Supporting Information

Aryldithiocarbamates as thiol alternatives in Cu-catalyzed C(aryl)-S coupling reactions using aryldiazonium tetrafluoroborate salts

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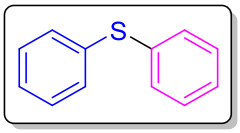
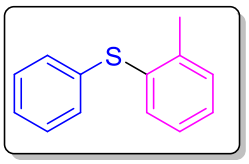
A. Characterization Data of Synthesized Compounds

Diphenylsulfide (Table 2, 3a)



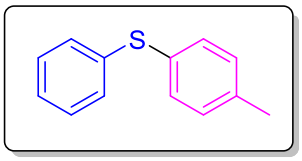
Yellow oil (148 mg, 5h, 80% yield); R_f - 0.6 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.38-7.21 (m, 10*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 135.79, 131.05, 129.22, 127.17 ppm.

Phenyl(o-tolyl)sulfide (Table 2, 3b)



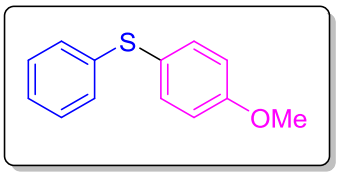
Yellow oil (168 mg, 6h, 84% yield); R_f - 0.5 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.26-7.06 (m, 9*H*), 2.30 (s, 3*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 140.13, 136.34, 133.91, 133.17, 130.73, 129.77, 129.19, 128.04, 126.84, 126.46 ppm.

Phenyl(p-tolyl)sulfide (Table 2, 3c)



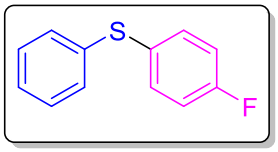
Yellow oil (164 mg, 6h, 82% yield); R_f - 0.64 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.32-7.10 (m, 9*H*), 2.30 (s, 3*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 137.59, 137.18, 132.40, 131.33, 130.19, 129.97, 129.17, 126.55, 21.14. ppm.

(4-methoxyphenyl)(phenyl)sulfide (Table 2, 3d)



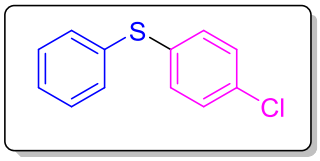
Yellow oil (183 mg, 5h, 85% yield); R_f - 0.54 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42 (d, J = 8 Hz, 2*H*), 7.24 (t, J = 8 Hz, 2*H*), 7.18-7.12 (m, 3*H*), 6.90 (d, J = 8 Hz, 2*H*), 3.82 (s, 3*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.00, 138.74, 135.47, 129.07, 128.42, 125.93, 124.55, 115.15, 55.51 ppm.

(4-fluorophenyl)(phenyl)sulfide (Table 2, 3e)



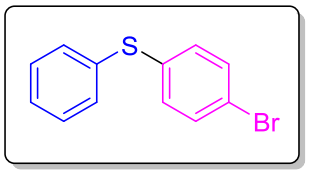
Colourless oil (173 mg, 5h, 85% yield); R_f - 0.52 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.51(d, J = 8 Hz, 2*H*), 7.30-7.22 (m, 5*H*), 7.03-7.00 (m, 2*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 163.74, 161.27, 136.76, 134.24, 134.16, 130.08, 129.30, 126.88, 116.63, 116.41 ppm.

(4-chlorophenyl)(phenyl)sulfide (Table 2, 3f)



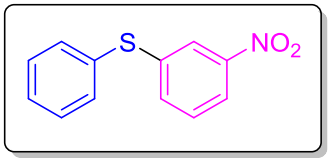
Yellow oil (180 mg, 5h, 82% yield); R_f - 0.64 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.35-7.29 (m, 5*H*), 7.27-7.21 (m, 4*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 135.27, 134.80, 133.15, 132.16, 131.47, 129.48, 129.45, 127.30 ppm.

(4-bromophenyl)(phenyl)sulfide (Table 2, 3g)



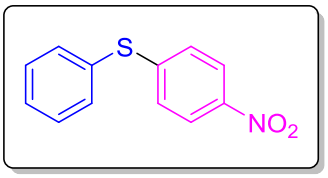
Colourless oil (232 mg, 5h, 88% yield); R_f - 0.68 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.44-7.18 (m, 7*H*), 7.04 (d, J = 9 Hz, 2*H*) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ 135.61, 134.94, 132.34, 132.19, 131.67, 129.49, 127.67, 120.98 ppm.

(3-nitrophenyl)(phenyl)sulfide (Table 2, 3h)



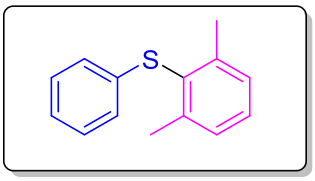
Yellow solid (180 mg, 5h, 78% yield); R_f - 0.48 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v); melting point: 92°C. ^{1}H NMR ($CDCl_3$, 300 MHz) δ 8.03-8.01 (m, 2*H*), 7.48-7.26 (m, 7*H*) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ 148.79, 140.67, 134.34, 133.52, 132.21, 129.95, 129.77, 129.04, 123.23, 121.00 ppm.

(4-nitrophenyl)(phenyl)sulfide (Table 2, 3i)



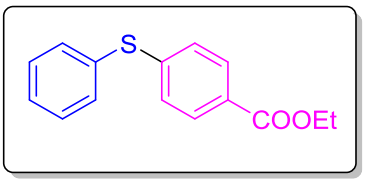
Yellow solid (187 mg, 5h, 81% yield); R_f - 0.46 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v); melting point: 56°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.06 (d, J = 8 Hz, 2*H*), 7.55-7.53 (m, 2*H*), 7.46-7.45 (m, 3*H*), 7.18 (d, J = 8 Hz, 2*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.60, 145.57, 134.87, 130.68, 130.17, 129.79, 126.90, 124.18 ppm.

(2,6-dimethylphenyl)(phenyl)sulfide (Table 2, 3j)



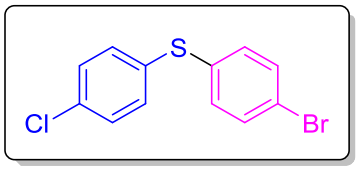
Yellow oil (166 mg, 6h, 78% yield); R_f - 0.40 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.36-7.22 (m, 5*H*), 7.09 (d, J = 8 Hz, 1*H*), 6.97 (d, J = 8 Hz, 2*H*), 2.47 (s, 6*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 144.04, 138.19, 130.69, 129.38, 129.03, 128.58, 125.84, 124.77, 21.96 ppm.

Ethyl 4-(phenylthio)benzoate (Table 2, 3k)



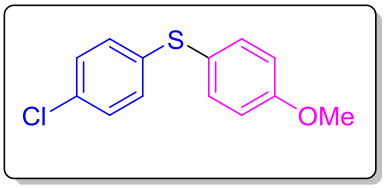
Colourless oil (216 mg, 5h, 84% yield); R_f - 0.32 (in 2% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 2/8, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.81 (d, J = 8 Hz, 2*H*), 7.39-7.27 (m, 5*H*), 7.11 (d, J = 8 Hz, 2*H*), 4.27 (q, J = 8 Hz, 2*H*), 1.27 (t, J = 8 Hz, 3*H*), 1.61 (s, 6*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 166.20, 144.16, 133.61, 132.83, 130.12, 129.66, 128.62, 127.98, 127.75, 60.96, 14.38 ppm.

(4-bromophenyl)(4-chlorophenyl)sulfide (Table 3, 3l)



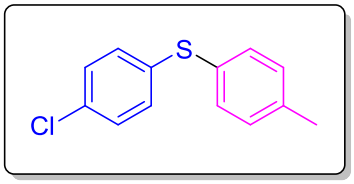
Colourless oil (242 mg, 5h, 81% yield); R_f - 0.64 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42 (d, J = 8 Hz, 2*H*), 7.28-7.26 (m, 4*H*), 7.18 (d, J = 8 Hz, 2*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 134.96, 133.85, 132.57, 132.48, 132.40, 129.59, 129.38, 121.49 ppm.

(4-chlorophenyl)(4-methoxyphenyl)sulfide (Table 3, 3m)



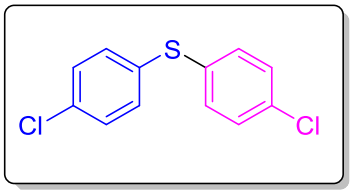
White solid (212 mg, 6h, 85% yield); R_f - 0.54 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v); melting point: 64- 66°C. ^{1}H NMR ($CDCl_3$, 500 MHz) δ 7.41 (d, J = 8.8 Hz, 2H), 7.19 (d, J = 8.6 Hz, 2H), 7.08 (d, J = 8.6 Hz, 2H), 6.91 (d, J = 8.8 Hz, 2H), 3.82 (s, 3H) ppm. ^{13}C NMR ($CDCl_3$, 125 MHz) δ 160.16, 137.50, 135.60, 131.68, 129.40, 129.10, 123.83, 115.23, 55.46 ppm.

(4-chlorophenyl)(p-tolyl)sulfide (Table 3, 3n)



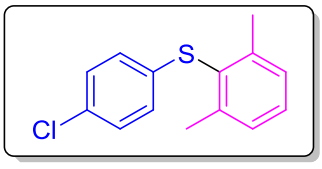
White solid (196 mg, 6h, 84% yield); R_f - 0.66 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v); melting point: 70- 72°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.35-7.29 (m, 4*H*), 7.24-7.17 (m, 4*H*), 2.39 (s, 3*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 138.03, 136.23, 132.67, 132.51, 130.95, 130.33, 129.45, 129.28, 21.27 ppm.

bis(4-chlorophenyl)sulfide (Table 3, 3o)



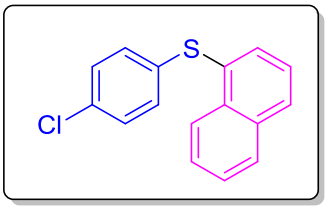
White solid (209 mg, 5h, 82% yield); R_f - 0.64 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v); melting point: 94-96 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33-7.30 (m, 4*H*), 7.28-7.26 (m, 4*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 134.22, 133.72, 132.46, 129.64 ppm.

(4-chlorophenyl)(2,6-dimethylphenyl)sulfide (Table 3, 3p)



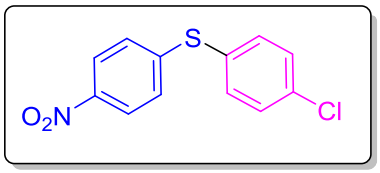
Colourless oil (200 mg, 6h, 81% yield); R_f - 0.58 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.42-7.40 (m, 1*H*), 7.29-7.23 (m, 2*H*), 7.19 (d, J = 8 Hz, 2*H*), 7.17 (d, J = 8 Hz, 2*H*), 2.44 (s, 6*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 143.88, 136.79, 130.56, 129.59, 129.38, 129.09, 128.67, 126.93, 21.87 ppm. HRMS: calcd for $C_{14}H_{13}ClS$ $[M+H]^+$ 249.0426; found 249.1790.

(4-chlorophenyl)(naphthalen-1-yl)sulfide (Table 3, 3q)



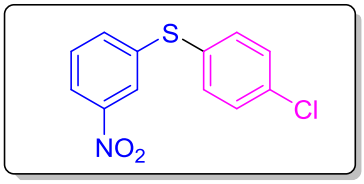
Yellow oil (221 mg, 6h, 82% yield); R_f - 0.54 (in hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.38-8.36 (m, 1*H*), 7.80 (d, *J* = 8 Hz, 2*H*), 7.72 (d, *J* = 4 Hz, 1*H*), 7.56-7.54 (m, 2*H*), 7.47-7.41 (m, 1*H*), 7.19 (d, *J* = 8 Hz, 2*H*), 7.11 (d, *J* = 8 Hz, 2*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 135.89, 134.44, 133.69, 133.15, 132.09, 130.64, 130.01, 129.79, 129.29, 128.77, 127.25, 126.66, 125.95, 125.64 ppm.

(4-chlorophenyl)(4-nitrophenyl)sulfide (Table 3, 3r)



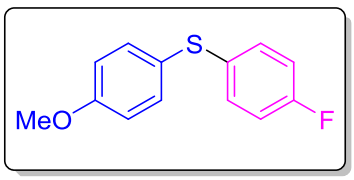
Yellow solid (198 mg, 5h, 75% yield); R_f - 0.36 (in 2% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 2/8, v/v); melting point: 58-60°C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.07 (d, *J* = 8 Hz, 2*H*), 7.47-7.40 (m, 4*H*), 7.18 (d, *J* = 8 Hz, 2*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 147.64, 145.76, 136.13, 135.89, 130.36, 129.34, 127.12, 124.24 ppm.

(4-chlorophenyl)(3-nitrophenyl)sulfide (Table 3, 3s)



Yellow oil (204 mg, 5h, 77% yield); R_f - 0.38 (in 2% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 2/8, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.05-8.03 (m, 2*H*), 7.58-7.51 (m, 1*H*), 7.47-7.37 (m, 5*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 148.80, 139.79, 135.21, 134.65, 134.47, 131.05, 130.10, 129.95, 123.55, 121.39 ppm.

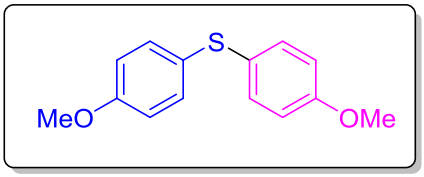
(4-fluorophenyl)(4-methoxyphenyl)sulfide (Table 3, 3t)



Yellow oil (191 mg, 6h, 82% yield); R_f - 0.46 (in 2% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.40 (d, *J* = 8 Hz, 2*H*), 7.26-7.22 (m, 2*H*), 7.01-6.96 (m, 2*H*), 6.91 (d, *J* = 8 Hz, 2*H*), 3.84 (s, 3*H*) ppm.

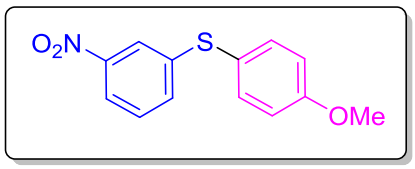
^{13}C NMR ($CDCl_3$, 100 MHz) δ 162.96, 160.51, 159.82, 134.59, 133.24, 132.75, 131.25, 131.17, 125.43, 116.27, 116.05, 115.13, 55.45 ppm.

bis(4-methoxyphenyl)sulfide (Table 3, 3u)



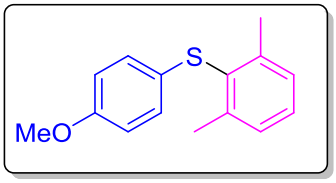
Colourless oil (198 mg, 5h, 81% yield); R_f - 0.48 (in 5% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 2/8, v/v). ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.31-7.28 (m, 4*H*), 6.86-6.83 (m, 4*H*), 3.77 (s, 6*H*) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ 159.13, 132.87, 127.56, 114.92, 55.42 ppm.

(4-methoxyphenyl)(3-nitrophenyl)sulfide (Table 3, 3v)



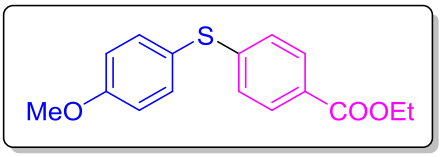
Yellow oil (203 mg, 6h, 78% yield); R_f - 0.34 (in 2% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 2/8, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ7.90-7.87 (m, 2*H*), 7.45 (d, *J* = 8 Hz, 2*H*), 7.38-7.36 (m, 2*H*), 6.94 (d, *J* = 8 Hz, 2*H*), 3.82 (s, 3*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 160.02, 142.71, 136.74, 132.44, 129.57, 123.54, 121.29, 120.12, 115.66, 114.72, 55.43 ppm.

(2,6-dimethylphenyl)(4-methoxyphenyl)sulfide (Table 3, 3w)



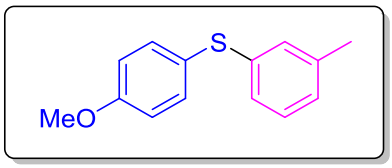
White solid (198 mg, 6h, 81% yield); R_f - 0.22 (in 2% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 2/8, v/v), melting point: 52°C. ^{1}H NMR ($CDCl_3$, 100 MHz) δ 7.24-7.19 (m, 3*H*), 6.98 (d, *J* = 8 Hz, 2*H*), 6.80 (d, *J* = 8 Hz, 2*H*), 3.77 (s, 3*H*), 2.50 (s, 6*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 157.69, 143.65, 132.07, 129.08, 128.76, 128.56, 128.11, 114.84, 55.40, 22.11 ppm.

Ethyl 4-((4-methoxyphenyl)thio)benzoate (Table 3, 3x)



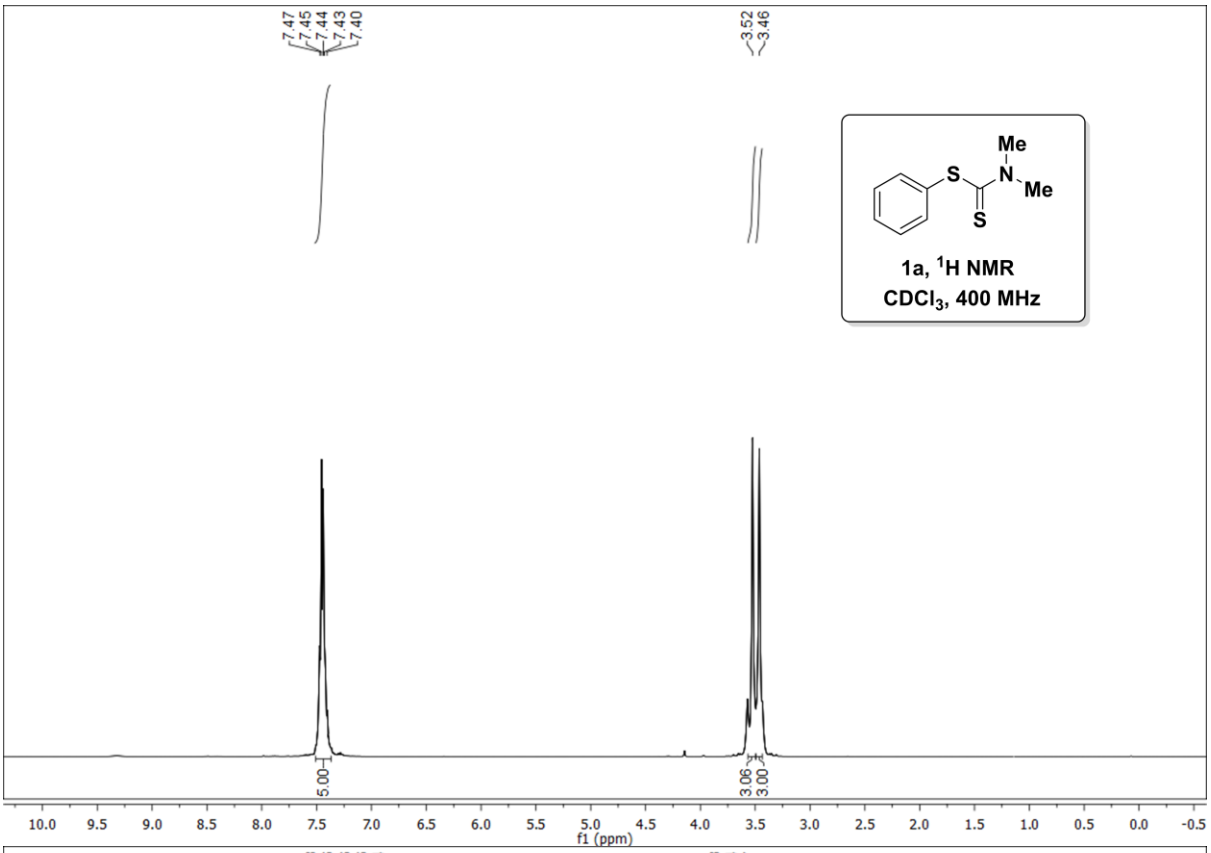
Yellow oil (236 mg, 5h, 82% yield); R_f - 0.42 (in 5% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 2/8, v/v). ^{1}H NMR ($CDCl_3$, 300 MHz) δ 7.83 (d, J = 9 Hz, 2*H*), 7.41 (d, J = 9 Hz, 2*H*), 7.01 (d, J = 9 Hz, 2*H*), 6.85 (d, J = 9 Hz, 2*H*), 4.28 (q, J = 6 Hz, 2*H*), 3.78 (s, 3*H*), 1.27 (t, J = 6 Hz, 3*H*) ppm. ^{13}C NMR ($CDCl_3$, 75 MHz) δ 165.91, 159.31, 146.25, 137.15, 130.52, 127.95, 126.20, 122.02, 114.55, 61.31, 55.39, 14.61 ppm.

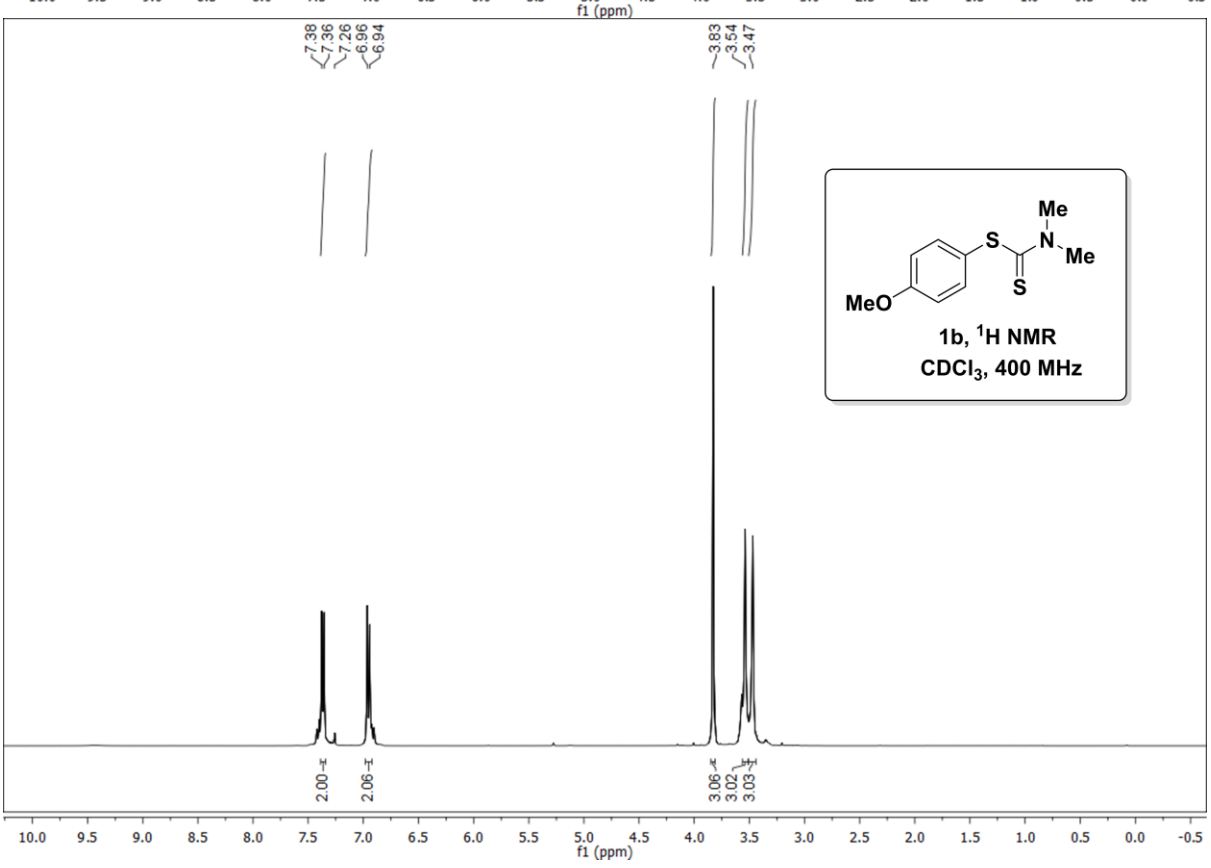
(4-methoxyphenyl)(m-tolyl)sulfide (Table 3, 3y)

