Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Copper-catalyzed efficient access to 2,4,6-triphenyl pyridines via oxidative decarboxylation coupling of aryl acetic acids with oxime acetates

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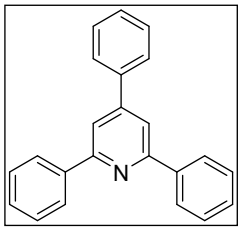
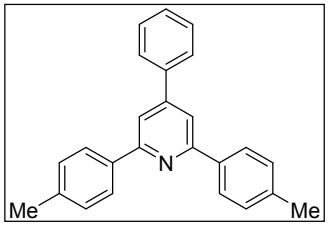
General section: The ^{1}H and ^{13}C NMR spectra of all synthesized compounds were recorded in Bruker 400 or 500 MHz NMR machine using their solutions in $CDCl_3$. The ^{1}H NMR was referred to TMS used as an internal standard and ^{13}C NMR was referred to the central line of $CDCl_3$ (δ = 0.00 and δ = 77.00 ppm respectively). The mass data was obtained from GC-MS. HRMS (High resolution mass spectra) were recorded using electro spray ionization in Bruker waters machine. For TLC, aluminium plates coated with silica gel containing F254 indicator were used which are purchased from Merck and the spots were visualized by UV light and/or by heating the plates sprayed with Seebach solution (phosphomolybdic acid (2.5 g), $Ce(SO_4)_2$ (1.0 g), conc. H_2SO_4 (6 mL) and H_2O (94 mL). The crude products were purified by column chromatography on 100-200 mesh silica gel using mixture of hexanes and ethyl acetate as eluent. Unless otherwise noted, all commercial reagents were used without purification. The oxime esters are synthesised according to the literature procedure.

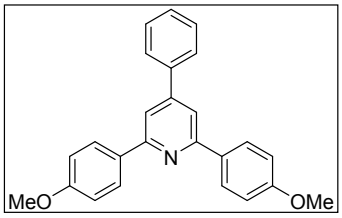
General procedure for the synthesis of 2,4,6-triphenyl substituted pyridines (3): The round bottom flask charged with oxime acetate **1** (0.2 mmol), phenylacetic acid **2** (0.15 mmol), CuCl (20 mol%) and $NaHSO_3$ (0.5 equiv.) in DMF (2 mL) under oxygen atmosphere. The mixture was allowed to stir at 150 ℃ for 2-4 h. The reaction progress was monitored by TLC. After completion of the reaction mixture cooled to room temperature and diluted with ethyl acetate (10 mL) and water. Both layers were separated and aqueous fraction washed with ethyl acetate (10 mL). The organic layer was dried over anhydrous Na_2SO_4 and the solvents were removed using rotary evaporator. The crude residue was purified by column chromatography using silica gel as stationary phase, Hexane/EtoAc (98:2) as a mobile phase to obtain the corresponding **3**.[1]



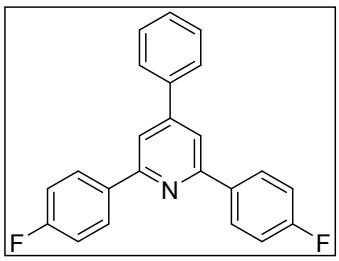
2,4,6-Triphenyl-pyridine (3aa).[1] White solid, 90% yield, mp 101-102 ℃ (lit.[1,2] mp 102-104 ℃); H^1 NMR (400 MHz, $CDCl_3$) δ 8.21 (d, J = 7.1 Hz, 4H), 7.90 (s, 2H), 7.76 (d, J = 6.9 Hz, 2H), 7.60 -7.41 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 150.2, 139.6, 139.1, 129.2, 129.0, 129.0, 128.5, 127.2, 127.1, 117.1; HRMS (ESI) calc. for $C_{23}H_{18}N$ $(M+H)^+$, 308.1437, found 308.1441.



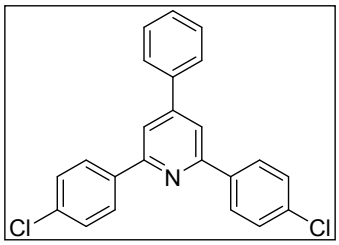
2,6-Bis(4-methylphenyl)-4-phenylpyridine (3ab). White solid, 92% yield, mp 150 -154 ℃ (lit.[1] mp 157.4- 157.9 ℃); H^1 NMR (400 MHz, $CDCl_3$) δ 8.11- 8.09 (m, 4H), 7.84 (s, 2H), 7.75 (m, 2H), 7.55-7.45 (m, 3H), 7.31 (d, J = 4.0 Hz, 4H), 2.42 (d, J = 7.4 Hz, 6H);^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 150.0, 139.3, 138.9, 136.9, 129.4, 129.1,128.8, 127.2, 127.1, 116.5, 21.2; HRMS (ESI) calc. for $C_{25}H_{22}N$ $(M+H)^+$, 336.1747, found 336.1752.



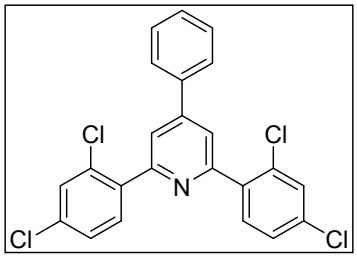
2,6-Bis(4-methoxyphenyl)-4-phenylpyridine (3ac). White solid, 94% yield, mp 96-98 ℃ (lit.[1,2] mp 98-98 ℃); H[1] NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.7 Hz, 2H), 7.94 (d, *J* = 1.2 Hz, 4H), 7.78 (s, 2H), 7.53-7.44 (m, 2H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 3H), 3.88 (d, *J* = 5.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 156.8, 150.0, 139.3, 132.2, 130.6, 128.8, 128.3, 127.1, 115.7, 114.0. 55.5; HRMS (ESI) calc. for $C_{25}H_{22}NO_2$ $(M+H)^+$, 368.1644, found 368.1649.



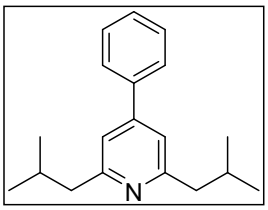
2,6-Bis(4-fluorophenyl)-4-phenylpyridine (3ad). White solid, 88% yield, mp 149-150 ℃ (lit.[1] mp 150-152℃); H[1] NMR (400 MHz, $CDCl_3$) 8.08 (m, 4H), 7.84 (d, *J* = 15.6 Hz, 2H), 7.66 (m, 2H), 7.44(d, *J* = 6.4 Hz, 3H), 7.19 (d, *J* = 17.2 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4 (d, $J_{C\text{-}F}$ = 16 Hz), 155.6,145.0, 134.7, 134.5(d, $J_{C\text{-}F}$ = 3.0 Hz), 131.1, (d, $J_{C\text{-}F}$ = 10.0 Hz), 130.9, 130.6, 129.0, 128.4, 121.5, 115.6.; HRMS (ESI) calc. for $C_{23}H_{16}NF_2$ $(M+H)^+$, 344.1247, found 344.1251.



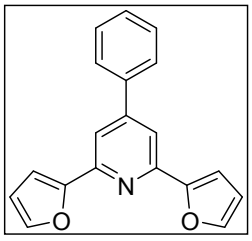
2,6-Bis(4-chlorophenyl)-4-phenylpyridine (3ae). White solid, 86% yield, mp 162-164 ℃ (lit.[1] mp 160-164℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.7 Hz, 4H), 7.87 (s, 2H), 7.73 (d, *J* = 6.9 Hz, 2H), 7.51-7.46 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.3, 150.2, 137.8, 137.1, 135.3, 129.3, 129.2, 128.9, 128.3, 127.2, 117.1; HRMS (ESI) calc. for $C_{23}H_{16}NCl_2$ $(M+H)^+$, 376.0656, found 376.0659.



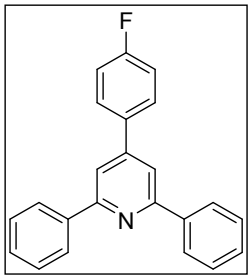
2,6-Bis(2,4-chlorophenyl)-4-phenylpyridine (3af). White solid, 82% yield, mp 159-160 ℃ (lit.[5] mp 163-164℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 2H), 7.75 -7.66 (m, 4H), 7.53 (dd, *J* = 6.8, 1.8 Hz, 4H), 7.49 (d, *J* = 1.7 Hz, 1H), 7.38 (dd, *J* = 8.3, 2.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.2, 148.8, 137.5 , 135.0, 133.0 , 132.7, 130.0, 129.2, 127.5, 127.2, 121.7; HRMS (ESI) calc. for $C_{23}H_{14}NCl_4$ $(M+H)^+$, 444.9891, found 444.9897.



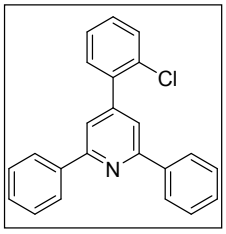
2,6-Bis(isobutyl)-4-phenylpyridine (3ah). Yellow oil, 78% yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.54 (s, 1H), 7.41(t, *J* = 2.8 Hz, 5H), 2.56 (d, *J* = 7.2 Hz, 4H), 1.70 (s, 2H), 1.0 (d, *J* = 6.4 Hz, 12H),); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 142.4, 137.3, 134.6, 130.4, 128.9, 126.6, 49.6, 29.7, 25.2, 22.7; HRMS (ESI) calc. for $C_{19}H_{26}N$ $(M+H)^+$, 264.1708, found 264.1711.



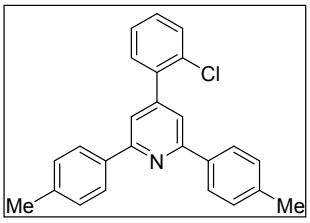
2,6-Bis(furan-2 yl)-4-phenylpyridine (3ai). Yellow solid, 45% yield, mp 104-107 ℃ (lit.[4] mp 102-104℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 4.0 Hz 2H), 7.79 (t, *J* = 1.6 Hz, 2H), 7.57 (t, *J* = 0.8 Hz, 2H), 7.51 (t, *J* = 7.2 Hz, 3H), 7.21(m, 2H), 6.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.8, 149.7, 143.3, 129.1, 129.0, 127.0, 114.8, 112.0, 109.1; HRMS (ESI) calc. for $C_{19}H_{14}NO_2$ $(M+H)^+$, 288.1021, found 288.1018.



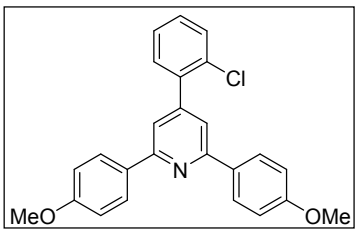
4-(4-Fluorophenyl)2,6-diphenylpyridine (3ba). White solid, 80% yield, mp 135-136 ℃ (lit.[1] mp 138-140℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 7.2 Hz, 4H), 7.86 (s, 2H), 7.62 (m, 2H), 7.53 (t, *J* = 7.2 Hz, 4H), 7.48 (d, *J* = 6.0 Hz, 2H), 7.23 (d, *J* = 32.8 Hz, 2H); HRMS (ESI) calc. for $C_{23}H_{17}NF$ $(M+H)^+$; 326.1342, found 342.1339.



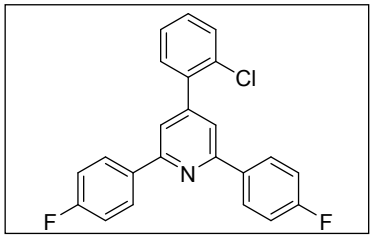
4-(2-Chlorophenyl)2,6-diphenylpyridine (3ca). Yellow solid, 72% yield, mp 112-114 ℃ (lit.[1] mp 108-110℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 9.6 Hz, 4H), 7.78 (s, 2H), 7.56 (dd, *J* = 2.3, 1.8 Hz, 10 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 149.7, 139.3, 134.0, 132.0, 129.9, 129.0, 128.7, 128.5, 127.6, 127.1, 120.2, 119.5; HRMS (ESI) calc. for $C_{23}H_{17}NCl$ $(M+H)^+$; 342.1052, found 342.1062.



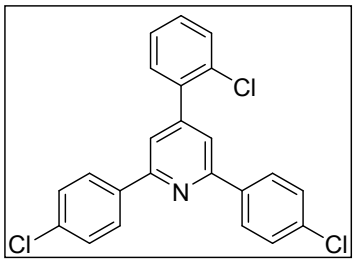
2,6-Bis(4-methylphenyl)-4-(2-chlorophenyl)pyridine (3cb). White solid, 75% yield, mp 182-184 ℃; H[1] NMR (400 MHz, $CDCl_3$) 8.11 (d, *J* = 8.0 Hz, 4H), 7.74 (s, 2H), 7.71 (d, *J* = 1.6 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 4H), 2.19 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 142.7, 137.9, 135.1, 134.0, 132.4, 132.0, 130.6, 130.0, 129.7, 129.4, 127.6, 127.3, 115.9, 21.3; HRMS (ESI) calc. for $C_{25}H_{21}NCl$ $(M+H)^+$, 370.1298, found 370.1294.



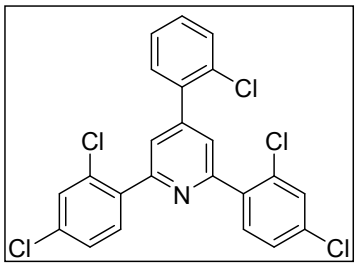
2,6-Bis(4-methoxyphenyl)-4-(2-chlorophenyl)pyridine (3cc). White solid, 71% yield, mp 138-140 ℃; H[1] NMR (400 MHz, $CDCl_3$) 8.16 (d, *J* = 8.8 Hz, 4H), 7.96 (d, *J* = 8.8 Hz, 2H), 7.67 (s, 2H), 7.04 (d, *J* = 8.8 Hz, 4H), 6.95 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 156.3, 148.4, 139.8, 138.8, 132.1, 130.8, 130.6, 129.5, 128.3, 127.1, 124.7, 118.0, 114.0, 113.7, 55.7; HRMS (ESI) calc. for $C_{25}H_{21}NO_2Cl$ $(M+H)^+$, 402.1205 found 402.1208.



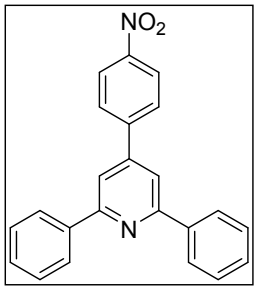
2,6-Bis(4-florophenyl)-4-(2-chlorophenyl)pyridine (3cd). Yellow oil, 68% yield; H^1 NMR (400 MHz, $CDCl_3$)) 8.20 (d, J = 15.6 Hz, 2H), 8.08 (m, 4H), 7.78 (s, 2H), 7.76 (d, J = 2.4 Hz, 2H), 7.50 (d, J = 16.0 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.9, 164.4 (d, J_{C-F} = 8.0 Hz), 157.9, 145.0, 140.8, 135.5, 134.2 (d, J_{C-F} = 3.0 Hz), 134.0, 133.1, 133.8, 131.2, 131.2 (d, J_{C-F} = 9.0 Hz), 130.3, 127.8, 127.1, 124.3, 115.7; HRMS (ESI) calc. for $C_{24}H_{15}NCl_2$ $(M+H)^+$, 378.0794, found 378.0805.



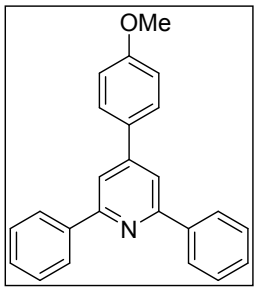
2,6-Bis(4-chlorophenyl)-4-(2-chlorophenyl)pyridine (3ce). White solid, 65% yield, mp 171-173 ℃ (lit.[3] mp 169-170 ℃); H^1 NMR (400 MHz, $CDCl_3$), 8.15 (d, J = 2.0 Hz, 4H), 8.14 (d, J = 8.0 Hz, 2H), 7.78 (s, 2H), 7.58 (m, 2H), 7.54 (m, 4H),; ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 148.9, 137.6, 135.3, 132.2, 130.8, 129.9, 128.9, 128.3, 127.2, 119.5; HRMS (ESI) calc.$C_{24}H_{15}NCl_3$ $(M+H)^+$, 410.0210, found 410.0232.



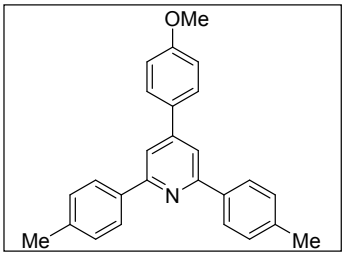
2,6-Bis(2,4-chlorophenyl)-4-(2-chlorophenyl)pyridine (3cf). White solid, 60% yield, mp 205-207 ℃ (lit.[5] mp 208-210 ℃); H^1 NMR (400 MHz, $CDCl_3$) 7.82(s, 2H),7.78 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 2.0 Hz, 2H), 7.45 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 155.6, 146.1, 137.8, 137.4, 134.9, 132.6, 130.9, 130.2, 129.9, 128.4, 127.7, 124.4, 119.8; HRMS (ESI) calc. for $C_{23}H_{13}NCl_5$ $(M+H)^+$, 479.9412, found 479.9419**.**



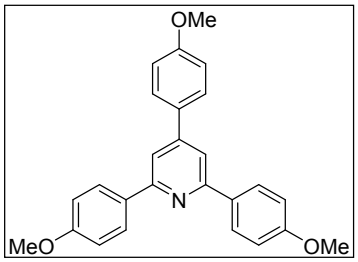
4-(4-Nitrophenyl)2,6-diphenylpyridine (3da). Yellow solid, 65% yield, mp 195-196 ℃ (lit.[2] mp 196-198℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (m, 2H), 8.18 (m, 4H), 7.84 (m, 2H), 7.73 (d, *J* = 7.6 Hz, 2H), 7.49 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 150.8, 142.7, 139.5, 137.4, 120.7, 128.9, 128.6, 127.3,127.1, 127.0, 118.6; HRMS (ESI) calc. for $C_{23}H_{17}N2O_2Cl$ $(M+H)^+$; 353.1249, found 353.1246.



