Electronic Supplementary Material (ESI) for Chemical Science.


# Electrochemical Radical-Mediated Selective C($sp^3$)-S Bond Activation

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# Supporting Information

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**General information**

All reactions were run under a nitrogen atmosphere in an undivided cell. All glassware was oven dried at 110 ºC for hours and cooled down under vacuum. Unless otherwise noted, sulfides and thiols were obtained from commercial suppliers and used without further purification. Some sulfides were synthesized according to the literature.[1] The Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. Flash chromatography columns were packed with 200-300 mesh silica gel in petroleum (bp. 60-90 ºC). GC-MS spectra were recorded on a Varian GC-MS 3900-2100T. All new compounds were characterized by $^{1}$H NMR, $^{13}$C NMR and HRMS. The known compounds were characterized by $^{1}$H NMR, $^{13}$C NMR. $^{1}$H and $^{13}$C NMR data were recorded with Bruker (400 MHz) NMR spectrometer with tetramethylsilane as an internal standard. High resolution mass spectra (HRMS) were measured with a Waters Micromass GCT instrument and accurate masses were reported for the molecular ion + Hydrogen (M+H), or + Sodium (M+Na). All chemical shifts (δ) were reported in ppm and coupling constants (*J*) in Hz. All chemical shifts were reported relative to tetramethylsilane (0 ppm for $^{1}$H), $CDCl_3$ (77.16 ppm for $^{13}$C) and DMSO (2.50 ppm for $^{1}$H, 39.52 ppm for $^{13}$C), respectively.

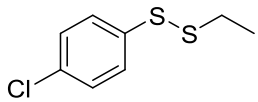
# Experimental section

## 1) Graphical guide for the set-up

As experimental set-up, a carbon rod electrode (Φ 6 mm), a platinum plate electrode (15 mm×15 mm×0.3 mm), a nickel plate electrode (15 mm×15 mm×1 mm), rubber plugs, an undivided three-necked bottle and a dual display potentiostat (DJS-292B) (made in China) were used.


**Figure S1.** Graphical Guide for the set-up

## 2) Analytical data of compounds.

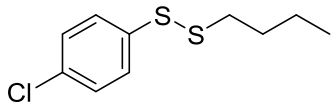


**1-(4-Chlorophenyl)-2-ethyldisulfane (3a).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 8.6, 1.9 Hz, 2H), 7.32 – 7.27 (m, 2H), 2.75 (qd, *J* = 7.4, 1.8 Hz, 2H), 1.31 (td, *J* = 7.4, 1.8 Hz, 3H).

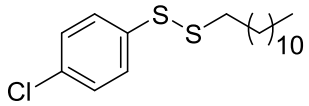
$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.44, 132.75, 129.17, 128.84, 32.86, 14.29.

**HRMS (APCI+)**: m/z calcd for $C_8H_9ClS_2$ $[M]^+$: 203.9829, found: 203.9831.



**1-Butyl-2-(4-chlorophenyl)disulfane (3b).**[2]

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.47 (dd, *J* = 8.6, 1.2 Hz, 2H), 7.29 (dd, *J* = 8.6, 1.2 Hz, 2H), 2.73 (t, *J* = 7.3 Hz, 2H), 1.64 (p, *J* = 7.4 Hz, 2H), 1.42 – 1.36 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H).
$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.43, 132.72, 129.16, 128.83, 38.77, 30.98, 21.73, 13.77.

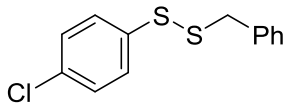


**1-(4-Chlorophenyl)-2-dodecyldisulfane (3c).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.42 (m, 2H), 7.32 – 7.26 (m, 2H), 2.75 – 2.69 (m, 2H), 1.65 (dt, *J* = 9.4, 5.8 Hz, 2H), 1.35 (d, *J* = 7.5 Hz, 2H), 1.27 – 1.23 (m, 16H), 0.87 (d, *J* = 7.0 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.45, 132.71, 129.16, 128.85, 39.12, 32.07, 29.79, 29.78, 29.72, 29.61, 29.50, 29.30, 28.90, 28.57, 22.85, 14.30.

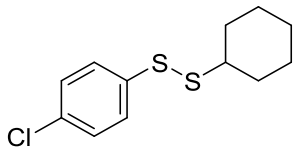
**HRMS (APCI+)**: m/z calcd for $C_{18}H_{29}ClS_2$ $[M]^+$: 344.1394, found: 344.1393.



**1-Benzyl-2-(4-chlorophenyl)disulfane (3d).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.18 (m, 9H), 3.92 (s, 2H).
$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.48, 135.77, 132.85, 129.49, 129.13, 129.06, 128.69, 127.74, 43.51.

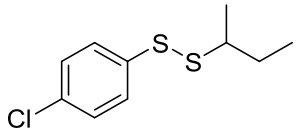
**HRMS (APCI+)**: m/z calcd for $C_{13}H_{11}ClS_2$ $[M]^+$: 265.9985, found: 265.9991.



**1-(4-Chlorophenyl)-2-cyclohexyldisulfane (3e).**

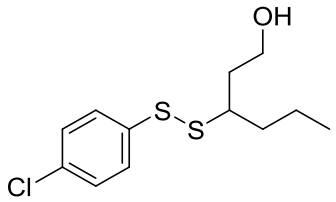
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.6 Hz, 2H), 7.26 (d, *J* = 8.6 Hz, 2H), 2.78 (tt, *J* = 10.8, 3.7 Hz, 1H), 1.98 (dd, *J* = 13.4, 3.4 Hz, 2H), 1.79 – 1.71 (m, 2H), 1.62 – 1.54 (m, 1H), 1.39 – 1.20 (m, 5H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 137.22, 132.25, 128.99, 128.19, 50.07, 32.70, 26.10, 25.62.
**HRMS (APCI+)**: m/z calcd for $C_{12}H_{15}ClS_2$ $[M]^+$: 258.0298, found: 258.0305.



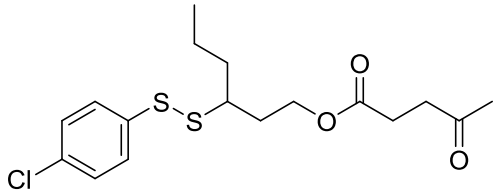
**1-(*sec*-Butyl)-2-(4-chlorophenyl)disulfane (3f).**[3]

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.44 (m, 2H), 7.29 – 7.26 (m, 2H), 2.82 (h, *J* = 6.8 Hz, 1H), 1.74 – 1.66 (m, 1H), 1.51 (dd, *J* = 14.2, 7.1 Hz, 1H), 1.27 (d, *J* = 6.8 Hz, 3H), 0.95 (t, *J* = 7.4 Hz, 3H).
$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 137.13, 132.48, 129.06, 128.59, 48.70, 28.91, 20.03, 11.58.



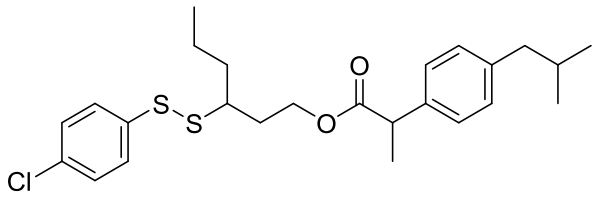
**3-((4-Chlorophenyl)disulfanyl)hexan-1-ol (3g).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.42 (m, 2H), 7.31 – 7.23 (m, 2H), 3.80 – 3.64 (m, 2H), 2.98 – 2.86 (m, 1H), 1.83 (q, *J* = 6.5 Hz, 2H), 1.61 – 1.50 (m, 2H), 1.45 – 1.33 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H).
$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.84, 132.86, 129.35, 129.06, 60.21, 49.38, 36.75, 36.37, 20.07, 13.87.
**HRMS (APCI+)**: m/z calcd for $C_{12}H_{18}ClOS_2$ $[M+H]^+$: 277.0482, found: 277.0487.



**3-((4-Chlorophenyl)disulfanyl)hexyl 4-oxopentanoate (3h).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 7.43 (m, 2H), 7.30 – 7.25 (m, 2H), 4.14 (t, *J* = 6.6 Hz, 2H), 2.86 – 2.78 (m, 1H), 2.73 (t, *J* = 6.5 Hz, 2H), 2.52 (t, *J* = 6.4 Hz, 2H), 2.18 (s, 3H), 1.90 (q, *J* = 6.6 Hz, 2H), 1.63 – 1.52 (m, 2H), 1.47 – 1.31 (m, 2H), 0.83 (t, *J* = 7.2 Hz, 3H).
$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 206.68, 172.73, 136.74, 132.91, 129.38, 129.11, 62.16, 49.23, 38.01, 36.11, 32.80, 30.00, 27.99, 20.07, 13.85.
**HRMS (APCI+)**: m/z calcd for $C_{17}H_{23}ClO_3S_2$ $[M]^+$: 374.0772, found: 374.0771.



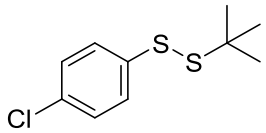
**3-((4-Chlorophenyl)disulfanyl)hexyl 2-(4-isobutylphenyl)propanoate (3i).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.39 (m, 2H), 7.28 – 7.21 (m, 2H), 7.17-7.12 (m, 2H), 7.08-7.02 (m, 2H), 4.18-4.05 (m, 2H), 3.68-3.59 (m, 1H), 2.61 (p, J = 6.8 Hz, 1H), 2.43 (dd, J = 7.0, 2.7 Hz,

2H), 1.83 (q, J = 6.2 Hz, 3H), 1.50-1.42 (m, 5H), 1.33-1.20 (m, 2H), 0.89 (d, J = 6.7 Hz, 6H), 0.79-0.72 (m, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 174.59, 140.61, 137.75, 137.74, 136.75, 136.74, 132.81, 129.40, 129.21, 129.05, 127.19, 127.17, 62.04, 61.94, 49.06, 49.04, 45.24, 45.16, 45.10, 35.96, 35.92, 32.86, 30.27, 22.50, 19.99, 18.46, 18.39, 13.77, 13.75.

HRMS (APCI+): m/z calcd for $C_{25}H_{33}ClO_2S_2$ $[M]^+$: 464.1605, found: 464.1602.

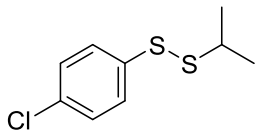



**1-(Tert-butyl)-2-(4-chlorophenyl)disulfane (3j).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.49 (dd, *J* = 8.7, 3.0 Hz, 2H), 7.36 – 7.19 (m, 2H), 1.29 (s, 9H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 137.58, 132.19, 128.94, 128.19, 49.59, 29.94.

**HRMS (APCI+)**: m/z calcd for $C_{10}H_{13}ClS_2$ $[M]^+$: 232.0142, found: 232.0138.

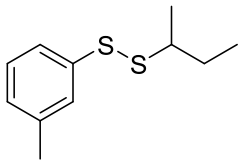



**1-(4-Chlorophenyl)-2-isopropyldisulfane (3k).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.44 (m, 2H), 7.29 – 7.25 (m, 2H), 3.05 (p, *J* = 6.7 Hz, 1H), 1.29 (d, *J* = 6.7 Hz, 6H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 137.07, 132.50, 129.08, 128.52, 41.85, 22.54.

**HRMS (APCI+)**: m/z calcd for $C_9H_{11}ClS_2$ $[M]^+$: 217.9985, found: 217.9991.

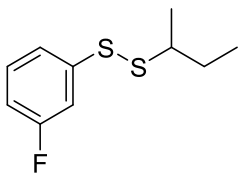



**1-(*sec*-Butyl)-2-(m-tolyl)disulfane (3l).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.30 (m, 2H), 7.19 (t, *J* = 7.9 Hz, 1H), 7.00 (d, *J* = 7.5 Hz, 1H), 2.82 (q, *J* = 6.7 Hz, 1H), 2.34 (s, 3H), 1.71 (dt, *J* = 14.1, 7.0 Hz, 1H), 1.55 – 1.49 (m, 1H), 1.28 (d, *J* = 6.8 Hz, 3H), 0.95 (t, *J* = 7.4 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 138.77, 138.12, 128.78, 127.71, 127.43, 124.24, 48.45, 28.89, 21.51, 20.01, 11.58.

**HRMS (APCI+)**: m/z calcd for $C_{11}H_{16}S_2$ $[M]^+$: 212.0688, found: 212.0685.




**1-(*sec*-Butyl)-2-(3-fluorophenyl)disulfane (3m).**

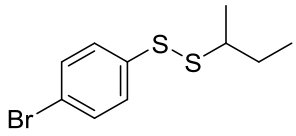
$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.23 (m, 3H), 6.95 – 6.80 (m, 1H), 2.83 (h, *J* = 6.8 Hz, 1H),

1.70 (dtd, *J* = 14.8, 7.4, 6.3 Hz, 1H), 1.53 (dt, *J* = 14.2, 7.2 Hz, 1H), 1.28 (d, *J* = 6.8 Hz, 3H), 0.96 (t, *J* = 7.4 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 164.44, 161.97, 141.17, 141.09, 130.24, 130.15, 122.24, 122.21, 113.69, 113.49, 113.45, 113.28, 48.68, 28.93, 19.98, 11.56.

$^{19}$F NMR (377 MHz, Chloroform-*d*) δ -111.82.

**HRMS (APCI+)**: m/z calcd for $C_{10}H_{13}FS_2$ $[M]^+$: 216.0437, found: 216.0442.

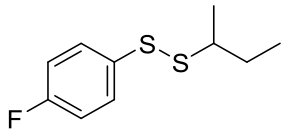



**1-(4-Bromophenyl)-2-(sec-butyl)disulfane (3n).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.41 (s, 4H), 2.82 (q, *J* = 6.7 Hz, 1H), 1.69 (dt, *J* = 14.1, 7.0 Hz, 1H), 1.51 (dt, *J* = 14.2, 7.2 Hz, 1H), 1.27 (d, *J* = 6.8 Hz, 3H), 0.95 (t, *J* = 7.4 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 137.78, 131.92, 128.70, 120.28, 48.67, 28.89, 20.02, 11.59.

**HRMS (APCI+)**: m/z calcd for $C_{10}H_{13}BrS_2$ $[M]^+$: 275.9637, found: 275.9637.



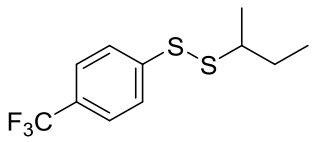

**1-(*sec*-Butyl)-2-(4-fluorophenyl)disulfane (3o).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.45 (m, 2H), 7.13 – 6.93 (m, 2H), 2.92-2.74 (m, 1H), 1.74 – 1.64 (m, 1H), 1.52 (dt, *J* = 14.2, 7.2 Hz, 1H), 1.27 (d, *J* = 6.8 Hz, 3H), 0.93 (t, *J* = 7.4 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 163.30, 160.85, 133.69, 133.66, 130.01, 129.93, 116.17, 115.95, 48.60, 28.86, 20.02, 11.54.

$^{19}$F NMR (377 MHz, Chloroform-*d*) δ -115.41.

**HRMS (APCI+)**: m/z calcd for $C_{10}H_{13}FS_2$ $[M]^+$: 216.0437, found: 216.0441.



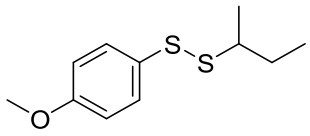

**1-(*sec*-Butyl)-2-(4-(trifluoromethyl)phenyl)disulfane (3p).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.64 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.3 Hz, 2H), 2.85 (h, *J* = 6.7 Hz, 1H), 1.72 (ddd, *J* = 13.8, 7.4, 6.4 Hz, 1H), 1.54 (dt, *J* = 14.2, 7.2 Hz, 1H), 1.29 (d, *J* = 6.8 Hz, 3H), 0.98 (t, *J* = 7.4 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 143.57, 128.42 (q, $^{1}J_{CF}$ = 32.3 Hz), 126.26, 125.78 (q, $^{3}J_{CF}$ = 3.0 Hz), 124.24 (q, $^{1}J_{CF}$ = 272.7 Hz), 48.82, 28.98, 20.02, 11.58.

$^{19}$F NMR (377 MHz, Chloroform-*d*) δ -62.37.

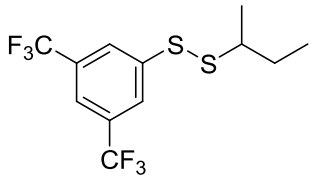
**HRMS (APCI+)**: m/z calcd for $C_{11}H_{13}F_3S_2$ $[M]^+$:266.0405, found: 266.0411.



**1-(*sec*-Butyl)-2-(4-methoxyphenyl)disulfane (3q).**[4]

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.54 – 7.43 (m, 2H), 6.89 – 6.81 (m, 2H), 3.79 (s, 3H), 2.82 (h, *J* = 6.8 Hz, 1H), 1.79 – 1.64 (m, 1H), 1.51 (dt, *J* = 14.2, 7.2 Hz, 1H), 1.27 (d, *J* = 6.8 Hz, 3H), 0.92 (t, *J* = 7.4 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 159.33, 131.14, 129.34, 114.64, 55.51, 48.36, 28.85, 20.00, 11.53.



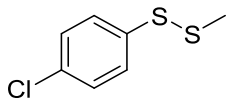
**1-(3,5-Bis(trifluoromethyl)phenyl)-2-(sec-butyl)disulfane (3r).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.99 (s, 2H), 7.67 (s, 1H), 2.87 (h, *J* = 6.7 Hz, 1H), 1.69 (dq, *J* = 14.4, 7.2 Hz, 1H), 1.56 (dt, *J* = 14.2, 7.1 Hz, 1H), 1.31 (d, *J* = 6.8 Hz, 3H), 1.00 (t, *J* = 7.4 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 142.55, 132.82, 132.48, 132.15, 131.82, 127.32, 126.11, 126.08, 126.04, 126.00, 124.61, 121.89, 120.07, 120.04, 120.00, 119.96, 119.92, 119.18, 49.39, 29.02, 20.22, 11.53.

$^{19}$F NMR (377 MHz, Chloroform-*d*) δ -63.14.

**HRMS (APCI+)**: m/z calcd for $C_{12}H_{12}F_6S_2$ $[M]^+$:334.0279, found: 334.0283.

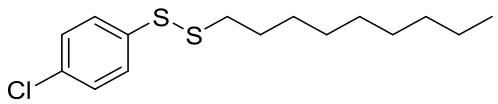


**1-(4-Chlorophenyl)-2-methyldisulfane (3s).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.50 – 7.43 (m, 2H), 7.32 – 7.28 (m, 2H), 2.44 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 135.65, 133.04, 129.29, 129.12, 22.98.

**HRMS (APCI+)**: m/z calcd for $C_7H_7ClS_2$ $[M]^+$: 189.9672, found: 189.9673.

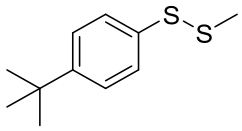


**1-(4-Chlorophenyl)-2-nonyldisulfane (3t).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.40 (m, 2H), 7.32 – 7.25 (m, 2H), 2.71 (t, *J* = 7.3 Hz, 2H), 1.63 (q, *J* = 7.4 Hz, 2H), 1.38 – 1.33 (m, 2H), 1.28 – 1.22 (m, 10H), 0.88 (t, *J* = 6.7 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.47, 132.71, 129.13, 128.84, 39.13, 31.98, 29.56, 29.37, 29.29, 28.90, 28.56, 22.80, 14.25.

**HRMS (APCI+)**: m/z calcd for $C_{15}H_{23}ClS_2$ $[M]^+$: 302.0924, found: 302.0927.

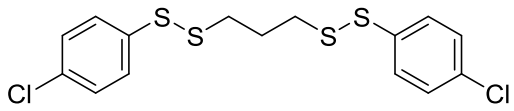


**1-(4-(*Tert*-butyl)phenyl)-2-methyldisulfane (3u).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.49 – 7.43 (m, 2H), 7.39 – 7.33 (m, 2H), 2.44 (s, 3H), 1.31 (s, 9H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 150.57, 133.67, 128.29, 126.26, 34.68, 31.42, 23.15.

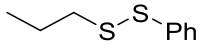
**HRMS (APCI+):** m/z calcd for $C_{11}H_{16}S_2$ $[M]^+$: 212.0688, found: 212.0689.



**4,6-Dimethyl-2-(*p*-tolyldisulfanyl)pyrimidine (3v).**[5]

1H NMR (400 MHz, Chloroform-d) δ 7.51 – 7.39 (m, 4H), 7.34 – 7.26 (m, 4H), 2.77 (t, J = 6.9 Hz, 4H), 2.05 (p, J = 6.9 Hz, 2H).

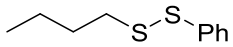
13C NMR (101 MHz, Chloroform-d) δ 135.82, 133.09, 129.28, 129.20, 36.82, 27.47.



**1-Phenyl-2-propyldisulfane (3w).**[6]

1H NMR (400 MHz, Chloroform-d) δ 7.53 (d, J = 7.7 Hz, 2H), 7.31 (t, J = 7.5 Hz, 2H), 7.20 (t, J = 7.2 Hz, 1H), 2.71 (t, J = 7.3 Hz, 2H), 1.70 (p, J = 7.3 Hz, 2H), 0.96 (t, J = 7.4 Hz, 3H).

13C NMR (101 MHz, Chloroform-d) δ 137.76, 129.03, 127.41, 126.72, 40.98, 22.29, 13.22.

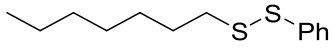


**1-Butyl-2-phenyldisulfane (3x).**

1H NMR (400 MHz, Chloroform-d) δ 7.61 – 7.49 (m, 2H), 7.36 – 7.28 (m, 2H), 7.25 – 7.16 (m, 1H), 2.78 – 2.71 (m, 2H), 1.69 – 1.63 (m, 2H), 1.43 – 1.36 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H).

13C NMR (101 MHz, Chloroform-d) δ 137.81, 129.06, 127.51, 126.77, 38.79, 31.00, 21.75, 13.78.

HRMS (APCI+): m/z calcd for $C_{10}H_{14}S_2$ $[M]^+$: 198.0531, found: 198.0530.

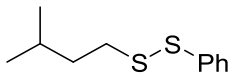


**1-Heptyl-2-phenyldisulfane (3y).**

1H NMR (400 MHz, Chloroform-d) δ 7.61-7.47 (m, 2H), 7.36-7.26 (m, 2H), 7.24 – 7.17 (m, 1H), 2.73 (t, J = 7.3 Hz, 2H), 1.66 (p, J = 7.3 Hz, 2H), 1.38 – 1.32 (m, 2H), 1.29 – 1.18 (m, 6H), 0.87 (t, J = 6.7 Hz, 3H).

13C NMR (101 MHz, Chloroform-d) δ 137.79, 129.03, 127.45, 126.72, 39.08, 31.80, 28.97, 28.91, 28.54, 22.72, 14.22.

HRMS (APCI+): m/z calcd for $C_{13}H_{20}S_2$ $[M]^+$: 240.1001, found: 240.1005.

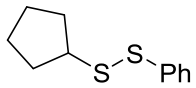


**1-Isopentyl-2-phenyldisulfane (3z).**

1H NMR (400 MHz, Chloroform-d) δ 7.58 – 7.47 (m, 2H), 7.32 (t, J = 7.6 Hz, 2H), 7.24 – 7.19 (m, 1H), 2.79 – 2.69 (m, 2H), 1.66 (dt, J = 13.2, 6.6 Hz, 1H), 1.58 – 1.53 (m, 2H), 0.87 (d, J = 6.6 Hz, 6H).

13C NMR (101 MHz, Chloroform-d) δ 137.78, 129.06, 127.57, 126.79, 37.90, 37.15, 27.26, 22.40.

HRMS (APCI+): m/z calcd for $C_{11}H_{16}S_2$ $[M]^+$: 212.0688, found: 212.0686.

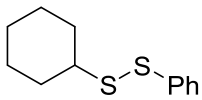



**1-Cyclopentyl-2-phenyldisulfane (3aa).**

1H NMR (400 MHz, Chloroform-d) δ 7.54 (d, J = 7.7 Hz, 2H), 7.31 (t, J = 7.7 Hz, 2H), 7.20 (t, J = 7.4 Hz, 1H), 3.33 (h, J = 5.3, 4.4 Hz, 1H), 1.94 (dq, J = 12.3, 7.0, 6.5 Hz, 2H), 1.71 (ddd, J = 21.5, 11.0, 5.6 Hz, 4H), 1.57 (d, J = 6.7 Hz, 2H).

13C NMR (101 MHz, Chloroform-d) δ 138.15, 128.98, 127.22, 126.59, 50.39, 32.88, 24.83.

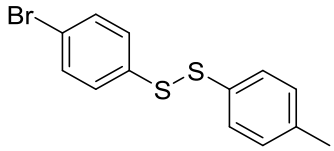
HRMS (APCI+): m/z calcd for $C_{11}H_{16}S_2$ $[M]^+$: 210.0531, found: 210.0529.




**1-Cyclohexyl-2-phenyldisulfane (3ab).**[7]

1H NMR (400 MHz, Chloroform-d) δ 7.53 (d, J = 7.6 Hz, 2H), 7.30 (t, J = 7.6 Hz, 2H), 7.19 (t, J = 7.3 Hz, 1H), 2.80 (tt, J = 10.9, 3.7 Hz, 1H), 2.01 (d, J = 10.3 Hz, 2H), 1.79-1.72 (m, 2H), 1.63 – 1.57 (m, 1H), 1.39 – 1.21 (m, 5H).

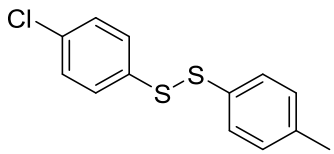
13C NMR (101 MHz, Chloroform-d) δ 138.56, 128.93, 126.88, 126.40, 49.95, 32.74, 26.14, 25.70.




**1-(4-Bromophenyl)-2-(*p*-tolyl)disulfane (3ac).**[8]

[1]H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.39 (m, 2H), 7.38 – 7.33 (m, 4H), 7.11 (d, *J* = 8.0 Hz, 2H), 2.32 (s, 3H).

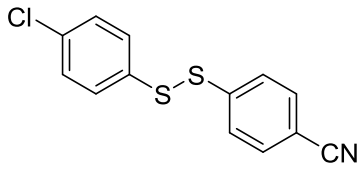
[13]C NMR (101 MHz, Chloroform-*d*) δ 138.04, 136.69, 133.23, 132.18, 130.07, 129.44, 128.80, 121.23, 21.22.




**1-(4-Chlorophenyl)-2-(*p*-tolyl)disulfane (3ad).**[8]

[1]H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.39 (m, 2H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.28 – 7.23 (m, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 2.31 (s, 3H).

[13]C NMR (101 MHz, Chloroform-*d*) δ 138.00, 135.99, 133.30, 133.26, 130.05, 129.28, 129.26, 128.79, 21.22.

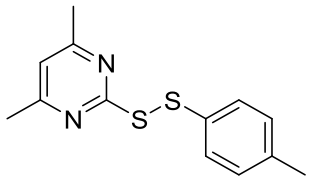



**4-((4-Chlorophenyl)disulfanyl)benzonitrile (3ae).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.57 (s, 4H), 7.44 – 7.35 (m, 2H), 7.31 – 7.24 (m, 2H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 143.29, 134.12, 134.05, 132.67, 129.55, 129.17, 126.56, 118.46, 110.44.

**HRMS (APCI+)**: m/z calcd for $C_{13}H_8ClNS_2$ $[M]^+$: 276.9781, found: 276.9779.

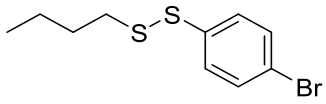



**4,6-Dimethyl-2-(*p*-tolyldisulfanyl)pyrimidine (3af).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.51 (m, 2H), 7.12 – 7.06 (m, 2H), 6.79 (s, 1H), 2.45 (s, 6H), 2.31 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 169.95, 167.96, 138.26, 133.60, 130.68, 129.74, 117.38, 24.04, 21.28.

**HRMS (APCI+)**: m/z calcd for $C_{13}H_{20}S_2$ $[M]^+$: 240.1001, found: 240.1005.

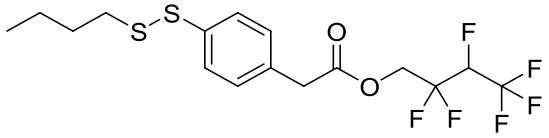



**1-(4-Bromophenyl)-2-butyldisulfane (3ag).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.47 – 7.35 (m, 4H), 2.72 (t, *J* = 7.4 Hz, 2H), 1.63 (p, *J* = 7.3 Hz, 2H), 1.38 (h, *J* = 7.3 Hz, 2H), 0.88 (t, *J* = 7.3 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 137.09, 132.02, 128.93, 120.52, 38.73, 30.96, 21.71, 13.75.

**HRMS (APCI+)**: m/z calcd for $C_{10}H_{13}BrS_2$ $[M]^+$: 275.9637, found: 275.9638.



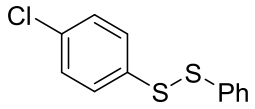

**2,2,3,4,4,4-Hexafluorobutyl 2-(4-(butyldisulfanyl)phenyl)acetate (3ah).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 7.58 – 7.48 (m, 2H), 7.26 – 7.19 (m, 2H), 4.78 (dddt, *J* = 43.6, 14.7, 11.6, 5.8 Hz, 1H), 4.56 – 4.40 (m, 2H), 3.70 (s, 2H), 2.79 – 2.66 (m, 2H), 1.69 – 1.60 (m, 2H), 1.39 (h, *J* = 7.3 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 169.76, 137.40, 131.30, 129.91, 127.75, 40.29, 38.73, 30.99, 21.74, 13.75.

$^{19}$F NMR (377 MHz, Chloroform-*d*) δ -73.88 – -74.30 (m), -115.08 (dqd, *J* = 279.4, 9.5, 7.2 Hz), -119.82 (ddq, *J* = 279.8, 12.2, 10.2 Hz), -212.64 (qd, *J* = 11.5, 7.2 Hz).

**HRMS (APCI+)**: m/z calcd for $C_{16}H_{18}F_6O_2S_2$ $[M]^+$: 420.0647, found: 420.0649.

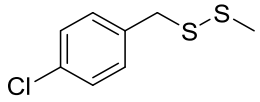


**1-(4-Chlorophenyl)-2-phenyldisulfane (3ai).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.45 (m, 2H), 7.45 – 7.39 (m, 2H), 7.33 – 7.24 (m, 5H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.68, 135.74, 133.41, 129.33, 129.30, 129.15, 127.90, 127.59.

**HRMS (APCI+)**: m/z calcd for $C_{12}H_9ClS_2$ $[M]^+$: 251.9829, found: 251.9832.

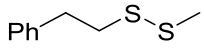


**1-(4-Chlorobenzyl)-2-methyldisulfane (3aj).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.23 (m, 4H), 3.85 (s, 2H), 2.13 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 136.29, 133.41, 130.74, 128.79, 42.25, 23.19.

