Electronic Supplementary Information (ESI) for

Oxidative nucleophilic strategy for synthesis of thiocyanates and trifluoromethyl sulfides from thiols

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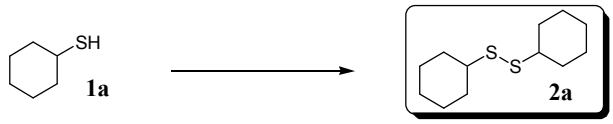
Preparation of OMS-2

An aqueous solution of $KMnO_4$ (5.89 g, 100 mL) was added to an aqueous solution (30 mL) containing $MnSO_4 \cdot H_2O$ (8.8 g) and concentrated HNO_3 (3 mL). The resulting mixture was refluxed at 100 °C for 24 h. Then, the dark brown solid formed was filtered off, washed with a large amount of water (ca. 3 L), and dried under air at 120 °C, affording 8.2 g of OMS-2. The content of Mn in OMS-2 was 58.8 wt%. The BET surface area was 94.0 $m^2 g^{-1}$. The structure and XRD pattern of OMS-2 are shown in Figs S4 and S7, respectively.

Table S1 Oxidative homocoupling of cyclohexanethiol (**1a**)[a]



Entry	Metal oxide or salt	Solvent	Yield (%)[b]
1	MgO	Acetonitrile	<1
2	Al_2O_3	Acetonitrile	<1
3	SiO_2	Acetonitrile	<1
4	Sc_2O_3	Acetonitrile	<1
5	TiO_2	Acetonitrile	<1
6	V_2O_5	Acetonitrile	<1
7	Cr_2O_3	Acetonitrile	<1
8	OMS-2	Acetonitrile	95
9[c]	OMS-2	Acetonitrile	80
10	OMS-2	THF	91
11	OMS-2	DMF	96
12	OMS-2	DMAc	>99
13	OMS-2	Ethanol	70
14	OMS-2	Dichloromethane	50
15	OMS-2	Chloroform	26
16	OMS-2	*n*-Hexane	35
17	OMS-2	Toluene	14
18	β-MnO_2	Acetonitrile	<1
19	Birnessite-type MnO_2	Acetonitrile	<1
20	Fe_2O_3	Acetonitrile	<1
21	Co_3O_4	Acetonitrile	2
22	NiO	Acetonitrile	5
23	CuO	Acetonitrile	17
24	ZnO	Acetonitrile	<1
25	MoO_3	Acetonitrile	<1
26	WO_3	Acetonitrile	<1
27[d]	KF	Acetonitrile	<1

[a] Reaction conditions: Metal oxide (50 mg), **1a** (0.5 mmol), solvent (2 mL), 30 °C, O_2 (1 atm), 5 min. [b] Yields were determined by GC using naphthalene as the internal standard. In all cases, **2a** was selectively produced without formation of any byproducts. [c] OMS-2 (10 mg), 60 °C. [d] KF (0.13 mmol).

Table S2 Metal oxides used in this study

Metal oxide	Literature or company; note
OMS-2	See the Experimental Section (see Refs. 13,14); BET: 94.0 m^2 g^{-1}
Birnessite-type MnO_2	Prepared according to Ref. 16; BET: 62.2 m^2 g^{-1}
β-MnO_2	Obtained from Aldrich (No. 529664-5G); BET: 2.6 m^2 g^{-1}
MgO	Obtained from Kanto (No. 25018-33)
Al_2O_3	Obtained from Sumitomo Chemical (No. KHS-24)
SiO_2	Obtained from Fuji Silysia Chemical (No. CARiACT Q-10)
Sc_2O_3	Obtained from Aldrich (No. 307874-1G)
TiO_2	Obtained from Ishihara Sangyo Kaisya (No. ST-01)
V_2O_5	Obtained from KANTO (No. 44017-30)
Cr_2O_3	Obtained from nacalai tesque (No. 08909-22)
Fe_2O_3	Obtained from Alfa Aesar (No. 12593)
Co_3O_4	Obtained from Wako (No. 039-08792)
NiO	Obtained from Aldrich (No. 637130-25G)
CuO	Obtained from Wako (No. 036-09461)
ZnO	Obtained from Wako (No. 260-01261)
MoO_3	Obtained from Wako (No. 138-03352)
WO_3	Obtained from Aldrich (No. 550086-5G)

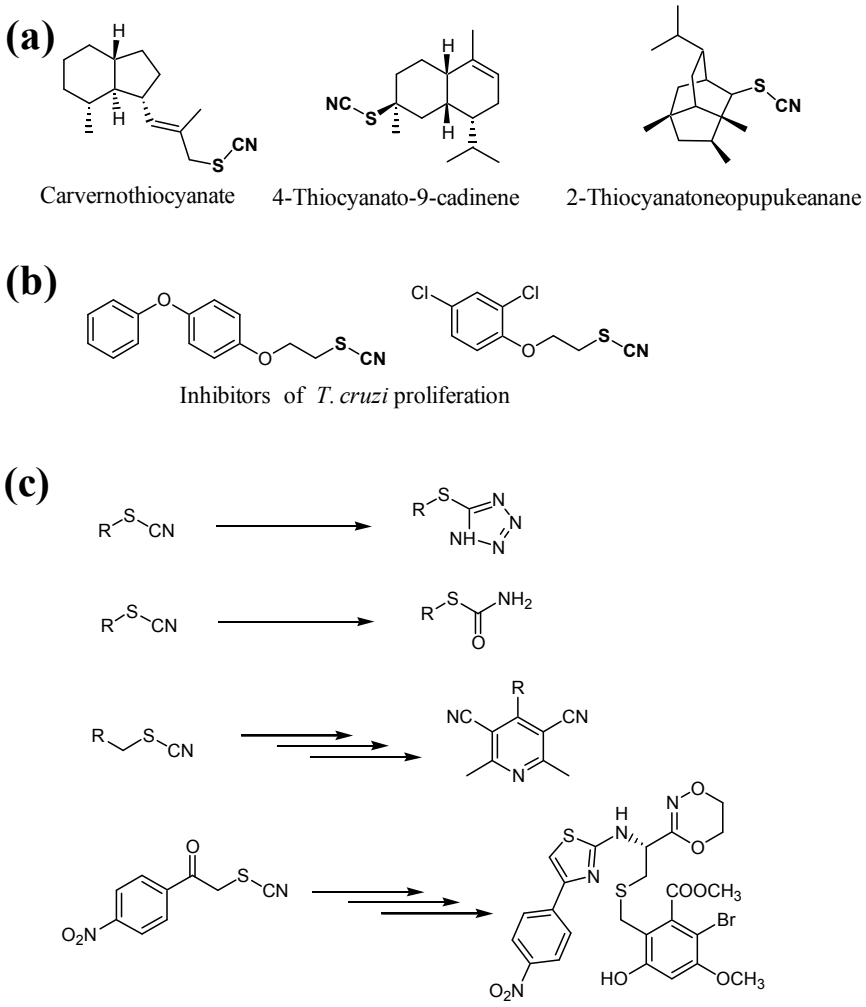


Fig. S1 Examples of (a) naturally found bioactive thiocyanates, (b) thiocyanate drugs, and (c) utilization of thiocyanates as synthons.[1]

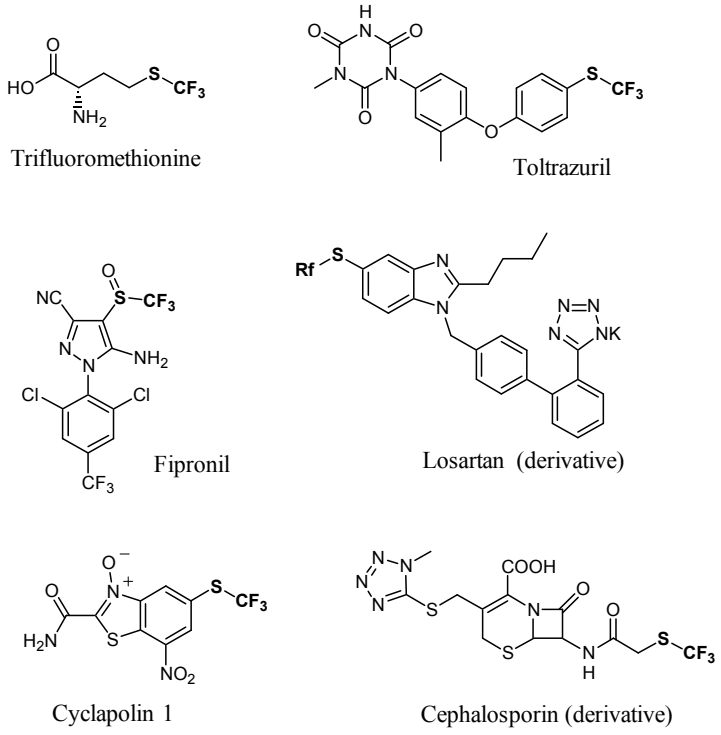


Fig. S2 Examples of trifluoromethyl sulfide-based drugs and drug candidates.[2,3]

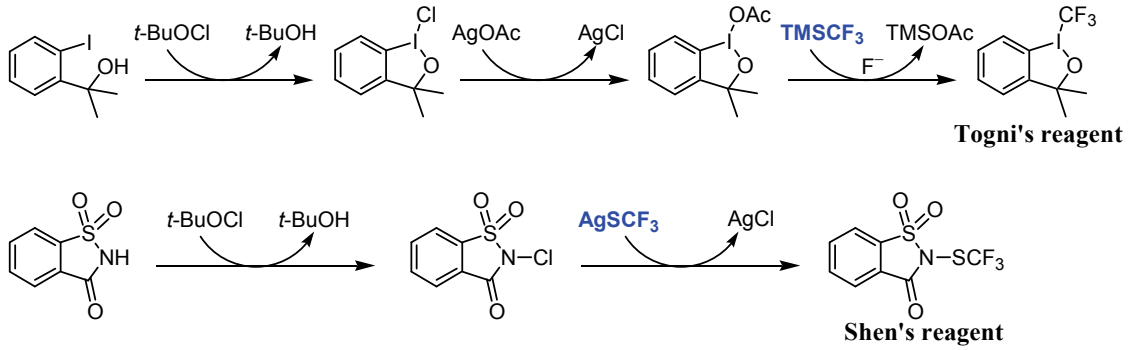


Fig. S3 Synthetic procedures of Togni's (trifluoromethylation)[11] and Shen's (trifluoromethylthiolation)[12a] reagents.

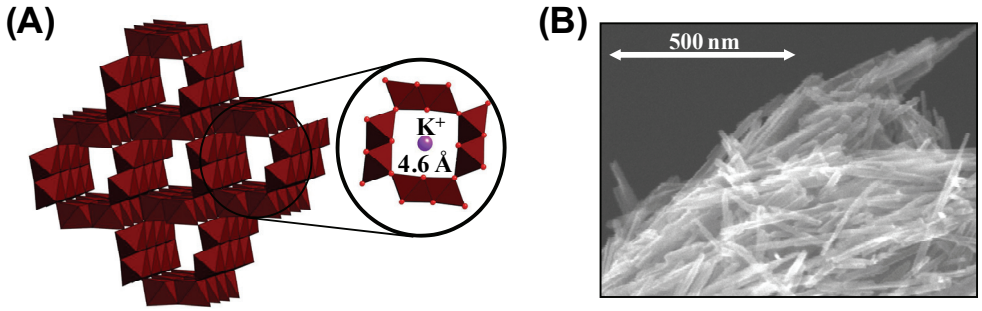


Fig. S4. (A) Structure and (B) SEM image of OMS-2. The octahedra indicate the {MnO_6} units.[13,14]

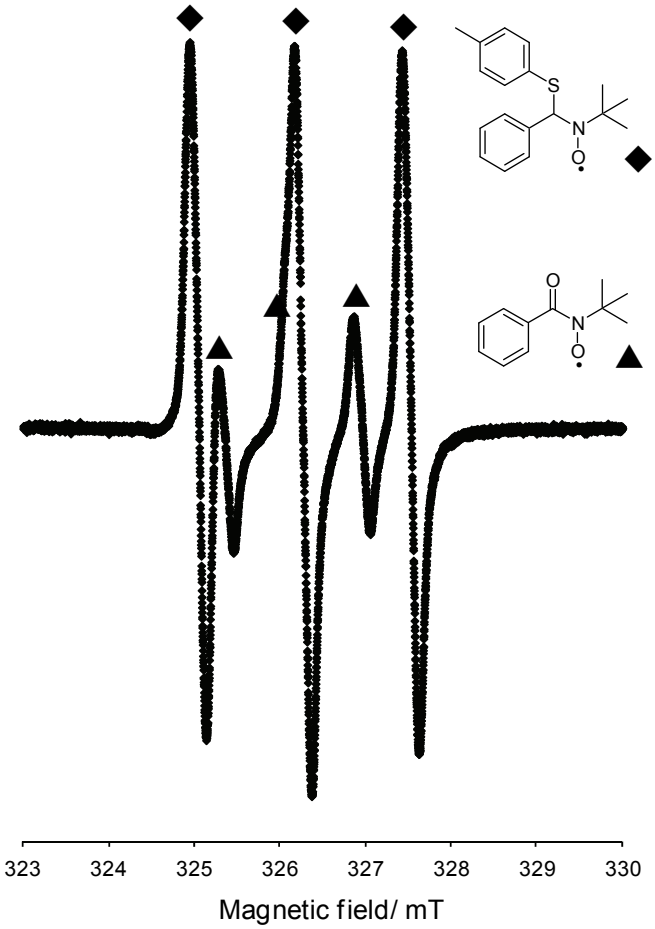


Fig. S5 ESR spectrum of the reaction mixture. OMS-2 was added into a quartz cell (4 mm ID). Then, a toluene solution of **1h** and α-phenyl-*tert*-butylnitron (PBN) (ca. 1 mL, 0.25 M) was added, and the spectrum was measured at measured at –20 °C (frequency: 9.16 GHz). Two sets of signals assignable to the spin adduct between PBN and the thiyl radical species (A_N = 1.3 mT, ◆) and the oxidized PBN (A_N = 0.85 mT, ▲). See: G. R. Buttner, *Free Radical Biol. Med.*, 1987, **3**, 259–303.

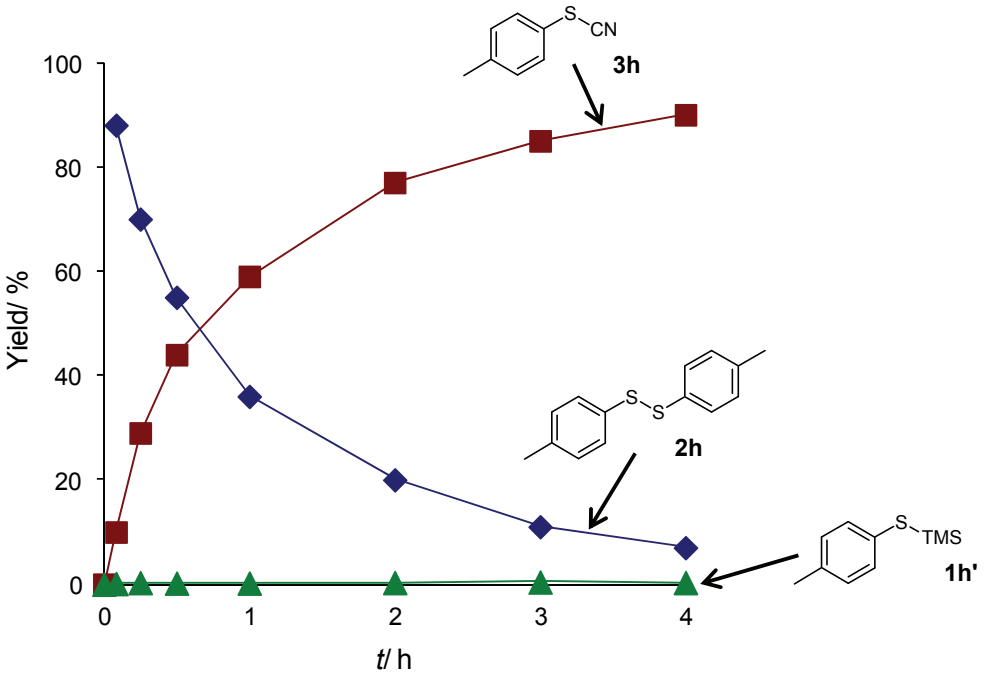


Fig. S6. Reaction profile for the cyanation of **1h**. Reaction conditions: OMS-2 (50 mg), **1h** (0.5 mmol), TMSCN (2 mmol), DMF (2 mL), 30 °C, O_2 (1 atm).

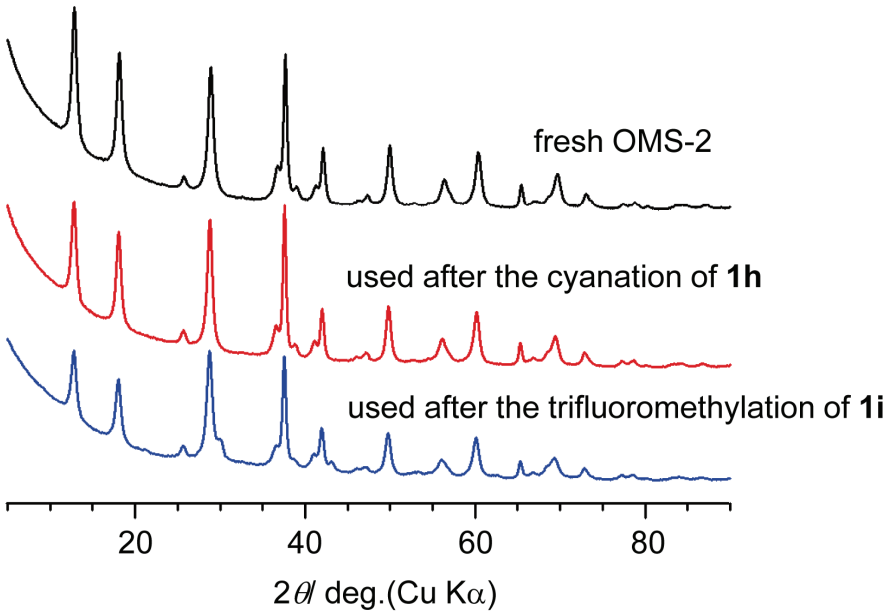
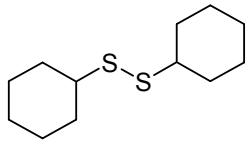
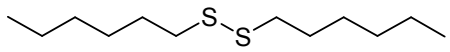


Fig. S7 XRD patterns of fresh and used OMS-2.

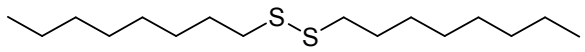
Spectral data of disulfides, thiocyanates, and trifluoromethyl sulfides



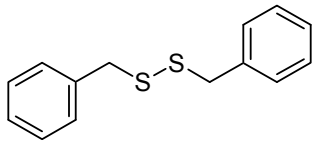
Compound 2a (Table 1, entries 1 and 2): MS (EI): *m*/*z* (%): 230 (8) [M^+], 148 (30), 84 (6), 83 (90), 81 (6), 67 (6), 55 (100), 54 (5), 53 (9).



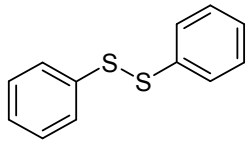
Compound 2b (Table 1, entry 3): MS (EI): *m*/*z* (%): 235 (7), 234 (45) [M^+], 152 (8), 151 (7), 150 (80), 118 (6), 117 (64), 115 (6), 87 (11), 86 (7), 85 (100), 83 (13), 82 (6), 81 (9), 79 (11), 73 (7), 69 (9), 67 (6), 61 (9), 60 (8), 59 (9), 57 (74), 56 (12), 55 (76), 53 (8).