4-(4-Methoxyphenyl)-2,6-diphenylpyridine (3ea). White solid, 88% yield, mp 98-99 ℃ (lit.[1,4] mp 100-102 ℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 9.3 Hz, 4H), 7.85 (s, 2H), 7.70 (d, *J* = 8.8 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 4H), 7.44 (t, *J* = 6.6 Hz, 2H), 7.05 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 157.5, 149.6, 139.7, 131.3, 129.0, 128.71, 128.3, 127.1, 116.6, 114.4, 55.4; HRMS (ESI) calc. for $C_{24}H_{20}NO$ $(M+H)^+$, 338.1538, found 338.1542.

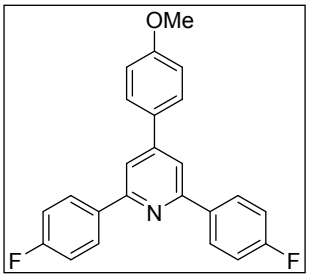


2**,6-Bis(4-methyl phenyl)-4-(4-methoxyphenyl)pyridine (3eb)**. White solid, 86% yield, mp 152-154 ℃ (lit.[1b] mp 155-157 ℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.1 Hz, 4H), 7.80 (s, 2H), 7.70 (d, *J* = 8.7 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 4H), 7.04 (d, *J* = 8.7 Hz, 2H), 3.88 (s, 3H), 2.43 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 157.3, 149.5, 138.9, 137.0, 131.5, 129.4, 128.3, 127.0, 116.0, 114.5, 55.4, 21.3; HRMS (ESI) calc. for $C_{26}H_{24}NO$ $(M+H)^+$, 366.1851, found 366.1854.

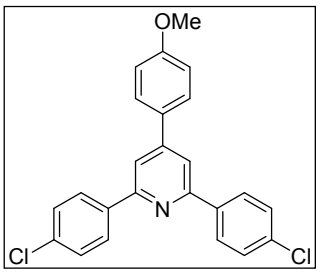


2,4,6-Tris(4-methoxyphenyl)pyridine (3ec). White solid, 84% yield, mp 132-134 ℃ (lit.[1b] mp 138-139 ℃); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.9 Hz, 2H), 7.94 (d, *J* = 9.0 Hz, 2H), 7.74 (s, 2H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.09-7.01 (m, 5H), 6.94 (d, *J* = 9.0 Hz, 2H), 3.89 (s, 9H); ^{13}C NMR

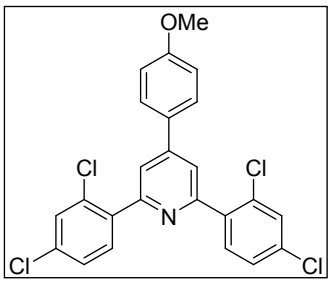
(100 MHz, $CDCl_3$) δ 158.4, 155.5, 153.6, 149.0, 139.2, 136.3, 134.3, 128.3, 128.3, 115.2, 114.5, 114.0, 55.4; HRMS (ESI) calc. for $C_{26}H_{24}NO_3$ $(M+H)^+$, 398.1751, found 398.1761.



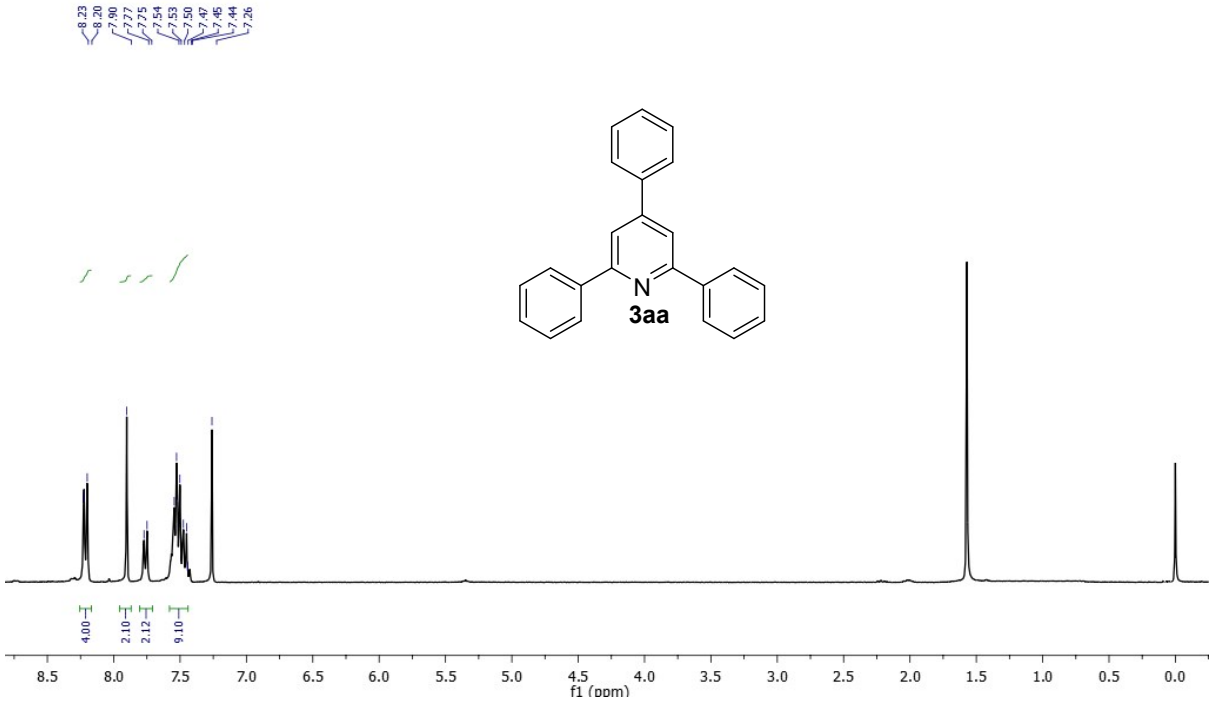
2,6-Bis(4-fluorophenyl)-4-(4-methoxyphenyl)pyridine (3ed). White solid, 76% yield, mp 122-123 ℃ (lit.[1b] mp 124-126 ℃); H^1 NMR (400 MHz, $CDCl_3$), 8.11(d, J = 1.6 Hz, 2H), 8.09 (d, J = 3.6 Hz, 2H), 7.88 (s, 2H), 7.77 (m, 2H), 7.18 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 155.8, 146.3, 135.5, 130.5, 129.5 (d, $J_{C\text{-}F}$ = 12 Hz), 129.3, 129.2, 128.7, 128.8, 128.52(d, $J_{C\text{-}F}$ = 8.0 Hz), 128.2, 118.2, 116.1, 115.9, 55.6; HRMS (ESI) calc. for $C_{24}H_{18}NOF_2$ $(M+H)^+$, 374.1350, found 374.1358.

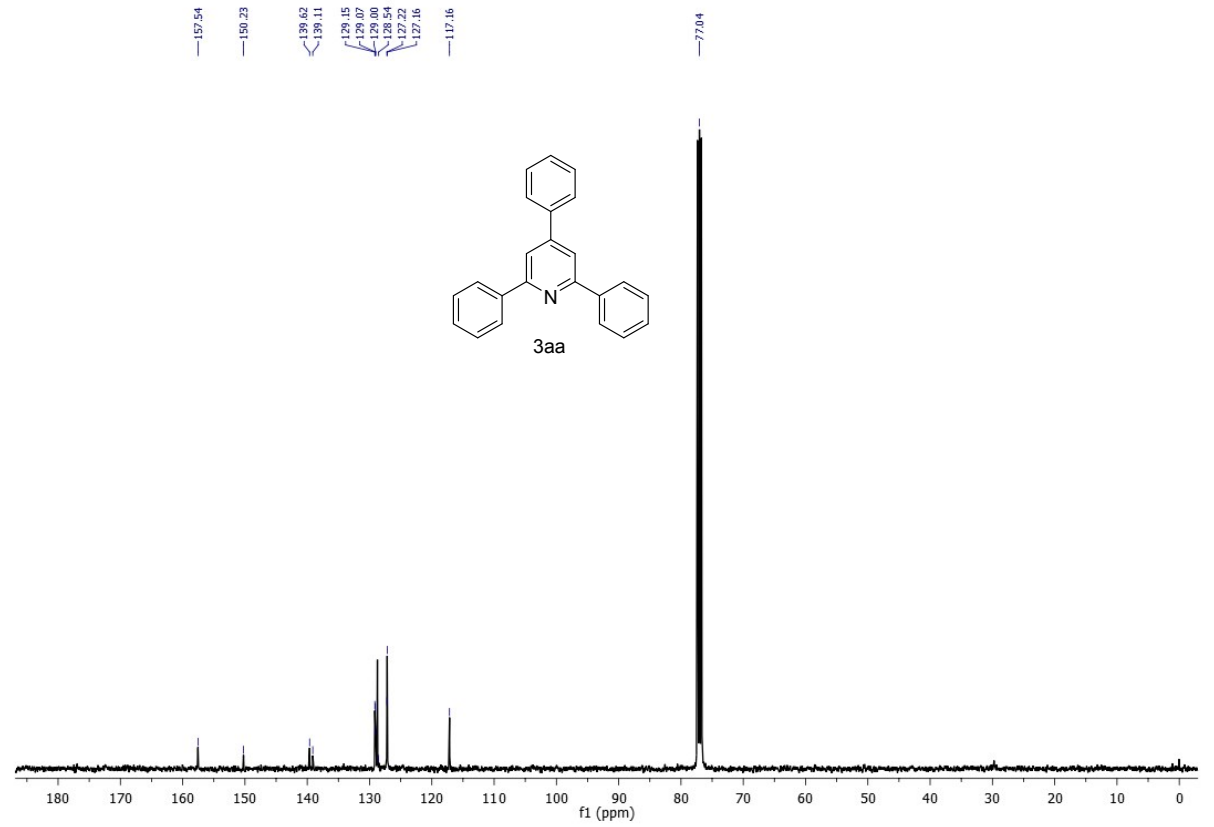


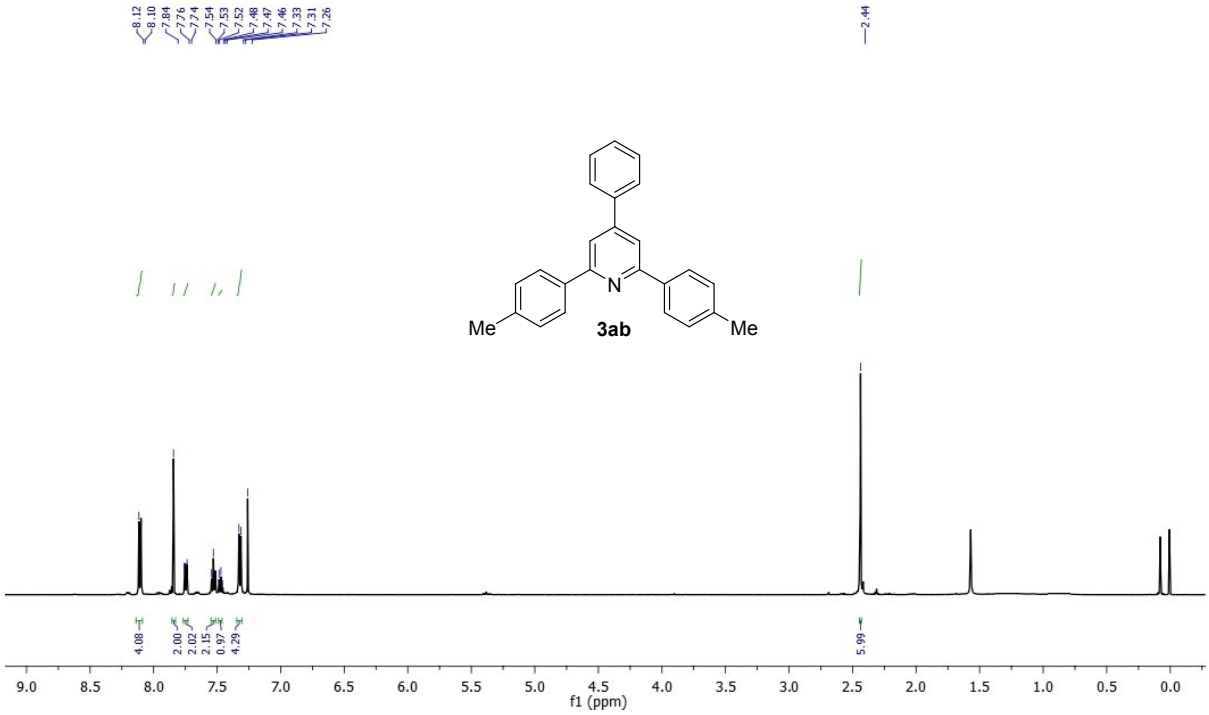
2,6-Bis(4-chlorophenyl)-4-(4-methoxyphenyl)pyridine(3ee). White solid, 72% yield, mp 178-180 ℃ (lit.[1b] mp 180-182 ℃); ^1H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, J = 8.7 Hz, 4H), 7.82 (s, 2H), 7.69 (d, J = 8.8 Hz, 2H), 7.55-7.41 (m, 4H), 7.06 (d, J = 8.8 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 156.3, 150.0, 137.9, 135.2, 133.5, 130.9, 128.9, 128.3, 116.6, 114.6, 55.4; HRMS (ESI) calc. for $C_{24}H_{18}NOCl_2$ $(M+H)^+$, 406.0750, found 406.0765.

