Electronic Supplementary Material (ESI) for Chemical Communications

$Pd(OAc)_2$ Catalyzed Direct Arylation of Electron-Deficient Arenes without Ligands or with Monoprotected Amino Acid Ligands Assistance

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General Experimental Section

All reactions were carried out under nitrogen atmosphere using standard Schlenk techniques. N, N-dimethylacetamide (DMA) was distilled under nitrogen from calcium hydride and stored under nitrogen. All other chemical reagents were obtained from commercial sources and used without further purification. Nuclear magnetic resonance (NMR) spectra were recorded using Bruker spectrometers operating at 400 MHz (^{1}H), 100 MHz (^{13}C) and 377 MHz (^{19}F) at room temperature in $CDCl_3$. High resolution mass spectrometry (HRMS) was performed using the Waters Micromass GCT Permier. A gas chromatography-mass spectra (Thermo Focus ISQ) was also used.

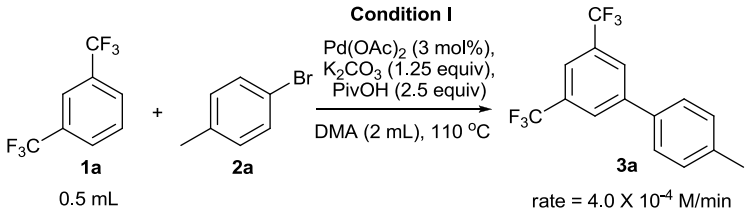
General Experimental Procedures

Under air atmosphere, $Pd(OAc)_2$ (0.006 mmol, 1.3 mg), mono-N-protected amino acid ligand (0.006 mmol), K_2CO_3 (0.25 mmol, 34 mg), pivalic acid (6-51 mg) and 1,3,5-trimethoxybenzene (0.2 mmol, 33.6 mg) were added into a dried Schlenk tube. The reaction vessel was evacuated and backfilled with nitrogen for three times. Then the arene (0.5 mL), aryl halide (0.2 mmol) and DMA (2 mL) were added by syringe. The reaction mixture was heated at 110 °C for 24 h. After cooling down, the mixture was diluted with petroleum ether (10 mL), filtered through a pad of silica gel, followed by washing the pad of the silica gel with the same solvent (20 mL). The filtrate was washed with water (15 mL × 3). The organic phase was dried over Na_2SO_4, filtered, and then concentrated under reduced pressure. The residue was analyzed by ^{1}H NMR spectroscopy directly, or purified by flash chromatography to afford the corresponding product.

Initial Rate Measurements

Under air atmosphere, $Pd(OAc)_2$ (0.006 mmol, 1.3 mg), Ac-Ile-OH (0.006 mmol, 1.0 mg, under condition II), K_2CO_3 (0.25 mmol, 34 mg), pivalic acid (6 or 51 mg) were added into a dried Schlenk tube. The reaction vessel was evacuated and backfilled with nitrogen for three times. Then the **1a** or **1a'** (0.5 mL), 4-bromotoluene **2a** (0.2 mmol, 34 mg) and DMA (2 mL) were added

by syringe. The reaction mixture was stirred at room temperature for 5 min, and then at 110 °C for the appropriate time. At regular intervals, one of the reactions would be removed from hot plate to 0 °C in an ice bath. A 2.0 N HCl solution (4 mL) and petroleum ether (10 mL) were added. Then the reaction mixture was filtered through a pad of silica gel, followed by washing the pad of the silica gel with the same solvent (20 mL). The filtrate was washed with water (15 mL × 3). The organic phase was dried over Na_2SO_4, filtered, and then concentrated under reduced pressure. The residue was analyzed by ^1H NMR spectroscopy directly. The conversion was determined by integration of the benzyl proton signals, which appears as singlets (approximately 2.28 ppm for **2a**, 2.42 ppm for **3a** and 2.40 ppm for **3a'**). Each reaction was repeated three times. The resulting data was plotted, and linear regression established the initial rate. The determinations of initial rate for the arylation of substrate **1a** under both conditions are shown in Figure S1 and Figure S2.



entry	time (min)	% conv. (T1)	% conv. (T2)	% conv. (T3)	average	Std. Dev.
1	0	0	0	0	0	0
2	10	2.4	1.2	2.6	2.1	0.8
3	20	10.0	9.8	7.5	9.1	1.4
4	30	12.7	12.9	10.0	11.9	1.6
5	40	20.5	16.2	21.6	19.4	2.9

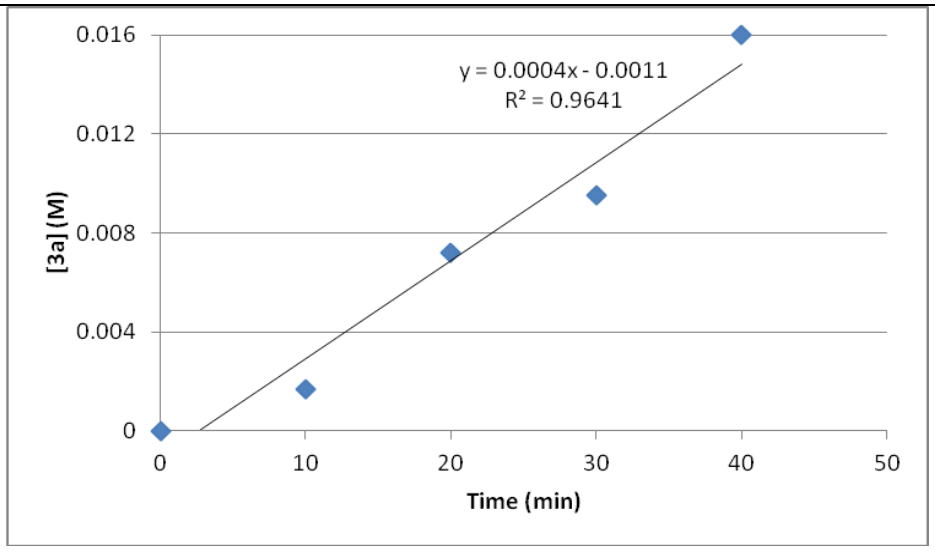
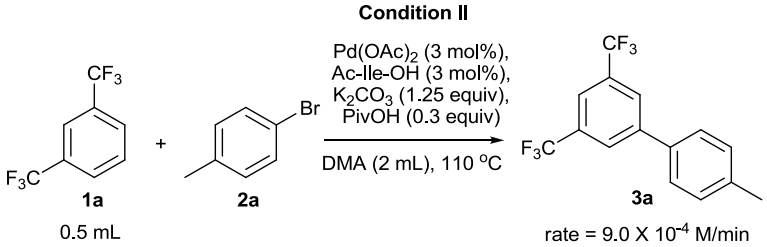


Figure S1: The initial rate data for arylation of substrate **1a** under condition I. Each data point represents the average of three trials.



entry	time (min)	% conv. (T1)	% conv. (T2)	% conv. (T3)	average	Std. Dev.
1	0	0	0	0	0	0
2	5	4.2	3.7	5.3	4.4	0.8
3	10	8.9	10.6	8.4	9.3	1.2
4	15	21.8	14.4	14.7	17	4.2
5	20	29.9	16.4	25.2	23.1	6.9

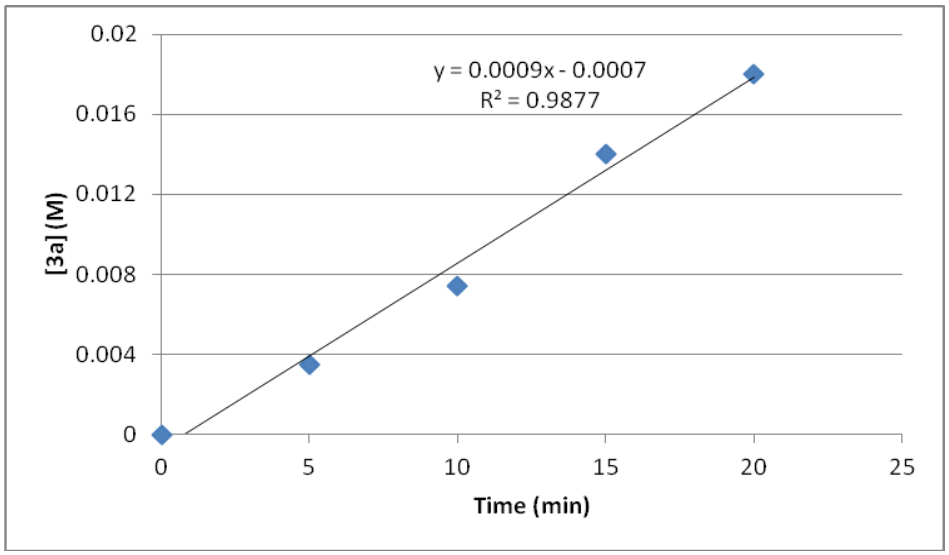
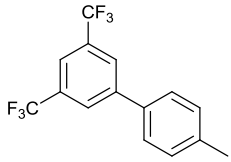


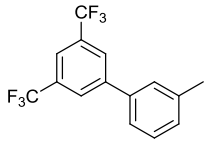
Figure S2: The initial rate data for arylation of substrate **1a** under condition II. Each data point represents the average of three trials.

Experimental Data



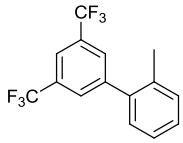
4'-Methyl-3,5-bis(trifluoromethyl)biphenyl (**3a**)[1,2]

^{1}H NMR (500 MHz, $CDCl_3$): δ 7.99 (s, 1H), 7.82 (s, 1H), 7.50 (d, J = 10.5 Hz, 2H), 7.30 (d, J = 10.0 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.32, 139.06, 135.42, 132.13 (q, J = 32.9 Hz), 130.06, 127.11, 127.03, 123.51 (d, J = 271.5 Hz), 120.67-120.56 (m), 21.22; ^{19}F NMR (377 MHz, $CDCl_3$): δ -61.72 (s, 6F); GC/MS: M/Z = 304. 23.



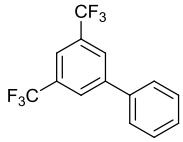
3'-Methyl-3,5-bis(trifluoromethyl)biphenyl (**3b**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.00 (s, 2H), 7.84 (s, 1H), 7.40 (s, 3H), 7.26 (s, 1H), 2.45 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.45, 139.06, 138.12, 132.18 (q, J = 33.0 Hz), 129.60, 129.16, 127.93, 127.20, 124.76 (d, J = 271.2 Hz), 124.34, 120.77 (m), 21.47; ^{19}F NMR (377 MHz, $CDCl_3$): δ -62.75 (s, 6F); HRMS (EI) calcd for $C_{15}H_{10}F_6$: 304.0687 (M^+), found: 304.0688.



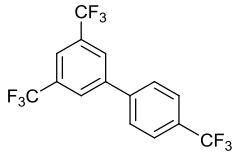
2-Methyl-3',5'-bis(trifluoromethyl)biphenyl (**3c**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (s, 1H), 7.80 (s, 2H), 7.29 (m, 3H), 7.24 (d, J = 7.2 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.94, 138.81, 135.15, 131.51 (q, J = 33 Hz), 130.79, 129.59, 129.34, 128.65, 126.28, 123.38 (d, J = 271.2 Hz), 120.76 (m), 20.20; ^{19}F NMR (377 MHz, $CDCl_3$): δ -62.69 (s, 6F); HRMS (EI) calcd for $C_{15}H_{10}F_6$: 304.0687 (M^+), found: 304.0690.



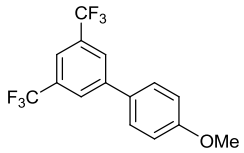
3,5-Bis(trifluoromethyl)biphenyl (**3d**)[3, 4]

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.43 (m, 3H), 7.59 (m, 2H), 7.85 (s, 1H), 8.01 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.30, 138.22, 132.24 (q, J = 33.2 Hz), 129.26, 128.86, 127.23, 124.72, 121.94, 120.88 (m); ^{19}F NMR (377 MHz, $CDCl_3$): δ -62.73(s, 6F); GC/MS: M/Z = 290.12.



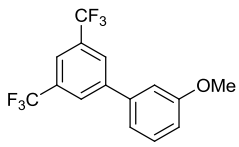
3,4',5-Tris(trifluoromethyl)biphenyl (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (s, 1H), 7.93 (s, 2H), 7,77 (d, J = 8.0 Hz, 2H), 7.72 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.87, 141.69, 131.96 (q, J = 32.8 Hz), 130.44 (q, J = 32.8 Hz), 127.69, 127.39, 126.27, 126.24, 125.96 (d, J = 141.8 Hz), 121.83; ^{19}F NMR (377 MHz, $CDCl_3$): δ - 78.20 (s, 3F), -78.40 (s, 6F); HRMS (EI) calcd for $C_{15}H_7F_9$: 358.0404 (M^+), found: 358.0401.



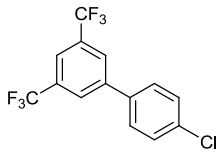
4'-Methoxy-3,5-bis(trifluoromethyl)biphenyl (**3f**)[2]

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (s, 2H), 7.80 (s, 1H), 7.57 (d, J = 8.4 Hz, 2H), 7.04 (d, J = 8.4 Hz, 2H),3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.33, 142.88, 132.18 (q, J = 32.8 Hz), 130.60, 128.37, 126.62, 124.79 (d, J = 271.6 Hz), 120.18 (m), 114.69, 55.40; ^{19}F NMR (377 MHz, $CDCl_3$): δ -62.75 (s, 6F); GC/MS: M/Z = 320.13.



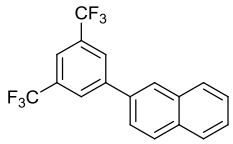
3'-Methoxy-3,5-bis(trifluoromethyl)biphenyl (**3g**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 3.89 (s, 3H), 6.98 (d, *J*=8.4 Hz, 1H), 7.10 (s, 1H), 7.17 (d, *J*=7.6 Hz, 1H), 7.42 (t, *J*=7.6, 1H), 7.99 (s.2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.24, 143.18, 139.66, 131.55 (q, *J*=32.4 Hz), 130.34, 127.25, 124.72 (d, *J*=252.8 Hz), 121.01 (m), 119, 62, 114.04, 113.11, 55.41; ^{19}F NMR (377 MHz, $CDCl_3$): δ - 62.75 (s, 6F); HRMS (EI) calcd for $C_{15}H_{10}F_6O$: 320.0636 (M^+), found: 320.0634.



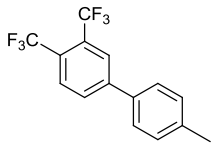
4'-Chloro-3,5-bis(trifluoromethyl)biphenyl (**3h**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (s, 2H), 7.87 (s, 1H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.49 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.07, 136.61, 135.25, 131.78 (q, *J* = 33.2 Hz), 129.49, 128.49, 127.02, 124.62 (q, *J* = 271.2 Hz), 121.20 (m); ^{19}F NMR (377 MHz, $CDCl_3$): δ – 62.78 (s, 6F); HRMS (EI) calcd for $C_{14}H_7ClF_6$: 324.0140 (M^+), found: 324.0138.



2-(3,5-Bis(trifluoromethyl)phenyl)naphthalene (**3i**)

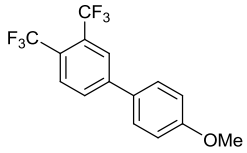
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (s, 2H), 8.07 (s, 1H), 8.04 (m, 4H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 143.22, 140.36, 135.40, 133.47, 133.16, 132.34 (q, *J* = 33.2 Hz), 129.18, 128.36, 127.73, 127.41, 126.89, 126.56, 124.67, 122.60 (d, *J* = 54.2 Hz), 120.91(m); ^{19}F NMR (377 MHz, $CDCl_3$): δ -62.66; HRMS (EI) calcd for $C_{18}H_{10}F_6$: 340.0687 (M^+), found: 340.0684.



4'-Methyl-3,4-bis(trifluoromethyl)biphenyl (**3j**)

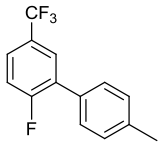
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (s, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 7.2 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ

145.14, 139.14, 135.25, 129.95, 129.88, 128.48, 128.42, 127.07, 126.34, 126.28, 126.22, 126.17, 21.17; ^{19}F NMR (377 MHz, $CDCl_3$): δ -59.00 (s, 3F), -59.33 (s, 3F); HRMS (EI) calcd for $C_{15}H_{10}F_6$: 304.0687 (M^+), found: 304.0685.



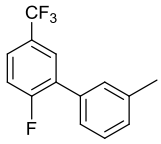
4'-Methoxy-3,4-bis(trifluoromethyl)biphenyl (**3k**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.99 (s, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 7.2 Hz, 2H), 7.03 (d, J = 8.4 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.46, 144.77, 130.46, 129.49, 128.40, 125.98, 125.92, 125.86, 125.81, 124.23, 121.52, 114.67, 55.39; ^{19}F NMR (377 MHz, $CDCl_3$): δ -59.97 (s, 3F), -59.32 (s, 3F); HRMS (EI) calcd for $C_{15}H_{10}F_6O$: 320.0636 (M^+), found: 320.0641.



2-Fluoro-4'-methyl-5-(trifluoromethyl)biphenyl (**3l**)

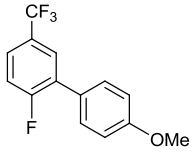
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, J = 5.2 Hz, 1H), 7.62 (m, 1H), 7.49 (d. J = 6.8 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.28 (s, 1H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.50 (d, J = 251.3 Hz), 138.40, 131.36, 129.88 (d, J = 14.8 Hz), 129.39, 128.81, 128.13 (m), 126.96 (d, J = 33.0 Hz), 125.88 (m), 123.84 (d, J = 270.6 Hz), 116.70 (d, J = 24.3 Hz), 21.20; ^{19}F NMR (377 MHz, $CDCl_3$): δ -61.85 (s, 3F), -112.48 (s, 1F); HRMS (EI) calcd for $C_{14}H_{10}F_4$: 254.0719 (M^+), found: 254.0720.



2-Fluoro-3'-methyl-5-(trifluoromethyl)biphenyl (**3m**)

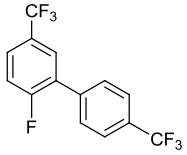
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, J = 7.2 Hz, 1H), 7.57 (s, 1H), 7.35 (s, 3H), 7.23 (d, J = 8.4 Hz, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.48 (d, J = 252 Hz), 138.38, 134.23,

130.06 (d, J = 14.9 Hz), 129.61, 129.17, 128.55, 128.26, 127.14, 126.06, 125.19, 122.48, 116.70 (d, J = 24.7 Hz), 21.44; ^{19}F NMR (377 MHz, $CDCl_3$): δ -77.20 (s, 3F), -140.18 (s, 1F); HRMS (EI) calcd for $C_{14}H_{10}F_4$: 254.0719 (M^+), found: 254.0714.



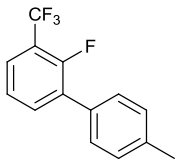
2-Fluoro-4'-methoxy-5-(trifluoromethyl)biphenyl (**3n**)

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, J = 5.2 Hz, 1H), 7.54 (s, 1H), 7.49 (d, J = 7.2 Hz, 2H), 7.22 (d, J = 9.2 Hz, 1H), 7.00 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.53 (d, J = 250.5 Hz), 159.89, 130.23, 129.64 (d, J = 14.1 Hz), 128.00, 126.69, 125.68, 125.60, 123.95 (d, J = 270.5 Hz), 116.81 (d, J = 23.5 Hz), 114.26, 55.46; ^{19}F NMR (377 MHz, $CDCl_3$): δ -77.21 (s, 3F), -140.67 (s, 1F); HRMS (EI) calcd for $C_{14}H_{10}F_4O$: 270.0668 (M^+), found: 270.0670.



2-Fluoro-4',5-bis(trifluoromethyl)biphenyl (**3o**)

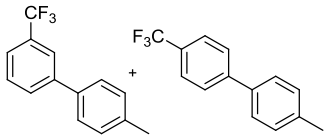
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (s, 1H), 7.73 (s, 2H), 7.67 (d, J = 8.0 Hz, 3H), 7.33-7.28 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.41 (d, J = 252.9 Hz), 137.82, 130.56 (d, J = 32.1 Hz), 129.37, 128.51 (d, J = 14.5 Hz), 128.13, 127.18, 125.66, 125.63, 125.16 (d, J = 36.7 Hz), 122.45 (d, J = 36.2), 117.04 (d, J = 24 Hz); ^{19}F NMR (377 MHz, $CDCl_3$): δ -77.33 (s, 3F), -78.21 (s, 3F), -140.02 (s, 1F); HRMS (EI) calcd for $C_{14}H_7F_7$: 308.0436 (M^+), found: 308.0440.



2-Fluoro-4'-methyl-3-(trifluoromethyl)biphenyl (**3p**)

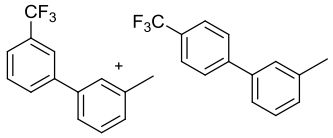
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.54 (m, 2H), 7.43 (d, J = 7.6 Hz, 2H), 7.28 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 138.41, 134.70, 131.45, 130.76 (d, J = 13.3 Hz), 129.89 (d, J

= 7.7 Hz), 129.45 , 129.02, 127.02 (d, *J* = 11.9 Hz), 125.87 (d, *J* = 4.0 Hz), 124.13, 121.54, 21.31; ^{19}F NMR (377 MHz, $CDCl_3$): δ -76.45 (s, 3F), -149.54 (s, 1F); HRMS (EI) calcd for $C_{14}H_{10}F_4$: 254.0719 (M^+), found: 254.0717.



4'-Methyl-3-(trifluoromethyl)biphenyl (**3q**) and 4-methyl-4'-(trifluoromethyl)biphenyl (**3q'**) [5]

^{1}H NMR(400 MHz, $CDCl_3$): δ 7.83 (s, 1H), 7.77 (m, 1H), 7.68 (s, 1H), 7.58 (m, 1H), 7.50 (m, 2H), 7.30 (d, *J* = 7.6, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.7, 141.91, 138.12, 137.93, 136.85, 130.18, 129.69, 129.15, 127.15, 127.09, 126.99, 125.66 (m), 123.71 (m); GC/MS: M/Z = 236.18.



