Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Metal Free Access to Quinolines *via* C-C Bond Cleavage of Styrenes

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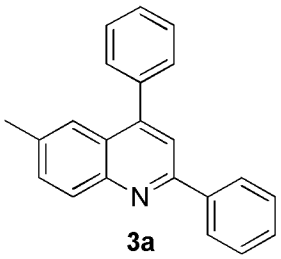
General Experimental:

All chemicals were obtained from Sigma-Aldrich Company and used as received. ^{1}H and ^{13}C NMR spectras were recorded on Brucker-Avance DPX FT-NMR 500 and 400 MHz instruments. Chemical data for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent ($CDCl_3$, 7.26 ppm). Carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 125 MHz or 100 MHz: chemical data for carbons are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent. ESI-MS and HRMS spectra were recorded on Agilent 1100 LC-Q-TOF and HRMS-6540-UHD machines.

Experimental procedures:

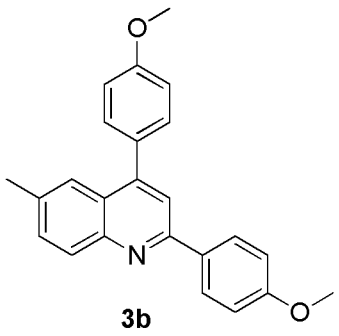
General procedure for synthesis of 2,4-disubstituted quinolines; Iodine (1 mmol) was added to a solution of styrene **1** (1 mmol) in DMSO (2 ml) followed by the addition *p*-methyl aniline **2** (0.5 mmol). The reaction mixture was then heated at 80 °C for 18 h and the product formation was monitored by TLC. After completion, reaction mixture was extracted with ethyl acetate (3 x 50ml). The combined organic layers were washed with brine solution, concentrated on rotary evaporator and purified by chromatography on a basic alumina column using ethyl acetate and hexane (2:98) to afford **3a** in 81% yields.

Spectroscopic Data:



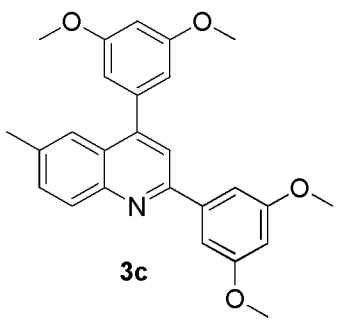
3a

6-methyl-2,4-diphenylquinoline (3a). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 – 8.11 (m, 3H), 7.77 (s, 1H), 7.65 (s, 1H), 7.57 – 7.43 (m, 9H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.1, 148.5, 147.4, 139.8, 138.6, 136.3, 131.8, 129.8, 129.5, 129.1, 128.8, 128.6, 128.3, 127.5, 125.7, 124.4, 119.4, 21.8; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{22}H_{18}N$ 296.1434 found 296.1424.



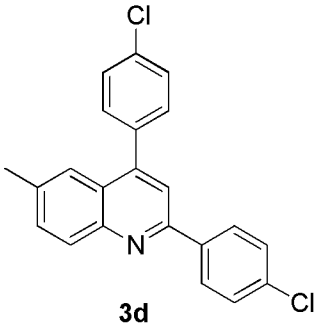
3b

2,4-bis(4-methoxyphenyl)-6-methylquinoline (3b). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.5 Hz, 2H), 8.09 (d, J = 8.5 Hz, 1H), 7.70 (s, 1H), 7.66 (s, 1H), 7.53 (d, J = 8.5 Hz, 1H), 7.49 (d, J = 8.4 Hz, 2H), 7.07 (t, J = 7.6 Hz, 2H), 7.03 (d, J = 8.6 Hz, 2H), 3.91 (s, 3H), 3.87 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 159.7, 155.6, 148.0, 147.4, 135.7, 132.4, 131.6, 131.0, 130.8, 129.6, 128.8, 125.6, 124.4, 118.9, 114.2, 114.0, 55.42, 55.40, 21.8; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{24}H_{22}NO_2$ 356.1645 found 356.1642.



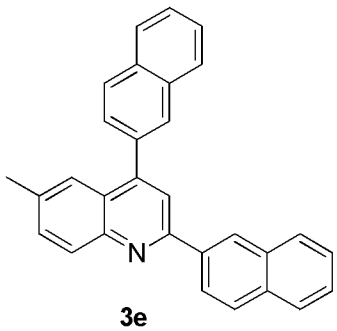
3c

2,4-bis(3,5-dimethoxyphenyl)-6-methylquinoline (3c). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.6 Hz, 1H), 7.74 (s, 1H), 7.69 (s, 1H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.31 (d, *J* = 15.7 Hz, 2H), 6.68 (s, 2H), 6.59 (d, *J* = 16.8 Hz, 2H), 3.90 (s, 6H), 3.86 (s, 6H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.2, 160.8, 155.7, 148.3, 147.2, 141.8, 140.5, 136.4, 131.8, 129.8, 125.8, 124.4, 119.2, 107.7, 105.4, 101.7, 100.2, 55.58, 55.56, 21.9; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{26}H_{26}NO_4$ 416.1856 found 416.1864.



3d

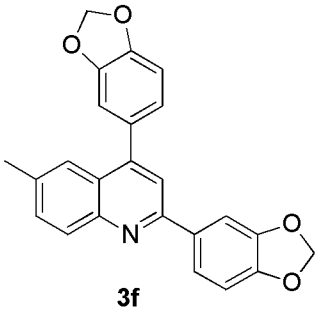
2,4-bis(4-chlorophenyl)-6-methylquinoline (3d). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 7.9, 5.9 Hz, 3H), 7.70 (s, 1H), 7.58 (d, *J* = 8.1 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.48 (dd, *J* = 8.4, 1.5 Hz, 4H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.3, 146.1, 146.0, 136.6, 135.5, 134.1, 133.3, 130.8, 129.5, 128.5, 127.7, 127.6, 127.4, 124.2, 122.7, 117.5, 20.5; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{22}H_{16}Cl_2N$ 364.0654 found 364.0652.



3e

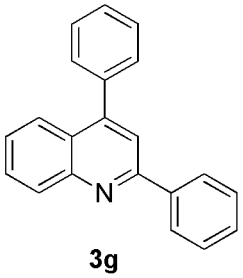
6-methyl-2,4-di(naphthalen-2-yl)quinoline (3e). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (s, 1H), 8.42 (d, *J* = 8.5 Hz, 1H), 8.21 (d, *J* = 8.5 Hz, 1H), 8.10 – 7.83 (m, 8H), 7.71 (d, *J* = 9.2 Hz, 2H), 7.65 – 7.44 (m, 5H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 148.5, 147.5, 137.0, 136.5, 136.2, 133.8, 133.6, 133.3, 133.1, 131.9, 129.9, 128.8, 128.6, 128.5, 128.3, 128.2, 127.8, 127.7,

127.51, 127.0, 126.7, 126.67, 126.63, 126.3, 125.9, 125.1, 124.5, 119.8, 21.8; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{30}H_{22}N$ 396.1747 found 396.1719.



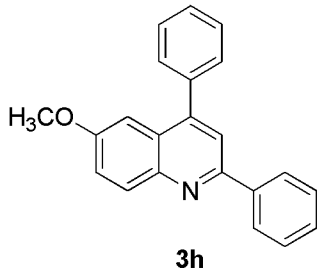
3f

2,4-bis(benzo[d][1,3]dioxol-5-yl)-6-methylquinoline (3f). ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.5 Hz, 1H), 7.74 (s, 1H), 7.69 – 7.61 (m, 3H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.05 – 6.88 (m, 4H), 6.09 (s, 2H), 6.04 (s, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 148.7, 148.4, 148.0, 147.8, 147.7, 147.31, 136.0, 134.2, 132.4, 131.7, 129.7, 125.6, 124.3, 123.2, 121.6, 118.9, 110.0, 108.5,108.4, 107.8, 101.4, 101.3, 21.8; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{24}H_{18}NO_4$ 384.1230 found 384.1238.



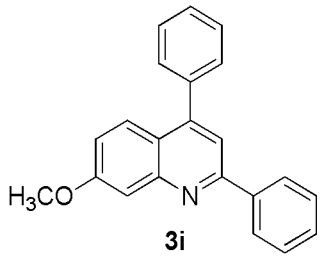
3g

2,4-diphenylquinoline (3g). ^1H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.4 Hz, 1H), 8.20 (d, *J* = 7.7 Hz, 2H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.83 (s, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 7.60 – 7.42 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.9, 149.2, 148.8, 139.7, 138.4, 130.1, 129.6, 129.5, 129.3, 128.8, 128.6, 128.4, 127.6, 126.3, 125.8, 125.6, 119.3; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{21}H_{16}N$ 282.1277 found 282.1279.



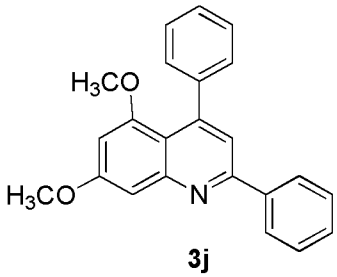
3h

6-methoxy-2,4-diphenylquinoline (3h). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, J = 7.0 Hz, 3H), 7.77 (s, 1H), 7.61 – 7.35 (m, 10H), 7.19 (d, J = 2.8, 1H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 154.7, 147.8, 144.9, 139.8, 138.8, 131.7, 129.4, 129.1, 128.8, 128.7, 128.4, 127.3, 126.7, 121.8, 119.7, 103.7, 55.5; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{22}H_{18}NO$ 312.1383 found 312.1368.



3i

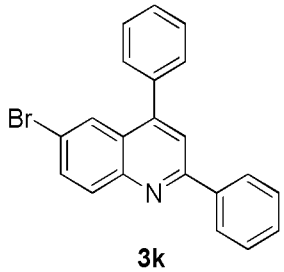
7-methoxy-2,4-diphenylquinoline (3i). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.76 (d, J = 8.9 Hz, 1H), 7.53 (d, J = 2.4 Hz, 2H), 7.46 – 7.40 (m, 2H), 7.31 – 7.19 (m, 9H), 3.98 (s, 3H); ^{13}C NMR (125 MHz, CDCl3) δ 160.9, 158.5, 148.9, 140.6, 140.1, 137.3, 132.4, 129.9, 129.8, 128.5, 128.2, 127.94, 127.90, 126.9, 122.4, 120.1, 107.3 55.6.



3j

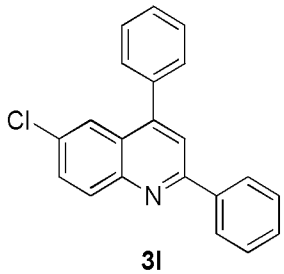
5,7-dimethoxy-2,4-diphenylquinoline (3j). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.48 – 7.38 (m, 2H), 7.26 (dd, J = 8.0, 4.3 Hz, 9H), 6.54 (d, J = 1.6 Hz, 1H), 3.99 (s, 3H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 158.8, 156.1, 149.3, 140.7, 140.4, 132.6, 131.5, 129.9,

129.8, 128.1, 127.9, 127.8, 126.8, 115.7, 99.7, 98.3 55.8, 55.7; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{23}H_{20}NO_2$ 342.1489 found 342.1484.



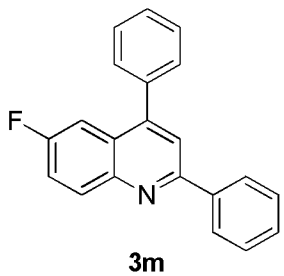
3k

6-bromo-2,4-diphenylquinoline (3k). ^1H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 7.9 Hz, 2H), 8.10 (d, J = 9.0 Hz, 1H), 8.04 (s, 1H), 7.86 – 7.76 (m, 2H), 7.60 – 7.46 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 148.4, 147.4, 139.2, 137.7, 133.0, 131.8, 129.6, 129.4, 128.9, 128.8, 128.7, 127.8, 127.5, 127.0, 120.4, 120.0; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{21}H_{15}BrN$ 360.0382 found 360.0372.



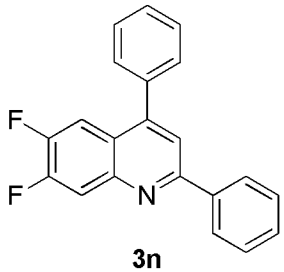
3l

6-chloro-2,4-diphenylquinoline (3l). ^1H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, J = 8.0, 4.5 Hz, 3H), 7.85 (s, 1H), 7.81 (s, 1H), 7.64 (d, J = 8.9 Hz, 1H), 7.58 – 7.44 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 148.4, 147.2, 139.2, 137.7, 132.2, 131.7, 130.4, 129.6, 129.4, 128.9, 128.8, 128.7, 127.6, 126.5, 124.5, 120.0; HRMS (TOF) m/z $[M + H]^+$ Calcd for $C_{21}H_{15}ClN$ 316.0888 found 316.0892.