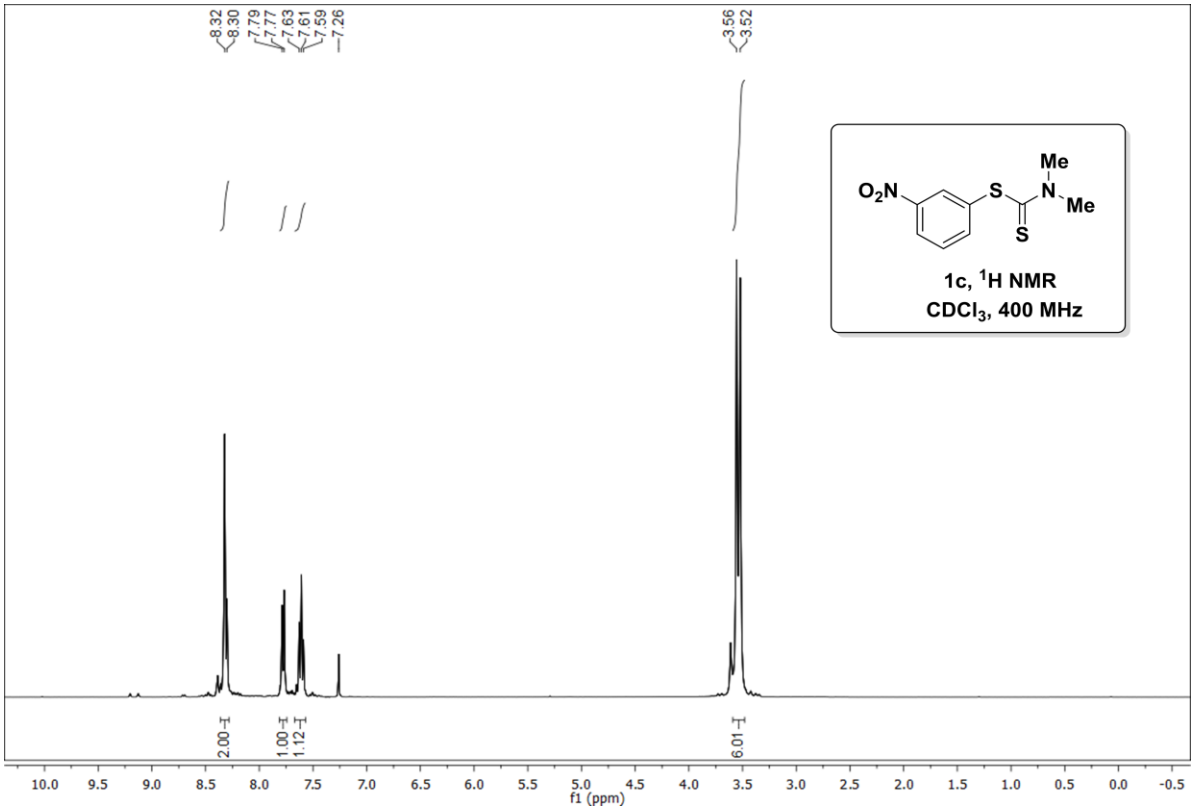


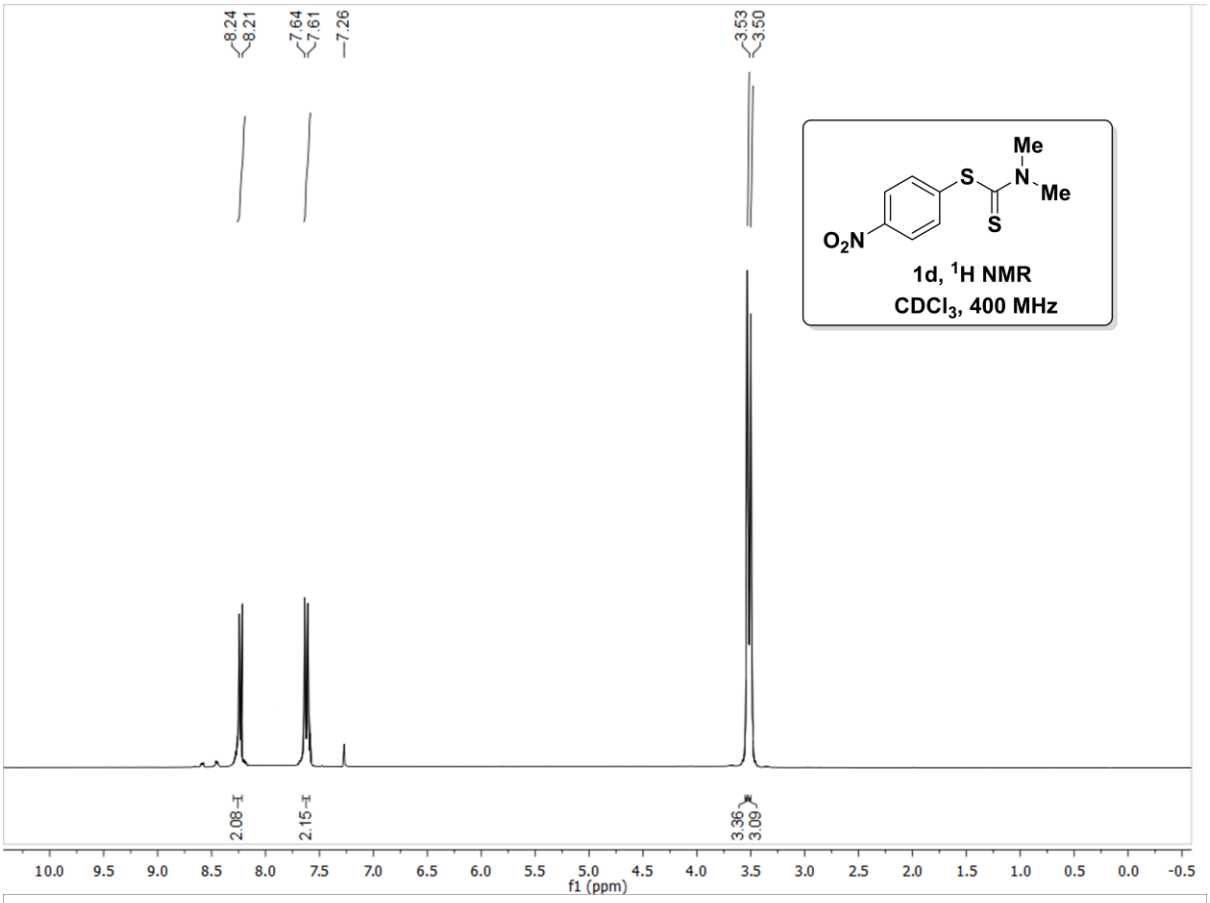
Yellow oil (195 mg, 6h, 85% yield); R_f - 0.58 (in 2% EtOAc-hexane); purified by column chromatography using (EtOAc/hexane = 1/9, v/v). ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.45-7.42 (m, 2*H*), 7.15 (t, J = 8 Hz, 1*H*), 7.06 (s, 1*H*), 7.02-6.97 (m, 2*H*), 6.91 (d, J = 8 Hz, 2*H*), 3.82 (s, 3*H*), 2.30 (s, 3*H*) ppm. ^{13}C NMR ($CDCl_3$, 100 MHz) δ 159.87, 138.87, 138.34, 135.30, 129.11, 128.95, 126.90, 125.63, 124.72, 115.08, 55.45, 21.47 ppm.

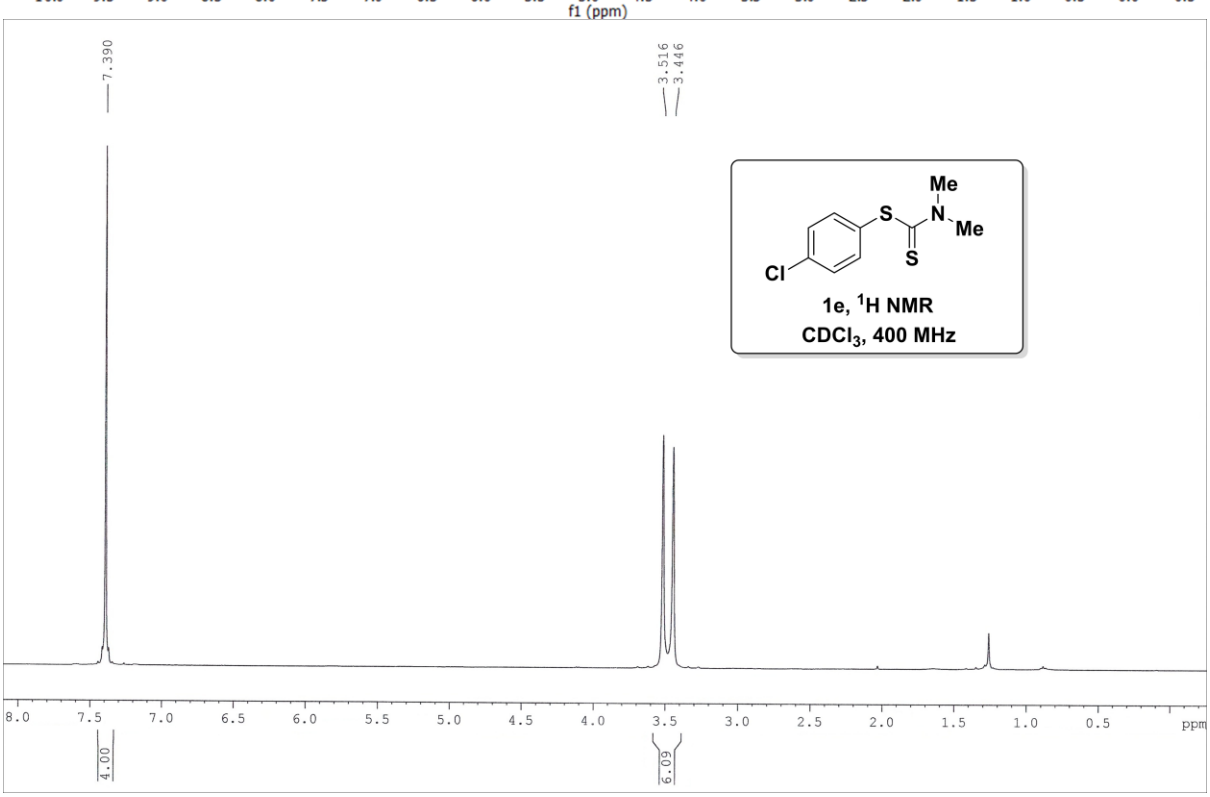
B. ^{1}H and ^{13}C Spectra of Synthesized Compounds

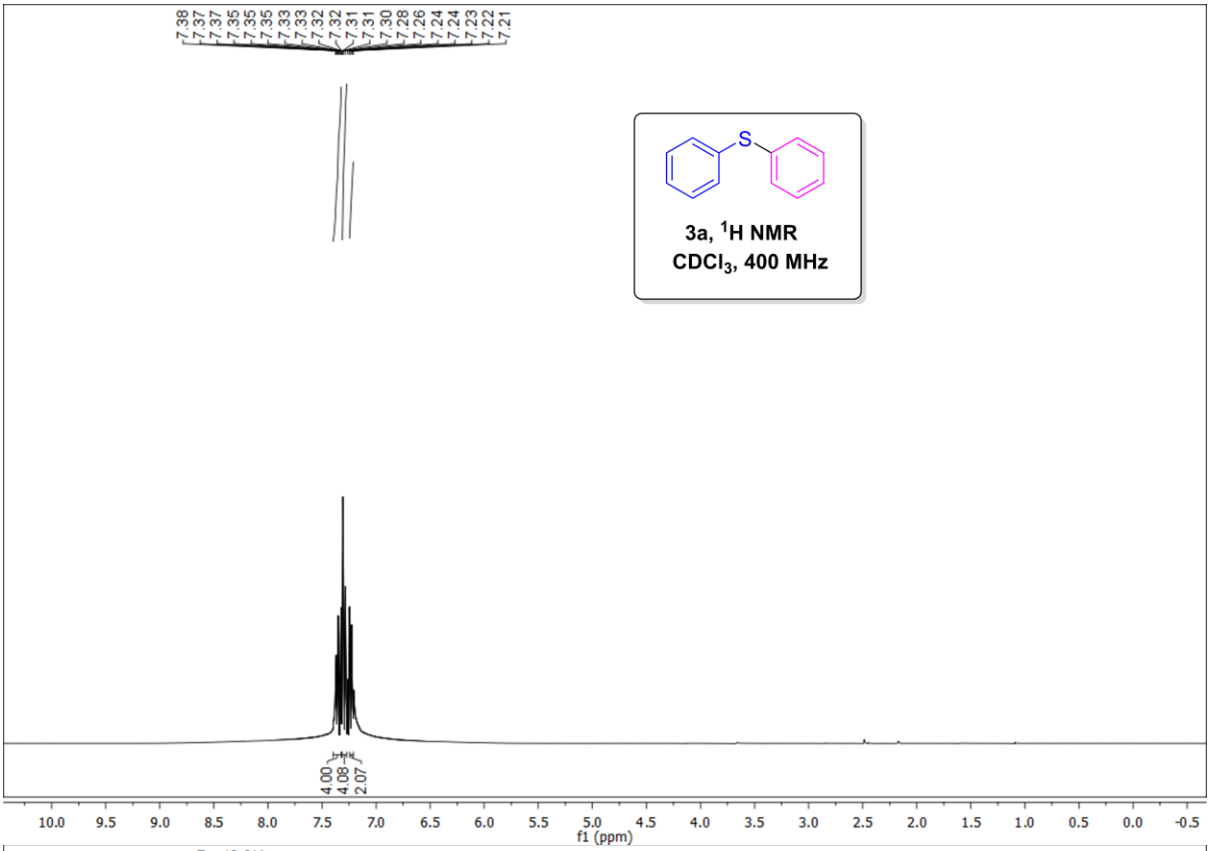


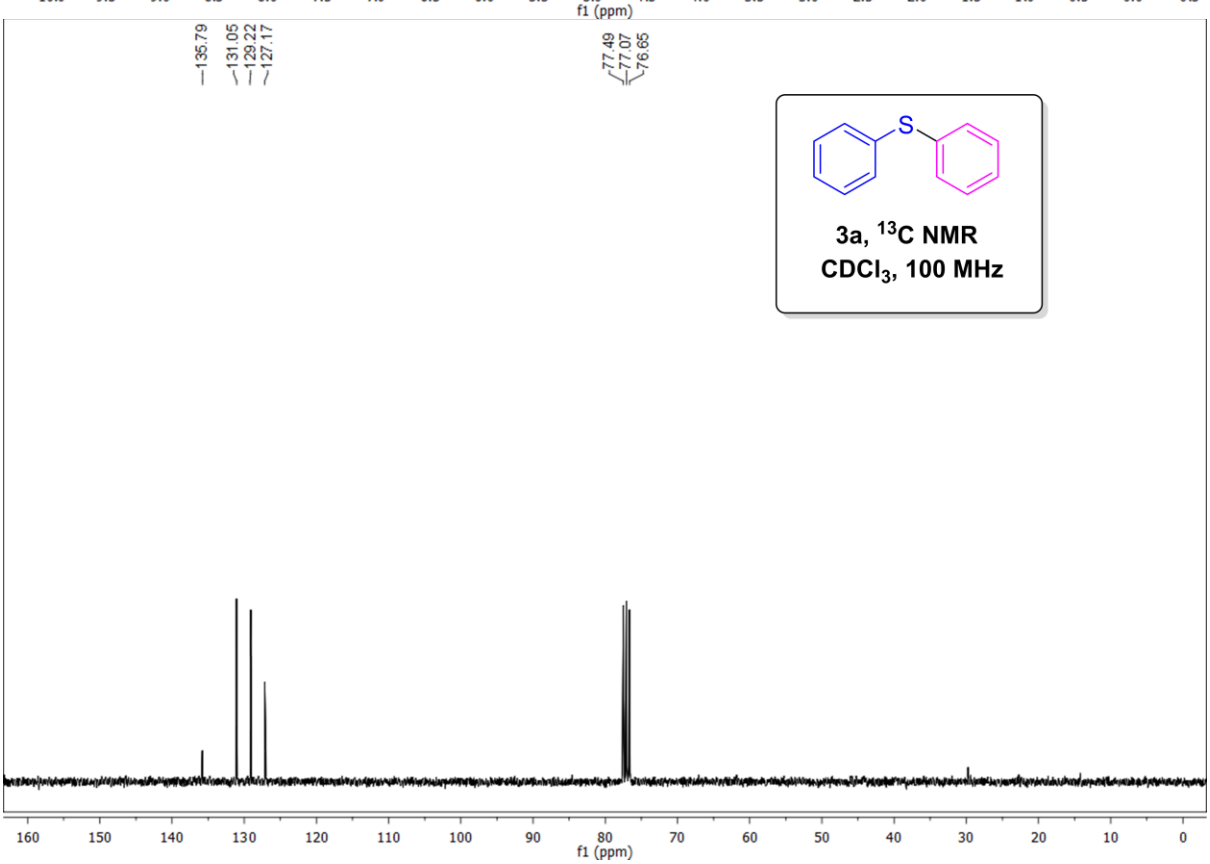


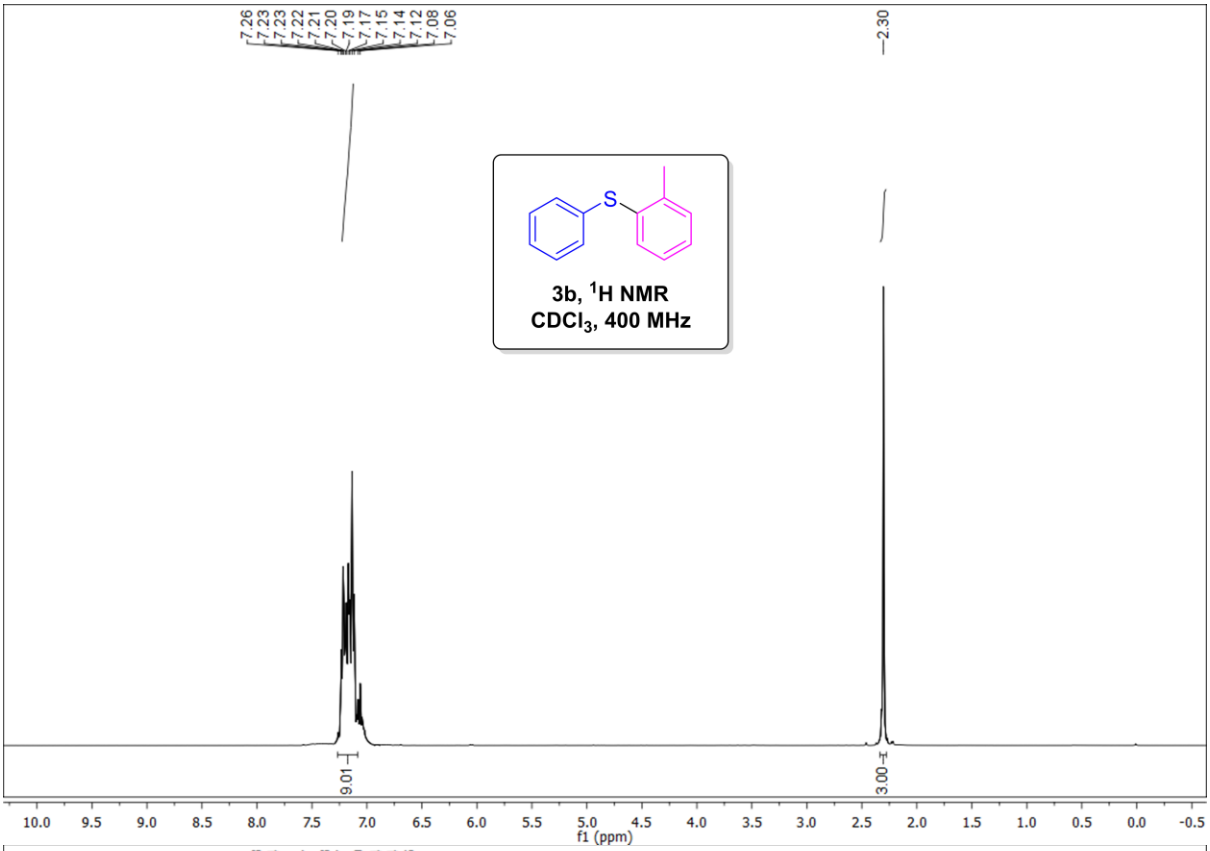

8.32
8.30
7.79
7.77
7.63
7.61
7.59
7.26
3.56
3.52
Me
O2N
S
N
Me
S
1c, 1H NMR
CDCl3, 400 MHz
2.00
1.00
1.12
6.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

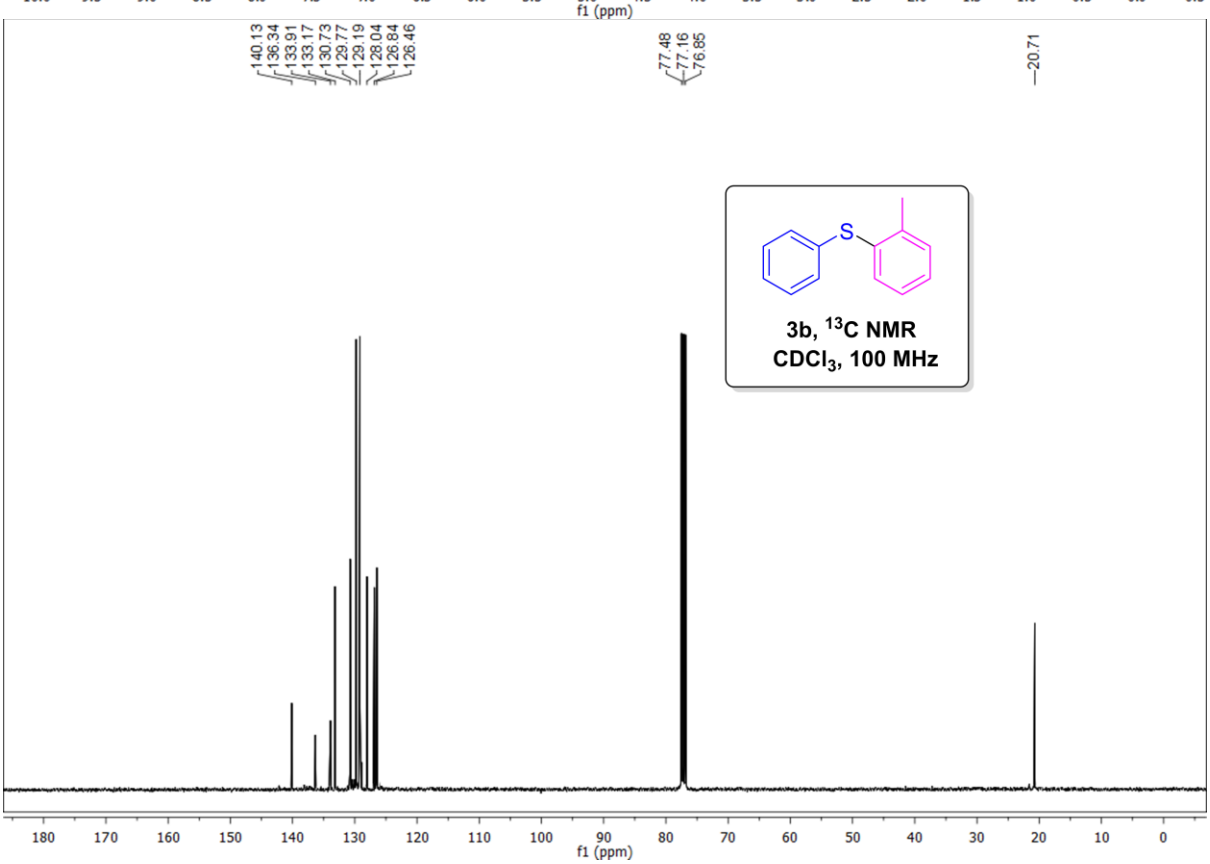

8.24
8.21
7.64
7.61
7.26
3.53
3.50
Me
N
Me
S
S
O_2N
1d, ^{1}H NMR
$CDCl_3$, 400 MHz
2.08
2.15
3.36
3.09
f1 (ppm)

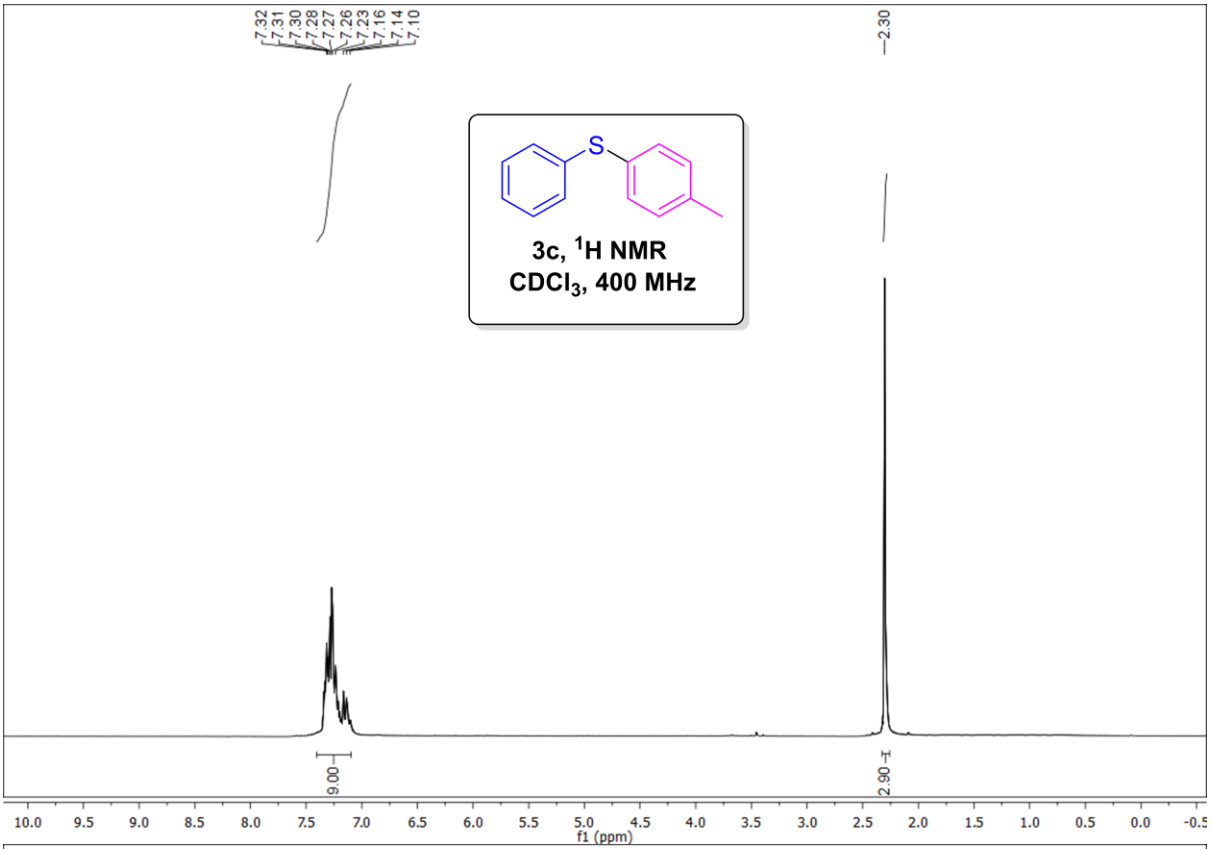

7.390
3.516
3.446
Me
N
Me
S
S
Cl
1e, ^{1}H NMR
$CDCl_3$, 400 MHz
4.00
6.09
ppm

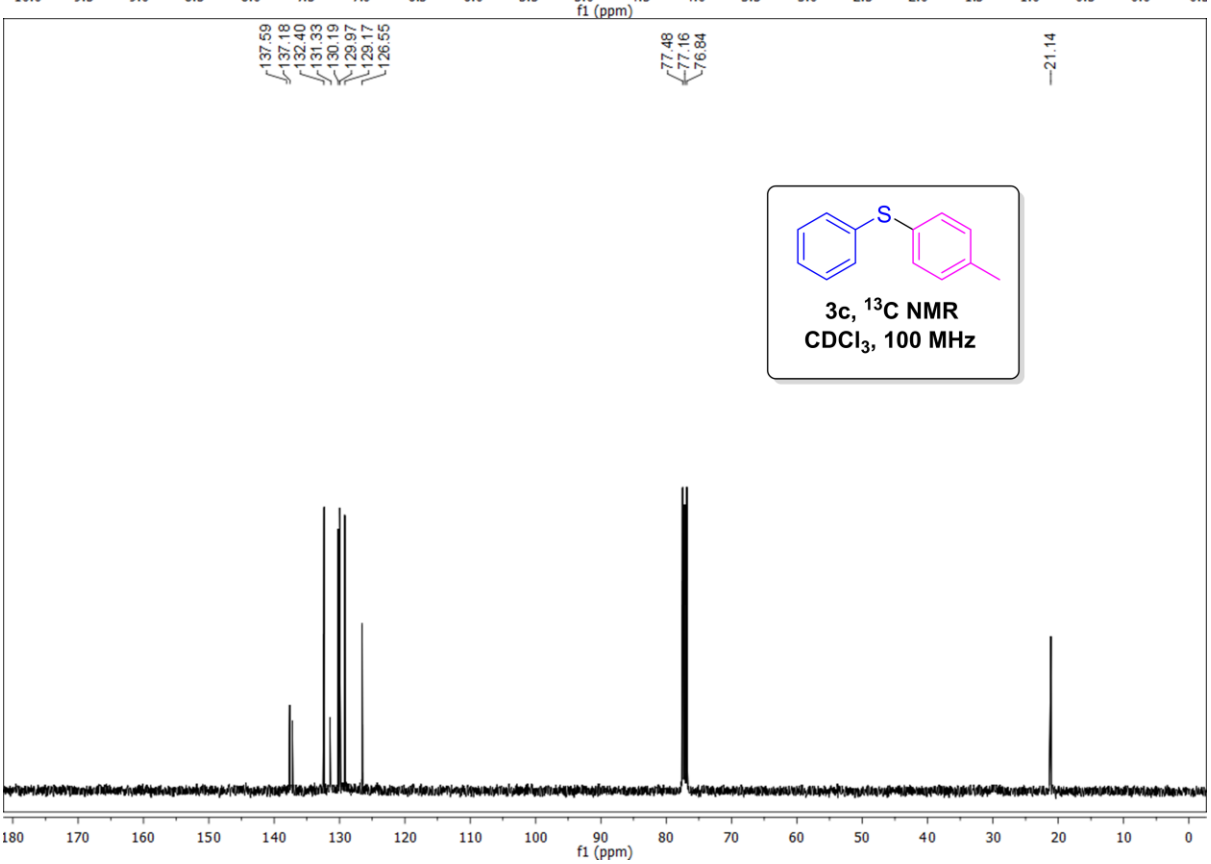

7.38
7.37
7.37
7.35
7.35
7.35
7.33
7.32
7.32
7.31
7.31
7.30
7.28
7.26
7.24
7.24
7.23
7.22
7.21
S
3a, 1H NMR
CDCl3, 400 MHz
4.00
4.08
2.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