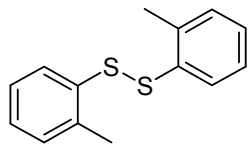
Compound 2c (Table 1, entry 4): MS (EI): *m*/*z* (%): 290 (18) [M^+], 178 (15), 145 (21), 87 (10), 71 (74), 70 (6), 69 (27), 67 (8), 57 (100), 56 (9), 55 (39).



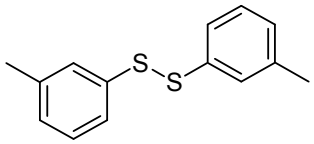
Compound 2d (Table 1, entry 5): MS (EI): *m*/*z* (%): 246 (3) [M^+], 92 (8), 91 (100), 65 (17).



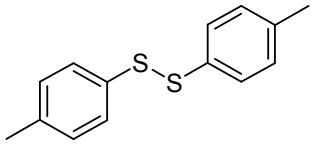
Compound 2e (Table 1, entries 6 and 7): MS (EI): *m*/*z* (%): 219 (7), 218 (47) [M^+], 185 (13), 154 (24), 140 (6), 111 (5), 110 (10), 109 (100), 108 (9), 77 (9), 69 (14), 65 (38), 51 (10).



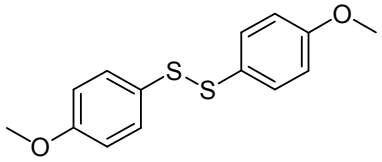
Compound 2f (Table 1, entry 8): MS (EI): *m*/*z* (%): 248 (5), 247 (9), 246 (51) [M^+], 125 (5), 124 (18), 123 (100), 122 (27), 121 (26), 97 (6), 91 (26), 89 (12), 79 (26), 78 (19), 77 (60), 69 (10), 65 (16), 63 (13), 53 (6), 51 (15).



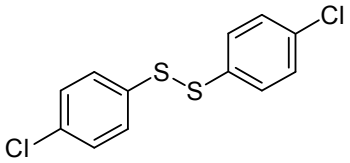
Compound 2g (Table 1, entry 9): MS (EI): *m*/*z* (%): 248 (6), 247 (10), 246 (59) [M^+], 213 (10), 198 (10), 182 (15), 167 (10), 125 (5), 124 (13), 123 (100), 122 (8), 121 (20), 97 (8), 91 (22), 89 (8), 79 (35), 78 (15), 77 (43), 69 (9), 65 (15), 63 (10), 53 (6), 51 (10).



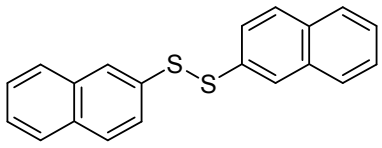
Compound 2h (Table 1, entry 10): MS (EI): *m*/*z* (%): 246 (22) [M^+], 125 (5), 124 (13), 123 (100), 122 (8), 121 (11), 108 (7), 97 (5), 91 (15), 89 (5), 79 (42), 78 (12), 77 (40), 69 (9), 65 (15), 63 (7), 51 (7).



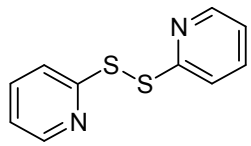
Compound 2i (Table 1, entry 11): MS (EI): *m*/*z* (%): 278 (20) [M^+], 141 (5), 140 (10), 139 (100), 124 (11), 96 (21), 95 (20), 77 (5), 70 (8), 69 (6).



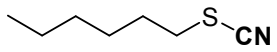
Compound 2j (Table 1, entry 12): MS (EI): *m*/*z* (%): 288 (12), 287 (2) [M^+], 286 (15), 145 (26), 144 (7), 143 (72), 110 (5), 109 (10), 108 (100), 107 (7), 101 (7), 99 (24), 82 (12), 75 (12), 73 (10), 69 (13), 63 (14).



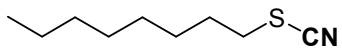
Compound 2k (Table 1, entry 13): MS (EI): *m*/*z* (%): 320 (6), 319 (12), 318 (49) [M^+], 285 (6), 255 (8), 254 (36), 253 (7), 160 (18), 159 (55), 128 (6), 116 (12), 115 (100), 114 (6), 89 (6).



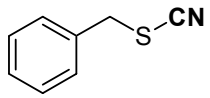
Compound 2l (Table 1, entry 14): MS (EI): *m*/*z* (%): 222 (5), 221 (7), 220 (52) [M^+], 187 (14), 156 (46), 155 (22), 142 (7), 130 (7), 129 (11), 110 (13), 84 (8), 83 (25), 82 (11), 79 (10), 78 (100), 69 (7), 67 (7), 58 (5), 57 (20), 52 (29), 51 (94), 50 (21).



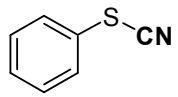
Compound 3b (Table 3, entry 1): MS (EI): *m*/*z* (%): 143 (0.14) [M^+], 142 (1.3), 128 (9), 117 (6), 116 (78), 115 (6), 114 (13), 110 (17), 101 (35), 100 (18), 96 (5), 88 (8), 87 (61), 86 (6), 85 (9), 84 (11), 83 (9), 82 (12), 72 (12), 69 (35), 68 (5), 67 (8), 60 (16), 59 (13), 58 (7), 57 (42), 56 (100), 55 (82), 54 (12), 53 (9).



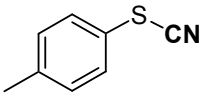
Compound 3c (Table 3, entry 2): MS (EI): *m*/*z* (%): 144 (34), 143 (7), 138 (5), 129 (7), 128 (6), 124 (11), 115 (21), 114 (9), 112 (6), 110 (16), 102 (7), 101 (61), 100 (8), 97 (5), 96 (10), 88 (6), 87 (33), 84 (15), 83 (40), 82 (12), 72 (9), 71 (27), 70 (42), 69 (59), 68 (20), 67 (12), 60 (12), 59 (7), 57 (53), 56 (64), 55 (100), 54 (12), 53 (8). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 2.95 (t, J = 7.0 Hz, 2H), 1.82 (quin, J = 7.0 Hz, 2H), 1.41–1.47 (m, 2H), 1.24–1.36 (m, 8H), 0.89 (t, J = 7.0 Hz, 3H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 112.43 (SCN), 34.14, 31.75, 29.95, 29.08, 28.90, 28.01, 22.65, 14,10.



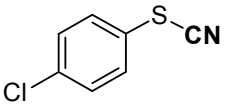
Compound 3d (Table 3, entry 3): MS (EI): *m*/*z* (%): 149 (6) [M^+], 92 (9), 91 (100) [$(M - SCN)^+$], 65 (16), 63 (5). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.33–7.39 (m, 5H), 4,13 (s, 2H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 134.44, 129.18, 129.03, 128.94, 112.04 (SCN), 38.38.



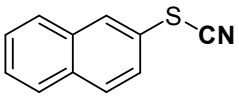
Compound 3e (Table 3, entries 4 and 5): MS (EI): *m*/*z* (%): 137 (5), 136 (9), 135 (100) [M^+], 108 (33), 91 (24), 84 (6), 77 (44), 74 (5), 69 (7), 65 (8), 51 (23), 50 (11). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.51–7.53 (m, 2H), 7.39–7.45 (m, 3H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 130.32, 130.15, 129.62, 124.52, 110.60 (SCN).



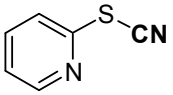
Compound 3h (Table 3, entries 6–9): MS (EI): *m*/*z* (%): 151 (5), 150 (11), 149 (100) [M^+], 148 (15), 123 (6), 122 (6), 121 (12), 117 (7), 116 (63), 92 (6), 91 (74), 90 (5), 89 (13), 78 (5), 77 (11), 68 (7), 65 (23), 63 (13), 62 (5), 51 (8), 50 (5). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.39–7.42 (m, 2H), 7.22 (d, J = 8.0 Hz, 2H), 2.36 (s, 3H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 140.29, 131.00, 130.72, 120.57, 111.07 (SCN), 21.19.



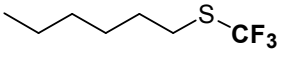
Compound 3j (Table 3, entry 10): MS (EI): *m*/*z* (%): 171 (37) [M^+], 170 (9), 169 (100) [M^+], 144 (5), 143 (7), 142 (13), 135 (6), 134 (56), 133 (10), 125 (13), 113 (6), 111 (18), 108 (15), 107 (6), 79 (5), 75 (29), 74 (10), 73 (6), 69 (9), 63 (9), 51 (5), 50 (13). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.45–7.48 (m, 2H), 7.40–7.42 (m, 2H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 136.25, 131.52, 130.52, 122.84, 110.02 (SCN).



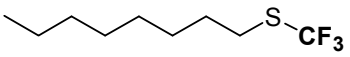
Compound 3k (Table 3, entry 11): MS (EI): *m*/*z* (%): 187 (5), 186 (13), 185 (100) [M^+], 159 (7), 158 (9), 153 (21), 141 (25), 140 (7), 127 (20), 126 (12), 115 (19), 114 (7), 79 (10), 77 (7), 75 (5), 63 (5). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.95 (d, J = 2.0 Hz, 1H), 7.84 (d, J = 8.5 Hz, 1H), 7.80–7.82 (m, 1H), 7.75–7.78 (m, 1H), 7.51–7.55 (m, 2H), 7.95 (dd, J = 8.5 Hz, 2.0 Hz, 1H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 133.65, 133.10, 130.32, 129.87, 128.00, 127.71, 127.66, 127.62, 126.25, 121.31, 110.68 (SCN).



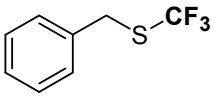
Compound 3l (Table 3, entry 12): MS (EI): *m*/*z* (%): 137 (5), 136 (56) [M^+], 79 (6), 78 (100) [$(M - SCN)^+$], 52 (8), 51 (30). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 8.53 (d, J = 5.0 Hz, 1H), 7.78 (ddd, J = 8.0 Hz, 7.3 Hz, 2.0 Hz, 1H), 7.61 (d, J = 8.0 Hz, 1H), 7.29 (dd, J = 7.3 Hz, 5.0 Hz, 1H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 150.62, 150.03, 138.55, 122.86, 122.11, 109.06 (SCN).



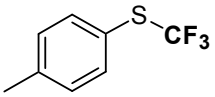
Compound 4b (Table 4, entry 1): MS (EI): *m*/*z* (%): 186 (0.29) [M^+], 129 (6), 118 (7), 117 (100) [$(M - CF_3)^+$], 115 (18), 85 (5), 84 (7), 83 (35), 69 (44), 60 (5), 59 (5), 57 (12), 56 (96), 55 (62).



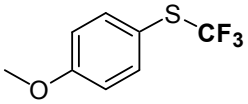
Compound 4c (Table 4, entry 2): MS (EI): *m*/*z* (%): 214 (0.08) [M^+], 157 (5), 147 (5), 146 (10), 145 (100) [$(M - CF_3)^+$], 115 (12), 84 (10), 83 (12), 71 (10), 70 (19), 69 (63), 68 (5), 57 (24), 56 (30), 55 (43). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 2.87 (t, J = 7.5 Hz, 2H), 1.69 (quin, J = 7.5 Hz, 2H), 1.37–1.42 (m, 2H), 1.26–1.34 (m, 8H), 0.89 (t, J = 7.5 Hz, 3H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 131.39 (q, J = 305.9 Hz, SCF_3), 31.90, 30.04, 29.56, 29.23, 29.09, 28.68, 22.77, 14.21. ^{19}F NMR (470.62 MHz, $CDCl_3$): δ –42.20 (s, 3F).



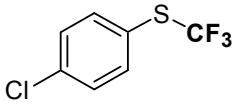
Compound 4d (Table 4, entry 3): MS (EI): *m*/*z* (%): 192 (17) [M^+], 92 (8), 91 (100) [$(M - SCF_3)^+$], 65 (13), 63 (5). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.36–7.27 (m, 5H), 4.11 (s, 2H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 135.16, 130.78 (q, J = 307.0 Hz, SCF_3), 129.07, 129.01, 128.16, 34.42. ^{19}F NMR (470.62 MHz, $CDCl_3$): δ –42.64 (s, 3F).



Compound 4h (Table 4, entries 4 and 5): MS (EI): *m*/*z* (%): 194 (5), 193 (9), 192 (97) [M^+], 173 (5), 125 (5), 124 (7), 123 (100) [$(M - CF_3)^+$], 122 (7), 121 (12), 91 (37), 79 (26), 78 (8), 77 (19), 69 (14), 65 (8), 63 (8), 51 (7). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.53 (d, J = 8.0 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 2.38 (s, 3H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 141.53, 136.54, 130.40, 129.89 (q, J = 308.3 Hz, SCF_3), 121.05, 21.47. ^{19}F NMR (470.62 MHz, $CDCl_3$): δ –44.17 (s, 3F).

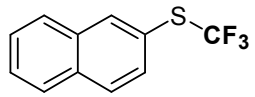


Compound 4i (Table 4, entries 6 and 7): MS (EI): *m*/*z* (%): 209 (6), 208 (63) [M^+], 141 (5), 140 (7), 139 (100) [$(M - CF_3)^+$], 124 (11), 96 (15), 95 (18), 77 (5), 70 (8), 69 (12), 63 (6). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.55–7.58 (m, 2H), 6.91–6.94 (m, 2H), 3.83 (s, 3H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 162.01, 138.43, 129.78 (q, J = 307.1 Hz, SCF_3), 115.16, 115.00, 55.56. ^{19}F NMR (470.62 MHz, $CDCl_3$): δ –44.92 (s, 3F).

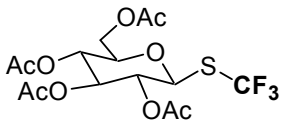


Compound 4j (Table 4, entries 8 and 9): MS (EI): *m*/*z* (%): 214 (32) [M^+], 213 (8), 212 (87) [M^+], 193 (6), 145 (36) [$(M - CF_3)^+$], 144 (8), 143 (100) [$(M - CF_3)^+$], 108 (55), 99 (9), 82 (6),

75 (9), 74 (6), 73 (6), 69 (17), 63 (11), 50 (7). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 7.57–7.59 (m, 2H), 7.38–7.41 (m, 2H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 137.86, 137.72, 129.96, 129.47 (q, J = 308.4 Hz, SCF_3), 122.95. ^{19}F NMR (470.62 MHz, $CDCl_3$): δ –43.78 (s, 3F).

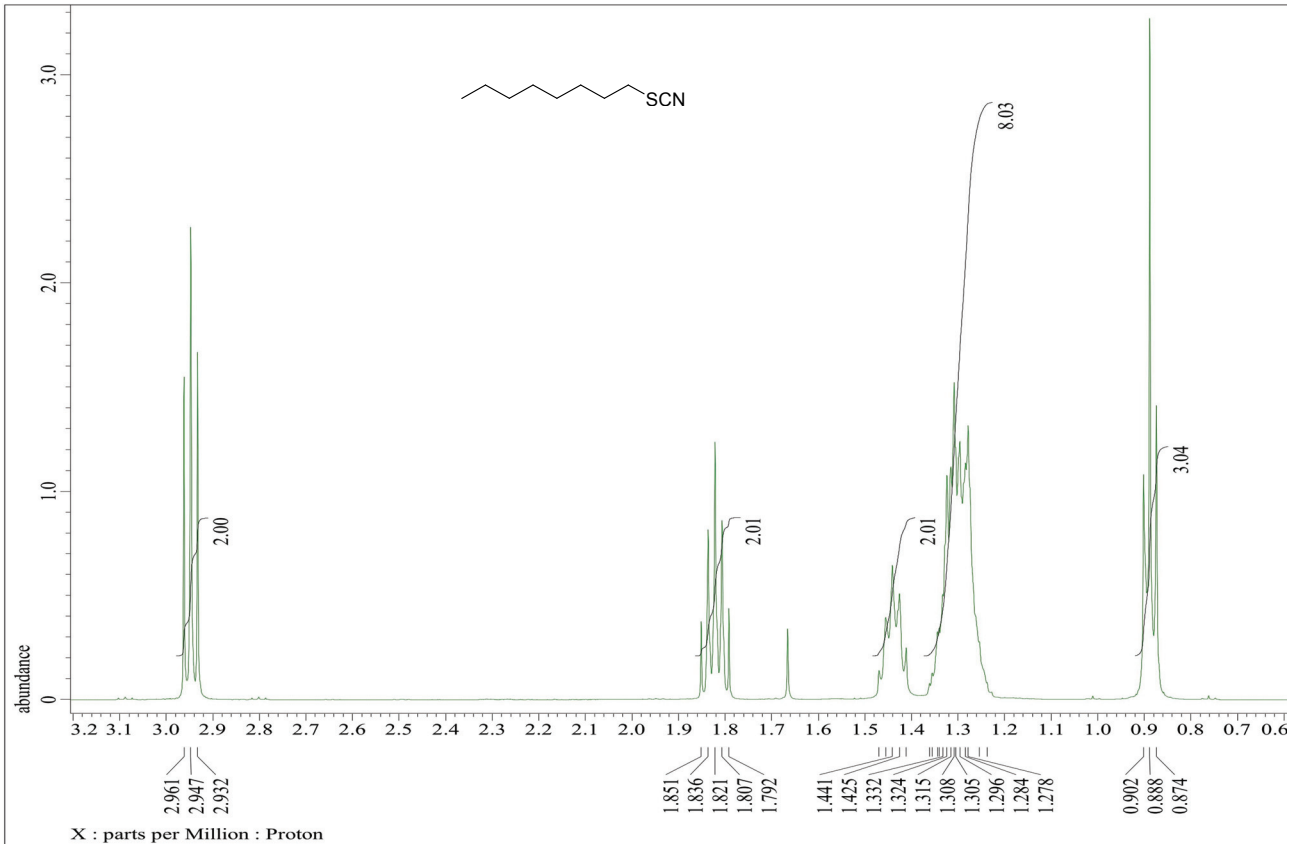


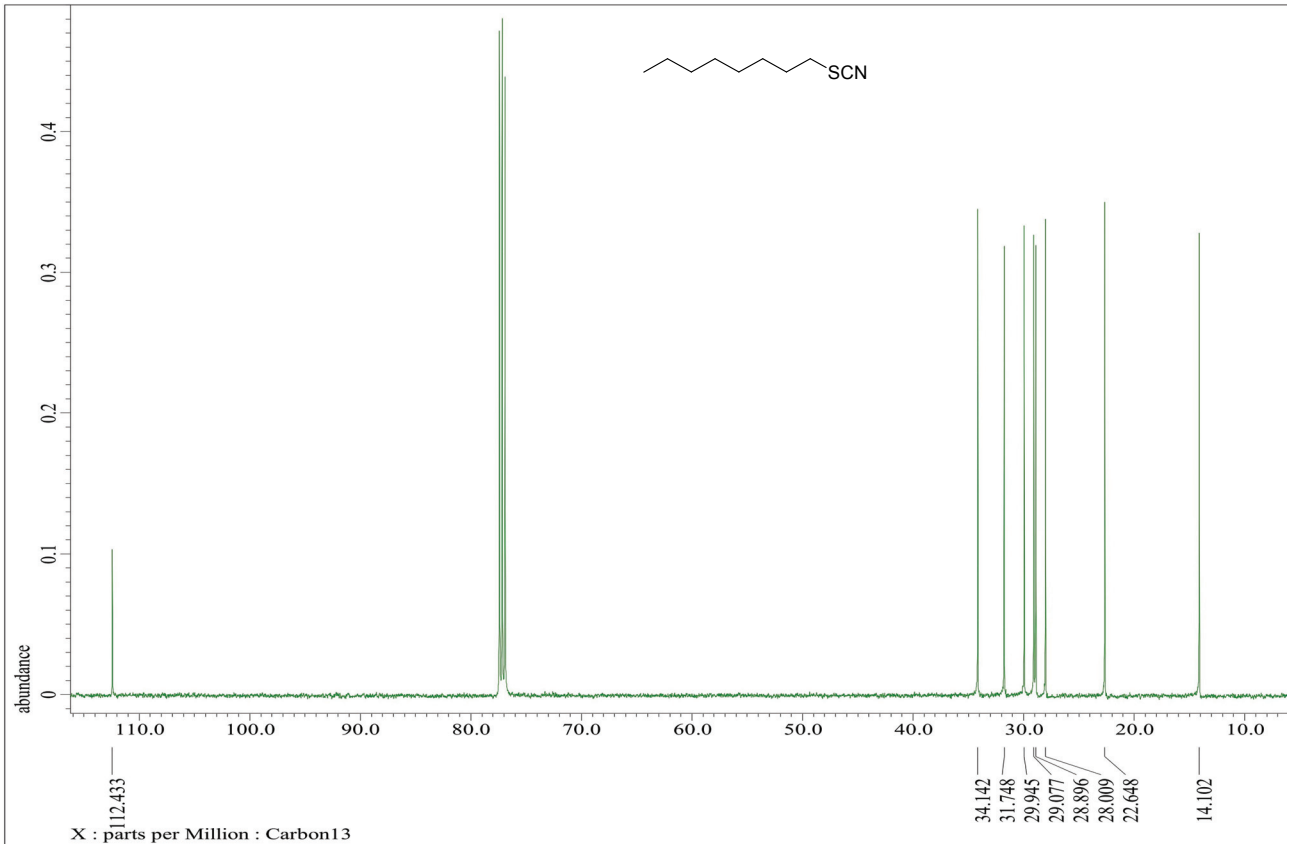
Compound 4k (Table 4, entry 10): MS (EI): *m*/*z* (%): 230 (5), 229 (14), 228 (100) [M^+], 160 (7), 159 (54) [$(M - CF_3)^+$], 158 (5), 116 (6), 115 (57), 114 (5). ^{1}H NMR (500.16 MHz, $CDCl_3$): δ 8.18 (s, 1H), 7.82–7.87 (m, 3H), 7.64–7.66 (m, 1H), 7.52–7.58 (m, 2H). ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 137.17, 134.03, 133.53, 131.94, 129.89 (q, J = 308.3 Hz, SCF_3), 129.36, 128.32, 128.07, 127.92, 127.15, 121.66. ^{19}F NMR (470.62 MHz, $CDCl_3$): δ –43.47 (s, 3F).