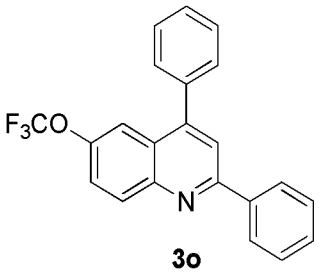
3m

6-fluoro-2,4-diphenylquinoline (3m). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21 (dd, J = 8.8, 5.7 Hz, 1H), 8.16 (d, J = 7.8 Hz, 2H), 7.81 (s, 1H), 7.55 – 7.42 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8 (d, $^{1}J_{C\text{-}F}$ = 245 Hz), 156.3, 148.7, 146.0, 139.4, 138.0, 132.6, 129.45, 129.41, 128.9, 128.8, 128.6, 127.5, 126.6, 119.8, 119.8 (d, $^{2}J_{C\text{-}F}$ =26 Hz), 109.2(d, $^{2}J_{C\text{-}F}$ =23 Hz); HRMS (TOF) m/z [M + H]$^{+}$ Calcd for $C_{21}H_{15}FN$ 300.1183 found 300.1194



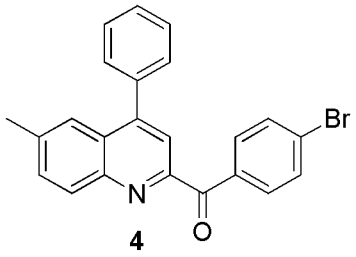
3n

6,7-difluoro-2,4-diphenylquinoline (3n). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (d, J = 7.2 Hz, 2H), 7.98 (dd, J = 11.3, 7.9 Hz, 1H), 7.82 (s, 1H), 7.67 – 7.46 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5, 151.5 (d, $^{1}J_{C\text{-}F}$ = 202 Hz), 151.4 (d, $^{1}J_{C\text{-}F}$ = 203 Hz), 149.2 (d, $^{2}J_{C\text{-}F}$ = 12 Hz), 147.2 (d, $^{2}J_{C\text{-}F}$ = 13 Hz), 146.9, 137.1, 135.8, 127.8, 127.4, 127.1, 127.06, 127.02, 121.0, 117.5, 114.3 (d, $^{2}J_{C\text{-}F}$ = 13 Hz), 109.6 (d, $^{2}J_{C\text{-}F}$ = 16 Hz); HRMS (TOF) m/z [M + H]$^{+}$ Calcd for $C_{21}H_{14}F_2N$ 318.1089 found 318.1083.



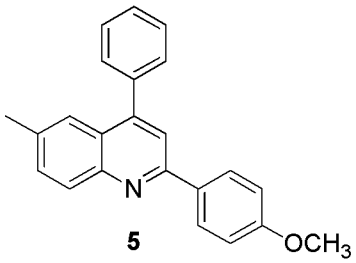
3o

2,4-diphenyl-6-(trifluoromethoxy)quinoline (3o). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, J = 9.2 Hz, 1H), 8.19 (d, J = 7.3 Hz, 2H), 7.88 (s, 1H), 7.74 (s, 1H), 7.63 – 7.45 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 149.1, 147.1, 146.9, 139.2, 137.6, 132.3, 129.6, 129.4, 128.9, 128.9, 128.8, 128.5, 127.6, 127.1, 126.0, 123.5, 120.1, 116.4; HRMS (TOF) m/z [M + H]$^{+}$ Calcd for $C_{22}H_{15}F_3NO$ 366.1100 found 366.1115.



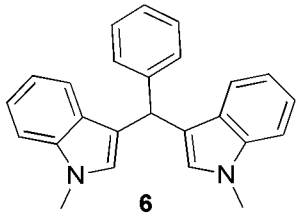
4

(4-bromophenyl)(4-phenylquinolin-2-yl)methanone (4). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (m, 3H), 8.04 (s, 1H), 7.75 (s, 1H), 7.66 (m, 3H), 7.59 – 7.50 (m, 5H), 2.52 (s, 3H).



5

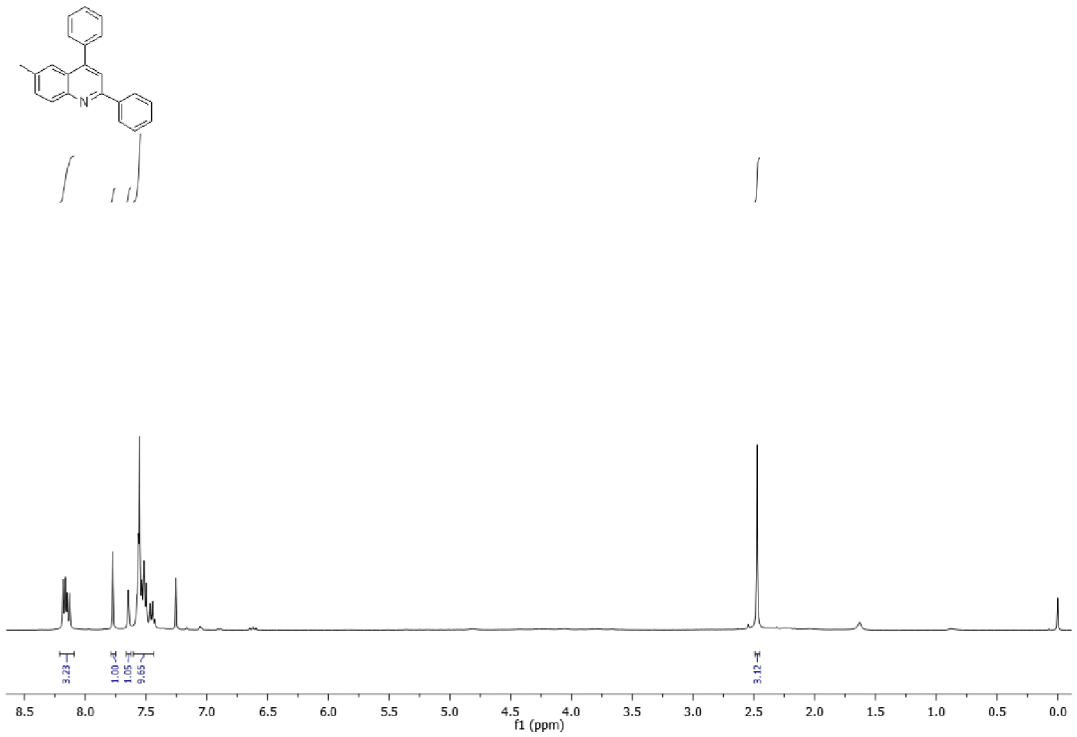
2-(4-methoxyphenyl)-6-methyl-4-phenylquinoline (5). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, J = 17.4, 8.7 Hz, 3H), 7.73 (s, 1H), 7.55 (m, 7H), 7.04 (d, J = 8.8 Hz, 2H), 3.88 (s, 3H), 2.48 (s, 3H).

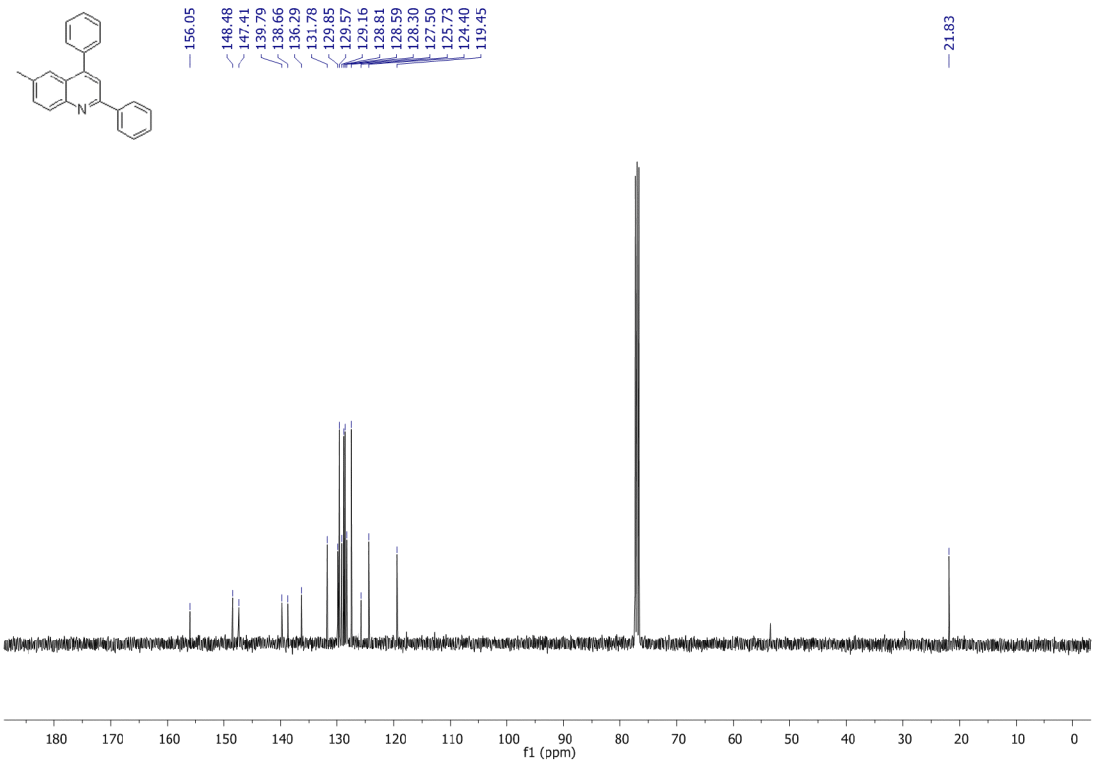


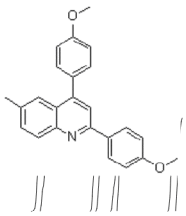
6

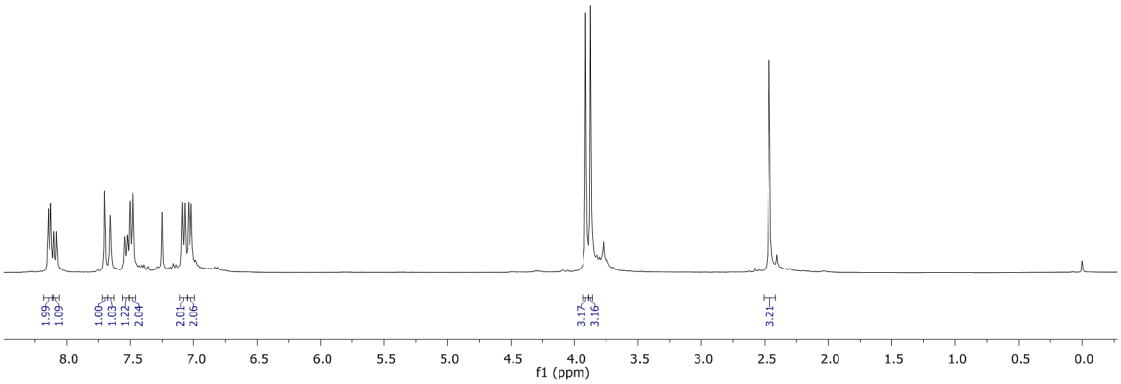
3,3'-(phenylmethylene)bis(1-methyl-1H-indole) (6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (m, 9H), 7.19 (m, 3H), 6.99 (t, J = 7.2 Hz, 2H), 6.52 (s, 2H), 5.88 (s, 1H), 3.67 (s, 6H).