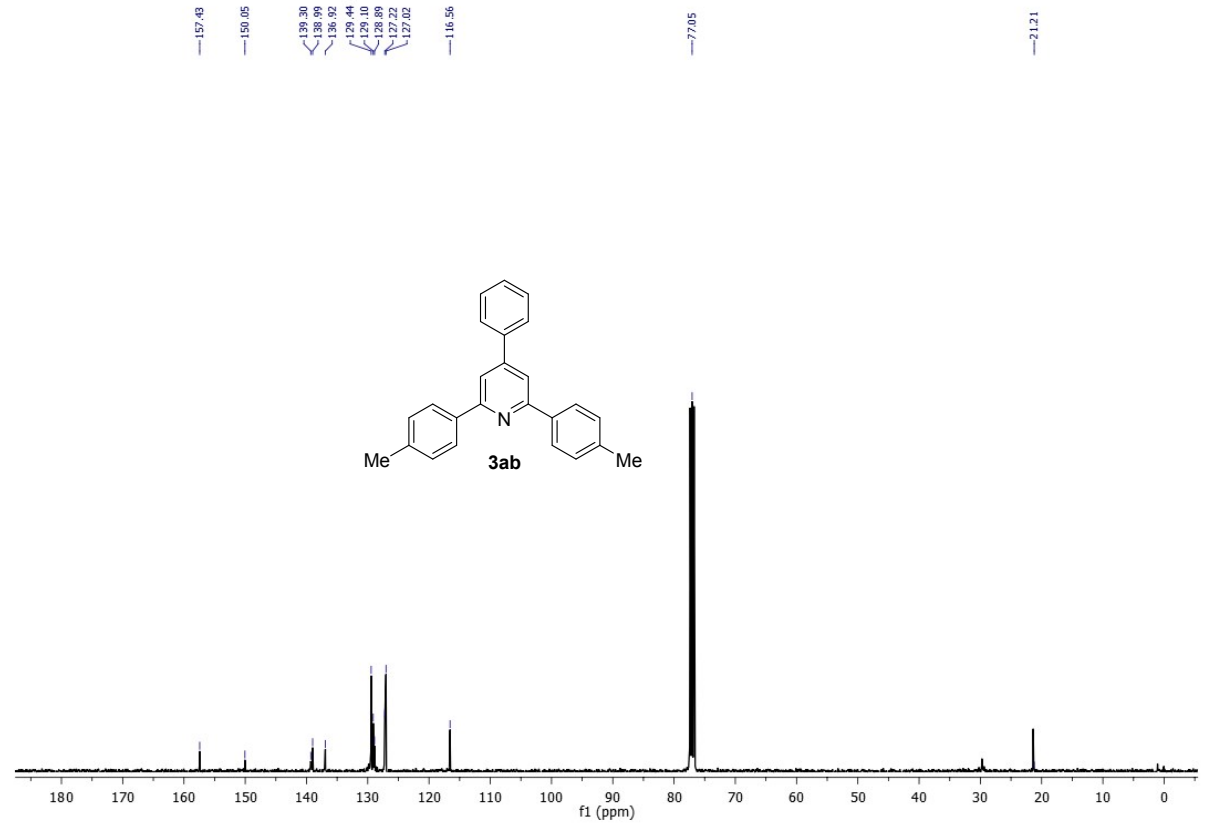


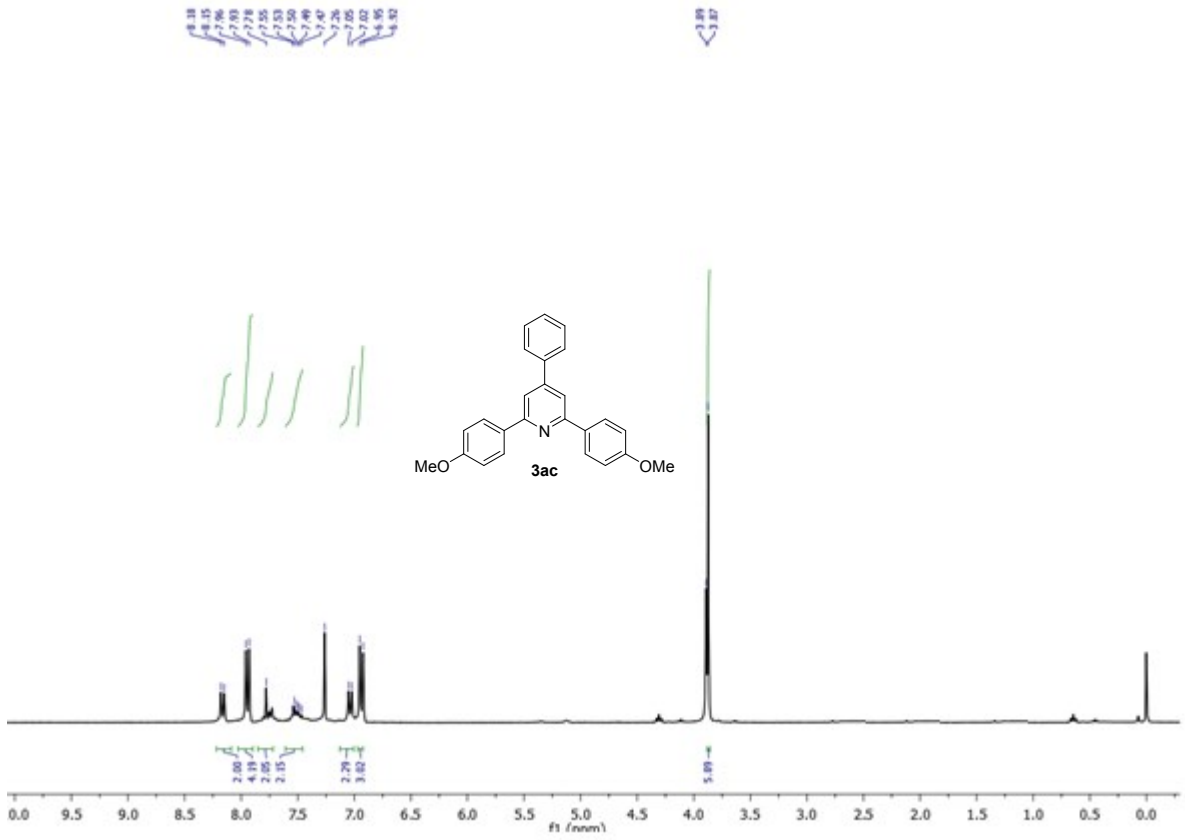
2,6-Bis(2,4-chlorophenyl)-4-(4-methoxyphenyl)pyridine (3ef). White solid, 67% yield, mp 178-180 ℃ (lit.[4] mp 168-169 ℃); H^1 NMR (400 MHz, $CDCl_3$), 7.83 (s, 2H), 7.68 (d, J = 8.0 Hz, 4H), 7.54 (d, J = 8.0 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.05 (d, J = 8.8 Hz, 2H), 3.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 156.2, 148.2, 138.2, 137.8, 135.0, 134.2, 129.8, 129.5, 127.3, 114.5, 55.5; HRMS (ESI) calc. for $C_{24}H_{16}NOCl_4$ $(M+H)^+$; 474.9892, found 474.9898.

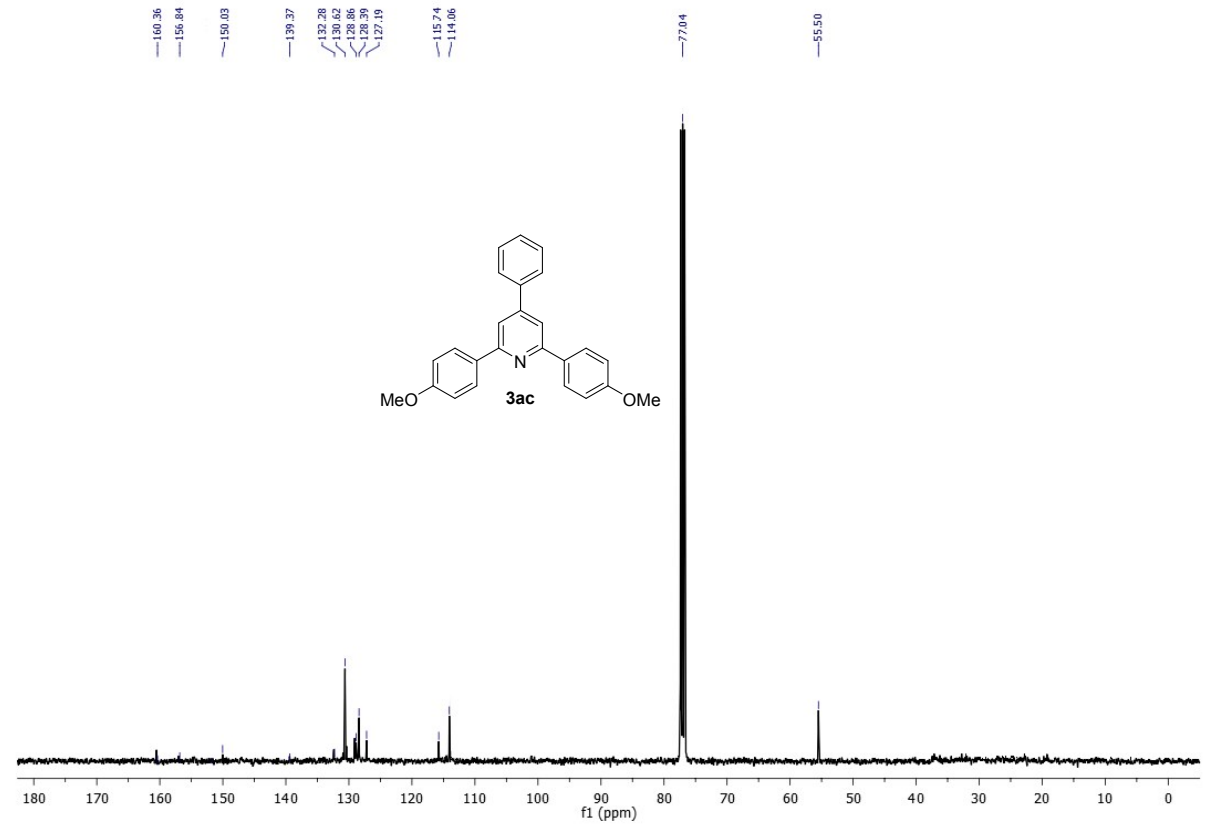

8.23
8.20
7.90
7.77
7.75
7.54
7.53
7.50
7.47
7.45
7.44
7.26
N
3aa
4.00
2.10
2.12
9.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

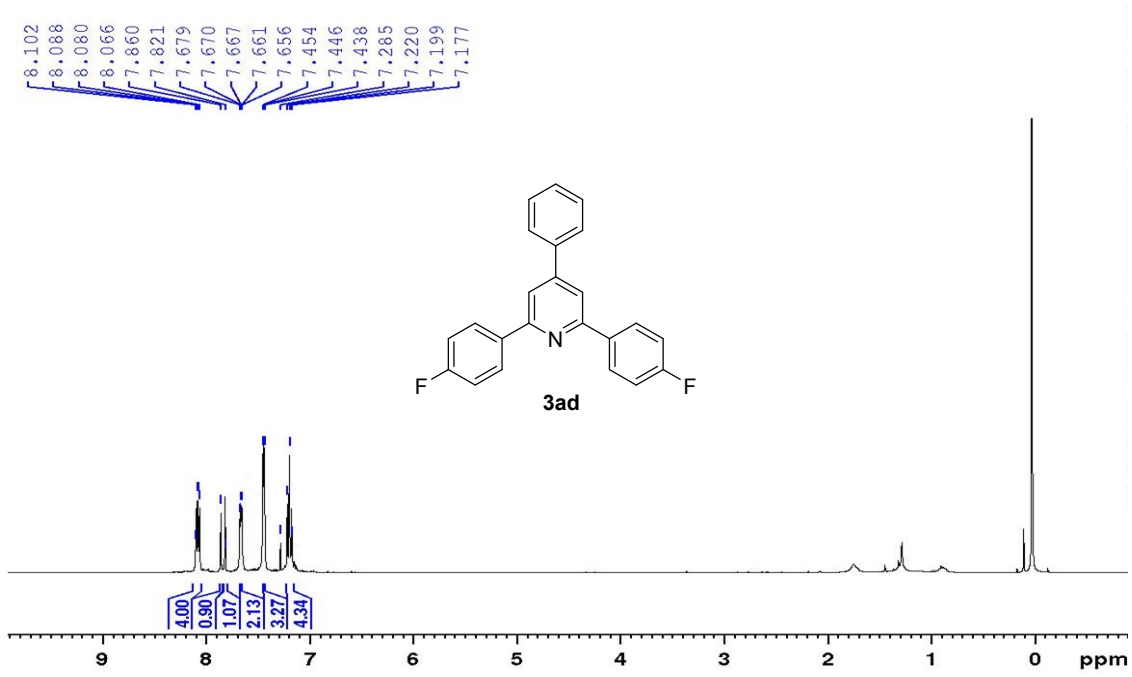

157.54
150.23
139.62
139.11
129.15
129.07
129.00
128.54
127.22
127.16
117.16
77.04
N
3aa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.12
8.10
7.84
7.76
7.74
7.54
7.53
7.52
7.48
7.47
7.46
7.33
7.31
7.26
2.44
Me
N
Me
3ab
4.08
2.00
2.02
2.15
0.97
4.29
5.99
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)


157.43
150.05
139.30
138.99
136.92
129.44
129.10
128.89
127.22
127.02
116.56
77.05
21.21
Me
N
Me
3ab
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MeO
OMe
3ac
f1 (ppm)


MeO
OMe
3ac
f1 (ppm)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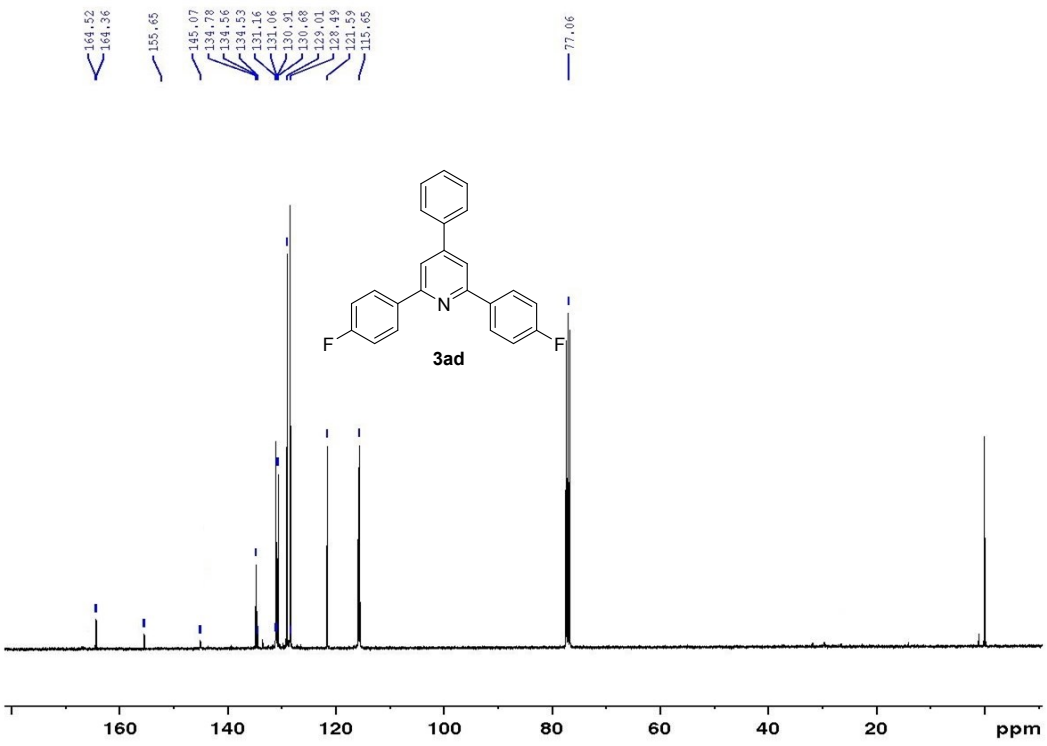
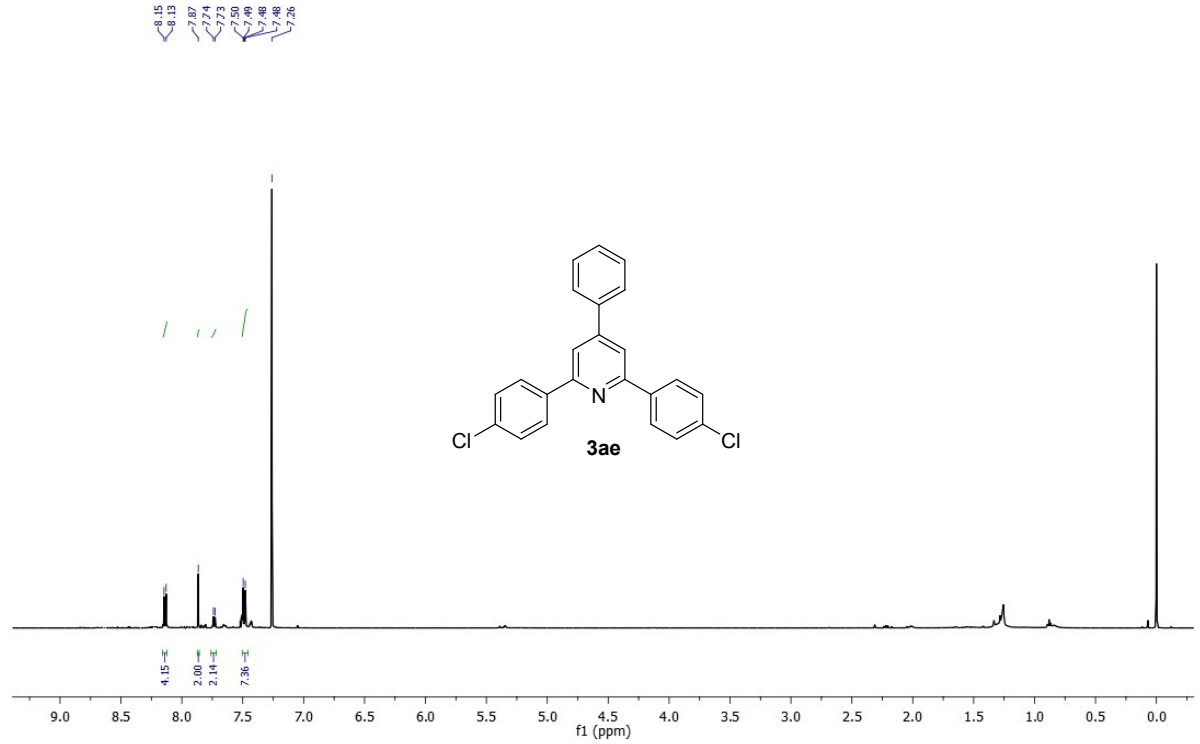
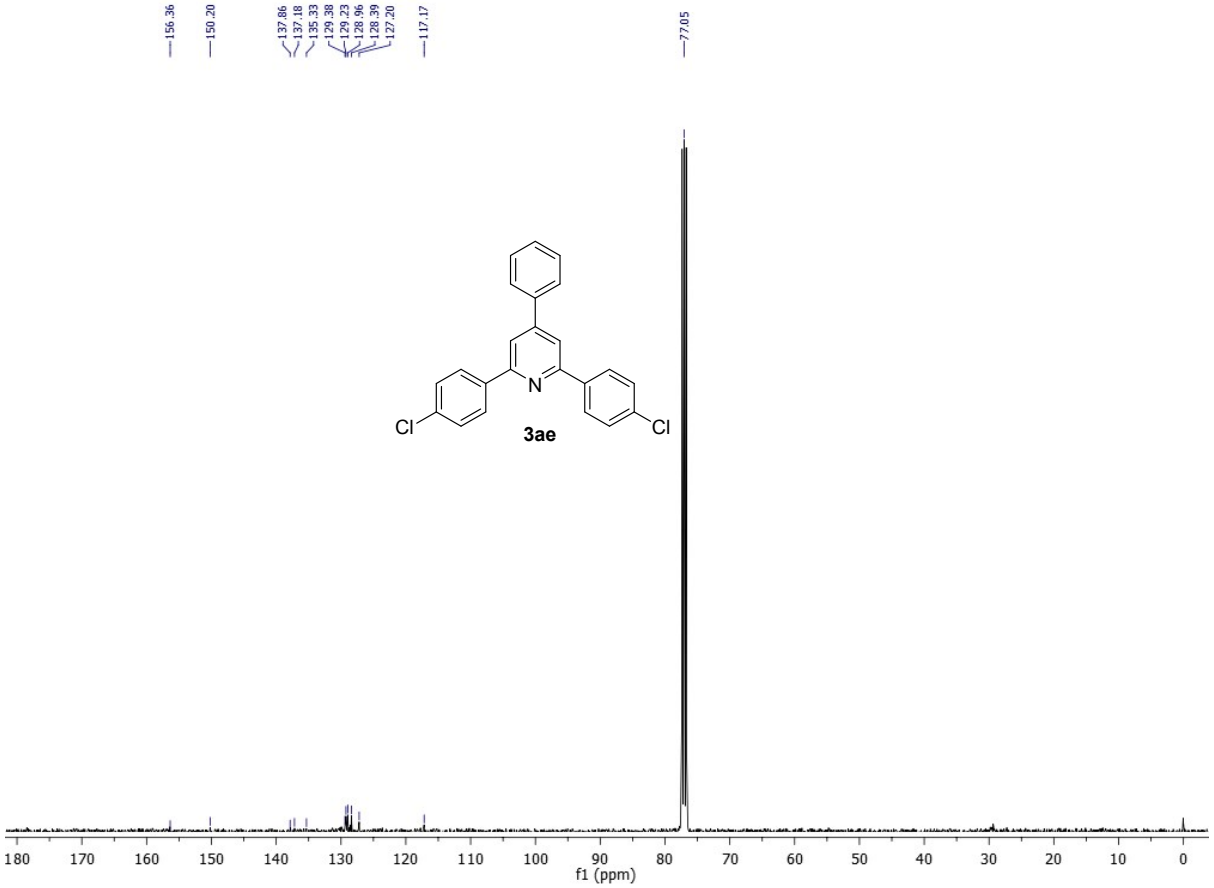
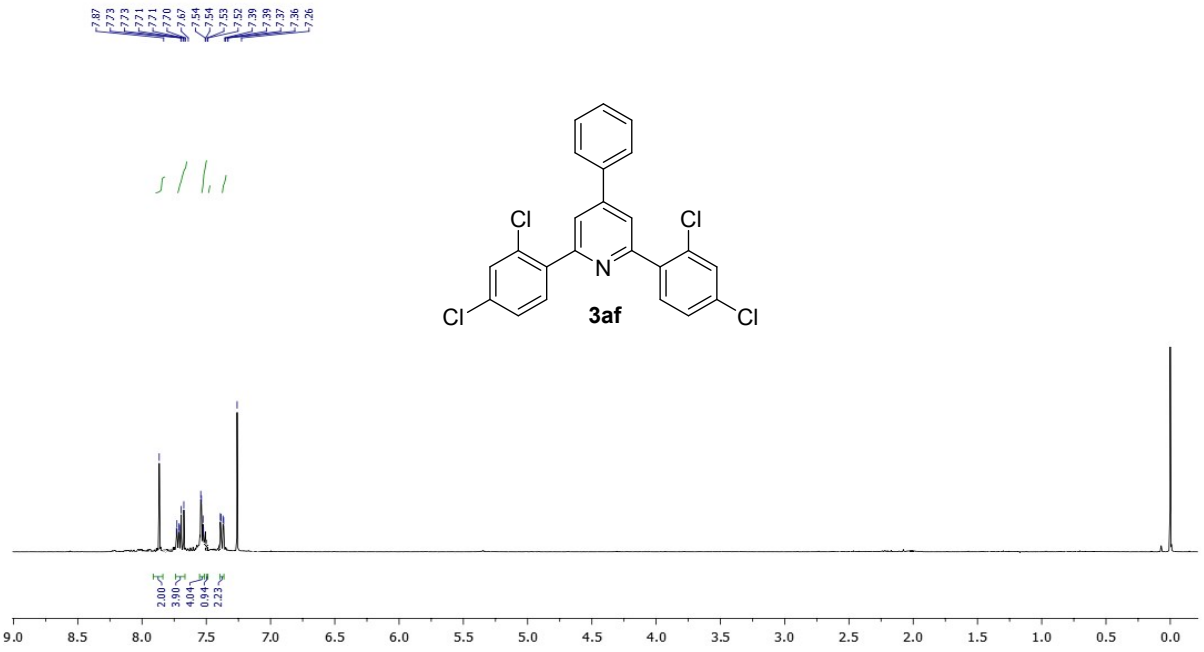
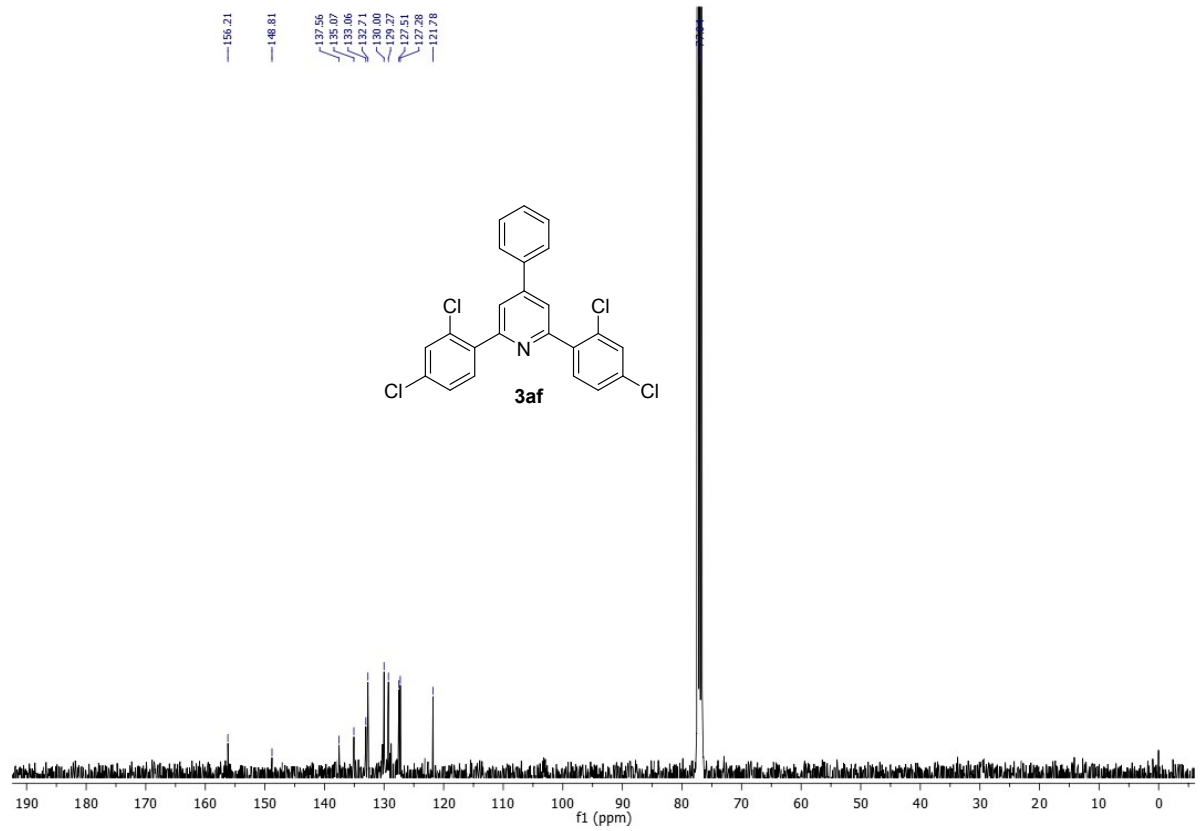
8.088
8.080
8.066
7.860
7.821
7.679
7.670
7.667
7.661
7.656
7.454
7.446
7.438
7.285
7.220
7.199
7.177
N
F
F
3ad
4.00
0.90
1.07
2.13
3.27
4.34
9
8
7
6
5
4
3
2
1
0
ppm

