Electronic Supplementary Material (ESI) for Catalysis Science & Technology.


# Supporting Information

# Trifluoromethylation of Thiophenols and Thiols with Sodium Trifluoromethanesulfinate and Iodine Pentoxide

Jing-Jing Ma[a], Wen-Bin Yi[a]*, Guo-Ping Lu[a] and Chun Cai[a]

*School of Chemical Engineering, Nanjing University of Science and Technology, Xiao Ling*

*Wei Street, Nanjing 210094, People's Republic of China*

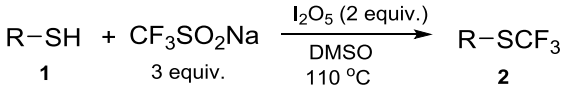
*Corresponding author. Fax: +86-25-84315030; Tel.: +86-25-84315514; E-mail: yiwenbin@mail.njust.edu.cn

## 1. General Information

Unless otherwise mentioned, solvents and reagents were purchased from commercial sources and used without further purification. $^{1}H$, $^{19}F$ and $^{13}C$ NMR spectra were recorded on a 500 MHz Bruker DRX 500 and tetramethylsilane (TMS) was used as a reference. Chemical shifts were reported in parts per million (ppm), $^{1}H$ NMR chemical shifts were determined relative to intermal $(CH_3)_4Si$ (TMS) at δ 0.0 (sometimes may be two points) or to the signal of a residual protonated solvent: $CDCl_3$ δ 7.26 (due to the quality of $CDCl_3$ the water peak may move to about 1.6 ppm). $^{13}C$ NMR chemical shifts were determined relative to internal TMS at δ 0.0. Data for $^{1}H$, $^{13}C$ and $^{19}F$ NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet, br = broad). GC-MS were performed on an ISQ Trace 1300 (electrospray ionization: EI).

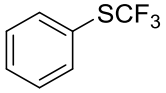
## 2. Representative Procedures and Analytical Data

### 2.1 General procedure for the trifluoromethylation of thiols or thiophenols



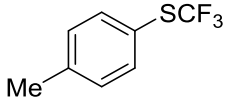

A reaction tube was charged with 4-Methyl-cinnamic acid (**1b**) (24.8 mg, 0.2 mmol) at room temperature, then trifluoromethanesulfinate (93.6 mg, 0.6 mmol) and iodine pentoxide (133.6 mg, 0.4 mmol), DMSO (2.0 mL) were added. The resulting mixture was stirred at 110 ℃ in this sealed tube equipped with a Teflon plug for 24 h. After cooling to room temperature, the reaction mixture was quenched and purified by flash silica gel column chromatography (eluent: hexane/EtOAc) to afford the desired product **2b** (34.2 mg, 89%).

### 2.2 Analytical data of compounds 2.



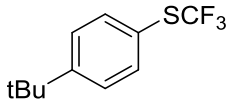

Chemical Formula: $C_7H_5F_3S$
Exact Mass: 178.02

Phenyl(trifluoromethyl)sulfane (**2a**)[1]: 26.3 mg, 74 % yield, colorless oil. $^{1}H$ NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.3 Hz, 2H), 7.52–7.46 (m, 1H), 7.46–7.38 (m, 2H); $^{19}F$ NMR (470 MHz, $CDCl_3$) δ -42.77 (s); GC-MS (EI) Calcd. for $C_7H_5F_3S$ 178.01, found 178.02.



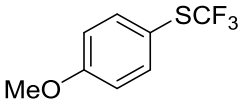

Chemical Formula: $C_8H_7F_3S$
Exact Mass: 192.02

(4-methylphenyl)(trifluoromethyl)sulfane (**2b**)[1]: 34.2 mg, 89% yield, colorless oil. $^{1}H$ NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.9 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 2.39 (s, 3H); $^{13}C$ NMR (126 MHz, $CDCl_3$) δ 141.42 (s), 136.42 (s), 133.19 (q, *J* = 308.7), 130.28 (s), 120.90 (s), 21.32 (s); $^{19}F$ NMR (470 MHz, $CDCl_3$) δ -43.22 (s). GC-MS (EI) Calcd. for $C_8H_7F_3S$ 192.02, found 192.02.



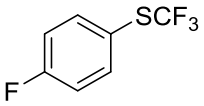

Chemical Formula: $C_{11}H_{13}F_3S$
Exact Mass: 234.26

(4-*tert*-butylphenyl)(trifluoromethyl)sulfane (**2c**)[1]: 39.3 mg, 84% yield, colorless oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.47–7.40 (m, 2H), 1.33 (s, 9H); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.99 (s). GC-MS (EI) Calcd. for $C_{11}H_{13}F_3S$ 234.07, found 234.26.



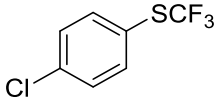

Chemical Formula: $C_8H_7F_3OS$
Exact Mass: 208.01

(4-methoxyphenyl)(trifluoromethyl)sulfane (**2d**)[1]: 37.8 mg, 91% yield, yellow oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.58 (t, *J* = 5.8 Hz, 2H), 7.03 – 6.82 (m, 2H), 3.84 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) $^{13}$C NMR (126 MHz, $CDCl_3$) δ 133.39, 130.94, 128.49, 126.04; δ 161.95 (s), 138.39 (s), 133.40 (q, *J* = 308.7), 115.02 (s), 55.52 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -43.94 (s). GC-MS (EI) Calcd. for $C_8H_7F_3OS$ 208.02, found 208.01.



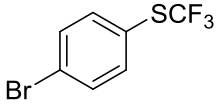

Chemical Formula: $C_7H_4F_4S$
Exact Mass: 196.01

(4-fluorophenyl)(trifluoromethyl)sulfane (**2e**)[2]: 29.8 mg, 76% yield, colorless oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.61 (m, 2H), 7.16 – 7.09 (m, 2H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 165.51 (d, *J* = 252.0), 138.76 (s), 138.69 (s), 130.61 (q, *J* = 302.4), 116.89(s), 116.71(s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -43.37 (s), -108.66 (s). GC-MS (EI) Calcd. for $C_7H_4F_4S$ 196.00, found 196.01.



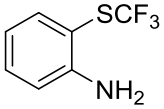

Chemical Formula: $C_7H_4ClF_3S$
Exact Mass: 211.99

(4-chlorophenyl)(trifluoromethyl)sulfane (**2f**)[1]: 34.6 mg, 82%, colorless oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.5 Hz, 2H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 137.71 (s), 137.60 (s), 130.55 (q, *J* = 308.7), 129.82 (s), 122.80 (s), 122.78 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.85 (s). GC-MS (EI) Calcd. for $C_7H_4ClF_3S$ 211.97, found 211.99.



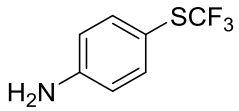

Chemical Formula: $C_7H_4BrF_3S$
Exact Mass: 255.95

(4-bromophenyl)(trifluoromethyl)sulfane (**2g**)[3]: 44.5 mg, 87%, yellow oil.. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.60 – 7.54 (m, 2H), 7.52 (d, *J* = 8.5 Hz, 2H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 137.75, 132.90 (q, *J* = 308.7 Hz), 132.81, 126.02, 123.44, 123.42; $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.74 (s). GC-MS (EI) Calcd. for $C_7H_4BrF_3S$ 255.92, found 255.95.



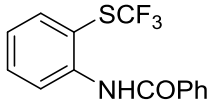

Chemical Formula: $C_7H_6F_3NS$
Exact Mass: 193.05

2-(trifluoromethylthio)aniline (**2h**)[4]: 22.8 mg, 59%, brown oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.8 Hz, 1H), 7.31 – 7.26 (m, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.77 – 6.71 (m, 1H); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.78 (s). GC-MS (EI) Calcd. for $C_7H_6F_3NS$ 193.02 , found .193.05.



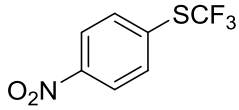

Chemical Formula: $C_7H_6F_3NS$
Exact Mass: 193.08

4-((trifluoromethyl)thio)aniline (**2i**)[8]: 29.3 mg, 76%, brown oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.4 Hz, 2H), 6.67-6.52 (m, 2H); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -44.44. GC-MS (EI) Calcd. for $C_7H_6F_3NS$ 193.05, found 193.08.



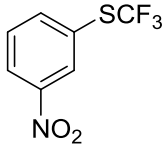

Chemical Formula: $C_{14}H_{10}F_3NOS$
Exact Mass: 297.13

*N*-(2-((trifluoromethyl)thio)phenyl)benzamide (**2j**): 89%, 52.8 mg, yellow power. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.97 (s, 1H), 8.62 (d, *J* = 8.4 Hz, 1H), 7.90-7.80 (m, 2H), 7.68-7.59 (m, 1H), 7.55 -7.48 (m, 2H), 7.45 (t, *J* = 7.5 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 165.37 (s), 141.62 (s) , 138.91 (s) , 134.63 (s) , 133.59 (s) , 132.42 (s) , 130 (q, *J* = 308.8), 129.16 (s) , 127.15 (s) , 124.72 (s) , 121.31(s) , 112.04 (s) ; $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.29. GC-MS (EI) Calcd. for $C_{14}H_{10}F_3NOS$ 297.04 , found 297.13.



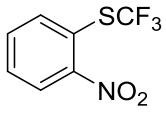

Chemical Formula: $C_7H_4F_3NO_2S$
Exact Mass: 223.03

(4-nitrophenyl)(trifluoromethyl)sulfane (**2k**)[5]: 39.2 mg, 88%, yellow oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.8 Hz, 2H), 7.83 (d, *J* = 8.7 Hz, 2H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 149.16 (s), 136.10 (s), 132.57 (q, J = 300.0), 124.37 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -41.31 (s). GC-MS (EI) Calcd. for $C_7H_4F_3NO_2S$ 222.09, found 223.03.




Chemical Formula: $C_7H_4F_3NO_2S$
Exact Mass: 222.98

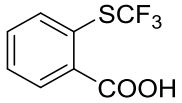
(*E*)-1-bromo-4-(3,3,3-trifluoroprop-1-en-1-yl)benzene (**2l**)[5]: 36.6 mg, 82%, yellow oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.55 (t, *J* = 1.9 Hz, 1H), 8.38 (ddd, *J* = 8.3, 2.2, 1.0 Hz, 1H), 8.01 (d, *J* = 7.8 Hz, 1H), 7.67 (t, *J* = 8.0 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 148.60 (s), 141.74 (s), 132.74 (q, *J* = 313.7), 130.79 (s), 130.44 (s), 126.78 (s), 125.74 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.03 (s). GC-MS (EI) Calcd. for $C_7H_4F_3NO_2S$ 222.99, found 222.98.




Chemical Formula: $C_7H_4F_3NO_2S$
Exact Mass: 223.00

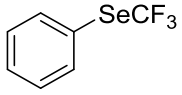
(2-nitrophenyl)(trifluoromethyl)sulfane (**2m**)[5]: 29.9 mg, 67%, yellow oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.67 (td, *J* = 7.9, 1.4 Hz, 1H),

7.59–7.52 (m, 1H); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -41.21 (s). GC-MS (EI) Calcd. for $C_7H_4F_3NO_2S$ 222.99, found 223.00.



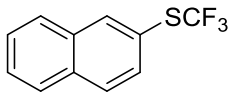

Chemical Formula: $C_8H_5F_3O_2S$
Exact Mass: 222.00

2-(trifluoromethylthio)benzoic acid (**2n**)[4]: 34.6 mg, 78%, yellow oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 6.9 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.66–7.55 (m, 1H), 7.48 (t, *J* = 7.5 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 171.45 (s), 134.13 (q, *J* = 297.4), 133.63 (s), 132.17 (s), 132.02 (s), 130.36 (s), 130.19 (s), 128.49 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.20 (s). GC-MS (EI) Calcd. for $C_8H_5F_3O_2S$ 222.00, found 222.00.



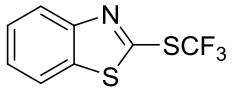

Chemical Formula: $C_7H_5F_3Se$
Exact Mass: 225.94

(*E*)-1-nitro-4-(3,3,3-trifluoroprop-1-en-1-yl)benzene (**2o**)[9]: 33.3 mg, 74%, yellow solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.3 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.5 Hz, 2H); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -36.11 (s). GC-MS (EI) Calcd. for $C_7H_5F_3Se$ 225.95, found 225.94.



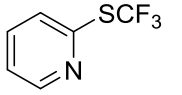

Chemical Formula: $C_{11}H_7F_3S$
Exact Mass: 228.03

Naphthalen-2-yl(trifluoromethyl)sulfane (**2p**)[2]: 37.8 mg, 83%, yellow oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.21 (s, 1H), 7.88 (d, *J* = 8.2 Hz, 3H), 7.67 (d, *J* = 8.5 Hz, 1H), 7.63–7.51 (m, 2H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 137.14 (s), 133.97 (s), 133.47 (s), 132.80 (q, *J* = 308.4), 131.92 (s), 129.32 (s), 128.29 (s), 128.04 (s), 127.89 (s), 127.11 (s), 121.61(s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -42.49 (s). GC-MS (EI) Calcd. for $C_{11}H_7F_3S$ 228.02, found 228.03.




Chemical Formula: $C_8H_4F_3NS_2$
Exact Mass: 235.01

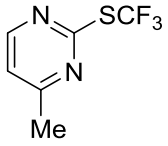
2-(trifluoromethylthio)benzo[d]thiazole (**2q**)[6]: 38.0 mg, 81%, brown solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.2 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.61–7.53 (m, 1H), 7.53–7.44 (m, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 166.63 (s), 153.10 (s), 151.74 (s), 137.89 (s), 134.05 (q, *J* = 312.5), 126.99 (s), 126.69 (s), 124.14 (s), 121.31 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -40.17 (d, *J* = 5.6 Hz). GC-MS (EI) Calcd. for $C_8H_4F_3NS_2$ 234.97, found 235.01.




Chemical Formula: $C_6H_4F_3NS$
Exact Mass: 179.07

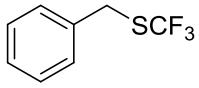
2-((trifluoromethyl)thio)pyridine (**2r**)[4]: 30.8 mg, 86%, red oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.62 (dd, *J* = 5.0, 1.9 Hz, 1H), 7.74 (td, *J* = 7.7, 2.0 Hz, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.33 (ddd, *J* = 7.6, 4.8, 1.1 Hz, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 150.65 (s), 149.26 (s), 137.83 (s), 136.42 (q,

*J* = 308.7), 128.26 (s), 123.95 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -40.38. GC-MS (EI) Calcd. for $C_6H_4F_3NS$ 179.00, found 179.07.



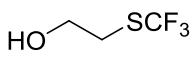

Chemical Formula: $C_6H_5F_3N_2S$
Exact Mass: 194.06

4-methyl-2-((trifluoromethyl)thio)pyrimidine (**2s**): 28.7 mg, 74%, red oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.42 – 6.73 (m, 1H), 2.51 (s, 3H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 168.97 (s), 165.23 (s), 157.48 (s), 132.12 (q, *J* = 307.4), 118.74 (s), 24.05 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -40.97. GC-MS (EI) Calcd. for $C_6H_5F_3N_2S$ 194.01, found 194.06.



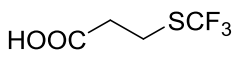

Chemical Formula: $C_8H_7F_3S$
Exact Mass: 192.04

Benzyl(trifluoromethyl)sulfane (**2t**)[7]: 32.2 mg, 84%, colorless oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 7.39 – 7.28 (m, 5H), 4.12 (s, 2H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 135.10 (s), 131.92 (q, *J* = 307.4), 129.00 (s), 128.94 (s), 128.10 (s), 34.37 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -41.66 (s). GC-MS (EI) Calcd. for $C_8H_7F_3S$ 192.02, found 192.04.



