 3H); **^{13}C NMR**δ 121.044, 123.294, 127.744, 129.460, 132.399, 134.321, 149.758, 166.834, 176.054.[2]

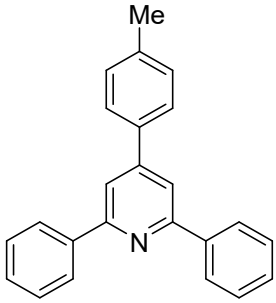


5-methyl-3-phenyl-1,2,4-oxadiazole (3 m): Yield 120 mg (75%), colourless liquid:BP>200 °C; **^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 2.57 (s, 3H), 7.36-7.38 (m, 3H), 7.95-7.98 (m, 2H); **^{13}C**

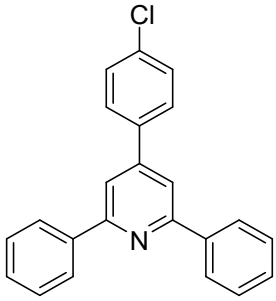
NMRδ 12.36, 126.82, 127.33, 128.84, 131.11, 168.35, 177.28; LCMS (ESI-APCI) $C_9H_8N_2O$ for: 161$[M+H]^+$, Anal. Calcd for$C_9H_8N_2O$**:** C= 67.39, H= 5.09, N= 17.49.[2, 4]



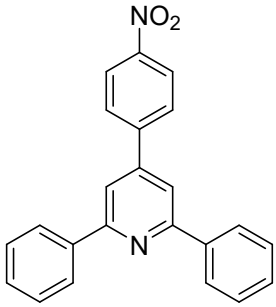
2,4,6-triphenylpyridine (6a): Yield 282 mg (92 %), white solid: MP 132-133 °C; **^{1}H NMR (300 MHz, $CDCl_3$)** δ ppm: 7.42-7.48 (m, 9H), 7.77 (d, 2H, *J*= 7.2 Hz), 8.136 (s, 2H), 8.28 (d, 4H, *J*=7.8Hz);**^{13}C NMR**δ 117.16, 127.20, 127.23, 128.08, 128.76, 129.02, 129.10, 129.16, 139.11, 139.65, 150.23, 157.55.[5]



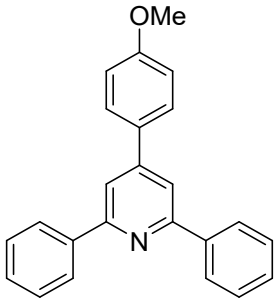
2,6-diphenyl-4-(p-tolyl)pyridine (6b): Yield 276 mg (86%), light yellow solid: MP 118-119 °C; **^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 2.49 (s, 3H), 7.45-7.56 (m, 8H), 7.90 (d, 2H, *J*= 7.2Hz), 8.11 (s, 2H), 8.23 (d, 4H, *J*= 7.8Hz); **^{13}C NMR**δ 21.01, 116.36, 126.65, 127.98, 128.08, 128.47, 129.21, 137.92, 139.22, 140.56, 150.42, 157.37.[6]



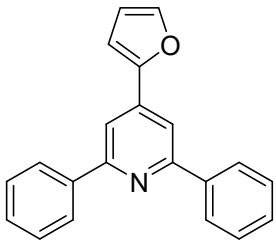
4-(4-chlorophenyl)-2,6-diphenylpyridine (6c): Yield 317 mg (93%), white solid: MP 121-123 °C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.39-7.48 (m, 8H), 7.80 (d, 2H, *J*= 7.2 Hz), 8.13 (s, 2H), 8.30 (d, 4H, *J*= 7.8Hz); **^{13}C NMR δ** 116.59, 127.15, 128.07, 128.41, 128.67, 129.04, 129.42, 138.91, 139.77, 148.77, 157.45.[5]



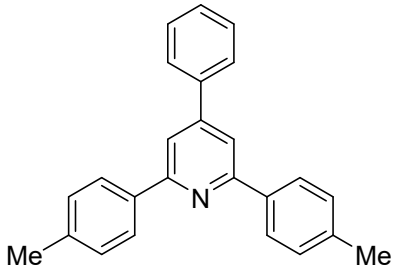
4-(4-nitrophenyl)-2,6-diphenylpyridine (6d): Yield 310 mg (88%), off white solid: MP 192-193 °C; **^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.46-7.56 (m, 8H), 7.89 (d, 2H, *J*=8.1Hz), 8.21 (s, 2H), 8.40 (d, 4H, *J*= 7.8Hz); **^{13}C NMR**δ 116.42, 123.85, 126.64, 127.67, 128.31, 128.93, 133.11, 133.65, 143.53, 147.37, 157.52.[5]



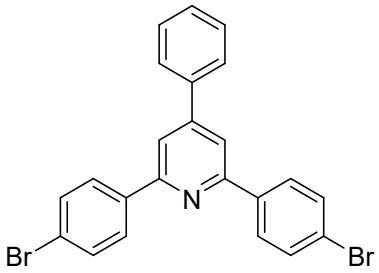
4-(4-methoxyphenyl)-2,6-diphenylpyridine (6e): Yield 280 mg (83%), white solid: MP 100-102 °C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 3.74 (s, 3H), 7.10 (d, 2H, *J*= 7.8 Hz), 7.29-7.51 (m, 8H), 7.72 (s,2H), 7.92 (d, 4H, *J*= 6.9 Hz); **^{13}C NMR**δ 54.90, 119.35, 127.16, 127.92, 128.06, 129.73, 132.04, 138.05, 140.37, 144.18, 151.72, 161.22.[5]



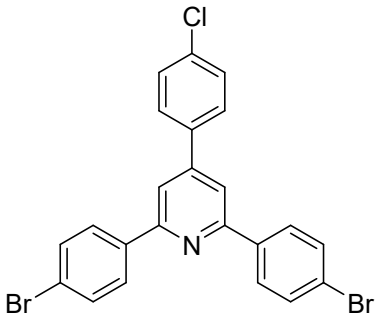
4-(furan-2-yl)-2,6-diphenylpyridine (6f): Yield 231 mg (78%), light brown solid: MP 112-13 °C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 6.56 (d, 1H, *J*=1.5Hz), 6.96 (d, 1H, *J*= 3Hz), 7.44-7.58 (m, 7H), 7.92 (s, 2H), 8.19 (d, 4H, *J*= 8.1 Hz);**^{13}C NMR** δ 107.96, 111.61, 112.51, 126.58, 128.18, 128.59, 138.57, 138.99, 143.12, 151.51, 157.03.[5]



4-phenyl-2,6-di-p-tolylpyridine (6g): Yield 291 mg (87%), white solid: MP 152-154 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 2.37 (s, 6H), 7.21 (d, 4H, *J*=7.2Hz), 7.38-7.43 (m, 3H), 7.61-7.72 (m, 2H), 7.74 (s, 2H), 7.99 (d, 4H, *J*=8.1Hz); **^{13}C NMR** δ 21.40, 116.56, 127.05, 127.23, 128.54, 128.92, 129.12, 136.94, 139.00, 139.30, 150.04, 157.43.[5]

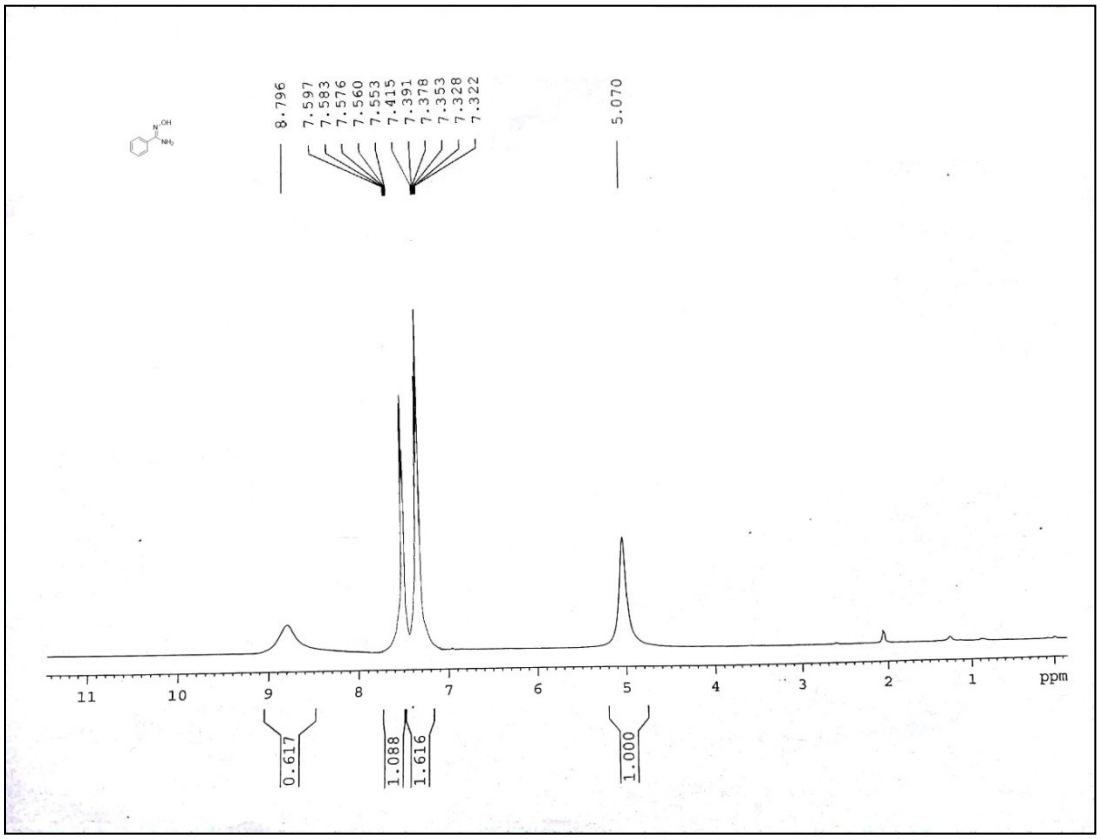


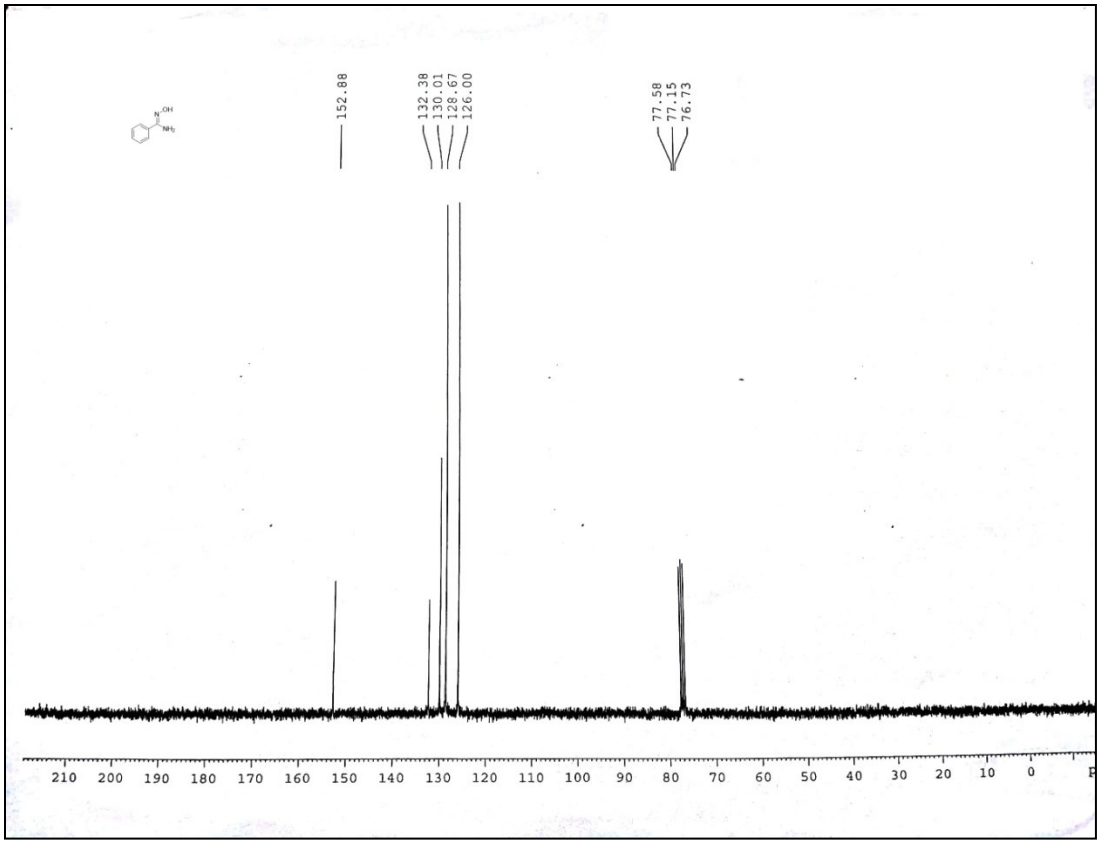
2,6-bis(4-bromophenyl)-4-phenylpyridine (6h): Yield 418 mg (90%), white solid: MP 105-106 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.09-7.36 (m, 5H), 7.49 (s, 2H), 7.76 (d, 4H, *J*= 7.8 Hz), 8.10 (d, 4H, *J*=8.1 Hz); **^{13}C NMR**δ 116.46, 123.05, 127.05, 128.40, 128.94, 129.49, 132.94, 135.19, 139.60, 149.07, 154.16.[6]



2,6-bis(4-bromophenyl)-4-(4-chlorophenyl)pyridine (6i): Yield 469 mg (94%), white solid: MP> 250 ^{o}C;**^{1}H NMR (300 MHz, $CDCl_3$)**δ ppm: 7.02-7.06 (m, 4H), 7.34 (d, 2H. *J*= 7.2 Hz), 7.73 (d, 2H, *J*= 7.5 Hz), 7.87 (s, 2H), 8.13 (d, 4H, *J*= 8.4 Hz); **^{13}C NMR**δ 116.32, 122.89, 128.68, 128.87, 129.10, 130.59, 137.58, 138.07, 149.38, 156.62.[7]