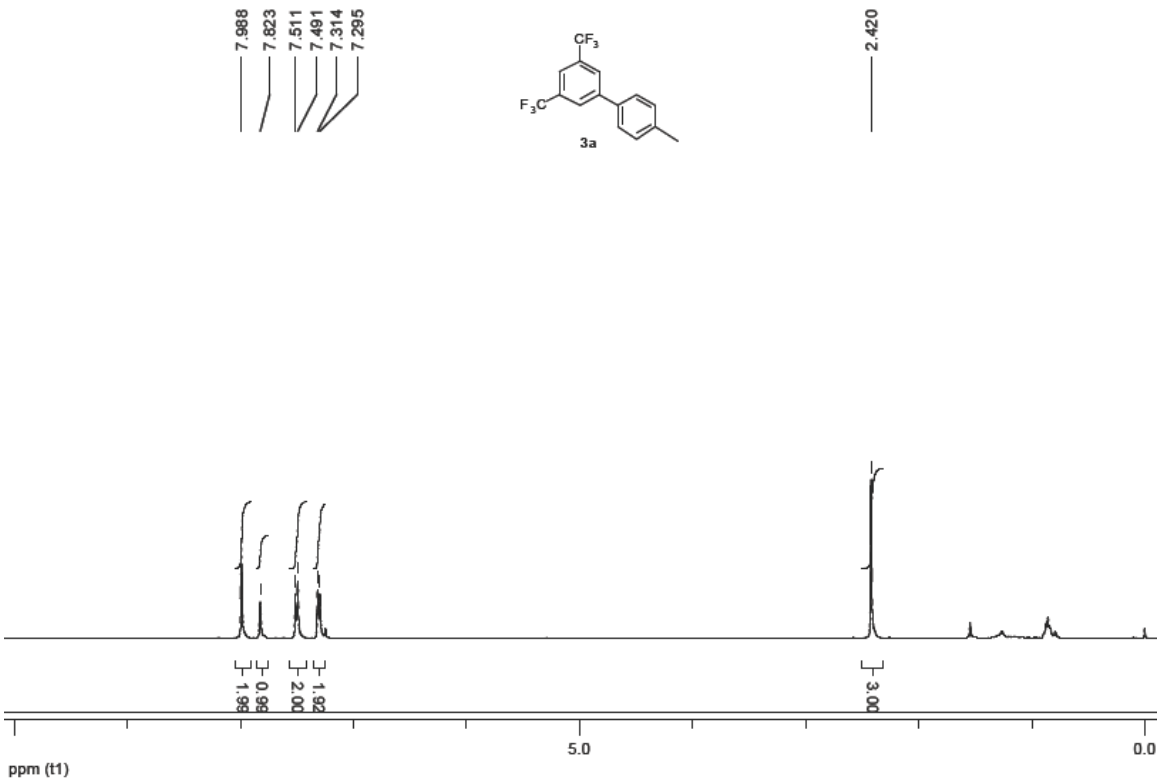
3-methyl-3'-(trifluoromethyl)biphenyl (**3r**) and 3-methyl-4'-(trifluoromethyl)biphenyl (**3r'**)[6]

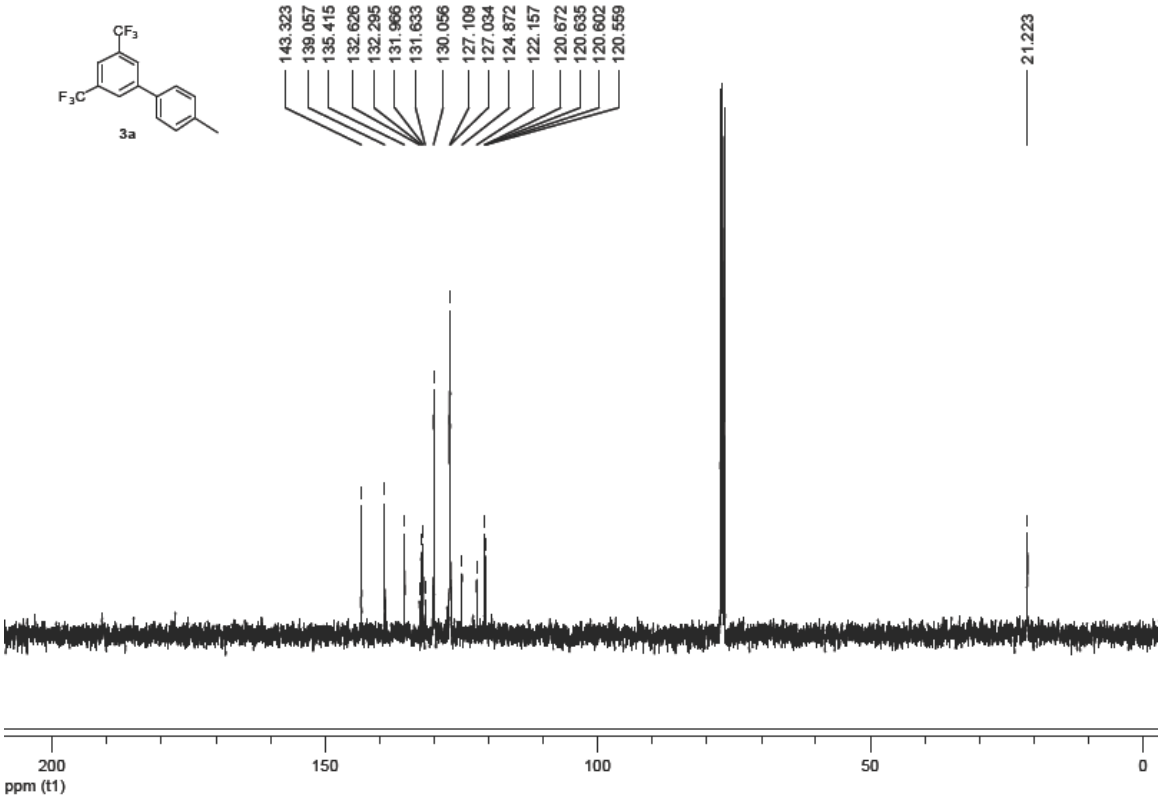
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (s, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.68 (s, 1H), 7.60 (m, 1H), 7.40 (m, 3H), 7.22 (d, *J* = 6.4 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.12, 139.73, 138.66, 130.41, 129.13, 128.88, 128.75, 128.02, 127.93, 127.39, 125.67 (m), 124.37, 124.28, 123.93 (m), 21.48; GC/MS: M/Z = 236.20.

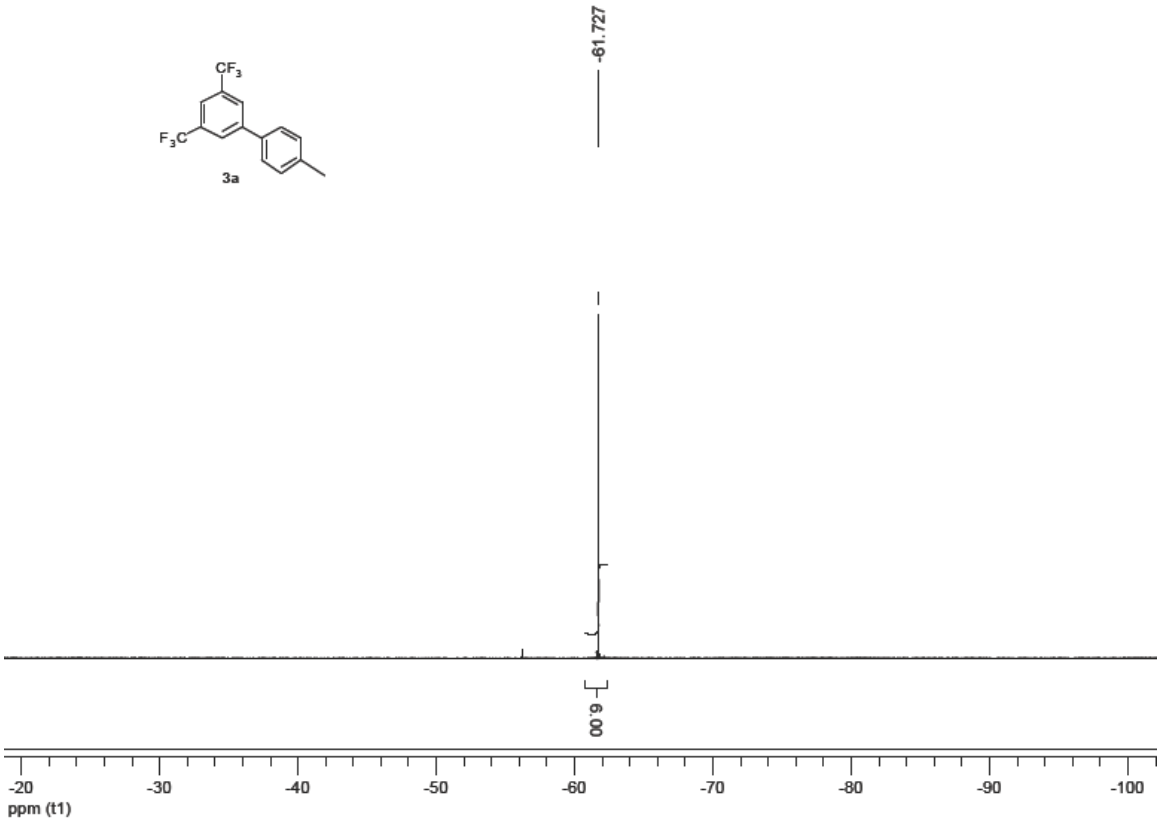
References for known compounds

(1) H.A.Chiong, Q. -N. Pham and O. Daugulis, *J. Am. Chem.Soc.*, 2007, **129**, 9879.
(2) A. C. Spivey, C. J.G. Gripton, J. P. Hannah, C. -C. Tseng, P. Fraine, N. J. Parr and J. J. Scicinski, *Appl. Organometal. Chem.*, 2007, **21**, 572.
(3) T. Tu, X. Feng, Z. Wang and X. Liu, *Dalton Trans.*, 2010, **39**, 10598.
(4) Z. Liu, T. Zhang and M. Shi, *Orgnometallic*, 2008, **27**, 2668.
(5) L. Ackermann and A. Althammer, *Org. Lett.*, 2006, **8**, 3457.
(6) S. Bhunia, S. Md. A. Sohel, C. -C. Yang, S. -F. Lush, F. -M. Shen and R. -S. Liu, *J. Organometal. Chem.*, 2009, **694**, 566.

Spectra of products (^{1}H, ^{13}C, ^{19}F)



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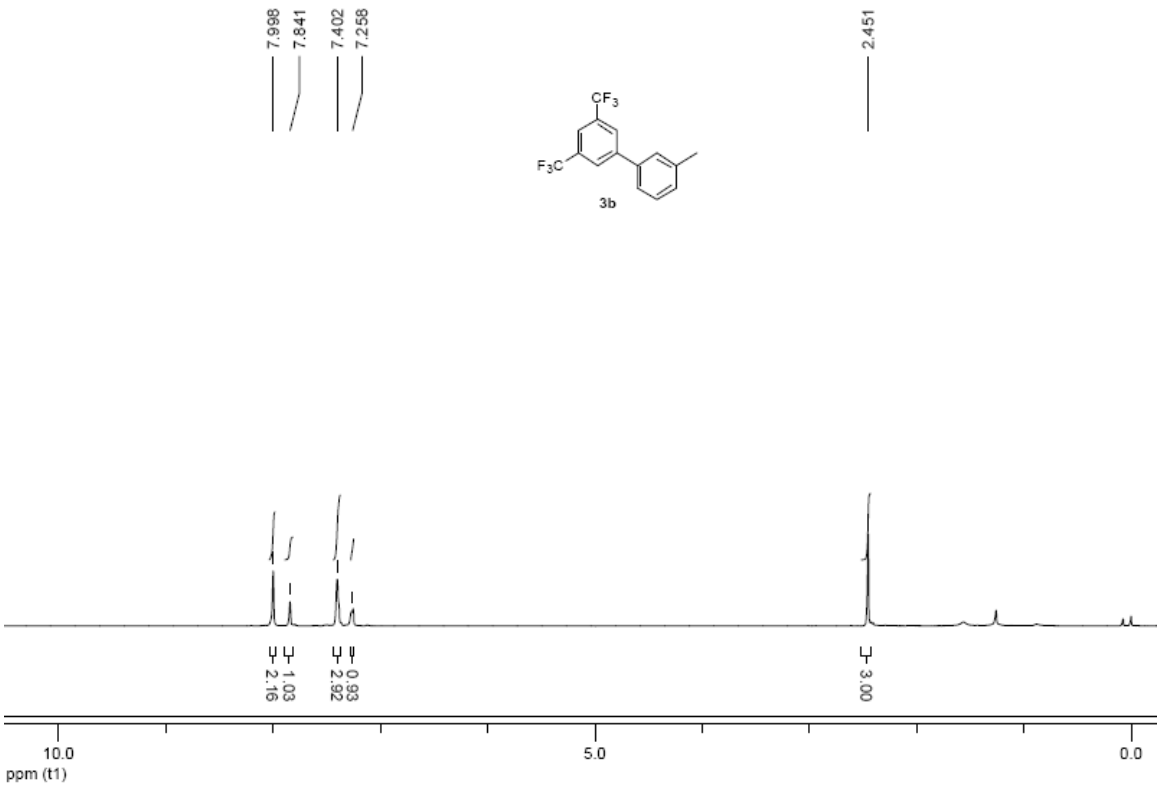
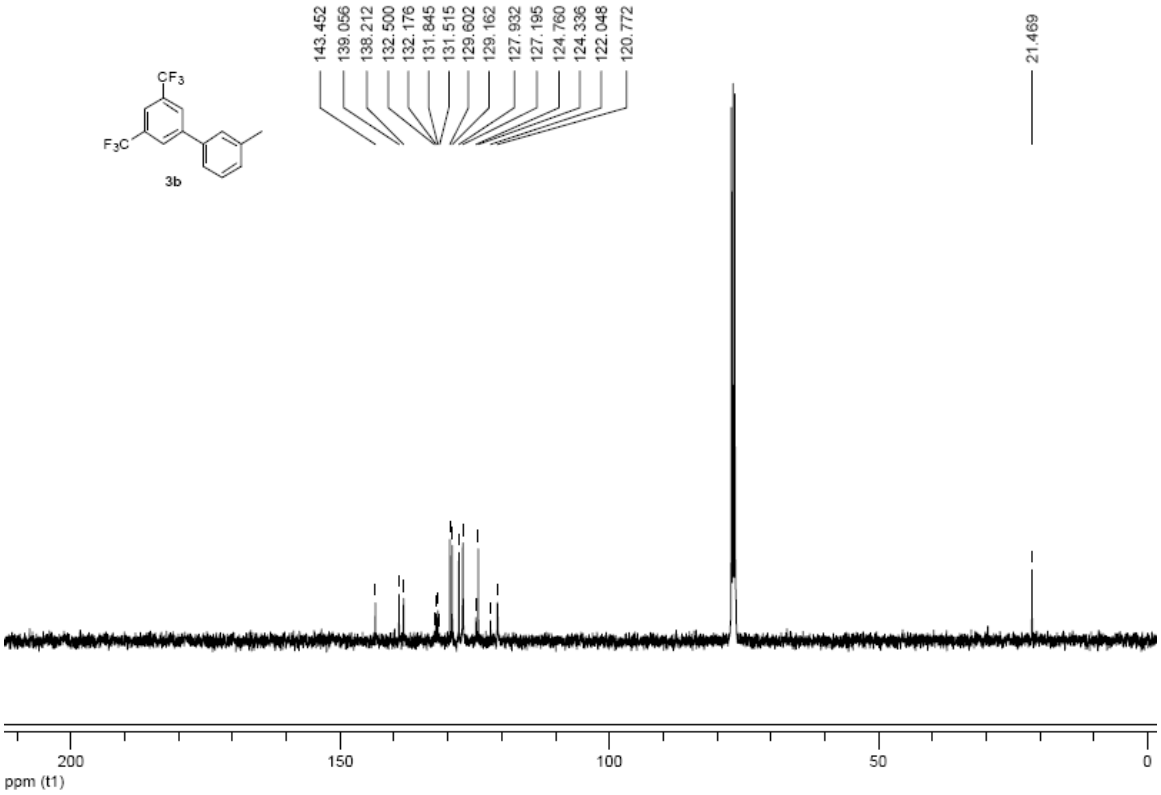
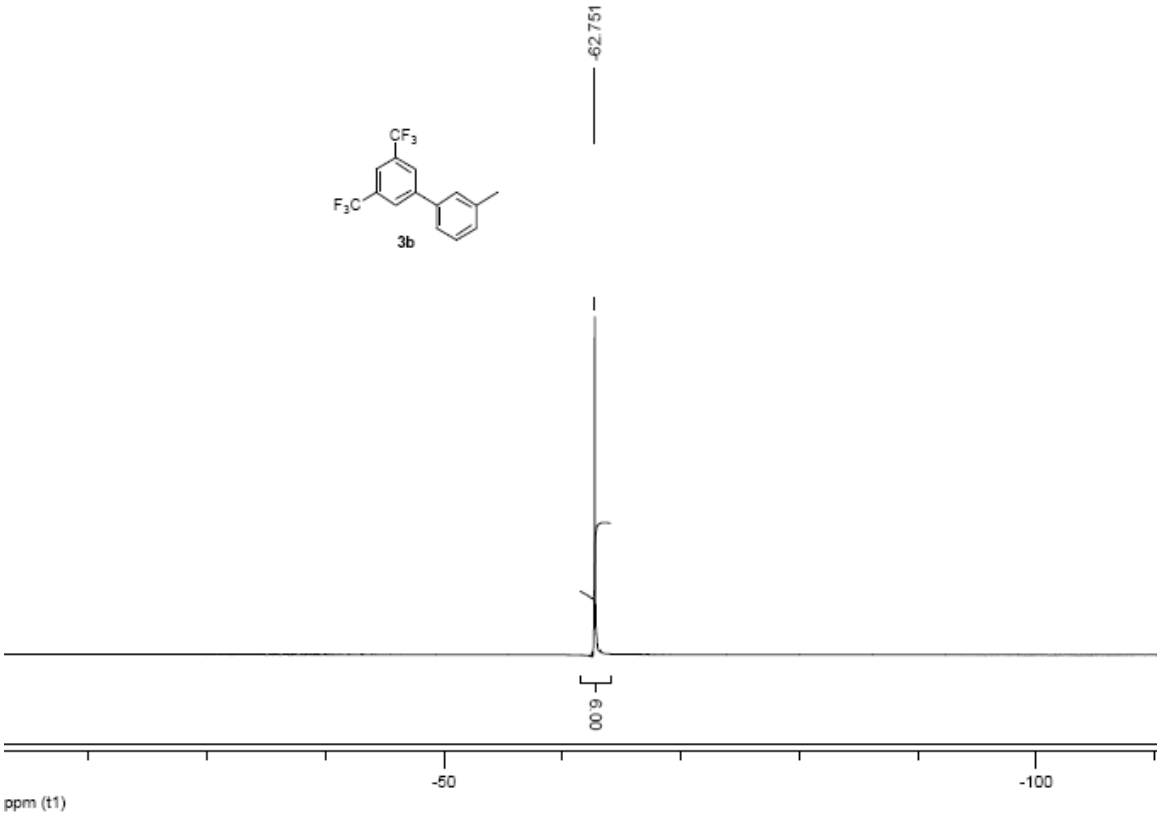
6.00
-20
-30
-40
-50
-60
-70
-80
-90
-100
ppm (t1)

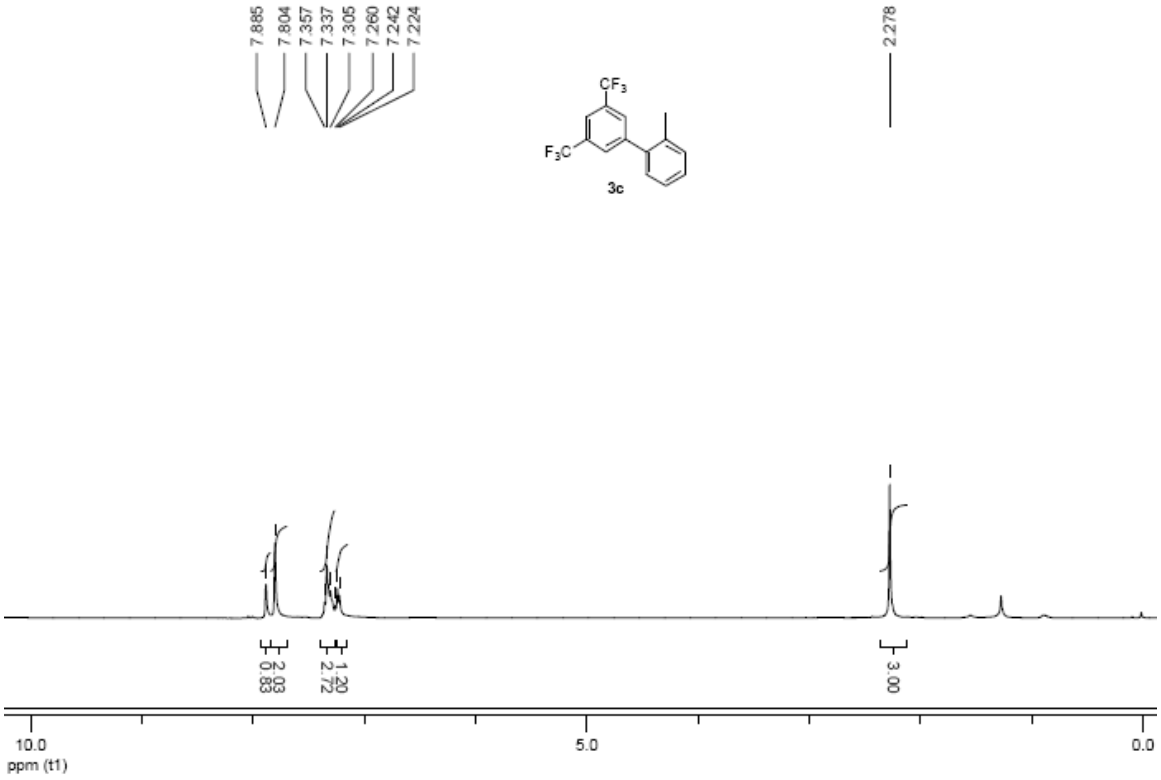
3a


7.998
7.841
7.402
7.258
2.451
2.16
1.03
2.32
0.83
3.00
10.0
5.0
0.0
ppm (t1)