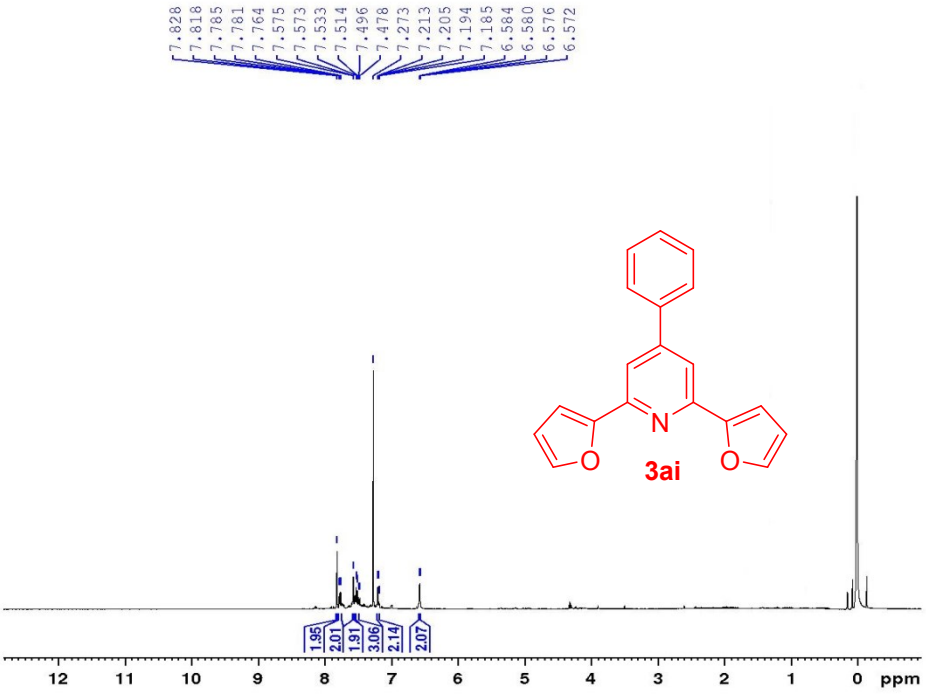

164.52
164.36
155.65
145.07
134.78
134.56
134.53
131.16
131.06
130.91
130.68
129.01
128.49
121.59
115.65
77.06
N
F
F
3ad
160
140
120
100
80
60
40
20
ppm

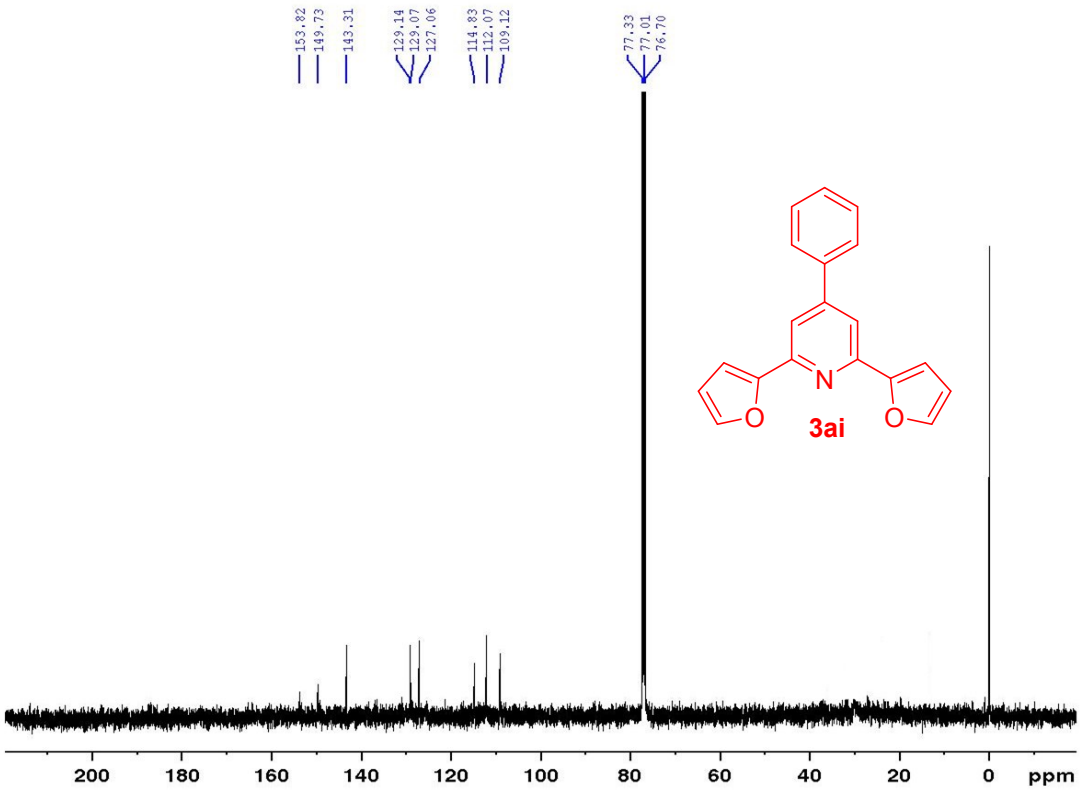

8.15
8.13
7.87
7.74
7.73
7.50
7.49
7.48
7.48
7.26
Cl
N
Cl
3ae
4.15
2.00
2.14
7.36
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

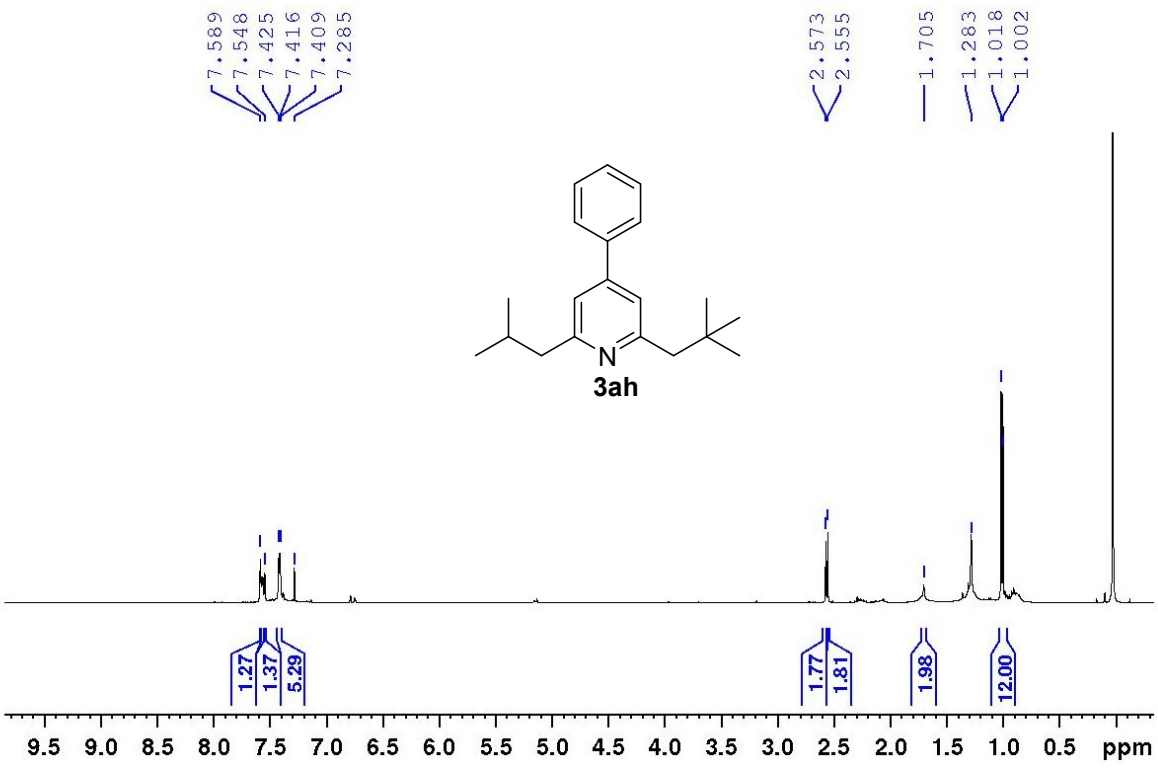

156.36
150.20
137.86
137.18
135.33
129.38
129.23
128.96
128.39
127.20
117.17
77.05
Cl
N
Cl
3ae
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.87
7.73
7.73
7.71
7.71
7.70
7.67
7.54
7.54
7.53
7.52
7.39
7.39
7.37
7.36
7.26
Cl
Cl
N
Cl
Cl
3af
2.00
3.90
4.04
0.94
2.23
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


156.21
148.81
137.56
135.07
133.06
132.71
130.00
129.27
127.51
127.28
121.78
Cl
Cl
N
Cl
Cl
3af
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.828
7.818
7.785
7.781
7.764
7.575
7.573
7.533
7.514
7.496
7.478
7.273
7.213
7.205
7.194
7.185
6.584
6.580
6.576
6.572
N
O
O
3ai
1.95
2.01
1.91
3.06
2.14
2.07
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm


153.82
149.73
143.31
129.14
129.07
127.06
114.83
112.07
109.12
77.33
77.01
76.70
N
O
O
3ai
200
180
160
140
120
100
80
60
40
20
0
ppm