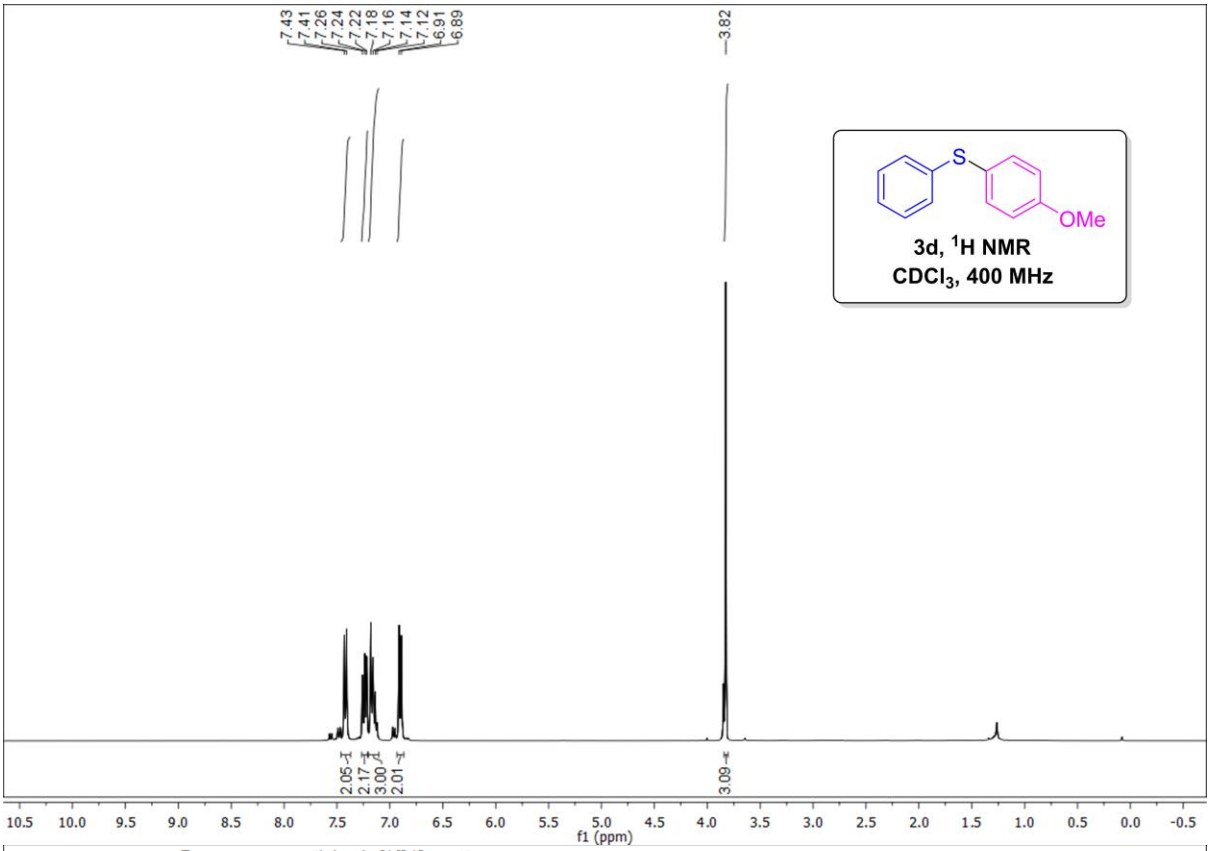

135.79
131.05
129.22
127.17
77.49
77.07
76.65
S
3a, 13C NMR
CDCl3, 100 MHz
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

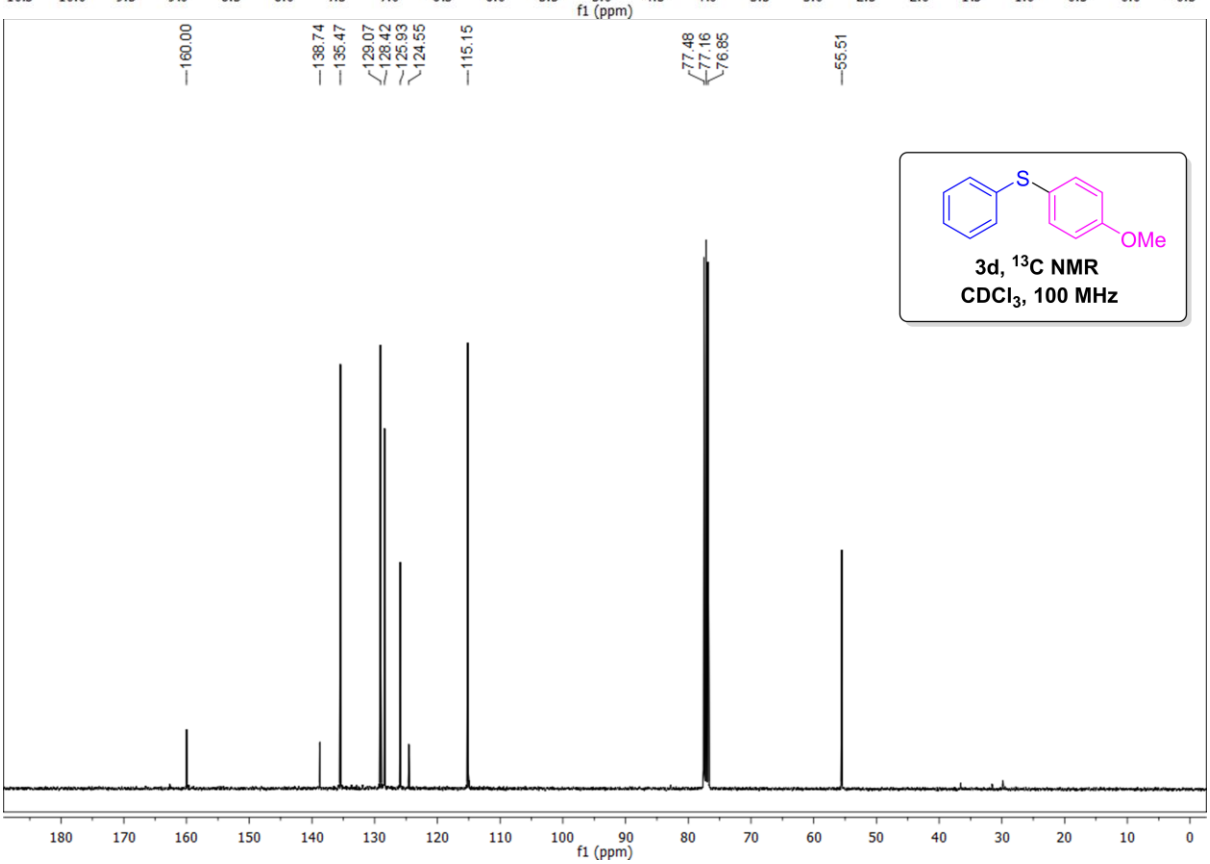

7.26
7.23
7.23
7.22
7.21
7.20
7.19
7.17
7.15
7.14
7.12
7.08
7.06
2.30
S
3b, 1H NMR
CDCl3, 400 MHz
9.01
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

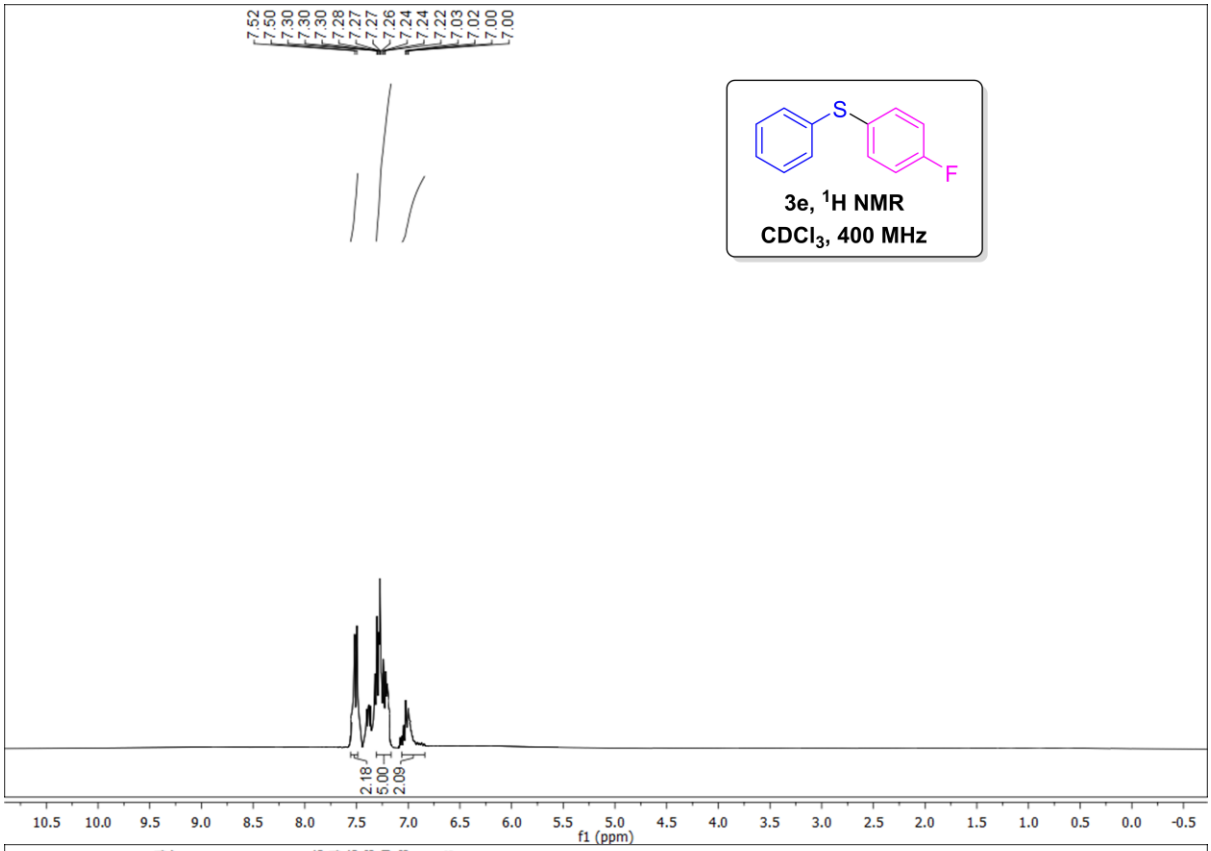

140.13
136.34
133.91
133.17
130.73
129.77
129.19
128.04
126.84
126.46
77.48
77.16
76.85
20.71
S
3b, 13C NMR
CDCl3, 100 MHz
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

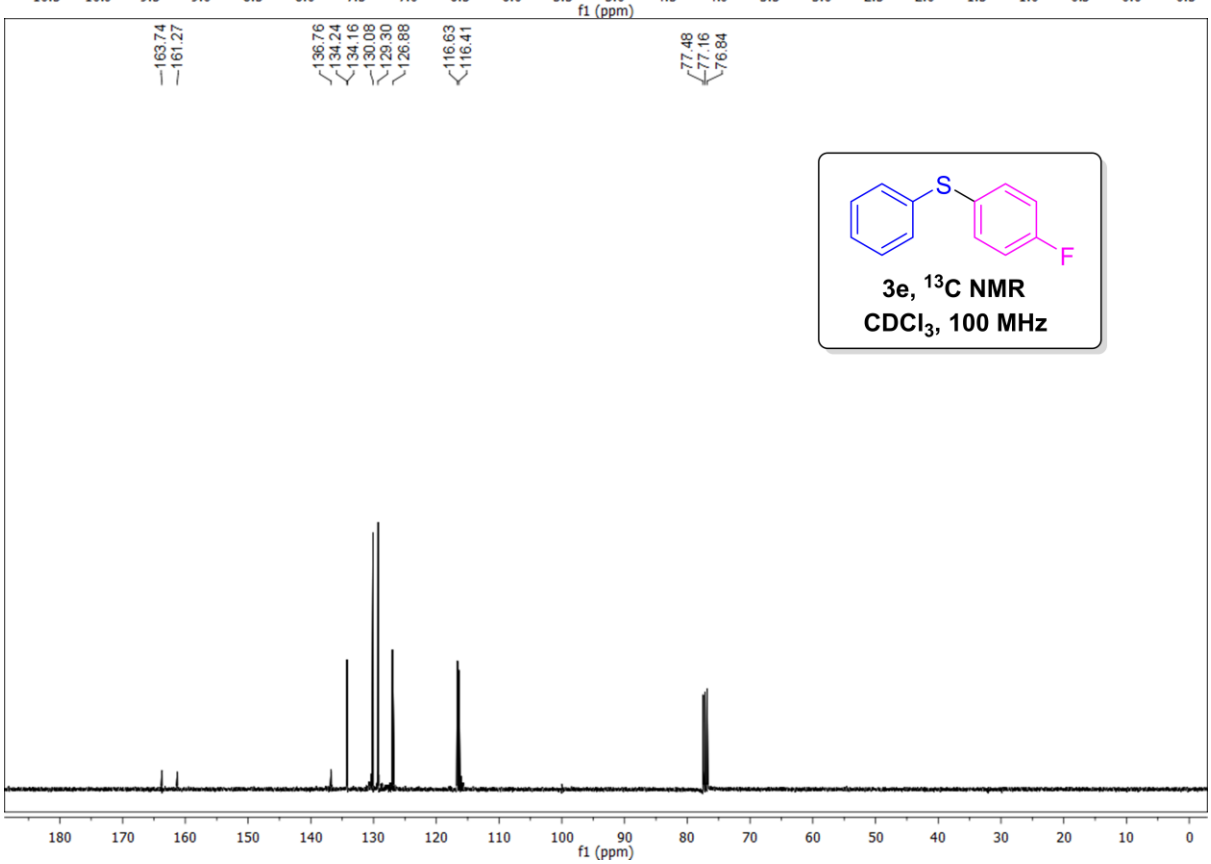

7.32
7.31
7.30
7.28
7.27
7.26
7.23
7.16
7.14
7.10
2.30
S
3c, ^{1}H NMR
$CDCl_3$, 400 MHz
9.00
2.90
f1 (ppm)

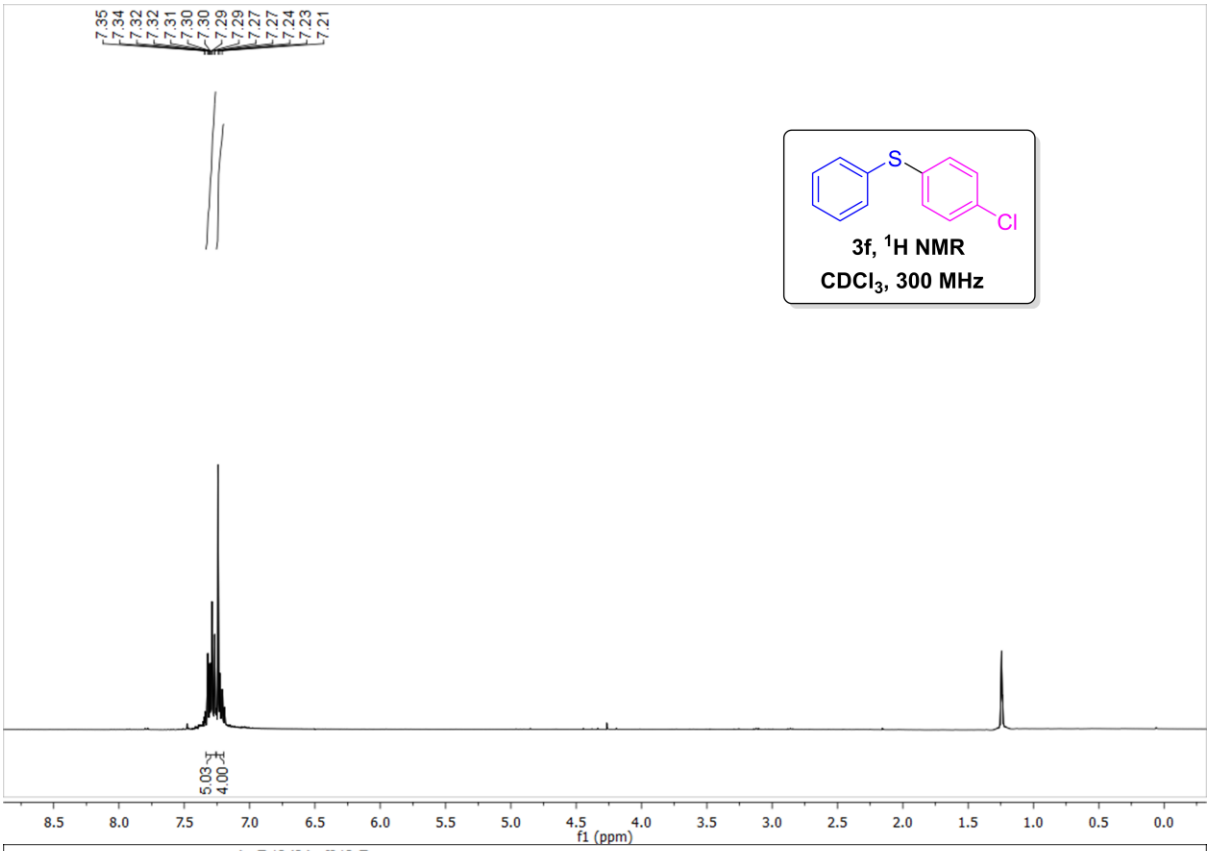

137.59
137.18
132.40
131.33
130.19
129.97
129.17
126.55
77.48
77.16
76.84
21.14
S
3c, ^{13}C NMR
$CDCl_3$, 100 MHz
f1 (ppm)

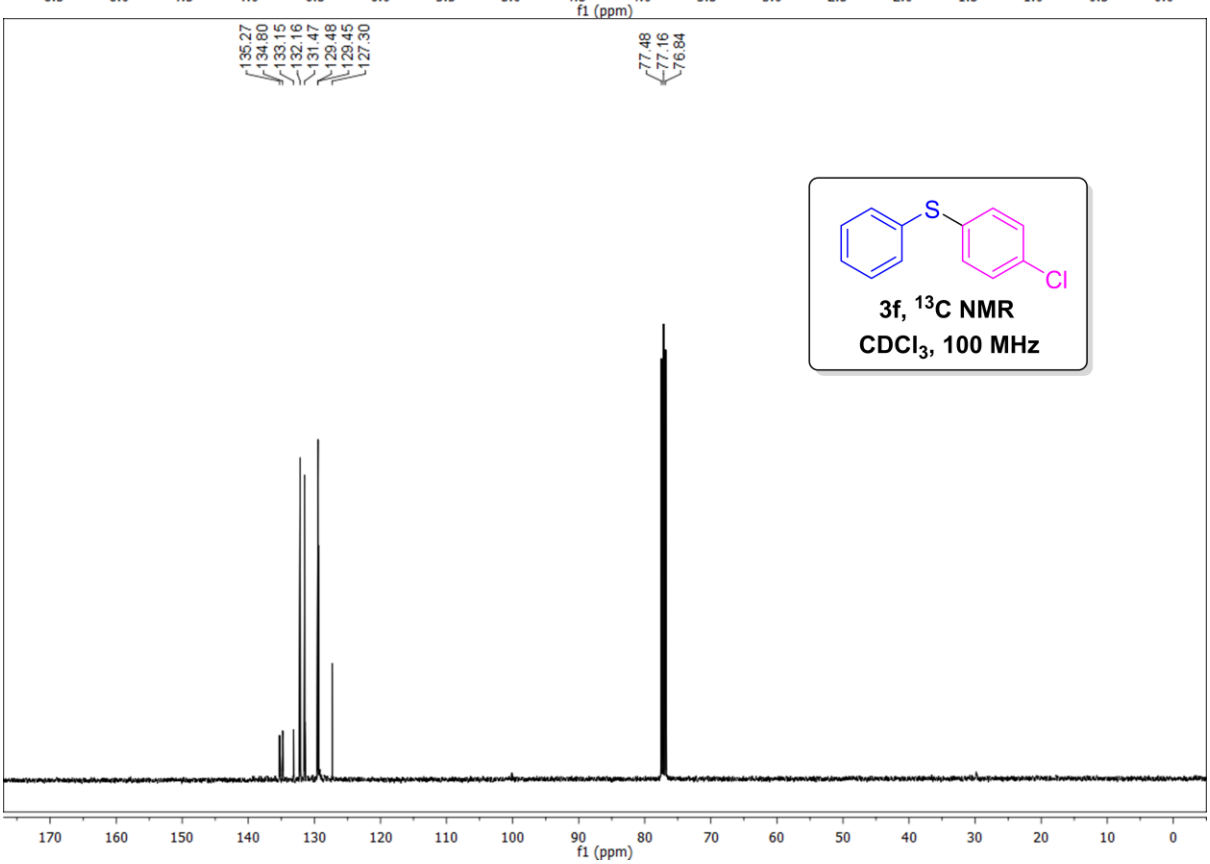

7.43
7.41
7.26
7.24
7.22
7.18
7.16
7.14
7.12
6.91
6.89
3.82
2.05
2.17
3.00
2.01
3.09
S
OMe
3d, 1H NMR
CDCl3, 400 MHz
f1 (ppm)

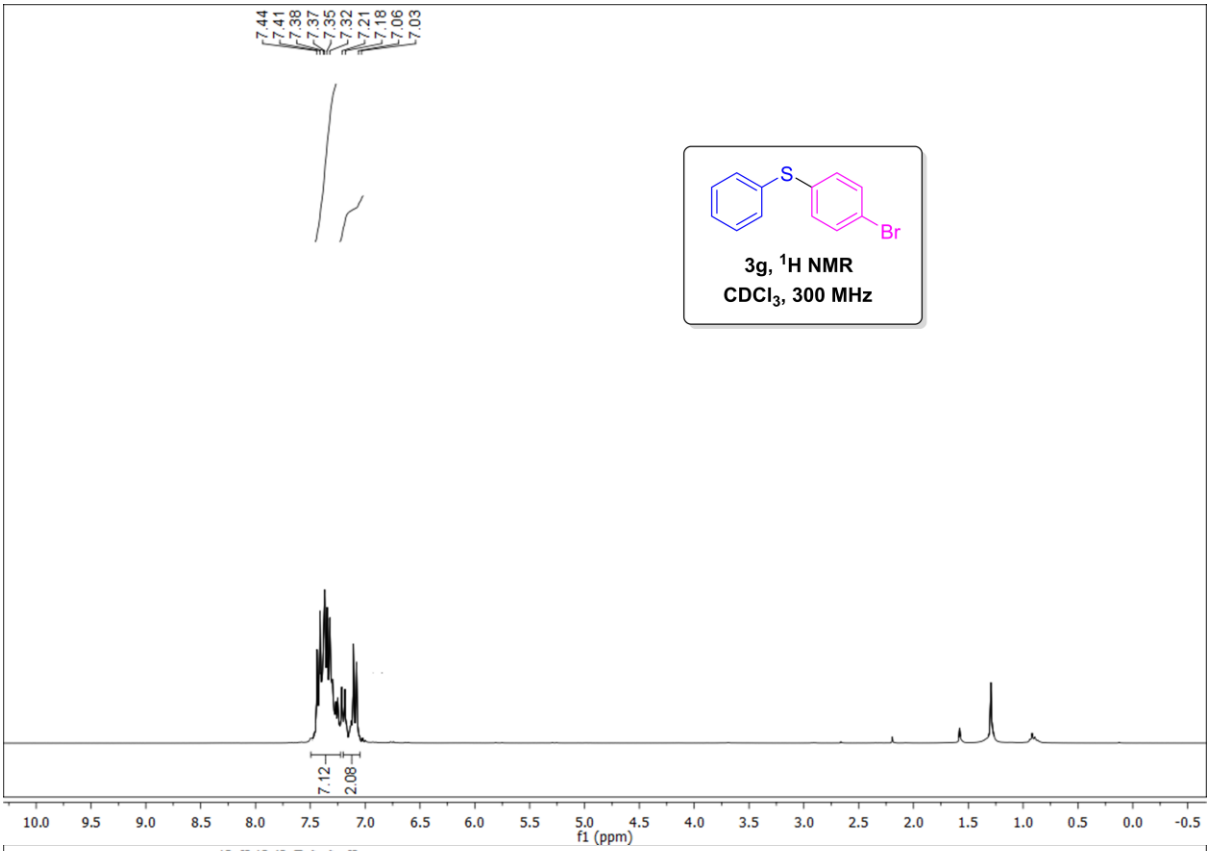

160.00
138.74
135.47
129.07
128.42
125.93
124.55
115.15
77.48
77.16
76.85
55.51
S
OMe
3d, 13C NMR
CDCl3, 100 MHz
f1 (ppm)