3b



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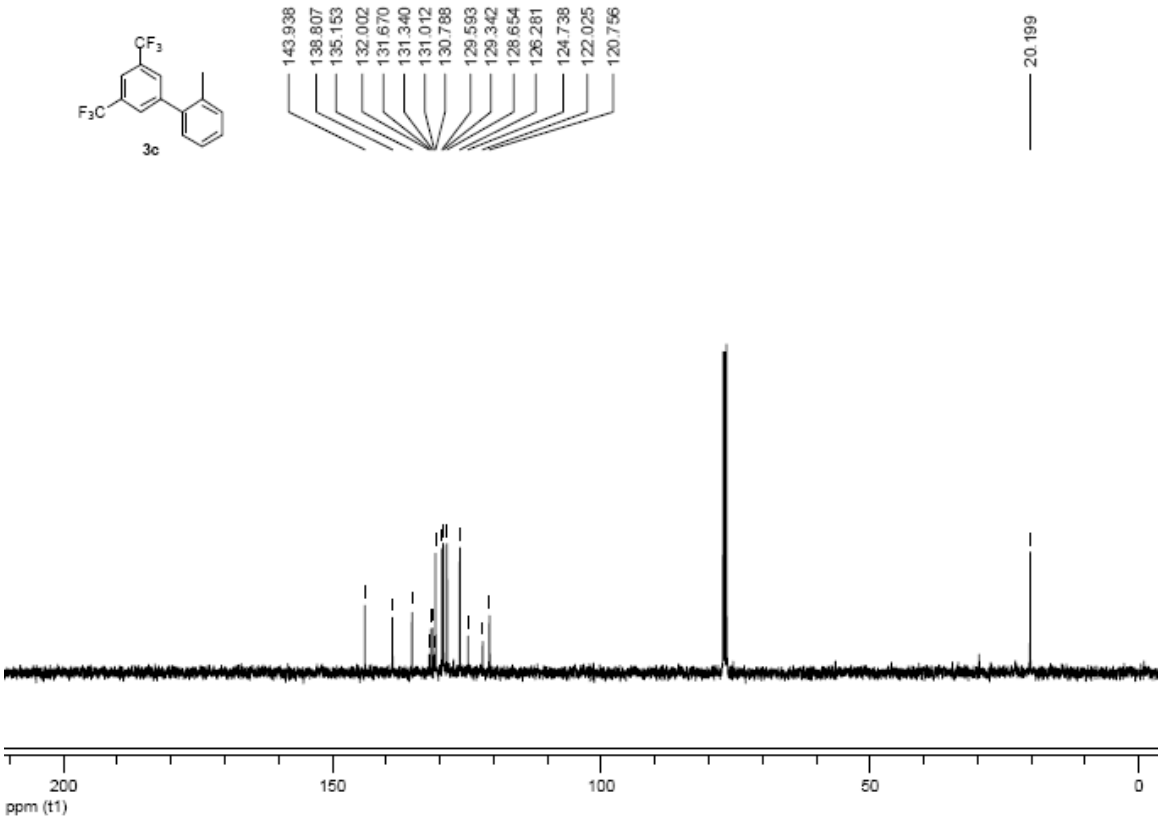
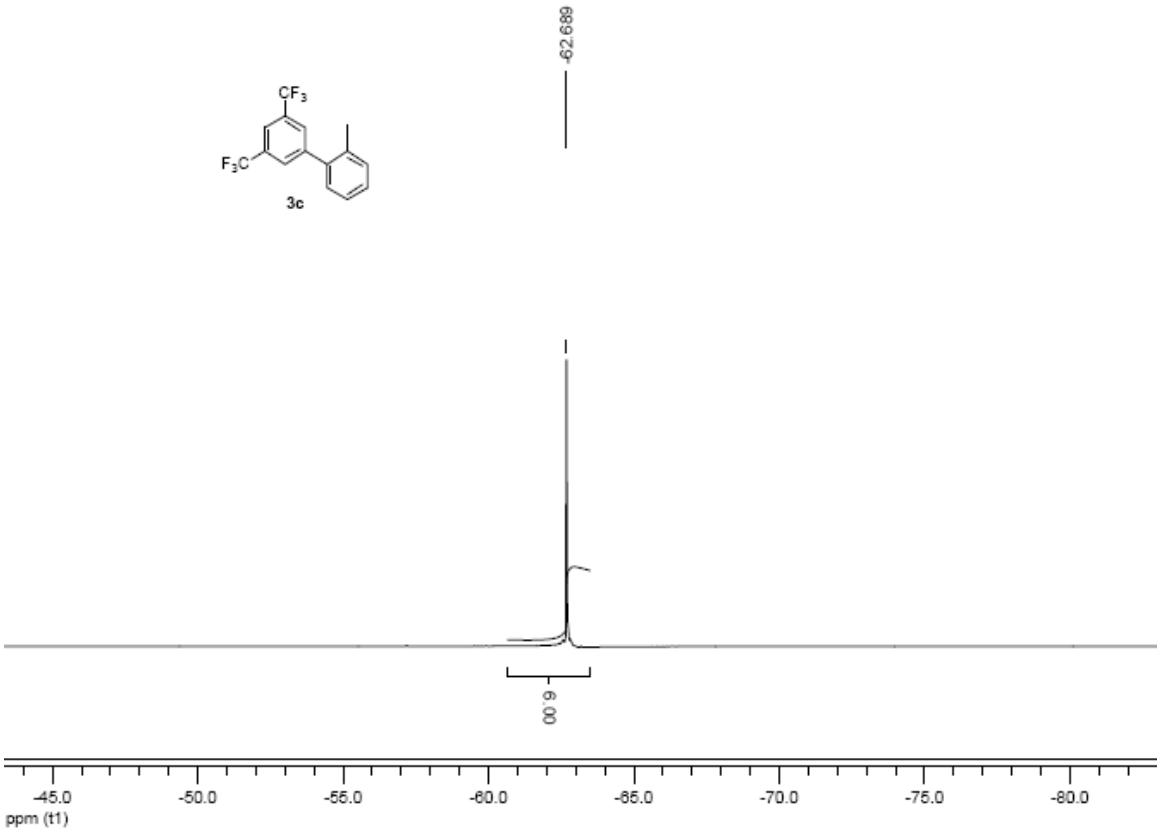
7.804
7.357
7.337
7.305
7.260
7.242
7.224
2.278
CF3
F3C
3c
0.83
0.88
2.72
1.20
3.00
10.0
5.0
0.0
ppm (t1)


CF3
F3C
3c
143.938
138.807
135.153
132.002
131.670
131.340
131.012
130.788
129.593
129.342
128.654
126.281
124.738
122.025
120.756
20.199
200
150
100
50
0
ppm (t1)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F3C
3c
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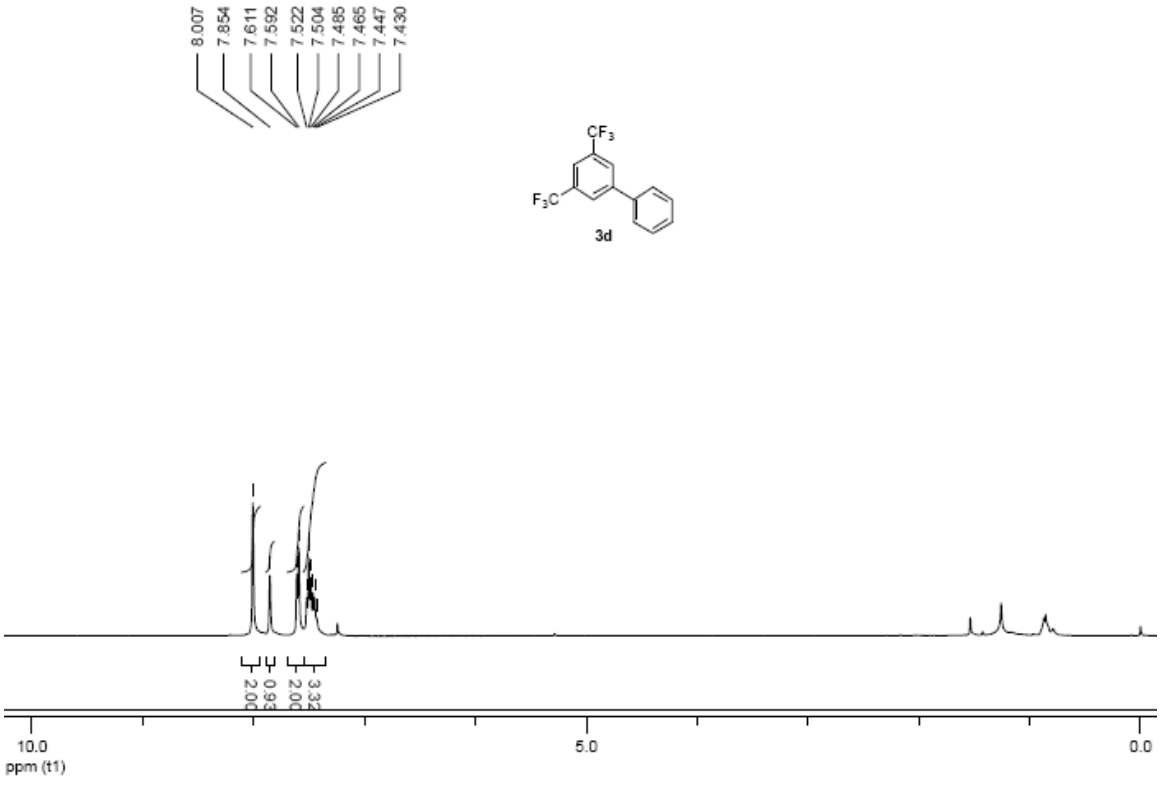
-75.0
-80.0
ppm (t1)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7.854
7.611
7.592
7.522
7.504
7.485
7.465
7.447
7.430
CF3
F3C
3d
2.00
0.93
2.00
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10.0
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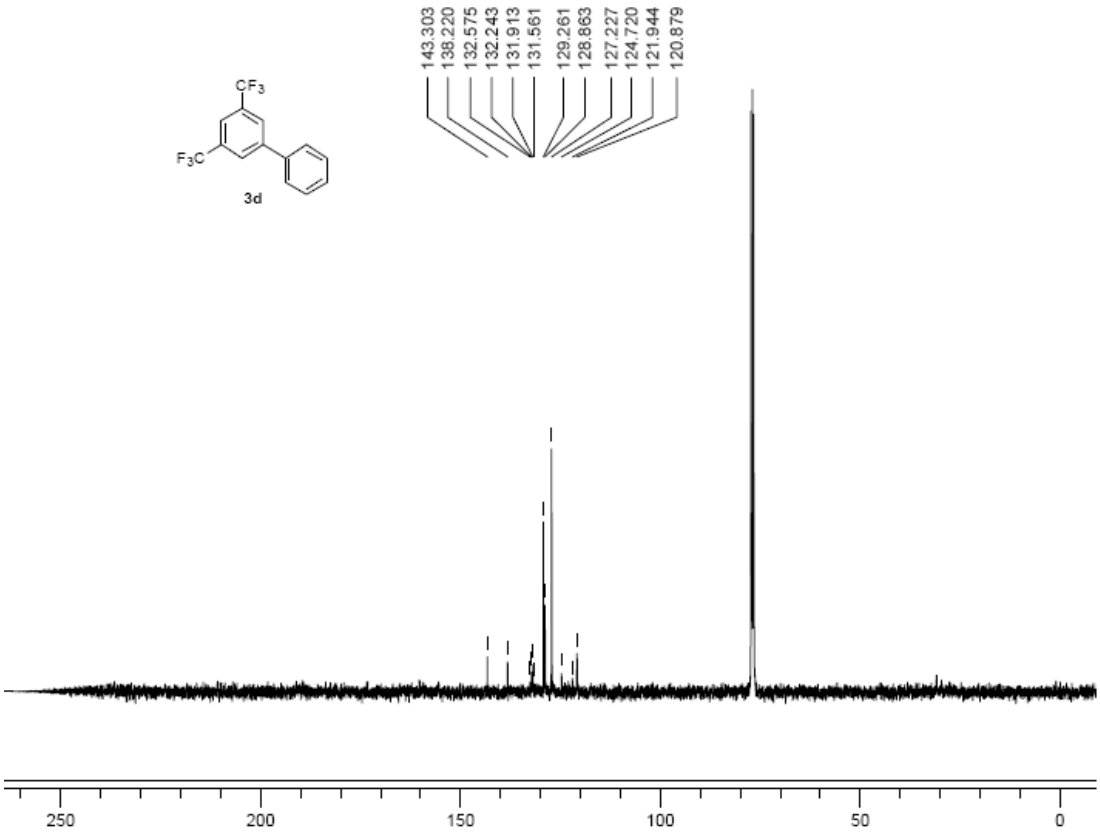
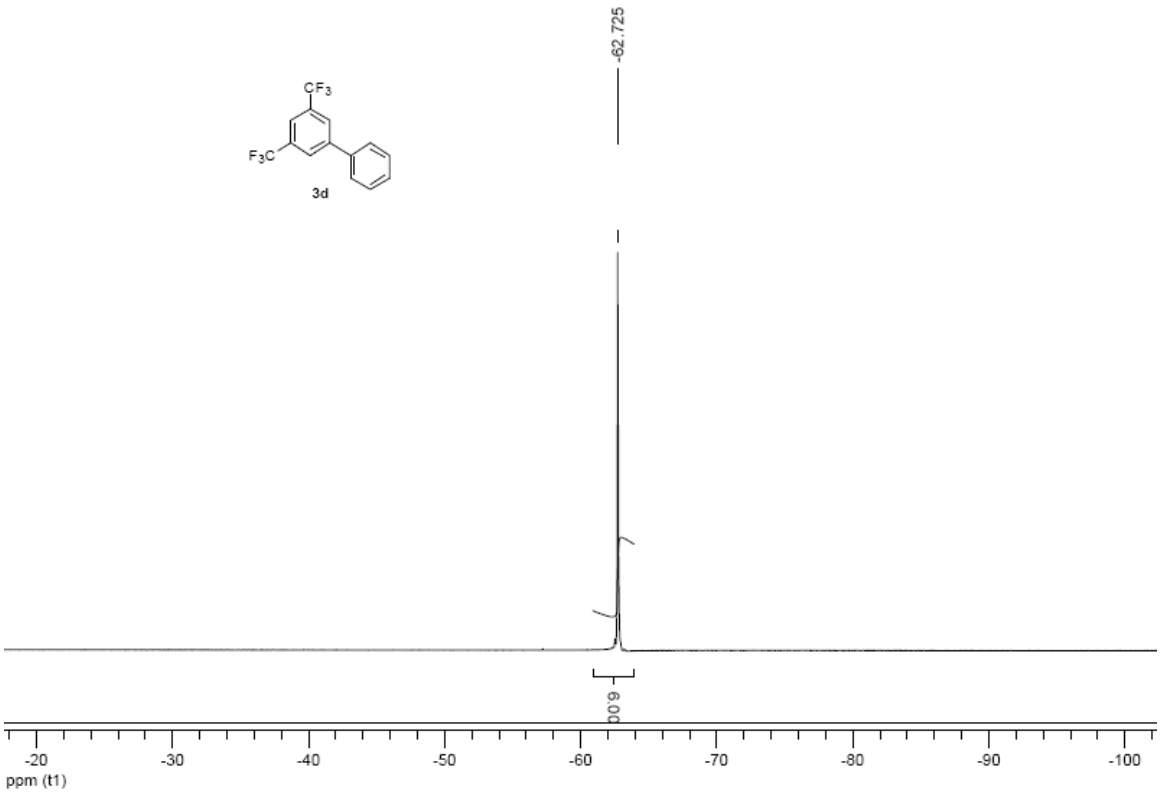
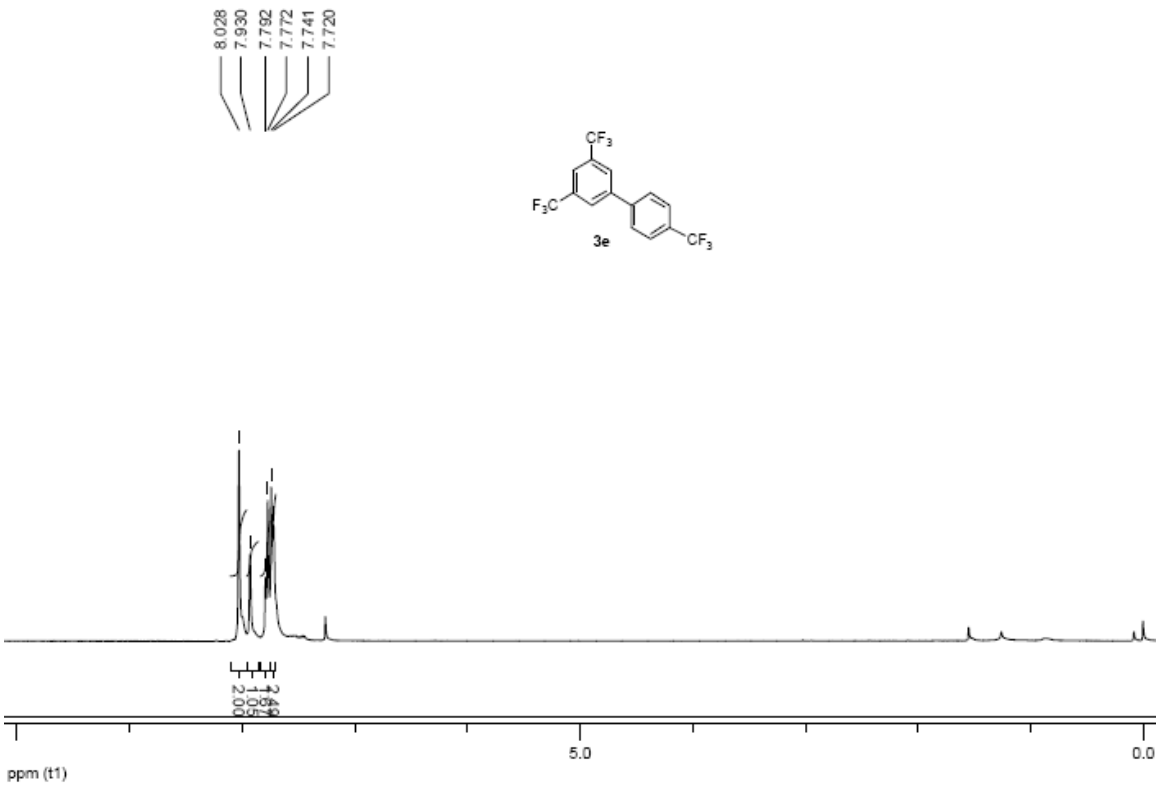
0.0
ppm (t1)