**HRMS (APCI+)**: m/z calcd for $C_8H_9ClS_2$ $[M]^+$: 203.9829, found: 203.9832.

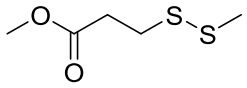


**1-Methyl-2-phenethyldisulfane (3ak).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.27 (m, 2H), 7.26 – 7.19 (m, 3H), 3.04 – 2.92 (m, 4H), 2.42 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 140.20, 128.74, 128.64, 126.53, 39.51, 35.86, 23.44.

**HRMS (APCI+)**: m/z calcd for $C_9H_{12}S_2$ $[M]^+$: 184.0375, found: 184.0373.

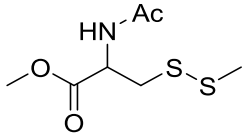


**Methyl 3-(methyldisulfanyl)propanoate (3al).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 3.71 (s, 3H), 2.95 (t, *J* = 7.2 Hz, 2H), 2.77 (t, *J* = 7.2 Hz, 2H), 2.41 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 172.36, 51.97, 34.07, 32.48, 23.27.

**HRMS (APCI+)**: m/z calcd for $C_5H_{10}O_2S_2$ $[M]^+$: 166.0117, found: 166.0115.

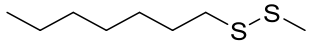


**Methyl N-acetyl-S-(methylthio)-L-cysteinate (3am).**

$^1$H NMR (400 MHz, Chloroform-*d*) δ 6.48 (d, *J* = 7.6 Hz, 1H), 4.92 (dt, *J* = 7.7, 5.1 Hz, 1H), 3.78 (s, 3H), 3.29 – 3.09 (m, 2H), 2.42 (s, 3H), 2.07 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 171.17, 170.02, 52.79, 51.77, 39.54, 23.22, 23.11.

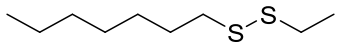
**HRMS (APCI+)**: m/z calcd for $C_7H_{13}NO_3S_2$ $[M]^+$: 223.0331, found: 223.0328.



**1-Heptyl-2-methyldisulfane (3an).**[9]

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 2.71 (t, *J* = 2.0 Hz, 2H), 2.41 (s, 3H), 1.69 (p, *J* = 7.3 Hz, 2H), 1.42 – 1.35 (m, 2H), 1.33 – 1.26 (m, 6H), 0.89 (t, *J* = 6.7 Hz, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 38.51, 31.86, 29.36, 29.07, 28.63, 23.52, 22.76, 14.23.



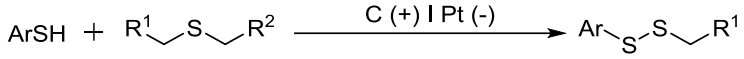

**1-Ethyl-2-heptyldisulfane (3ao).**

$^{1}$H NMR (400 MHz, Chloroform-*d*) δ 2.70 (q, *J* = 7.5 Hz, 4H), 1.67 (p, *J* = 7.3 Hz, 2H), 1.32 (td, *J* = 13.8, 10.8, 6.3 Hz, 11H), 0.92 – 0.84 (m, 3H).

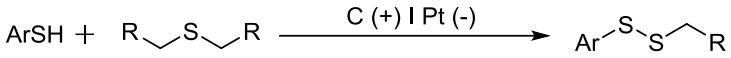
$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 39.45, 32.95, 31.86, 29.40, 29.05, 28.64, 22.75, 14.61, 14.23.

**HRMS (APCI+)**: m/z calcd for $C_9H_{20}S_2$ $[M]^+$: 192.1001, found: 192.1002.

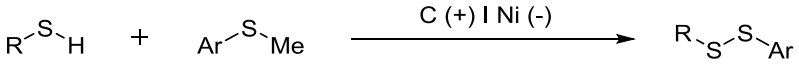
## 3) General reaction for the synthesis of disulfides



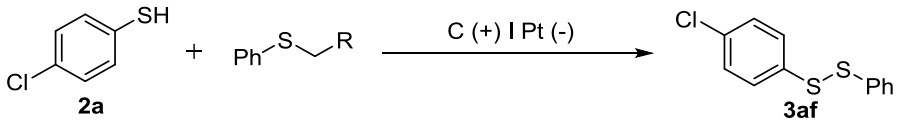

**Typical procedure for substrate scope with unsymmetrical alkyl thioethers:** A mixture of thiol (0.6 mmol), thioether (3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 12 h at 37 °C. Then, the system was concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product.



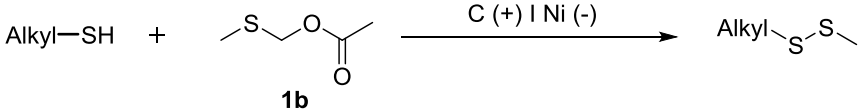

**Typical procedure for substrate scope with symmetrical alkyl thioethers:** A mixture of thiol (0.6 mmol), thioether (3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 12 h at 37 °C. Then, the system was concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product.




**Typical procedure for substrate scope with aryl methyl thioethers:** A mixture of thiol (0.6 mmol), thioether (3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, nickel plate cathode, was electrolyzed at constant current of 25 mA for 12 h at 37 °C. Then, the system was concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product.



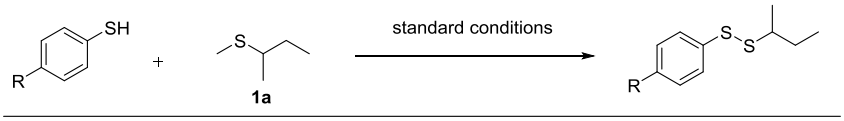

**Typical procedure for investigation of different kinds of C-S bonds:** A mixture of thiol (**2a**, 0.6 mmol), thioether (3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/CH_3OH$ (10/1, 11 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 12 h at 60 °C. Then, the system was concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product.

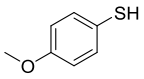


**Typical procedure for construction of unsymmetrical alkyl sulfides:** A mixture of thiol (0.6 mmol), (methylthio)methyl acetate (**1b**, 3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/CH_3OH$ (10/0.1, 10.1 mL), in an undivided cell at air atmosphere with carbon electrode anode, nickel plate cathode, was electrolyzed at constant current of 15 mA for 8 h at 60 °C. Then, the system was concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product.

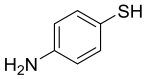
**Note:**

These thiols were not compatible with this protocol.

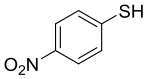



n.d.

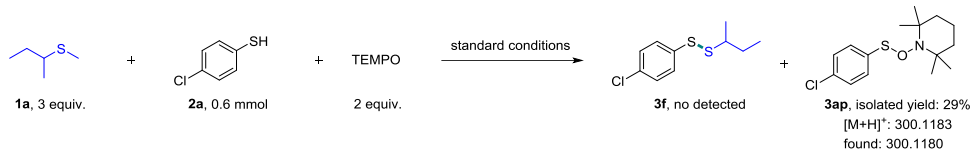



n.d.

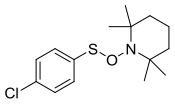



n.d.

# 4) Radical trapping experiment




**Typical procedure using TEMPO as capture reagent:** A mixture of thiol (**2a**, 0.6 mmol), thioether (**1a**, 3 equiv.), TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl, 1.2 mmol), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 12 h at 37 °C. Then, the system was detected by HRMS.[10]



$^1$H NMR (400 MHz, Chloroform-*d*) δ 7.59 (d, *J* = 8.6 Hz, 2H), 7.40 (d, *J* = 8.6 Hz, 2H), 1.72 – 1.33 (m, 15H), 0.89 (s, 3H).

$^{13}$C NMR (101 MHz, Chloroform-*d*) δ 149.02, 135.76, 128.81, 127.55, 61.57, 59.08, 43.55, 41.44, 35.47, 32.82, 28.83, 28.01, 17.32.

**HRMS (APCI+)**: m/z calcd for $C_{15}H_{23}ClNOS$ $[M+H]^+$: 300.1183, found: 300.1180.

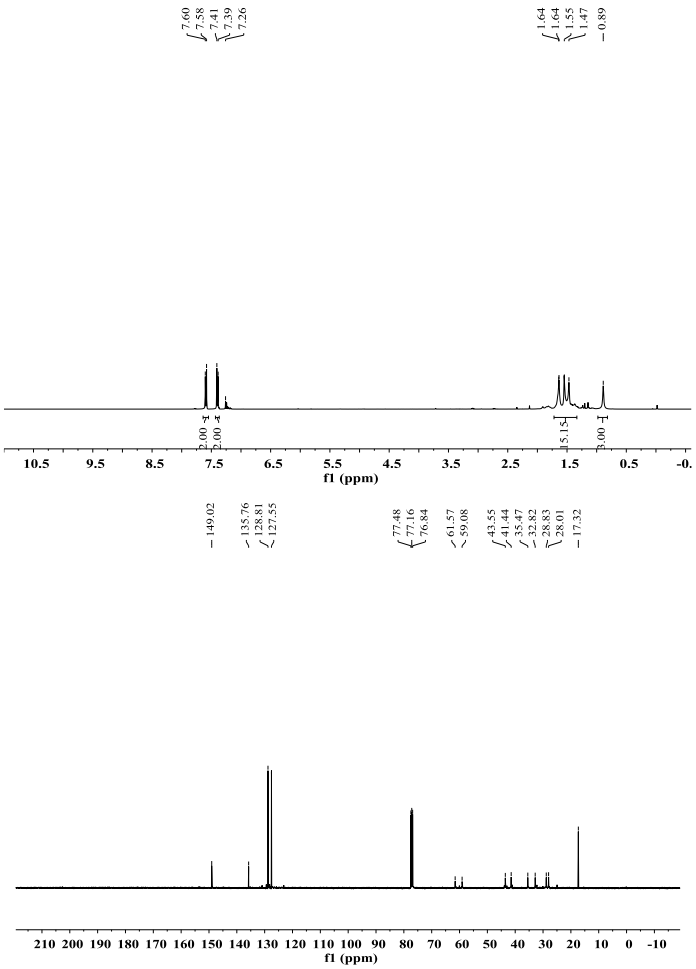



**Figure S2.** H[1] and C[12] NMR data of the compound **3ap**.

## 5) $F^{19}$ NMR experiments

**Typical procedure for $F^{19}$ NMR experiments:** A mixture of *p*-fluorothiophenol (0.6 mmol), thioether (**1a**, 3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA at 37 °C for different time. Then, the system was detected by $F^{19}$ NMR.

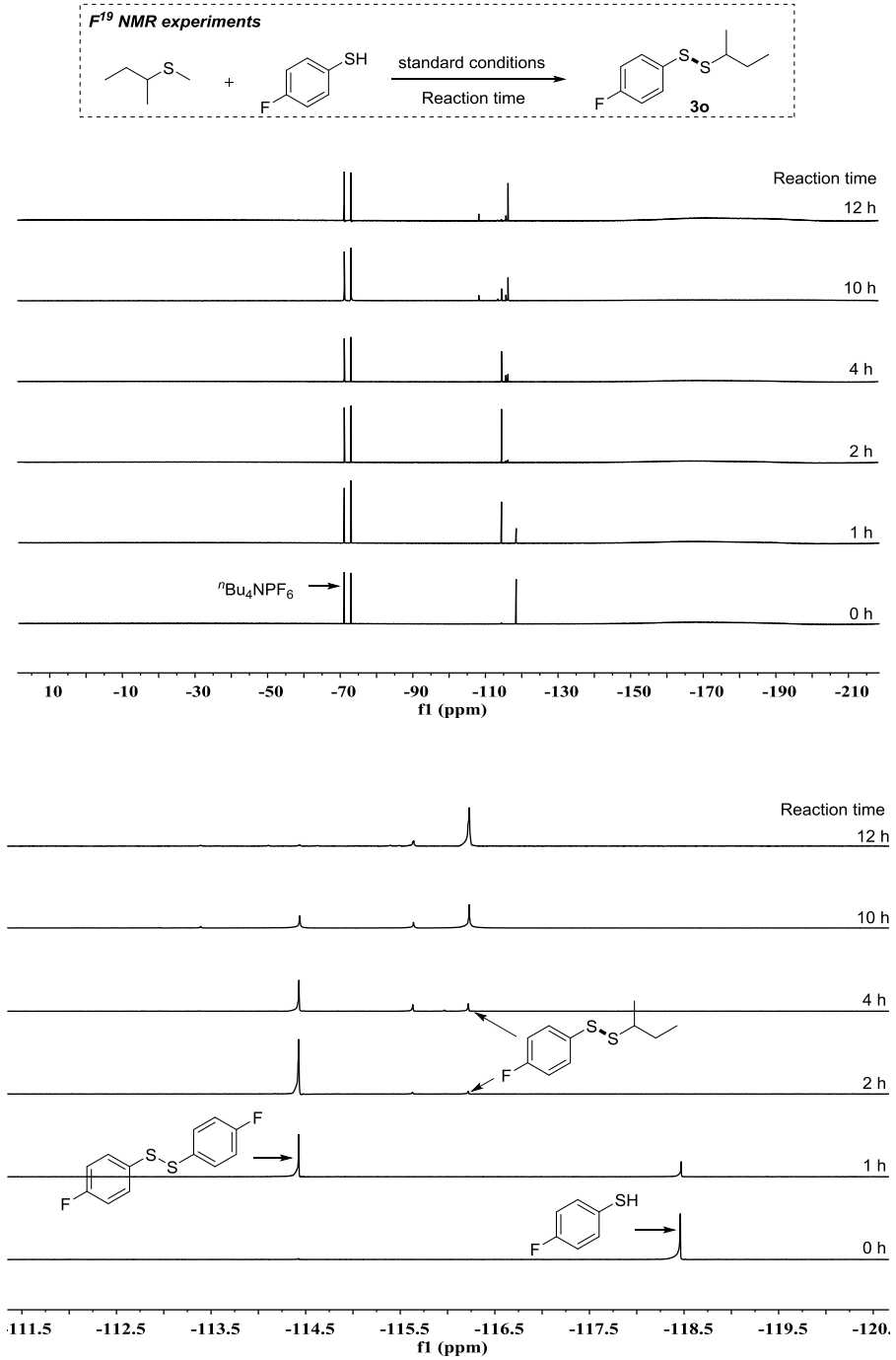
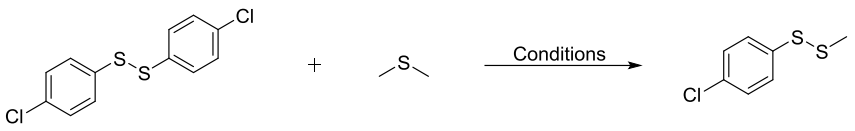


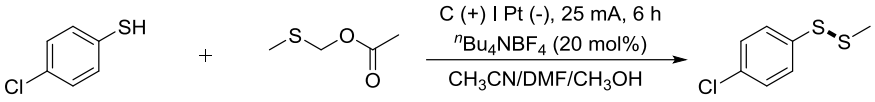

**Figure S3.** $F^{19}$ NMR experiments.

# 6) Intermediate experiments




**2aa** **1c** **3p**, 40%

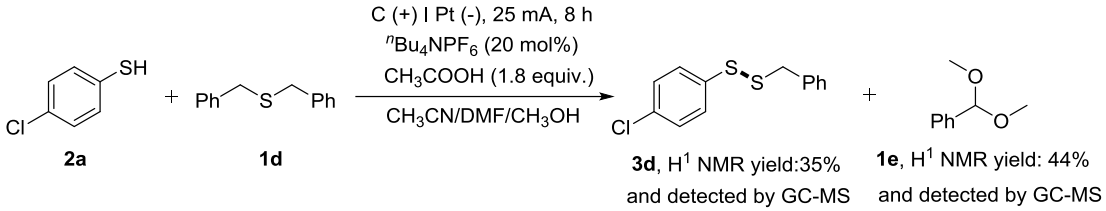
**Typical procedure for intermediate experiments:** A mixture of 1,2-bis(4-chlorophenyl)disulfane (**2aa**, 0.3 mmol), dimethyl sulfide (**1c**, 1.8 mmol), $CH_3COOH$ (1.08 mmol), $^nBu_4NPF_6$ (0.12 mmol), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 12 h at 37 °C. Then, the system was concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product.



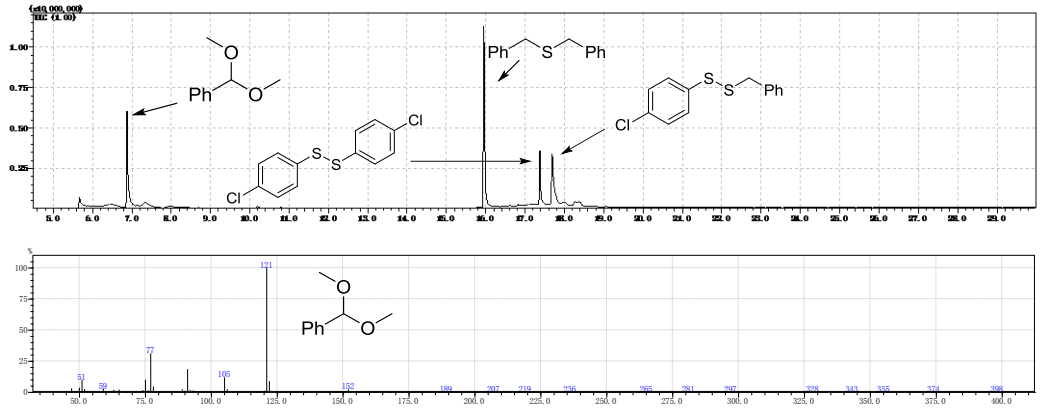

**2a** **1b** **3s**, 45%

**Typical procedure for intermediate experiments:** A mixture of 4-chlorobenzenethiol (**2a**, 0.6 mmol), (methylthio)methyl acetate (**1b**, 3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 6 h at 37 °C. Then, the system was concentrated under reduced pressure. The resulting crude product was separated on a silica gel column with petroleum ether and ethyl acetate as eluent to afford the desired product.

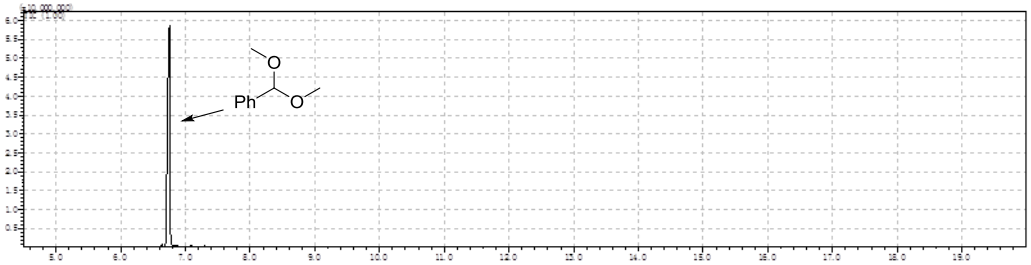
# 7) Control experiment



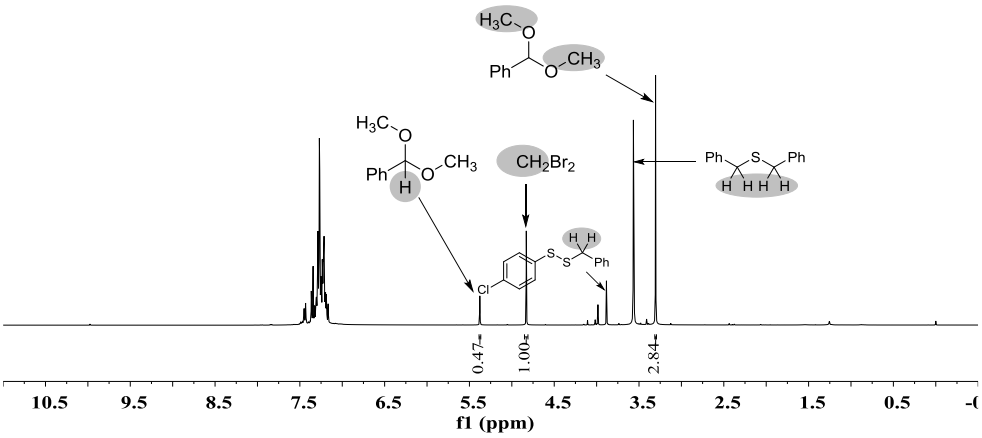

**Typical procedure for control experiments:** A mixture of 4-chlorobenzenethiol (**2a**, 0.6 mmol), dibenzylsulfane (**1d**, 3 equiv.), $CH_3COOH$ (1.8 equiv.), $^nBu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 8 h at 37 °C. Then, the system was concentrated under reduced pressure and using GC-MS to detect the system. In addition, the yields of **3d** and **1e** were detected by the NMR. (Note: compound **1e** is easily decomposed)



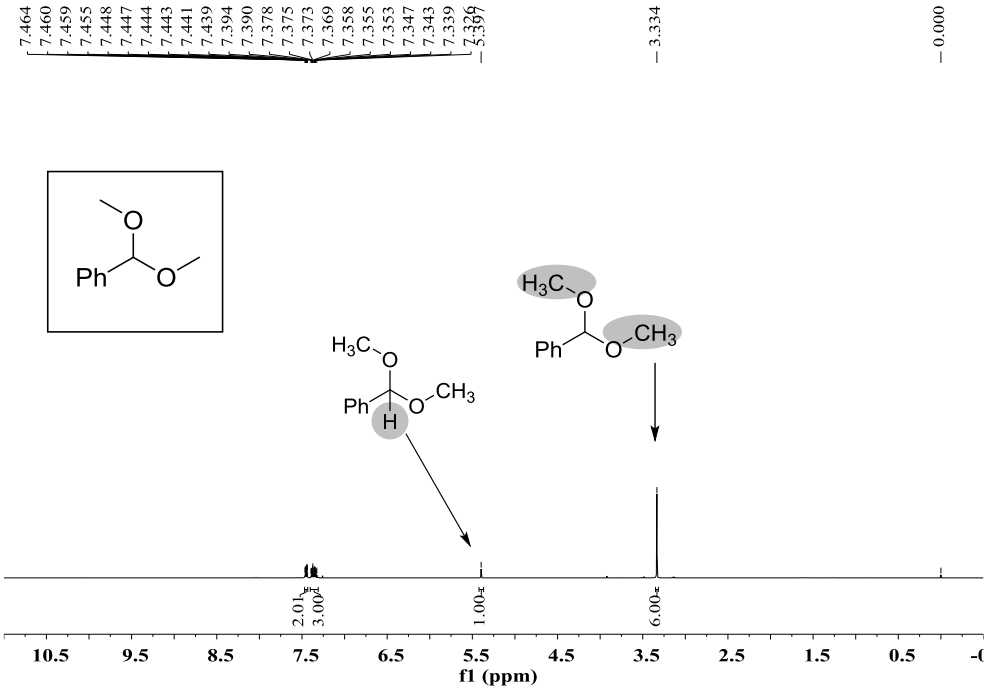
Scheme S1. GC-MS spectra of the reaction



Scheme S2. GC-MS spectra of the available commercial benzaldehyd-dimethylacetal (CAS:1125-88-8).



Scheme S3. $H^1$ NMR spectra of the reaction with $CH_2Br_2$ (50 mg) as internal standard ($H^1$ NMR yield of **1e**: 44%)




Scheme S4. $H^1$ NMR spectra of available commercial benzaldehyd-dimethylacetal (CAS:1125-88-8).

# 8) Cyclic voltammograms experiments

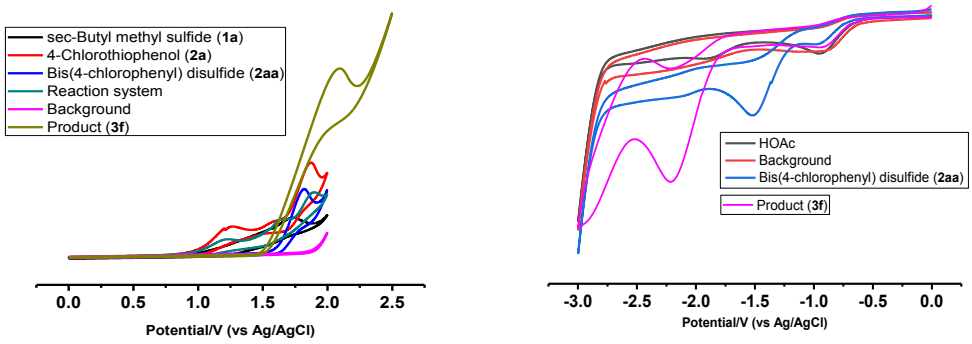
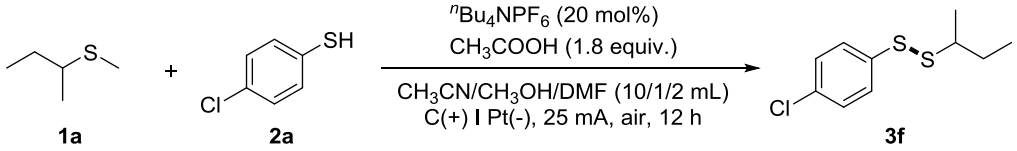



**Figure S4.** General procedure for cyclic voltammetry (CV): Cyclic voltammetry was performed in a three-electrode cell connected to a Schlenk line under air at room temperature. The working electrode was a glassy carbon electrode, the counter electrode a platinum wire. The reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution, and separated from reaction by a salt bridge. Related compounds (0.1 mmol) in $^{n}Bu_4NPF_6$ (1 mmol) in $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL) were poured into the electrochemical cell in all experiments. The scan rate is 0.05 V/s, ranging from 0 V to 2 V and -3 V to 0 V, respectively. The peak potentials vs. Ag/ AgCl was used.

# 9) Determination of hydrogen




**1a** **2a** **3f**

**Typical procedure for determination of hydrogen:** A mixture of 4-chlorothiophenol (**2a**, 0.6 mmol), *sec*-butyl methyl thioether (**1a**, 3 equiv.), $CH_3COOH$ (1.8 equiv.), $^{n}Bu_4NPF_6$ (20 mol%), $CH_3CN/DMF/CH_3OH$ (10/2/1, 13 mL), in an undivided cell at air atmosphere with carbon electrode anode, Pt plate cathode, was electrolyzed at constant current of 25 mA for 12 h at 37 °C. Then, using the GC machine to detect the gas atmosphere, and hydrogen was detected (shown below).

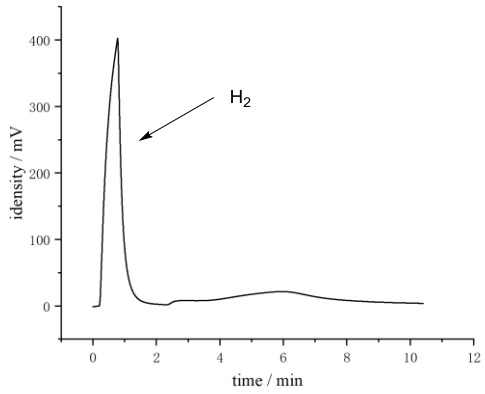



**Figure S5**. Determination of hydrogen

## References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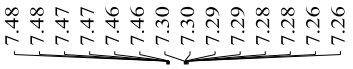
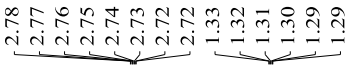
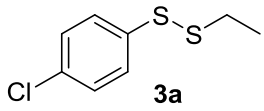
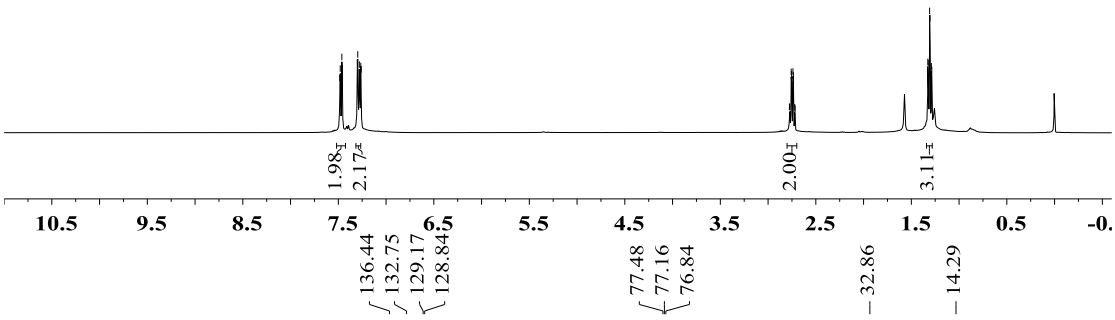
# NMR Spectra of Products

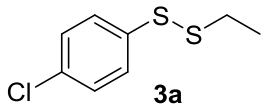



**3a**

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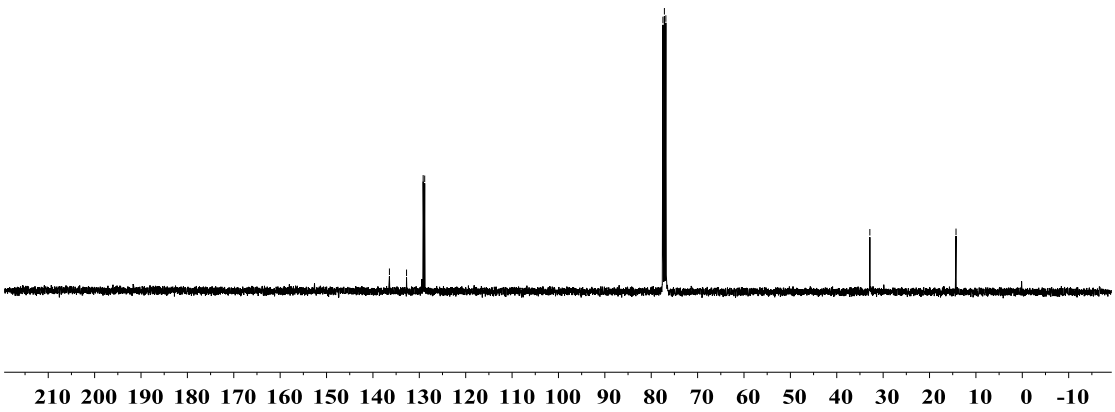