6. Scanned copies of ^{1}H and ^{13}C NMR spectra of synthesized compounds

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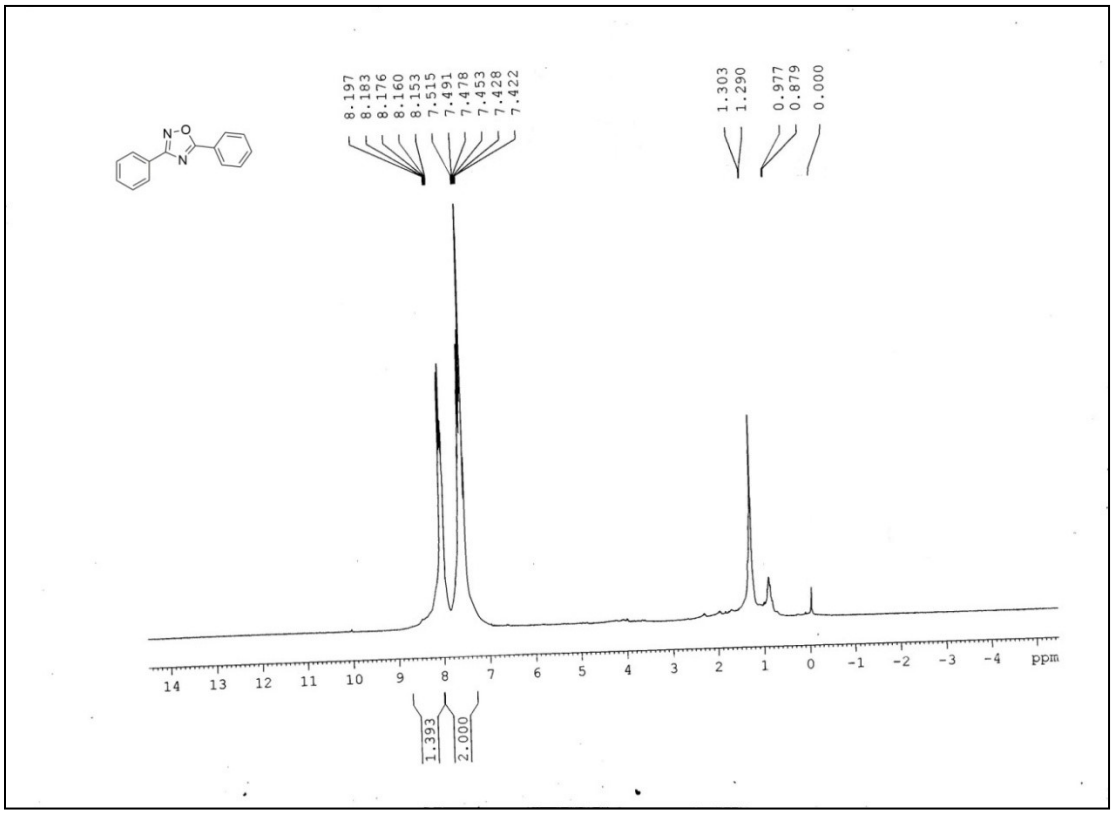
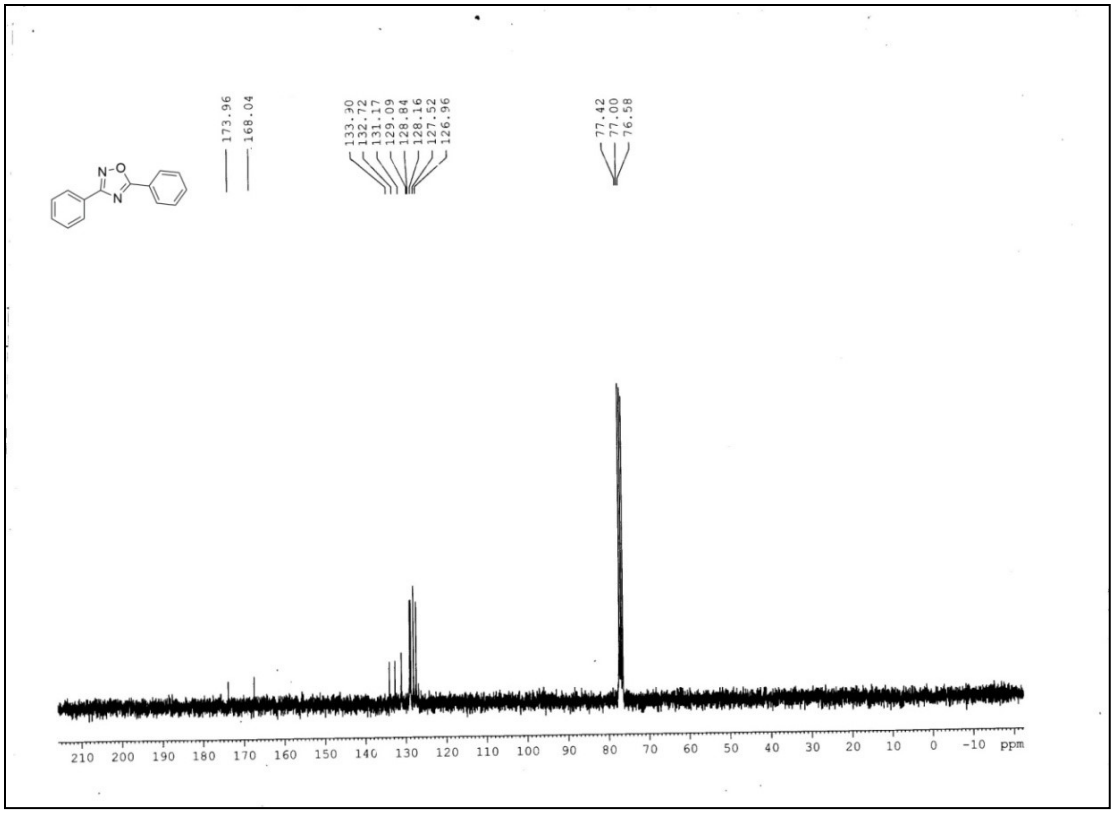
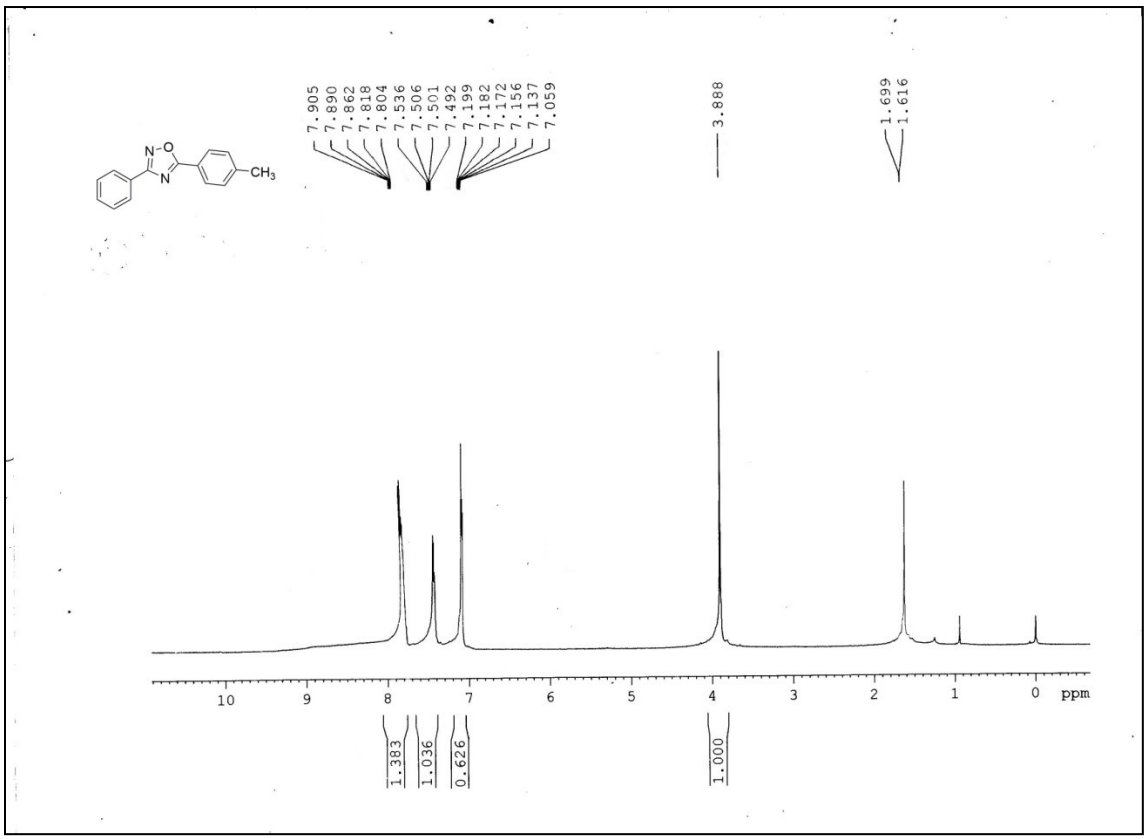
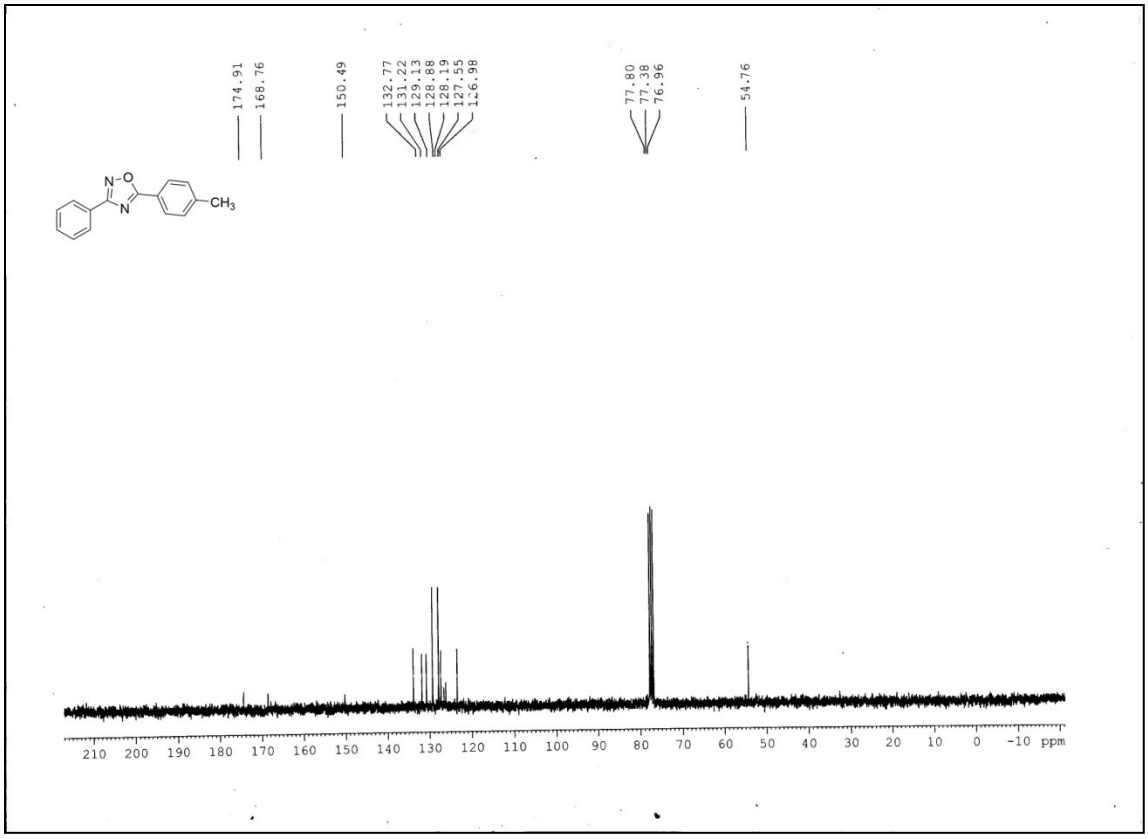
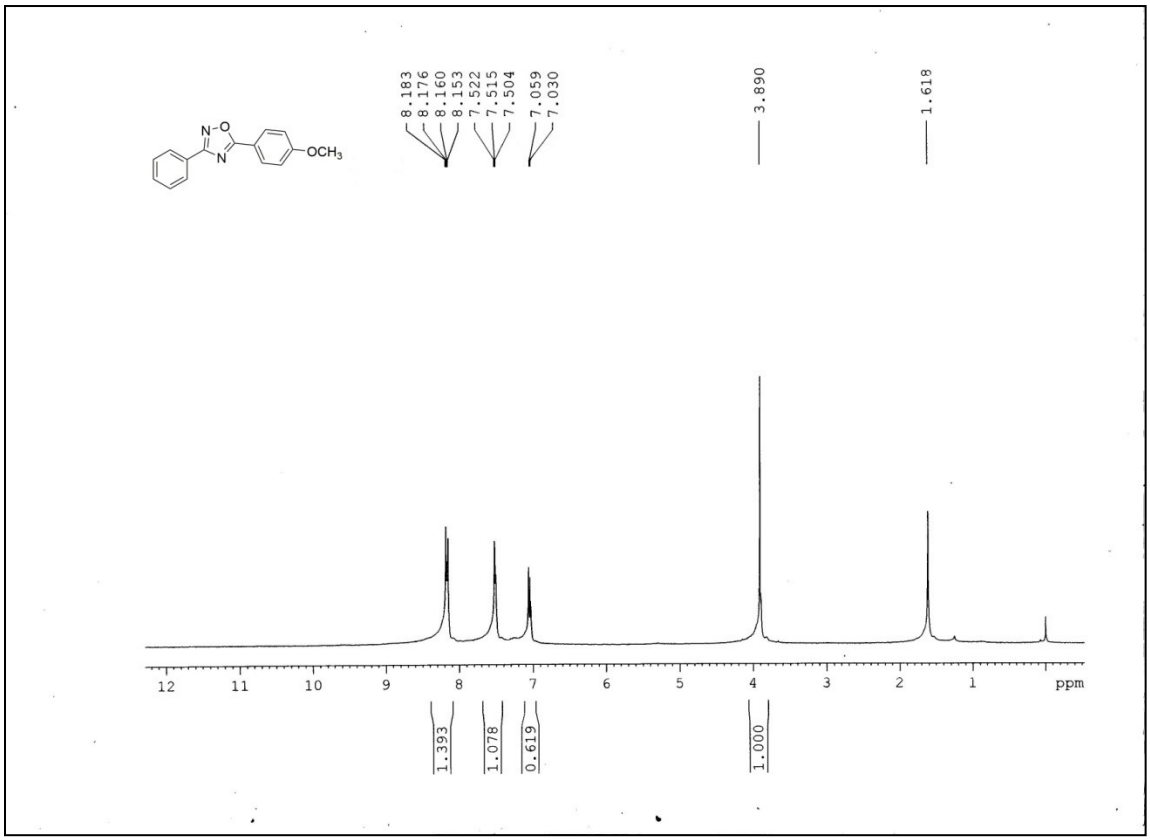
130.01
128.67
126.00
77.58
77.15
76.73
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

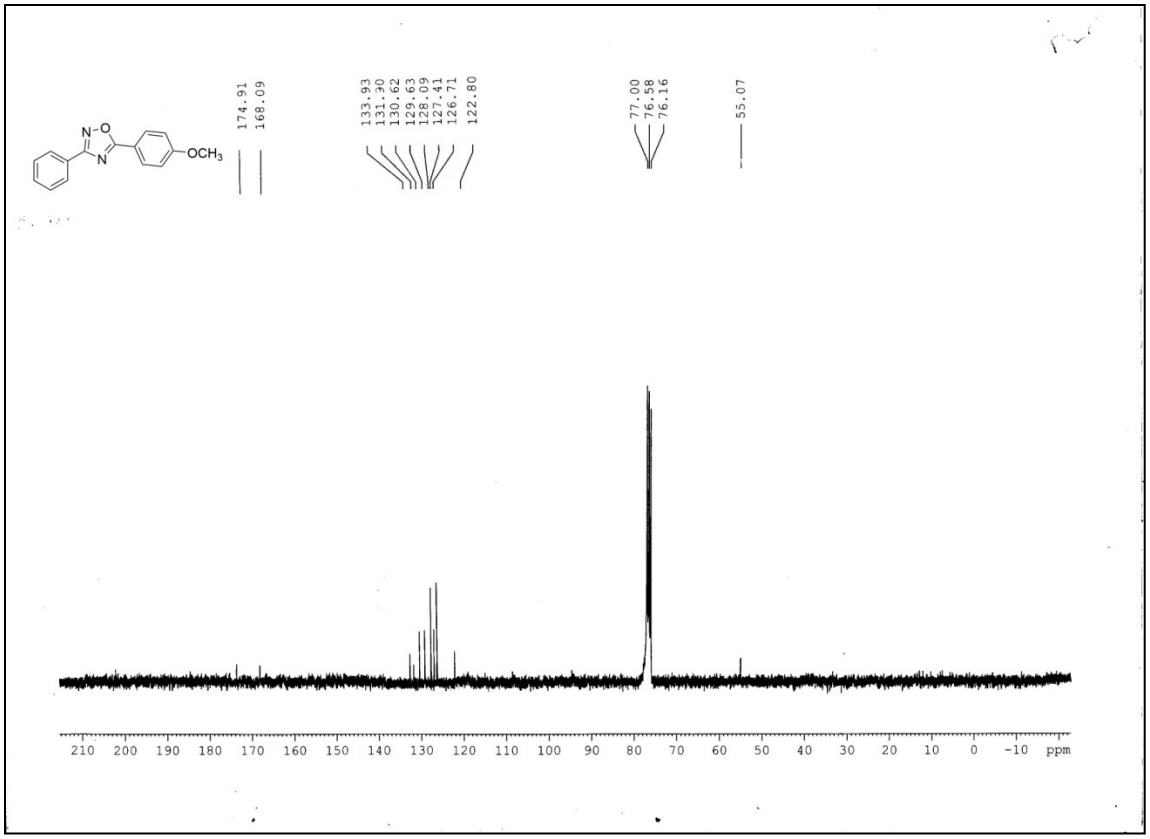

8.197
8.183
8.176
8.160
8.153
7.515
7.491
7.478
7.453
7.428
7.422
1.303
1.290
0.977
0.879
0.000
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 ppm
1.393
2.000

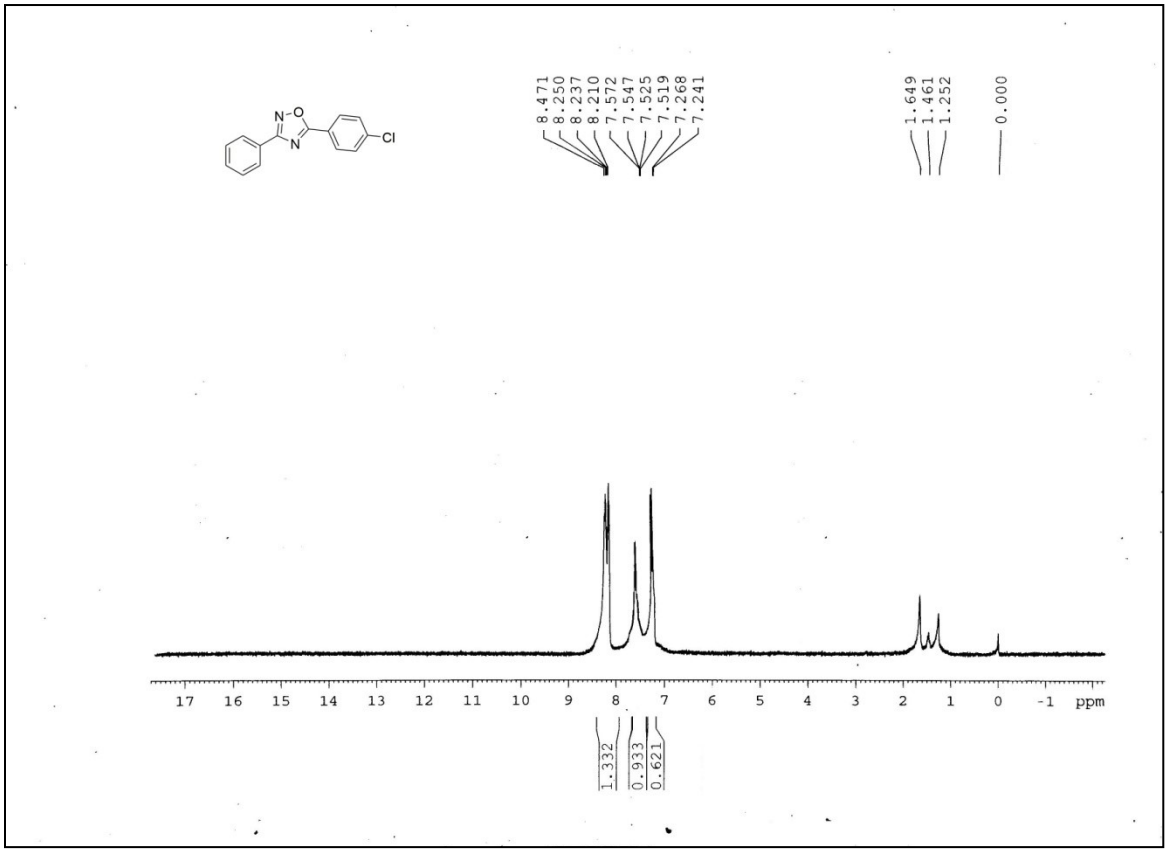

173.96
168.04
133.90
132.72
131.17
129.09
128.84
128.16
127.52
126.96
77.42
77.00
76.58
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

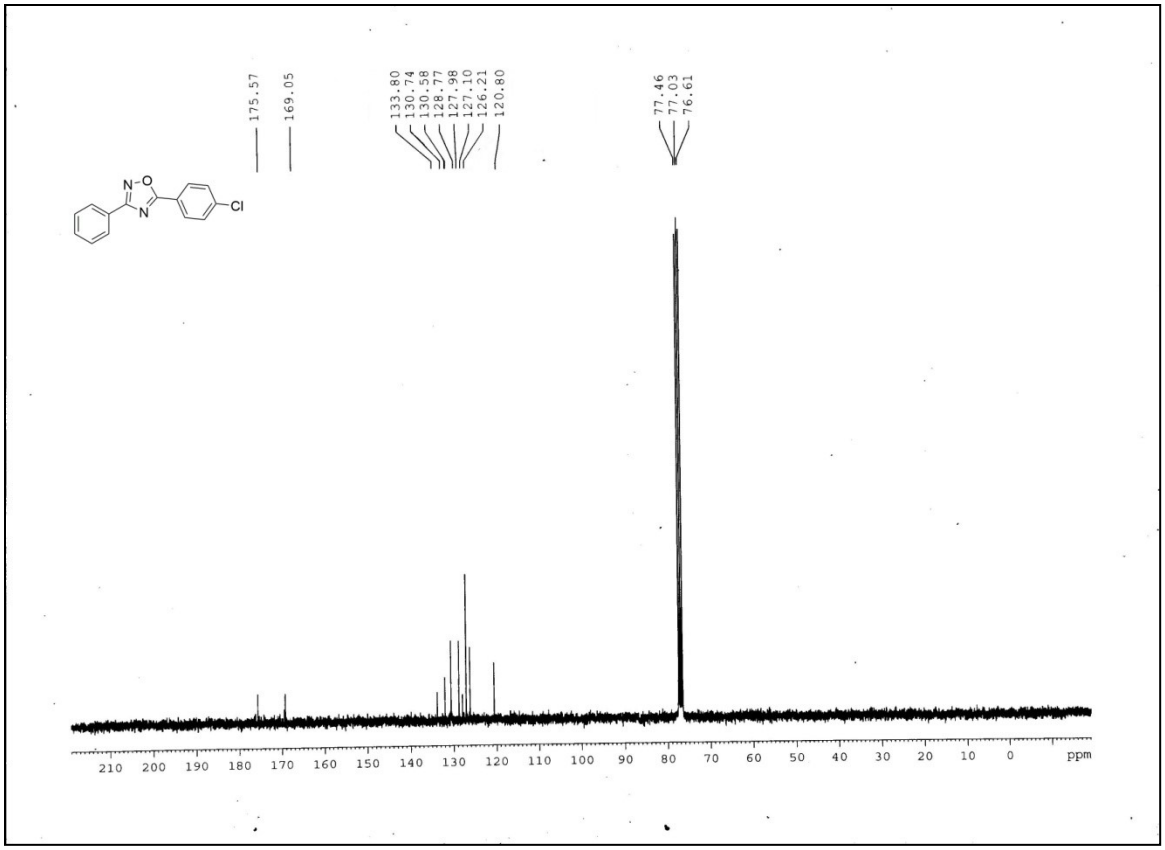

7.905
7.890
7.862
7.818
7.804
7.536
7.506
7.501
7.492
7.199
7.182
7.172
7.156
7.137
7.059
3.888
1.699
1.616
CH3
10 9 8 7 6 5 4 3 2 1 0 ppm
1.383
1.036
0.626
1.000