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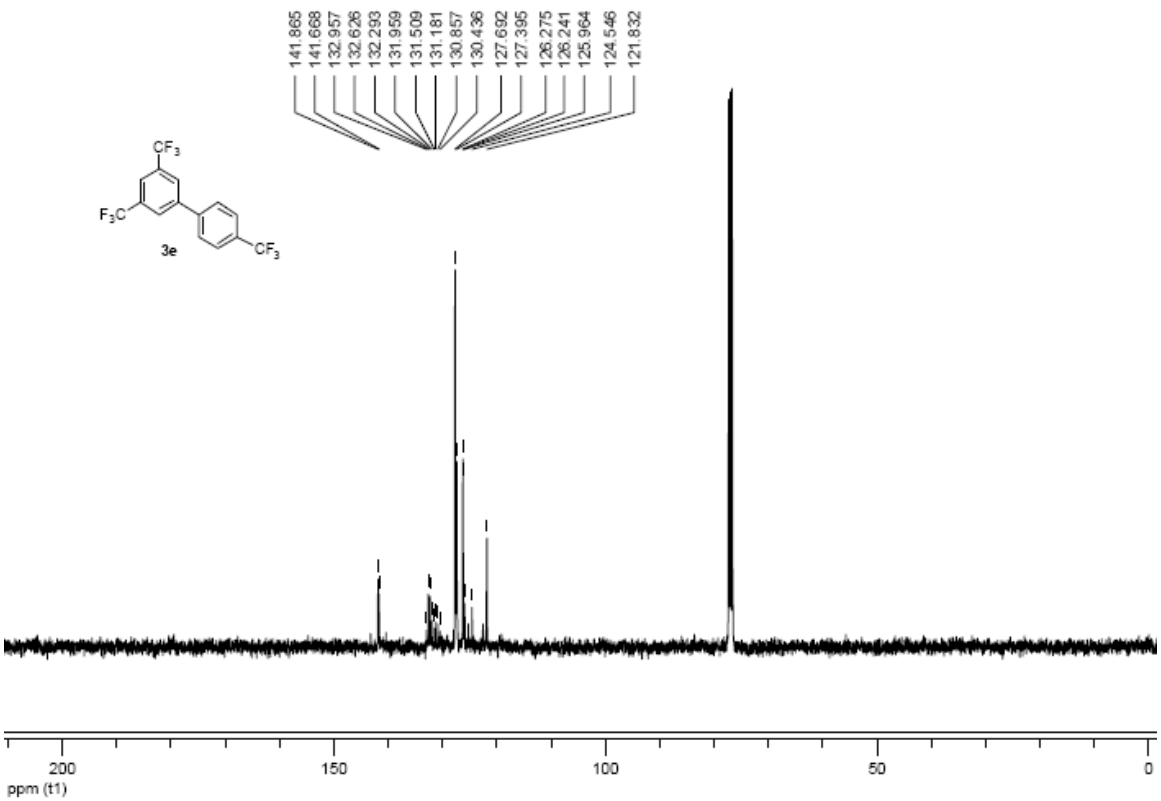
7.930
7.792
7.772
7.741
7.720
3e
2.00
1.05
2.19
2.19
5.0
0.0
ppm (t1)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141.668
132.957
132.626
132.293
131.959
131.509
131.181
130.857
130.436
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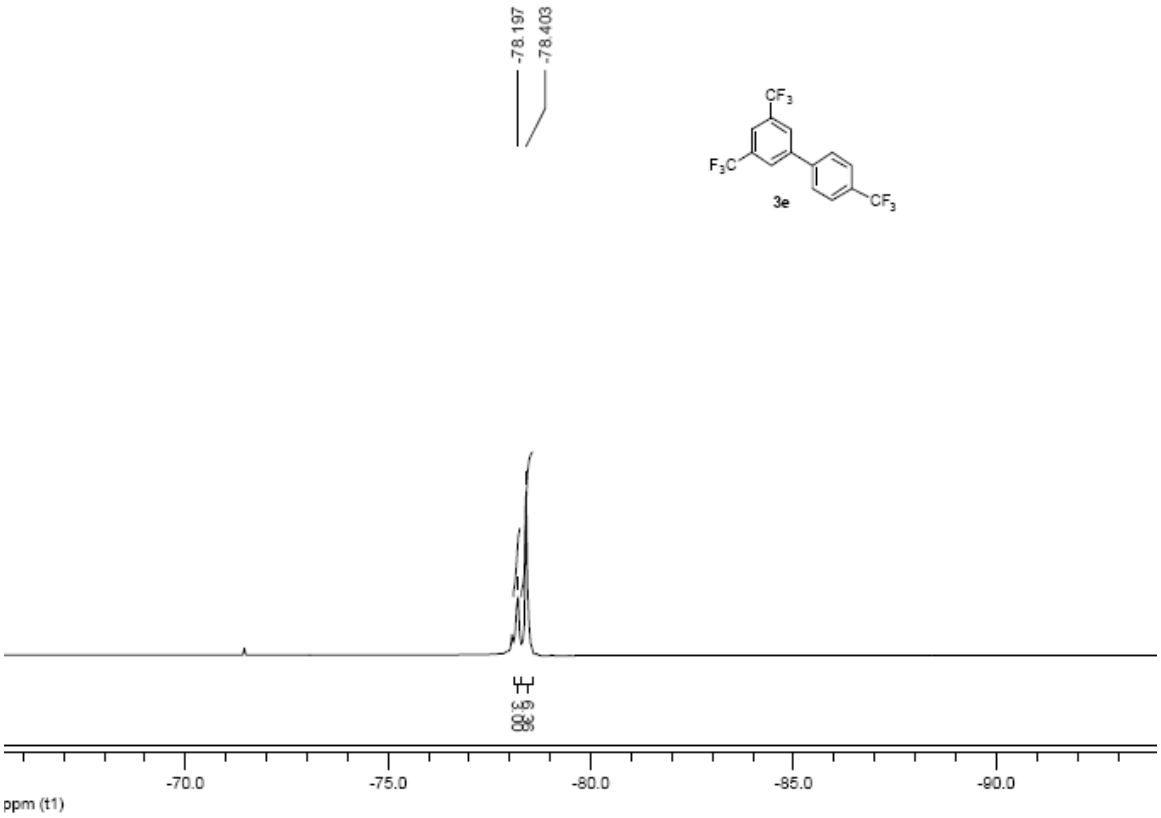
127.395
126.275
126.241
125.964
124.546
121.832
3e
200
150
100
50
0
ppm (t1)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CF3
F3C
CF3
3e
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-70.0
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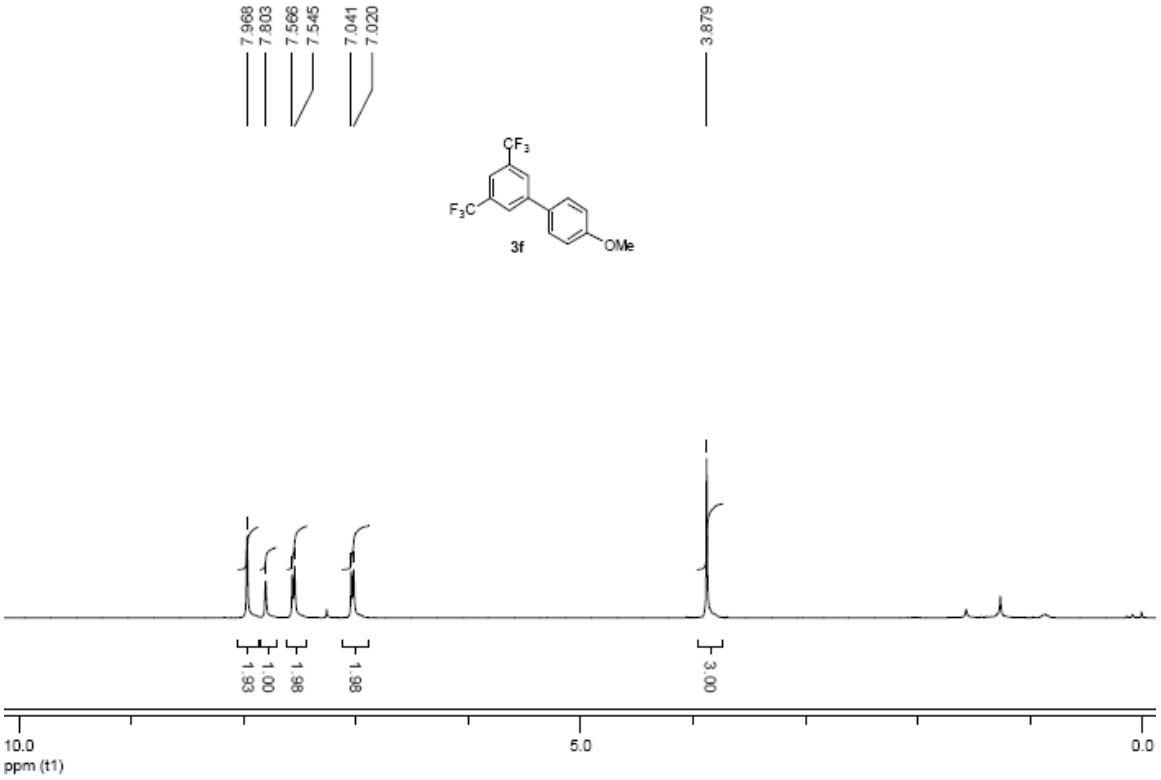
-90.0
ppm (t1)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7.041
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CF3
F3C
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3f
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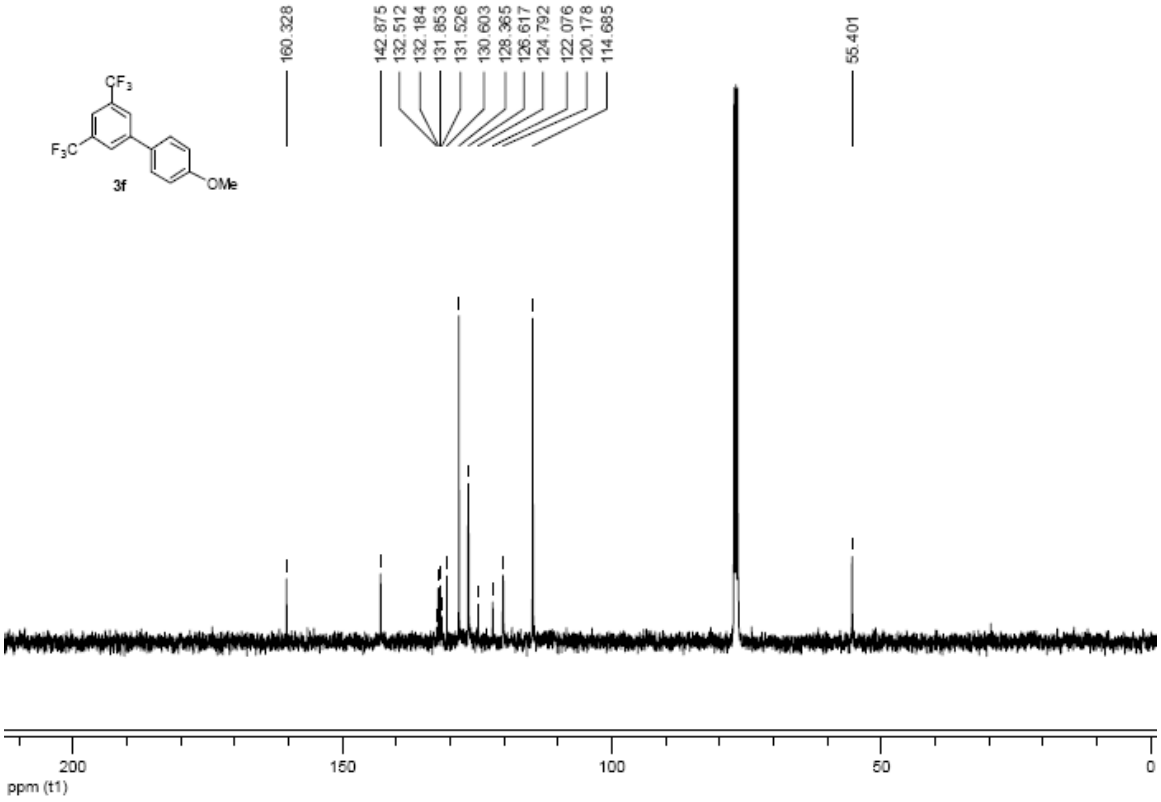
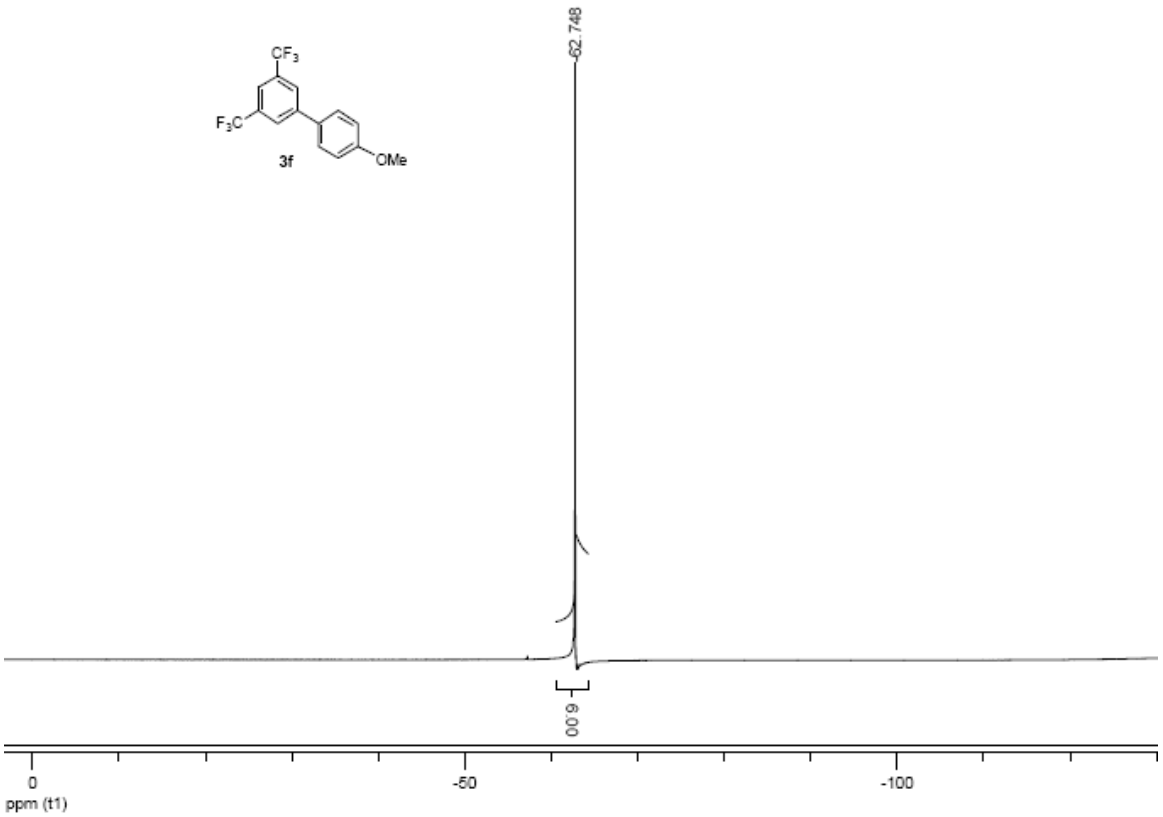
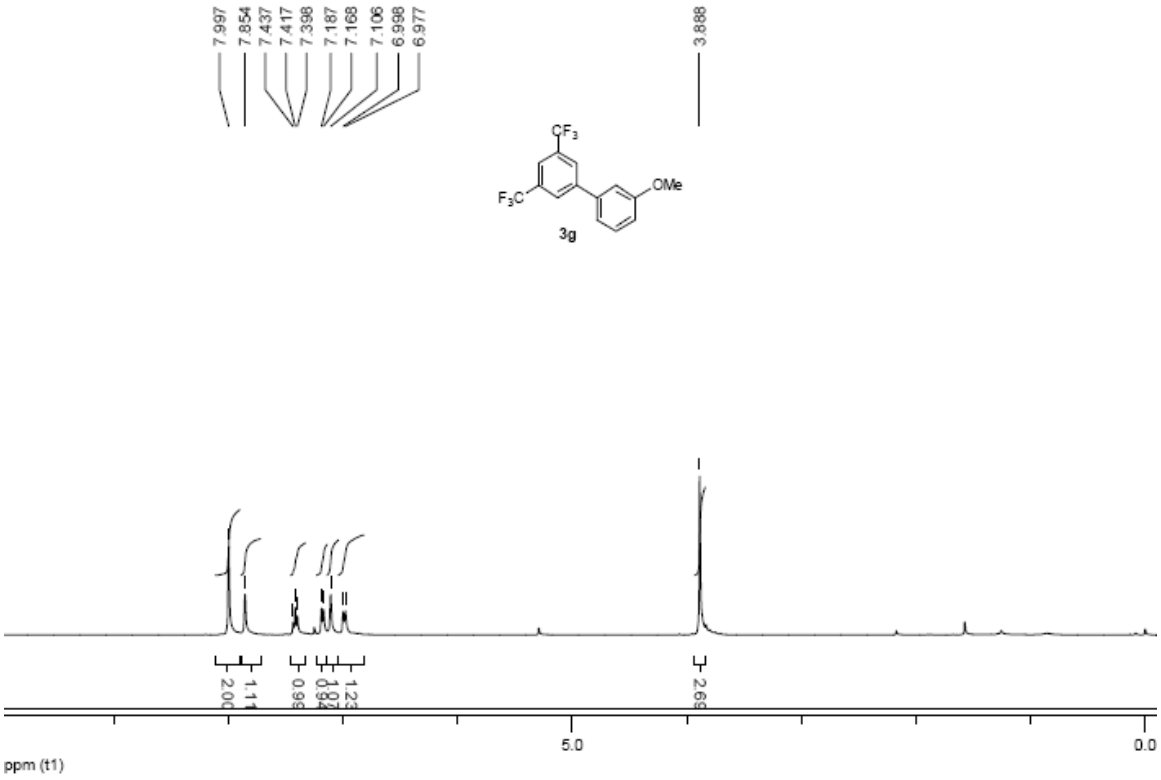
1.98
1.98
3.00
10.0
5.0
0.0
ppm (t1)



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7.398
7.187
7.168
7.106
6.998
6.977
3.888
CF3
F3C
OMe
3g
2.00
1.11
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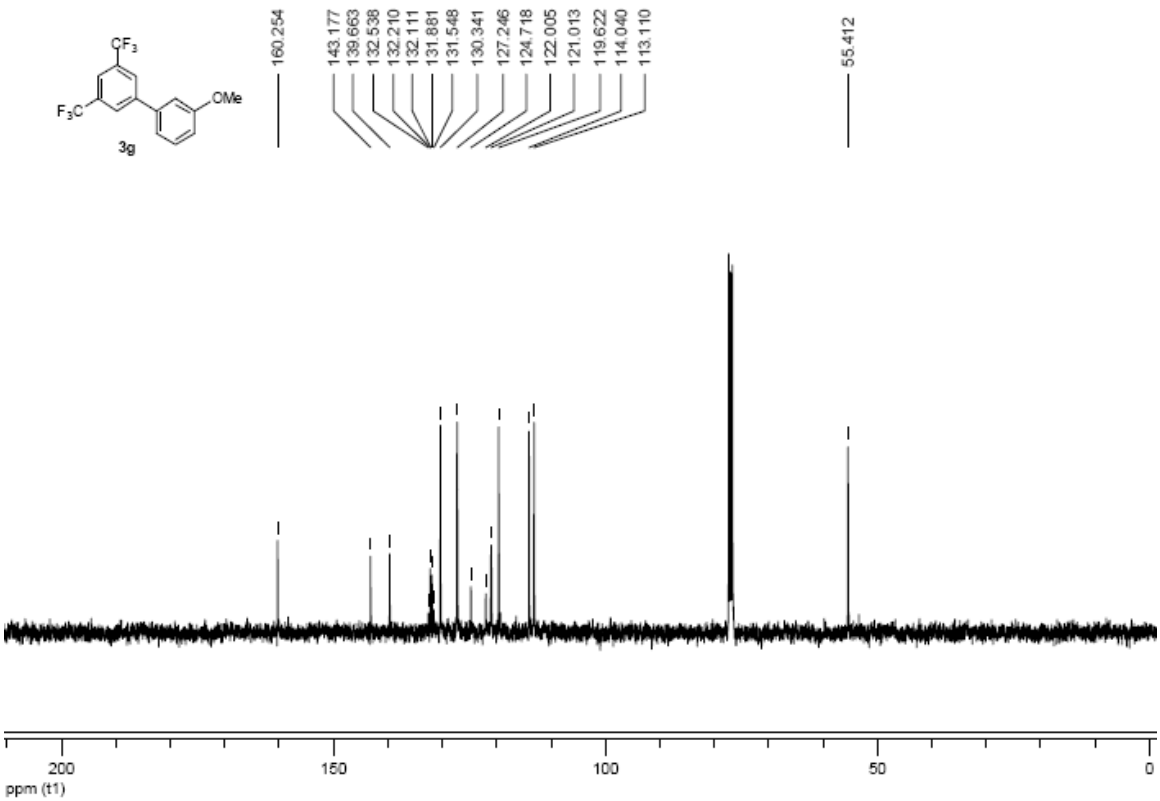
2.65
5.0
0.0
ppm (t1)


CF3
F3C
OMe
3g
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132.111
131.881
131.548
130.341
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121.013
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114.040
113.110
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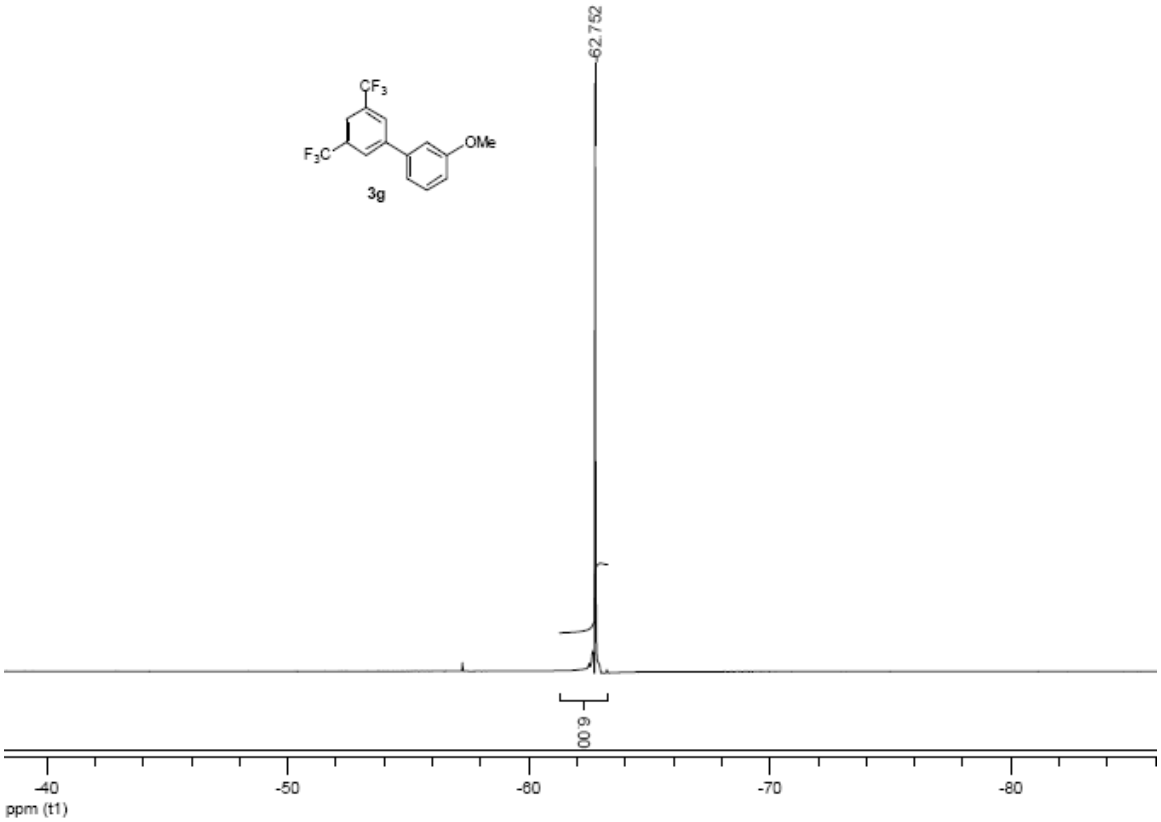
50
0
ppm (t1)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3g
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-60
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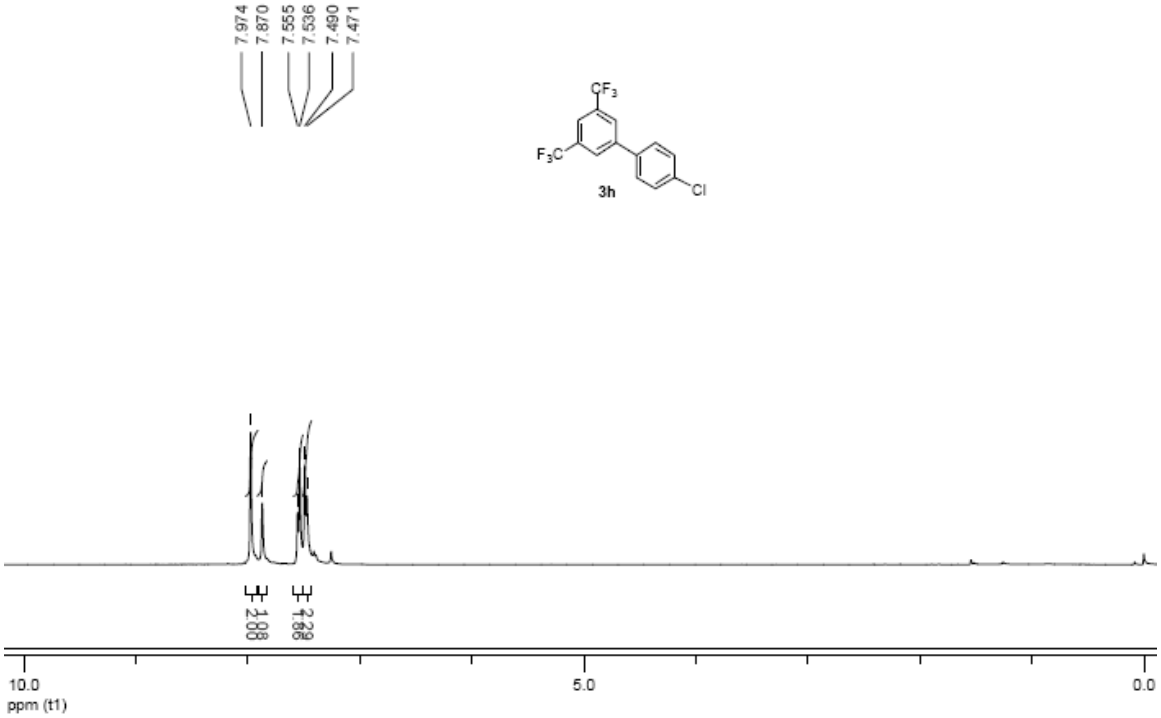
ppm (t1)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Cl
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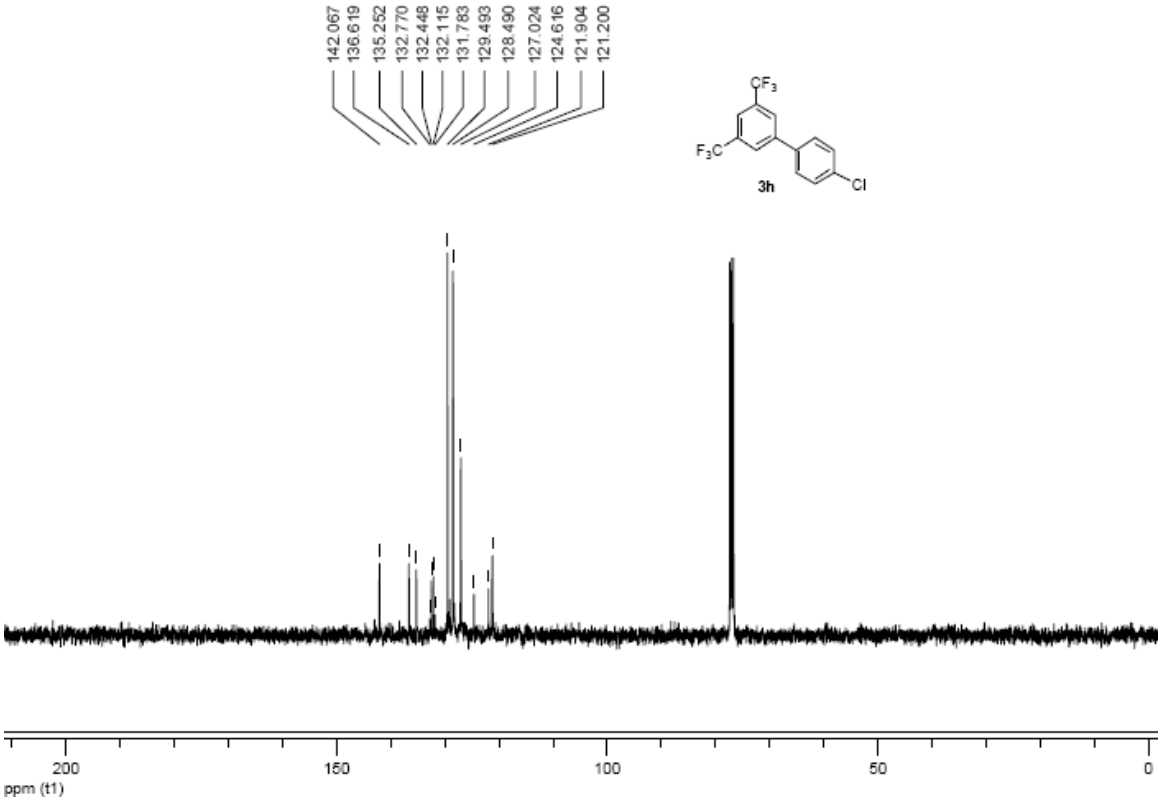
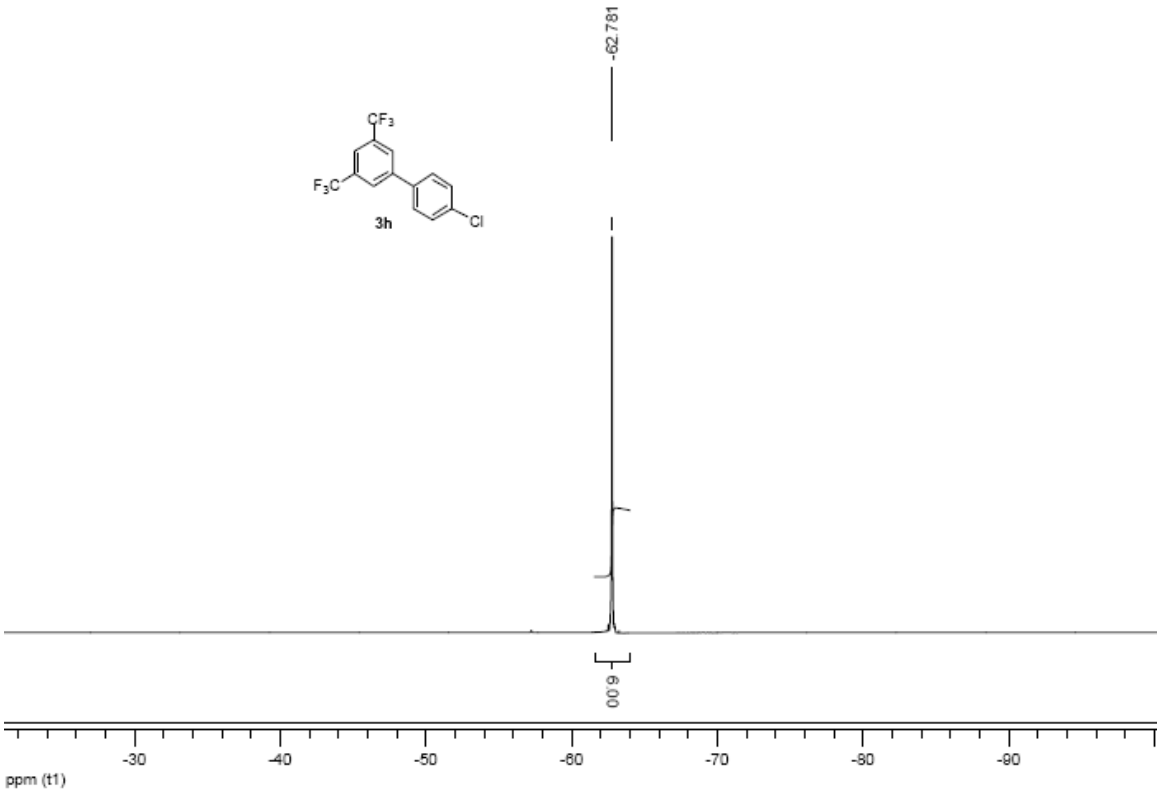
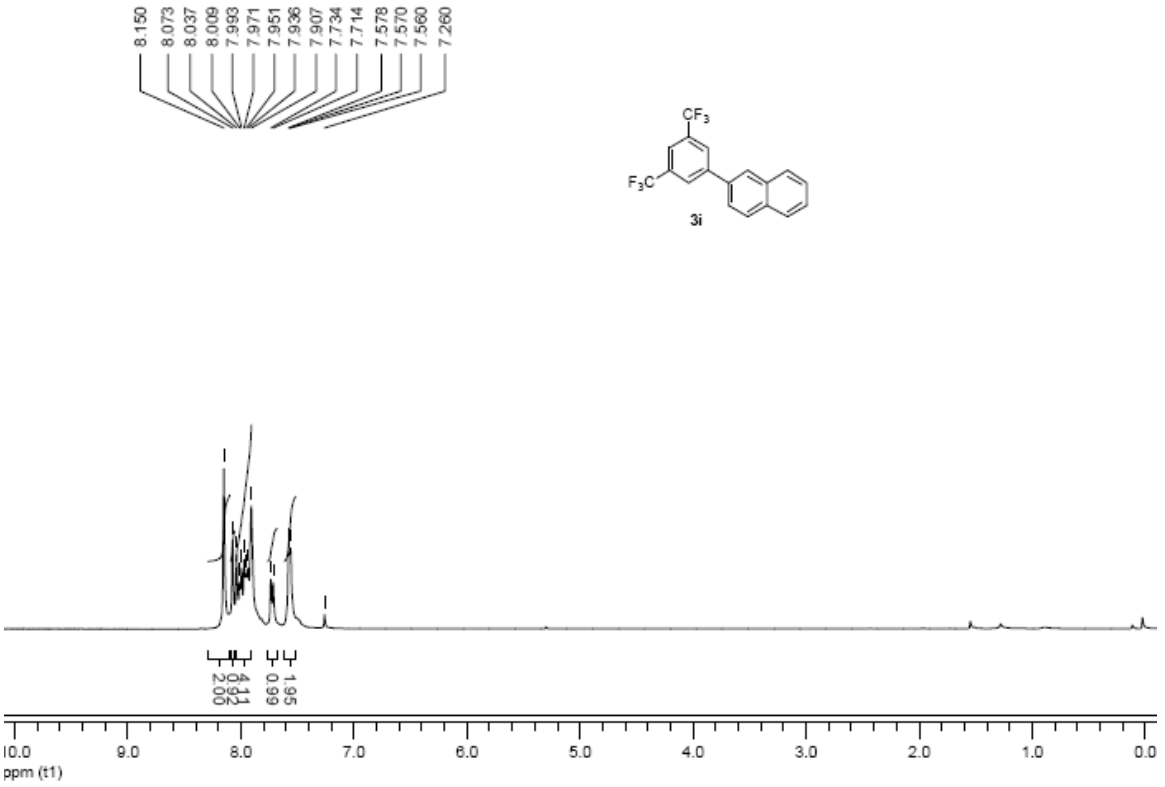
0.0
ppm (t1)