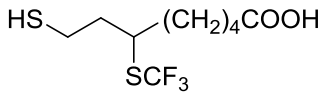

Chemical Formula: $C_3H_5F_3OS$
Exact Mass: 146.06

2-(trifluoromethylthio)ethanol (**2u**)[10]: 28.0 mg, 96%, colorless oil. $^1$H NMR (500 MHz, $CDCl_3$) δ 3.86 (t, *J* = 6.1 Hz, 2H), 3.06 (t, *J* = 6.1 Hz, 2H), 2.22 (s, 1H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 135.45 (q, *J* = 306.2), 61.13 (s), 32.77 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -40.83 (s). GC-MS (EI) Calcd. for $C_3H_5F_3OS$ 146.00, found 146.06.




Chemical Formula: $C_4H_5F_3O_2S$
Exact Mass: 174.01

3-(trifluoromethylthio)propanoic acid (**2v**)[4]: 34.4 mg, 99%, yellow solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 9.71 (s, 1H), 3.11 (t, *J* = 7.0 Hz, 2H), 2.81 (t, *J* = 7.0 Hz, 2H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 177.17 (s), 134.66 (q, *J* = 306.2), 34.68 (s), 24.34 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -41.59 (s). GC-MS (EI) Calcd. for $C_4H_5F_3O_2S$ 174.00, found 174.01.




Chemical Formula: $C_9H_{15}F_3O_2S_2$
Exact Mass: 276.02

8-mercapto-6-(trifluoromethylthio)octanoic acid (**2w**): 51.9 mg, 94%, yellow solid. $^1$H NMR (500 MHz, $CDCl_3$) δ 9.91 (d, *J* = 396.4 Hz, 1H), 3.16 – 2.90 (m, 2H), 2.76 (dd, *J* = 12.4, 6.1 Hz, 1H), 2.38 (t, *J* = 7.2 Hz, 2H), 2.10 (s, 1H), 1.98 (dt, *J* = 14.7, 7.5 Hz, 2H), 1.86–1.37 (m, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) δ 179.98 (s), 134.70 (q, *J* = 302.4), 50.89 (s), 50.78 (s), 34.11 (s), 33.96 (s), 33.87 (s), 27.35 (s), 27.25 (s), 26.37 (s), 26.29 (s), 24.43 (s), 20.89 (s); $^{19}$F NMR (470 MHz, $CDCl_3$) δ -40.98 (d, *J* = 3.5 Hz). GC-MS (EI) Calcd. for $C_9H_{15}F_3O_2S_2$ 276.05, found 276.02.

## Reference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[5] D. J. Adams, A. Goddard, D. J. Macquarrie, *Chem. Commun.*, 2000, 987–988.

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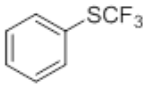
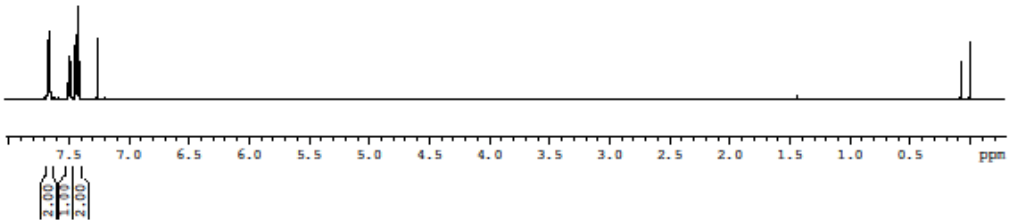
[10] C. Matheis, M.-Y. Wang, L. J. Goossen, *Synlett.* 2015, 26, 1628-1632.

## 3. NMR Spectra

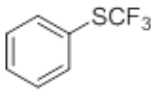




**500 MHz, $CDCl_3$**

**2a**

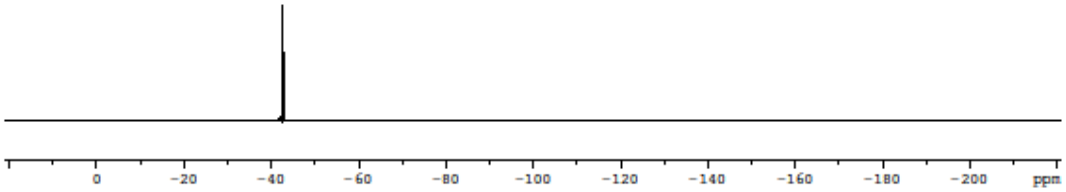


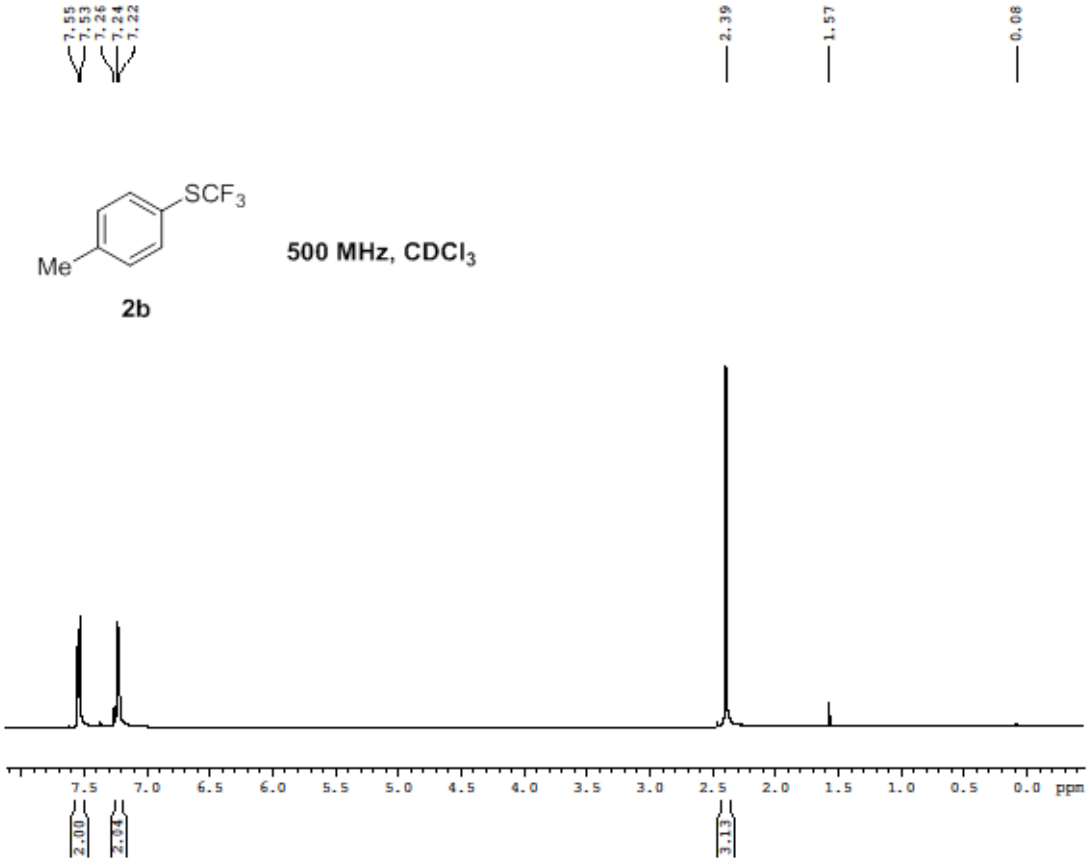


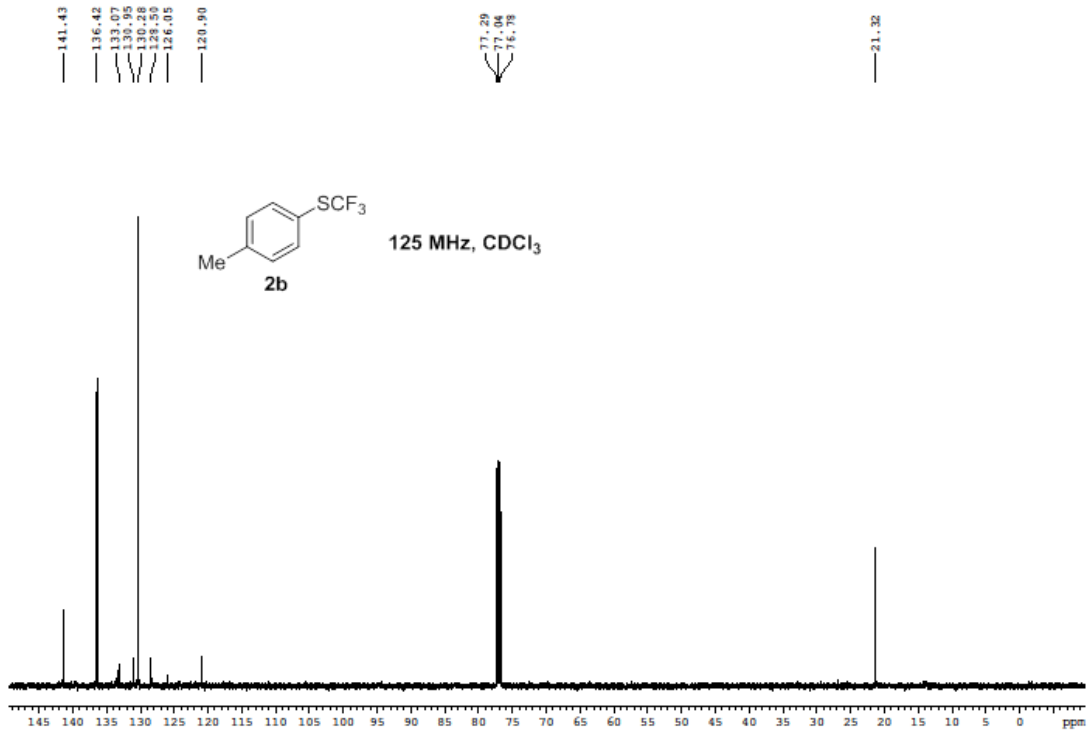


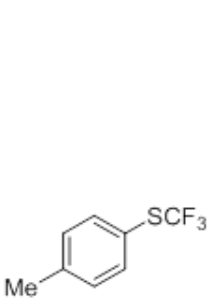

**470 MHz, $CDCl_3$**

**2a**



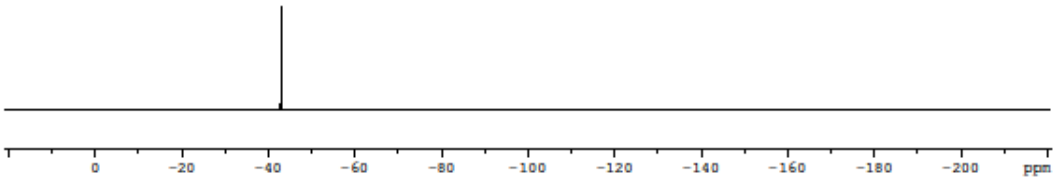

7.55
7.53
7.26
7.24
7.22
2.39
1.57
0.08
SCF3
Me
2b
500 MHz, CDCl3
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
2.04
3.13

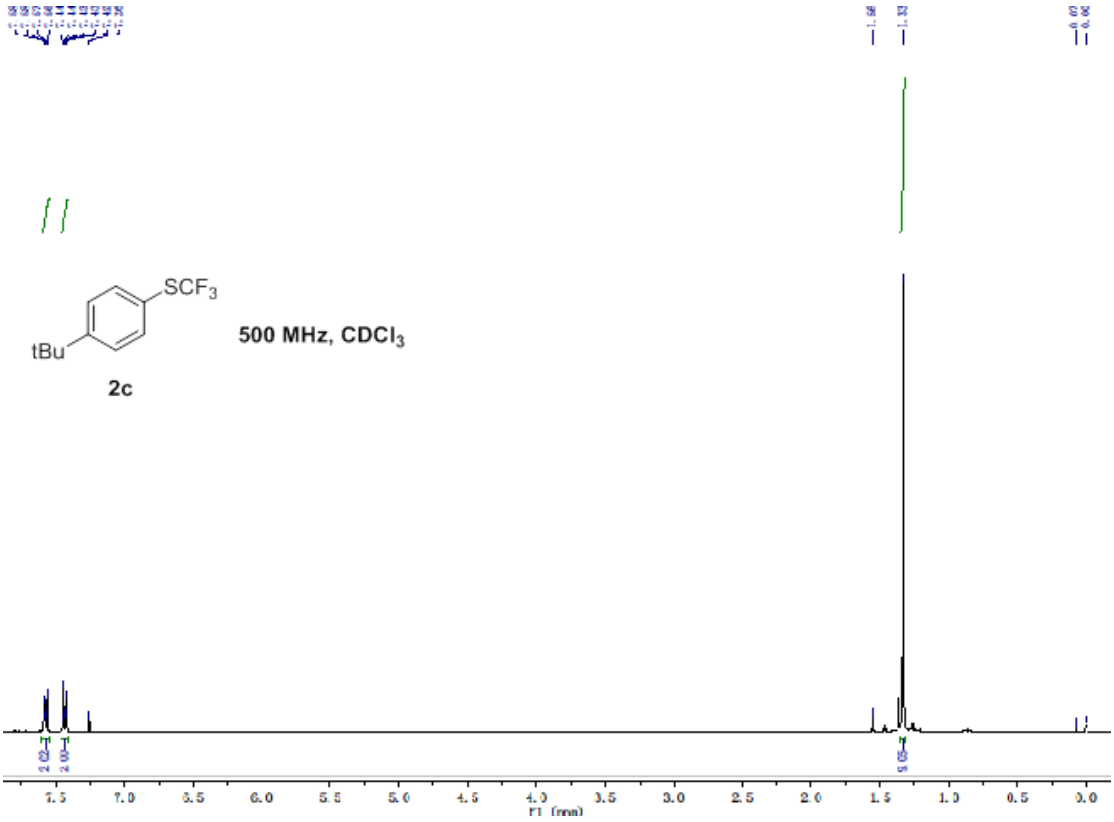

141.43
136.42
133.07
130.95
130.28
128.50
126.05
120.90
77.29
77.04
76.78
21.32
SCF3
Me
2b
125 MHz, CDCl3
145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 ppm