Spectral Graphs





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6.5
6.0
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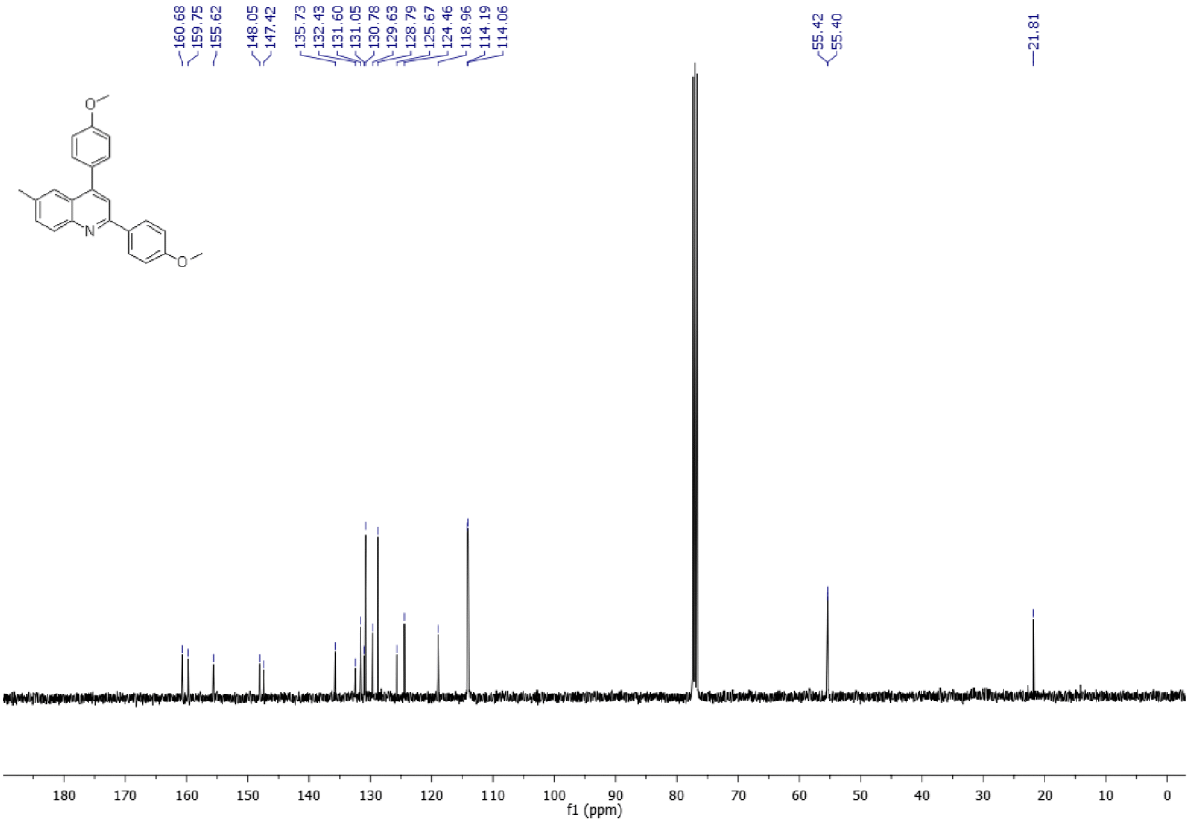
f1 (ppm)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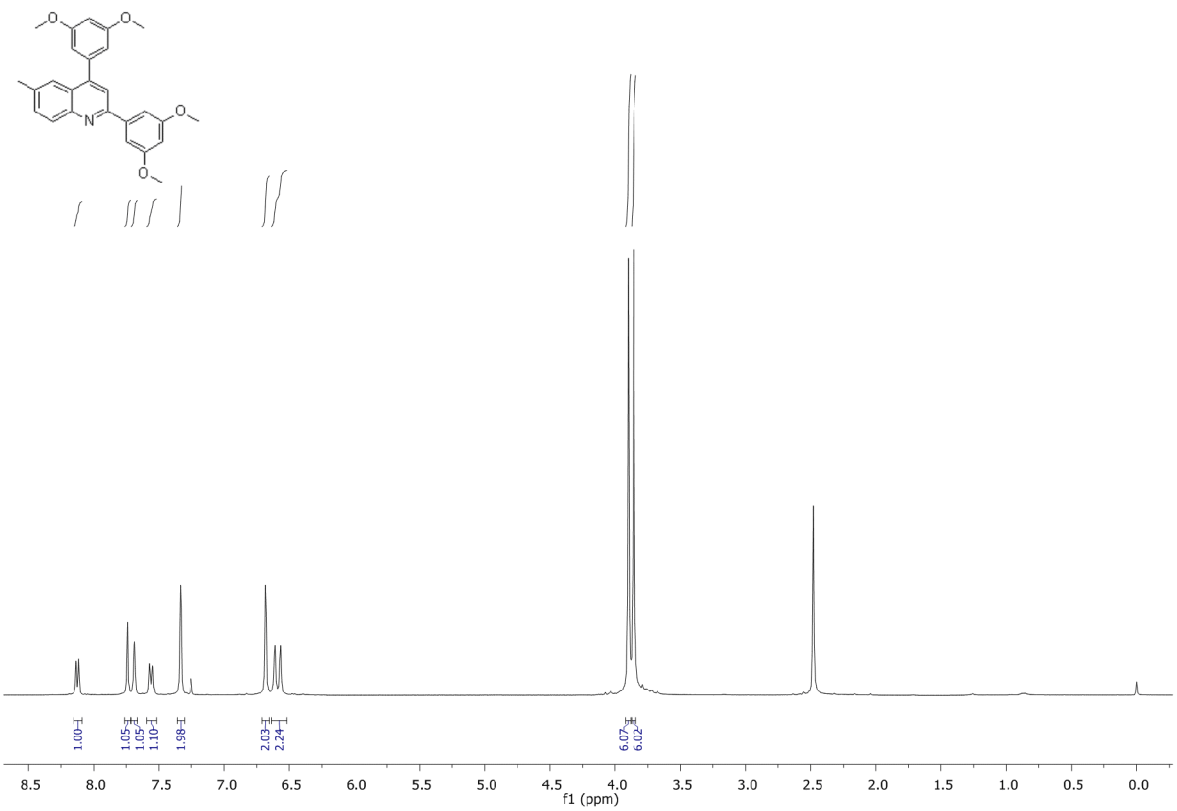
f1 (ppm)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6.0
5.5
5.0
4.5
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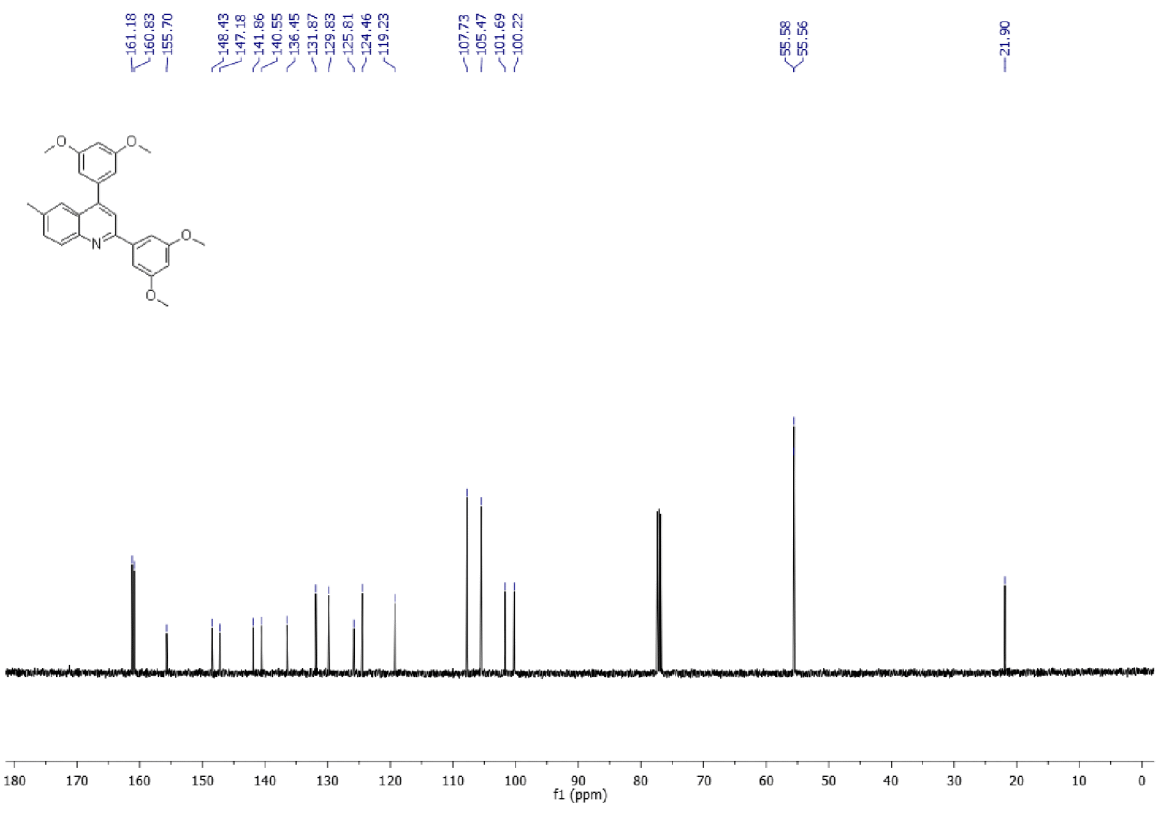
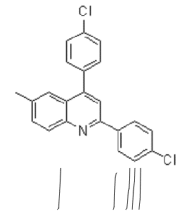
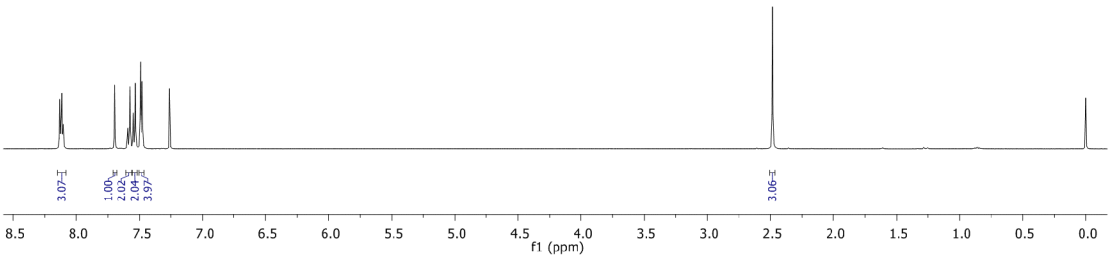
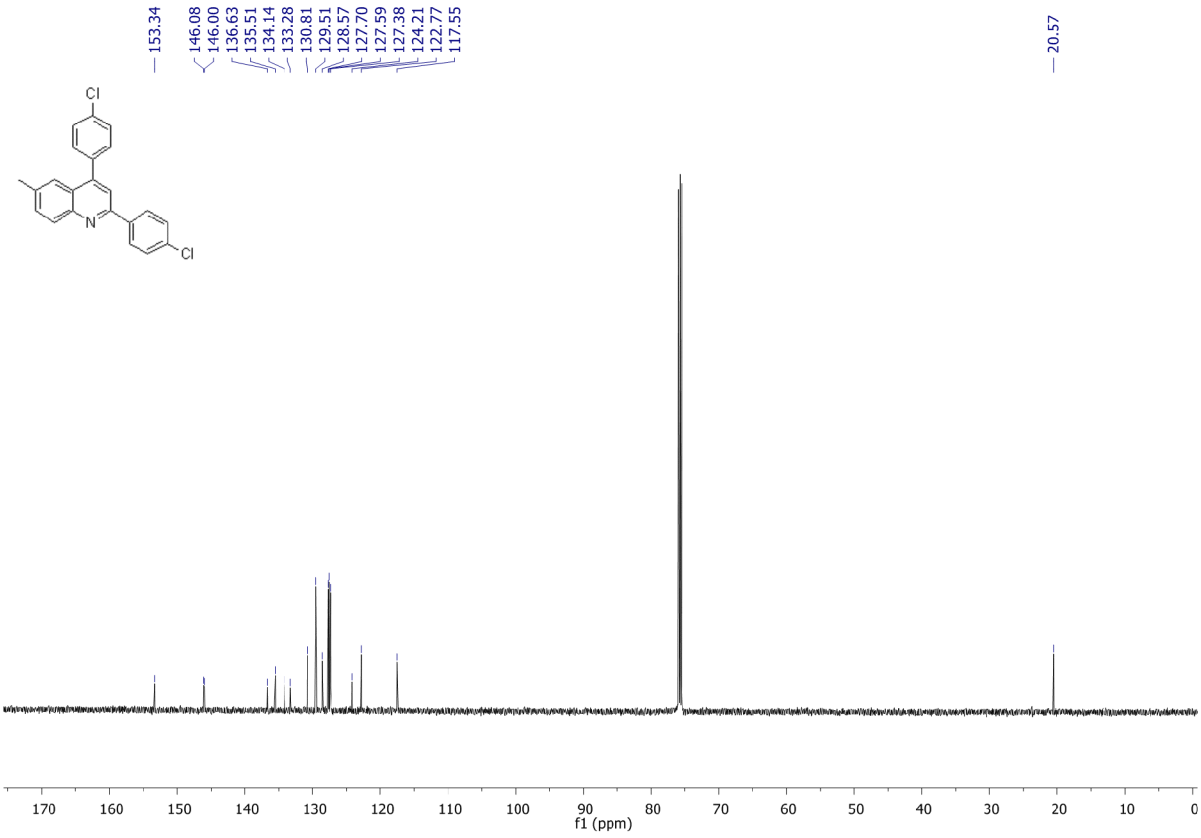
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.18
160.83
155.70
148.43
147.18
141.86
140.55
136.45
131.87
129.83
125.81
124.46
119.23
107.73
105.47
101.69
100.22
55.58
55.56
21.90
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Cl
N
Cl