Compound 4m (Table 4, entry 11): MS (EI): *m*/*z* (%): 363 (0.12) [$(M - SCF_3)^+$], 331 (2.4) [$(M - SCF_3)^+$], 211 (9), 210 (13), 197 (12), 170 (9), 169 (100), 139 (16), 127 (23), 115 (18), 110 (5), 109 (65), 103 (14), 102 (7), 99 (5), 98 (6), 97 (20), 85 (7), 81 (9), 70 (5), 69 (11).

NMR Spectra


SCN
8.03
3.04
2.00
2.01
2.01
abundance
3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.8 0.7 0.6
2.961 2.947 2.932
1.851 1.836 1.821 1.807 1.792
1.441 1.425 1.332 1.324 1.315 1.308 1.305 1.296 1.284 1.278
0.902 0.888 0.874
X : parts per Million : Proton


SCN
abundance
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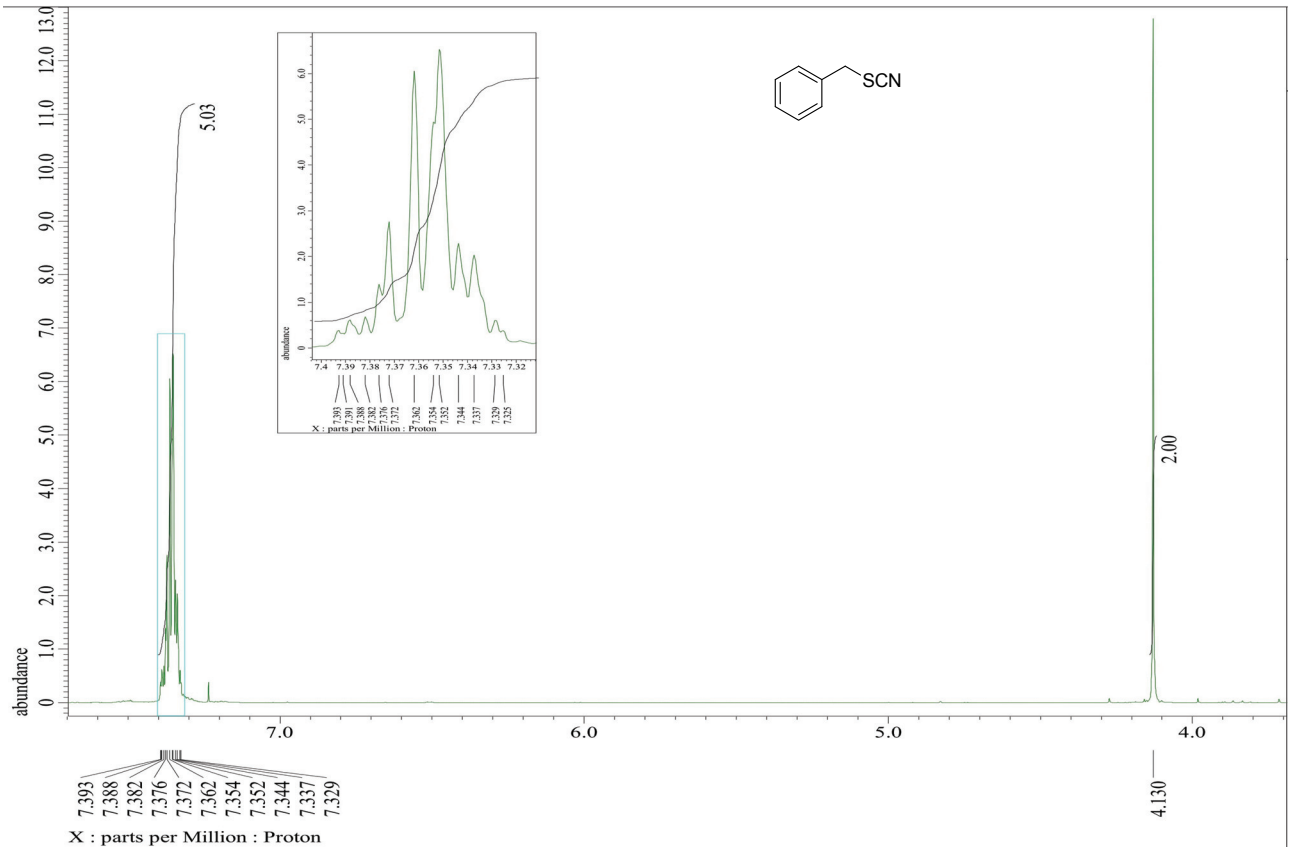
112.433
34.142 31.748 29.945 29.077 28.896 28.009 22.648 14.102
X : parts per Million : Carbon13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2.00
abundance
7.0
6.0
5.0
4.0
7.393
7.388
7.382
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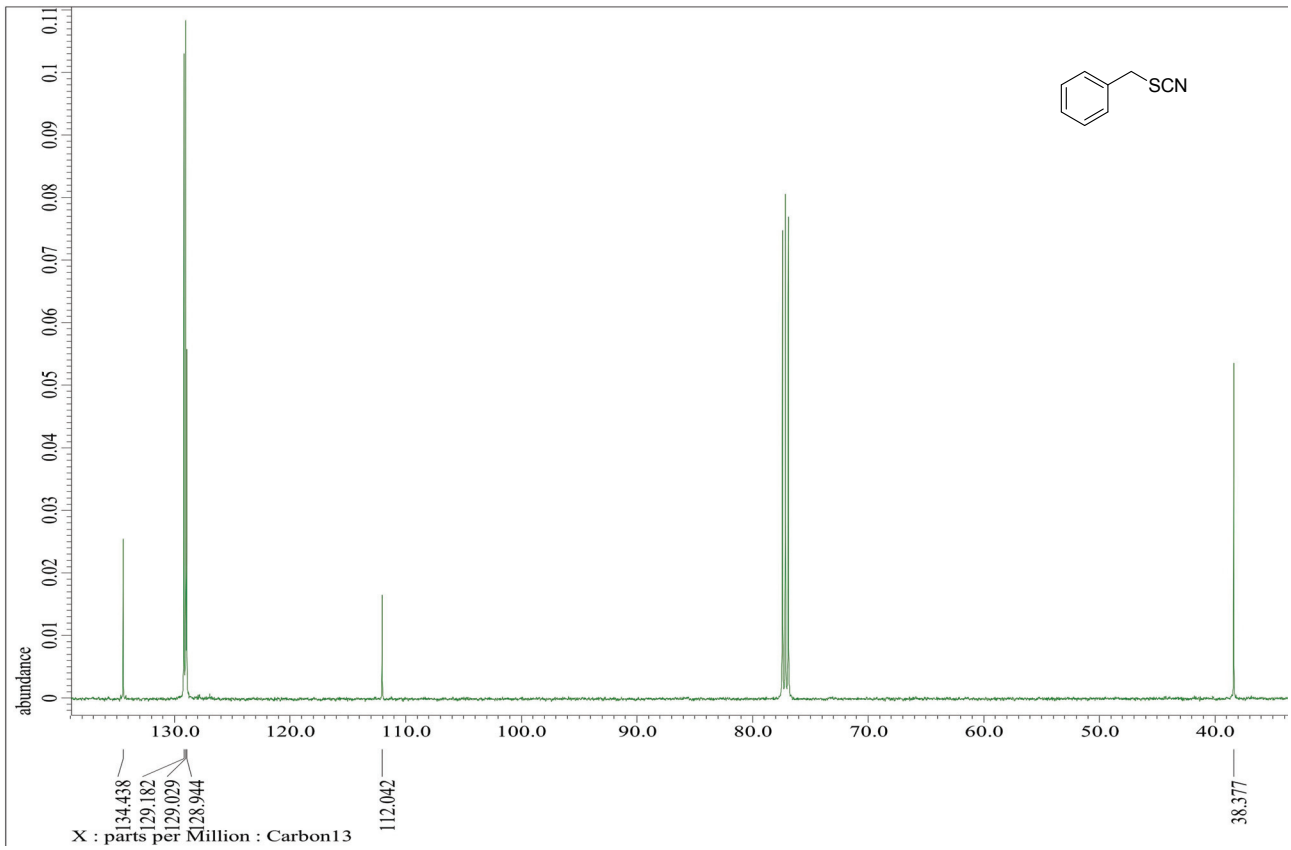
7.372
7.362
7.354
7.352
7.344
7.337
7.329
4.130
X : parts per Million : Proton


SCN
abundance
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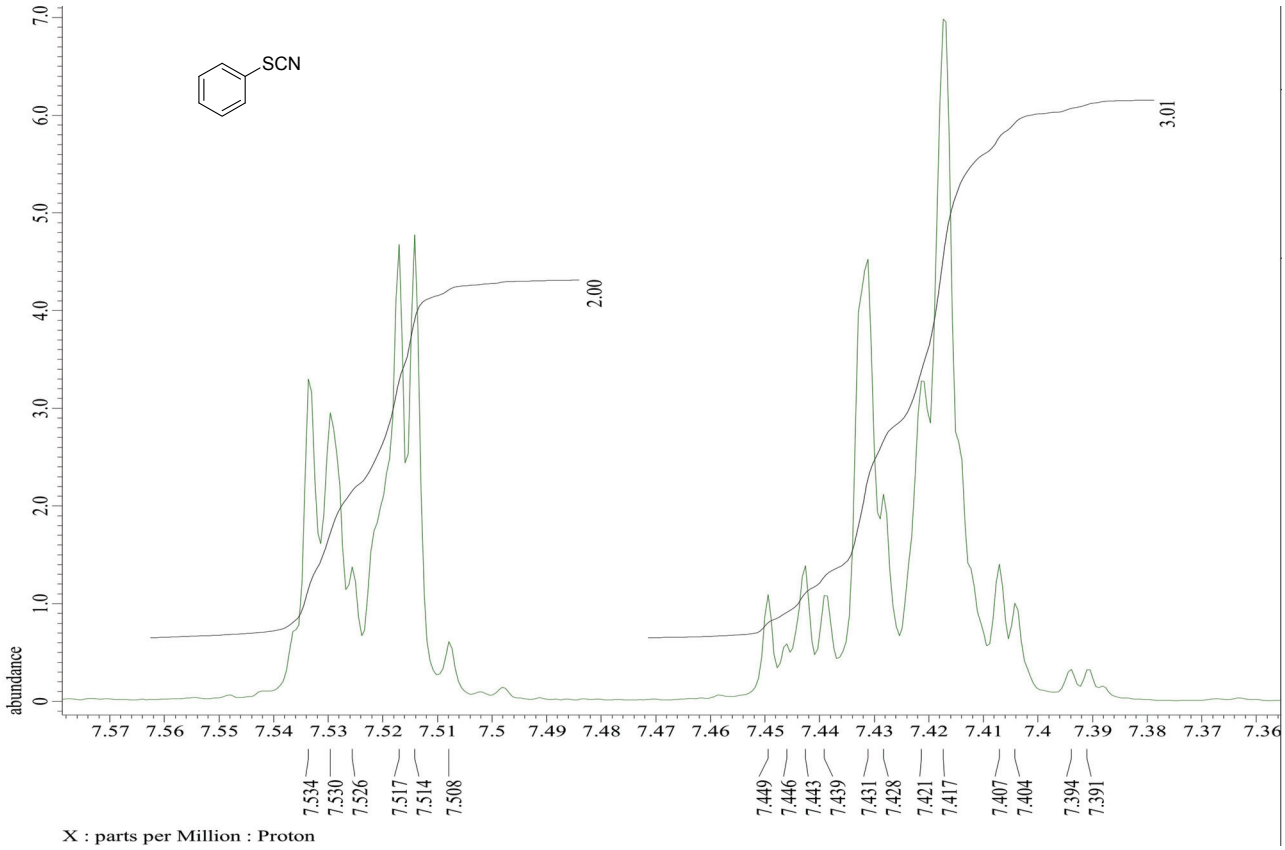
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
134.438
129.182
129.029
128.944
112.042
38.377
X : parts per Million : Carbon13


SCN
abundance
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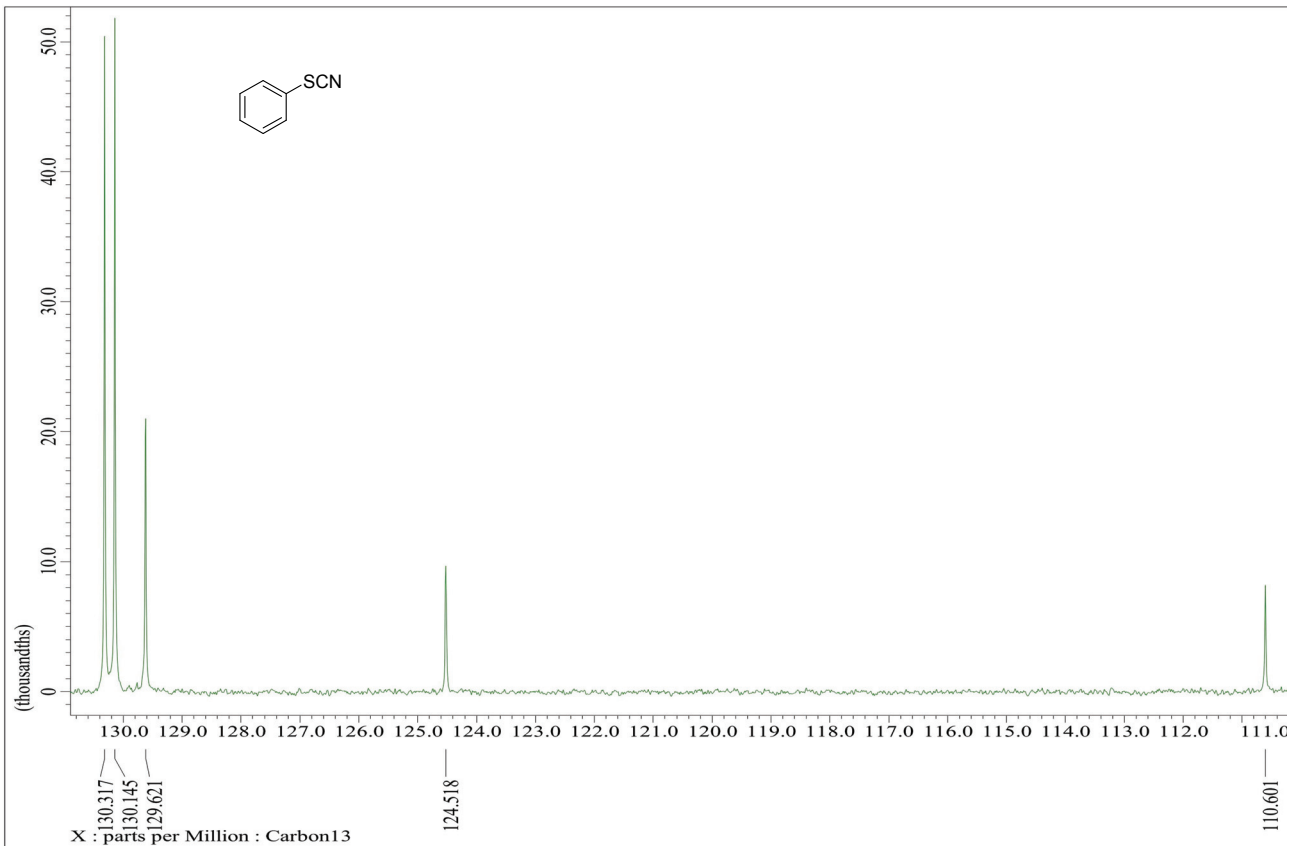
6.0
5.0
4.0
3.0
2.0
1.0
0
2.00
3.01
7.57 7.56 7.55 7.54 7.53 7.52 7.51 7.5 7.49 7.48 7.47 7.46 7.45 7.44 7.43 7.42 7.41 7.4 7.39 7.38 7.37 7.36
7.534
7.530
7.526
7.517
7.514
7.508
7.449
7.446
7.443
7.439
7.431
7.428
7.421
7.417
7.407
7.404
7.394
7.391
X : parts per Million : Proton