7.589
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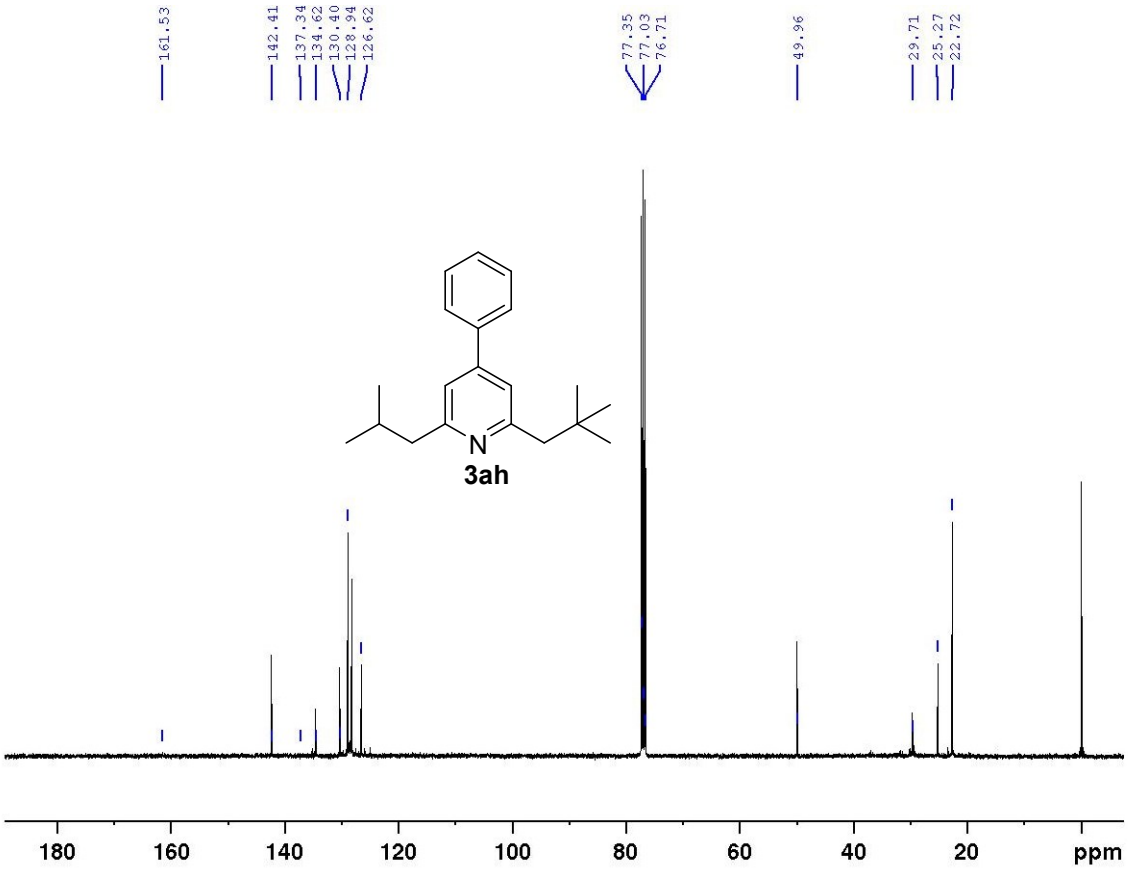
7.425
7.416
7.409
7.285
2.573
2.555
1.705
1.283
1.018
1.002
N
3ah
1.27
1.37
5.29
1.77
1.81
1.98
12.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm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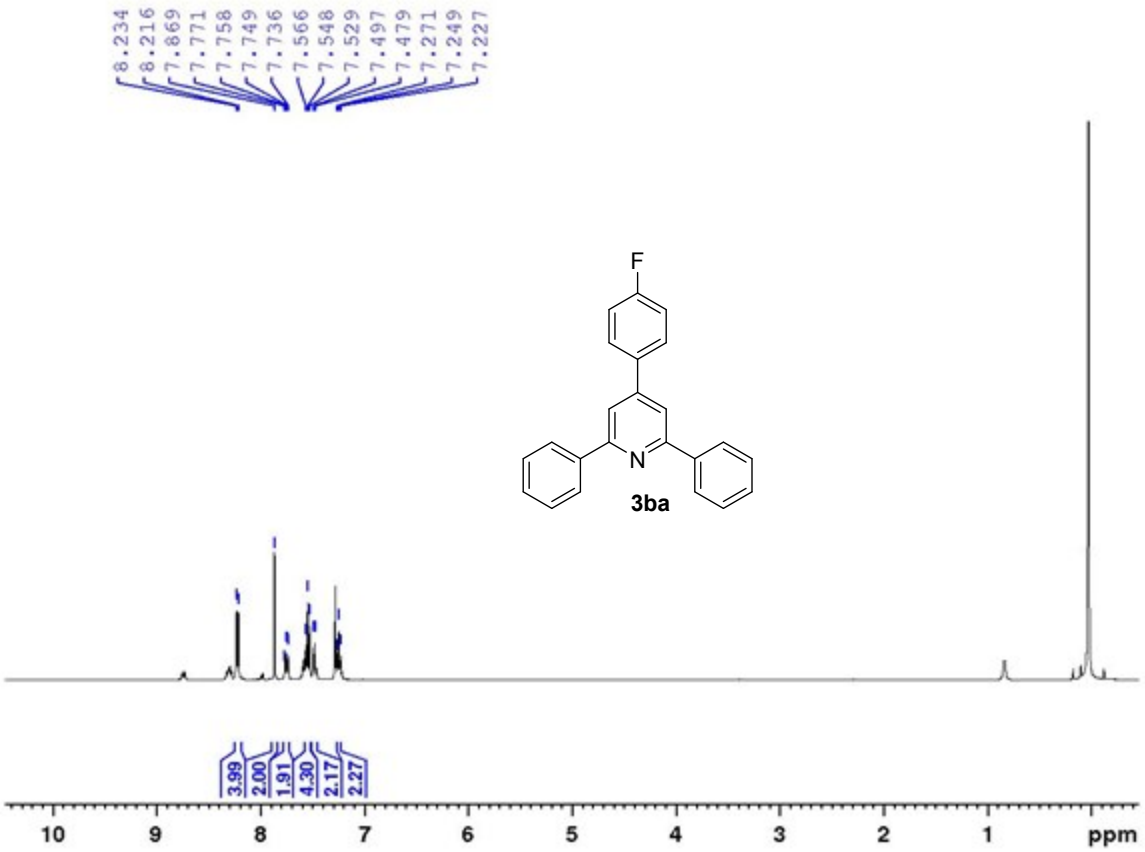
142.41
137.34
134.62
130.40
128.94
126.62
77.35
77.03
76.71
49.96
29.71
25.27
22.72
N
3ah
180 160 140 120 100 80 60 40 20 ppm


8.234
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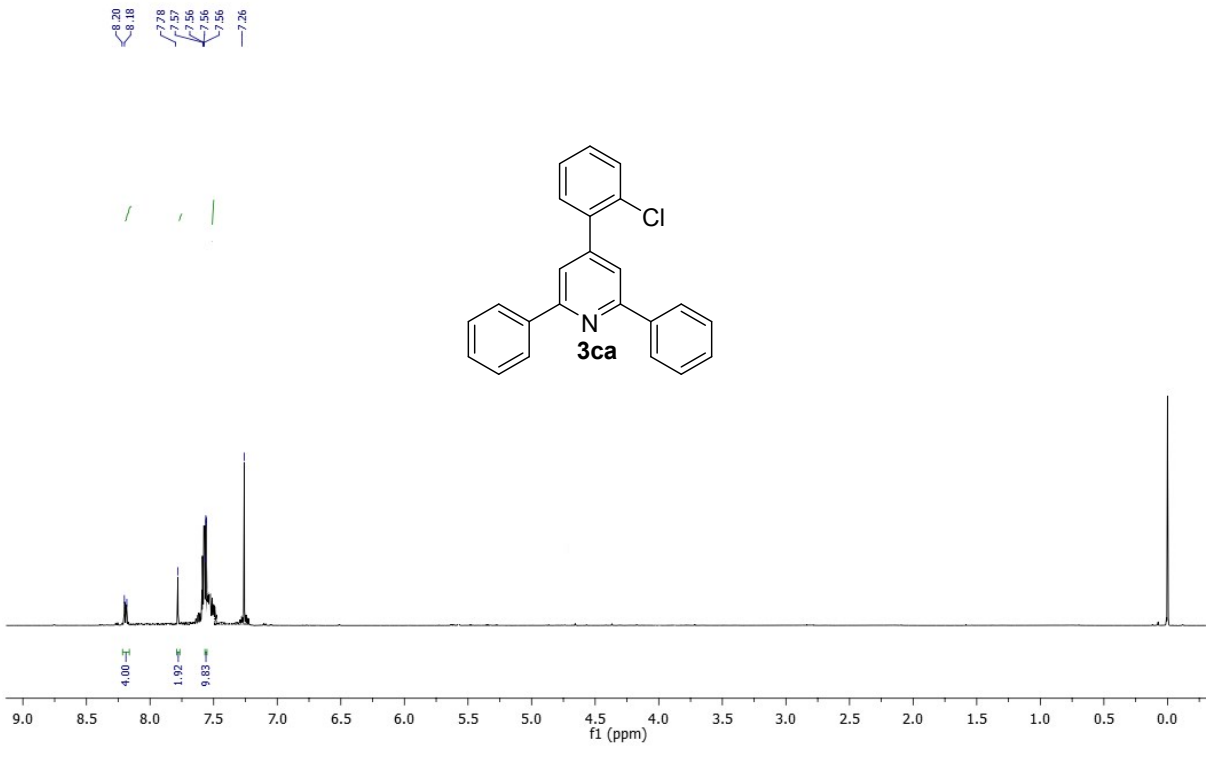
7.869
7.771
7.758
7.749
7.736
7.566
7.548
7.529
7.497
7.479
7.271
7.249
7.227
F
N
3ba
3.99
2.00
1.91
4.30
2.17
2.27
10
9
8
7
6
5
4
3
2
1
ppm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7.78
7.57
7.56
7.56
7.56
7.26
Cl
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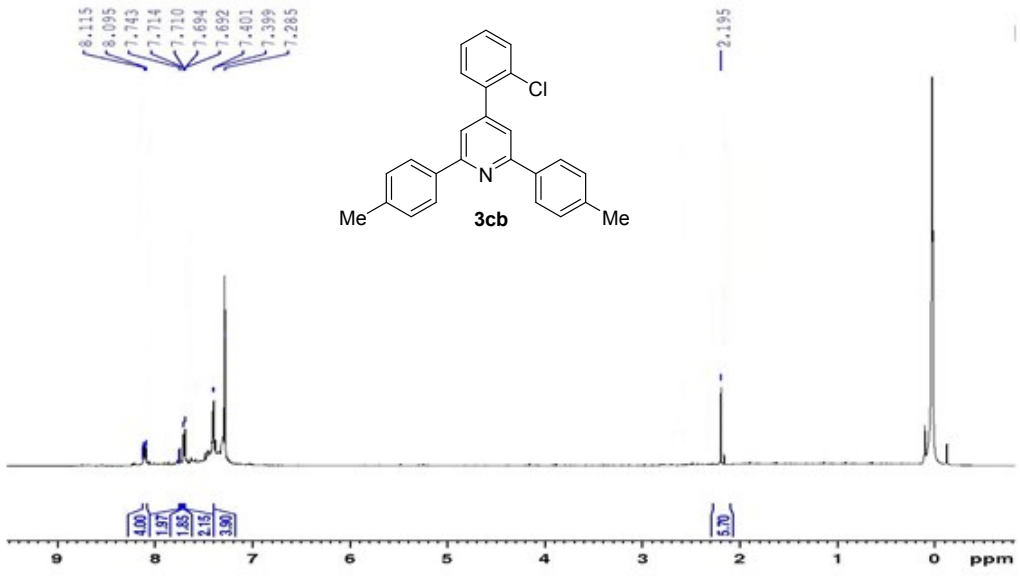
3ca
4.00
1.92
9.83
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