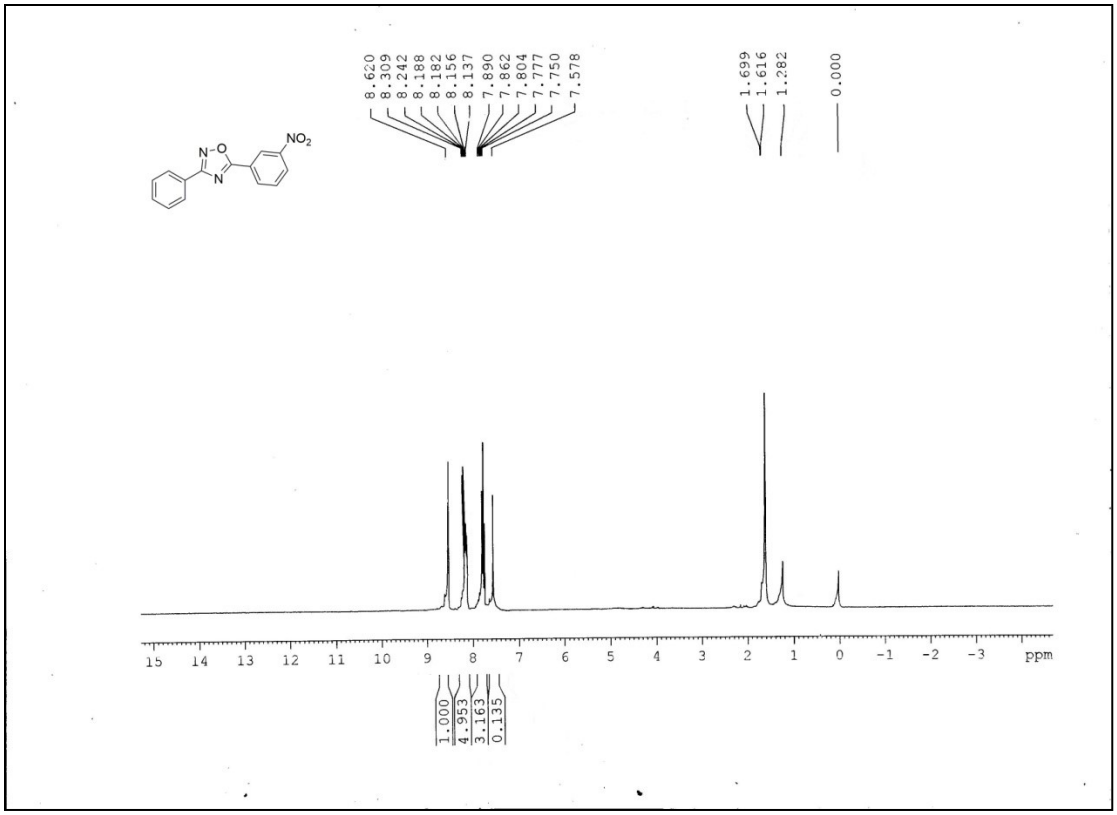

174.91
168.76
150.49
132.77
131.22
129.13
128.88
128.19
127.55
126.98
77.80
77.38
76.96
54.76
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm

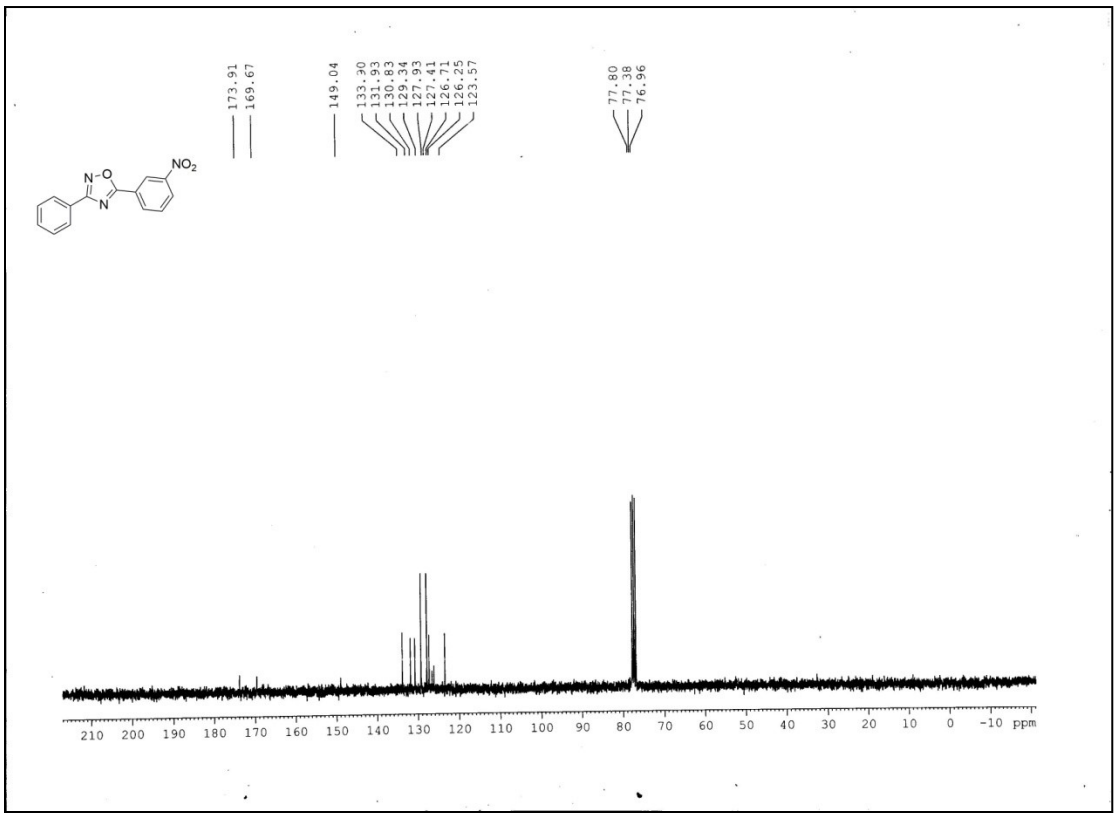

8.183
8.176
8.160
8.153
7.522
7.515
7.504
7.059
7.030
3.890
1.618
OCH3
12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.393
1.078
0.619
1.000

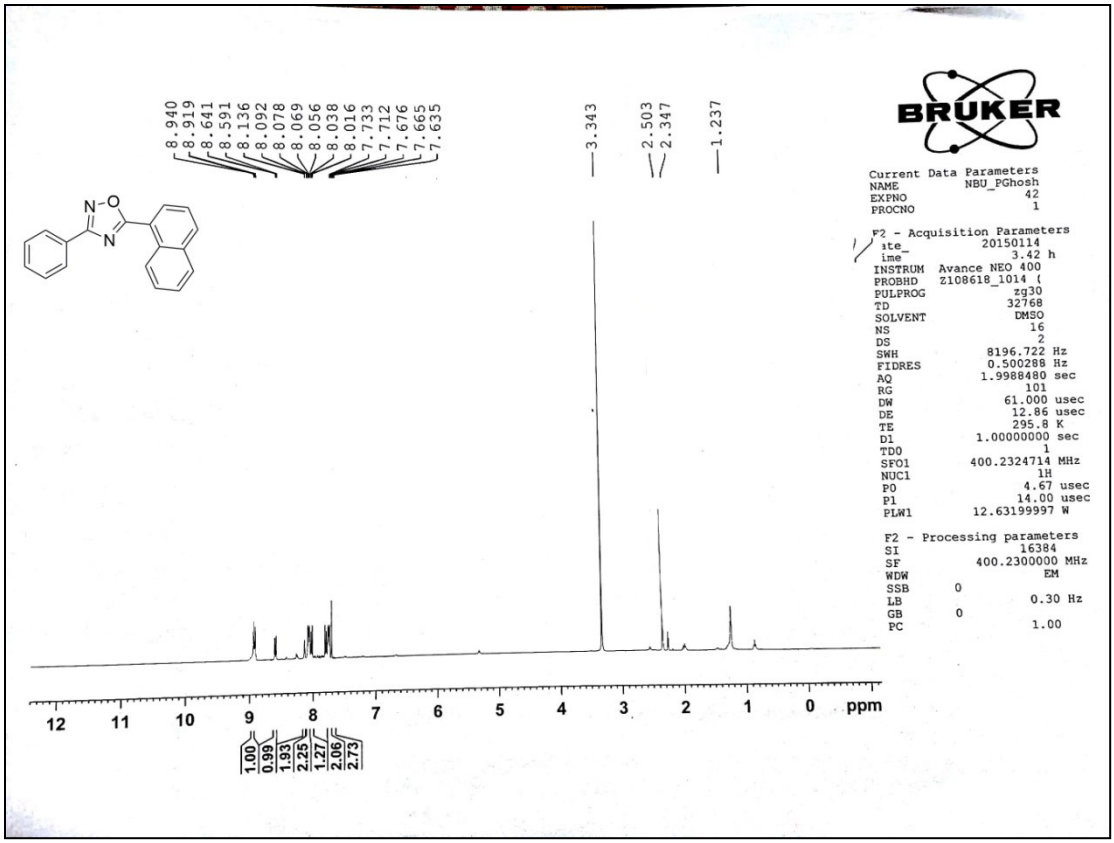

174.91
168.09
133.93
131.30
130.62
129.63
128.09
127.41
126.71
122.80
77.00
76.58
76.16
55.07
OCH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


8.471
8.250
8.237
8.210
7.572
7.547
7.525
7.519
7.268
7.241
1.649
1.461
1.252
0.000
Cl
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.332
0.933
0.621


175.57
169.05
133.80
130.74
130.58
128.77
127.98
127.10
126.21
120.80
77.46
77.03
76.61
N
O
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.620
8.309
8.242
8.188
8.182
8.156
8.137
7.890
7.862
7.804
7.777
7.750
7.578
1.699
1.616
1.282
0.000
NO2
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
1.000
4.953
3.163
0.135


173.91
169.67
149.04
133.90
131.93
130.83
129.34
127.93
127.41
126.71
126.25
123.57
77.80
77.38
76.96
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 ppm


8.940
8.919
8.641
8.591
8.136
8.092
8.078
8.069
8.056
8.038
8.016
7.733
7.712
7.676
7.665
7.635
3.343
2.503
2.347
1.237
BRUKER
Current Data Parameters
NAME NBU_PGhosh
EXPNO 42
PROCNO 1
F2 - Acquisition Parameters
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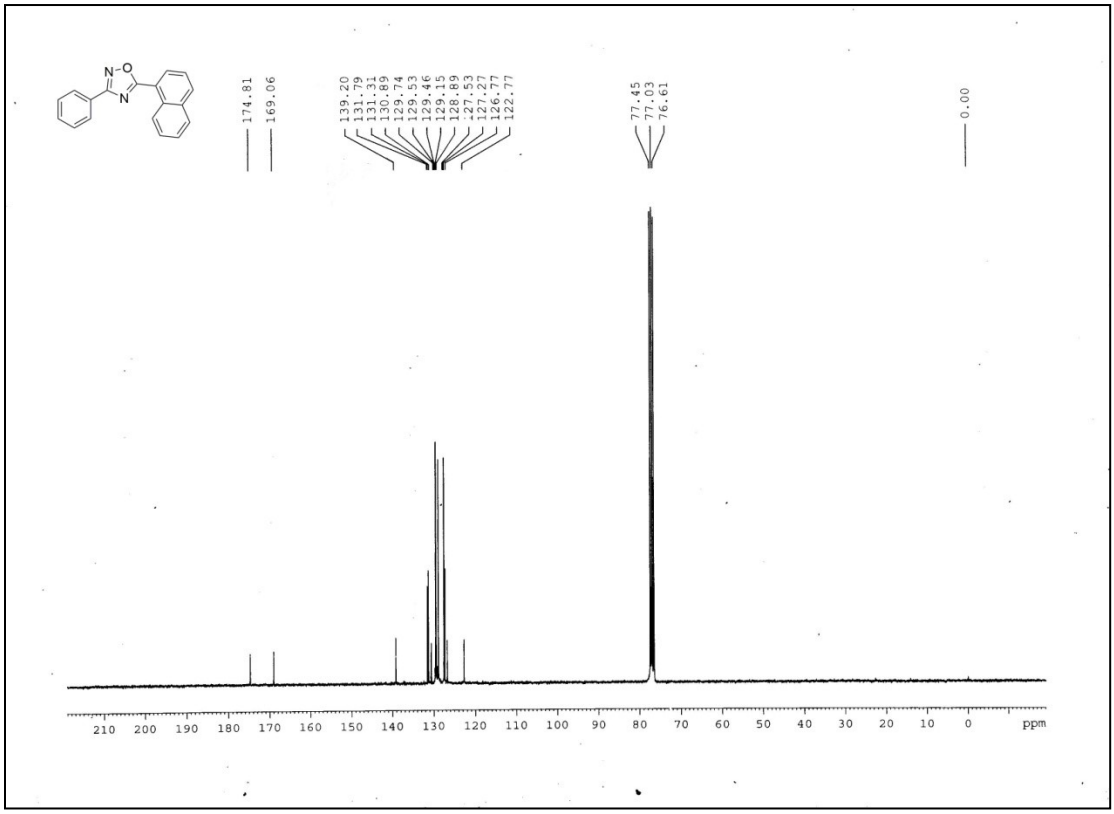
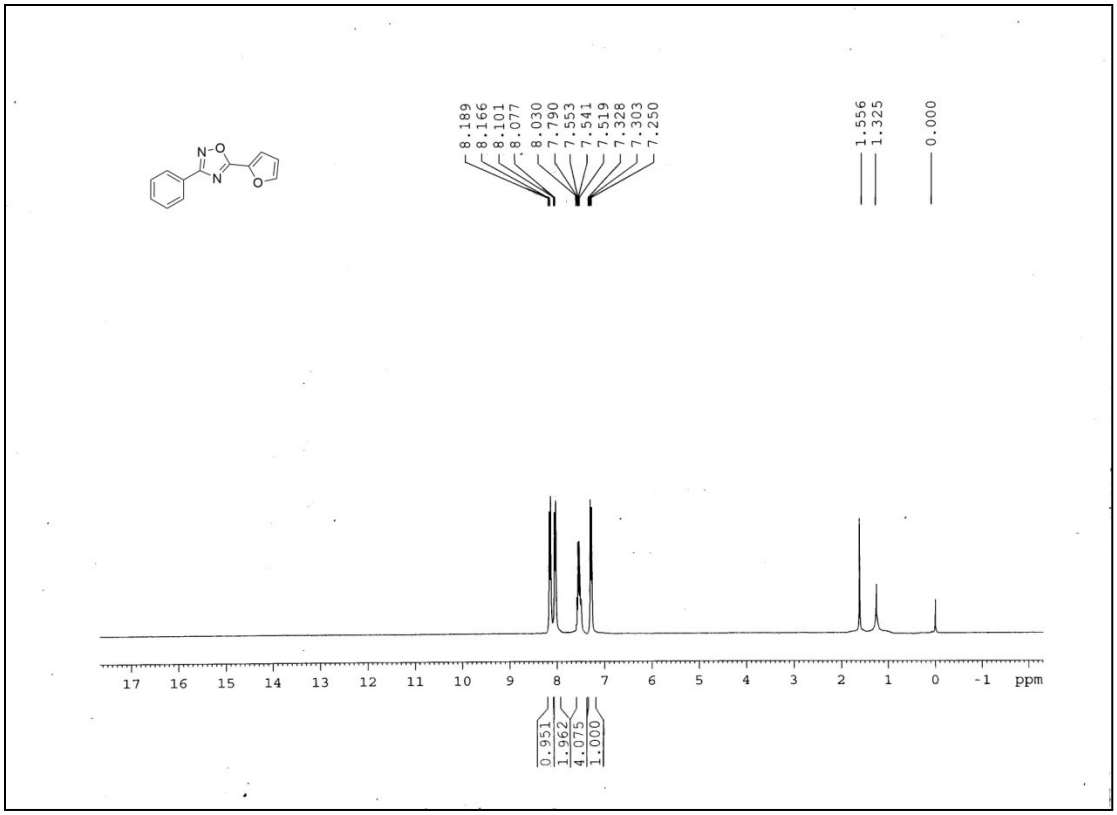
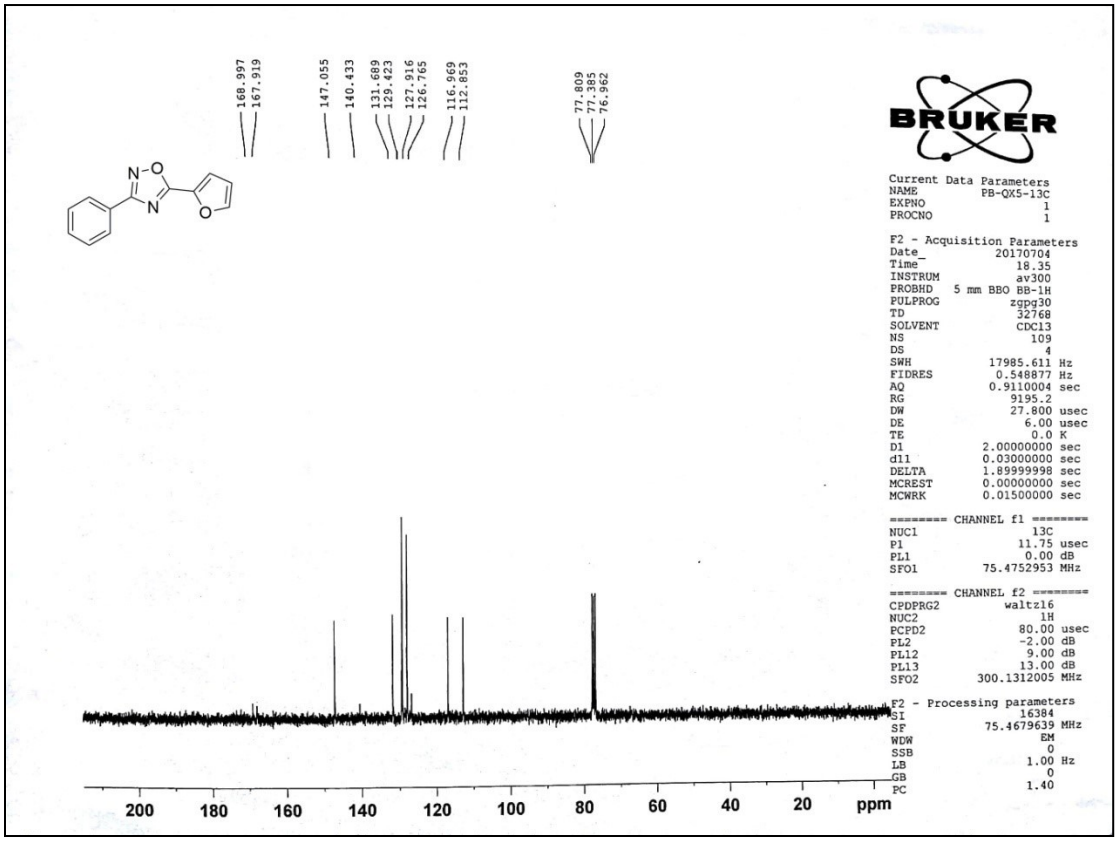
ime_ 3.42 h
INSTRUM Avance NEO 400
PROBHD Z108618_1014 (
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.500288 Hz
AQ 1.9988480 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 12.63199997 W
F2 - Processing parameters
SI 16384
SF 400.2300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00 0.99 1.93 2.25 1.27 2.06 2.73