SCN
(thousandths)
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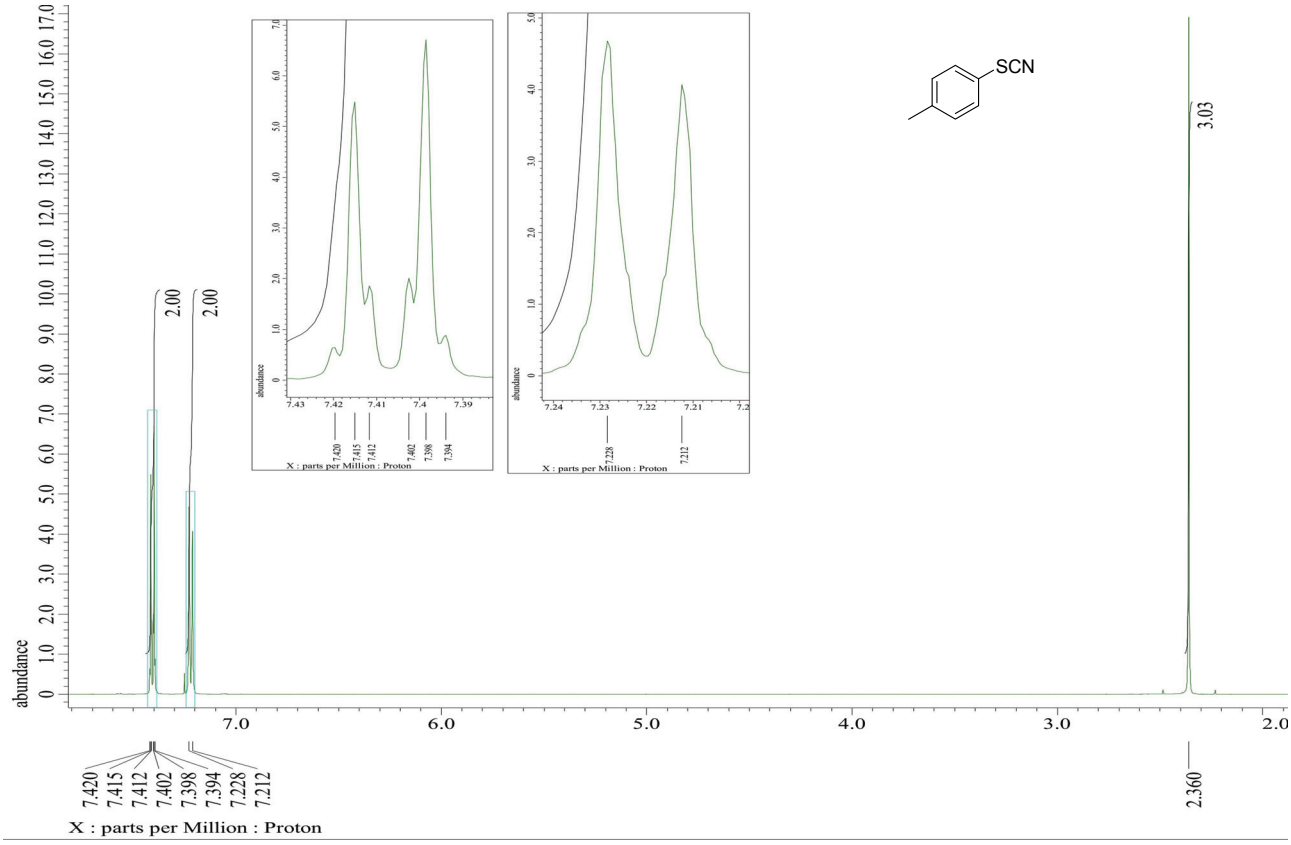
40.0
30.0
20.0
10.0
0
130.0 129.0 128.0 127.0 126.0 125.0 124.0 123.0 122.0 121.0 120.0 119.0 118.0 117.0 116.0 115.0 114.0 113.0 112.0
130.317
130.145
129.621
124.518
110.601
X : parts per Million : Carbon13


SCN
abundance
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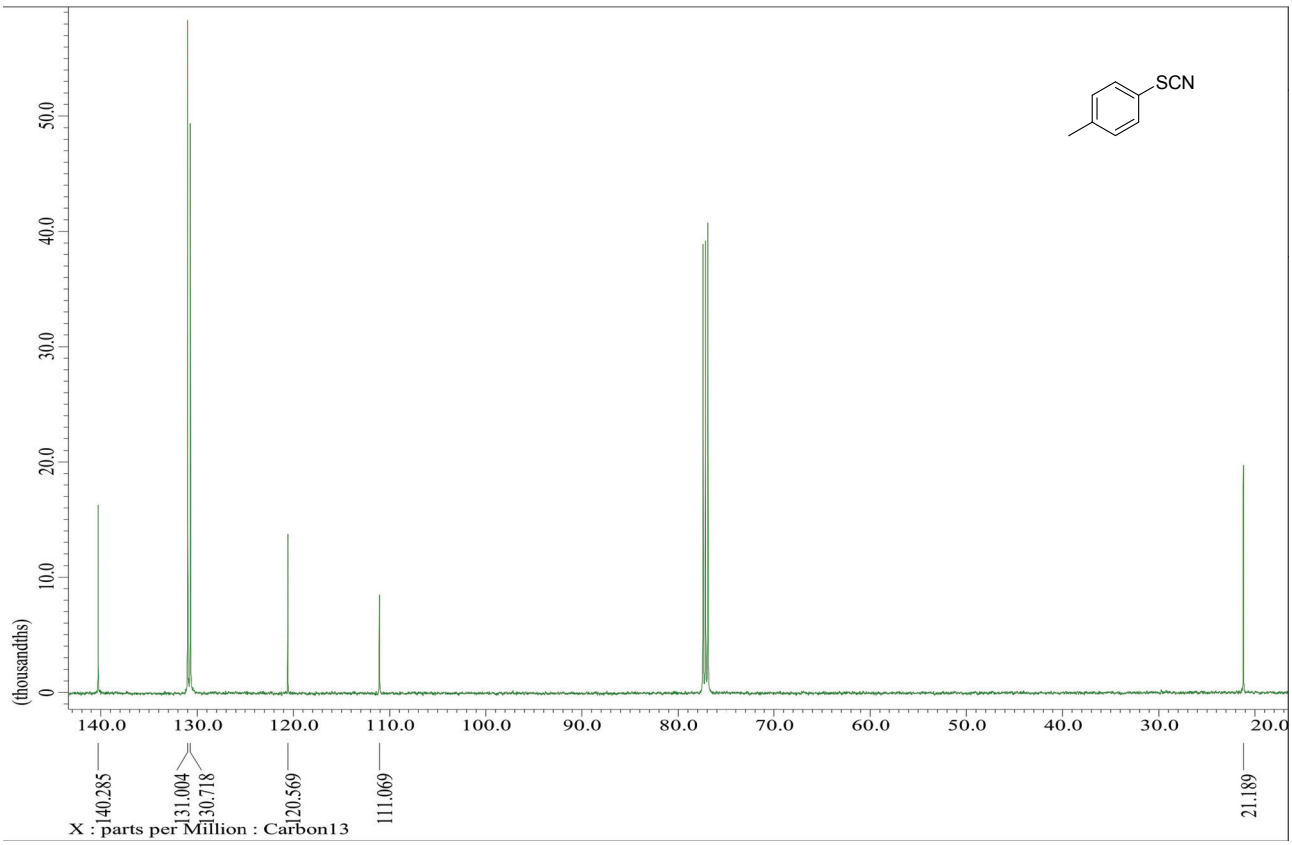
7.412
7.402
7.398
7.394
7.228
7.212
2.360
X : parts per Million : Proton


SCN
(thousandths)
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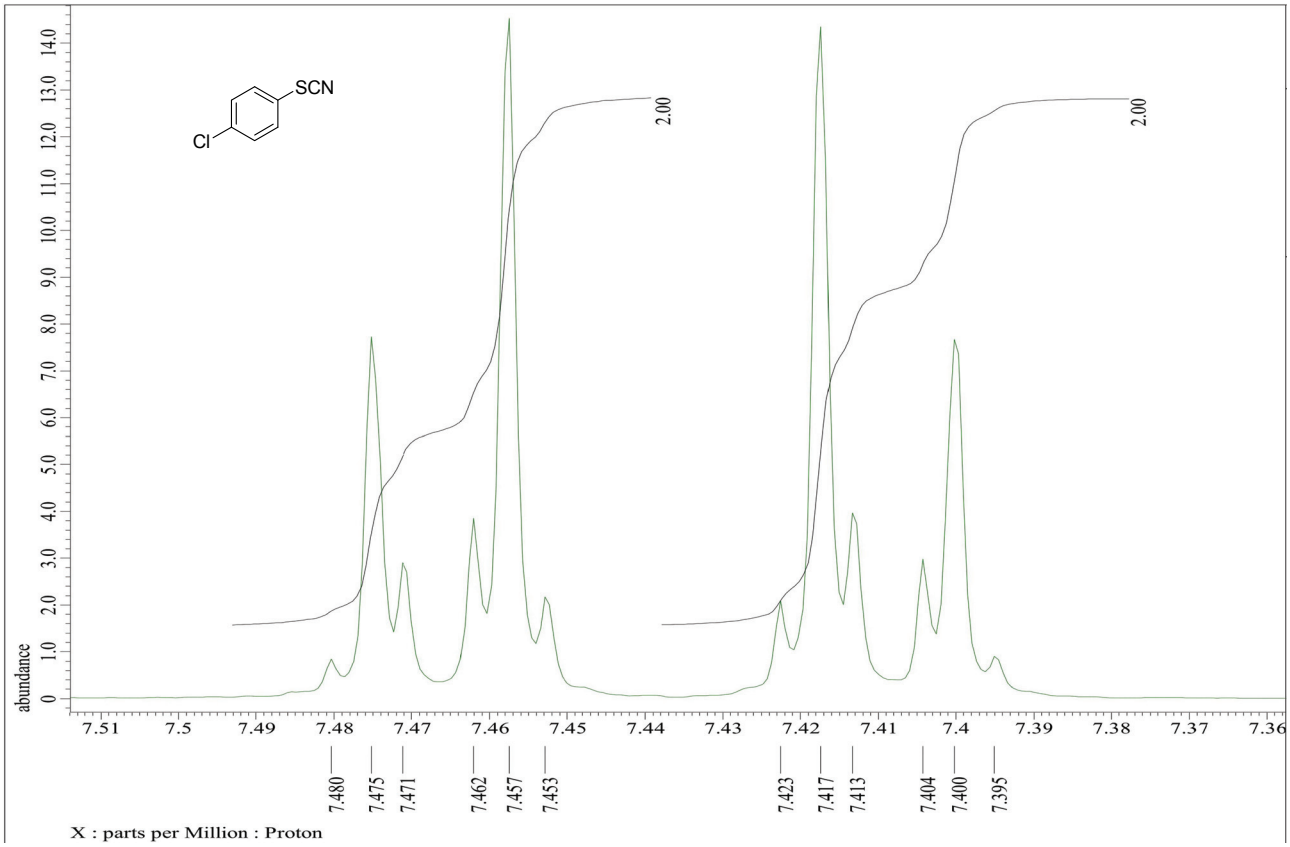
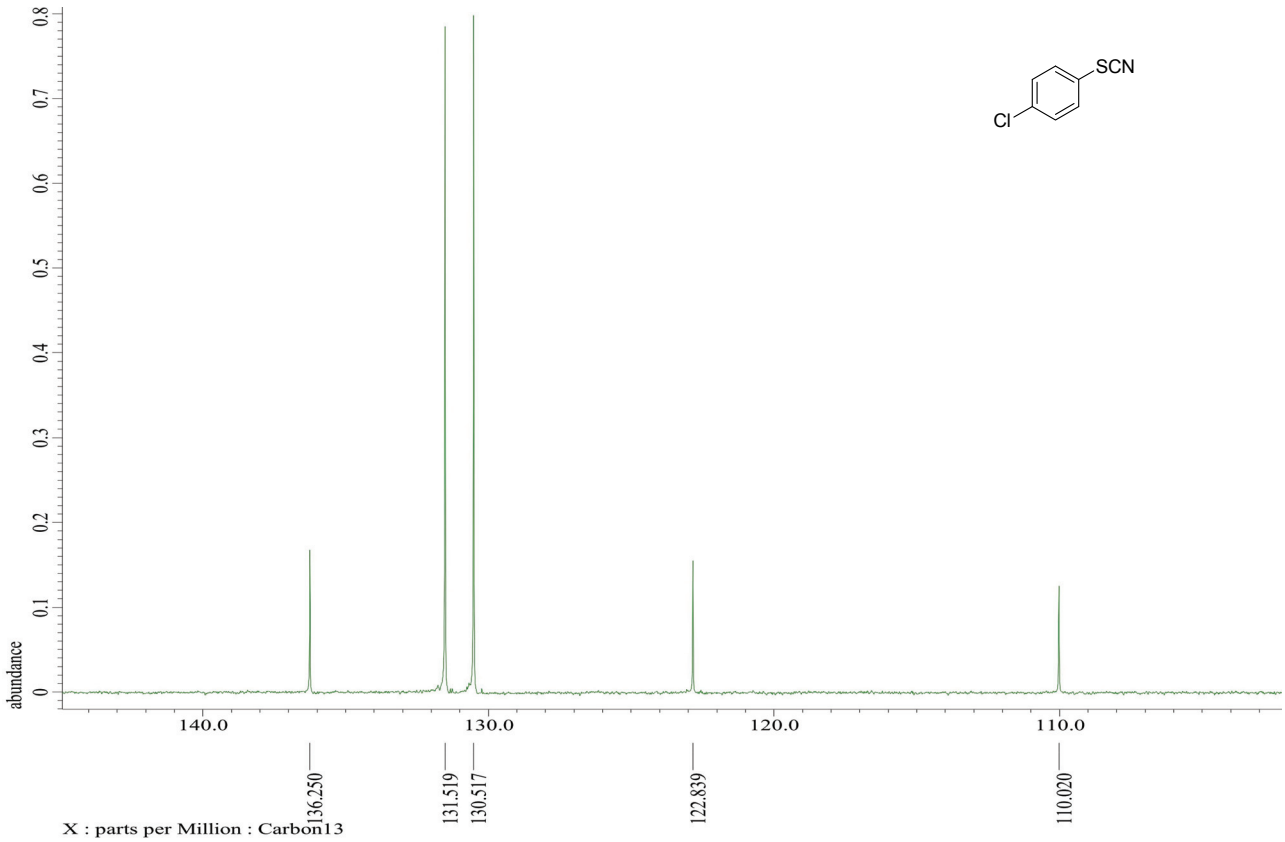
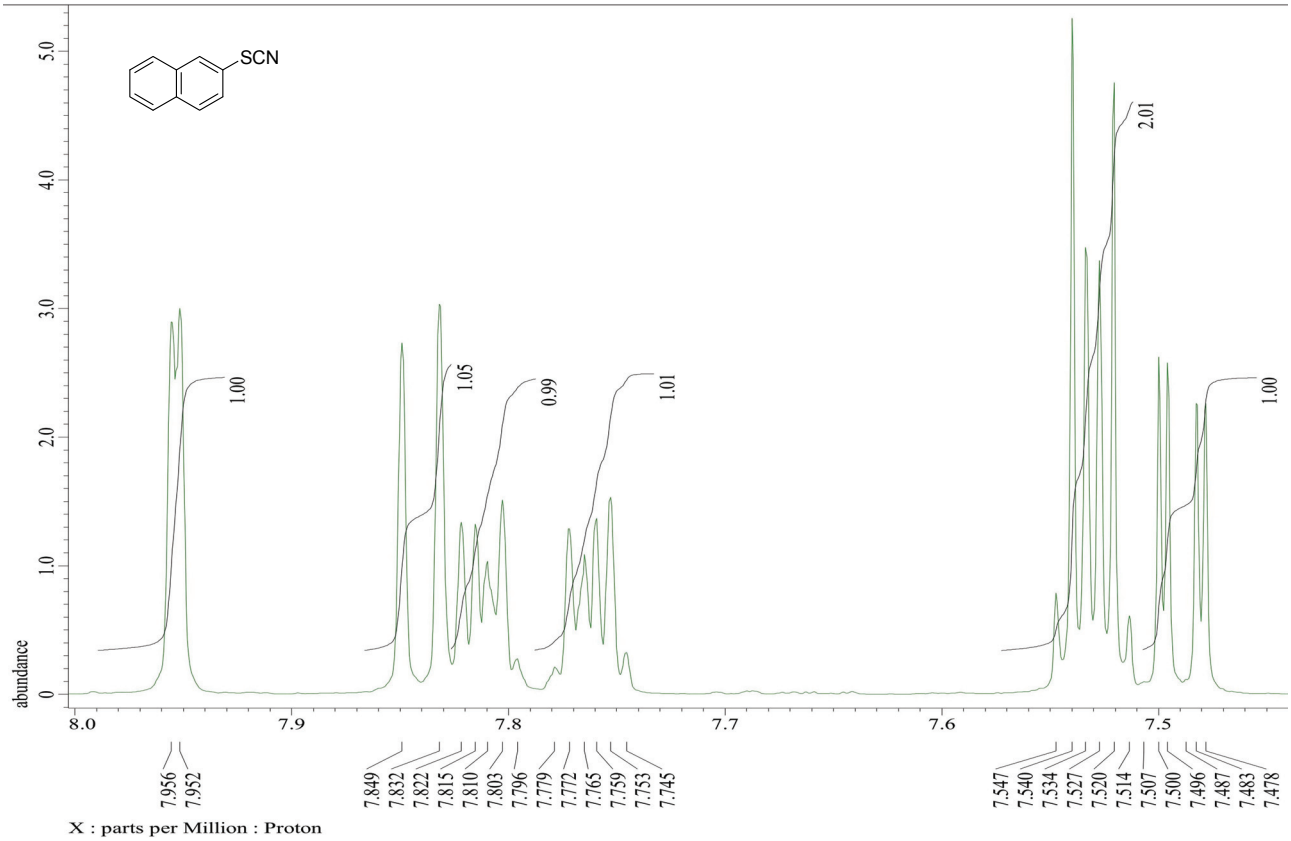
131.004
130.718
120.569
111.069
21.189
X : parts per Million : Carbon13


SCN
Cl
2.00
2.00
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0
7.51 7.5 7.49 7.48 7.47 7.46 7.45 7.44 7.43 7.42 7.41 7.4 7.39 7.38 7.37 7.36
7.480 7.475 7.471 7.462 7.457 7.453 7.423 7.417 7.413 7.404 7.400 7.395
X : parts per Million : Proton


SCN
Cl
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8
140.0 130.0 120.0 110.0
136.250 131.519 130.517 122.839 110.020
X : parts per Million : Carbon13


