Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

N-Thiocyanato-dibenzenesulfonimide：A New Electrophilic Thiocyanating Reagent with Enhanced Reactivity

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Contents

1. General Experimental Information.

All chemicals were bought from commercial companies and used directly unless noted. Reactions were carried out in a reaction tube with common solvents open to air. ^{1}H and ^{13}C HNMR spectra were recorded on a Bruker 400 or 700 instrument in $CDCl_3$ and DMSO-d_6. Chemical shifts are recorded in ppm. All of the MS of samples were analyzed on an Agilent (Q-TOF6520) unit with an ESI source. All IR spectra were measured on a Shimadzu IRAffinnity-1s spectrometer. Melting points were measured on a digital micro melting point apparatus unless otherwise indicated. Melting points were measured on a DSC-60 under a nitrogen flow (50 mL/min) at a heating rate of 5 ℃/min.

2. Synthesis of reagent R-5

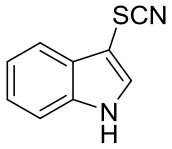
N-(Phenylsulfonyl)benzenesulfonamide (9.0 g, 30.30 mmol) and tert-butyl hypochlorite (33.33 mmol, 1.1 equiv) were stirred in methanol (50 mL) for **5** min at room temperature. Then the suspension was filtered giving the *N*-chloro-*N*-(phenylsulfonyl)-benzenesulfonamide as a white powder with a yield of 82 %. *N*-chloro-*N*-(phenylsulfonyl)-benzenesulfonamide (2.6 g, 7.9 mmol) was treated with AgSCN (2 g, 11.9 mmol, 1.5 equiv) in CH_2Cl_2 (25.0 mL) for 12 h at room temperature. Then the reaction mixture was filtered, and the filtrate was concentrated under reduced pressure to afford the product reagent R-**5** in 86% yield.

Thiocyanato-dibenzenesulfonimie (R-5): white solid (2.4 g, 86% yield), mp: 132-134^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 7.6 Hz, 4H, Ar-H), 7.66 (t, J = 7.6 Hz, 2H, Ar-H), 7.55 (t, J = 8 Hz, 4H, Ar-H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 134.1, 129.2, 127.8, 107.0, ppm; IR (KBr) 3126, 2158, 1448, 1363, 1083, 866 cm^{-1}; HRMS (ESI) m/z $[M\text{-}SCN]^-$ calcd for $C_{12}H_{10}NO_4S_2^-$ 296.0057 found 296.0057.

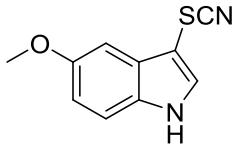
3. Reaction with substrates

Procedure for the Thiocyanation of Indoles

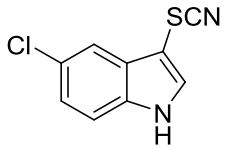
Indoles (0.2 mmol) and **R-5** (92 mg, 0.26 mmol, 1.3 equiv) were stirred in CH_3CN (1.0 mL) for 10 min at room temperature. After the reaction was completed (monitored by **TLC**), the reaction mixture was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the pure desired products.



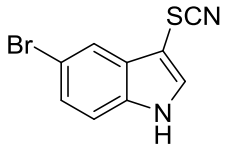
3-Thiocyanato-1H-indole (1a):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), off-white solid (34 mg, 98% yield), mp: 72-74 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (s, 1H, NH), 7.82-7.80 (m, 1H, Ar-H), 7.52 (d, J = 2.8 Hz, 1H, CH=CH), 7.45-7.43 (m, 1H, Ar-H), 7.33-7.31 (m, 2H, Ar-H) ppm; IR (KBr) 3286, 2154, 1714, 1456, 750 cm^{-1}.



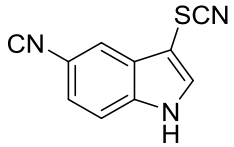
5-Methoxy-3-thiocyanato-1H-indole (1b):[1] eluent petroleum ether / ethyl acetate (4:1, v/v)，white solid (39 mg, 94% yield), mp: 119-121 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H, NH), 7.50 (d, J = 2.8 Hz, 1H, CH=CH), 7.32 (d, J = 8.8 Hz, 1H, Ar-H), 7.19 (d, J = 2.4 Hz, 1H, Ar-H), 6.98-6.95 (dd, J = 8.4, 2.4 Hz, 1H, Ar-H), 3.92 (s, 3H, CH_3) ppm; IR (KBr) 3283, 2156, 1632, 1554, 750 cm^{-1}.



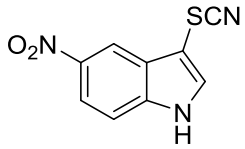
5-Cholor-3-thiocyanato-1H-indole (1c):[2] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (40 mg, 94% yield), mp: 132-134 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (s,1H, NH), 7.77 (d, J = 1.6 Hz, 1H, CH=CH), 7.54 (d, J = 2.8 Hz, 1H，Ar-H), 7.35 (d, J = 2.8 Hz, 1H, Ar-H), 7.28-7.25 (dd, J = 8.8, 2.0 Hz, 1H, Ar-H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.2, 132.1, 128.8, 127.9, 124.4, 118.3, 113.1, 111.4, 92.9, ppm; IR (KBr): 2954, 2154, 1750, 1460, 763 cm^{-1}.



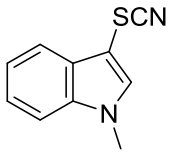
5-Bromo-3-thiocyanato-1H-indole(1d): [1] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (48 mg, 96% yield), mp: 140-142 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (s, 1H, NH), 7.93 (s, 1H, CH=CH), 7.53 (d, J = 2.4 Hz, 1H，Ar-H), 7.40 (d, J = 8.8 Hz, 1H, Ar-H), 7.30 (d, J = 8.8 Hz, 1H, Ar-H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.6, 132.0, 129.4, 127.1, 121.5, 115.5, 113.5, 111.4, 92.3. ppm; IR (KBr): 3260, 2920, 2152, 1593, 1463 cm^{-1}.



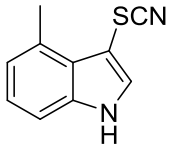
5-cyano-3-thiocyanato-1H-indole (1e):[3] eluent petroleum ether / ethyl acetate (4:1, v/v), white solid (48mg, 96% yield), mp: 210-212 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ 12.46 (s, 1H, NH), 8.19 (s, 1H, CH=CH), 8.17 (s, 1H, Ar-H), 7.67 (dd, J = 8.4, 0.8 Hz, 1H, Ar-H), 7.60 (dd, J =8.4 1.6 Hz, 1H, Ar-H), ppm; IR(KBr): 3263, 2920, 2156, 2104, 1601, 1461 cm^{-1}.



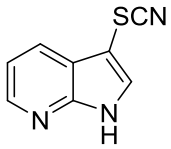
5-Nitro-3-thiocyanato-1H-indole(1f):[1] eluent petroleum ether / ethyl acetate (4:1, v/v), white solid (48 mg, 96% yield), mp: 140-142 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ 12.59 (s, 1H, NH), 8.51 (d, J =2.4 Hz, 1H, Ar-H), 8.26 (s, 1H, CH=CH), 8.12 (dd, J = 9.2, 2.4 Hz, 1H, Ar-H), 7.70 (d, J =9.2 Hz, 1H, Ar-H), ppm; IR (KBr): 3215, 2156, 1581, 1323, 750cm^{-1}.



1-Methyl-3-thiocyanato-1H-indole (1g):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (36 mg, 96% yield), mp: 83-85 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 7.2 Hz, 1H, Ar-H), 7.41 (s, 1H, CH=CH), 7.40-7.30 (m, 3H, Ar-H), 3.83 (s, 3H, CH_3), ppm; IR (KBr): 3121, 2156, 1649, 1532 cm^{-1}.



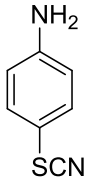
4-Methyl-3-thiocyanato-1H-indole (1h):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (40 mg, 95% yield), mp: 108-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H, NH), 7.47 (d, J = 2.8 Hz, 1H, CH=CH), 7.23 (d, J = 6.8 Hz, 1H, Ar-H), 7.15 (t, J = 7.6 Hz, 1H, Ar-H), 6.99 (d, J = 7.2 Hz, 1H, Ar-H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 132.0, 131.0, 125.5, 123.9, 123.5, 113.2, 109.9, 92.3, 19.1 ppm; IR (KBr): 3240, 2146, 1527, 1465 cm^{-1}.



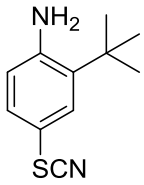
2-Thiocyanato-1H-pyrolo[2,3-b]pyridine (1i): [1] eluent petroleum ether / ethyl acetate (4:1, v/v), white solid (33 mg, 96% yield), mp: 200-202 °C. ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.59 (s, 1H, NH), 8.39 (dd, J = 4.8, 1.6 Hz, 1H, Ar-H), 8.17 (s, 1H, CH=CH), 8.12 (dd, J = 8,1, 6.0 Hz, 1H, Ar-H), 7.30 (dd. J = 7.6, 3.6 Hz, 1H, Ar-H) ppm; IR (KBr): 3254, 2922, 2152, 1595, 1496, 1274 cm^{-1}.

Procedure for the thiocyanation of anilines

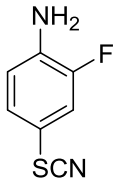
Anilines (0.2mmol) and **R-5** (92 mg, 0.206 mmol, 1.3 equiv) were stirred in CH_2Cl_2 (1.0mL) for 10 min at room temperature. After the reaction was completed (monitored by TLC), the reaction mixture was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the pure desired products.



4-Thiocyanatoaniline (2a):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (28 mg, 93% yield), mp: 49-51 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 8.4 Hz, 2H, Ar-H), 6.67 (d, J = 8.4 Hz, 2H, Ar-H), 3.97 (s, 2H, NH), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.7, 134.4, 116.0, 112.3, 109.7, ppm; IR (KBr): 3367, 2920, 2150, 1624, 1593, 1496 cm^{-1}.

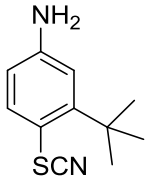


2-(tert-Butyl)-4-thiocyanatoaniline (2b):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), colorless liquid (37 mg, 90% yield), mp: 50−52 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 -7.39 (d, J = 2.0 Hz, 1H, Ar-H), 7.24 (dd, J = 8.4, 2.4 Hz, 1H, Ar-H), 6.62 (d, J = 8.4 Hz, 1H, Ar-H), 4.12 (s, 2 H, NH), 1.40 (s, 9 H, CH_3), ppm; IR (KBr): 3501, 3402, 2150, 1593, 1512 cm^{-1}.

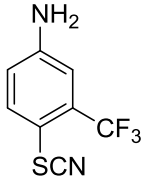


2-Fluoro-4-thiocyanatoaniline(2c):[4] eluent petroleum ether / ethyl acetate (8:1, v/v), colorless liquid (32 mg, 91% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 (dd, J = 10.4, 2.4 Hz, 1H, Ar-H), 7.18-7.15 (m, 1H, Ar-H), 6.77 (t, J = 8.8 Hz, 1H, Ar-H), 4.05 (s, 2H, NH), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9 (d, ^1J = 243 Hz), 137.4 (d, ^2J = 12 Hz), 129.7 (d, ^3J =

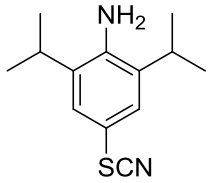
3.0 Hz), 119.74 (d, ^{2}J = 21 Hz), 117.2 (d, ^{3}J = 5.0 Hz), 111.61, 109.4 (d, ^{3}J = 7.0 Hz), ppm; IR(KBr): 3052, 3046, 2154, 1487, 1274 cm^{-1}.



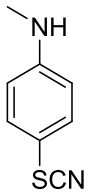
3-(tert-Butyl)-4-thiocyanatoaniline(2d):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), yellow liquid (37 mg, 90% yield), mp: 49−51 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d. J = 8.4 Hz, 1H, Ar-H), 6.74 (d, J = 2.8 Hz ,1H, Ar-H), 6.54 (dd, J = 8.4, 2.8 Hz, 1H, Ar-H), 3.89 (s, 2H, NH), 1.46 (s, 9H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 148.6, 139.2, 114.3, 113.7, 113.2, 108.9, 36.2, 30.7, ppm; IR (KBr): 3054, 3041, 2152, 1602, 1523 cm^{-1}.



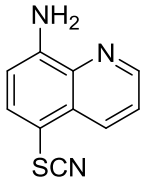
3-Trifluoromethyl-4-thiocyanatoaniline (2e):[4] eluent petroleum ether / ethyl acetate (8:1, v/v), yellow liquid (30 mg, 88% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 8.4 Hz, 1H, Ar-H), 7.01 (d, J = 2.8 Hz, 1H, Ar-H), 6.81 (dd, J = 8.8, 2.8 Hz, 1H, Ar-H); 4.20 (s, 2H, NH), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.9, 138.1, 124.1, 121.4, 118.0, 113.7, 111.2, 107.2, ppm; IR (KBr): 3212, 2920, 2154, 1750, 1498 cm^{-1}.



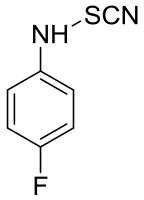
2.6-Diisopropyl-4-thiocyanatoaniline (2f):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), colorless liquid (44 mg, 96% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (s, 1H, Ar-H), 4.02 (s, 2H, NH), 2.87 (m, 2H, CH), 1.27 (d, J = 7.8 Hz, 12H, CH_3), ppm; IR (KBr): 3405, 2920, 2152, 1654 cm^{-1}.



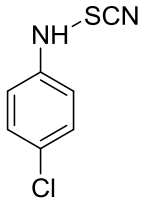
N-Methyl-4-thiocyanatoaniline (2g):[5] eluent petroleum ether / ethyl acetate (8:1, v/v), colorless liquid (28 mg, 88% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.4 Hz, 2H, Ar-H), 6.57 (d, J =8.8 Hz, 2H, Ar-H), 4.09 (s, 1H, NH), 2.84 (s. 3H, CH_3), ppm; IR (KBr): 3341, 2960, 2152, 1494, 1396 cm^{-1}.



5-Thiocyano-8-aminoquinoline (2h):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), yellow solid (28 mg, 70% yield), mp: 85-87 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (dd, J = 8.4, 1.6 Hz, 1H Ar-H), 8.60 (dd, J =8.4, 1.6 Hz, 1H, Ar-H), 7.74 (d, J = 8.4 Hz, 1H, Ar-H), 7.60 (dd, J =8.4, 4.4 Hz, 1H, Ar-H), 6.84 (d, J = 8.0 Hz, 1H, Ar-H), 5.45 (s, 1H, NH), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 147.9, 138.7, 137.4, 133.3, 129.6, 123.3, 111.8, 108.8, 103.0, ppm; IR (KBr): 3421, 2954, 2150, 1502, 1465 cm^{-1}.

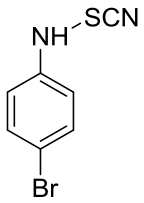


4-(Thiocyanatoamino)fluorobenzene (2i):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (24 mg,73% yield) mp: 78-80 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07-7.04 (m, 4 H, Ar-H), 5.03 (s, 1H, NH), ppm; IR (KBr): 3269, 2964, 2152, 1504, 1274 cm^{-1}.



4-(Thiocyanatoamino)chlorobenzene (2j):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), colorless liquid (28 mg, 78% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, J = 8.8 Hz,

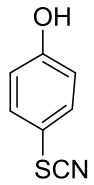
2H, Ar-H), 7.03 (d, J = 9.2 Hz, 2H, Ar-H), 5.21 (s, 1H, NH), ppm; IR (KBr): 3297, 2925, 2156, 1510, 1284 cm^{-1}.



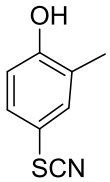
4-(Thiocyanatoamino)bromobenzene (2k):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), colorless solid (33 mg,73% yield); mp: 63-65°C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, J = 8.8 Hz, 2H, Ar-H), 6.99 (d, J = 8.4 Hz, 2H, Ar-H), 5.20 (s, 1H, NH), ppm; IR (KBr): 3294, 2966, 2144, 1485, 1267 cm^{-1}.

Procedure for the Thiocyanation of phenols and anisoles

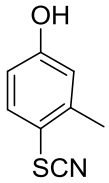
Phenols and anisoles (0.2mmol) and **R-5** (92 mg, 0.26 mmol, 1.3 equiv) were stirred in CH_3CN (1.0mL) for 10 min at room temperature. After the reaction was completed (monitored by TLC), the reaction mixture was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the pure desired products.



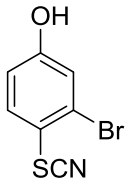
4-Thiocyanatophenol (3a):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), yellow solid (29 mg,97% yield); mp: 53-55 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.8 Hz, 2H, Ar-H), 6.89 (d, *J* = 8.8 Hz, 2H, Ar-H), 5.37 (s, 1H, OH), ppm; IR (KBr): 3420, 2924, 2160, 1583, 1494 cm^{-1}.



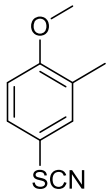
2-Methyl-4-thiocyanatophenol (3b):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (29 mg, 88% yield); mp: 60-62 °C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.34 (d, *J* = 2 Hz, 1H, Ar-H), 7.28 (dd, *J* = 8.4, 2.4 Hz, 1H, Ar-H), 6.80 (d, *J* = 7.6, 1H, Ar-H), 5.26 (s, 1H, OH), 2.25 (s, 3H, CH_3), ppm; IR (KBr): 3377, 2154, 1597, 1496 cm^{-1}.



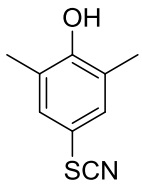
3-Methyl-4-thiocyanatophenol (3c):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), yellow solid (32 mg, 97% yield); mp: 75-77 °C; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.47 (d, *J* = 8.8 Hz, 1H, Ar-H), 6.79 (d, *J* =2.8 Hz, 1H, Ar-H), 6.70 (dd, *J* = 8.4, 2.8 Hz, 1H, Ar-H), 5.57 (s, 1H, OH), 2.48 (s, 1H, CH_3); ppm; IR (KBr): 3363, 2158, 1591, 1301 cm^{-1}.



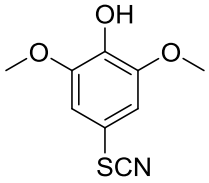
3-Bromo-4-thiocyanatophenol (3d):[5] eluent petroleum ether / ethyl acetate (8:1,v/ v), yellow solid (38 mg, 83% yield); mp: 89-91 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 8.4 Hz, 1H, Ar-H), 7.19 (d, J = 2.8 Hz, 1H, Ar-H), 6.88 (dd, J = 8.4, 2.4 Hz, 1H, Ar-H); 5.90 (s, 1H, OH), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 133.8, 126.0, 121.2, 116.6, 115.6, 110.8, ppm; IR (KBr): 3483, 2962, 2144, 1618, 1436 cm^{-1}.



1-Methoxy-2-methyl-4-thiocyanatobenzene (3e):[1] eluent petroleum ether / ethyl acetate (8:1,v/ v), colorless liquid (30 mg, 83% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 8.8 Hz, 1H, Ar-H), 7.34 (s, 1H, Ar-H), 6.83 (d, J = 8.4 Hz, 1H, Ar-H), 3.84 (s, 3H, CH_3), 2.22 (s, 3H, CH_3), ppm; IR (KBr): 3467, 2922, 2154, 1577, 1492, 1253 cm^{-1}.

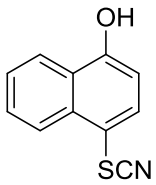


2,6-Dimethyl-2-methyl-4-thiocyanatobenzene (3f):[1] eluent petroleum ether / ethyl acetate (8:1,v/ v), white solid (29 mg, 81% yield); mp: 97-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (s, 2H, Ar-H), 4.89 (s, 3H, CH_3),2.25 (s, 3H, CH_3), ppm; IR(KBr): 3454, 2154, 1581, 1479, 1236 cm^{-1}.



2,6-Dimethoxy-4-thiocyanatophenol (3g):[1] eluent petroleum ether / ethyl acetate (8:1,v/v), colorless liquid (30 mg, 83% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.09 (s, 2H, Ar-H), 5.71 (s,

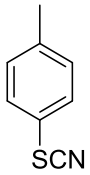
1H, OH), 3.85 (s, 6H, CH_3), ppm: 111-113 ^oC; ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 160.7, 112.4, 92.8, 89.2, 87.3, 56.3, ppm; IR (KBr): 3271, 2920, 2154, 1573, 1489 cm^{-1}.



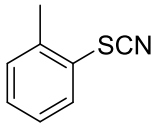
4-Thiocyanatonaphthalen-1-ol (3h):[6] eluent petroleum ether / ethyl acetate (10:1, v/v), yellow solid (36 mg, 92% yield); mp: 111-113 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, J = 8.8 Hz, 2H, Ar-H), 7.72 (t, J = 7.6 Hz, 2H, Ar-H), 7.60 (dt, J = 8.0, 1.2 Hz, 1H, Ar-H), 6.80 (d, J = 8.0 Hz, 1H, Ar-H), 6.25 (s, 1H, OH), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 135.2, 34.2, 128.8, 126.4, 125.6, 124.7, 123.0, 111.8, 110.7, 108.8, ppm; IR (KBr): 3412, 2924, 2158, 1668, 1558 cm^{-1}.

Procedure for the thiocyanation of unactivated arenes and heteroaromatics

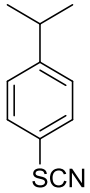
Unactivated arenes and heteroaromatics (0.2 mmol), CF_3SO_3H (30 mg. 0.2 mmol, 1.0 mmol) and **R-5** (92 mg, 0.26 mmol, 1.3 equiv) were stirred in CH_3CN (1.0 mL) for 12 h at 60 ^oC temperature. After the reaction was completed (monitored by TLC), the reaction mixture was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the pure desired products.



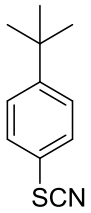
4-Thiocyanotoluene (4a):[7] eluent petroleum ether / ethyl acetate (10:1,v/v), colorless liquid (15 mg ,50% yield); ^1H NMR (400 MHz, $CDCl_3$) δ 7.43 (d, J = 8Hz, 2H, Ar-H), 7.23 (d, J = 8 Hz, 2H, Ar-H), 2.37 (s, 3H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.2, 130.9, 130.7, 127.7, 111.0, 21.1, ppm; IR (KBr): 2926, 2156, 1492, 1456 cm^{-1}.



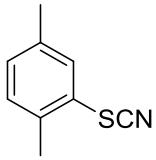
2-Thiocyanotoluene (4a'): [8] eluent petroleum ether / ethyl acetate (10:1,v/v), colorless liquid (7.5 mg, 25% yield); ^1H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, J = 7.6 Hz, 1H, Ar-H), 7.34 (t, J = 7.2 Hz, 1H, Ar-H), 7.29 (m, 2H, Ar-H), 2.48 (s, 3H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 132.0, 131.4, 130.2, 123.6, 120.6, 110.4, 20.4, ppm; IR (KBr): 2926, 2156, 1492, 1456 cm^{-1}.



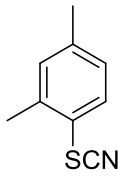
4-Isopropylphenyl thiocyanate (4b):[7] eluent petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (28 mg, 80% yield); ^1H NMR (400 MHz, $CDCl_3$) δ 7.46 (d, J = 8.4 Hz, 2H, Ar-H), 7.29 (d, J = 8.4 Hz, 2H, Ar-H), 2.96-2.89 (m, 1H, CH), 1.24 (d, J = 6.8, 6H, CH_3), ^{13}C NMR (100 MHz, $CDCl_3$) δ 151. 130.8, 128.4, 120.7, 111.0, 33.9, 23.7, ppm; IR (KBr): 2925, 2154, 1576, 1463 cm^{-1}.



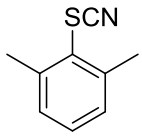
4-tert-Butylphenylthiocyanate (4c) : eluent petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (30 mg, 77% yield); ^{1}H NMR (400MHz, $CDCl_3$) δ 7.45 (m, 4H, Ar-H), 1.32 (s, 9H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 130.4, 127.3, 120.8, 111.0, 31.1, 30.5, ppm; IR (KBr): 2920, 2156, 1754, 1564 cm^{-1} .HRMS (ESI) m/z $[M + H]^+$ calcd for $C_{11}H_{14}NS^+$ 192.0841 found 192.0841.



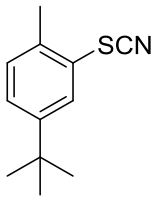
1.4-Dimrthyl-2-thiocyanatobenzene (4d):[9] eluent petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (21 mg, 64% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (s, 1H, Ar-H), 7.15 (m. 2H, Ar-H), 2.42 (s, 3H, CH_3), 2.34 (s, 3H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.7, 136.0, 132.3, 131.2, 131.0, 123.1, 110.6, 20.7, 19.8, ppm; IR (KBr): 2920, 2156, 1716, 1456 cm^{-1}.



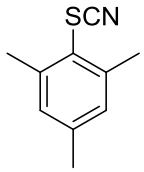
2,4-Dimethylphenylthiocyanateeluent (4e) petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (24 mg, 75% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8 Hz, 1H, Ar-H), 7.12 (s, 1H, Ar-H), 7.07 (d, J =8 Hz, 1H, Ar-H), 2.46 (s, 3H, CH_3), 2.34 (s, 3H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.9, 139.7, 132.7, 132.2, 128.4, 119.7, 110.8, 21.0, 20.4, ppm; IR (KBr): 2924, 2156, 1734, 1456 cm^{-1}. HRMS (ESI) m/z $[M + H]^+$ calcd for $C_9H_{10}NS^+$ 164.0528, found 164.0526.



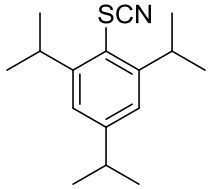
2,6-Dimethylphenylthiocyanate (4e'): eluent petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (3 mg, 7% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (t, J = 8 Hz, 1H, Ar-H), 7.18 (d, J =7.6 Hz, 2H, Ar-H), 2.60 (s, 6H, CH_3), ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.9, 131.0, 129.1, 122.6, 110.5, 21.9, ppm; IR (KBr): 2924, 2156, 1734, 1456 cm^{-1}. HRMS (ESI) m/z [M + H]$^{+}$ calcd for $C_9H_{10}NS^{+}$ 164.0528, found 164.0526.



4-tert-Butyl-1-methyl-2-thiocyanatobenzene(4f): eluent petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (28 mg, 68% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 2.0 Hz, 1H, Ar-H), 7.36 (dd, J =8.0, 2.0 Hz, 1H, Ar-H), 7.23 (d, J =8.0 Hz, 1H, Ar-H), 2.45 (s, 3H, CH_3), 1.32 (s, 9H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 136.6, 131.1, 129.4, 127.6, 122.9, 110.8, 34.7, 31,1, 19.9, ppm; IR (KBr): 2921, 2154, 1765, 1542 cm^{-1}. HRMS (ESI) m/z [M + H]$^{+}$ calcd for $C_{12}H_{16}NS^{+}$ 206.0998 found 206.0989.

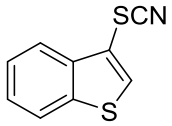


1.3.5-Trimethyl-2-thiocyanatobenzene (4g):[10] eluent petroleum ether / ethyl acetate (10:1,v/v), colorless liquid (30 mg, 83% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.00 (s,1H, Ar-H), 2.55 (s, 6H, CH_3), 2.30 (s, 6H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.7, 141.4, 130.0, 119.1, 110.9, 21.8, 21.0, ppm; IR (KBr): 2920, 2154, 1593, 1463 cm^{-1}.

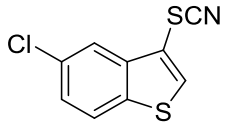


1.3.5-Triisopropyl-2-thiocyanatobenzene(4h):[11] eluent petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (38 mg, 73% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.10 (s, 2H,

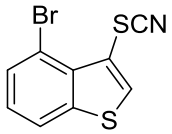
Ar-H), 3.79-3.73 (m, 2H, CH), 2.94-287 (m, 1H), 1.31 (d, J = 2.8 Hz, 12H, CH_3), 1.25 (d, J = 2.8 Hz, 6H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 152.9, 123.1, 117.7, 112.2, 34.4, 32.4, 23.86, 23.81, ppm; IR (KBr): 2964, 2153, 1595, 1463 cm^{-1}.



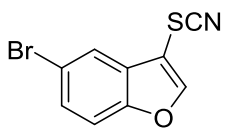
3-Thiocyanatobenzo[b]thiophene (4i):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (36 mg, 95% yield); mp: 90-92 ^oC, ^1H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.0 Hz, 1H, Ar-H), 7.92 (d, J = 8.0 Hz, 1H, Ar-H), 7.91 (s, 1H, CH=CH), 7.57 (t, J = 7.2 Hz, 1H, Ar-H), 7.50 (t, J = 7.6 Hz, 1H, Ar-H), ppm; IR (KBr): 2926, 2150, 1724, 1454 cm^{-1}.



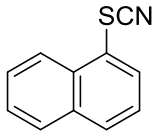
***5-Chloro-3-thiocyanatobenzo[b]thiophene(4j)*:** eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (37 mg, 86% yield); mp: 151-153 ^oC, ^1H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 2.0 Hz, 1H, Ar-H), 7.97 (s, 1H, CH=CH), 7.77 (d, J = 8.4 Hz, 1H, Ar-H), 7.59 (dd, J = 8.8, 2.0 Hz, 1H, Ar-H), ppm; ^{13}C NMR(100 MHz, $CDCl_3$) δ 138.9,138.1, 136.1, 129.2. 125.0, 124.4, 120.1, 111.5, 109.1, ppm; IR (KBr): 2993, 2156, 1770, 1274 cm^{-1}. HRMS (ESI) m/z $[M + H]^+$ calcd for $C_9H_5ClNS_2^+$ 225.9546 found 225.9547, 227.9571.



4-Bromo-3-thiocyanatobenzo[b]thiophene (4k): eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (45 mg, 80% yield); mp: 90-92 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H, CH=CH), 7.84 (dd, J = 8.0, 0.8 Hz, 1H, Ar-H), 7.64 (dd, J =8.0, 0.8 Hz, 1H, Ar-H), 7.27 (t, J = 8.0 Hz, 1H, Ar-H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.3, 133.7, 130.5, 130.1, 126.5, 112.8, 116.0, 114.6, 110.4, ppm; IR (KBr): 3005, 2158, 1770, 1757, 1274 cm^{-1}. HRMS (ESI) m/z $[M + H]^+$ calcd for $C_9H_5BrNS_2^+$ 269.9041 found 269.9044, 270.9019.



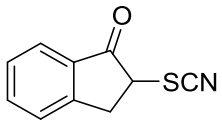
4-Bromo-3-thiocyanatobenzofuran (4l): eluent petroleum ether / ethyl acetate (10:1, v/v), brown solid (30 mg, 60% yield); mp: 51-52 ^{o}C ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H, CH=CH), 7.91 (d,*J* =2.0 Hz, 1H, Ar-H), 7.55 (dd, *J* = 8.8, 2.0 Hz, 1H, Ar-H), 7.46 (d, *J* = 8.8 Hz, 1H, Ar-H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.1, 150.4, 129.5, 128.1, 122.4, 117.8, 113.8, 108.8, ppm; IR (KBr): 3358, 2920, 2158, 1770, 1247, 764 cm^{-1}. HRMS (ESI) m/z $[M+H]^+$ calcd for $C_9H_5BrNOS^+$ 253.9270 found 253.9271, 255.9242.



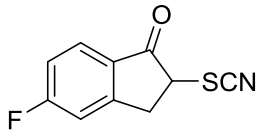
1-Thiocyanonaphthalene (4m):[7] eluent petroleum ether / ethyl acetate ((10:1, v/v), light yellow liquid (24 mg, 67% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.98 (d, *J* = 7.6 Hz, 1H, Ar-H), 7.93 (d, *J* = 7.6 Hz, 2H, Ar-H), 7.70 (t, *J* = 6.8 Hz, 1H, Ar-H), 7.62 (t, *J* = 8.0 Hz, 1H, Ar-H), 7.51 (t, *J* = 8.0 Hz, 1H, Ar-H), ppm; ^{13}C NMR(100 MHz, $CDCl_3$) δ 134.3, 32.4, 132.2, 131.6, 129.0, 128.1, 127.2, 125.9, 124.2, 120.8, 110.6, ppm; IR (KBr): 2920, 2148, 1751, 1274 cm^{-1}.

Procedure for the Thiocyanation of ketones

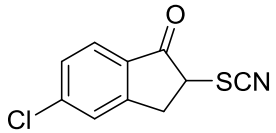
Ketones (0.2 mmol), $Zn(OTf)_2$ (14.5 mg, 0.04 mmol, 0.2 equiv) and **R-5** (141 mg, 0.4 mmol, 2.0 equiv) were stirred in CH_3CN (1.0 mL) for 24 h at 40 °C. After the reaction was completed (monitored by TLC), the reaction mixture was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the pure desired products.



2-Thiocyanato-2,3-dihydro-1H-inden-1-one (5a):[1] eluent petroleum ether / ethyl acetate (8:1, v/v), red liquid (34 mg, 91% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, J = 7.6 Hz, 1H, Ar-H), 7.71 (dt, J = 7.6, 0.8 Hz, 1H, Ar-H), 7.50 (m, 2H, Ar-H), 4.14 (dd, J = 8.0, 4.0 Hz, 1H, CH), 3.83 (dd, J_{AB} =18, 8.0 Hz, 1H, CH_2), 3.37 (dd, J_{AB} =18, 4.0 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz , $CDCl_3$) δ 197.9, 151.0, 136.4, 134.1, 128.6, 126.5, 125.1, 109.9, 48.2, 34.8, ppm; IR(KBr): 2924, 2156, 1650, 1467, 1255, 750 cm^{-1}.

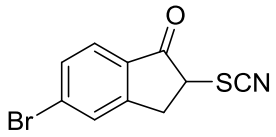


5-Fluoro-2-thiocyanato-2,3-dihydro-1H-inden-1-one (5b):[12] eluent petroleum ether / ethyl acetate (8:1, v/v), red solid (30 mg, 73%); mp: 80-82 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.84 (dd, J =9.2, 6.0 Hz, 1H, Ar-H), 7.19-7.15 (m, 1H, Ar-H), 4.12 (dd, J = 8.0, 4.4 Hz, 1H, CH), 3.82 (dd, J_{AB} =18.0, 8.4 Hz, 1H, CH_2), 3.40-3.34 (dd, J_{AB} =18.0, 4.0 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz , $CDCl_3$) δ 196.0, 196.6 (d, ^1J = 258 Hz), 154.0 (d, ^2J = 10.0 Hz), 130.6 (d, ^3J = 2.0 Hz), 127.6 (d, ^2J = 10 Hz), 117.1 (d, ^2J = 24 Hz), 113.3 (d, ^2J = 23 Hz), 109.5, 48.2, 34.7, ppm; IR (KBr): 2923, 2158, 1724, 1602, 1265 cm^{-1}.

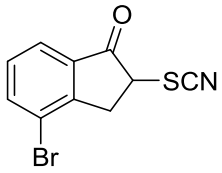


5-Chloro-2-thiocyanato-2,3-dihydro-1H-inden-1-one (5c):[12] eluent petroleum ether / ethyl acetate (8:1,v/v), white solid (32 mg, 74% yield); mp: 124-126 °C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78-7.76 (d, J = 8.4 Hz, 1H, Ar-H), 7.51 (s, 1H, Ar-H), 7.45 (d, J = 8.8 Hz, 1H, Ar-H), 4.11 (dd, J = 8.4, 4.4 Hz, 1H, CH), 3.80 (dd, J_{AB} =18, 8.0 Hz, 1H, CH_3), 3.35 (dd, J_{AB} =

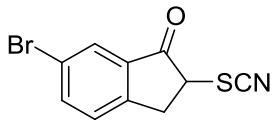
18, 4.4 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.5, 152.3, 143.3, 132.6, 129.6, 126.7, 126.1, 109.5, 48.1, 34.5, ppm; IR (KBr): 2920, 2154, 1714, 1591, 1261 cm^{-1}.



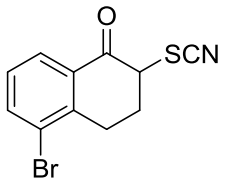
***5-Bromo-2-thiocyanato-2,3-dihydro-1H-inden-1-one (5d)*:[1]** eluent petroleum ether / ethyl acetate (8:1, v/v), brown solid (40 mg, 76% yield); mp: 128-130 °C, ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, J = 8 Hz, 1H, Ar-H), 7.69 (s, 1H, Ar-H) 7.61 (d, J = 8 Hz, 1H, Ar-H), 4.10 (dd, J = 8 4, 4 Hz, 1H, CH), 3.81 (dd, J_{AB} = 18, 8 Hz, 1H, CH_2), 3.36 (dd, J_{AB} = 18, 4 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz , $CDCl_3$) δ 196.8, 152.4, 132.9, 132.4, 132.2, 129.7, 126.1, 109.5, 48.0, 34.4, ppm; IR (KBr): 2910, 2154, 1714, 1612, 1245 cm^{-1}.



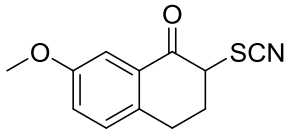
***4-Bromo-2-thiocyanato-2,3-dihydro-1H-inden-1-one(5e)*:**[1] eluent petroleum ether / ethyl acetate (8:1, v/v), red liquid (43 mg, 80% yield); mp: 93-95 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J =7.6 Hz, 1H, Ar-H), 7.89 (d, J = 7.6 Hz, 1H, Ar-H), 7.38 (t, J = 8 Hz, 1H, Ar-H), 4.14 (dd, J =8.4, 4.4 Hz, 1H, CH), 3.79 (dd, J_{AB} = 18, 8.0 Hz, 1H, CH_2), 3.32 (dd, J_{AB} = 18, 4.4 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.4, 150.8, 139.1, 136.1, 130.4, 123.8, 121.8, 109.4, 47.8, 35.7, ppm; IR (KBr): 2921, 2154, 1632, 1261, 914 cm^{-1}.



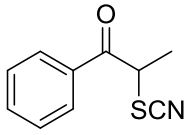
***4-Bromo-2-thiocyanato-2,3-dihydro-1H-inden-1-one(5f)*:**[1] eluent petroleum ether / ethyl acetate (8:1, v/v), red liquid (50 mg, 84% yield); mp: 91-93 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, J = 2.0 Hz, 1H, Ar-H), 7.80 (dd, J =8.0, 1.6 Hz, 1H, Ar-H), 7.40 (d, J = 8.4 Hz, 1H, Ar-H), 4.12 (dd, J = 8.0, 3.6 Hz, 1H, CH), 3.78 (dd, J_{AB} = 18, 8.0 Hz, 1H, CH_2), 3.30 (dd, J_{AB} =18, 8.0 Hz, 1H, CH_2), ppm; IR (KBr): 2922, 2156, 1625, 1268, 915 cm^{-1}.



5-Bromo-2-thiocyanato-3,4-dihydronaphthalen-1(2H)-one (5g): eluent petroleum ether / ethyl acetate (8:1, v/v), white solid (47 mg, 84% yield); mp: 137-139 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (dd, J =7.6, 0.8 Hz, 1H, Ar-H), 7.83 (dd, J = 7.6, 0.8 Hz, 1H, Ar-H), 7.27 (t, J = 8..0 Hz,1H, Ar-H), 4.55 (dd, J = 13.6, 4.8 Hz, 1H, CH), 3.35-3.34 (m, 1H, CH_2), 3.09-3.00 (m, 1H, CH_2), 2.93-2.87 (m, 1H, CH_2), 2.48-2.47 (m, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.9, 142.4, 138.7, 132.5, 128.5, 127.3, 124.8, 111.3, 54.8, 30.3, 29.7, ppm; IR (KBr); 3005, 2152, 1676, 1274, 912 cm^{-1}. HRMS (ESI) m/z $[M+H]^+$ calcd for $C_{11}H_9BrNOS^+$ 281.9583 found 281.9583.