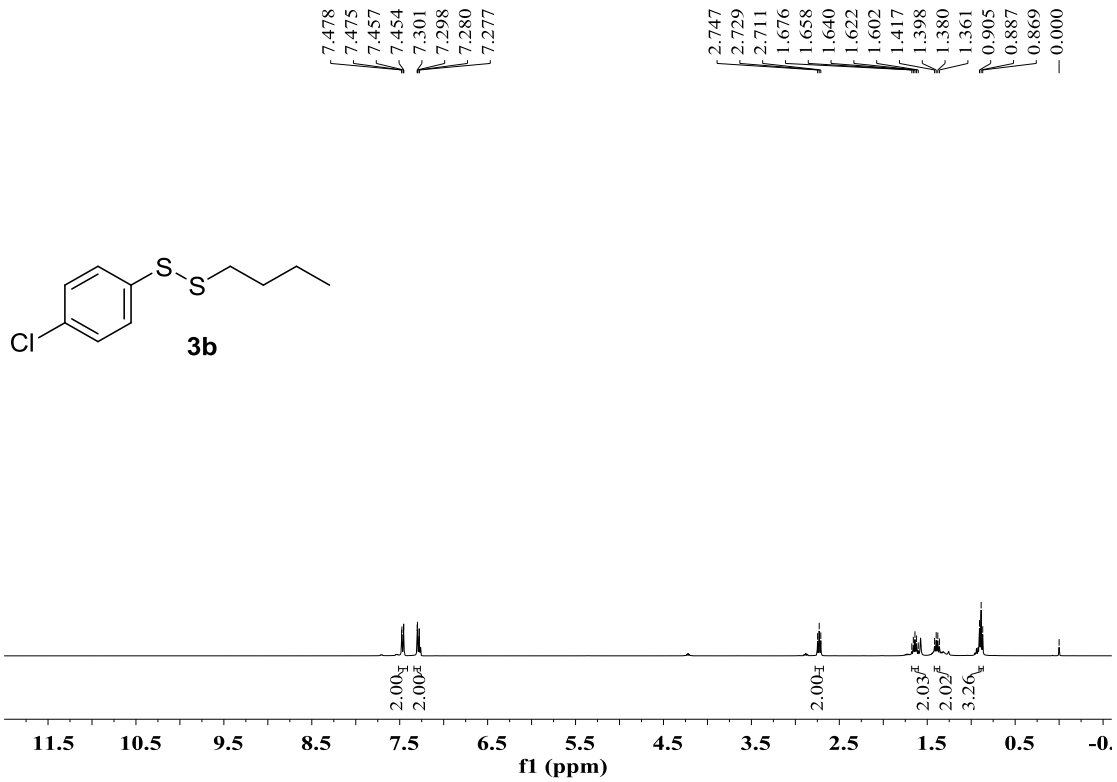
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2.729
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1.658
1.640
1.622
1.602
1.417
1.398
1.380
1.361
0.905
0.887
0.869
0.000
S
S
Cl
3b
2.00
2.00
2.00
2.03
2.02
3.26
11.5
10.5
9.5
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7.5
6.5
5.5
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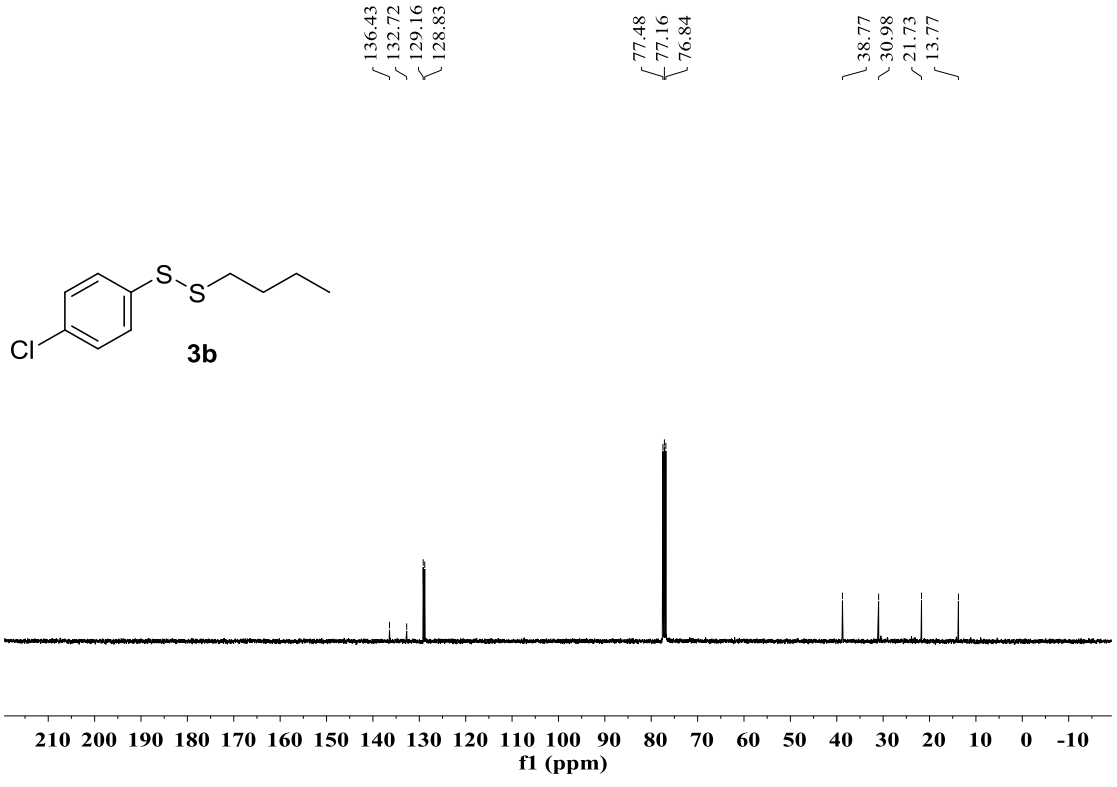
2.5
1.5
0.5
f1 (ppm)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S
S
Cl
3b
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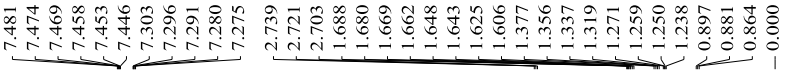
f1 (ppm)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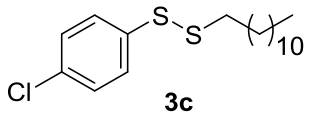
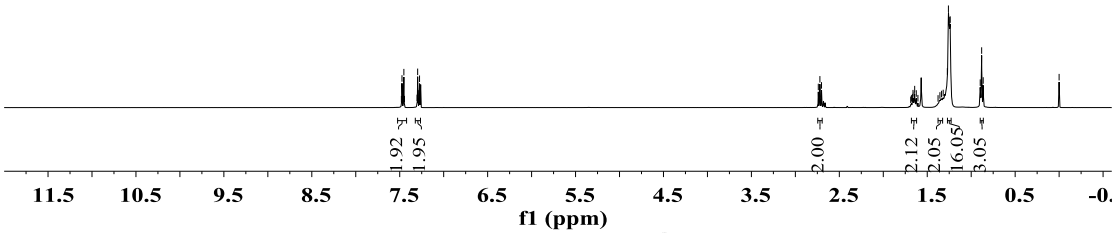

S
S
10
Cl

**3c**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1.5
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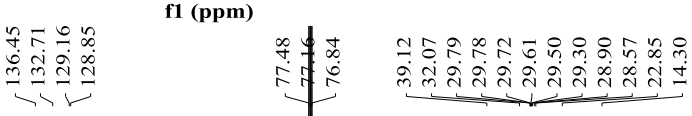
f1 (ppm)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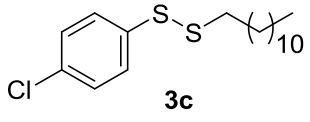
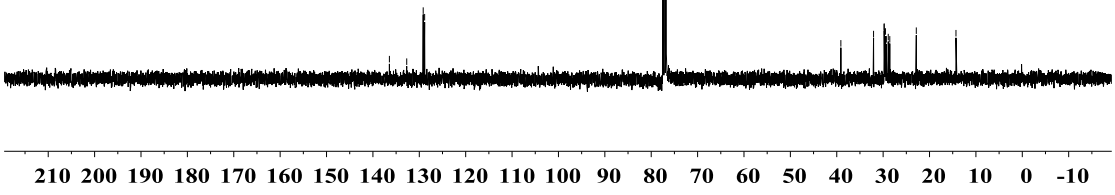
14.30


S
S
10
Cl

**3c**


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


7.32
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7.31
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7.27
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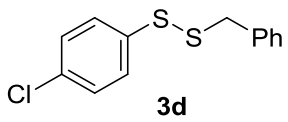
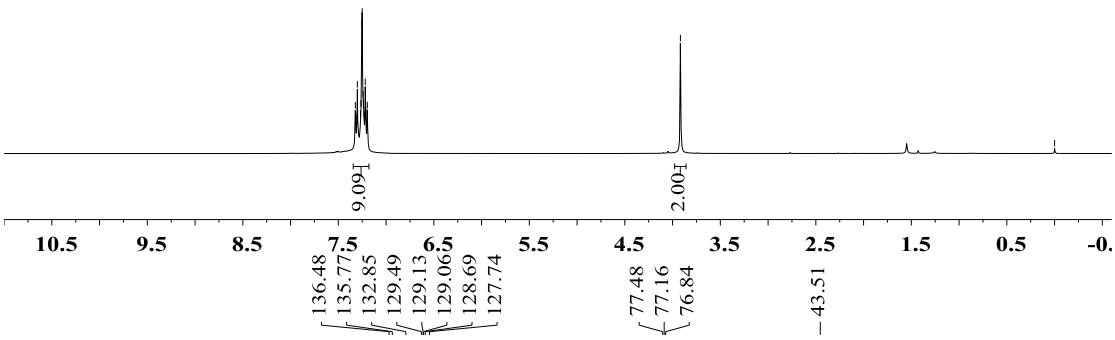
7.25
7.24
7.24
7.23
7.22
7.22
7.21
7.20
3.92
0.00


S
S
Ph
Cl

**3d**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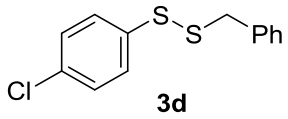
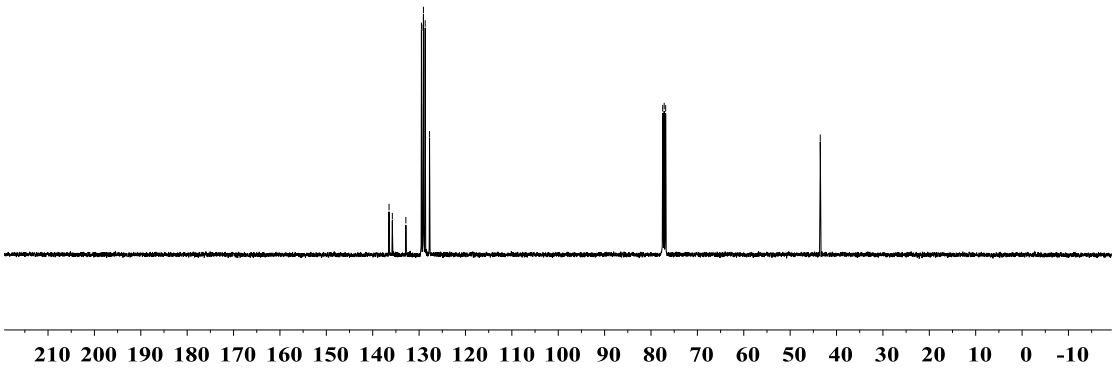
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.


136.48
135.77
132.85
129.49
129.13
129.06
128.69
127.74
77.48
77.16
76.84
43.51


S
S
Ph
Cl

**3d**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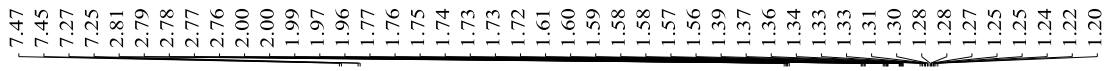
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2.79
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2.77
2.76
2.00
2.00
1.99
1.97
1.96
1.77
1.76
1.75
1.74
1.73
1.73
1.72
1.61
1.60
1.59
1.58
1.58
1.57
1.56
1.39
1.37
1.36
1.34
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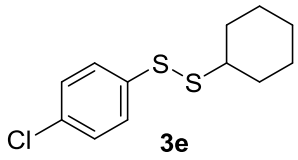
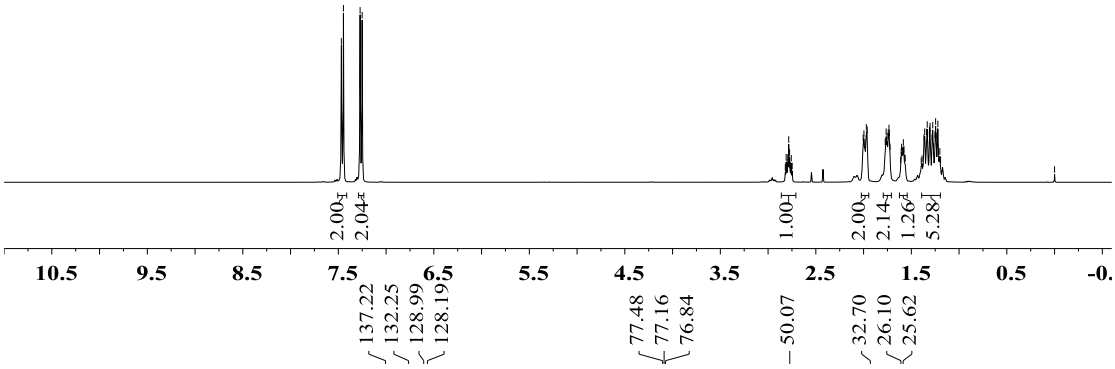
1.27
1.25
1.25
1.24
1.22
1.20


S
S
Cl

**3e**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1.00
2.00
2.14
1.26
5.28
10.5
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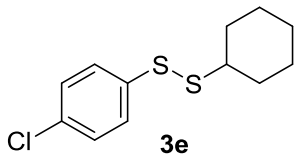
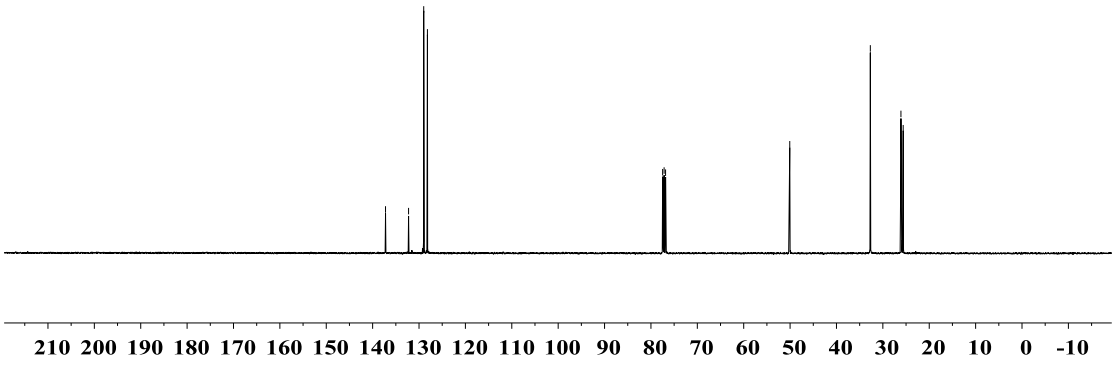
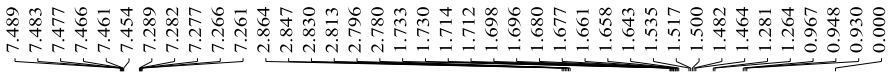
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.


137.22
132.25
128.99
128.19
77.48
77.16
76.84
50.07
32.70
26.10
25.62


S
S
Cl

**3e**


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.483
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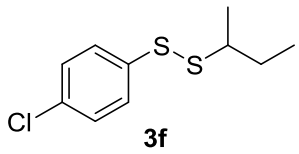
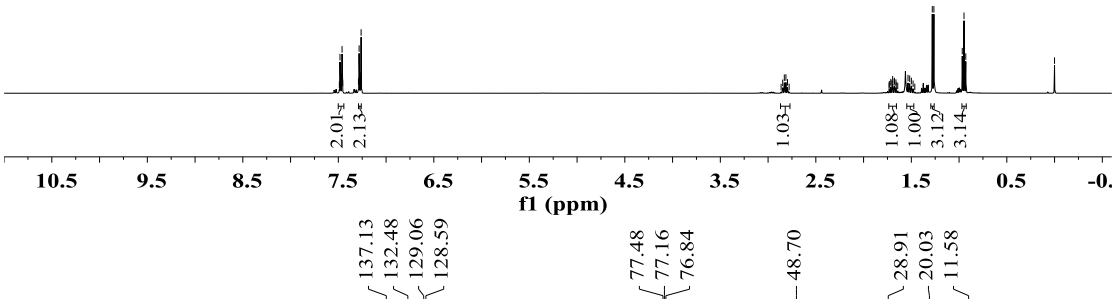
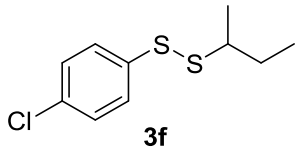
7.454
7.289
7.282
7.277
7.266
7.261
2.864
2.847
2.830
2.813
2.796
2.780
1.733
1.730
1.714
1.712
1.698
1.696
1.680
1.677
1.661
1.658
1.643
1.535
1.517
1.500
1.482
1.464
1.281
1.264
0.967
0.948
0.930
0.000


S
S
Cl

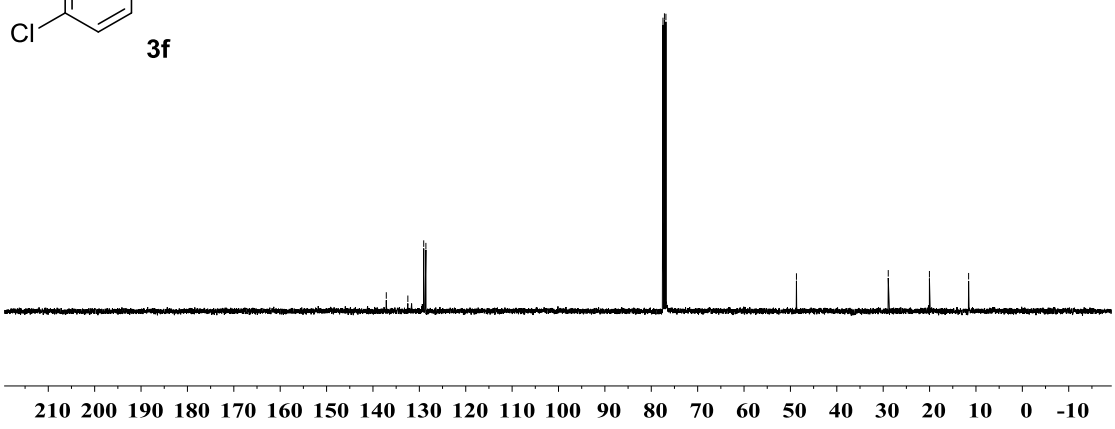
**3f**


2.01
2.13
1.03
1.08
1.00
3.12
3.14
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
f1 (ppm)


137.13
132.48
129.06
128.59
77.48
77.16
76.84
48.70
28.91
20.03
11.58


S
S
Cl

**3f**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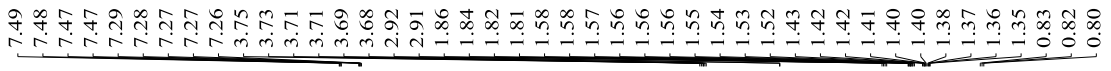
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7.48
7.47
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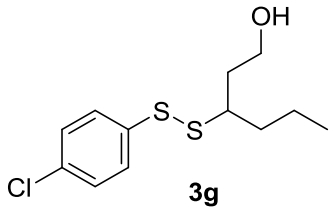
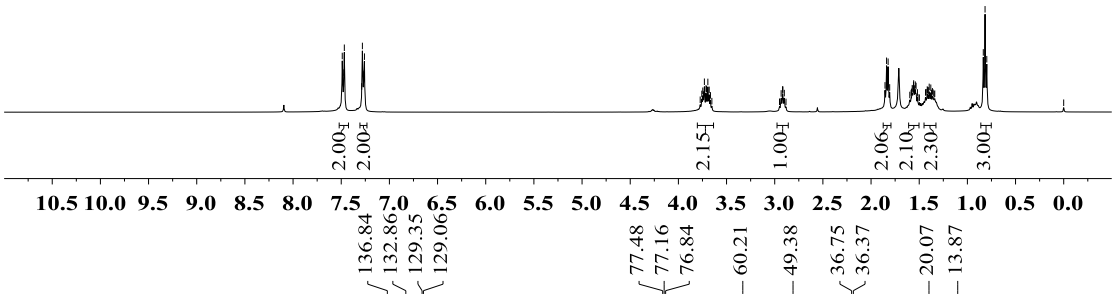
7.28
7.27
7.27
7.26
3.75
3.73
3.71
3.71
3.69
3.68
2.92
2.91
1.86
1.84
1.82
1.81
1.58
1.58
1.57
1.56
1.56
1.56
1.55
1.54
1.53
1.52
1.43
1.42
1.42
1.41
1.40
1.40
1.38
1.37
1.36
1.35
0.83
0.82
0.80


OH
S
S
Cl

**3g**


2.00
2.00
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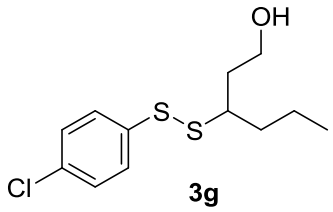
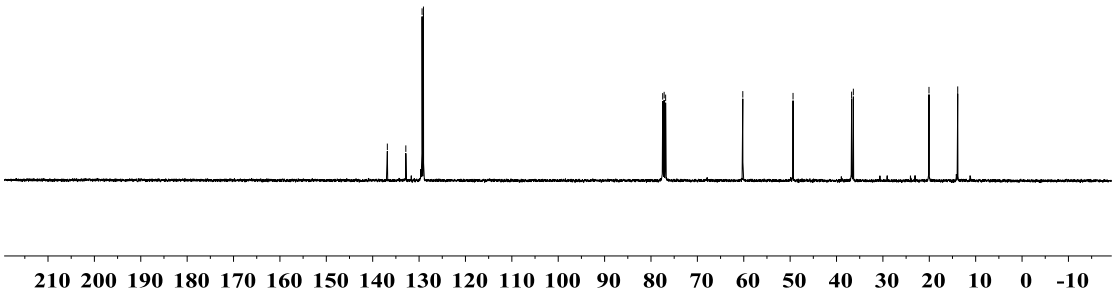
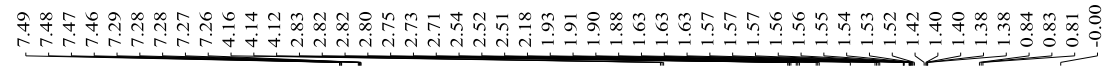
1.00
2.06
2.10
2.30
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


136.84
132.86
129.35
129.06
77.48
77.16
76.84
60.21
49.38
36.75
36.37
20.07
13.87


OH
S
S
Cl

**3g**


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


7.49
7.48
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7.29
7.28
7.28
7.27
7.26
4.16
4.14
4.12
2.83
2.82
2.82
2.80
2.75
2.73
2.71
2.54
2.52
2.51
2.18
1.93
1.91
1.90
1.88
1.63
1.63
1.57
1.57
1.57
1.56
1.56
1.55
1.54
1.53
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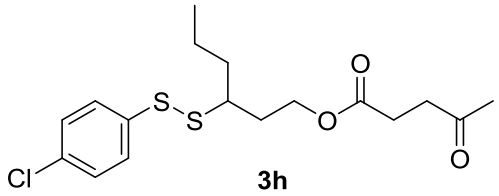
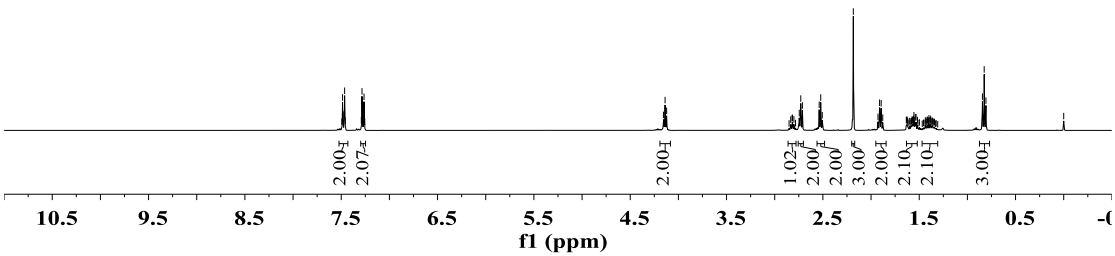
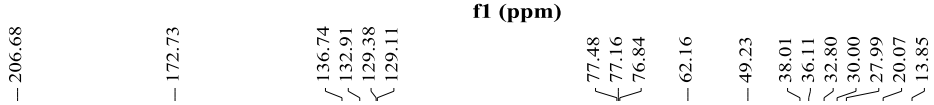
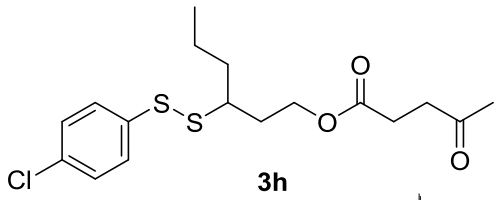
1.42
1.40
1.40
1.38
1.38
0.84
0.83
0.81
-0.00


S
S
O
O
O
Cl

3h

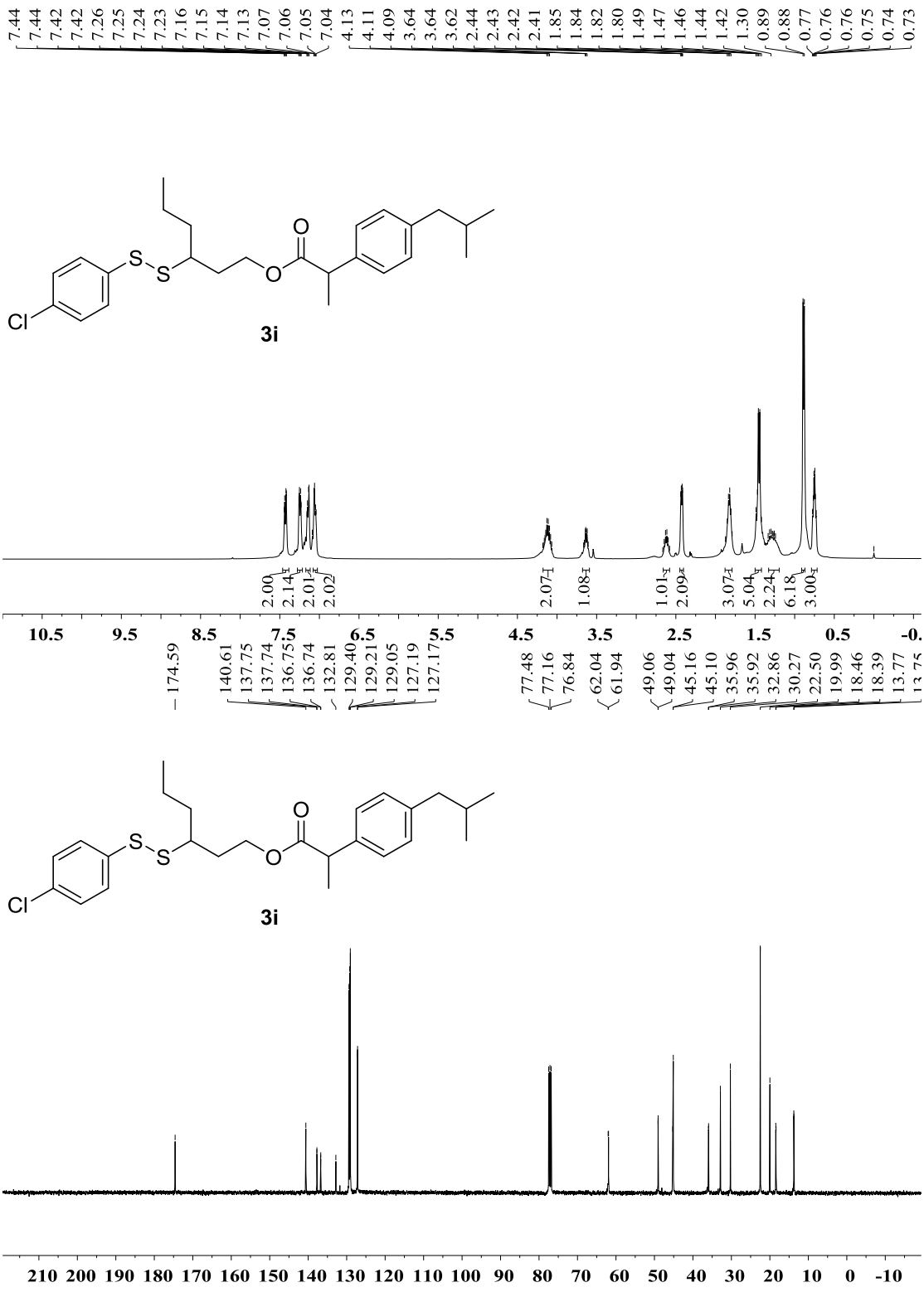

2.00
2.07
2.00
1.02
2.00
3.00
2.00
2.10
2.10
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

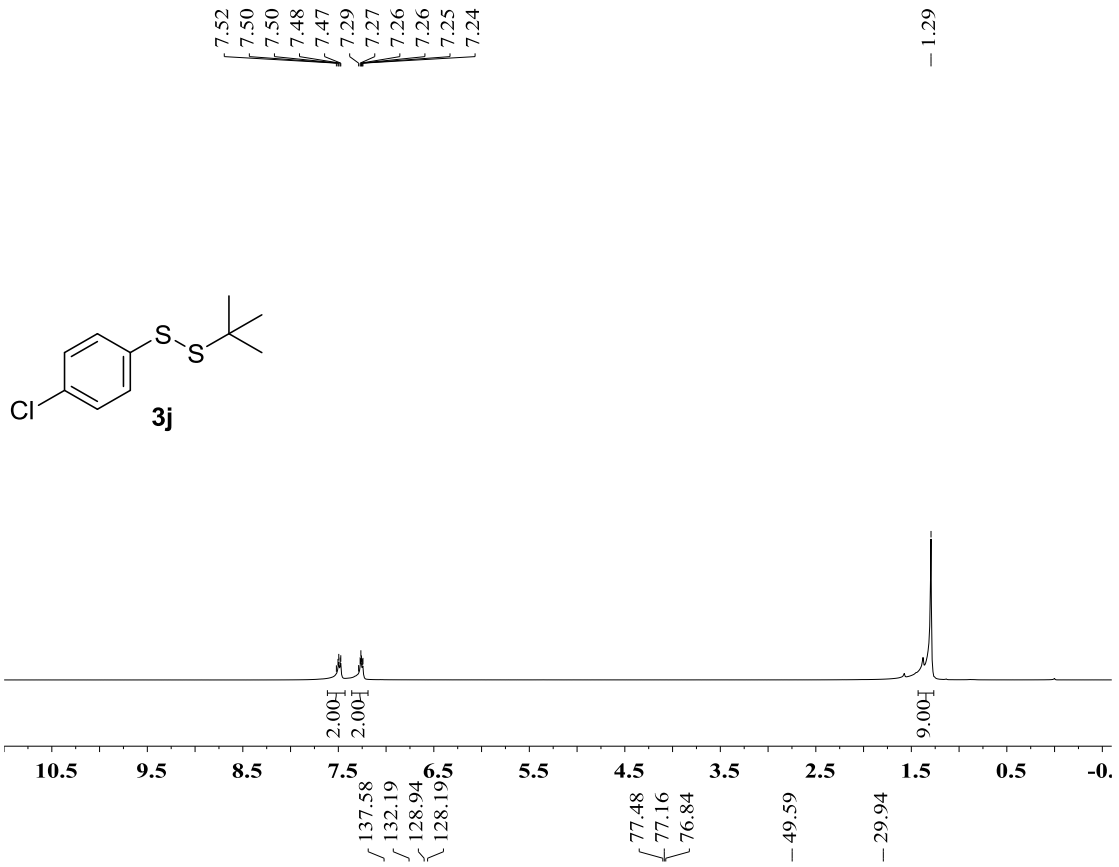

206.68
172.73
136.74
132.91
129.38
129.11
77.48
77.16
76.84
62.16
49.23
38.01
36.11
32.80
30.00
27.99
20.07
13.85