**470 MHz, $CDCl_3$**

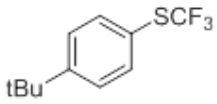
**2b**



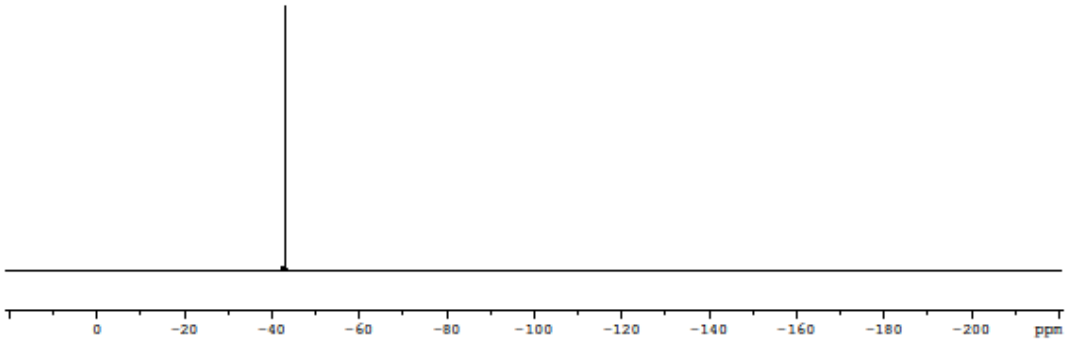

**500 MHz, $CDCl_3$**

**2c**

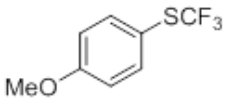




**470 MHz, $CDCl_3$**

**2c**

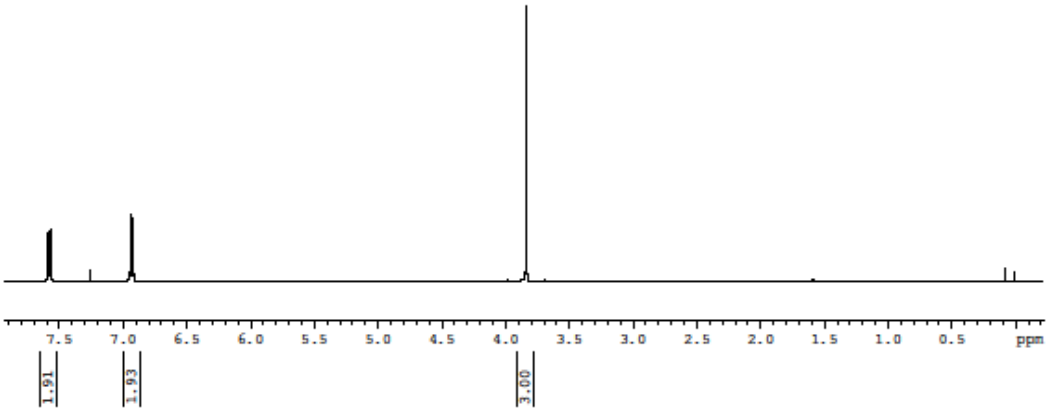


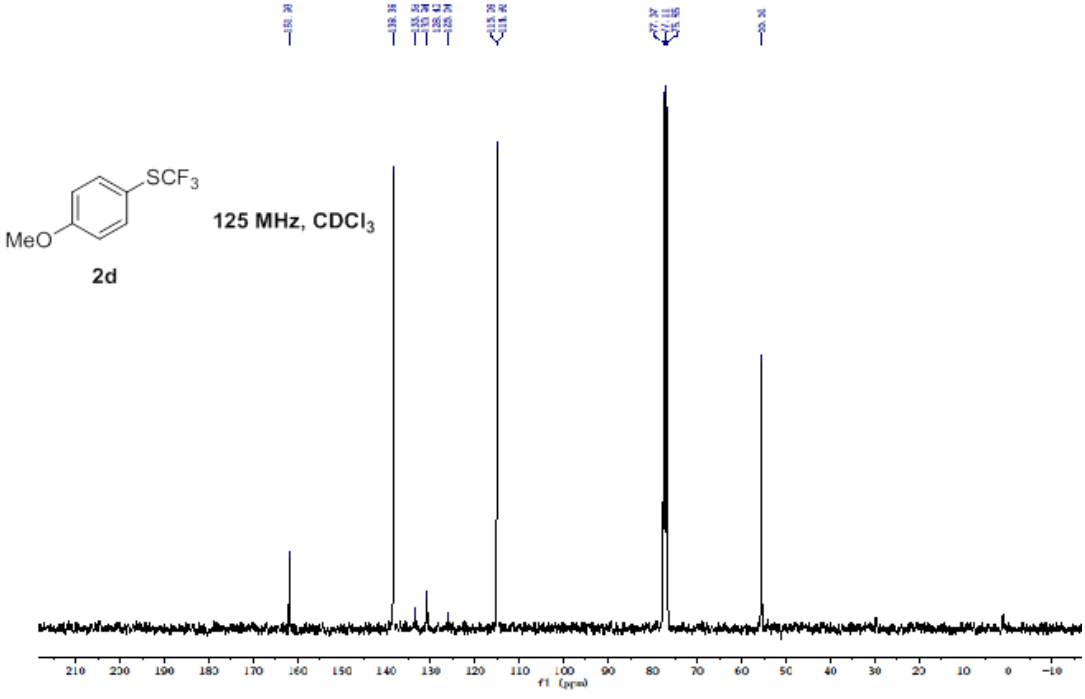


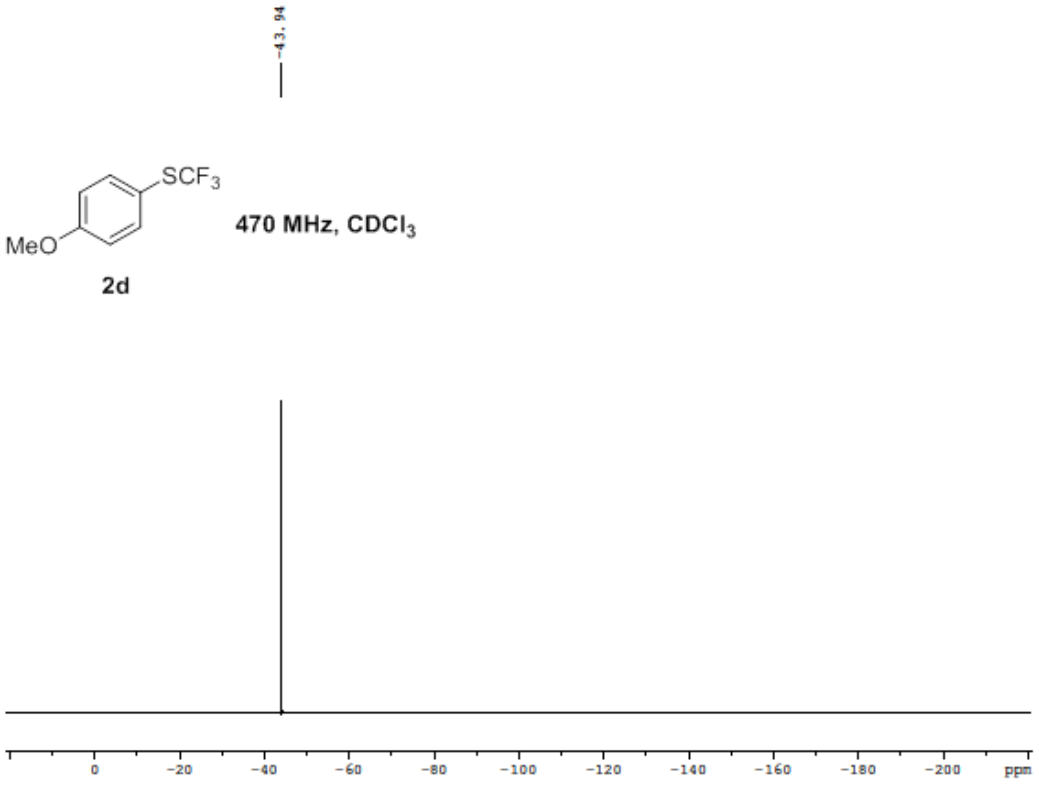



**500 MHz, $CDCl_3$**

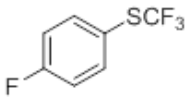
**2d**




SCF3
MeO
2d
125 MHz, CDCl3
f1 (ppm)

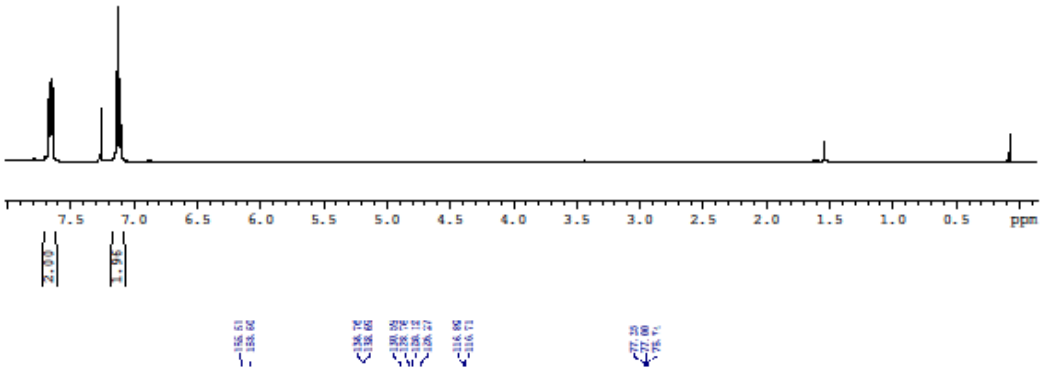

-43.94
SCF3
MeO
2d
470 MHz, CDCl3
ppm



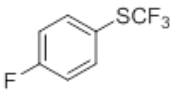



**500 MHz, $CDCl_3$**

**2e**

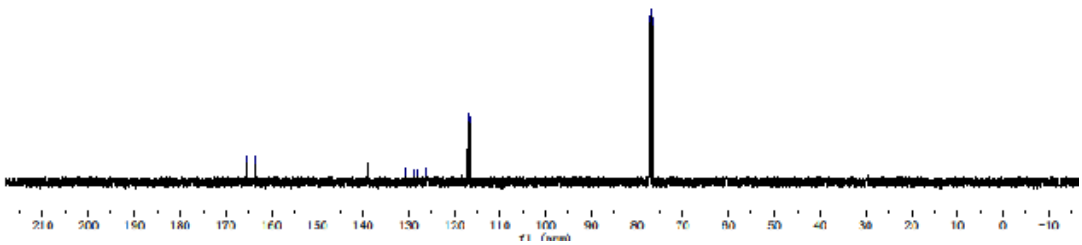


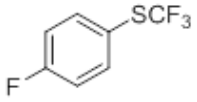



**125 MHz, $CDCl_3$**

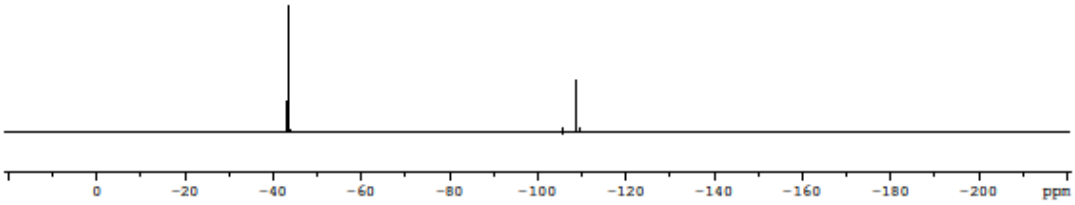
**2e**



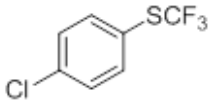




**470 MHz, $CDCl_3$**

**2e**

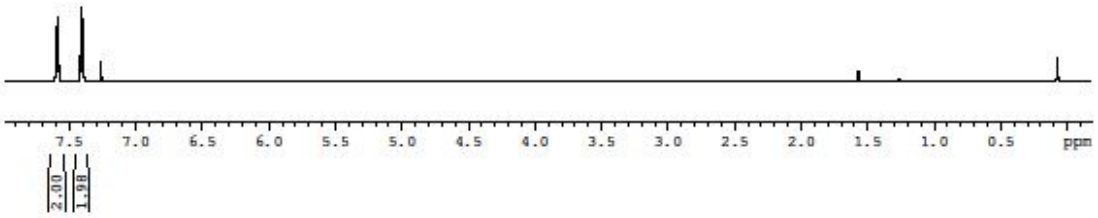


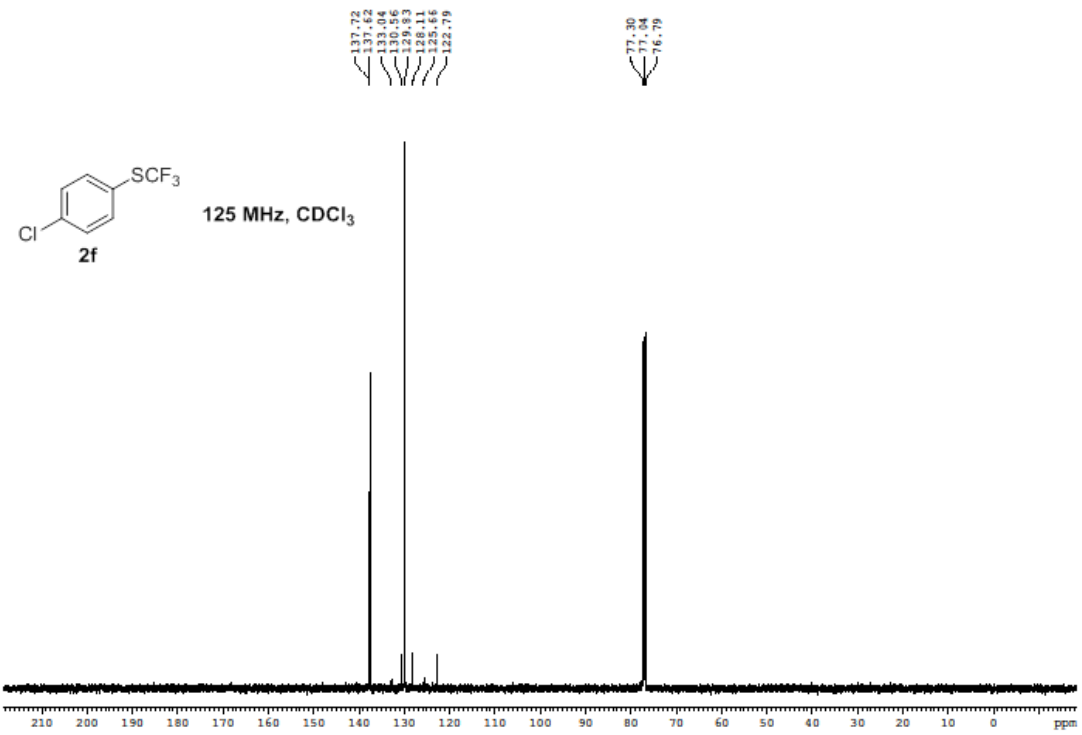


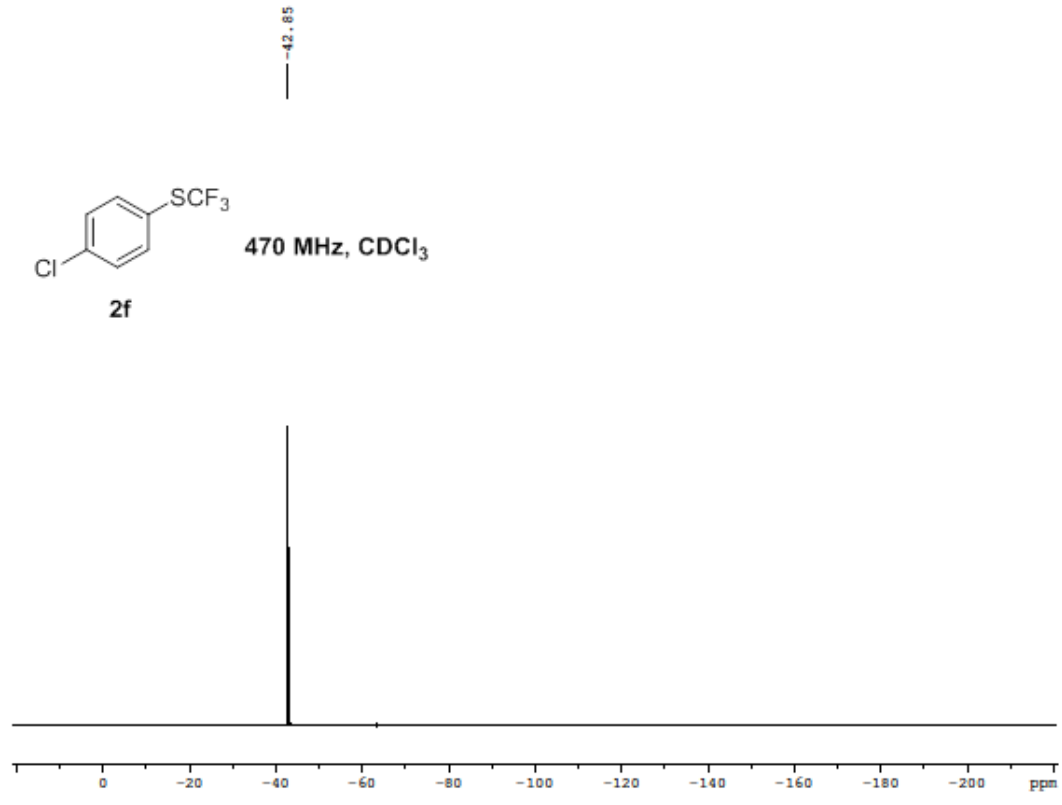



**500 MHz, $CDCl_3$**

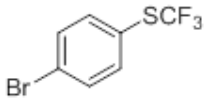
**2f**




137.72
137.62
133.04
130.56
129.83
128.11
125.46
122.79
77.30
77.04
76.79
SCF3
Cl
2f
125 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