3.07
1.00
2.02
2.04
3.97
3.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


153.34
146.08
146.00
136.63
135.51
134.14
133.28
130.81
129.51
128.57
127.70
127.59
127.38
124.21
122.77
117.55
20.57
Cl
N
Cl
170
160
150
140
130
120
110
100
90
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70
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50
40
30
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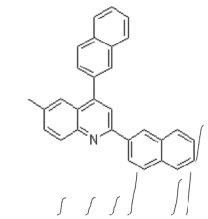
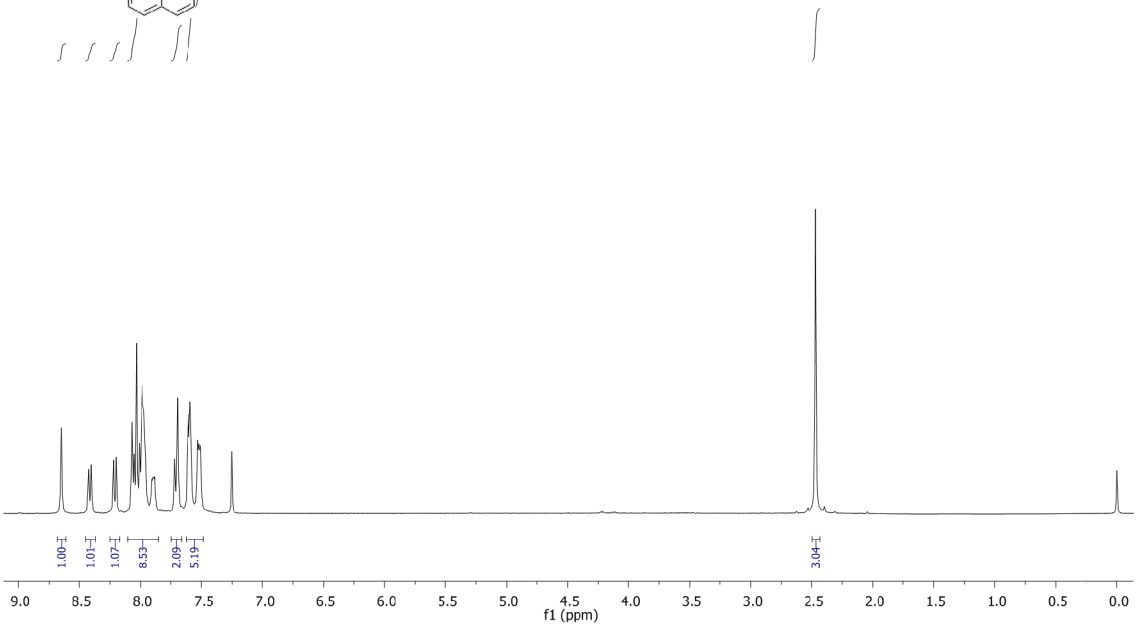
10
0
f1 (ppm)




1.00
1.01
1.07
8.53
2.09
5.19
3.04
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


155.83
148.54
147.54
137.06
136.48
136.24
133.86
133.58
133.36
133.07
131.91
129.93
128.82
128.66
128.57
128.29
128.18
127.89
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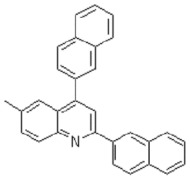
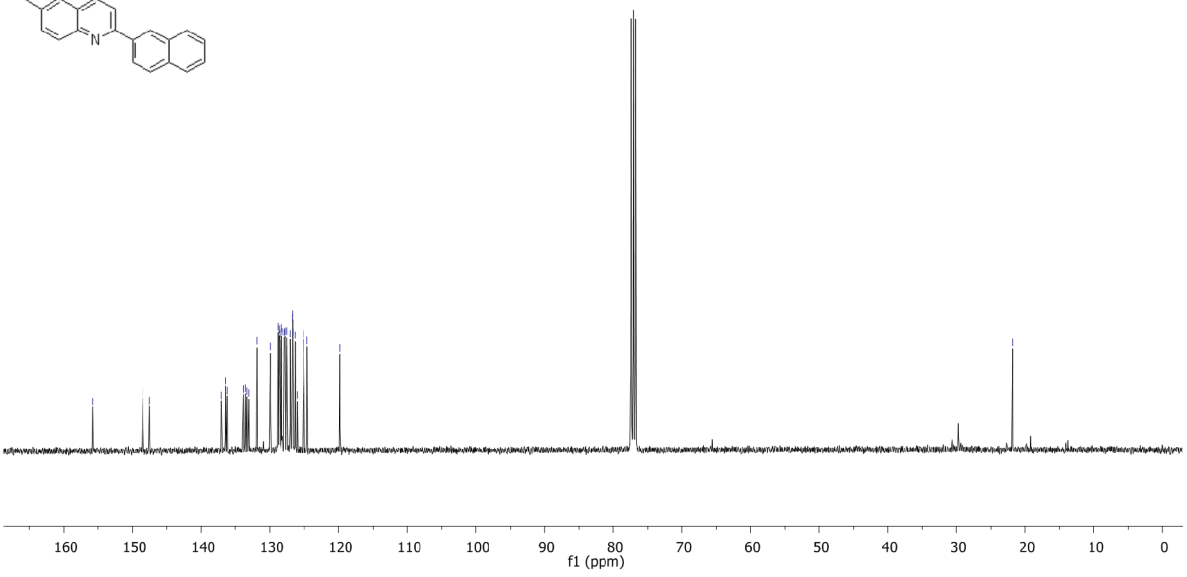
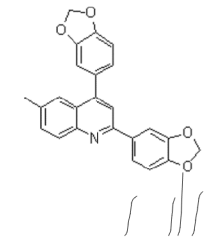
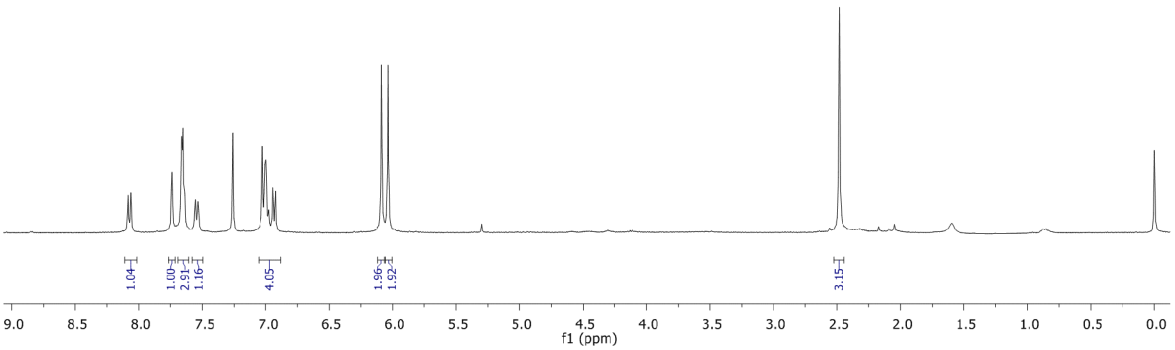
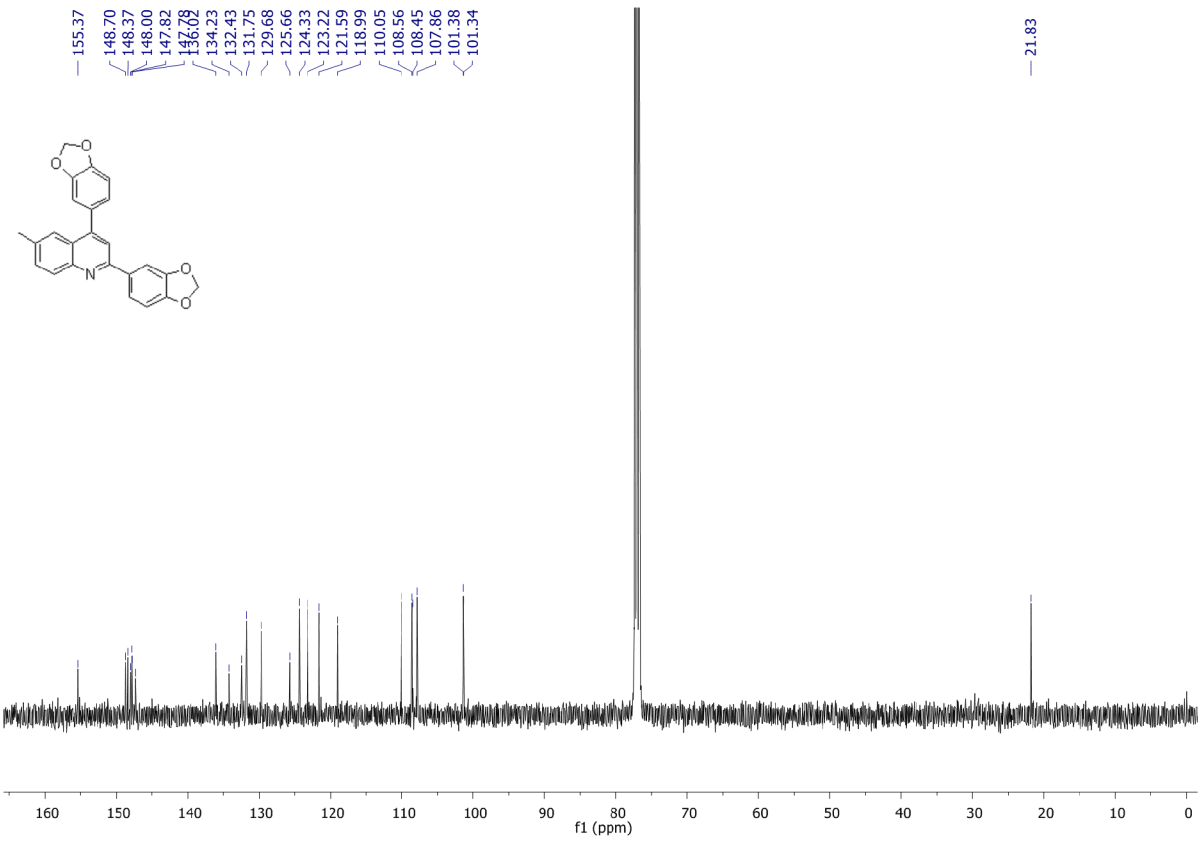
126.31
125.98
125.09
124.57
119.82
21.86

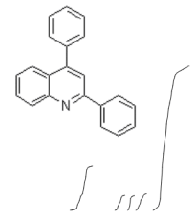


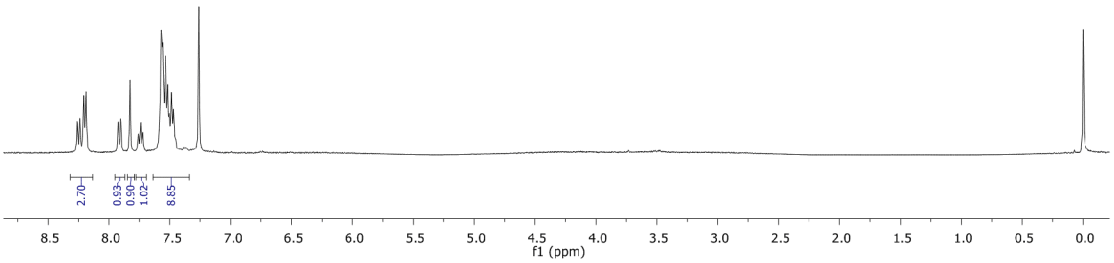

160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

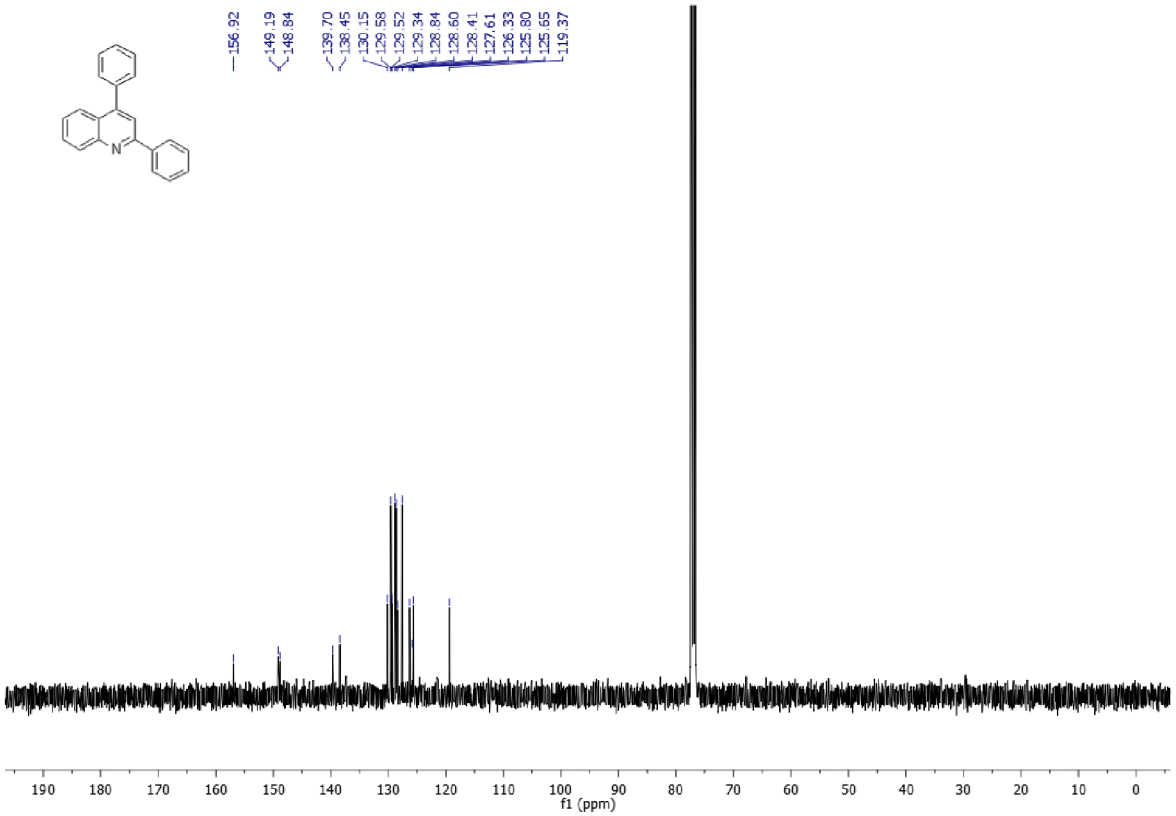


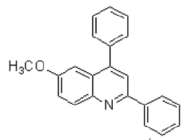

1.04
1.00
2.91
1.16
4.05
1.96
1.92
3.15
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

