Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

AIBN-Initiated Direct Thiocyanation of Benzylic sp^3 C–H with *N*-Thiocyanatosaccharin

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Table of Content

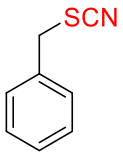
1. General Information

All reactions were carried out under air atmosphere, unless otherwise stated. All chemicals were purchased from commercial companies. All solvents were used directly. ^{1}H NMR spectra were recorded on a Brucker Avance400 (400 MHz) spectrometer, all signals are reported in ppm with the internal chloroform signal at 7.26 ppm as the standard. $^{13}C\{^{1}H\}$ NMR spectra were recorded on a Brucker Avance400 (100 MHz) spectrometer, all signals are reported in ppm with the internal chloroform signal at 77.0 ppm as the standard. The data is reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, coupling constant(s) in Hz, integration, assignment). Other analyses were carried out on the following instruments. Infrared spectrometer: Bruker ALPHA FT-IR-Spektrometer. High resolution mass spectrum: AGILENT 7890A/5975C. Melting point detector: Binocular microscope XT4A melting point apparatus (without correct).

2. General procedure

1 (1.00 mmol, 5.0 equiv), AIBN (0.04 mmol, 20 mol%) and benzene (1.0 mL) was added to a glass tube, Then, **R3** (0.20 mmol, 1.0 equiv) was added to the system, and the reaction system was continuely stirred 4 h at 80 °C. The reaction mixture was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (10:1, v/v) to afford the pure desired product.

3. Spectral data of the products



2a

(Thiocyanatomethyl)benzene (**2a**)[1] was synthesized following the general procedure: Yellow oil (27 mg, 93% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40 – 7.36 (m, 5H), 4.17 (s, 2H), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 134.3, 129.1, 128.9, 128.9, 111.9, 38.3.

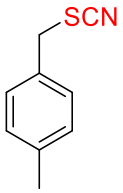
2b

1-Methyl-2-(thiocyanatomethyl)benzene (**2b**)[2] was synthesized following the general procedure: Colourless oil (30 mg, 92% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.25 – 7.17 (m, 4H), 4.18 (s, 2H), 2.37 (s, 3H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 136.8, 131.9, 131.0, 130.2, 129.3, 126.7, 111.9, 36.6, 19.0.

2c

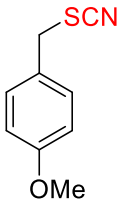
1-Methyl-3-(thiocyanatomethyl)benzene (**2c**)[3] was synthesized following the general procedure: colourless oil (33 mg, 100% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.25 – 7.11 (m, 4H), 4.09 (s, 2H),

2.33 (s, 3H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 138.9, 134.1, 129.7, 129.6, 129.0, 126.0, 112.0, 38.4, 21.3.



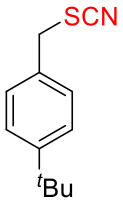
2d

1-Methyl-4-(thiocyanatomethyl)benzene (**2d**)[1] was synthesized following the general procedure: Colourless oil (32 mg, 98% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (d, J = 8.0 Hz, 2H), 7.19 (d, J = 8.0 Hz, 2H), 4.14 (s, 2H), 2.36 (s, 3H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 138.9, 131.2, 129.8, 128.9, 112.1, 38.2, 21.2.



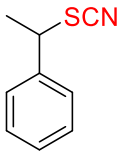
2e

1-Methoxy-4-(thiocyanatomethyl)benzene (**2e**)[1] was synthesized following the general procedure: Yellow oil (36 mg, 100% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.29 (d, J = 8.4 Hz, 2H), 6.90 (d, J = 8.4 Hz, 2H), 4.15 (s, 2H), 3.82 (s, J = 3H), $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 160.0, 130.3, 128.2, 114.5, 112.2, 55.3, 38.2.



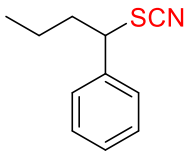
2f

1-(*tert*-Butyl)-4-(thiocyanatomethyl)benzene (**2f**)[4] was synthesized following the general procedure: Colourless oil (38 mg, 93% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (d, J = 8.4 Hz, 2H), 7.30 (d, J = 8.4 Hz, 2H), 4.16 (s, 2H), 1.33 (s, 9H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 152.0, 131.2, 128.7, 126.1, 38.2, 34.7, 31.2.



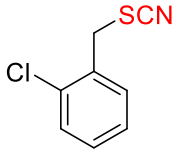
2g

(1-Thiocyanatoethyl)benzene (**2g**)[1] was synthesized following the general procedure: Colourless oil (33 mg, 100% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40 – 7.35 (m, 5H), 6.61 (q, J = 6.8 Hz, 1H), 1.89 (d, J = 6.8 Hz, 3H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 139.0, 129.0, 128.9, 127.0, 111.7, 48.4, 21.9.



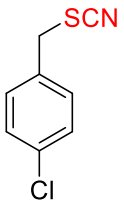
2h

(1-Thiocyanatobutyl)benzene (**2h**)[5] was synthesized following the general procedure: Colourless oil (36 mg, 94% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 – 7.33 (m, 5H), 4.35 (t, J = 7.6 Hz, 1H), 2.17 – 2.11 (m, 2H), 1.45 – 1.29 (m, 2H), 0.95 (t, J = 7.2 Hz, 3H). ^{13}C{^{1}H} NMR (175 MHz, $CDCl_3$) δ: 138.3, 129.0, 128.8, 127.4, 111.7, 53.4, 37.7, 20.6, 13.4.



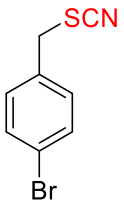
2i

1-Chloro-2-(thiocyanatomethyl)benzene (**2i**)[2] was synthesized following the general procedure: Colourless oil (14 mg, 38% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 – 7.40 (m, 2H), 7.36 – 7.29 (m, 2H), 4.25 (s, 2H), ^{13}C{^{1}H} NMR (175 MHz, $CDCl_3$) δ: 134.2, 132.3, 131.1, 130.5, 130.1, 127.5, 111.8, 36.2.



2j

1-Chloro-4-(thiocyanatomethyl)benzene (**2j**)[2] was synthesized following the general procedure: Yellow oil (19 mg, 52% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37 (d, J = 8.8 Hz, 2H), 7.30 (d, J = 8.8 Hz, 2H), 4.12 (s, 2H), ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 135.0, 132.9, 130.3, 129.4, 111.5, 37.6.

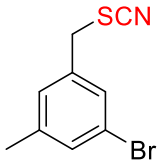


2k

1-Bromo-4-(thiocyanatomethyl)benzene (**2k**)[2] was synthesized following the general procedure: colourless oil (30 mg, 66% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.53 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 4.10 (s, 2H), ^{13}C{^{1}H} NMR (175 MHz, $CDCl_3$) δ: 133.4, 132.3, 130.5, 123.1, 111.5, 37.6.

2l

1-Bromo-3-(thiocyanatomethyl)benzene (**2l**)[6] was synthesized following the general procedure: Colourless oil (21 mg, 46% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.54 – 7.52 (m, 2H), 7.35 – 7.28 (m, 2H), 4.13 (s, 2H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 136.5, 132.1, 131.9, 127.6, 123.0, 111.4, 37.4.

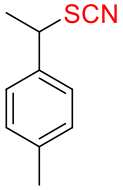


2m

1-Bromo-3-methyl-5-(thiocyanatomethyl)benzene (**2m**) was synthesized following the general procedure: White solid, mp. 50 – 52 °C, (44 mg, 91% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33 (s, 1H), 7.31 (s, 1H), 7.10 (s, 1H), 4.07 (s, 2H), 2.35 (s, 3H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 141.0, 136.1, 132.7, 128.9, 122.7, 111.5, 37.5, 21.1. IR (KBr): 2916, 2152 (SCN), 1597, 1566, 1442, 1257 cm^{-1}. HRMS (APCI) m/z calcd C_9H_9BrNS for $[M + H]^+$: 241.9634, found: 241.9634.

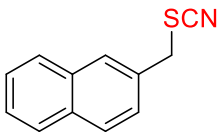
2n

1,3-Dimethyl-5-(thiocyanatomethyl)benzene (**2n**) was synthesized following the general procedure: White solid, mp. 47 – 49 °C, (35 mg, 99% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 6.99 (s, 1H), 6.97 (s, 2H), 4.11 (s, 2H), 2.33 (s, 6H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 138.8, 134.0, 130.6, 126.7, 112.2, 38.4, 21.2. IR (KBr): 2916, 2152 (SCN), 1604, 1466 cm^{-1}. HRMS (APCI) m/z calcd $C_{10}H_{12}NS$ for $[M + H]^+$: 178.0685, found 178.0678.



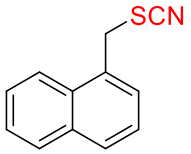
2o

1-Methyl-4-(1-thiocyanatoethyl)benzene (**2o**)[7] was synthesized following the general procedure: Colourless oil (31 mg, 88% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.28 (d, J = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 4.60 (q, *J* = 7.2 Hz, 1H), 2.36 (s, 3H), 1.87 (d, *J* = 7.2 Hz, 3H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 138.9, 136.0, 129.7, 126.9, 111.9, 48.4, 22.0, 21.1.



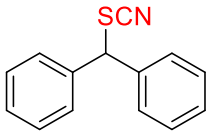
2p

2-(Thiocyanatomethyl)naphthalene (**2p**)[8] was synthesized following the general procedure: White solid, mp. 96 – 98 ^{o}C, (30 mg, 75% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.89 – 7.82 (m, 4H), 7.55 – 7.52 (m, 2H), 7.45 (dd, J = 8.4, 1.6 Hz, 1H), 4.32 (s, 2H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 133.1, 133.1, 131.5, 129.2, 128.3, 128.0, 127.7, 126.8, 126.7, 126.0, 111.9, 38.7.



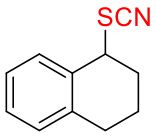
2q

1-(Thiocyanatomethyl)naphthalene (**2q**)[9] was synthesized following the general procedure: White solid, mp. 81 – 83 ^{o}C, (33 mg, 83% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.98 – 7.88 (m, 3H), 7.65 – 7.45 (m, 4H), 4.66 (s, 2H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 134.0, 130.6, 130.2, 129.4, 129.2, 128.6, 127.0, 126.3, 125.3, 122.7, 112.0. 36.4.



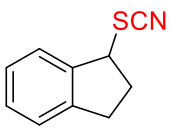
2r

(Thiocyanatomethylene)dibenzene (**2r**)[9] was synthesized following the general procedure: Colourless oil (36 mg, 80% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 – 7.33 (m, 10H, 5.83 (s, 1H), $^{13}C\{^{1}H\}$ NMR (175 MHz, $CDCl_3$) δ: 137.5, 129.1, 128.8, 128.2, 111.7, 57.4.



2s

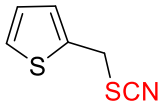
1-Thiocyanato-1,2,3,4-tetrahydronaphthalene (**2s**) was synthesized following the general procedure: Colourless oil (37 mg, 98% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33 (d, J = 7.6 Hz, 1H), 7,25 – 7.18 (m, 2H), 7.12 (d, J = 8.4 Hz, 1H), 4.91 (t, J = 3.6 Hz, 1H), 2.92 – 2.75 (m, 2H), 2.43 – 1.91 (m, 4H). $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) δ: 137.9, 131.5, 130.3, 129.7, 128.8, 126.4, 112.4, 49.7, 29.7, 28.6, 18.2. IR (KBr): 2931, 2145 (SCN), 1489, 1450, 1265 cm^{-1}. HRMS (APCI) m/z calcd $C_{11}H_{12}NS$ for $[M + H]^{+}$: 190.0685, found 190.0676.



2t

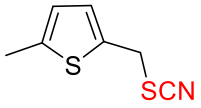
1-Thiocyanato-2,3-dihydro-1H-indene (**2t**) was synthesized following the general procedure: Colourless oil (32 mg, 91% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.43 (d, J = 7.2 Hz, 1H), 7.31 – 7.25 (m,

3H), 4.93 (dd, J = 7.2, 2.8 Hz, 1H), 3.24 – 3.16 (m, 1H), 3.00 – 2.93 (m, 1H), 2.71 – 2.62 (m, 1H), 2.43 – 2.36 (m, 1H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 143.8, 139.4, 129.4, 127.2, 125.1, 124.9, 112.2, 53.3, 34.1, 30.4. IR (KBr): 2939, 2144 (SCN), 1465, 1319 cm^{-1}. HRMS (APCI) m/z calcd $C_{10}H_{10}NS$ for $[M + H]^+$: 176.0528, found 176.0524.



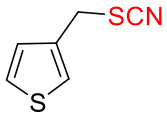
2u

2-(Thiocyanatomethyl)thiophene (**2u**)[7] was synthesized following the general procedure: Yellow oil (29 mg, 94% yield). eluent PE/EtOAc (10:1, v/v). ^1H NMR (400 MHz, $CDCl_3$) δ: 7.34 (dd, J = 5.2, 0.8 Hz, 1H), 7.14 (d, J = 3.2 Hz, 1H), 6.99 (dd, J = 5.2, 3.2 Hz, 1H), 4.42 (s, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 136.0, 128.7, 127.4, 127.3, 111.6, 33.2.



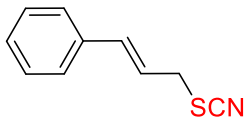
2v

2-Methyl-5-(thiocyanatomethyl)thiophene (**2v**) was synthesized following the general procedure: Yellow oil (33 mg, 98% yield). eluent PE/EtOAc (10:1, v/v). ^1H NMR (400 MHz, $CDCl_3$) δ: 6.91 (d, J = 3.2 Hz, 1H), 6.62 (d, J = 3.2 Hz, 1H), 4.35 (s, 2H), 2.47 (s, 3H), $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 142.3, 133.5, 128.8, 125.4, 111.8, 33.8, 15.4. IR (KBr): 2973, 2912, 2152 (SCN), 1666, 1427, 1249 cm^{-1}. HRMS (APCI) m/z calcd $C_7H_8NS_2$ for $[M + H]^+$: 170.0093, found 170.0085.



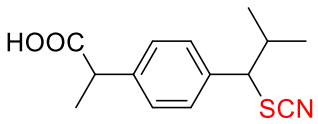
2w

3-(Thiocyanatomethyl)thiophene (**2w**) was synthesized following the general procedure: Yellow oil (28 mg, 90% yield). eluent PE/EtOAc (10:1, v/v). ^1H NMR (400 MHz, $CDCl_3$) δ: 7.38 – 7.33 (m, 2H), 7.11 (dd, J = 4.8, 1.2 Hz, 1H), 4.22 (s, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 134.4, 127.4, 127.3, 125.1, 112.0, 32.9. IR (KBr): 2970, 2923, 2154 (SCN), 1667, 1521, 1420, 1250 cm^{-1}. HRMS (APCI) m/z calcd $C_6H_6NS_2$ for $[M + H]^+$: 155.9936, found 155.9932.



2x

(E)-(3-thiocyanatoprop-1-en-1-yl)benzene (**2x**)[10] was synthesized folloeing the general procedure: Yellow oil (33 mg, 94%). eluent PE/EtOAc (10:1, v/v).^1H NMR (400 MHz, $CDCl_3$) δ: 7.42 – 7.30 (m, 5H), 6.70 (d, J = 15.6 Hz, 1H), 6.30 – 6.25 (m, 1H), 3.76 (d, J = 7.2 Hz, 2H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ: 136.5, 135.4, 128.7, 12.6, 126.8, 121.2, 111.8, 36.9.



2y

2-(4-(2-methyl-1-thiocyanatopropyl)phenyl)propanoic acid (**2y**) was synthesized folloeing the general procedure: Colourless oil (46 mg, 87%). eluent PE/EtOAc (2:1, v/v).^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33 (d, J = 8.4 Hz, 2H), 7.26 (d, J = 8.4 Hz, 2H), 4.06 (d, J = 9.2 Hz, 1H), 3.75 (q, J = 7.2 Hz, 1H), 2.38 – 2.30 (m, 1H), 1.52 (d, J = 7.2 Hz, 3H), 1.17 (d, J = 7.2 Hz, 3H), 0.89 (d, J = 6.4 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 180.1, 140.0, 137.6, 128.1, 128.0, 111.9, 61.4, 44.9, 33.5, 21.0, 20.5, 18.0. IR (KBr): 2970, 2931, 2152, 1705, 1512, 1458, 1226 cm^{-1}. HRMS (APCI) m/z calcd $C_{14}H_{16}NO_2S$ for $[M - H]^-$: 262.0907, found 262.0915.

2z

(Selenocyanatomethyl)benzene (**2z**)[11] was synthesized following the general procedure: Yellow oil (23 mg, 58% yield). eluent PE/EtOAc (10:1, v/v). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38 – 7.32 (m, 5H), 4.32 (s, 2H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ: 135.3, 129.1, 129.0, 128.7, 101.8, 32.8.