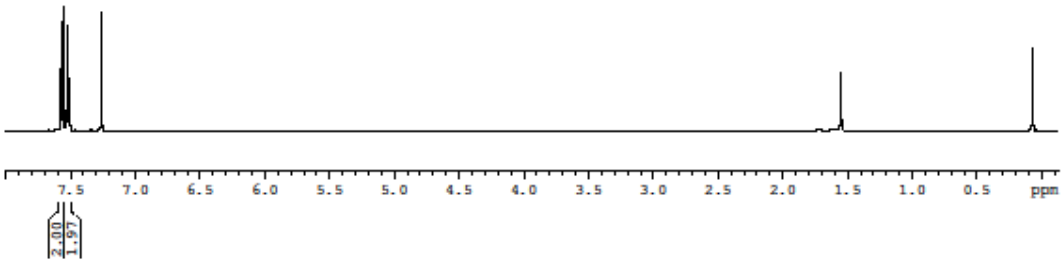

-42.85
SCF3
Cl
2f
470 MHz, CDCl3
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

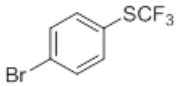



**500 MHz, $CDCl_3$**

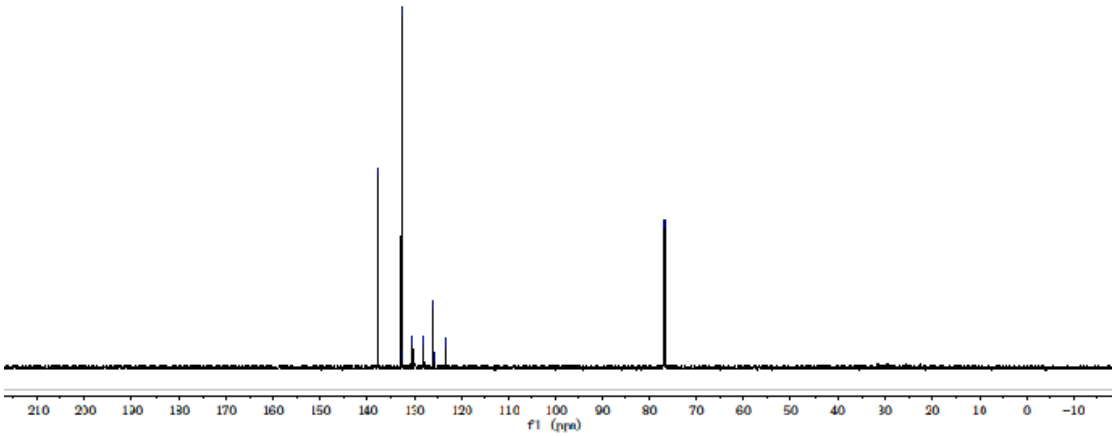
**2g**

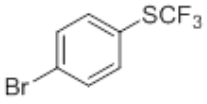



**125 MHz, $CDCl_3$**

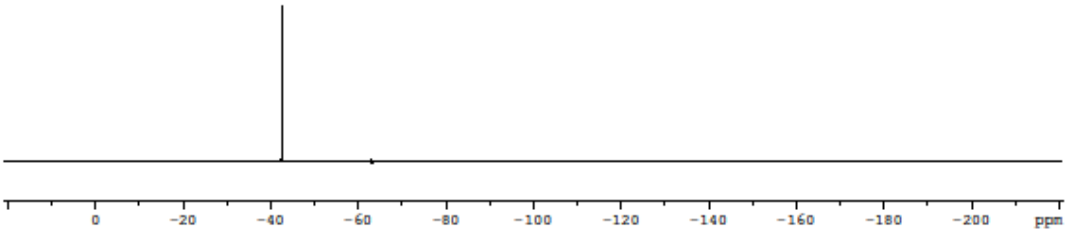
**2g**



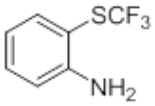




**470 MHz, $CDCl_3$**

**2g**

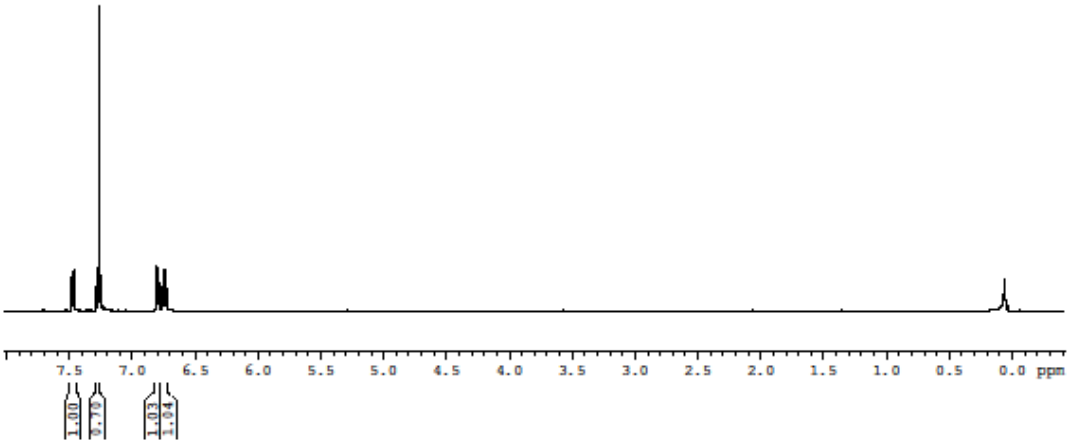


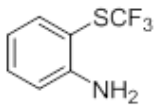



**500 MHz, $CDCl_3$**

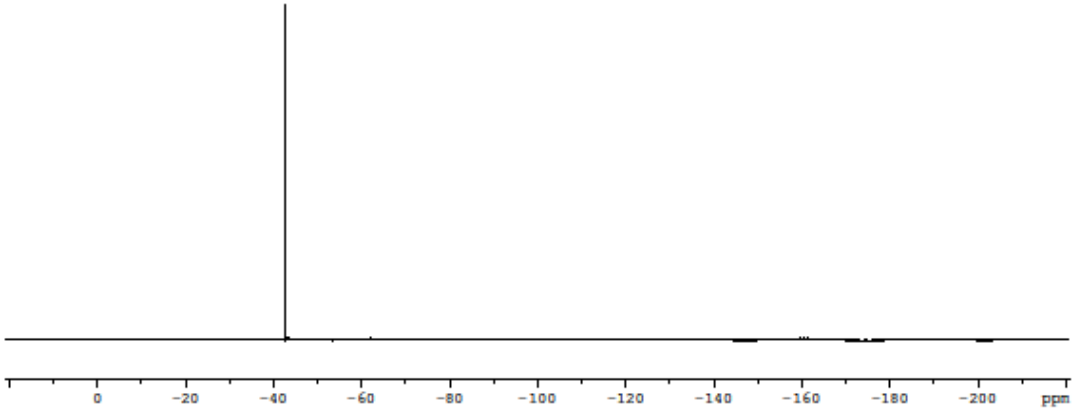
**2h**



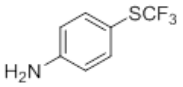




**470 MHz, $CDCl_3$**

**2h**

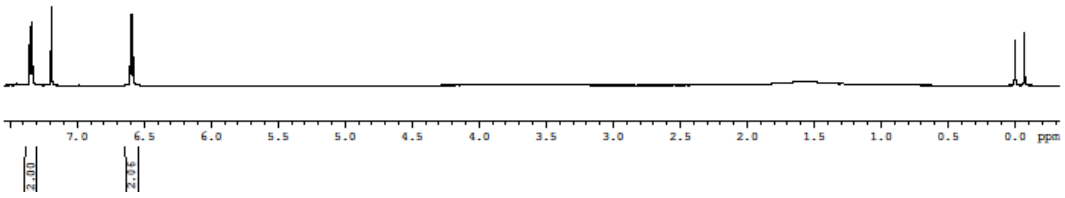


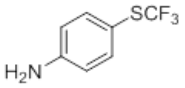





**500 MHz, $CDCl_3$**

**2i**

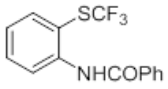




**470 MHz, $CDCl_3$**

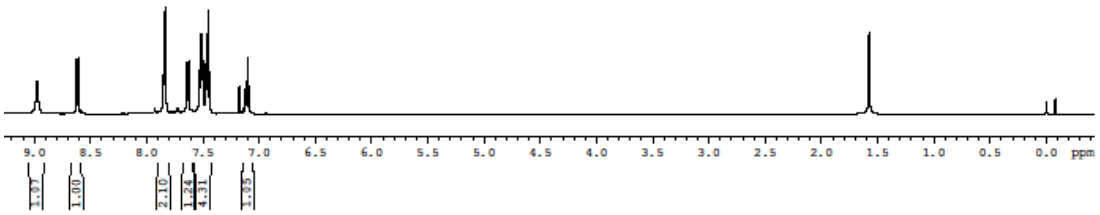
**2i**

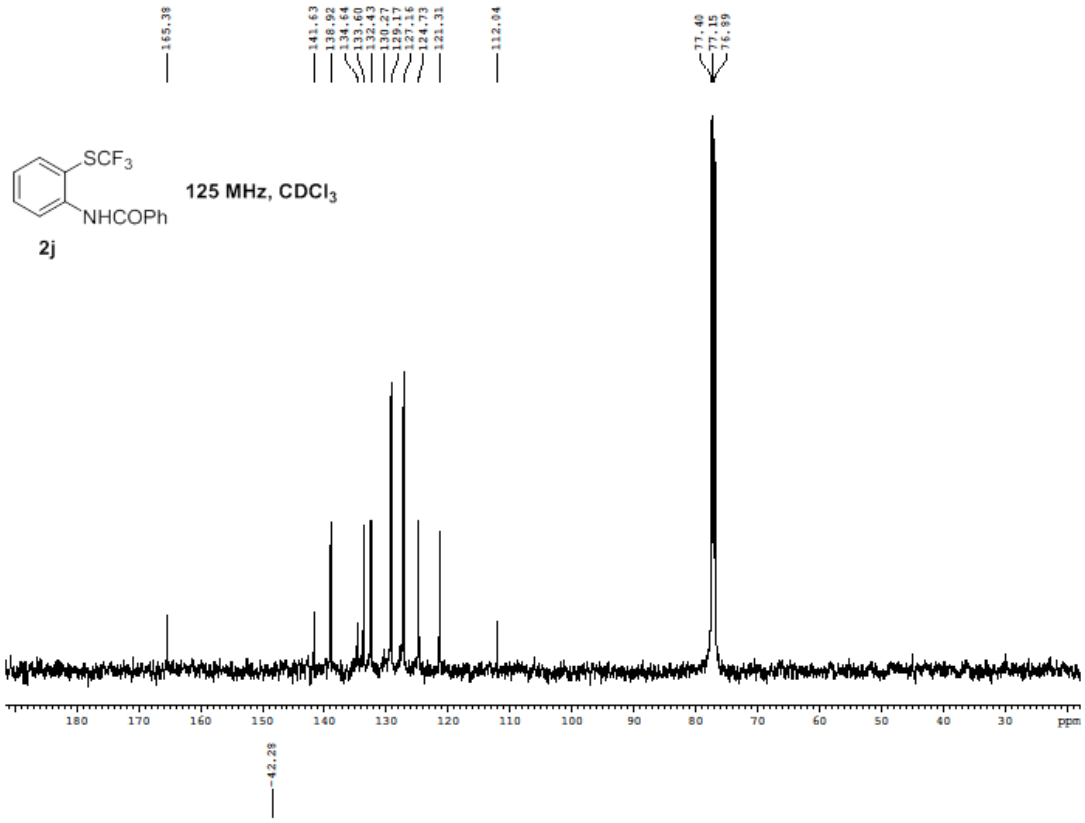


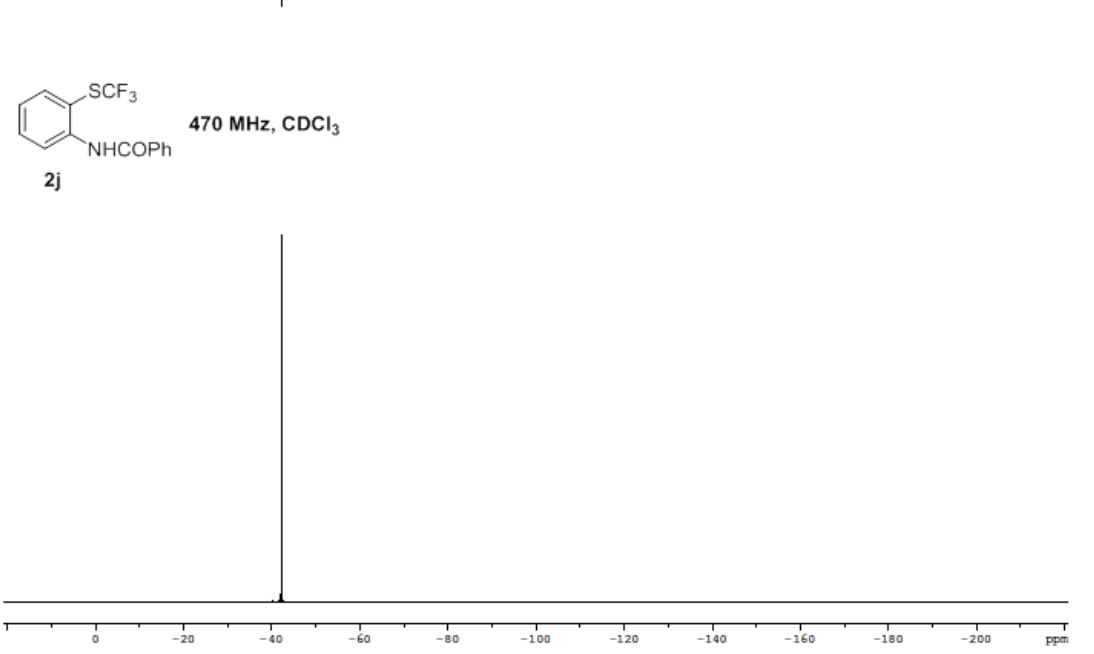



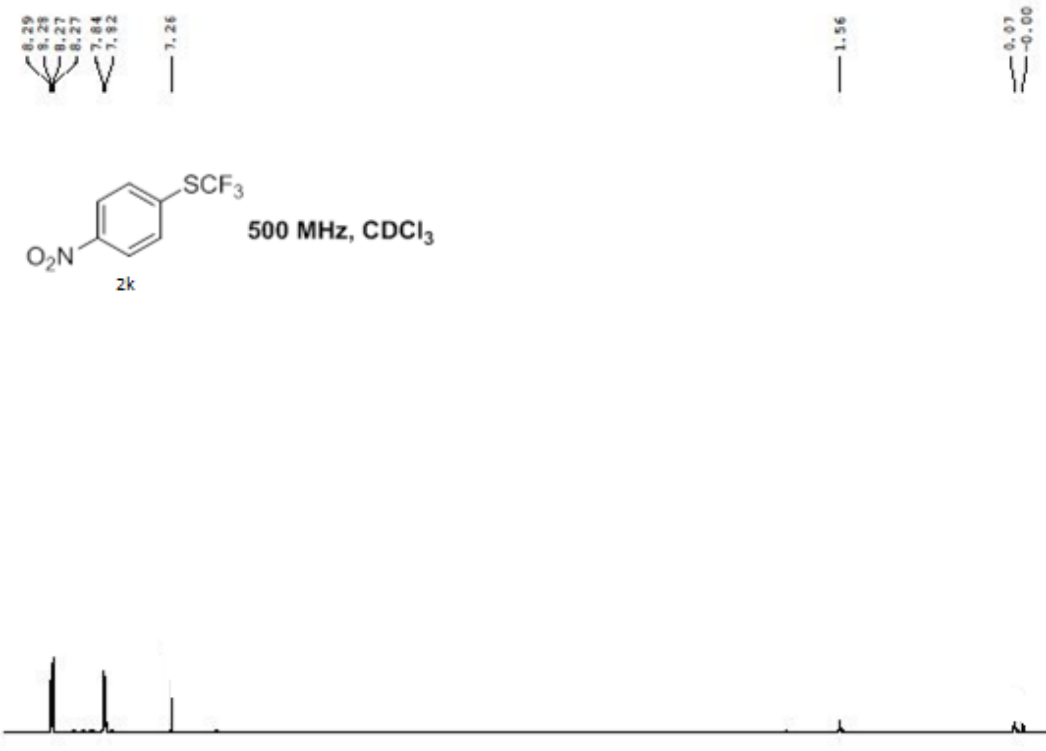