.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7.714
7.710
7.694
7.692
7.401
7.399
7.285
2.195
Cl
N
Me
Me
3cb
4.00
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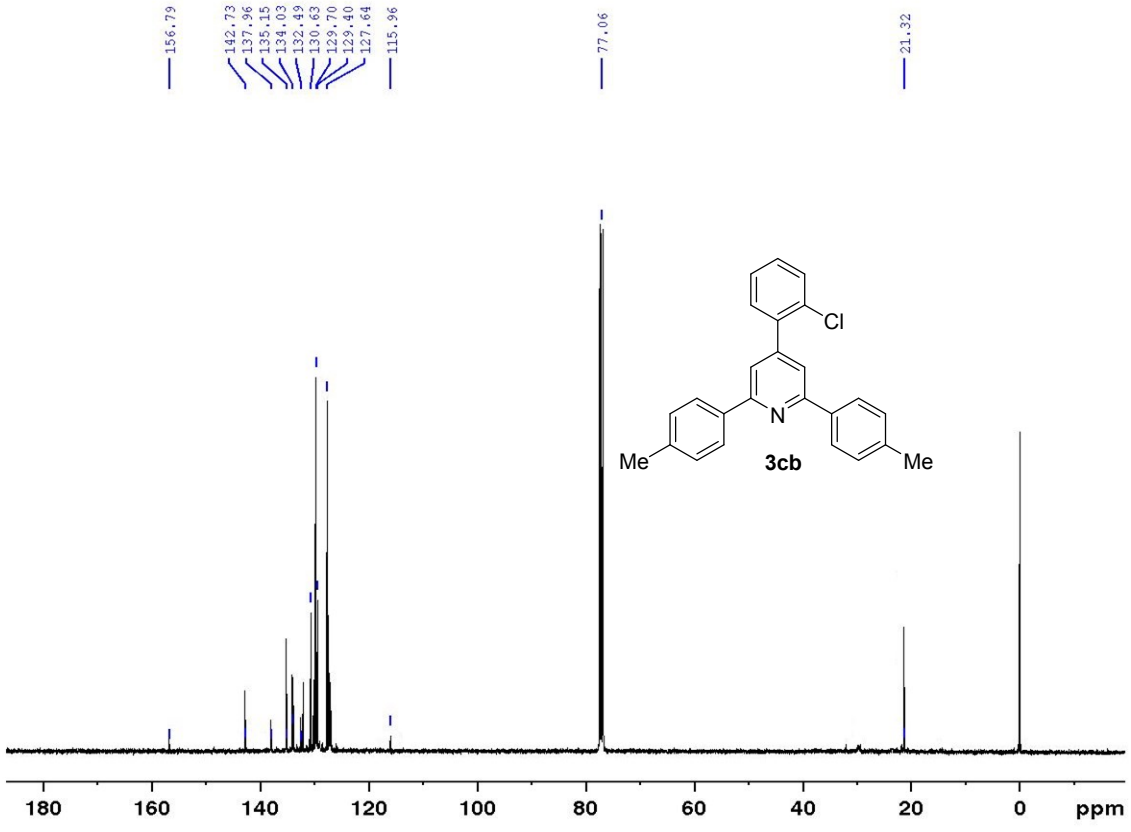
2.15
3.90
5.70
9
8
7
6
5
4
3
2
1
0
ppm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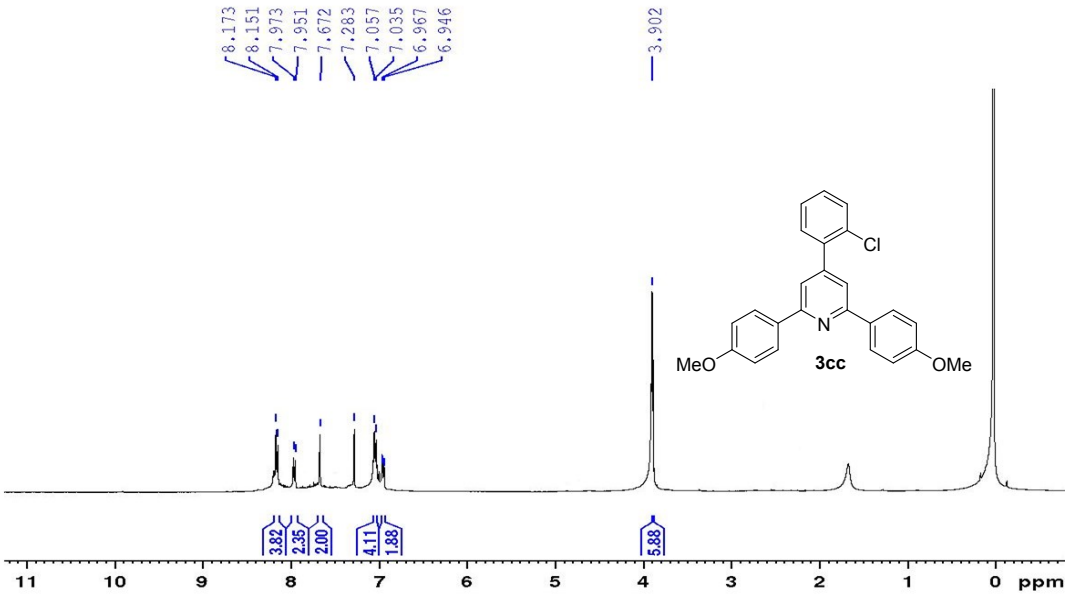
135.15
134.03
132.49
130.63
129.70
129.40
127.64
115.96
77.06
21.32
Cl
N
Me
Me
3cb
180
160
140
120
100
80
60
40
20
0
ppm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7.672
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7.057
7.035
6.967
6.946
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Cl
N
MeO
OMe
3cc
3.82
2.35
2.00
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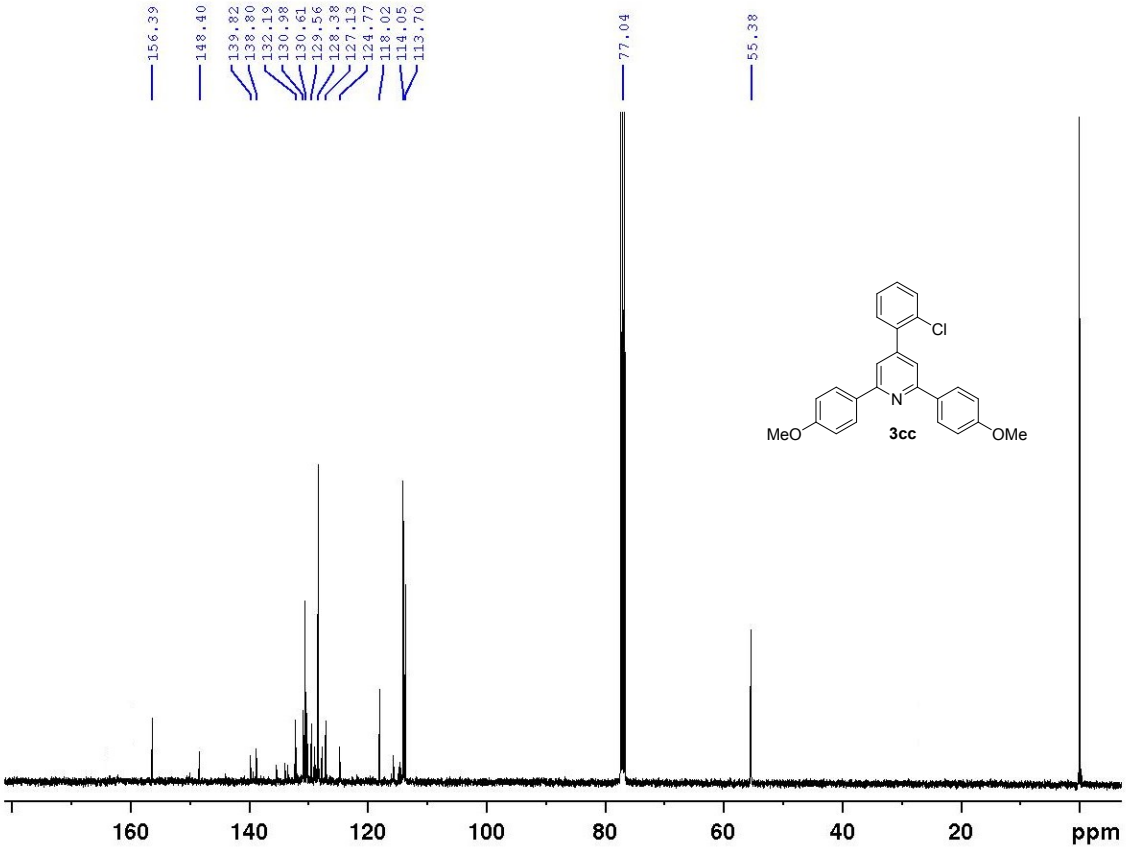
1.88
5.88
11
10
9
8
7
6
5
4
3
2
1
0
ppm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132.19
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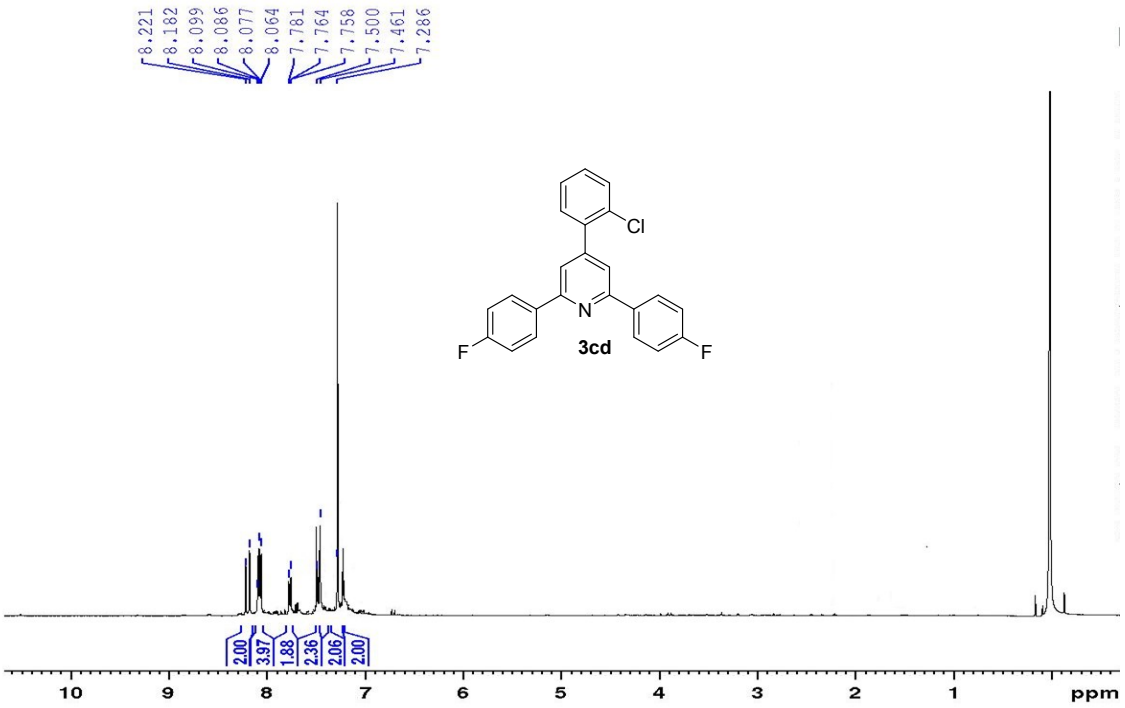
130.61
129.56
128.38
127.13
124.77
118.02
114.05
113.70
77.04
55.38
Cl
N
MeO
OMe
3cc
160
140
120
100
80
60
40
20
ppm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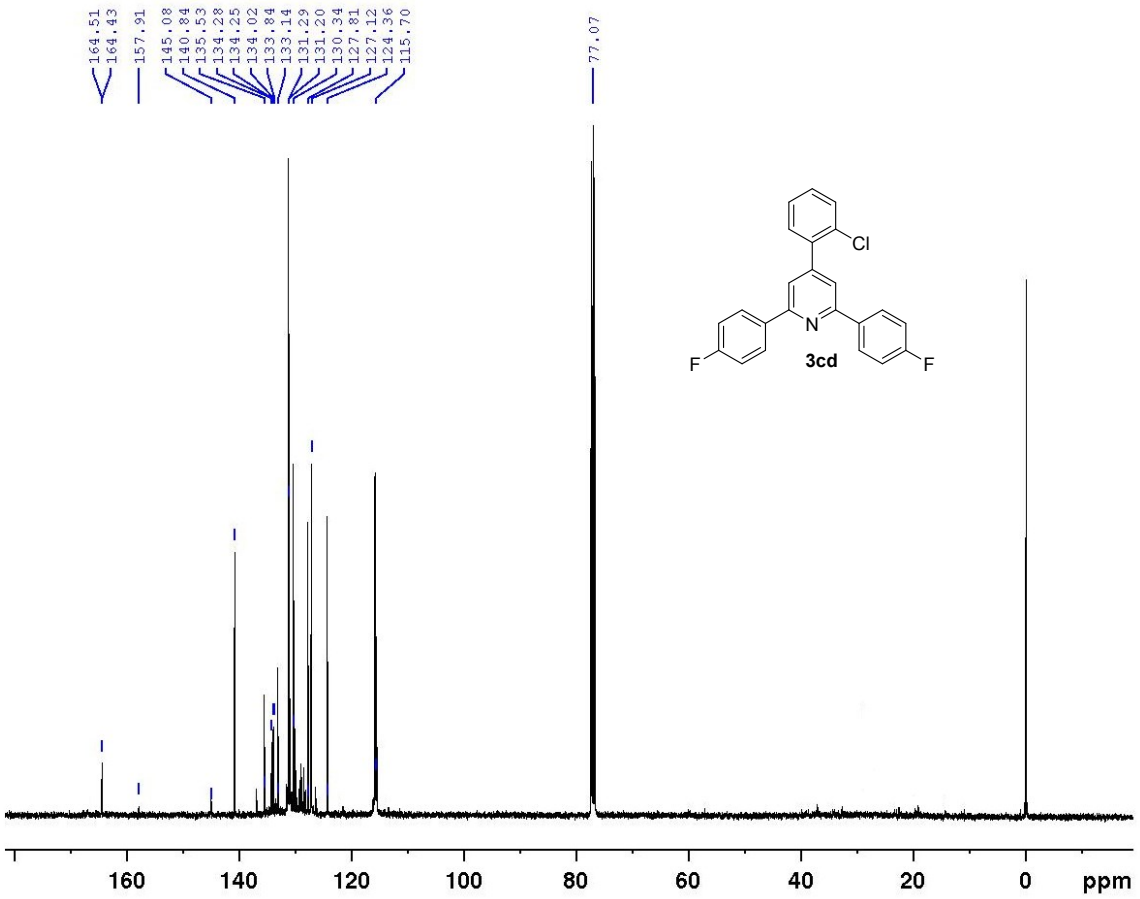
8.099
8.086
8.077
8.064
7.781
7.764
7.758
7.500
7.461
7.286
Cl
N
F
F
3cd
2.00
3.97
1.88
2.36
2.06
2.00
10
9
8
7
6
5
4
3
2
1
ppm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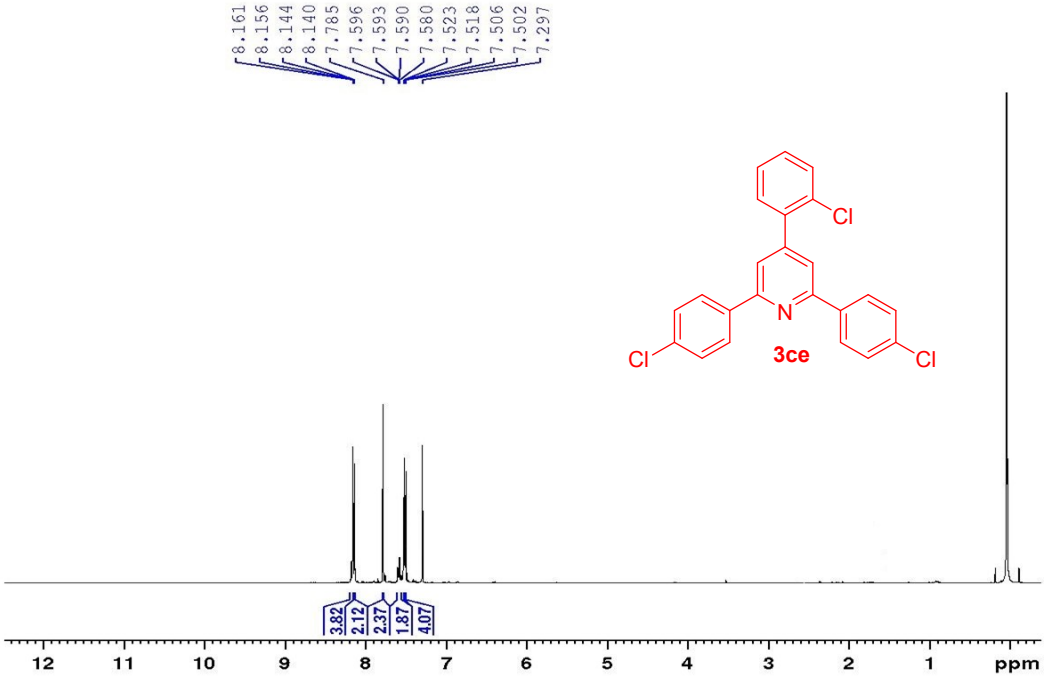
134.28
134.25
134.02
133.84
133.14
131.29
131.20
130.34
127.81
127.12
124.36
115.70
77.07
Cl
N
F
F
3cd
160
140
120
100
80
60
40
20
0
ppm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8.140
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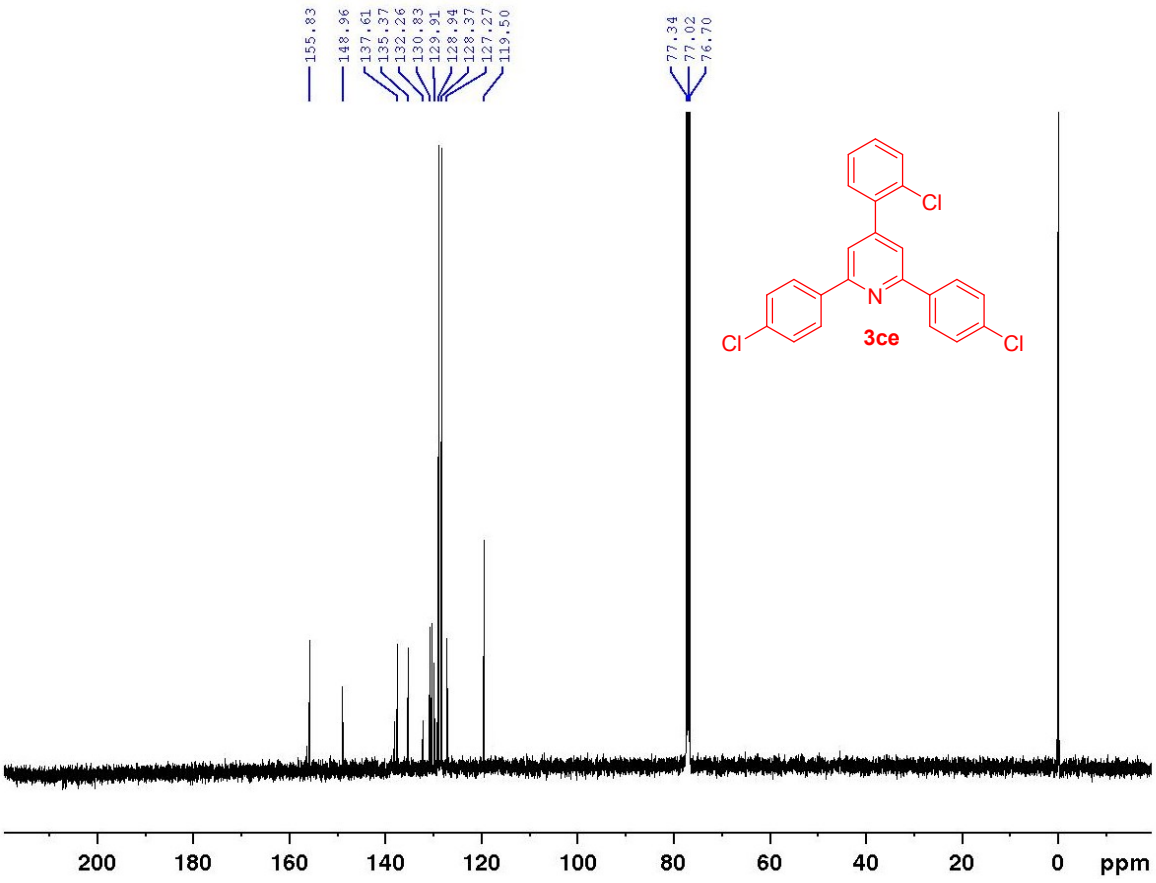
7.596
7.593
7.590
7.580
7.523
7.518
7.506
7.502
7.297
Cl
N
Cl
Cl
3ce
3.82
2.12
2.37
1.87
4.07
12
11
10
9
8
7
6
5
4
3
2
1
ppm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135.37
132.26
130.83
129.91
128.94
128.37
127.27
119.50
77.34
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Cl
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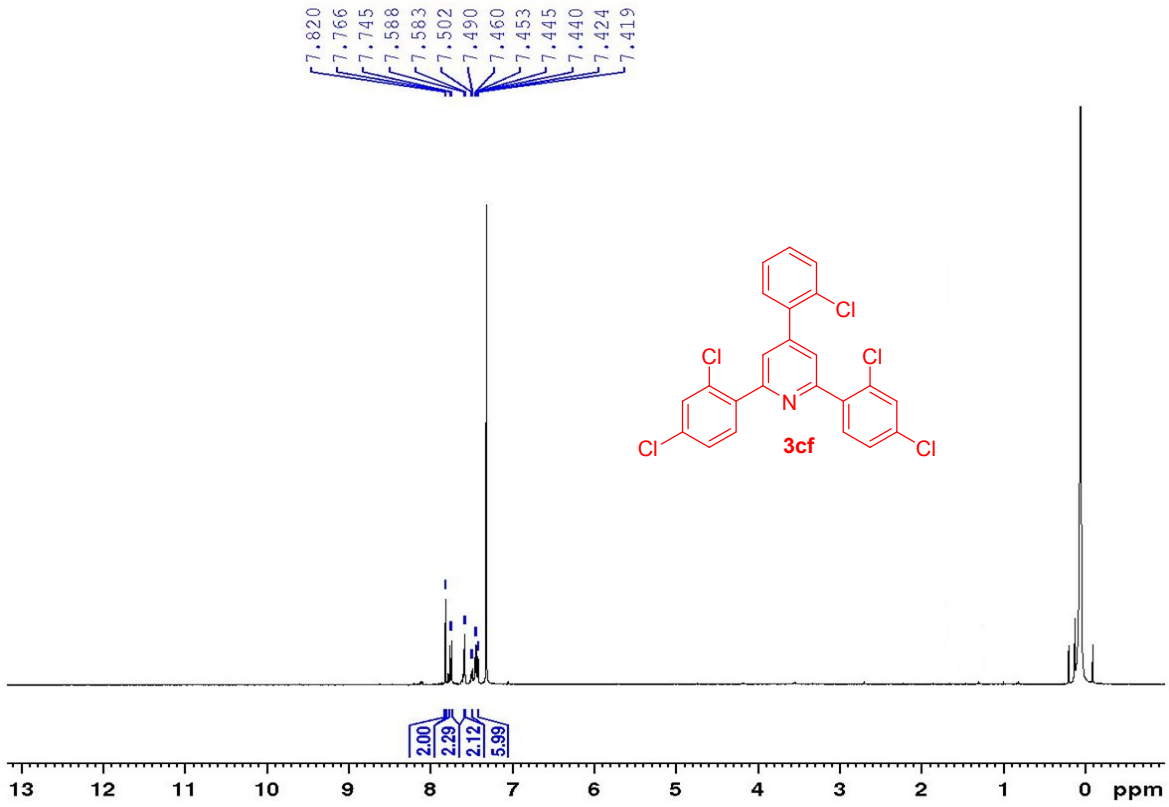
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Cl
Cl
Cl