4. References

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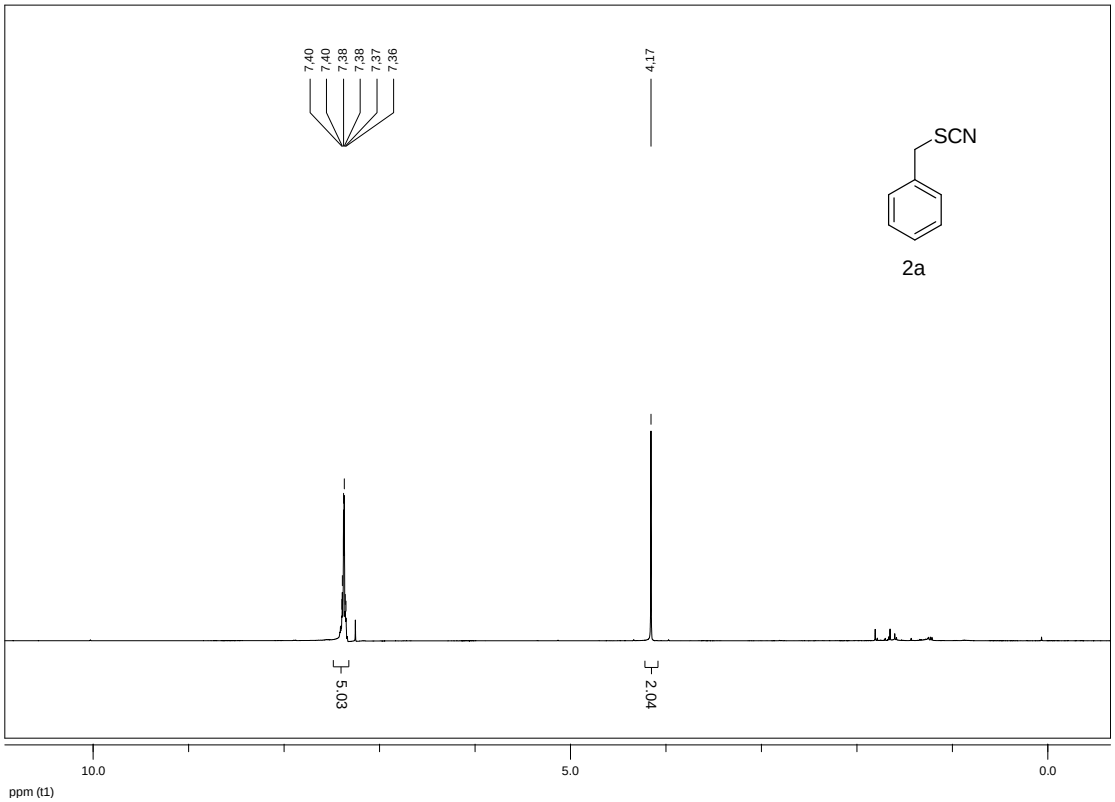
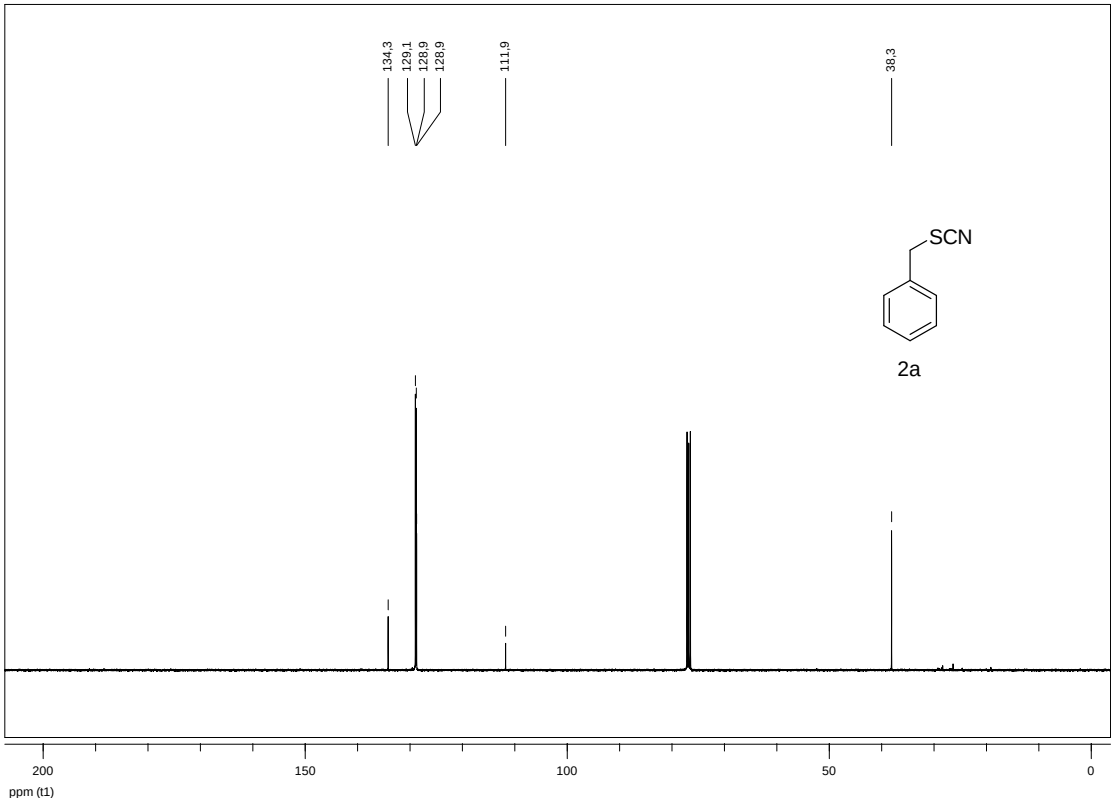
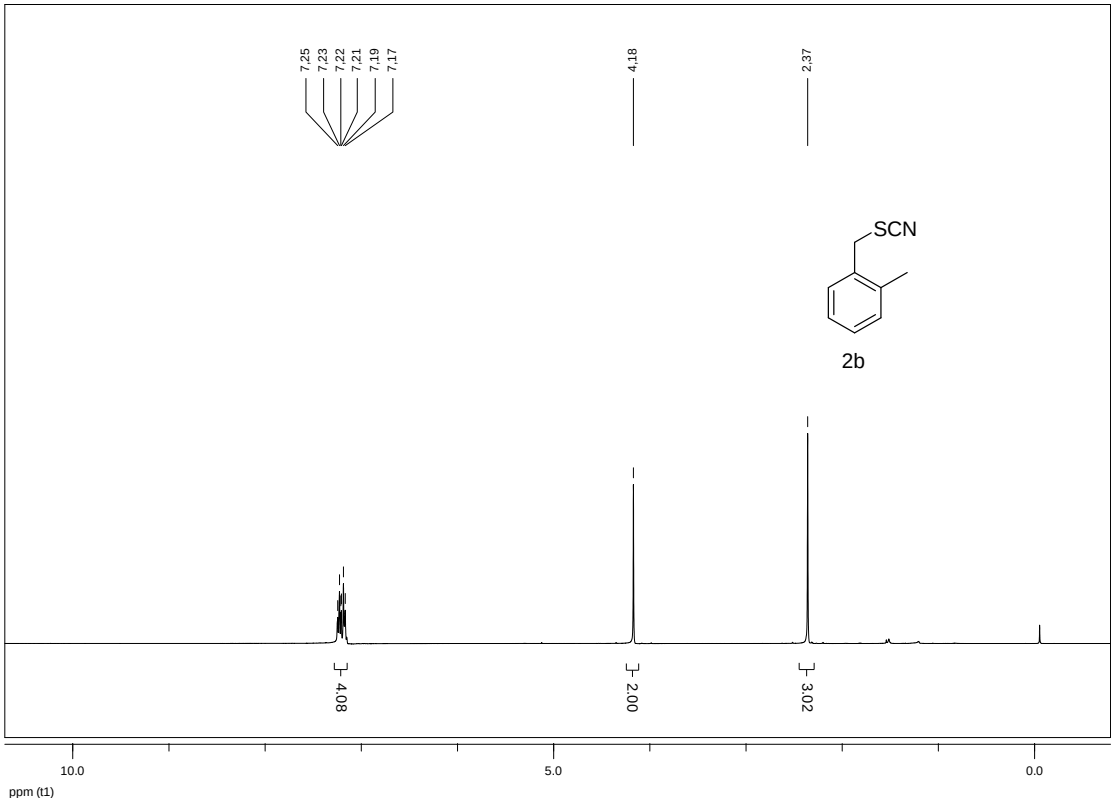
5. NMR spectra of products