S
S
O
O
O
Cl

3h


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.44 7.44 7.42 7.42 7.26 7.25 7.24 7.23 7.16 7.15 7.14 7.13 7.07 7.06 7.05 7.04
4.13 4.11 4.09 3.64 3.64 3.62 2.44 2.43 2.42 2.41 1.85 1.84 1.82 1.80 1.49 1.47 1.46 1.44 1.42 1.30 0.89 0.88 0.77 0.76 0.76 0.75 0.74 0.73
S S O O Cl
3i
2.00 2.14 2.01 2.02 2.07 1.08 1.01 2.09 3.07 5.04 2.24 6.18 3.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.
174.59 140.61 137.75 137.74 136.75 136.74 132.81 129.40 129.21 129.05 127.19 127.17 77.48 77.16 76.84 62.04 61.94 49.06 49.04 45.16 45.10 35.96 35.92 32.86 30.27 22.50 19.99 18.46 18.39 13.77
S S O O Cl
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.47
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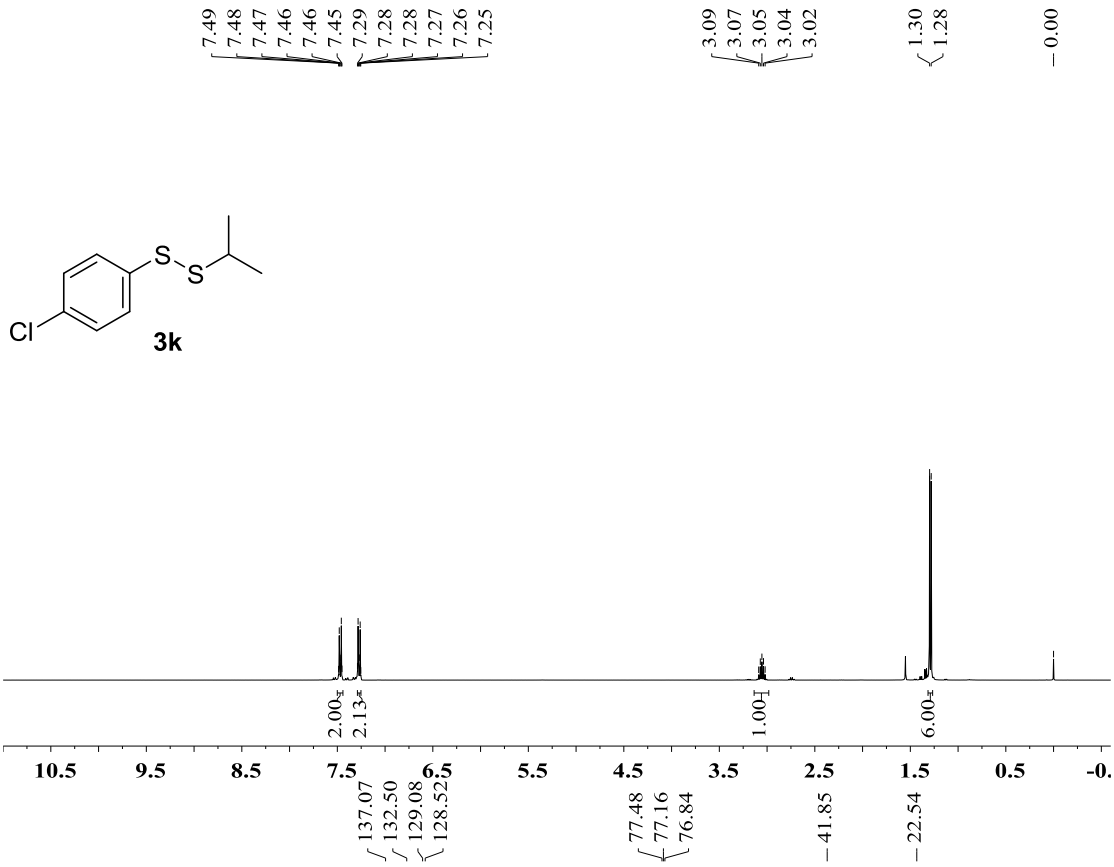
7.27
7.26
7.26
7.25
7.24
1.29
S
S
Cl
3j
2.00
2.00
9.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
137.58
132.19
128.94
128.19
77.48
77.16
76.84
49.59
29.94
S
S
Cl
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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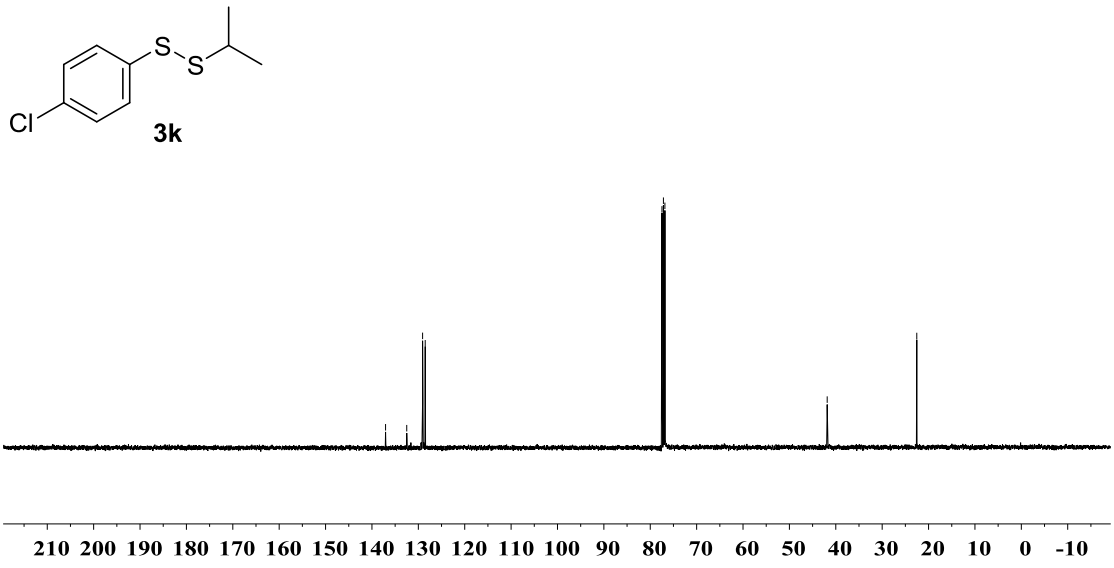
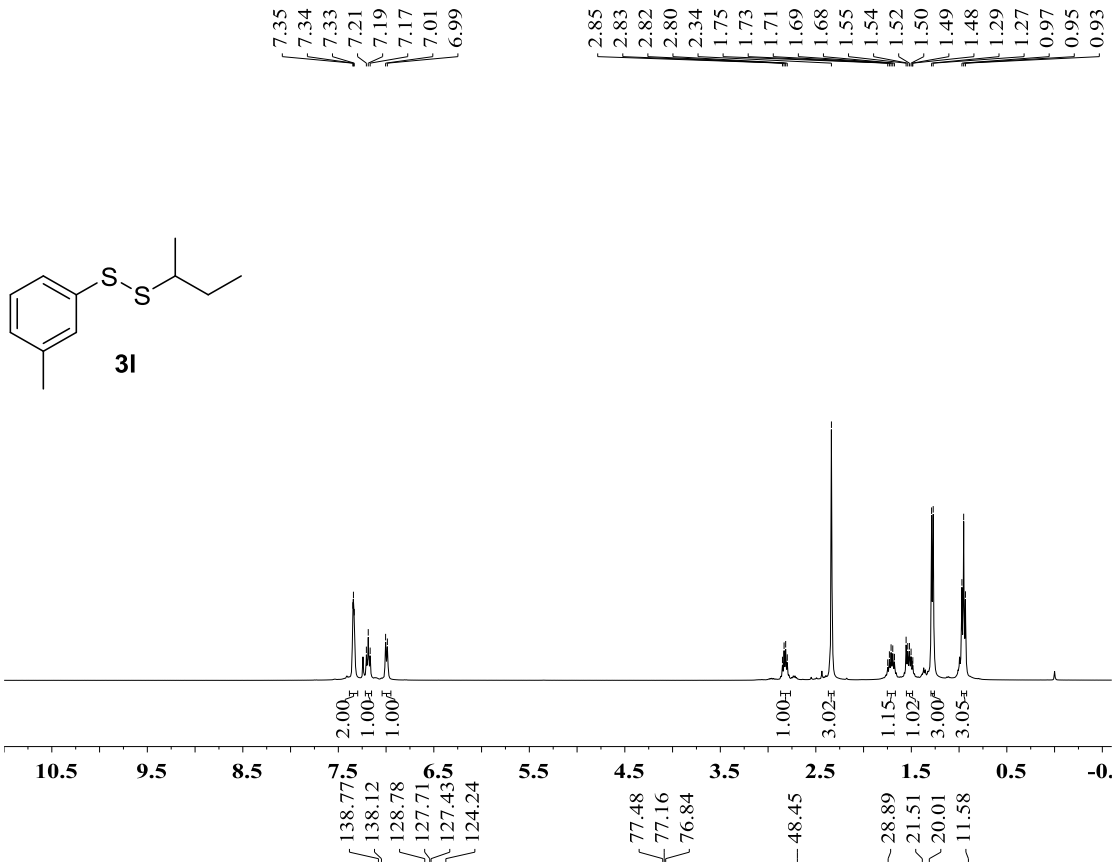
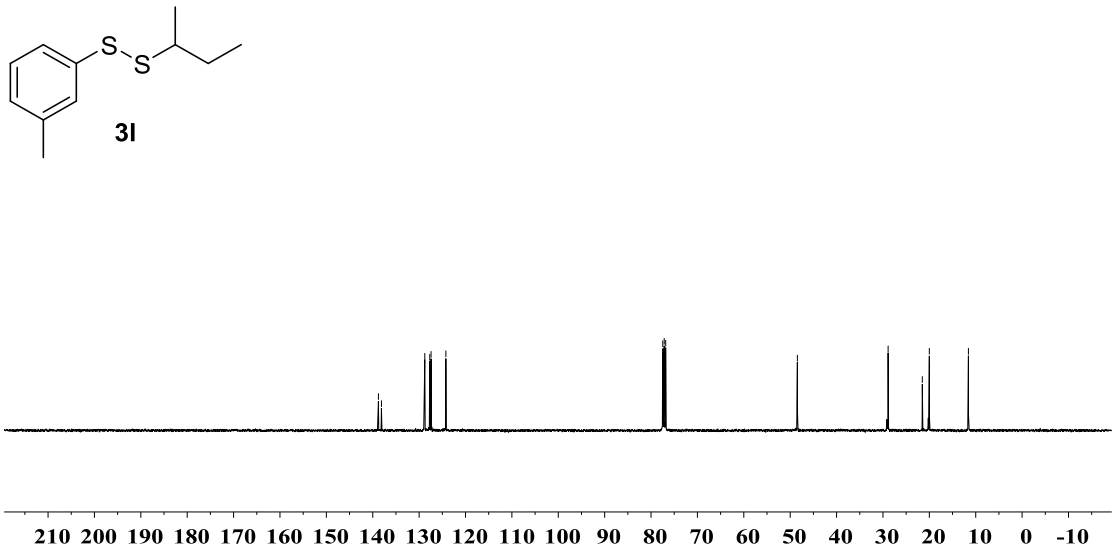
7.47
7.46
7.46
7.45
7.29
7.28
7.28
7.27
7.26
7.25
3.09
3.07
3.05
3.04
3.02
1.30
1.28
0.00
S
S
Cl
3k
2.00
2.13
1.00
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
137.07
132.50
129.08
128.52
77.48
77.16
76.84
41.85
22.54


S
S
Cl
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


7.35
7.34
7.33
7.21
7.19
7.17
7.01
6.99
2.85
2.83
2.82
2.80
2.34
1.75
1.73
1.71
1.69
1.68
1.55
1.54
1.52
1.50
1.49
1.48
1.29
1.27
0.97
0.95
0.93
S
S
3l
2.00
1.00
1.00
1.00
3.02
1.15
1.02
3.00
3.05
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
138.77
138.12
128.78
127.71
127.43
124.24
77.48
77.16
76.84
48.45
28.89
21.51
20.01
11.58


S
S
3l
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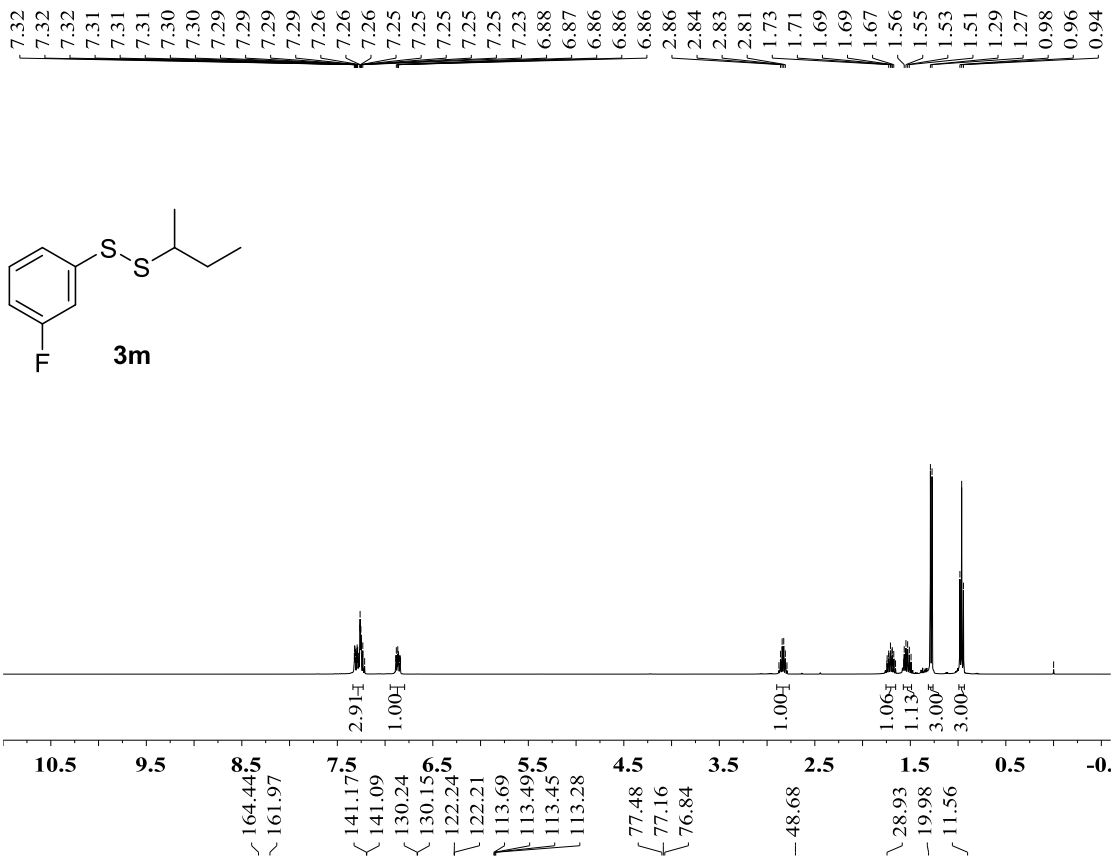
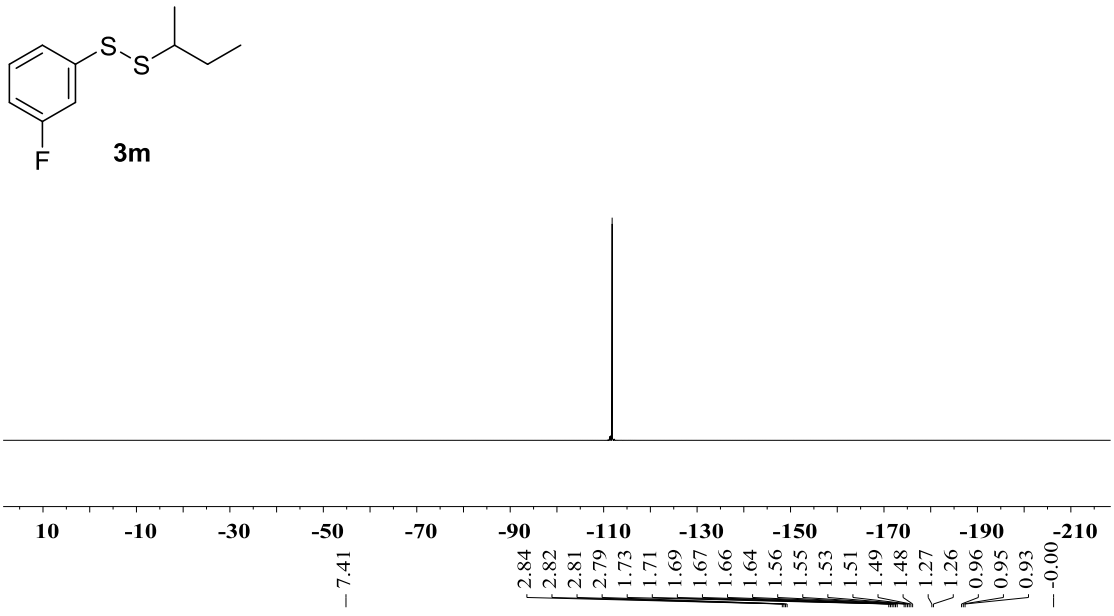
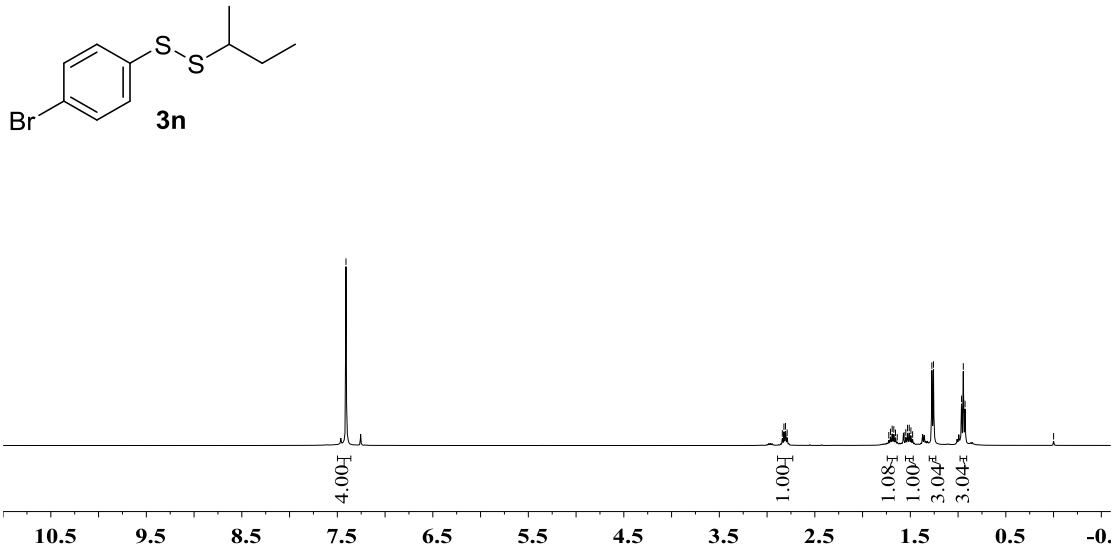

7.32 7.32 7.32 7.31 7.31 7.31 7.30 7.30 7.29 7.29 7.29 7.29 7.26 7.26 7.26 7.25 7.25 7.25 7.25 7.25 7.23 6.88 6.87 6.86 6.86 6.86
2.86 2.84 2.83 2.81 1.73 1.71 1.69 1.69 1.67 1.56 1.55 1.53 1.51 1.29 1.27 0.98 0.96 0.94
S
S
F
3m
2.91
1.00
1.00
1.06
1.13
3.00
3.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.
164.44 161.97 141.17 141.09 130.24 130.15 122.24 122.21 113.69 113.49 113.45 113.28 77.48 77.16 76.84 48.68 28.93 19.98 11.56
S
S
F
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


-111.82
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
7.41
2.84
2.82
2.81
2.79
1.73
1.71
1.69
1.67
1.66
1.64
1.56
1.55
1.53
1.51
1.49
1.48
1.27
1.26
0.96
0.95
0.93
-0.00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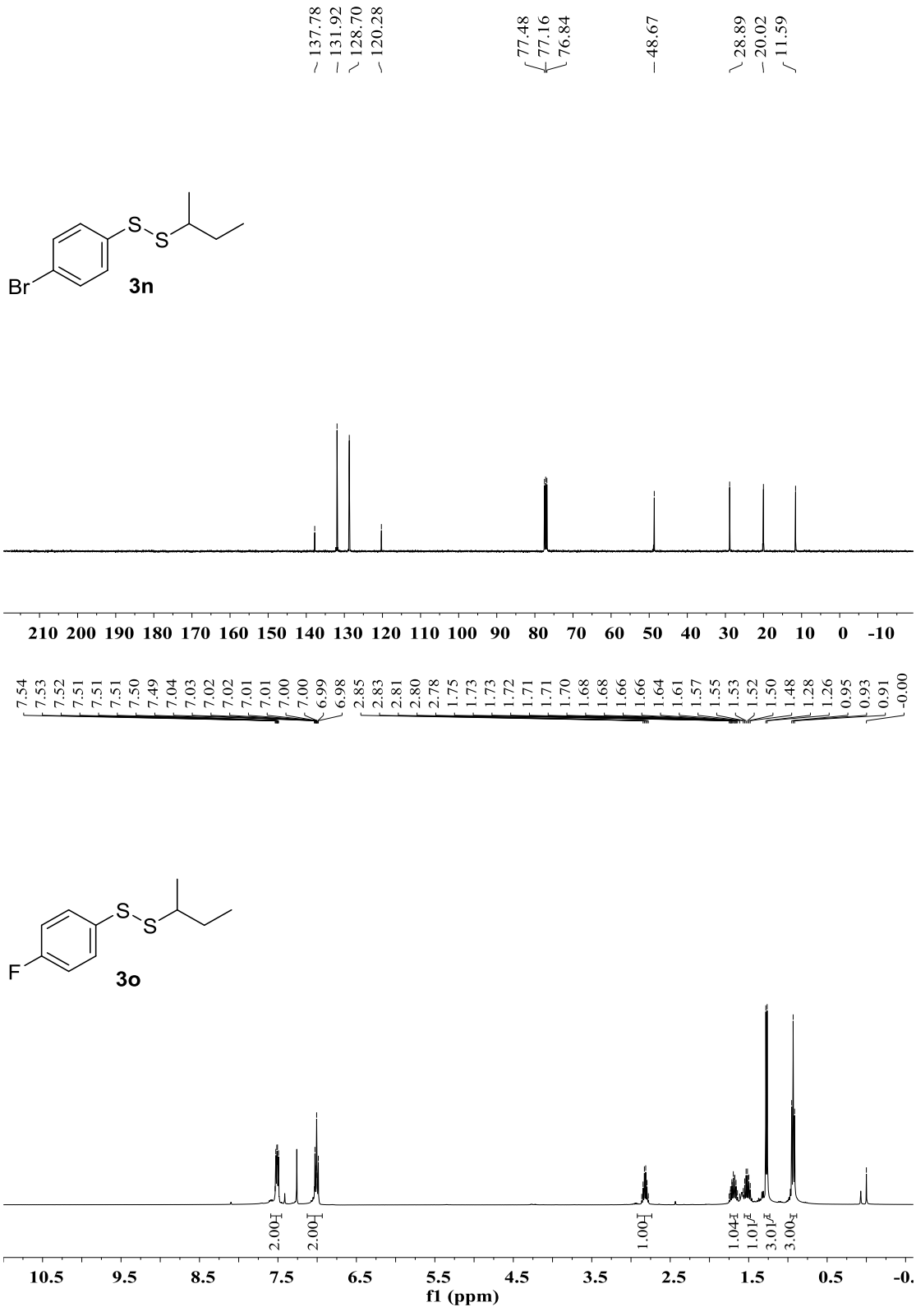
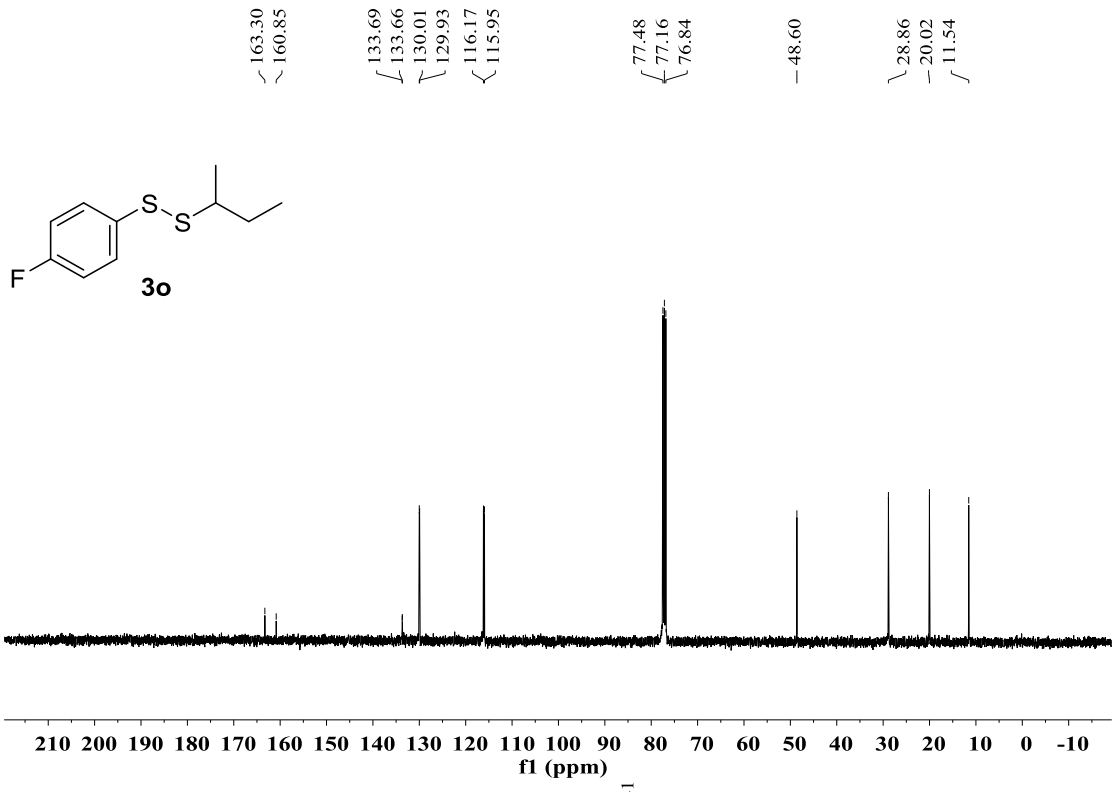
1.00
1.08
1.00
3.04
3.04
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.