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Cl
Cl
3cf
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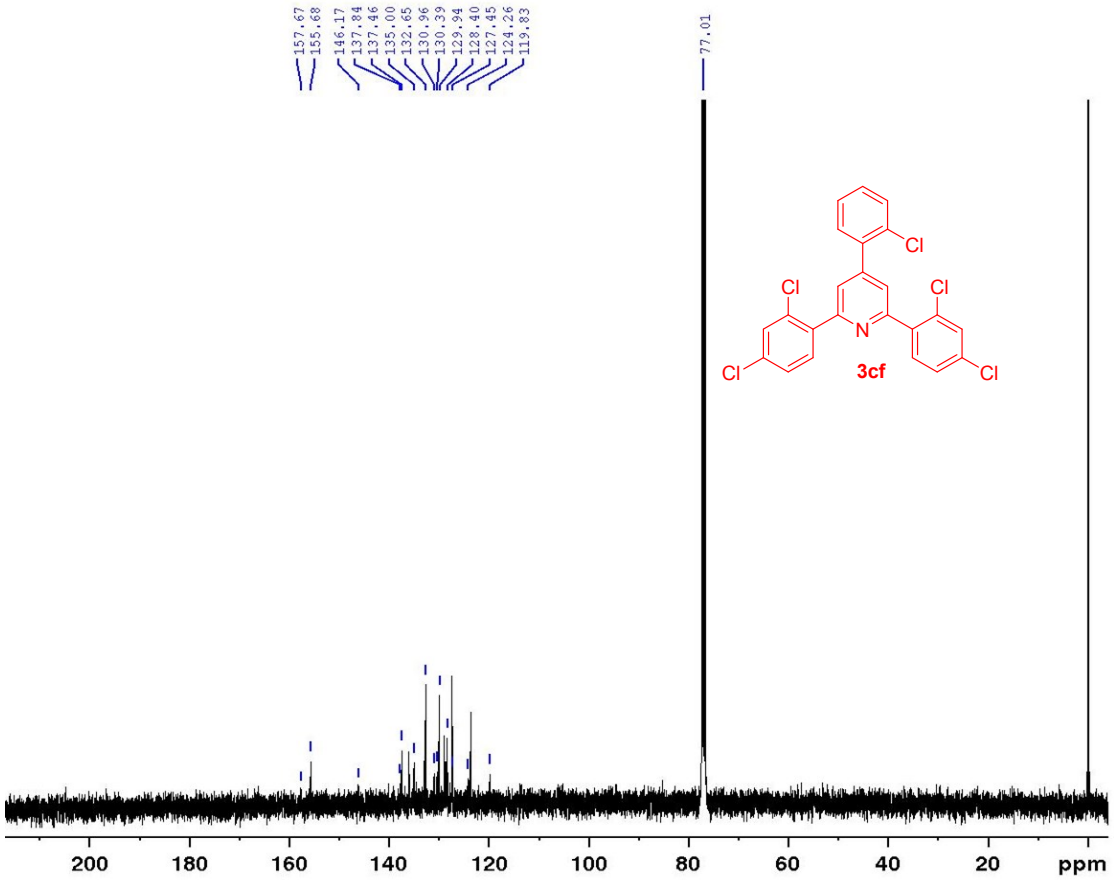
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127.45
124.26
119.83
77.01
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Cl
Cl
N
Cl
Cl
3cf
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140
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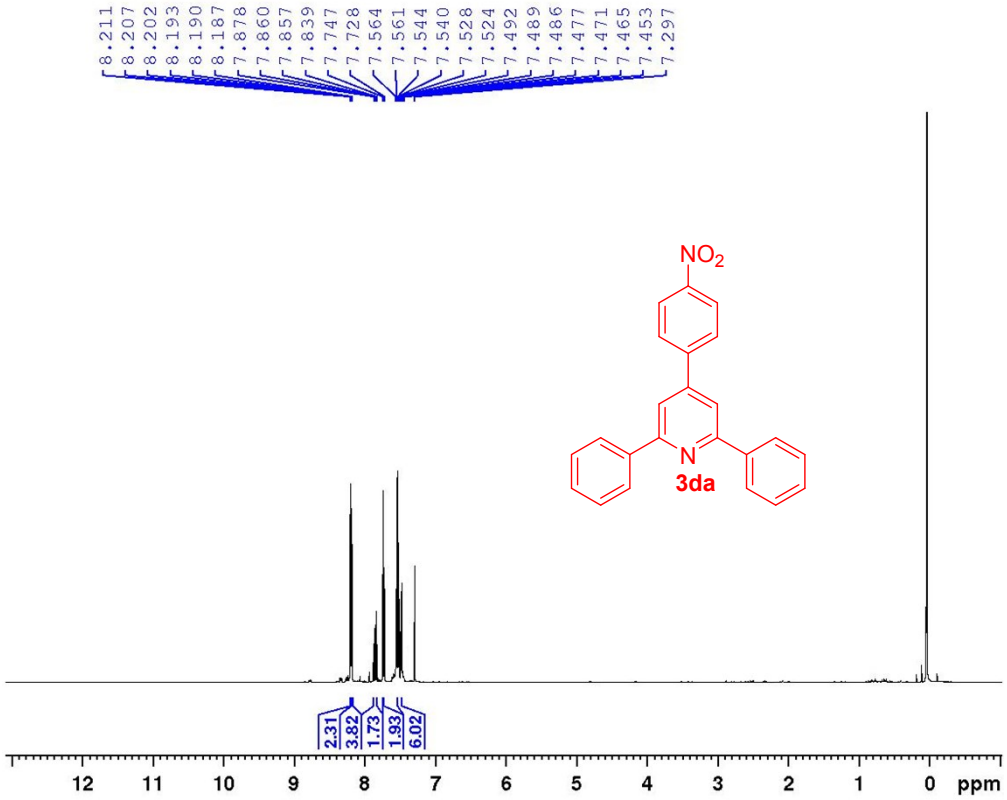
60
40
20
ppm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8.190
8.187
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7.860
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7.728
7.564
7.561
7.544
7.540
7.528
7.524
7.492
7.489
7.486
7.477
7.471
7.465
7.453
7.297
NO2
N
3da
2.31
3.82
1.73
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6.02
12
11
10
9
8
7
6
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4
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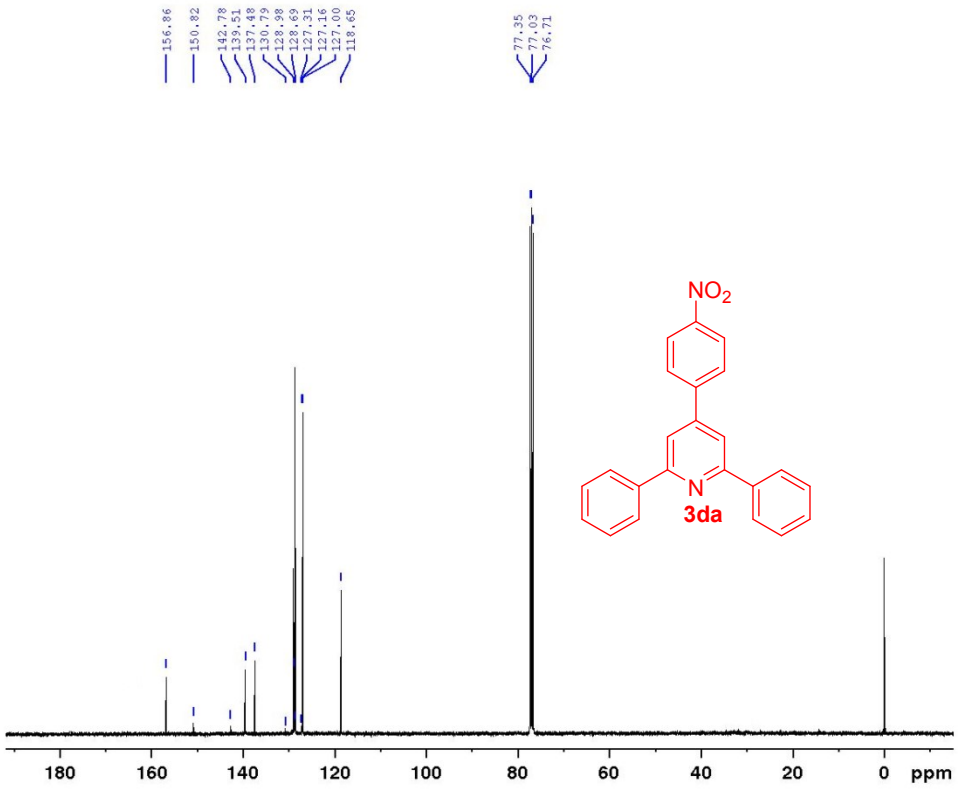
2
1
0
ppm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127.00
118.65
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76.71
NO2
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3da
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120
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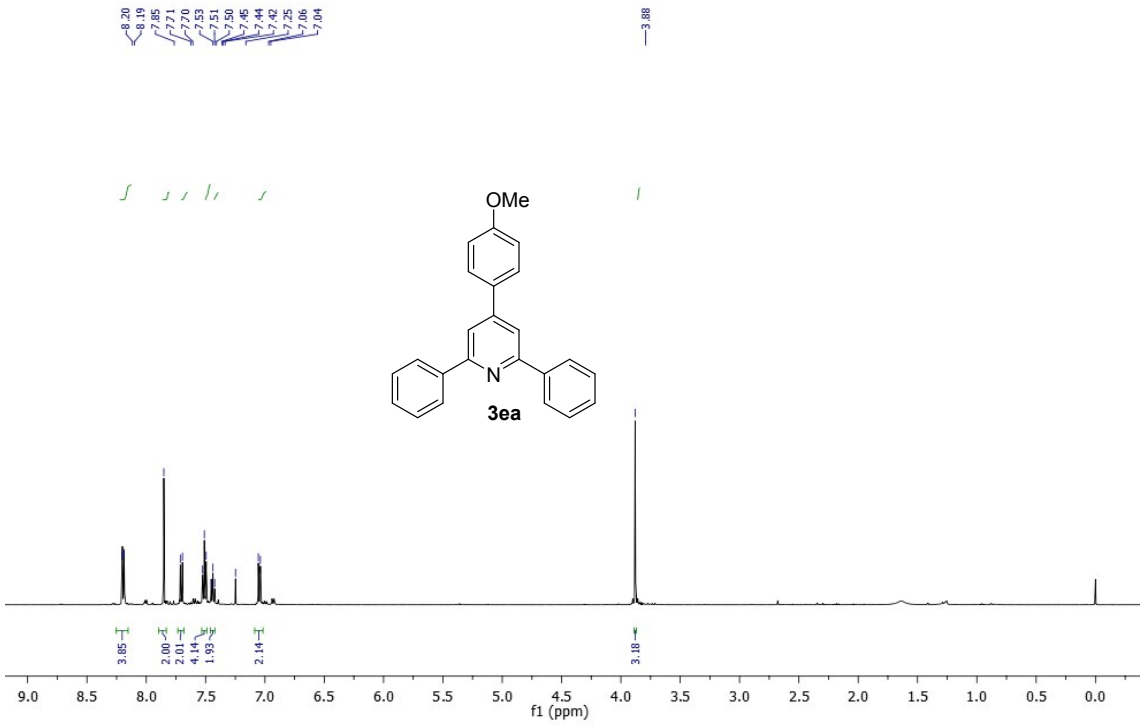
40
20
0
ppm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7.71
7.70
7.53
7.51
7.50
7.45
7.44
7.42
7.25
7.06
7.04
3.88
OMe
N
3ea
3.85
2.00
2.01
4.14
1.93
2.14
3.18
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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3.5
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2.5
2.0
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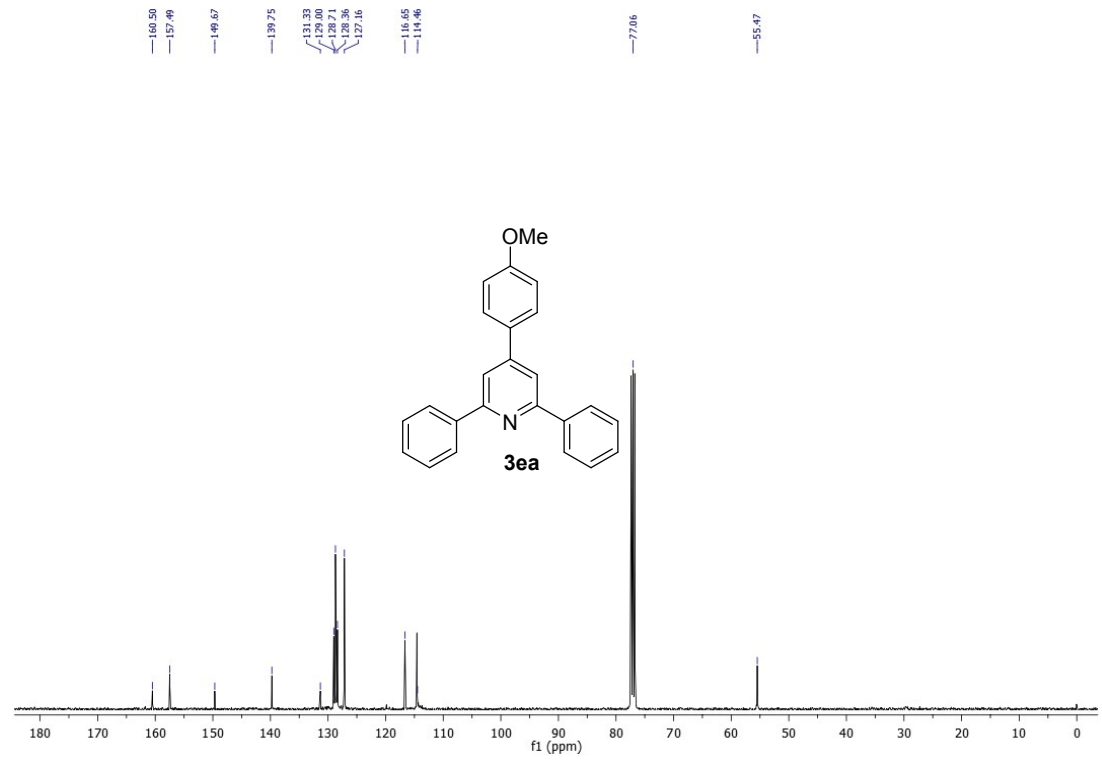
1.0
0.5
0.0
f1 (ppm)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129.00
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128.36
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116.65
114.46
77.06
55.47
OMe
N
3ea
180
170
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150
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130
120
110
100
90
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70