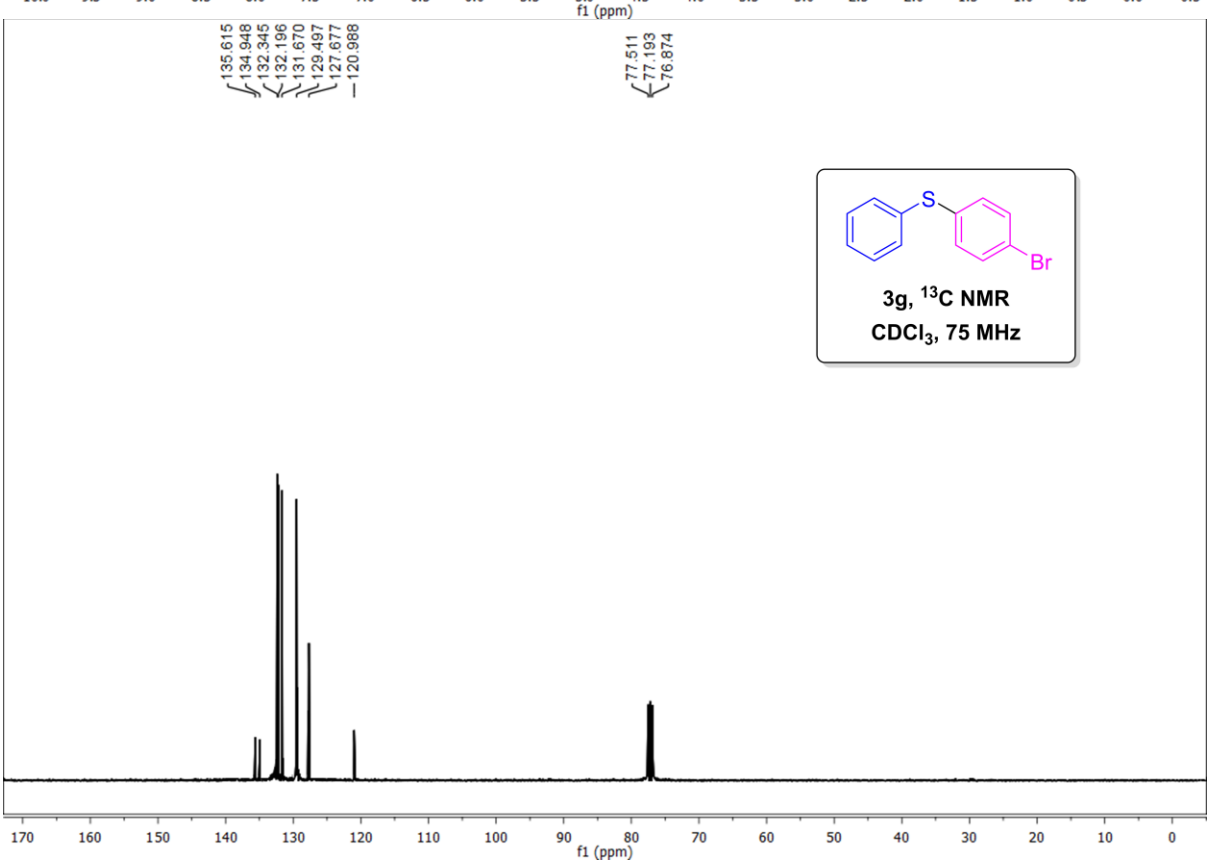

7.52
7.50
7.30
7.30
7.30
7.28
7.27
7.27
7.26
7.24
7.24
7.22
7.03
7.02
7.00
7.00
S
F
3e, 1H NMR
CDCl3, 400 MHz
2.18
5.00
2.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

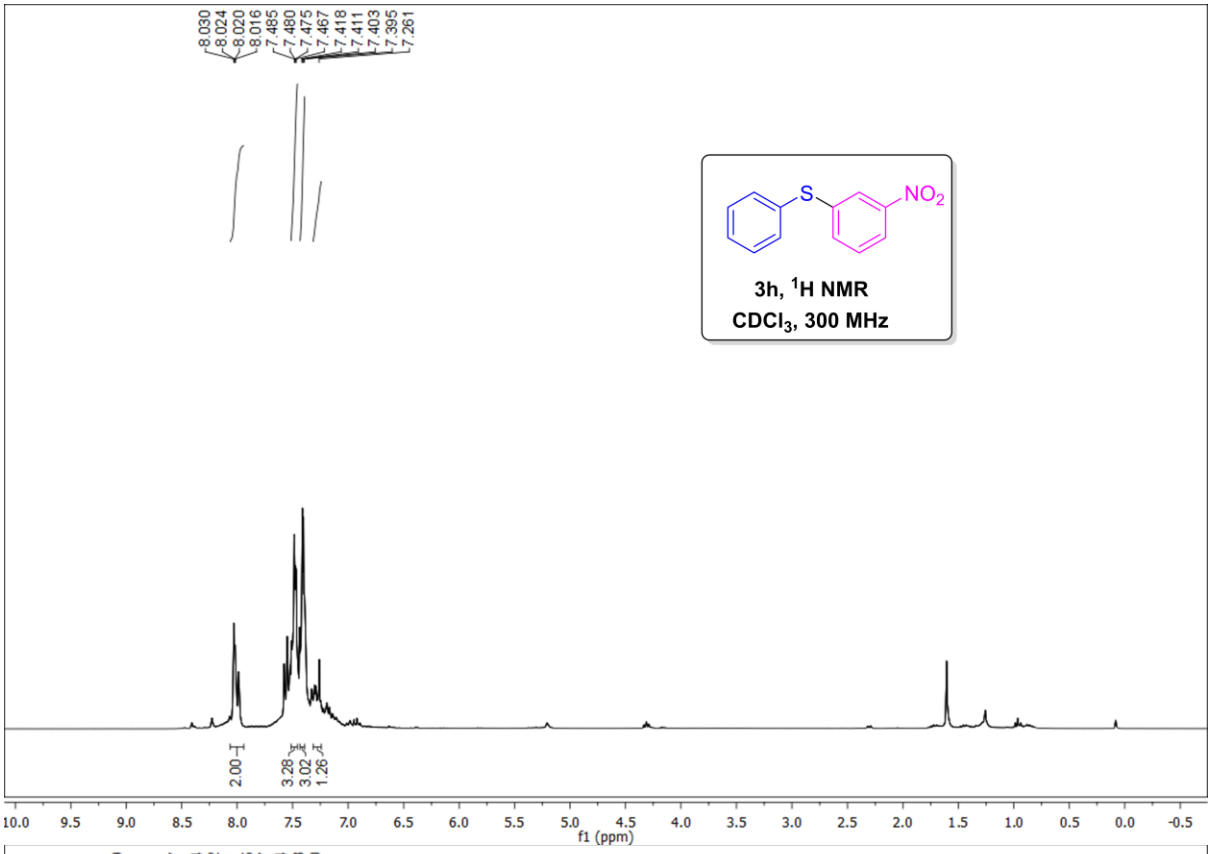

163.74
161.27
136.76
134.24
134.16
130.08
129.30
126.88
116.63
116.41
77.48
77.16
76.84
S
F
3e, 13C NMR
CDCl3, 100 MHz
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

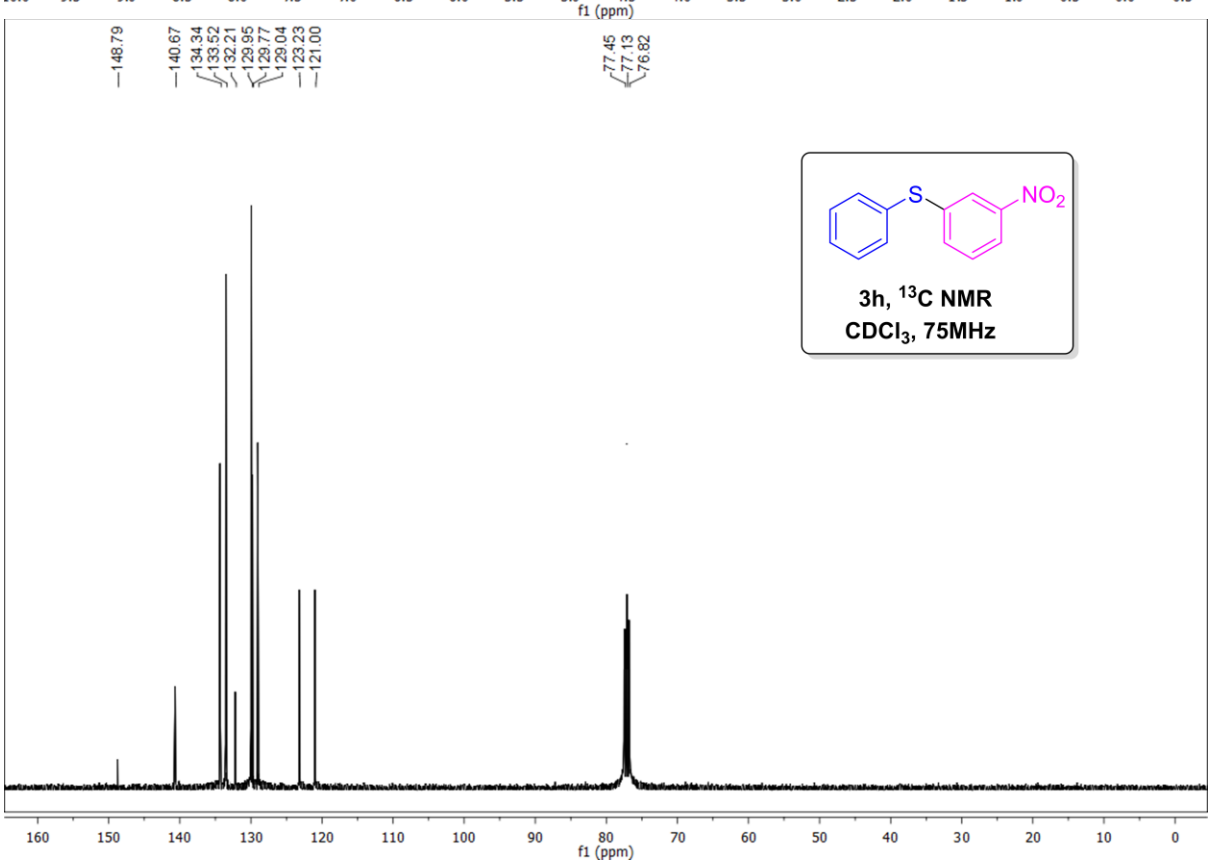

7.35
7.34
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.27
7.27
7.24
7.23
7.21
S
Cl
3f, 1H NMR
CDCl3, 300 MHz
5.03
4.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

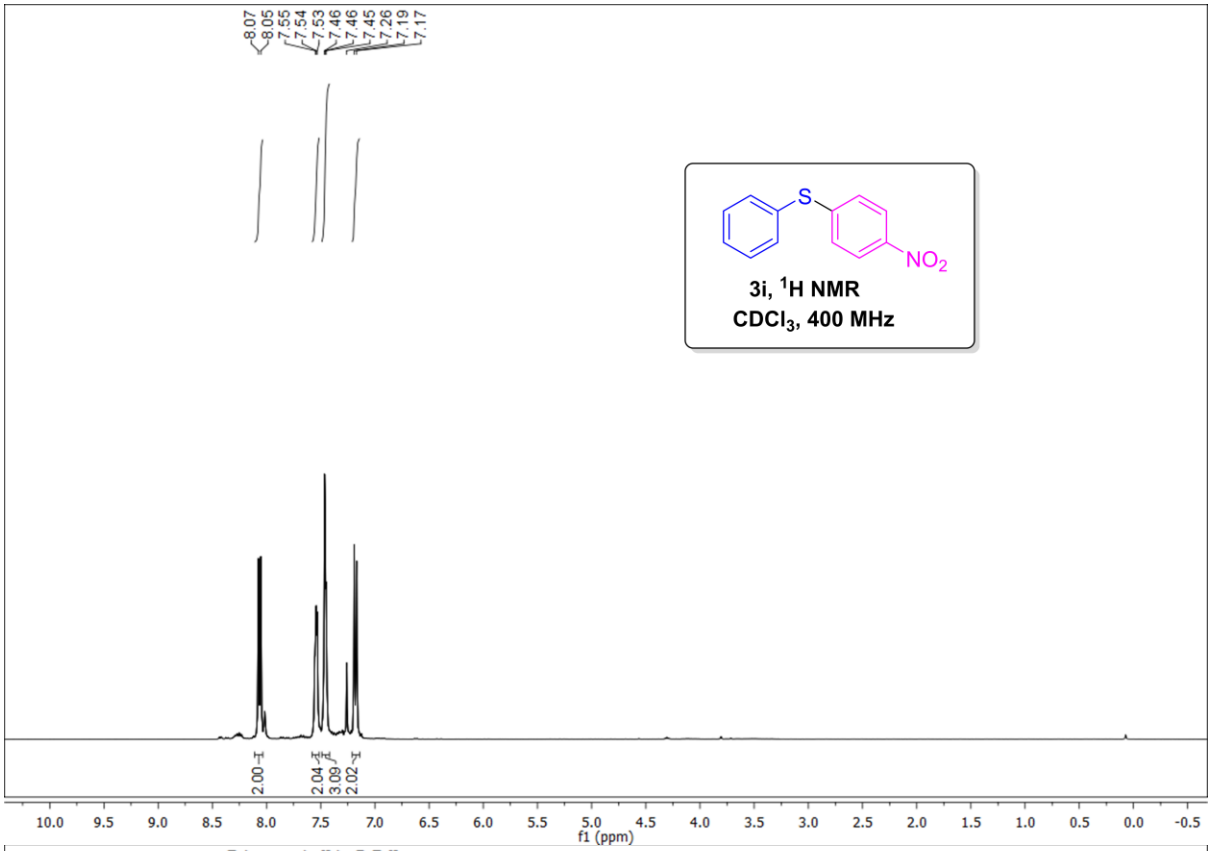

135.27
134.80
133.15
132.16
131.47
129.48
129.45
127.30
77.48
77.16
76.84
S
Cl
3f, 13C NMR
CDCl3, 100 MHz
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

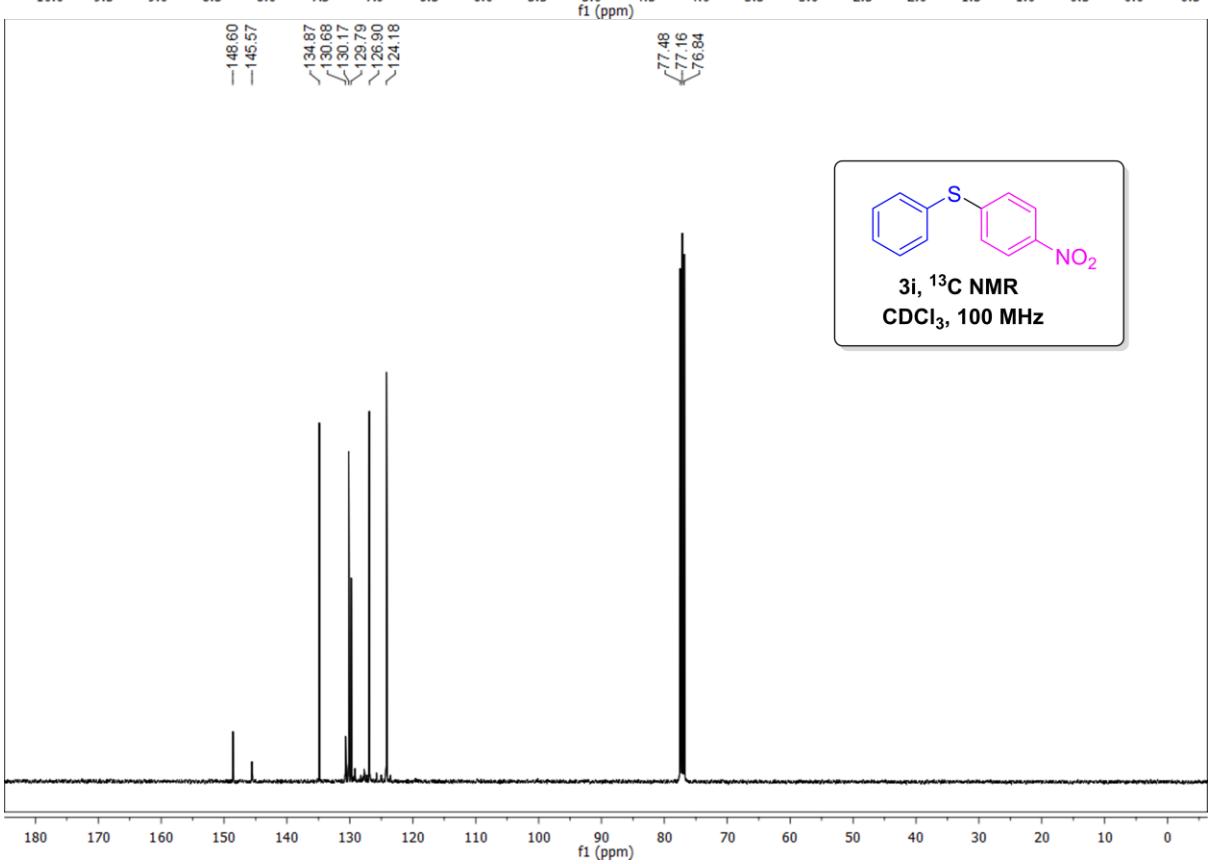

7.44
7.41
7.38
7.37
7.35
7.32
7.21
7.18
7.06
7.03
S
Br
3g, 1H NMR
CDCl3, 300 MHz
7.12
2.08
f1 (ppm)

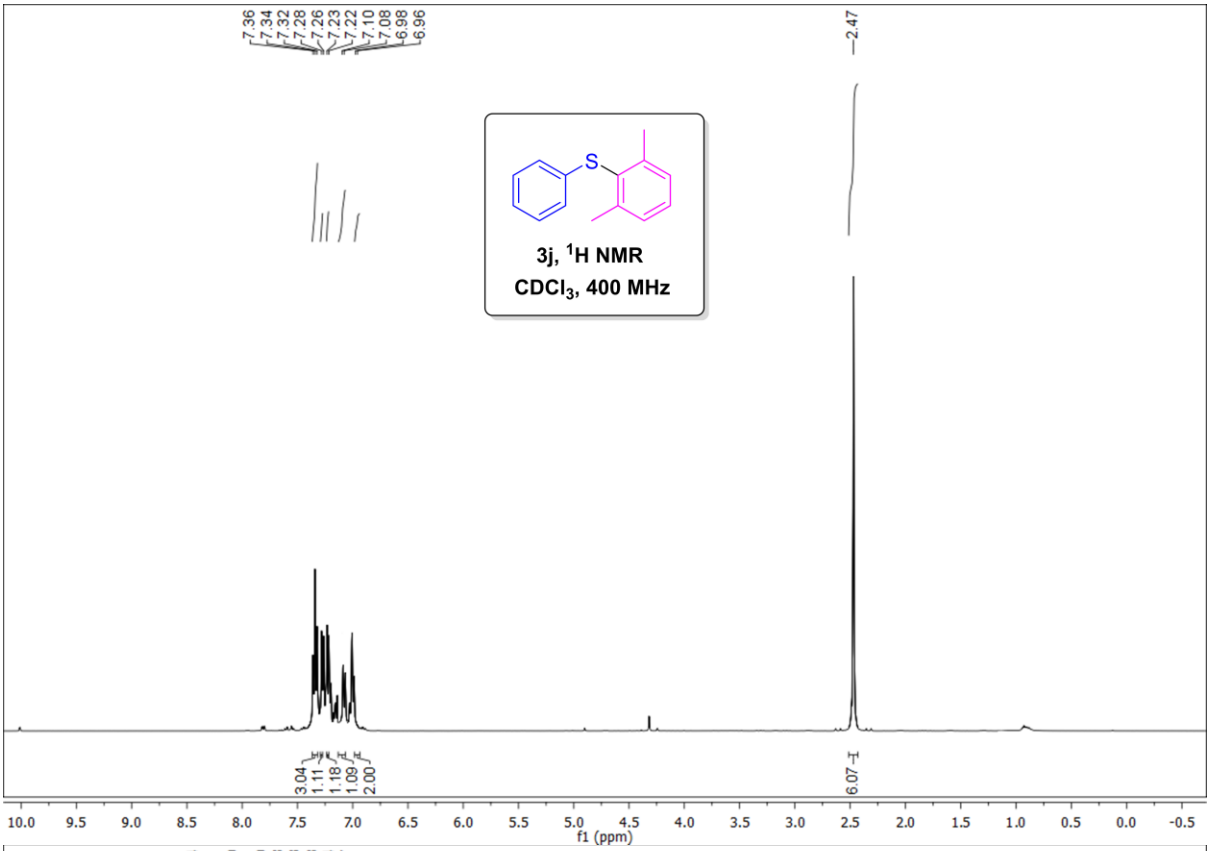

135.615
134.948
132.345
132.196
131.670
129.497
127.677
120.988
77.511
77.193
76.874
S
Br
3g, 13C NMR
CDCl3, 75 MHz
f1 (ppm)

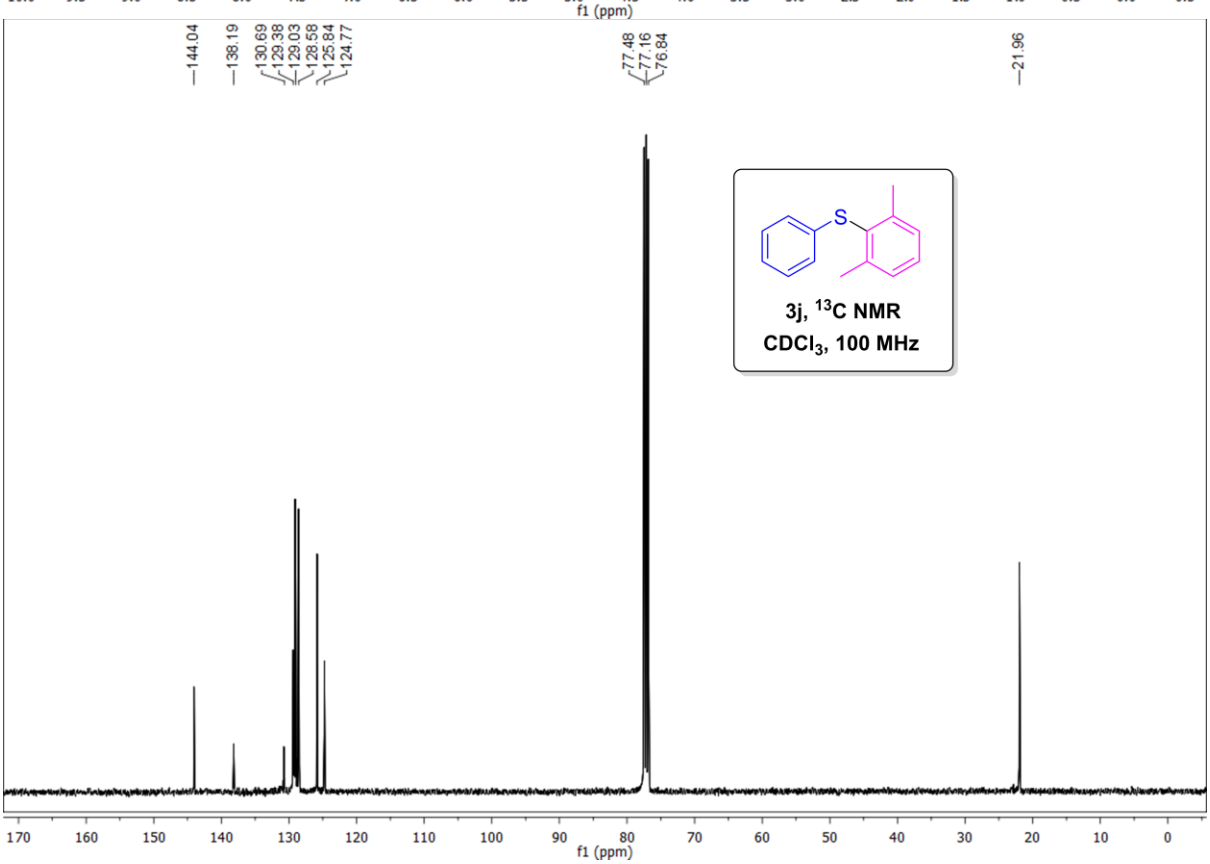

8.030
8.024
8.020
8.016
7.485
7.480
7.475
7.467
7.418
7.411
7.403
7.395
7.261
2.00
3.28
3.02
1.26
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
S
NO2
3h, 1H NMR
CDCl3, 300 MHz

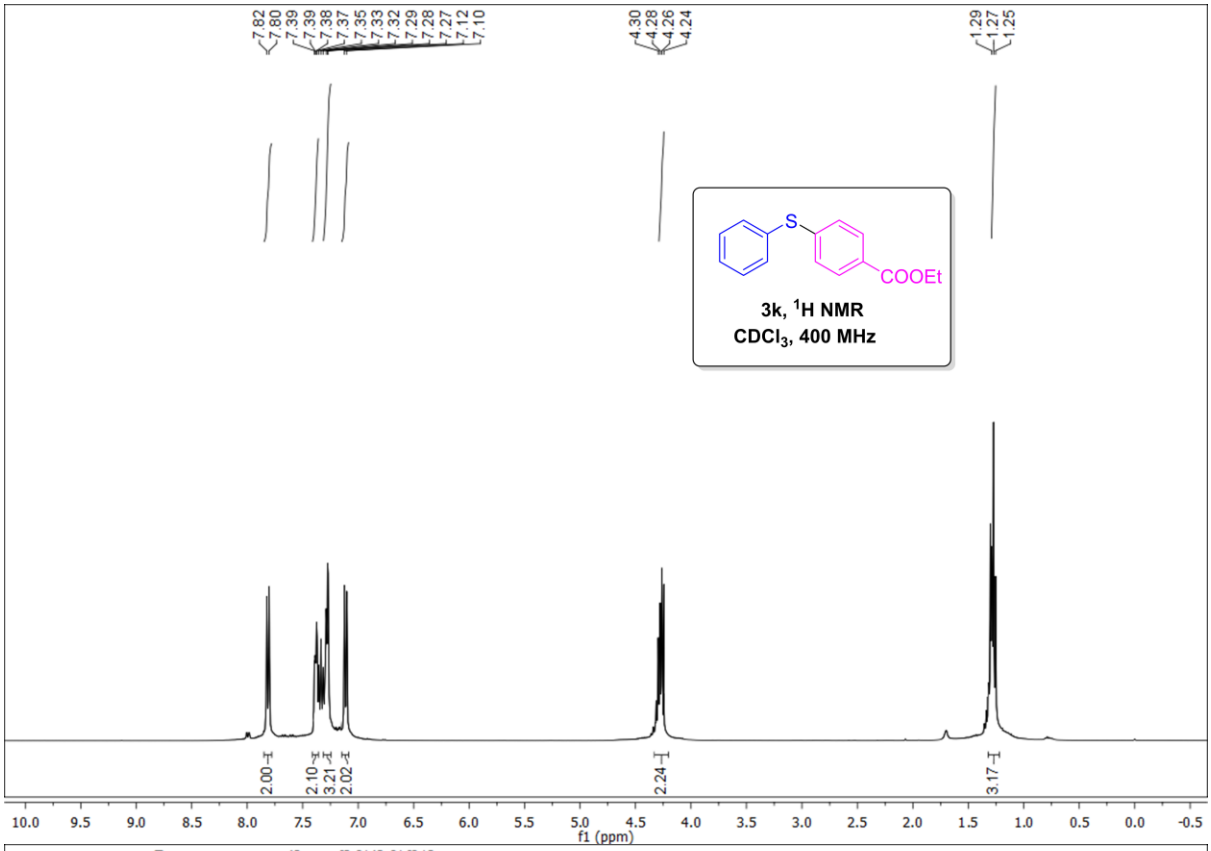

148.79
140.67
134.34
133.52
132.21
129.95
129.77
129.04
123.23
121.00
77.45
77.13
76.82
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
S
NO2
3h, 13C NMR
CDCl3, 75MHz