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2,37
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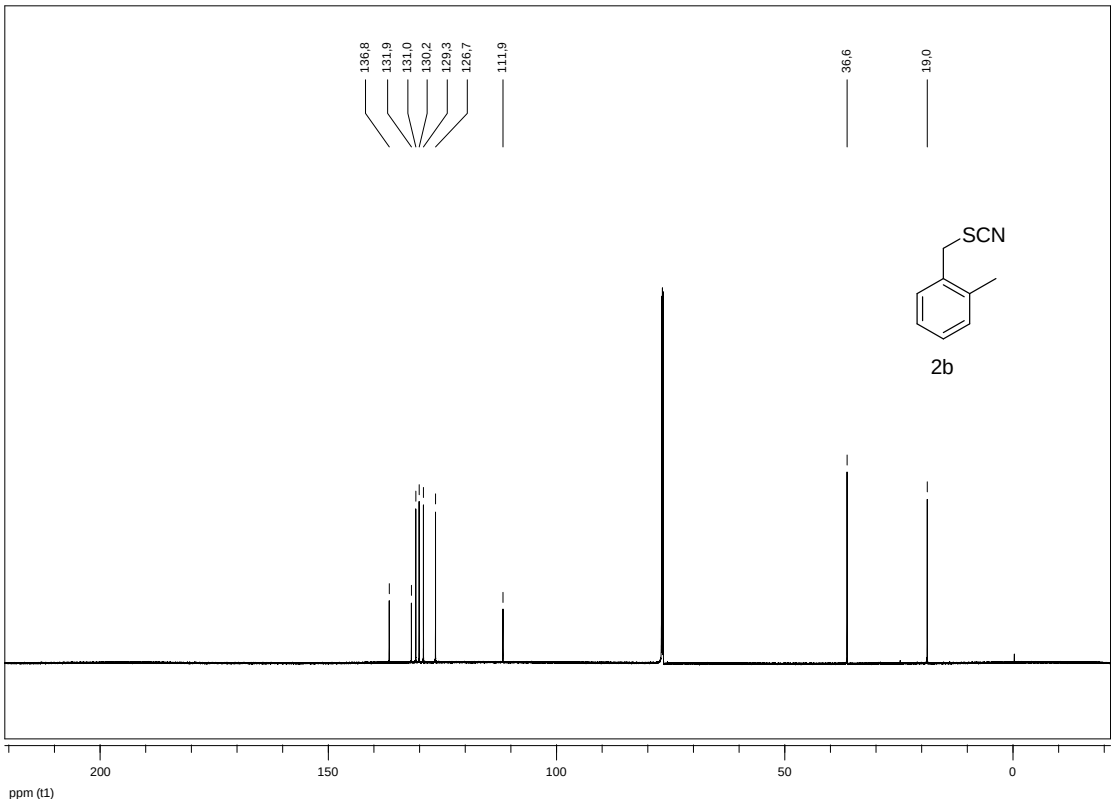
ppm (t1)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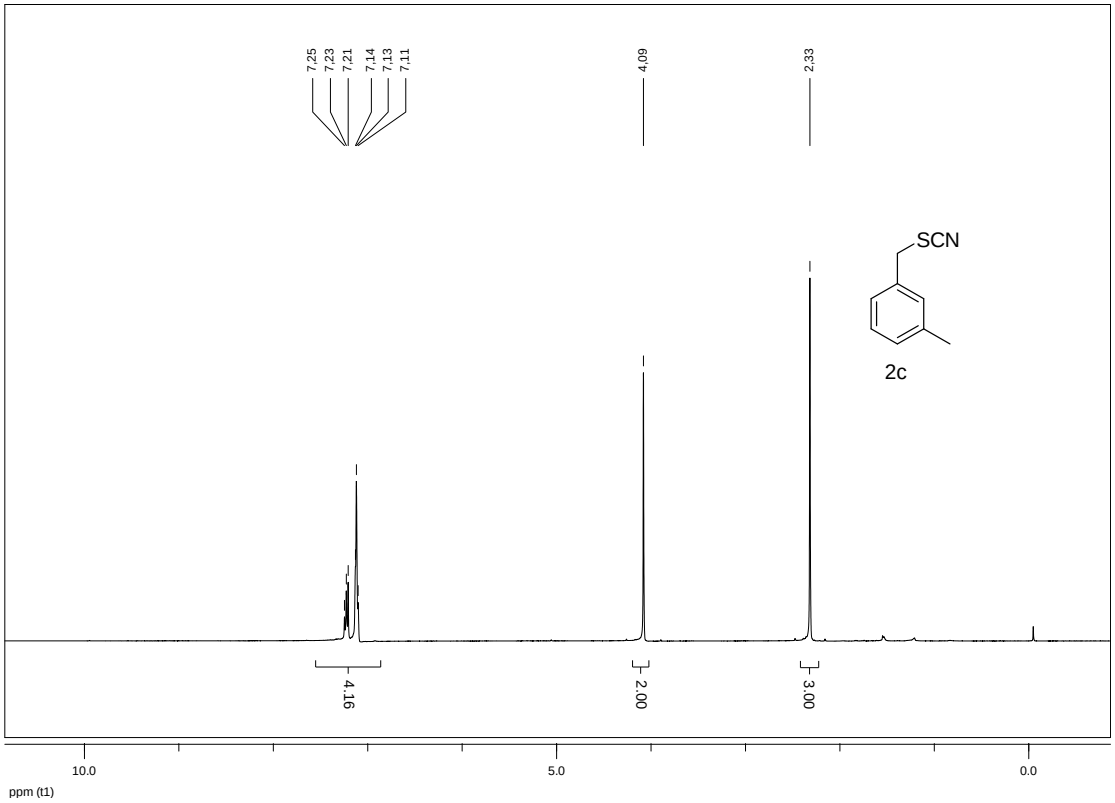
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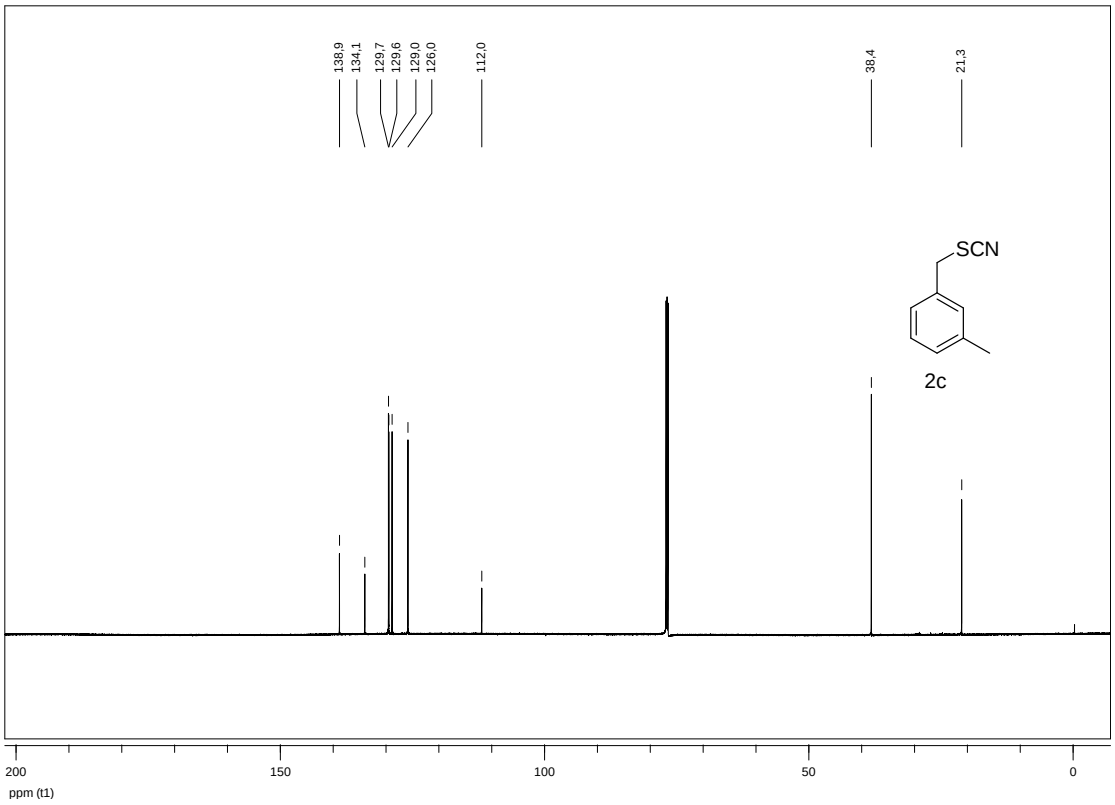
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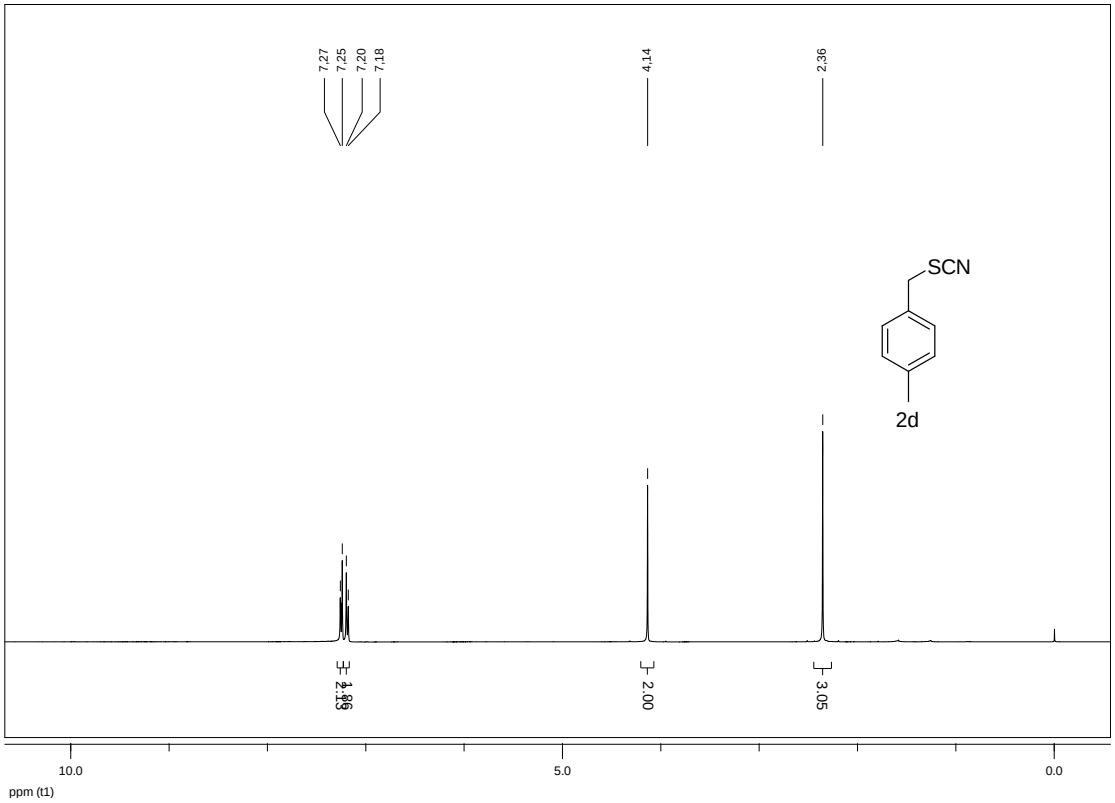
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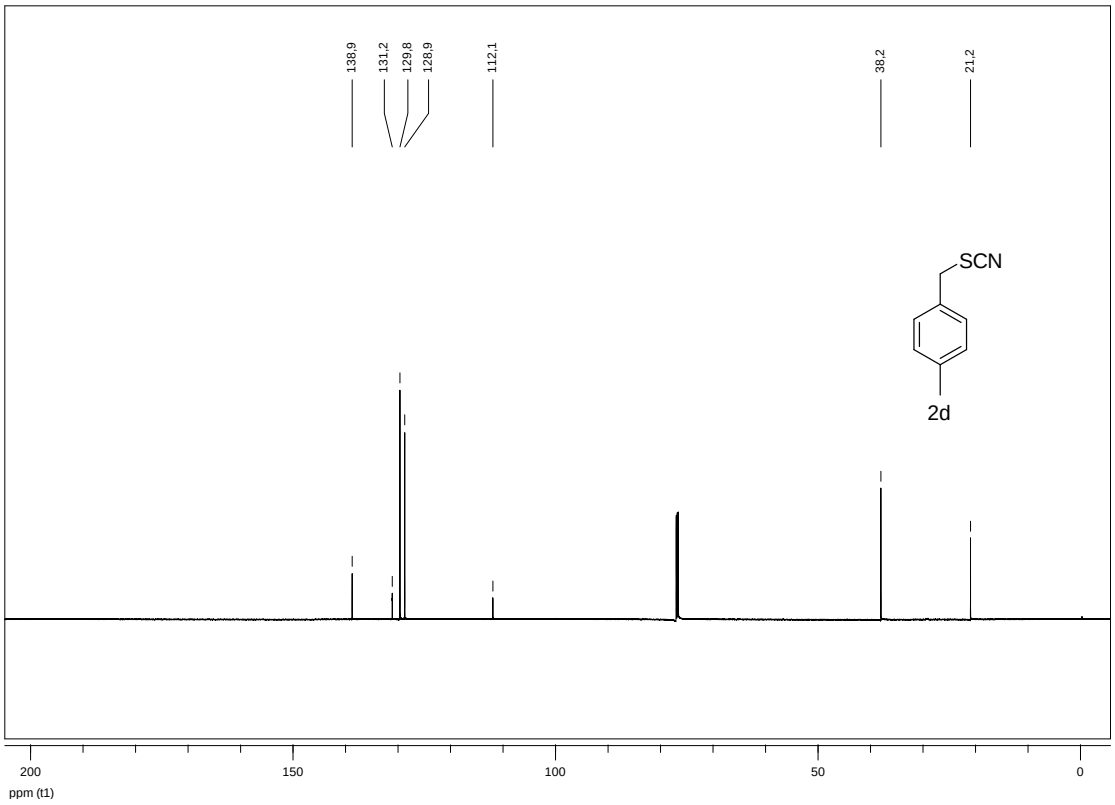
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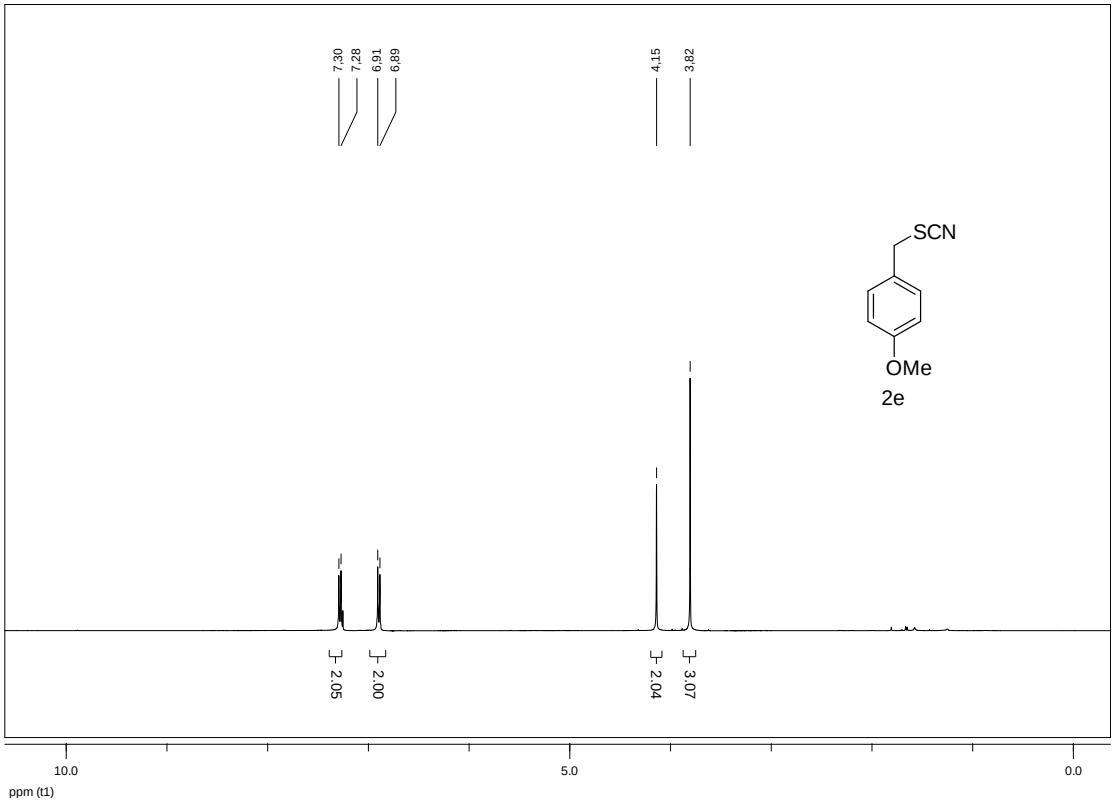
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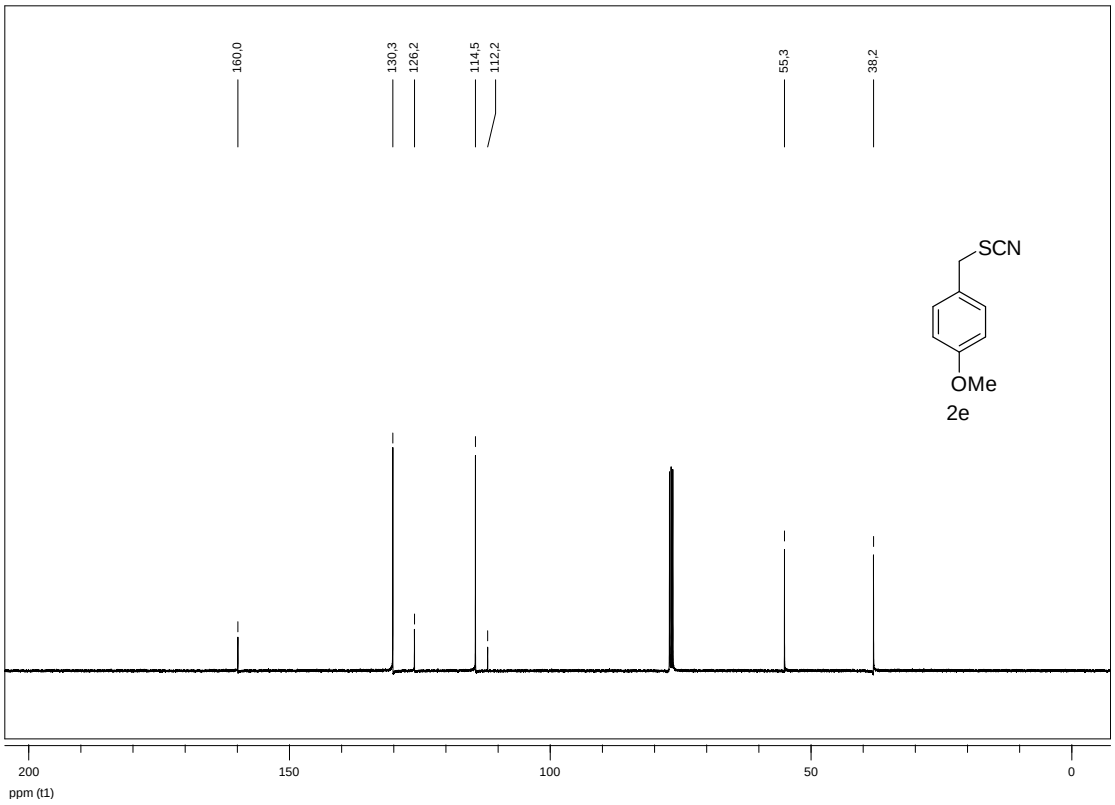
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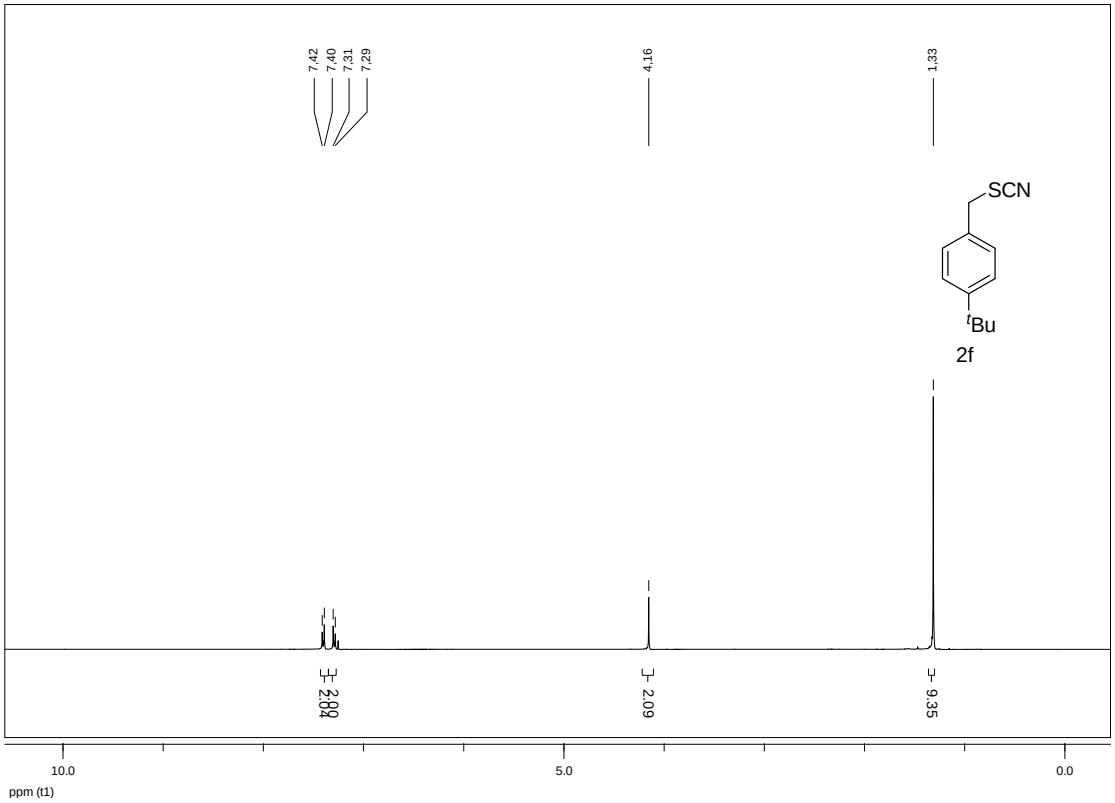
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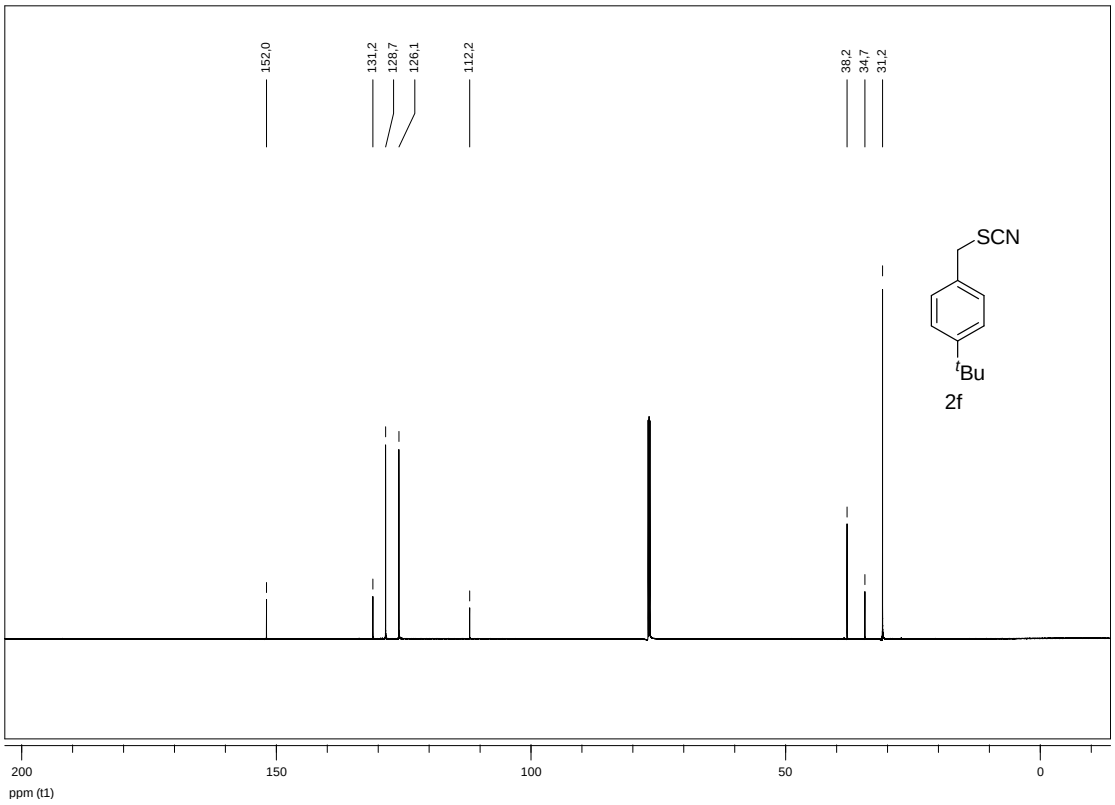
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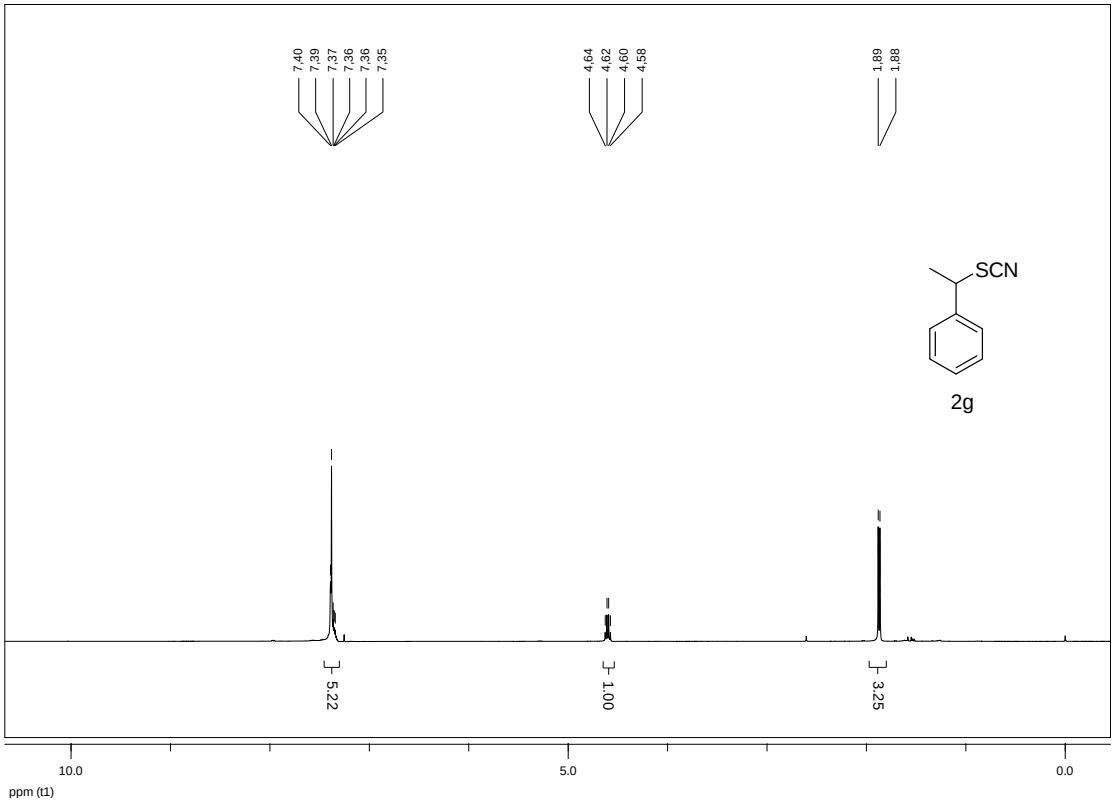