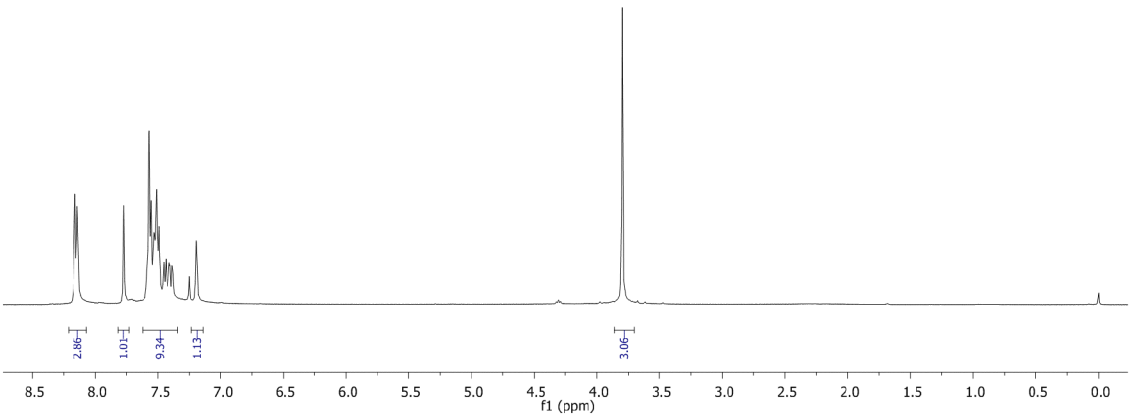

155.37
148.70
148.37
148.00
147.82
147.78
147.62
134.23
132.43
131.75
129.68
125.66
124.33
123.22
121.59
118.99
110.05
108.56
108.45
107.86
101.38
101.34
21.83
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

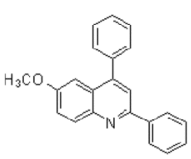



2.70
0.93
0.90
1.02
8.85
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

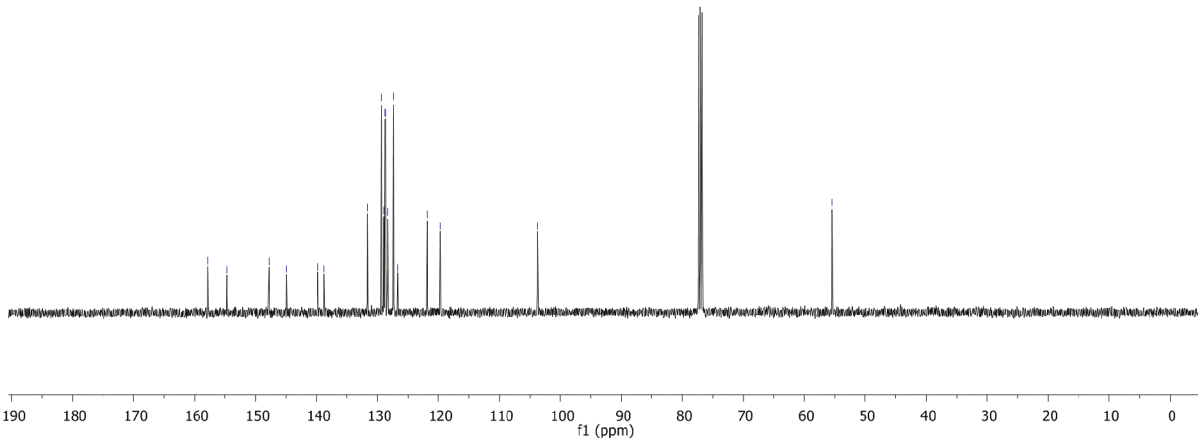

156.92
149.19
148.84
139.70
138.45
130.15
129.58
129.52
129.34
128.84
128.60
128.41
127.61
126.33
125.80
125.65
119.37
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

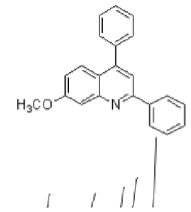


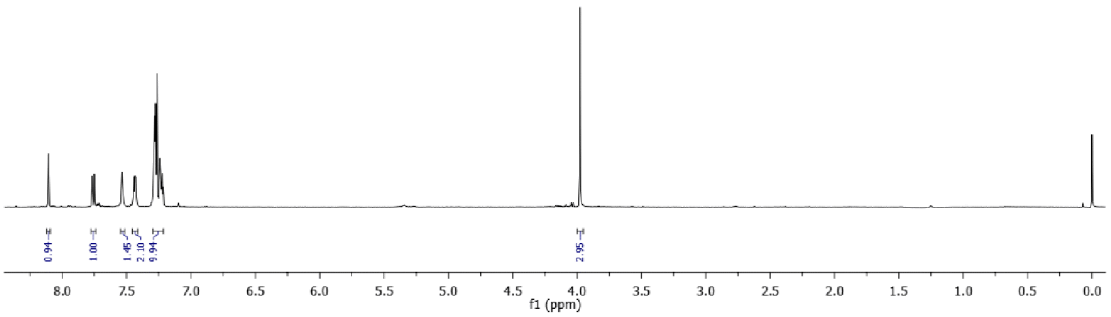


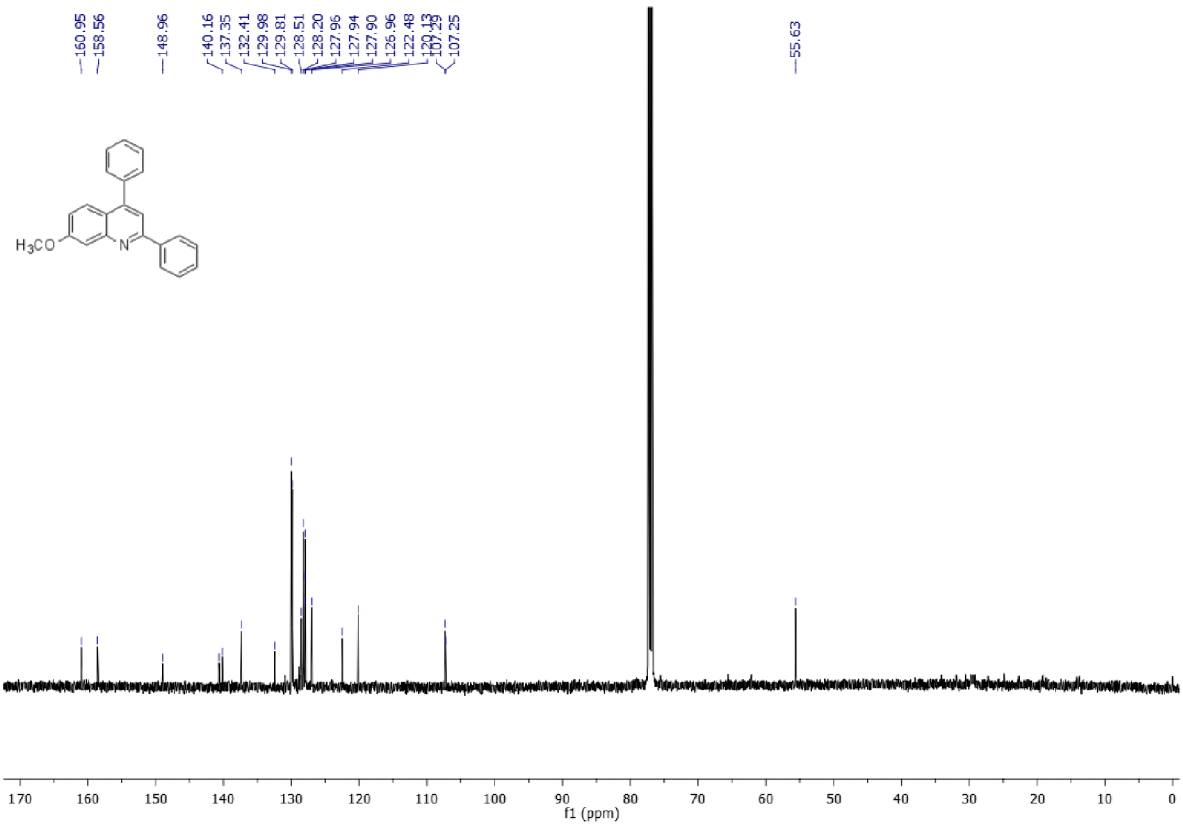


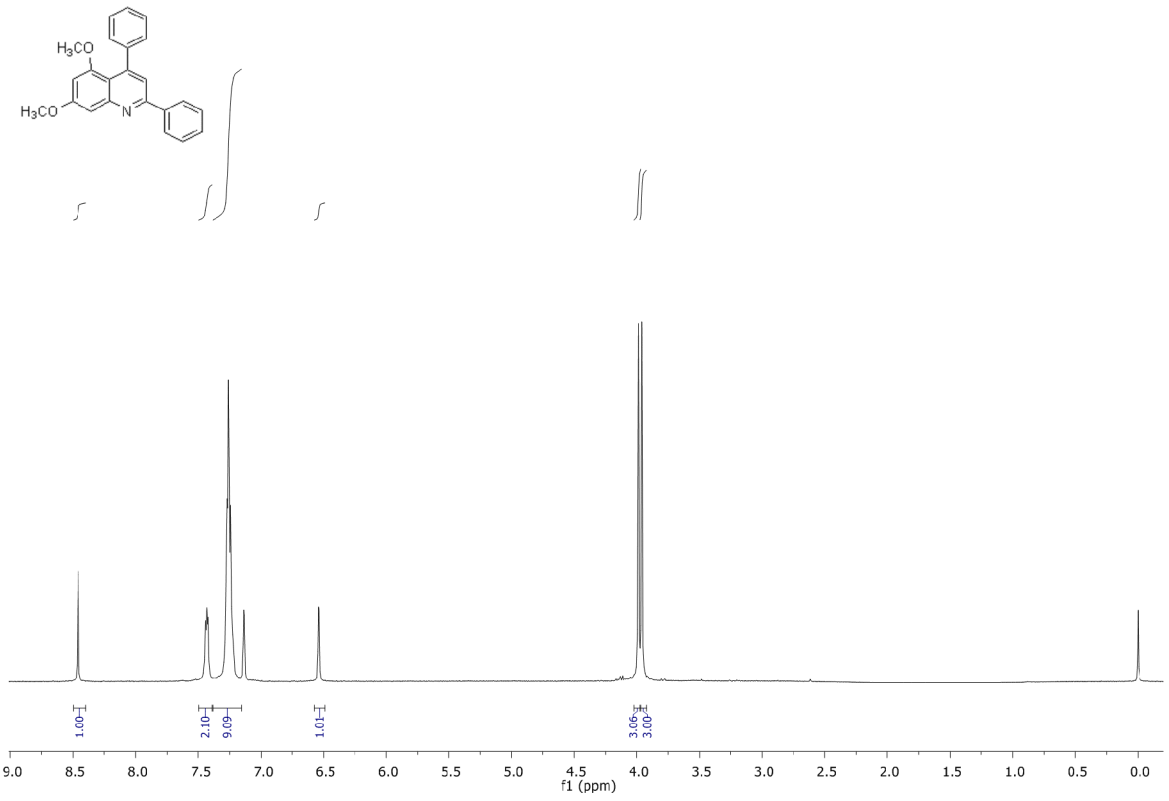
157.81
154.67
147.81
144.93
139.78
138.76
131.63
129.38
128.99
128.82
128.72
128.36
127.33
126.68
121.83
119.69
103.71
55.47