174.81
169.06
139.20
131.79
131.31
130.89
129.74
129.53
129.46
129.15
128.89
127.53
127.27
126.77
122.77
77.45
77.03
76.61
0.00
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.189
8.166
8.101
8.077
8.030
7.790
7.553
7.541
7.519
7.328
7.303
7.250
1.556
1.325
0.000
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.951
1.962
4.075
1.000


168.997
167.919
147.055
140.433
131.689
129.423
127.916
126.765
116.969
112.853
77.809
77.385
76.962
BRUKER
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PROCNO 1
F2 - Acquisition Parameters
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Time 18.35
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 109
DS 4
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 9195.2
DW 27.800 usec
DE 6.00 usec
TE 0.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.75 usec
PL1 0.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 9.00 dB
PL13 13.00 dB
SFO2 300.1312005 MHz
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SF 75.4679639 MHz
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LB 1.00 Hz
GB 0
PC 1.40
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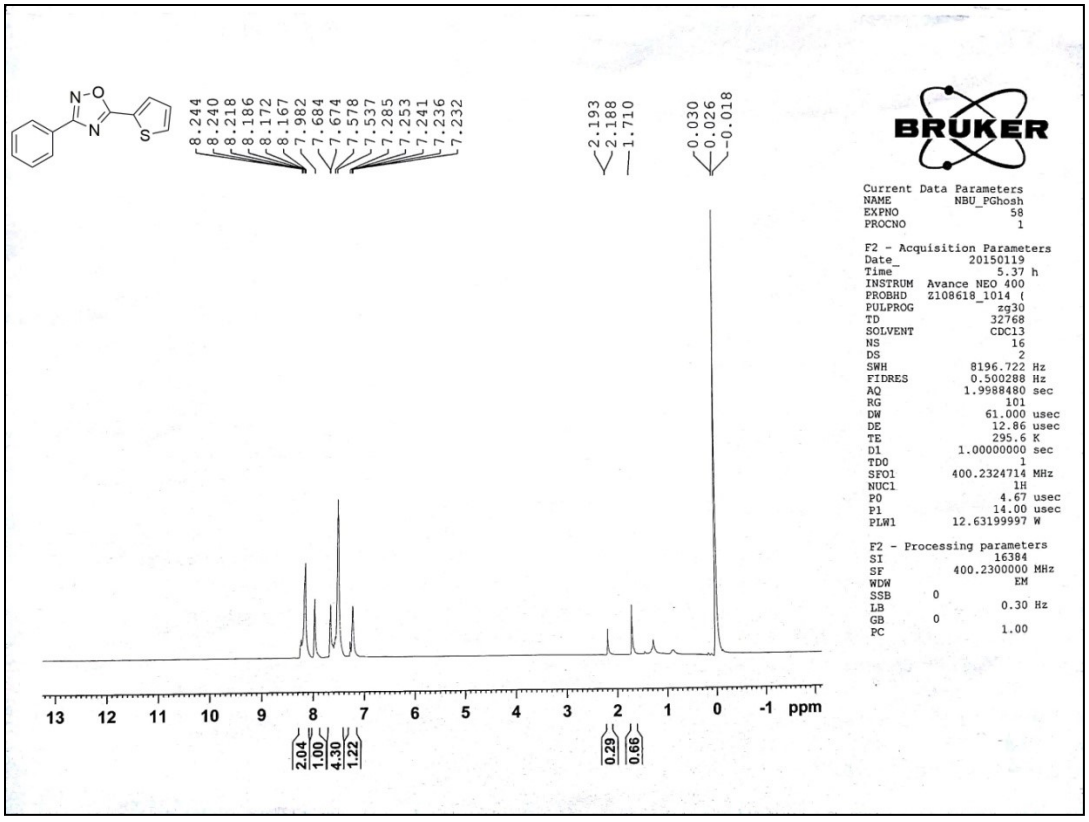
8.244
8.240
8.218
8.186
8.172
8.167
7.982
7.684
7.674
7.578
7.537
7.285
7.253
7.241
7.236
7.232
2.193
2.188
1.710
0.030
0.026
-0.018
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
2.04
1.00
4.30
1.22
0.29
0.66
BRUKER
Current Data Parameters
NAME NBU_PGhosh
EXPNO 58
PROCNO 1
F2 - Acquisition Parameters
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Time 5.37 h
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PROBHD Z108618_1014 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.500288 Hz
AQ 1.9988480 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 12.63199997 W
F2 - Processing parameters
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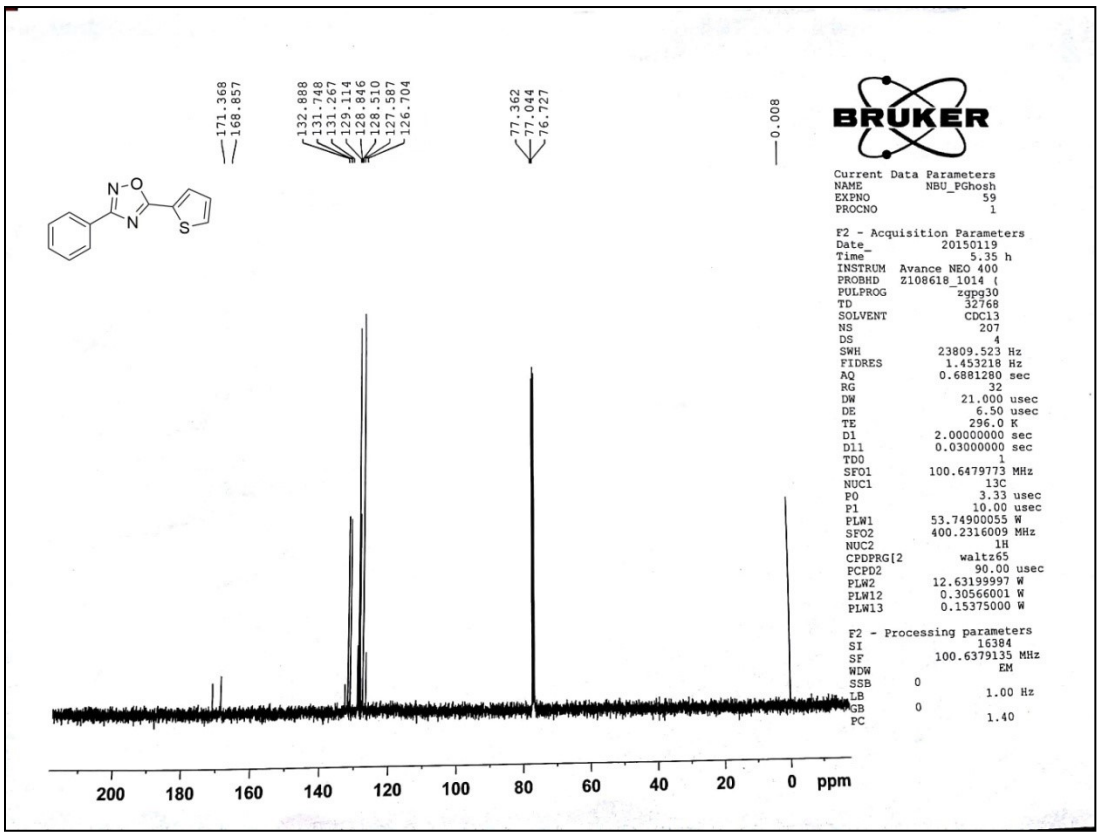
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


171.368
168.857
132.888
131.748
131.267
129.114
128.846
128.510
127.587
126.704
77.362
77.044
76.727
0.008
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
NAME NBU_PGhosh
EXPNO 59
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150119
Time 5.35 h
INSTRUM Avance NEO 400
PROBHD Z108618_1014 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
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DS 4
SWH 23809.523 Hz
FIDRES 1.453218 Hz
AQ 0.6881280 sec
RG 32
DW 21.000 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6479773 MHz
NUC1 13C
P0 3.33 usec
P1 10.00 usec
PLW1 53.74900055 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz65
PCPD2 90.00 usec
PLW2 12.63199997 W
PLW12 0.30566001 W
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SSB 0
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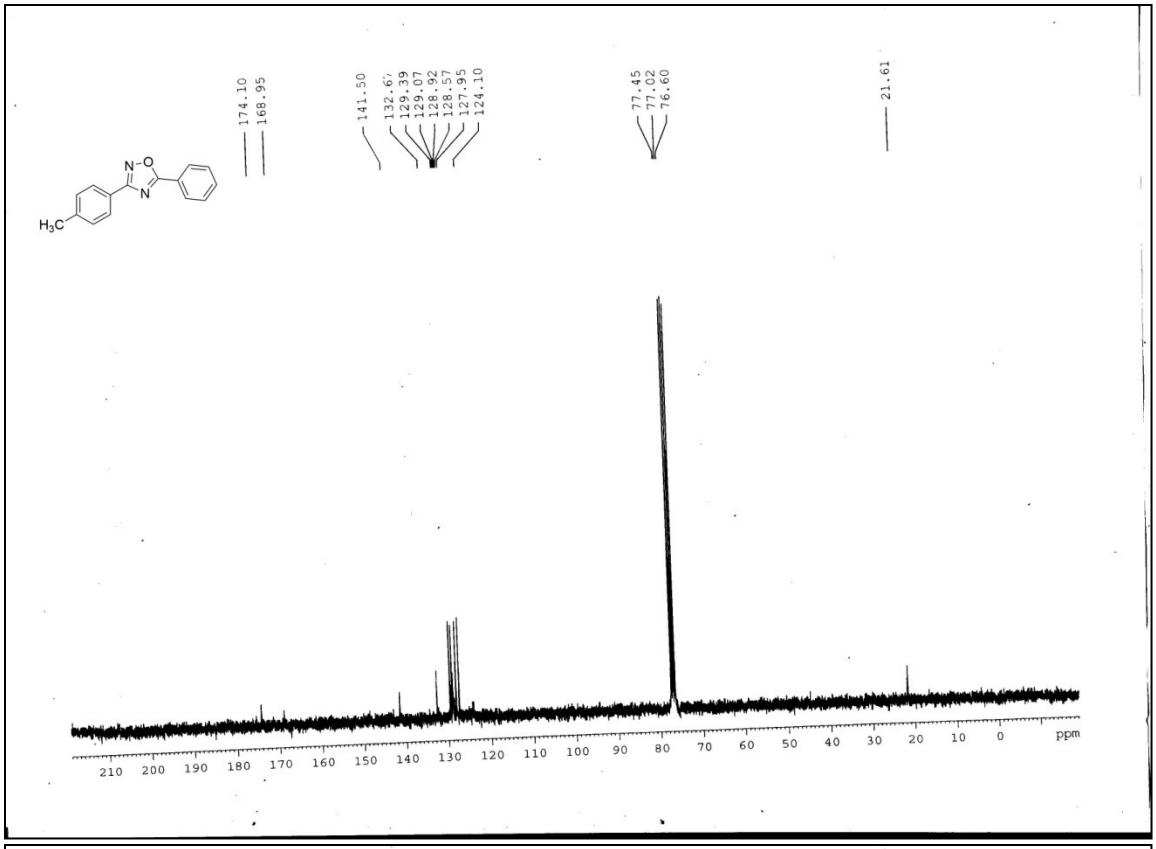
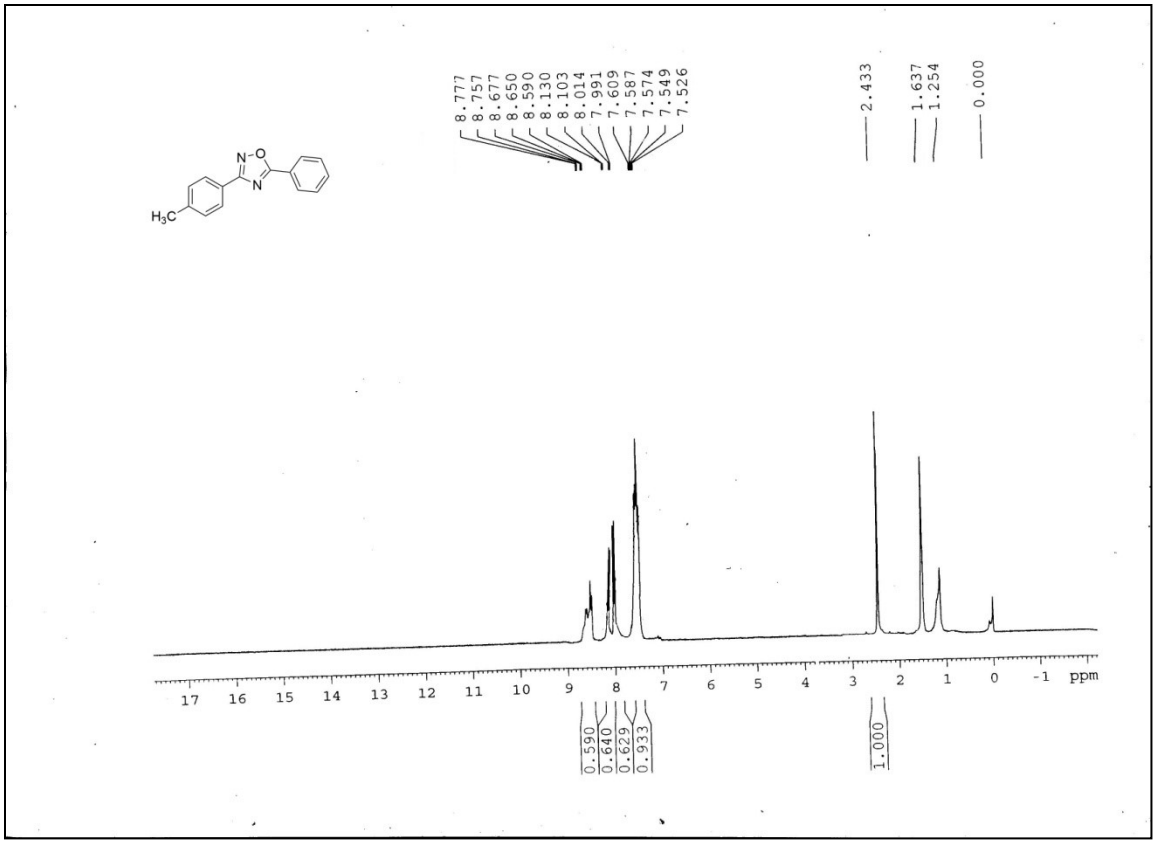
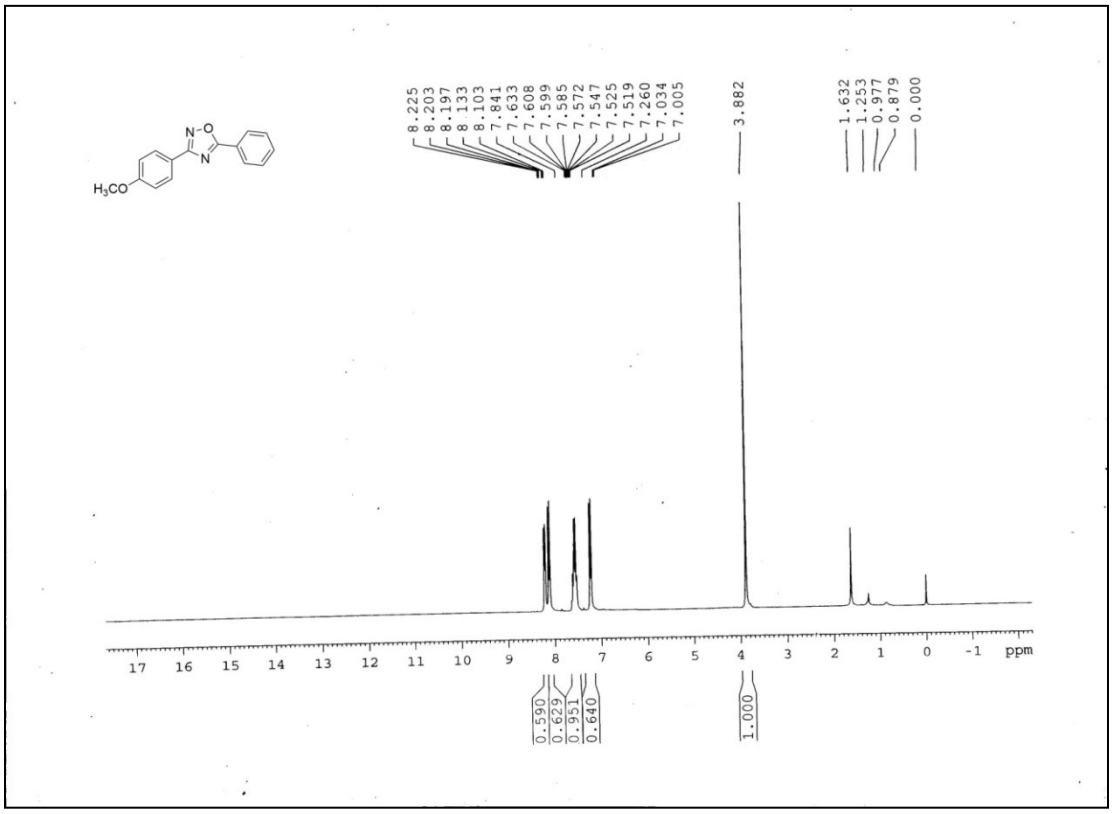
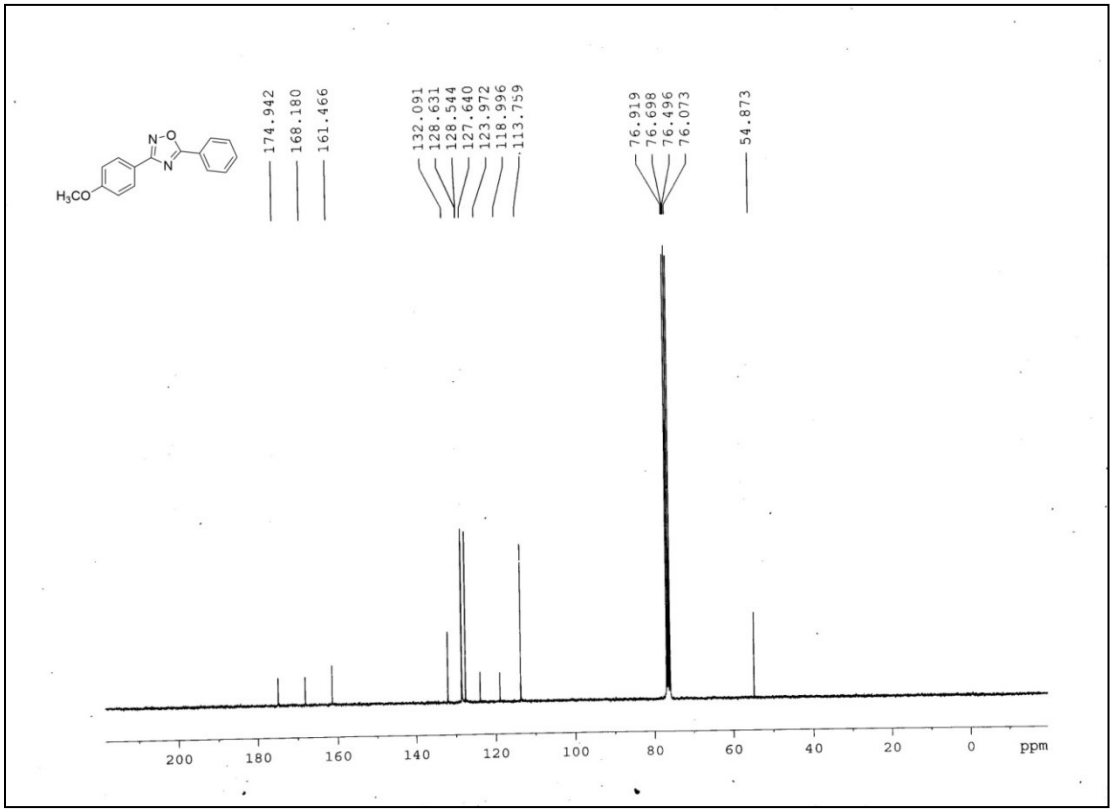
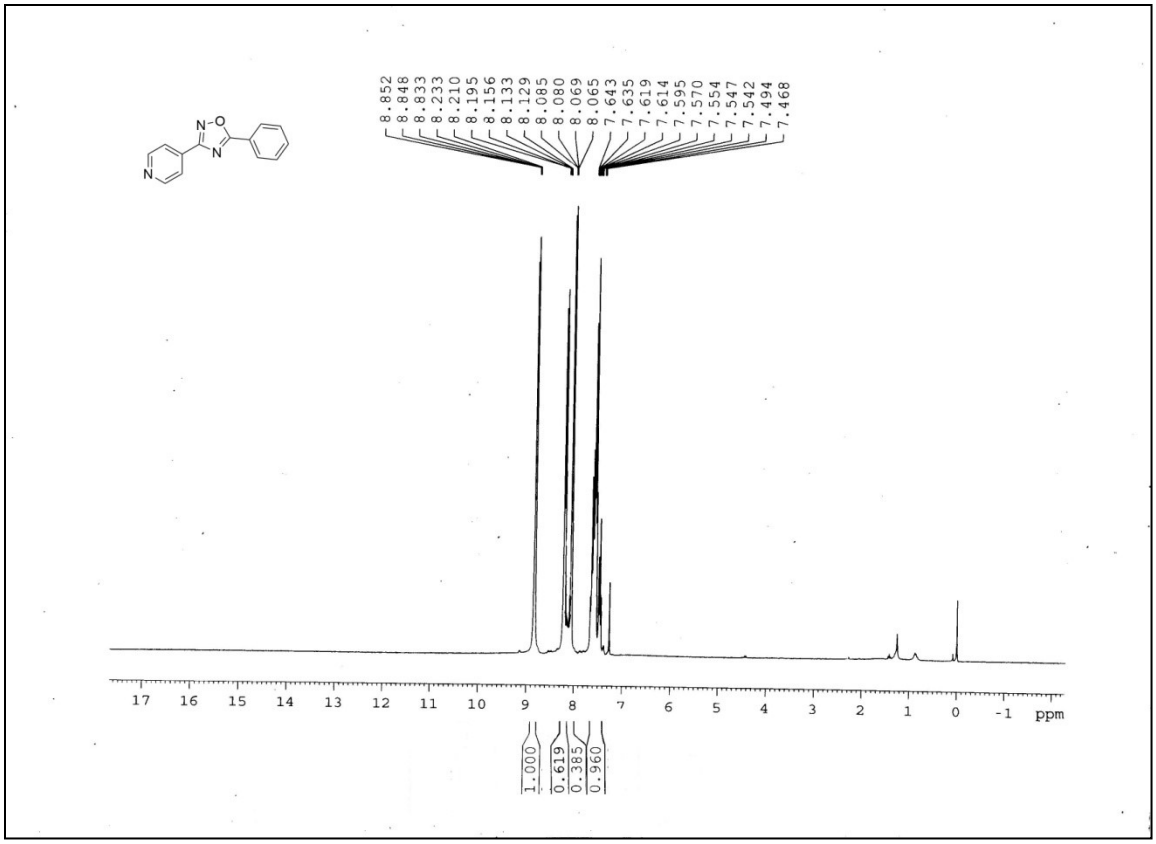
GB 0
PC 1.40