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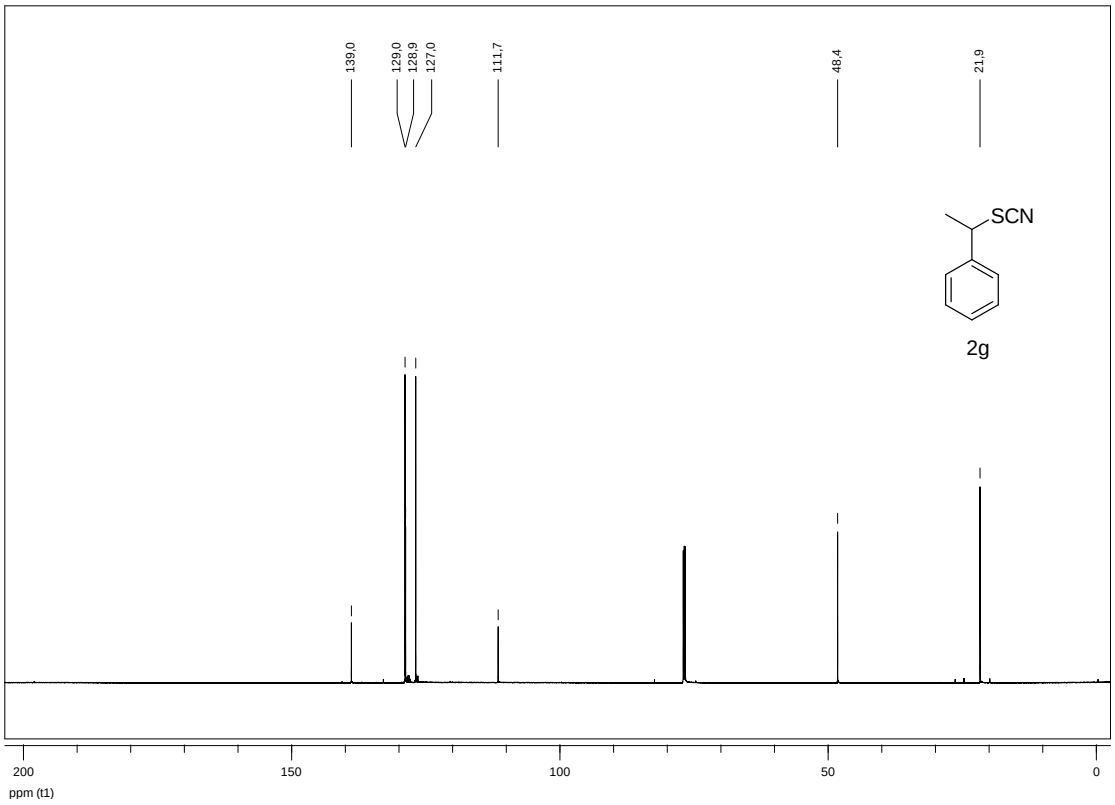
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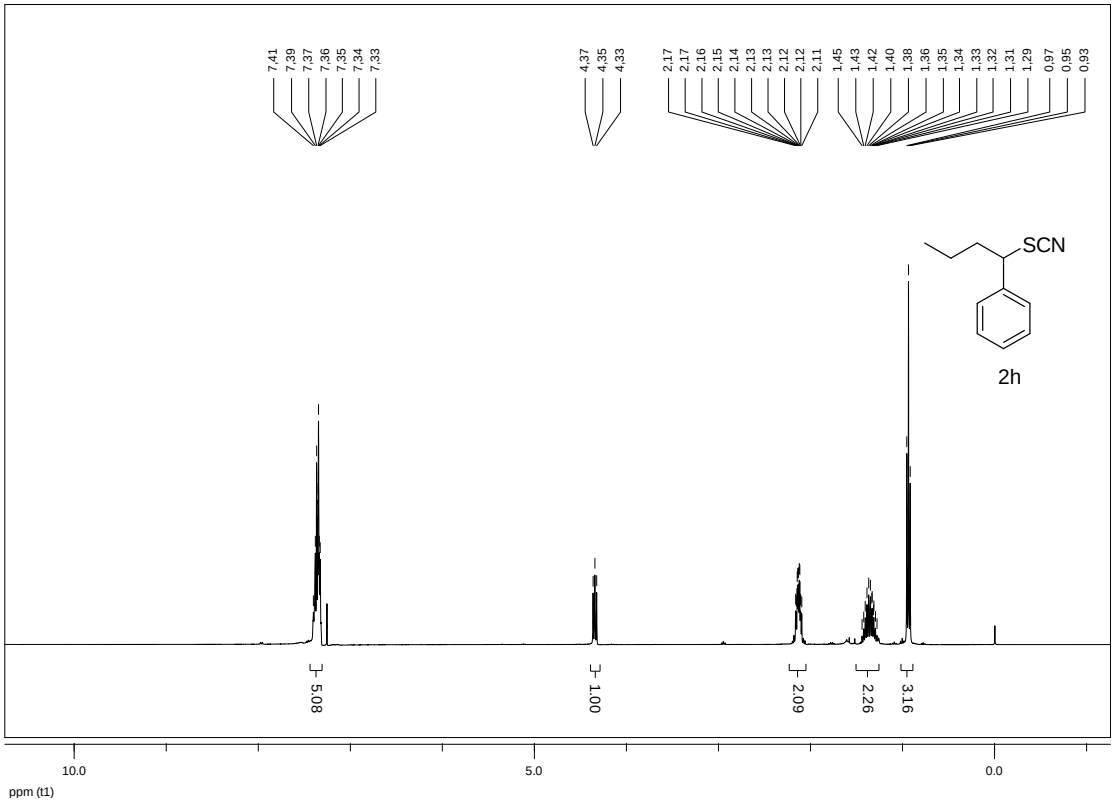
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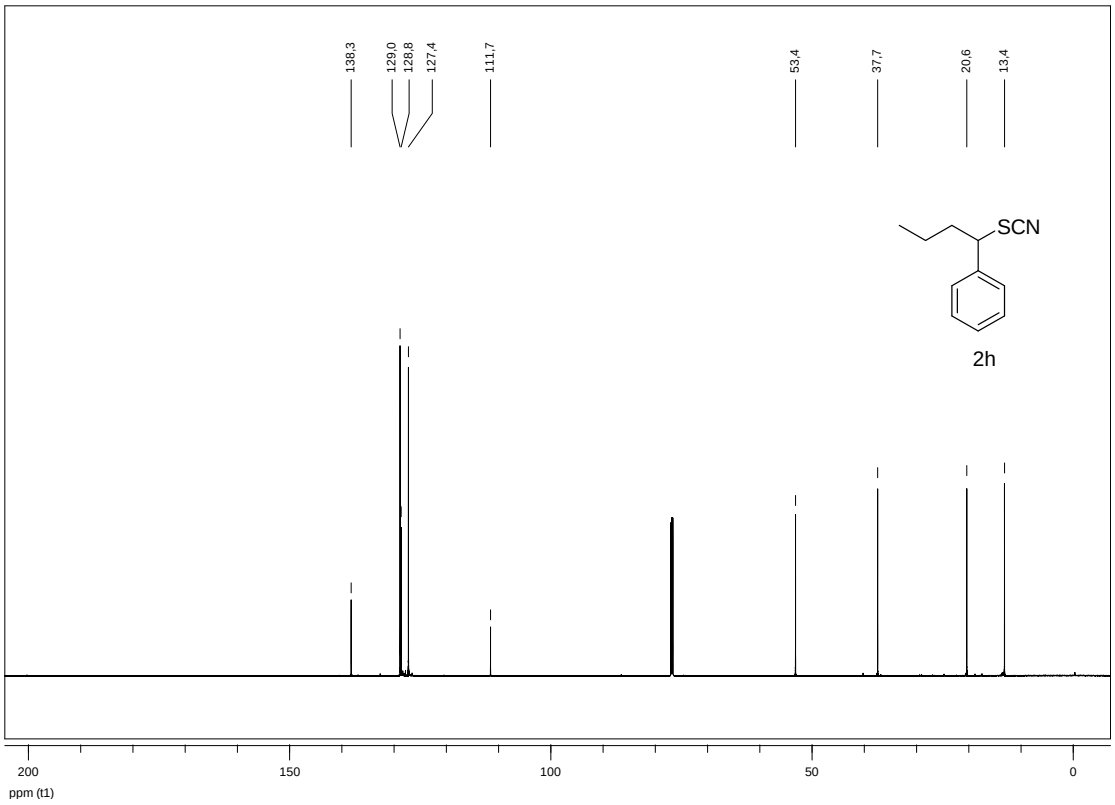
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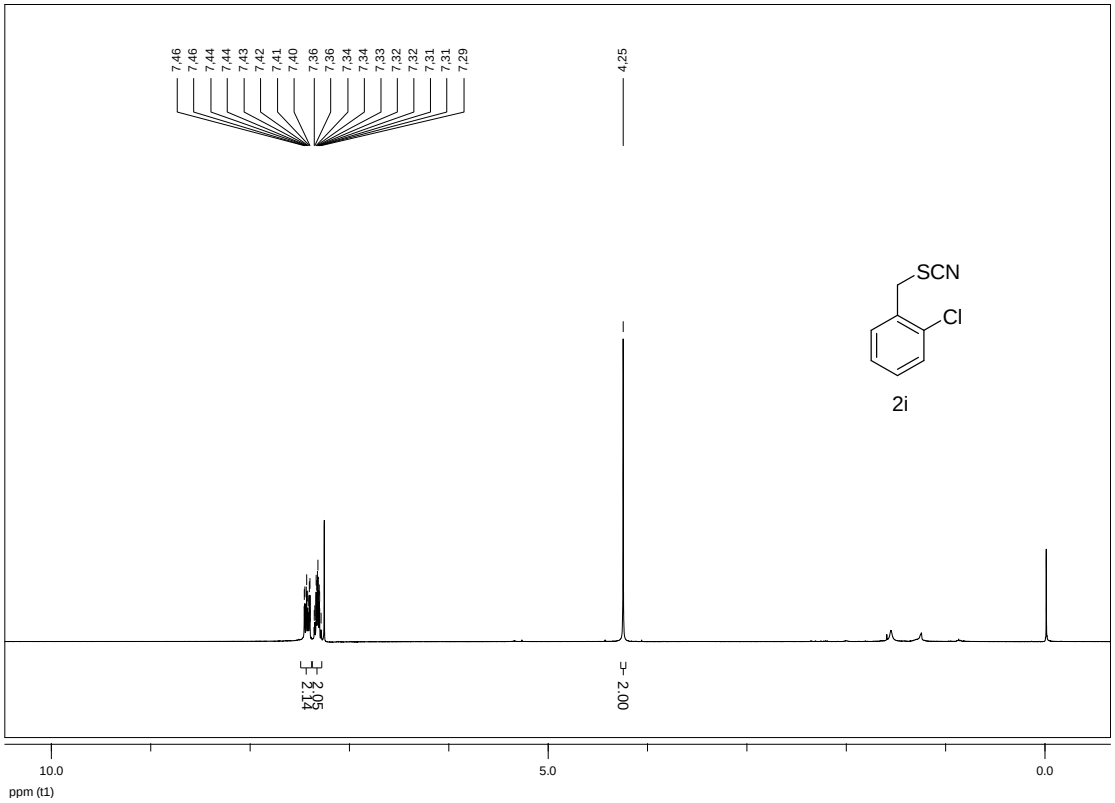
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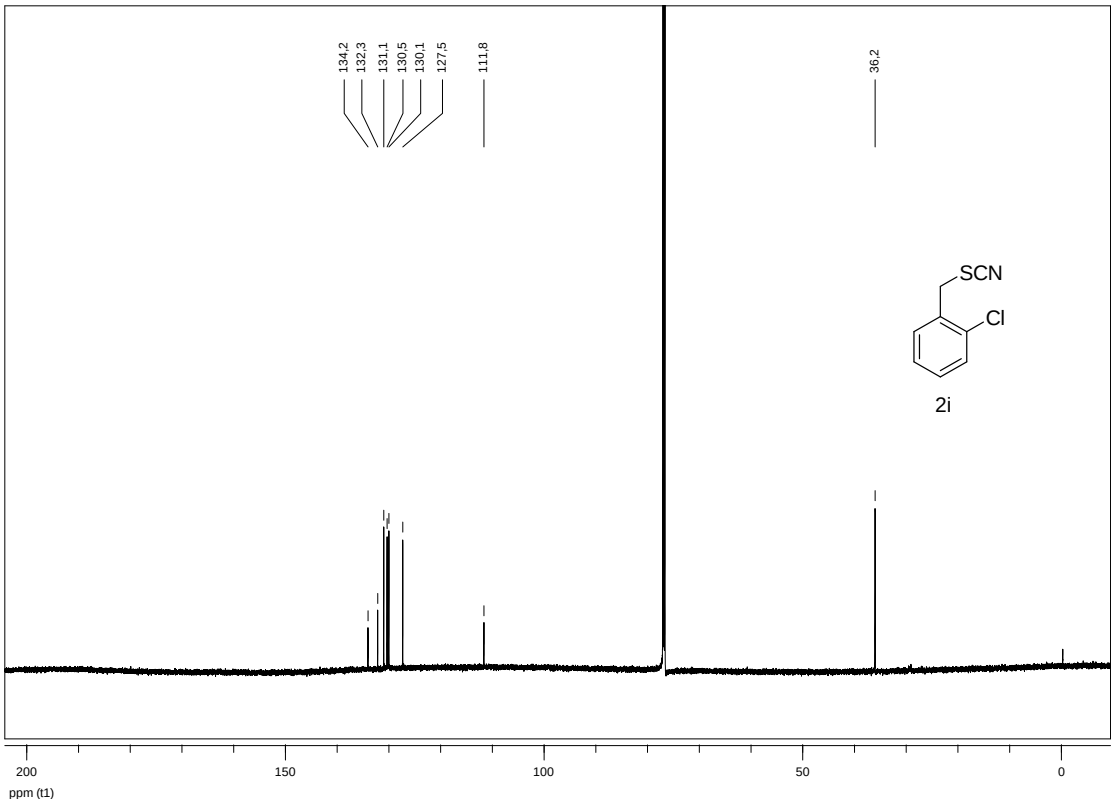
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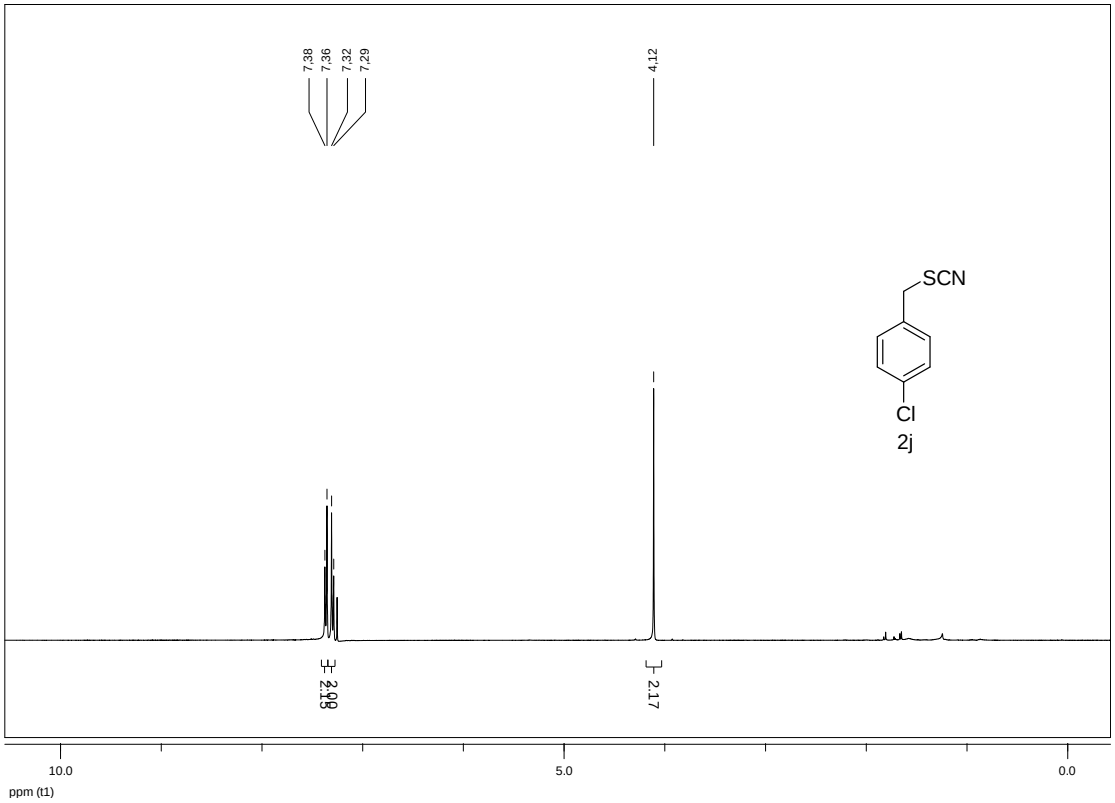
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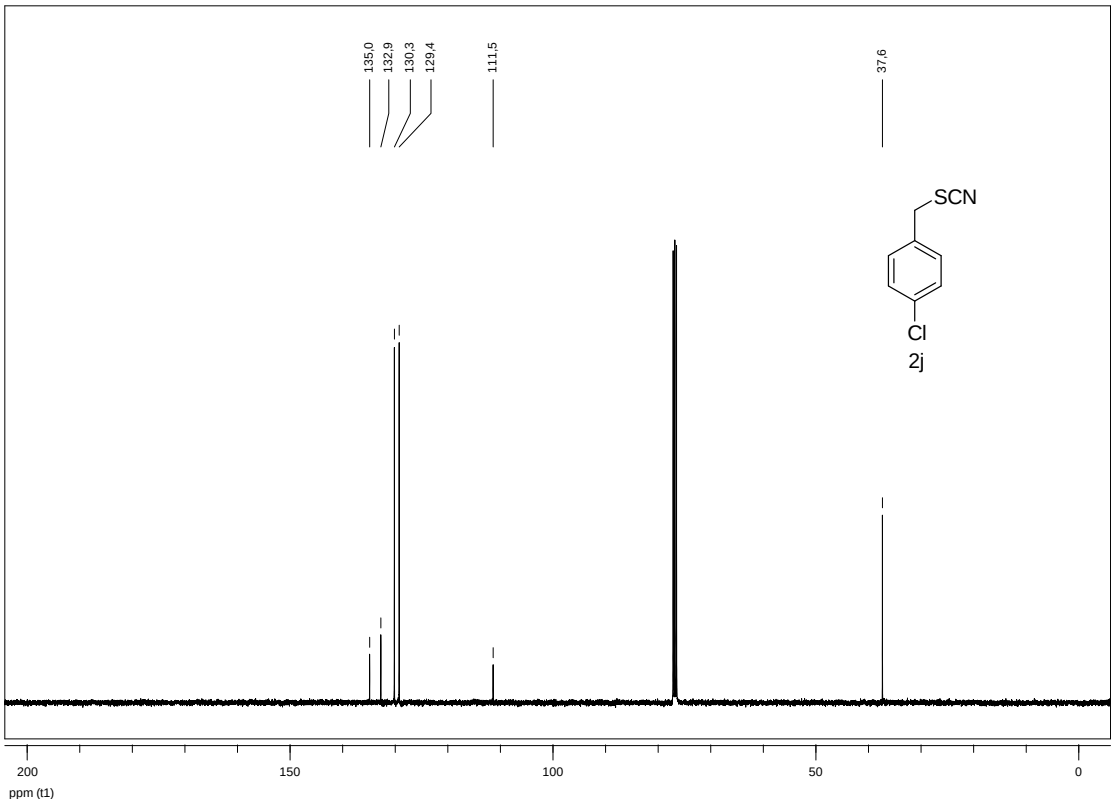
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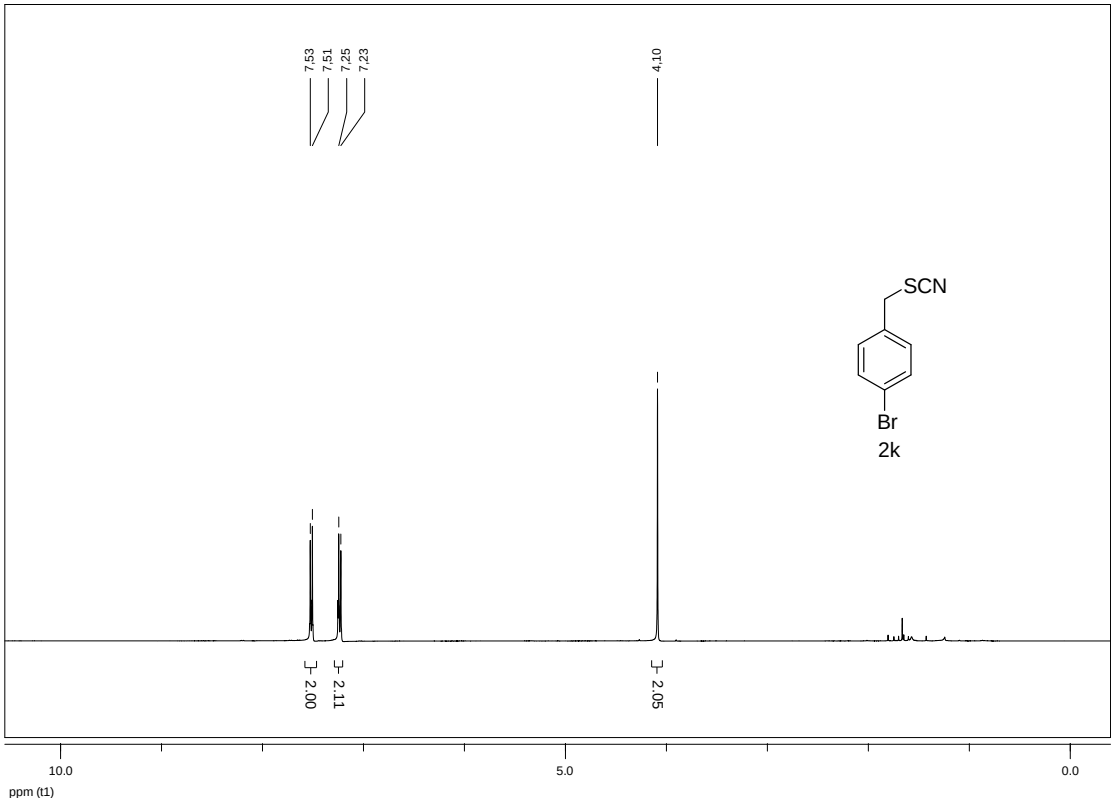
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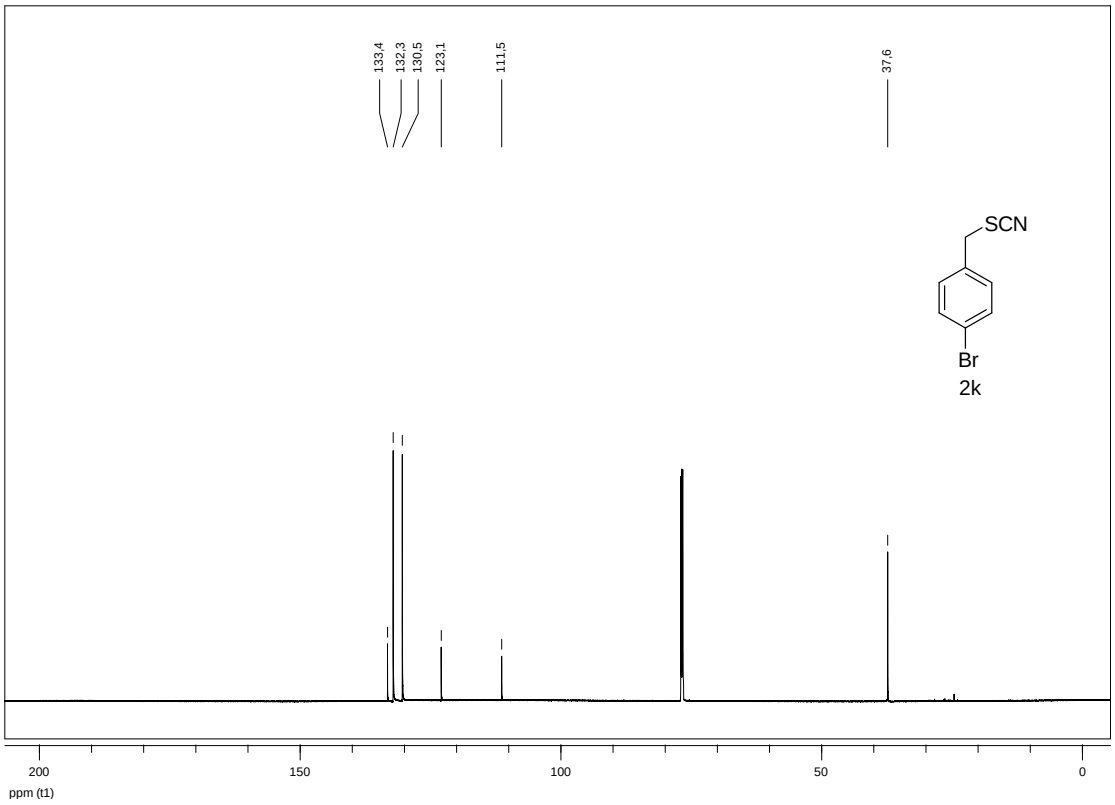
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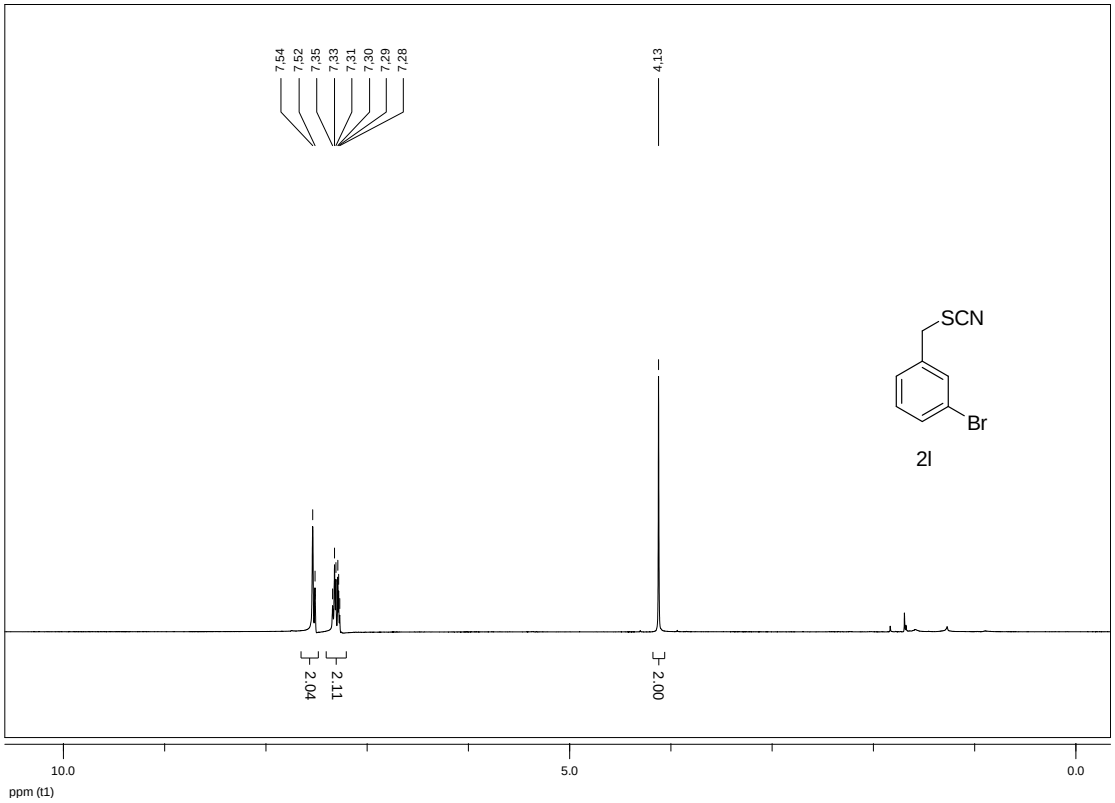
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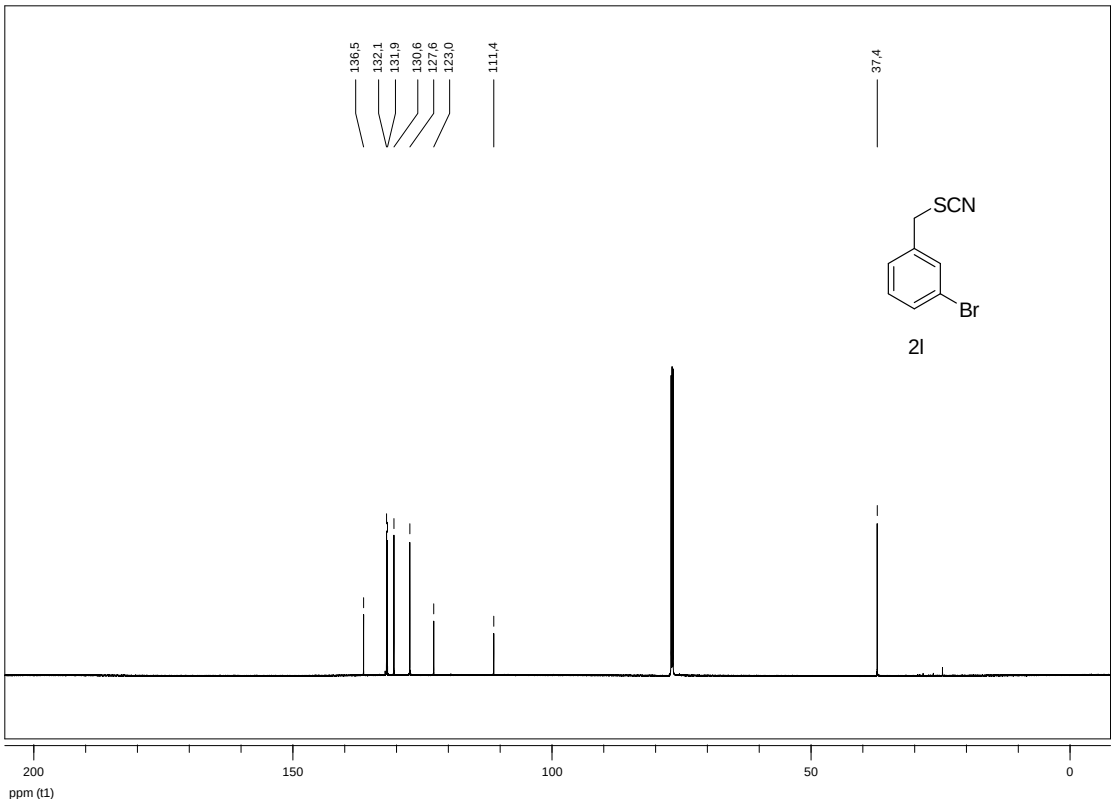