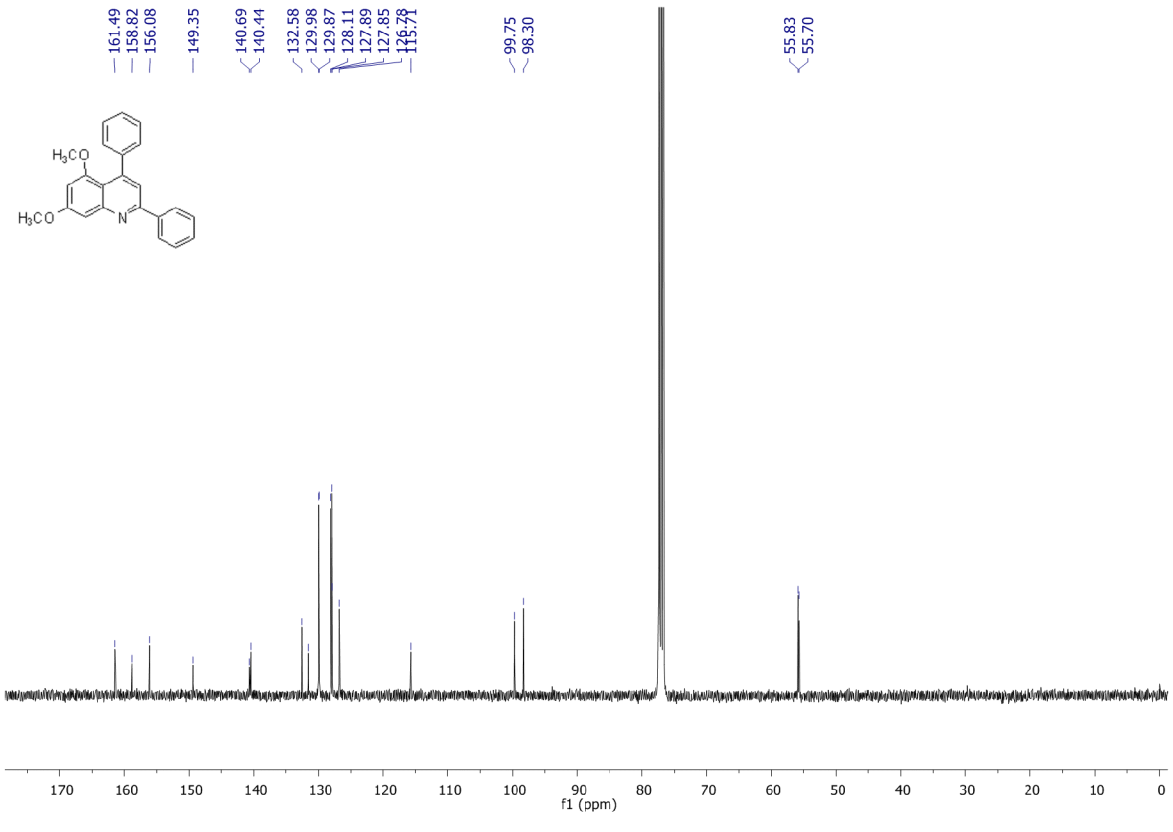


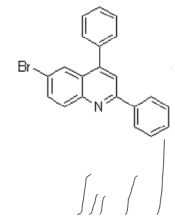

H3CO
N

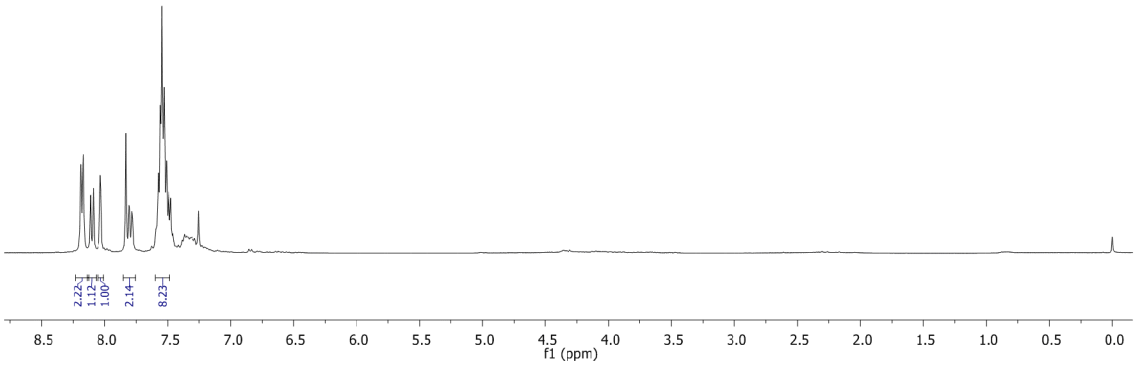

0.94
1.00
1.45
2.10
9.94
2.95
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

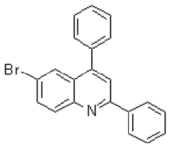

160.95
158.56
148.96
140.16
137.35
132.41
129.98
129.81
128.51
128.20
127.96
127.94
127.90
126.96
122.48
107.25
55.63
H3CO
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


H3CO
H3CO
N
1.00
2.10
9.09
1.01
3.06
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

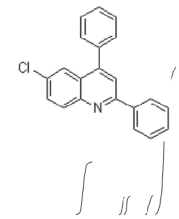

161.49
158.82
156.08
149.35
140.69
140.44
132.58
129.98
129.87
128.11
127.89
127.85
126.78
115.71
99.75
98.30
55.83
55.70
H3CO
H3CO
N
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

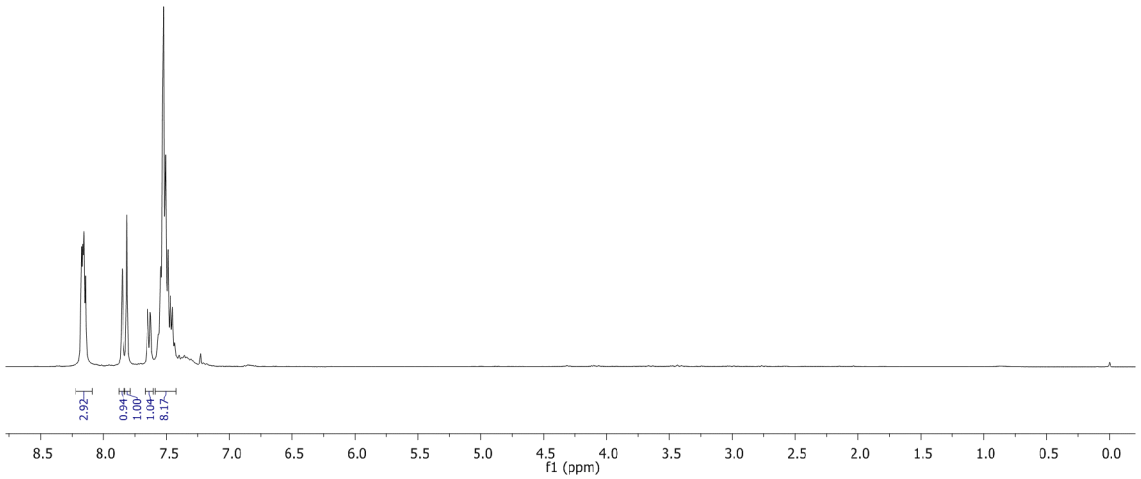

Br
N

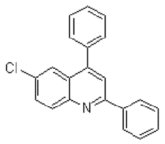

2.22
1.12
1.00
2.14
8.23
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Br
N

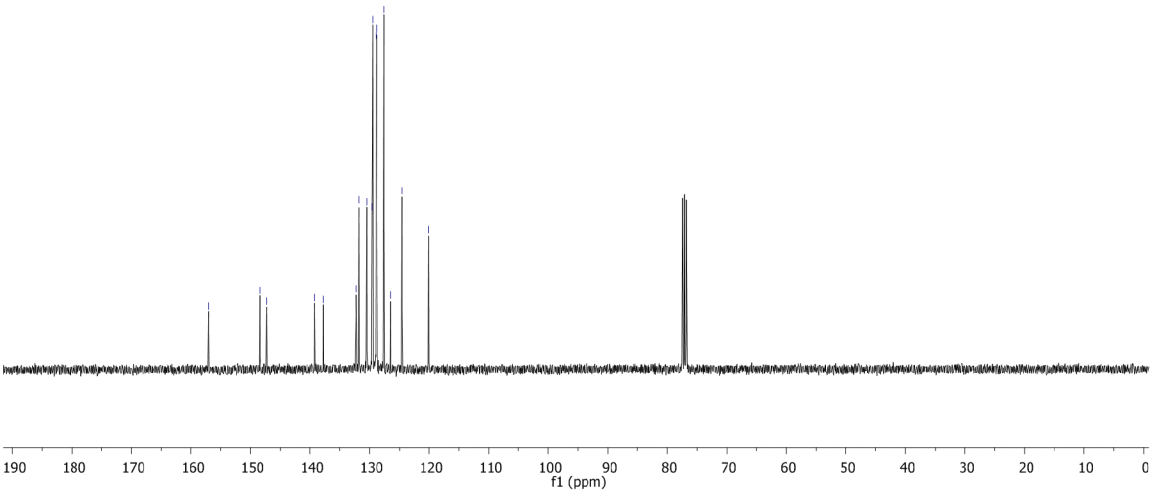
157.22
148.39
147.45
139.21
137.73
133.02
131.87
129.64
129.46
128.92
128.85
128.74
127.80
127.56
127.02
120.44
120.05
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