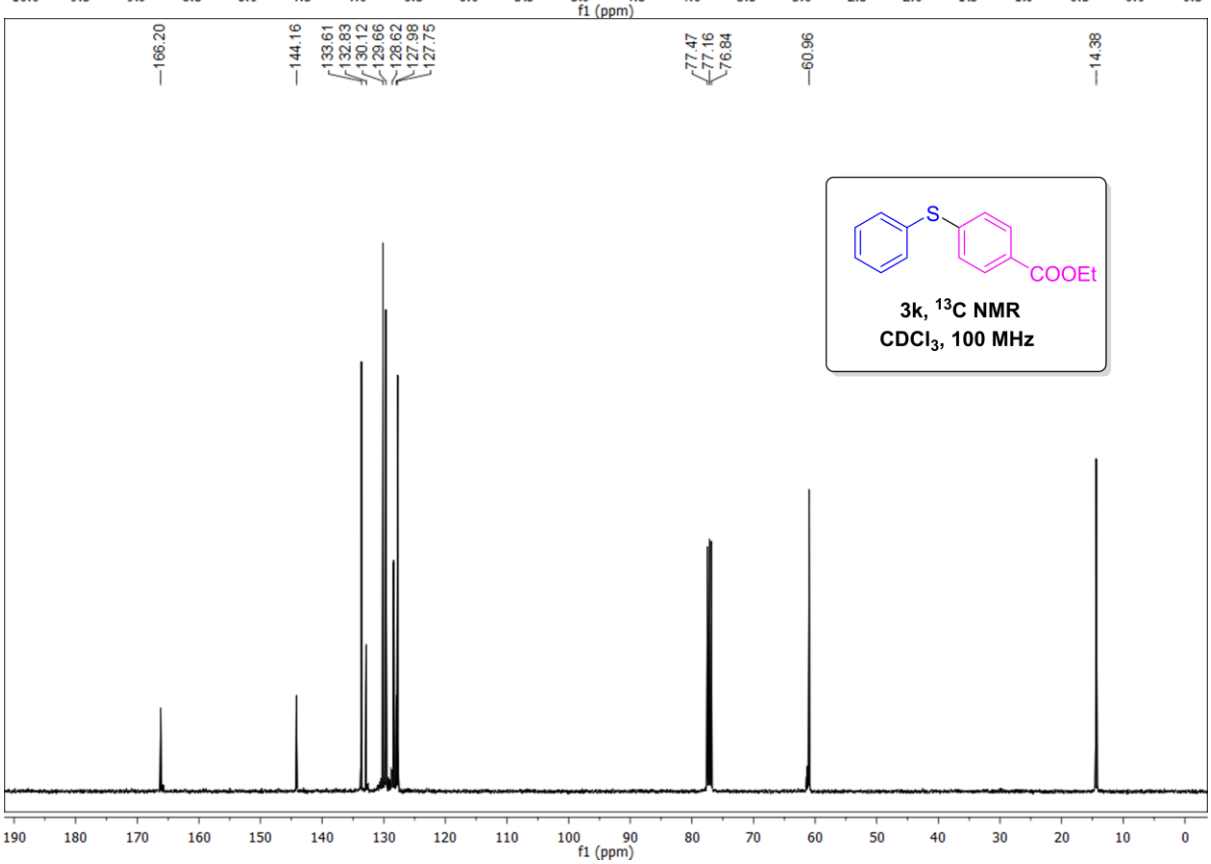

8.07
8.05
7.55
7.54
7.53
7.46
7.46
7.45
7.26
7.19
7.17
S
NO2
3i, 1H NMR
CDCl3, 400 MHz
2.00
2.04
3.09
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

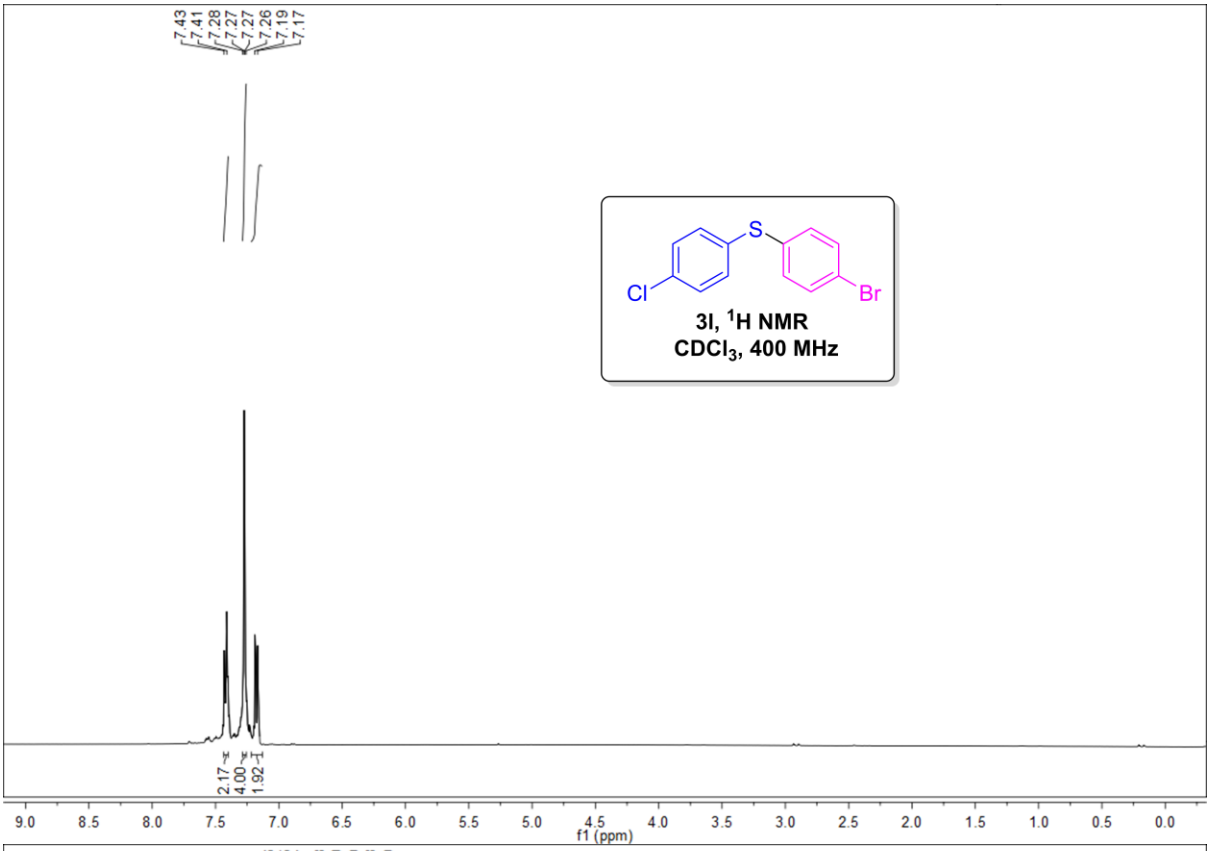

148.60
145.57
134.87
130.68
130.17
129.79
126.90
124.18
77.48
77.16
76.84
S
NO2
3i, 13C NMR
CDCl3, 100 MHz
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

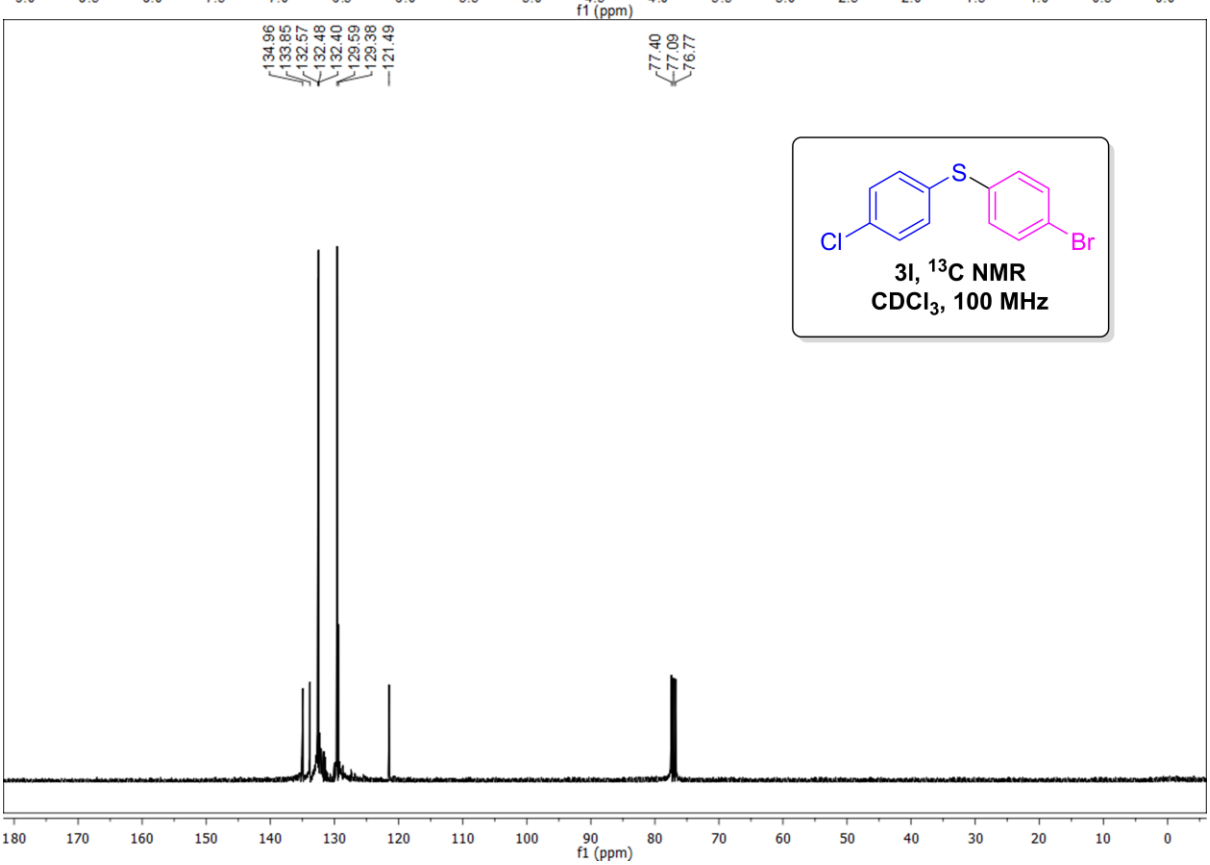

7.36
7.34
7.32
7.28
7.26
7.23
7.22
7.10
7.08
6.98
6.96
2.47
3j, ^{1}H NMR
$CDCl_3$, 400 MHz
3.04
1.11
1.18
1.09
2.00
6.07
f1 (ppm)

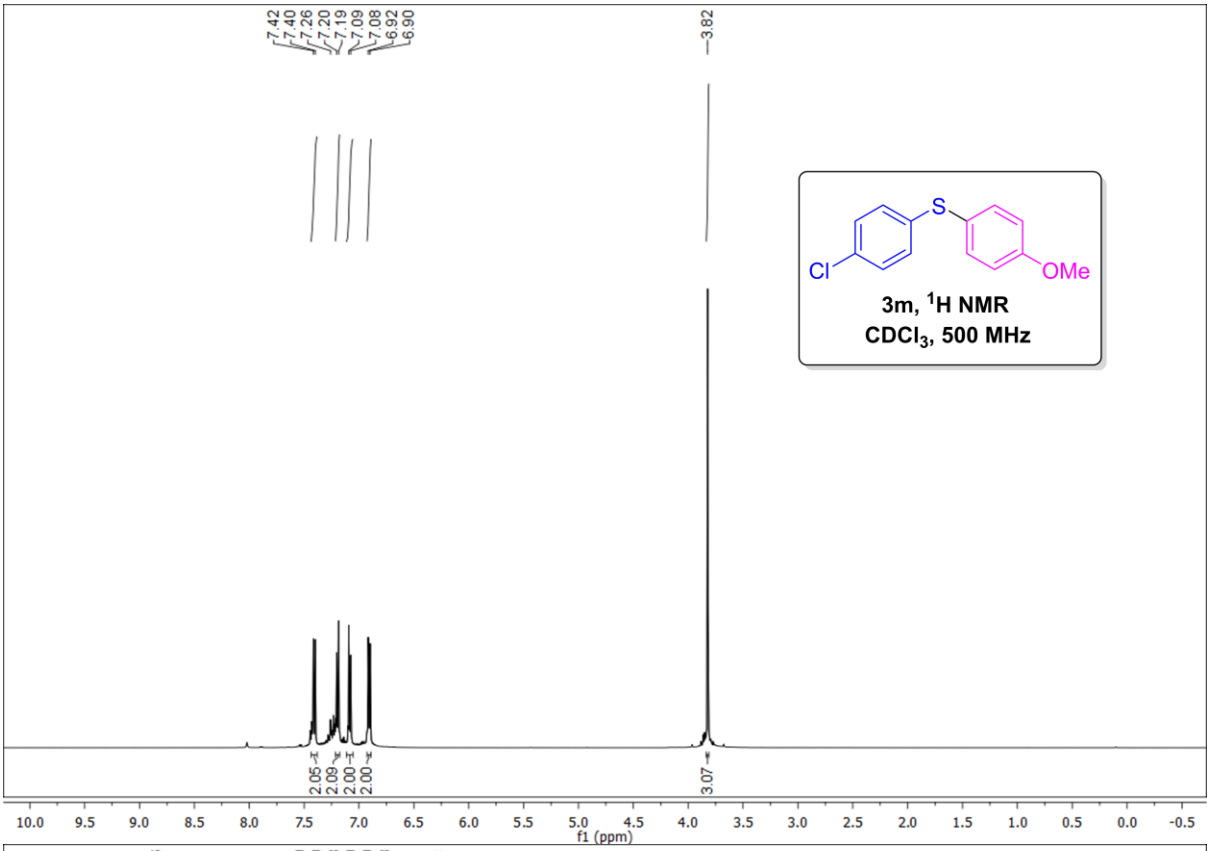

144.04
138.19
130.69
129.38
129.03
128.58
125.84
124.77
77.48
77.16
76.84
21.96
3j, ^{13}C NMR
$CDCl_3$, 100 MHz
f1 (ppm)

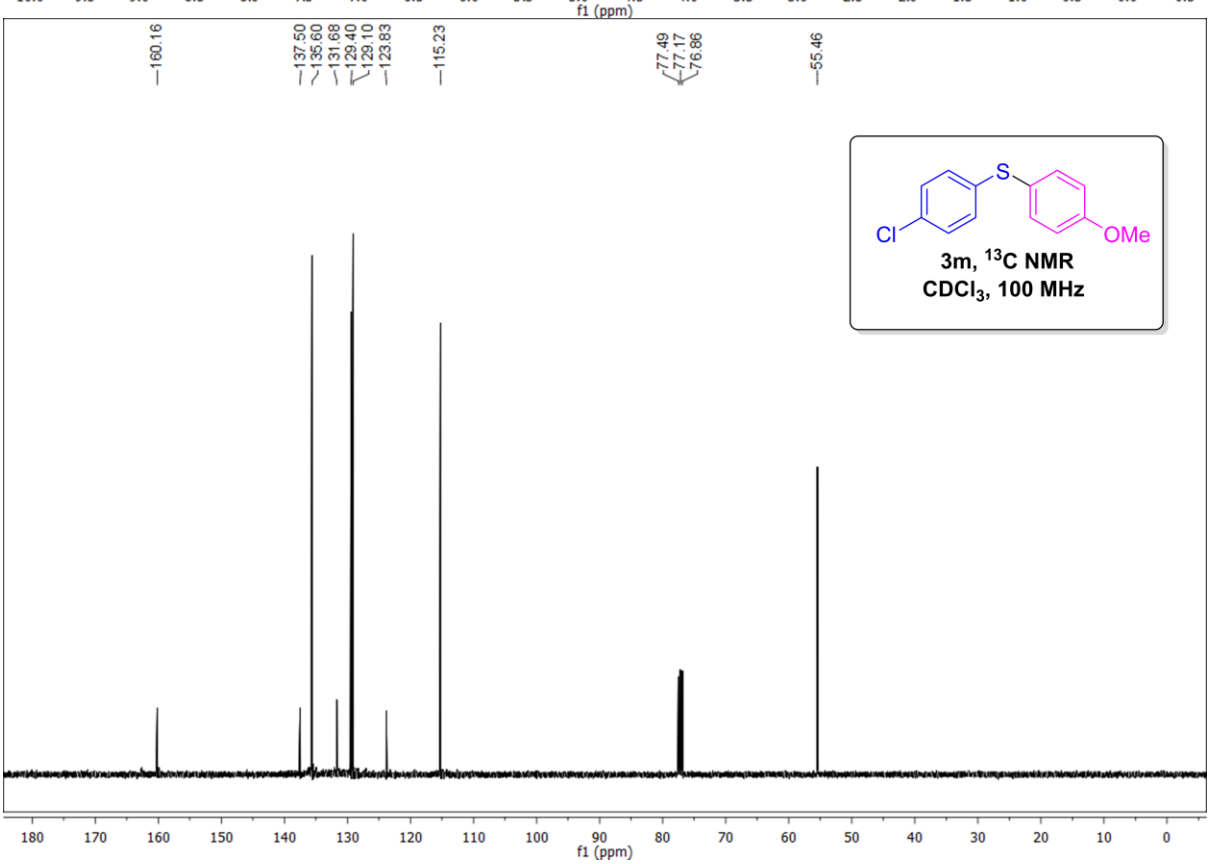

7.82
7.80
7.39
7.39
7.38
7.37
7.35
7.33
7.32
7.29
7.28
7.27
7.12
7.10
4.30
4.28
4.26
4.24
1.29
1.27
1.25
S
COOEt
3k, 1H NMR
CDCl3, 400 MHz
2.00
2.10
3.21
2.02
2.24
3.17
f1 (ppm)

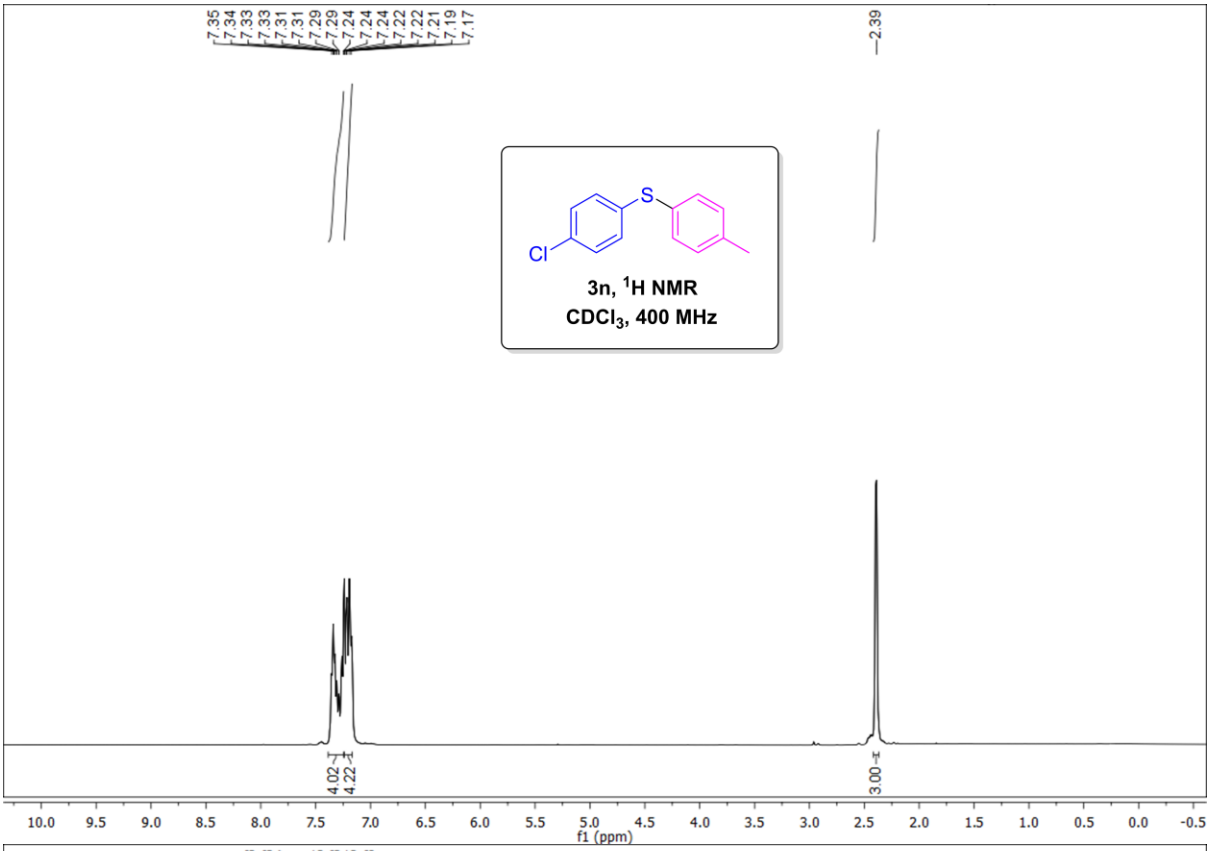

166.20
144.16
133.61
132.83
130.12
129.66
128.62
127.98
127.75
77.47
77.16
76.84
60.96
14.38
S
COOEt
3k, 13C NMR
CDCl3, 100 MHz
f1 (ppm)

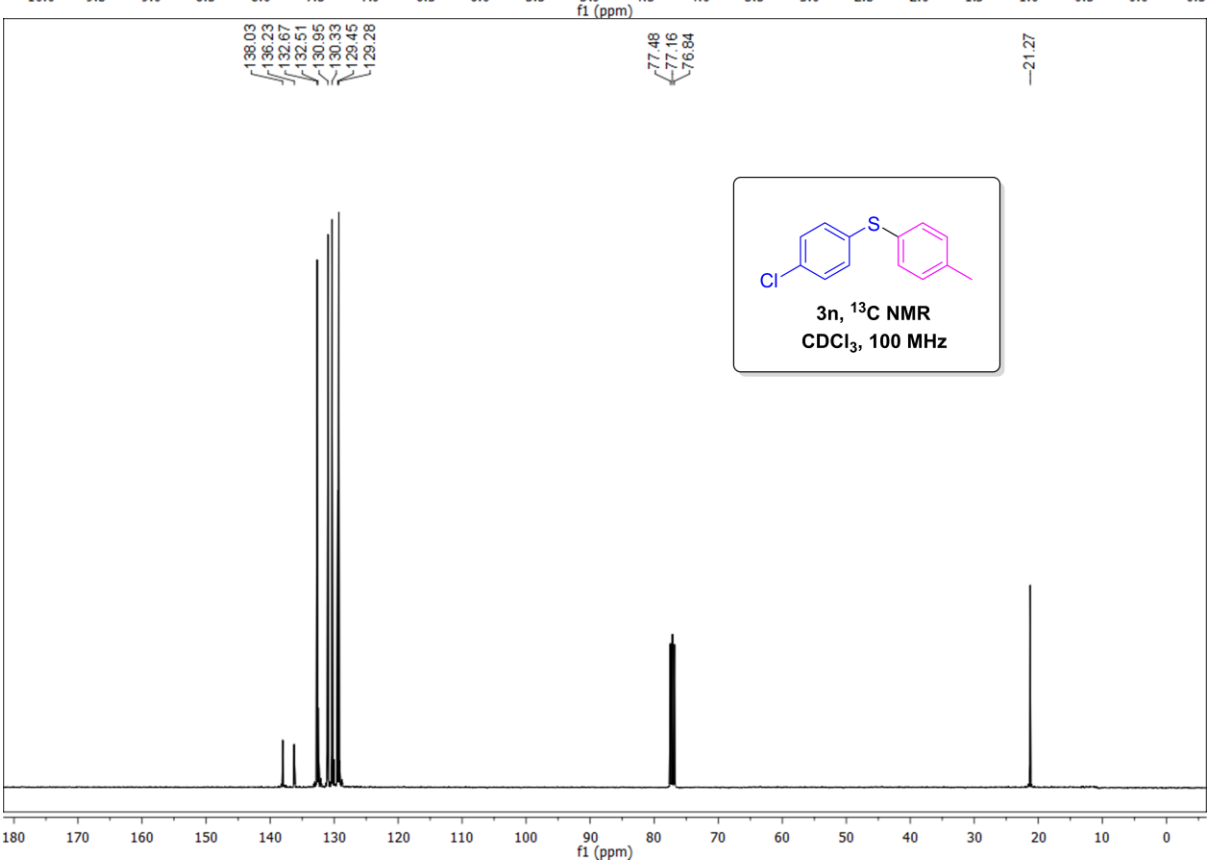

7.43
7.41
7.28
7.27
7.27
7.26
7.19
7.17
2.17
4.00
1.92
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
S
Cl
Br
3l, 1H NMR
CDCl3, 400 MHz

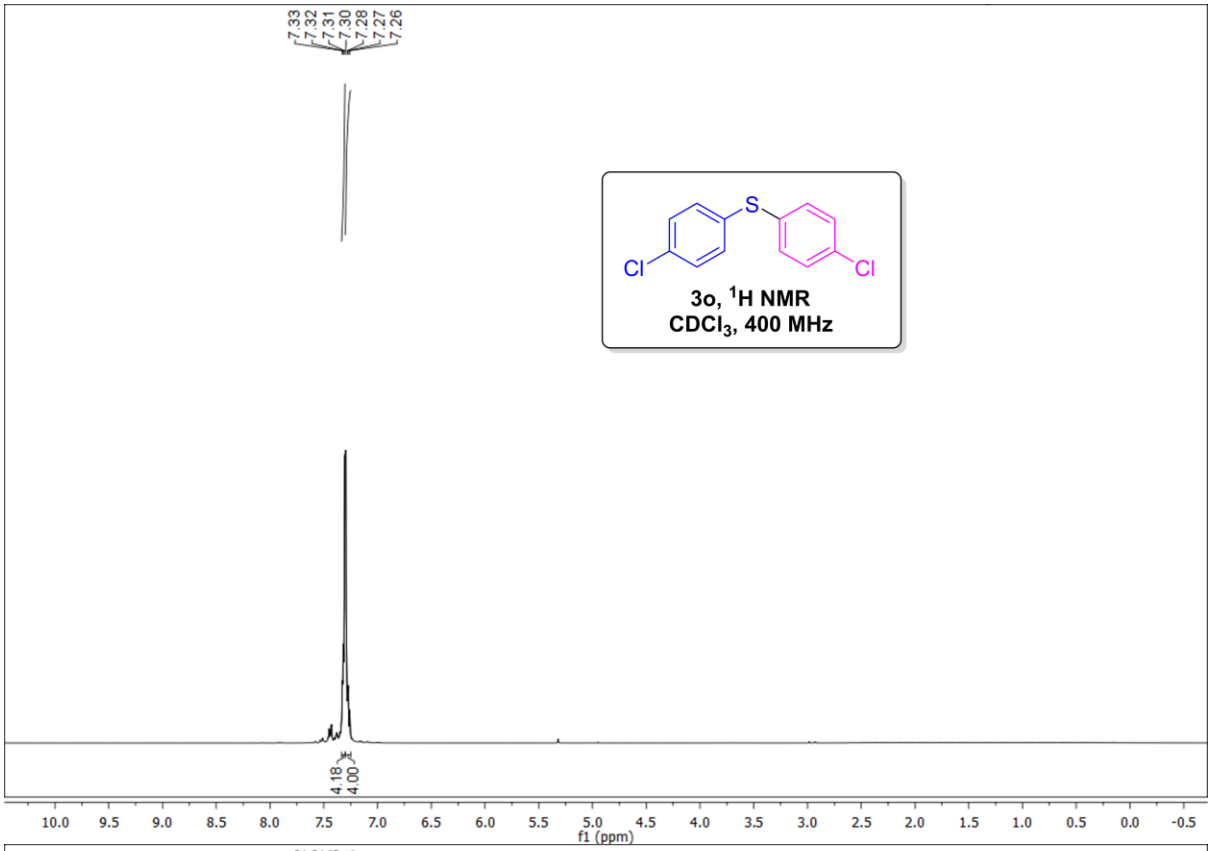

134.96
133.85
132.57
132.48
132.40
129.59
129.38
121.49
77.40
77.09
76.77
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
S
Cl
Br
3l, 13C NMR
CDCl3, 100 MHz