7-Methoxy-2-thiocyanato-3,4-dihydronaphthalen-1(2H)-one (5h):[13] eluent petroleum ether / ethyl acetate (8:1,v/v), white solid (47 mg, 84% yield); mp: 121-123 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 2.0 Hz, 1H, Ar-H), 7.21 (d, J = 8.4 Hz, 1H, Ar-H), 7.14 (dd, J =8.4, 2.8 Hz,1H, Ar-H), 4.53 (dd, J = 13.2, 4.8 Hz, 1H, Ar-H), 3.83 (s, 1H, CH_3), 3.11 (dd, J = 8.0, 4.0 Hz, 2H, CH_2), 2.87-2.80 (m, 1H, CH_2), 2.46-2.37 (m, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 191.6, 158.7, 136.1, 131.3, 130.1, 123.3, 111.6, 109.6, 55.6, 55.5, 31.7, 28.2, ppm; IR(KBr); 2953, 2152, 1670, 1494, 1274, 1028 cm^{-1}.



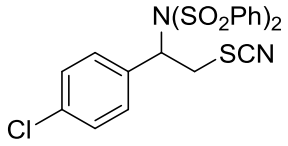
1-Phenyl-2-thiocyanatoethan-1-one (5i):[1] eluent petroleum ether / ethyl acetate (10:1, v/v), colorless liquid (31 mg, 82%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 7.2 Hz, 2H, Ar-H), 7.67 (t, J = 7.6 Hz, 1H, Ar-H), 7.53 (t, J = 7.6 Hz, 2H, Ar-H), 5.07 (m, 1H, CH) 1.87 (d, J = 7.2 Hz, 3H, CH_3), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.8, 134.8, 133.9, 129.2, 128.4, 111.8, 43.0, ppm; IR(KBr): 2920, 2156, 1683, 1558, 1274, 1001 cm^{-1}.

Procedure for the Thiocyanation of Alkenes

Alkenes (0.2 mmol) and **R-5** (92 mg, 0.26 mmol, 2 equiv) were stirred in CH_2Cl_2 (1.0 mL) for 1 h at room temperature. After the reaction was completed (monitored by TLC), the reaction mixture was purified by column chromatography on silica gel with petroleum ether/ethyl acetate to afford the pure desired products

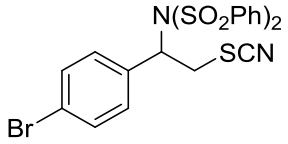
***N*-(1-Phenyl-2-thiocyanatoethyl)-*N*-(phenylsulfonyl)benzenesulfonamide (6a)**: eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (69 mg, 75% yield), mp:133-135 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.60-7.33 (m, 15H, Ar-H), 5.78-5.75 (dd, J = 11.2, 4.4 Hz, 1H, CH), 4.12-4.06 (dd,J = 14.0, 11.2 Hz, 1H, CH_2), 3.19-3.14 (dd, J = 14, 4.4 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 134.0, 132.1, 129.5, 129.2, 129.0, 128.7, 128.2, 110.9, 62.8, 34.5,IR (KBr): 3064, 2154, 1714, 1448, 1382, 1170cm^{-1}. HRMS (ESI) m/z $[M + NH_4]^+$ calcd for $C_{21}H_{22}N_3O_4S_3$ 476.0767 found 476.0767.

***N*-(1-(4-Fluorophenyl)-2-thiocyanatoethyl)-*N*-(phenylsulfonyl)benzenesulfonamide (6b)**: eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (60 mg, 62% yield), mp: 115-117 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.62-7.42 (m, 12H, Ar-H), 7.03 (t, J = 8.2 Hz, 2H, Ar-H), 5.72 (dd, J = 11.2, 4.4 Hz, 1H, CH), 4.02 (dd, J_{AB} = 14, 11.2, 1H, CH_2), 3.15 (dd, J_{AB} = 14, 4.4 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ ppm; 163.0 (d. ^1J = 249 Hz), 139.5, 134.1, 131.4 (d, ^2J = 9 Hz), 129.1, 128.1,128.1, 115.6 (d, ^3J = 2.2 Hz), 110.6, 62.2, 34.6, ppm; IR (KBr): 2926, 2156, 1637, 1512, 1384, 1170 cm^{-1}. HRMS (ESI) m/z $[M+NH_4]^+$ calcd for $C_{21}H_{21}FN_3O_4S_3^+$ 494.0673 found 494.0676.

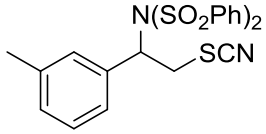


***N*-(1-(4-Chlorophenyl)-2-thiocyanatoethyl)-*N*-(phenylsulfonyl)benzenesulfonamide (6c)**: eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (56 mg, 56% yield), mp:133-135 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.63-7.28 (m, 14H, Ar-H), 5.70 (dd, J = 11.2, 4.4 Hz, 1H,

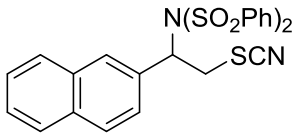
CH), 4.01 (dd, J_{AB} = 14, 11.2 Hz, 1H, CH_2), 3.13 (dd, J_{AB} = 14, 4.4 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 134.1, 131.8, 131.2, 131.1, 129.1, 128.1, 123.5, 110.6, 62.1, 34.3, ppm; IR(KBr): 2922, 2156, 1384, 1274, 1170 cm^{-1}. HRMS (ESI) m/z $[M+NH_4]^+$ calcd for $C_{21}H_{21}FN_3O_4S_3^+$ 494.0673, found 494.0676.



N-(1-(4-Bromophenyl)-2-thiocyanatoethyl)-N-(phenylsulfonyl)benzenesulfonamide (4d): eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (70 mg, 63% yield), mp:158-160 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.64-7.28 (m, 14H, Ar-H), 5.70 (dd, J = 10.8, 4.0 Hz, 1H, CH), 4.02 (dd, J = 14, 11.2 Hz, 1H, CH_2), 3.13 (dd, J = 14, 4.4 Hz, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.4, 134.1, 131.8, 131.2, 131.1, 129.1, 128.1, 123.5, 110.6, 62.1, 34.3, ppm; IR (KBr): 2924, 2156, 1489, 1382, 1168 cm^{-1}. HRMS (ESI) m/z $[M + NH_4]^+$ calcd for $C_{21}H_{21}BrN_3O_4S_3$ 553.9872 found 553.9876.



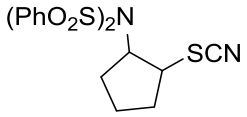
N-(Phenylsulfonyl)-N-(2-thiocyanato-1-(m-tolyl)ethyl)benzenesulfonamide (6e): eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (71 mg, 82% yield), mp: 122-124 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.59-7.44 (m, 10H, Ar-H), 7.24-7.16 (m, 4H, Ar-H), 5.74 (dd, J = 11.2, 4.4, 1H, CH), 4.06 (dd, J_{AB} = 13.6, 11.2, 1H, CH_2), 3.17 (dd, J_{AB} = 14, 4.4 Hz, 1H, CH_2), 2.24 (s, 3H), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ : 139.7, 138.6, 134.0, 131.9, 130.4, 129.8, 129.0, 128.5, 128.2, 126.1, 111.0, 62.8, 34.6, 21.3, ppm; IR (KBr): 3064, 2154, 1629, 1448, 1170 cm^{-1}. HRMS (ESI) m/z $[M+NH_4]^+$ calcd for $C_{22}H_{24}N_3O_4S_3^+$ 490.0929 found 490.0914.



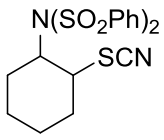
N-(1-(Naphthalen-2-yl)-2-thiocyanatoethyl)-N-(phenylsulfonyl)benzenesulfonamide (6f): eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (73 mg, 84% yield), mp: 127-129 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.85-7.74 (m, 17 H, Ar-H), 5.96 (dd, J = 11.2, 4.4 Hz, 1H, CH), 4.22 (dd, J_{AB} = 14, 11.2 Hz, 1H, CH_2), 3.28 (dd, J_{AB} =14, 4.4 Hz,1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ : 139.5, 133.9, 133.2, 132.7, 129.2, 128.9, 128.8, 128.5, 128.4,

128.2, 127.5, 127.2, 126.7, 126.2, 111.0, 63.0, 34.7, ppm; IR (KBr): 2924, 2156, 1689, 1170 cm^{-1}. HRMS (ESI) m/z $[M+NH_4]^+$ calcd for $C_{25}H_{20}N_2O_4S_3^+$ 508.0585 found 508.0580.

N-(Phenylsulfonyl)-N-(2-thiocyanato-1,2,3,4-tetrahydronaphthalen-1-yl)benzenesulfonamide (6g): eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (68 mg, 70 % yield), mp: 60-62 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.62-8.60 (m, 10H, Ar-H), 7.15 (d, J = 4.0 Hz, 2H, Ar-H), 7.04 (d, J = 8.0 Hz, 1H, Ar-H), 6.81-6.78 (m, 1H, Ar-H), 5.79 (d, J = 9.6 Hz, 1H, CH), 4.50-4.47 (m, 1H, CH), 3.24-3.15 (m, 1H, CH_2), 2.89-2.83 (m, 1H, CH), 2.55-2.50 (m, 1H, CH_2), 2.26-2.15 (m, 1H, CH_2), ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 137.45, 134.0, 131.8, 129.3, 129.3, 128.8, 128.6, 128.0, 126.6, 110.3, 66.2, 49.9, 32.8, 29.6, ppm; IR (KBr): 2954, 2156, 1490, 1382, 1170 cm^{-1}.HRMS (ESI) m/z $[M+NH_4]^+$ calcd for $C_{23}H_{24}N_3O_4S_3^+$ 502.0923, found 502.0926.

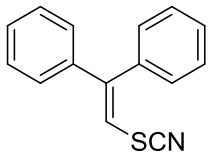


N-(Phenylsulfonyl)-N-(2-thiocyanatocyclopentyl)benzenesulfonamide (6h): eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (65 mg, 77 % yield), mp: 126-128 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 7.2 Hz, 4H, Ar-H), 7.69 (t, J = 7.6 Hz, 2H, Ar-H), 7.59 (t, J = 8.0 Hz, 4, Ar-H), 4.32 (dd, J = 18, 9.2 Hz, 1H, CH), 4.19 (dd, J = 17.2, 8.4 Hz, 1H, CH), 2.45-2.36 (m, 1H, CH_2), 2.20-2.13 (m, 1H, CH_2), 1.92-1.71 (m, 4H, CH_2),ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 134.2, 129.3, 128.3, 110.5, 66.9, 48.9, 32.7, 29.7, 21.9 IR (KBr): 2922, 2156, 1456, 1367, 1167 cm^{-1}. HRMS (ESI) m/z $[M+NH_4]^+$ calcd for $C_{18}H_{22}N_3O_4S_3^+$ 440.0767, found 440.0760.



N-(Phenylsulfonyl)-N-(2-thiocyanatocyclohexyl)benzenesulfonamide (6i): eluent petroleum ether / ethyl acetate (10:1, v/v), white solid (53 mg, 74 % yield), mp: 183-185 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 8.14-8.98 (dd, J = 17.6, 7.6 Hz, 4H, Ar-H), 7.69 (t, J = 7.2 Hz, 2H, Ar-H), 7.58 (dd, J = 17.6, 8,4 Hz, 4H, Ar-H), 4.13 (dt, J = 15.6, 4.0 Hz, 1H, CH), 3.88 (dt, J = 12, 4.0 Hz, 1H, CH), 2.47-2.42 (m, 1H, CH_2), 2.26-2.16 (m, 1H, CH_2), 1.83-1.64 (m, 4H, CH_2), 1.39-1.19 (m, 1H, CH_2), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 138.1, 134.5,

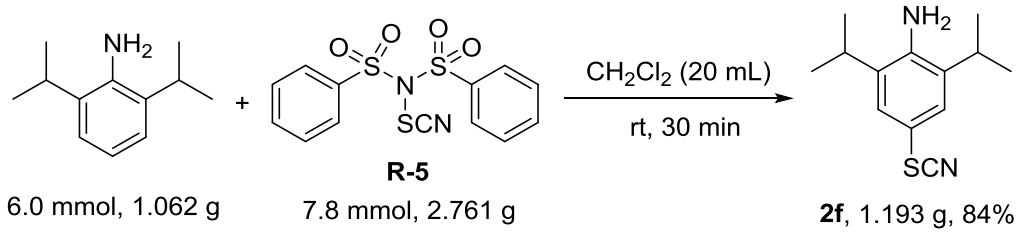
134.1, 129.4, 128.9, 128.8, 128.7, 110.5, 66.5, 49.5, 35.5, 32.7, 25.9, 25.6, ppm; IR (KBr): 2920, 2152, 1446, 1371, 1274, 1166 cm^{-1}. HRMS (ESI) m/z $[M+ H]^+$ calcd for $C_{19}H_{21}N_2O_4S_3$ 437.0658, found 437.0650.



(2-Thiocyanatoethene-1,1-diyl)dibenzene (6j):[14] eluent petroleum ether / ethyl acetate (10:1, v/v), yellow liquid (53 mg, 74 % yield); ^1H NMR (400 MHz, $CDCl_3$) δ 7.44-7.42 (m, 3H, Ar-H), 7.33-7.30 (m, 3H, Ar-H), 7.23-7.18 (m, 4H, Ar-H), 6.59 (s, 1H, CH), ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.3, 139.1, 136.6, 129.1,129.0, 128.9, 128.8, 128.5, 127.2, 111.1, 111.1, ppm; IR (KBr): 2921, 2156, 1654, 1566, 1478, 750 cm^{-1}.

Synthesis of 2f on a Gram Scale

Gram-scale reaction was carried out giving 1.193 g of **2f** in 84% yield from 2.6-diisopropylaniline (6.0 mmol) at room temperature for 30 min.



5. References

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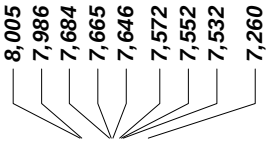
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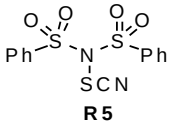
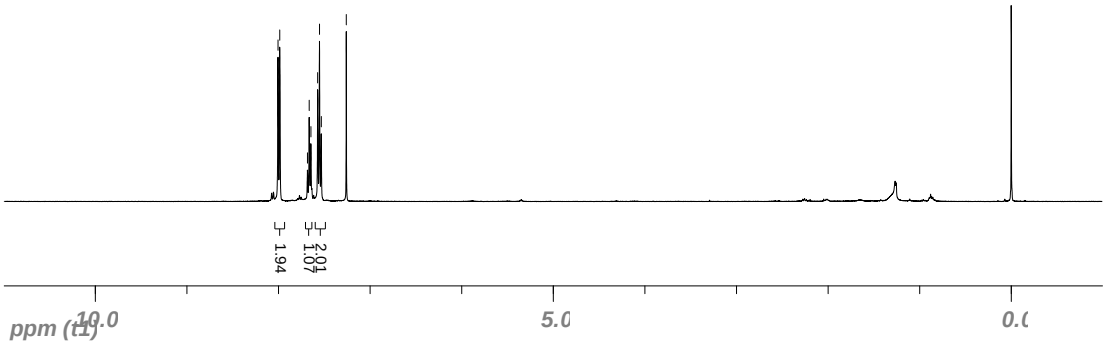
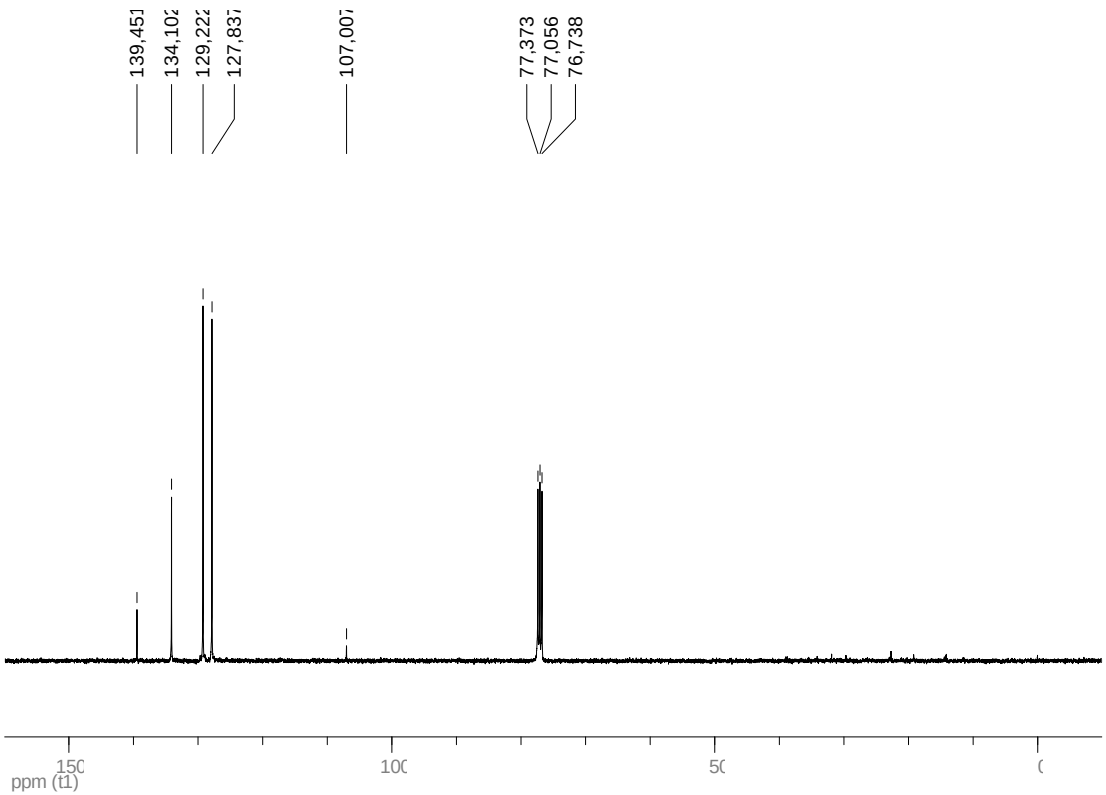
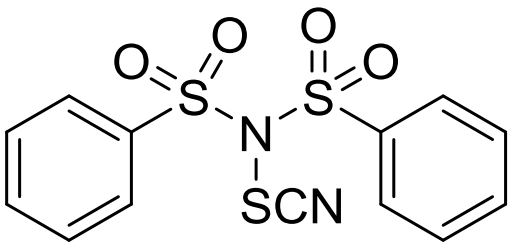
7,684
7,665
7,646
7,572
7,552
7,532
7,260


Ph
S
N
SCN
Ph
R5


1,94
2,01
1,07
ppm (t1)


139,451
134,102
129,222
127,837
107,007
77,373
77,056
76,738
ppm (t1)

6. X-ray Structure of reagent R-5 (CCDC1919695).



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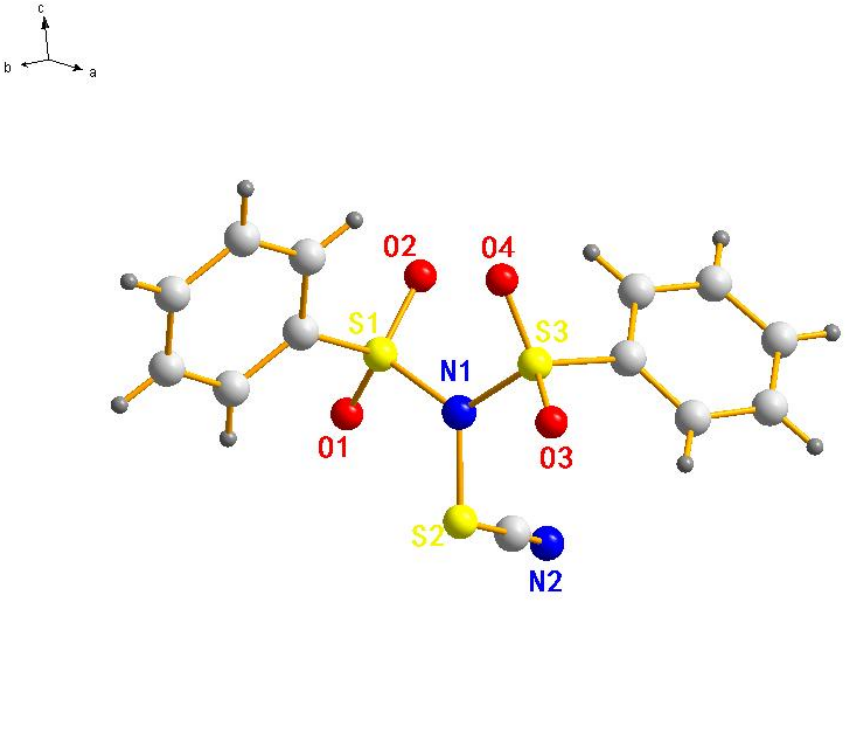
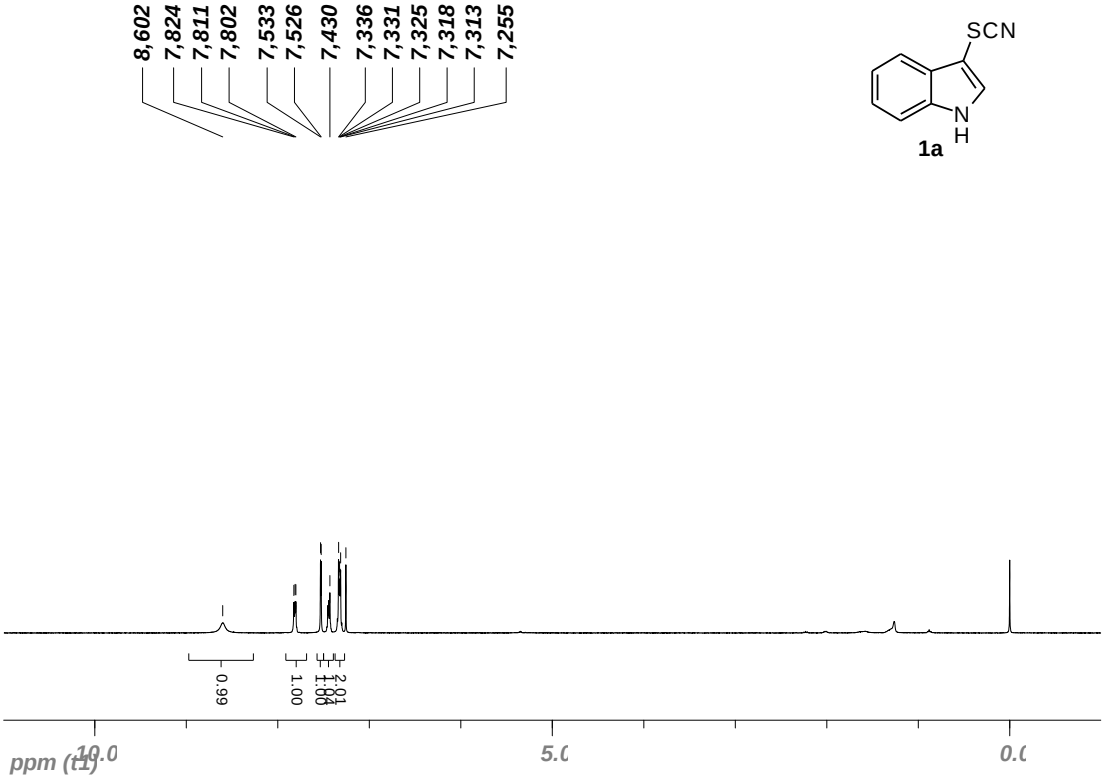
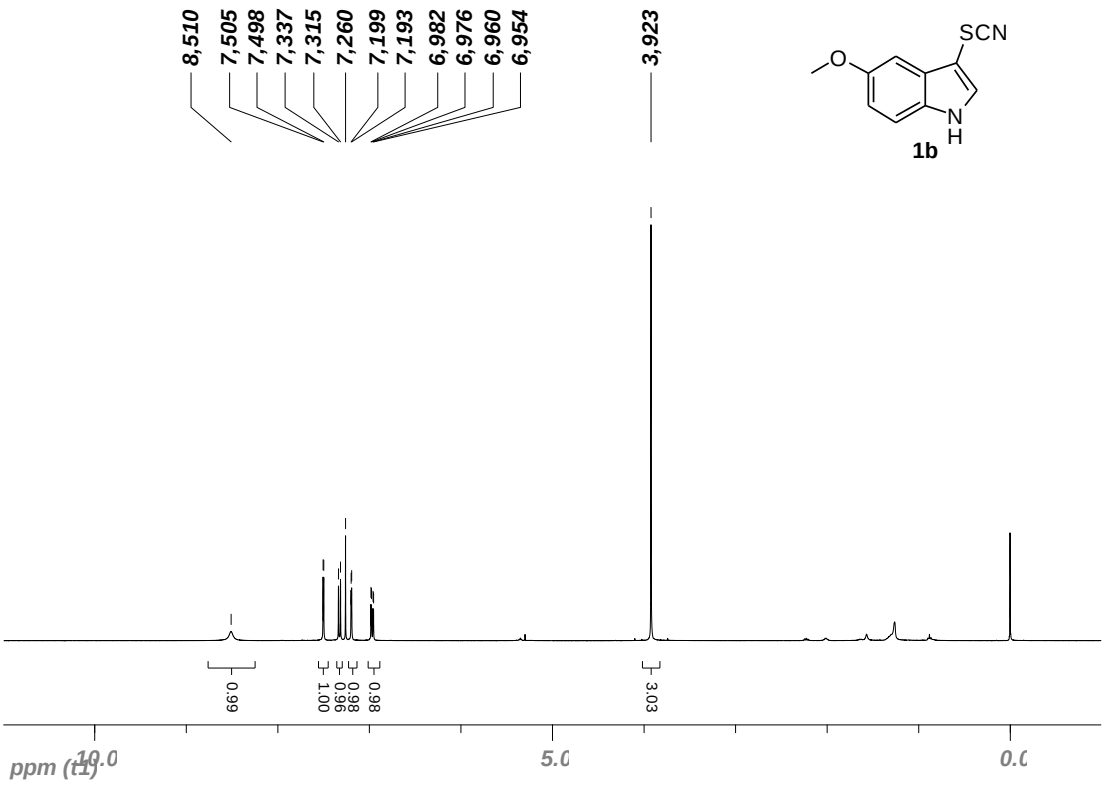


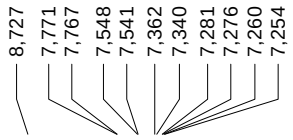
Table 1. Crystal data and structure refinement for reagent R-5 (CCDC1919695).

Identification code	lcq137
Empirical formula	$C_{13}H_{10}N_2O_4S_3$
Formula weight	354.41
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 11.5057(16) A alpha = 90 deg.
	b = 9.9709(14) A beta = 105.100(4) deg.
	c = 13.652(2) A gamma = 90 deg.
Volume	1512.1(4) A^3
Z, Calculated density	4, 1.557 Mg/m^3
Absorption coefficient	0.508 mm^-1
F(000)	728
Crystal size	? x ? x ? mm
Theta range for data collection	2.561 to 24.767 deg.
Limiting indices	-13<=h<=13, -11<=k<=11, -16<=l<=16
Reflections collected / unique	13844 / 2588 [R(int) = 0.0206]
Completeness to theta = 25.242	94.8 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2588 / 0 / 199
Goodness-of-fit on F^2	0.662
Final R indices [I>2sigma(I)]	R1 = 0.0243, wR2 = 0.0692
R indices (all data)	R1 = 0.0258, wR2 = 0.0715
Extinction coefficient	n/a
Largest diff. peak and hole	0.332 and -0.383 e.A^-3

7. Copies of ^{1}H and ^{13}C NMR spectra



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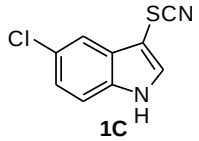
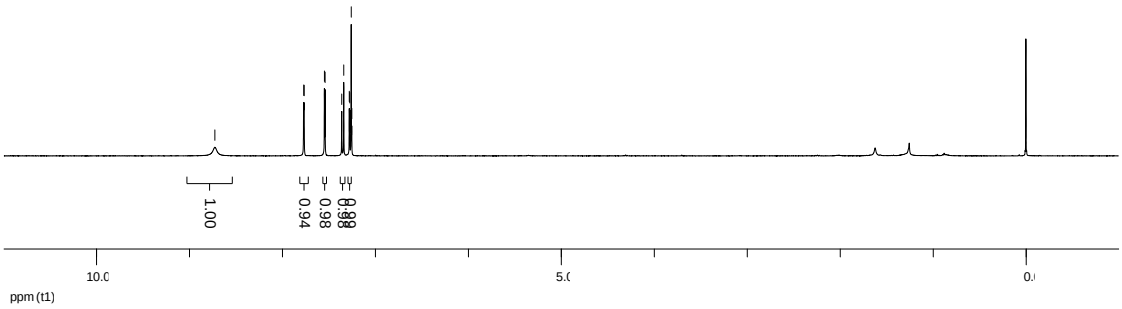
7,541
7,362
7,340
7,281
7,276
7,260
7,254


SCN
Cl
N
H

1C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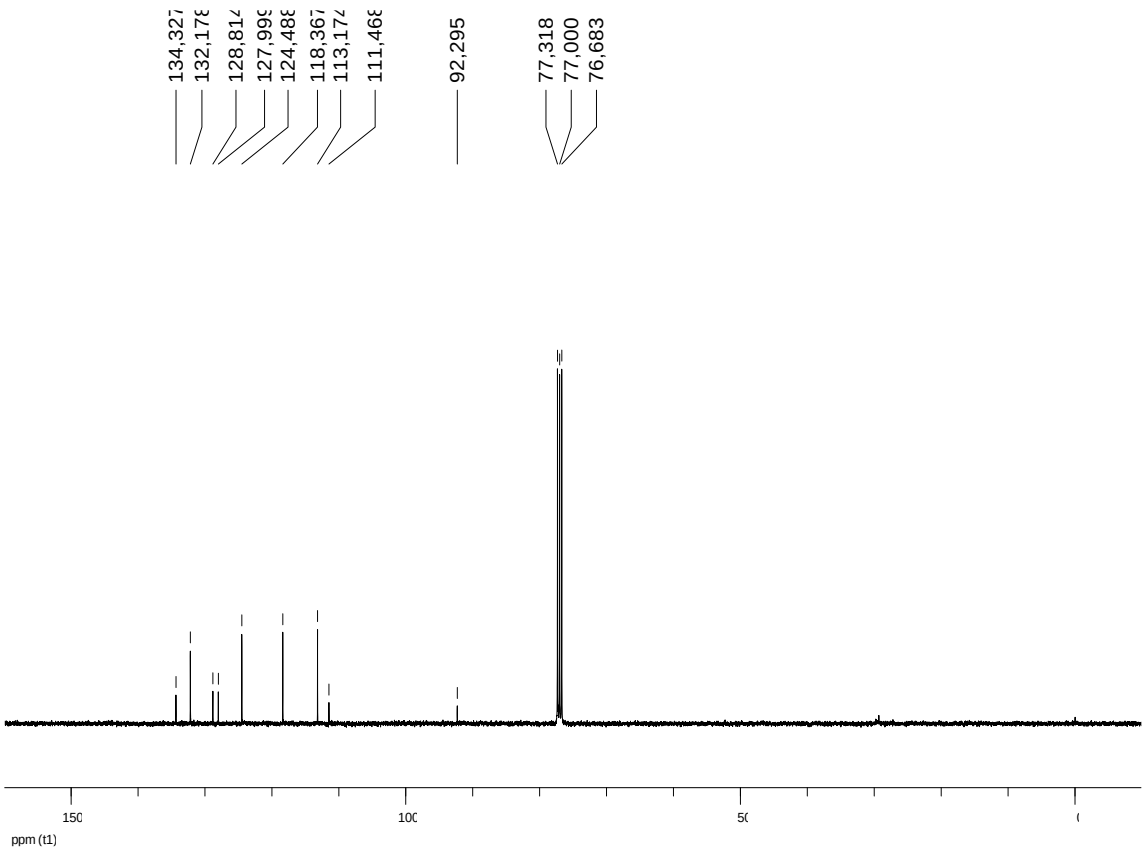
0,98
ppm (t1)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128,814
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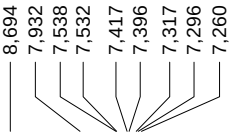
113,174
111,468
92,295
77,318
77,000
76,683
ppm (t1)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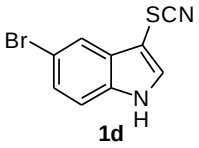
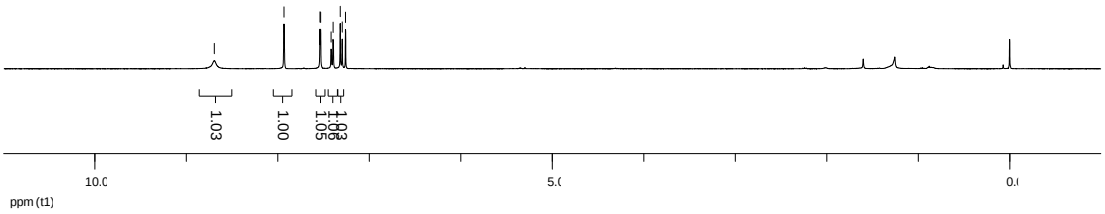
7,538
7,532
7,417
7,396
7,317
7,296
7,260