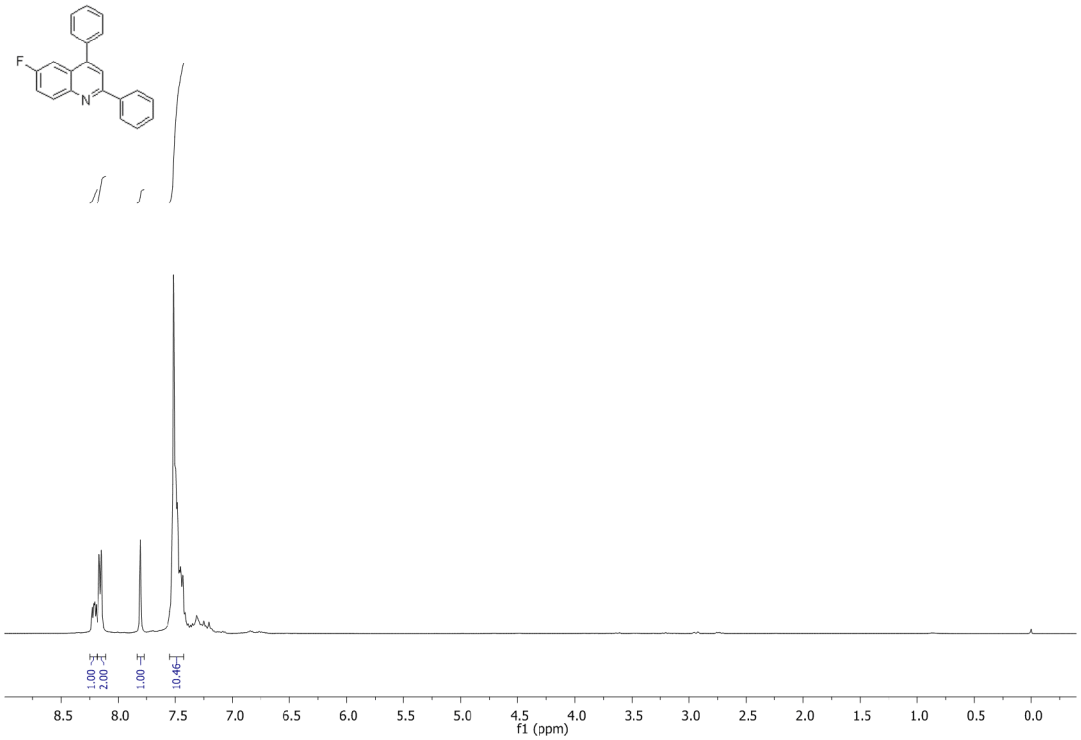


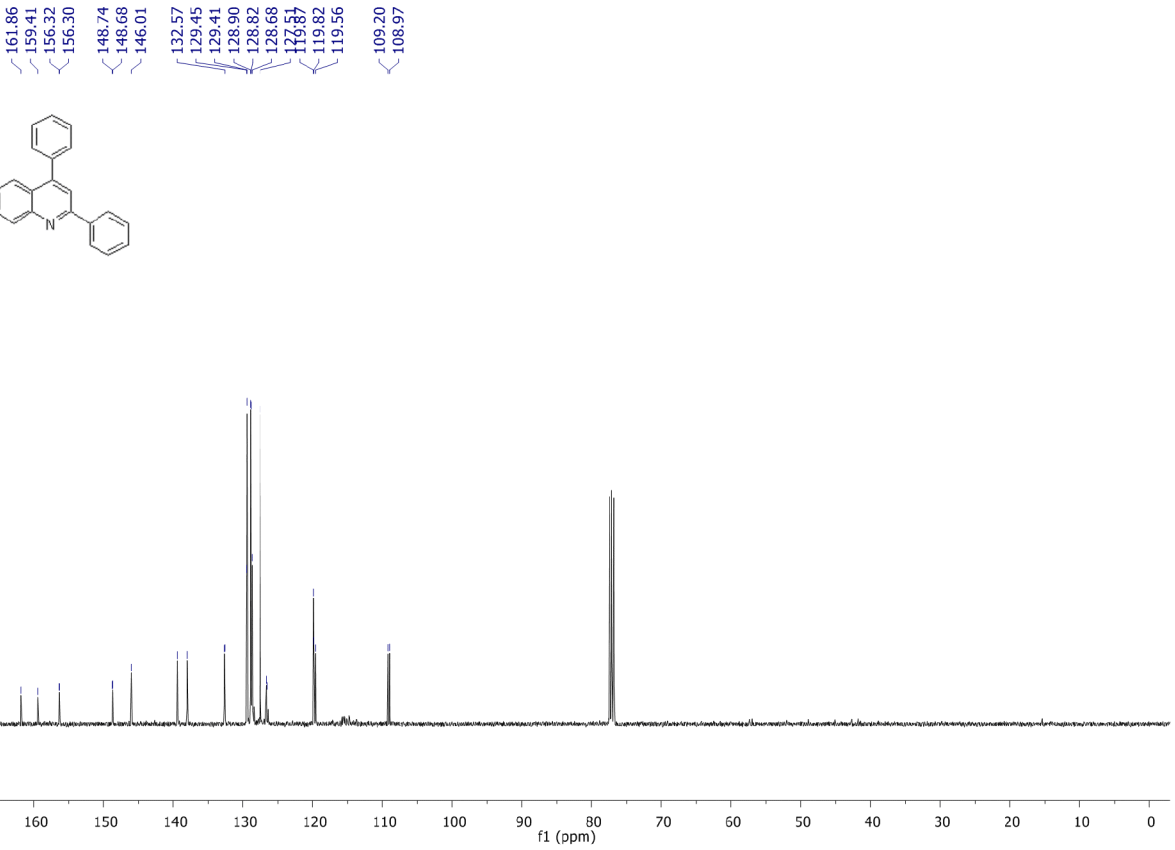




157.09
148.46
147.26
139.22
137.78
132.23
131.76
130.47
129.63
129.48
128.92
128.85
128.74
127.57
126.52
124.51
120.05




F
N
1.00
2.00
1.00
10.46
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.86
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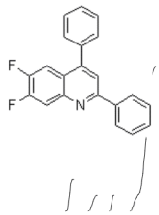
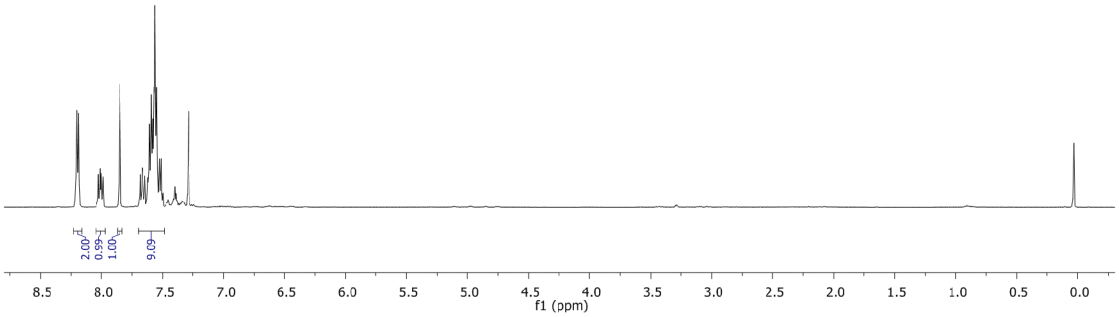
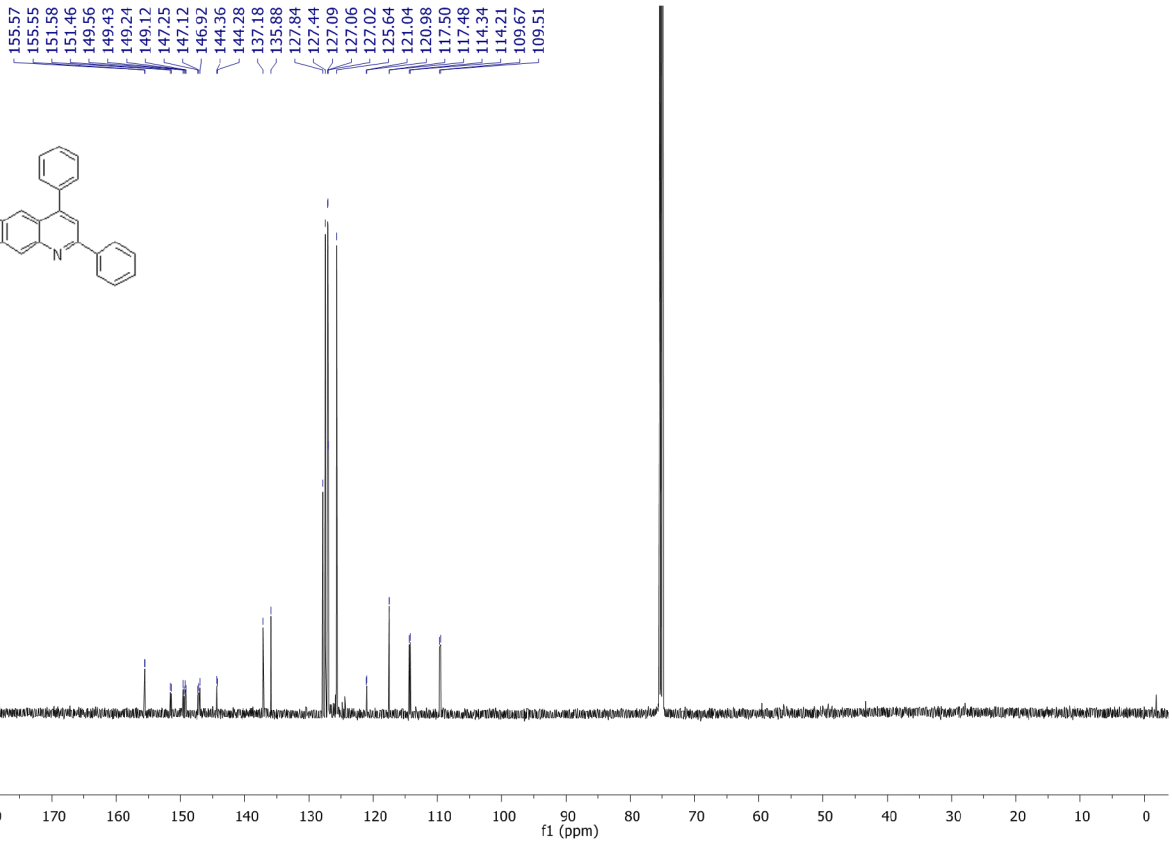
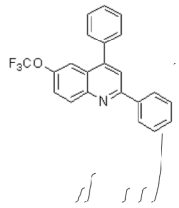
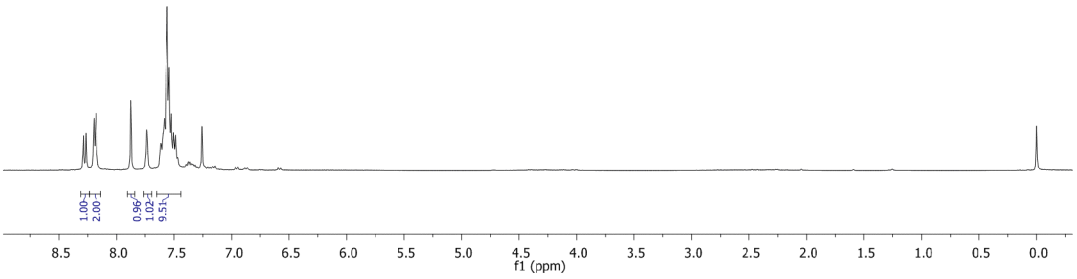
148.68
146.01
132.57
129.45
129.41
128.90
128.82
128.68
127.51
119.82
119.56
109.20
108.97
F
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

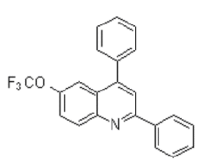

F
F
N


2.00
0.99
1.00
9.09
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


155.57
155.55
151.58
151.46
149.56
149.43
149.24
149.12
147.25
147.12
146.92
144.36
144.28
137.18
135.88
127.84
127.44
127.09
127.06
127.02
125.64
121.04
120.98
117.50
117.48
114.34
114.21
109.67
109.51
F
F
N
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)







157.45
149.17
147.16
139.19
137.65
132.29
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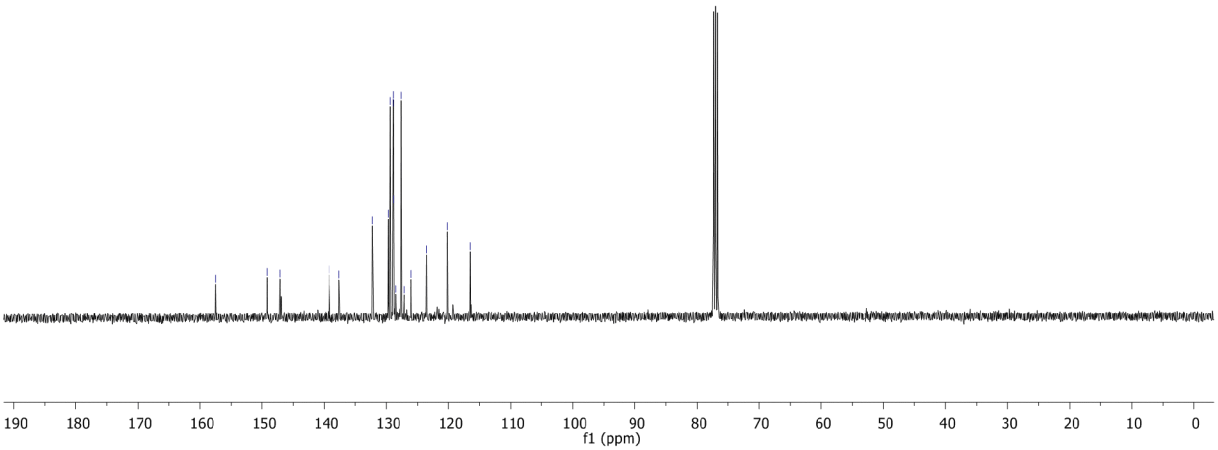
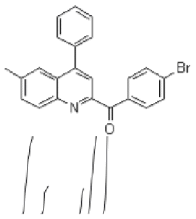
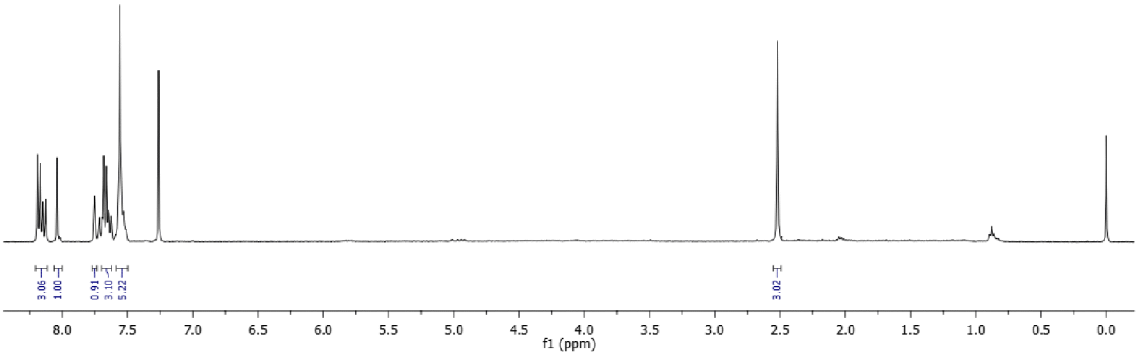
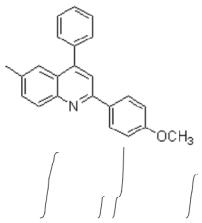
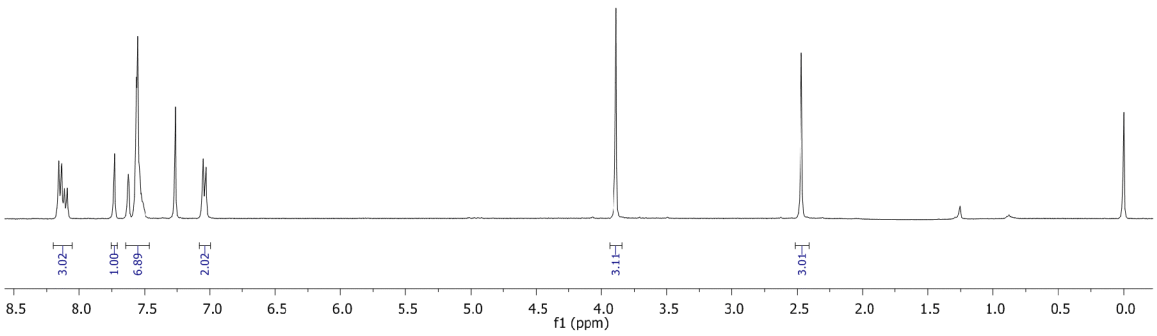
129.40
128.93
128.89
128.84
128.52
127.59
127.11
126.06
123.52
120.14
116.45