SCN
abundance
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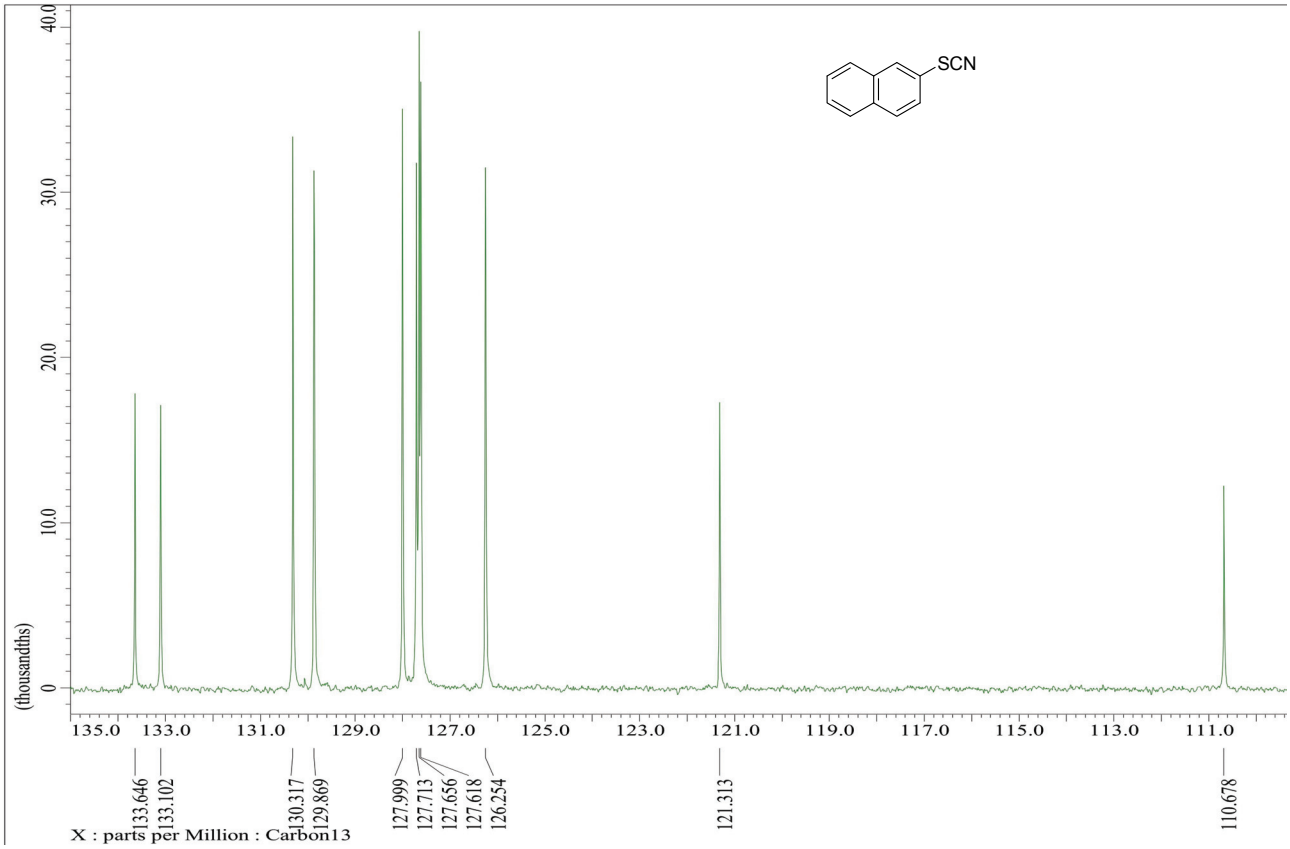
4.0
3.0
2.0
1.0
0
1.00
1.05
0.99
1.01
2.01
1.00
8.0
7.9
7.8
7.7
7.6
7.5
7.956
7.952
7.849
7.832
7.822
7.815
7.810
7.803
7.796
7.779
7.772
7.765
7.759
7.753
7.745
7.547
7.540
7.534
7.527
7.520
7.514
7.507
7.500
7.496
7.487
7.483
7.478
X : parts per Million : Proton


SCN
(thousandths)
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20.0
10.0
0
135.0
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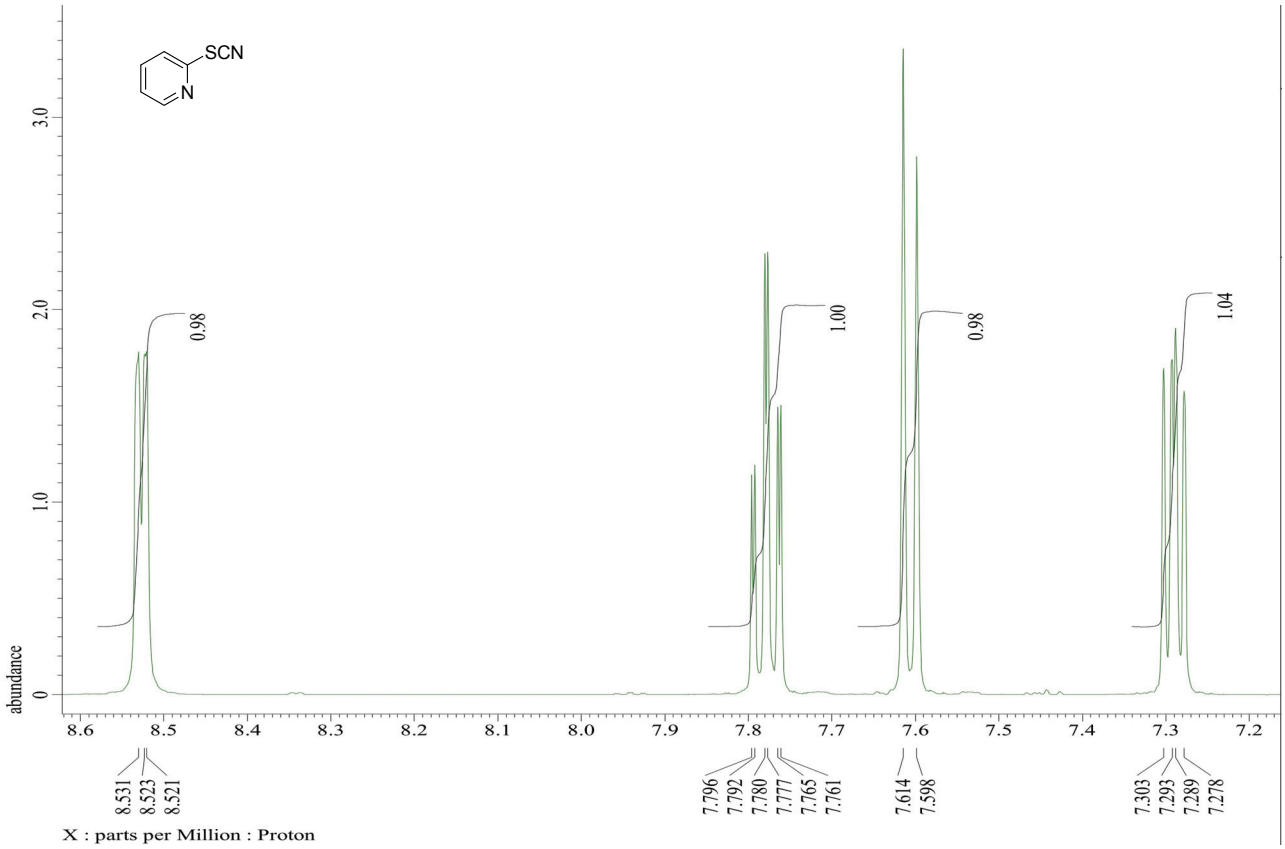
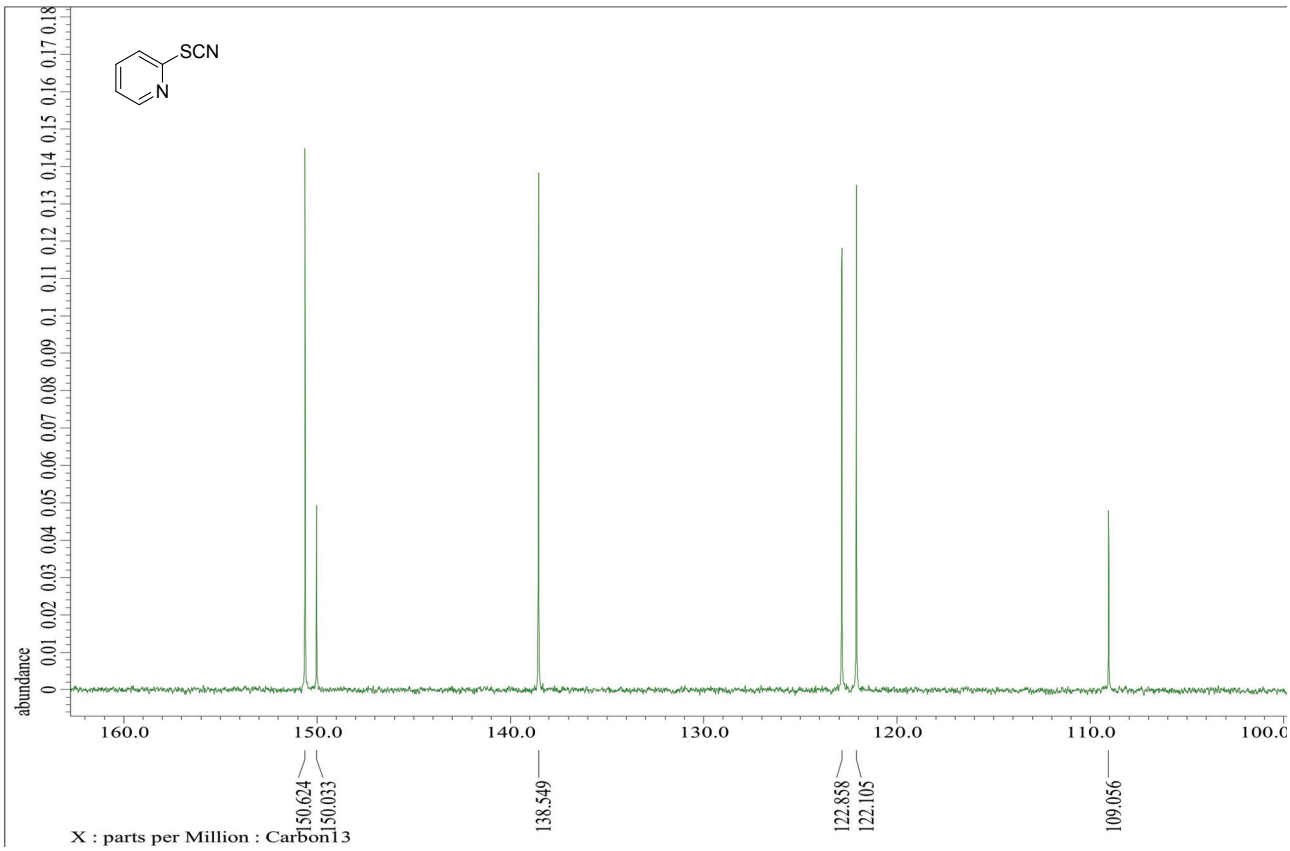
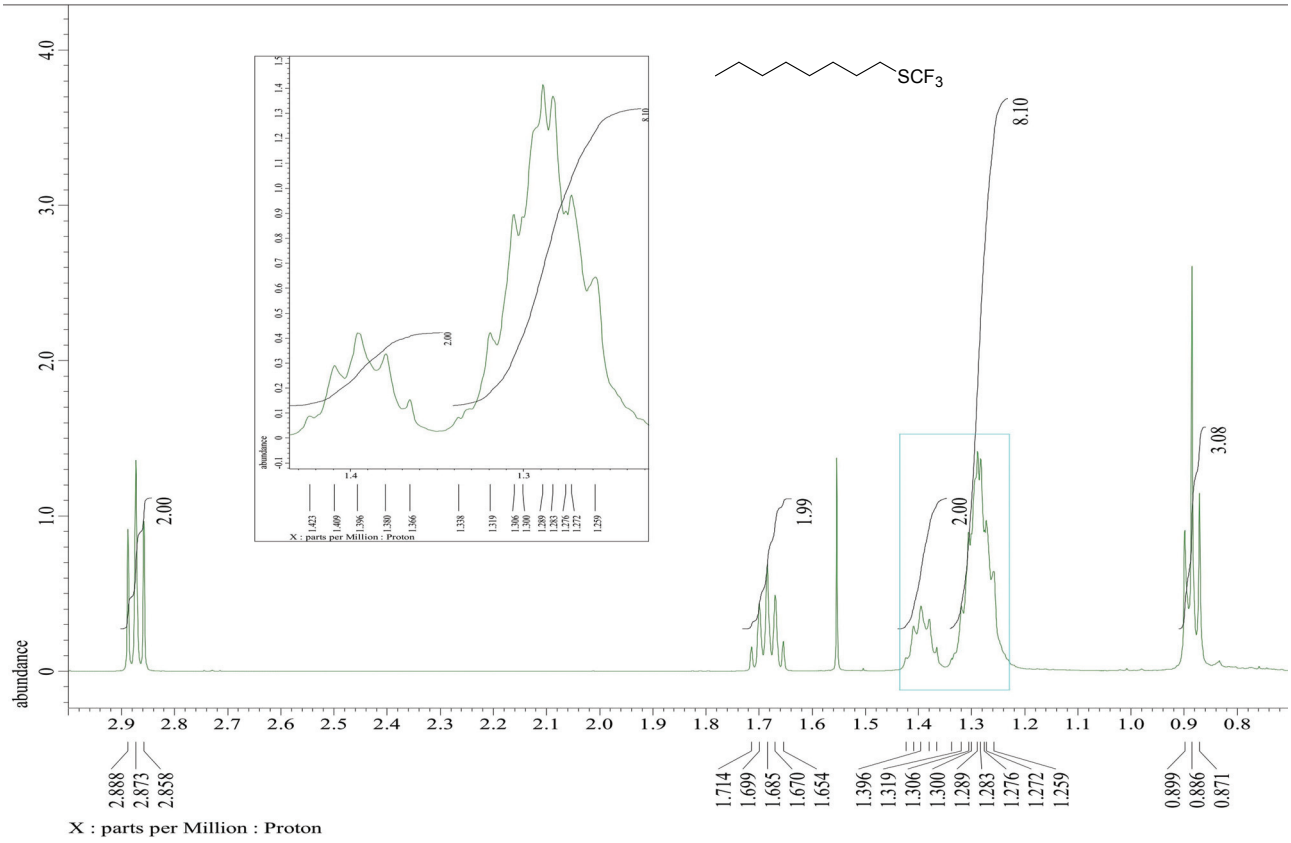
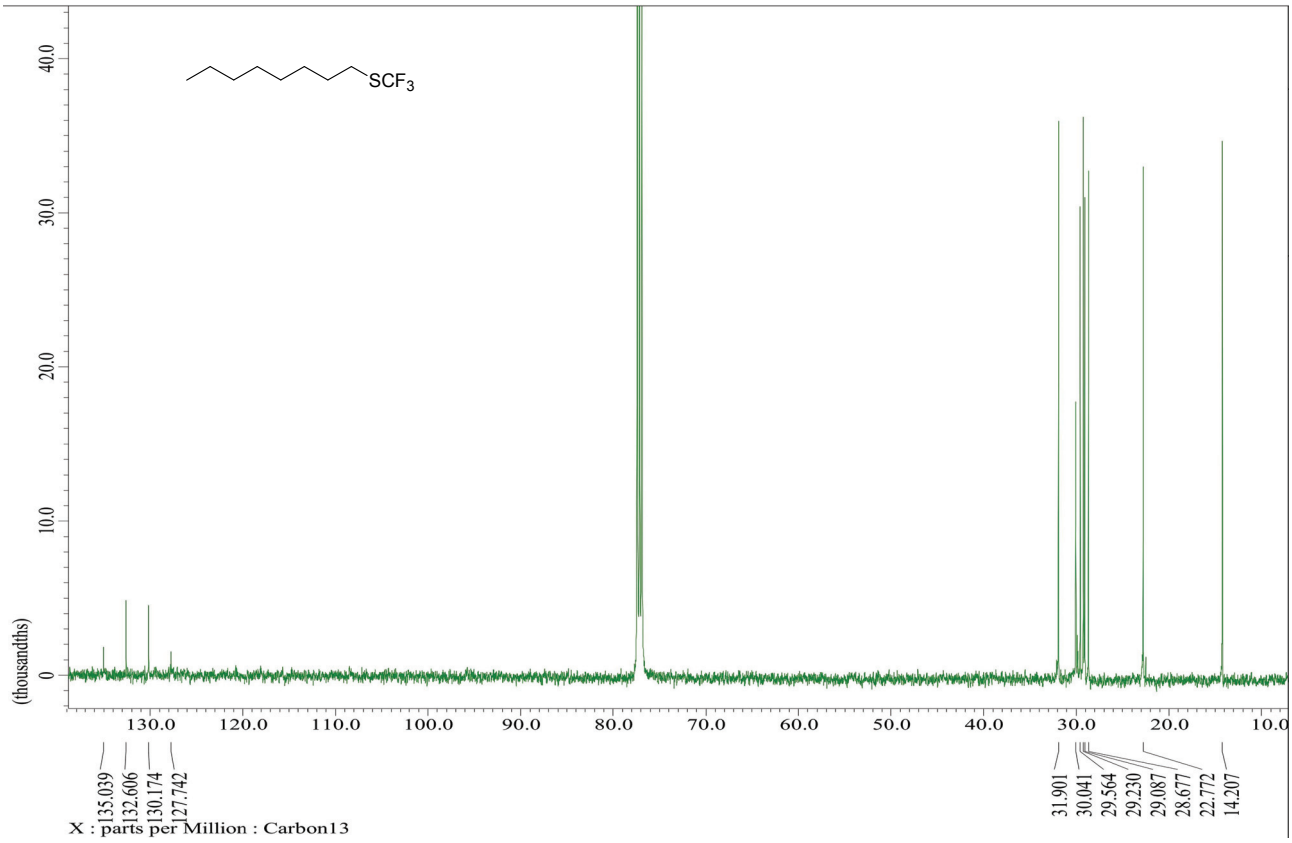
131.0
129.0
127.0
125.0
123.0
121.0
119.0
117.0
115.0
113.0
111.0
133.646
133.102
130.317
129.869
127.999
127.713
127.656
127.618
126.254
121.313
110.678
X : parts per Million : Carbon13


SCN
N
abundance
0
1.0
2.0
3.0
0.98
1.00
0.98
1.04
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
8.531
8.523
8.521
7.796
7.792
7.780
7.777
7.765
7.761
7.614
7.598
7.303
7.293
7.289
7.278
X : parts per Million : Proton


SCN
N
abundance
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
0.12
0.13
0.14
0.15
0.16
0.17
0.18
160.0
150.0
140.0
130.0
120.0
110.0
100.0
150.624
150.033
138.549
122.858
122.105
109.056
X : parts per Million : Carbon13


SCF3
8.10
3.08
2.00
1.99
2.00
2.00
abundance
X : parts per Million : Proton
2.888
2.873
2.858
1.714
1.699
1.685
1.670
1.654
1.396
1.319
1.306
1.300
1.289
1.283
1.276
1.272
1.259
0.899
0.886
0.871