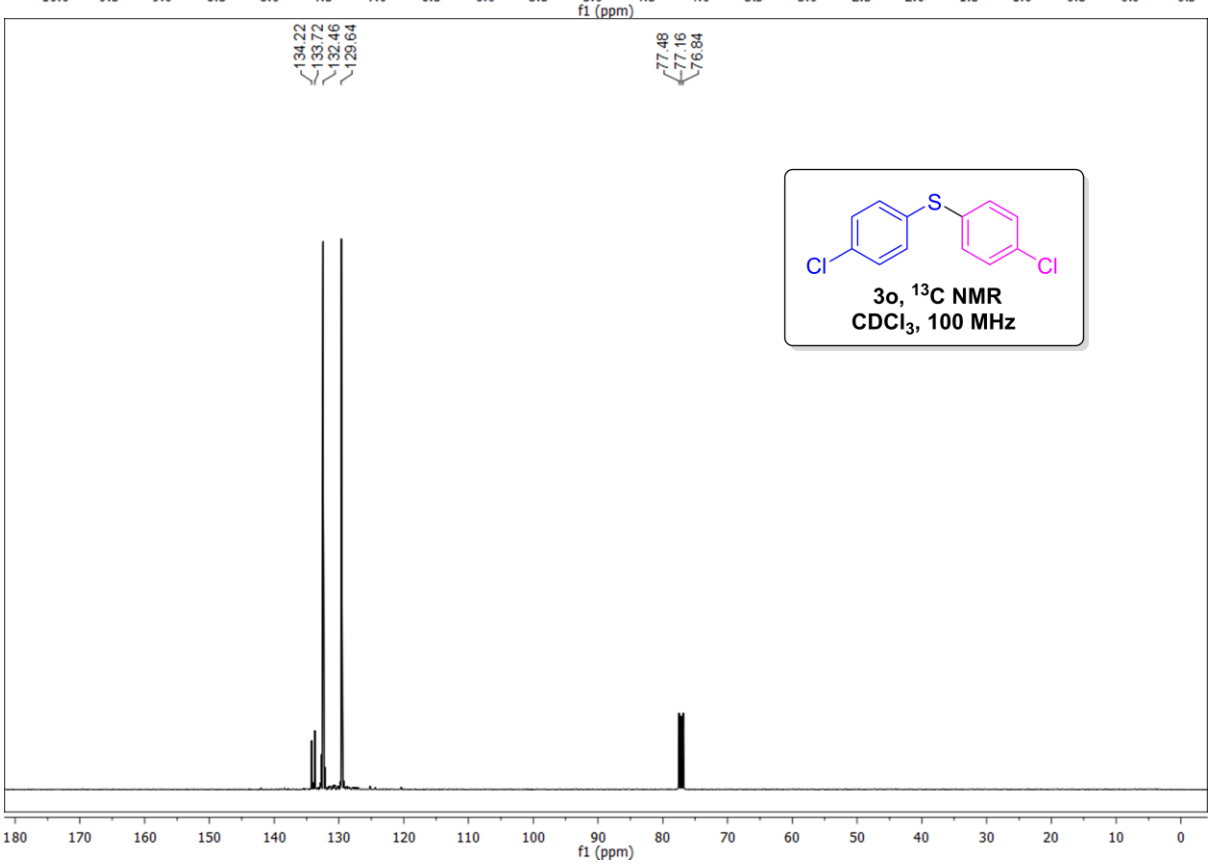

7.42
7.40
7.26
7.20
7.19
7.09
7.08
6.92
6.90
3.82
2.05
2.09
2.00
2.00
3.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
S
Cl
OMe
3m, ^{1}H NMR
$CDCl_3$, 500 MHz

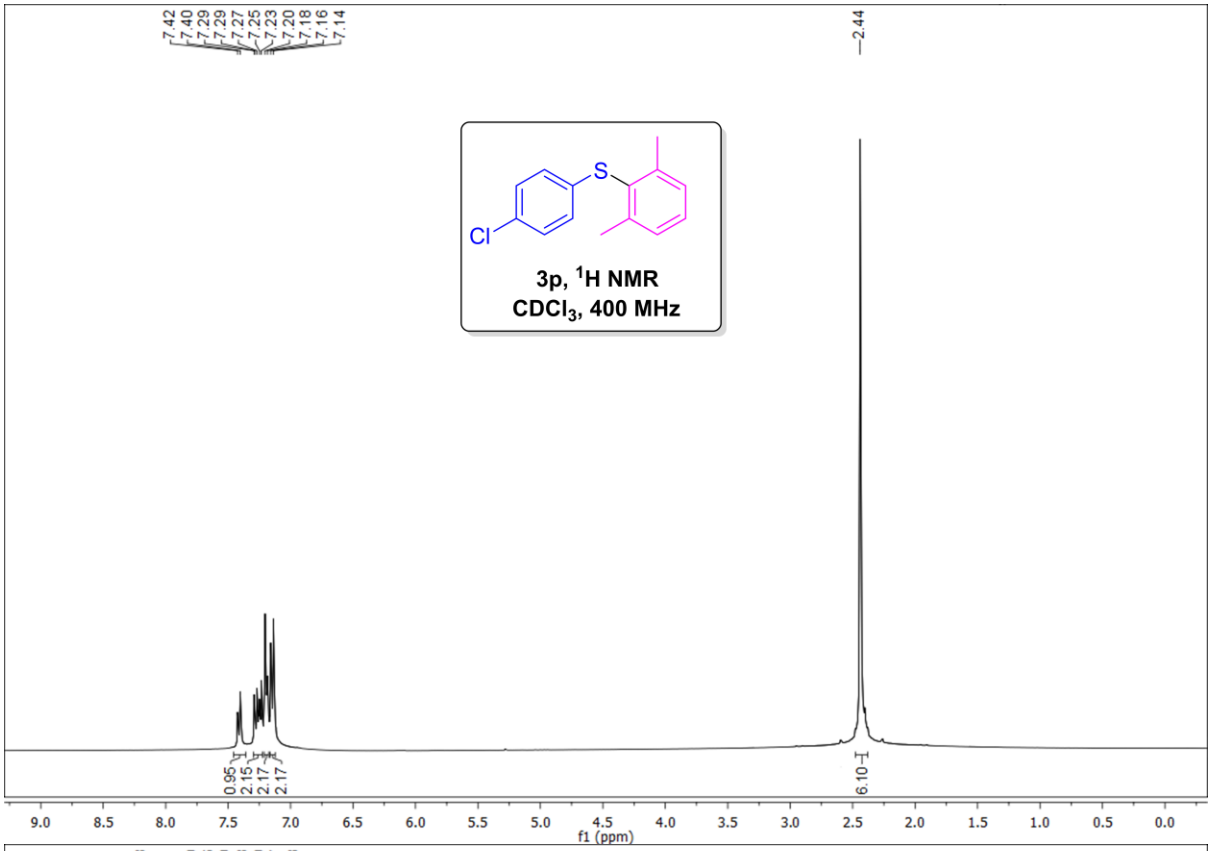

160.16
137.50
135.60
131.68
129.40
129.10
123.83
115.23
77.49
77.17
76.86
55.46
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
S
Cl
OMe
3m, ^{13}C NMR
$CDCl_3$, 100 MHz

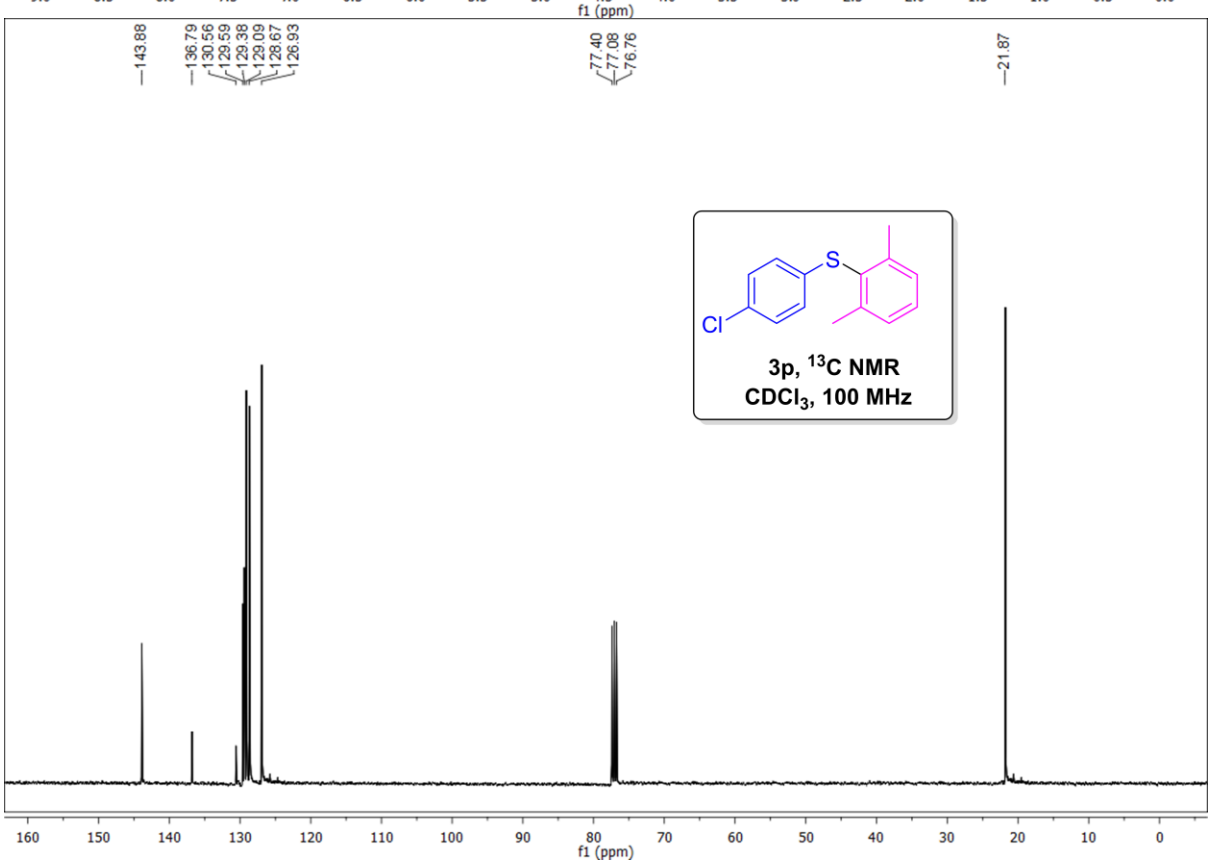

7.35
7.34
7.33
7.33
7.31
7.31
7.29
7.29
7.24
7.24
7.24
7.22
7.22
7.21
7.19
7.17
2.39
Cl
S
3n, 1H NMR
CDCl3, 400 MHz
4.02
4.22
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

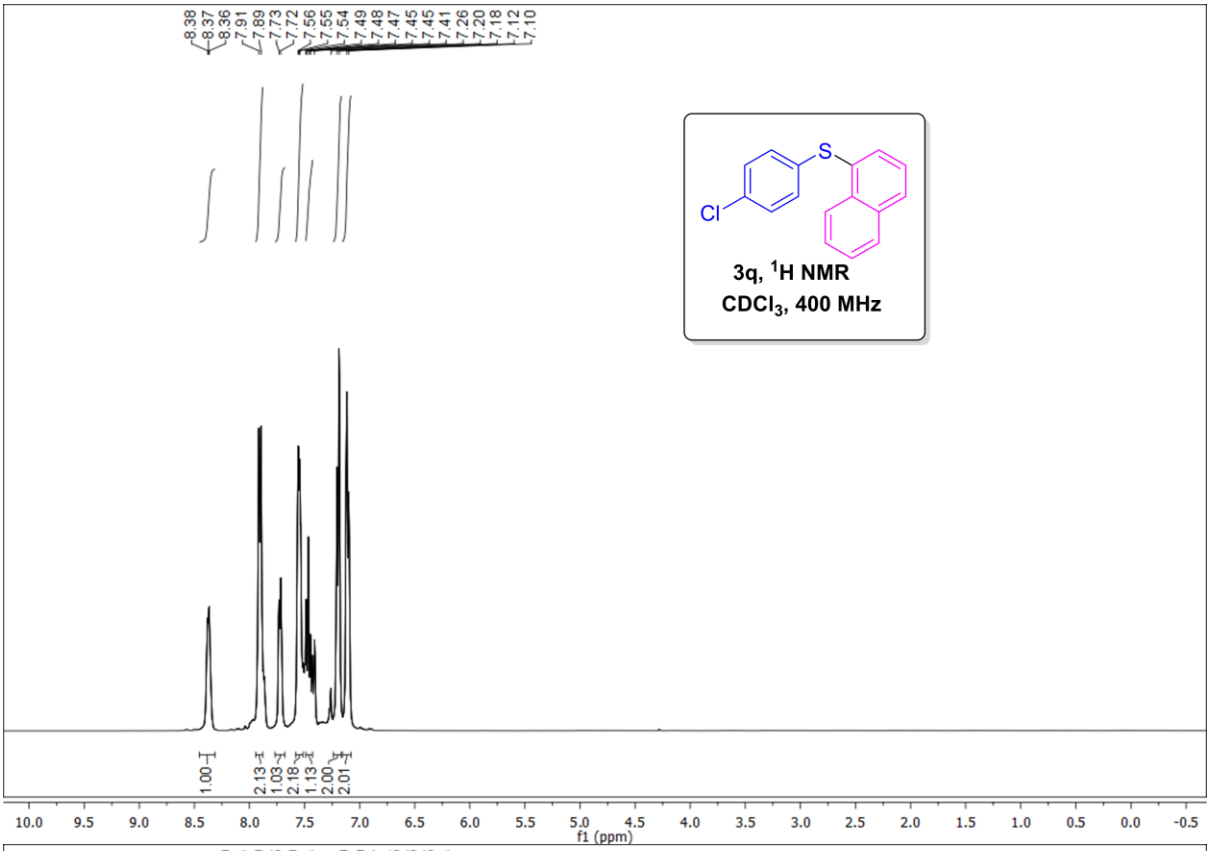

138.03
136.23
132.67
132.51
130.95
130.33
129.45
129.28
77.48
77.16
76.84
21.27
Cl
S
3n, 13C NMR
CDCl3, 100 MHz
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

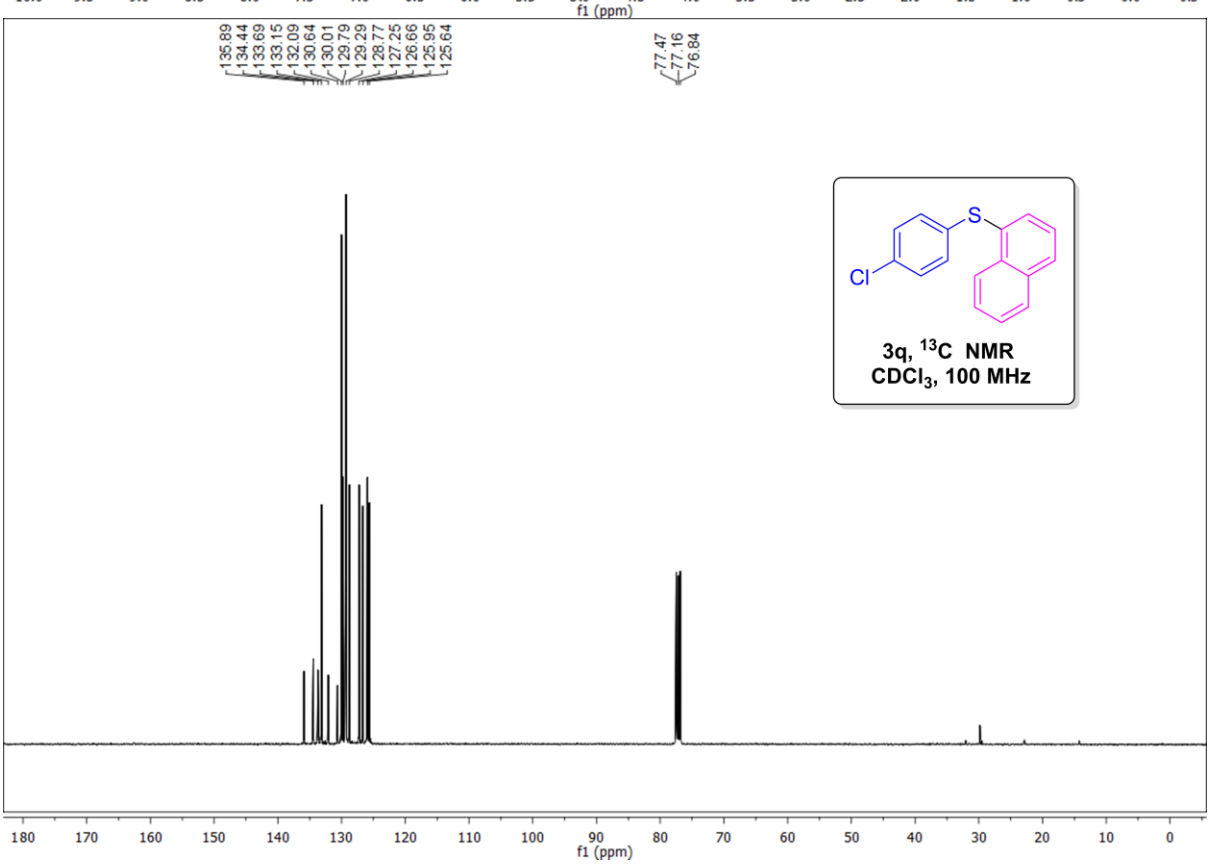

7.33
7.32
7.31
7.30
7.28
7.27
7.26
S
Cl
Cl
3o, 1H NMR
CDCl3, 400 MHz
4.18
4.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

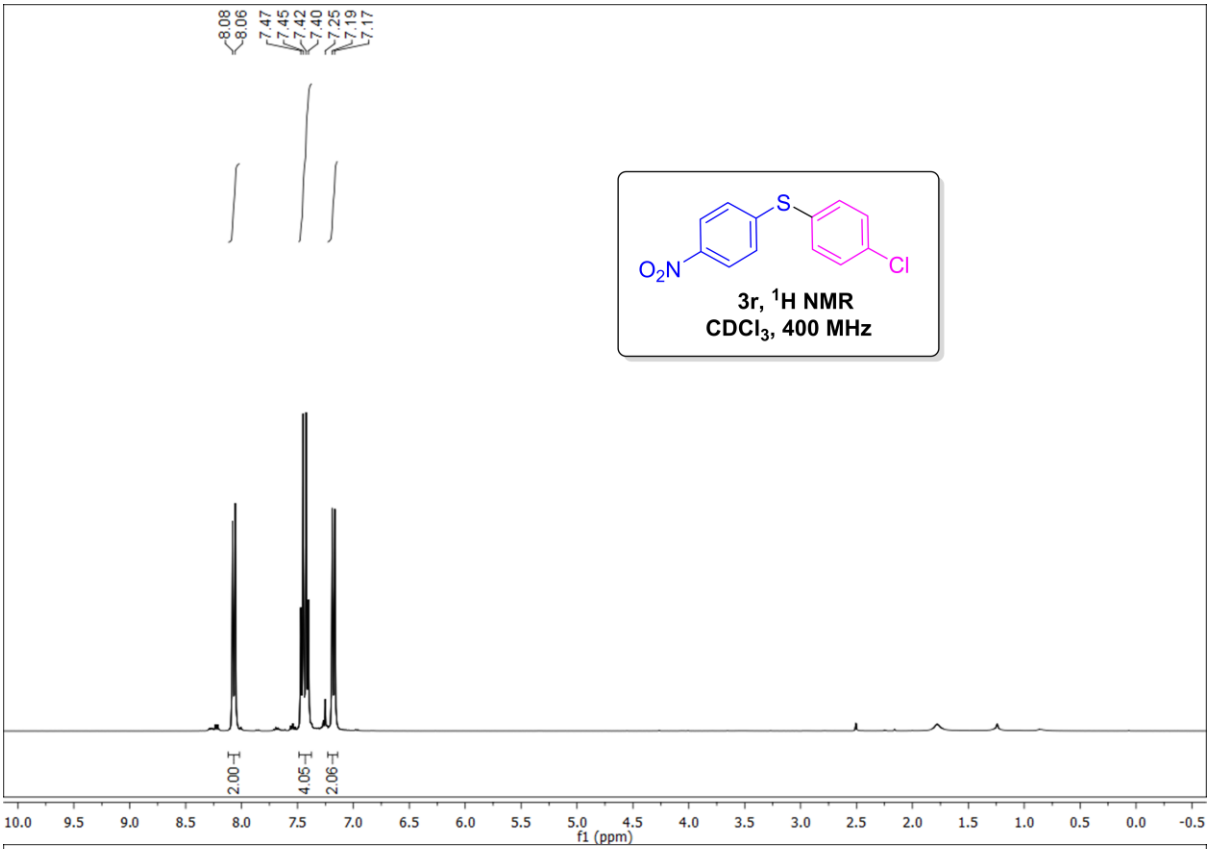

134.22
133.72
132.46
129.64
77.48
77.16
76.84
S
Cl
Cl
3o, 13C NMR
CDCl3, 100 MHz
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

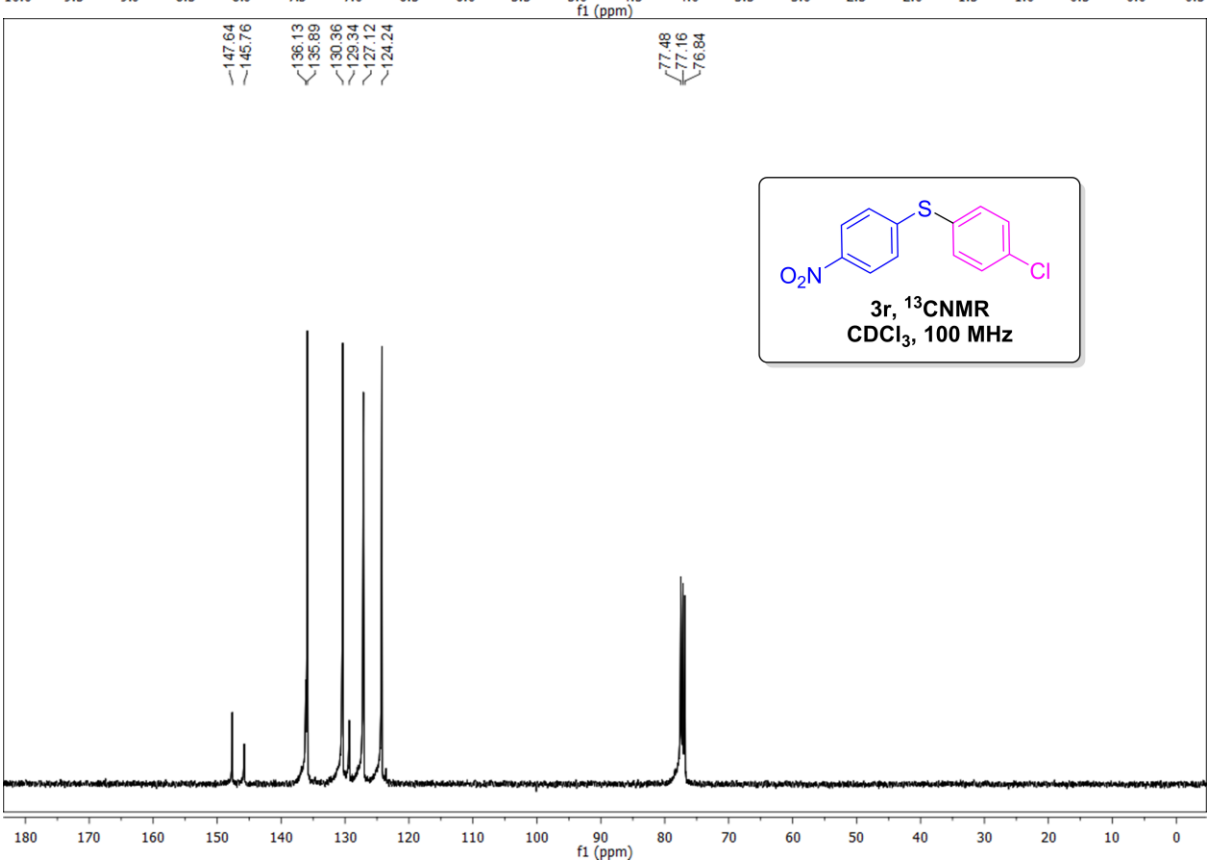

7.42
7.40
7.29
7.29
7.27
7.25
7.23
7.20
7.18
7.16
7.14
2.44
S
Cl
3p, 1H NMR
CDCl3, 400 MHz
0.95
2.15
2.17
2.17
6.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