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7.971
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7.936
7.907
7.734
7.714
7.578
7.570
7.560
7.260
CF3
F3C
3i
2.00
4.02
1.11
0.99
1.95
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7.0
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4.0
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2.0
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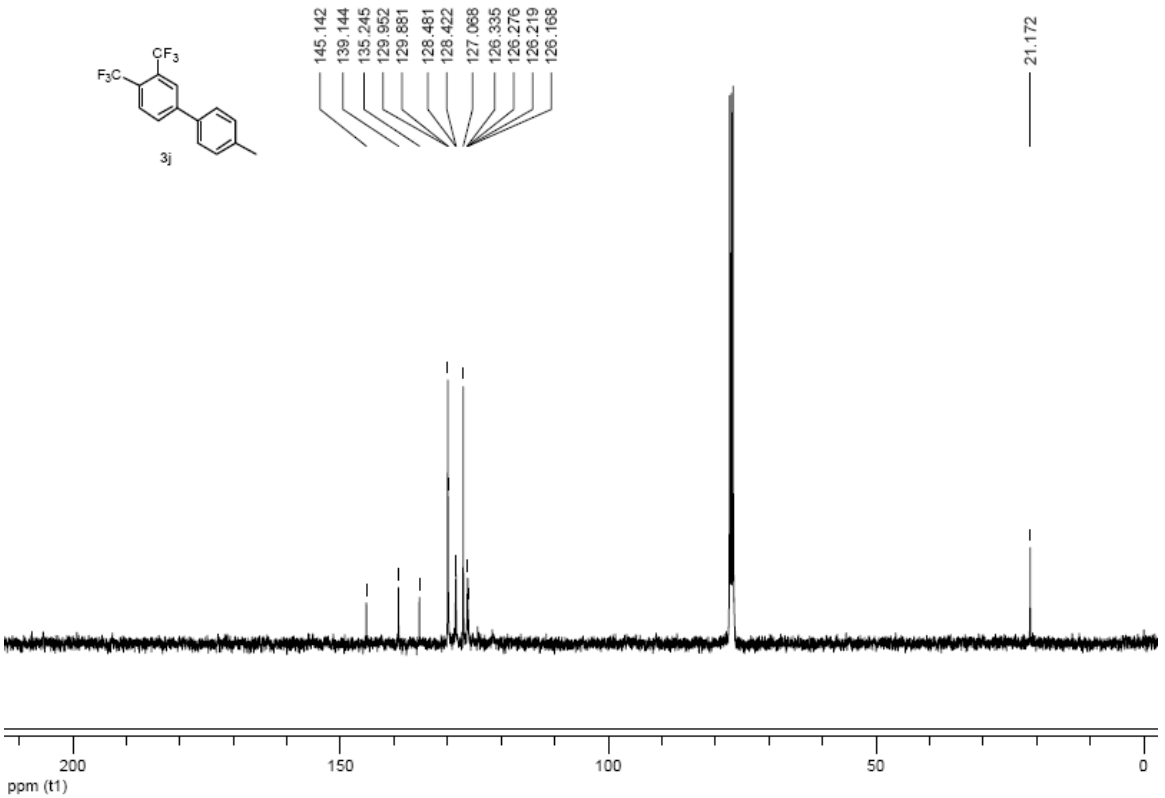
0.0
ppm (t1)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F3C
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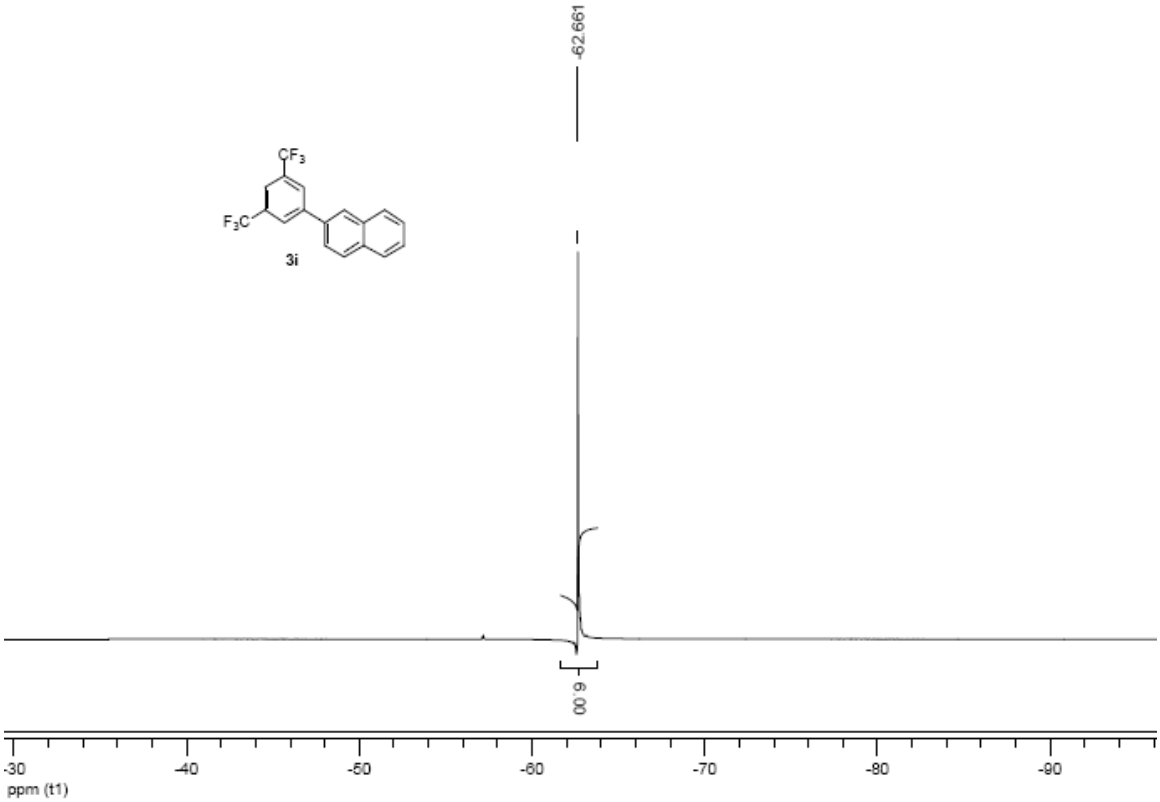
150
100
50
0
ppm (t1)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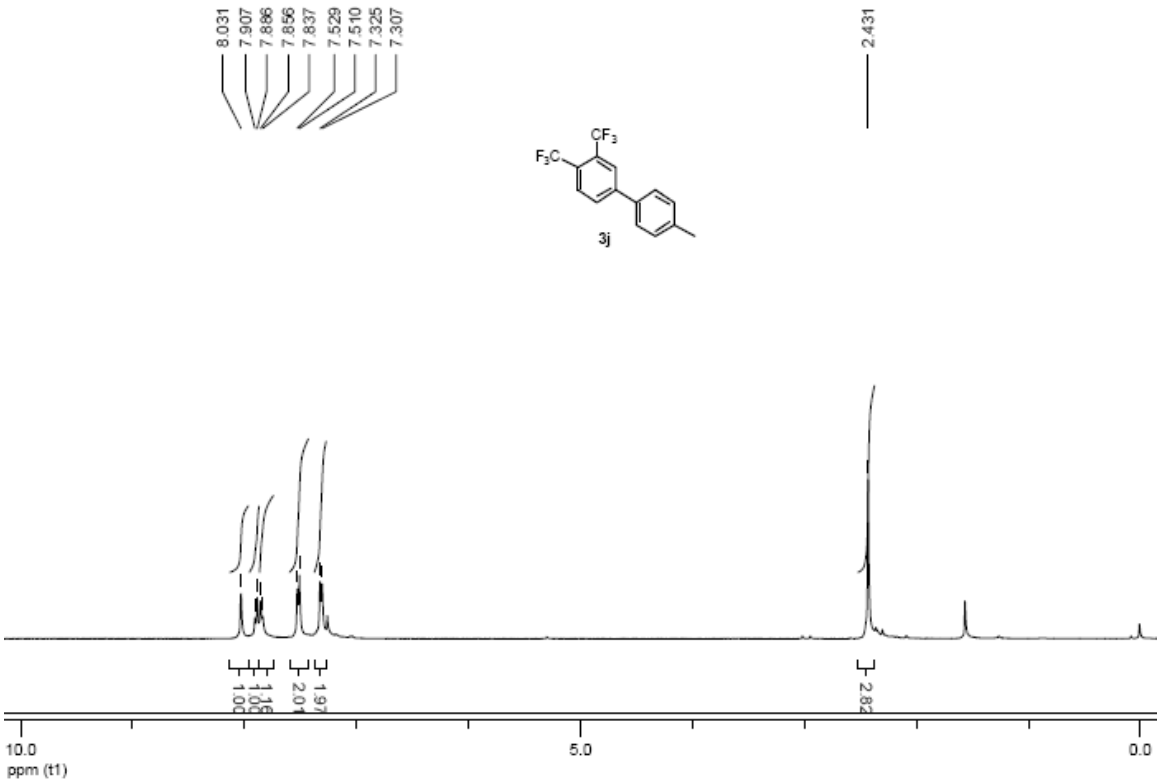
-90
ppm (t1)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7.325
7.307
2.431
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F3C
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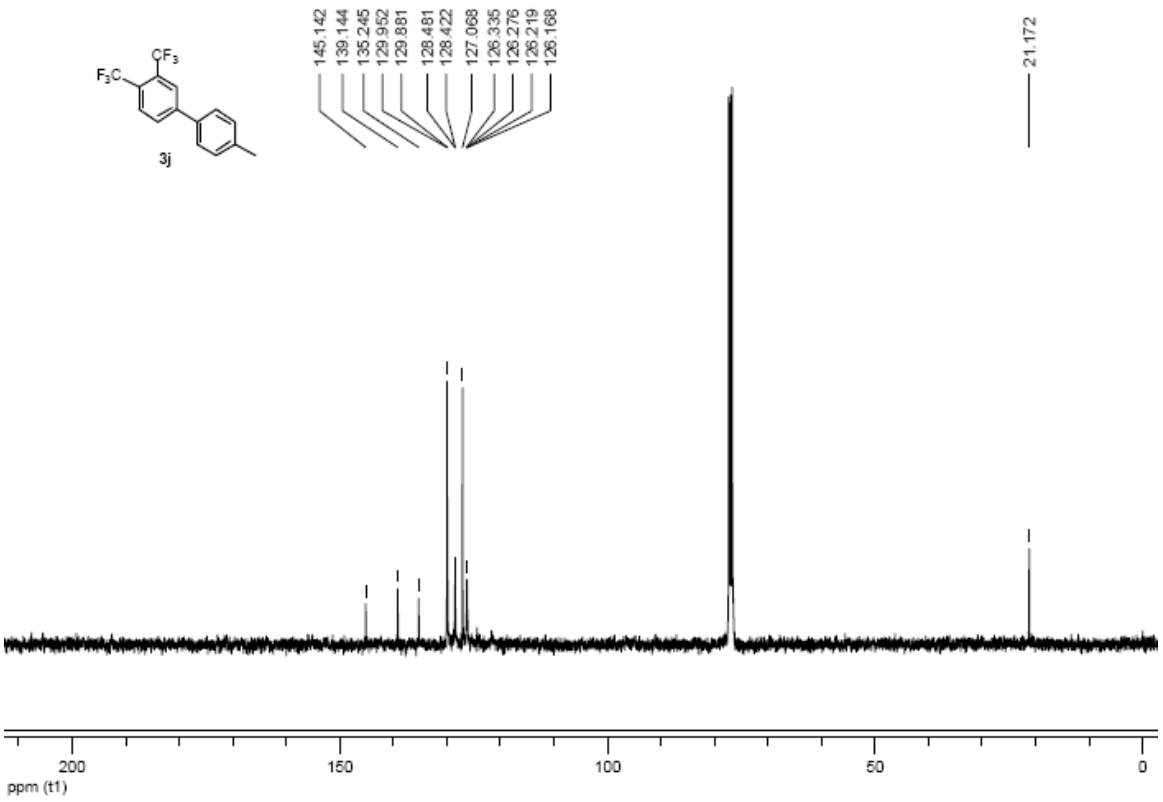
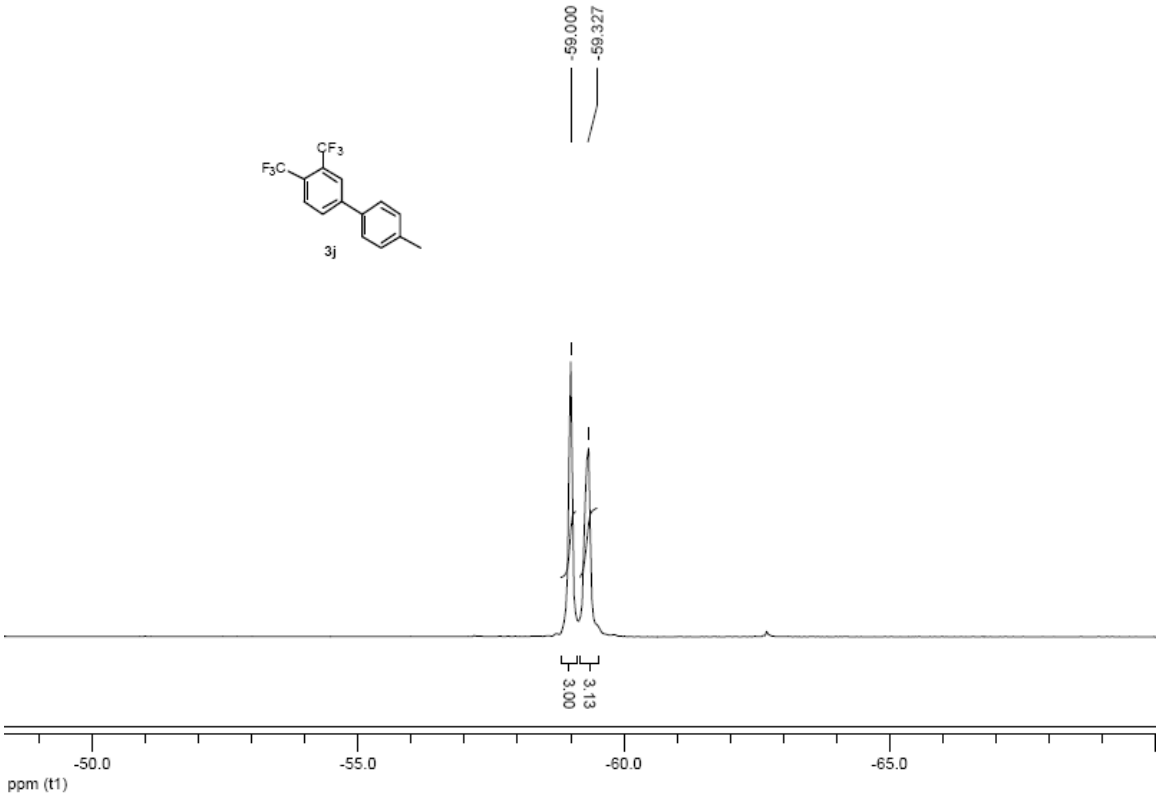
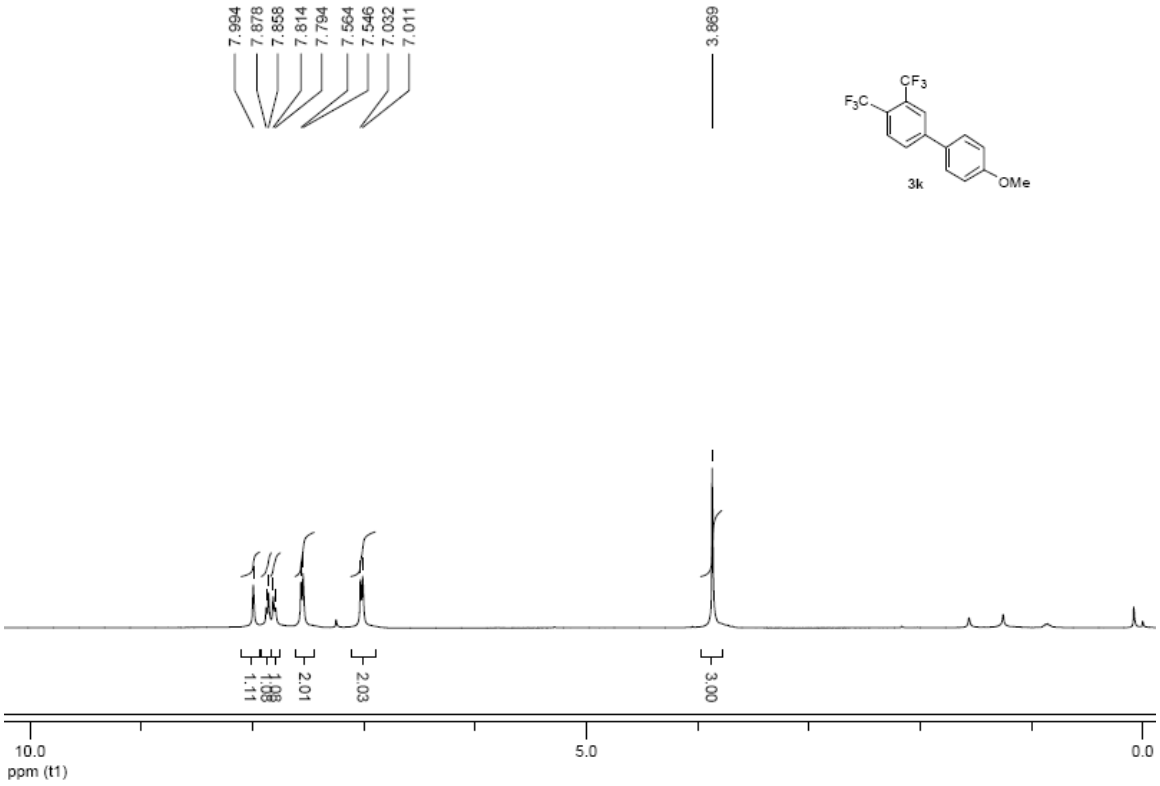
10.0
5.0
0.0
ppm (t1)