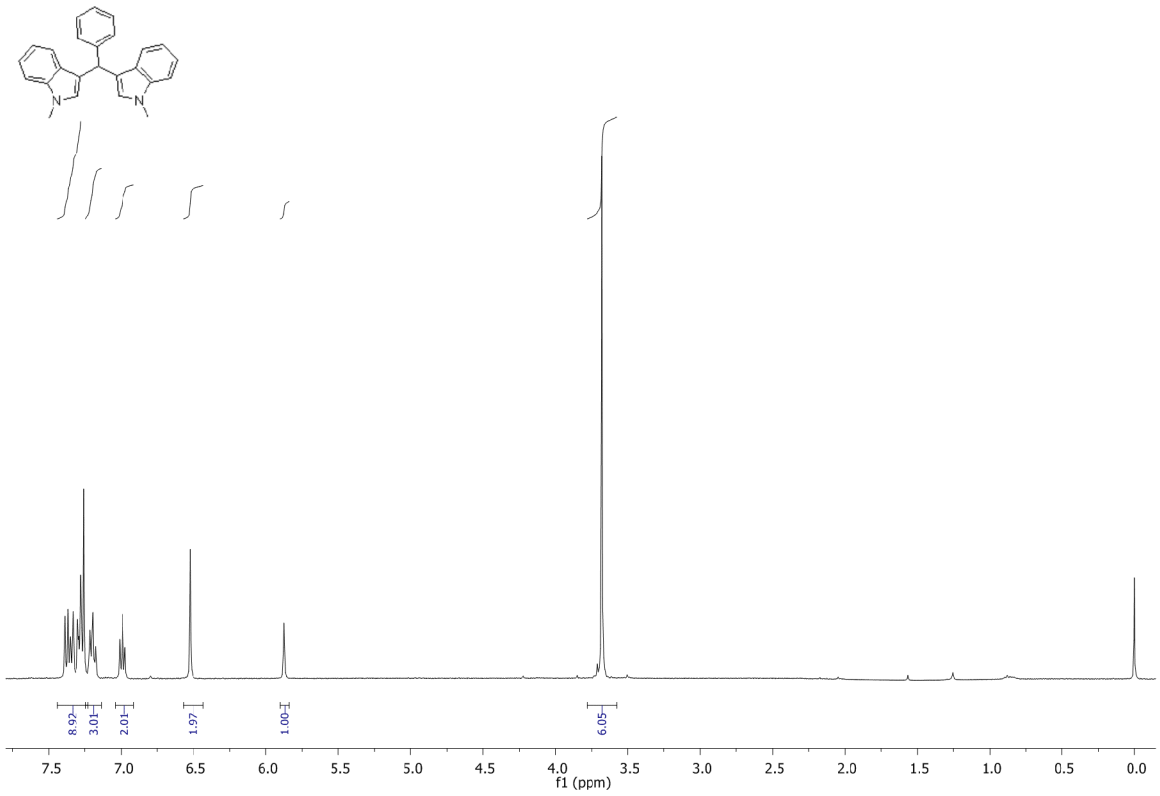



Br
N
O

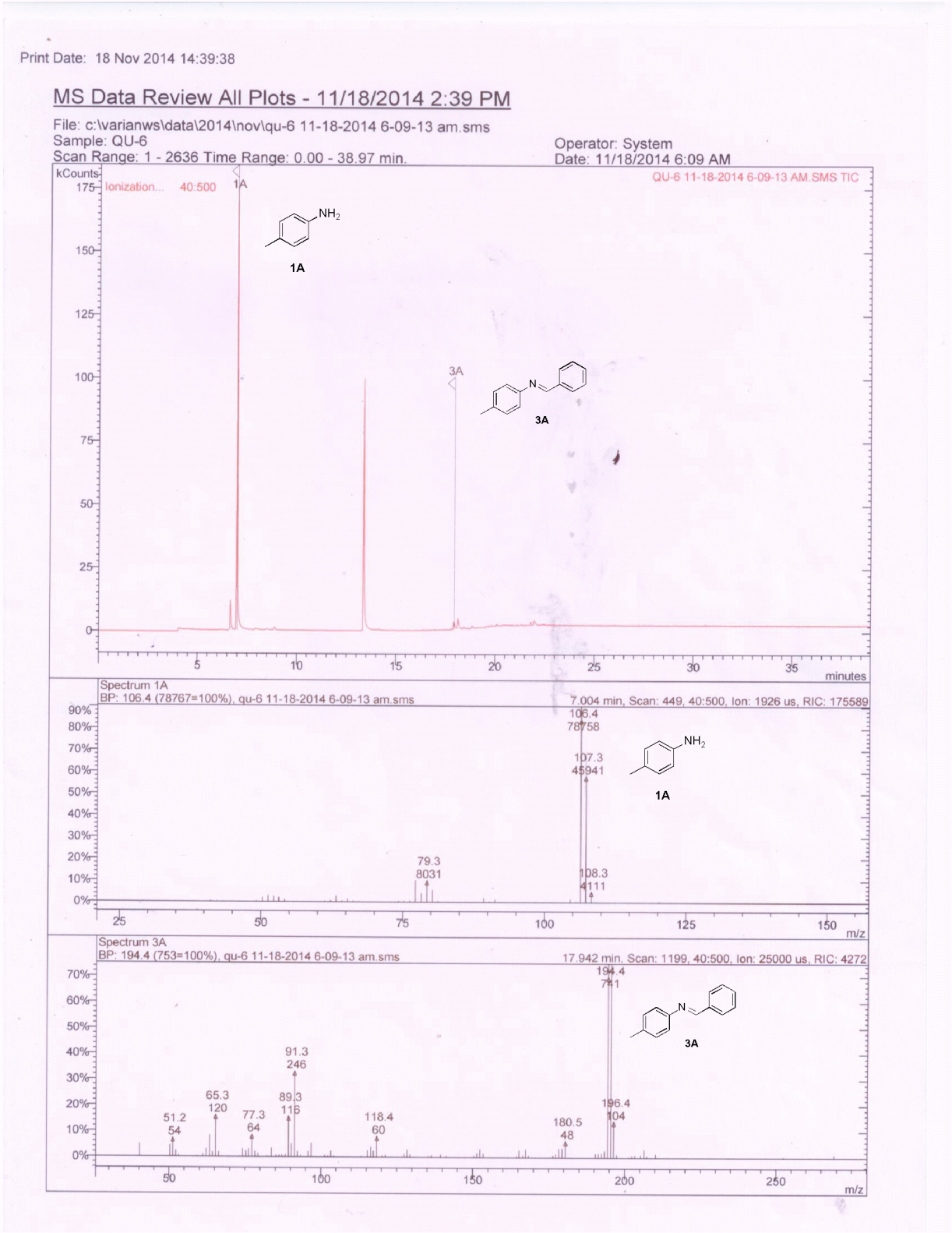

3.05
1.00
0.91
3.10
5.22
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


N
OCH3


3.02
1.00
6.89
2.02
3.11
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


8.92
3.01
2.01
1.97
1.00
6.05
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

GC-MS Spectra of Crude Reaction Mixture:

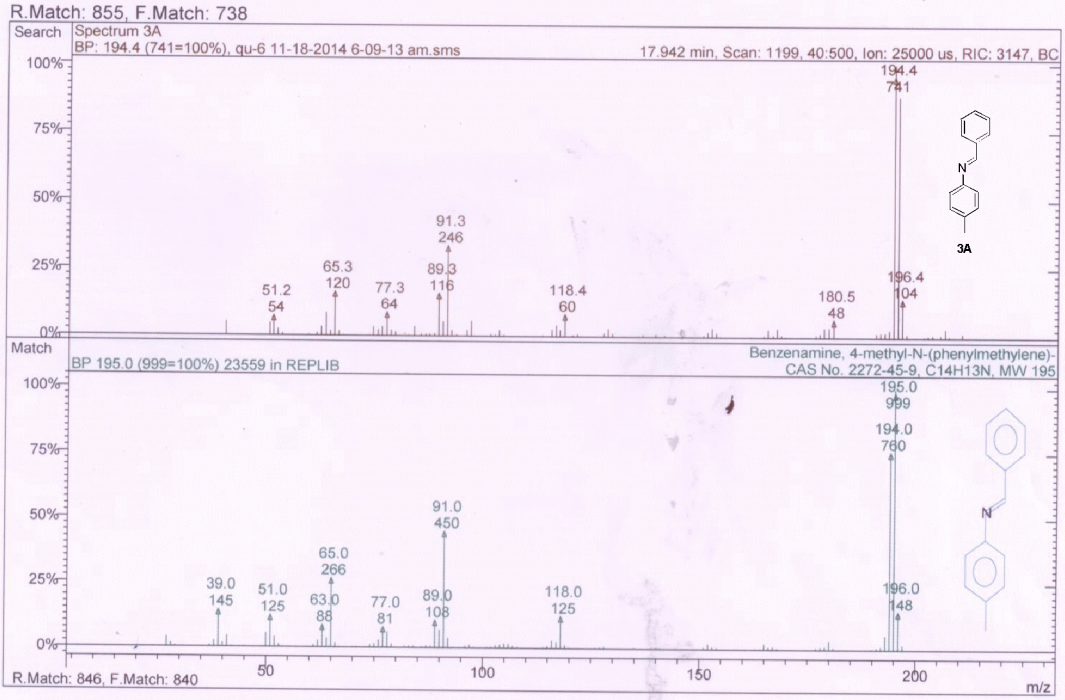


Print Date: 18 Nov 2014 14:44:58

Scan 1199 from c:\varianws\data\2014\nov\qu-6 11-18-2014 6-09-13 am.sms

Entry 23559 from REPLIB NIST Library

R.Match: 855, F.Match: 738



1st Spectrum from ...ws\data\2014\nov\qu-6 11-18-2014 6-09-13 am.sms
Scan No: 1199, Time: 17.942 minutes
No averaging. Background corrected.
Comment: 17.942 min. Scan: 1199 40:500 Ion: 25000 us RIC: 4272
Pair Count: 98 MW: 0 Formula: None
CAS No: None Acquired Range: 39.5 - 500.5 m/z

Method Internal EI and CI, Time: 0.00 - 39.00, Centroid
Seg 1, FIL/MUL DELAY , Time: 0.00- 4.00, Filament Off
Seg 2, <No Description>, Time: 4.00-39.00, Channels: 1
Chan 1, Full EI - Auto
Product Mass Range: 39.5 - 500.5 m/z

Ion	Int	Norm	Ion	Int	Norm	Ion	Int	Norm
40.2	36	49	92.3	15	20	165.3	20	27
50.3	33	44	93.4	4	5	166.5	5	7
51.2	54	73	95.8	15	20	167.4	23	31
52.2	17	23	96.8	39	53	168.4	5	7
53.2	5	7	101.3	5	7	169.4	1	1
59.2	2	3	102.3	3	4	176.4	5	7
61.2	7	9	103.3	16	22	177.3	9	12
62.2	23	31	104.3	3	4	178.3	25	34
63.3	61	82	113.3	2	3	179.4	25	34
64.3	13	18	115.4	18	24	180.5	48	65
65.3	120	162	116.4	29	39	181.4	1	1
66.3	13	18	117.3	17	23	190.4	11	15
67.3	1	1	118.4	60	81	191.4	12	16
73.3	1	1	120.2	3	4	192.4	12	16
74.2	23	31	121.3	6	8	193.4	19	26
75.3	16	22	127.4	9	12	194.4	741	999
76.2	23	31	128.4	21	28	195.4	654	882