174.10
168.95
141.50
132.67
129.39
129.07
128.92
128.57
127.95
124.10
77.45
77.02
76.60
21.61
H3C
ppm


8.777
8.757
8.677
8.650
8.590
8.130
8.103
8.014
7.991
7.609
7.587
7.574
7.549
7.526
2.433
1.637
1.254
0.000
H3C
ppm
0.590
0.640
0.629
0.933
1.000


8.225
8.203
8.197
8.133
8.103
7.841
7.633
7.608
7.599
7.585
7.572
7.547
7.525
7.519
7.260
7.034
7.005
3.882
1.632
1.253
0.977
0.879
0.000
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
0.590
0.629
0.951
0.640
1.000


174.942
168.180
161.466
132.091
128.631
128.544
127.640
123.972
118.996
113.759
76.919
76.698
76.496
76.073
54.873
200 180 160 140 120 100 80 60 40 20 0 ppm


8.852
8.848
8.833
8.233
8.210
8.195
8.156
8.133
8.129
8.085
8.080
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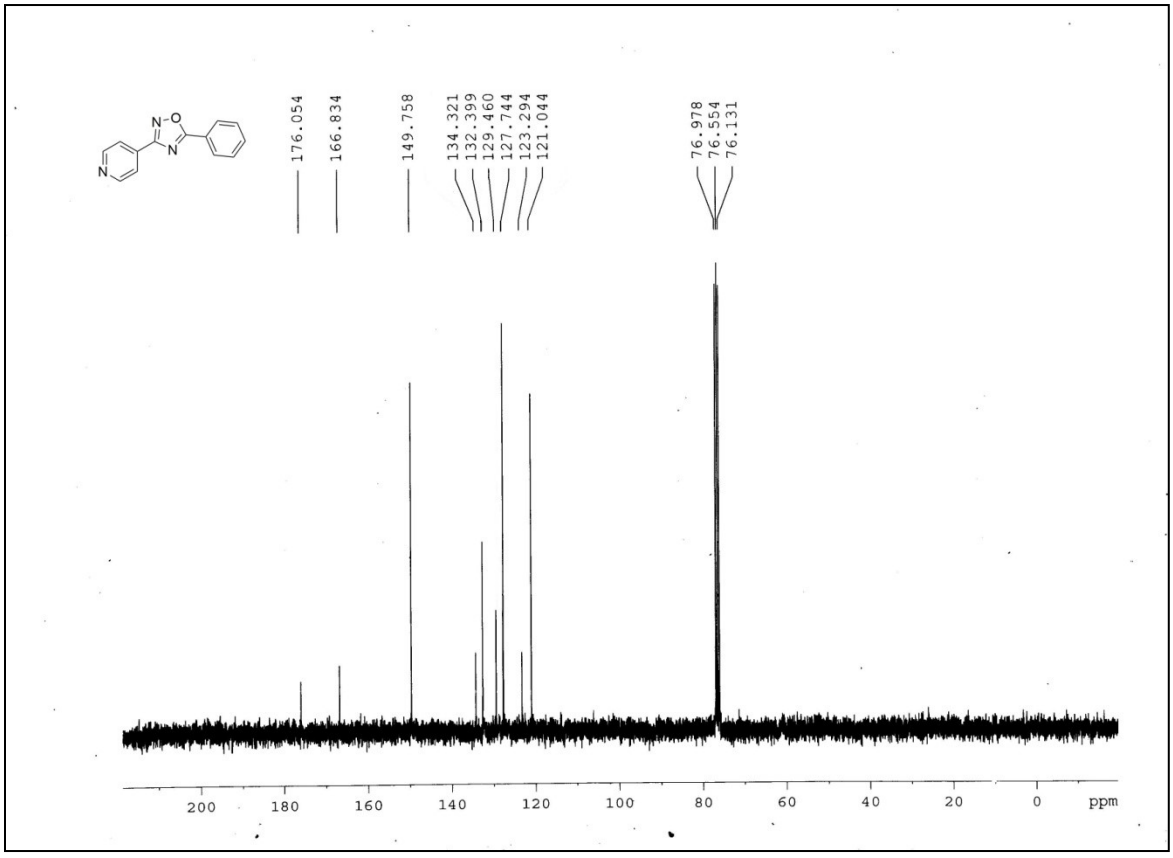
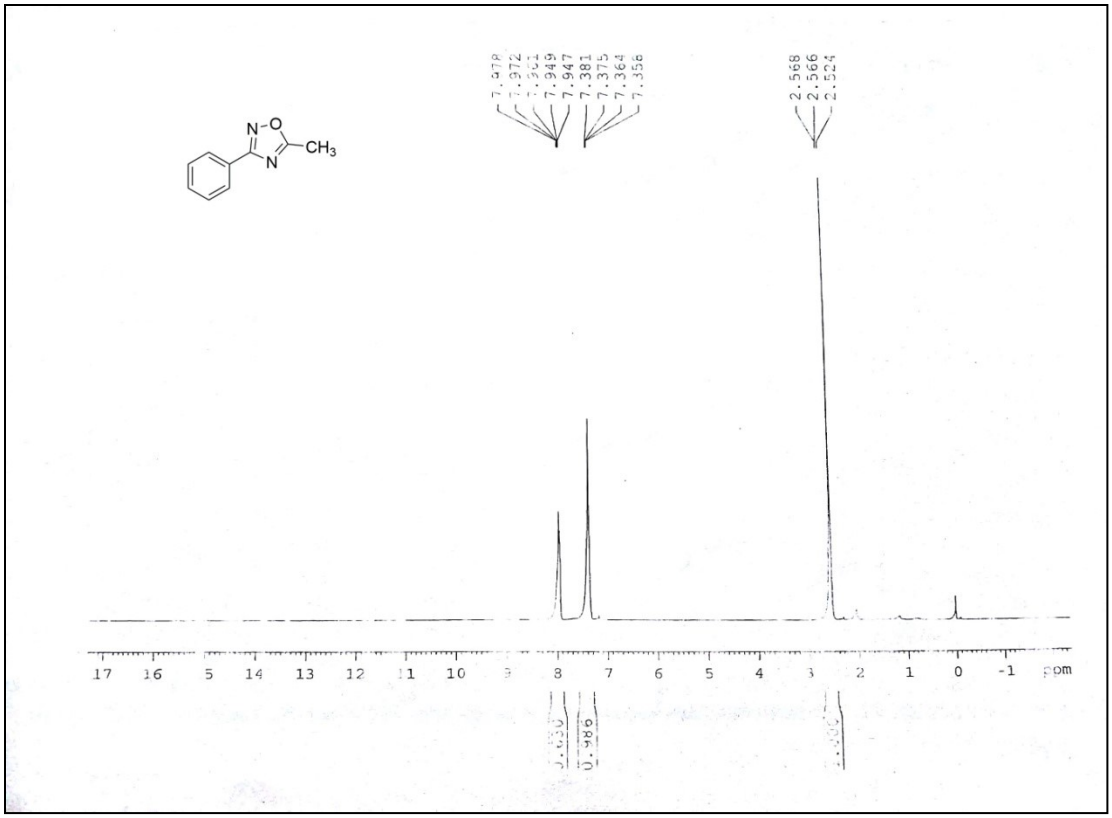
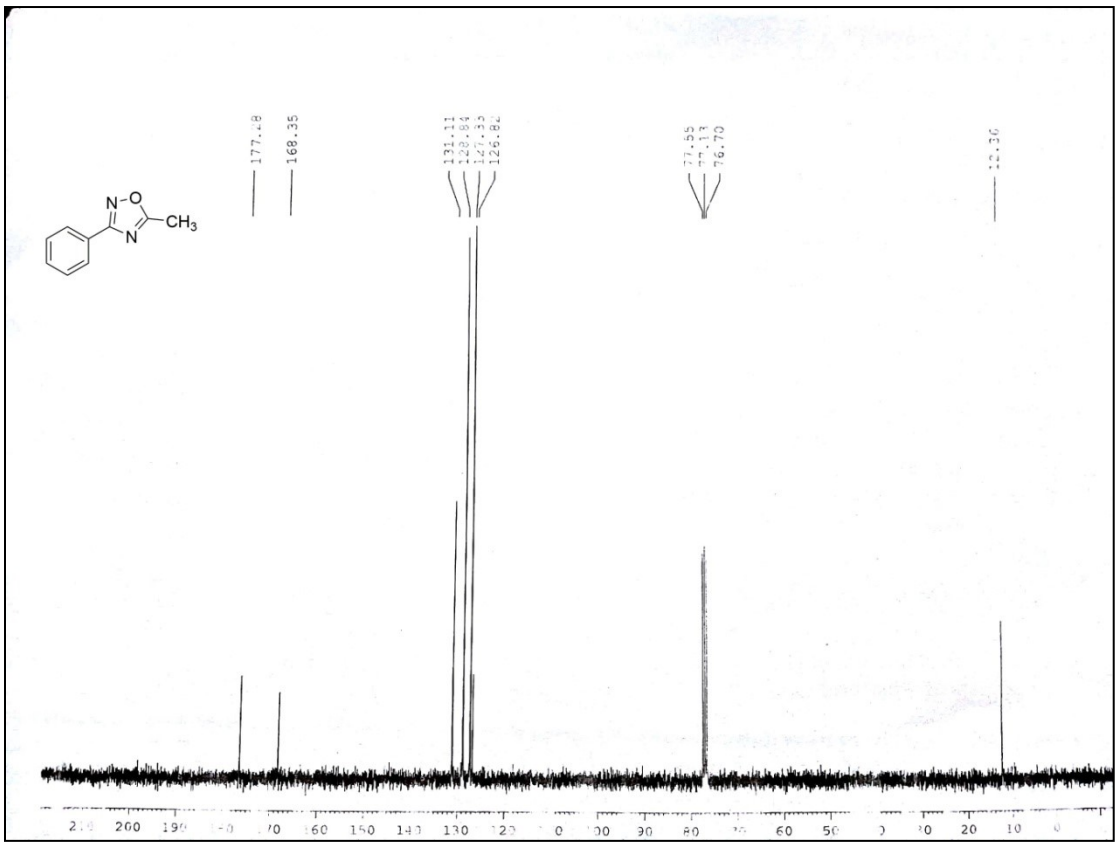
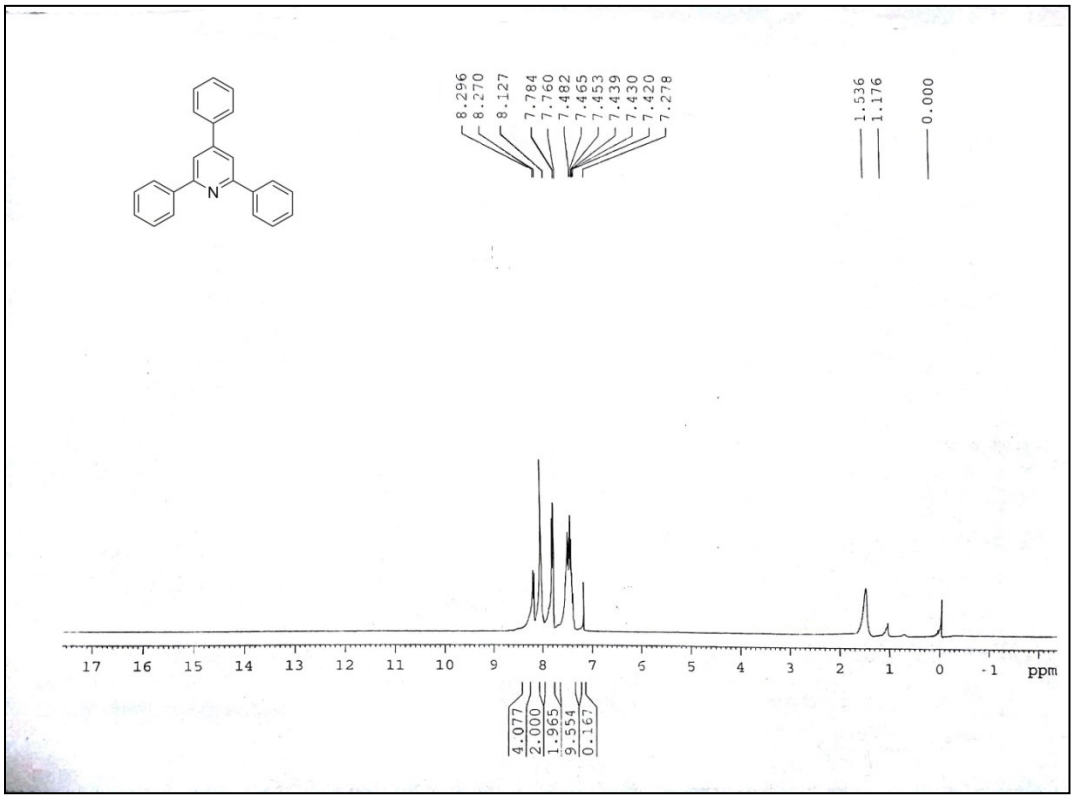
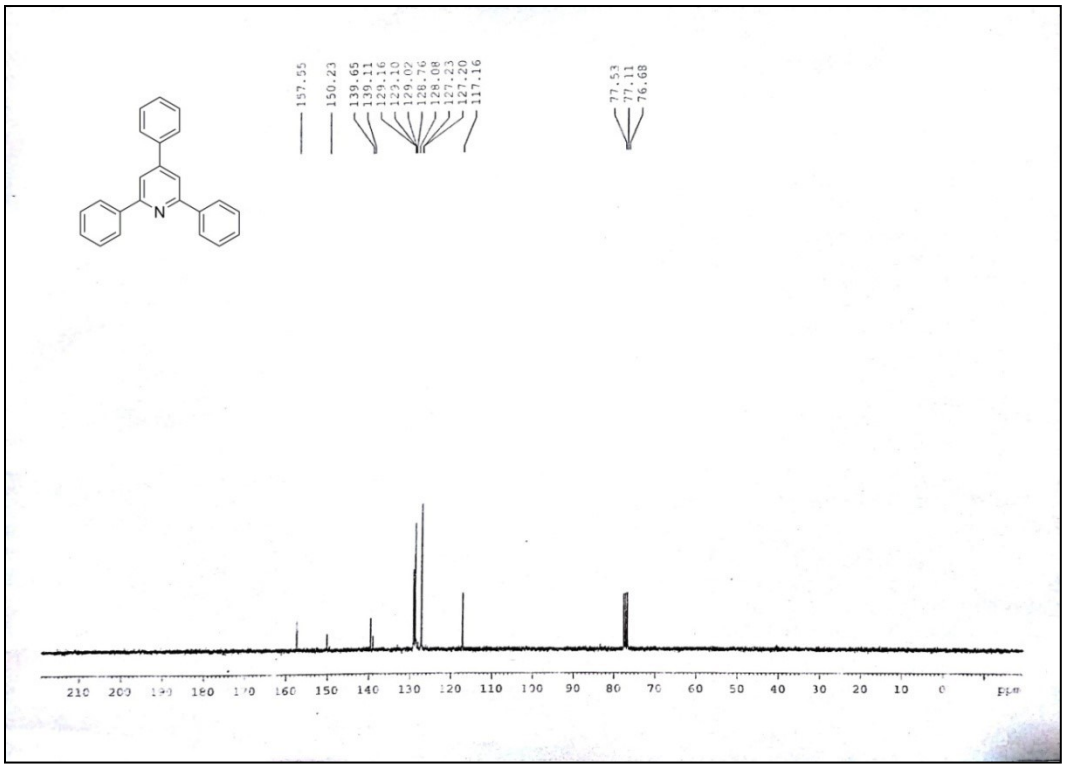
8.065
7.643
7.635
7.619
7.614
7.595
7.570
7.554
7.547
7.542
7.494
7.468
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.000
0.619
0.385
0.960