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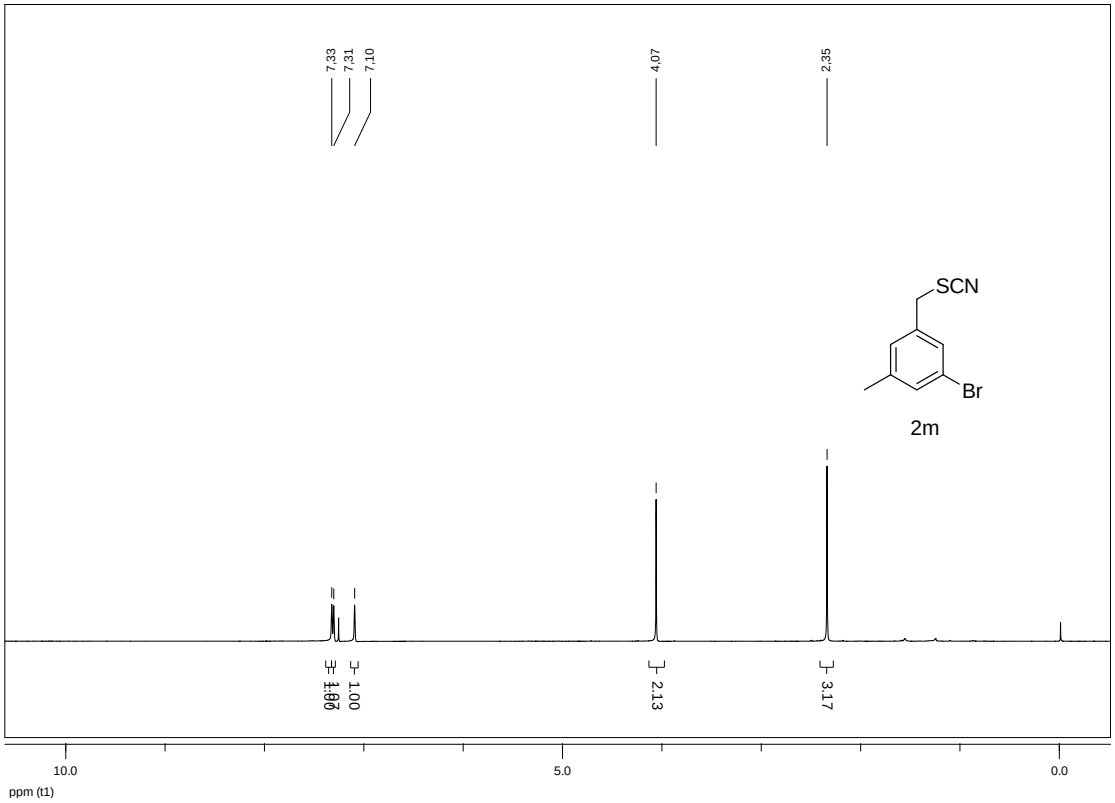
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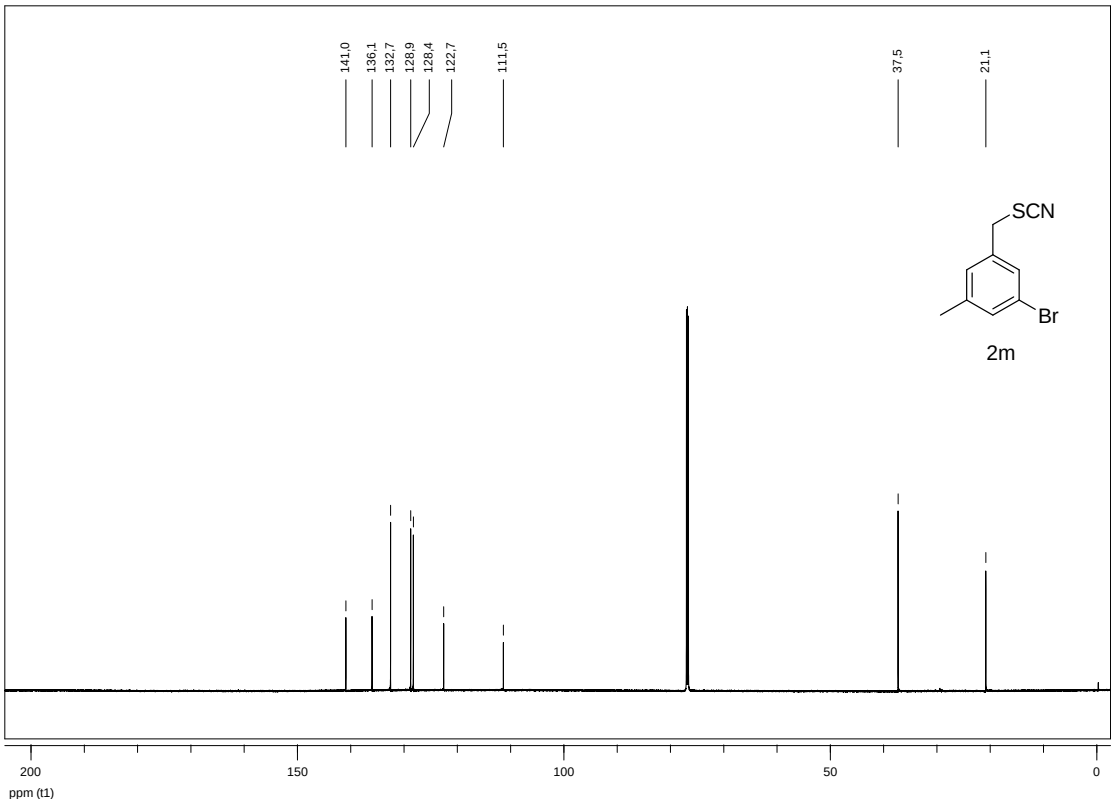
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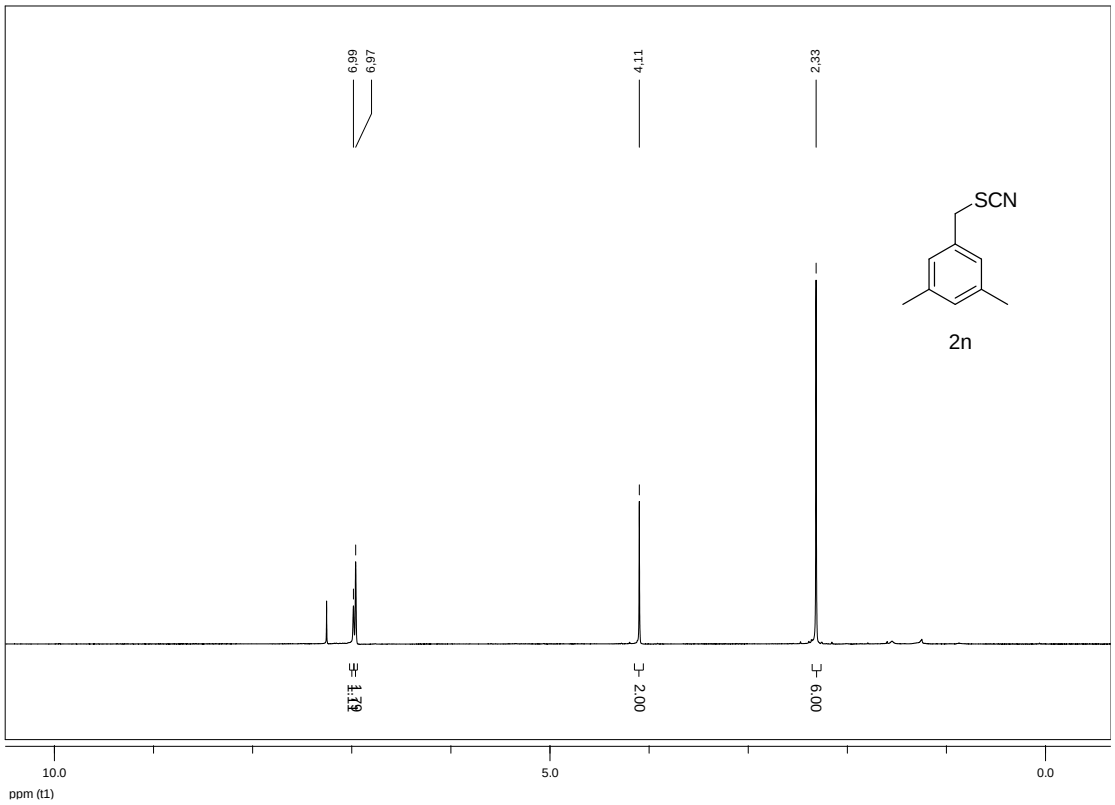
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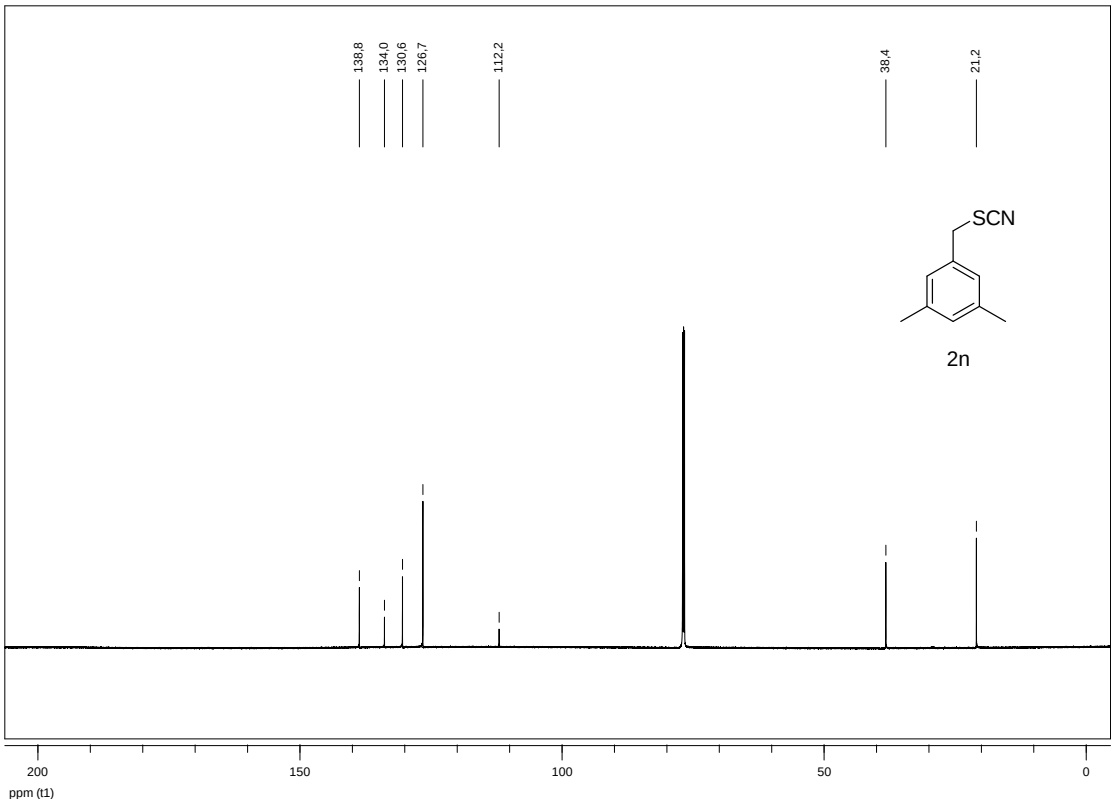
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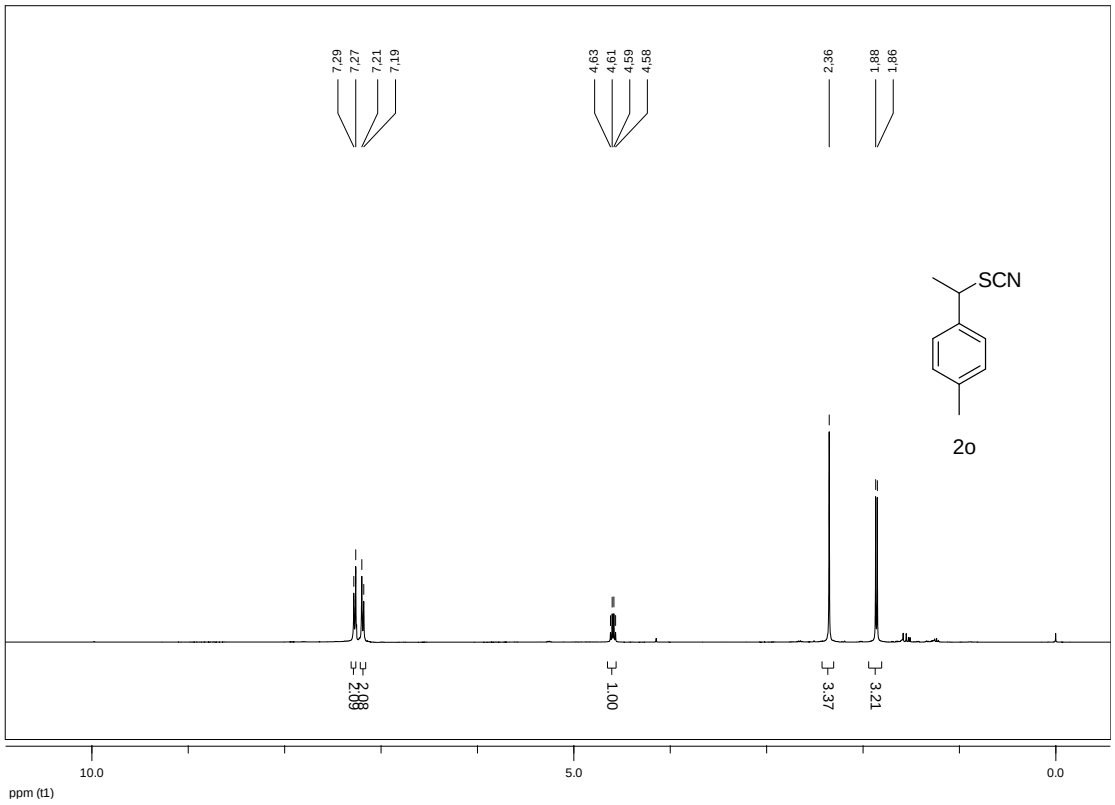
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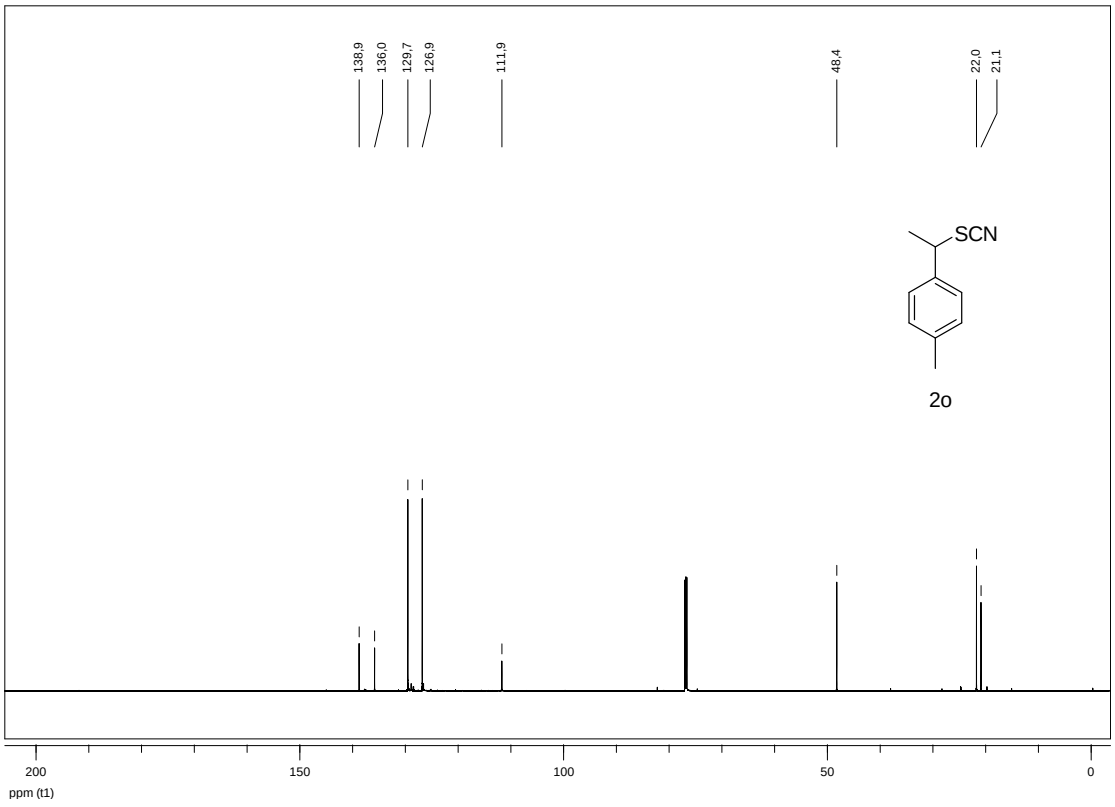
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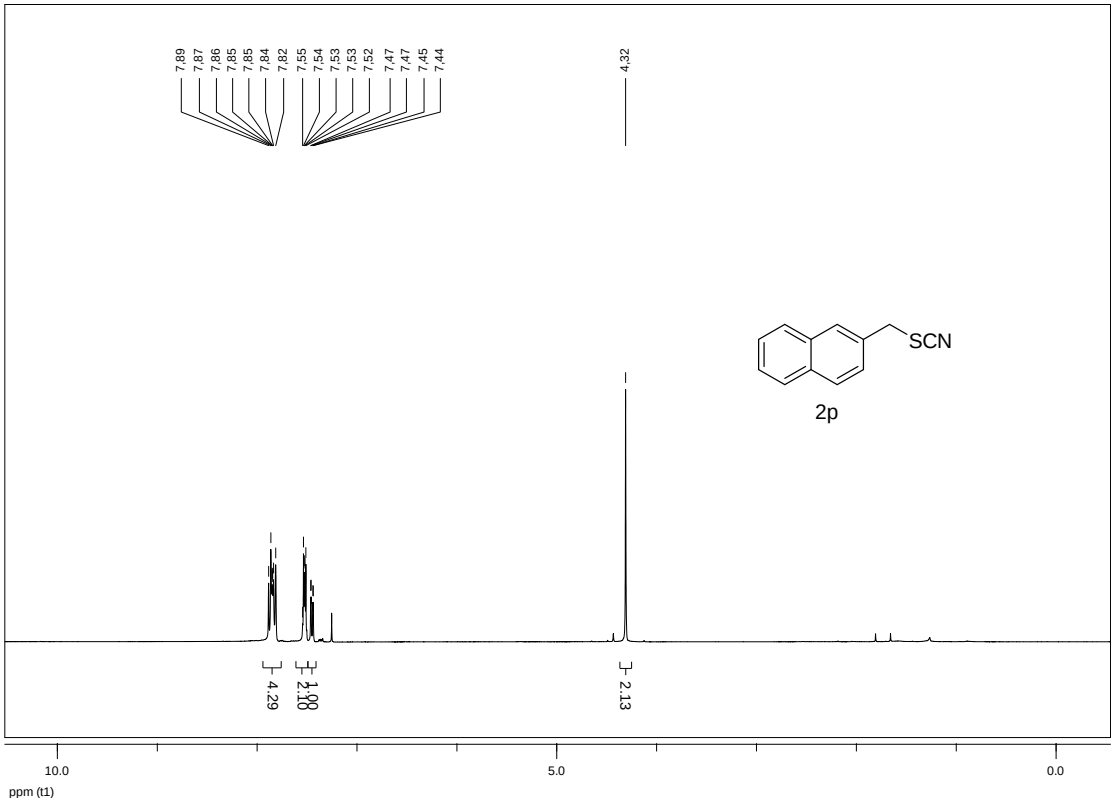
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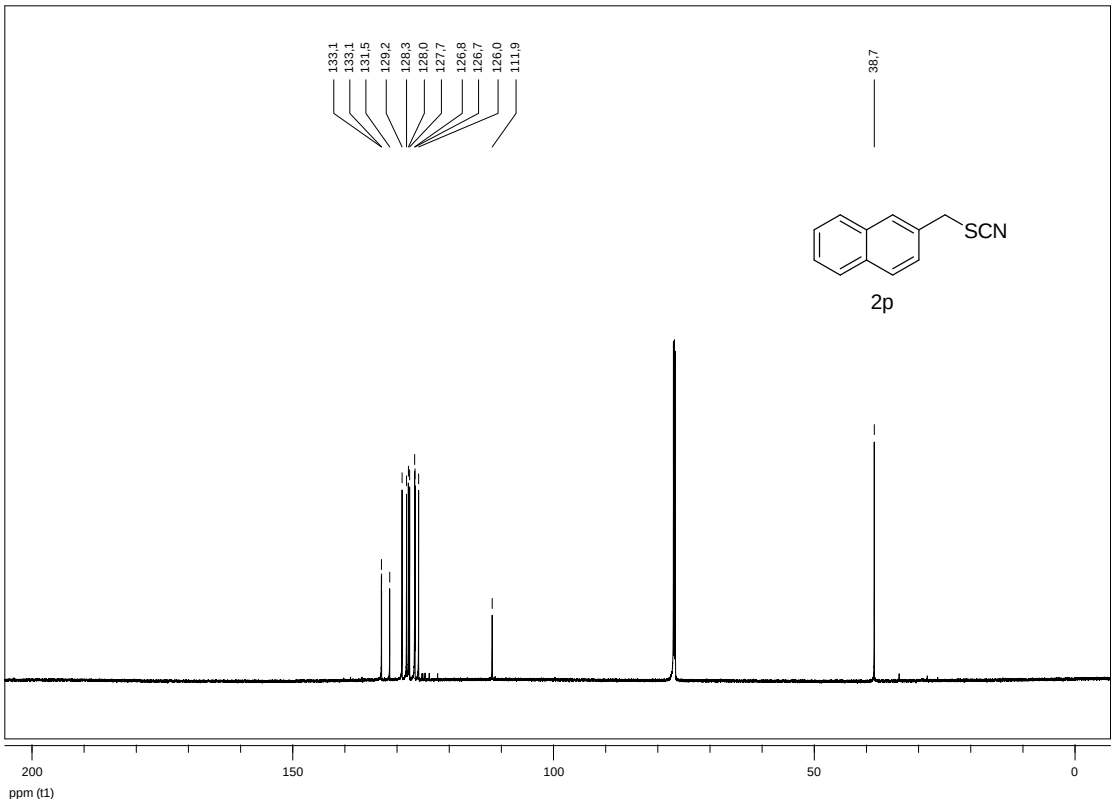
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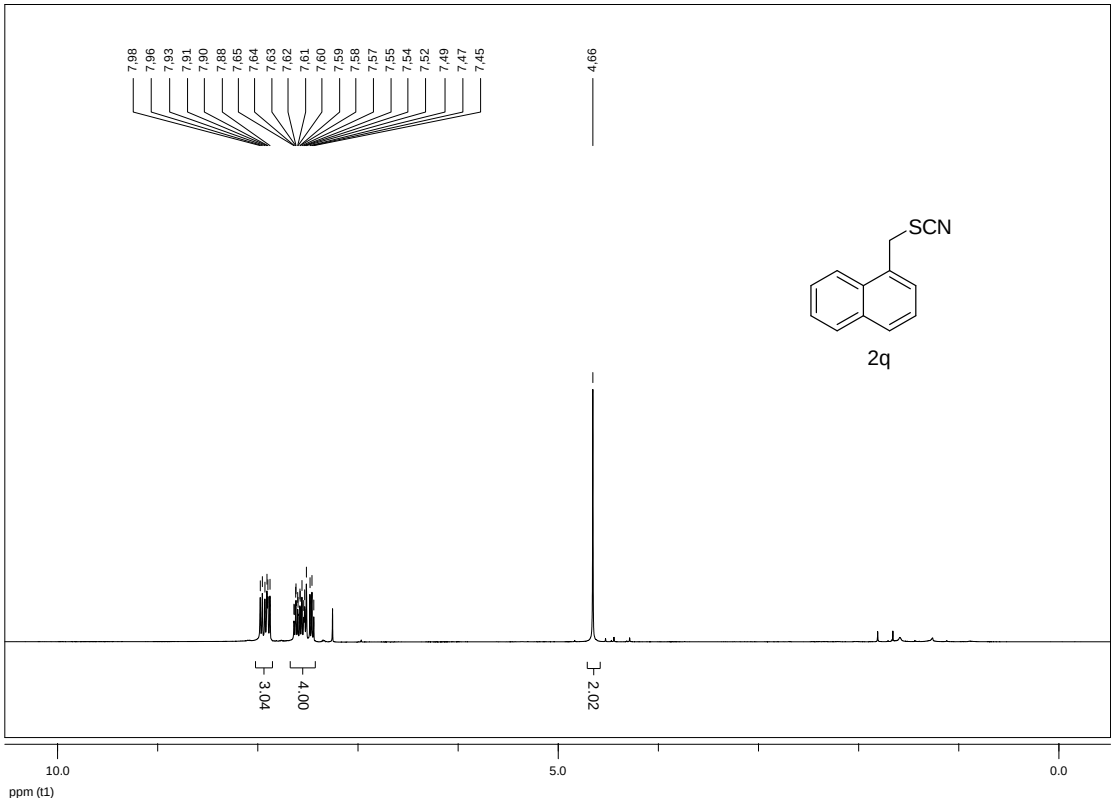
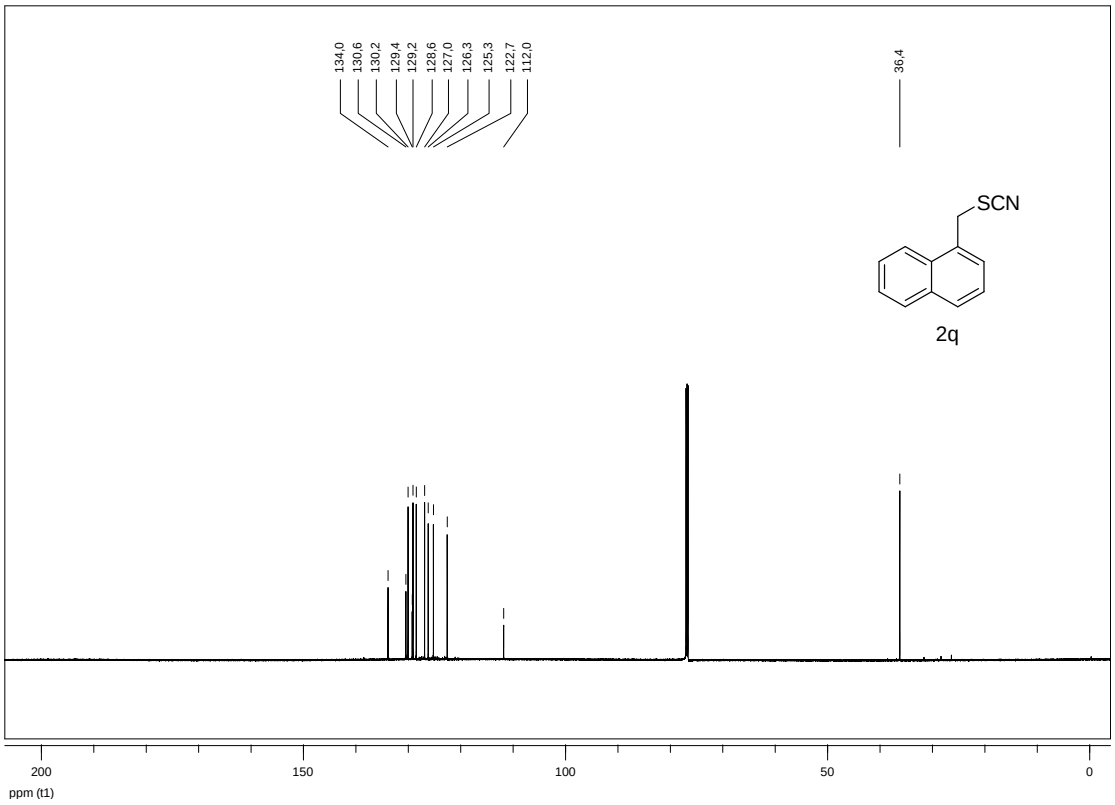
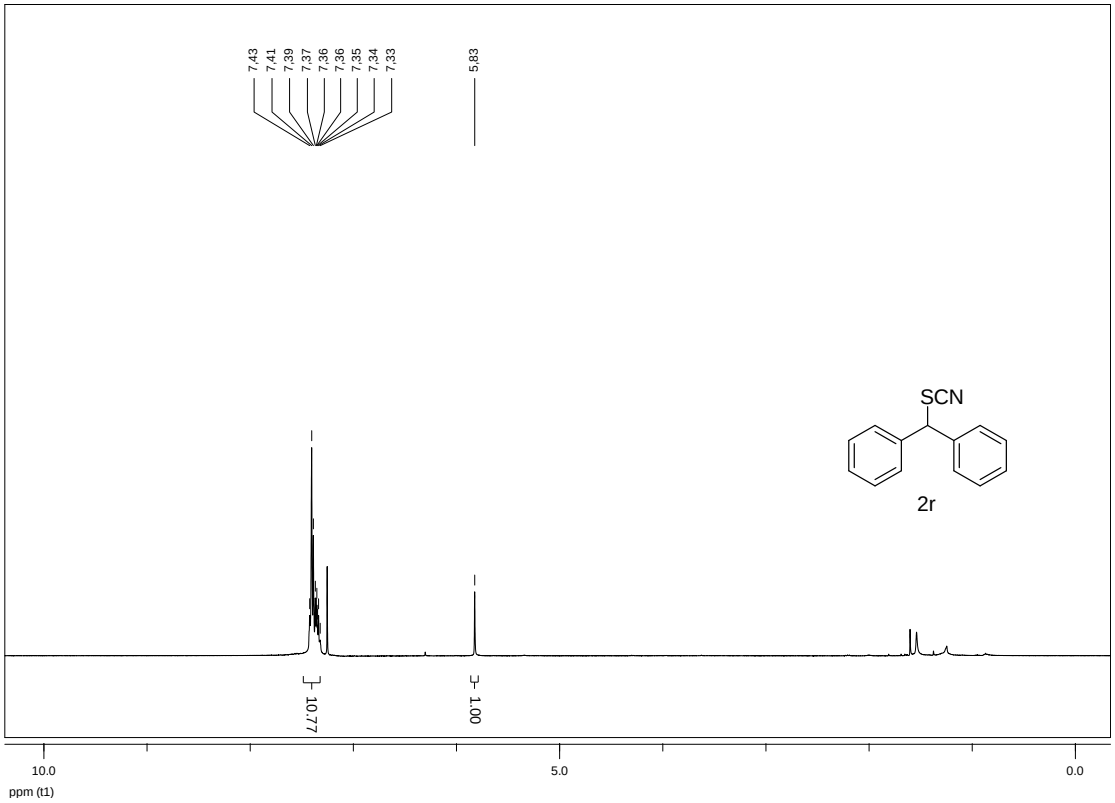
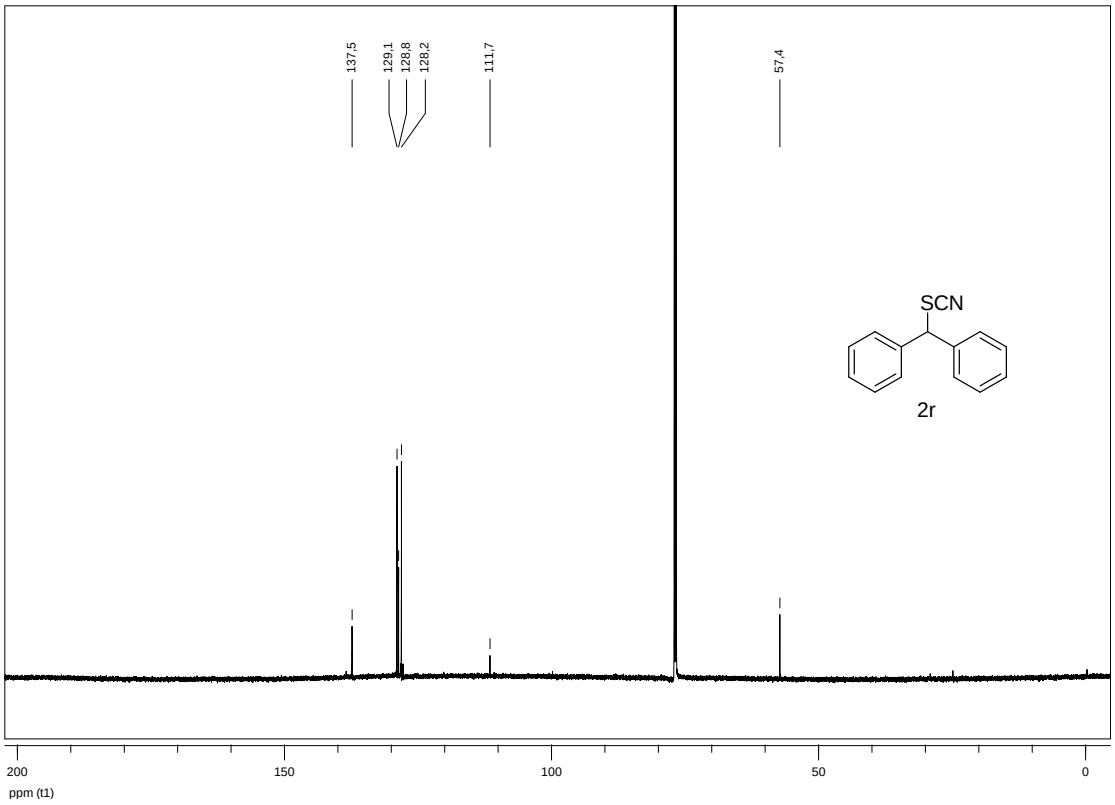
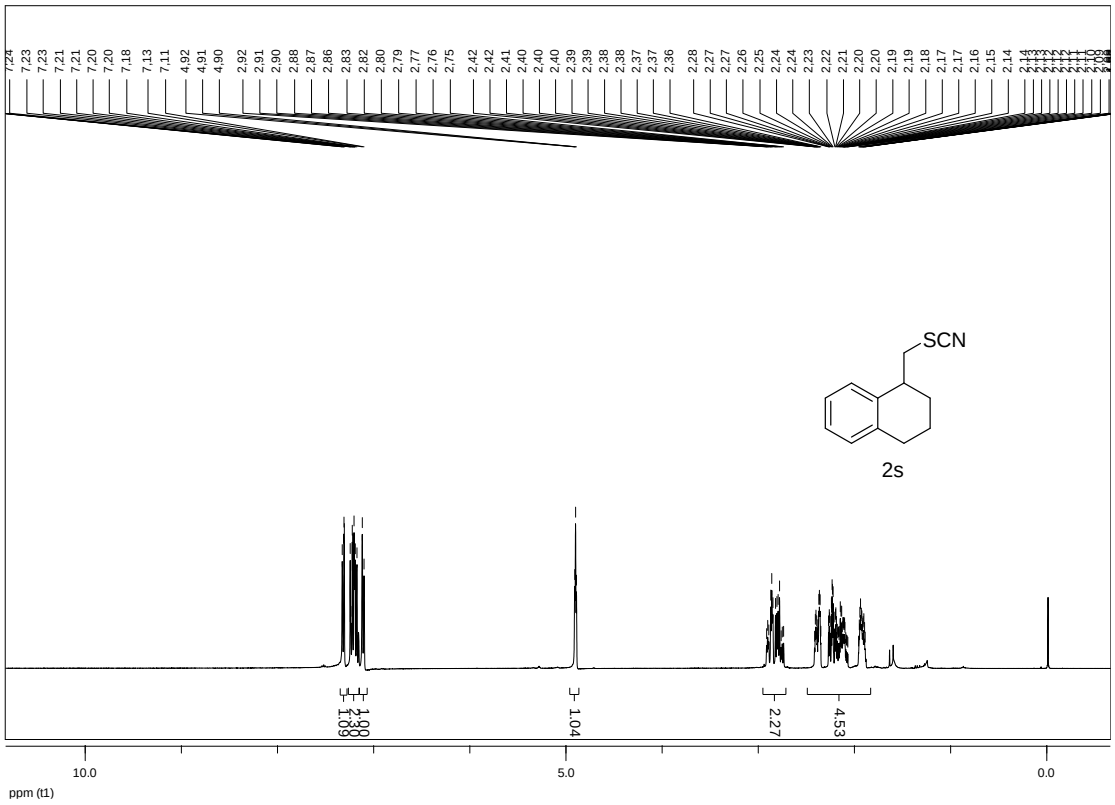
0
ppm (t1)