SCN
Br
N
H

1d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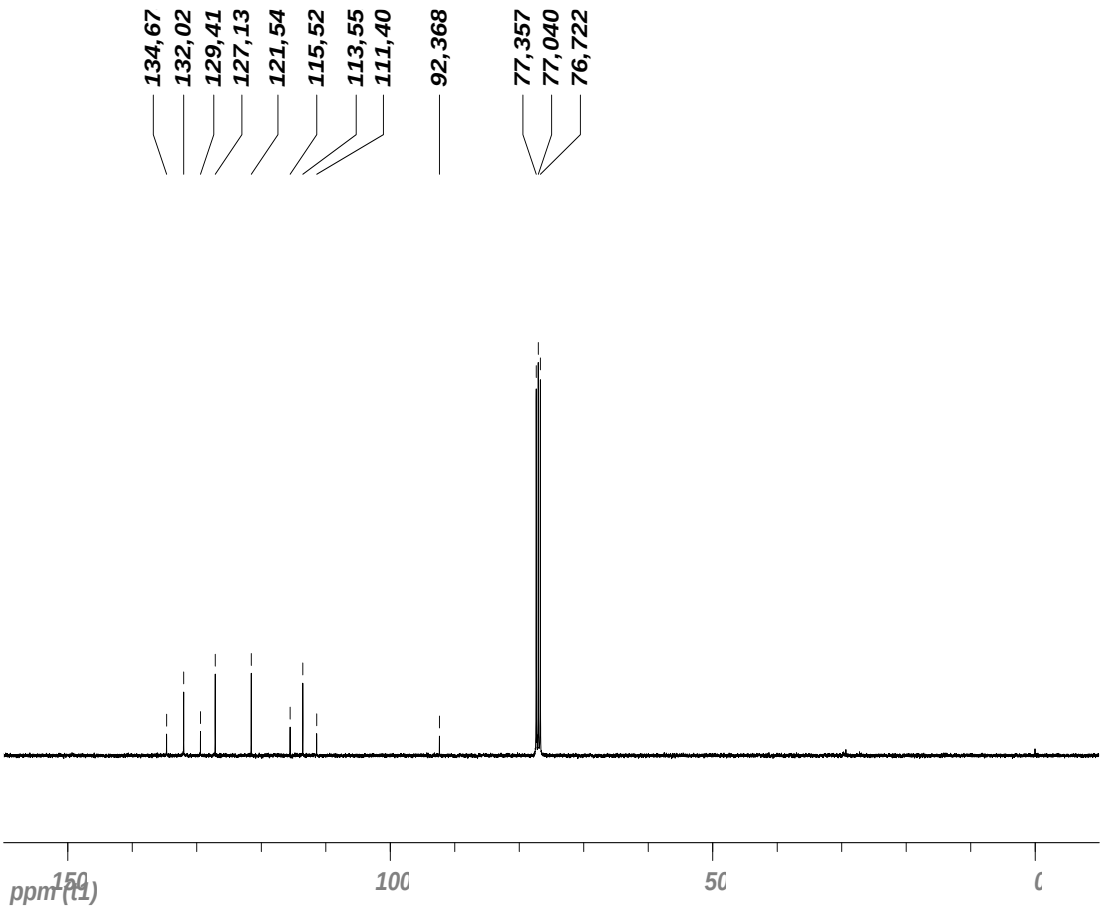
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111,40
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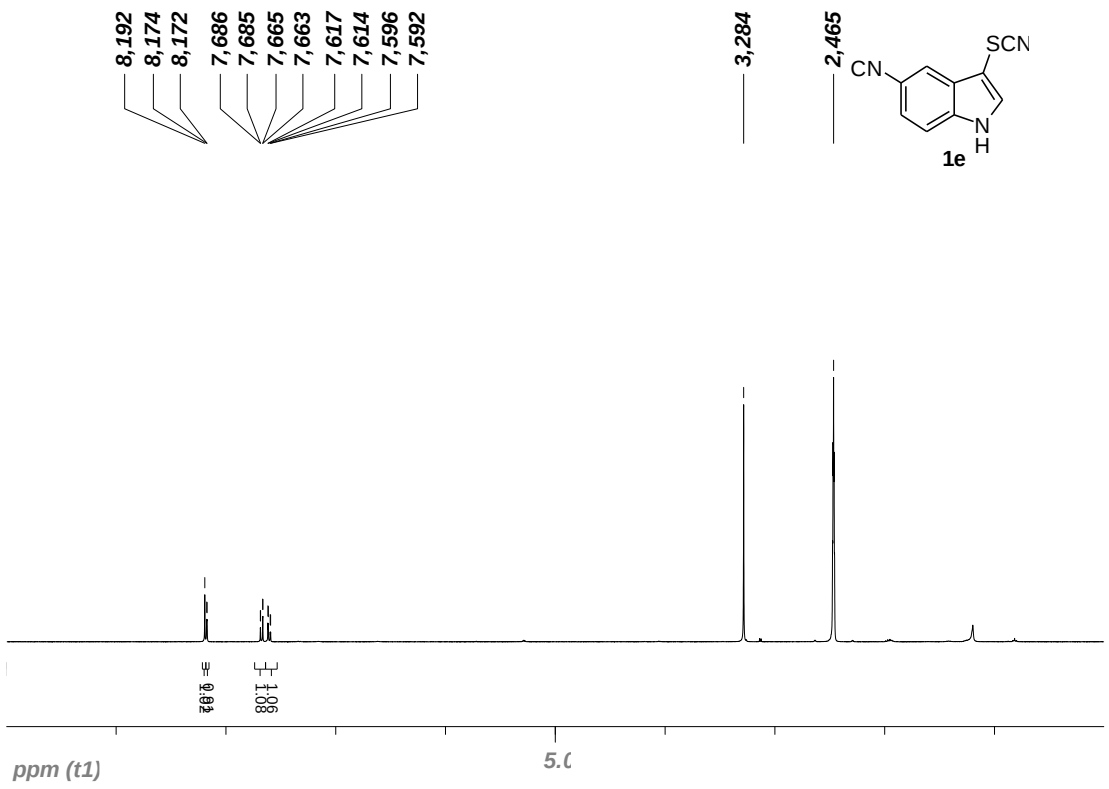
76,722
ppm (t1)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7,663
7,617
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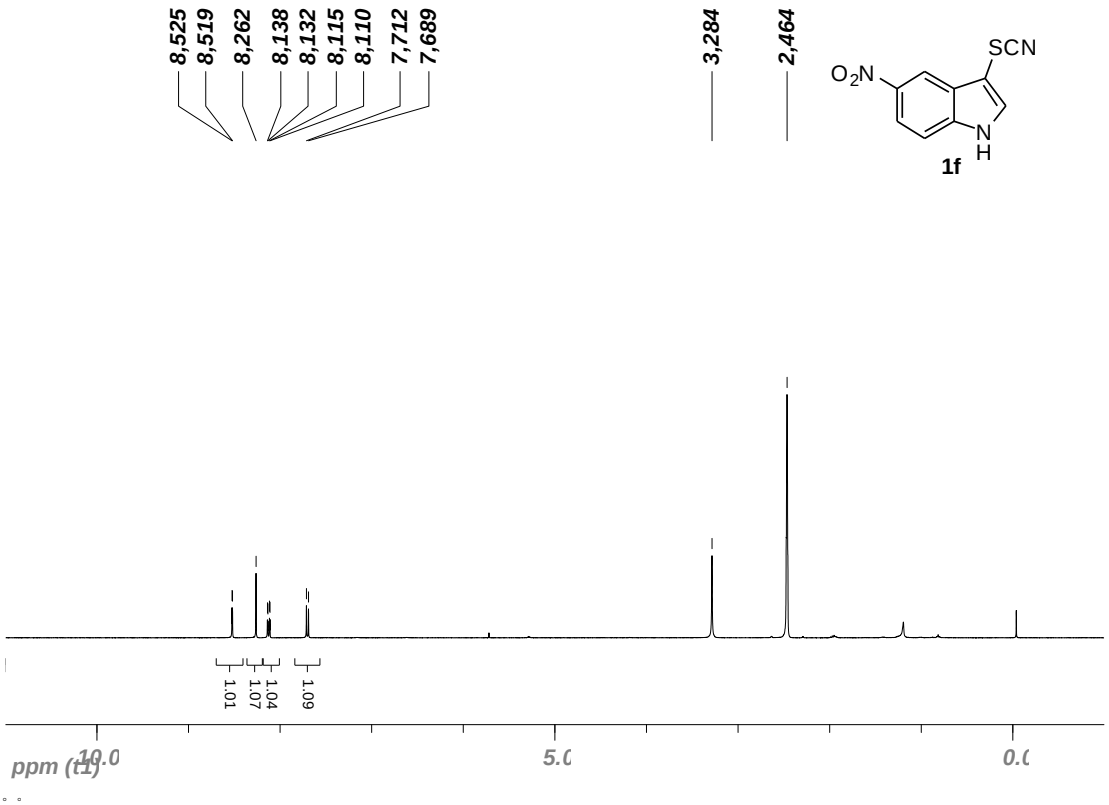
7,596
7,592
3,284
2,465
CN
SCN
N
H
1e
1.08
ppm (t1)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8,519
8,262
8,138
8,132
8,115
8,110
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2,464
O2N
SCN
N
H
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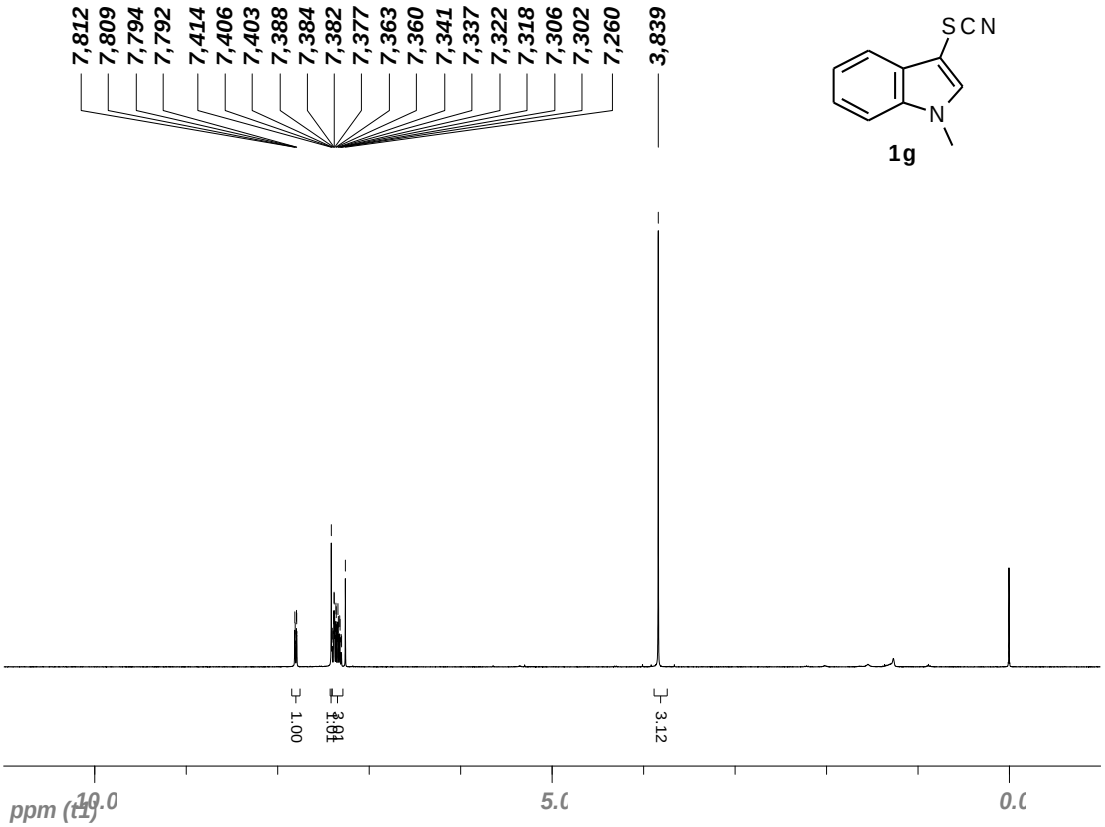
1.01
1.07
1.04
1.09
ppm (t1)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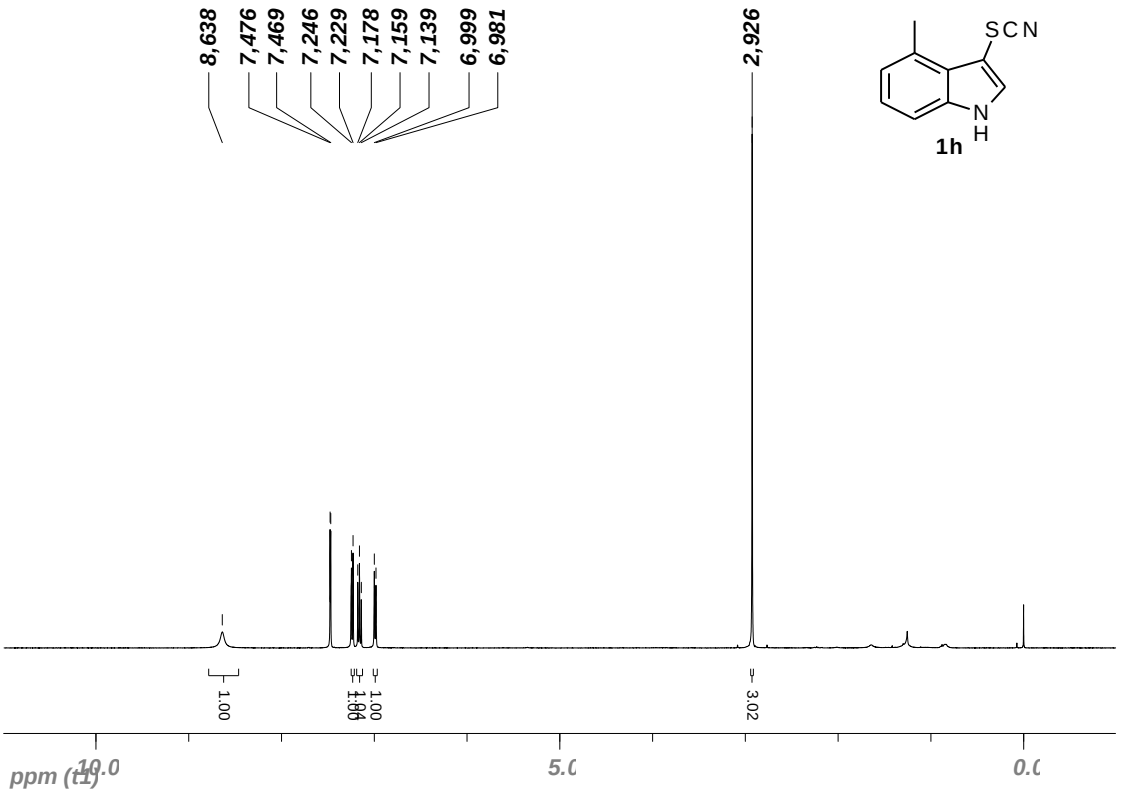
7,809
7,794
7,792
7,414
7,406
7,403
7,388
7,384
7,382
7,377
7,363
7,360
7,341
7,337
7,322
7,318
7,306
7,302
7,260
3,839
SCN
N
1g
1.00
1.01
1.01
3.12
10.0
5.0
0.0
ppm (t1)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7,229
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7,139
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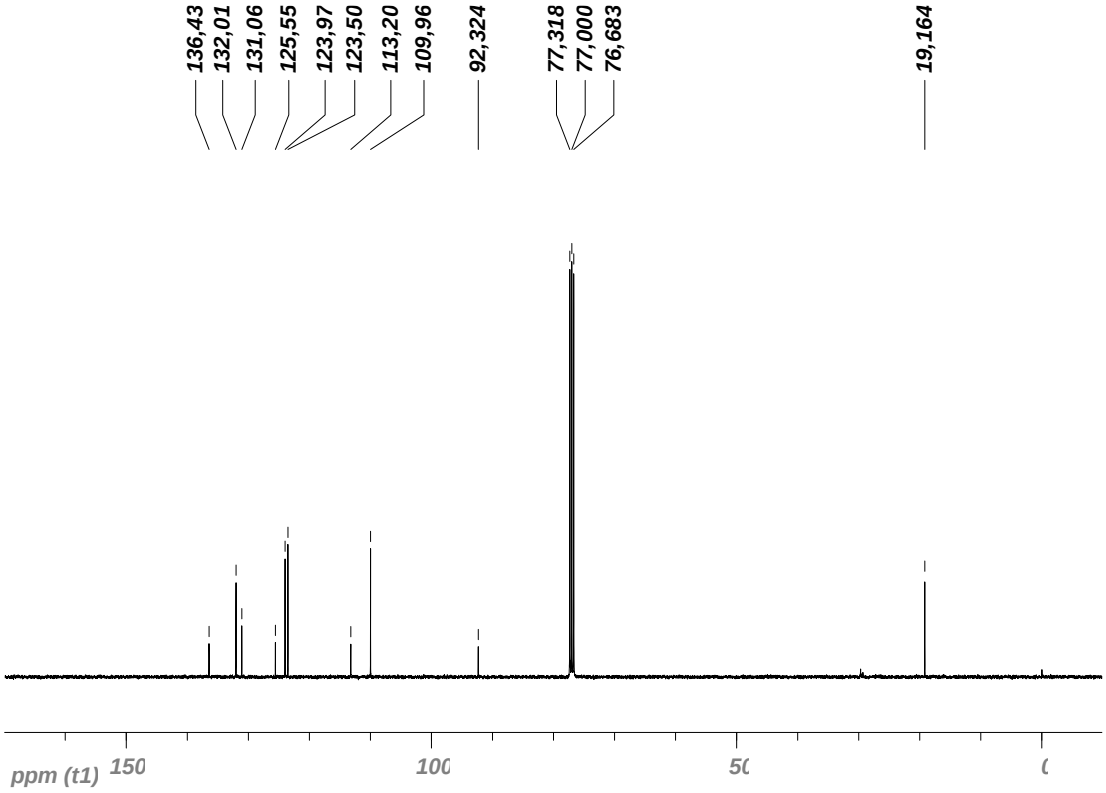
N
H
1h
1.00
1.00
1.00
3.02
10.0
5.0
0.0
ppm (t1)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76,683
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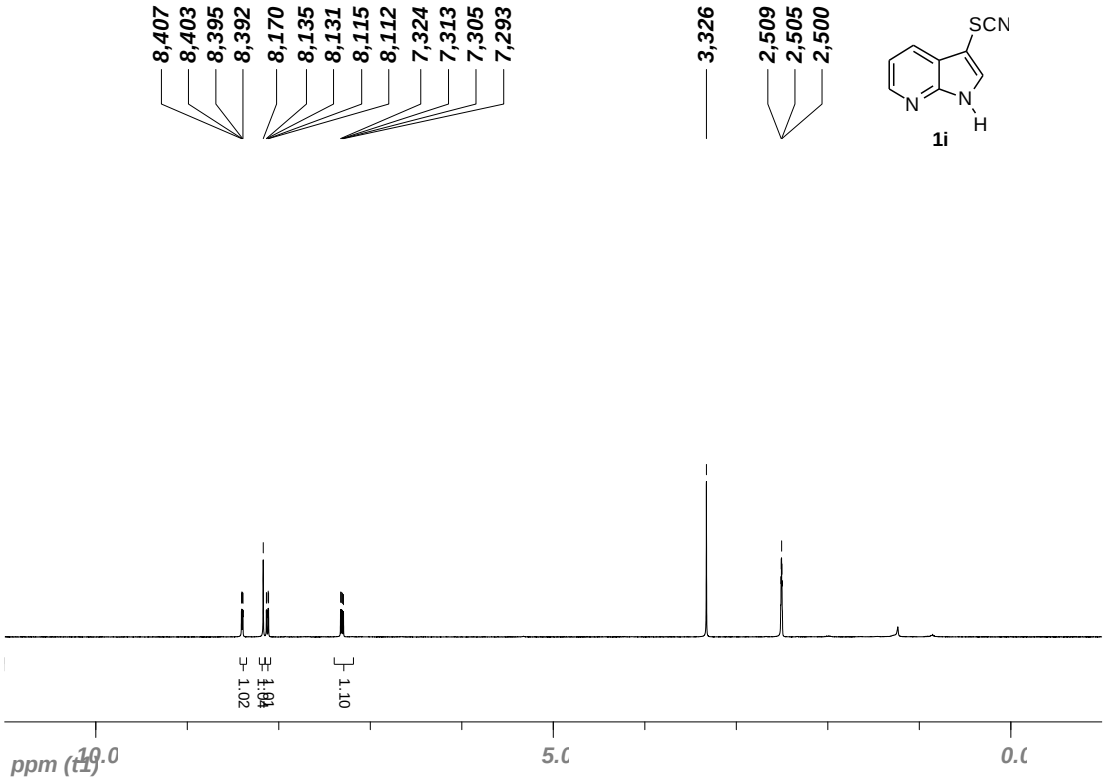
ppm (t1)
150
100
50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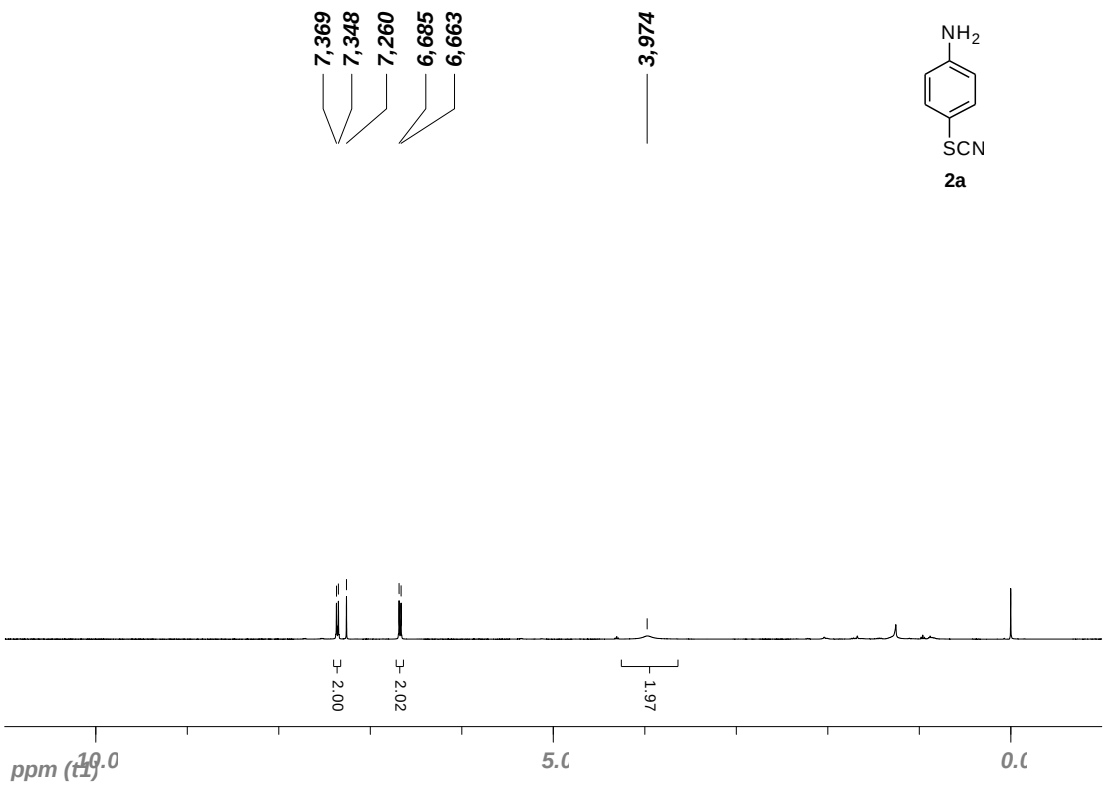
8,170
8,135
8,131
8,115
8,112
7,324
7,313
7,305
7,293
3,326
2,509
2,505
2,500
SCN
N
N
H
1i
1.02
1.04
1.10
10.0
5.0
0.0
ppm (t1)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6,685
6,663
3,974
NH2
SCN
2a
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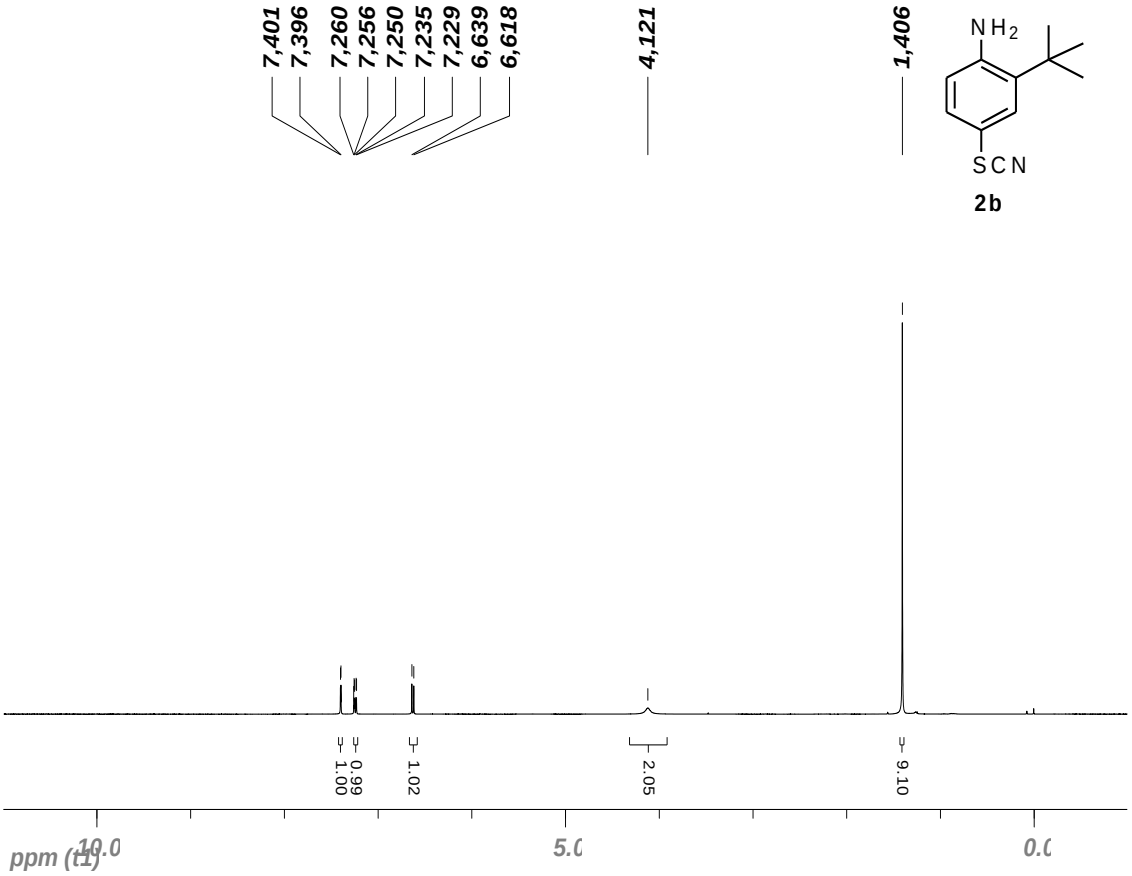
2.02
1.97
ppm (t1)
10.0
5.0
0.0
148,77
134,49
116,08
112,31
109,70
77,345
77,230
77,028
76,710
ppm (t1)
150
100
50
0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7,396
7,260
7,256
7,250
7,235
7,229
6,639
6,618
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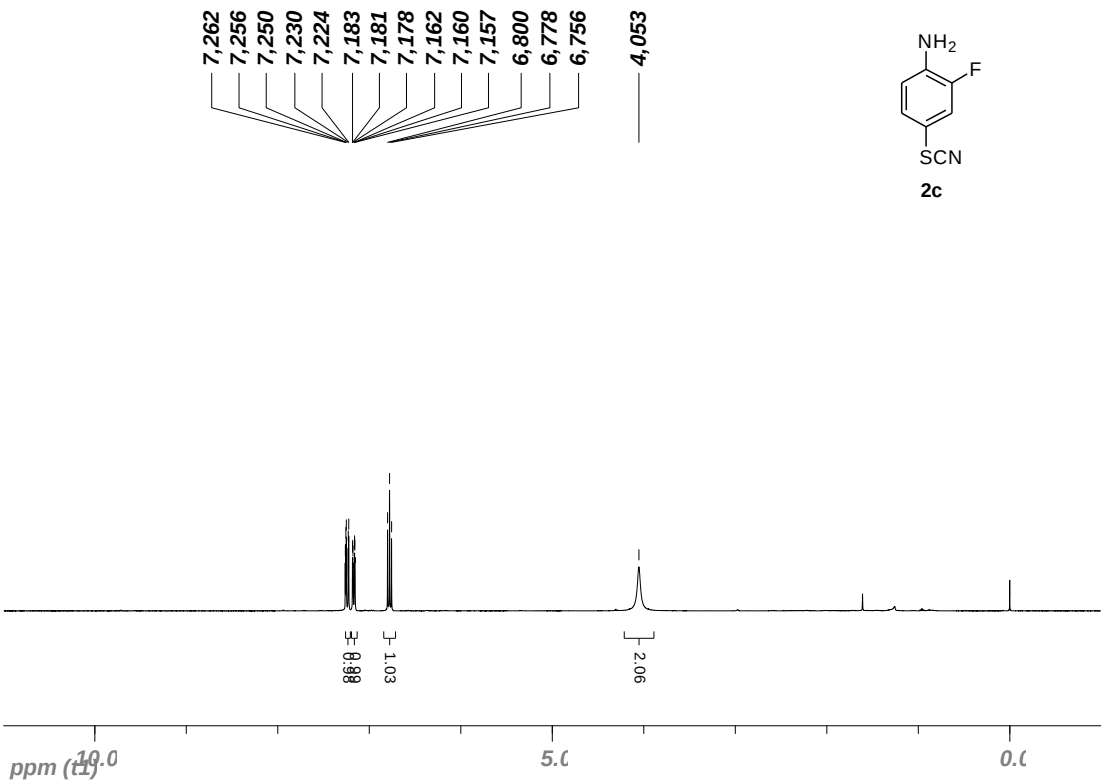
1,406
NH2
SCN
2b
1.00
0.99
1.02
2.05
9.10
ppm (t1)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7,250
7,230
7,224
7,183
7,181
7,178
7,162
7,160
7,157
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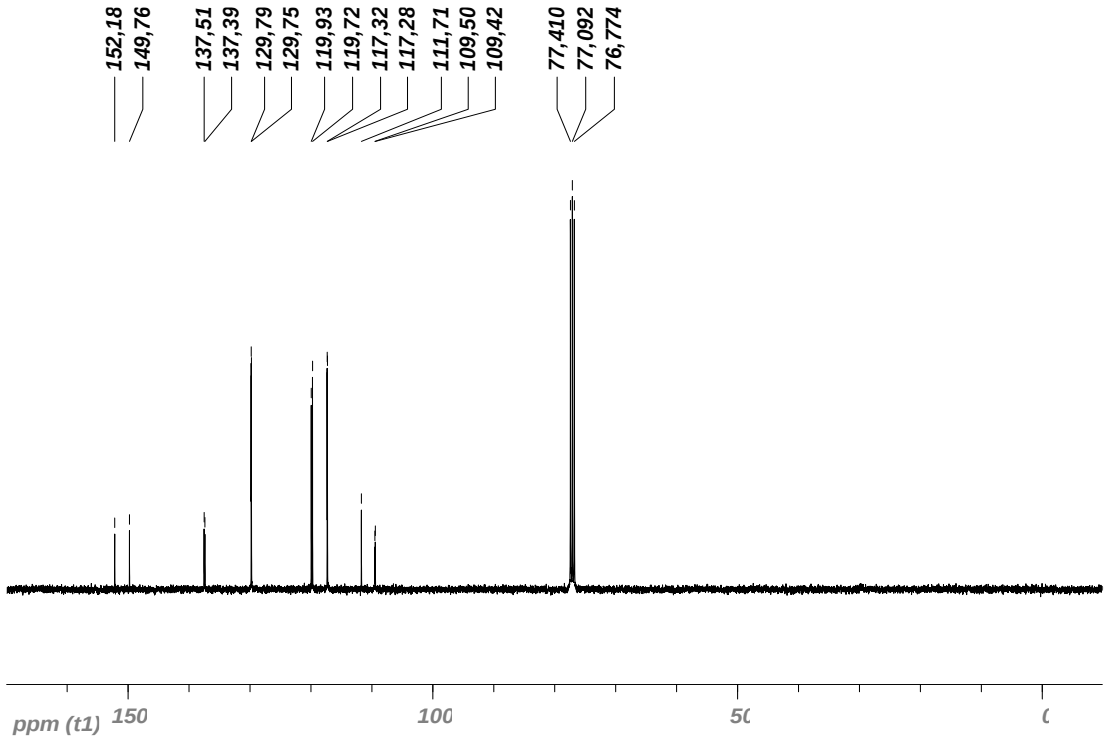
6,778
6,756
4,053
NH2
F
SCN
2c
1.03
2.06
ppm (t1)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137,51
137,39
129,79
129,75
119,93
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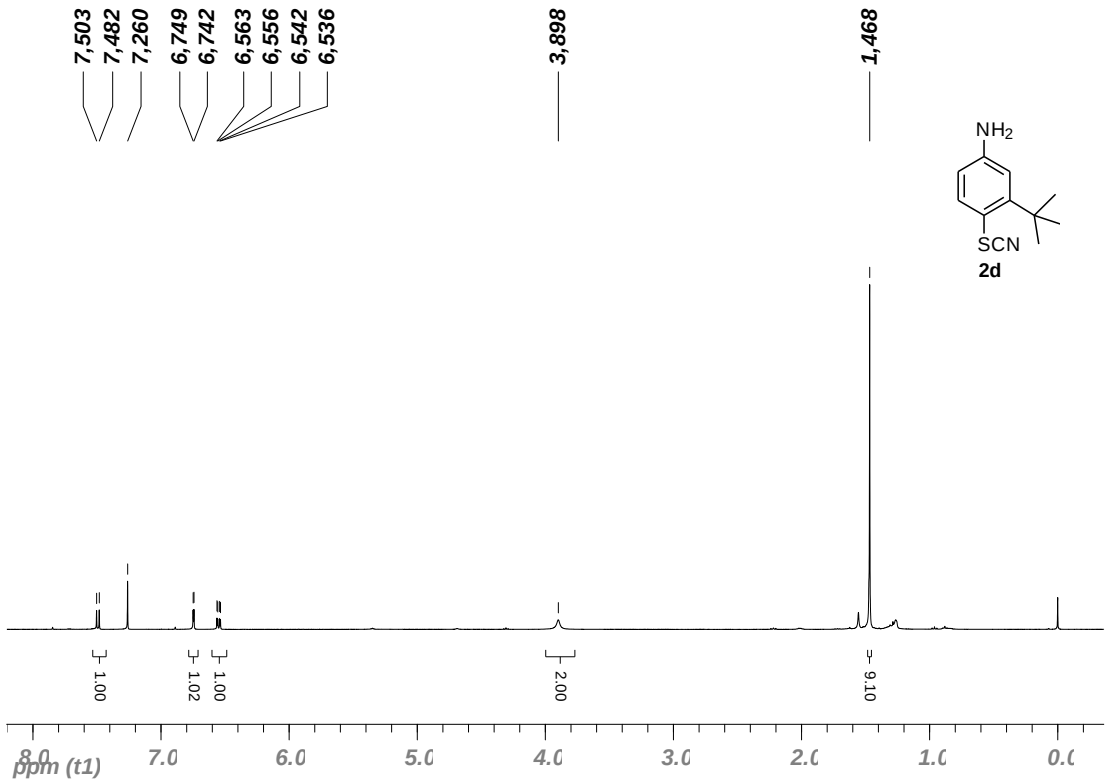
117,32
117,28
111,71
109,50
109,42
77,410
77,092
76,774
ppm (t1)
150
100
50


7,503
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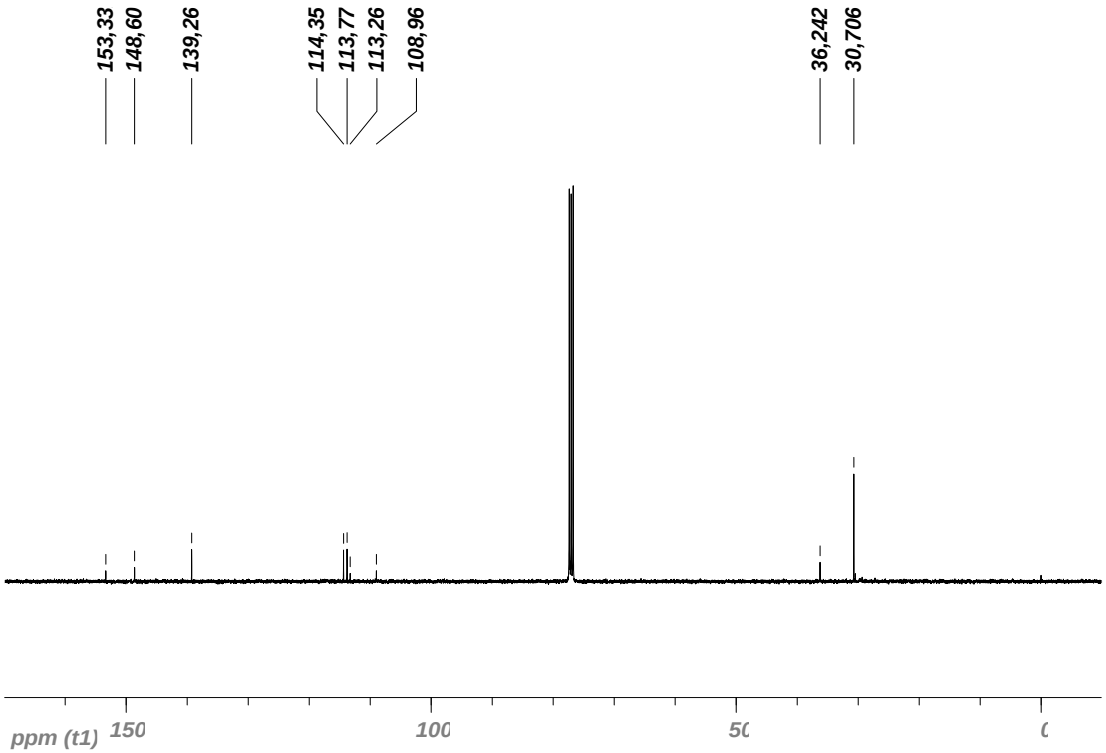
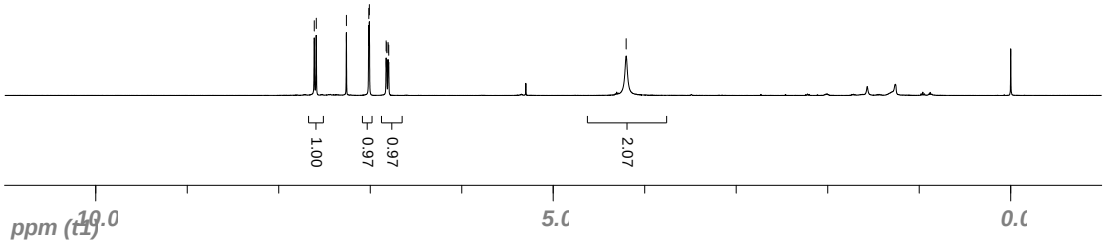
7,260
6,749
6,742
6,563
6,556
6,542
6,536
3,898
1,468
NH2
SCN
2d
1.00
1.02
1.00
2.00
9.10
ppm (t1)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0


153,33
148,60
139,26
114,35
113,77
113,26
108,96
36,242
30,706
ppm (t1)
150
100
50