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7.032
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3.869
CF3
F3C
3k
OMe
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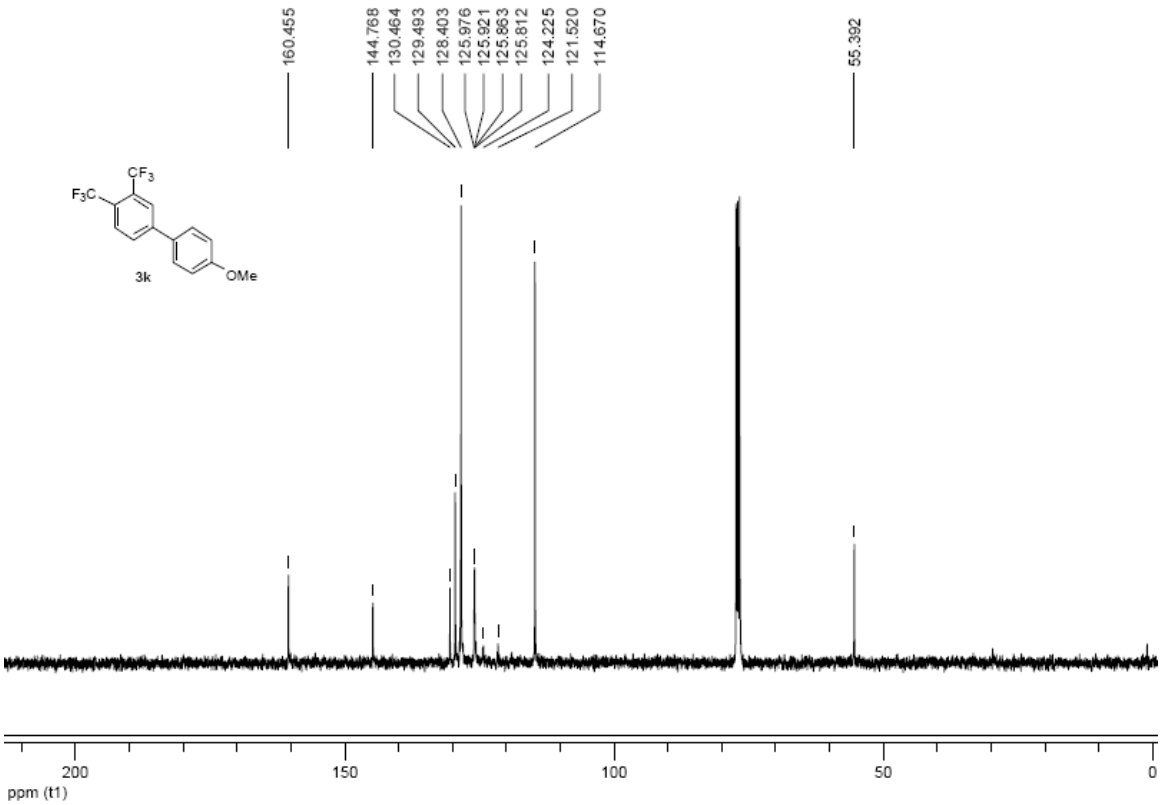
2.03
3.00
10.0
5.0
0.0
ppm (t1)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55.392
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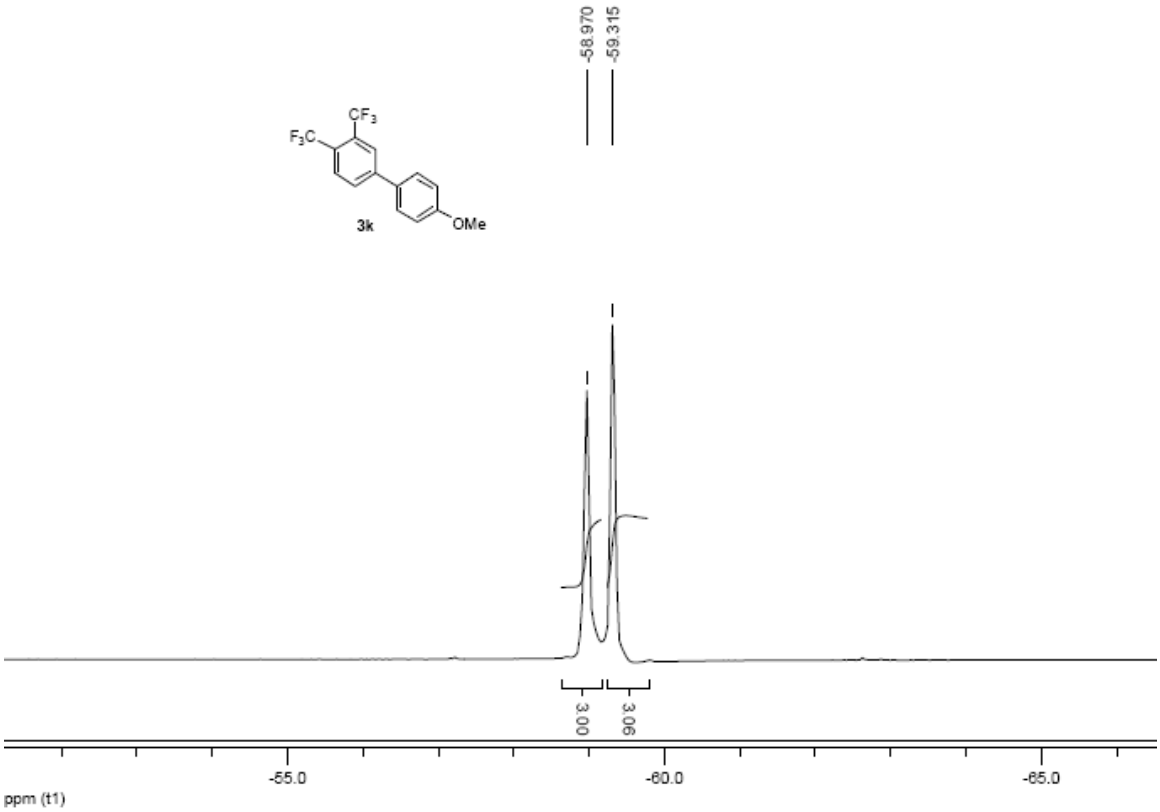
3k
OMe
200
150
100
50
0
ppm (t1)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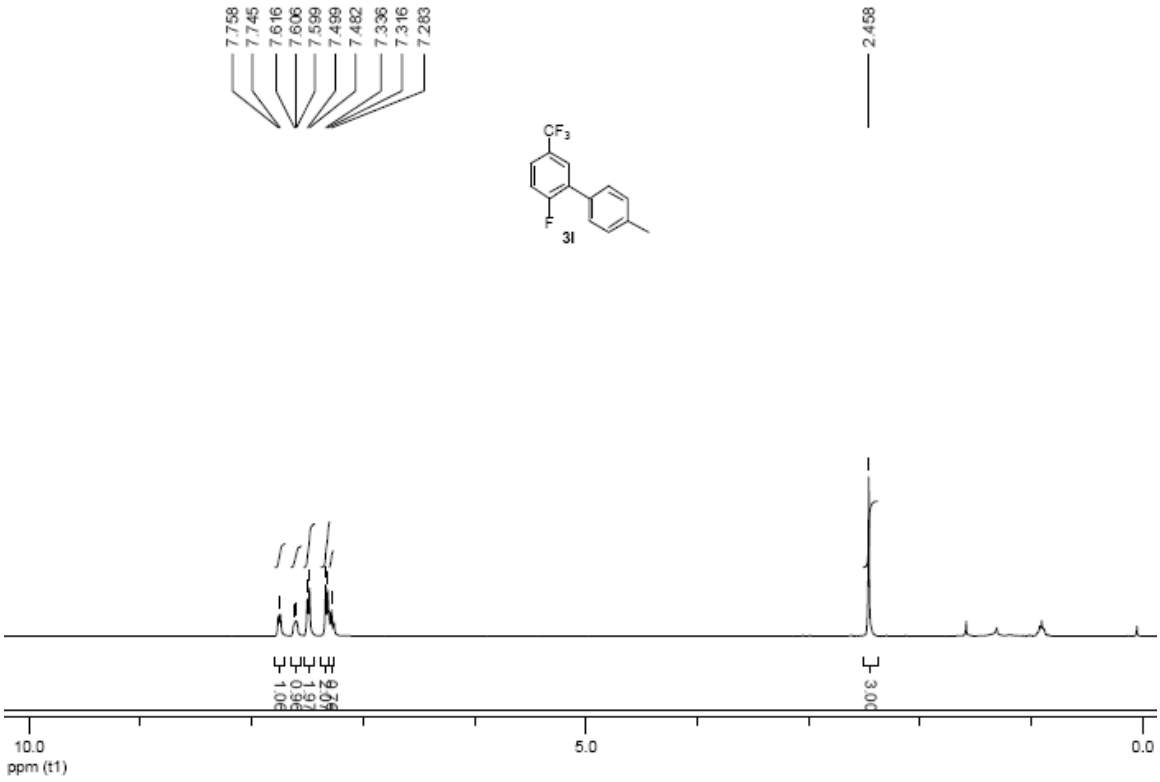
ppm (t1)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F
3l
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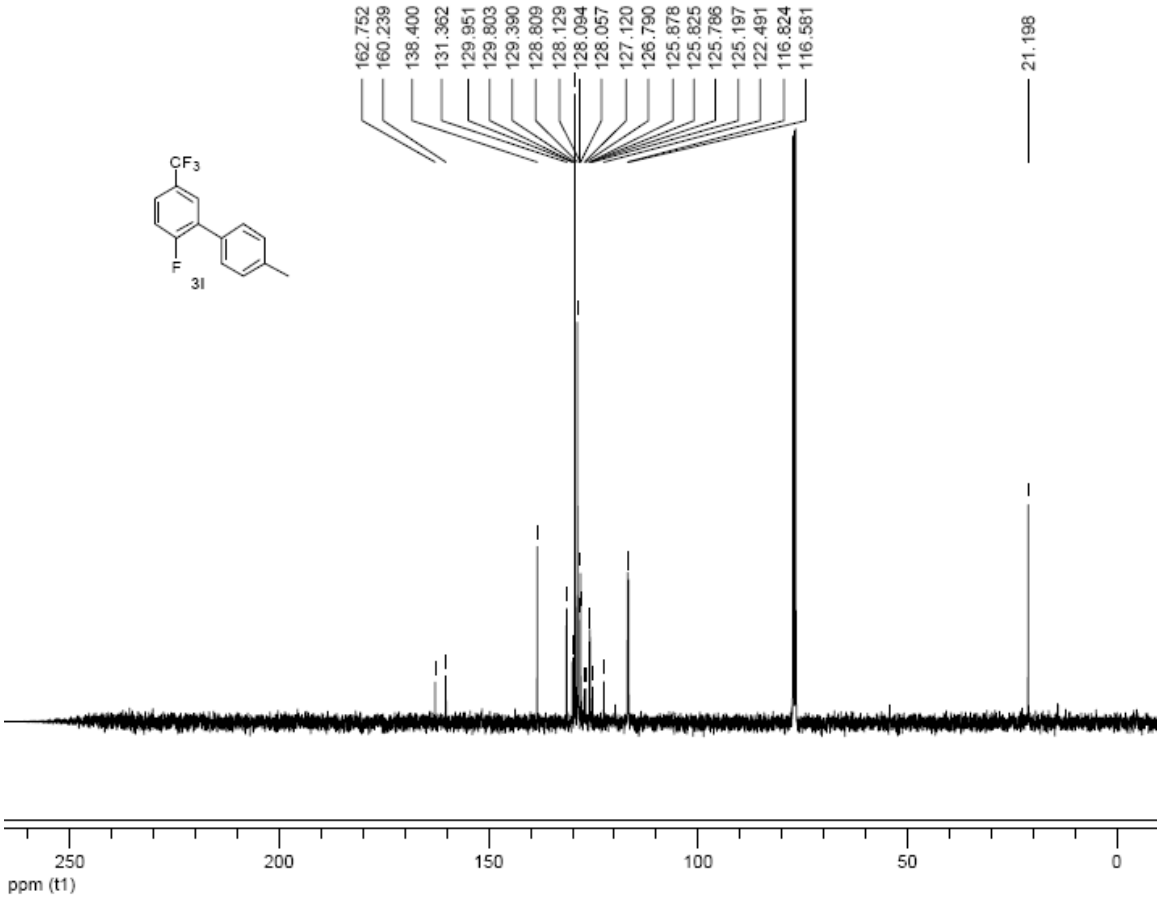
5.0
0.0
ppm (t1)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129.803
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128.094
128.057
127.120
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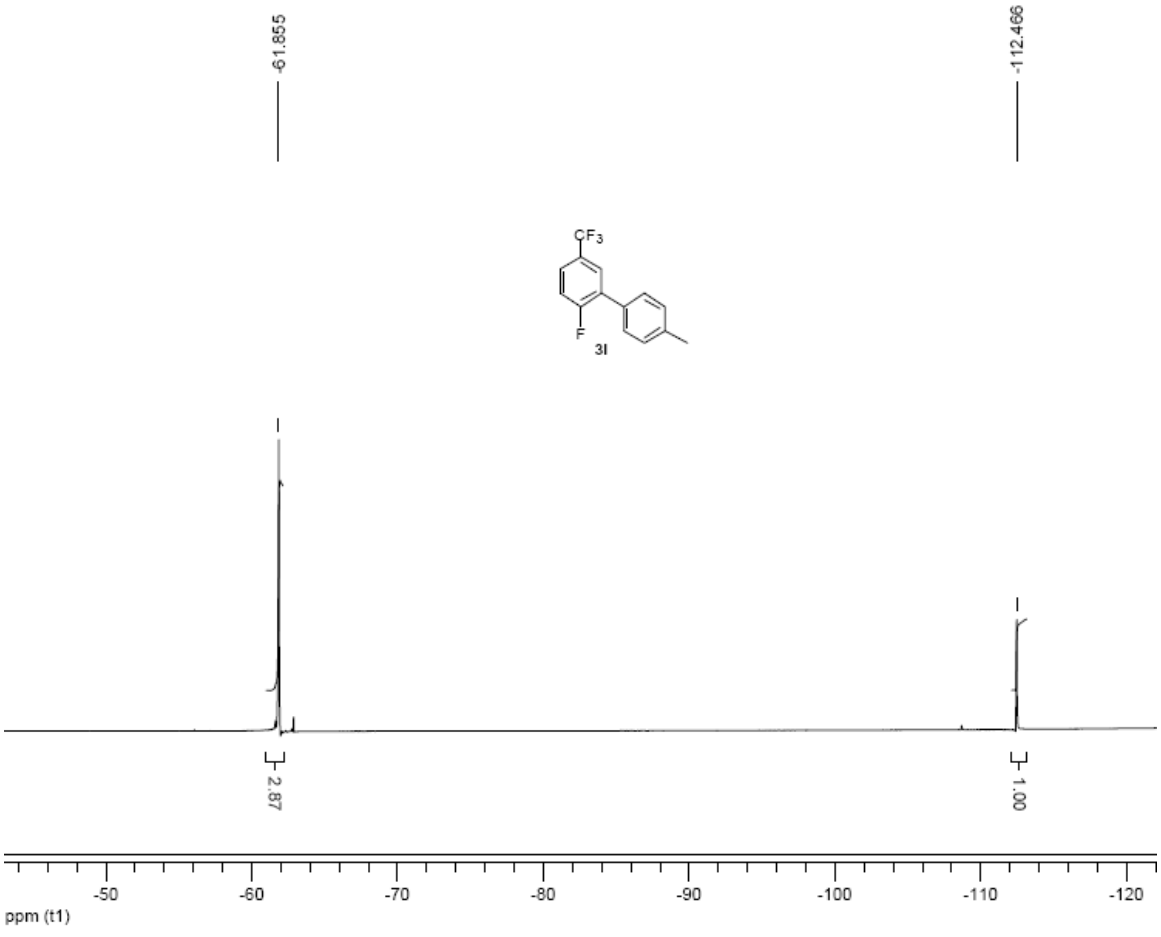
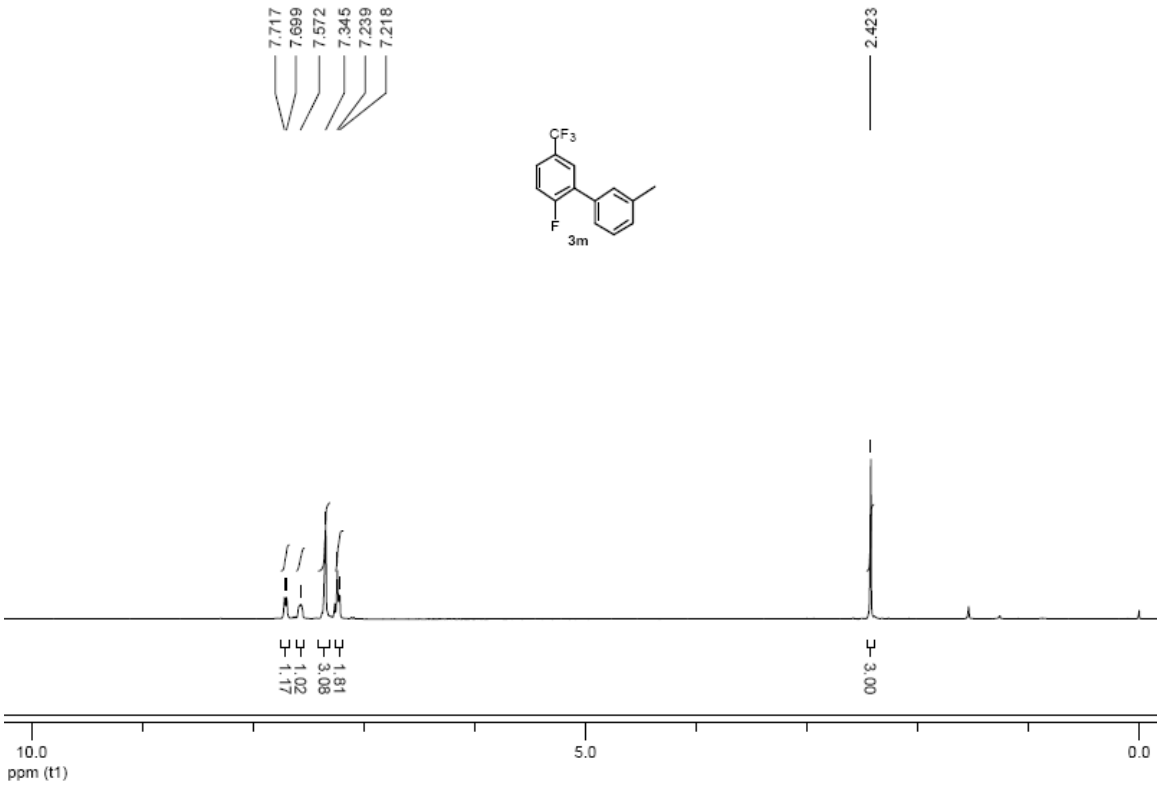
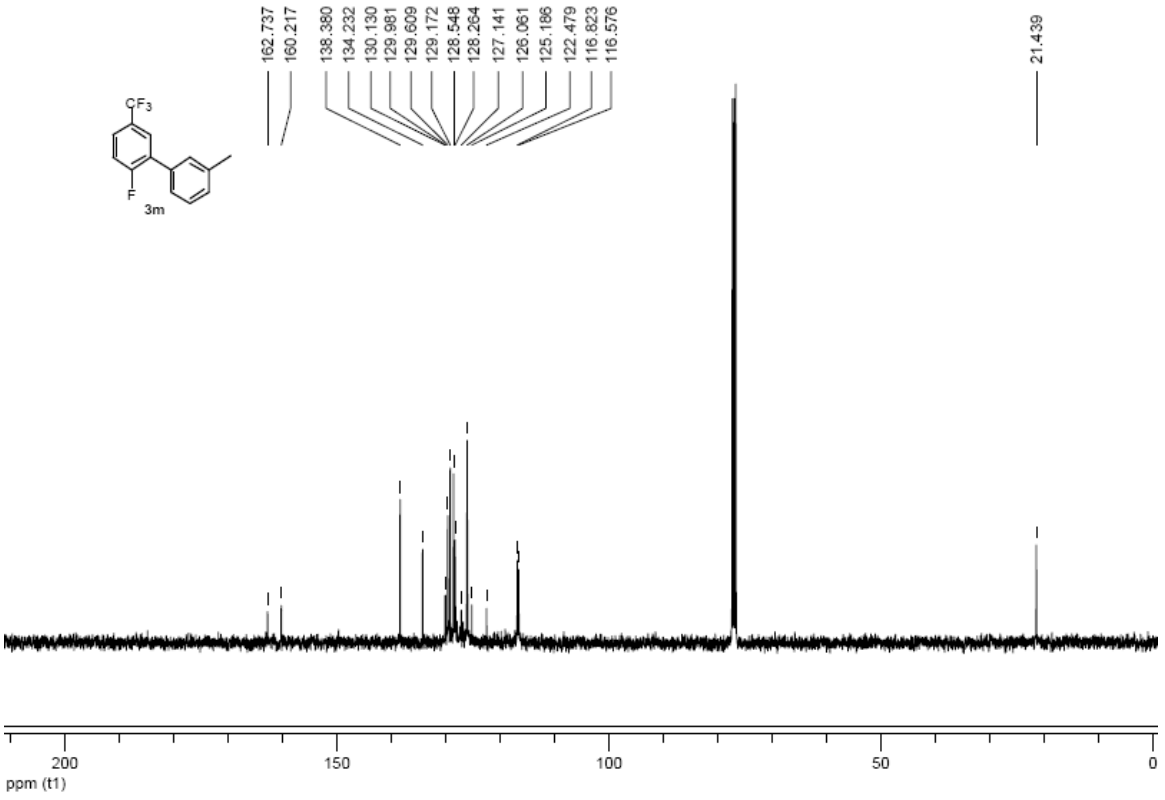
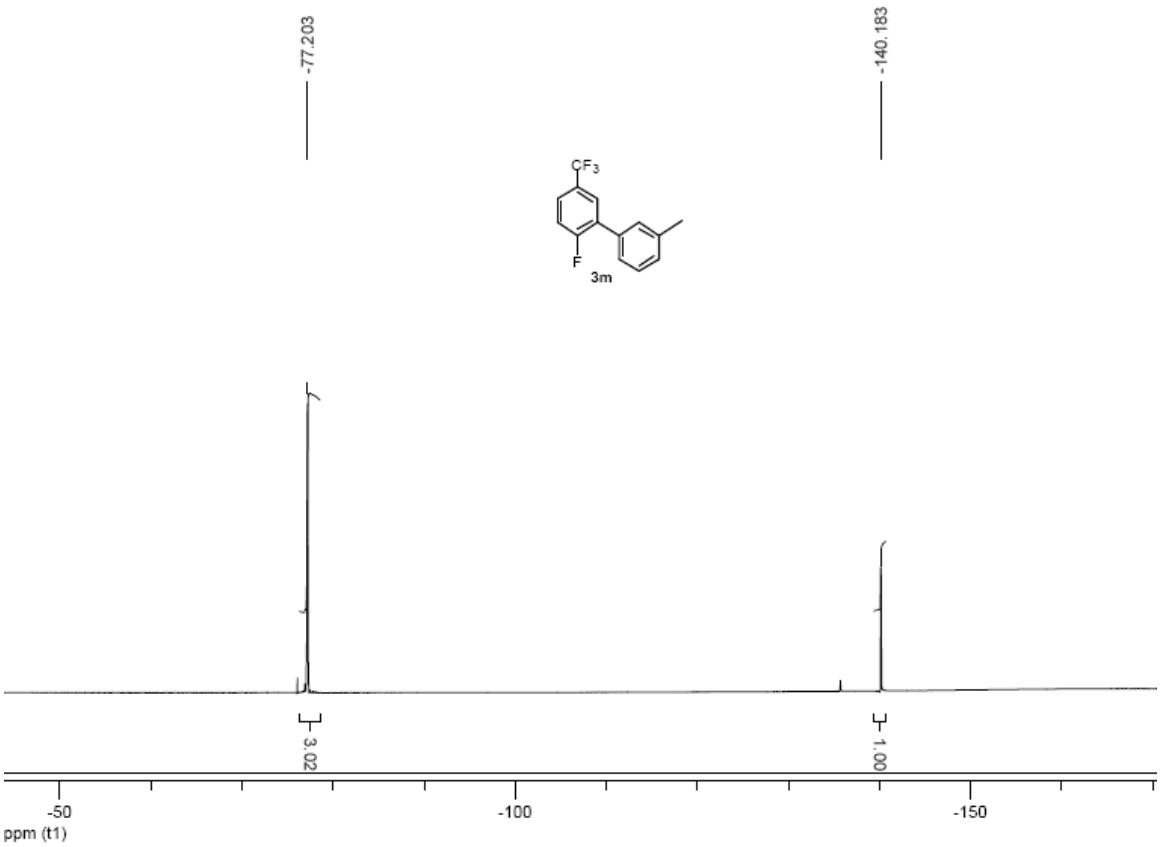
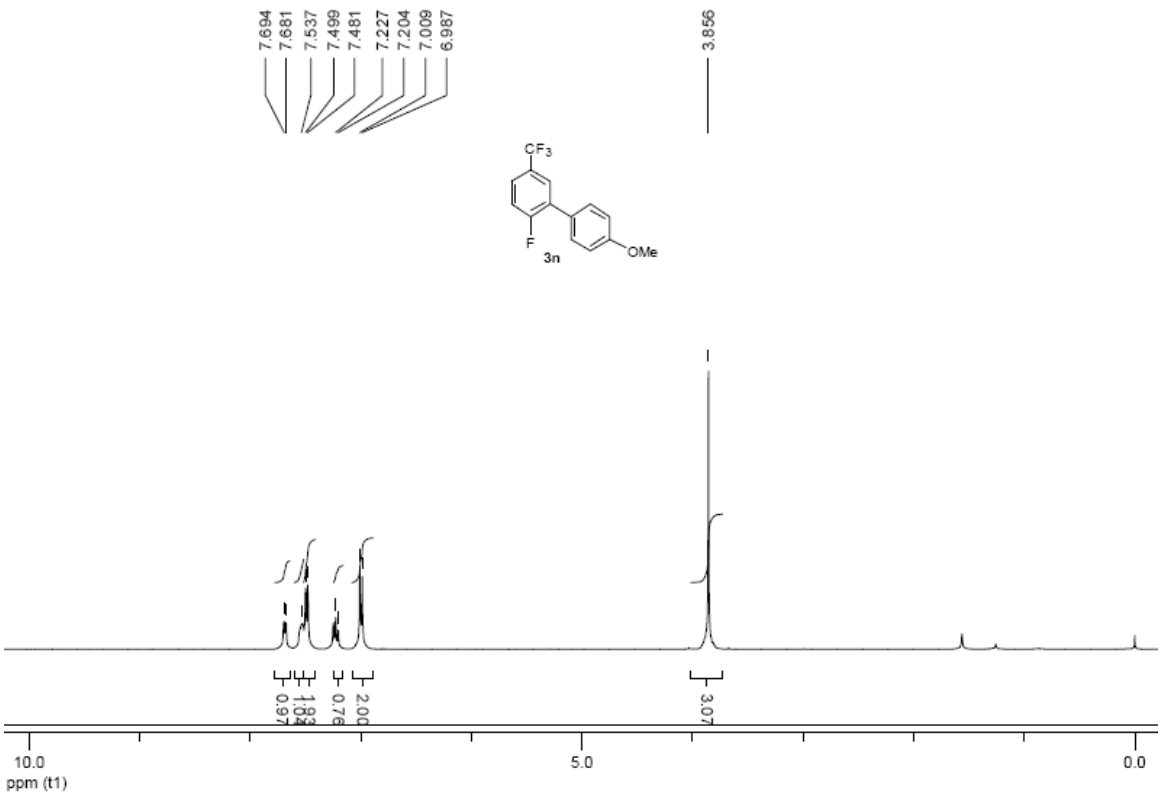
125.878
125.825
125.786
125.197
122.491
116.824
116.581
21.198
CF3
F
3l
250
200
150
100
50
0
ppm (t1)