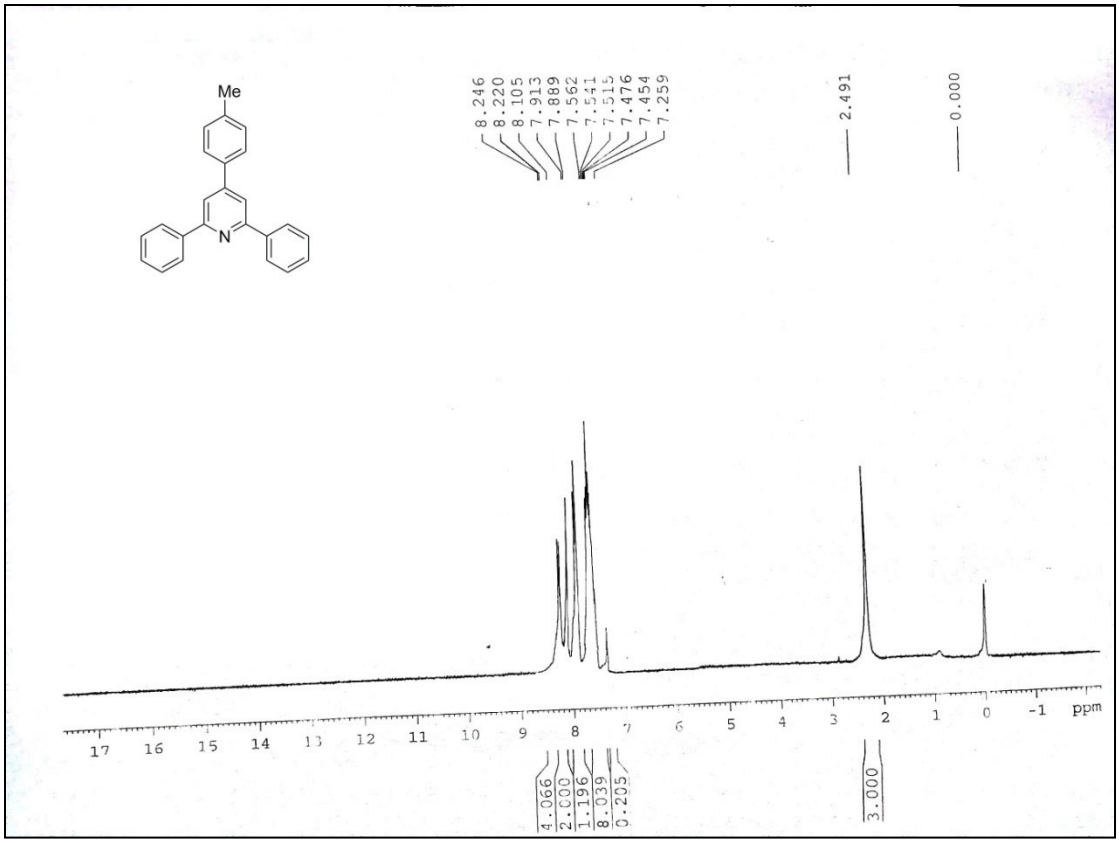

176.054
166.834
149.758
134.321
132.399
129.460
127.744
123.294
121.044
76.978
76.554
76.131
200 180 160 140 120 100 80 60 40 20 0 ppm

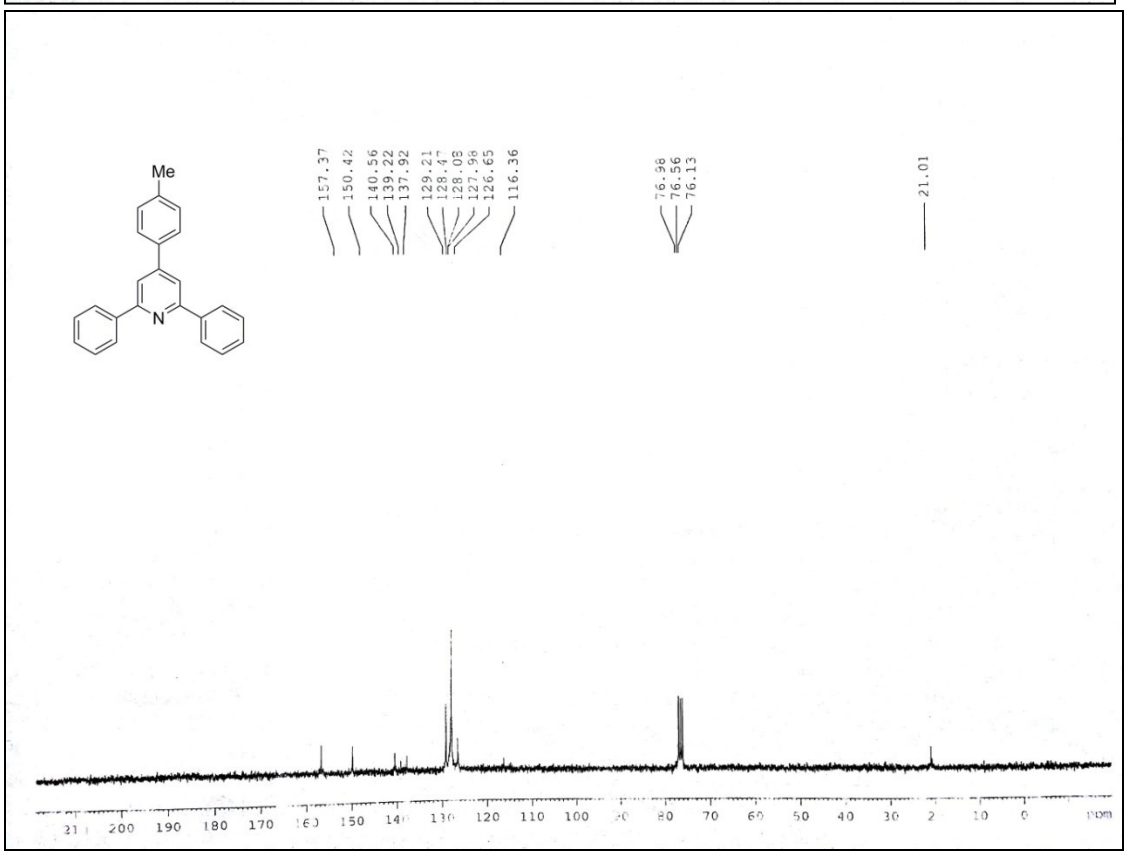

7.947
7.944
7.381
7.375
7.364
7.356
2.568
2.566
2.524
ppm

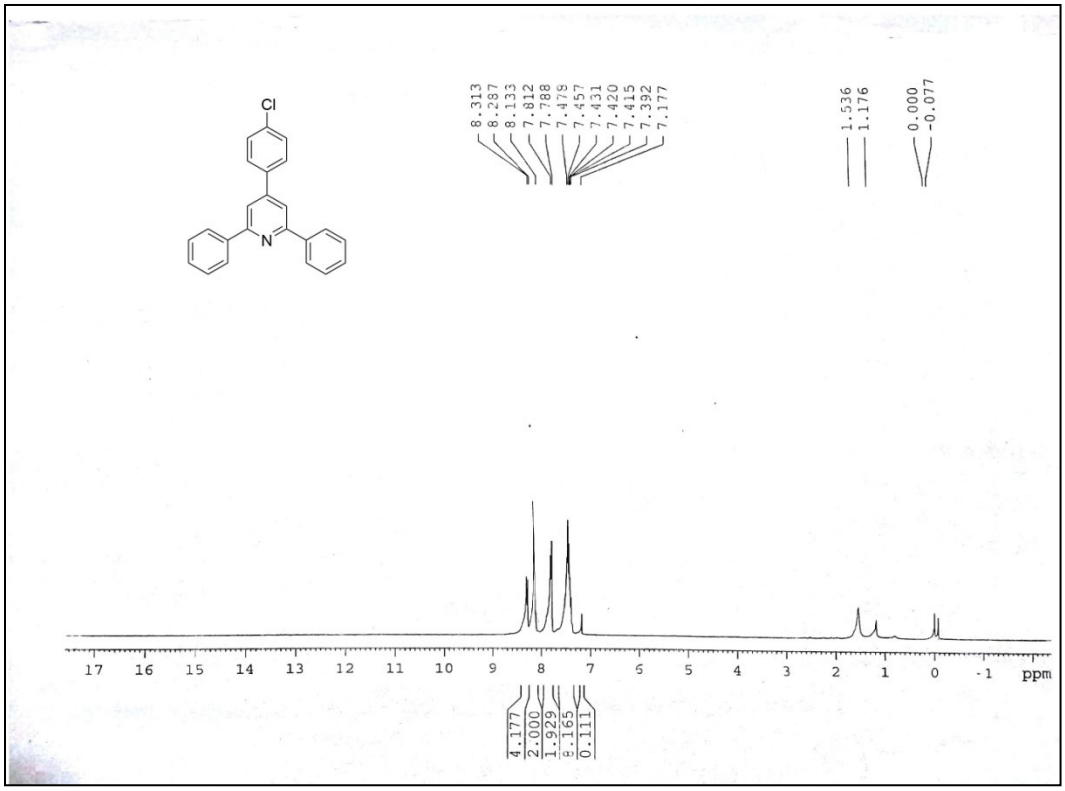

177.48
168.35
131.11
128.84
127.33
126.82
77.55
77.13
76.70
12.36

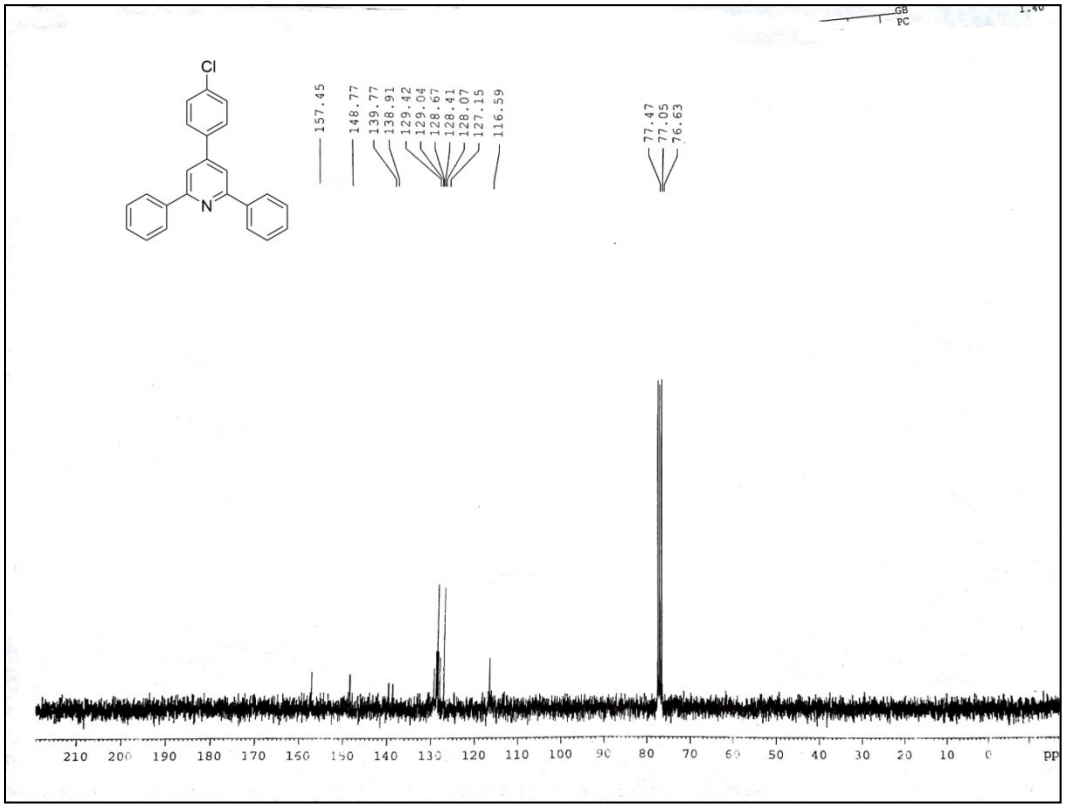

8.296
8.270
8.127
7.784
7.760
7.482
7.465
7.453
7.439
7.430
7.420
7.278
1.536
1.176
0.000
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
4.077
2.000
1.965
9.554
0.167

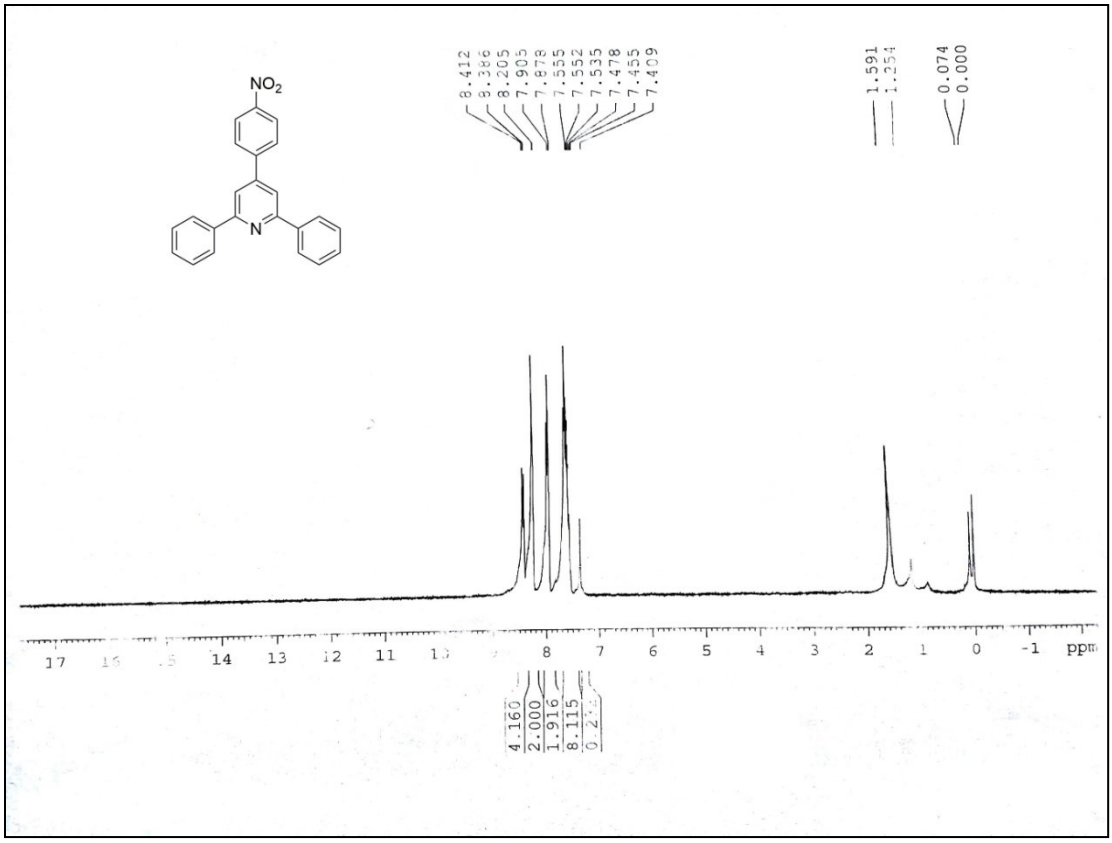

157.55
150.23
139.65
139.11
129.16
129.10
129.02
128.76
128.08
127.23
127.20
117.16
77.53
77.11
76.68
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