7,611
7,590
7,260
7,015
7,009
6,825
6,819
6,804
6,798
4,202
NH2
CF3
SCN

2e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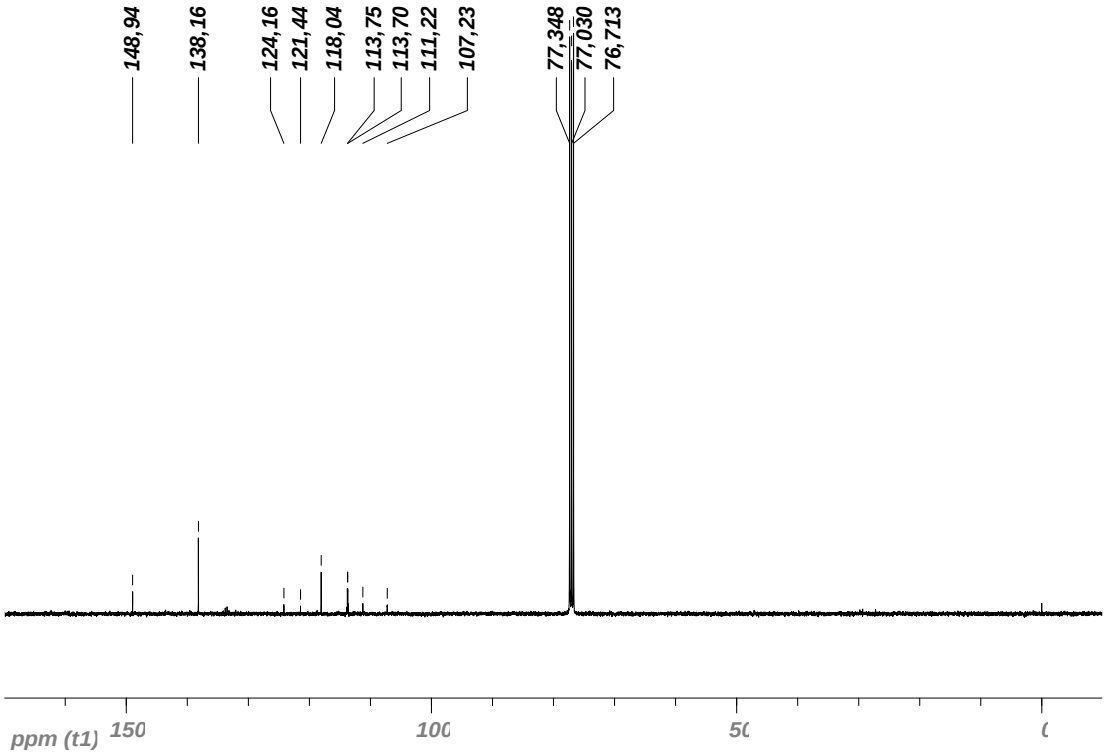
0,97
0,97
2,07
ppm (t1)
10.0
5.0
0.0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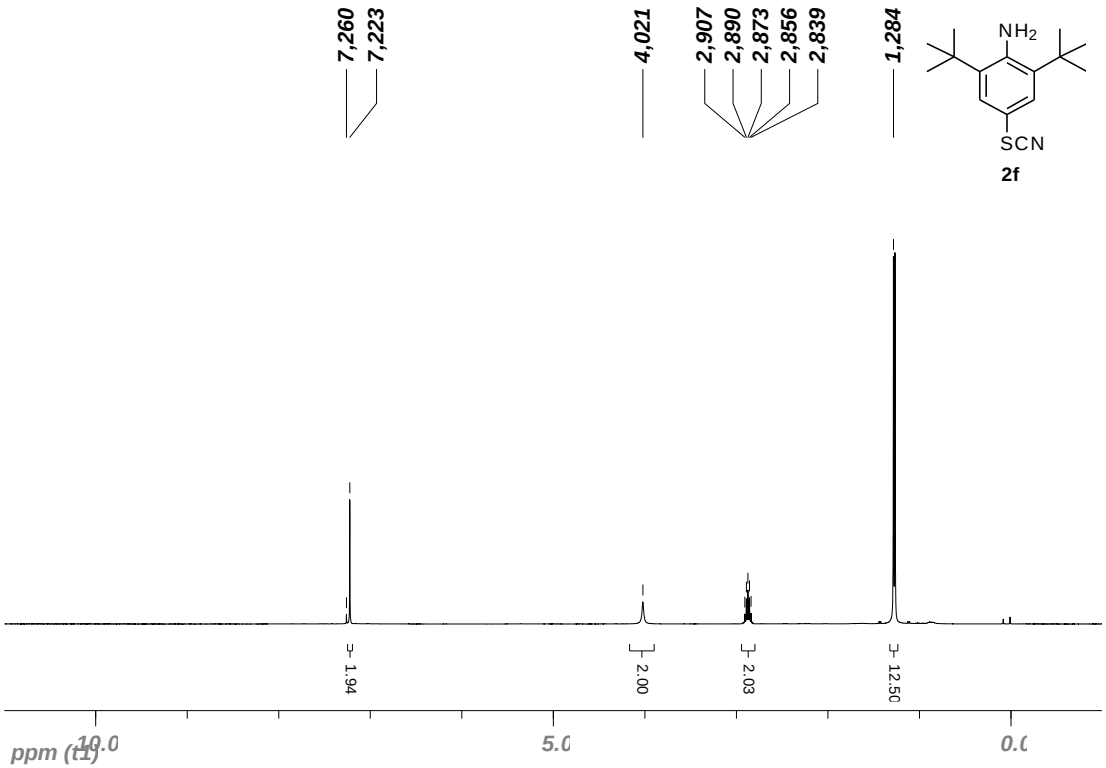
138,16
124,16
121,44
118,04
113,75
113,70
111,22
107,23
77,348
77,030
76,713
ppm (t1)
150
100
50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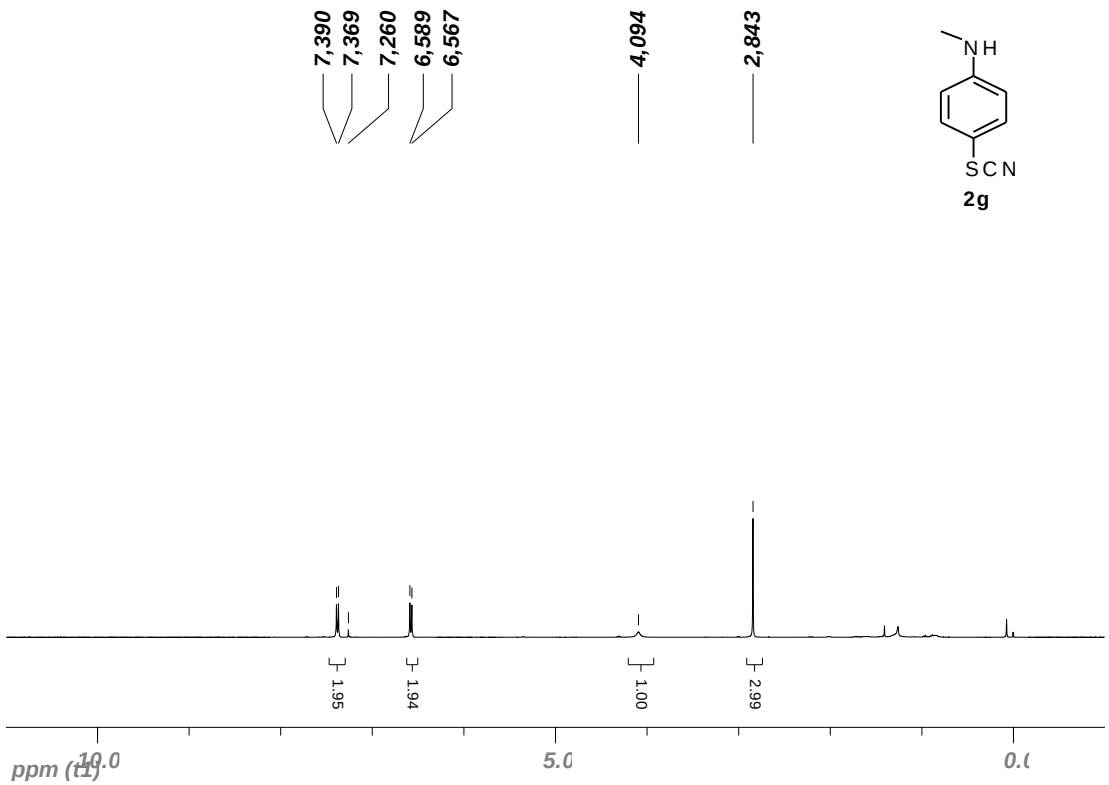
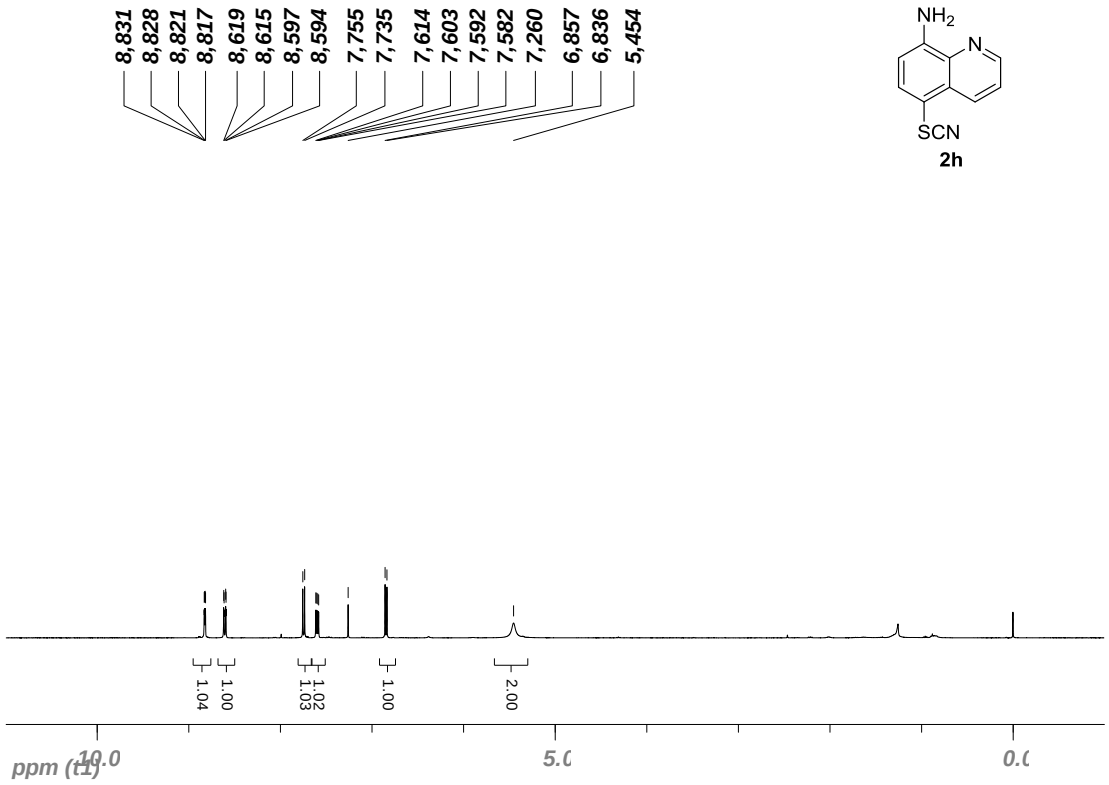
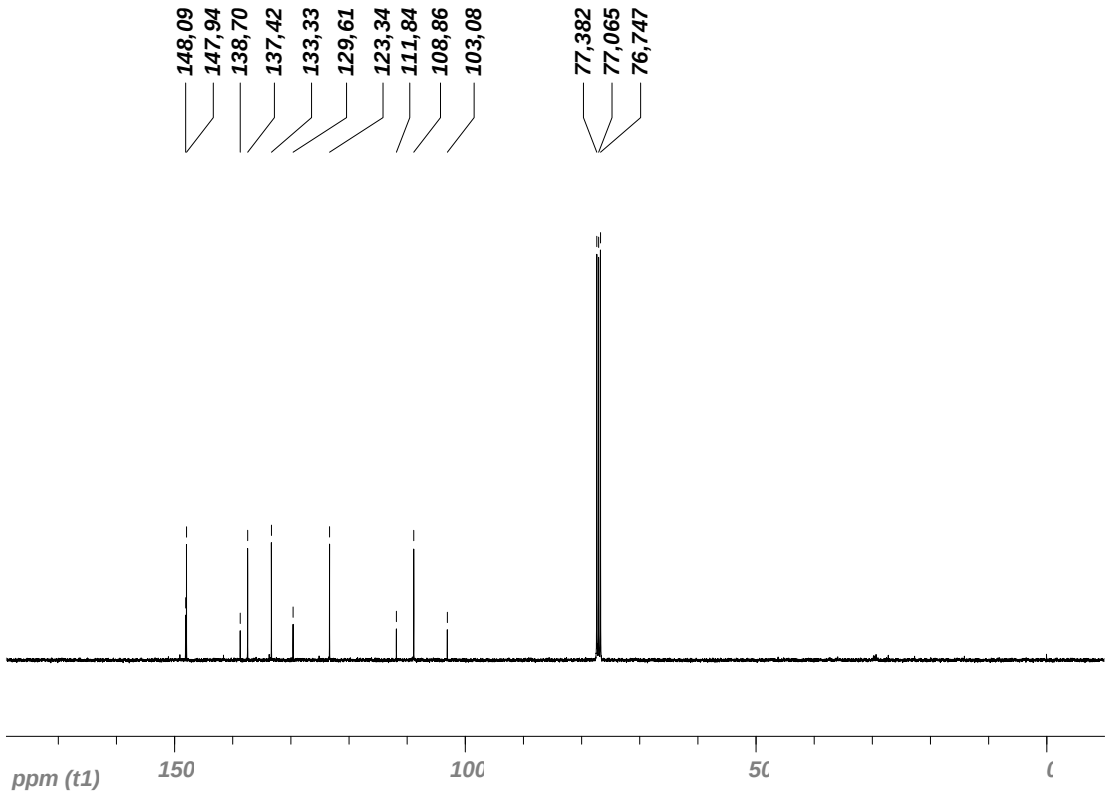
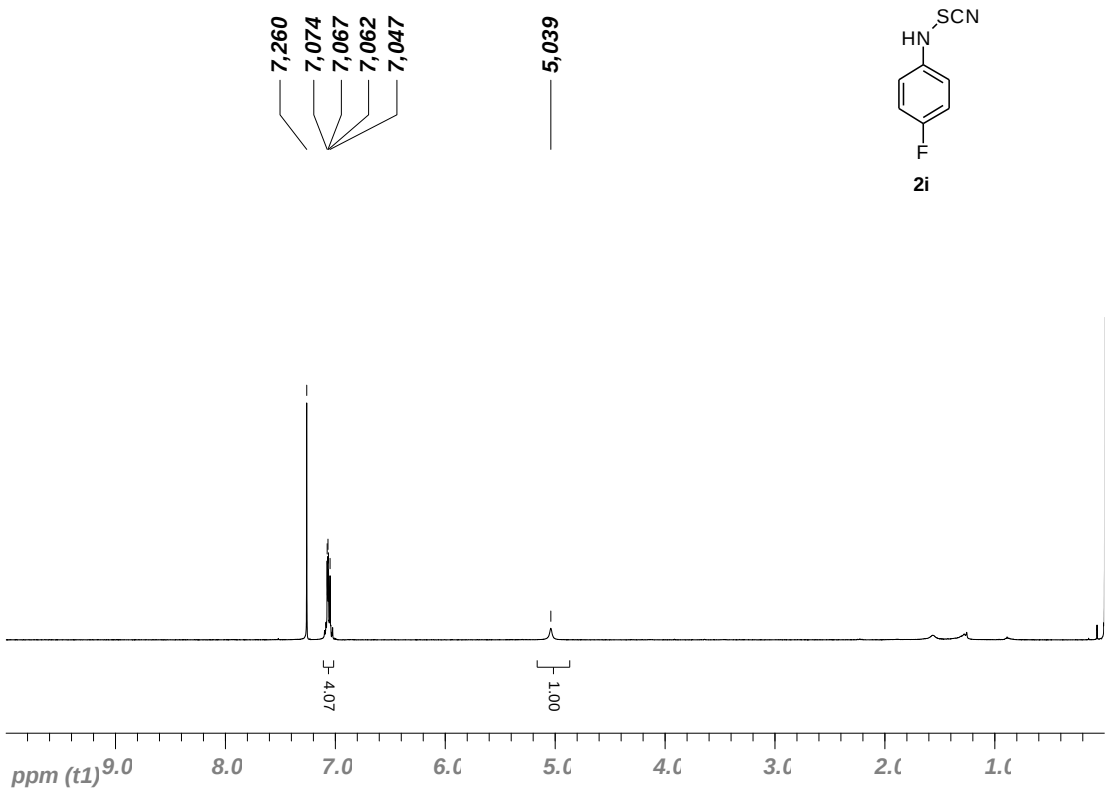
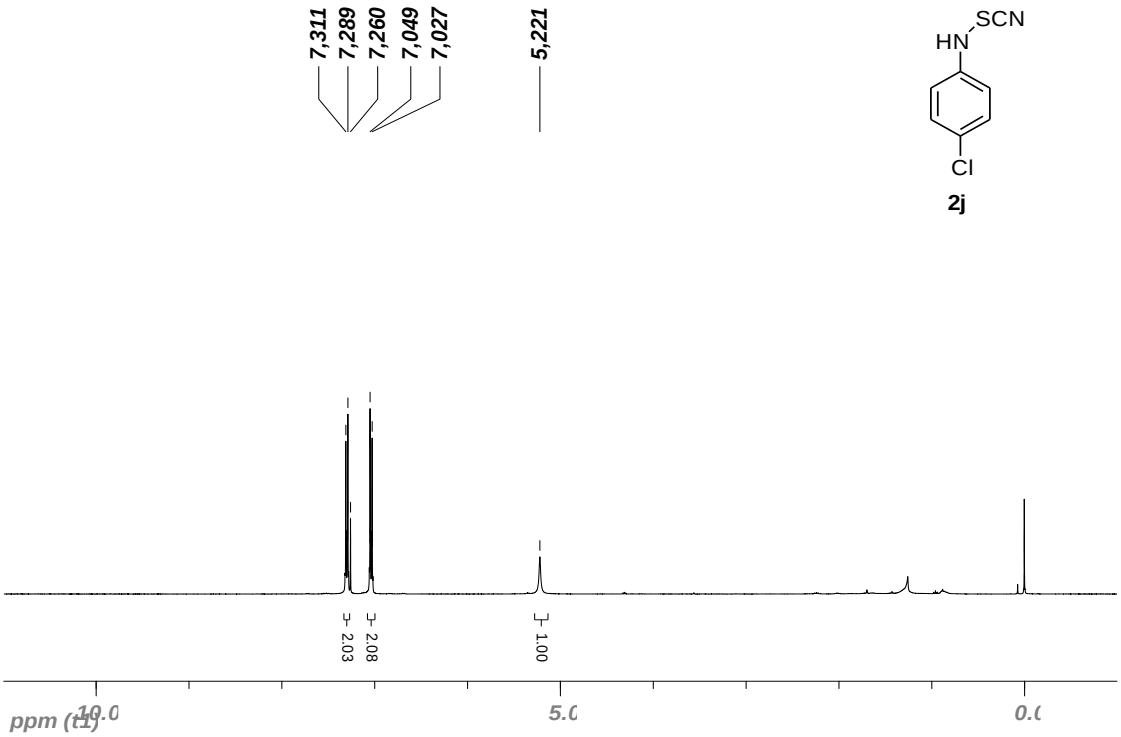
2,907
2,890
2,873
2,856
2,839
1,284
NH2
SCN
2f
1.94
2.00
2.03
12.50
ppm (t1)
10.0
5.0
0.0

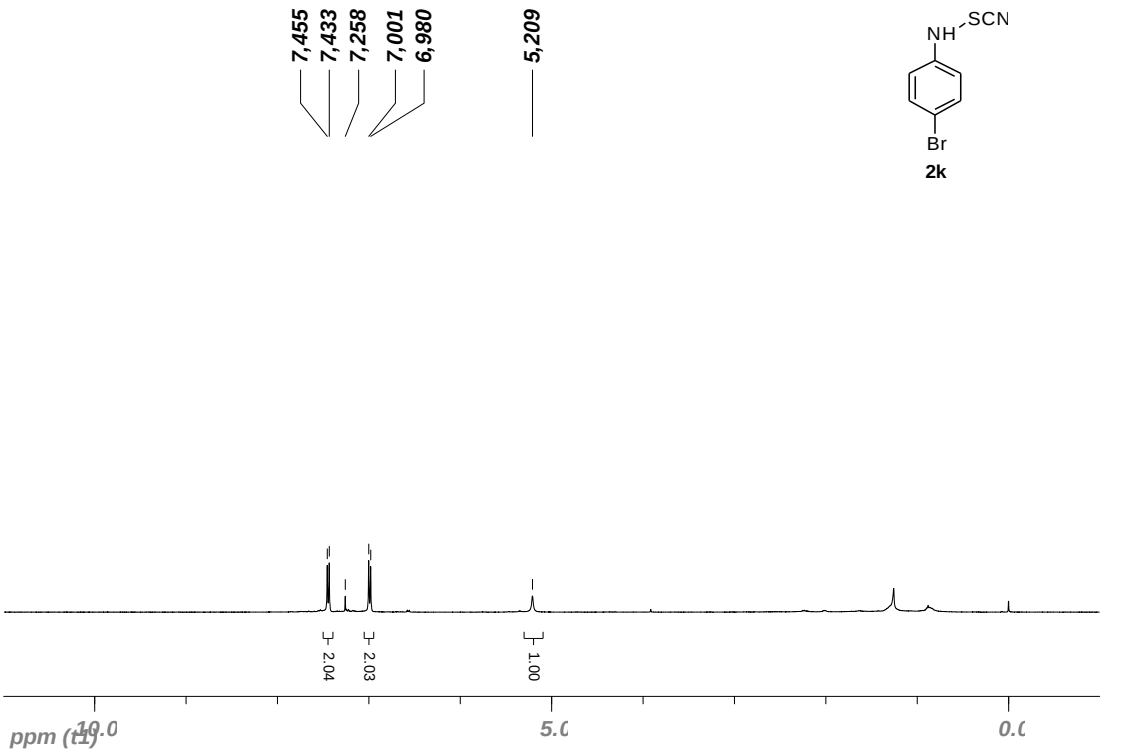

7,390
7,369
7,260
6,589
6,567
4,094
2,843
NH
SCN
2g
1.95
1.94
1.00
2.99
ppm (t1)

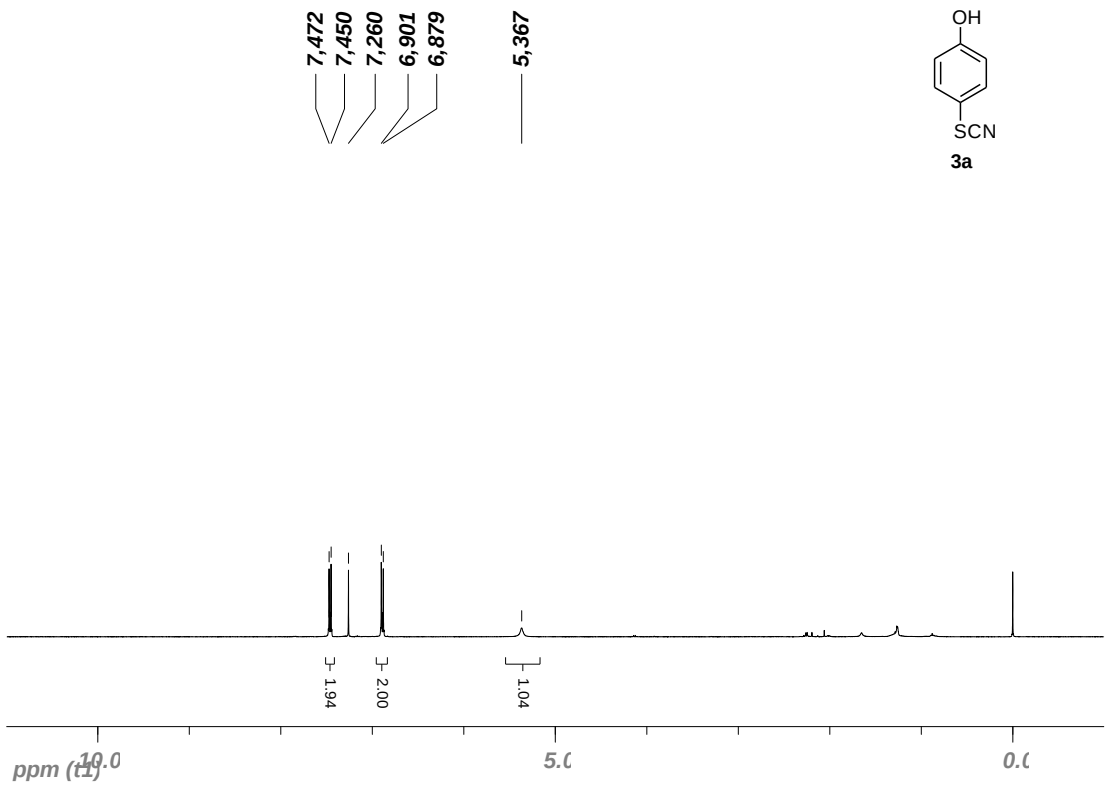

8,831
8,828
8,821
8,817
8,619
8,615
8,597
8,594
7,755
7,735
7,614
7,603
7,592
7,582
7,260
6,857
6,836
5,454
NH2
N
SCN
2h
1.04
1.00
1.02
1.03
1.00
2.00
ppm (t1)

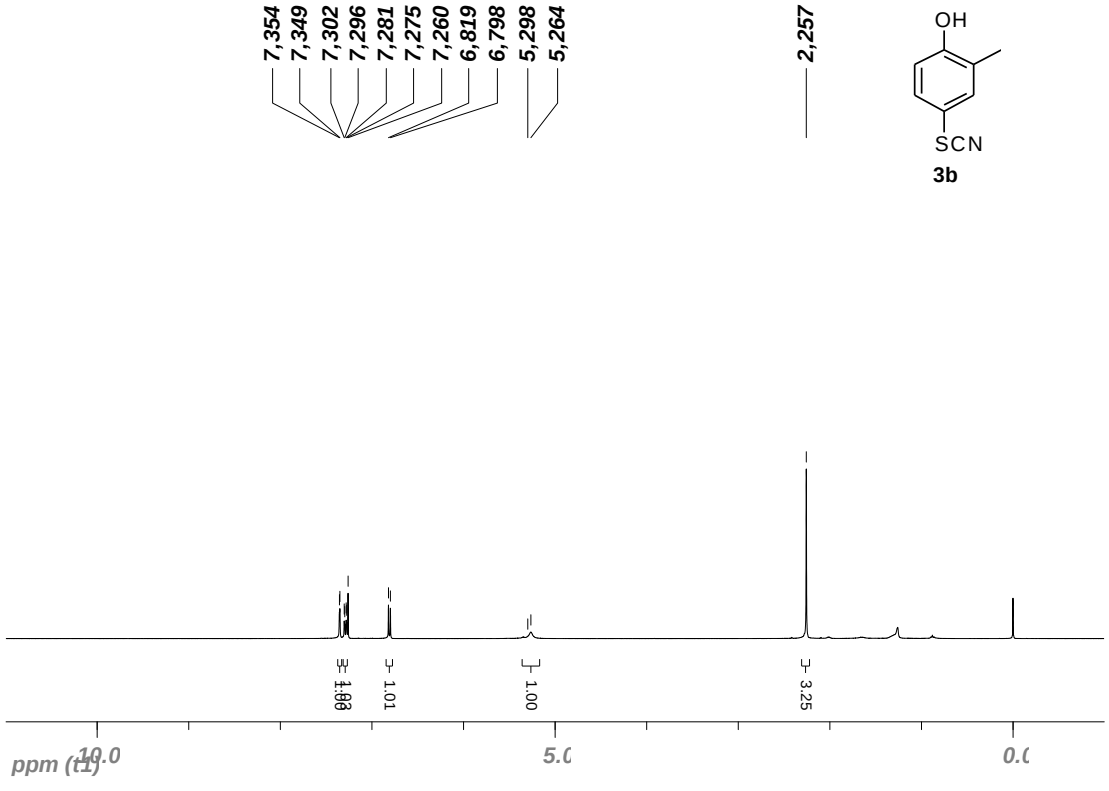

148,09
147,94
138,70
137,42
133,33
129,61
123,34
111,84
108,86
103,08
77,382
77,065
76,747
ppm (t1)
150
100
50

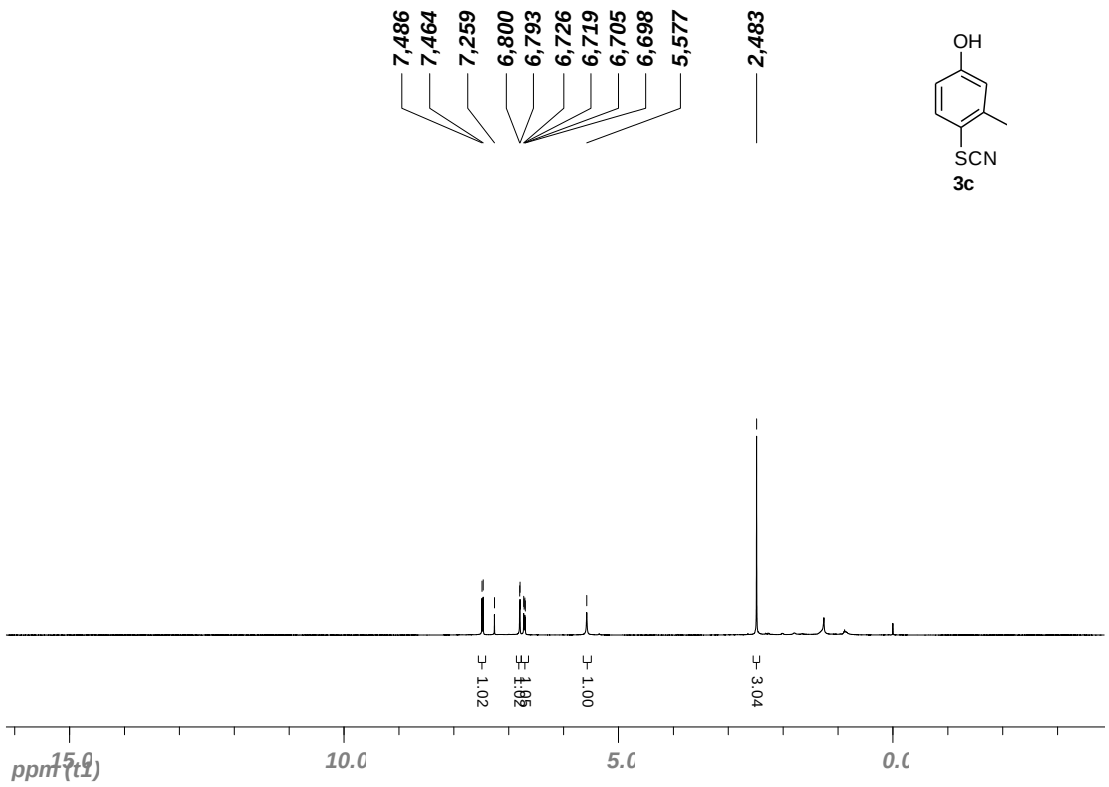

7,260
7,074
7,067
7,062
7,047
5,039
SCN
HN
F
2i
4,07
1,00
ppm (t1)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0

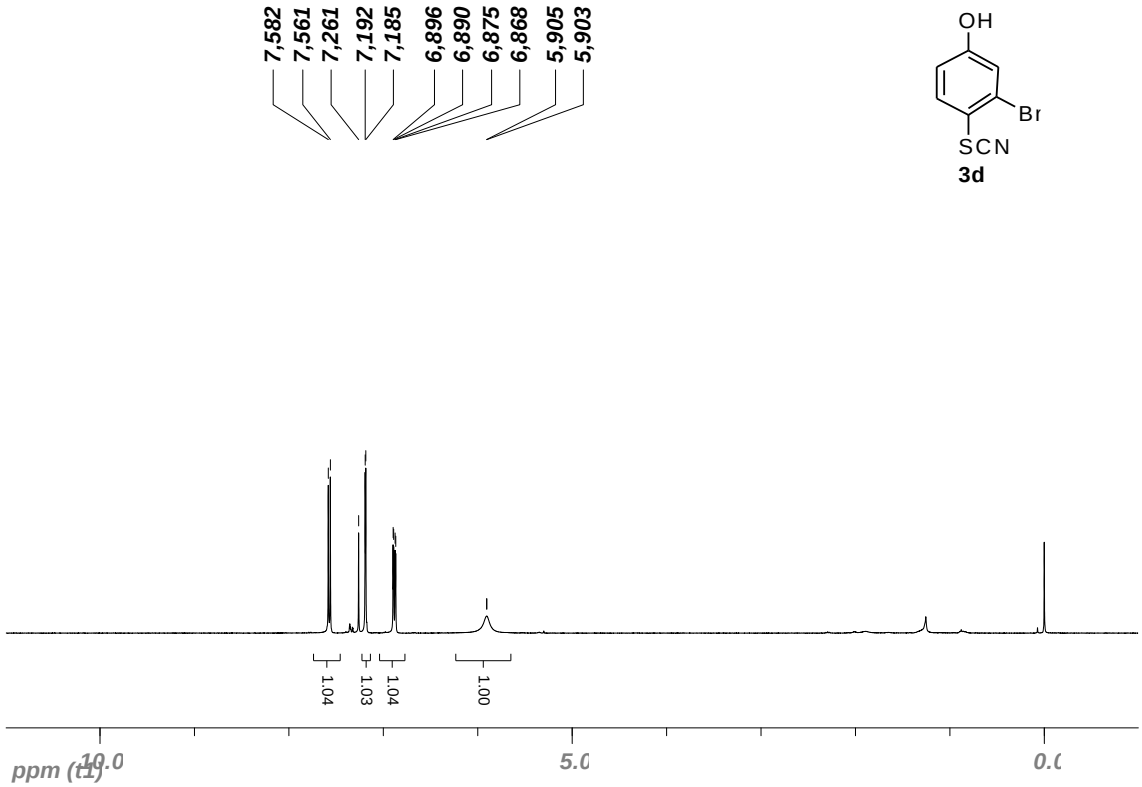

7,311
7,289
7,260
7,049
7,027
5,221
SCN
HN
Cl
2j
2.03
2.08
1.00
ppm (t1)

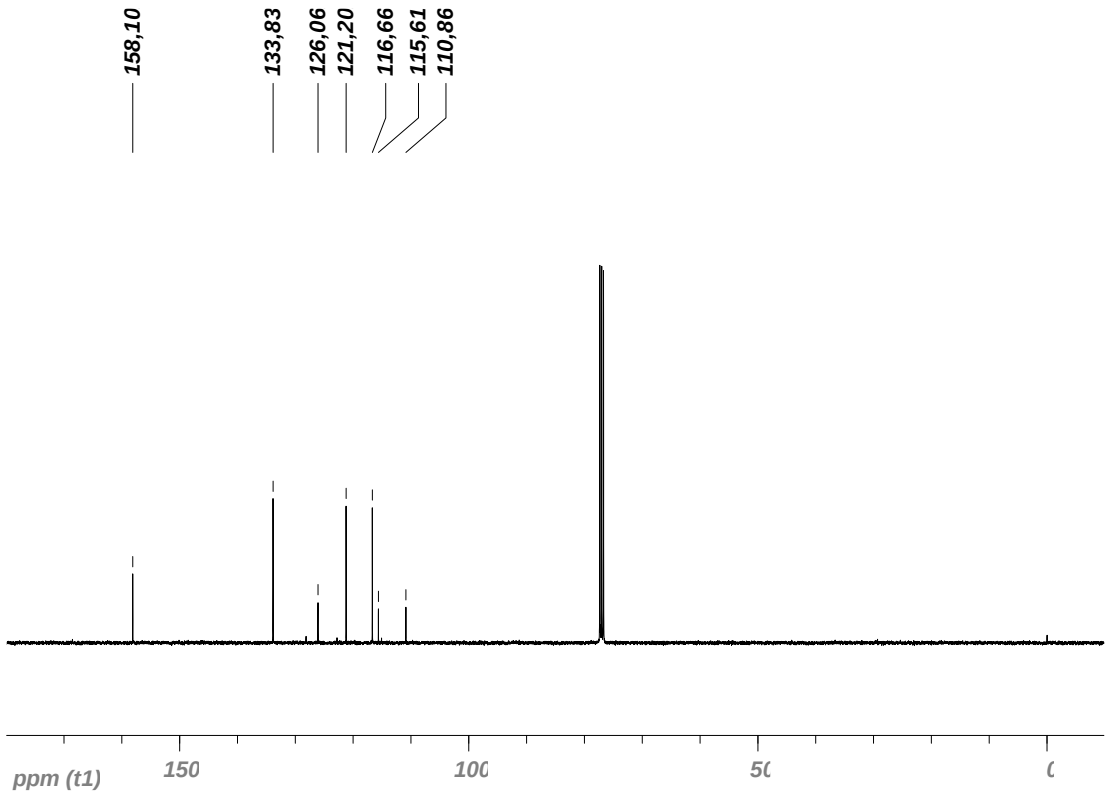

7,455
7,433
7,258
7,001
6,980
5,209
SCN
NH
Br
2k
2.04
2.03
1.00
ppm (t1)

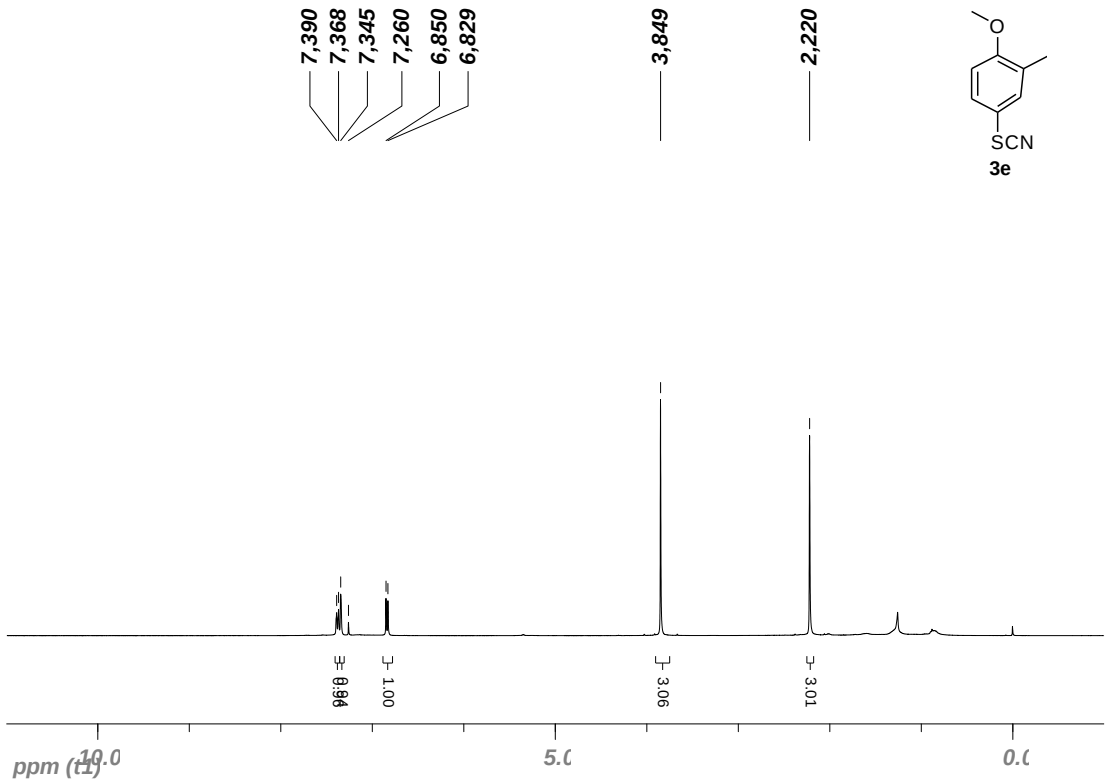

7,472
7,450
7,260
6,901
6,879
5,367
OH
SCN
3a
1.94
2.00
1.04
ppm (t1)

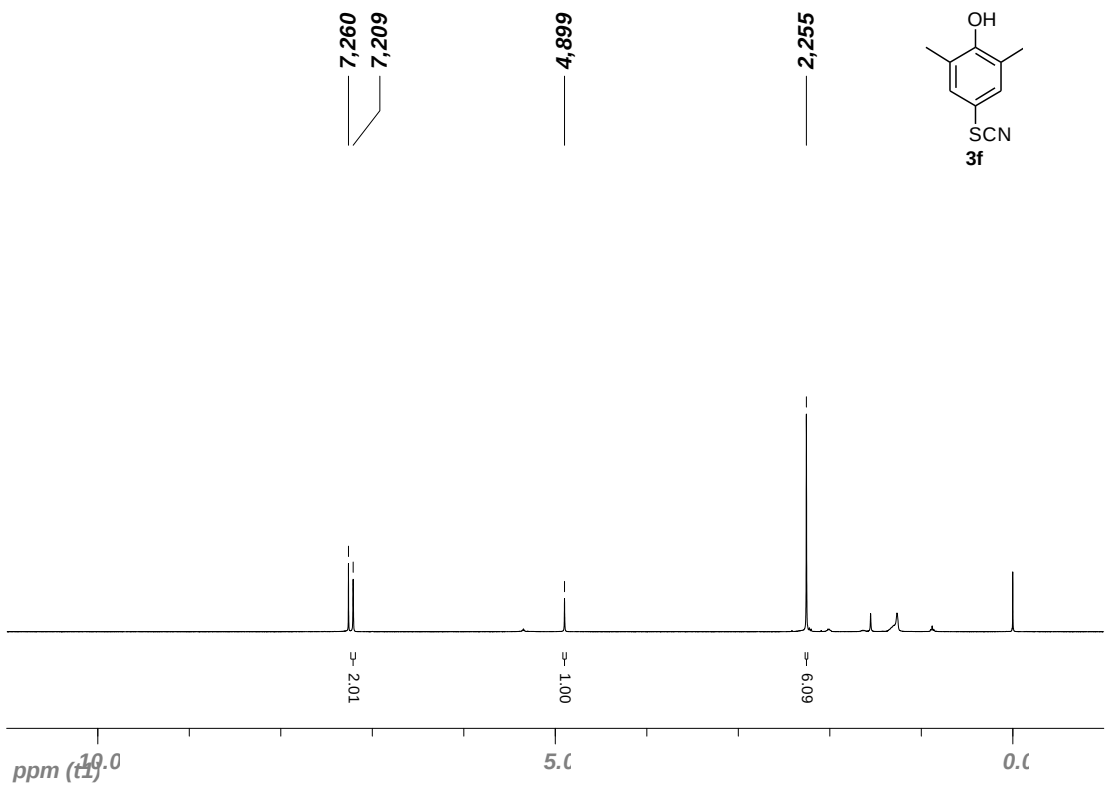

7,354
7,349
7,302
7,296
7,281
7,275
7,260
6,819
6,798
5,298
5,264
2,257
OH
SCN
3b
1.01
1.00
3.25
ppm (t1)

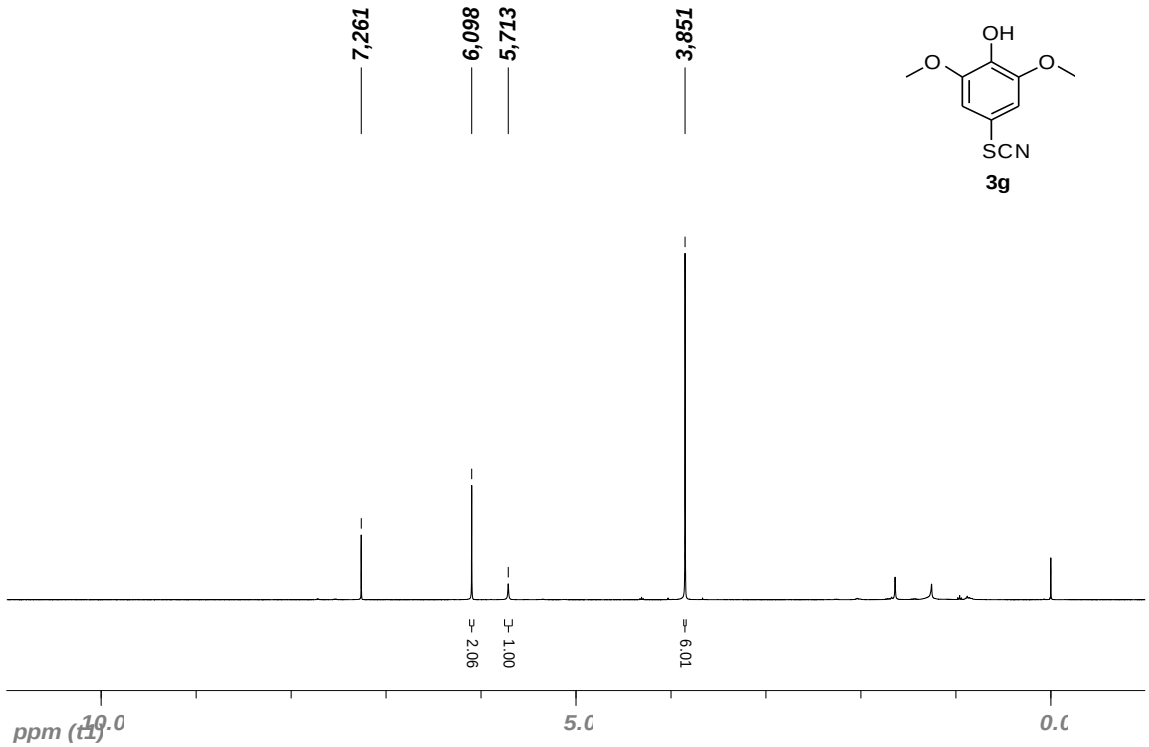

7,486
7,464
7,259
6,800
6,793
6,726
6,719
6,705
6,698
5,577
2,483
OH
SCN
3c
1.02
1.05
1.00
3.04
ppm (t1)