**500 MHz, $CDCl_3$**

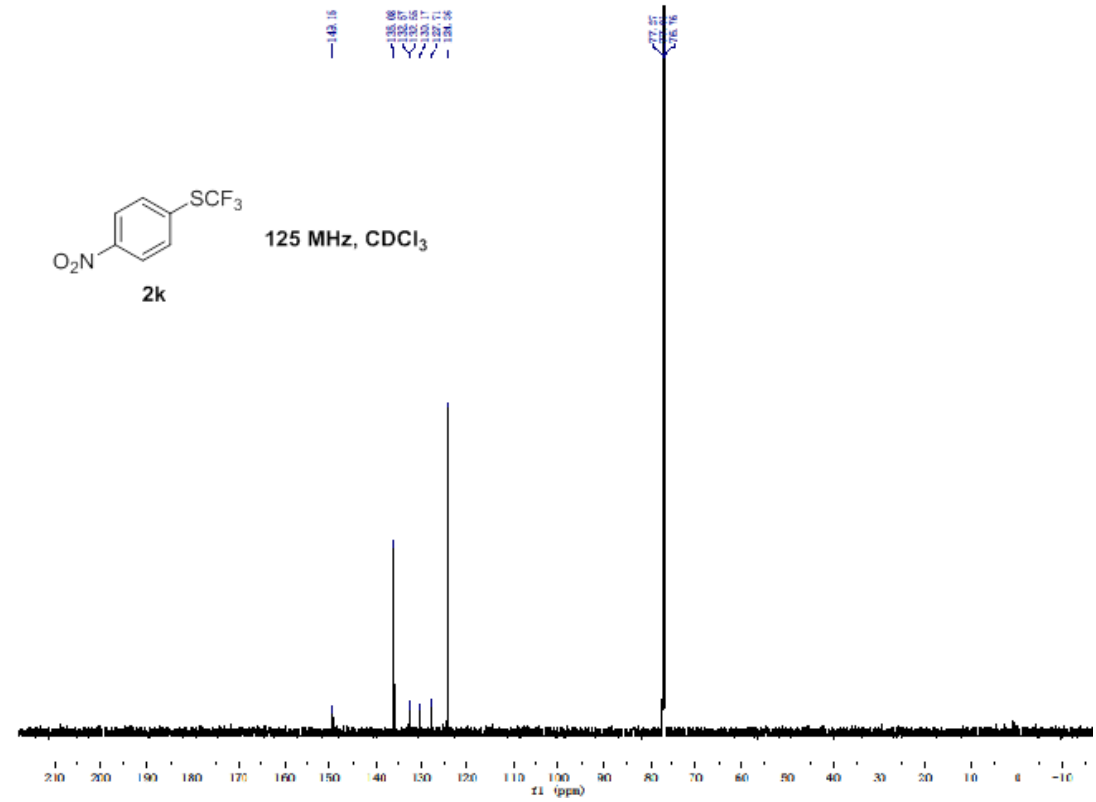
**2j**

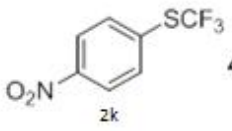



165.38
141.63
138.92
134.64
133.40
133.43
130.27
129.17
127.16
124.73
121.31
112.84
77.40
77.15
76.89
SCF3
NHCOPh
2j
125 MHz, CDCl3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm


-42.28
SCF3
NHCOPh
2j
470 MHz, CDCl3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

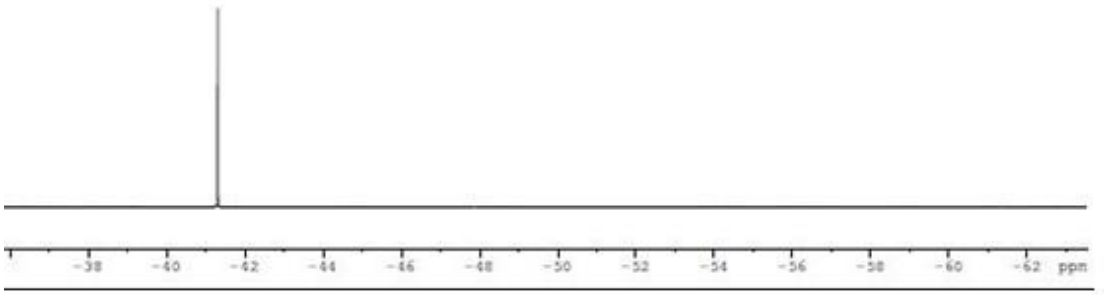

8.29
8.28
8.27
8.27
7.84
7.82
7.26
1.56
0.07
-0.00
SCF3
O2N
2k
500 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
2.00
1.96


SCF3
O2N
2k
125 MHz, CDCl3
f1 (ppm)

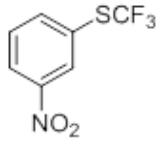



2k

**470 MHz, $CDCl_3$**

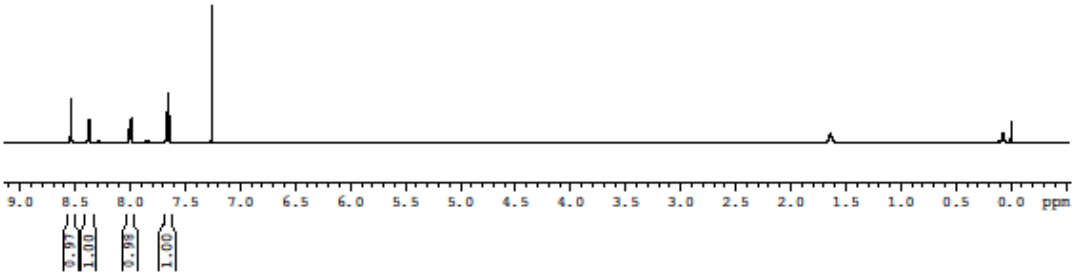


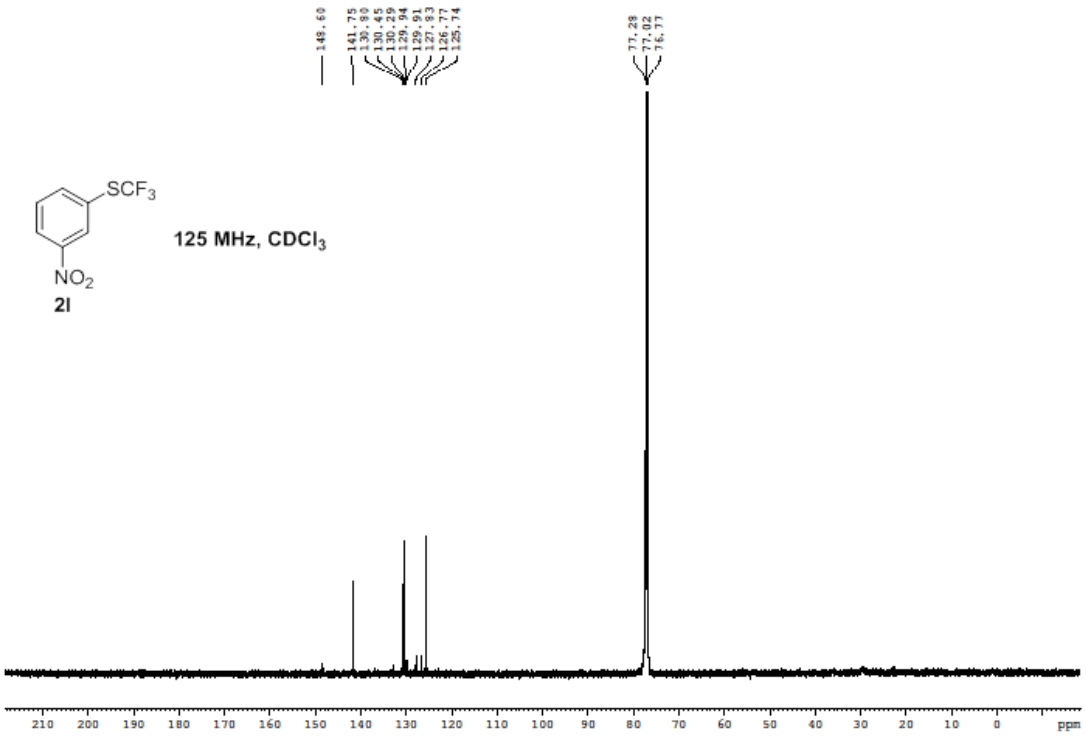


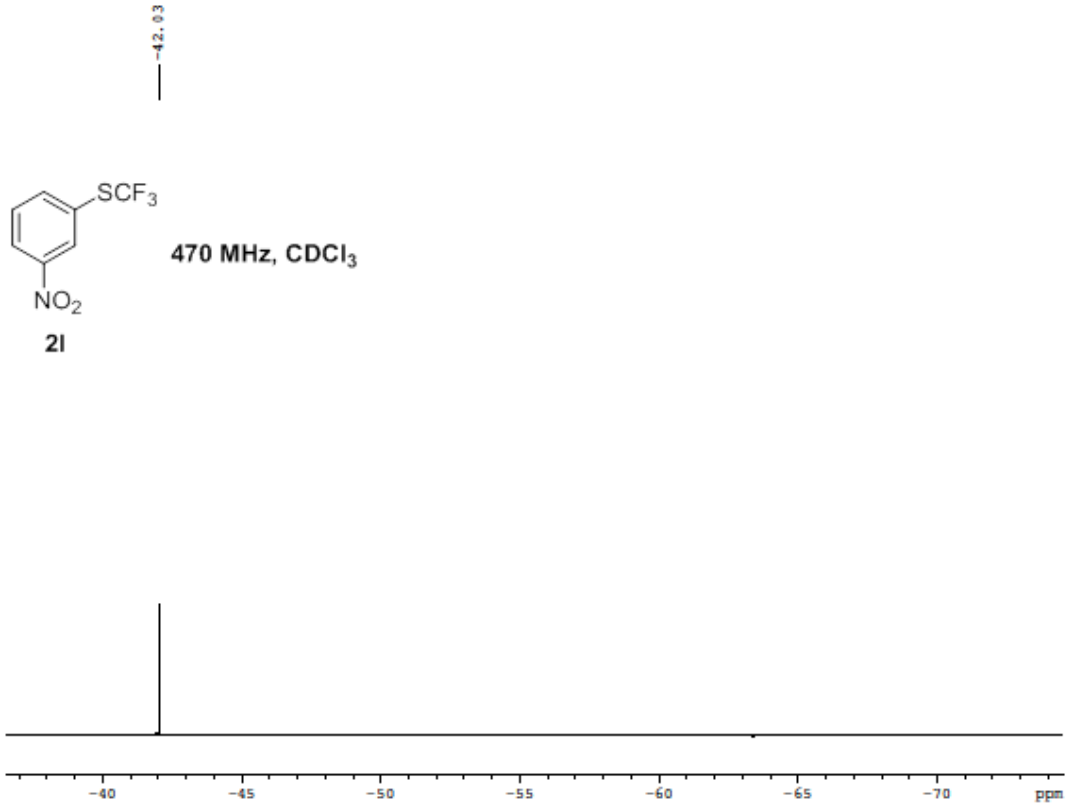



**2l**

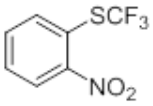
**500 MHz, $CDCl_3$**




148.60
141.75
130.90
130.45
130.29
129.94
129.91
127.93
126.77
125.74
77.28
77.02
76.77
SCF3
NO2
125 MHz, CDCl3
2l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