SCF3
(thousandths)
X : parts per Million : Carbon13
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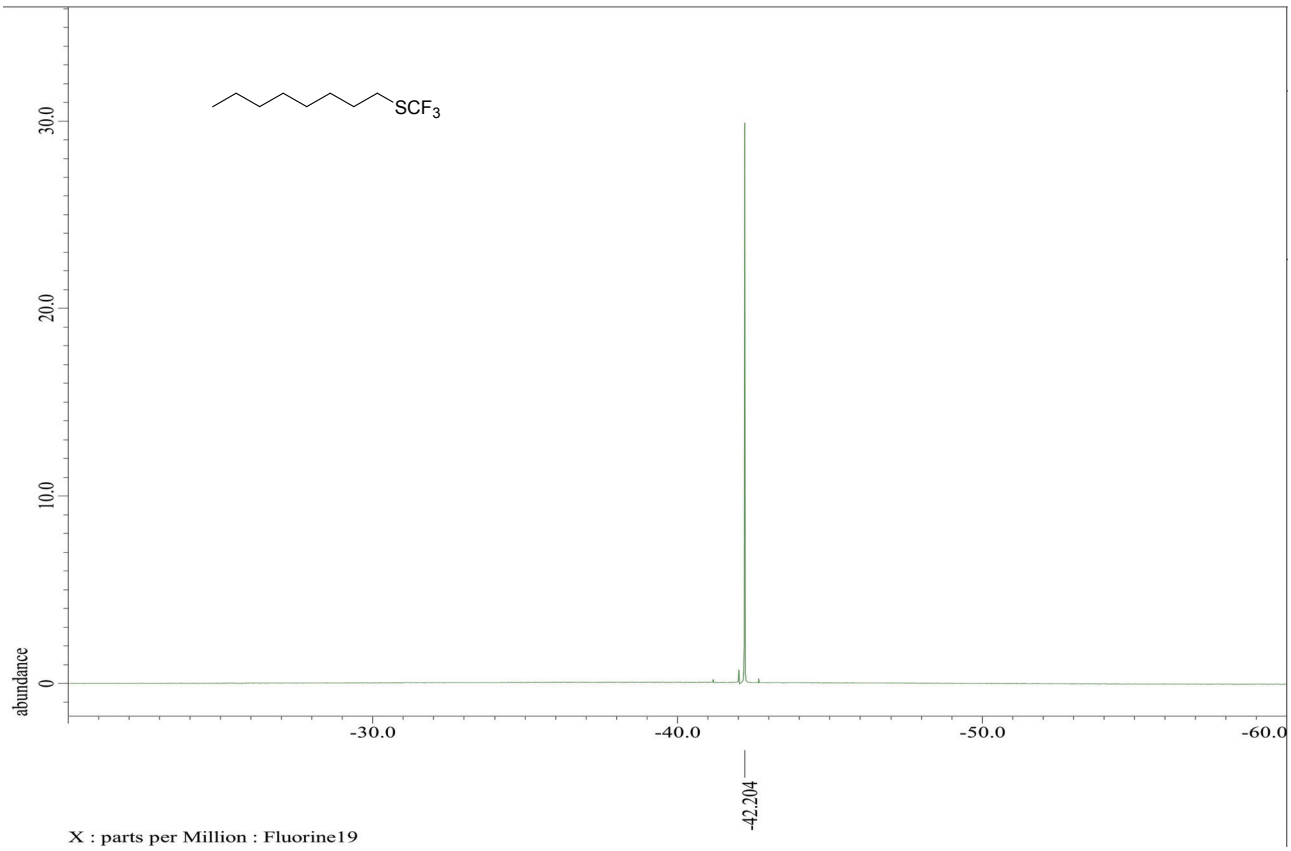
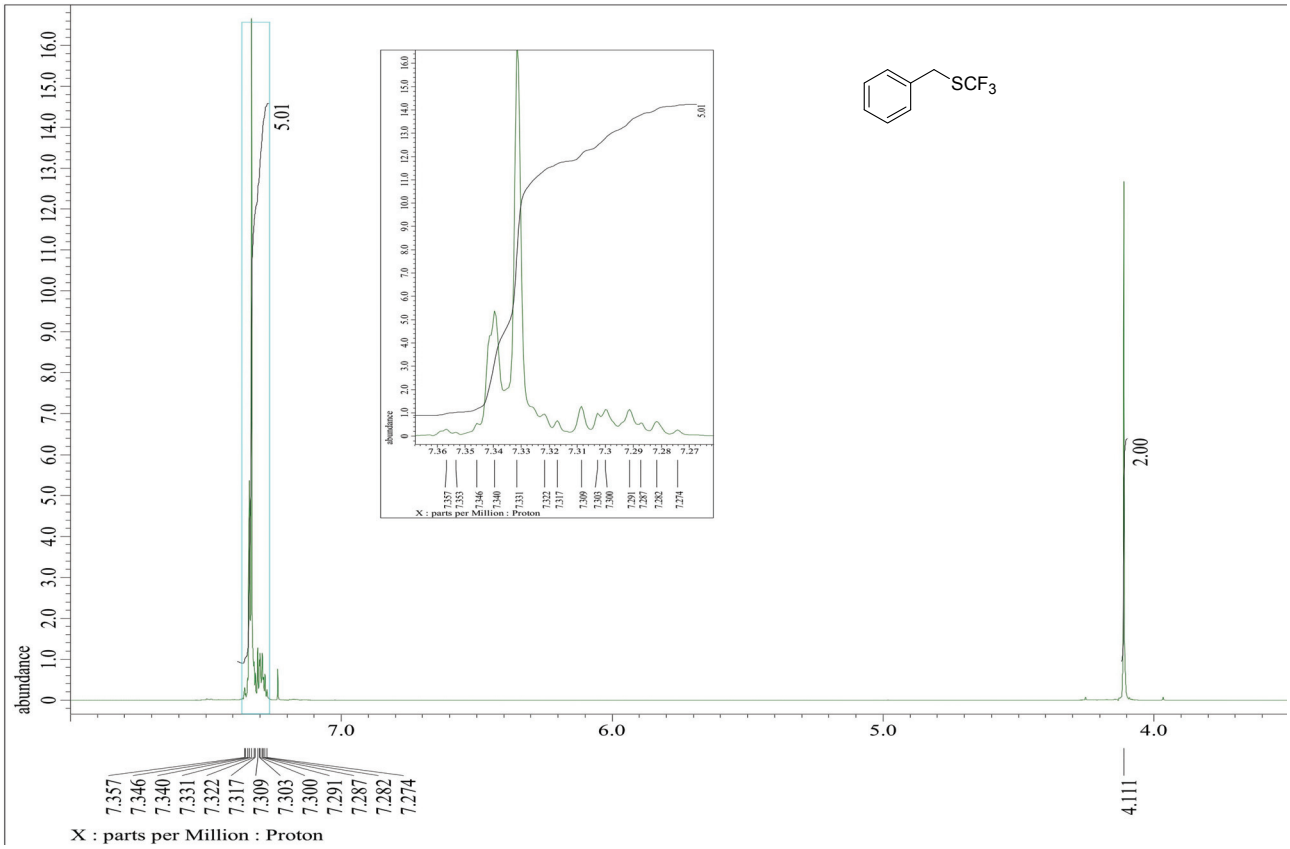
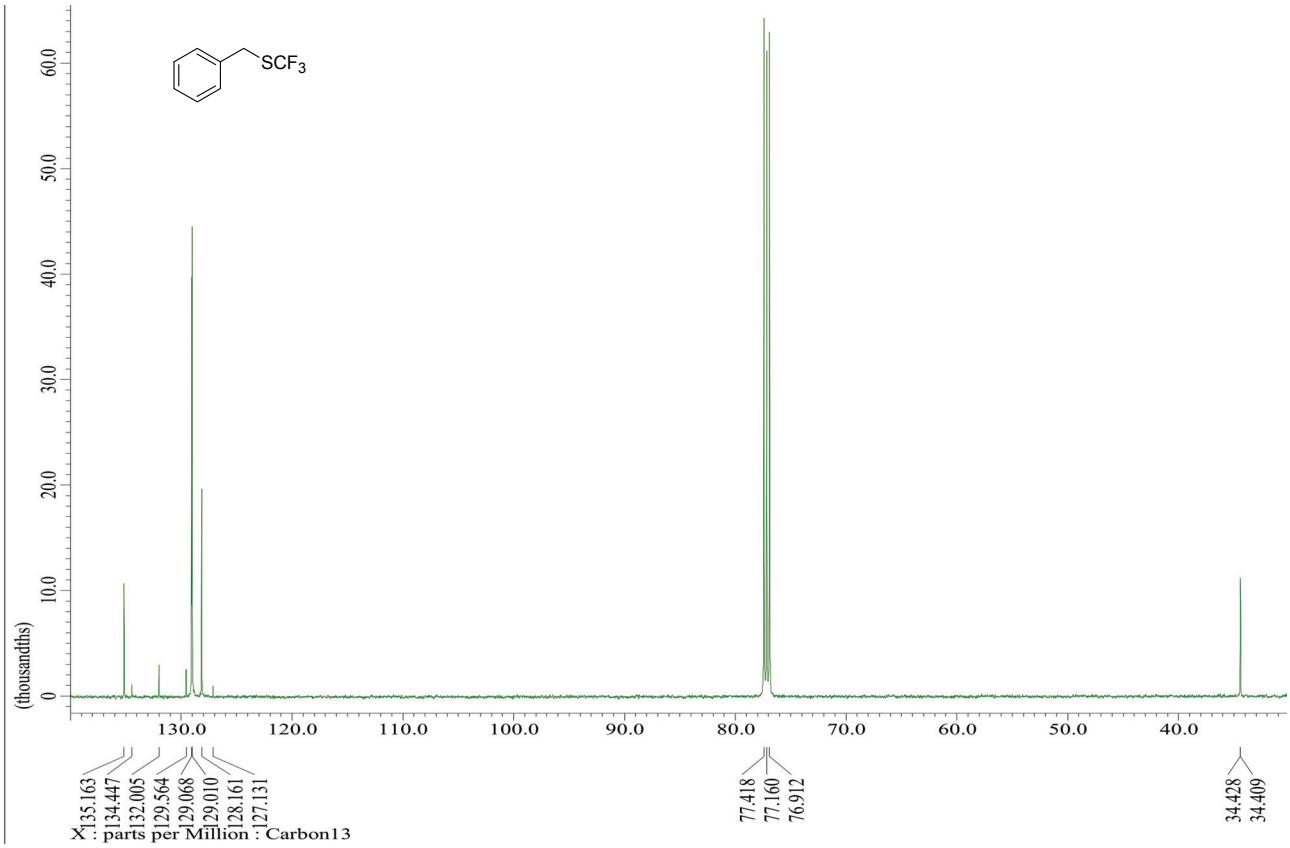
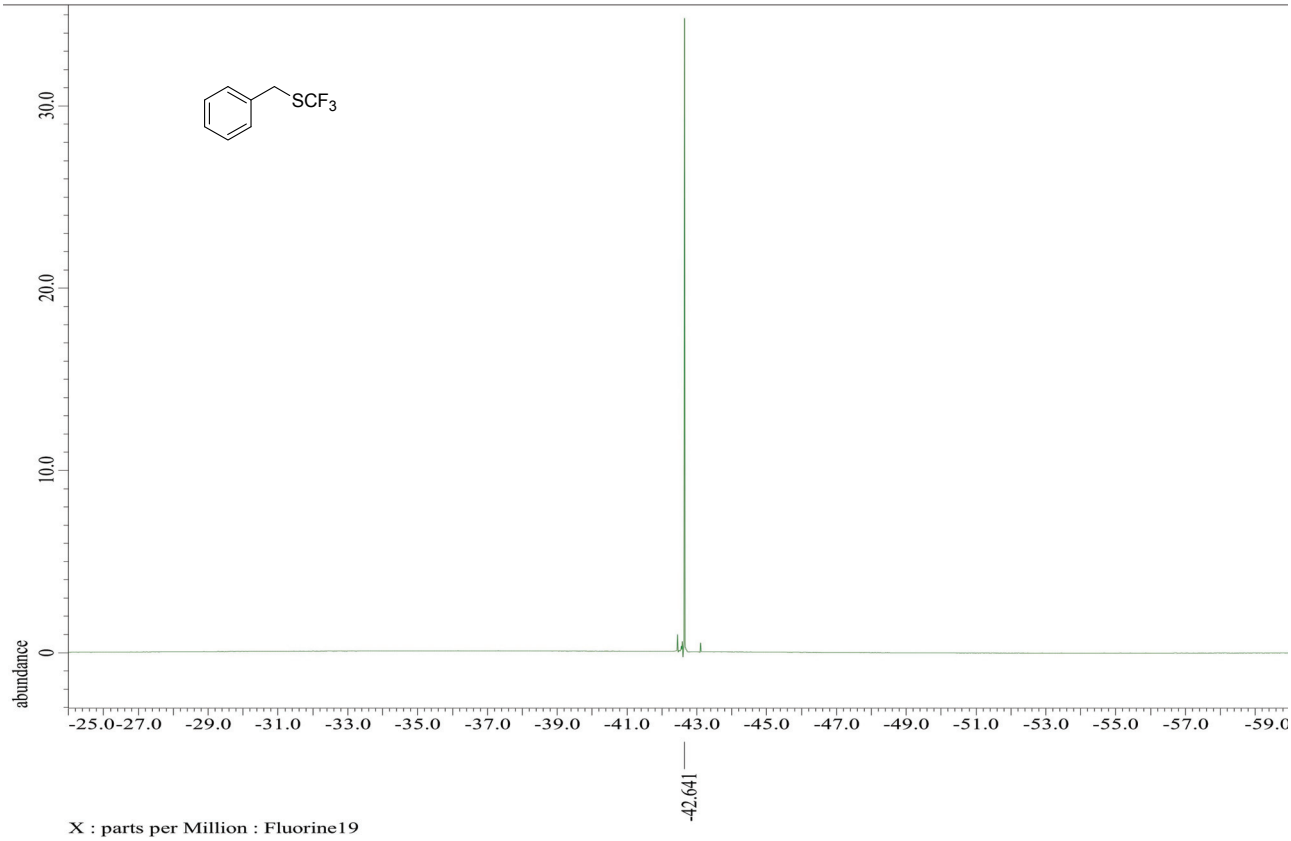
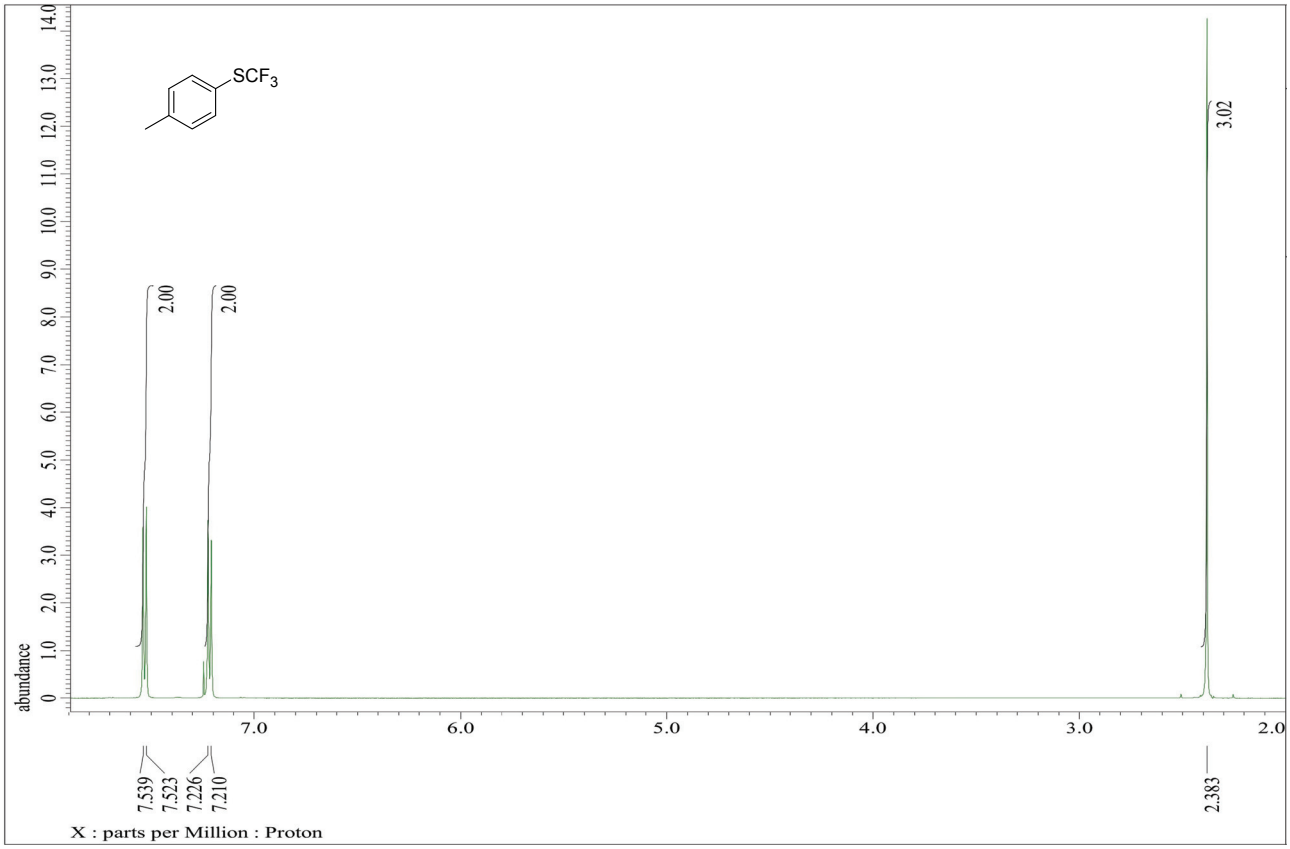
130.174
127.742
31.901
30.041
29.564
29.230
29.087
28.677
22.772
14.207

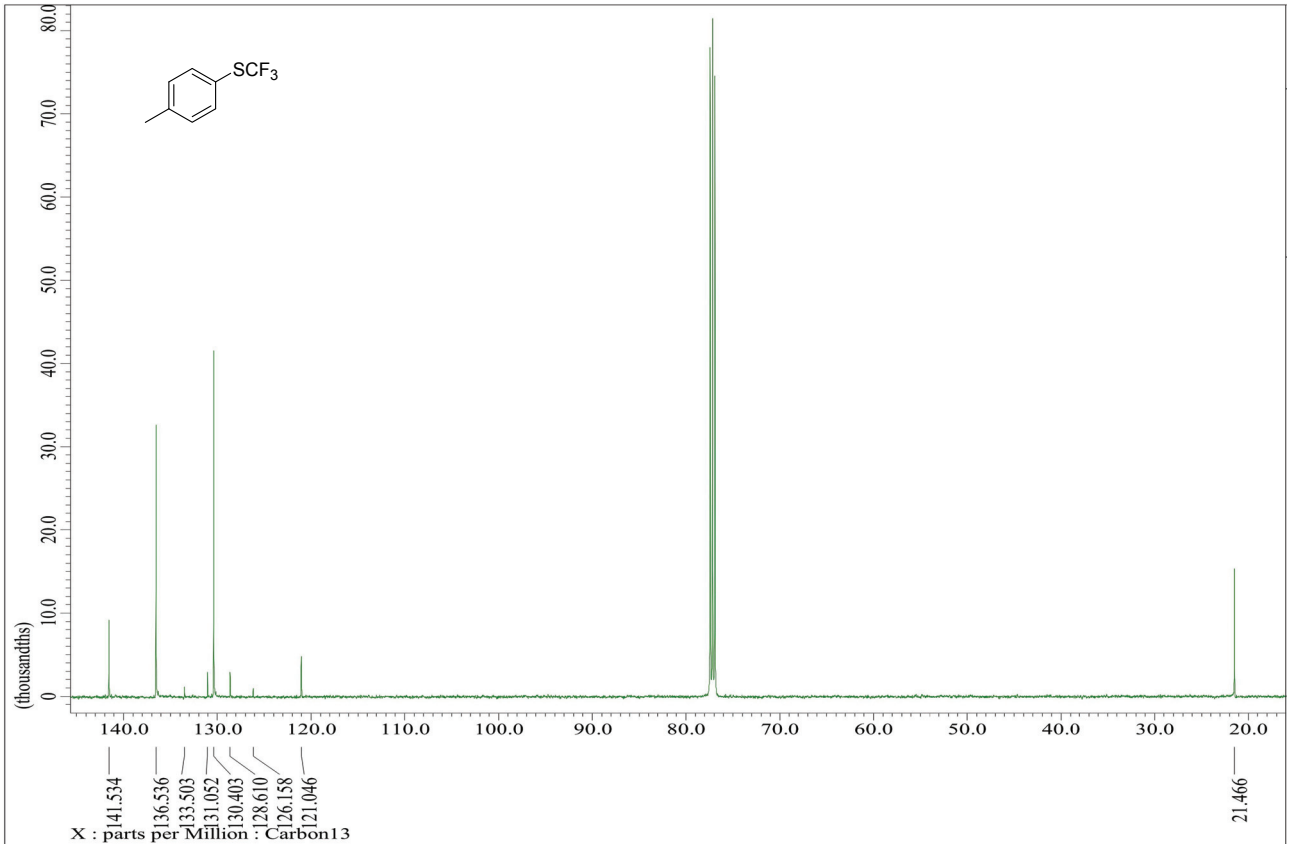

SCF3
30.0
20.0
10.0
0
abundance
-30.0
-40.0
-50.0
-60.0
-42.204
X : parts per Million : Fluorine19