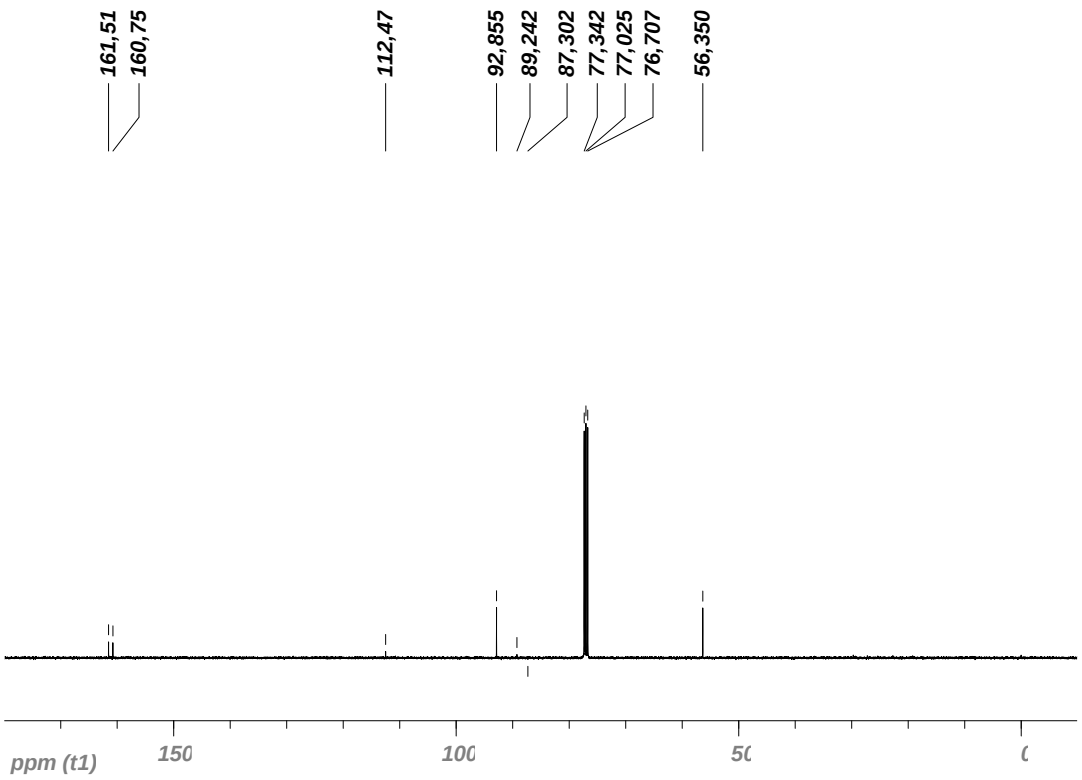

7,582
7,561
7,261
7,192
7,185
6,896
6,890
6,875
6,868
5,905
5,903
OH
Br
SCN
3d
1.04
1.03
1.04
1.00
ppm (t1)

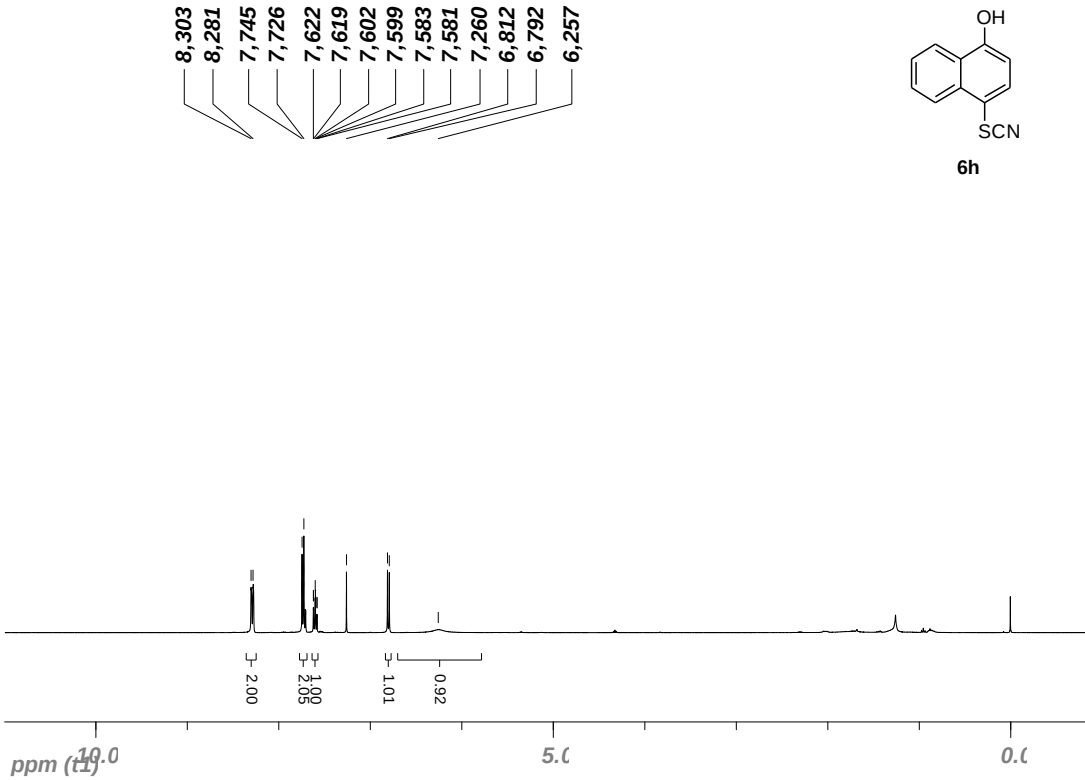

158,10
133,83
126,06
121,20
116,66
115,61
110,86
ppm (t1)
150
100
50
0


7,390
7,368
7,345
7,260
6,850
6,829
3,849
2,220
O
SCN
3e
1.00
3.06
3.01
ppm (t1)
10.0
5.0
0.0


7,260
7,209
4,899
2,255
OH
SCN
3f
2.01
1.00
6.09
ppm (t1)

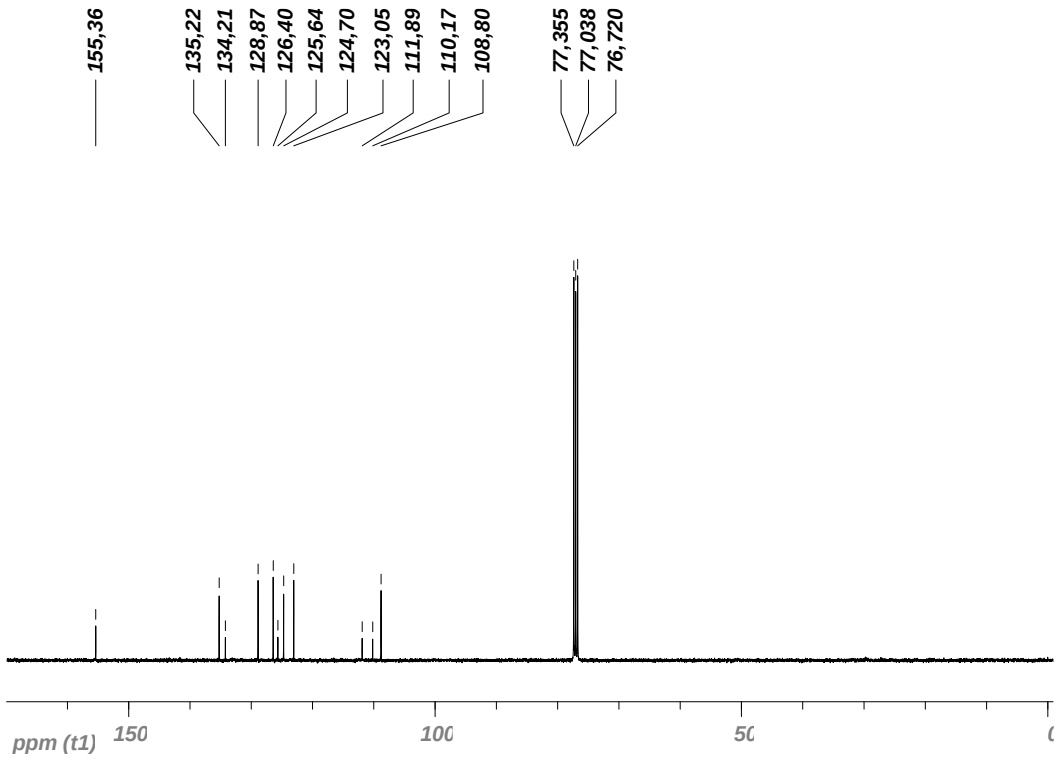

7,261
6,098
5,713
3,851
OH
O
O
SCN
3g
2.06
1.00
6.01
ppm (t1)

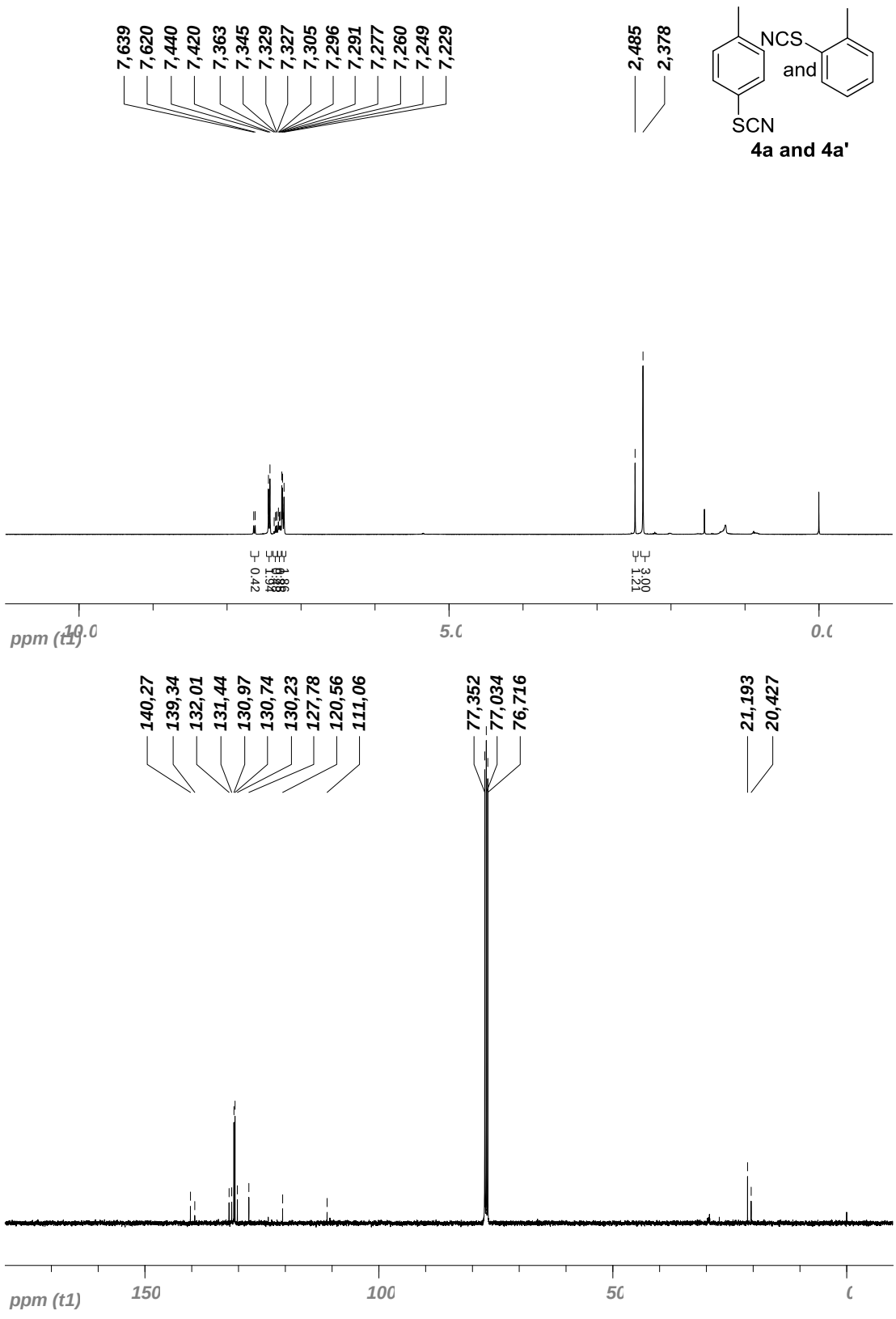

161,51
160,75
112,47
92,855
89,242
87,302
77,342
77,025
76,707
56,350
ppm (t1)
150
100
50
0

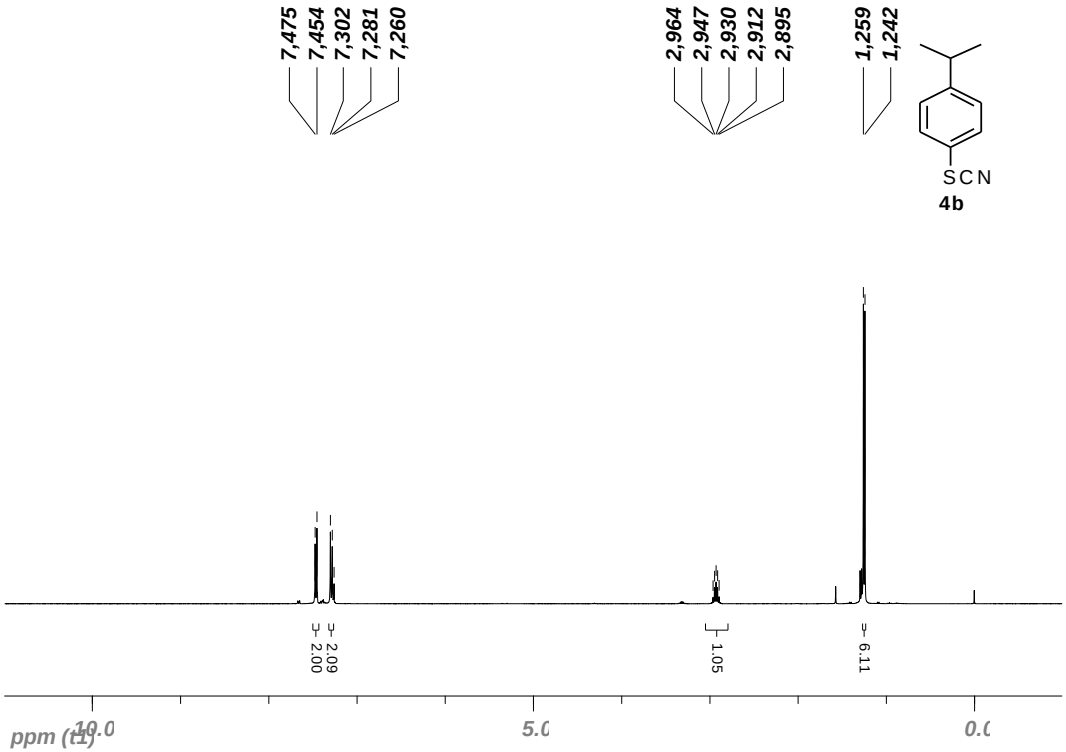

8,303
8,281
7,745
7,726
7,622
7,619
7,602
7,599
7,583
7,581
7,260
6,812
6,792
6,257
2.00
1.00
2.05
1.01
0.92
ppm (t1)
10.0
5.0
0.0

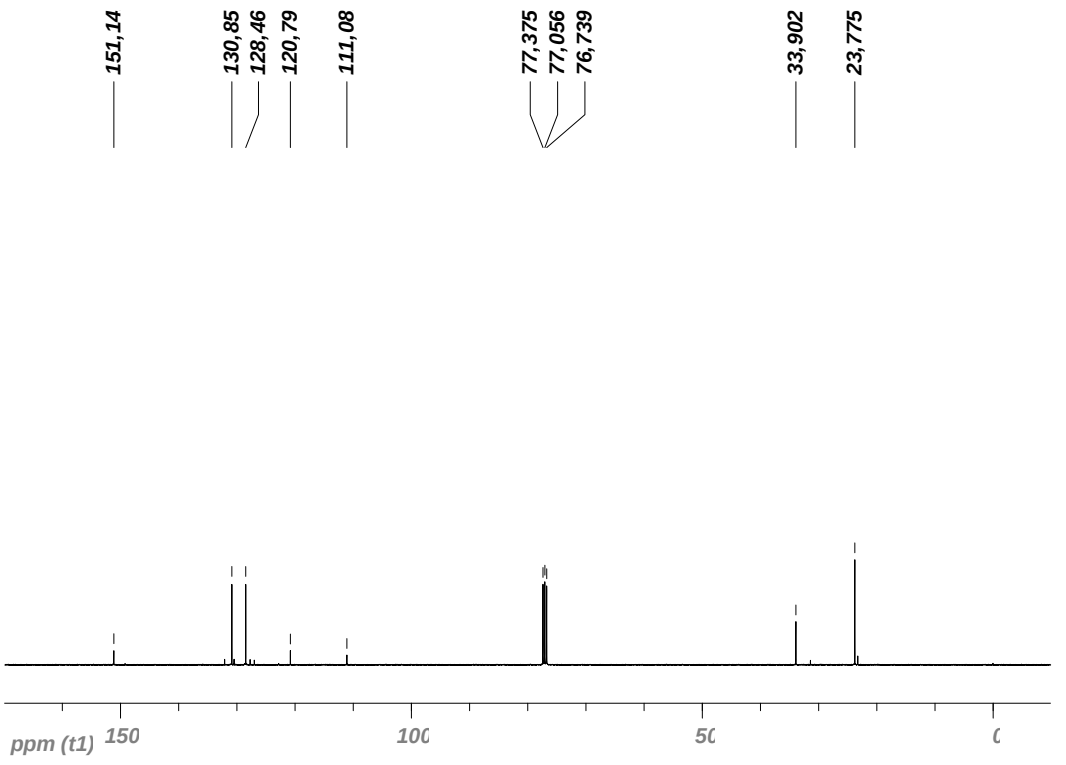
OH
SCN

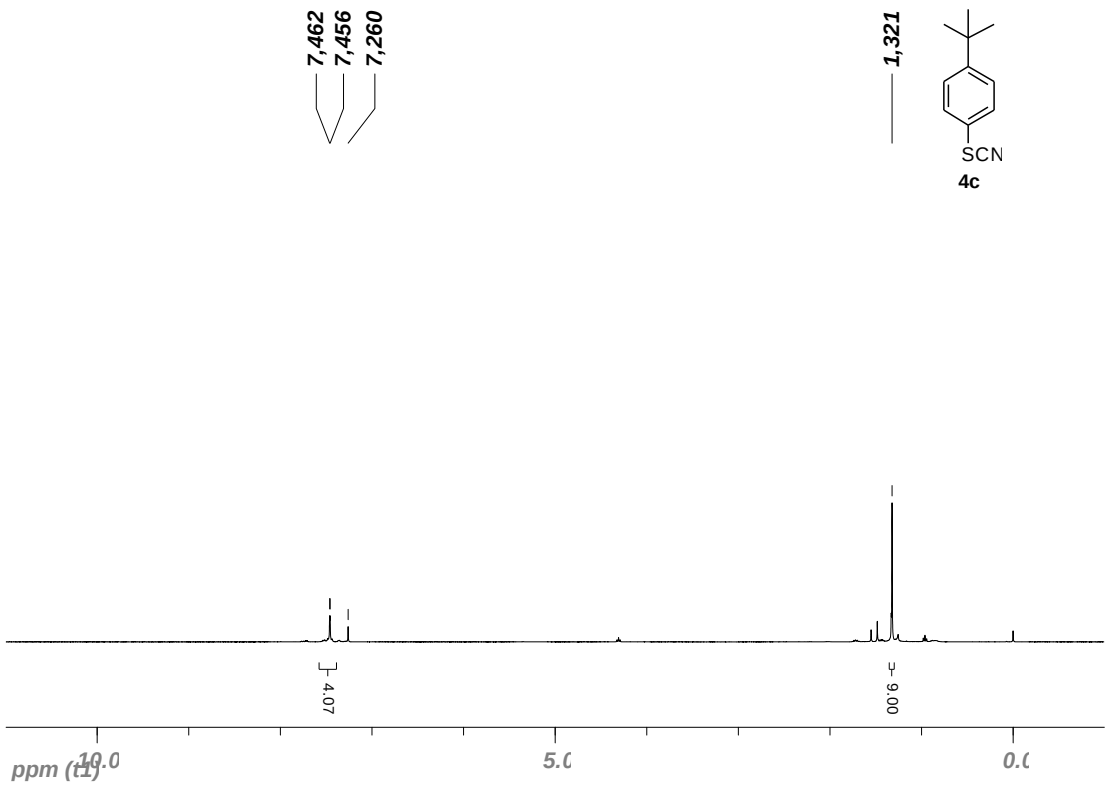
6h


155,36
135,22
134,21
128,87
126,40
125,64
124,70
123,05
111,89
110,17
108,80
77,355
77,038
76,720
ppm (t1)
150
100
50


7,639
7,620
7,440
7,420
7,363
7,345
7,329
7,327
7,305
7,296
7,291
7,277
7,260
7,249
7,229
2,485
2,378
NCS
and
SCN
4a and 4a'
0,42
1,94
1,86
3,00
1,21
ppm (t1)
140,27
139,34
132,01
131,44
130,97
130,74
130,23
127,78
120,56
111,06
77,352
77,034
76,716
21,193
20,427
ppm (t1)


7,475
7,454
7,302
7,281
7,260
2,964
2,947
2,930
2,912
2,895
1,259
1,242
SCN
4b
2,09
2,00
1,05
6,11
ppm (t1)


151,14
130,85
128,46
120,79
111,08
77,375
77,056
76,739
33,902
23,775
ppm (t1)


7,462
7,456
7,260
1,321
SCN
4c
4,07
9,00
ppm (t1)
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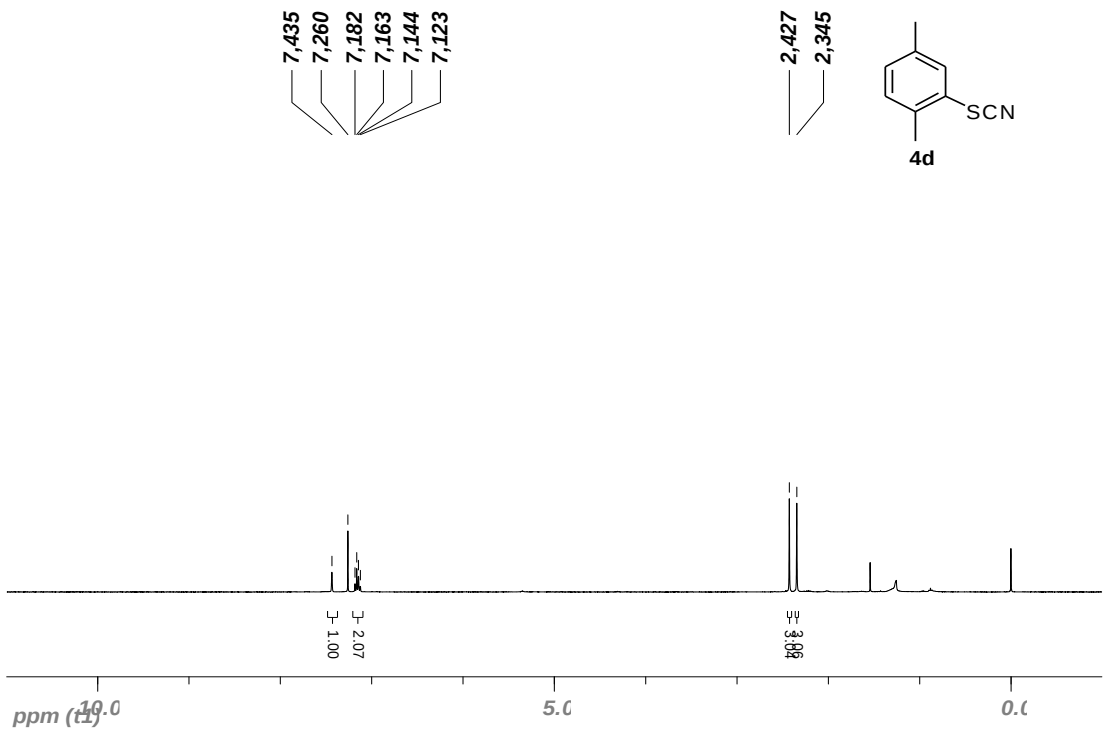
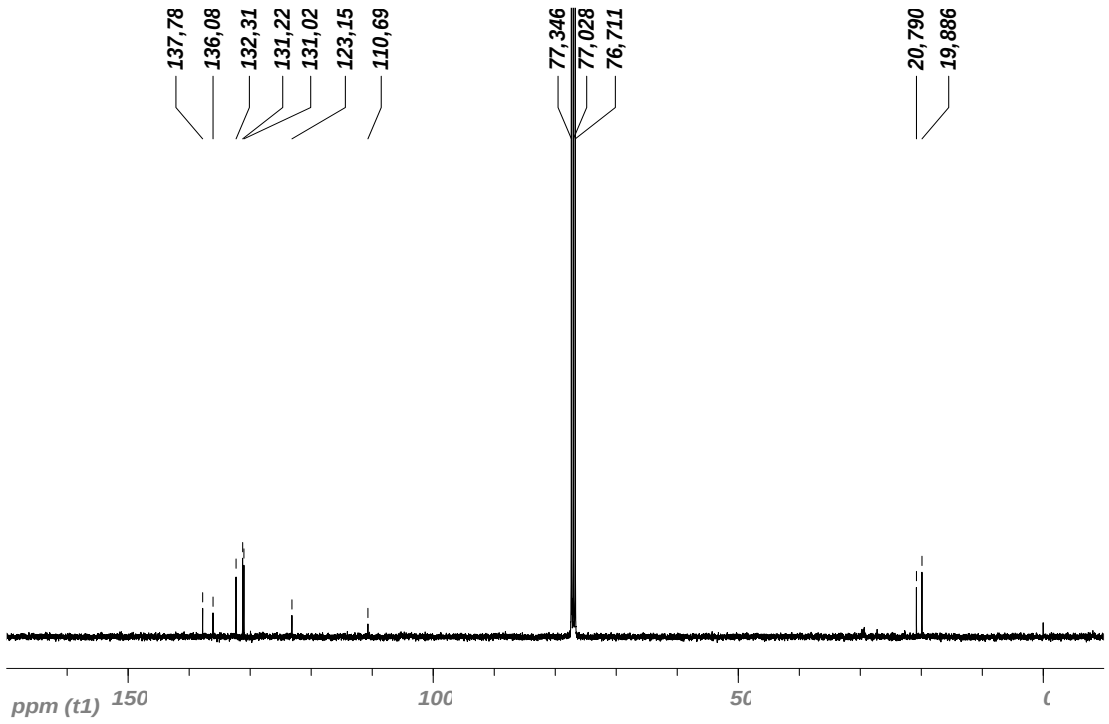
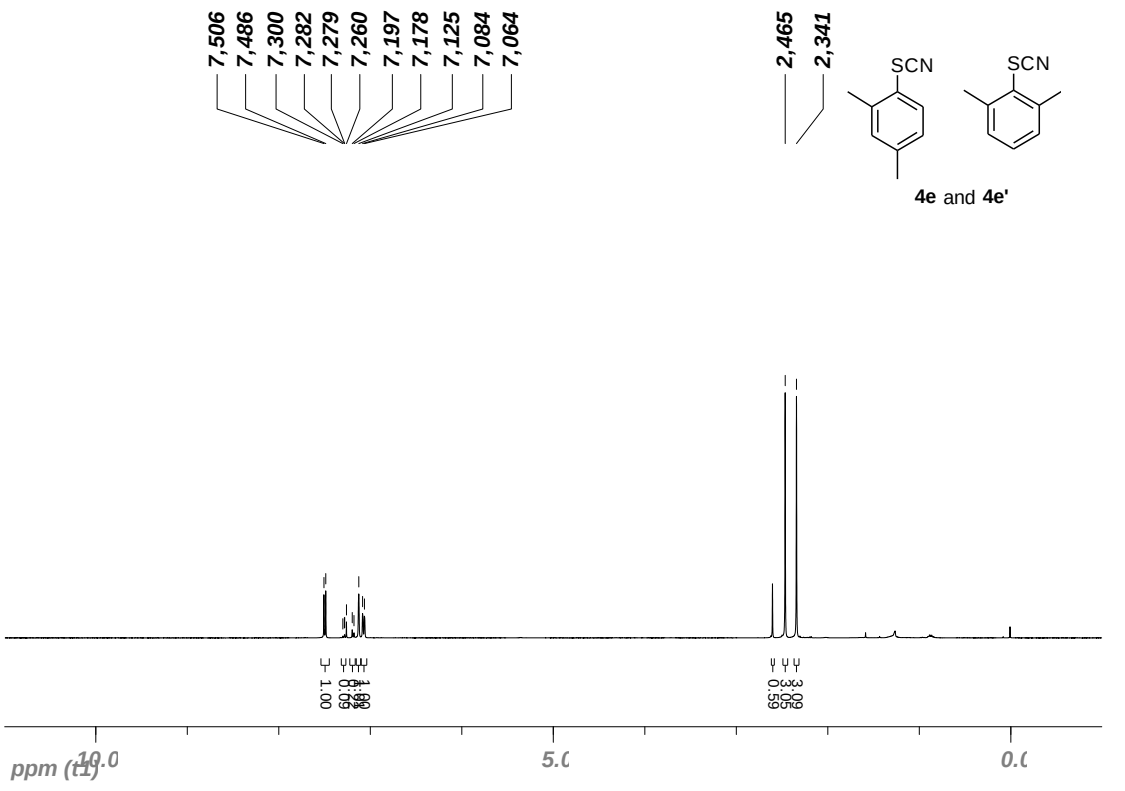
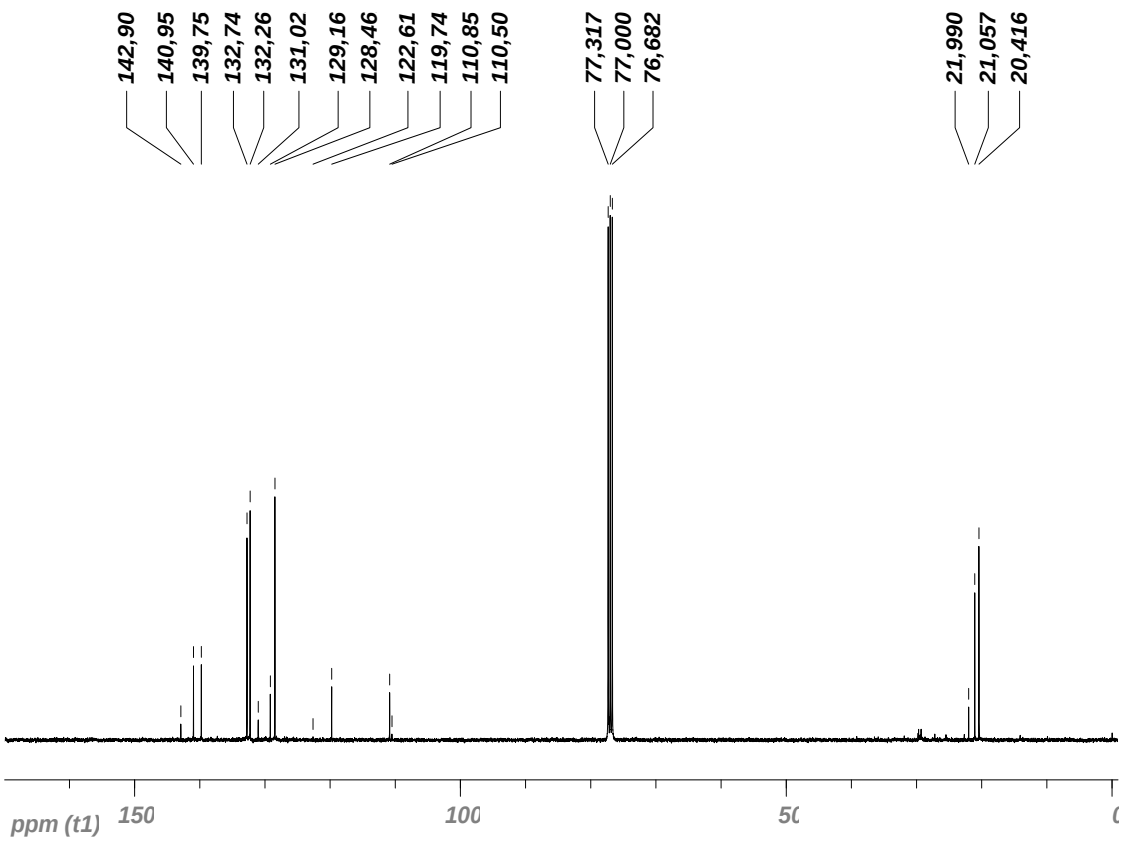
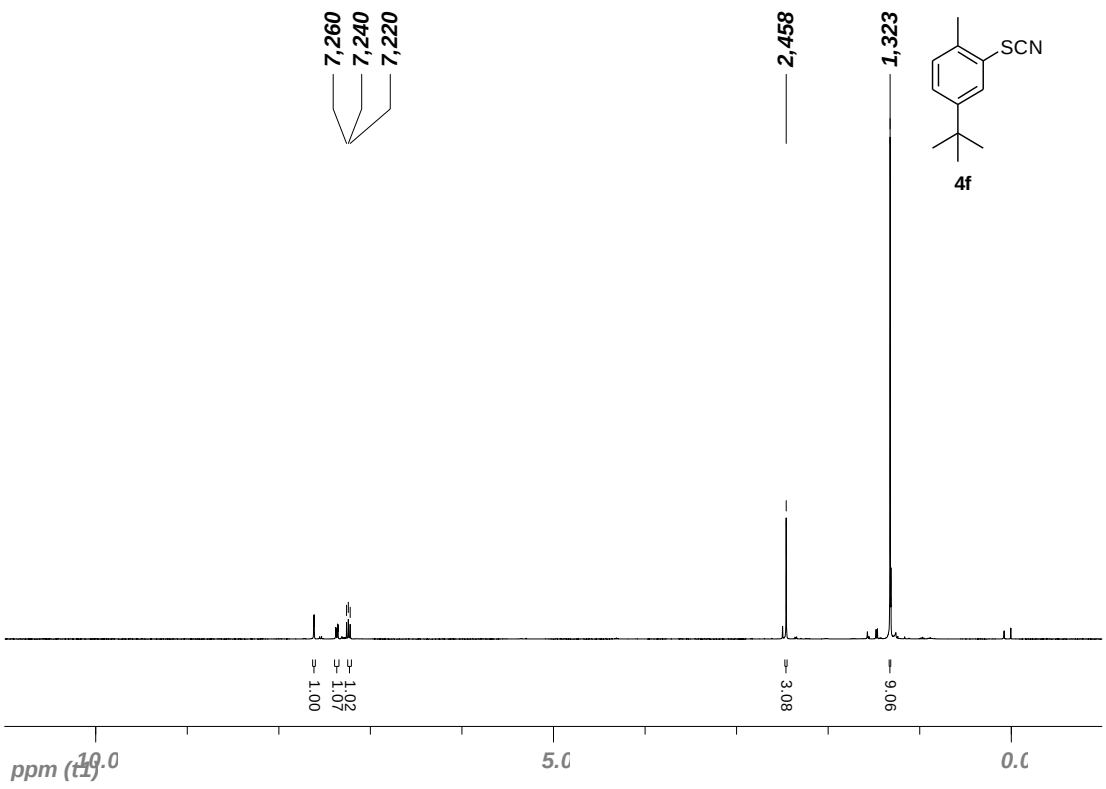
130,48
127,38
120,59
111,03
34,838
31,137
ppm (t1)

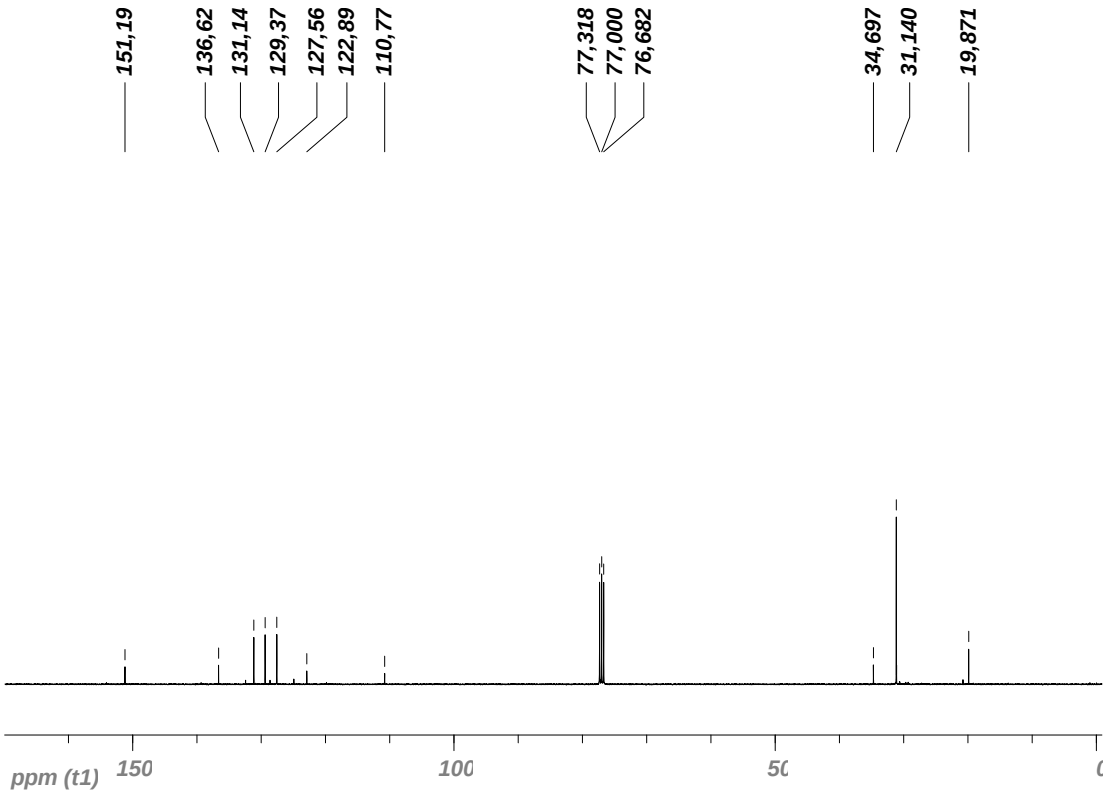

7,435
7,260
7,182
7,163
7,144
7,123
2,427
2,345
SCN
4d
1.00
2.07
3.06
3.04
ppm (t1)

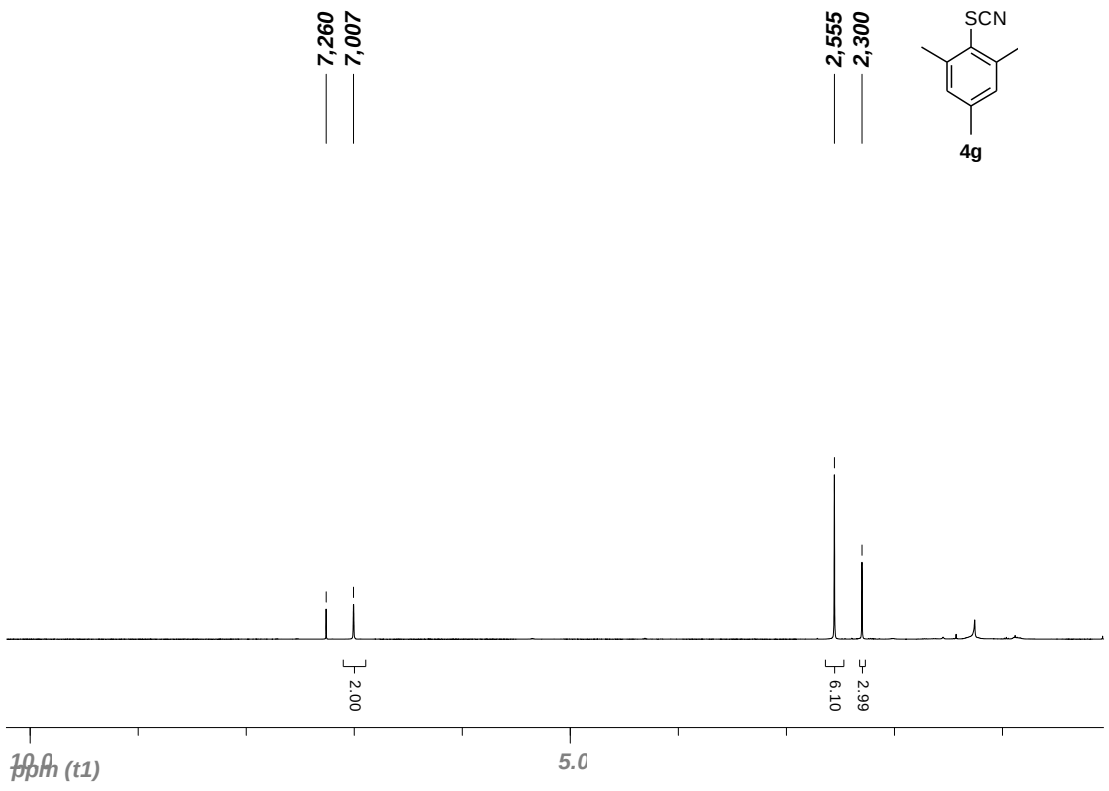

137,78
136,08
132,31
131,22
131,02
123,15
110,69
77,346
77,028
76,711
20,790
19,886
ppm (t1)