137.78
131.92
128.70
120.28
77.48
77.16
76.84
48.67
28.89
20.02
11.59
Br
S
S
3n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
7.54
7.53
7.52
7.51
7.51
7.51
7.50
7.49
7.04
7.03
7.02
7.02
7.01
7.01
7.00
7.00
6.99
6.98
2.85
2.83
2.81
2.80
2.78
1.75
1.73
1.73
1.72
1.71
1.71
1.70
1.68
1.68
1.66
1.66
1.64
1.61
1.57
1.55
1.53
1.52
1.50
1.48
1.28
1.26
0.95
0.93
0.91
-0.00
F
S
S
3o
2.00
2.00
1.00
1.04
1.01
3.01
3.00
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.
f1 (ppm)


163.30
160.85
133.69
133.66
130.01
129.93
116.17
115.95
77.48
77.16
76.84
48.60
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F
3o
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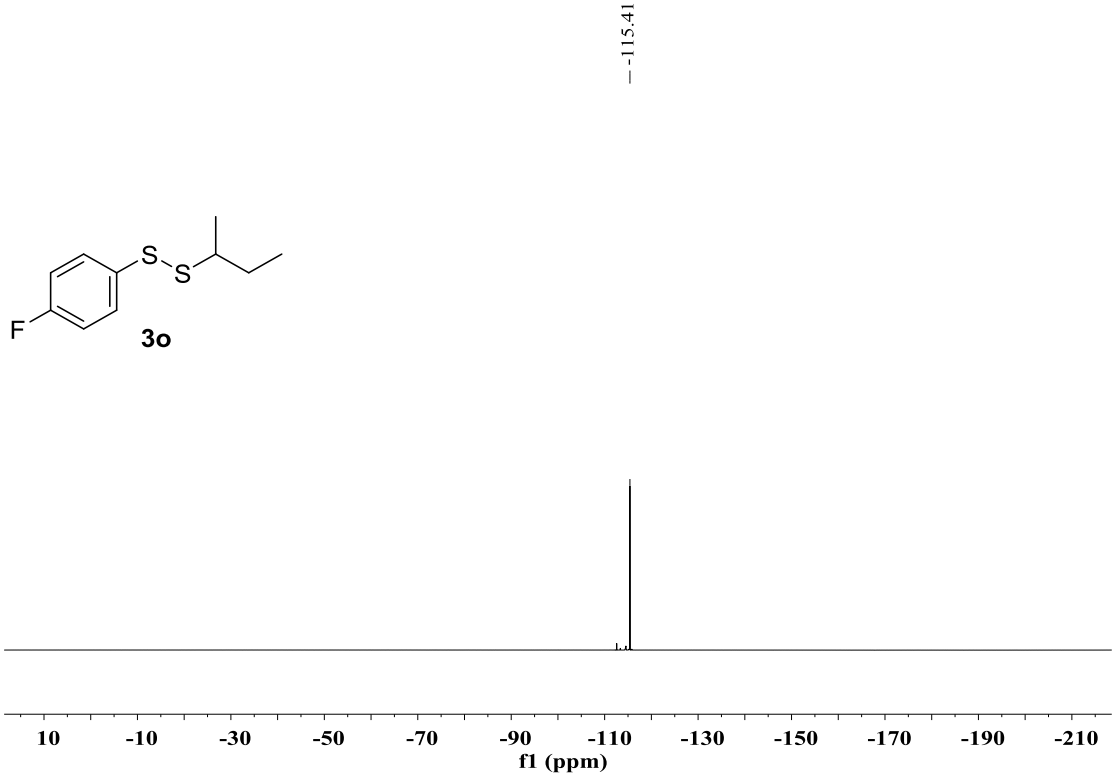
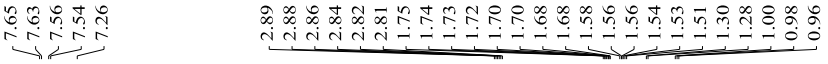
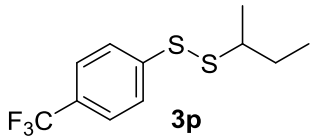
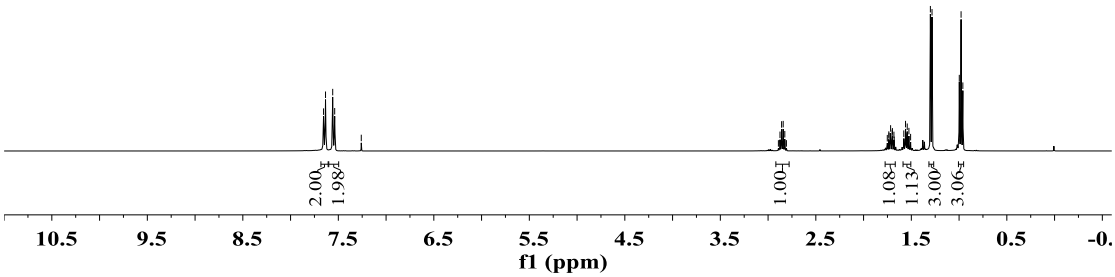
f1 (ppm)

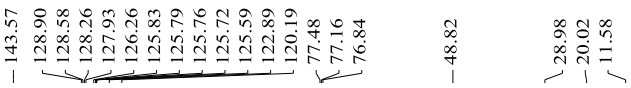

-115.41
S
S
F
3o
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

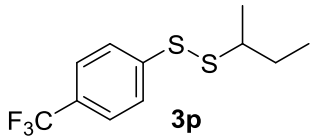

7.65
7.63
7.56
7.54
7.26
2.89
2.88
2.86
2.84
2.82
2.81
1.75
1.74
1.73
1.72
1.70
1.70
1.68
1.68
1.58
1.56
1.56
1.54
1.53
1.51
1.30
1.28
1.00
0.98
0.96


S
S
F3C

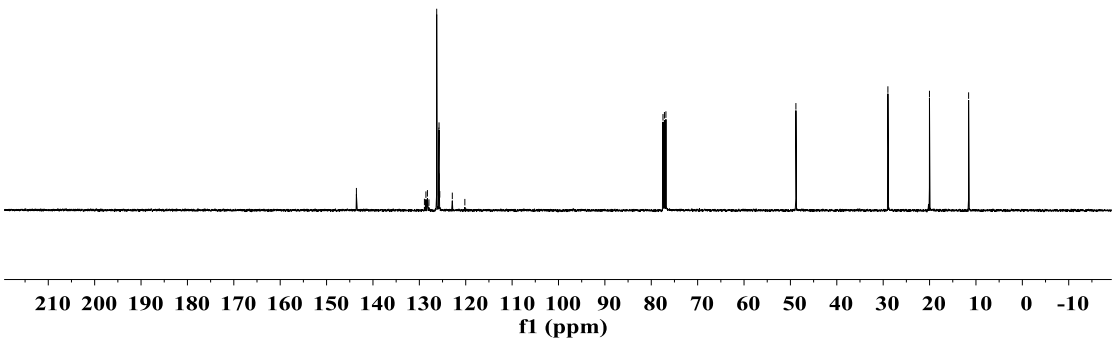
**3p**

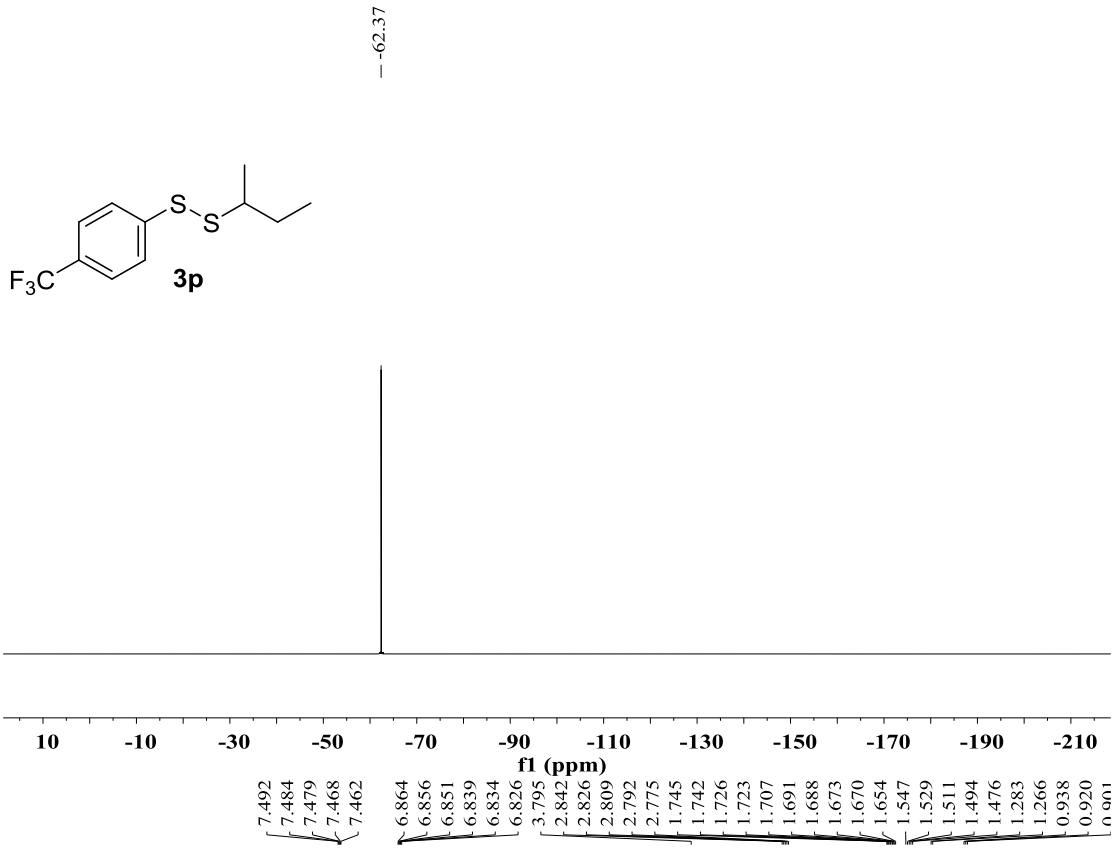

2.00
1.98
1.00
1.08
1.13
3.00
3.06
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
f1 (ppm)

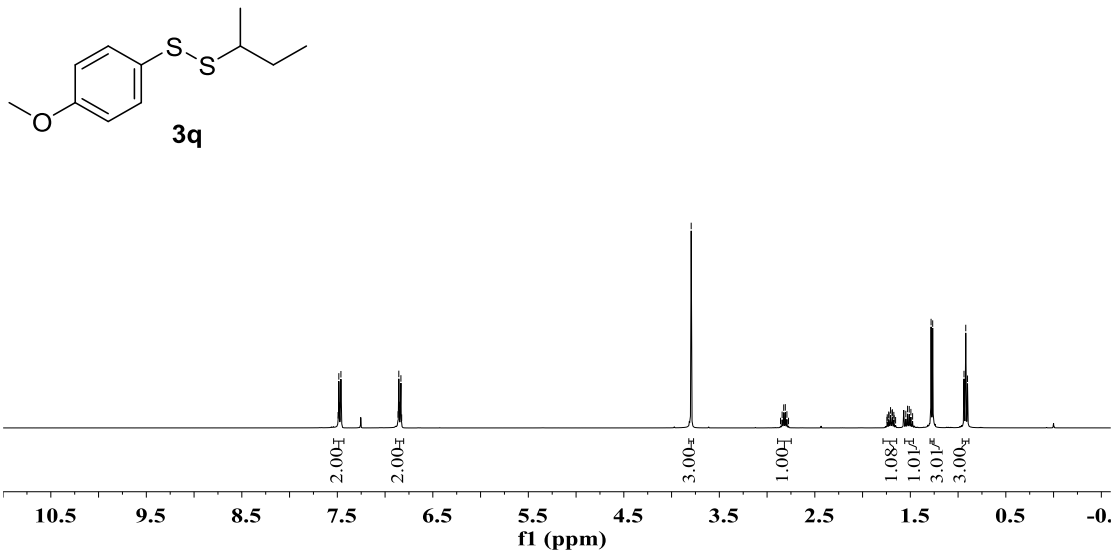

143.57
128.90
128.58
128.26
127.93
126.26
125.83
125.79
125.76
125.72
125.59
122.89
120.19
77.48
77.16
76.84
48.82
28.98
20.02
11.58

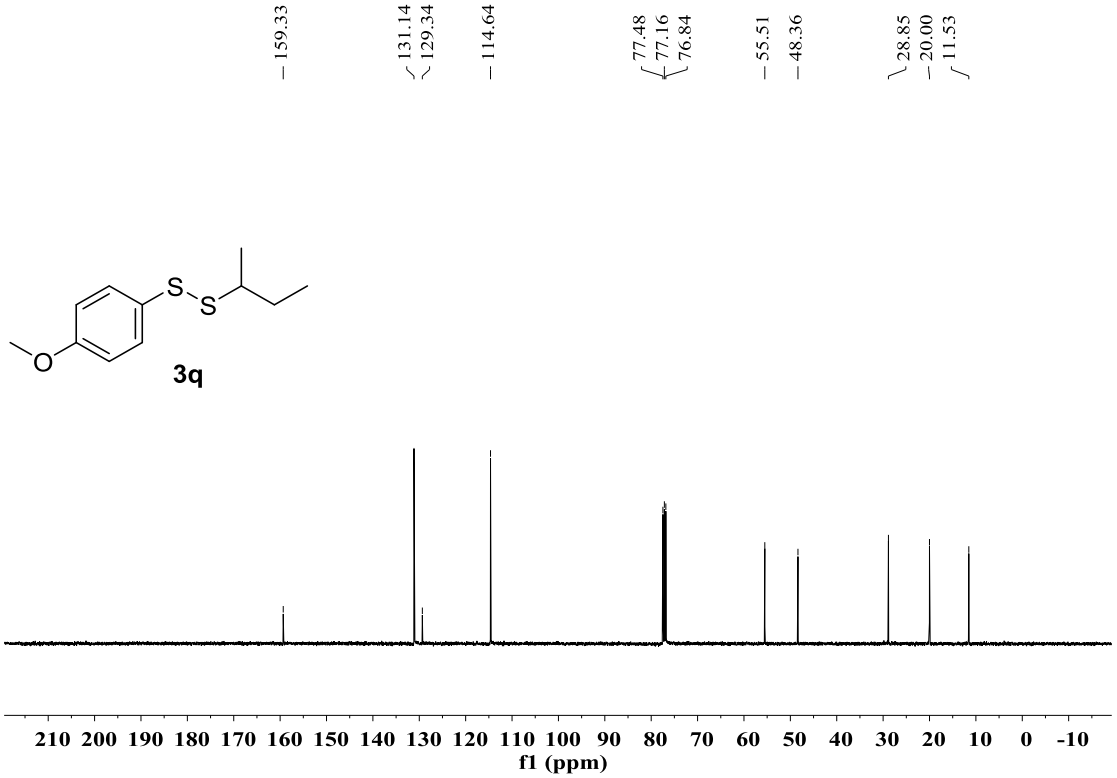

S
S
F3C

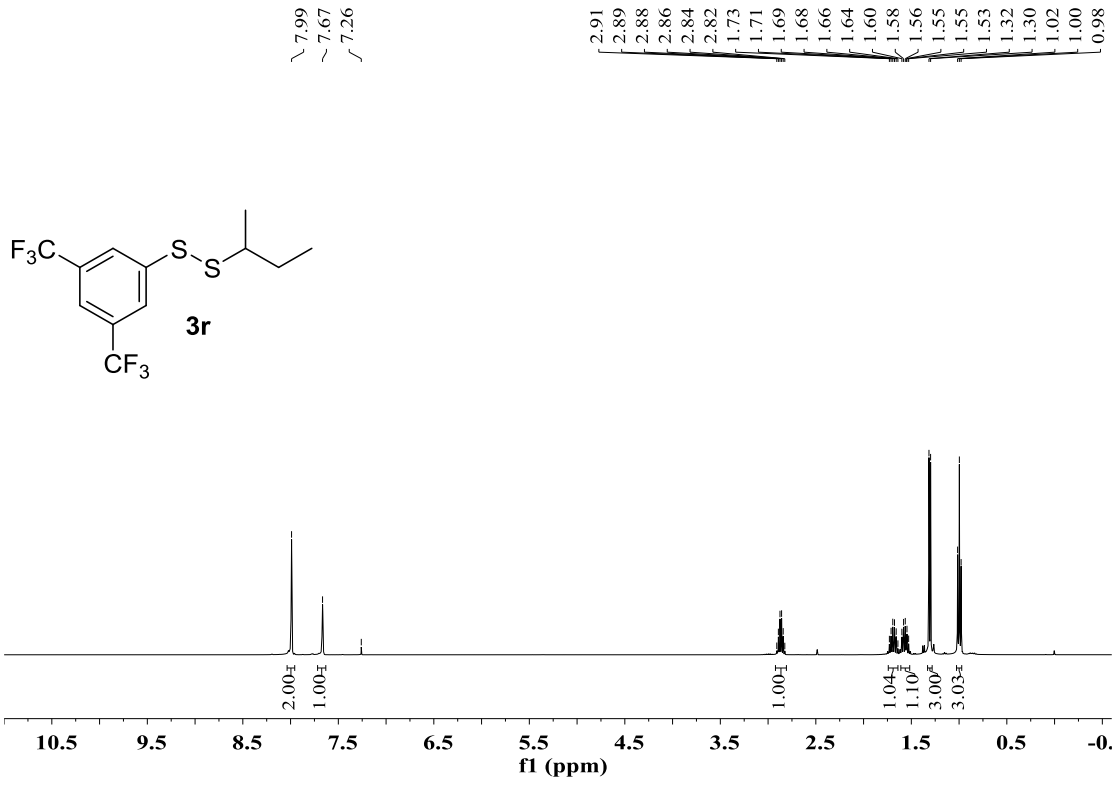
**3p**


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-62.37
S
S
F3C
3p
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)
7.492
7.484
7.479
7.468
7.462
6.864
6.856
6.851
6.839
6.834
6.826
3.795
2.842
2.826
2.809
2.792
2.775
1.745
1.742
1.726
1.723
1.707
1.691
1.688
1.673
1.670
1.654
1.547
1.529
1.511
1.494
1.476
1.283
1.266
0.938
0.920


S
S
O
3q
2.00
2.00
3.00
1.00
1.08
1.01
3.01
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
f1 (ppm)


159.33
131.14
129.34
114.64
77.48
77.16
76.84
55.51
48.36
28.85
20.00
11.53
S
S
O
3q
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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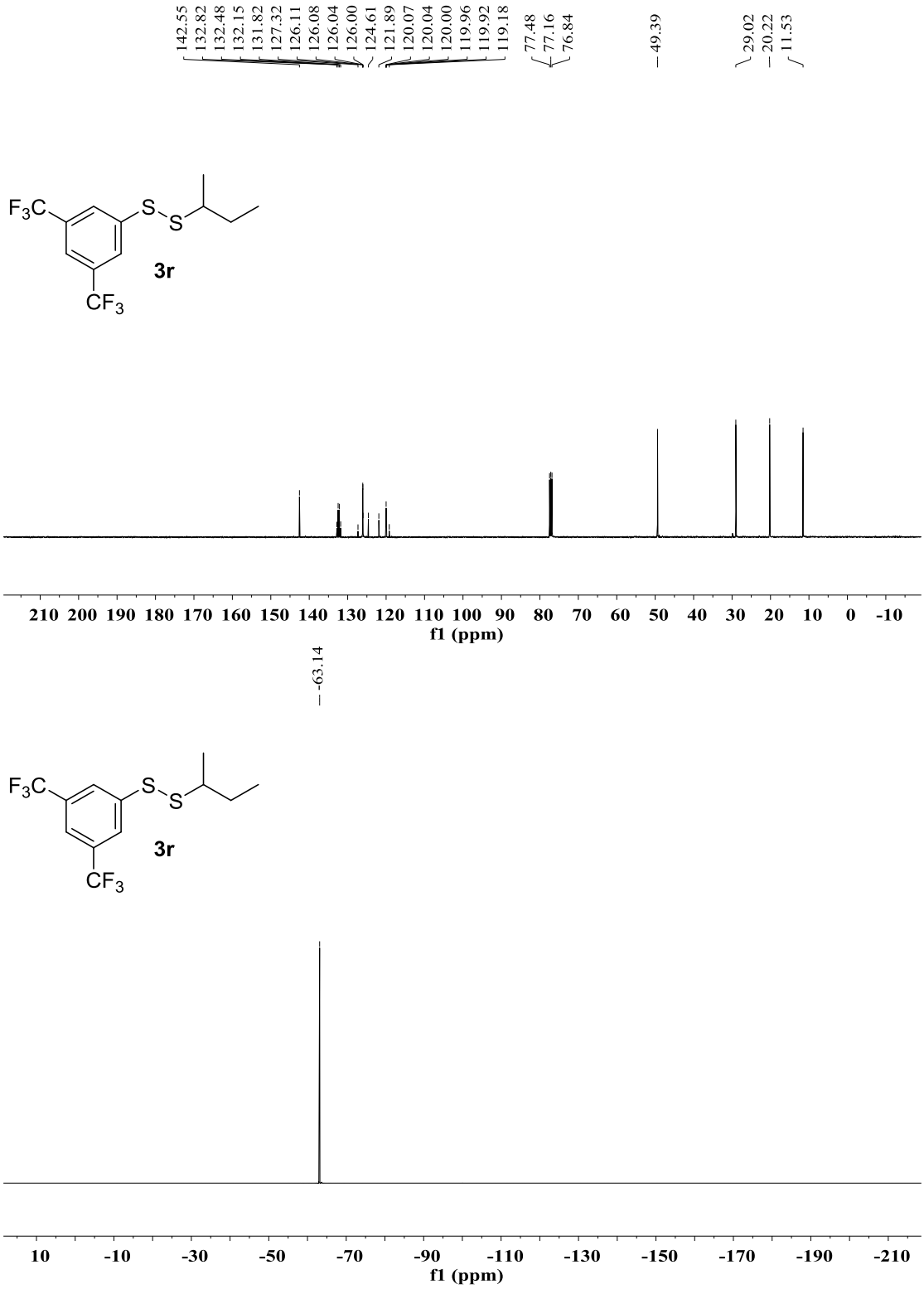
7.67
7.26
2.91
2.89
2.88
2.86
2.84
2.82
1.73
1.71
1.69
1.68
1.66
1.64
1.60
1.58
1.56
1.55
1.55
1.53
1.32
1.30
1.02
1.00
0.98
F3C
S
S
CF3
3r
2.00
1.00
1.00
1.04
1.10
3.00
3.03
10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.
f1 (ppm)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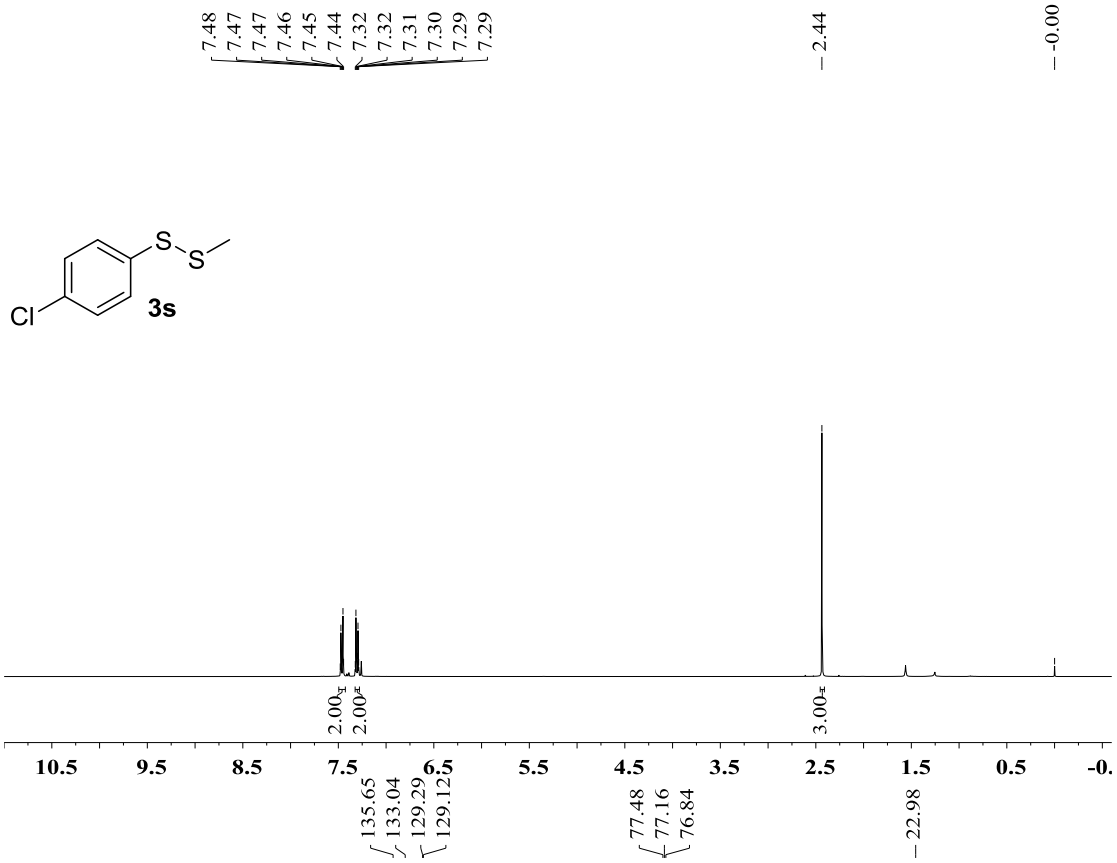
132.82
132.48
132.15
131.82
127.32
126.11
126.08
126.04
126.00
124.61
121.89
120.07
120.04
120.00
119.96
119.92
119.18
77.48
77.16
76.84
49.39
29.02
20.22
11.53
F3C
S
S
3r
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
-63.14
F3C
S
S
3r
CF3
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)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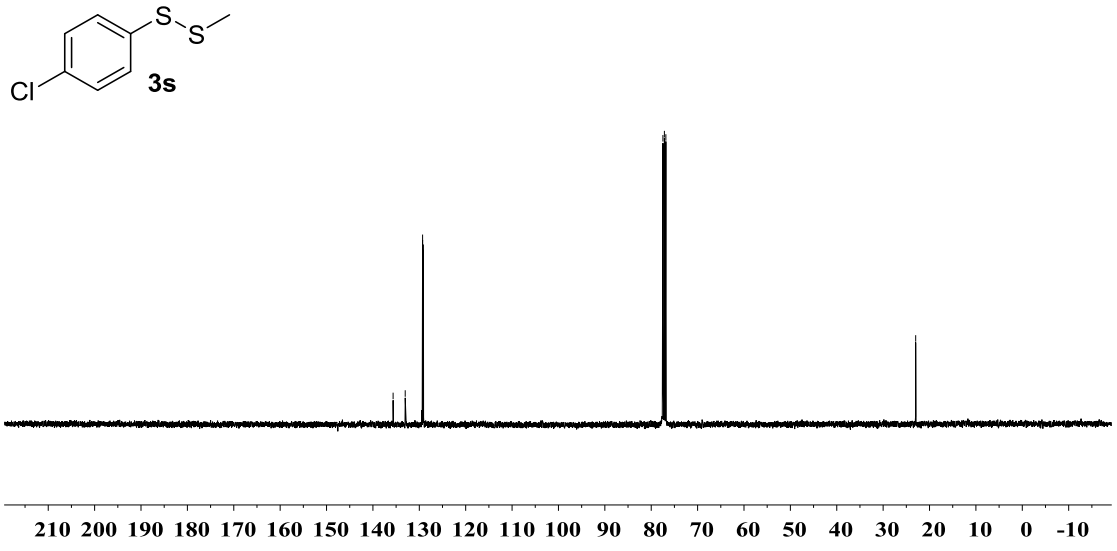
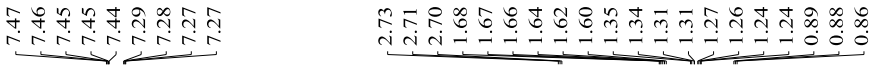
7.47
7.47
7.46
7.45
7.44
7.32
7.32
7.31
7.30
7.29
7.29
2.44
-0.00
S
S
Cl
3s
2.00
2.00
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.
135.65
133.04
129.29
129.12
77.48
77.16
76.84
22.98


S
S
Cl
3s
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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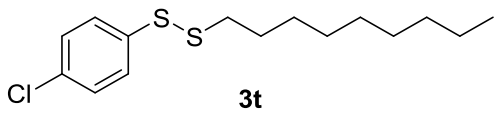
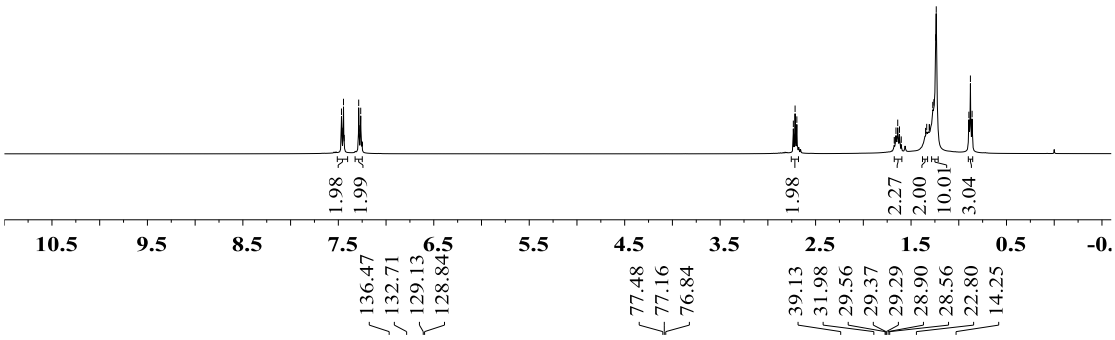
7.46
7.45
7.45
7.44
7.29
7.28
7.27
7.27
2.73
2.71
2.70
1.68
1.67
1.66
1.64
1.62
1.60
1.35
1.34
1.31
1.31
1.27
1.26
1.24
1.24
0.89
0.88
0.86


S
S
Cl

**3t**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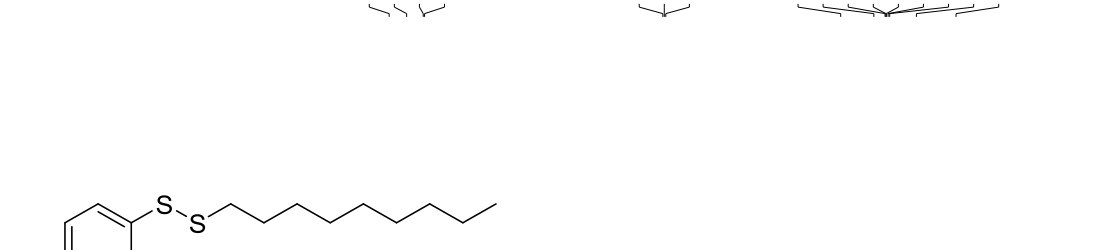
1.99
1.98
2.27
2.00
10.01
3.04
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.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132.71
129.13
128.84
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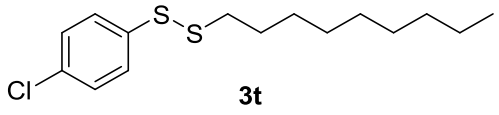
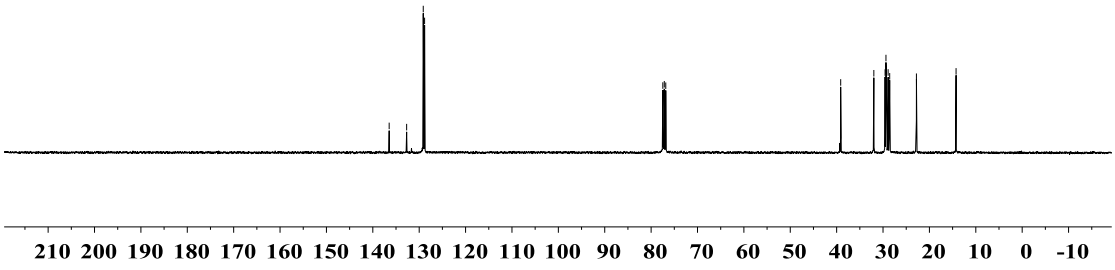
76.84
39.13
31.98
29.56
29.37
29.29
28.90
28.56
22.80
14.25