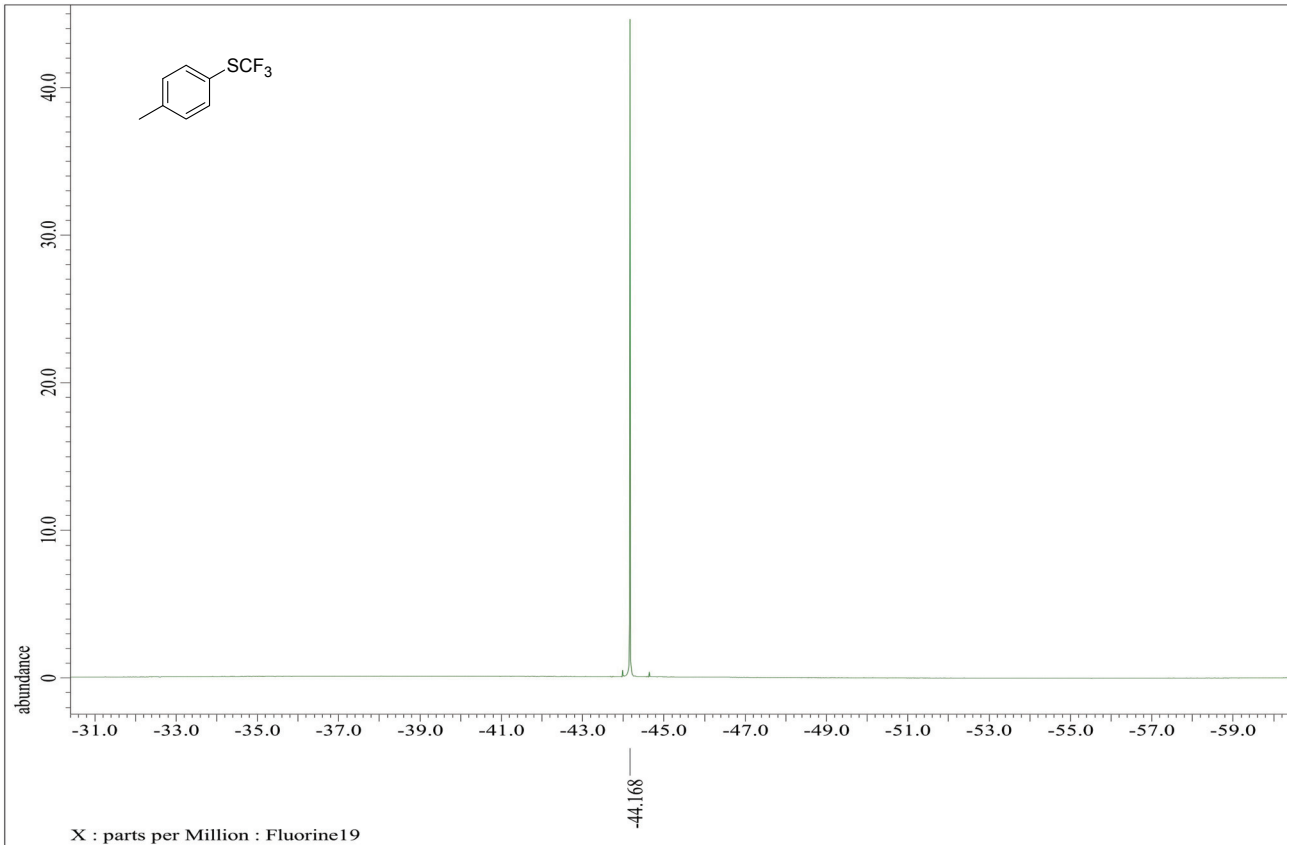

SCF3
5.01
2.00
abundance
7.357
7.346
7.340
7.331
7.322
7.317
7.309
7.303
7.300
7.291
7.287
7.282
7.274
4.111
X : parts per Million : Proton

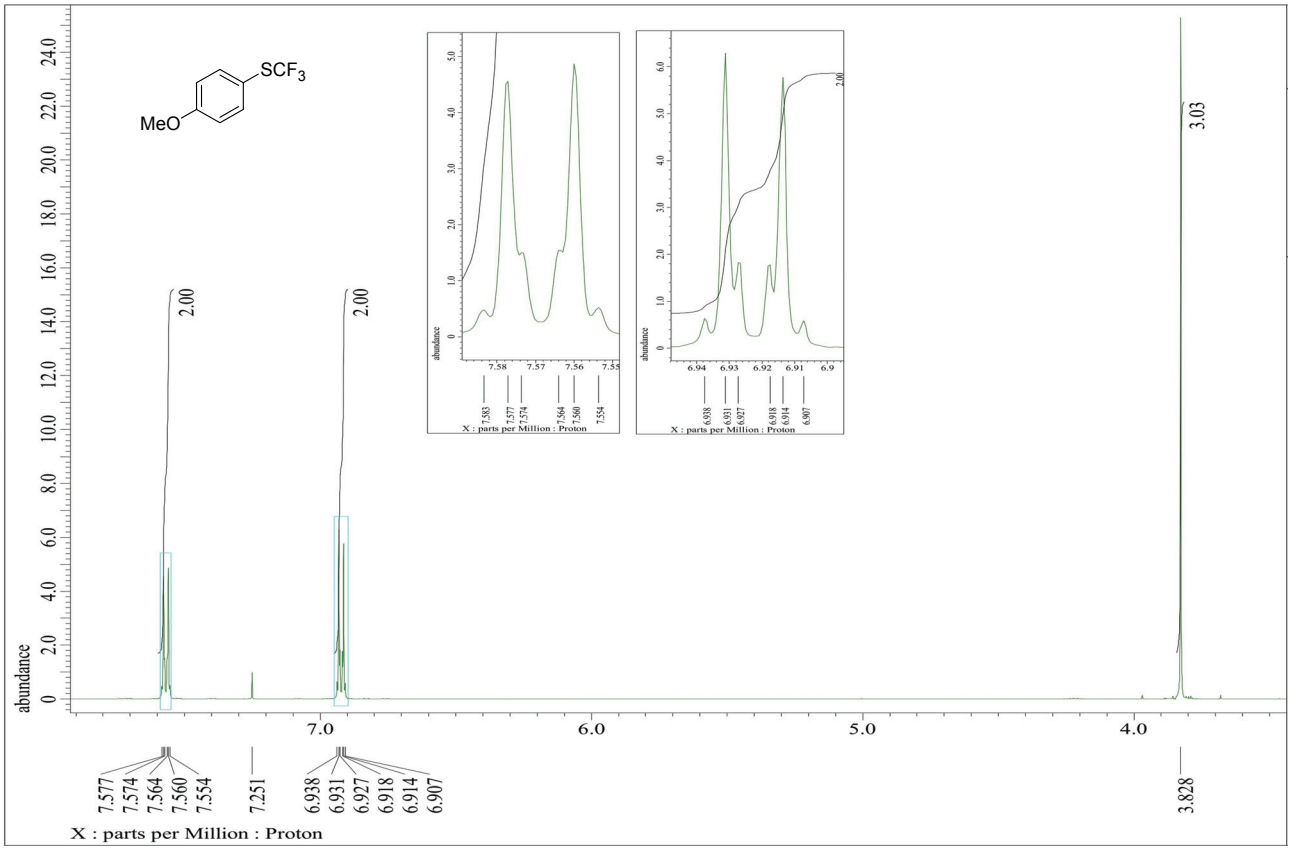

SCF3
(thousandths)
135.163
134.447
132.005
129.564
129.068
129.010
128.161
127.131
77.418
77.160
76.912
34.428
34.409
X : parts per Million : Carbon13

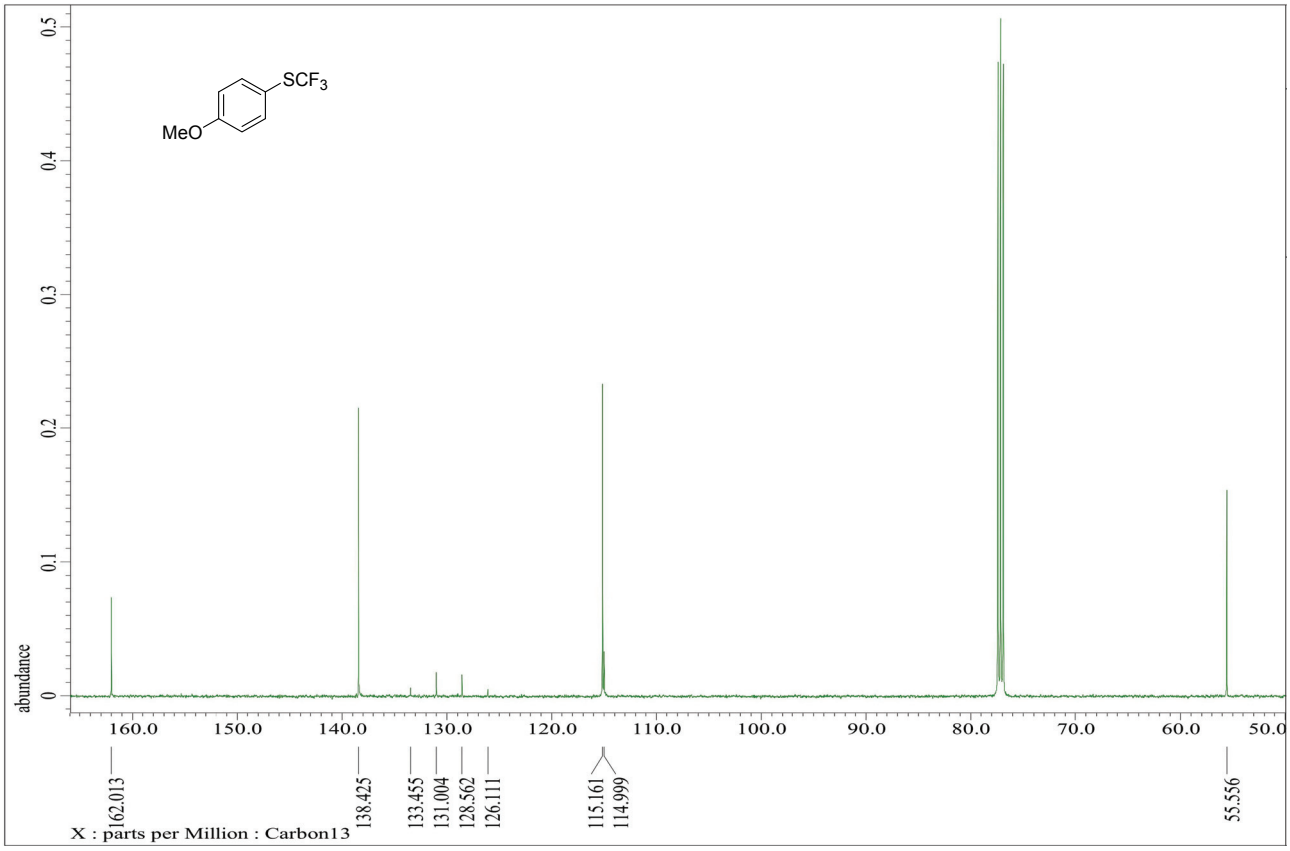

SCF3
30.0
20.0
10.0
0
abundance
-25.0 -27.0 -29.0 -31.0 -33.0 -35.0 -37.0 -39.0 -41.0 -43.0 -45.0 -47.0 -49.0 -51.0 -53.0 -55.0 -57.0 -59.0
-42.641
X : parts per Million : Fluorine19

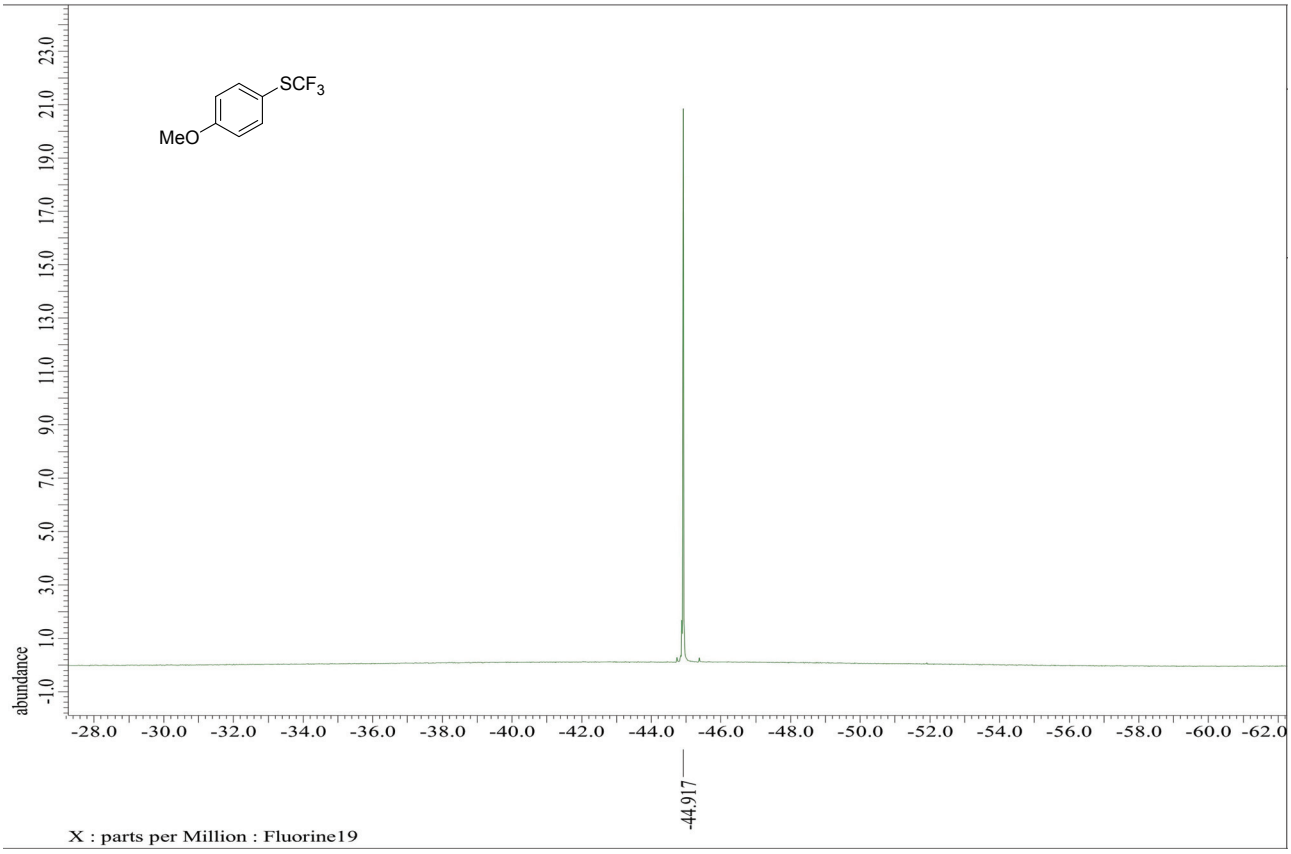

SCF3
abundance
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2.00
2.00
3.02
7.0
6.0
5.0
4.0
3.0
2.0
7.539
7.523
7.226
7.210
2.383
X : parts per Million : Proton

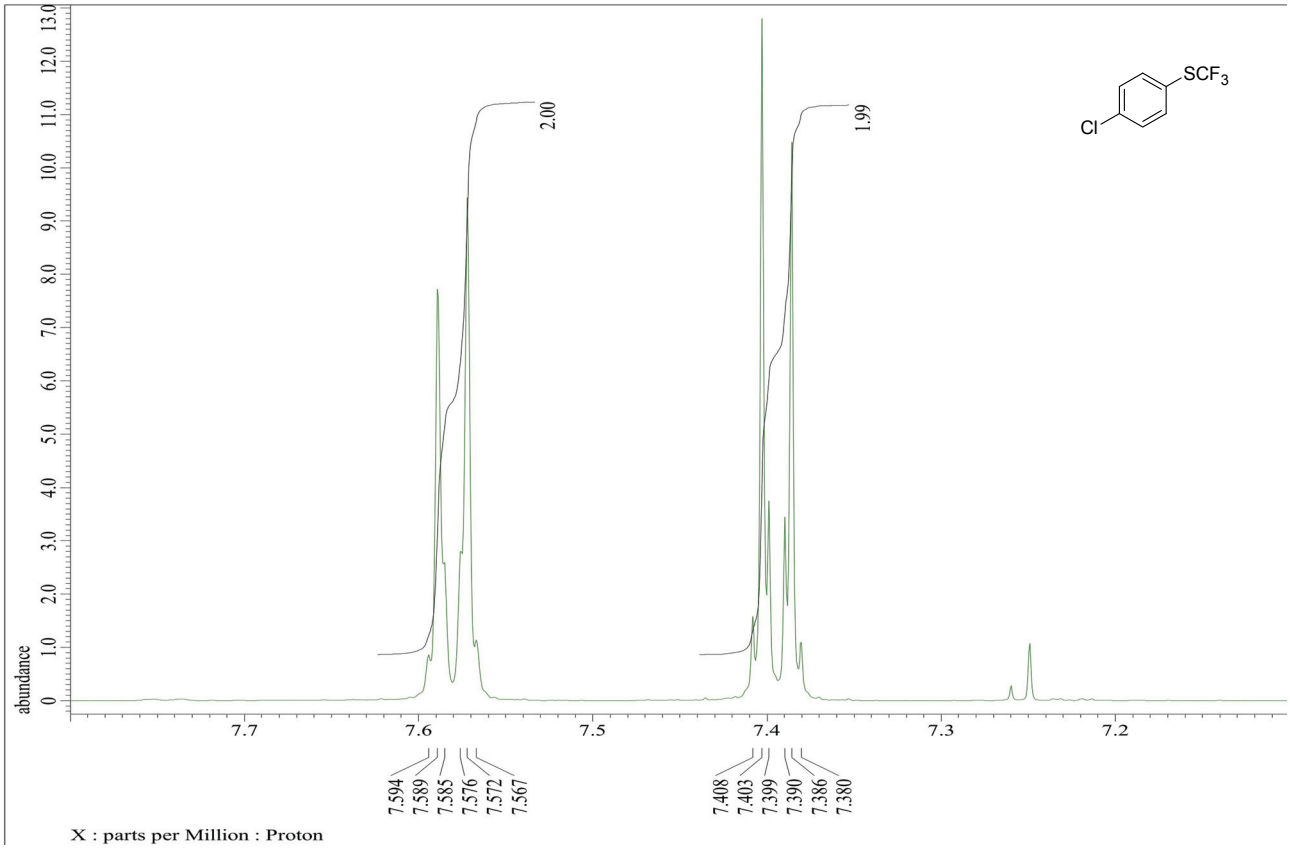

SCF3
(thousandths)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
141.534
136.536
133.503
131.052
130.403
128.610
126.158
121.046
21.466
X : parts per Million : Carbon13