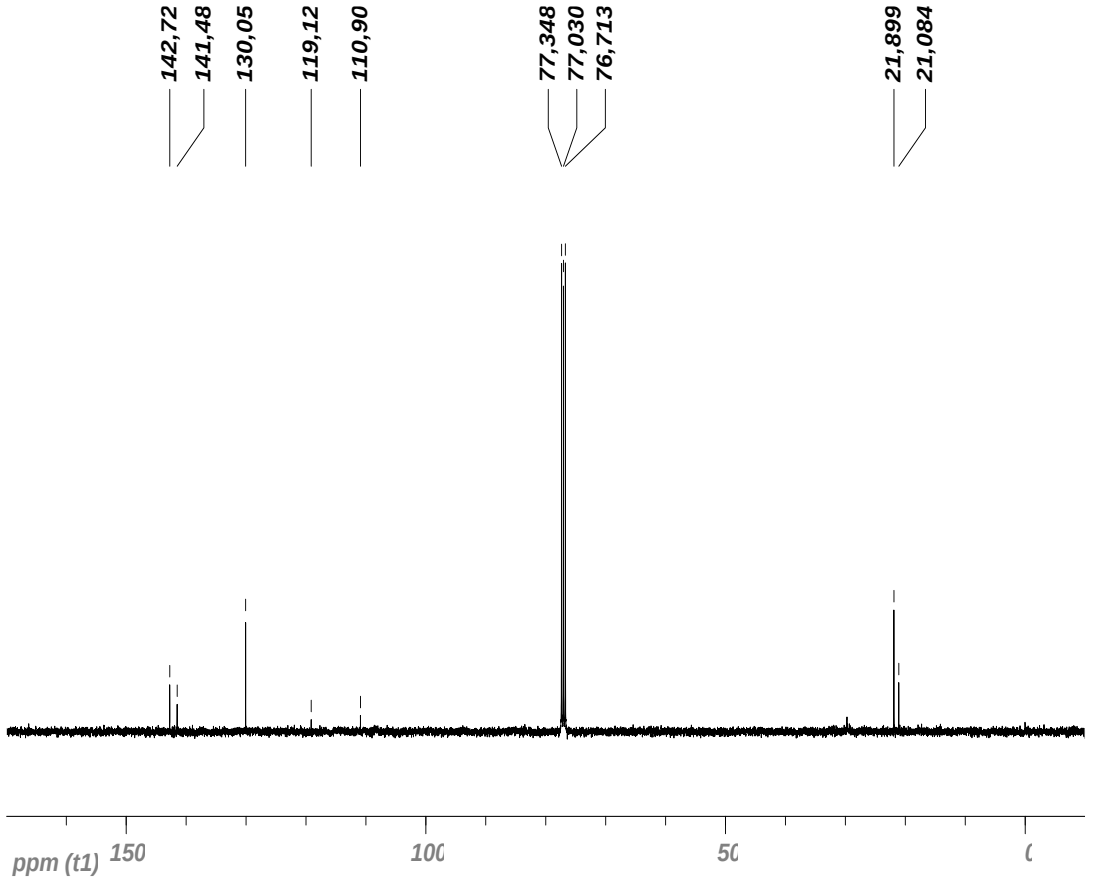

7,506
7,486
7,300
7,282
7,279
7,260
7,197
7,178
7,125
7,084
7,064
2,465
2,341
SCN
SCN
4e and 4e'
1,00
0,69
3,05
0,59
ppm (t1)

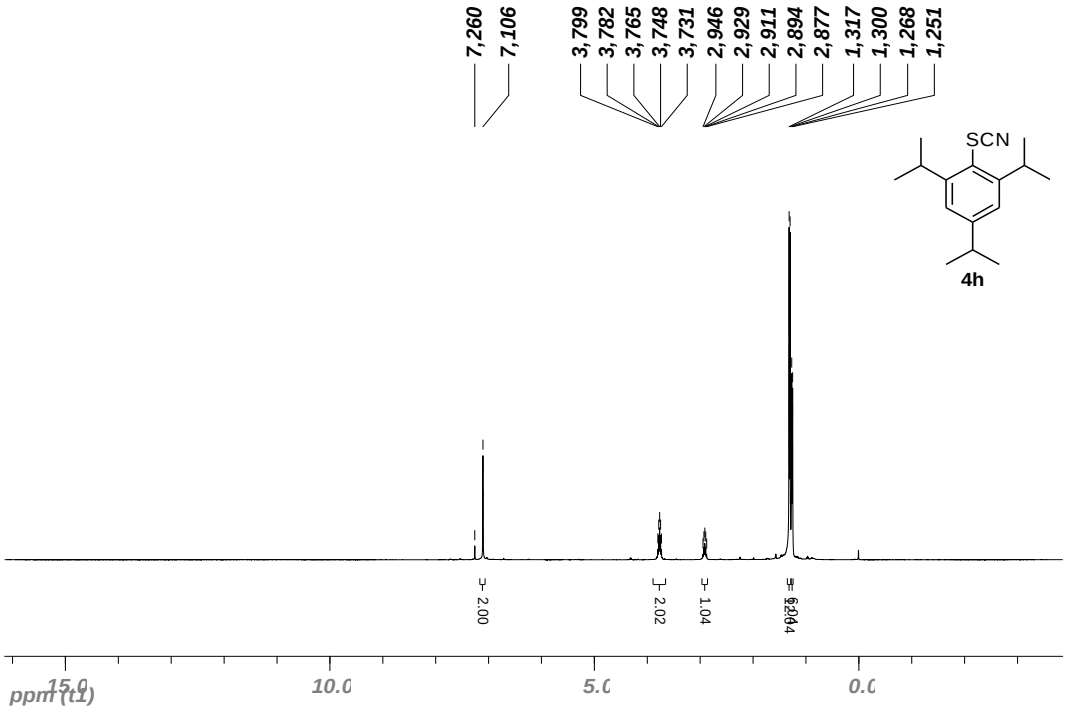

142,90
140,95
139,75
132,74
132,26
131,02
129,16
128,46
122,61
119,74
110,85
110,50
77,317
77,000
76,682
21,990
21,057
20,416
ppm (t1)
150
100
50

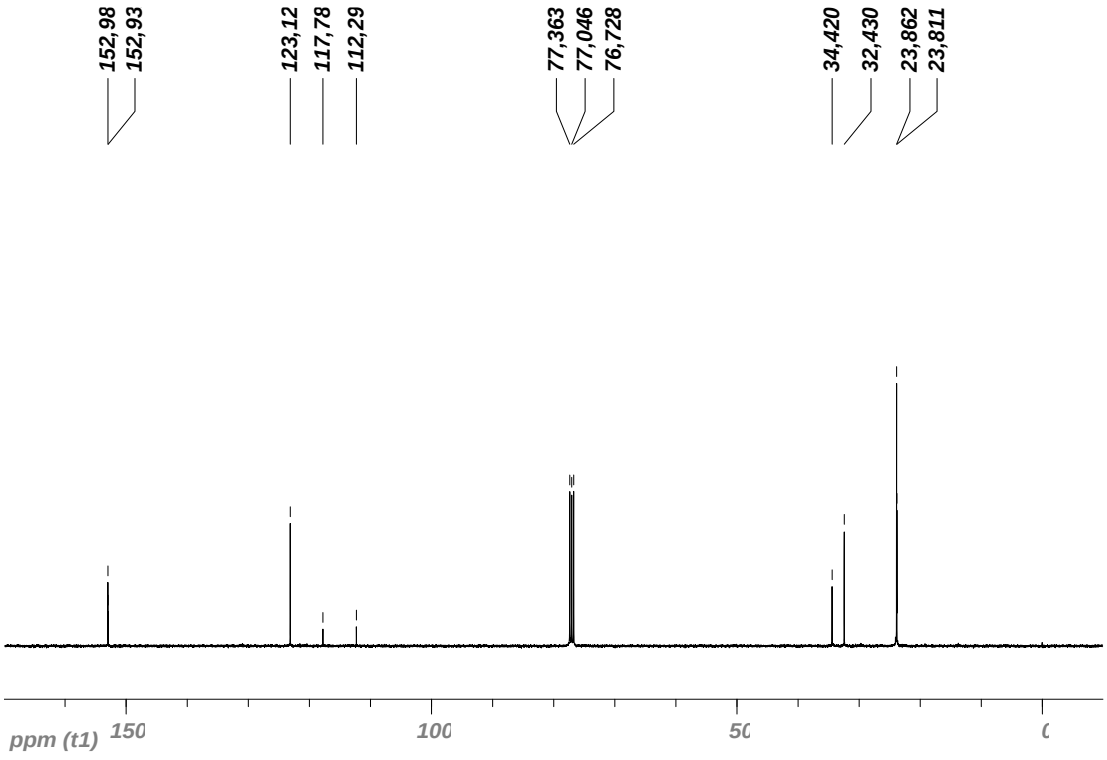

7,260
7,240
7,220
2,458
1,323
SCN
4f
1,00
1,07
1,02
3,08
9,06
ppm (t1)


151,19
136,62
131,14
129,37
127,56
122,89
110,77
77,318
77,000
76,682
34,697
31,140
19,871
ppm (t1)


7,260
7,007
2,555
2,300
SCN
4g
2.00
6.10
2.99
10.0
5.0
ppm (t1)


142,72
141,48
130,05
119,12
110,90
77,348
77,030
76,713
21,899
21,084
150
100
50
ppm (t1)


7,260
7,106
3,799
3,782
3,765
3,748
3,731
2,946
2,929
2,911
2,894
2,877
1,317
1,300
1,268
1,251
SCN
4h
2.00
2.02
1.04
6.04
ppm (t1)


152,98
152,93
123,12
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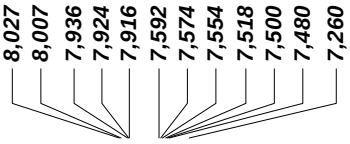
112,29
77,363
77,046
76,728
34,420
32,430
23,862
23,811
ppm (t1)


8,027
8,007
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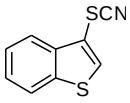
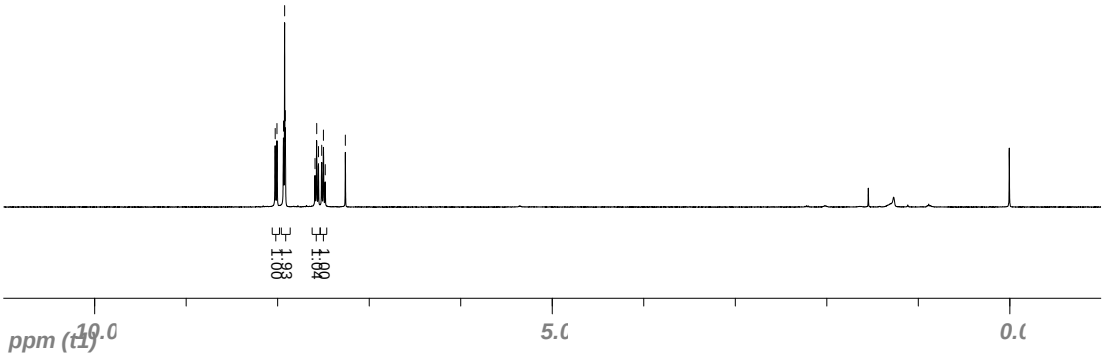
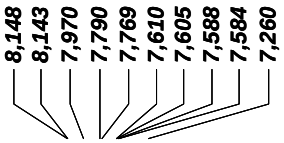
7,924
7,916
7,592
7,574
7,554
7,518
7,500
7,480
7,260


SCN
S

4i


1.93
1.00
ppm (t1)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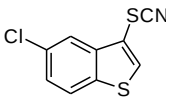
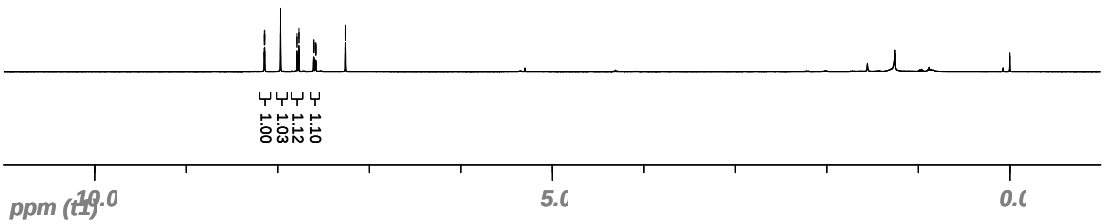
8,143
7,970
7,790
7,769
7,610
7,605
7,588
7,584
7,260


SCN
Cl
S

4j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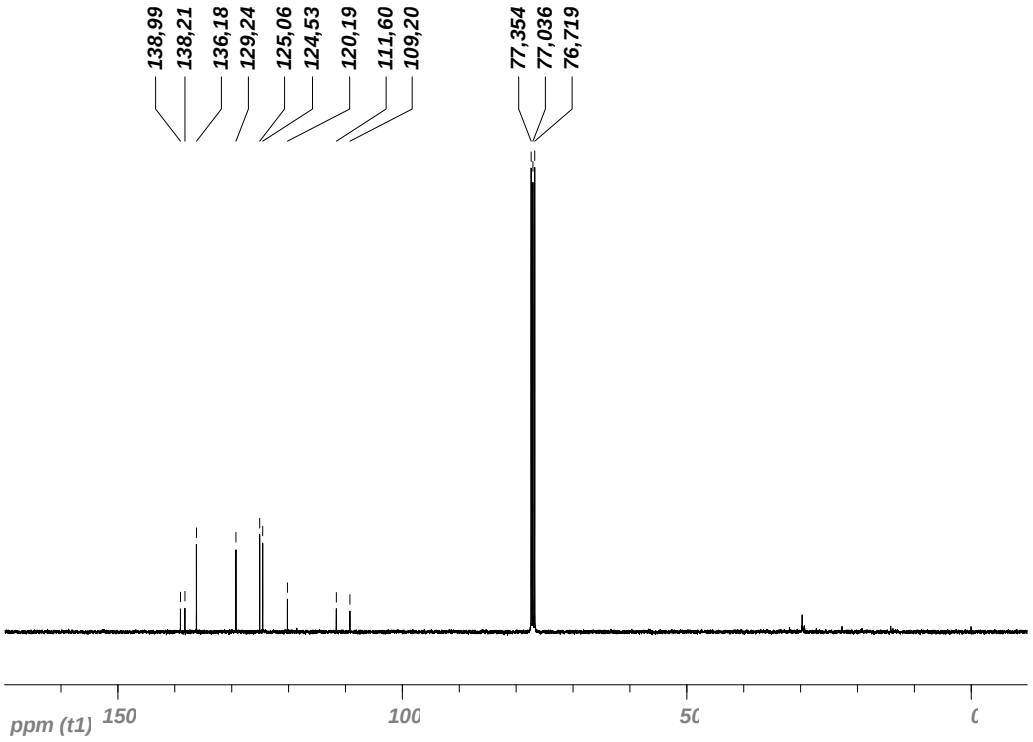
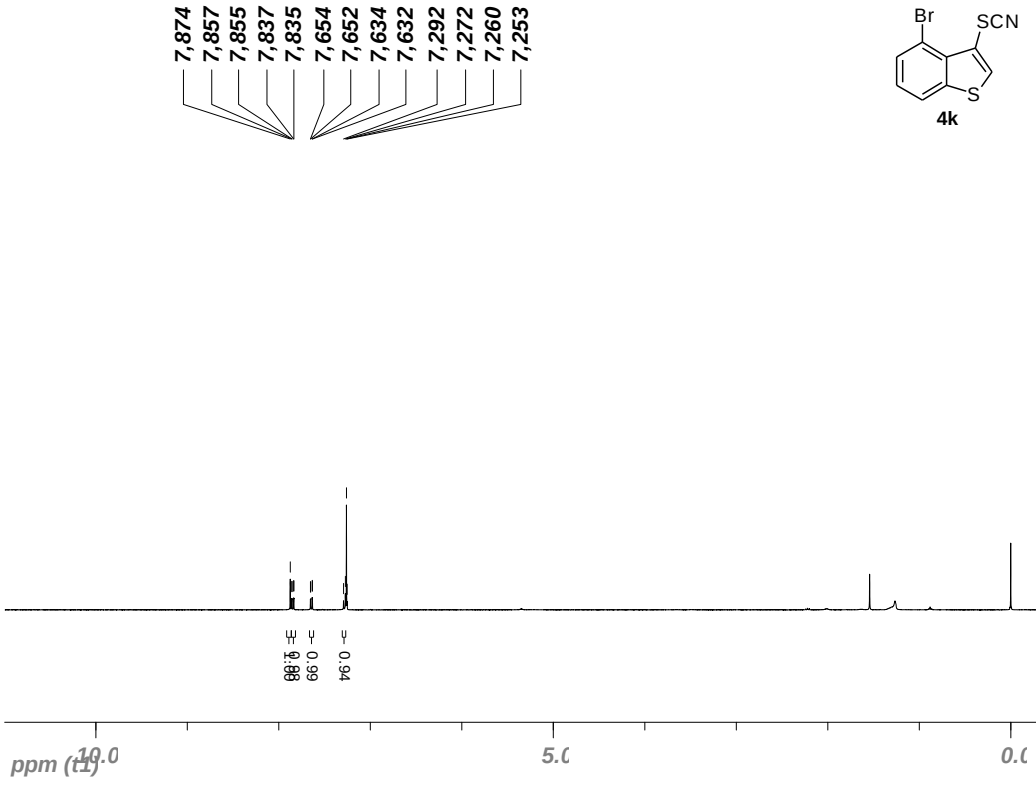
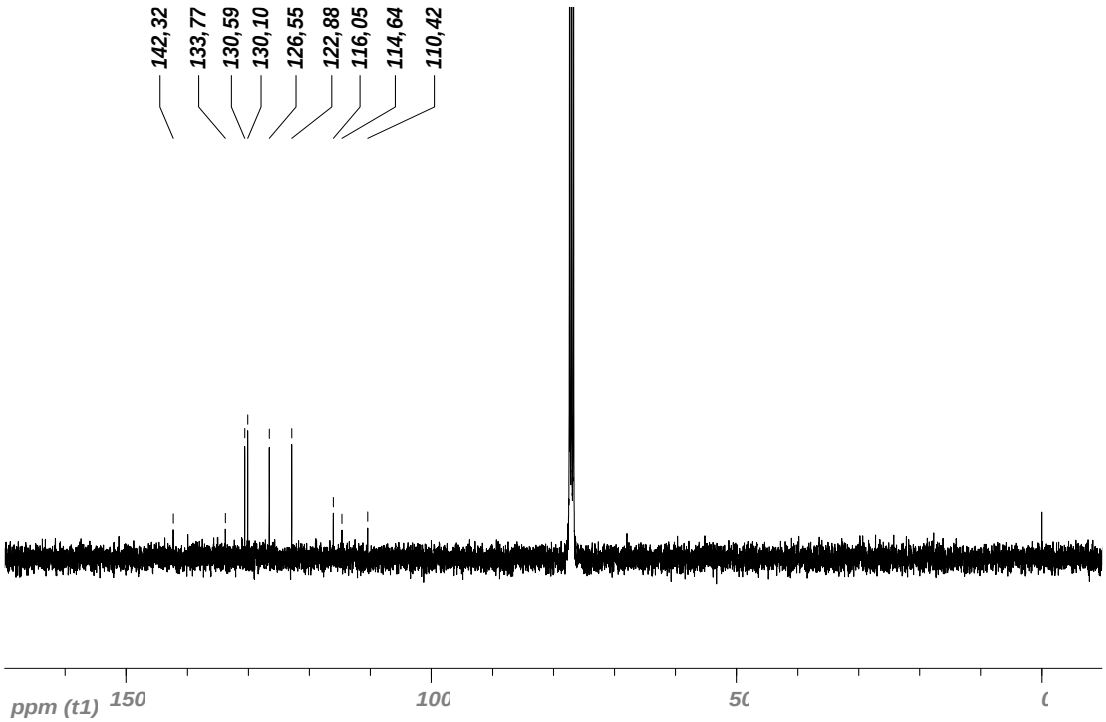
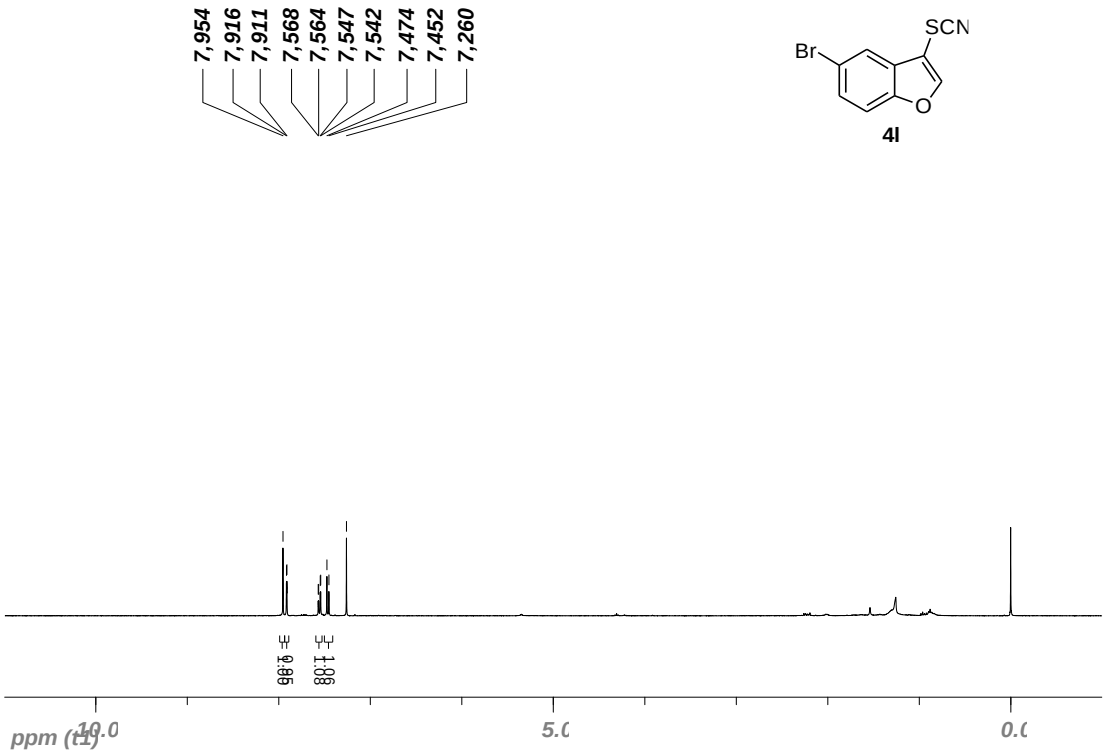
1.03
1.12
1.10
ppm (t1)


138,99
138,21
136,18
129,24
125,06
124,53
120,19
111,60
109,20
77,354
77,036
76,719
ppm (t1)
150
100
50
0

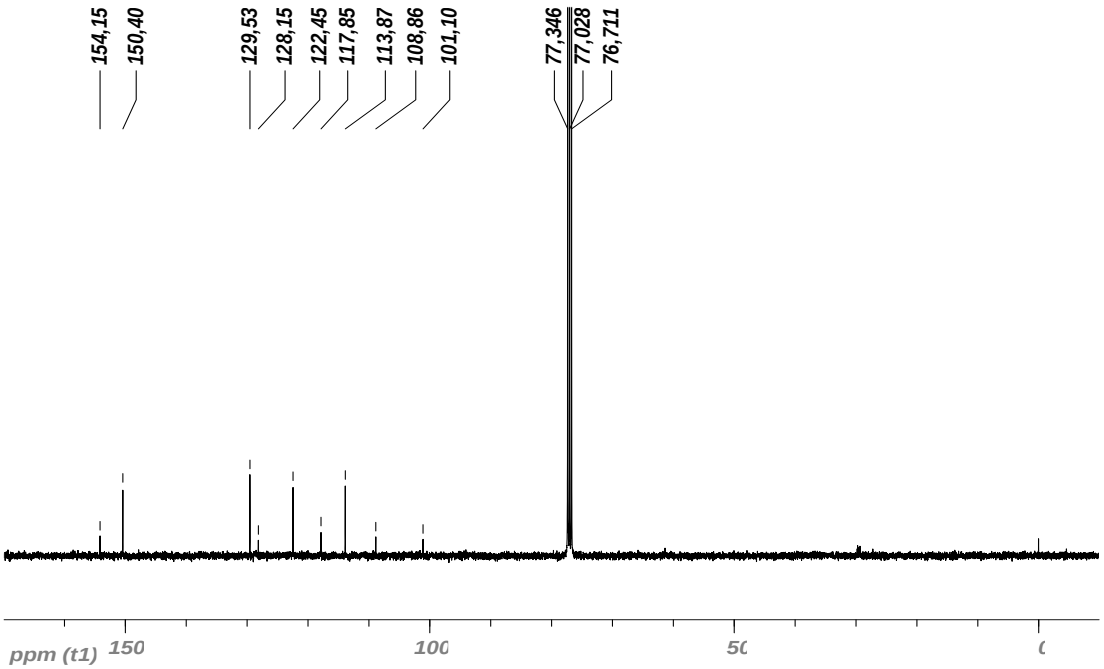

7,874
7,857
7,855
7,837
7,835
7,654
7,652
7,634
7,632
7,292
7,272
7,260
7,253
Br
SCN
S
4k
1,00
0,99
0,94
10.0
5.0
0.0
ppm (t1)

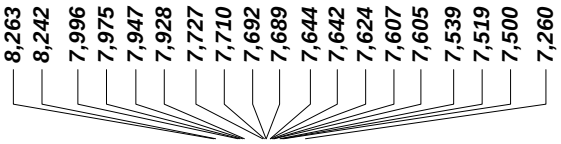

142,32
133,77
130,59
130,10
126,55
122,88
116,05
114,64
110,42
ppm (t1)
150
100
50
0


7,954
7,916
7,911
7,568
7,564
7,547
7,542
7,474
7,452
7,260
ppm (t1)
10.0
5.0
0.0

SCN
Br
O

4l


154,15
150,40
129,53
128,15
122,45
117,85
113,87
108,86
101,10
77,346
77,028
76,711
ppm (t1)
150
100
50


8,263
8,242
7,996
7,975
7,947
7,928
7,727
7,710
7,692
7,689
7,644
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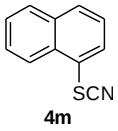
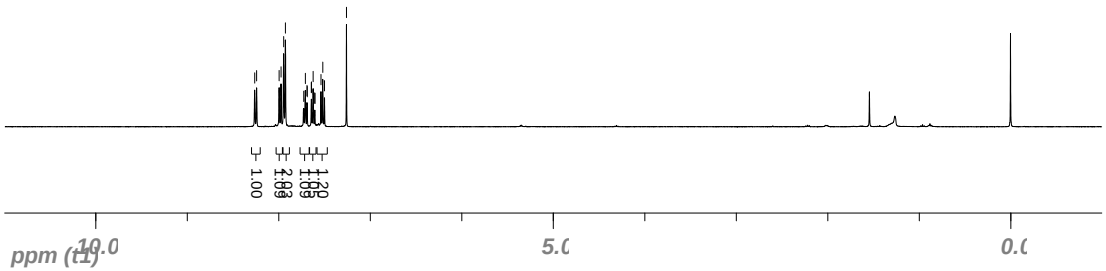
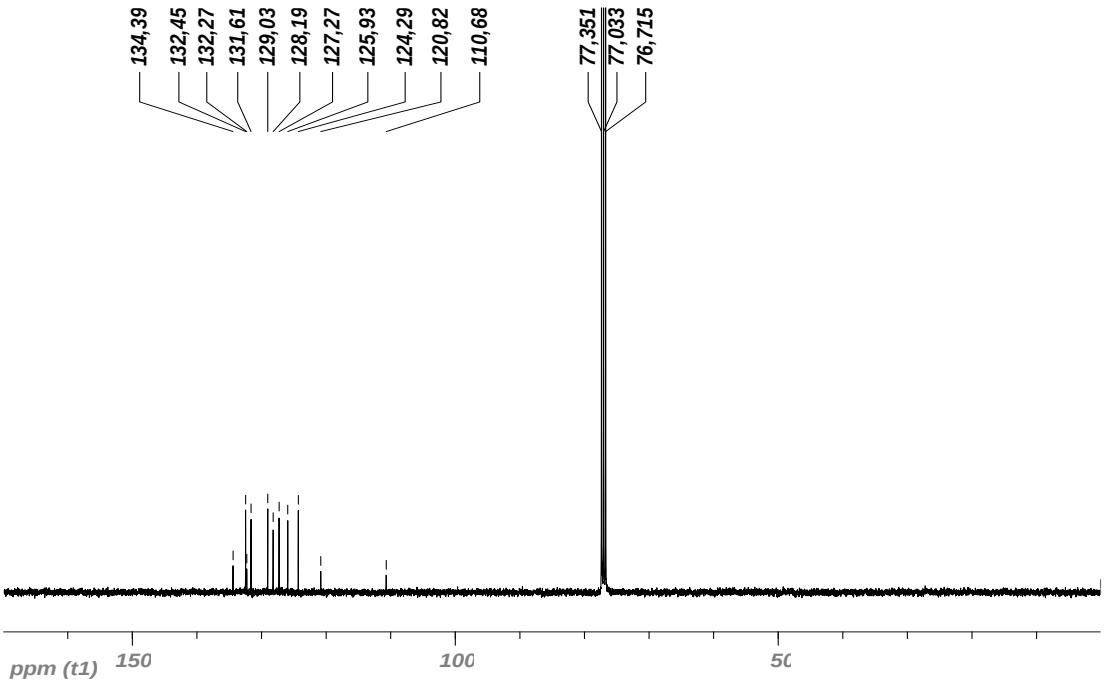
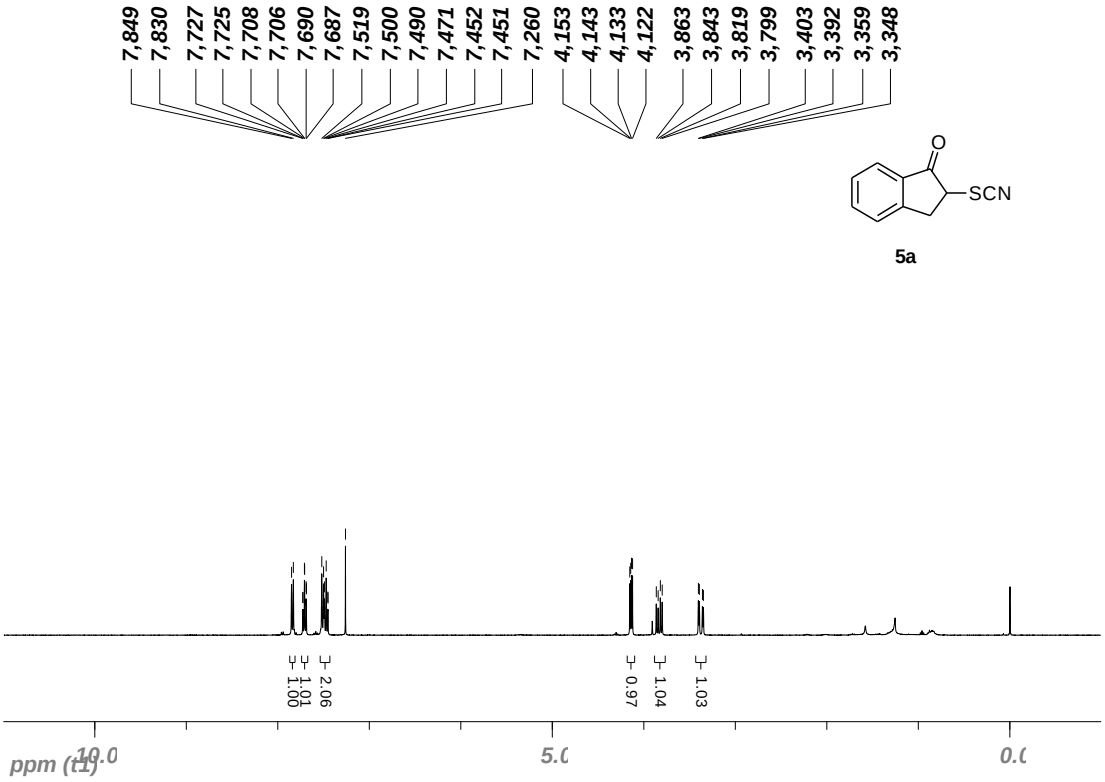
7,624
7,607
7,605
7,539
7,519
7,500
7,260


SCN

4m


1.00
2.09
1.89
1.20
ppm (t1)
10.0
5.0
0.0


134,39
132,45
132,27
131,61
129,03
128,19
127,27
125,93
124,29
120,82
110,68
77,351
77,033
76,715
ppm (t1)
150
100
50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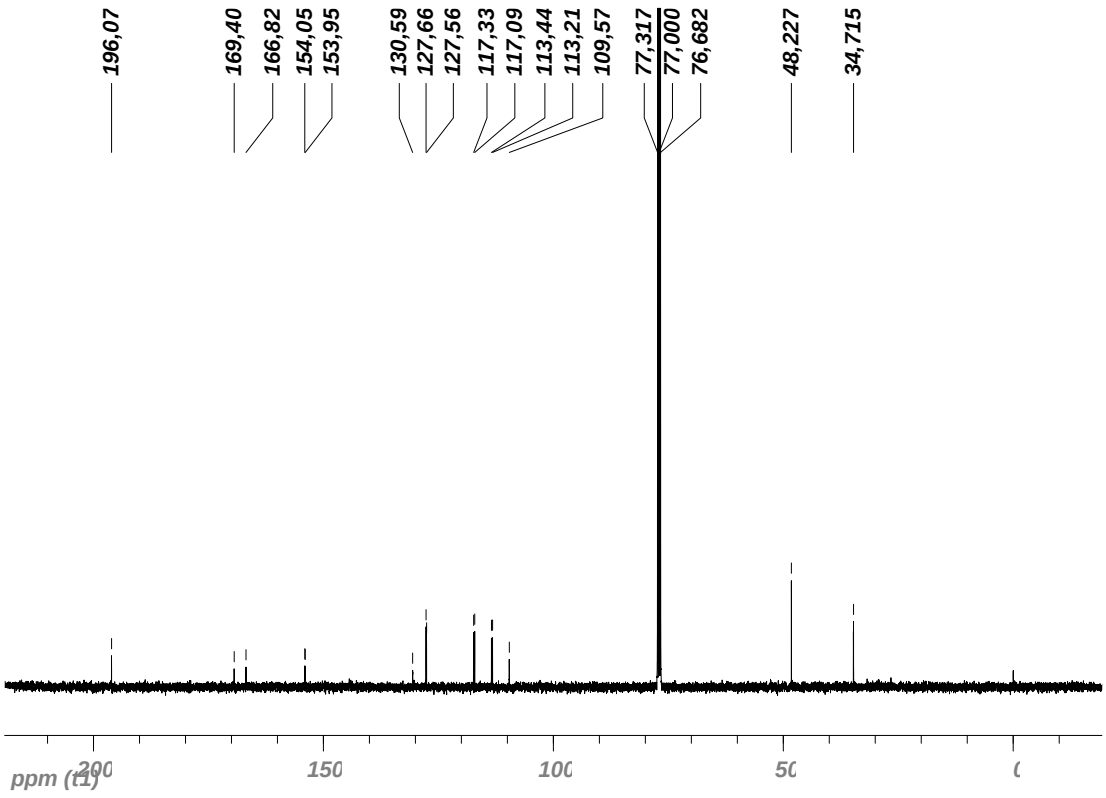
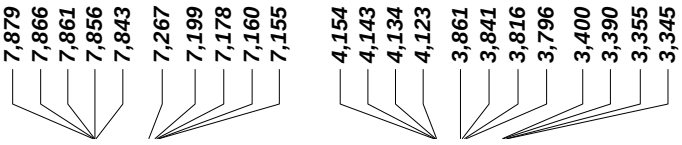
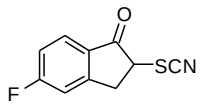
7,830
7,727
7,725
7,708
7,706
7,690
7,687
7,519
7,500
7,490
7,471
7,452
7,451
7,260
4,153
4,143
4,133
4,122
3,863
3,843
3,819
3,799
3,403
3,392
3,359
3,348
O
SCN
1.00
1.01
2.06
0.97
1.04
1.03
ppm (t1)
10.0
5.0
0.0

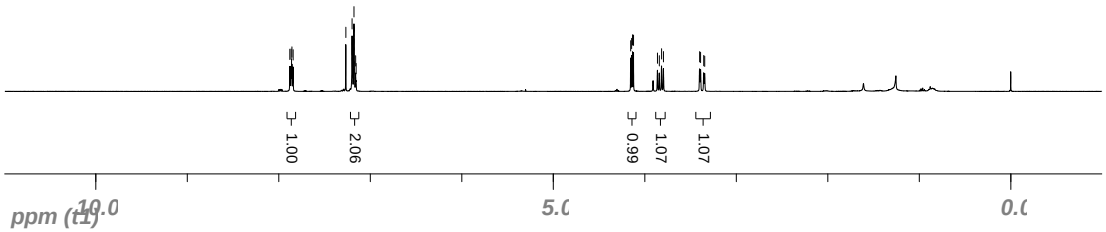
5a

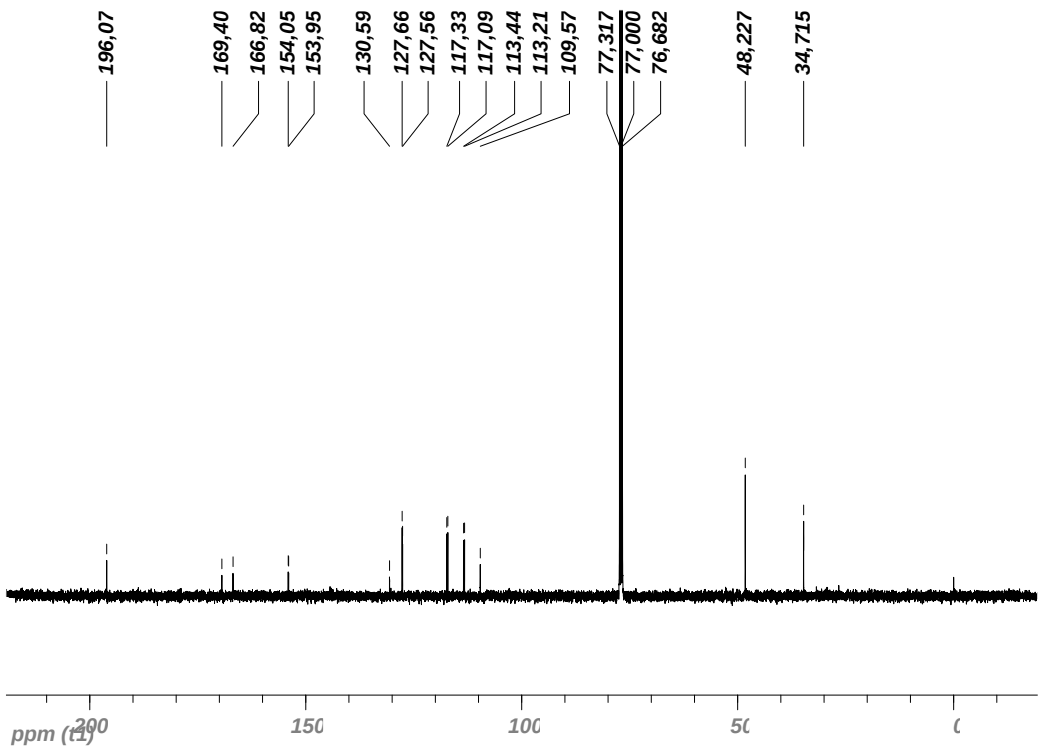

196,07
169,40
166,82
154,05
153,95
130,59
127,66
127,56
117,33
117,09
113,44
113,21
109,57
77,317
77,000
76,682
48,227
34,715
ppm (t1)