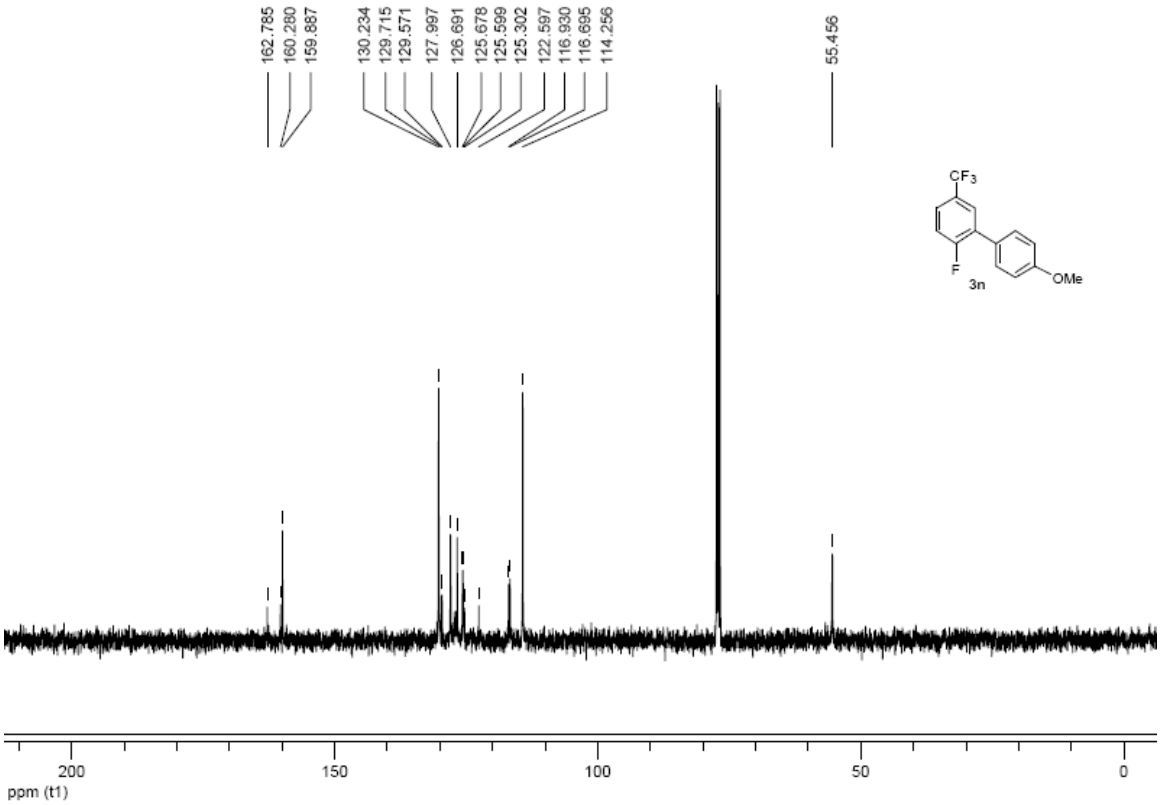

-61.855
-112.466
CF3
F
3l
2.87
1.00
-50
-60
-70
-80
-90
-100
-110
-120
ppm (t1)

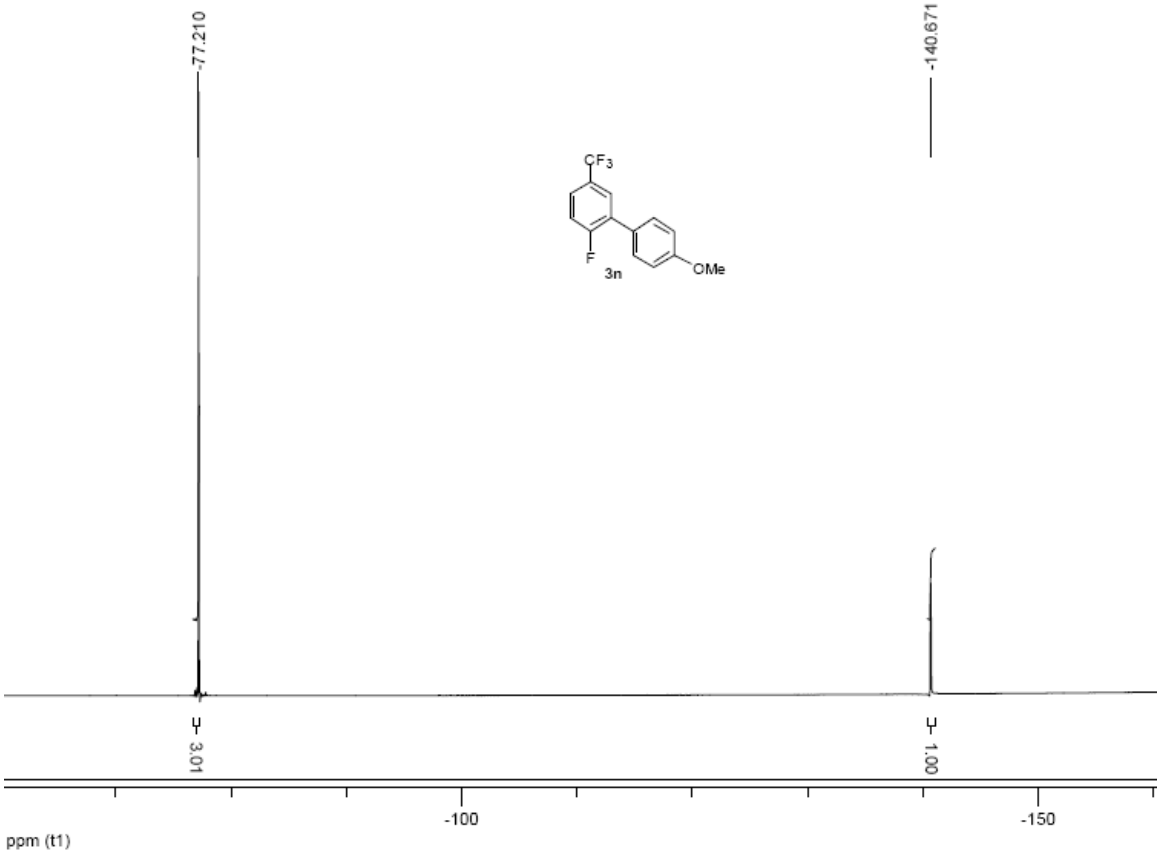

7.717
7.699
7.572
7.345
7.239
7.218
2.423
CF3
F
3m
1.17
1.02
3.08
1.81
3.00
10.0
ppm (t1)
5.0
0.0

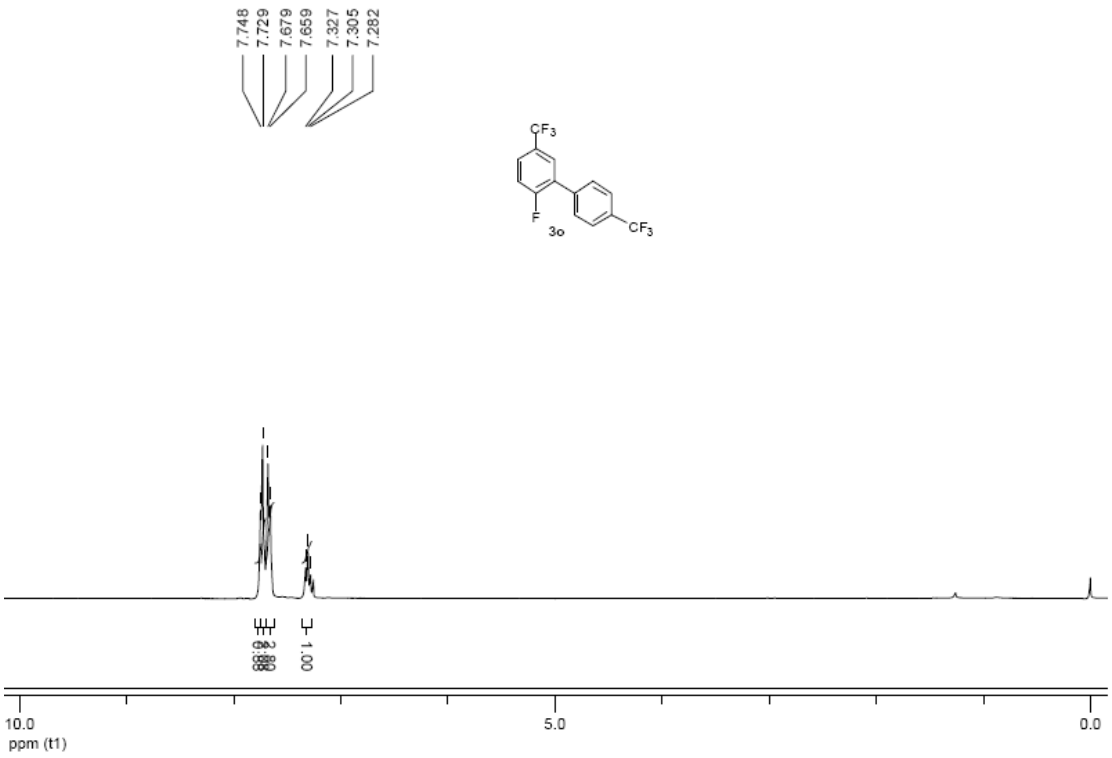

162.737
160.217
138.380
134.232
130.130
129.981
129.609
129.172
128.548
128.264
127.141
126.061
125.186
122.479
116.823
116.576
21.439
CF3
F
3m
200
150
100
50
0
ppm (t1)

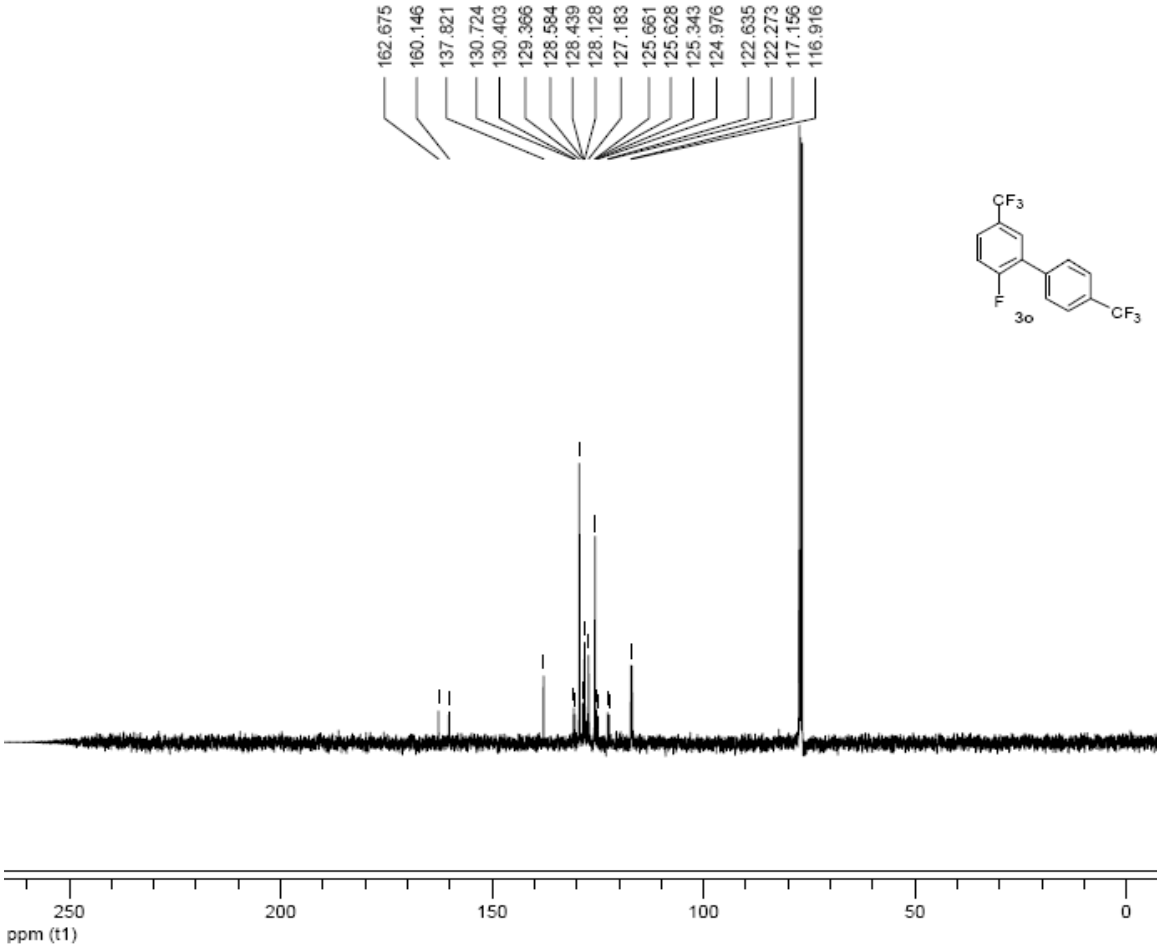

-77.203
-140.183
CF3
F
3m
3.02
1.00
-50
-100
-150
ppm (t1)

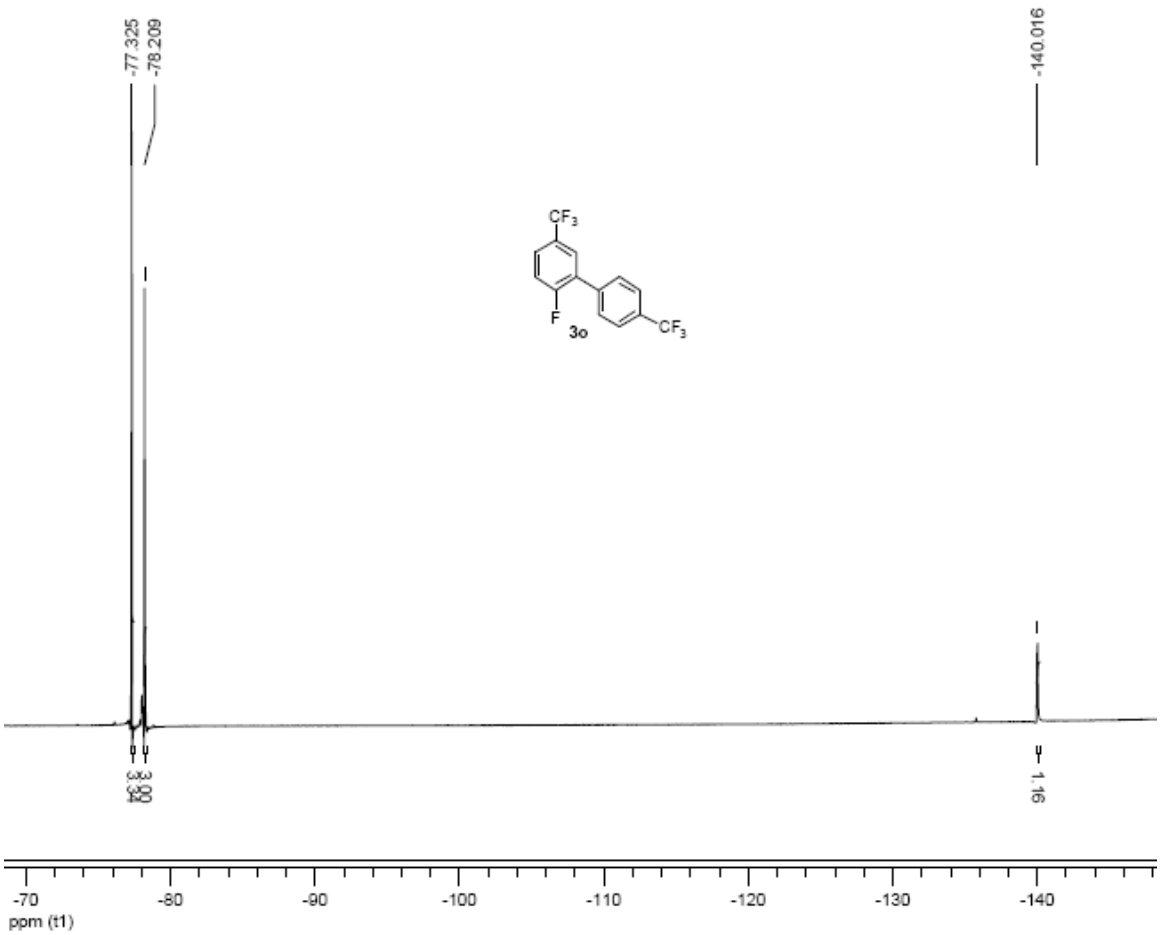

7.694
7.681
7.537
7.499
7.481
7.227
7.204
7.009
6.987
3.856
CF3
F
3n
OMe
0.97
1.04
1.13
0.76
2.00
3.07
10.0
5.0
0.0
ppm (t1)