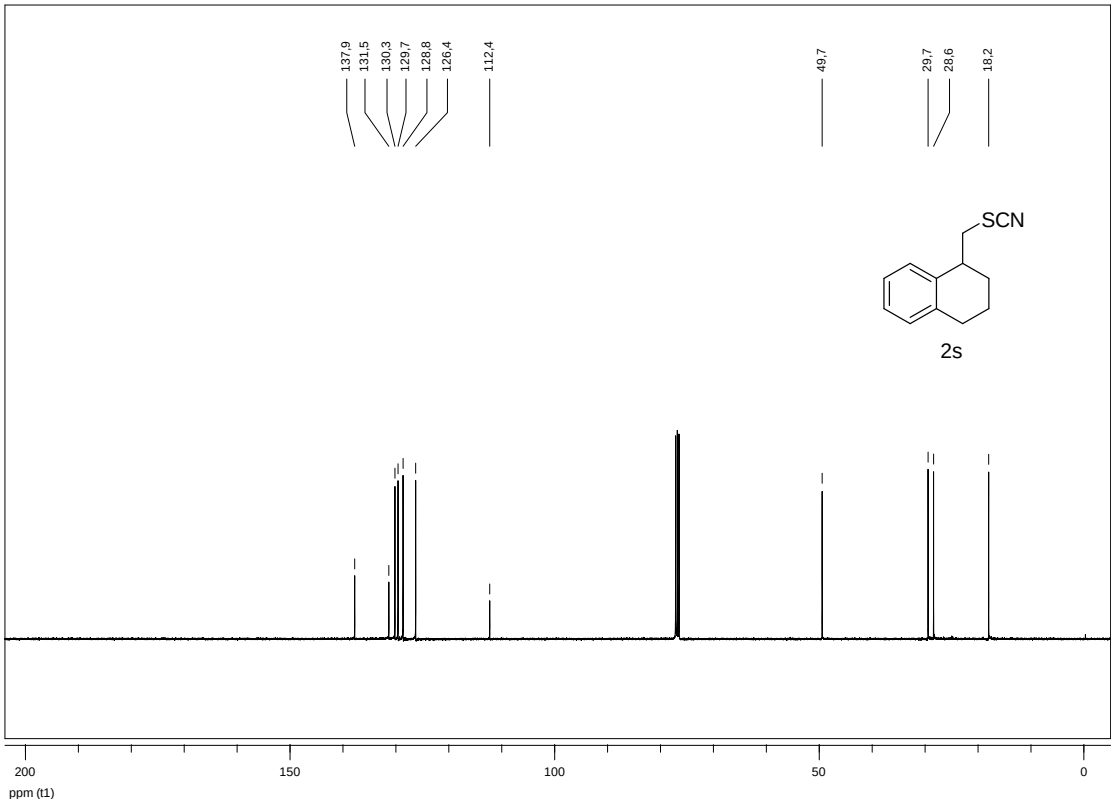

7,98
7,96
7,93
7,91
7,90
7,88
7,65
7,64
7,63
7,62
7,61
7,60
7,59
7,58
7,57
7,55
7,54
7,52
7,49
7,47
7,45
4,66
SCN
2q
3,04
4,00
2,02
10.0
5.0
0.0
ppm (t1)