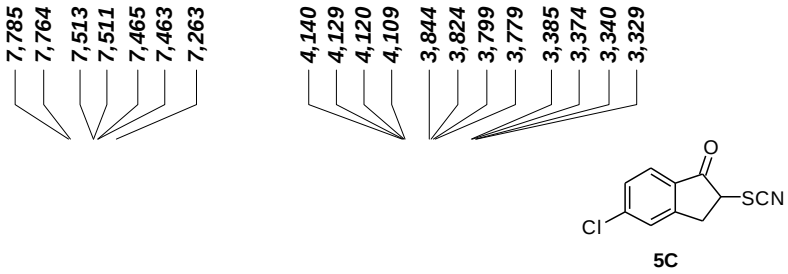

7,879
7,866
7,861
7,856
7,843
7,267
7,199
7,178
7,160
7,155
4,154
4,143
4,134
4,123
3,861
3,841
3,816
3,796
3,400
3,390
3,355
3,345


O
SCN
F

5b

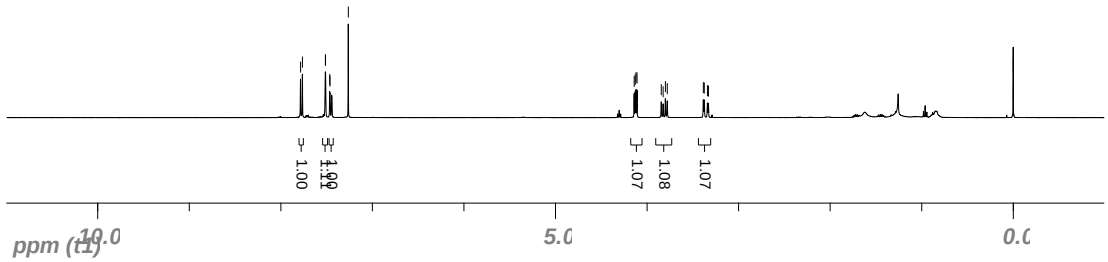

1.00
2.06
0.99
1.07
1.07
ppm (t1)

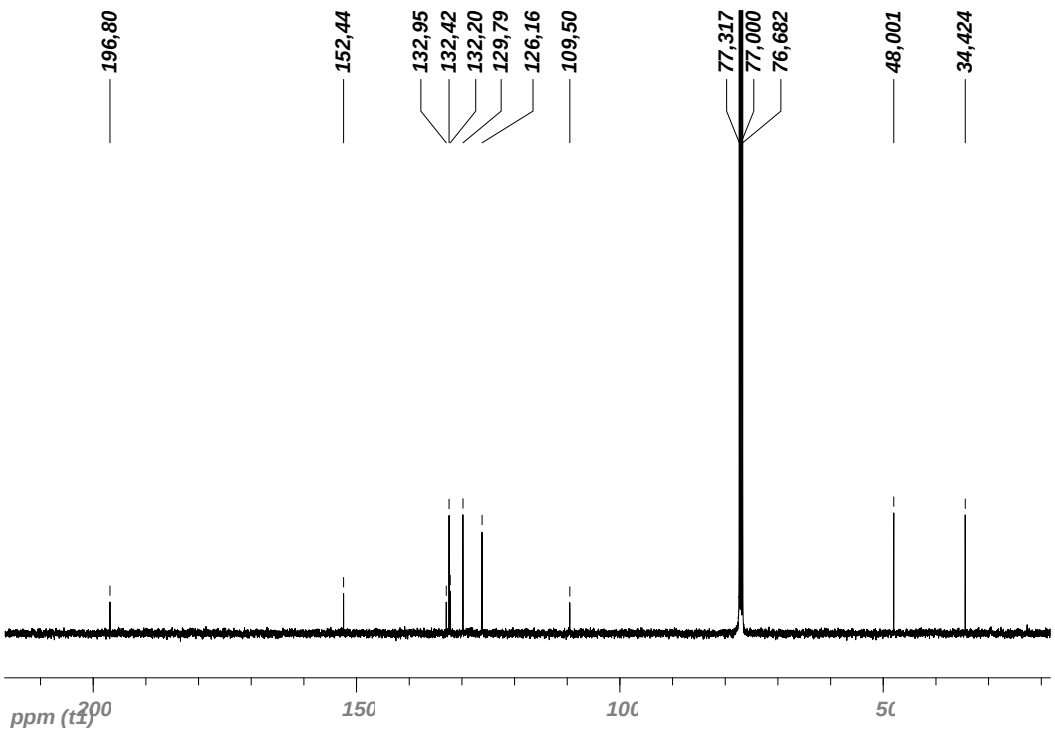

196,07
169,40
166,82
154,05
153,95
130,59
127,66
127,56
117,33
117,09
113,44
113,21
109,57
77,317
77,000
76,682
48,227
34,715
ppm (t1)

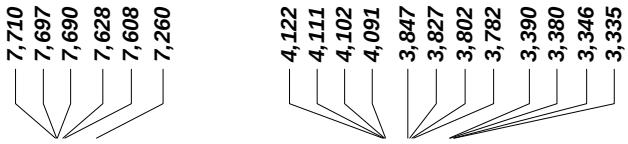

7,785
7,764
7,513
7,511
7,465
7,463
7,263
4,140
4,129
4,120
4,109
3,844
3,824
3,799
3,779
3,385
3,374
3,340
3,329

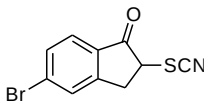
O
SCN
Cl

5C

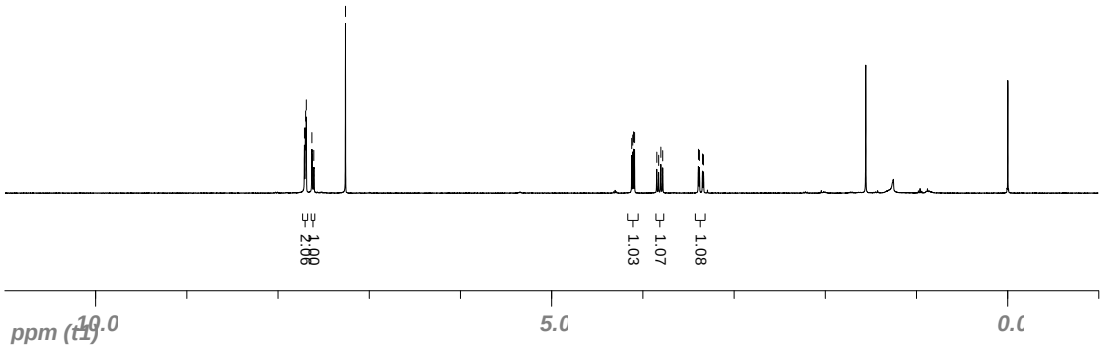

1.00
1.07
1.08
1.07
ppm (t1)

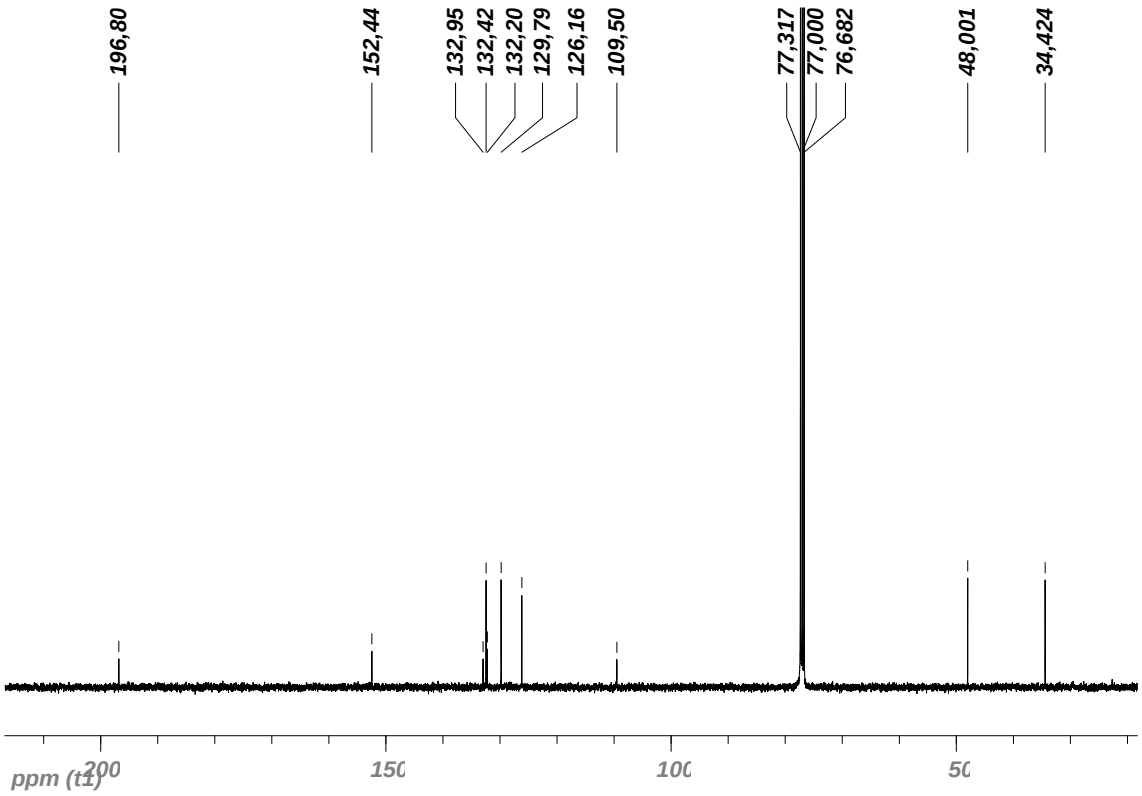

196,80
152,44
132,95
132,42
132,20
129,79
126,16
109,50
77,317
77,000
76,682
48,001
34,424
ppm (t1)

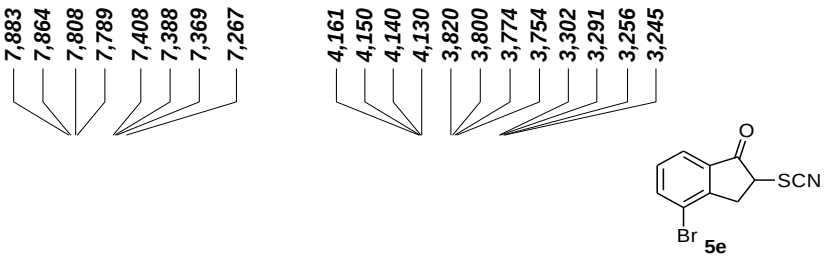

7,710
7,697
7,690
7,628
7,608
7,260
4,122
4,111
4,102
4,091
3,847
3,827
3,802
3,782
3,390
3,380
3,346
3,335


O
SCN
Br

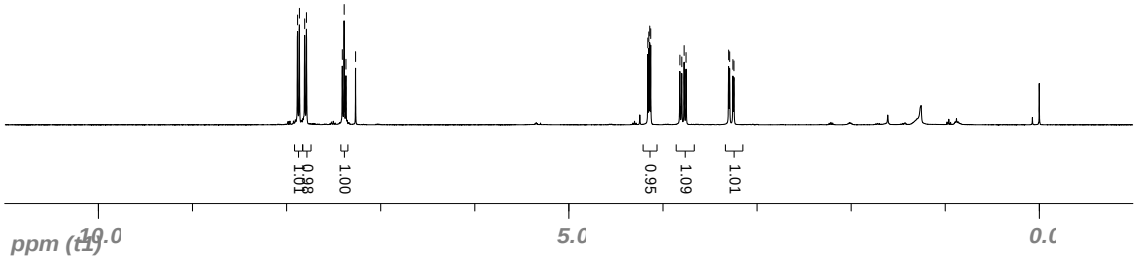
5d

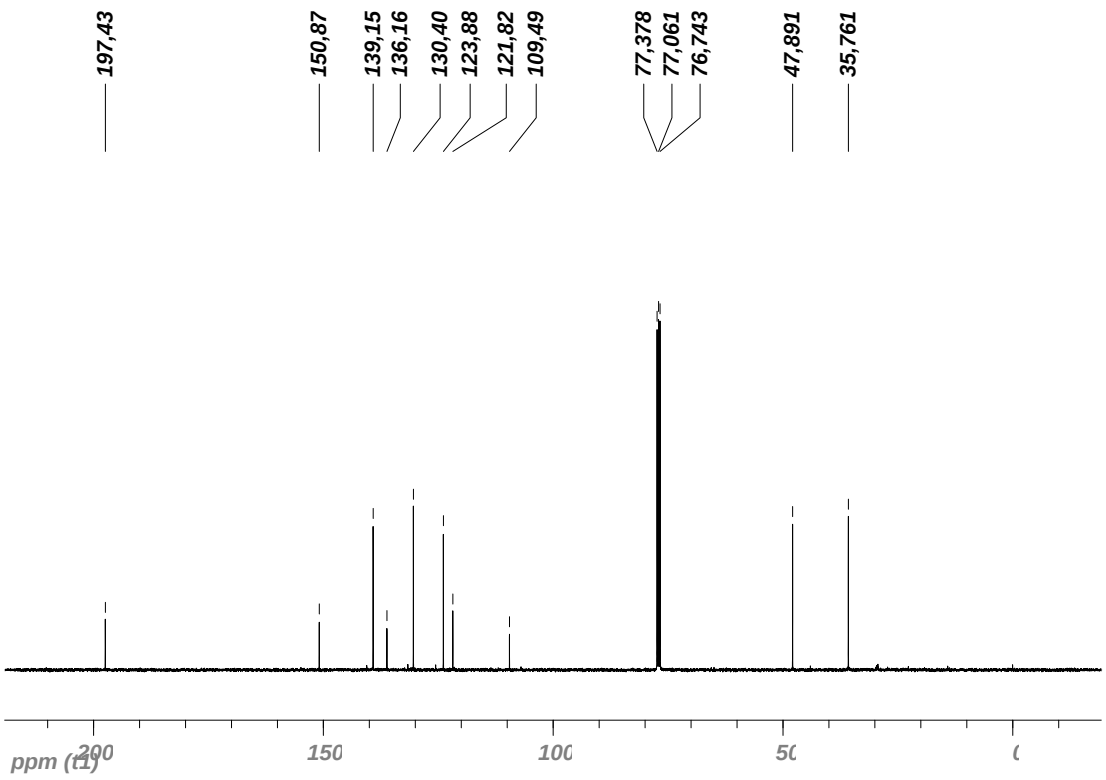

2.00
1.03
1.07
1.08
ppm (t1)

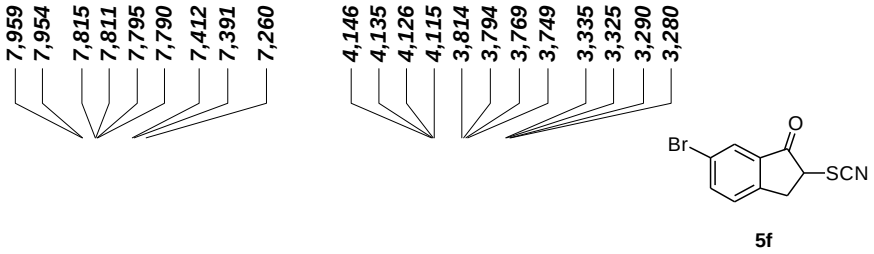

196,80
152,44
132,95
132,42
132,20
129,79
126,16
109,50
77,317
77,000
76,682
48,001
34,424
ppm (t1)
200
150
100
50


7,883
7,864
7,808
7,789
7,408
7,388
7,369
7,267
4,161
4,150
4,140
4,130
3,820
3,800
3,774
3,754
3,302
3,291
3,256
3,245
O
SCN
Br

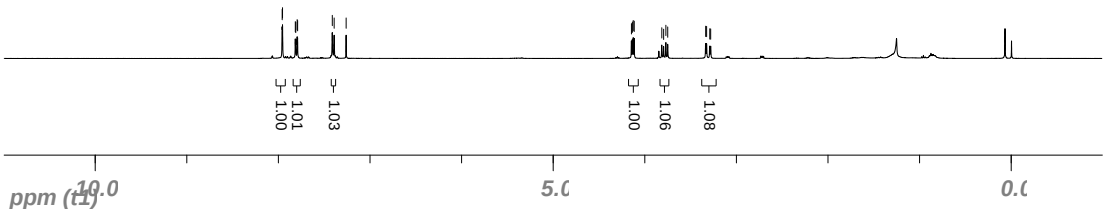
5e

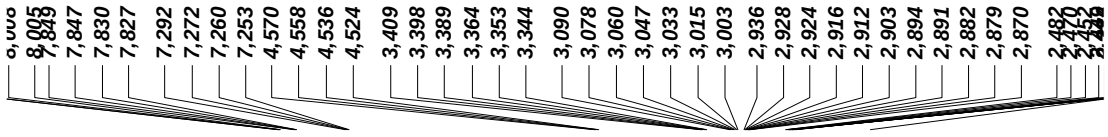

1.01
0.98
1.00
0.95
1.09
1.01
ppm (t1)
10.0
5.0
0.0

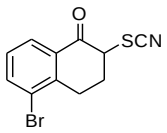

197,43
150,87
139,15
136,16
130,40
123,88
121,82
109,49
77,378
77,061
76,743
47,891
35,761
ppm (t1)


7,959
7,954
7,815
7,811
7,795
7,790
7,412
7,391
7,260
4,146
4,135
4,126
4,115
3,814
3,794
3,769
3,749
3,335
3,325
3,290
3,280
Br
O
SCN

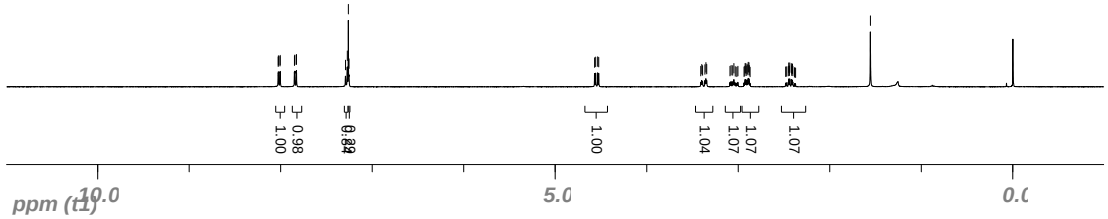
5f

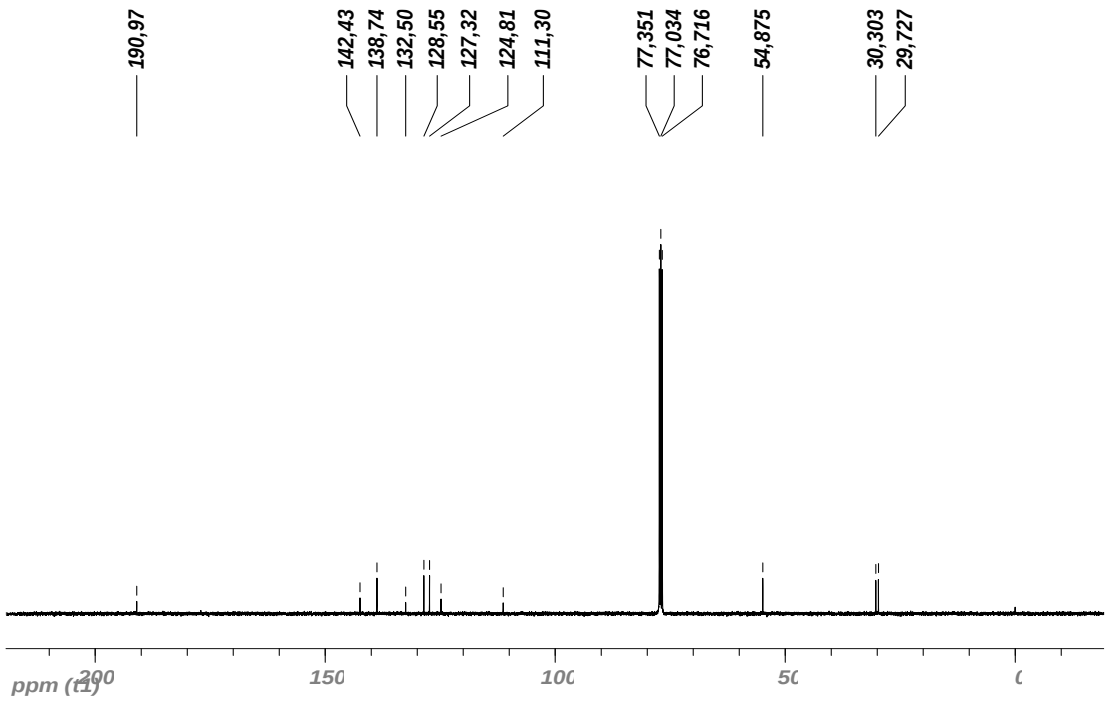

1.00
1.01
1.03
1.00
1.06
1.08
ppm (t1)

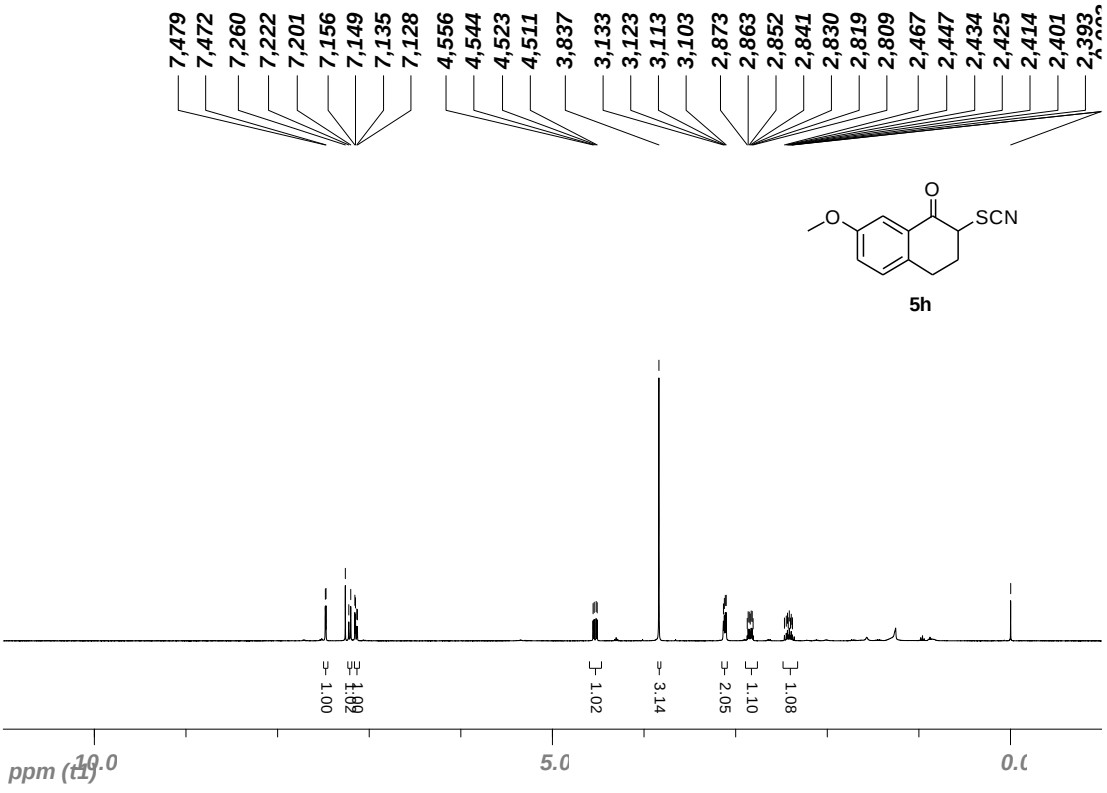



O
SCN
Br

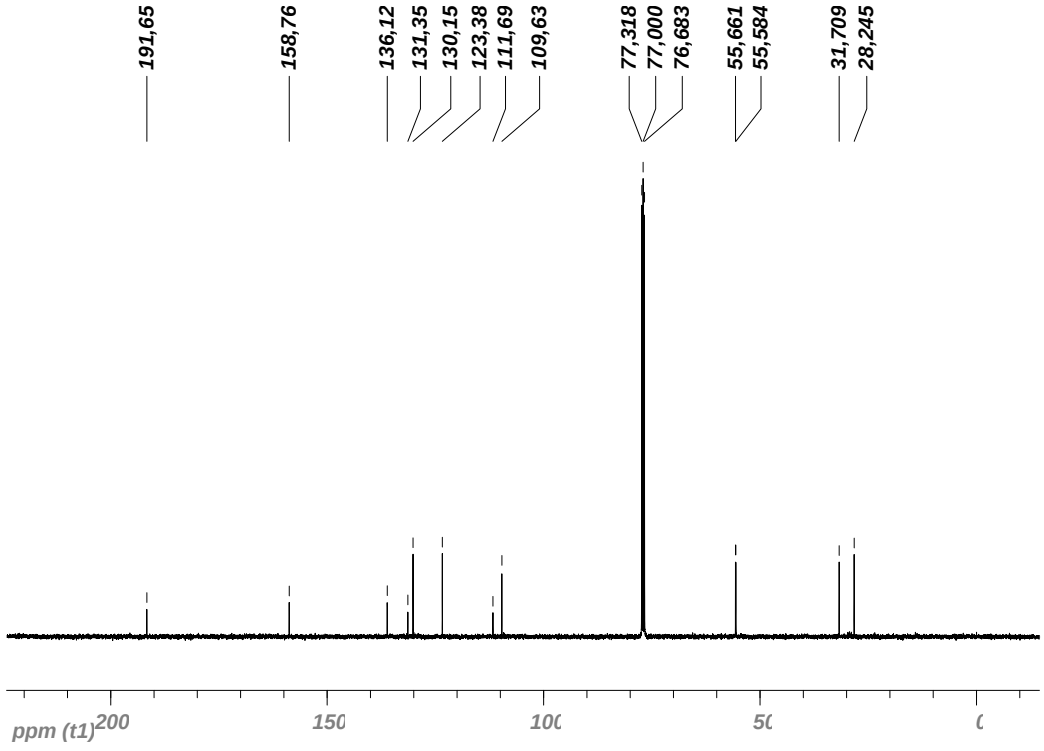
5g

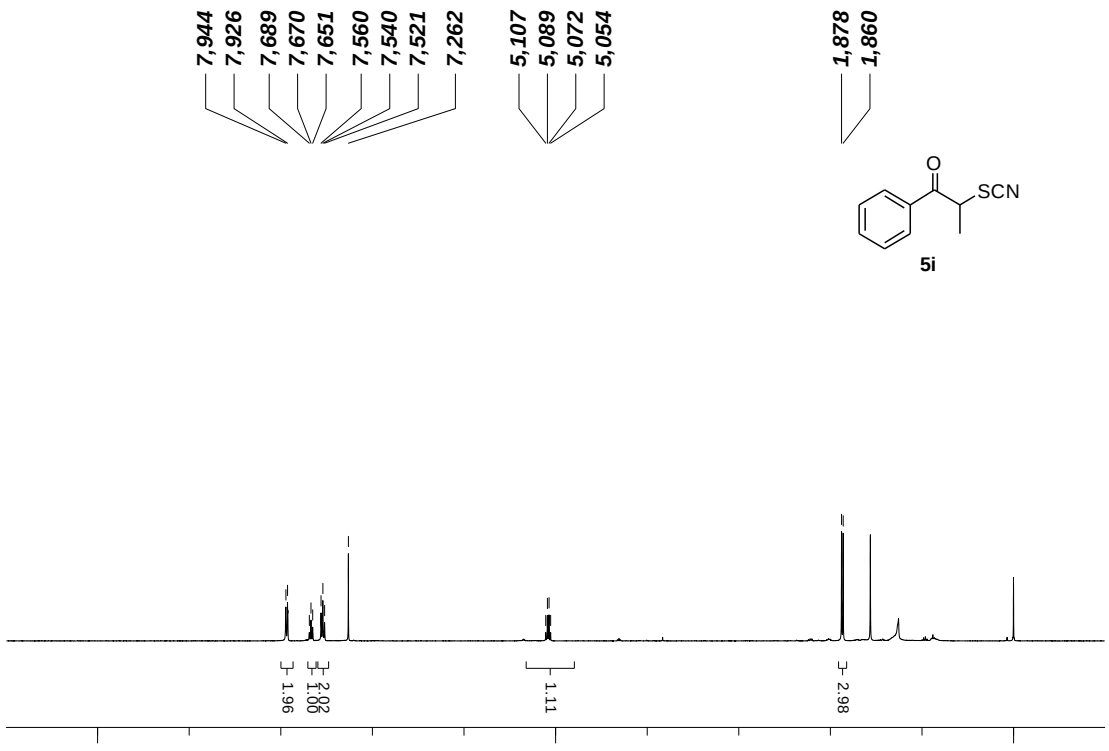

1.00
0.98
1.00
1.04
1.07
1.01
1.07
ppm (t1)

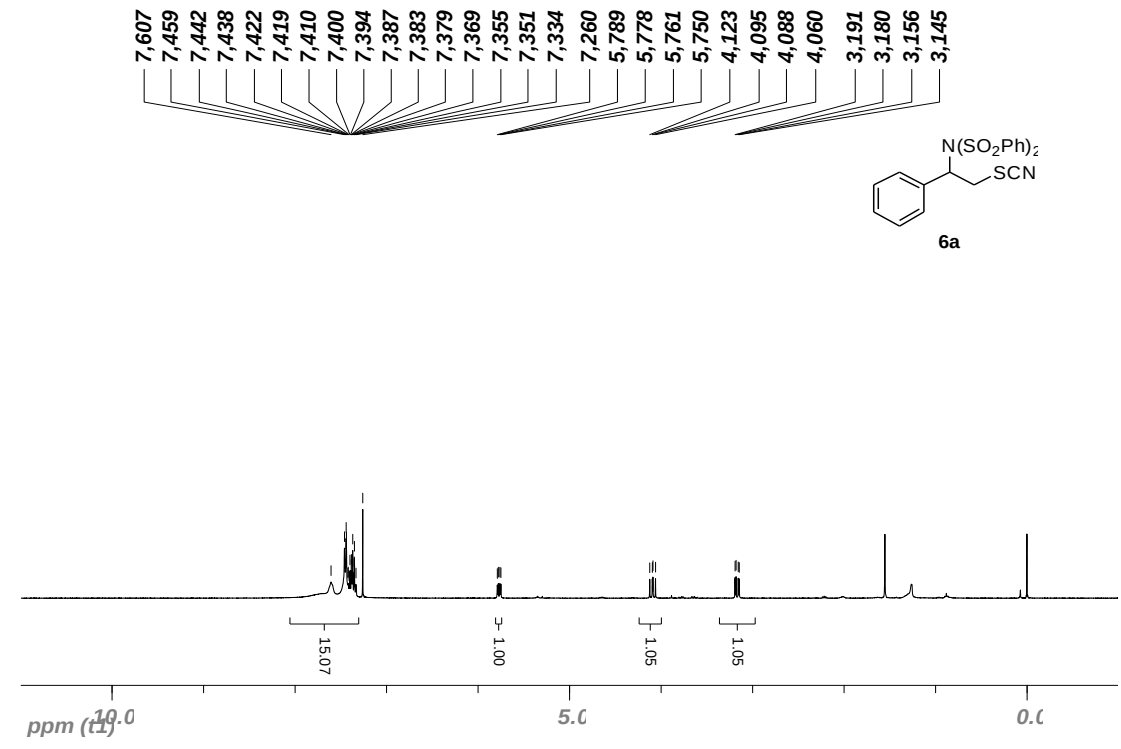

190,97
142,43
138,74
132,50
128,55
127,32
124,81
111,30
77,351
77,034
76,716
54,875
30,303
29,727
ppm (t1)

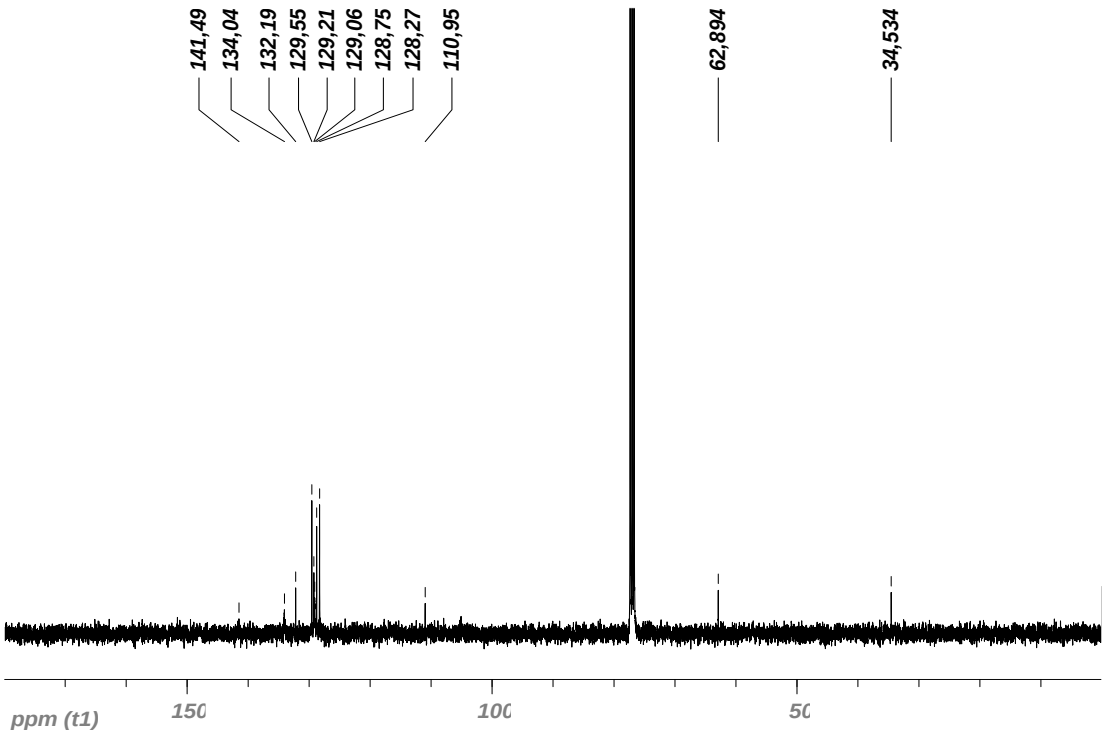

7,479
7,472
7,260
7,222
7,201
7,156
7,149
7,135
7,128
4,556
4,544
4,523
4,511
3,837
3,133
3,123
3,113
3,103
2,873
2,863
2,852
2,841
2,830
2,819
2,809
2,467
2,447
2,434
2,425
2,414
2,401
2,393
O
O
SCN
1.00
1.02
3.14
2.05
1.10
1.08
ppm (t1)
10.0
5.0
0.0

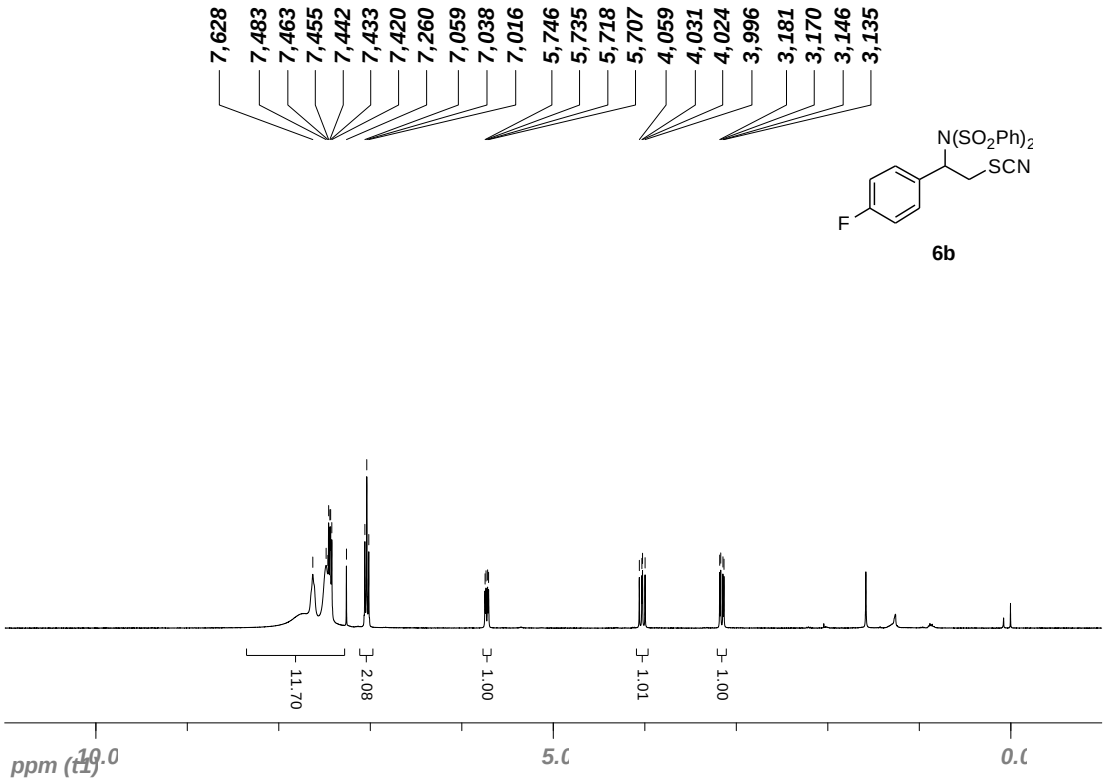
5h

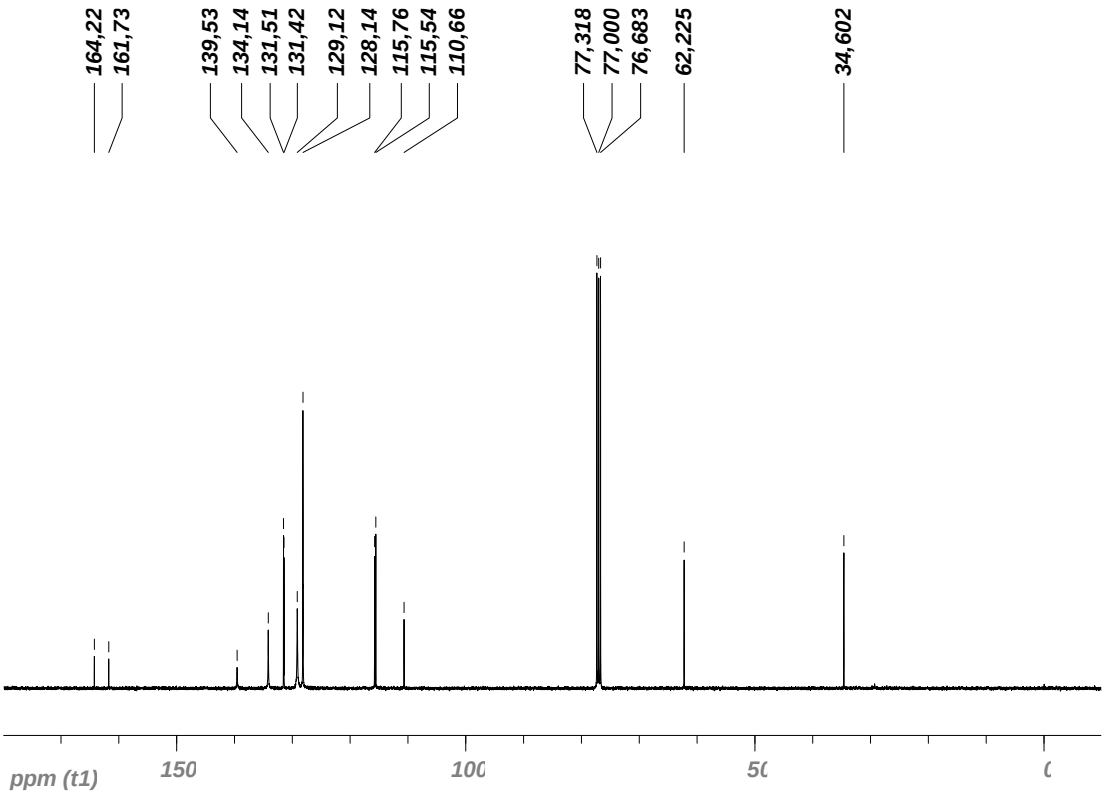

191,65
158,76
136,12
131,35
130,15
123,38
111,69
109,63
77,318
77,000
76,683
55,661
55,584
31,709
28,245
ppm (t1)
200
150
100
50
0