162.785
160.280
159.887
130.234
129.715
129.571
127.997
126.691
125.678
125.599
125.302
122.597
116.930
116.695
114.256
55.456
CF3
F
3n
OMe
200
150
100
50
0
ppm (t1)

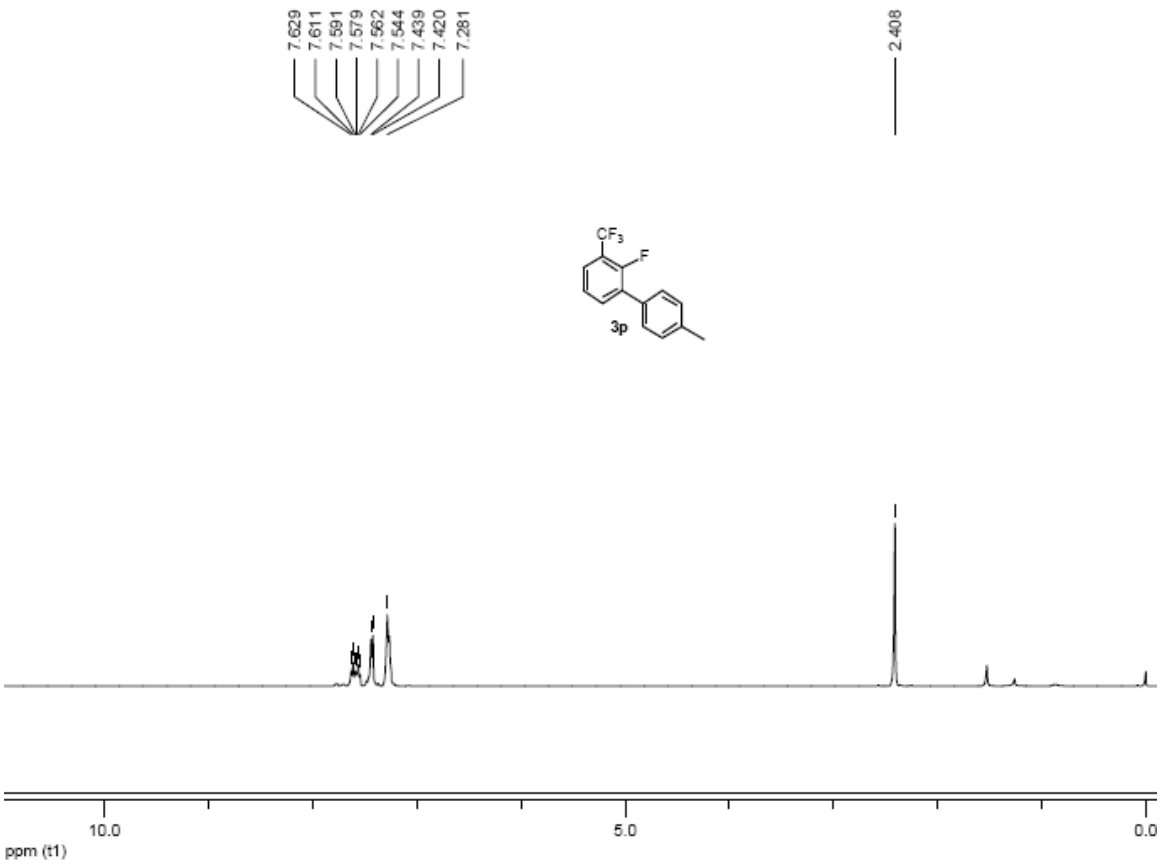

-77.210
-140.671
CF3
F
3n
OMe
3.01
1.00
-100
-150
ppm (t1)


7.748
7.729
7.679
7.659
7.327
7.305
7.282
CF3
F
3o
CF3
2.00
1.00
10.0
5.0
0.0
ppm (t1)

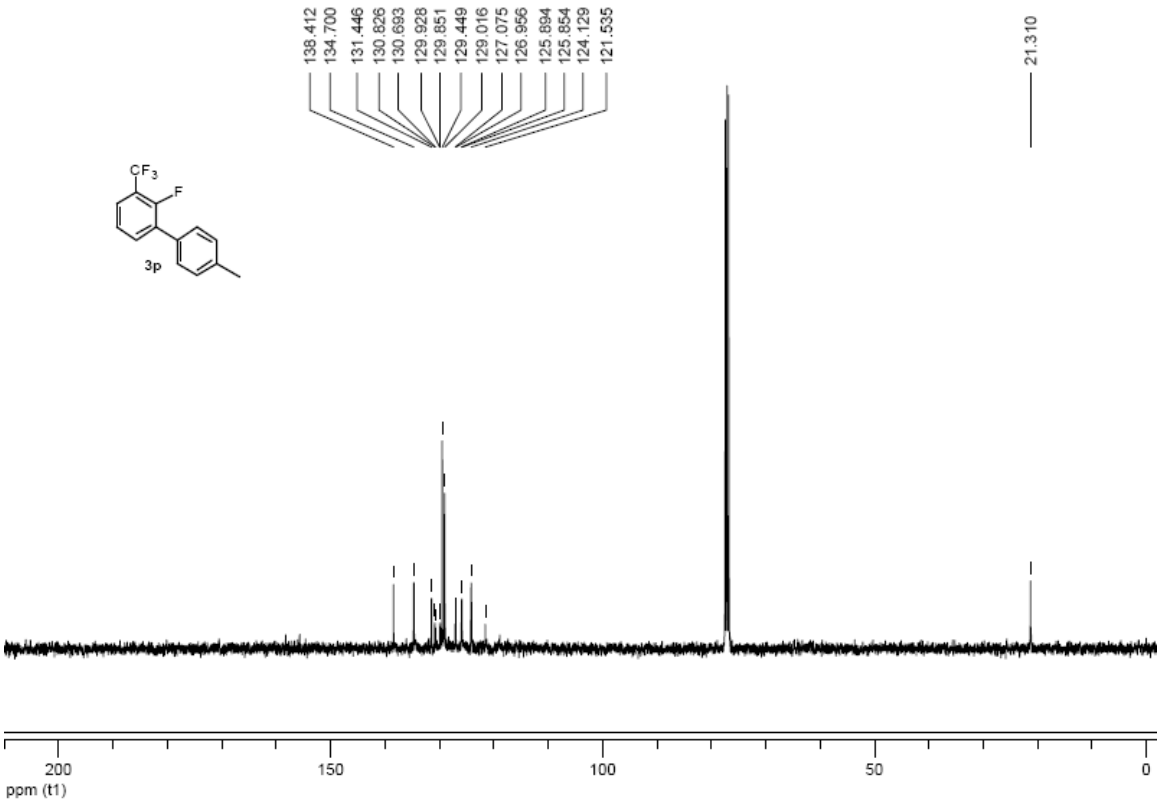

162.675
160.146
137.821
130.724
130.403
129.366
128.584
128.439
128.128
127.183
125.661
125.628
125.343
124.976
122.635
122.273
117.156
116.916
CF3
F
3o
CF3
250
200
150
100
50
0
ppm (t1)

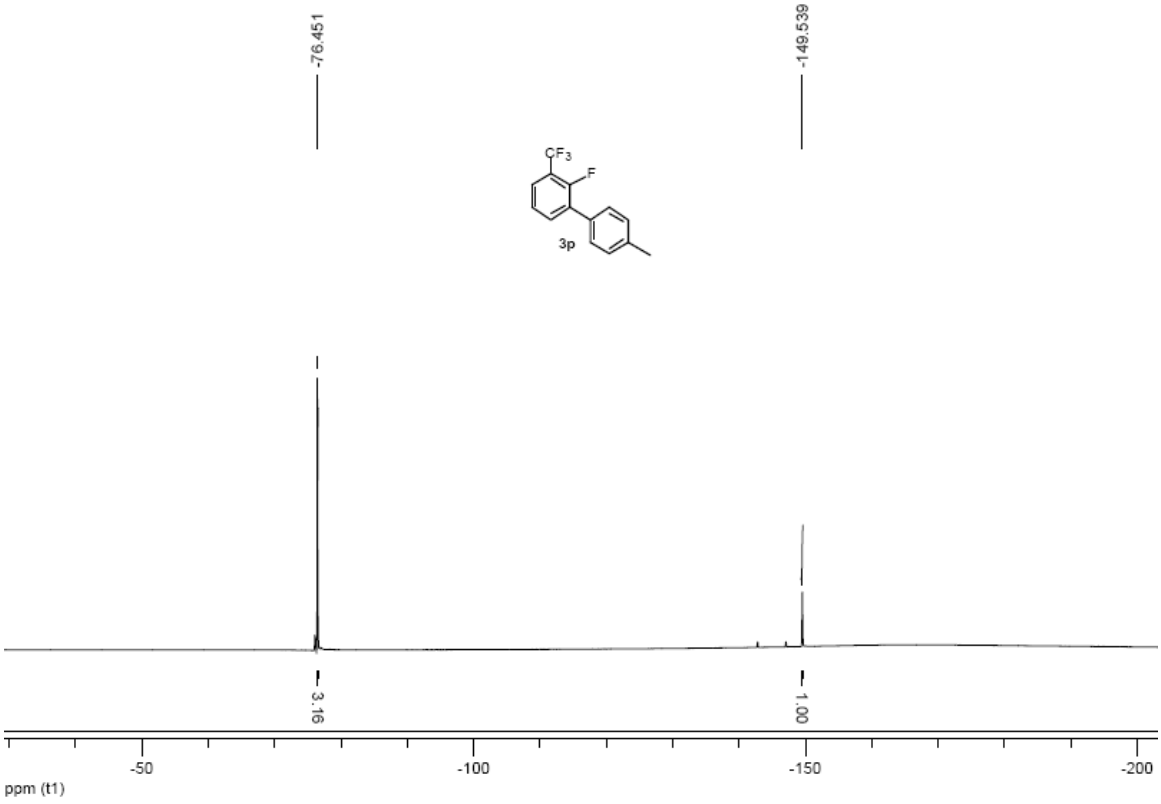

-77.325
-78.209
-140.016
3.00
3.94
1.16
-70
-80
-90
-100
-110
-120
-130
-140
ppm (t1)

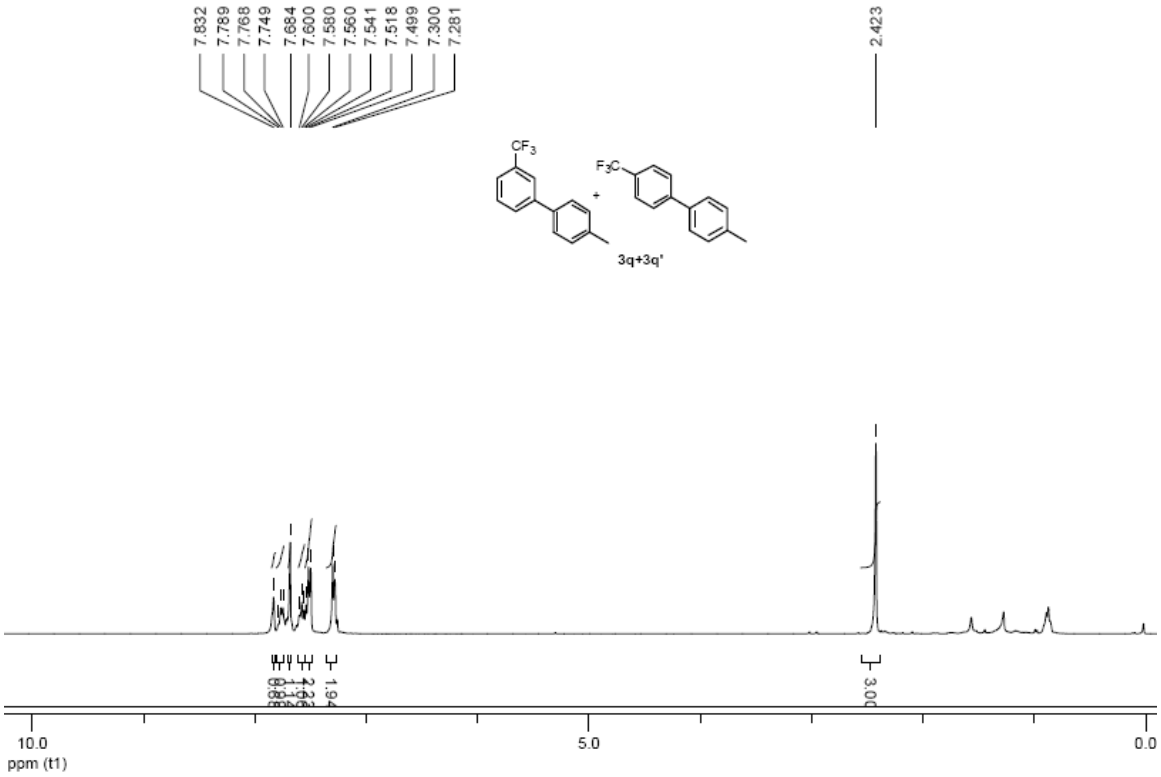
3o

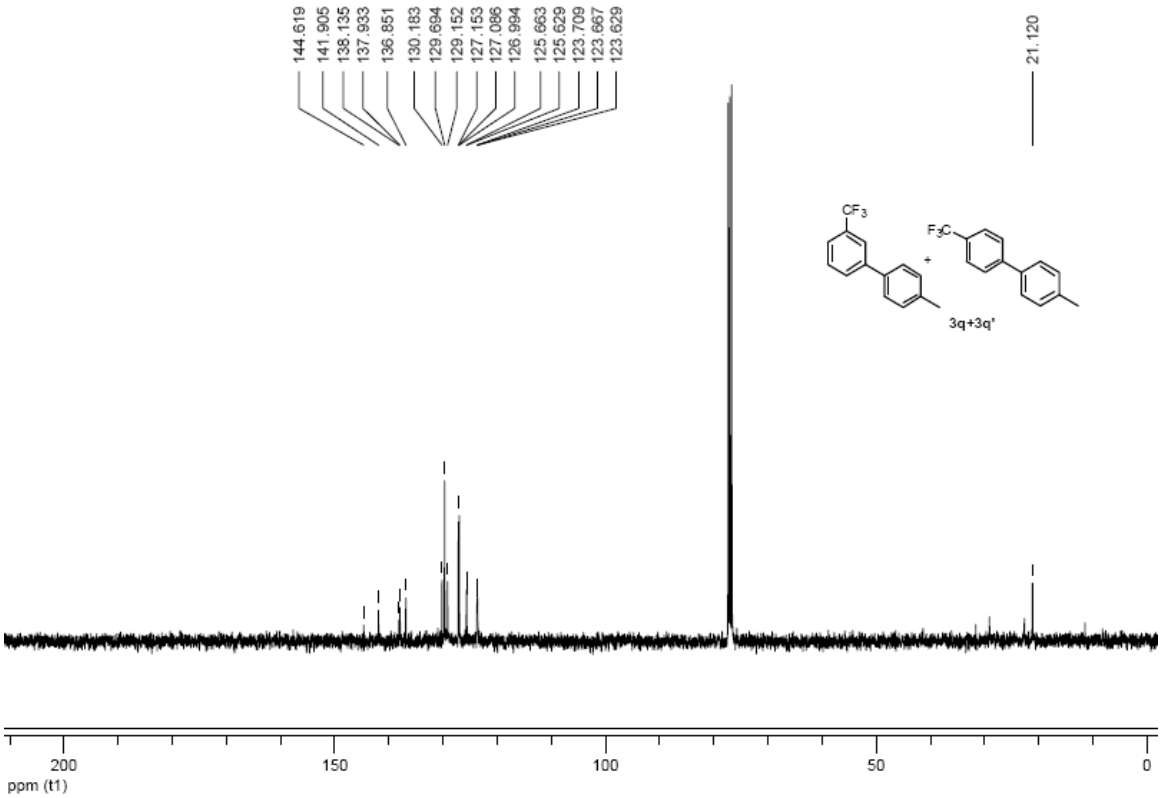

7.629
7.611
7.591
7.579
7.562
7.544
7.439
7.420
7.281
2.408
10.0
5.0
0.0
ppm (t1)

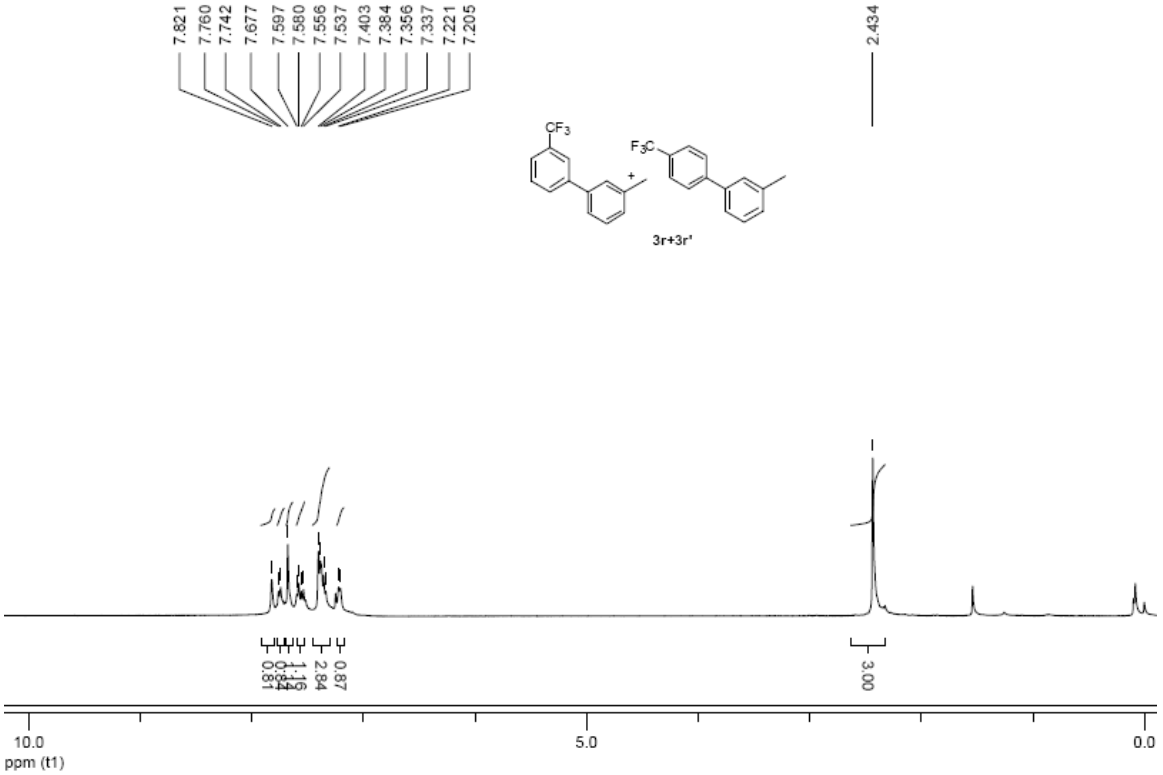
3p

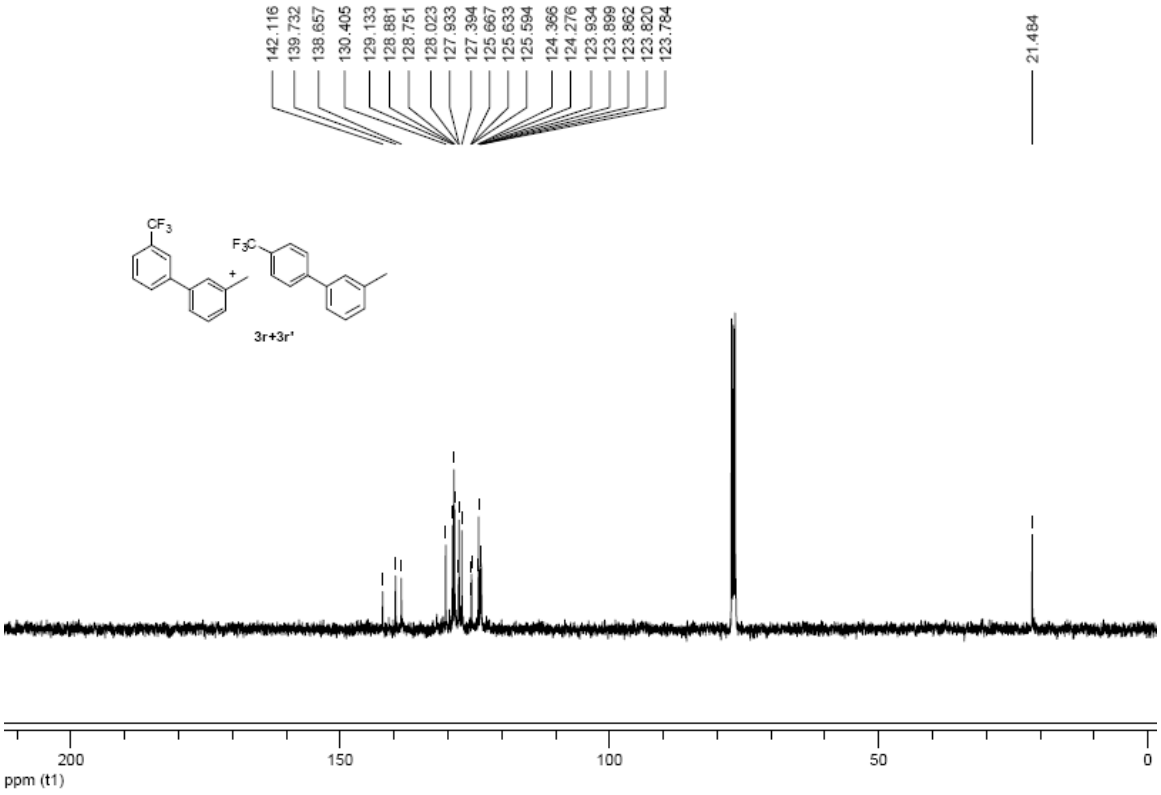

138.412
134.700
131.446
130.826
130.693
129.928
129.851
129.449
129.016
127.075
126.956
125.894
125.854
124.129
121.535
21.310
CF3
F
3p
200
150
100
50
0
ppm (t1)


-76.451
-149.539
CF3
F
3p
3.16
1.00
-50
-100
-150
-200
ppm (t1)


7.832
7.789
7.768
7.749
7.684
7.600
7.580
7.560
7.541
7.518
7.499
7.300
7.281
2.423
CF3
F3C
3q+3q'
10.0
5.0
0.0
ppm (t1)


144.619
141.905
138.135
137.933
136.851
130.183
129.694
129.152
127.153
127.086
126.994
125.663
125.629
123.709
123.667
123.629
21.120
CF3
F3C
3q+3q'
200
150
100
50
0
ppm (t1)


7.821
7.760
7.742
7.677
7.597
7.580
7.556
7.537
7.403
7.384
7.356
7.337
7.221
7.205
2.434
CF3
F3C
3r+3r'
0.81
0.84
1.15
2.84
0.87
3.00
10.0
5.0
0.0
ppm (t1)


142.116
139.732
138.657
130.405
129.133
128.881
128.751
128.023
127.933
127.394
125.667
125.633
125.594
124.366
124.276
123.934
123.899
123.862
123.820
123.784
21.484
CF3
F3C
3r+3r'
200
150
100
50
0
ppm (t1)