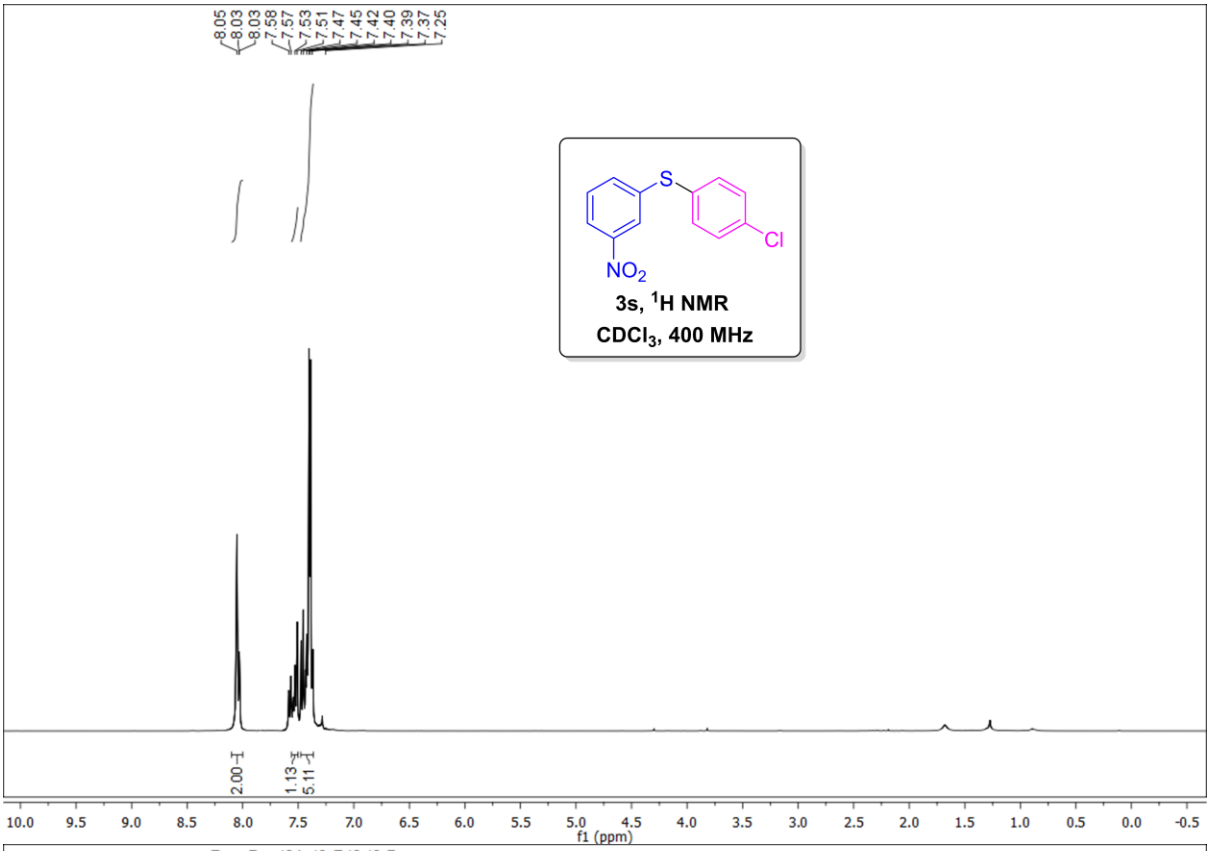

143.88
136.79
130.56
129.59
129.38
129.09
128.67
126.93
77.40
77.08
76.76
21.87
S
Cl
3p, 13C NMR
CDCl3, 100 MHz
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.38
8.37
8.36
7.91
7.89
7.73
7.72
7.56
7.55
7.54
7.49
7.48
7.47
7.45
7.45
7.41
7.26
7.20
7.18
7.12
7.10
1.00
2.13
1.03
2.18
1.13
2.00
2.01
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 -0.5
f1 (ppm)
Cl
S
3q, 1H NMR
CDCl3, 400 MHz

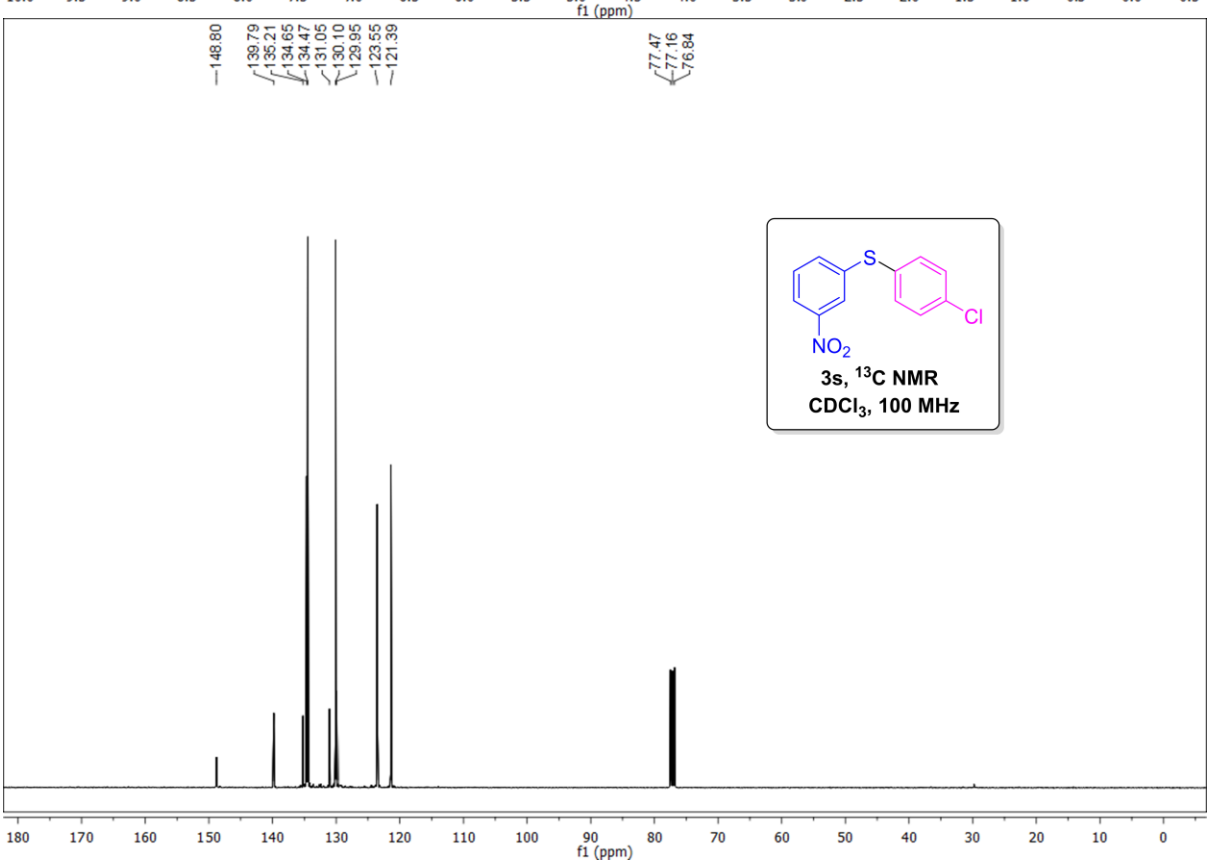

135.89
134.44
133.69
133.15
132.09
130.64
130.01
129.79
129.29
128.77
127.25
126.66
125.95
125.64
77.47
77.16
76.84
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Cl
S
3q, 13C NMR
CDCl3, 100 MHz


8.08
8.06
7.47
7.45
7.42
7.40
7.25
7.19
7.17
S
O2N
Cl
3r, 1H NMR
CDCl3, 400 MHz
2.00
4.05
2.06
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 -0.5
f1 (ppm)

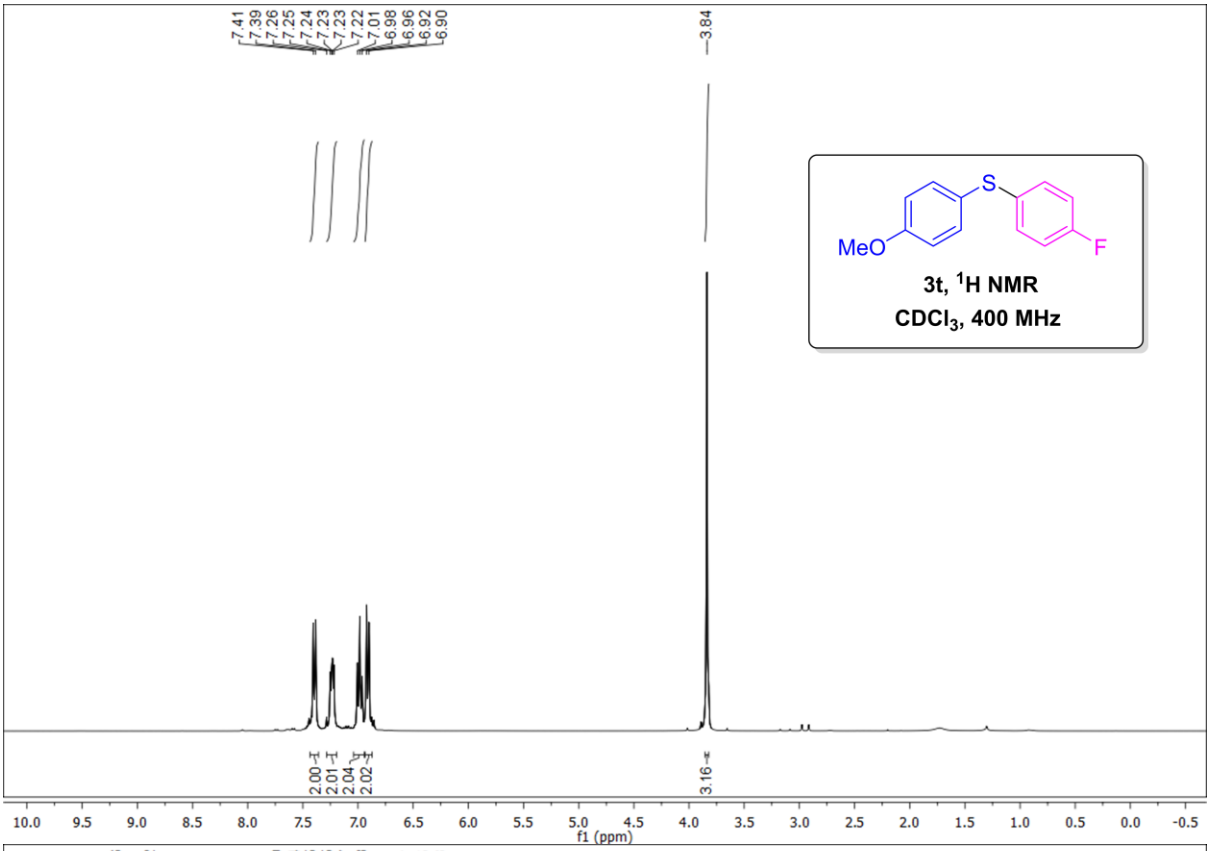

147.64
145.76
136.13
135.89
130.36
129.34
127.12
124.24
77.48
77.16
76.84
S
O2N
Cl
3r, 13CNMR
CDCl3, 100 MHz
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

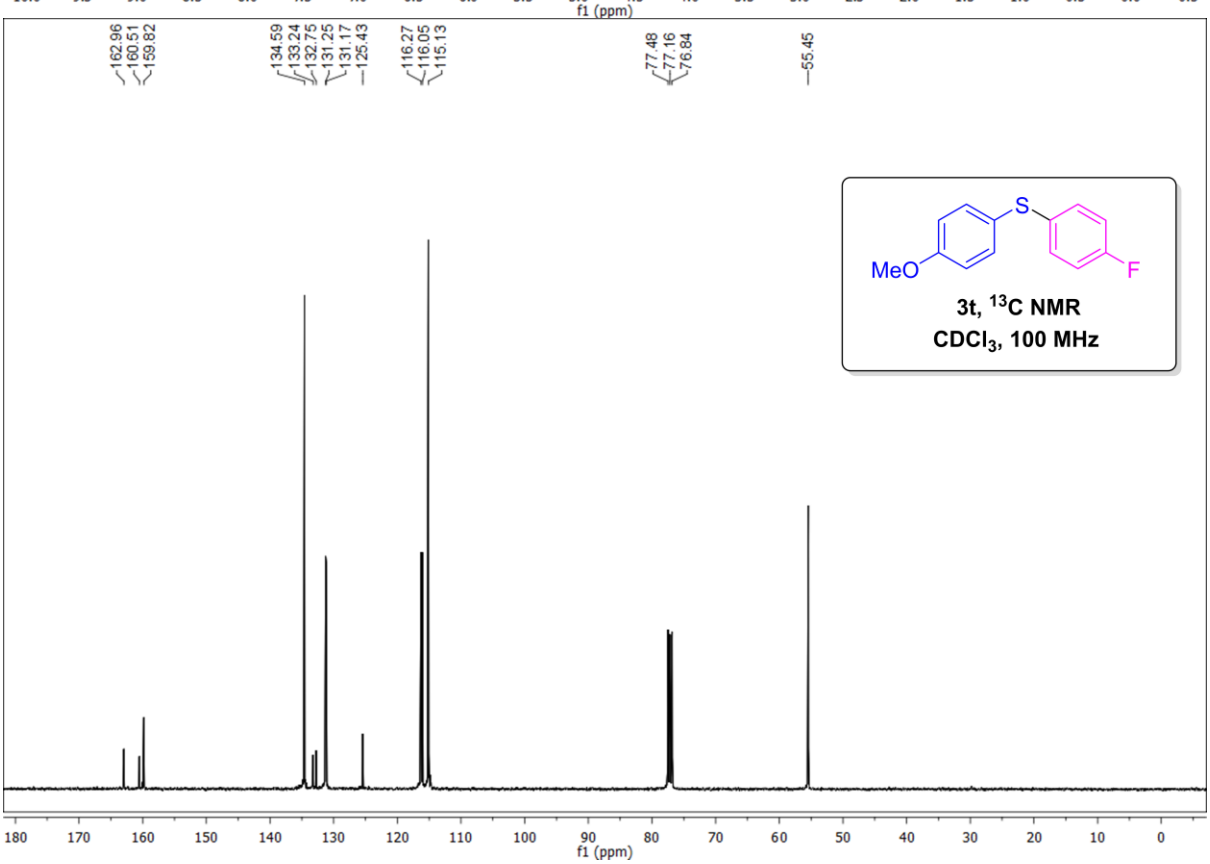


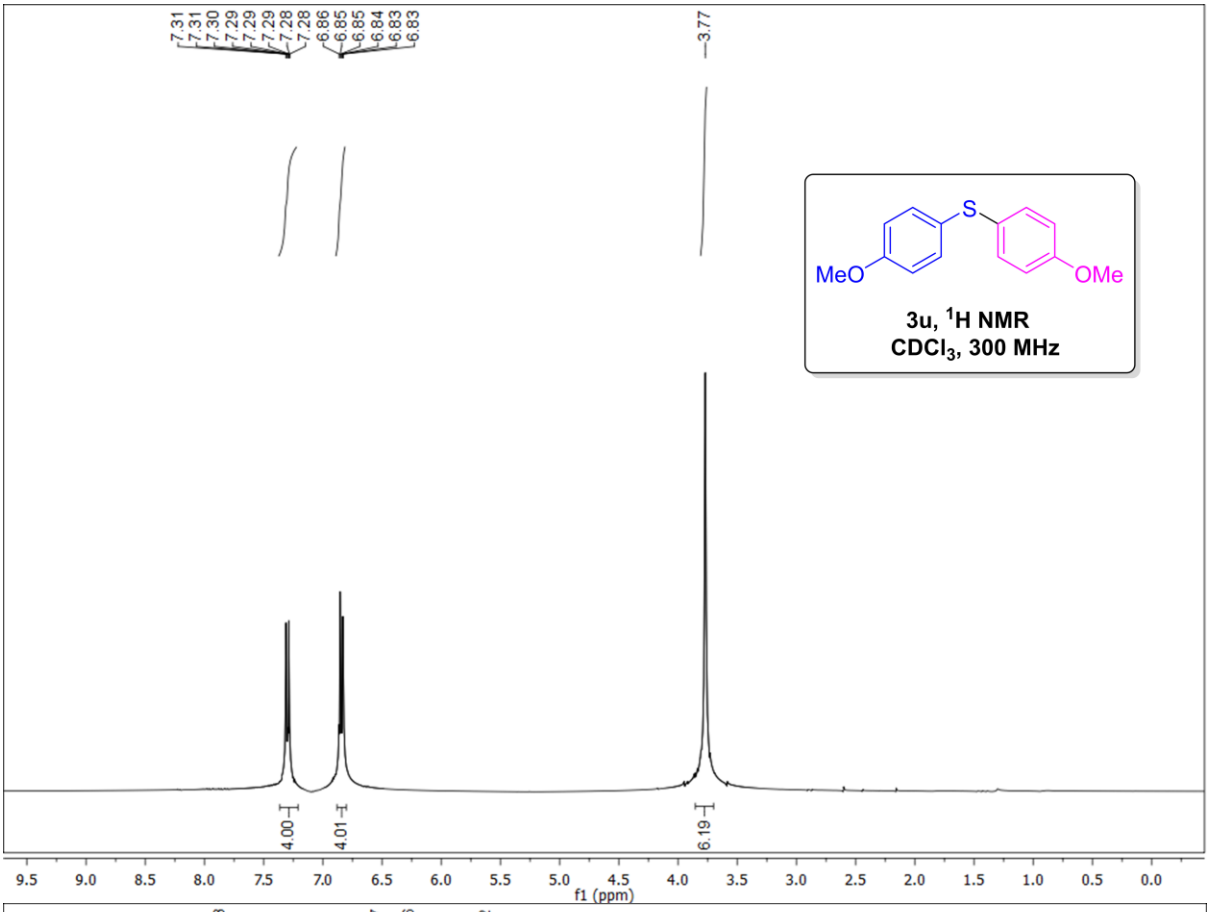
3s, ^{1}H NMR
$CDCl_3$, 400 MHz



3s, ^{13}C NMR
$CDCl_3$, 100 MHz


7.41
7.39
7.26
7.25
7.24
7.23
7.23
7.22
7.01
6.98
6.96
6.92
6.90
3.84
2.00
2.01
2.04
2.02
3.16
MeO
S
F
3t, 1H NMR
CDCl3, 400 MHz
f1 (ppm)


162.96
160.51
159.82
134.59
133.24
132.75
131.25
131.17
125.43
116.27
116.05
115.13
77.48
77.16
76.84
55.45
MeO
S
F
3t, 13C NMR
CDCl3, 100 MHz
f1 (ppm)


7.31
7.31
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7.29
7.29
7.28
7.28
6.86
6.85
6.85
6.84
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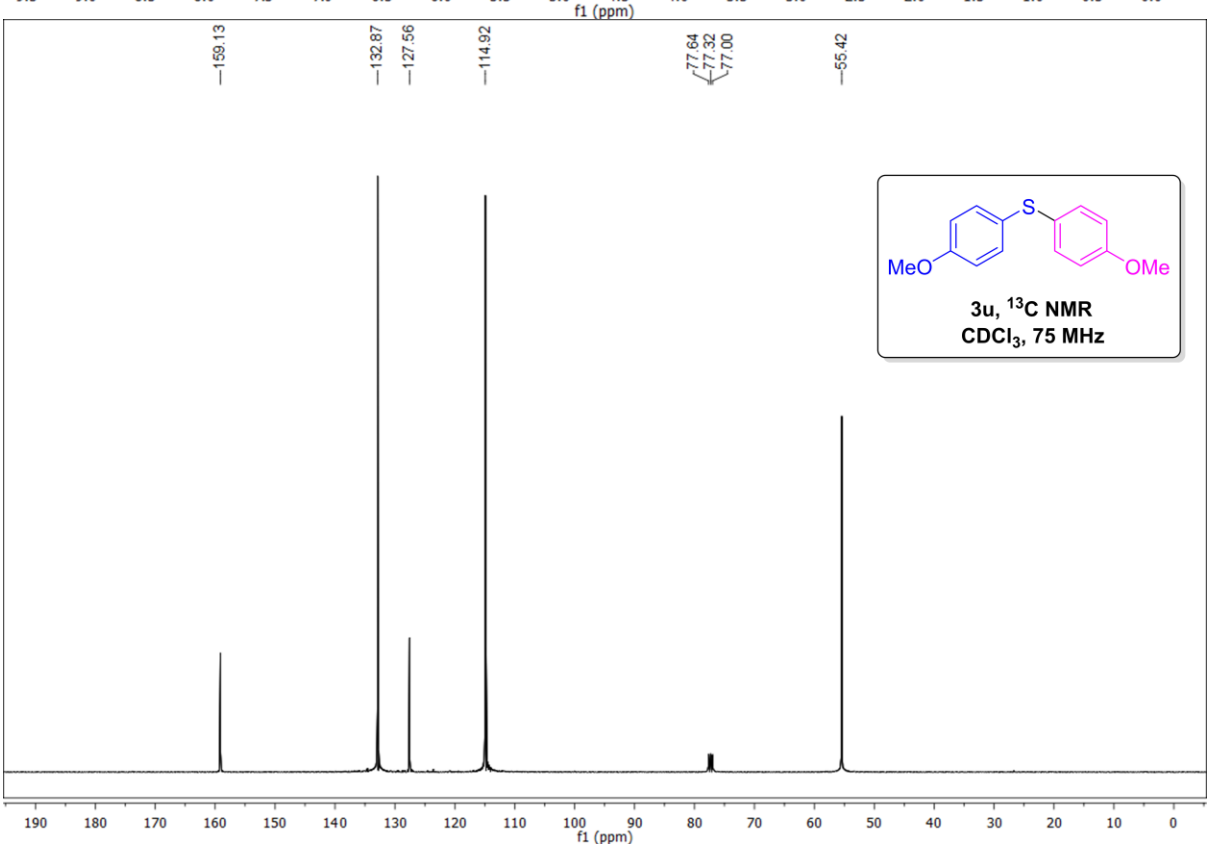
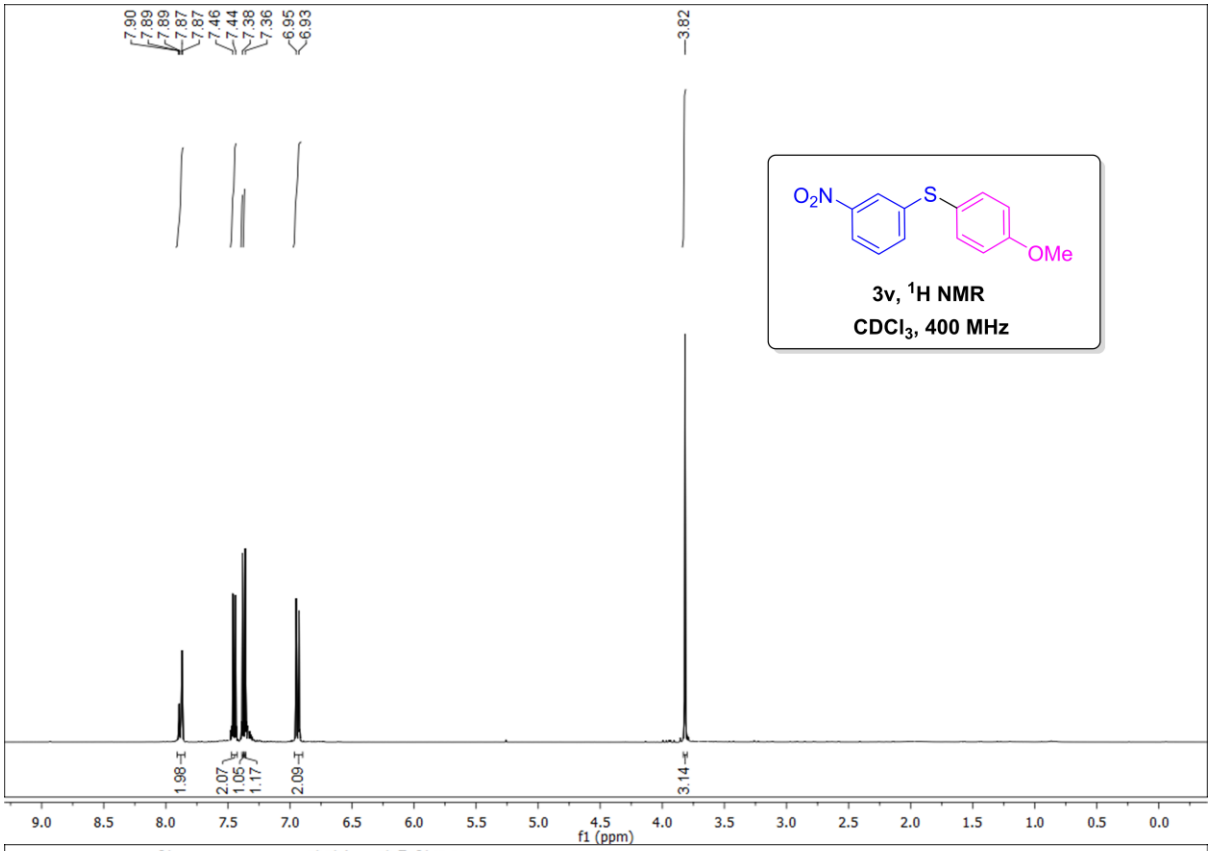
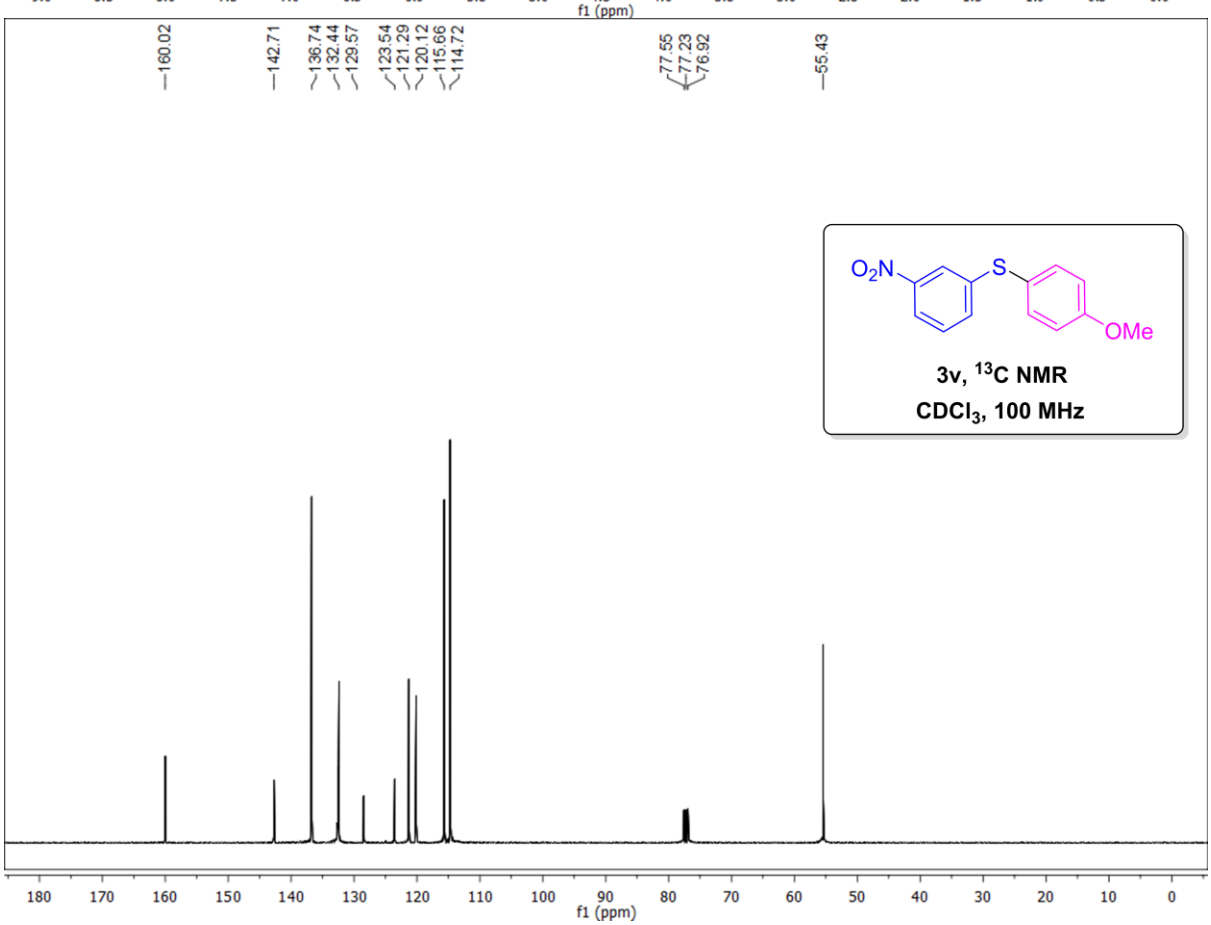
6.83
3.77
4.00
4.01
6.19
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
MeO
S
OMe
3u, 1H NMR
CDCl3, 300 MHz