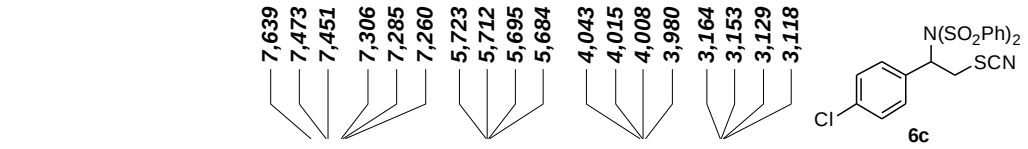

7,944
7,926
7,689
7,670
7,651
7,560
7,540
7,521
7,262
5,107
5,089
5,072
5,054
1,878
1,860
O
SCN
5i
1.96
2.02
1.00
1.11
2.98
ppm (t1)


7,607
7,459
7,442
7,438
7,422
7,419
7,410
7,400
7,394
7,387
7,383
7,379
7,369
7,355
7,351
7,334
7,260
5,789
5,778
5,761
5,750
4,123
4,095
4,088
4,060
3,191
3,180
3,156
3,145
N(SO2Ph)2
SCN
6a
15.07
1.00
1.05
1.05
ppm (t1)


141,49
134,04
132,19
129,55
129,21
129,06
128,75
128,27
110,95
62,894
34,534
ppm (t1)
150
100
50

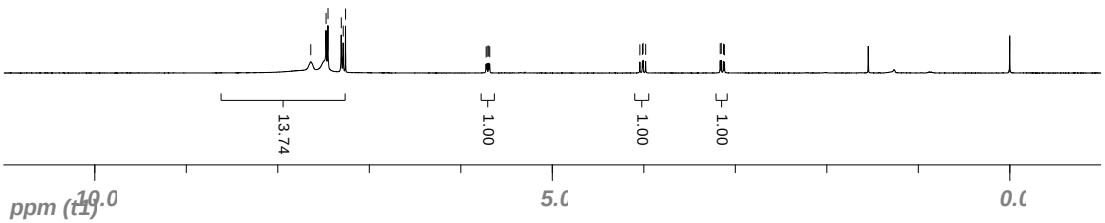

7,628
7,483
7,463
7,455
7,442
7,433
7,420
7,260
7,059
7,038
7,016
5,746
5,735
5,718
5,707
4,059
4,031
4,024
3,996
3,181
3,170
3,146
3,135
N(SO2Ph)2
SCN
F
6b
11.70
2.08
1.00
1.01
1.00
ppm (t1)
10.0
5.0
0.0

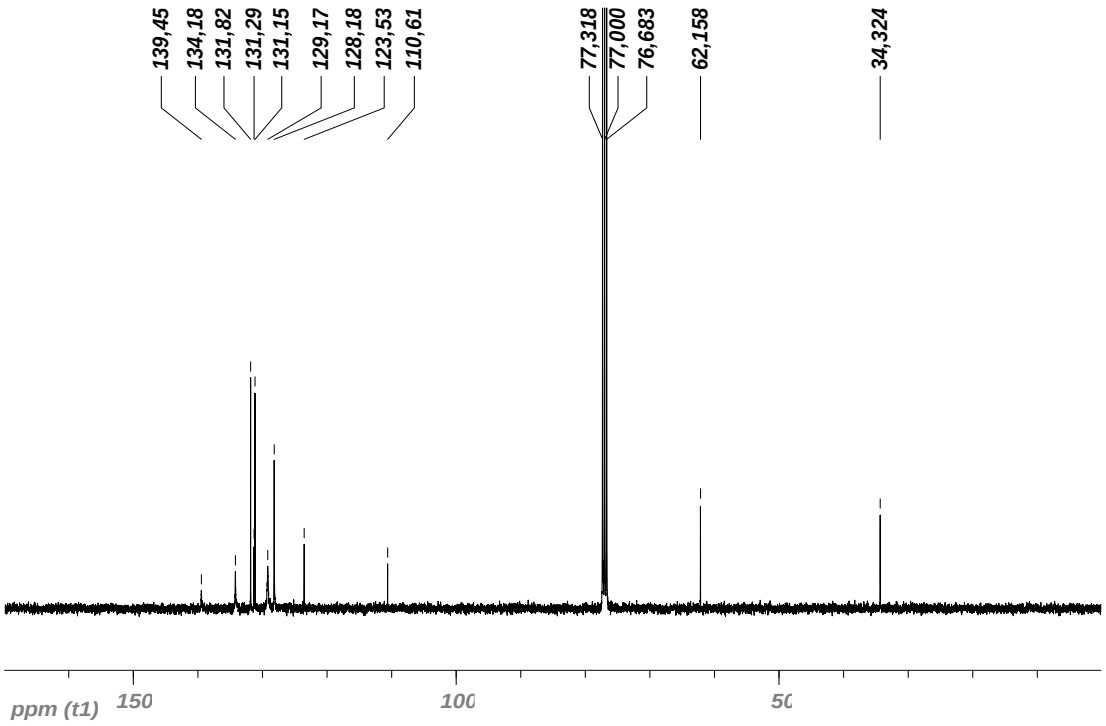

164,22
161,73
139,53
134,14
131,51
131,42
129,12
128,14
115,76
115,54
110,66
77,318
77,000
76,683
62,225
34,602
ppm (t1)
150
100
50
0

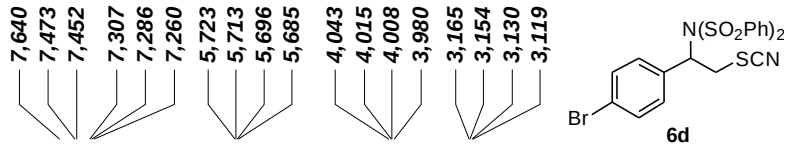

7,639
7,473
7,451
7,306
7,285
7,260
5,723
5,712
5,695
5,684
4,043
4,015
4,008
3,980
3,164
3,153
3,129
3,118

N(SO2Ph)2
SCN
Cl

6c

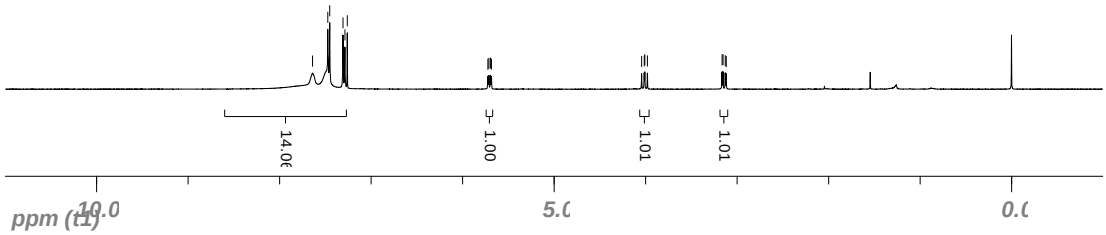

13,74
1,00
1,00
1,00
ppm (t1)
10.0
5.0
0.0

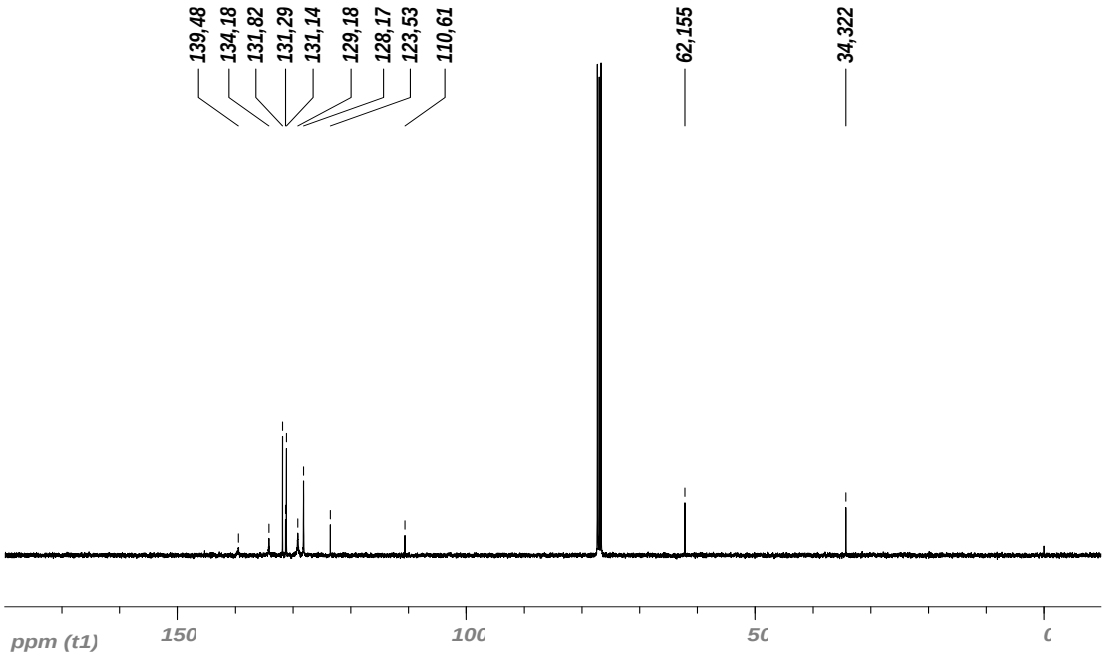

139,45
134,18
131,82
131,29
131,15
129,17
128,18
123,53
110,61
77,318
77,000
76,683
62,158
34,324
ppm (t1)
150
100
50

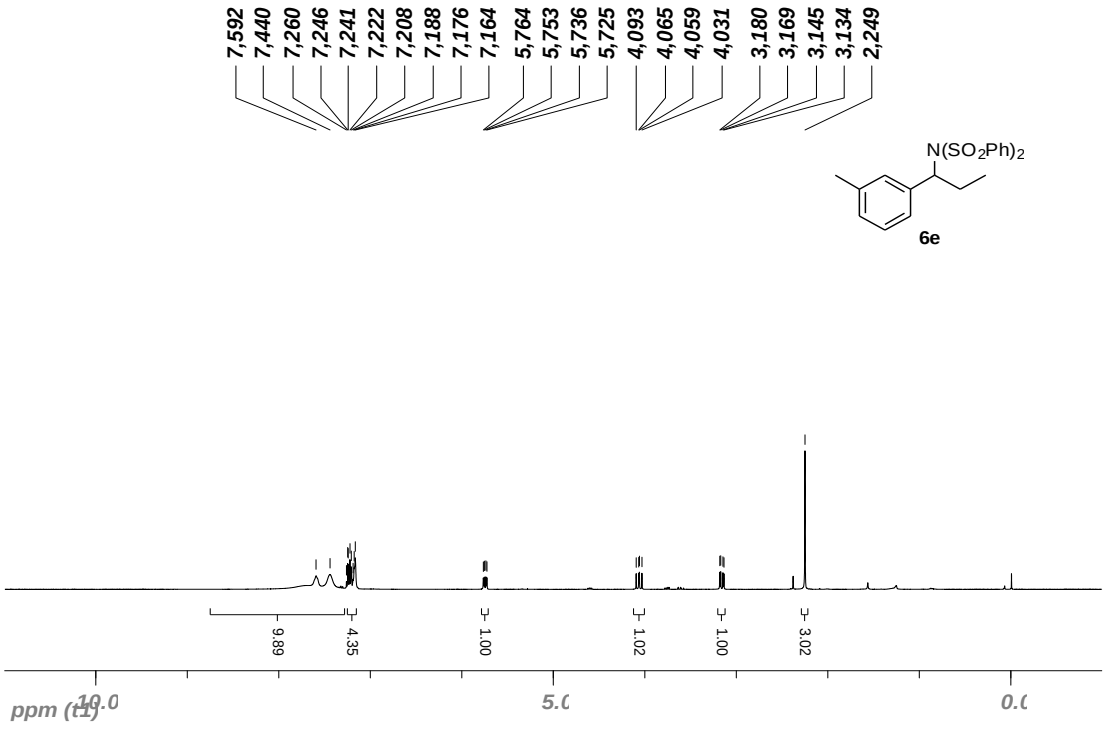

7,640
7,473
7,452
7,307
7,286
7,260
5,723
5,713
5,696
5,685
4,043
4,015
4,008
3,980
3,165
3,154
3,130
3,119

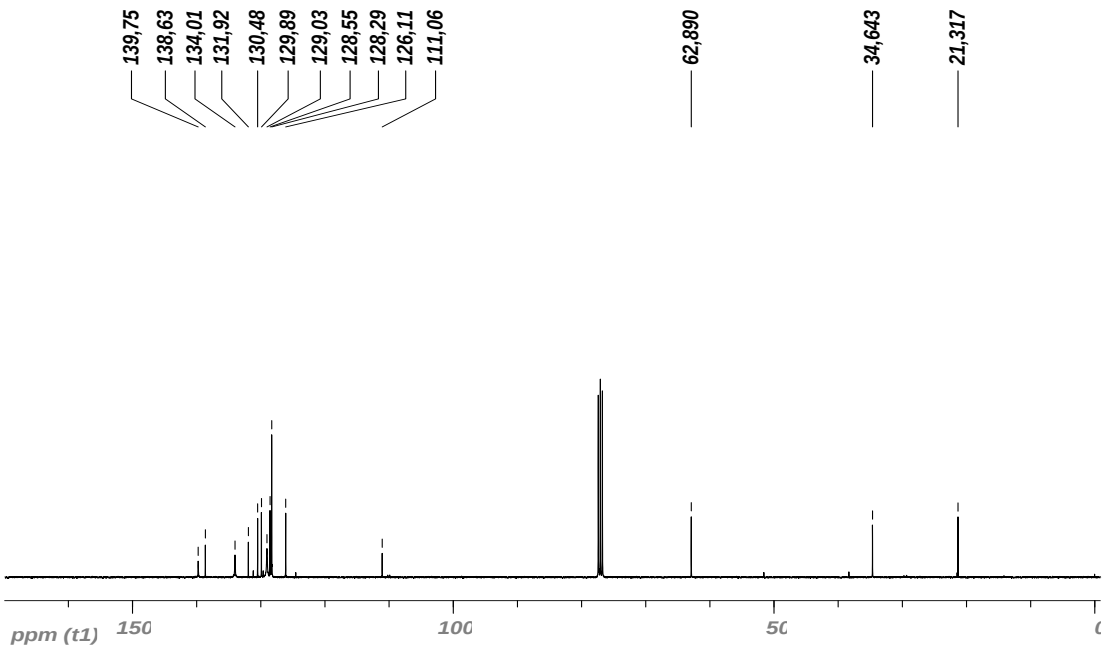
N(SO2Ph)2
SCN
Br

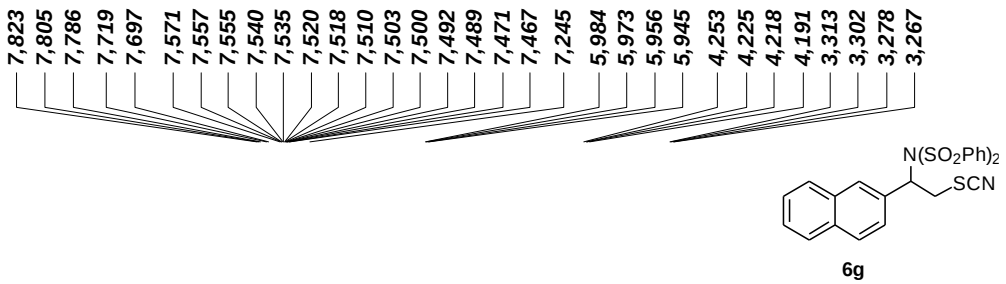
6d


14.06
1.00
1.01
1.01
ppm (t1)
10.0
5.0
0.0

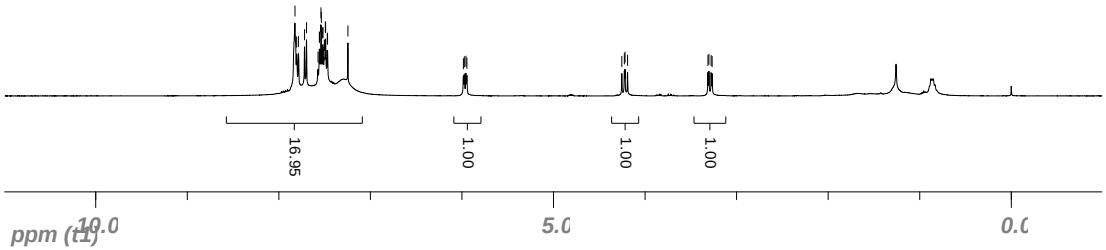

139,48
134,18
131,82
131,29
131,14
129,18
128,17
123,53
110,61
62,155
34,322
ppm (t1)
150
100
50
0

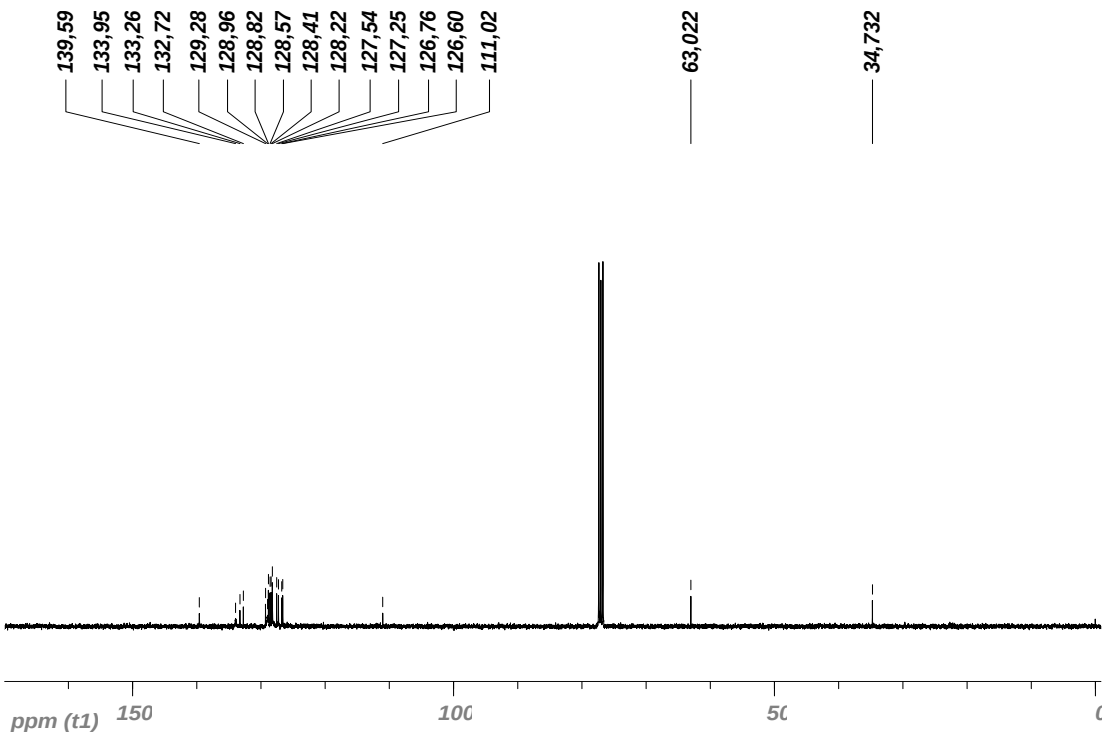

7,592
7,440
7,260
7,246
7,241
7,222
7,208
7,188
7,176
7,164
5,764
5,753
5,736
5,725
4,093
4,065
4,059
4,031
3,180
3,169
3,145
3,134
2,249
N(SO2Ph)2
6e
9.89
4.35
1.00
1.02
1.00
3.02
ppm (t1)
10.0
5.0
0.0

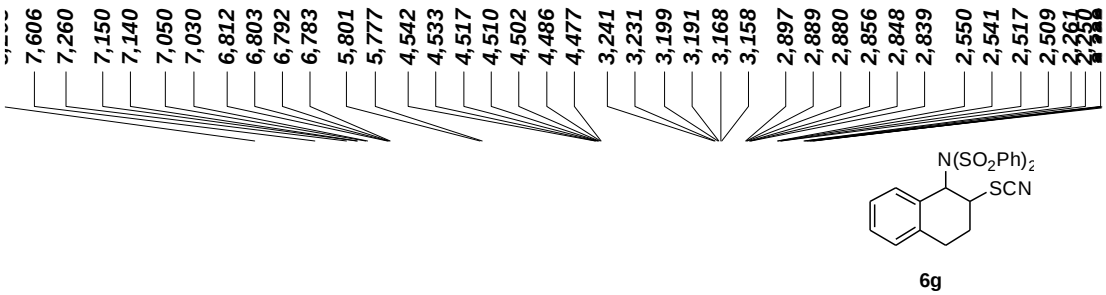

139,75
138,63
134,01
131,92
130,48
129,89
129,03
128,55
128,29
126,11
111,06
62,890
34,643
21,317
ppm (t1)
150
100
50


7,823
7,805
7,786
7,719
7,697
7,571
7,557
7,555
7,540
7,535
7,520
7,518
7,510
7,503
7,500
7,492
7,489
7,471
7,467
7,245
5,984
5,973
5,956
5,945
4,253
4,225
4,218
4,191
3,313
3,302
3,278
3,267
N(SO2Ph)2
SCN

6g

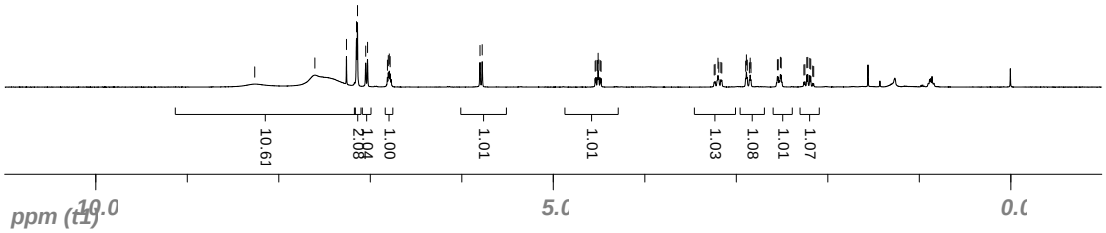

19,95
1,00
1,00
1,00
ppm (t1)
10.0
5.0
0.0

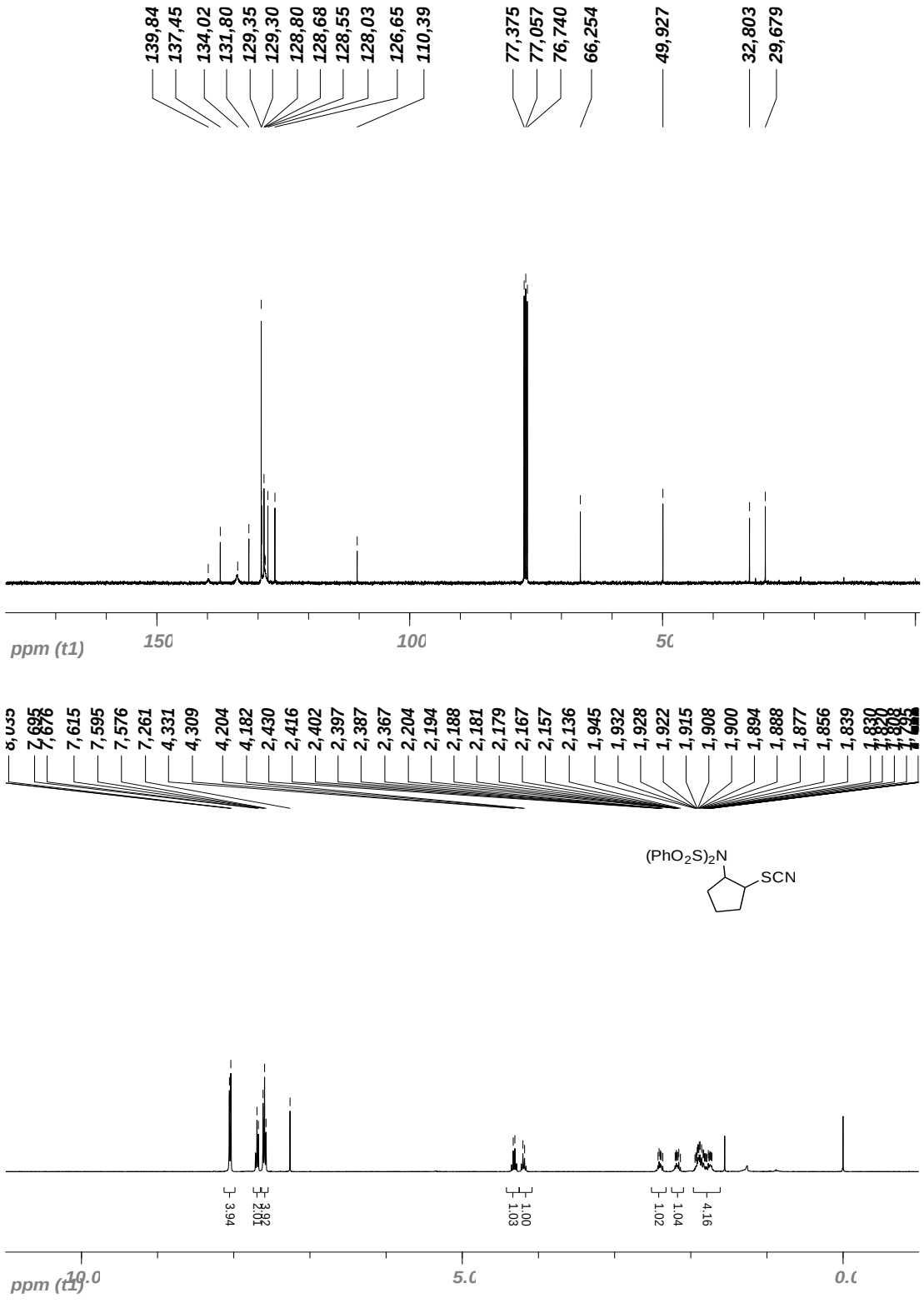

139,59
133,95
133,26
132,72
129,28
128,96
128,82
128,57
128,41
128,22
127,54
127,25
126,76
126,60
111,02
63,022
34,732
ppm (t1)
150
100
50

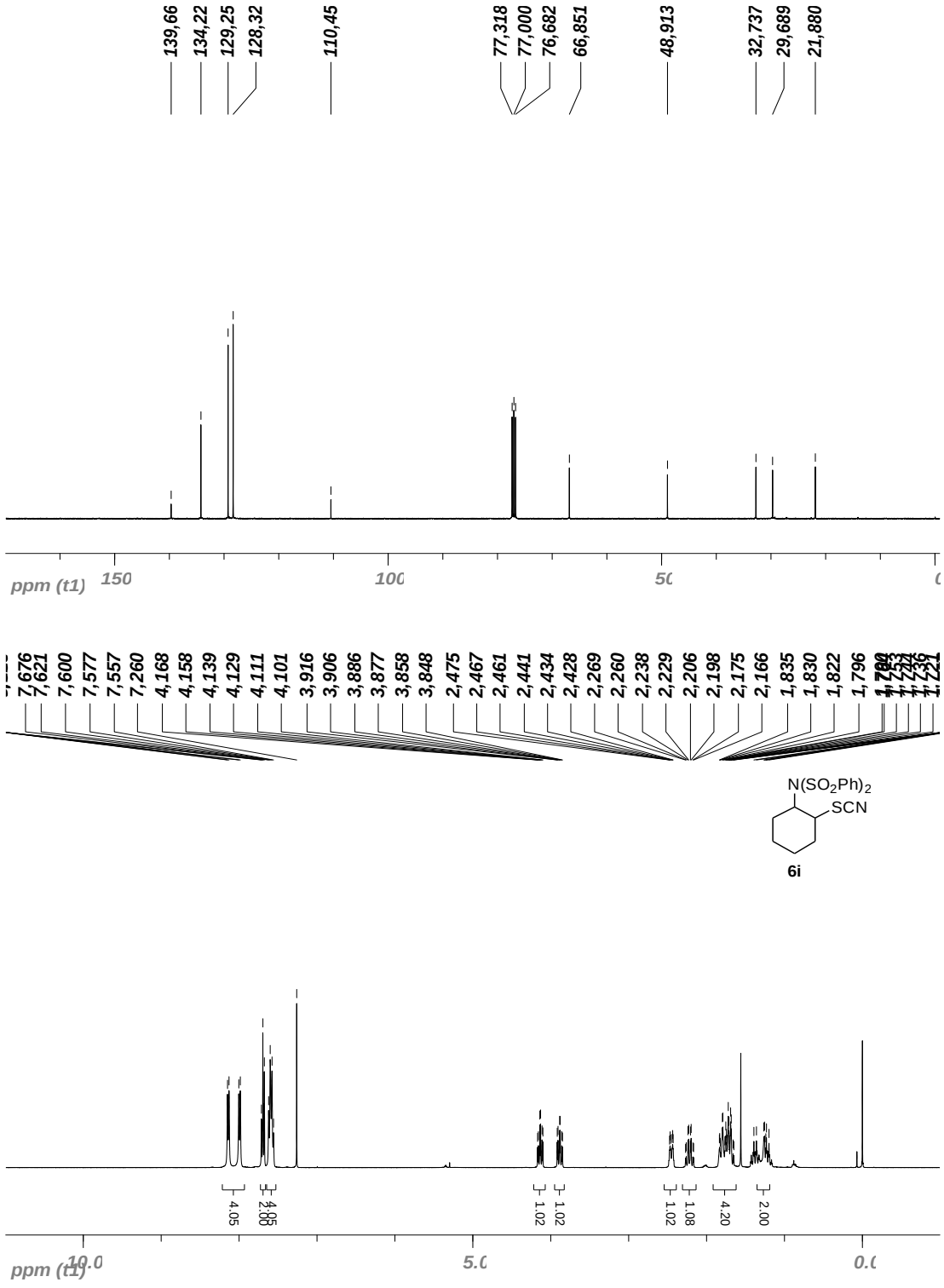

7,606
7,260
7,150
7,140
7,050
7,030
6,812
6,803
6,792
6,783
5,801
5,777
4,542
4,533
4,517
4,510
4,502
4,486
4,477
3,241
3,231
3,199
3,191
3,168
3,158
2,897
2,889
2,880
2,856
2,848
2,839
2,550
2,541
2,517
2,509

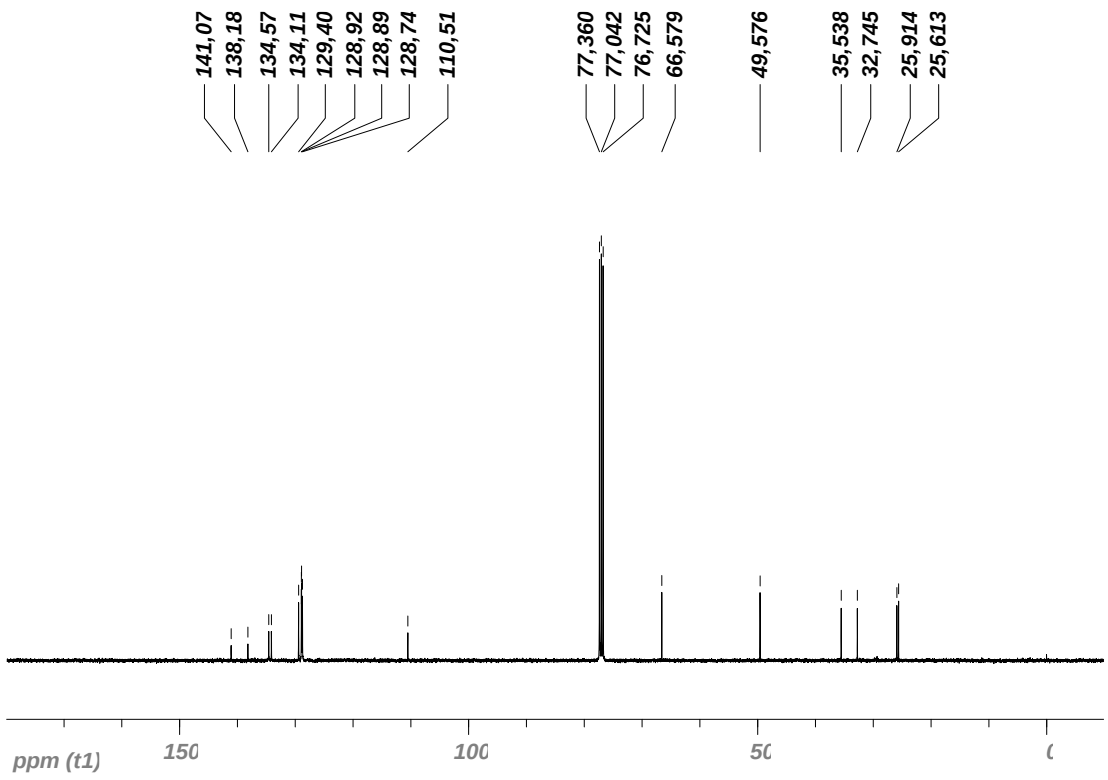
N(SO2Ph)2
SCN

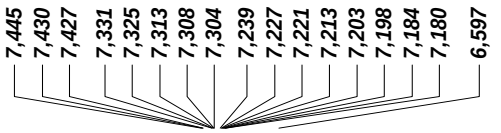
6g

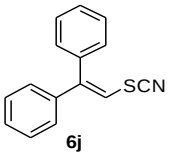

10.61
2.08
2.04
1.00
1.01
1.01
1.03
1.08
1.01
1.07
ppm (t1)
10.0
5.0
0.0


139,84
137,45
134,02
131,80
129,35
129,30
128,80
128,68
128,55
128,03
126,65
110,39
77,375
77,057
76,740
66,254
49,927
32,803
29,679
ppm (t1)
150
100
50
(PhO2S)2N
SCN
3.94
2.82
2.81
1.00
1.03
1.02
1.04
4.16
10.0
5.0
0.0
ppm (t1)

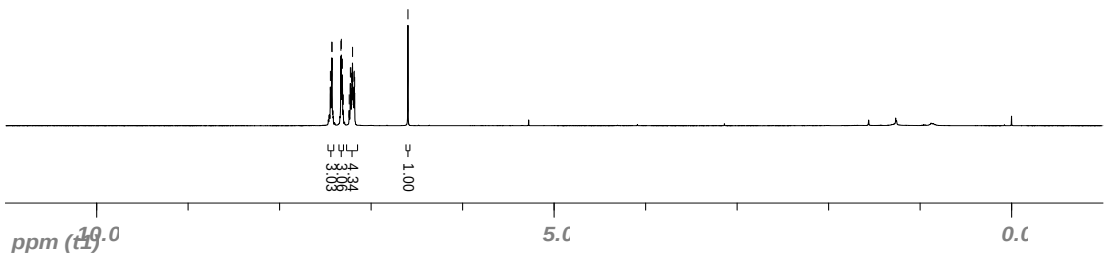

139,66
134,22
129,25
128,32
110,45
77,318
77,000
76,682
66,851
48,913
32,737
29,689
21,880
ppm (t1)
150
100
50
7,676
7,621
7,600
7,577
7,557
7,260
4,168
4,158
4,139
4,129
4,111
4,101
3,916
3,906
3,886
3,877
3,858
3,848
2,475
2,467
2,461
2,441
2,434
2,428
2,269
2,260
2,238
2,229
2,206
2,198
2,175
2,166
1,835
1,830
1,822
1,796
N(SO2Ph)2
SCN
6i
4.05
2.08
1.02
1.02
1.08
4.20
2.00
10.0
5.0
0.0

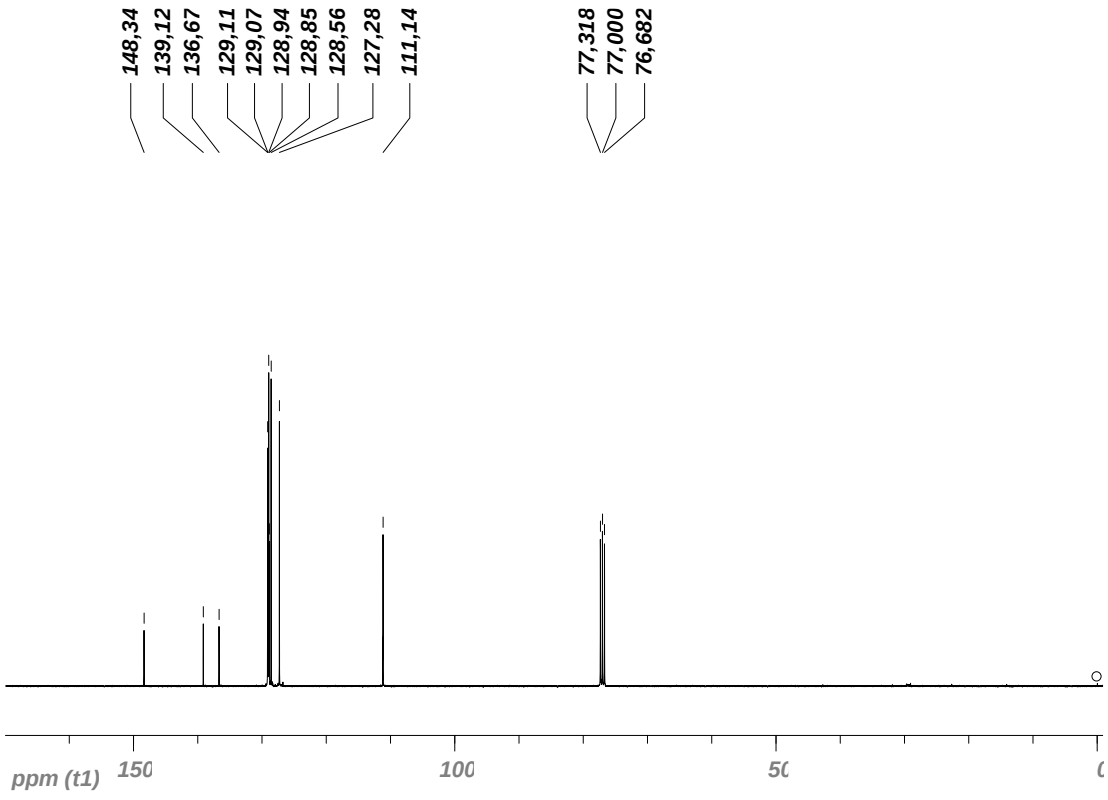

141,07
138,18
134,57
134,11
129,40
128,92
128,89
128,74
110,51
77,360
77,042
76,725
66,579
49,576
35,538
32,745
25,914
25,613
ppm (t1)
150
100
50
0


7,445
7,430
7,427
7,331
7,325
7,313
7,308
7,304
7,239
7,227
7,221
7,213
7,203
7,198
7,184
7,180
6,597


SCN

6j


4.34
3.06
3.03
1.00
ppm (t1)
10.0
5.0
0.0


148,34
139,12
136,67
129,11
129,07
128,94
128,85
128,56
127,28
111,14
77,318
77,000
76,682
ppm (t1)
150
100
50