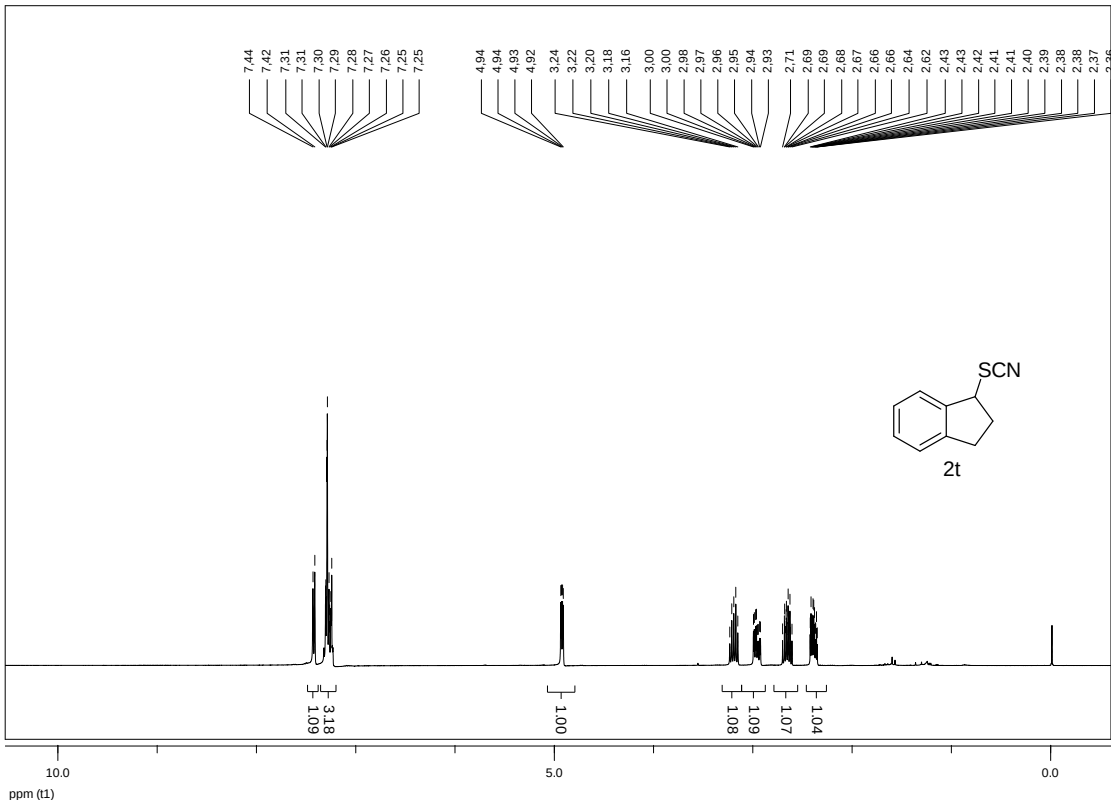

134,0
130,6
130,2
129,4
129,2
128,6
127,0
126,3
125,3
122,7
112,0
36,4
SCN
2q
200
150
100
50
0
ppm (t1)

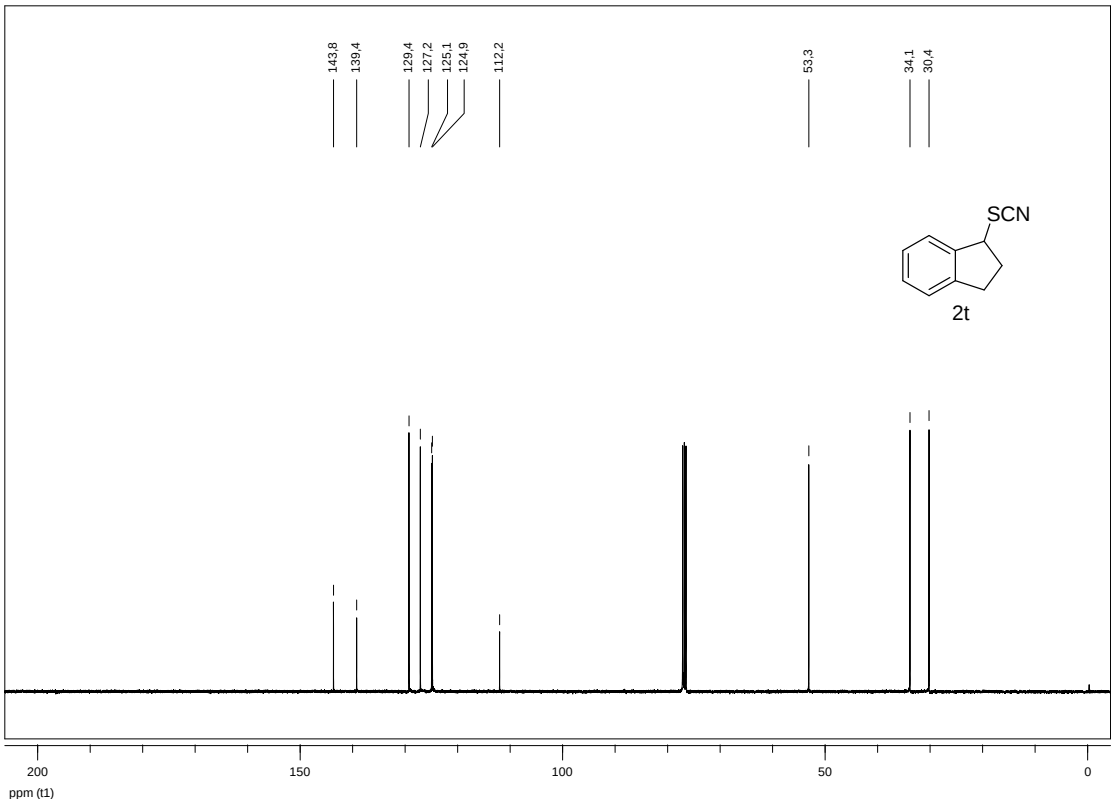

7.43
7.41
7.39
7.37
7.36
7.36
7.35
7.34
7.33
5.83
SCN
2r
10.77
1.00
10.0
5.0
0.0
ppm (t1)

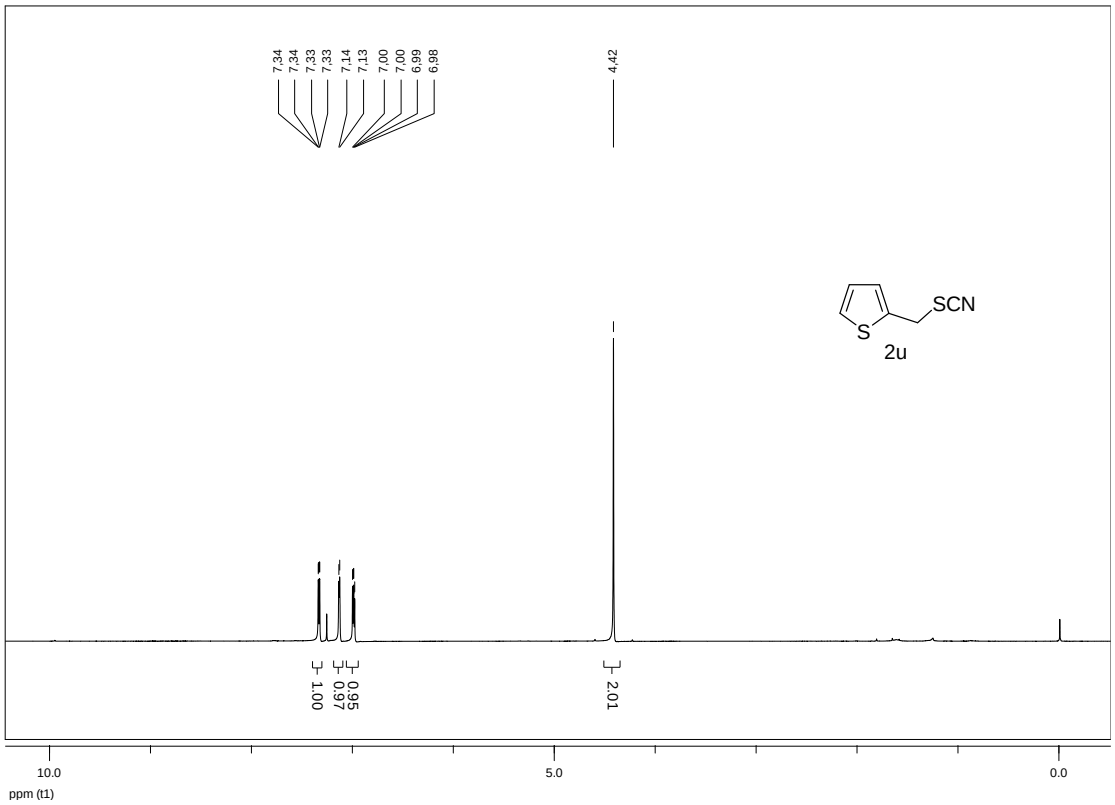

137.5
129.1
128.8
128.2
111.7
57.4
SCN
2r
200
150
100
50
0
ppm (t1)

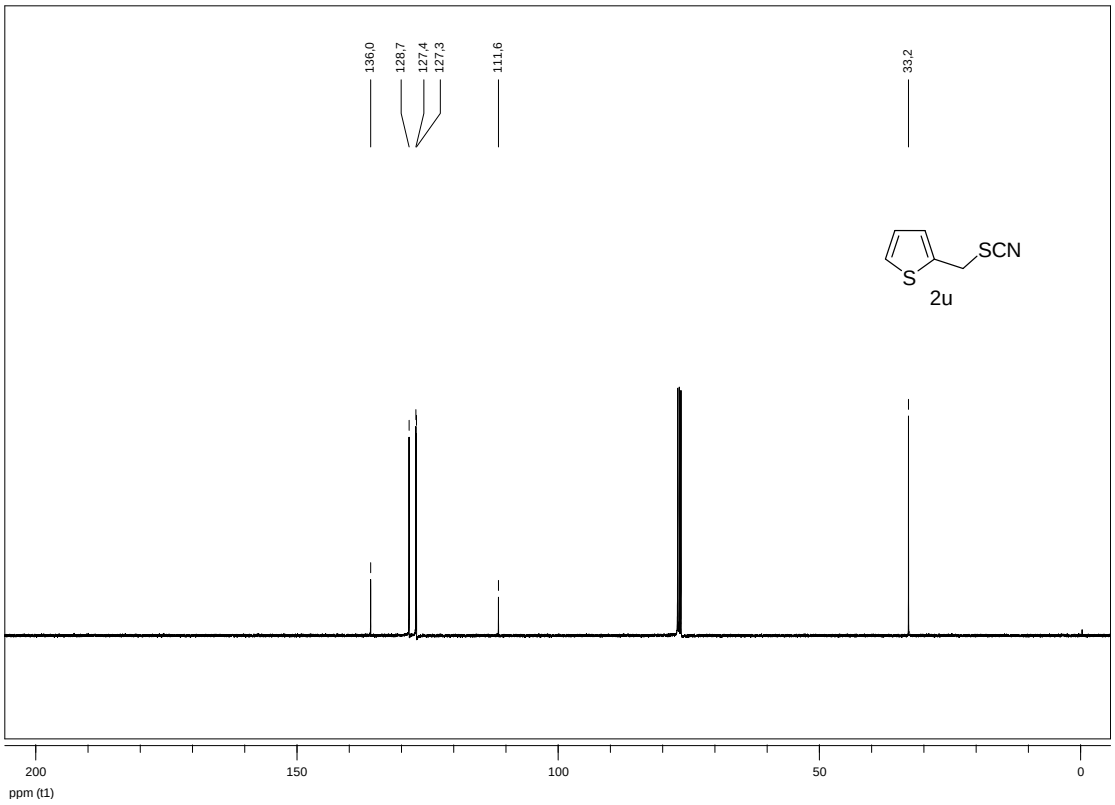

SCN
2s
1.09
1.38
1.00
1.04
2.27
4.53
10.0
5.0
0.0
ppm (t1)

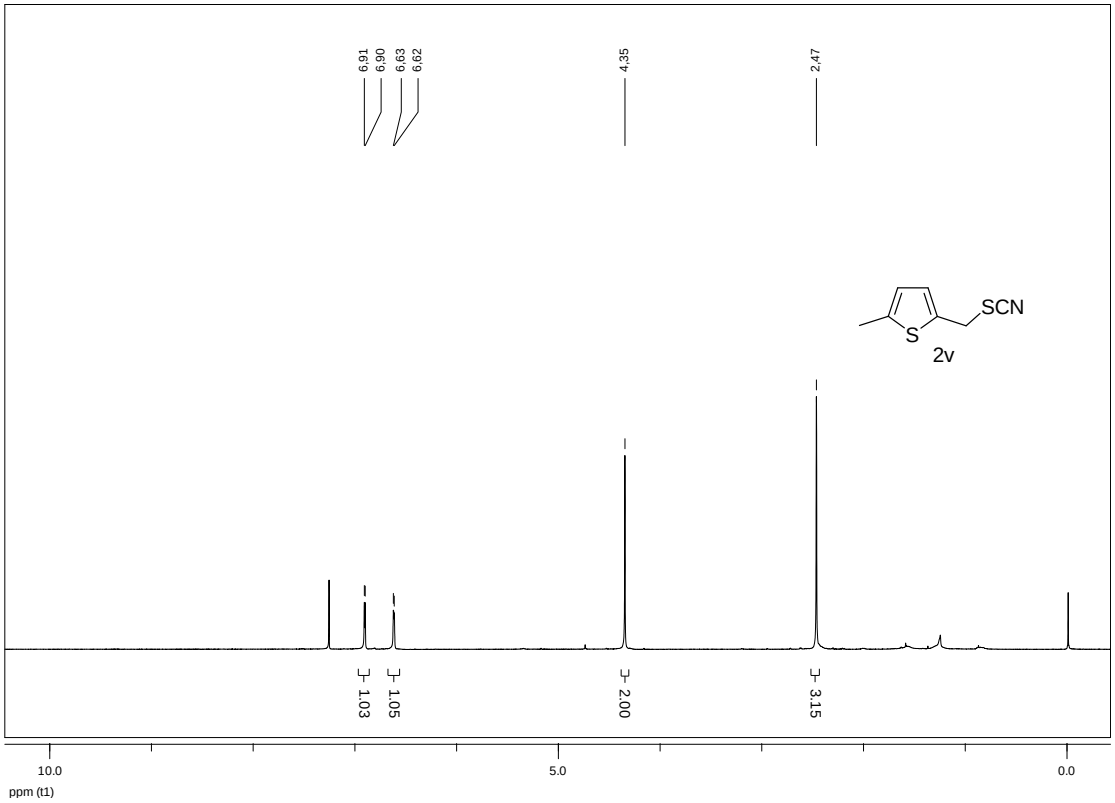

137.9
131.5
130.3
129.7
128.8
126.4
112.4
49.7
29.7
28.6
18.2
SCN
2s
200
150
100
50
0
ppm (t1)

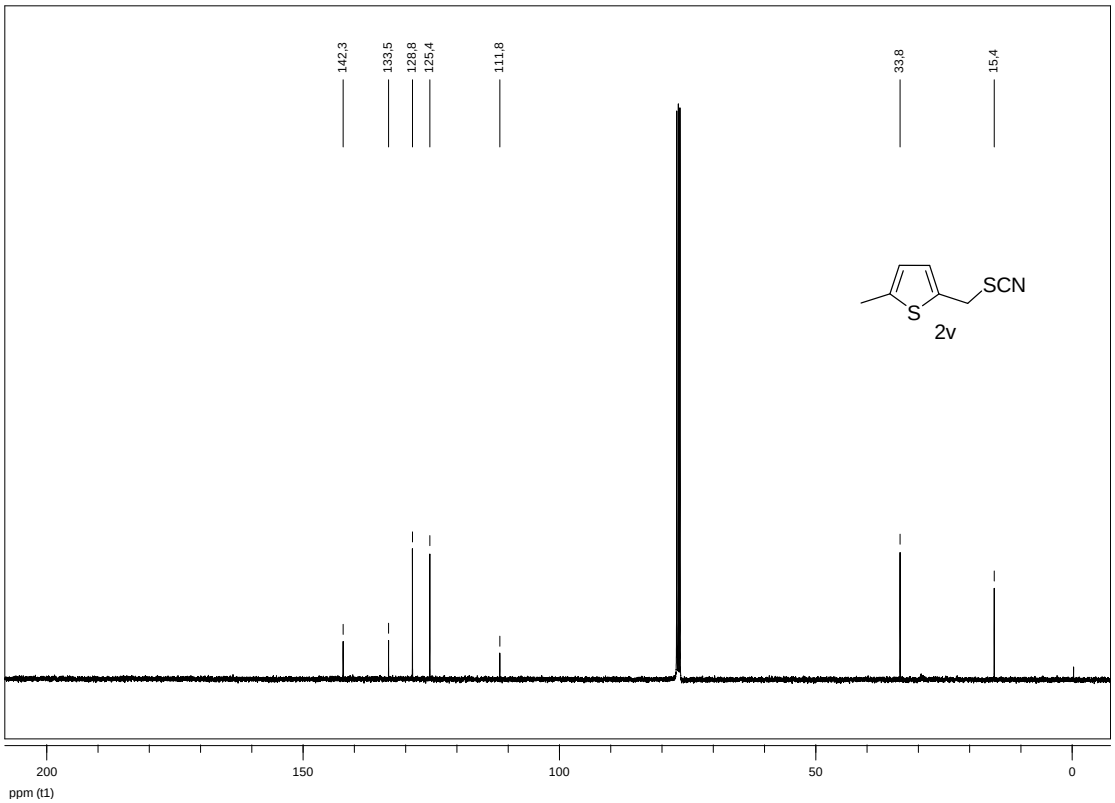

7,44
7,42
7,31
7,31
7,30
7,29
7,28
7,27
7,26
7,25
7,25
4,94
4,94
4,93
4,92
3,24
3,22
3,20
3,18
3,16
3,00
3,00
2,98
2,97
2,96
2,95
2,94
2,93
2,71
2,69
2,69
2,68
2,67
2,66
2,66
2,64
2,62
2,43
2,43
2,42
2,41
2,41
2,40
2,39
2,38
2,38
2,37
SCN
2t
1,09
3,18
1,00
1,08
1,09
1,07
1,04
10.0
5.0
0.0
ppm (t1)

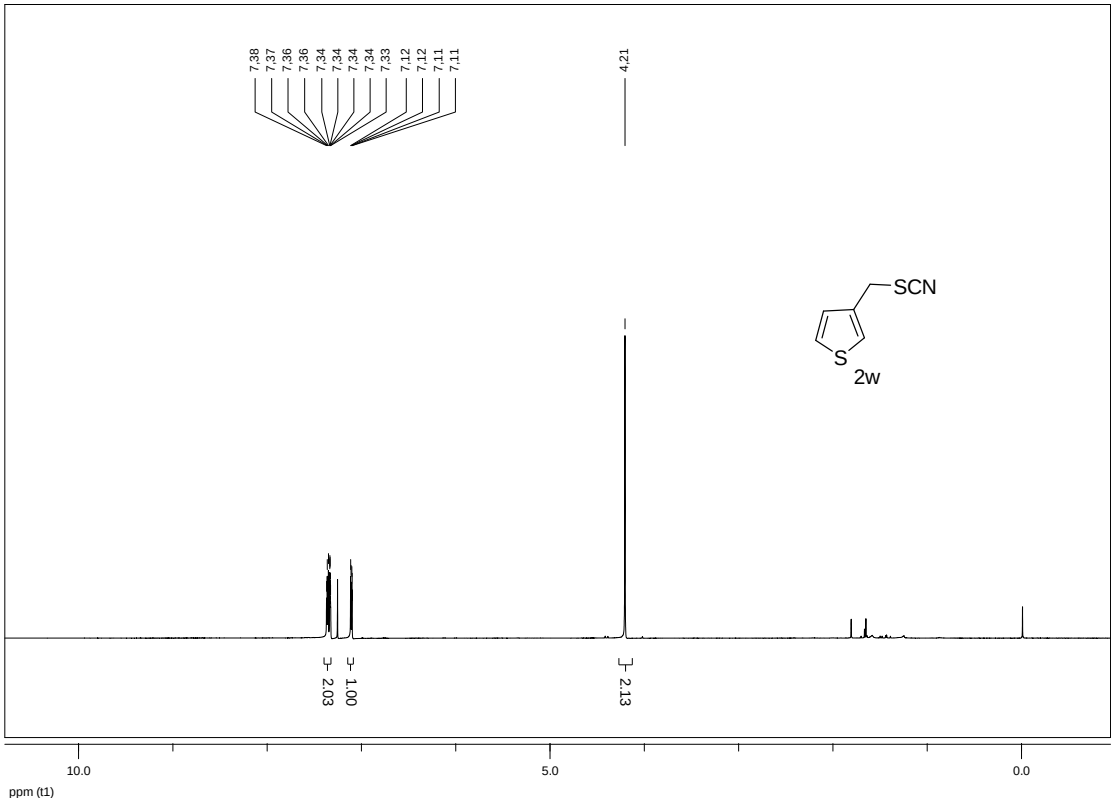

143,8
139,4
129,4
127,2
125,1
124,9
112,2
53,3
34,1
30,4
SCN
2t
200
150
100
50
0
ppm (t1)