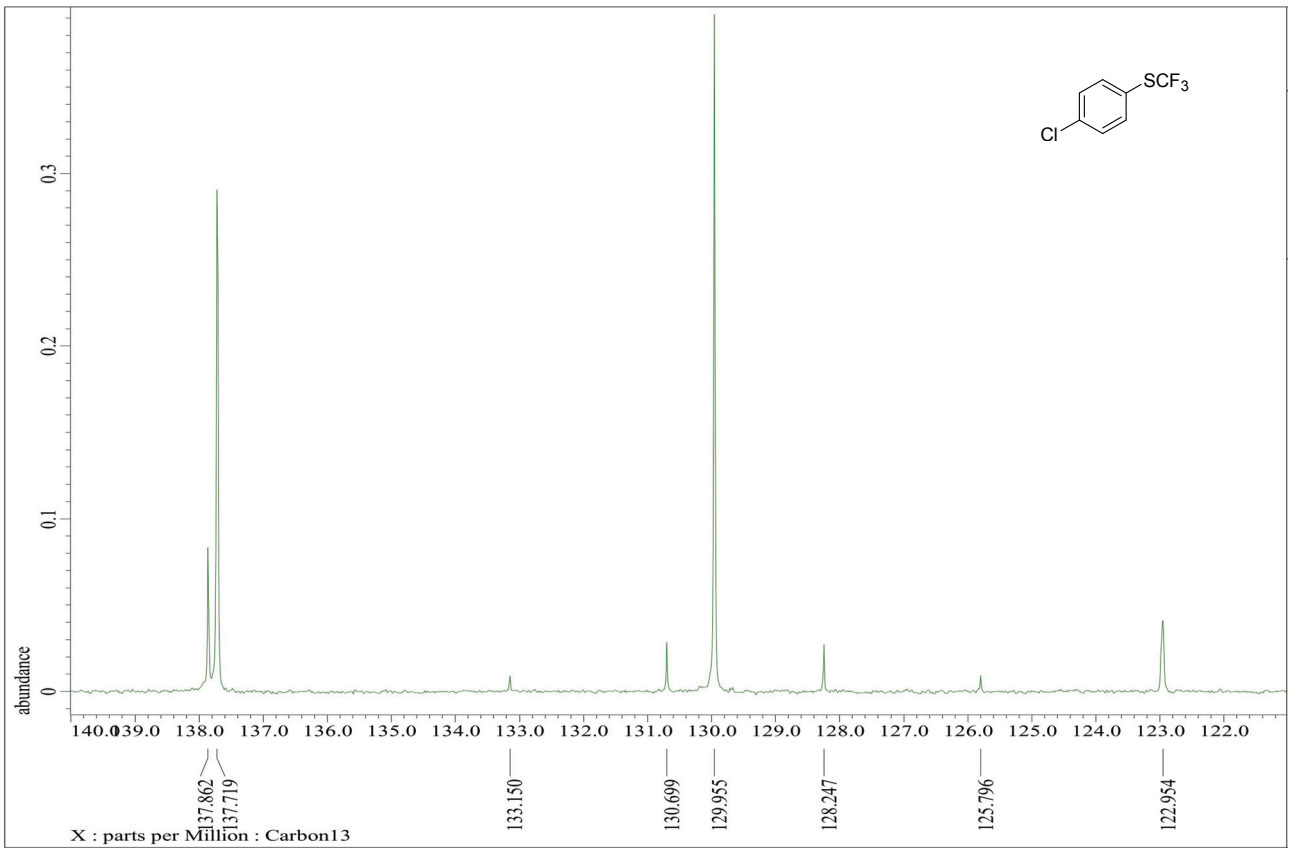

SCF3
abundance
40.0
30.0
20.0
10.0
0
-31.0
-33.0
-35.0
-37.0
-39.0
-41.0
-43.0
-45.0
-47.0
-49.0
-51.0
-53.0
-55.0
-57.0
-59.0
-44.168
X : parts per Million : Fluorine19

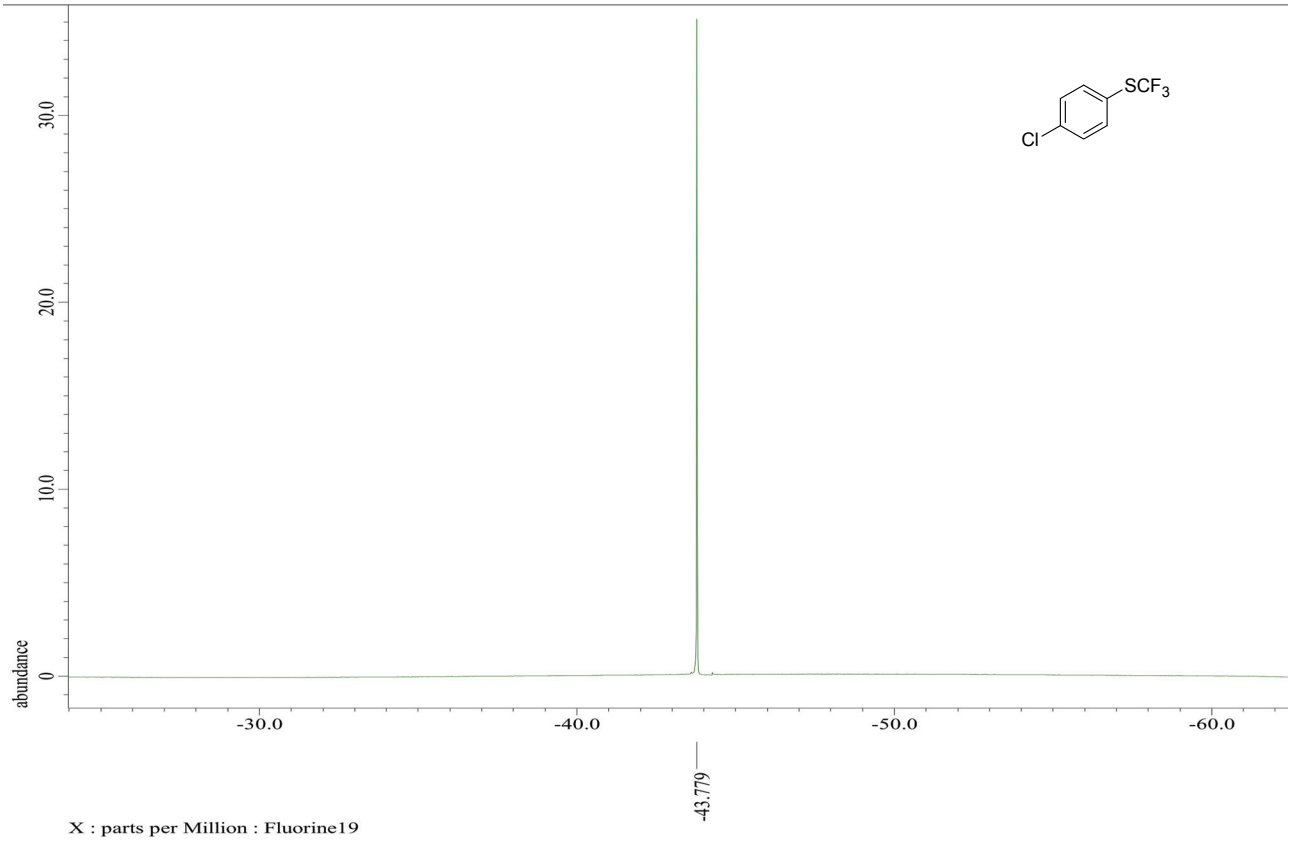

SCF3
MeO
2.00
2.00
3.03
abundance
X : parts per Million : Proton
7.577
7.574
7.564
7.560
7.554
7.251
6.938
6.931
6.927
6.918
6.914
6.907
3.828


SCF3
MeO
abundance
X : parts per Million : Carbon13
162.013
138.425
133.455
131.004
128.562
126.111
115.161
114.999
55.556

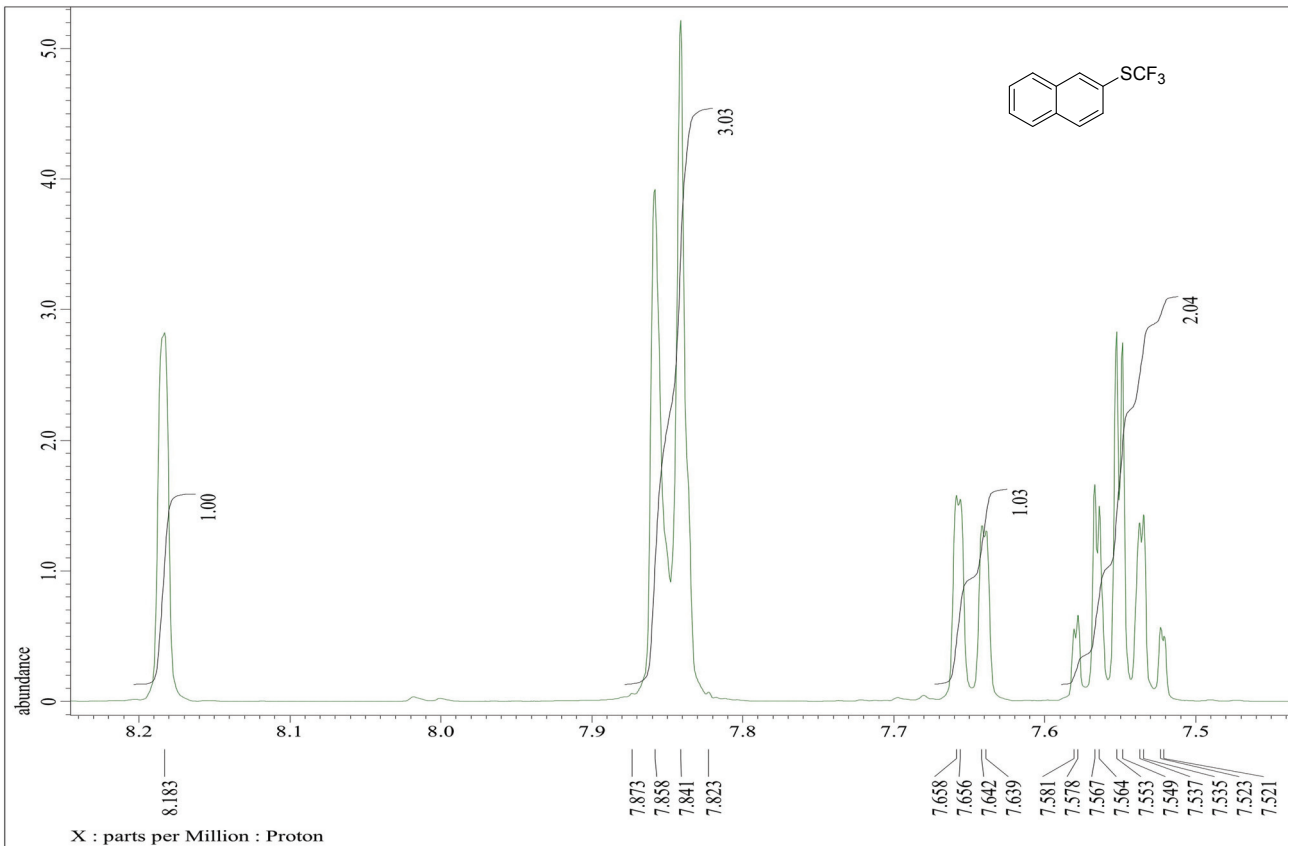

SCF3
MeO
abundance
23.0
21.0
19.0
17.0
15.0
13.0
11.0
9.0
7.0
5.0
3.0
1.0
-1.0
-28.0
-30.0
-32.0
-34.0
-36.0
-38.0
-40.0
-42.0
-44.0
-46.0
-48.0
-50.0
-52.0
-54.0
-56.0
-58.0
-60.0
-62.0
-44.917
X : parts per Million : Fluorine19

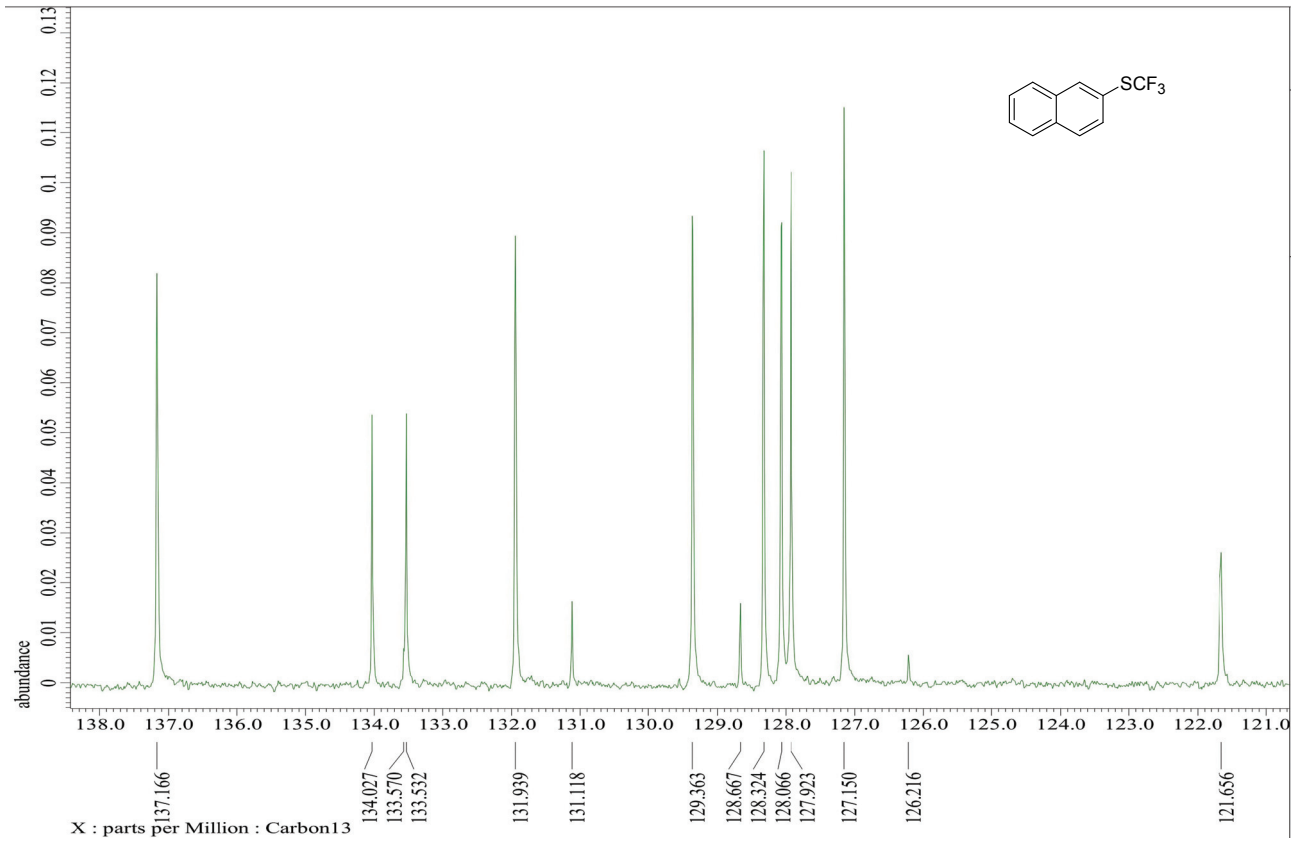

abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0
7.7
7.6
7.5
7.4
7.3
7.2
2.00
1.99
7.594
7.589
7.585
7.576
7.572
7.567
7.408
7.403
7.399
7.390
7.386
7.380
SCF3
Cl
X : parts per Million : Proton

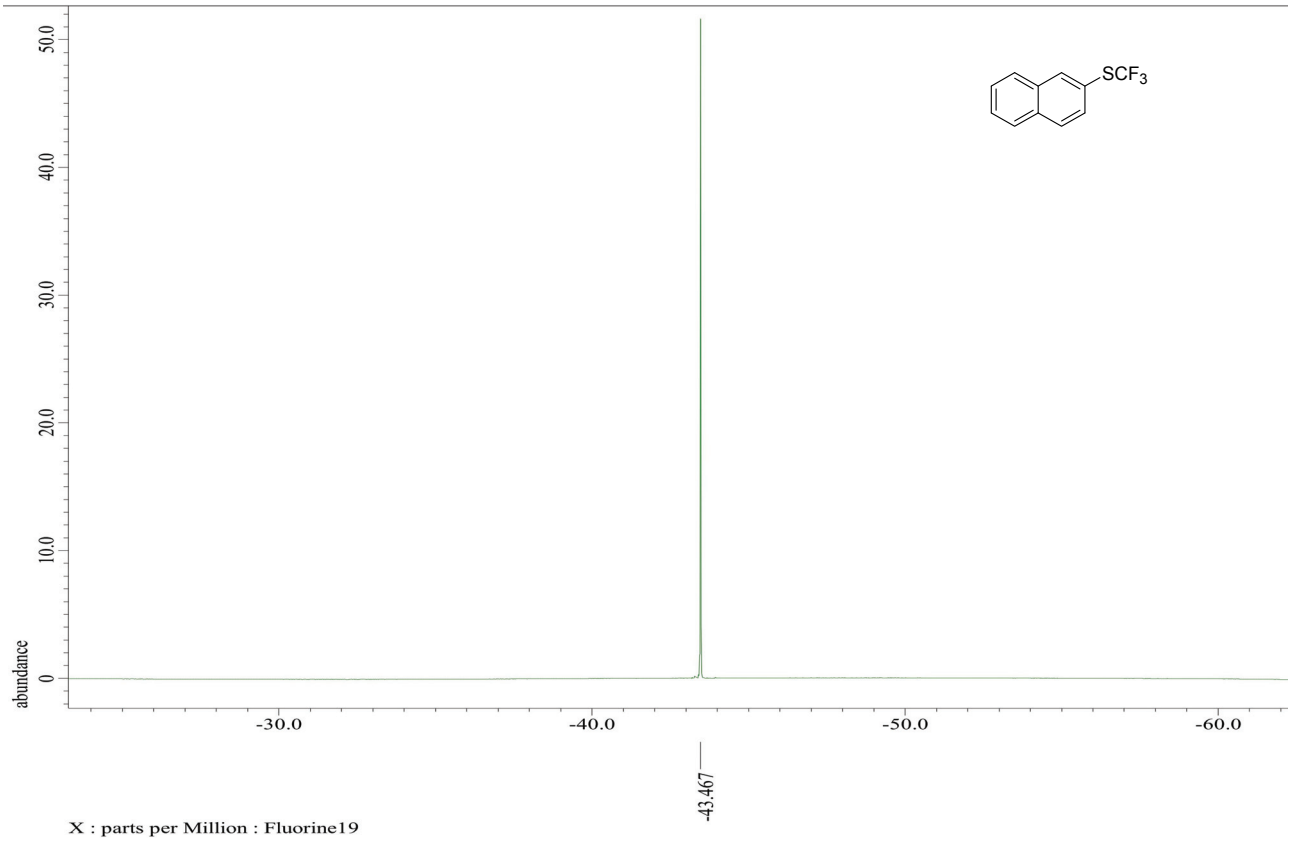

abundance
0 0.1 0.2 0.3
140.0 139.0 138.0 137.0 136.0 135.0 134.0 133.0 132.0 131.0 130.0 129.0 128.0 127.0 126.0 125.0 124.0 123.0 122.0
137.862
137.719
133.150
130.699
129.955
128.247
125.796
122.954
SCF3
Cl
X : parts per Million : Carbon13



X : parts per Million : Fluorine19


SCF3
abundance
5.0
4.0
3.0
2.0
1.0
0
1.00
3.03
1.03
2.04
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
8.183
7.873
7.858
7.841
7.823
7.658
7.656
7.642
7.639
7.581
7.578
7.567
7.564
7.553
7.549
7.537
7.535
7.523
7.521
X : parts per Million : Proton


SCF3
abundance
0.13
0.12
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
138.0
137.0
136.0
135.0
134.0
133.0
132.0
131.0
130.0
129.0
128.0
127.0
126.0
125.0
124.0
123.0
122.0
121.0
137.166
134.027
133.570
133.532
131.939
131.118
129.363
128.667
128.324
128.066
127.923
127.150
126.216
121.656
X : parts per Million : Carbon13



X : parts per Million : Fluorine19