S
S
Cl

**3t**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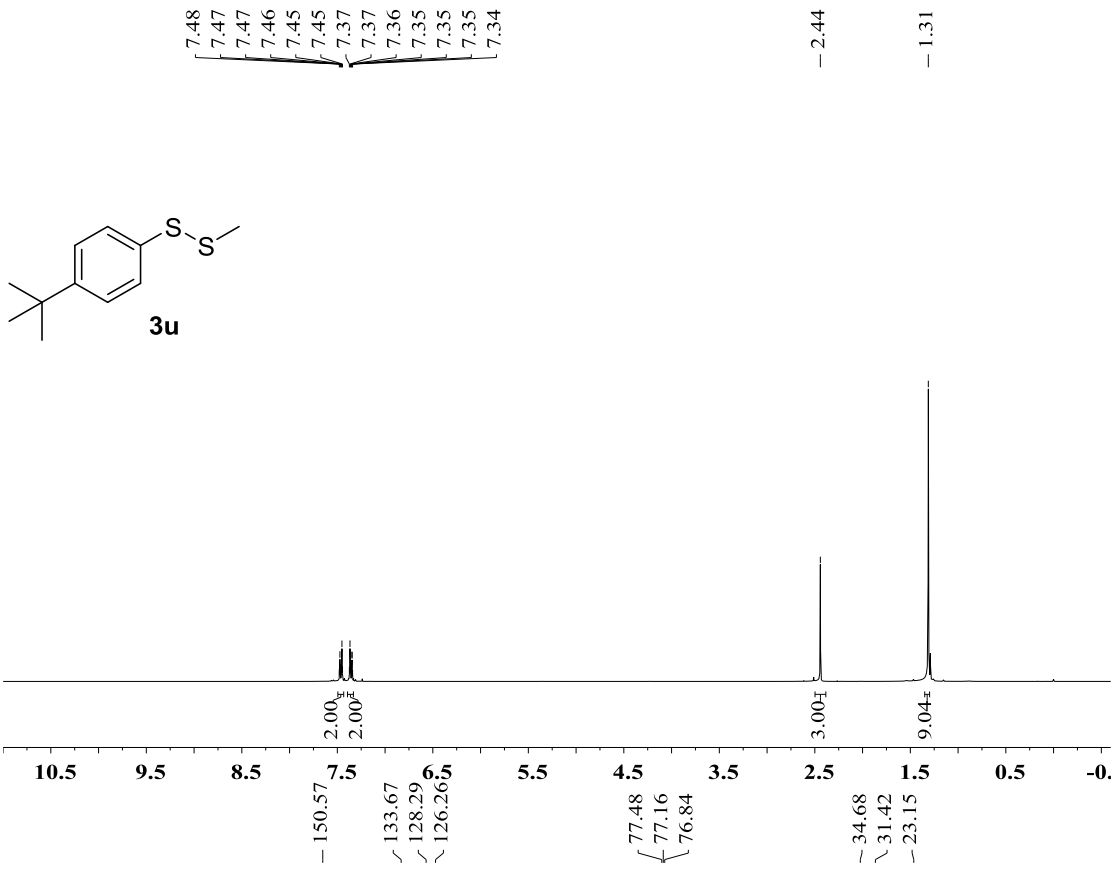
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7.47
7.47
7.46
7.45
7.45
7.37
7.37
7.36
7.35
7.35
7.35
7.34
2.44
1.31
S
S
3u
2.00
2.00
3.00
9.04
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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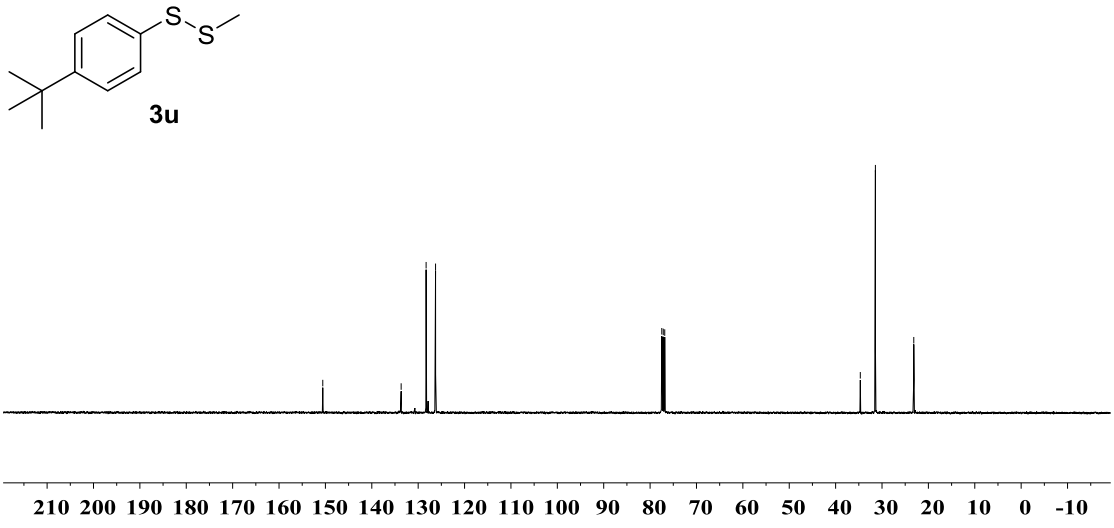
126.26
77.48
77.16
76.84
34.68
31.42
23.15


S
S
3u
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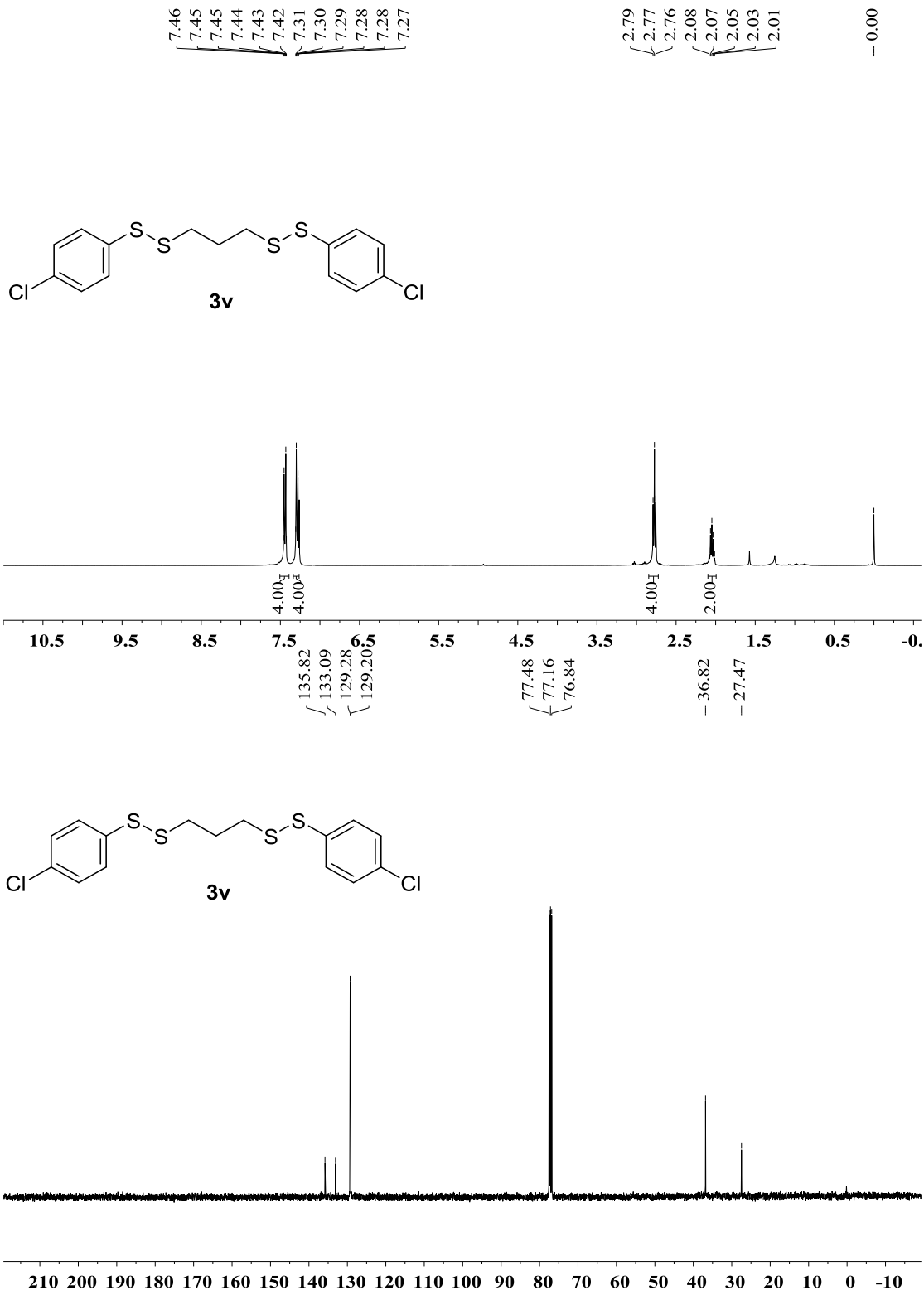
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7.30
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7.28
7.28
7.27
2.79
2.77
2.76
2.08
2.07
2.05
2.03
2.01
0.00
Cl
S
S
S
S
Cl
3v
4.00
4.00
4.00
2.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
135.82
133.09
129.28
129.20
77.48
77.16
76.84
36.82
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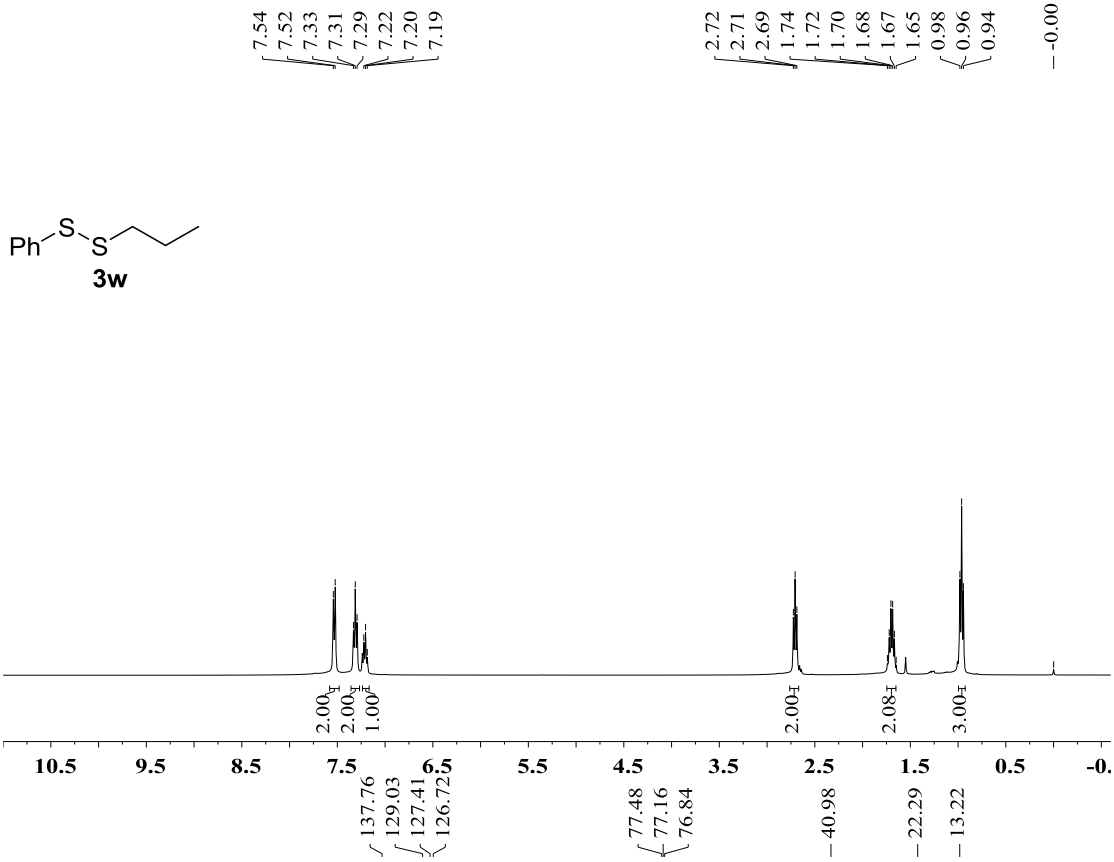
Cl
S
S
S
S
Cl
3v
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.29
7.22
7.20
7.19
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2.71
2.69
1.74
1.72
1.70
1.68
1.67
1.65
0.98
0.96
0.94
-0.00
Ph
S
S
3w
2.00
2.00
1.00
2.00
2.08
3.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
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77.16
76.84
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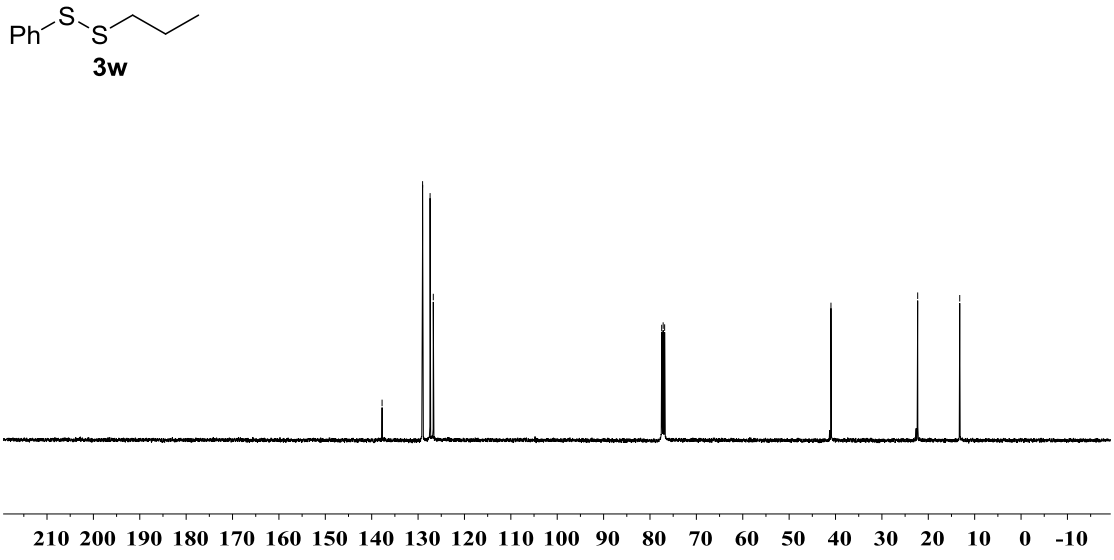
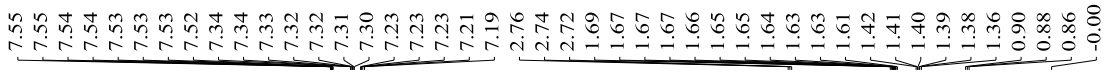
22.29
13.22


Ph
S
S
3w
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.32
7.32
7.31
7.30
7.23
7.23
7.23
7.21
7.19
2.76
2.74
2.72
1.69
1.67
1.67
1.67
1.66
1.65
1.65
1.64
1.63
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1.61
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1.39
1.38
1.36
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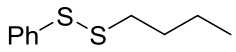
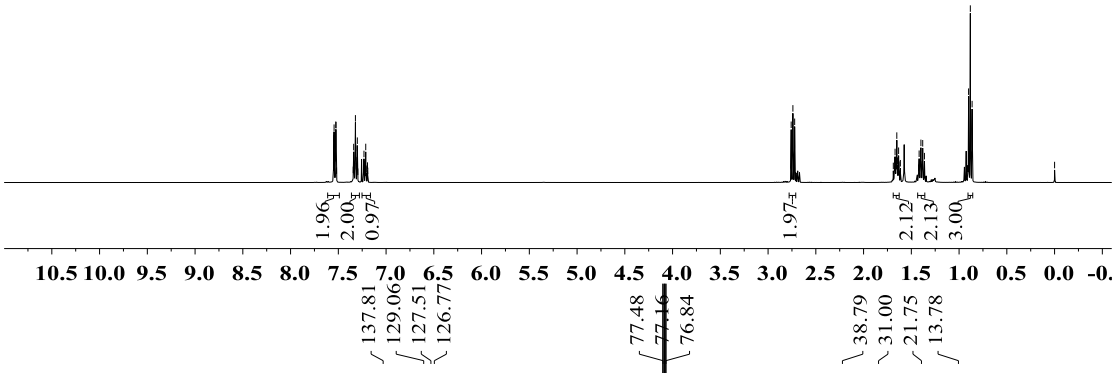
0.88
0.86
-0.00


Ph
S
S

**3x**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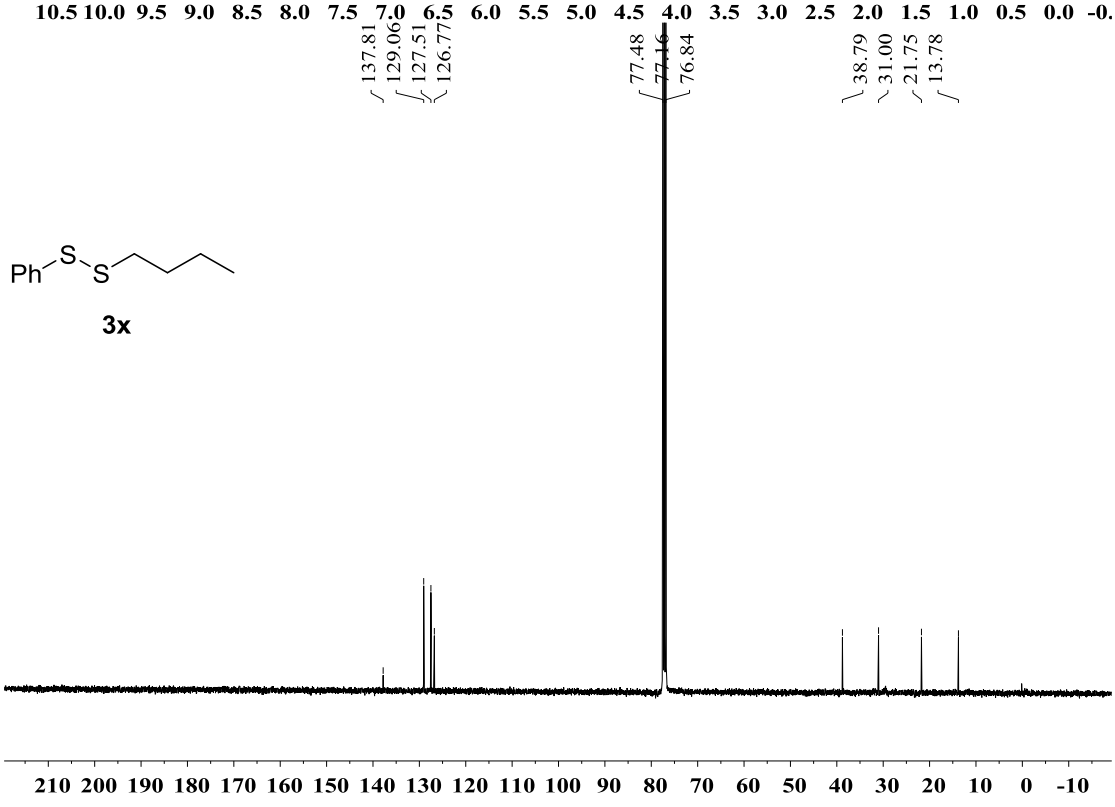
2.00
0.97
1.97
2.12
2.13
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.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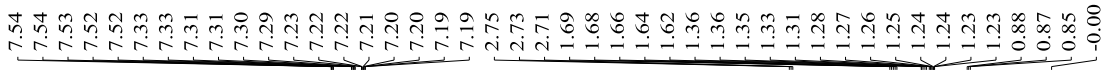
127.51
126.77
77.48
77.16
76.84
38.79
31.00
21.75
13.78
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10