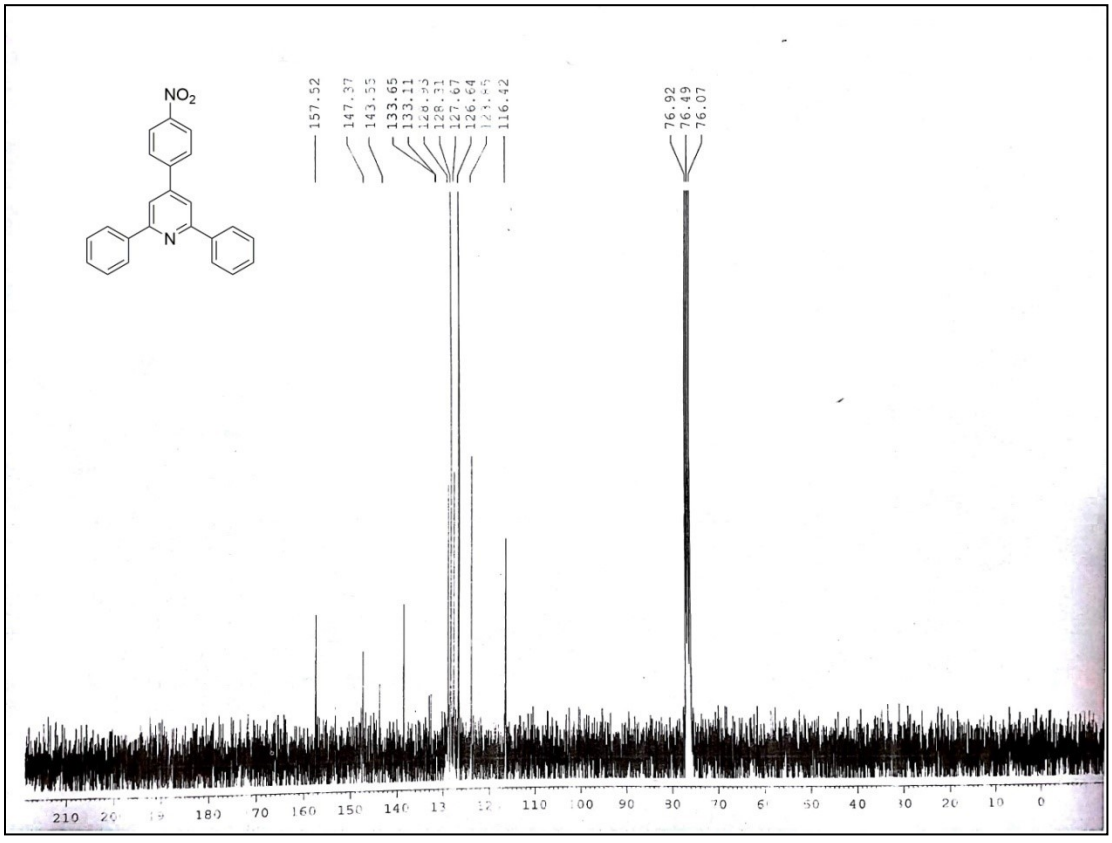

Me
N
8.246
8.220
8.105
7.913
7.889
7.562
7.541
7.515
7.476
7.454
7.259
2.491
0.000
ppm
4.066
2.000
1.196
8.039
0.205
3.000

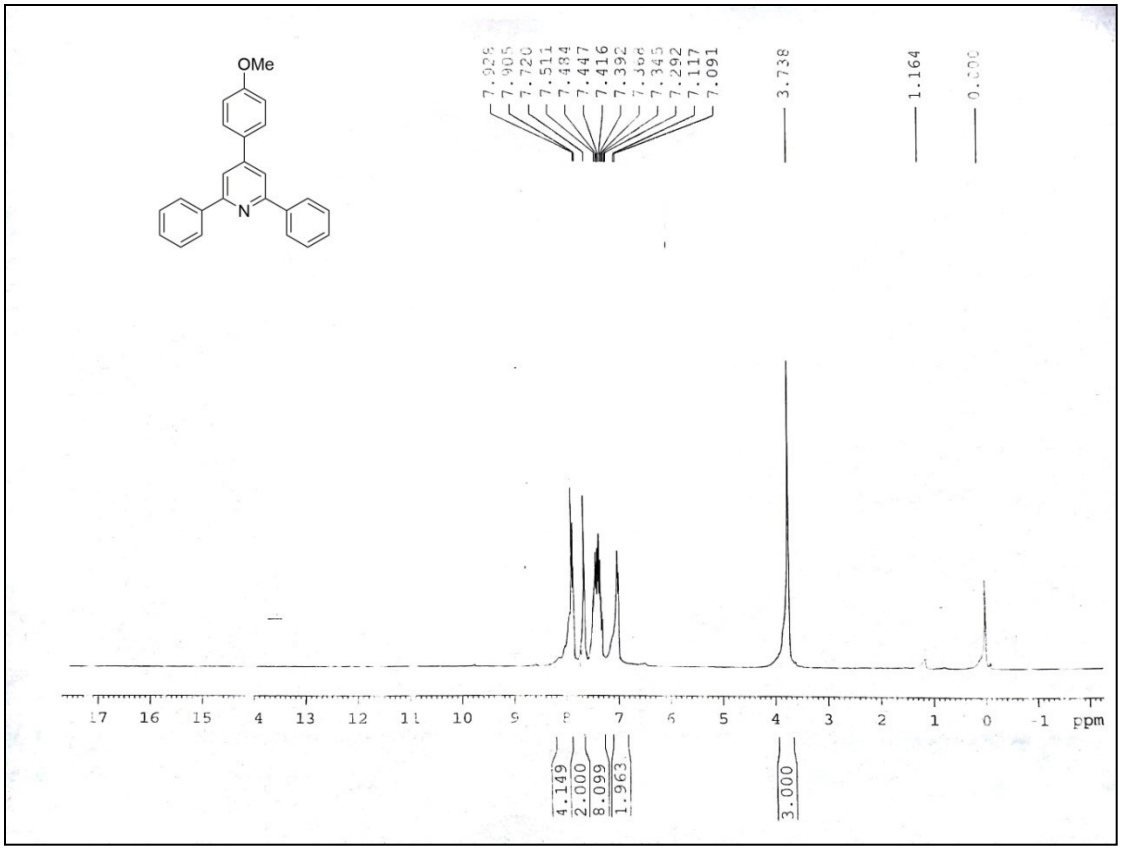

Me
N
157.37
150.42
140.56
139.22
137.92
129.21
128.47
128.08
127.98
126.65
116.36
76.98
76.56
76.13
21.01
ppm

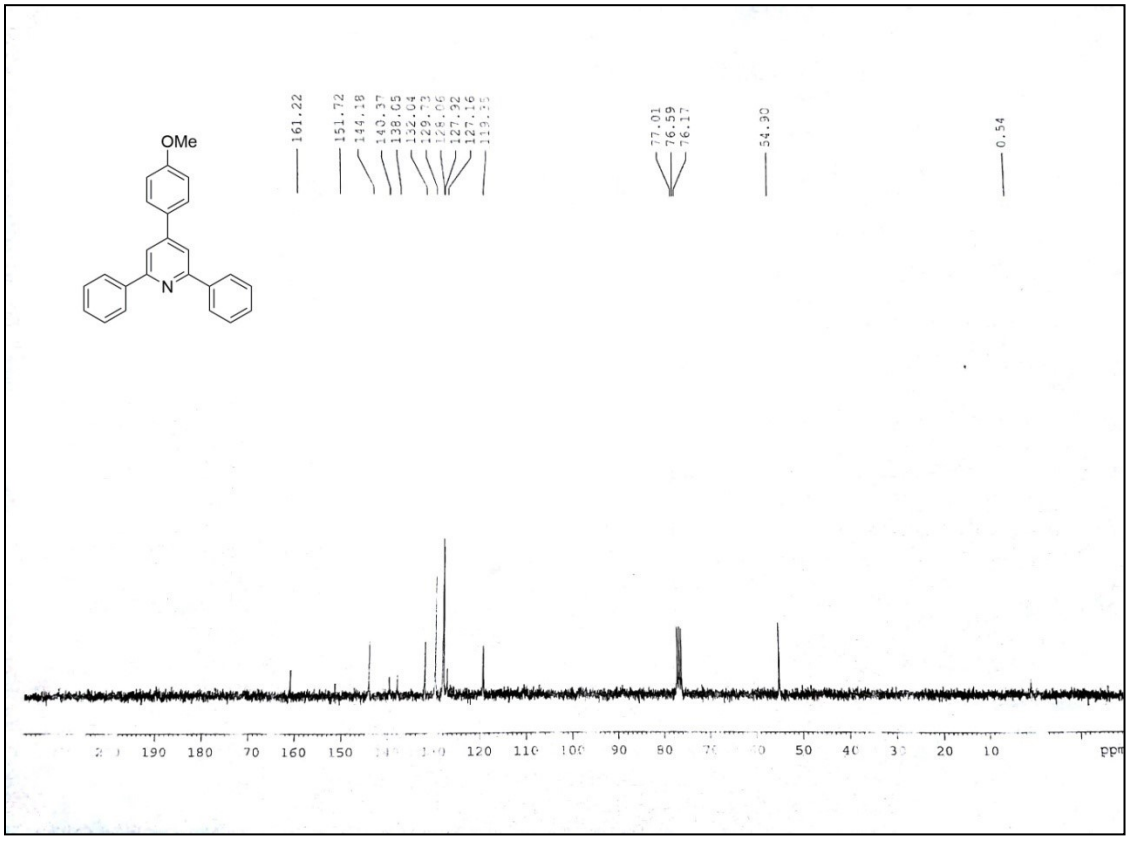

Cl
N
8.313
8.287
8.133
7.812
7.788
7.479
7.457
7.431
7.420
7.415
7.392
7.177
1.536
1.176
0.000
-0.077
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
4.177
2.000
1.929
2.165
0.111

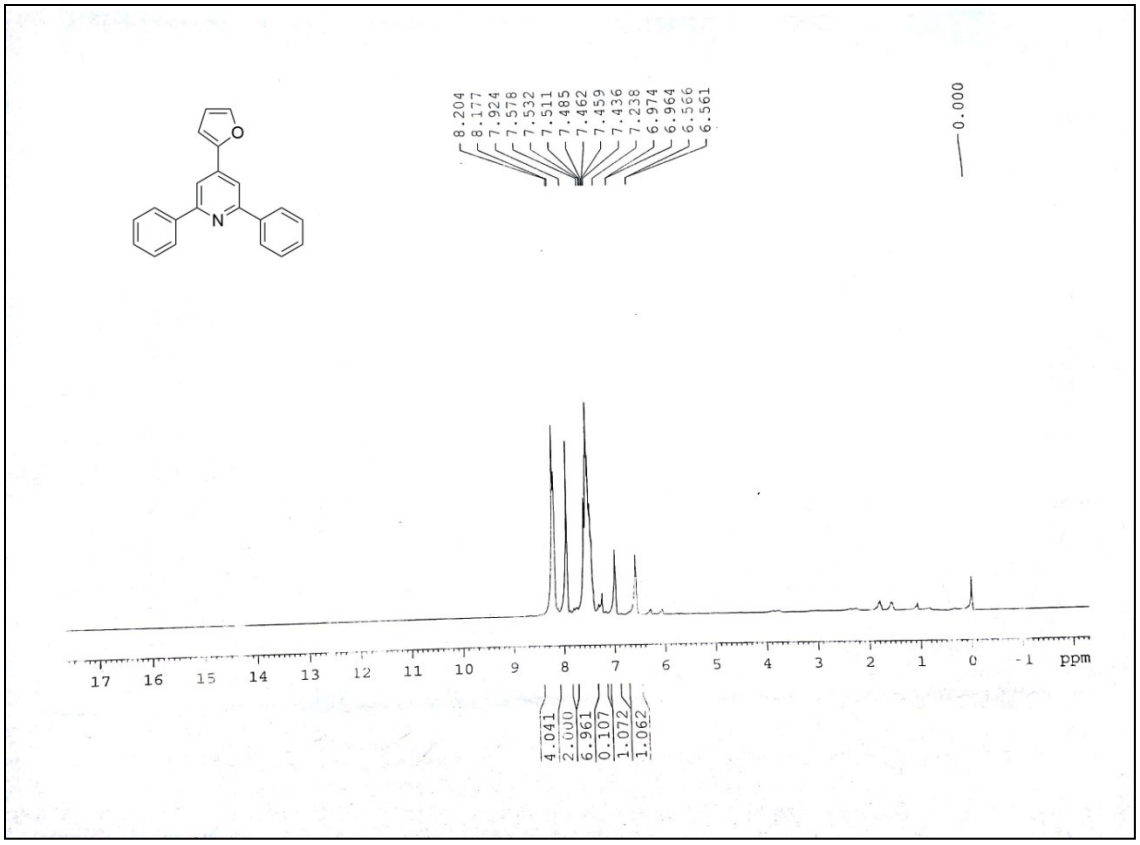

Cl
N
157.45
148.77
139.77
138.91
129.42
129.04
128.67
128.41
128.07
127.15
116.59
77.47
77.05
76.63
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

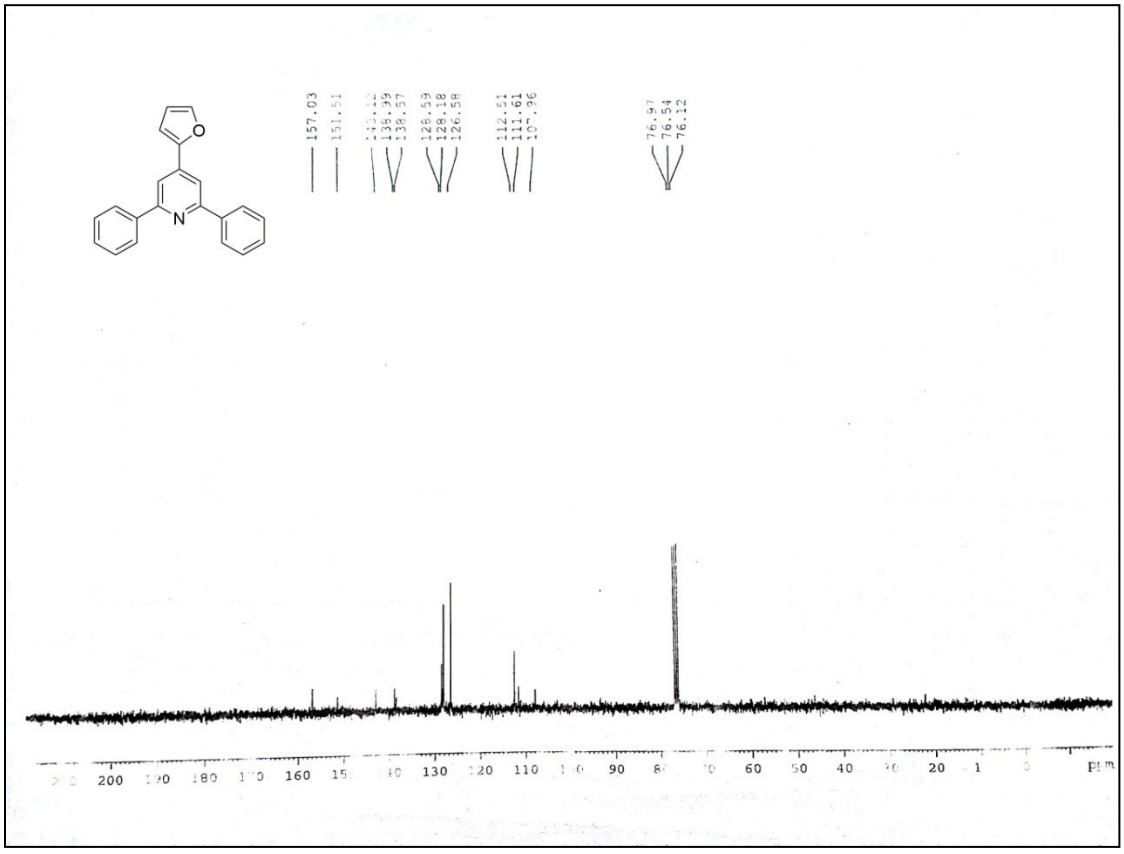

NO2
N
8.412
8.386
8.205
7.905
7.878
7.555
7.552
7.535
7.478
7.455
7.409
1.591
1.254
0.074
0.000
4.160
2.000
1.916
8.115
ppm