159.13
132.87
127.56
114.92
77.64
77.32
77.00
55.42
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
MeO
S
OMe
3u, 13C NMR
CDCl3, 75 MHz


7.90
7.89
7.89
7.89
7.87
7.87
7.46
7.44
7.38
7.36
6.95
6.93
3.82
1.98
2.07
1.05
1.17
2.09
3.14
f1 (ppm)
O2N
S
OMe
3v, 1H NMR
CDCl3, 400 MHz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142.71
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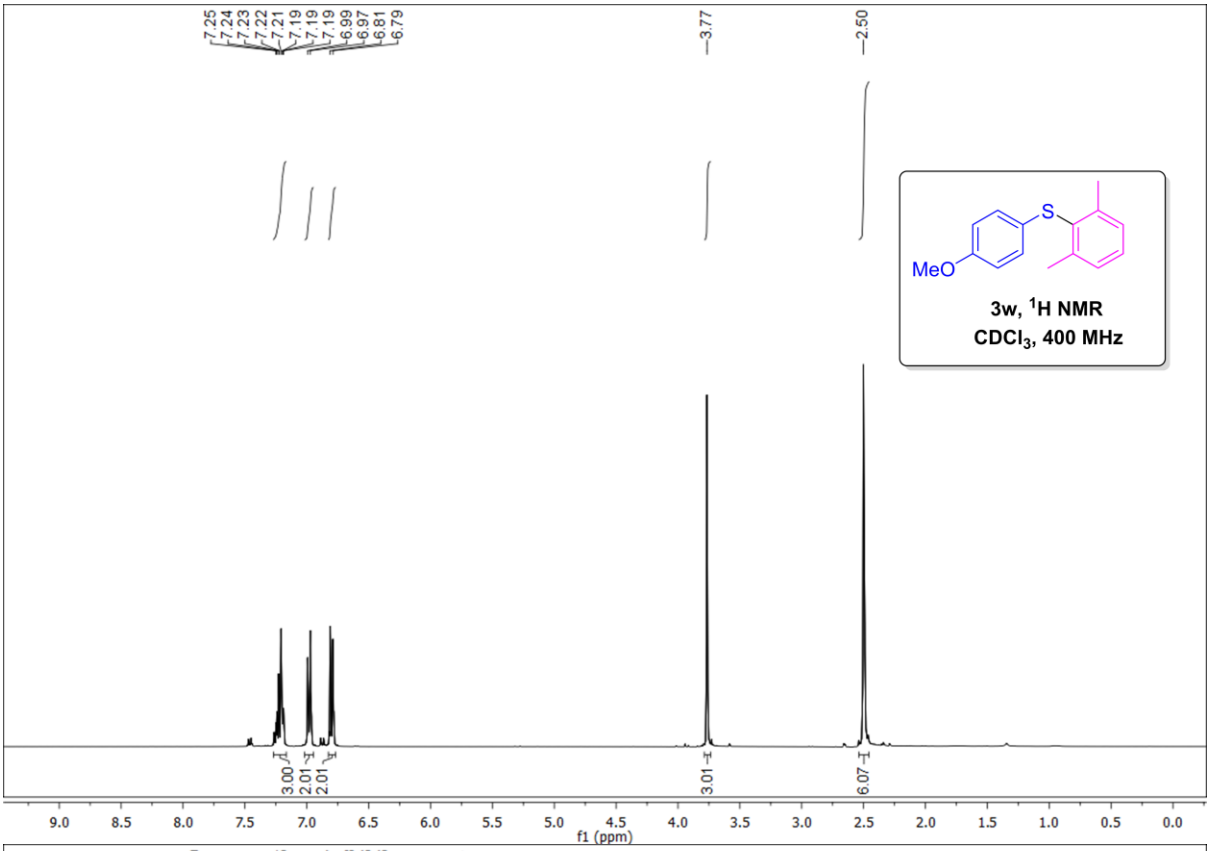
129.57
123.54
121.29
120.12
115.66
114.72
77.55
77.23
76.92
55.43
f1 (ppm)
O2N
S
OMe
3v, 13C NMR
CDCl3, 100 MHz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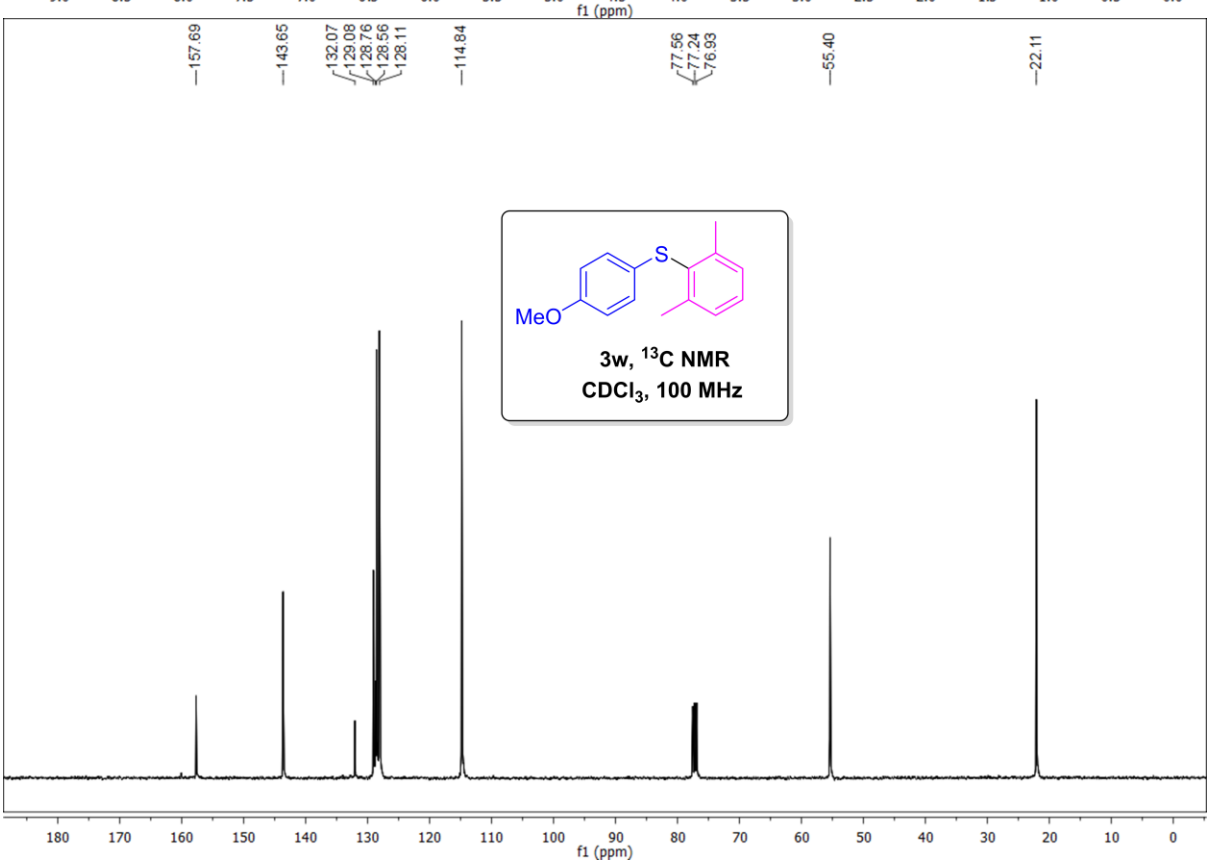
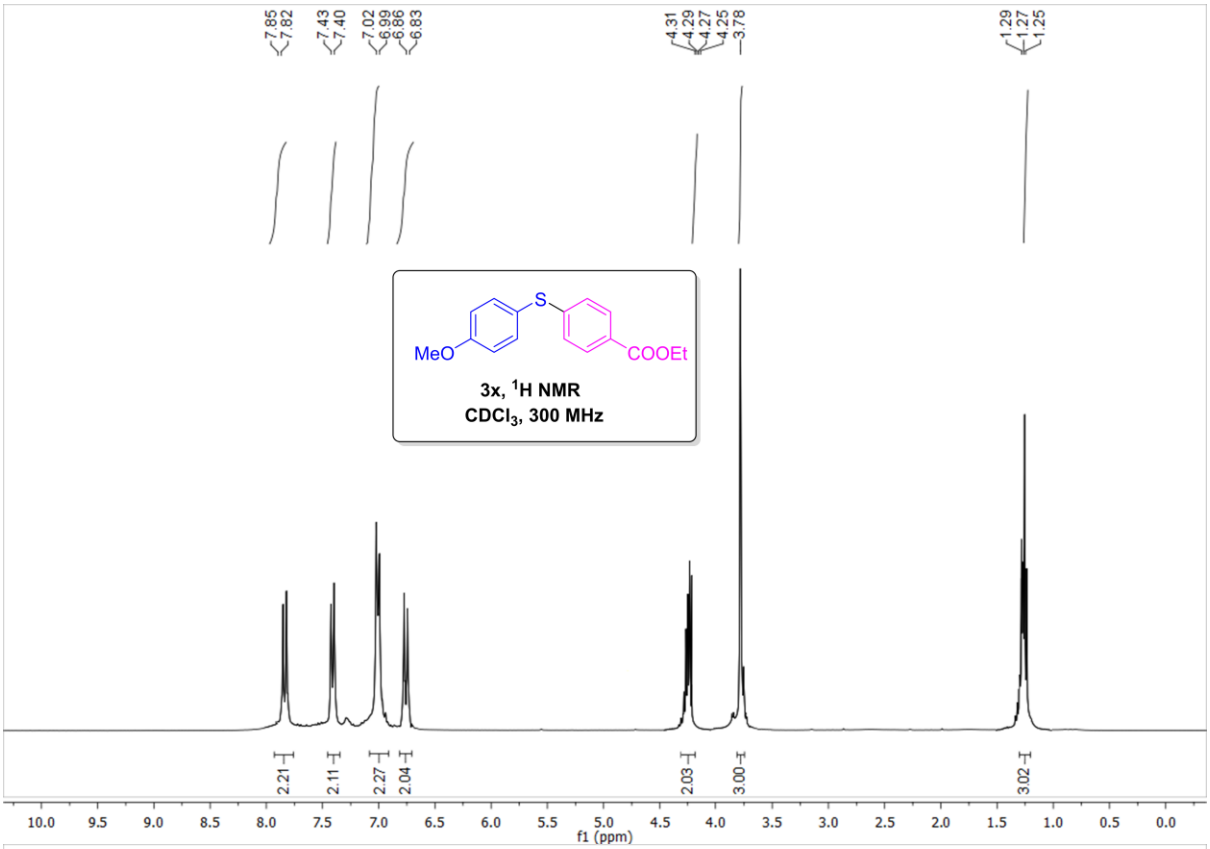
7.24
7.23
7.22
7.21
7.19
7.19
7.19
6.99
6.97
6.81
6.79
3.77
2.50
3.00
2.01
2.01
3.01
6.07
f1 (ppm)
MeO
S
3w, 1H NMR
CDCl3, 400 MHz


157.69
143.65
132.07
129.08
128.76
128.56
128.11
114.84
77.56
77.24
76.93
55.40
22.11
f1 (ppm)
MeO
S
3w, 13C NMR
CDCl3, 100 MHz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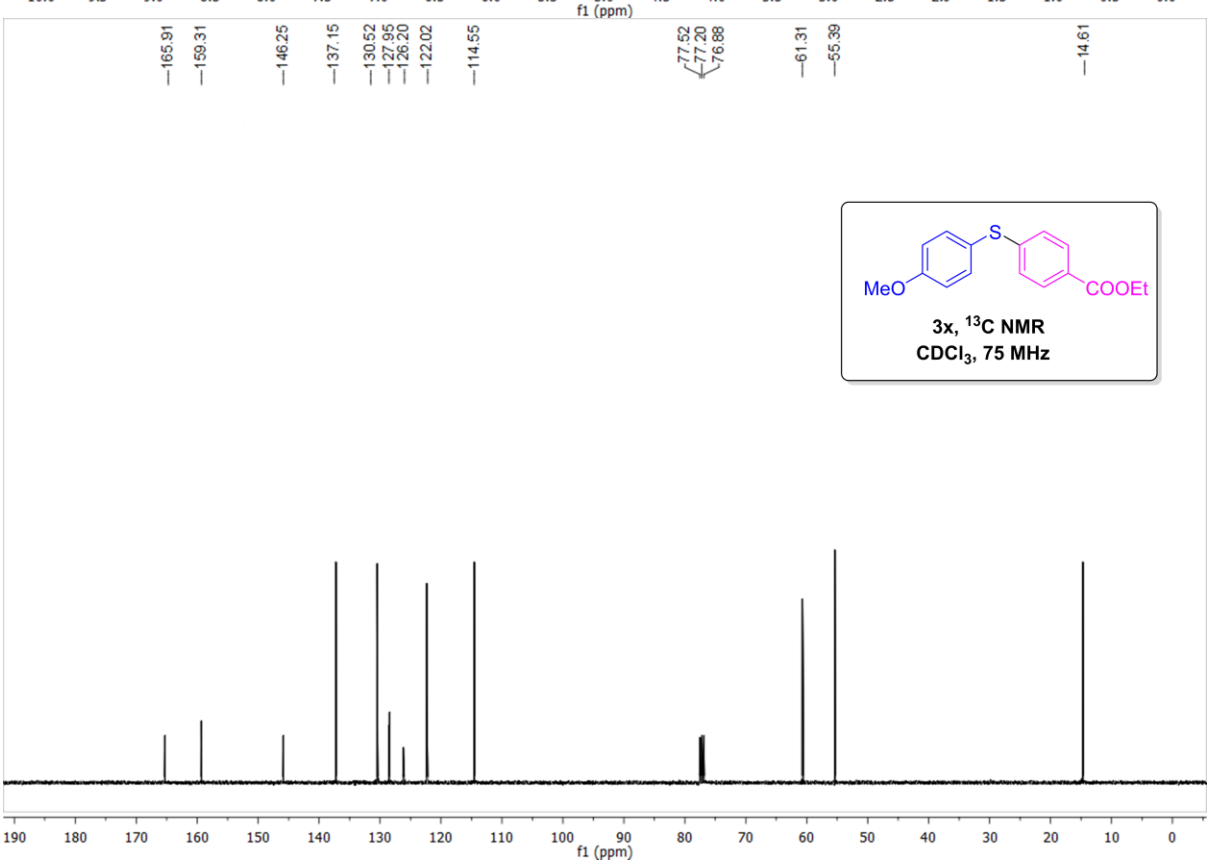
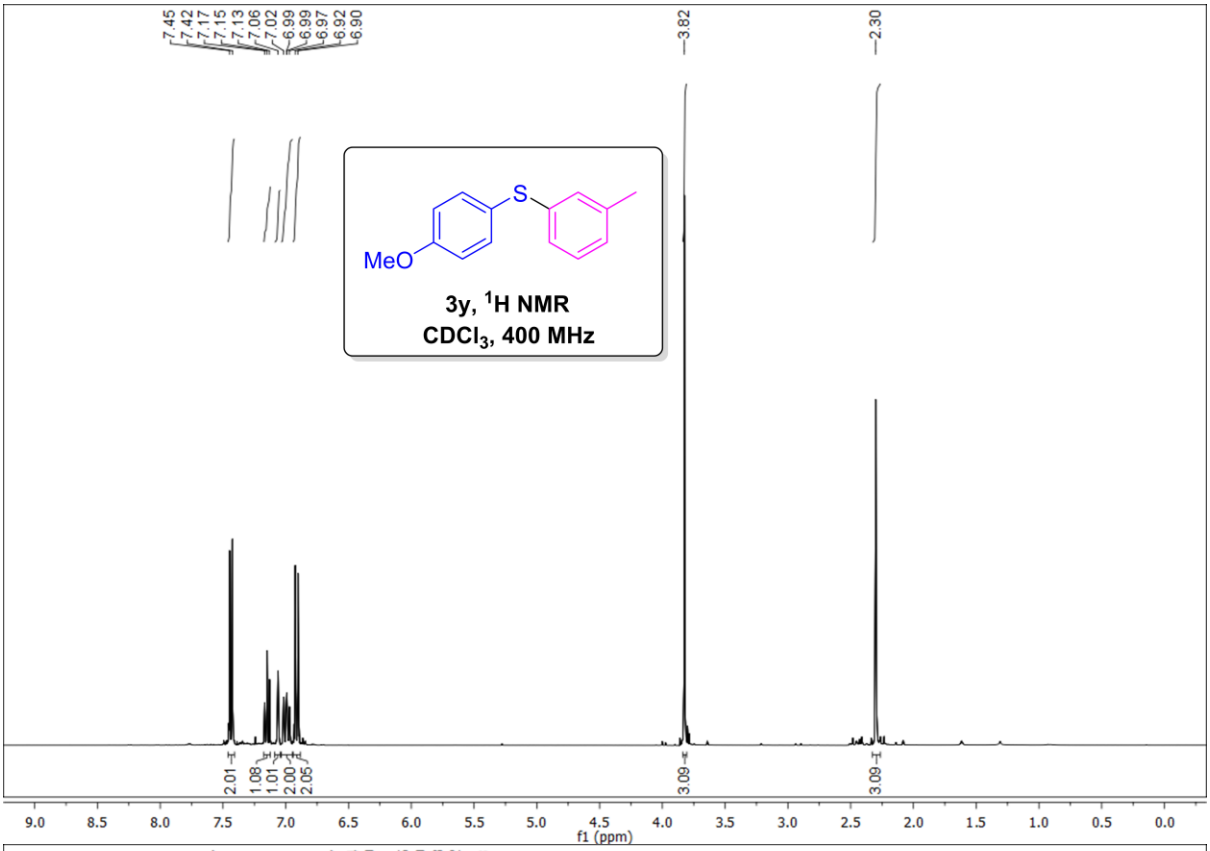
7.82
7.43
7.40
7.02
6.99
6.86
6.83
4.31
4.29
4.27
4.25
3.78
1.29
1.27
1.25
MeO
S
COOEt
3x, 1H NMR
CDCl3, 300 MHz
2.21
2.11
2.27
2.04
2.03
3.00
3.02
f1 (ppm)


165.91
159.31
146.25
137.15
130.52
127.95
126.20
122.02
114.55
77.52
77.20
76.88
61.31
55.39
14.61
MeO
S
COOEt
3x, 13C NMR
CDCl3, 75 MHz
f1 (ppm)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7.42
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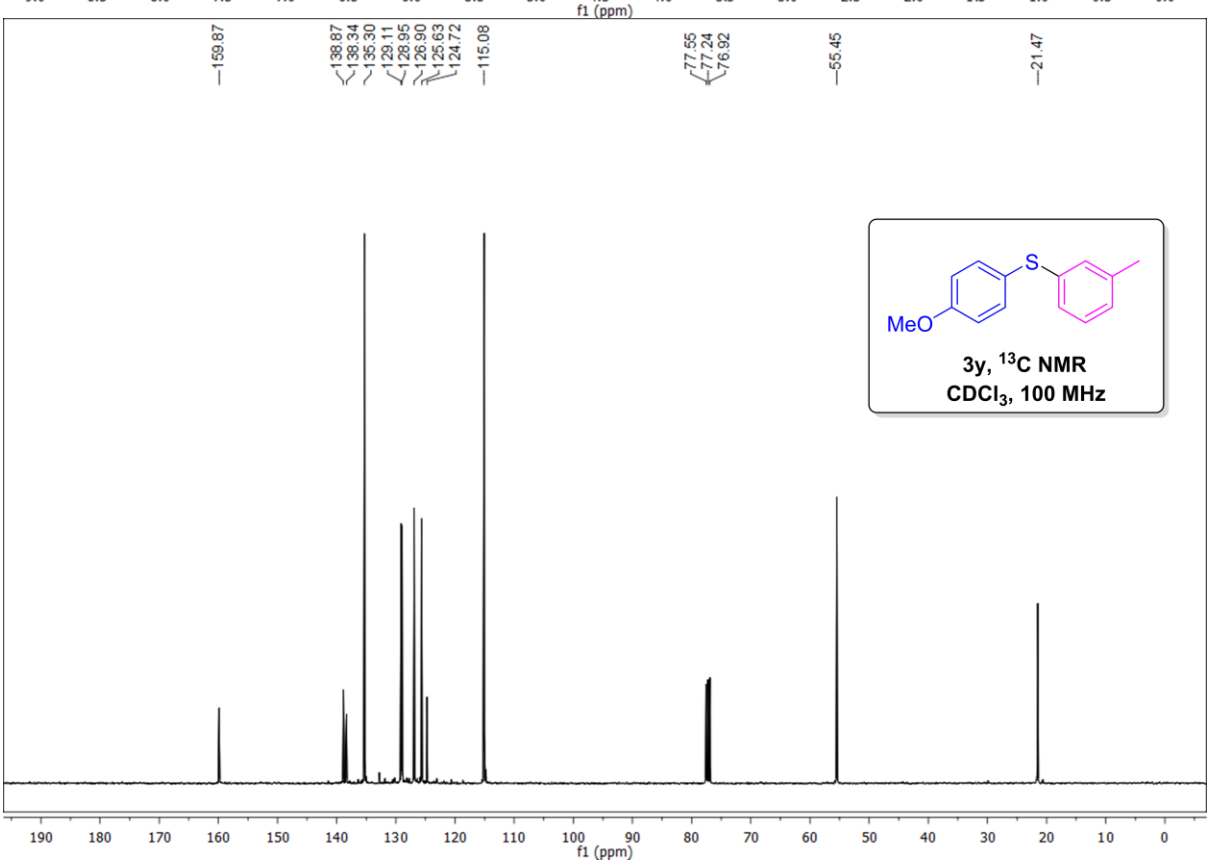
7.15
7.13
7.06
7.02
6.99
6.99
6.97
6.92
6.90
3.82
2.30
S
MeO
3y, 1H NMR
CDCl3, 400 MHz
2.01
1.08
1.01
2.00
2.05
3.09
3.09
f1 (ppm)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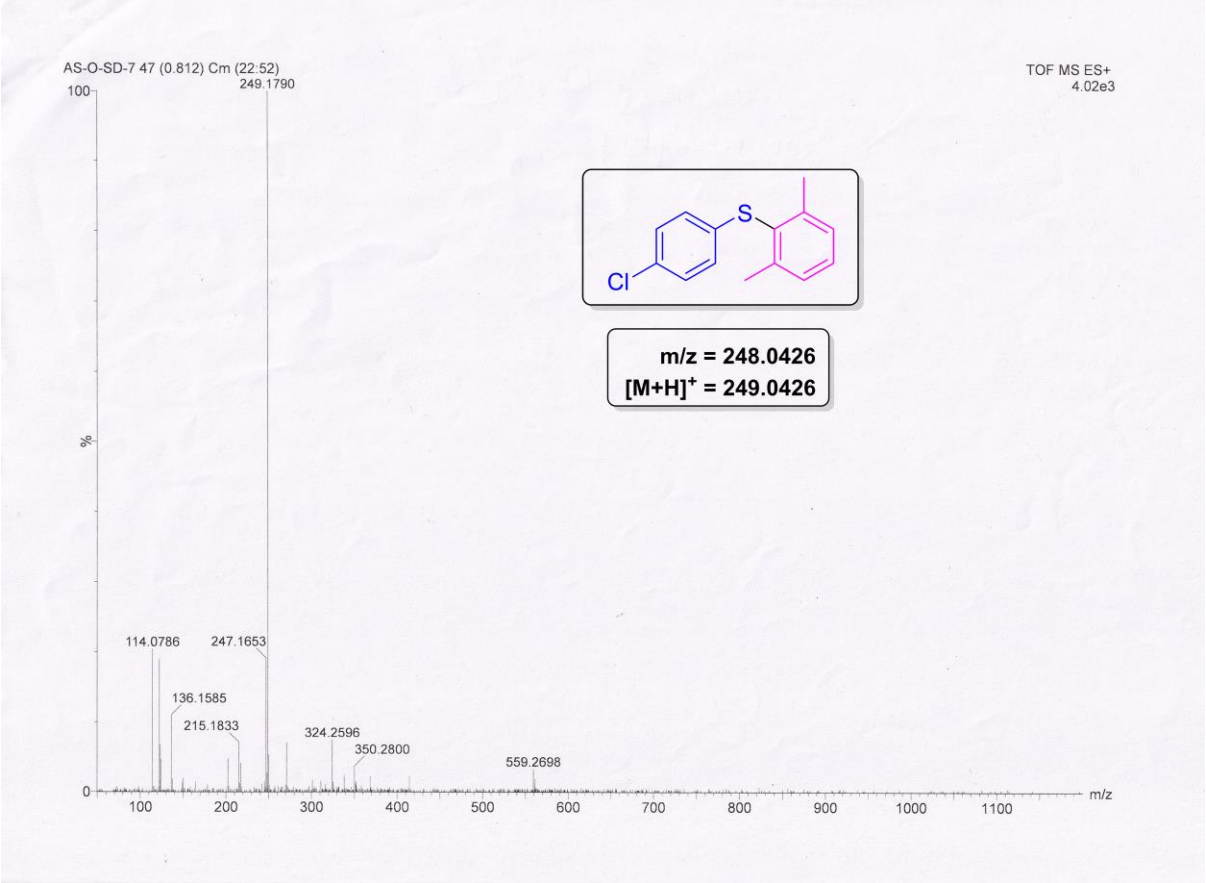
138.87
138.34
135.30
129.11
128.95
126.90
125.63
124.72
115.08
77.55
77.24
76.92
55.45
21.47
S
MeO
3y, 13C NMR
CDCl3, 100 MHz
f1 (ppm)


AS-O-SD-7 47 (0.812) Cm (22:52)
TOF MS ES+
4.02e3
249.1790
100
%
0
114.0786
247.1653
136.1585
215.1833
324.2596
350.2800
559.2698
100
200
300
400
500
600
700
800
900
1000
1100
m/z
S
Cl
m/z = 248.0426
[M+H]+ = 249.0426