Ph
S
S

**3x**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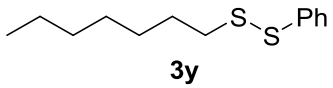
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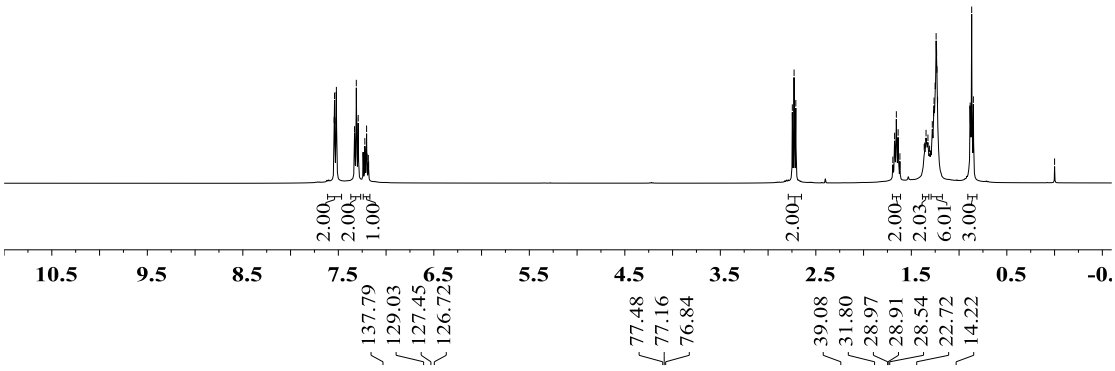
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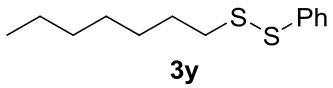
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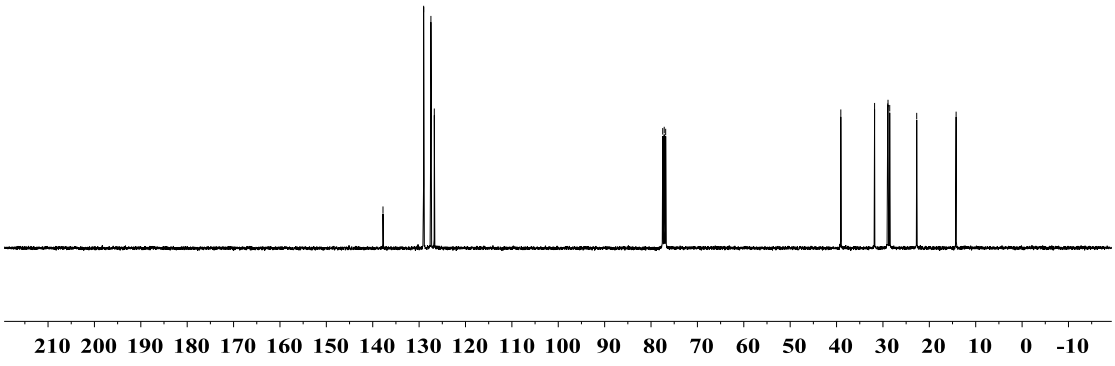
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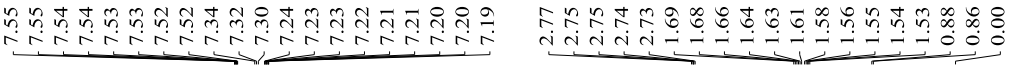
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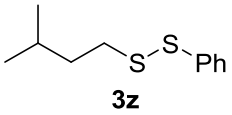
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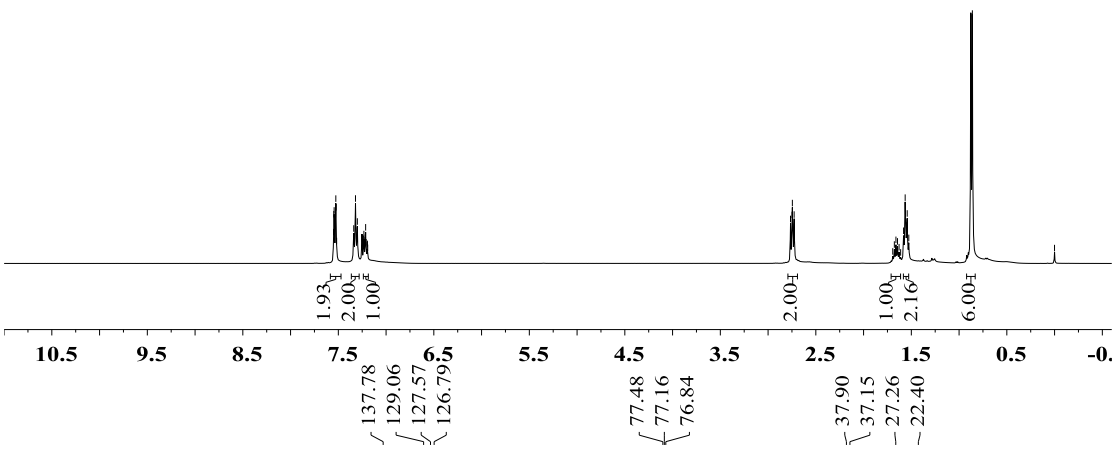
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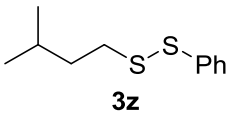
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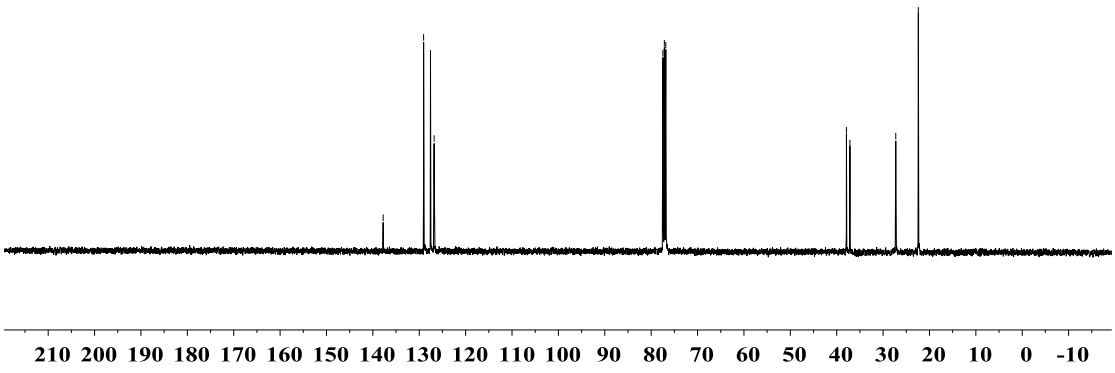
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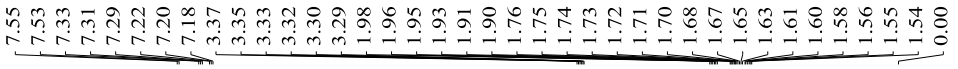
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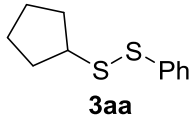
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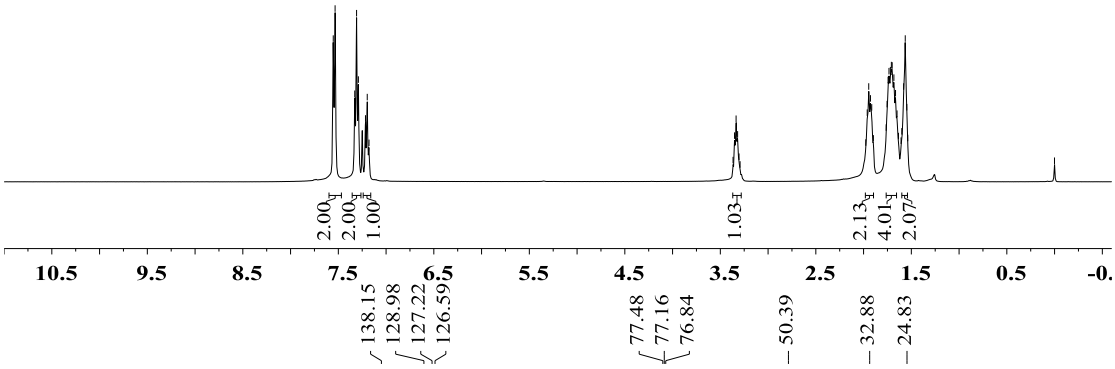
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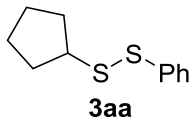
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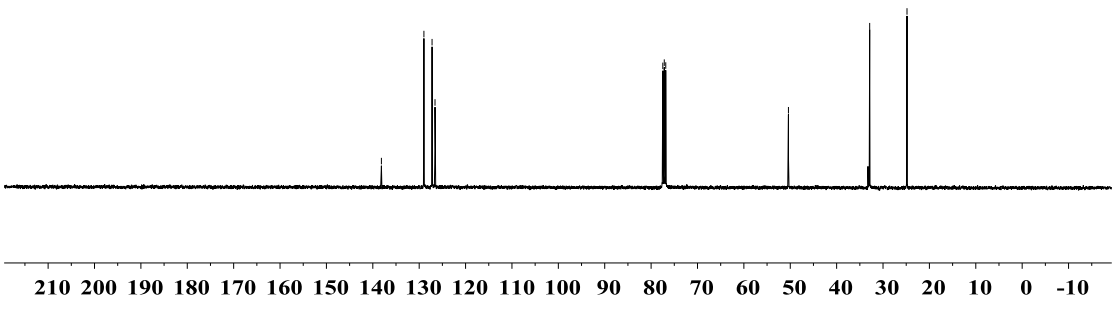
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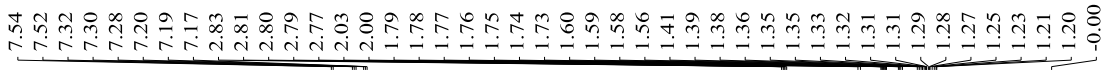
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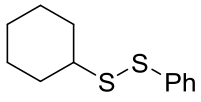
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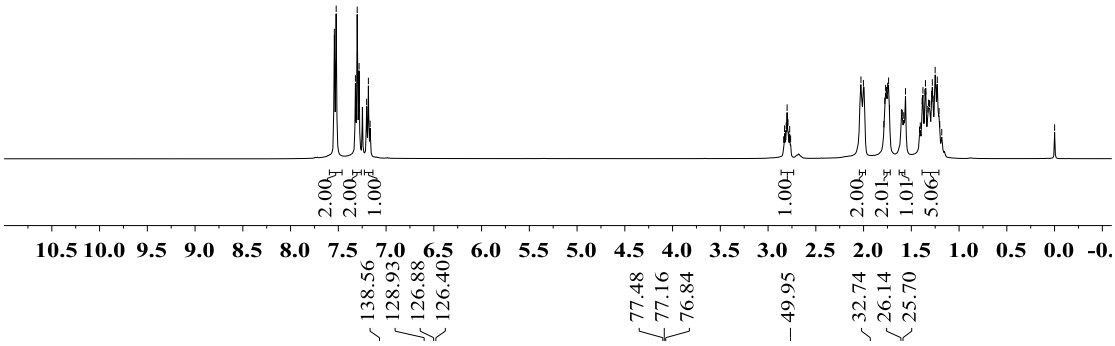
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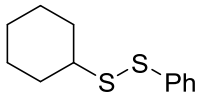
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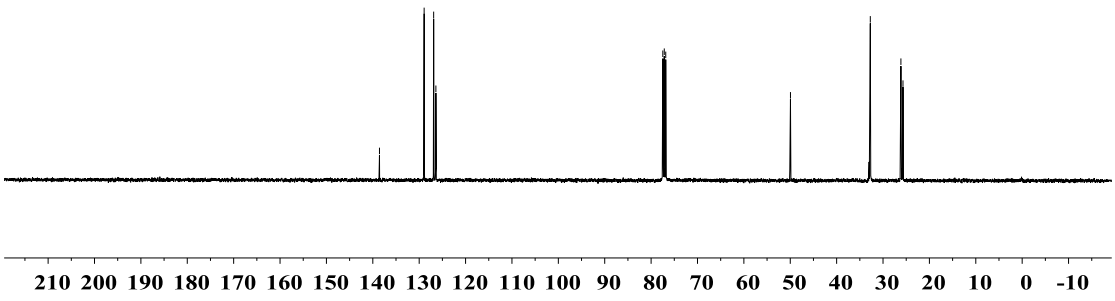
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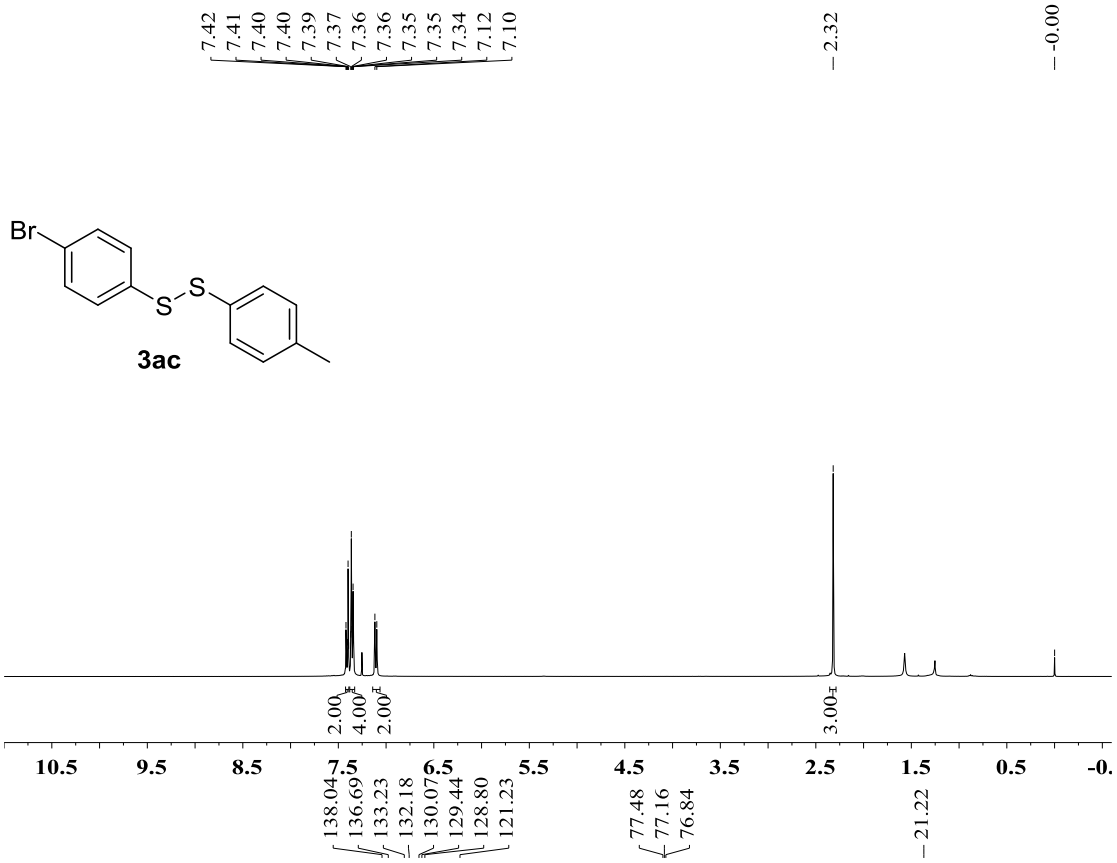
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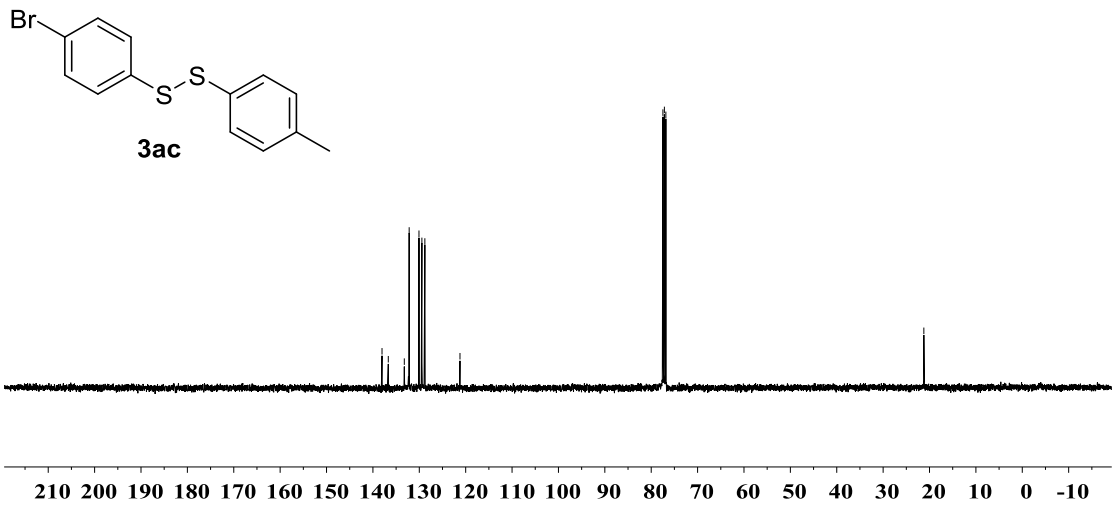
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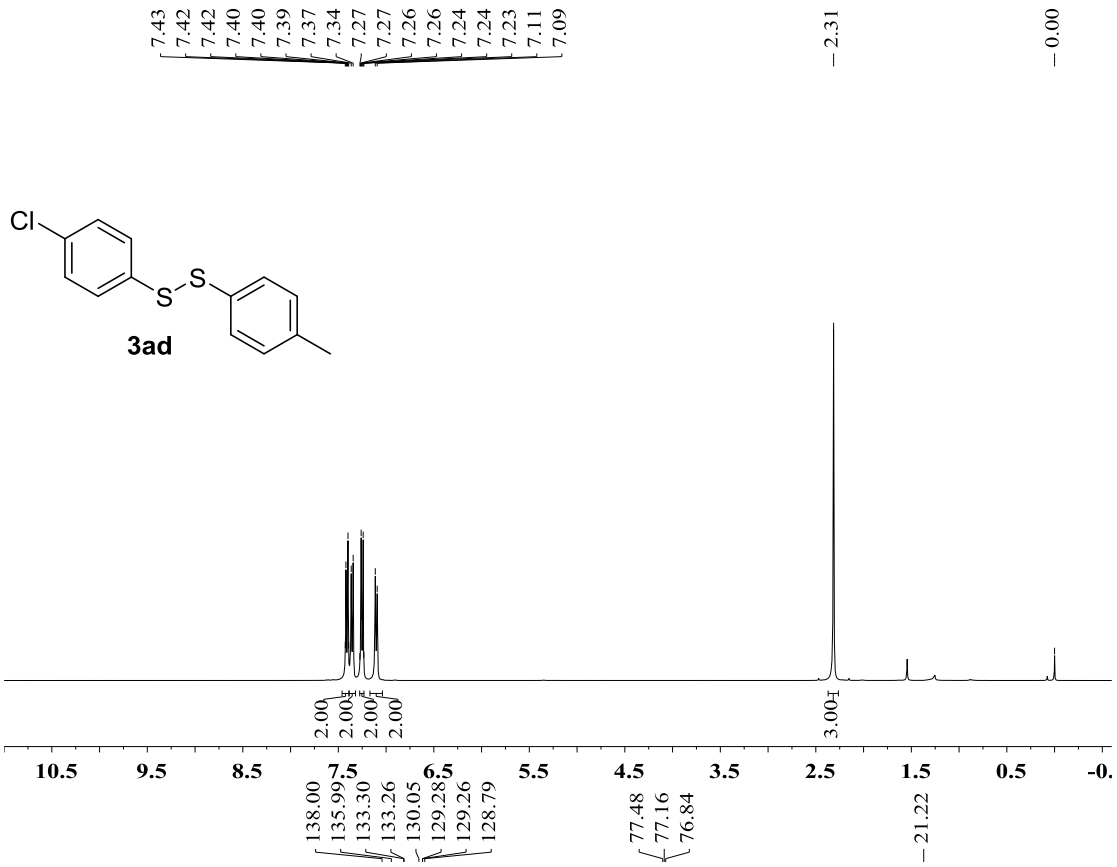
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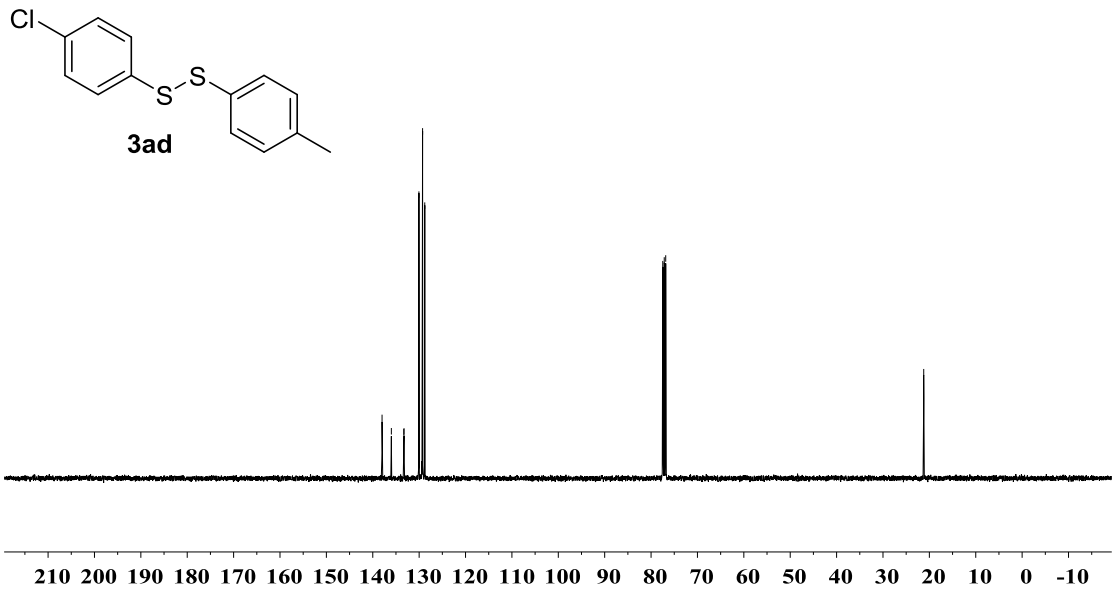
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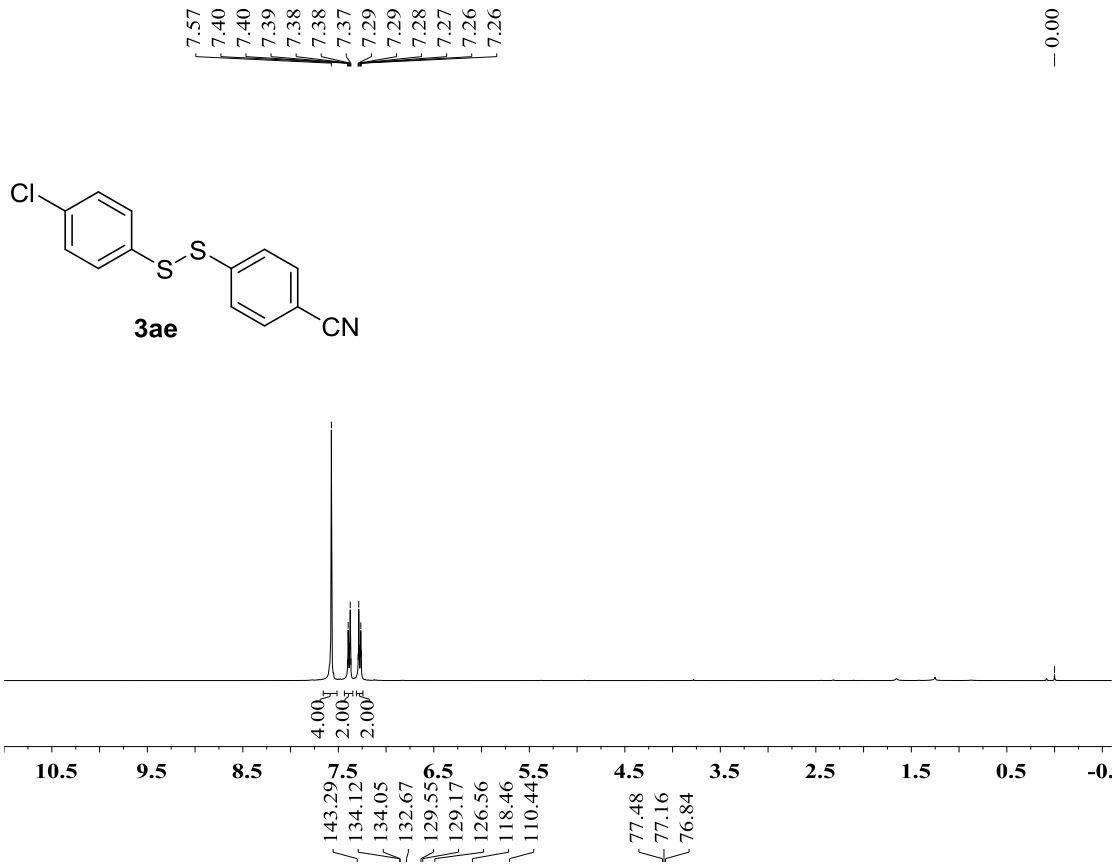
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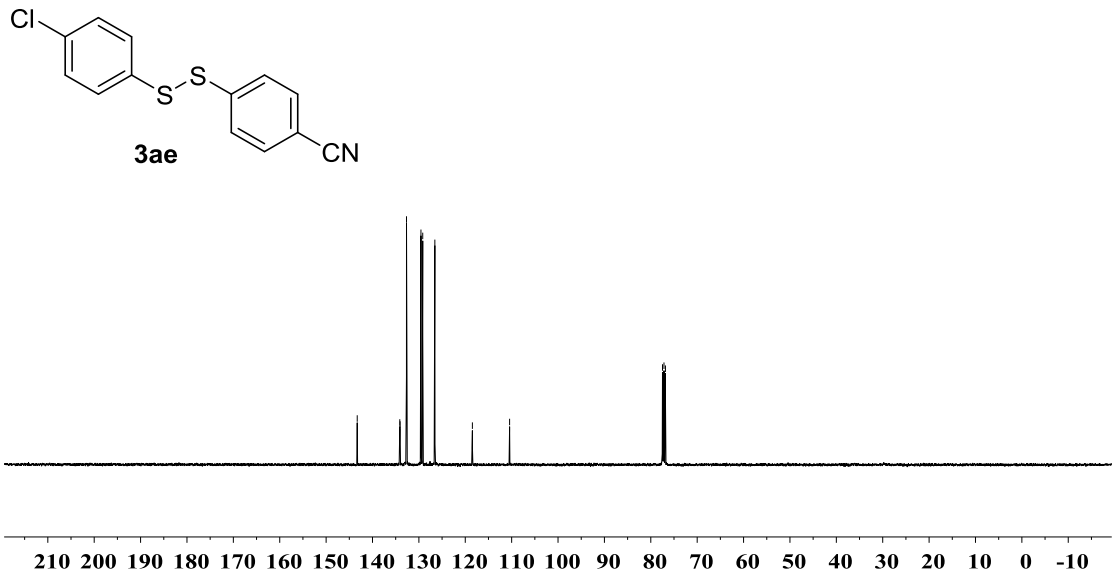
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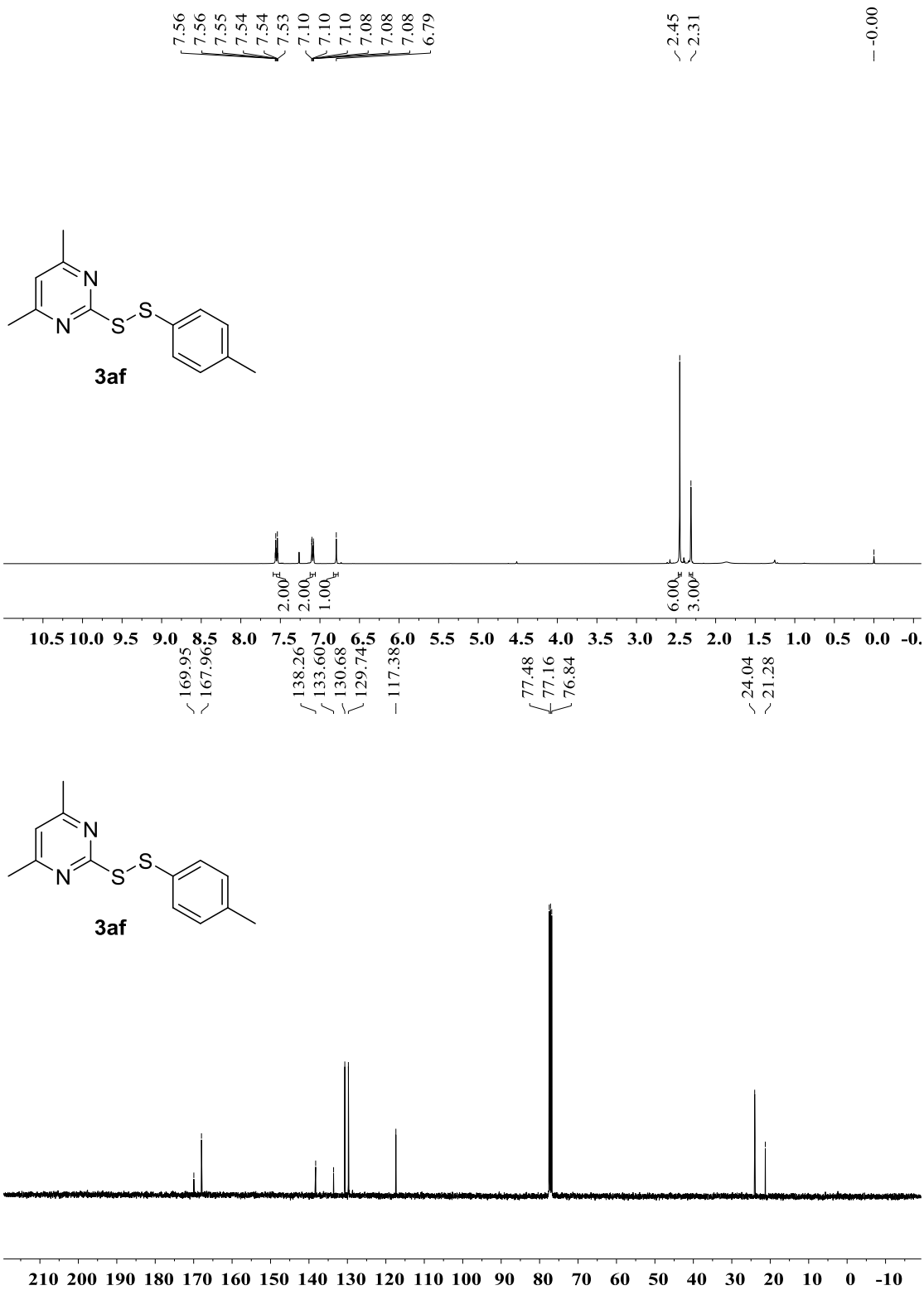
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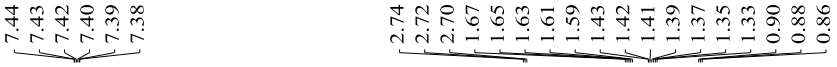
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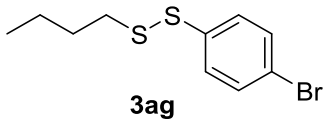
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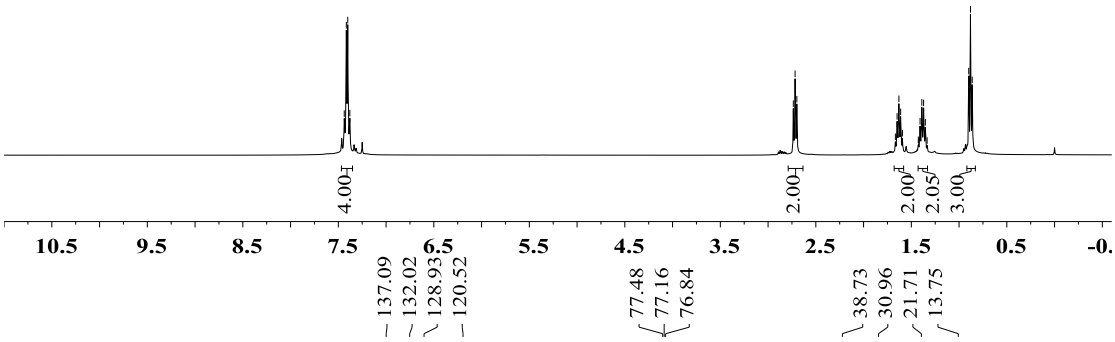
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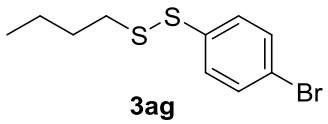
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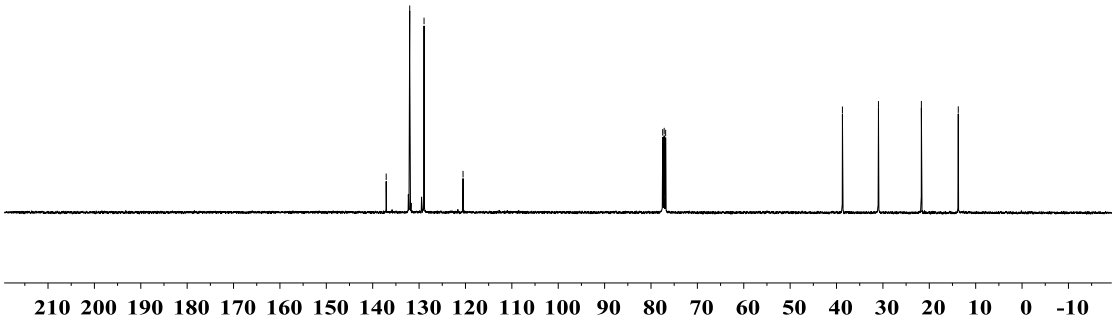
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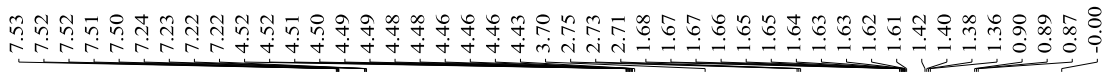
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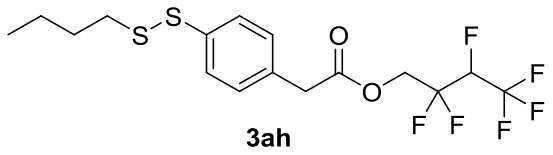
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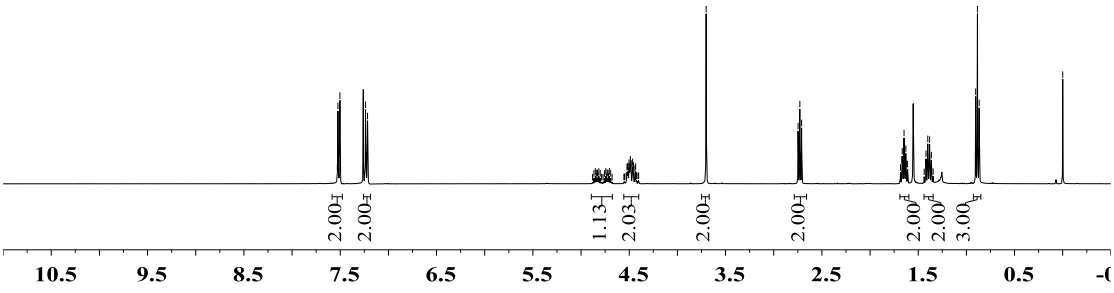
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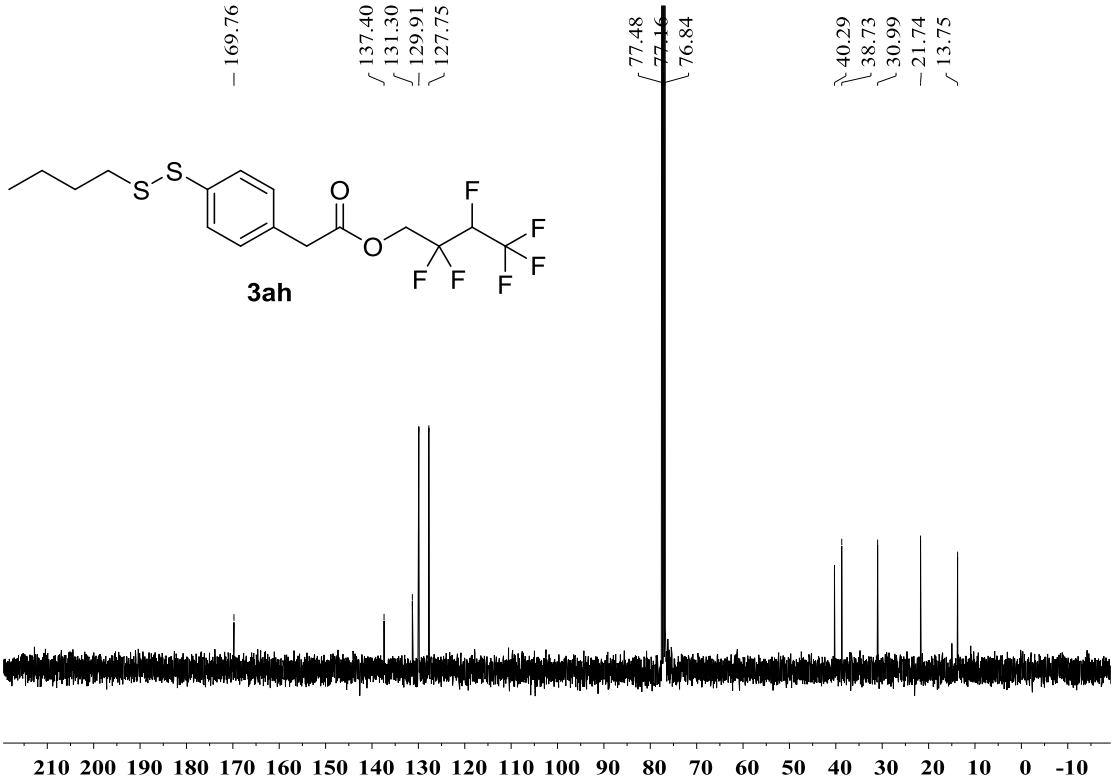
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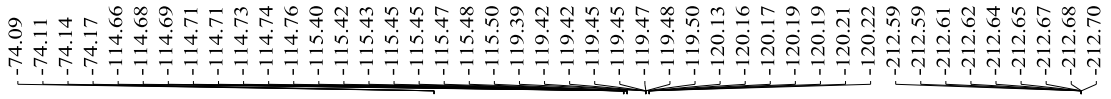
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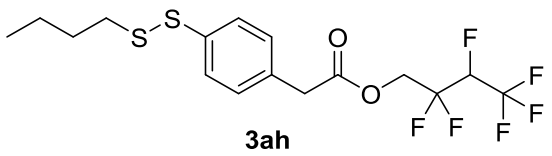
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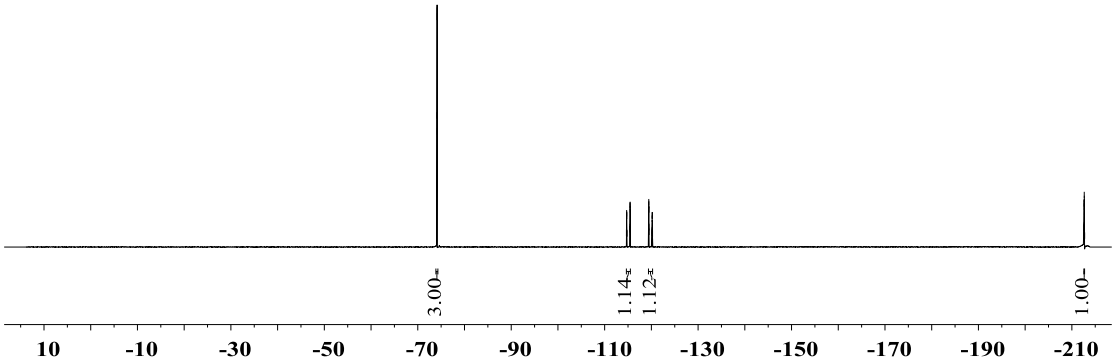
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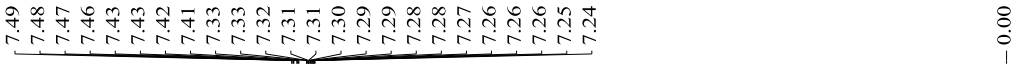
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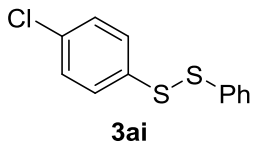
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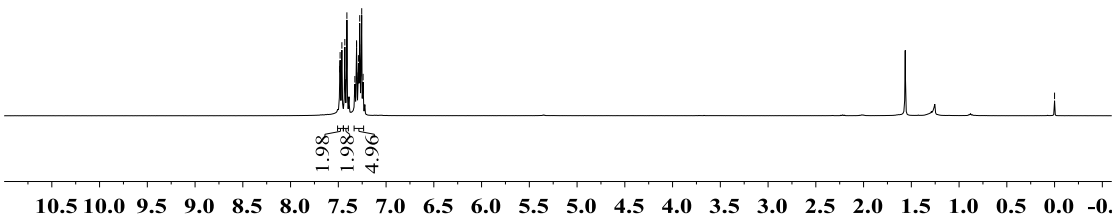
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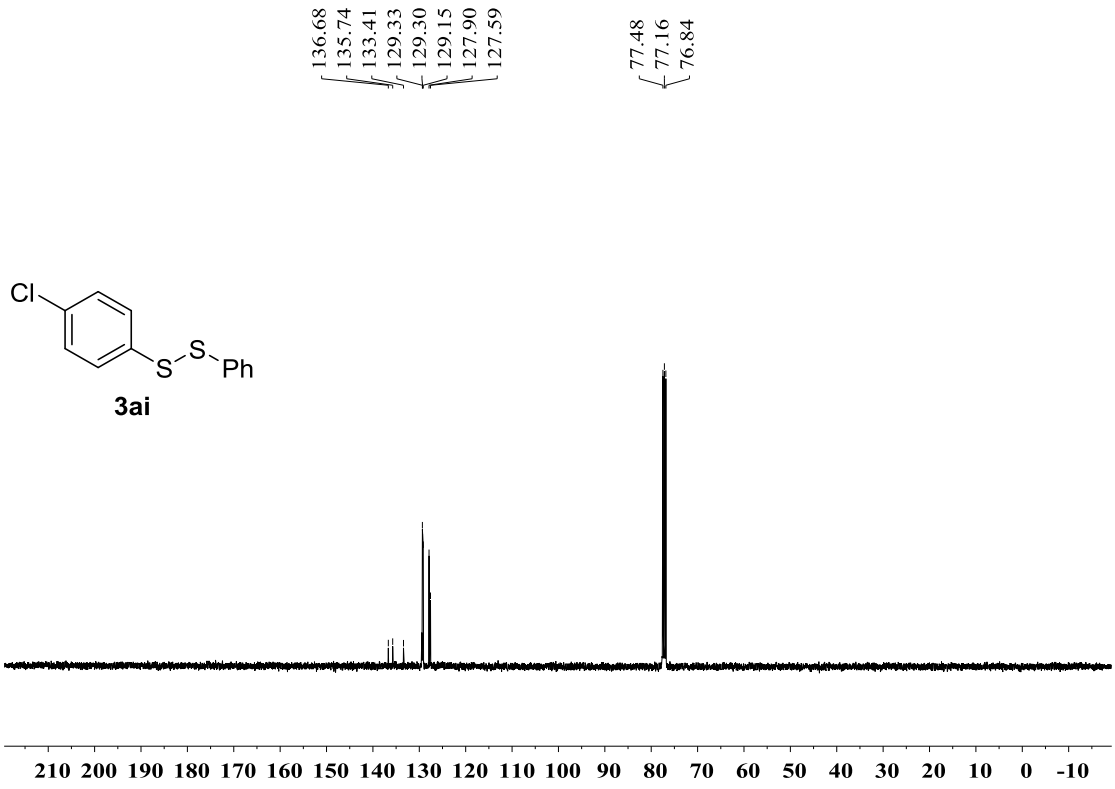
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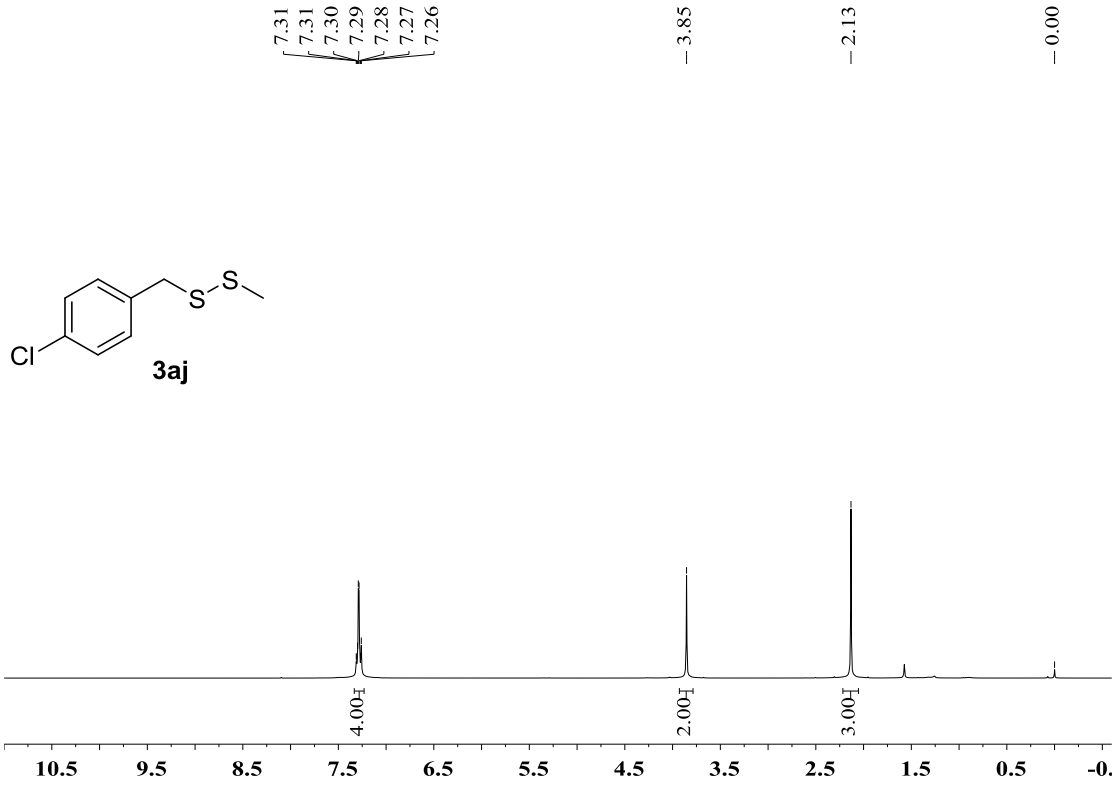
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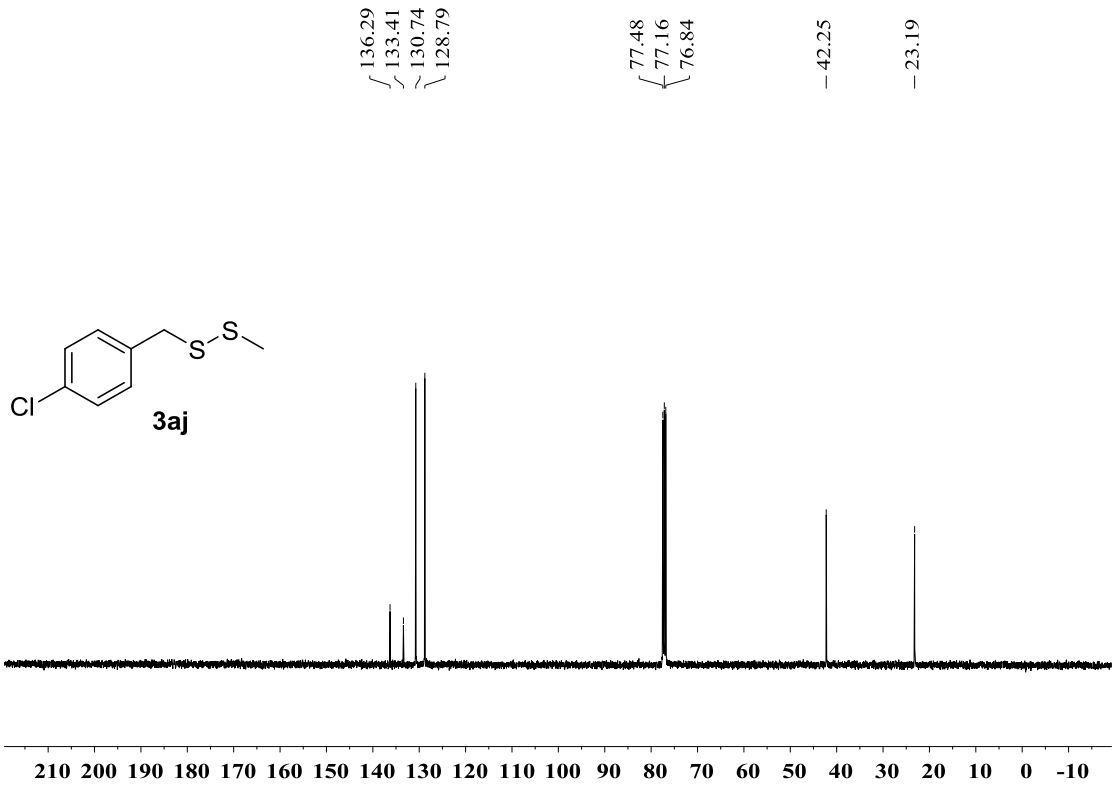
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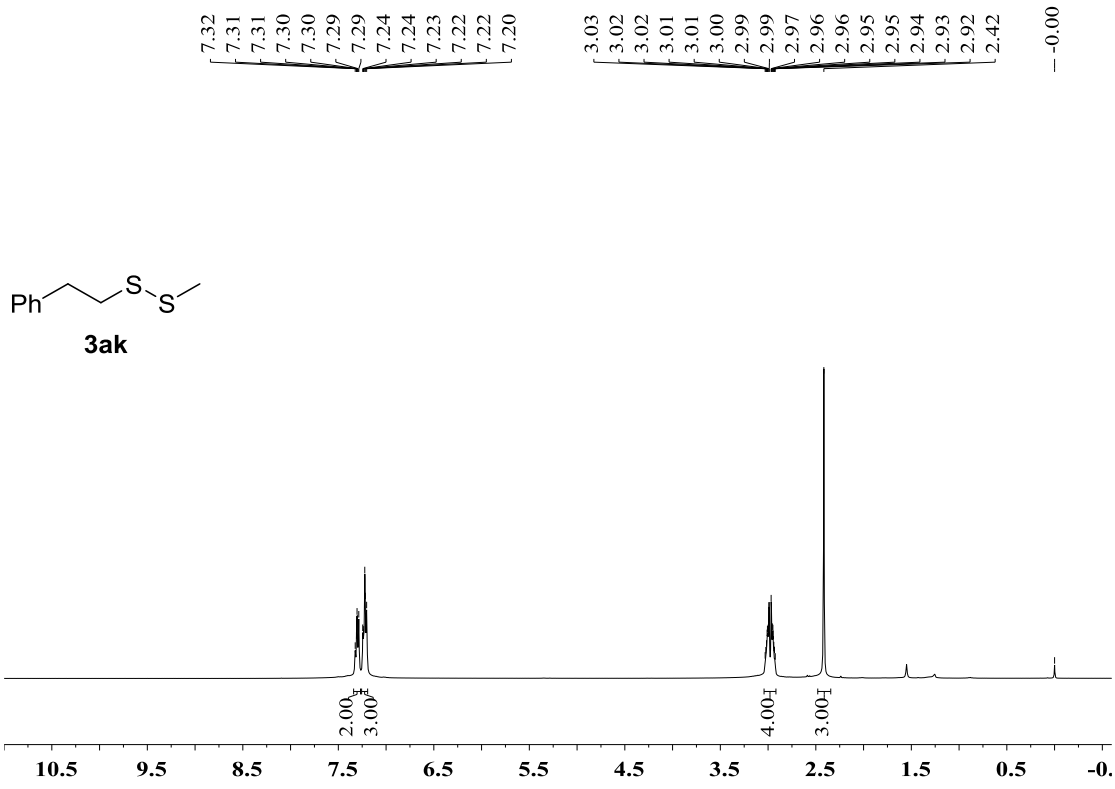
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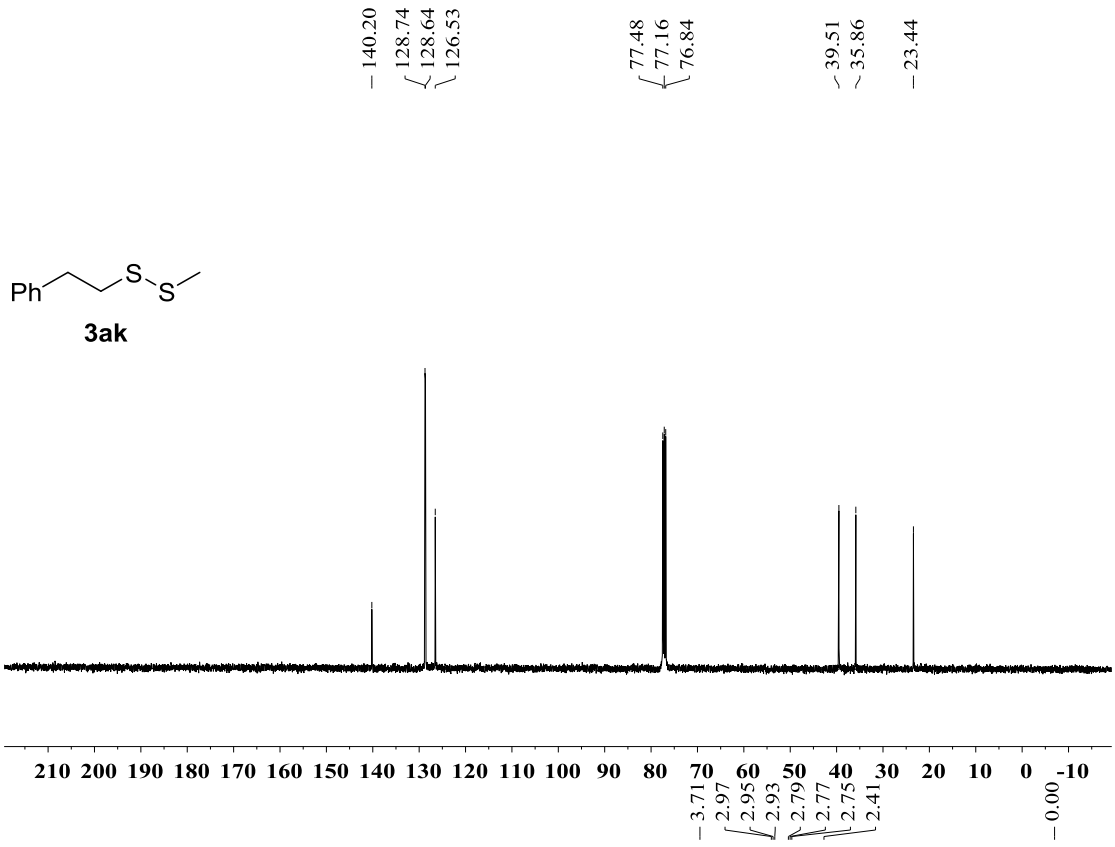
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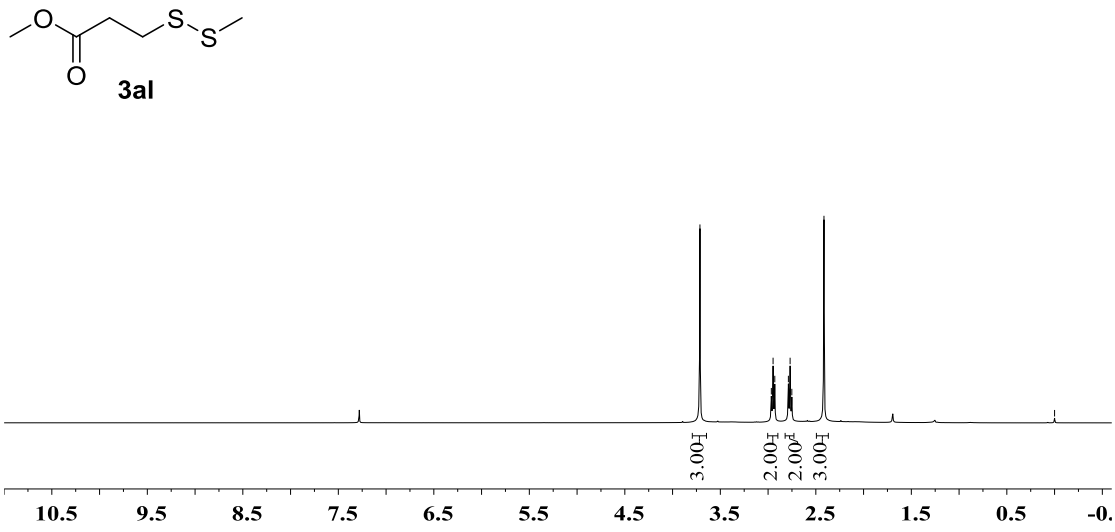
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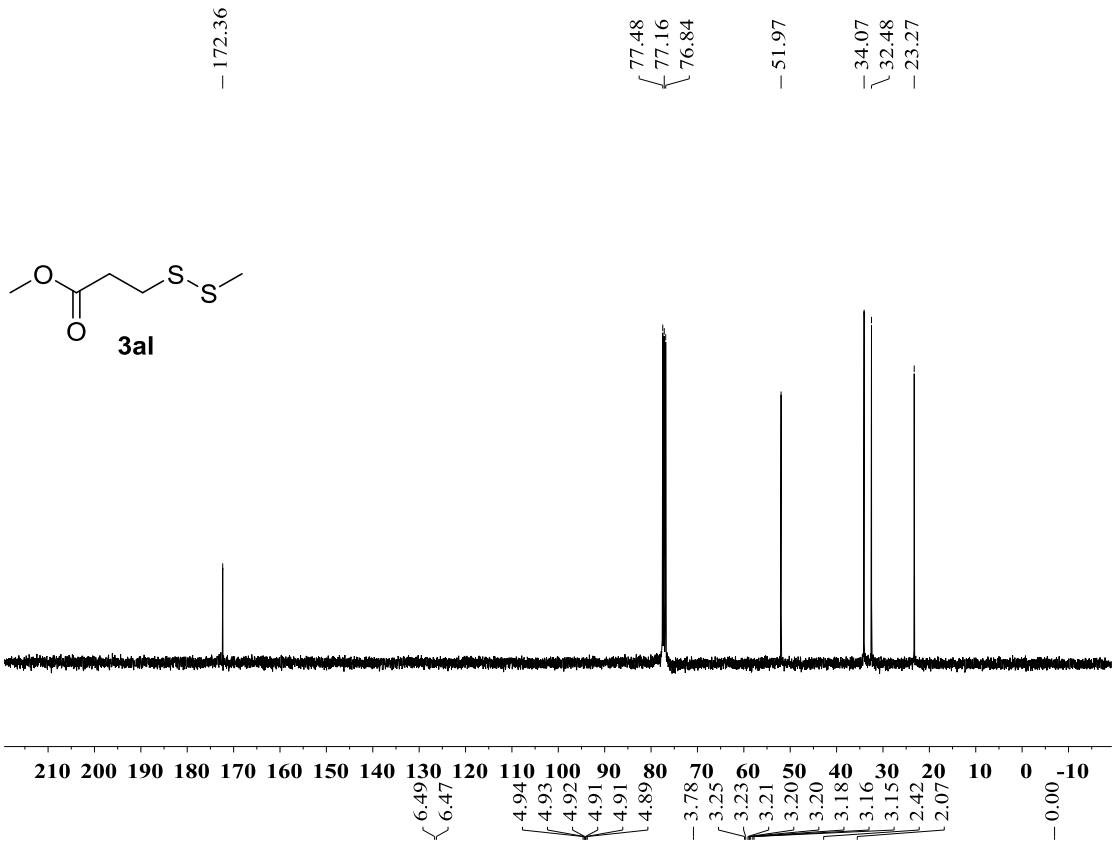
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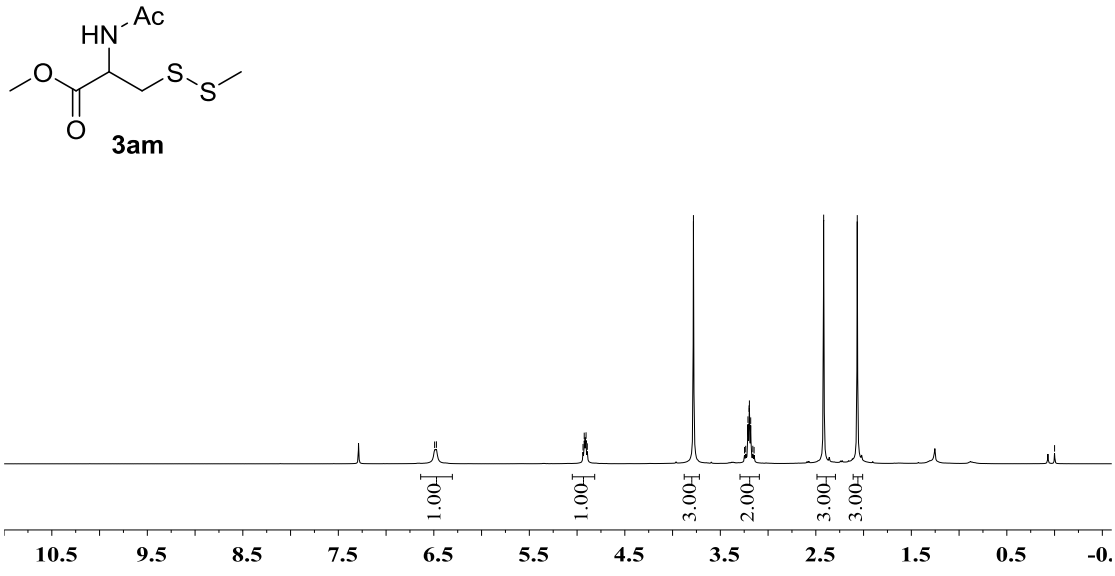
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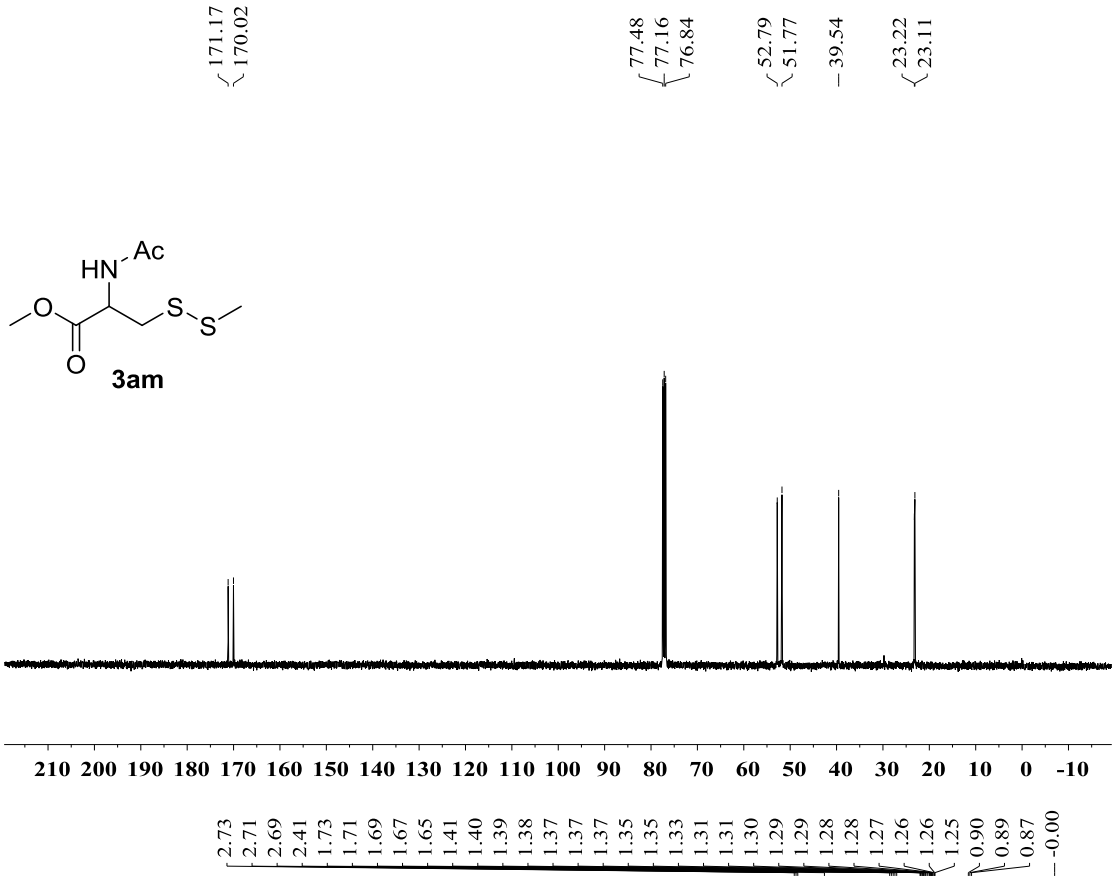
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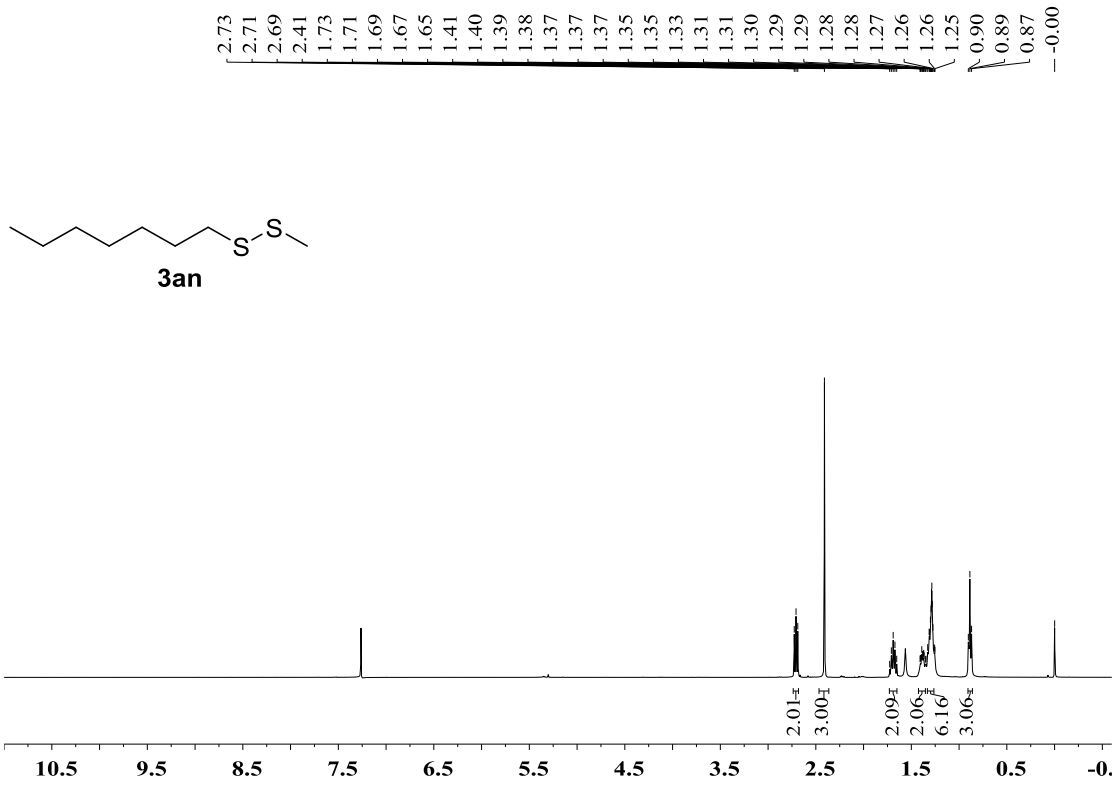
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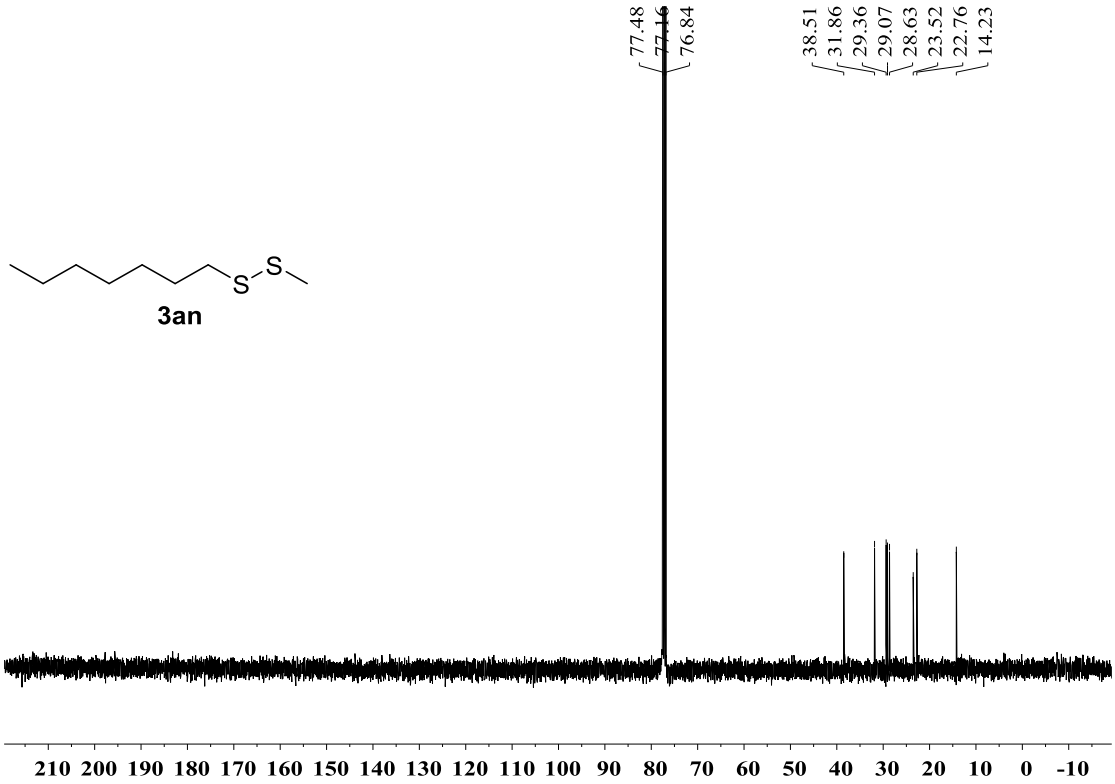
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**3an**