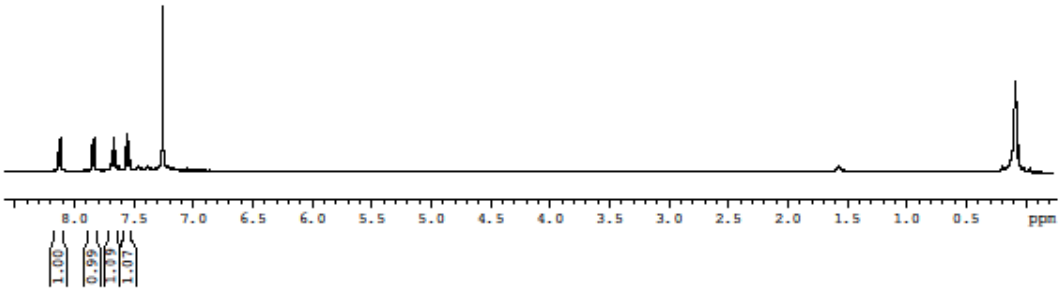

-42.03
SCF3
NO2
470 MHz, CDCl3
2l
-40 -45 -50 -55 -60 -65 -70 ppm



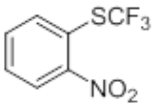



**500 MHz, $CDCl_3$**

**2m**

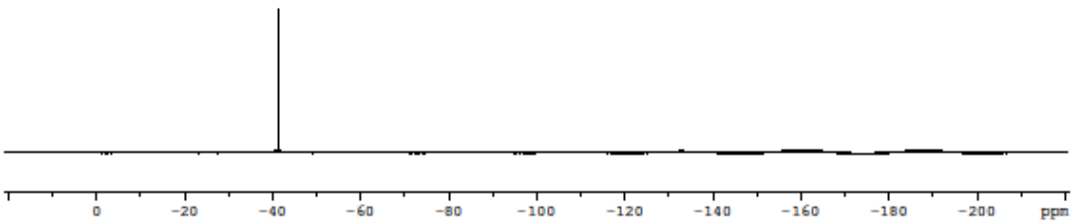


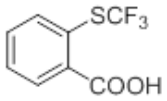





**470 MHz, $CDCl_3$**

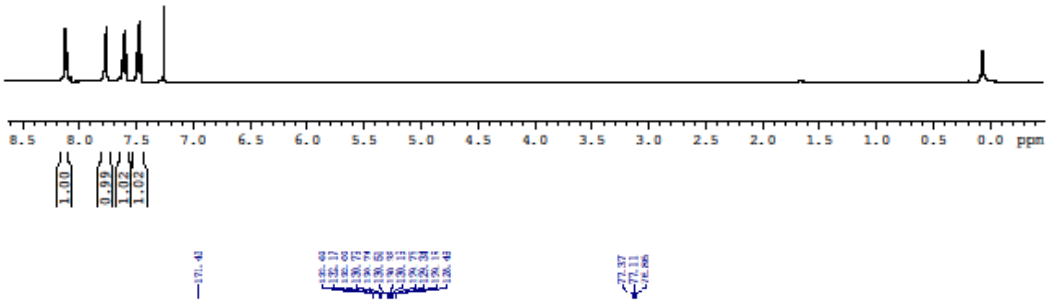
**2m**

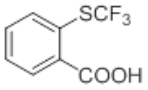



**500 MHz, $CDCl_3$**

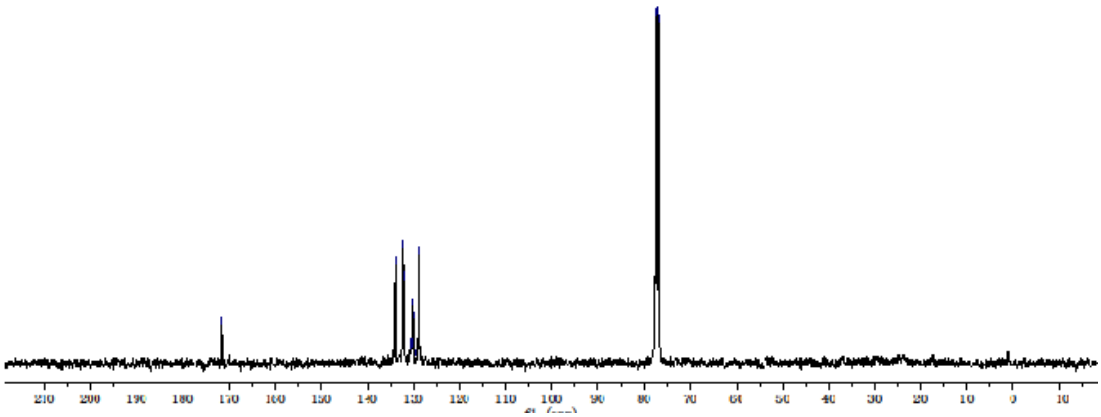
**2n**

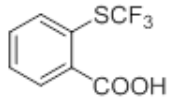



**125 MHz, $CDCl_3$**

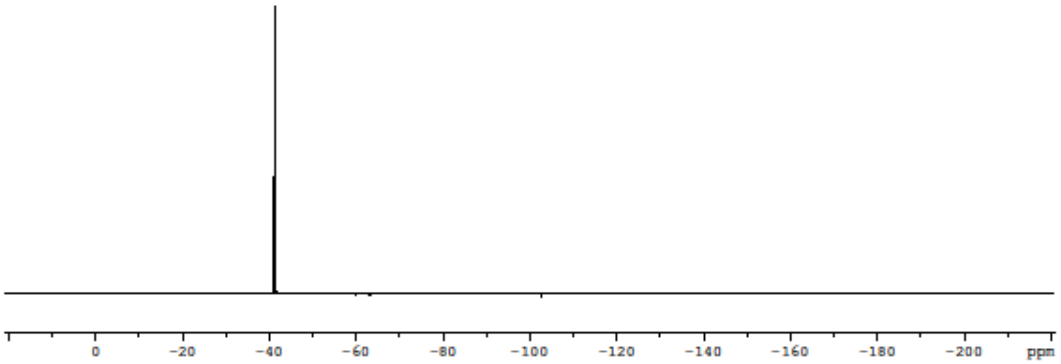
**2n**




**470 MHz, $CDCl_3$**

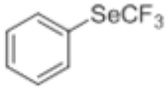
**2n**





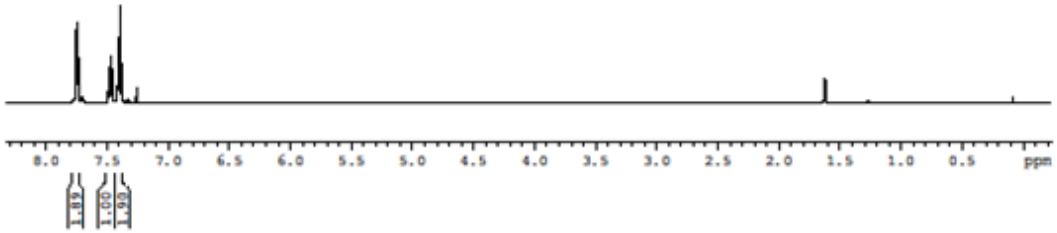


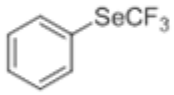





**500 MHz, $CDCl_3$**

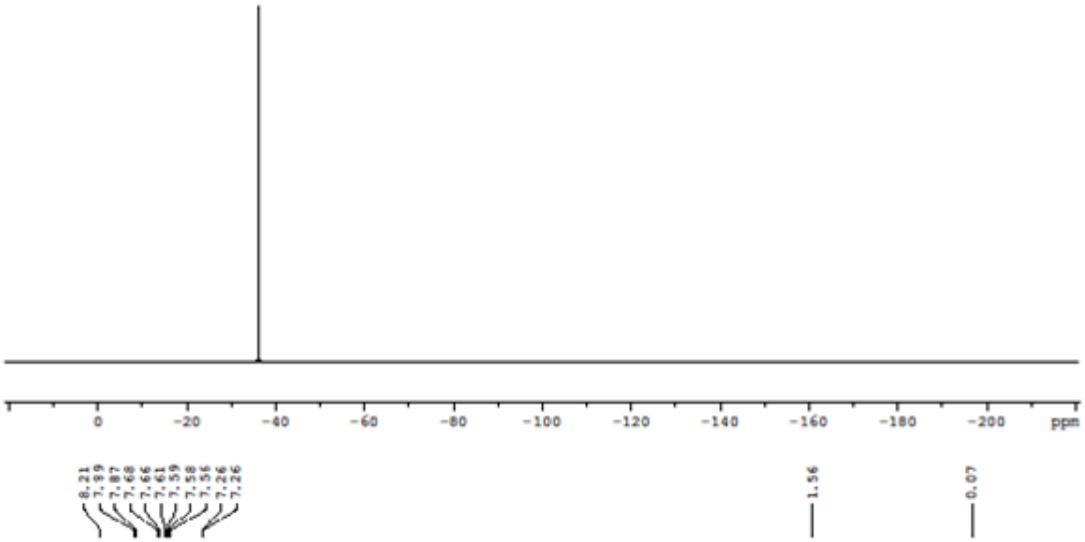
2o

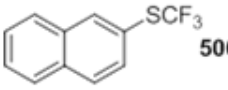





**470 MHz, $CDCl_3$**

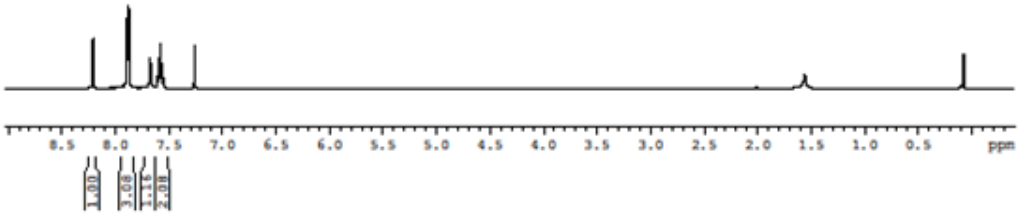
2o

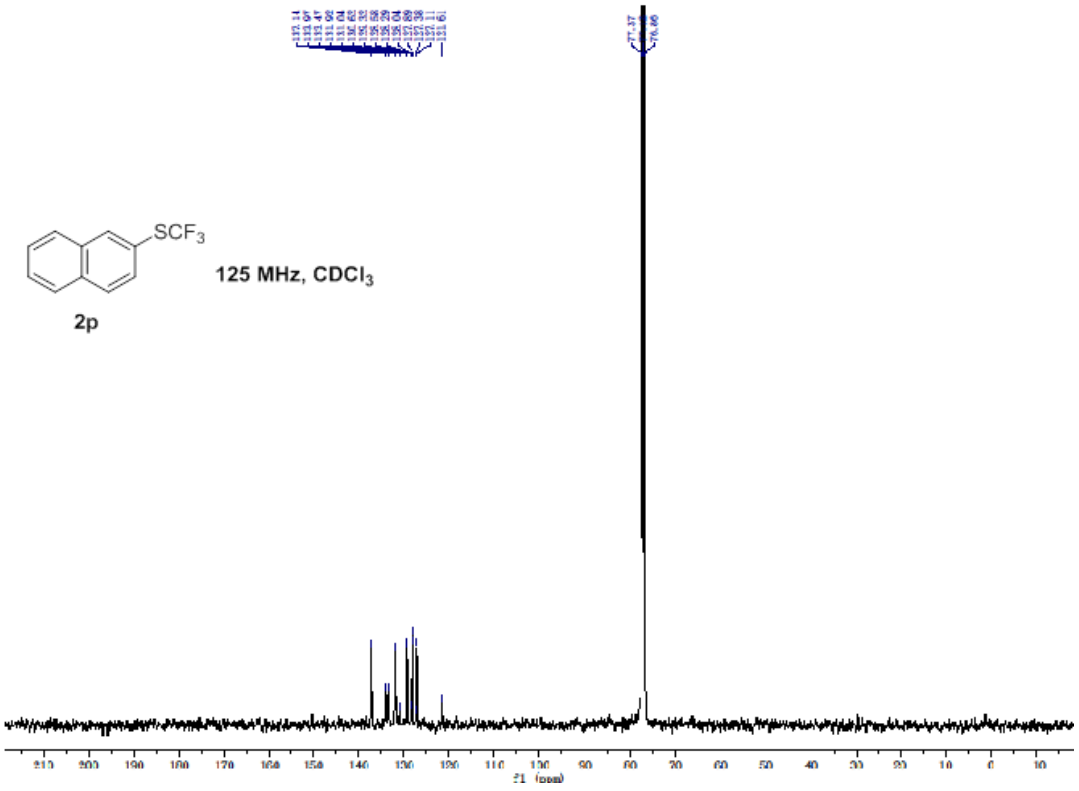


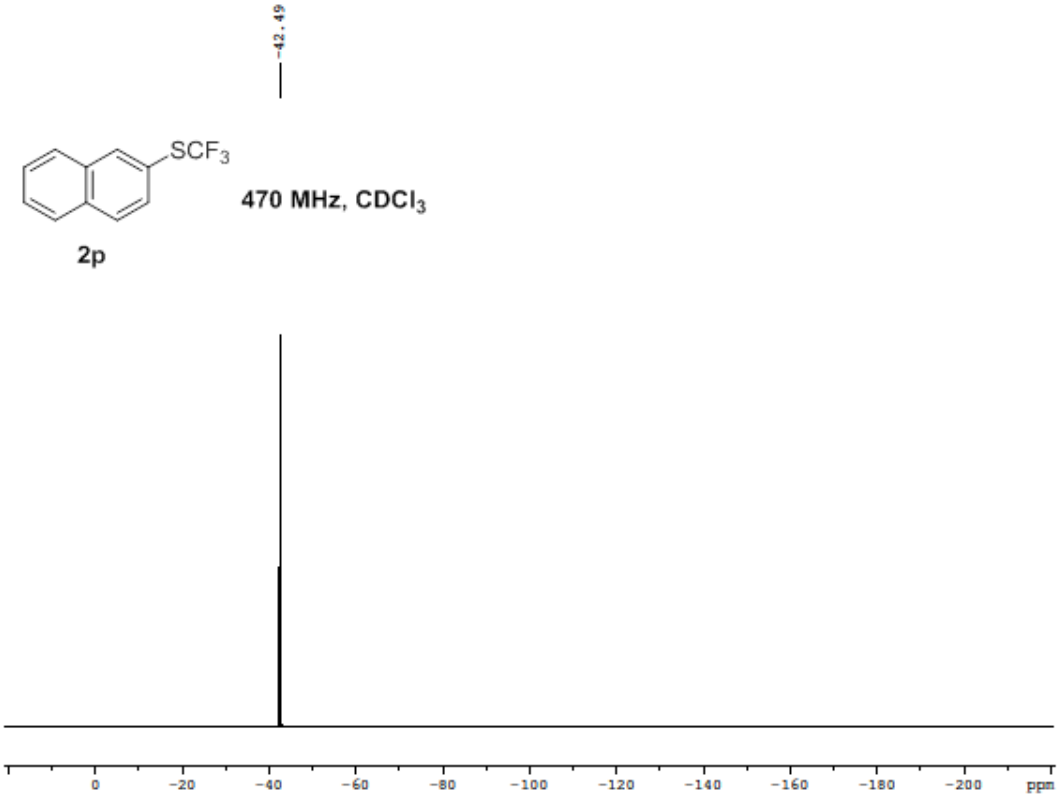



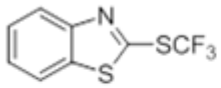

**500 MHz, $CDCl_3$**

2p



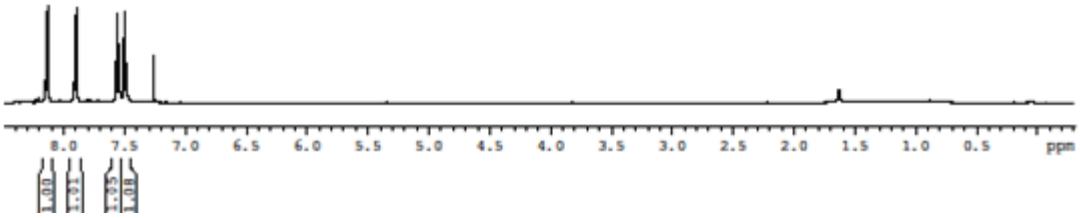

SCF3
125 MHz, CDCl3
2p
77.37
76.66
21 (ppm)


-42.49
SCF3
470 MHz, CDCl3
2p
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