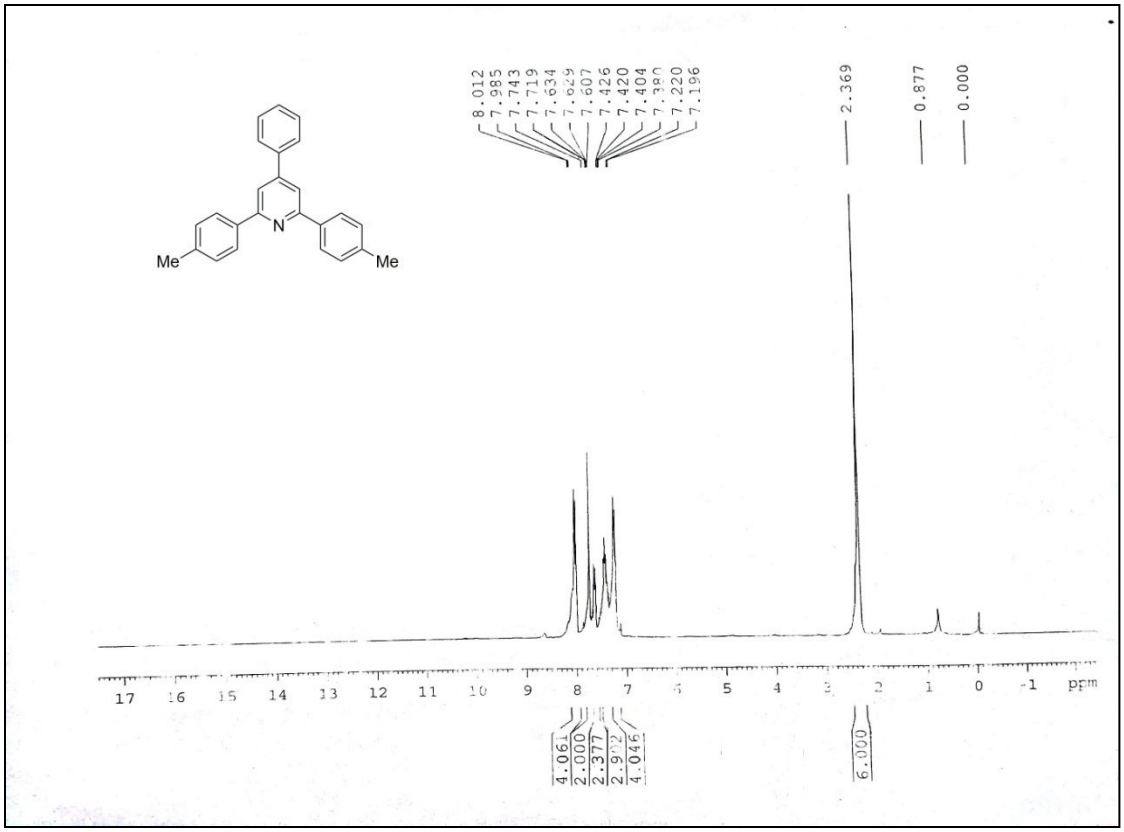

NO2
N
157.52
147.37
143.55
133.65
133.11
128.31
127.67
126.64
116.42
76.92
76.49
76.07

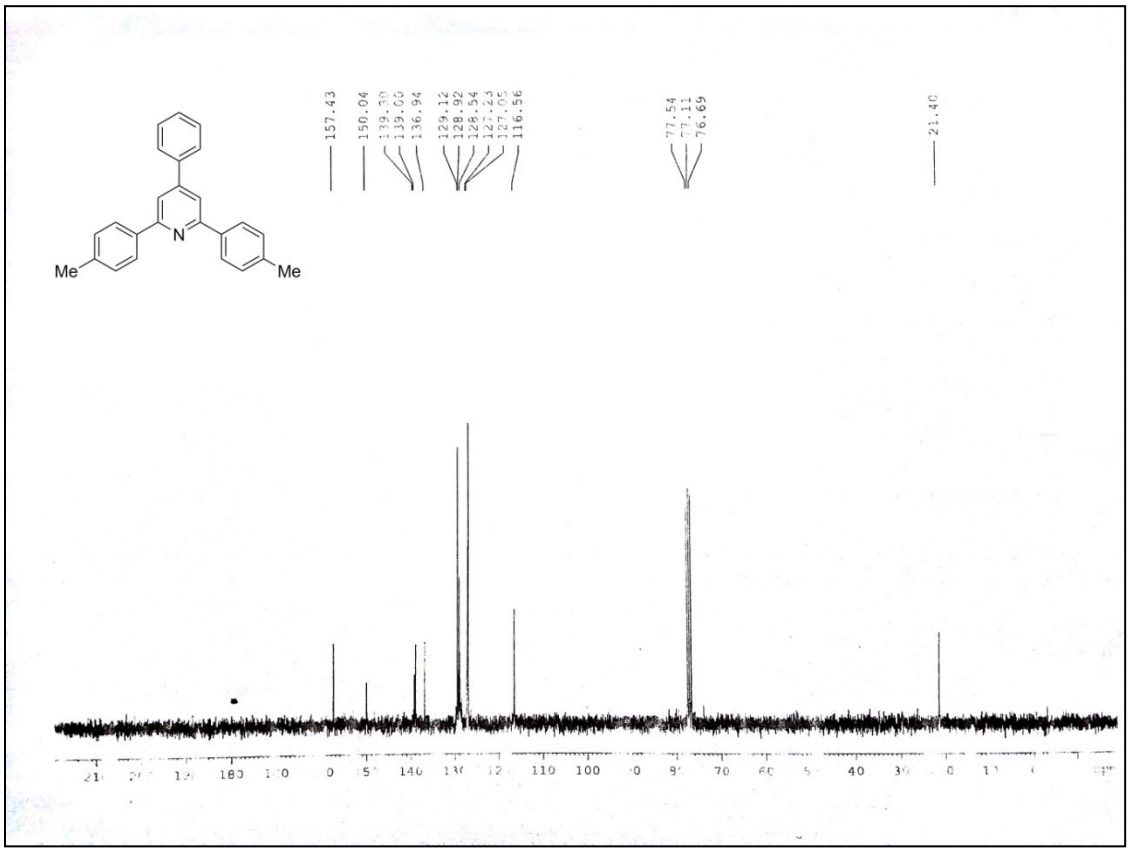

OMe
N
7.925
7.905
7.720
7.511
7.484
7.447
7.416
7.392
7.366
7.345
7.292
7.117
7.091
3.738
1.164
0.000
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
4.149
2.000
8.099
1.963
3.000

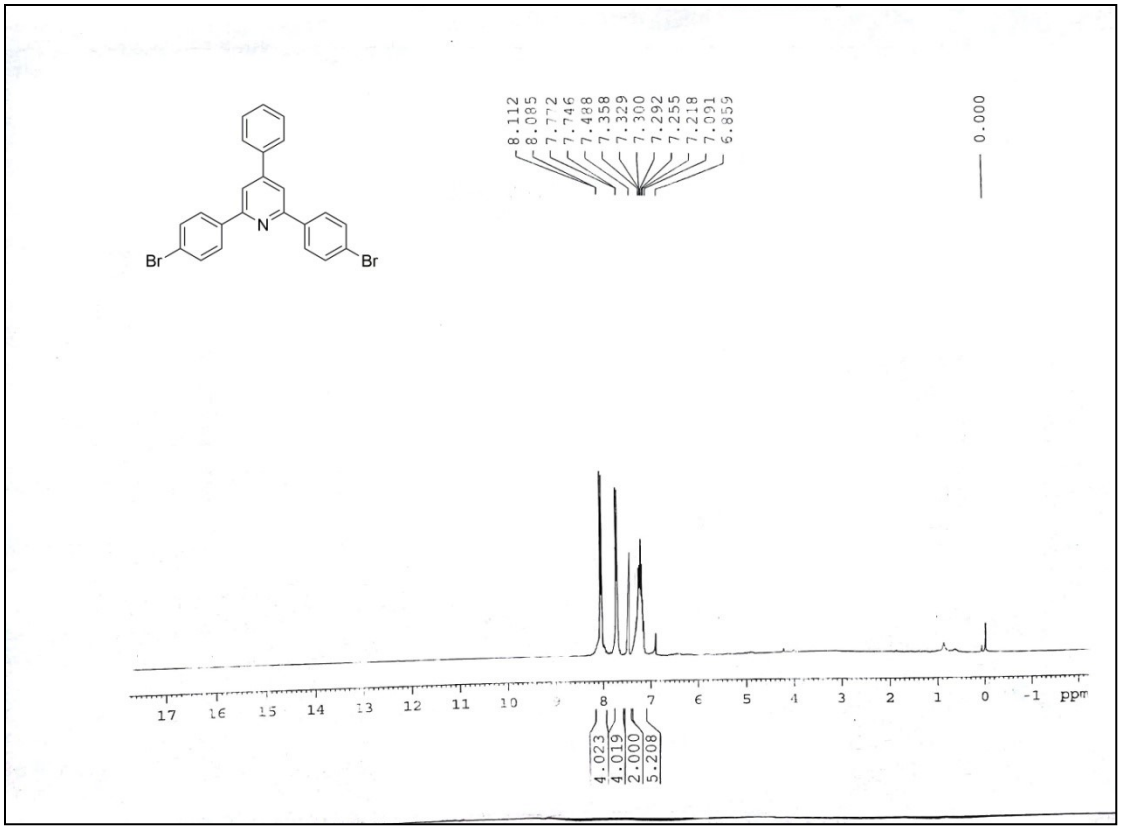

OMe
N
161.22
151.72
144.18
140.37
138.65
132.54
129.13
128.66
127.92
127.16
119.35
77.01
76.59
76.17
54.90
0.54
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

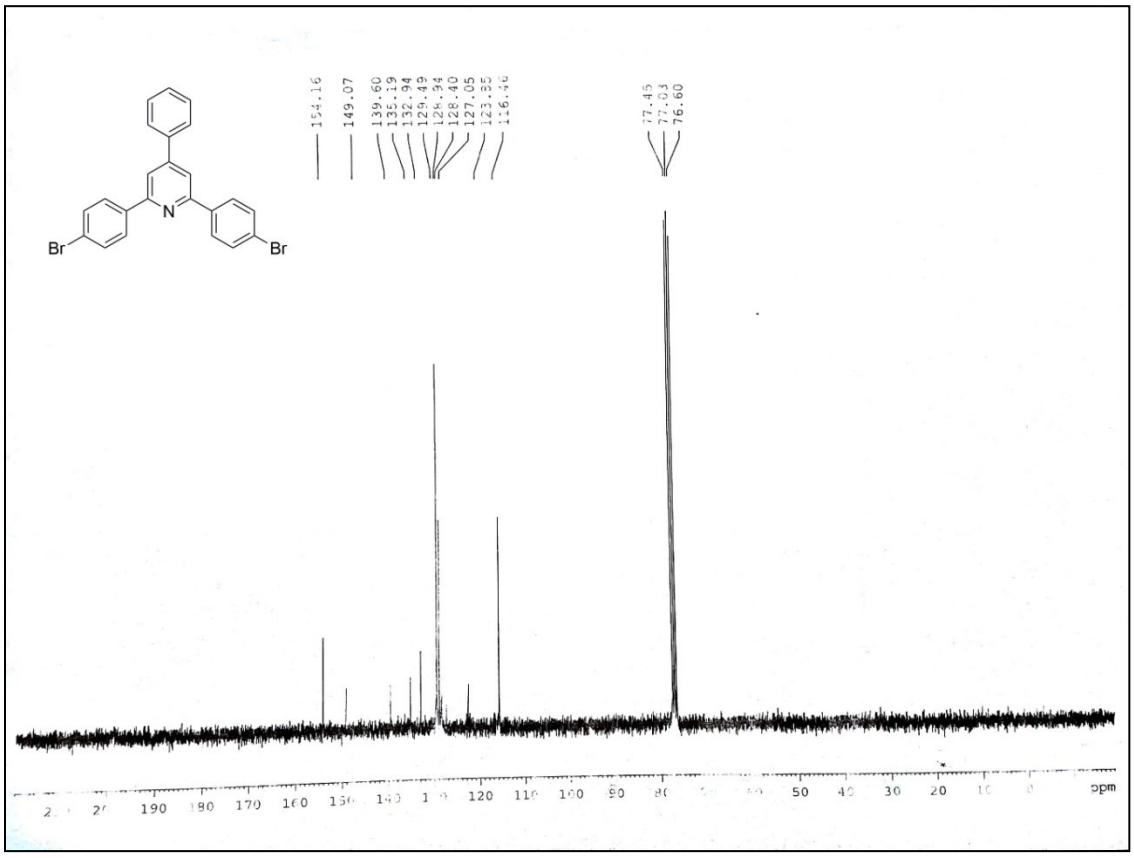

8.204
8.177
7.924
7.578
7.532
7.511
7.485
7.462
7.459
7.436
7.238
6.974
6.964
6.566
6.561
0.000
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
4.041
2.000
6.961
0.107
1.072
1.062

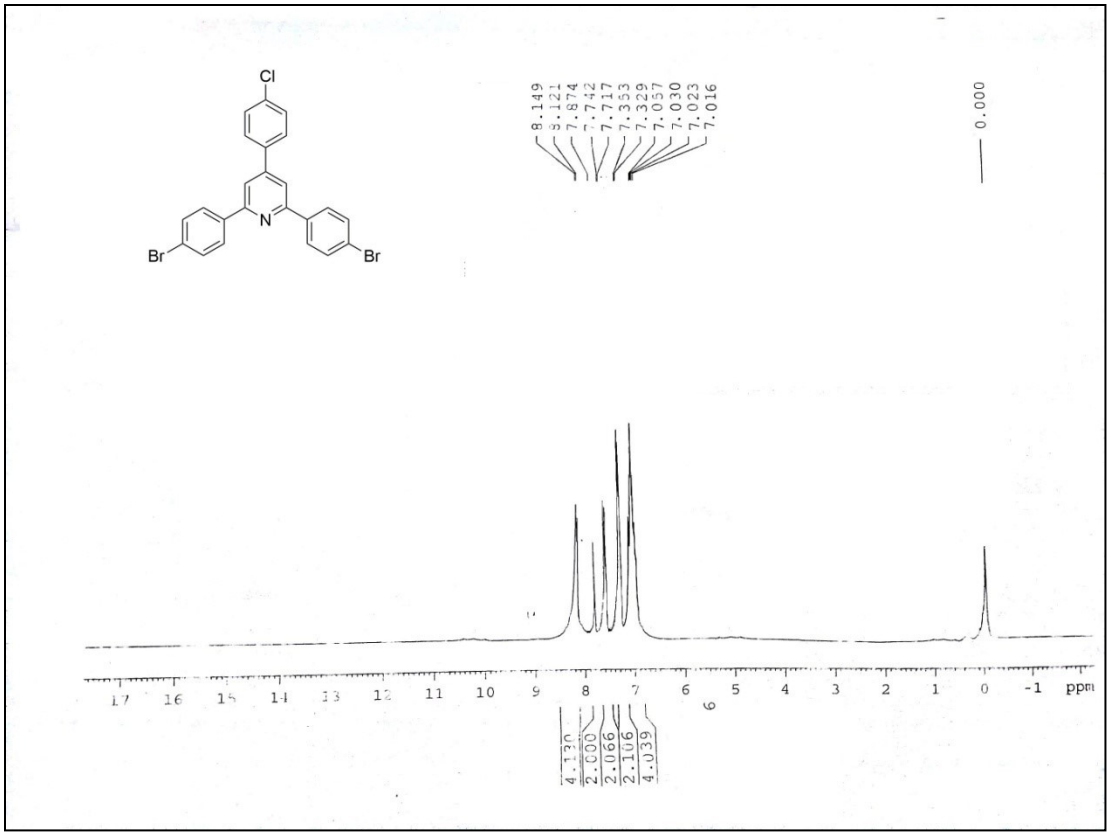

157.03
151.51
128.59
128.18
126.58
112.51
111.61
76.97
76.54
76.12
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

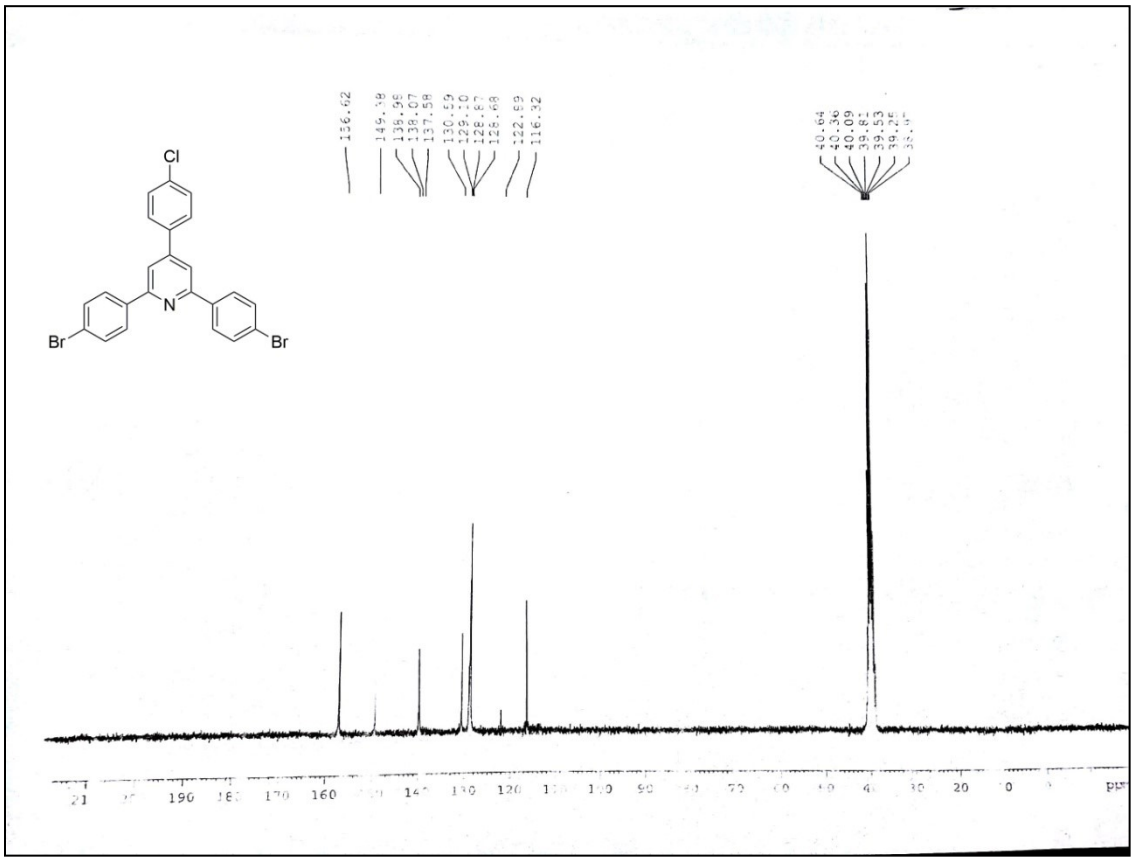

8.012
7.985
7.743
7.719
7.634
7.607
7.426
7.420
7.404
7.220
7.196
2.369
0.877
0.000
Me
N
Me
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
4.061
2.000
2.377
2.902
4.046
6.000


157.43
150.04
139.30
139.00
136.94
129.12
128.92
128.54
127.23
127.05
116.56
77.54
77.11
76.69
21.40
Me
N
Me


Br
N
Br
8.112
8.085
7.772
7.746
7.488
7.358
7.329
7.300
7.292
7.255
7.218
7.091
6.859
0.000
17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
4.023
4.019
2.000
5.208


Br
N
Br
154.16
149.07
139.60
135.19
132.94
129.49
128.40
127.05
77.45
77.03
76.60
190 180 170 160 150 140 120 110 100 90 50 40 30 20 ppm


Cl
Br
Br
N
8.149
8.121
7.874
7.742
7.717
7.353
7.329
7.057
7.030
7.023
7.016
0.000
4.130
2.000
2.066
2.106
4.039
ppm


Cl
Br
Br
N
136.62
149.38
138.96
138.07
137.58
130.59
129.10
128.87
128.68
122.69
116.32
40.64
40.36
40.09
39.81
39.53

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