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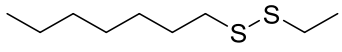

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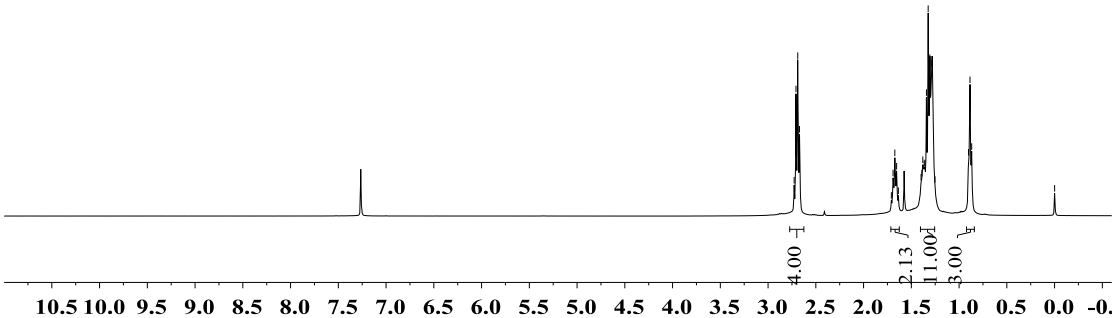
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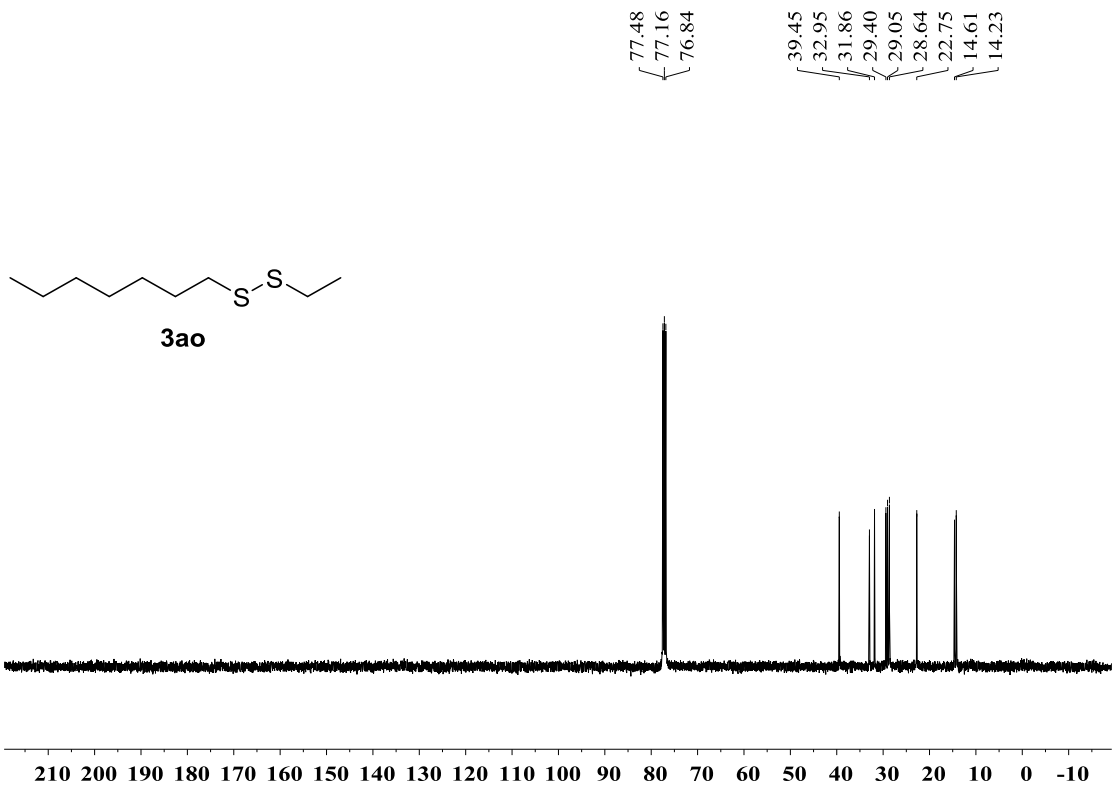
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