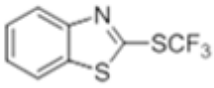




**500 MHz, $CDCl_3$**

2q

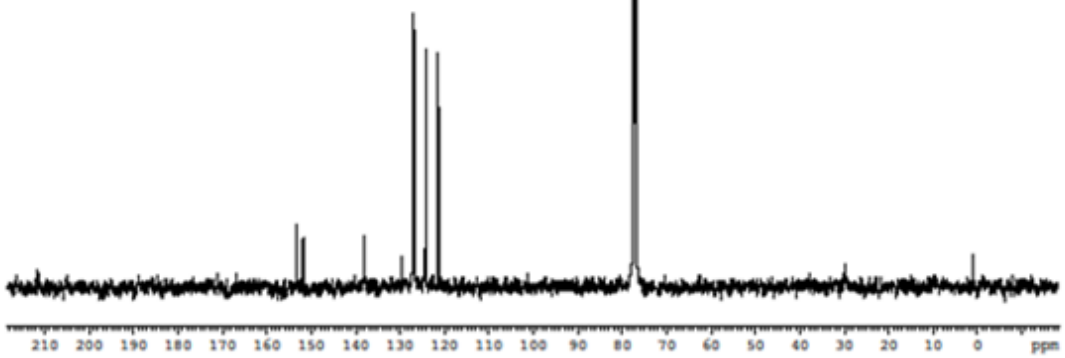


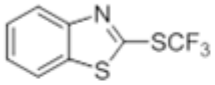





**125 MHz, $CDCl_3$**

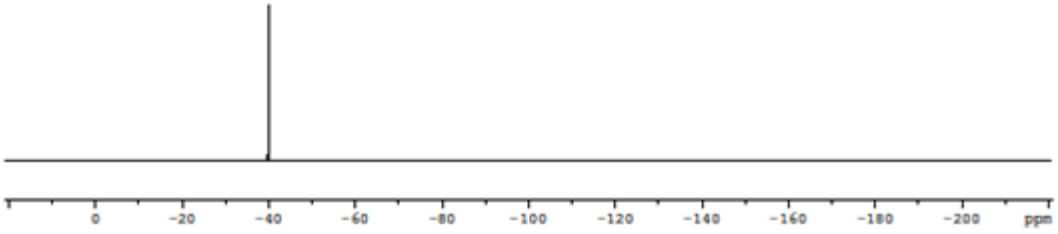
2q



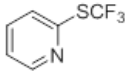




**470 MHz, $CDCl_3$**

**2q**

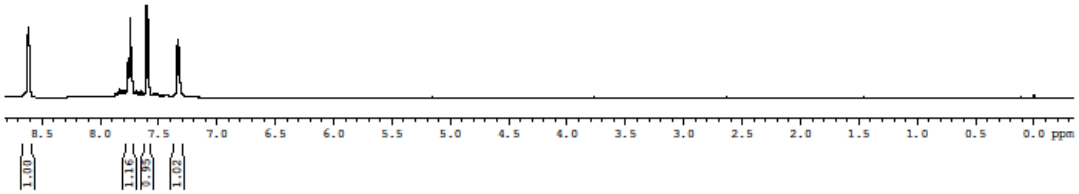


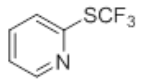



**500 MHz, $CDCl_3$**

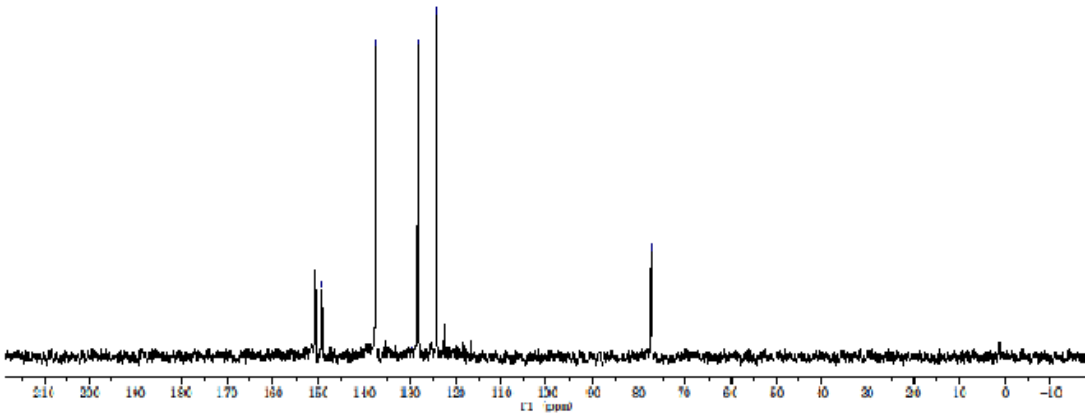
**2r**



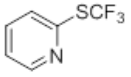



**125 MHz, $CDCl_3$**

**2r**

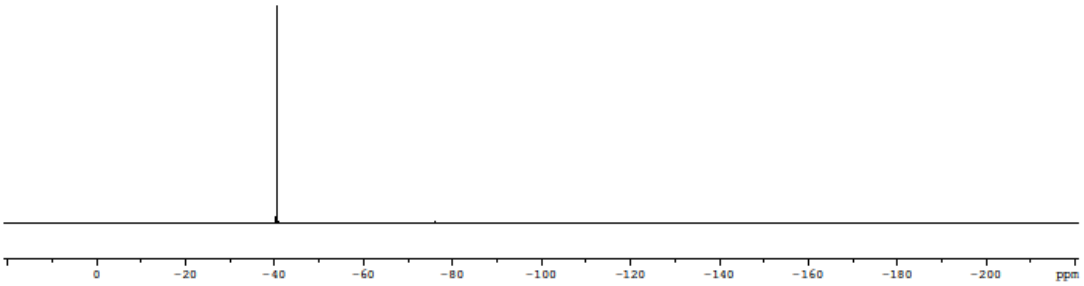


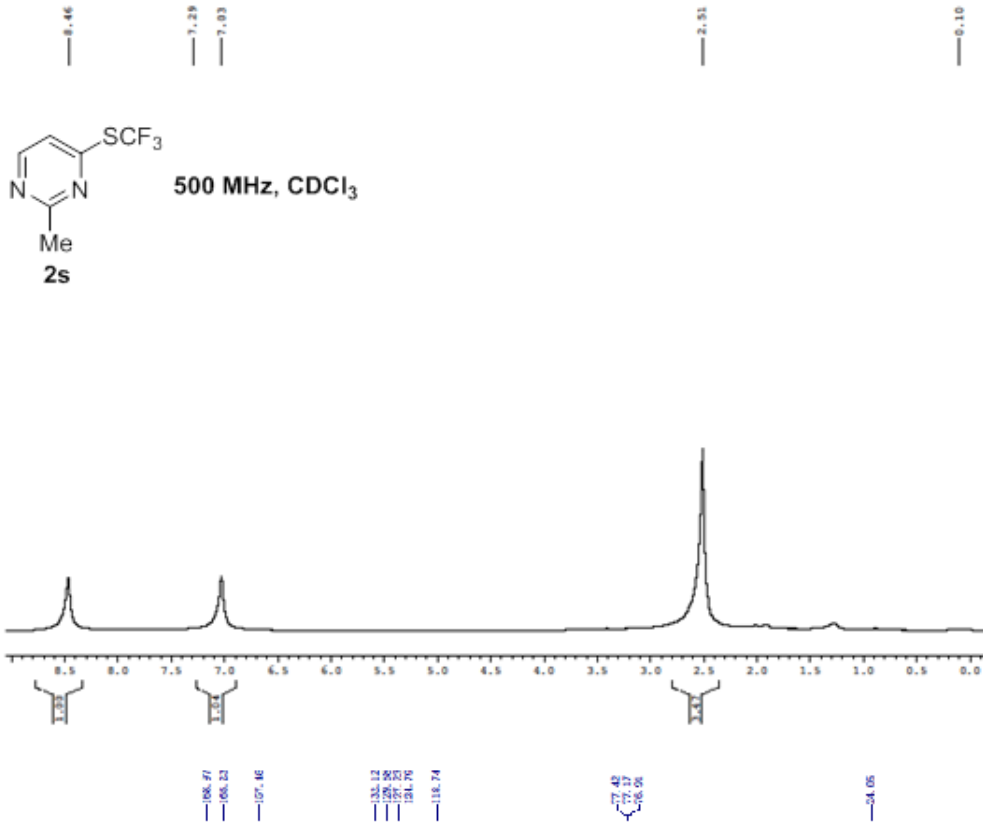


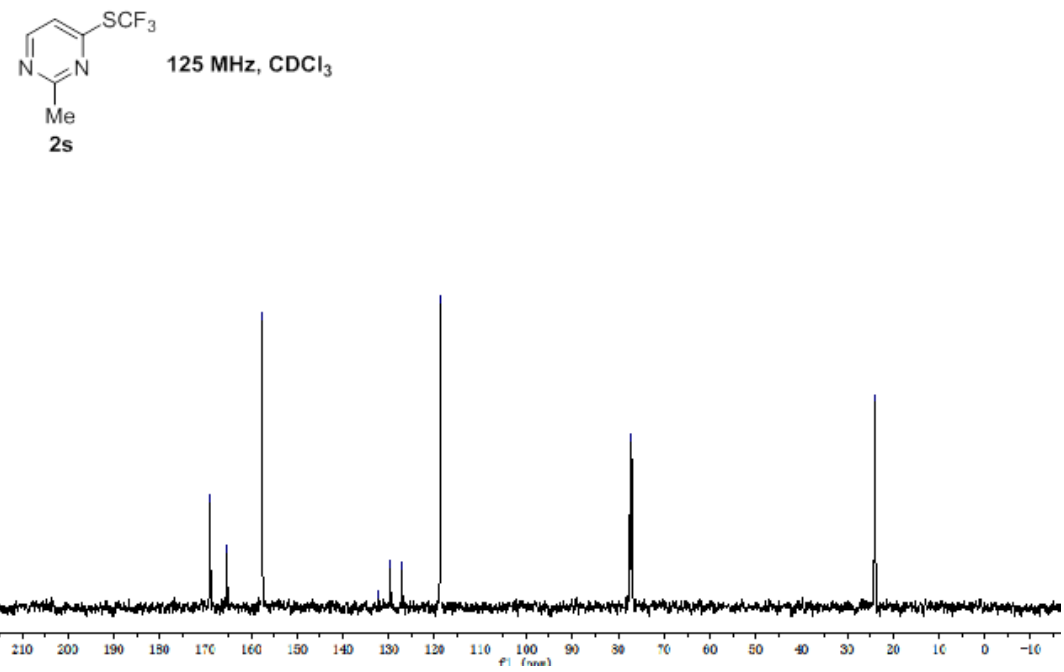



**470 MHz, $CDCl_3$**

**2r**

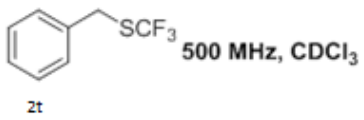


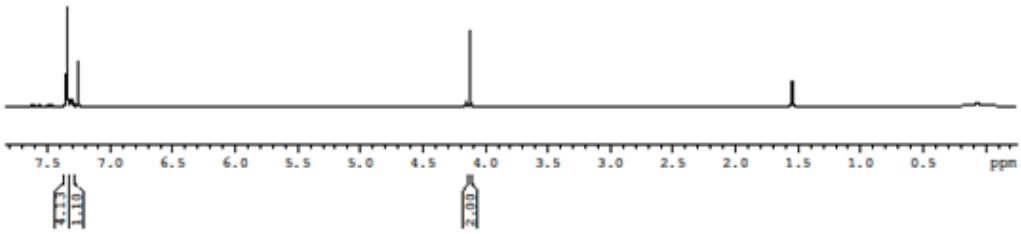

8.46
7.29
7.03
2.51
0.10
SCF3
N
N
Me
2s
500 MHz, CDCl3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
168.97
156.32
157.46
133.12
129.98
127.53
124.76
118.74
77.42
77.17
76.91
24.05

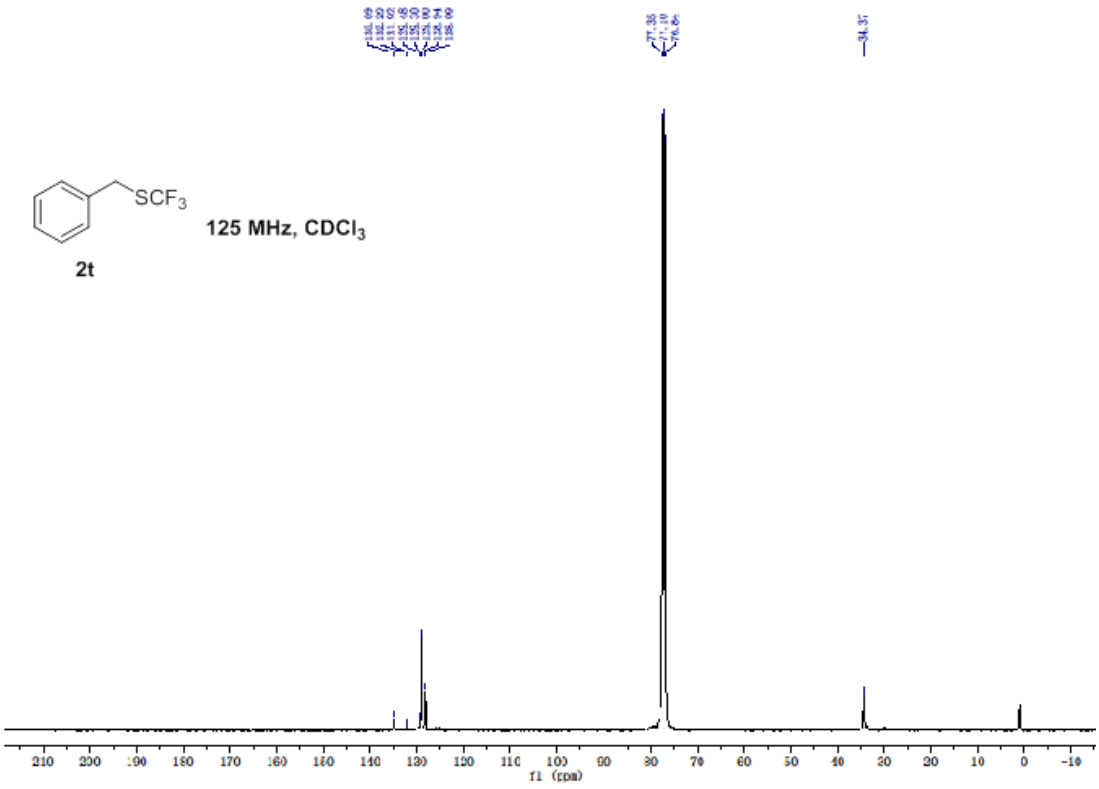

SCF3
N
N
Me
2s
125 MHz, CDCl3
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10

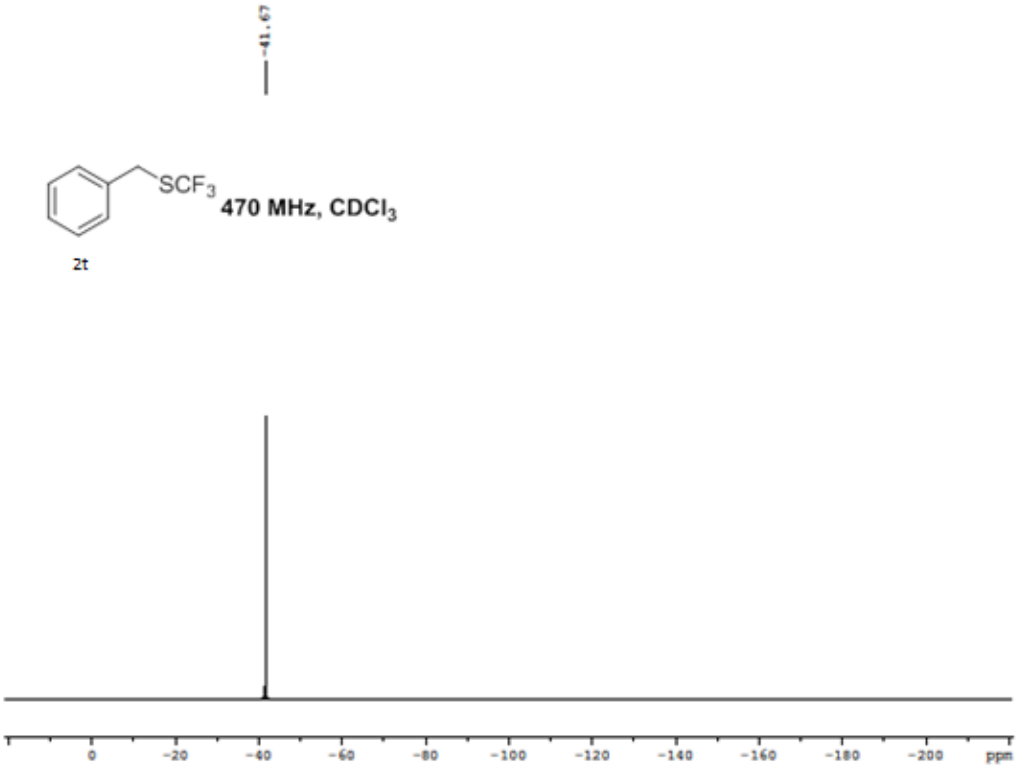

-40.97
SCF3
N
N
Me
470 MHz, CDCl3
2s
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


7.35
7.34
7.26
4.12
1.54
0.07


SCF3
500 MHz, CDCl3
2t


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
4.73
1.10
2.00

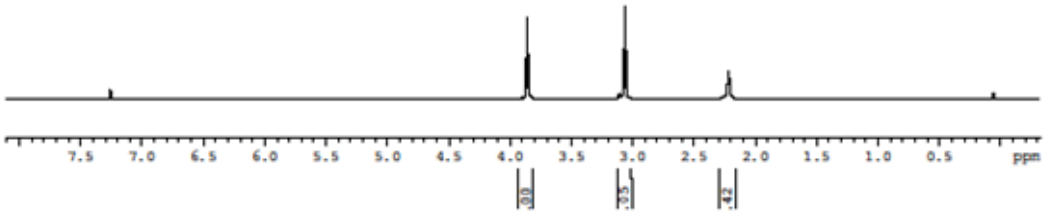

SCF3
125 MHz, CDCl3
2t
f1 (ppm)