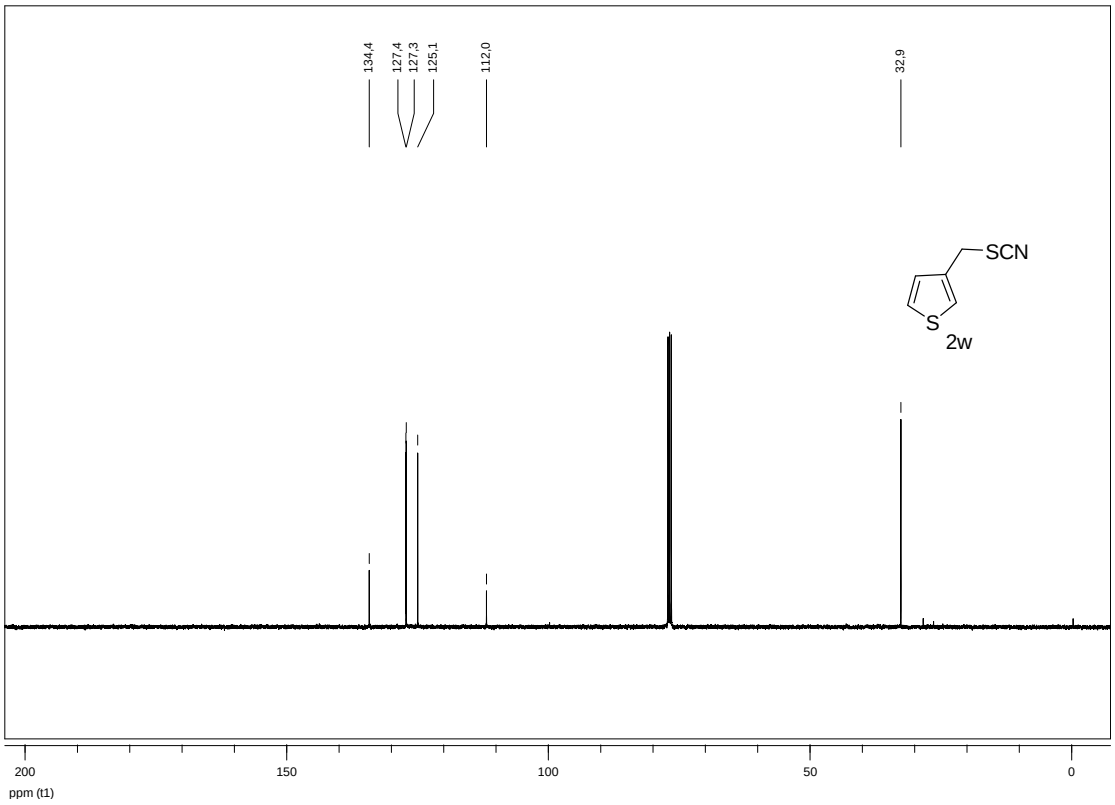

7,34
7,34
7,33
7,33
7,14
7,13
7,00
7,00
6,99
6,98
4,42
SCN
S
2u
1,00
0,97
0,95
2,01
10.0
5.0
0.0
ppm (t1)

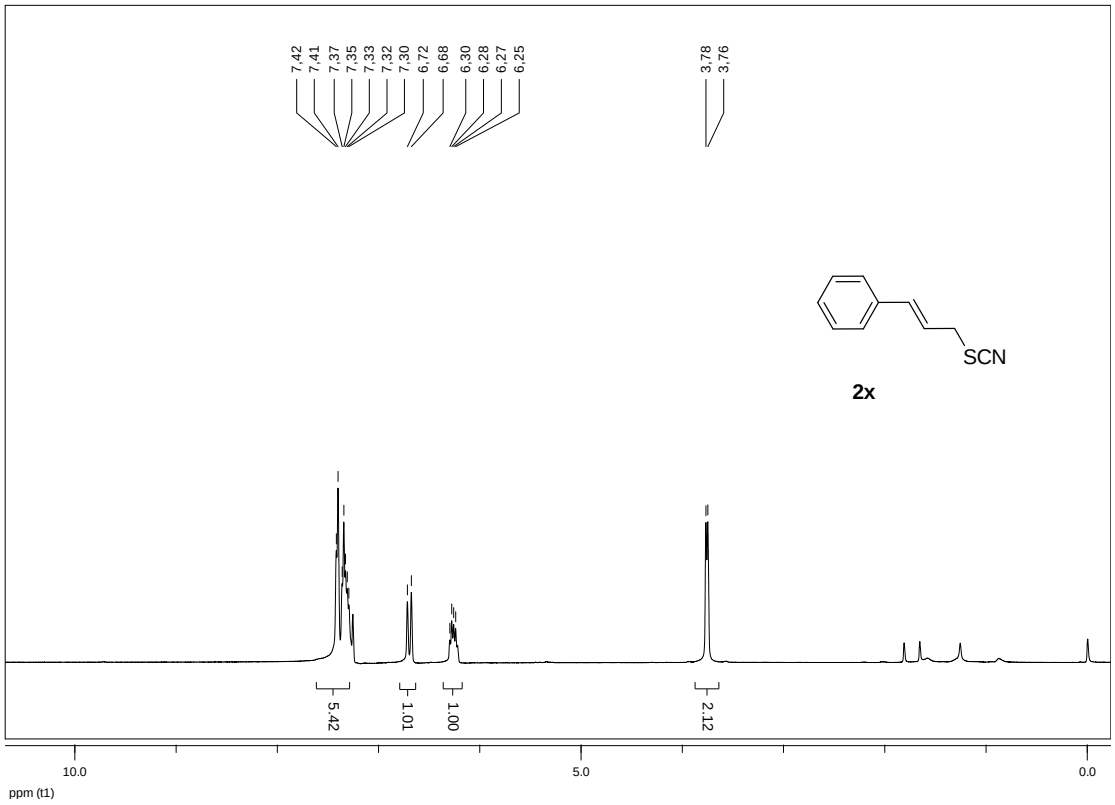

136,0
128,7
127,4
127,3
111,6
33,2
SCN
S
2u
200
150
100
50
0
ppm (t1)

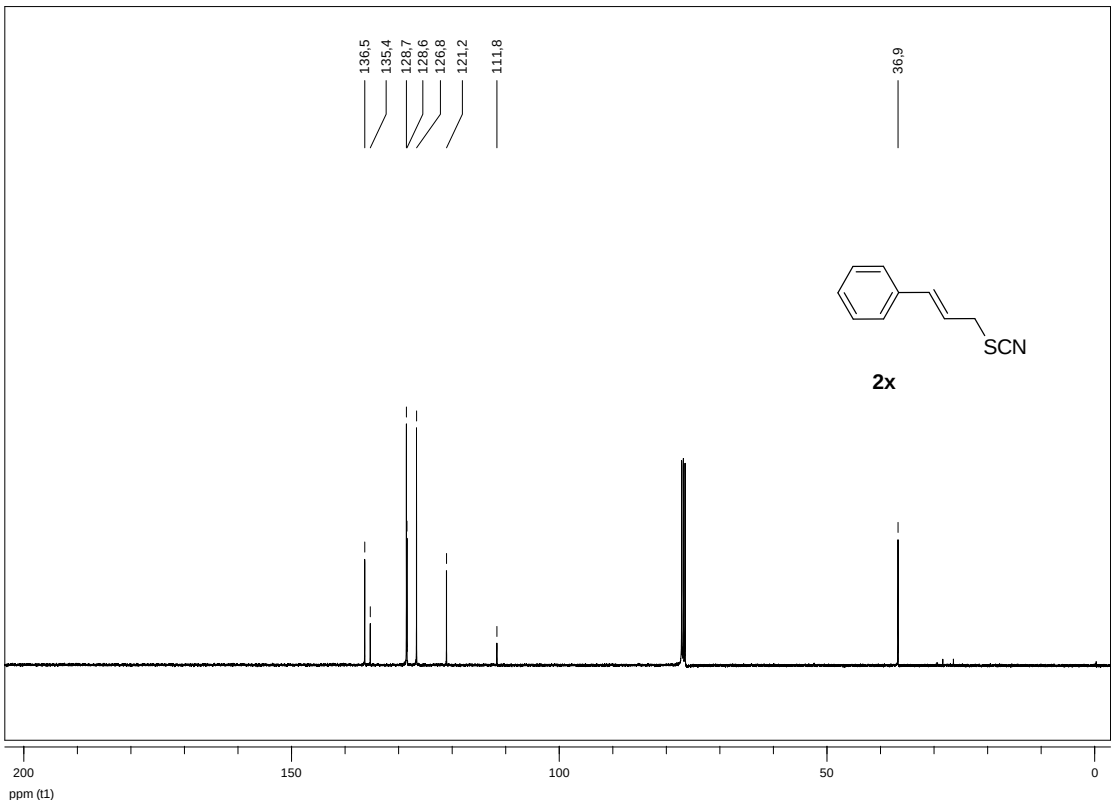

6,91
6,90
6,63
6,62
4,35
2,47
SCN
S
2v
1.03
1.05
2.00
3.15
10.0
5.0
0.0
ppm (t1)

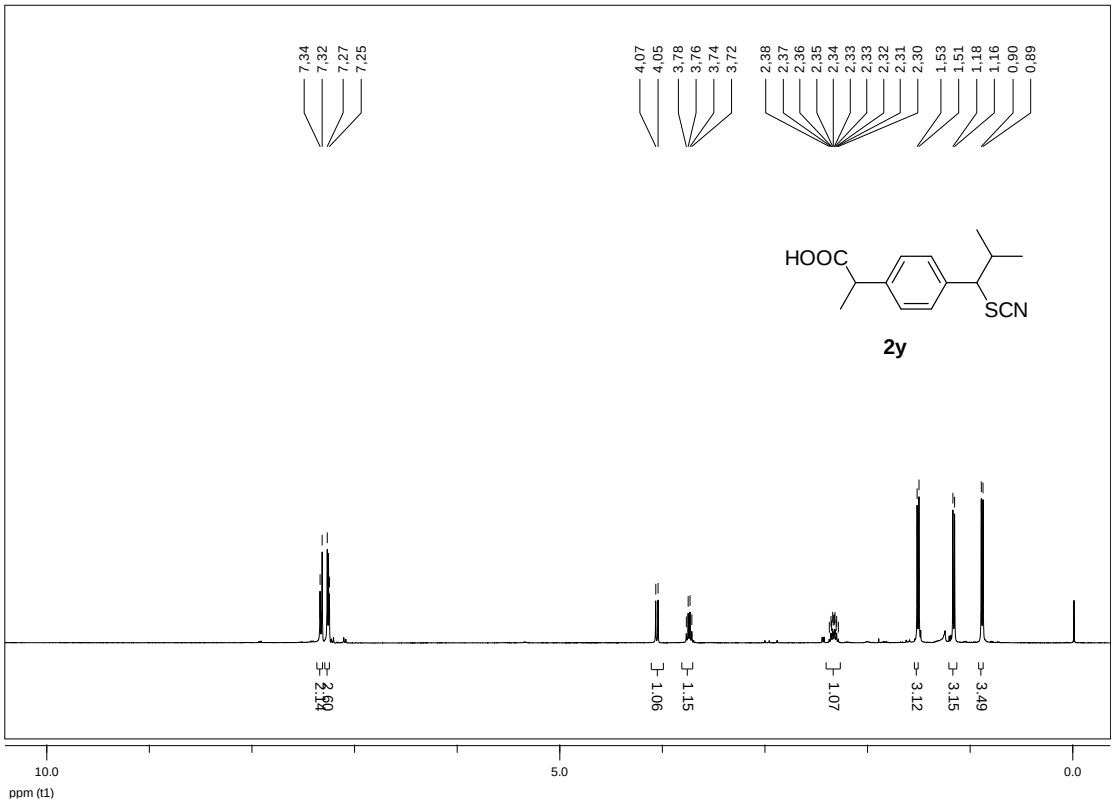

142,3
133,5
128,8
125,4
111,8
33,8
15,4
SCN
S
2v
200
150
100
50
0
ppm (t1)

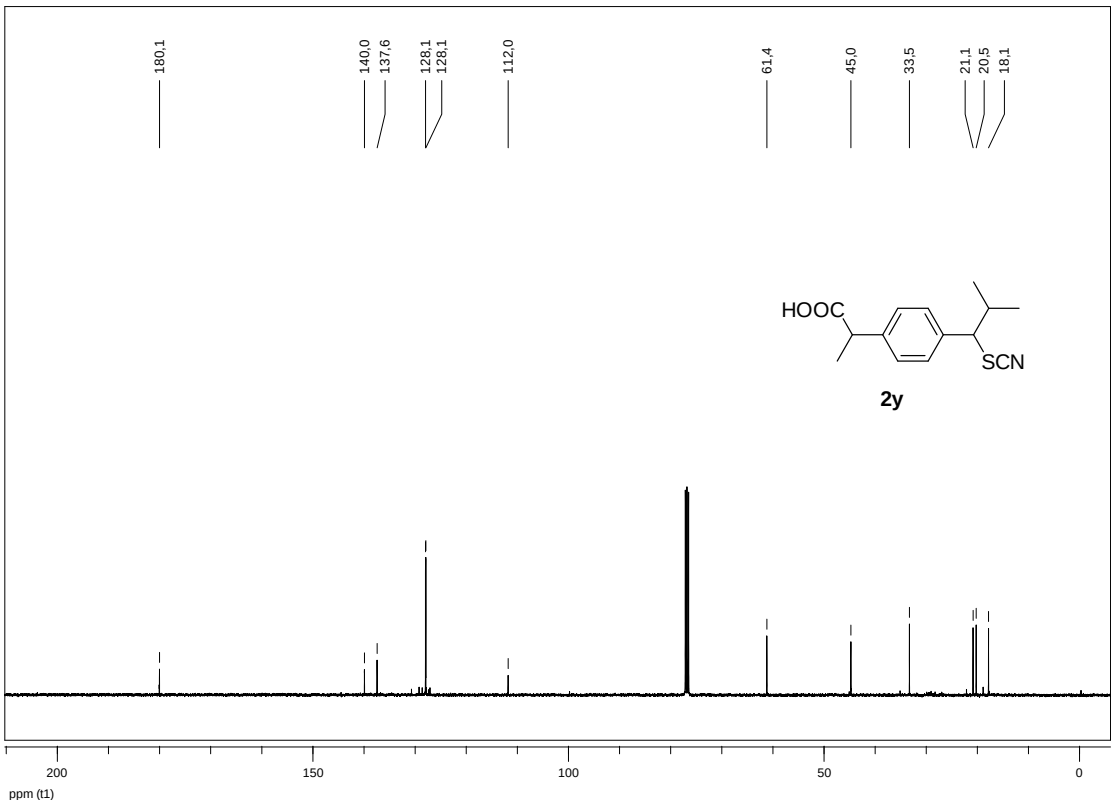

7.38
7.37
7.36
7.36
7.34
7.34
7.34
7.34
7.33
7.12
7.12
7.11
7.11
4.21
SCN
S
2w
2.03
1.00
2.13
10.0
5.0
0.0
ppm (t1)

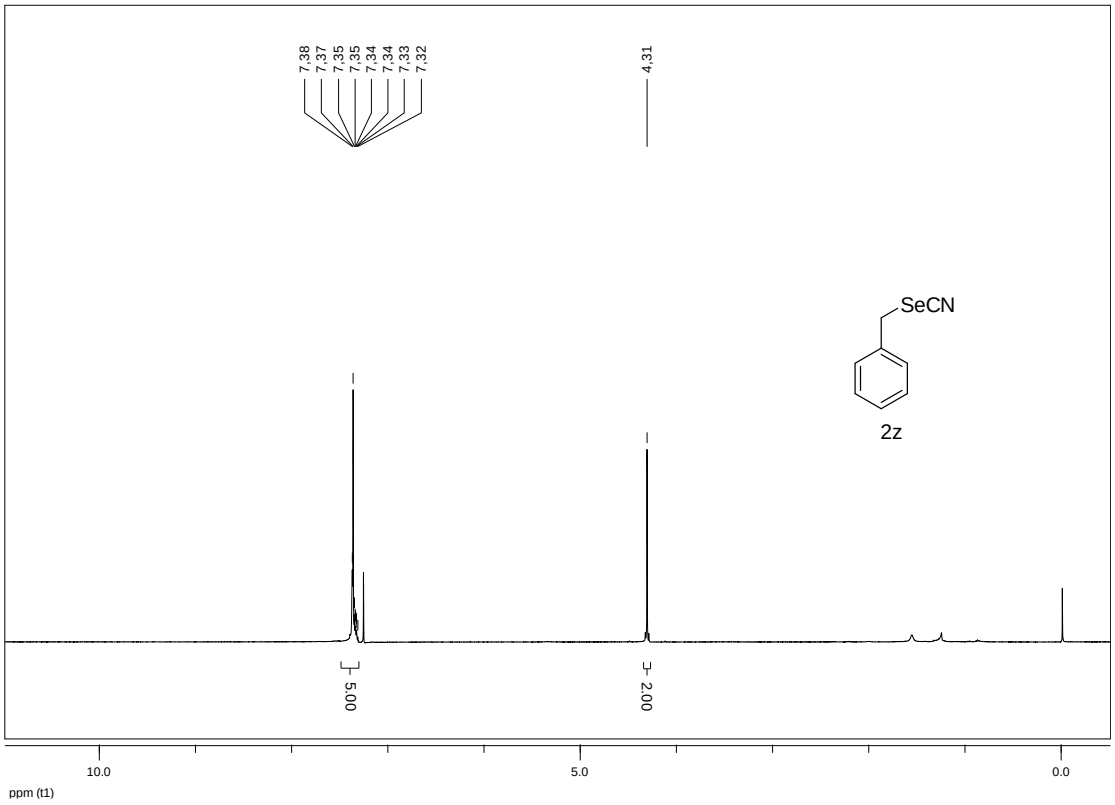

134.4
127.4
127.3
125.1
112.0
32.9
SCN
S
2w
200
150
100
50
0
ppm (t1)

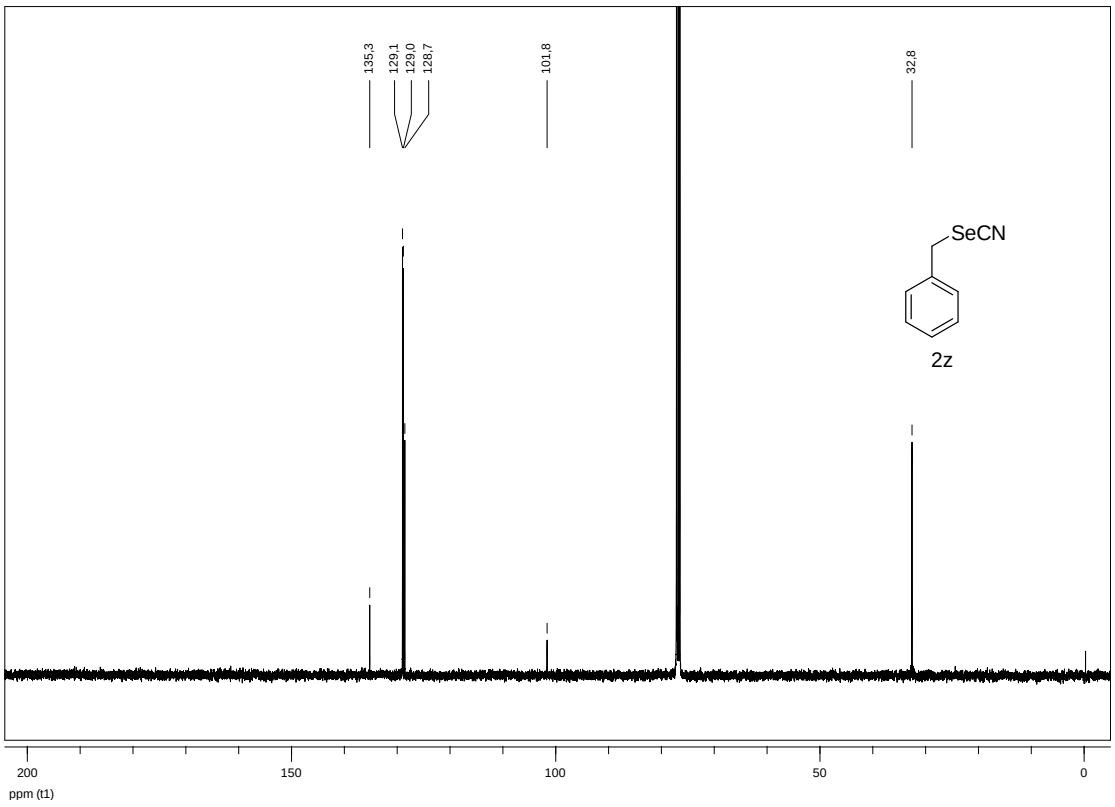

7,42
7,41
7,37
7,35
7,33
7,32
7,30
6,72
6,68
6,30
6,28
6,27
6,25
3,78
3,76
SCN
2x
5,42
1,01
1,00
2,12
10.0
5.0
0.0
ppm (t1)


136,5
135,4
128,7
128,6
126,8
121,2
111,8
36,9
SCN
2x
200
150
100
50
0
ppm (t1)


7.34
7.32
7.27
7.25
4.07
4.05
3.78
3.76
3.74
3.72
2.38
2.37
2.36
2.35
2.34
2.33
2.32
2.31
2.30
1.53
1.51
1.18
1.16
0.90
0.89
HOOC
SCN
2y
2.00
2.14
1.06
1.15
1.07
3.12
3.15
3.49
10.0
5.0
0.0
ppm (t1)


180.1
140.0
137.6
128.1
128.1
112.0
61.4
45.0
33.5
21.1
20.5
18.1
HOOC
SCN
2y
200
150
100
50
0
ppm (t1)


7,38
7,37
7,35
7,35
7,34
7,34
7,33
7,32
4,31
SeCN
2z
5,00
2,00
10.0
5.0
0.0
ppm (t1)


135,3
129,1
129,0
128,7
101,8
32,8
SeCN
2z
200
150
100
50
0
ppm (t1)