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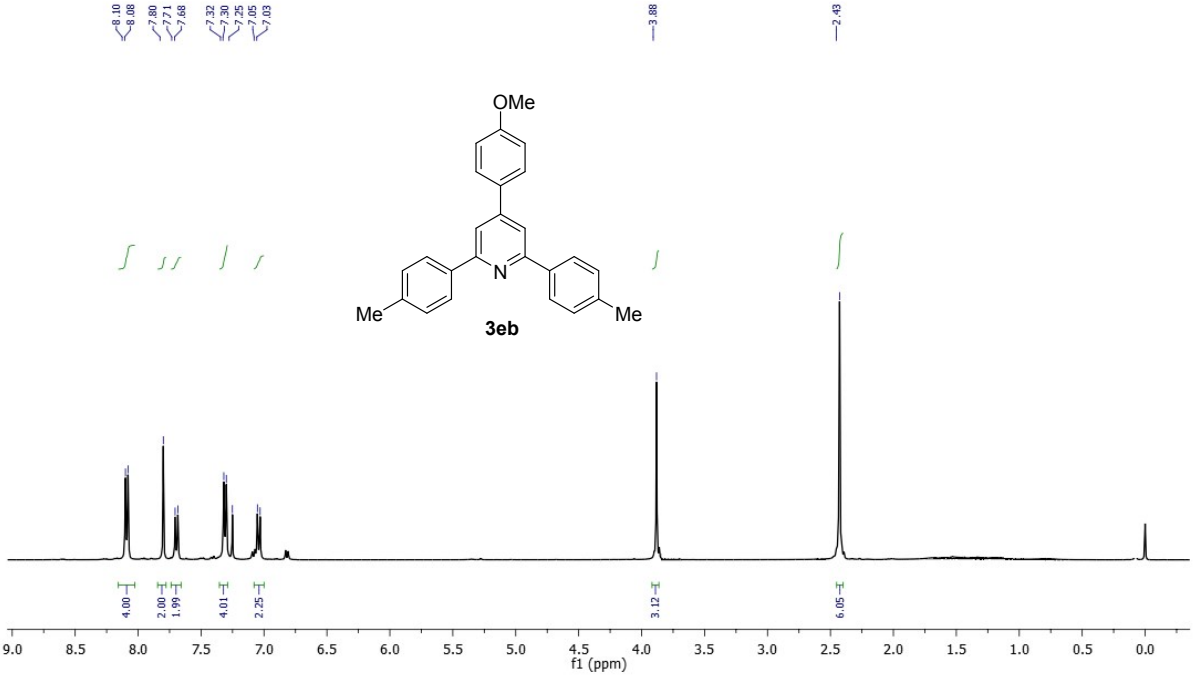
50
40
30
20
10
0
f1 (ppm)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7.80
7.71
7.68
7.32
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7.25
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7.03
3.88
2.43
OMe
N
Me
Me
3eb
4.00
2.00
1.99
4.01
2.25
3.12
6.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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2.0
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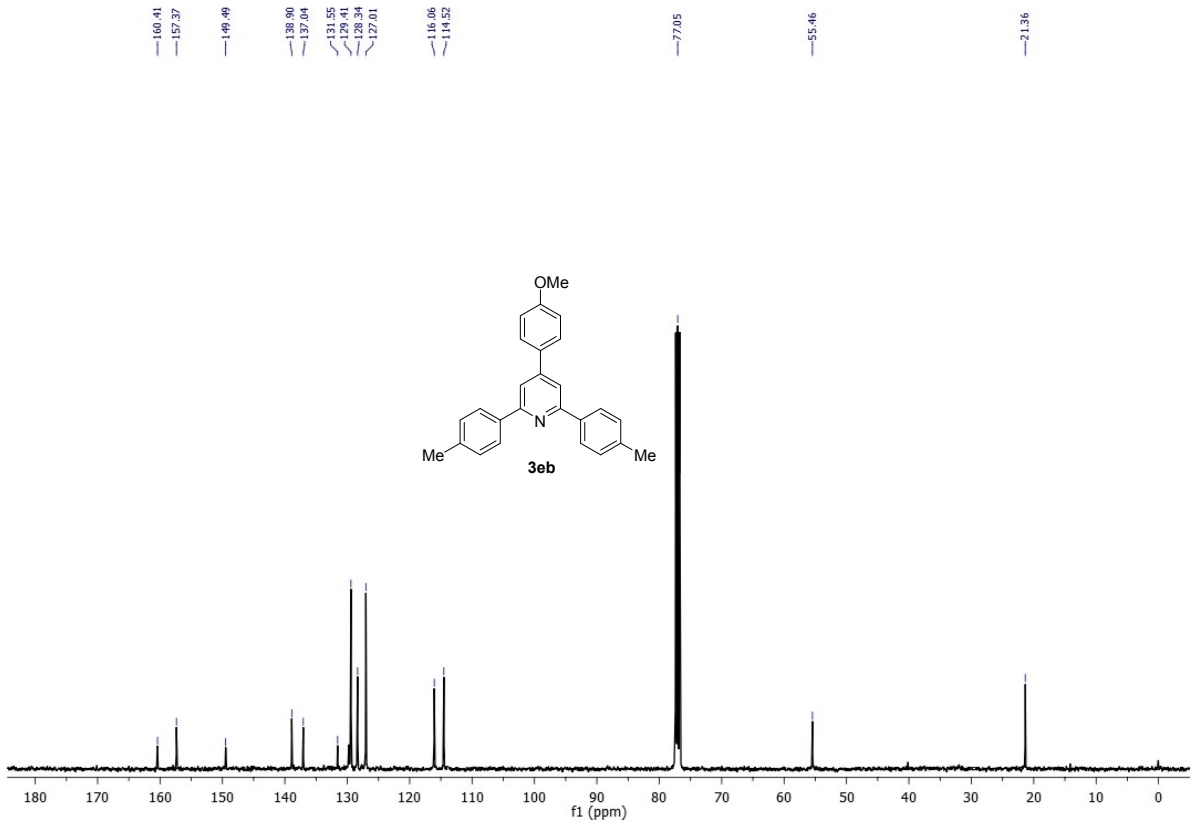
1.0
0.5
0.0
f1 (ppm)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157.37
149.49
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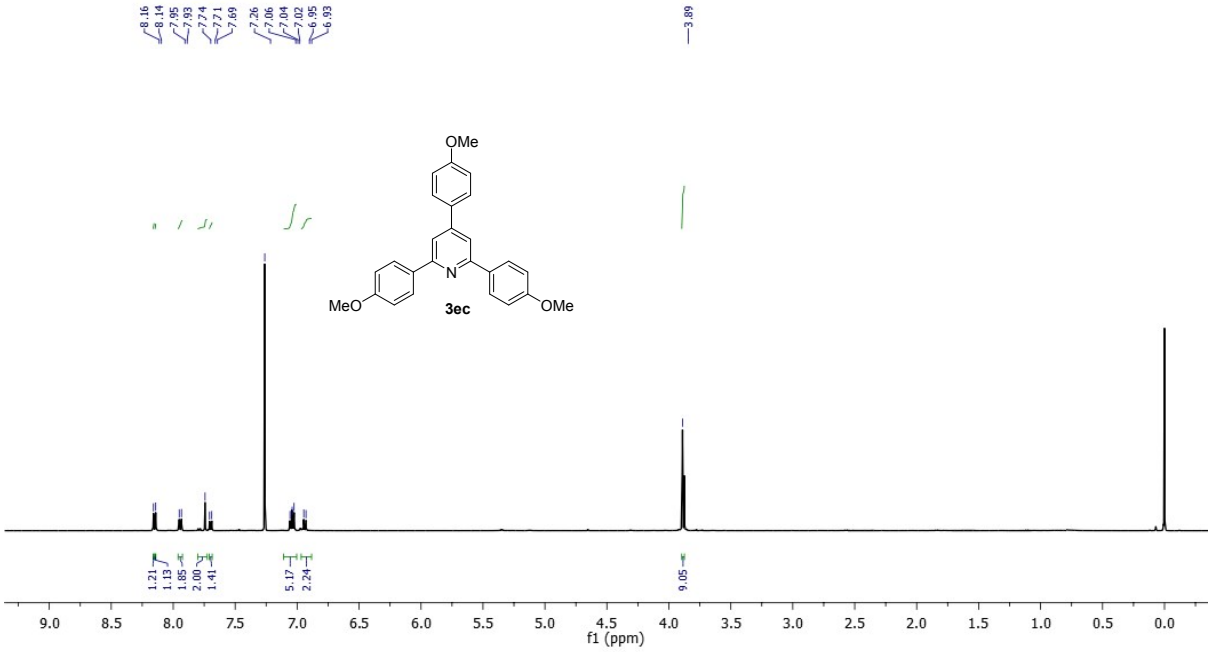
137.04
131.55
129.41
128.34
127.01
116.06
114.52
77.05
55.46
21.36
OMe
N
Me
Me
3eb
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.14
7.95
7.93
7.74
7.71
7.69
7.26
7.06
7.04
7.02
6.95
6.93
3.89
OMe
N
MeO
OMe
3ec
1.21
1.13
1.85
2.00
1.41
5.17
2.24
9.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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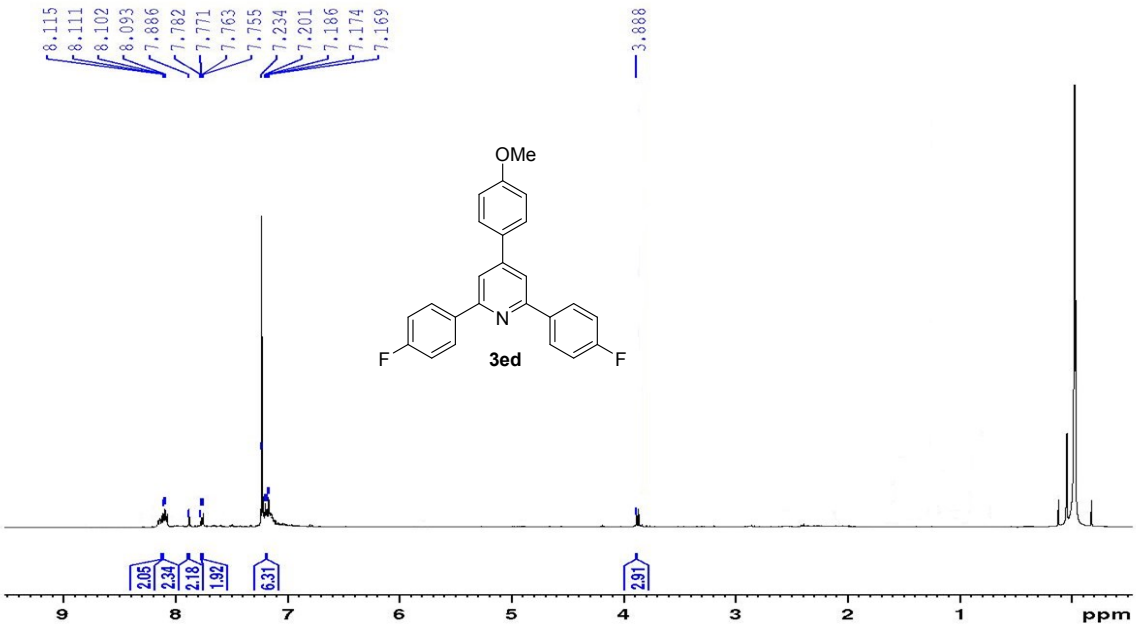
0.0
f1 (ppm)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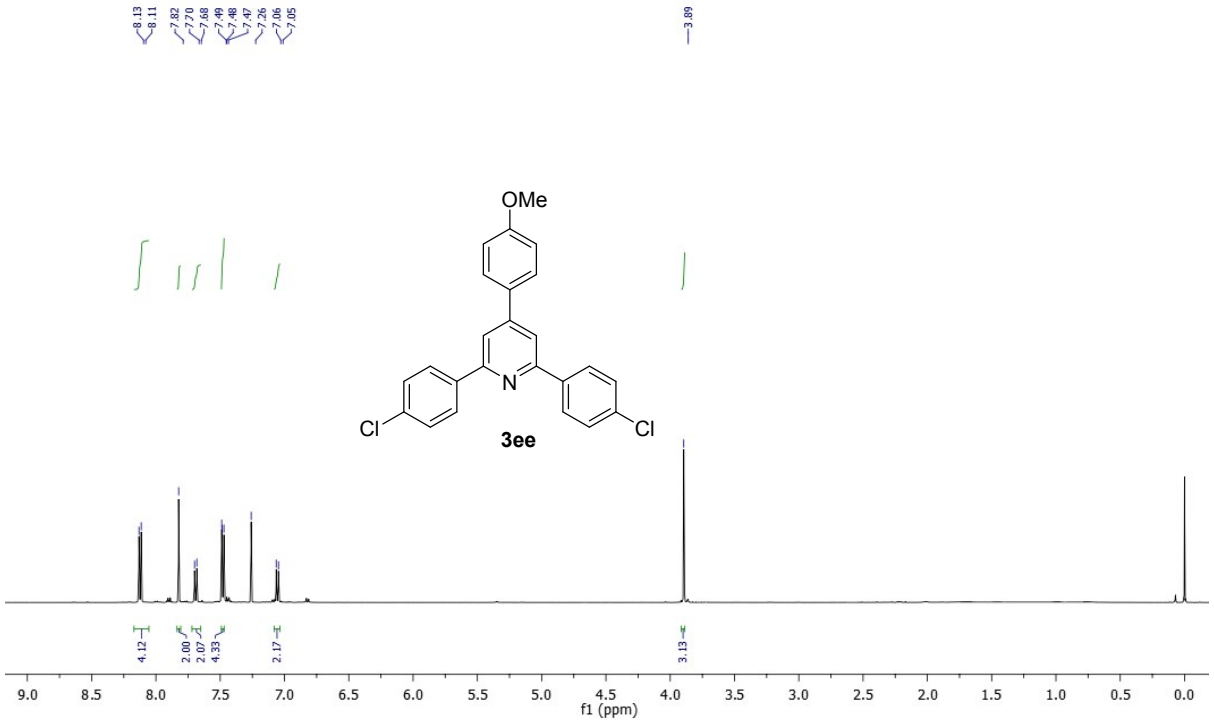
8.111
8.102
8.093
7.886
7.782
7.771
7.763
7.755
7.234
7.201
7.186
7.174
7.169
3.888
OMe
N
F
F
3ed
2.05
2.34
2.18
1.92
6.31
2.91
9
8
7
6
5
4
3
2
1
ppm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8.11
7.82
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7.68
7.49
7.48
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7.06
7.05
3.89
OMe
N
Cl
Cl
3ee
4.12
2.00
2.07
4.33
2.17
3.13
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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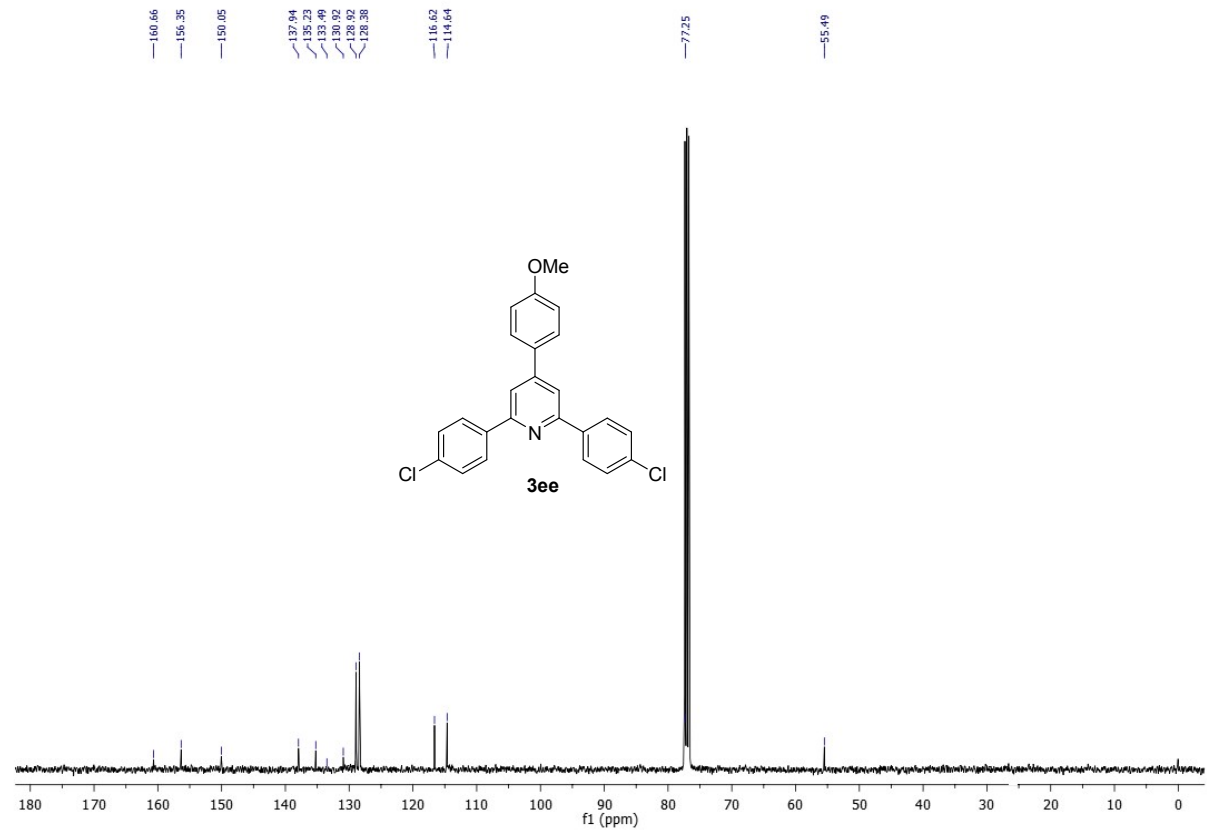
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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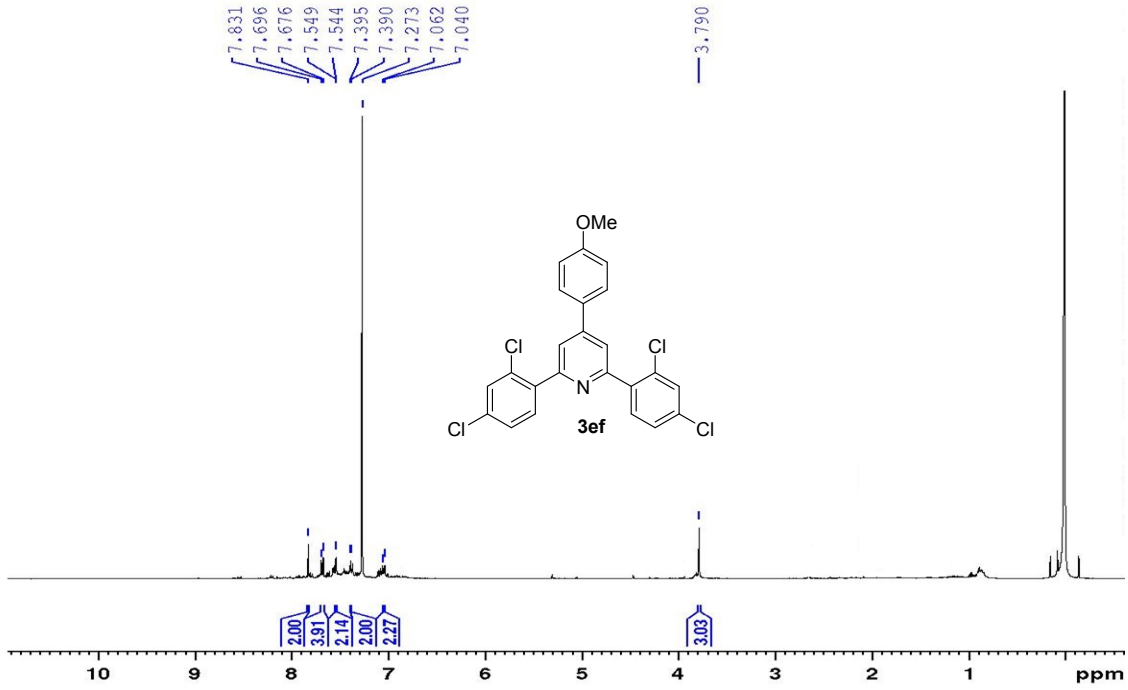
137.94
135.23
133.49
130.92
128.92
128.38
116.62
114.64
77.25
55.49
OMe
N
Cl
Cl
3ee
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



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