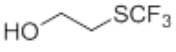

-41.67
SCF3
470 MHz, CDCl3
2t
ppm



2u

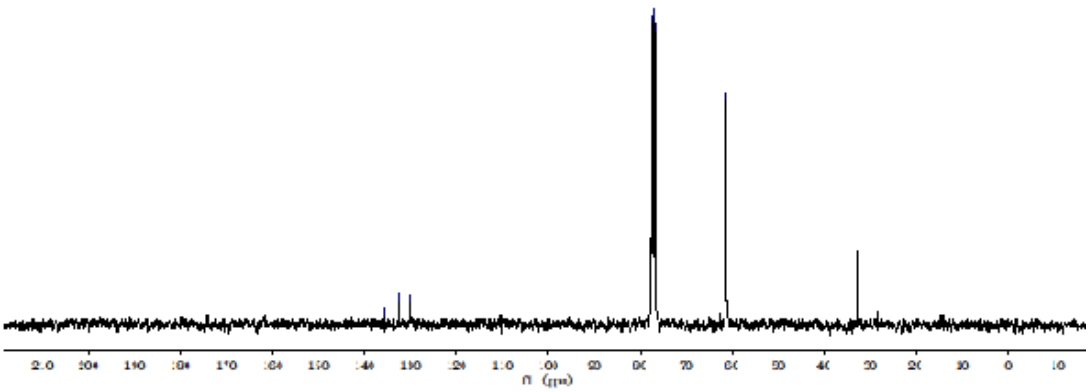
**500 MHz, $CDCl_3$**




**2u**

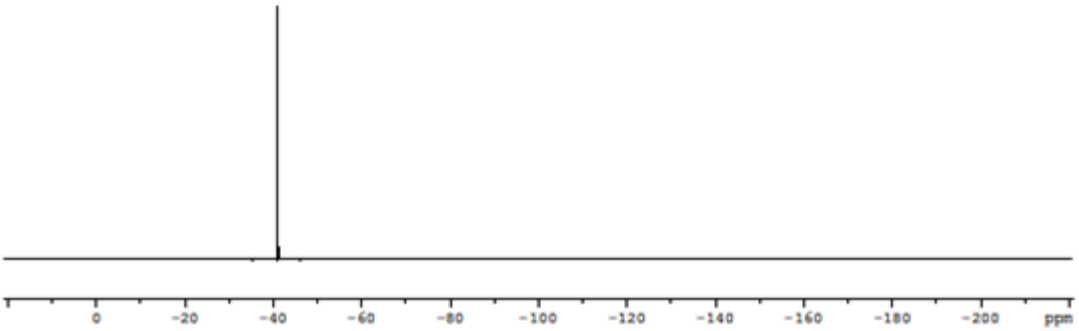
**125 MHz, $CDCl_3$**



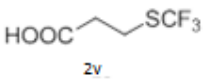


2u

**470 MHz, $CDCl_3$**

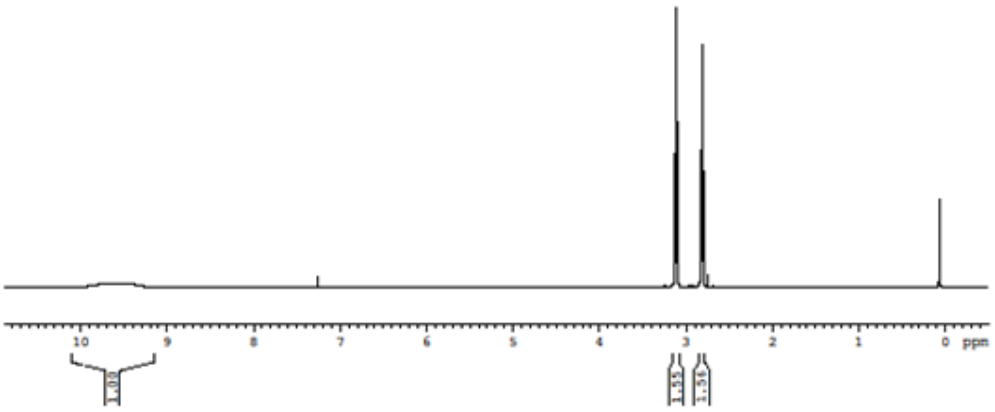


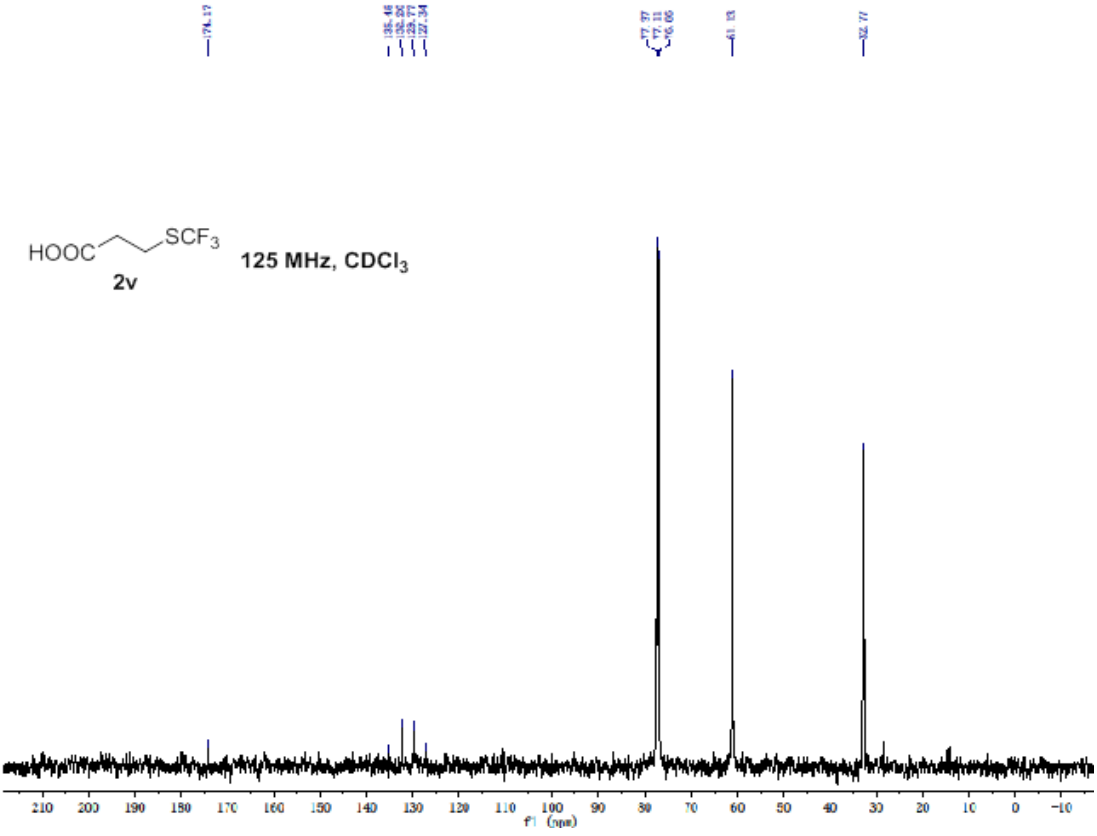


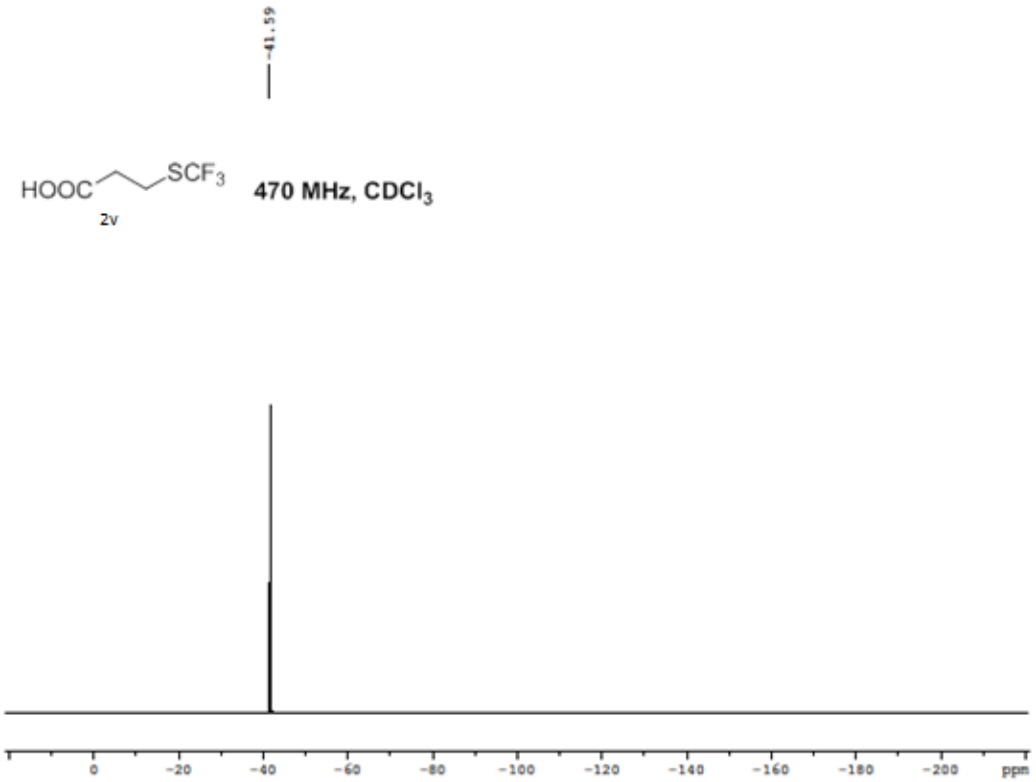


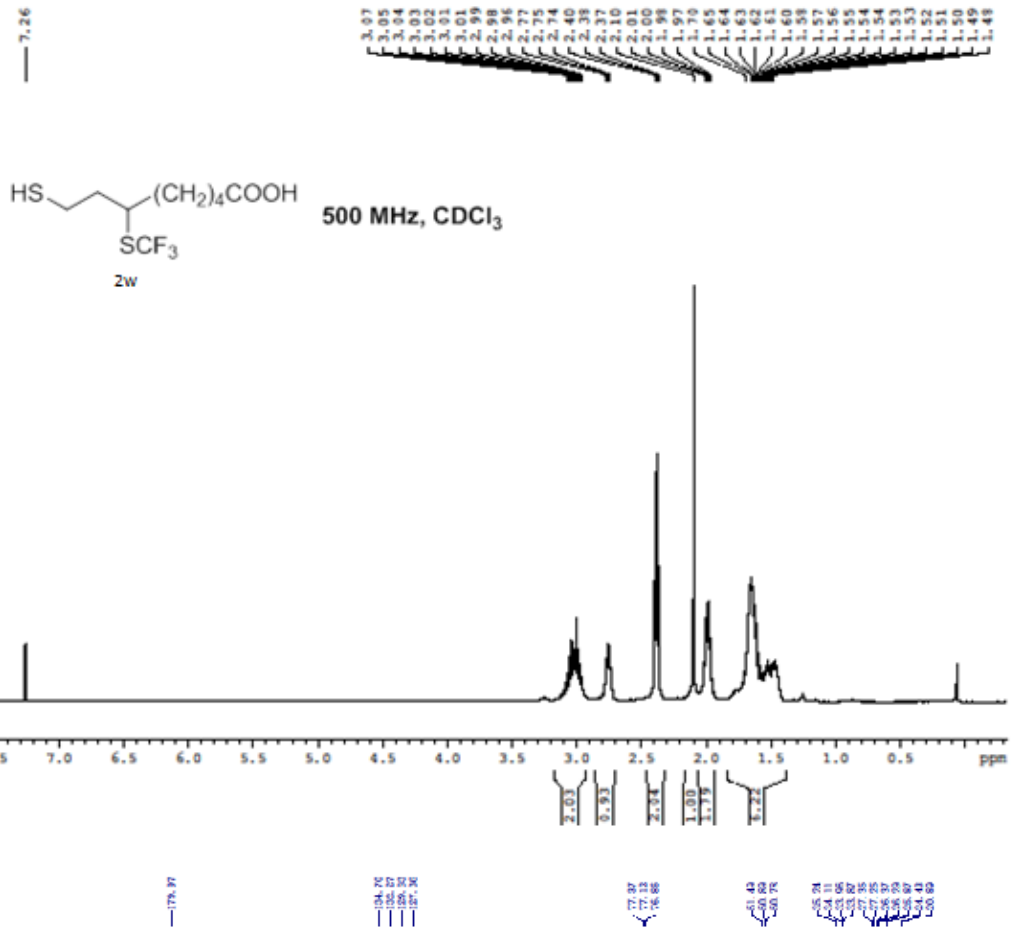

2v

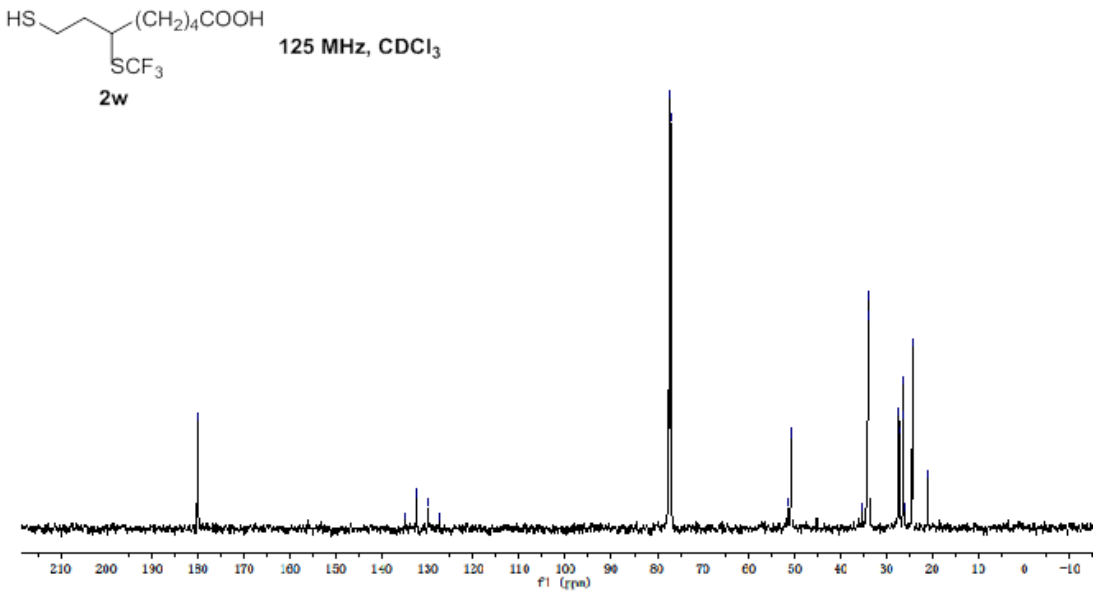
**500 MHz, $CDCl_3$**

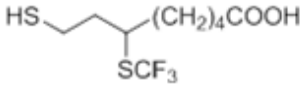



HOOC
SCF3
2v
125 MHz, CDCl3
f1 (ppm)


-41.59
HOOC
SCF3
2v
470 MHz, CDCl3
ppm


HS
(CH2)4COOH
SCF3
2w
500 MHz, CDCl3
ppm


HS
(CH2)4COOH
SCF3
2w
125 MHz, CDCl3
f1 (ppm)


**470 MHz, $CDCl_3$**

2w