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Supporting Information

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An Efficient CuO Nanoparticle Catalyzed *C-S* Cross Coupling of Thiols with Iodobenzene

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Materials and Methods

Thiols, aryl halides and CuO nanoparticle (particle size 33 nm, surface area 29 m^2/g and purity 99.99%) were purchased from Aldrich. NMR spectra (400 MHz for ^1H and 100 MHz for ^{13}C) were recorded using DRX-400 Varian spectrometer using $CDCl_3$ as solvent and Me_4Si as internal standard. Flash column chromatography was performed on silica gel (230-400 mesh) using ethyl acetate and hexane as eluent. Melting points were determined on Buchi B-540 and uncorrected. Centrifugation was carried out using SIGMA 3K30 Sartorius for 1 h with 10000 rpm.

General Procedure for *C-S* Coupling Reaction

Thiol (1 mmol), aryl halide (1.1 mmol), CuO nanoparticle (1.26 mol%) and KOH (1.5 mmol) were stirred in DMSO (1 mL) at 80 ^oC under N_2 atmosphere for the appropriate time. The progress of the reaction was monitored by TLC using ethyl acetate and hexane as eluent. After completion, the reaction mixture was treated with ethyl acetate (10 mL) and water (3 mL). The organic layer was separated and the aqeous layer was extracted with ethyl acetate (3 x 5 mL). The combined organic solution was washed with brine (3 x 5 mL) and water (1 x 5 mL). Drying (Na_2SO_4) and evaporation of the solvent provided a residue which was purified on short pad of silica gel using ethyl acetate and hexane.

4-Tolylphenyl sulfide (Table 4, entry 2). [1]

Colorless oil; H NMR ($CDCl_3$, 400 MHz) d 7.30-7.25 (m, 6H), 7.20-7.12 (m, 3H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$,100 MHz) d 137.80, 137.31, 132.48, 131.43, 130.26, 129.94, 129.24, 126.59, 21.34.

***p*-Anisyl phenyl sulfide (Table 4, entry 3).** [1]

Colorless oil; ^1H NMR ($CDCl_3$, 400 MHz) d 7.39-7.37 (dd, *J* = 8.8, 2.8 Hz, 2H), 7.2 3-7.12 (m, 5H), 6.88-6.85 (dd, *J* = 8.8, 2.4 Hz, 2H), 3.78 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) d 159.99, 138.79, 135.56, 129.10, 128.32, 125.91, 124.41, 115.15, 55.52.

4-Nitrophenyl phenyl sulfide (Table 4, entry 4).[2]

Yellow solid; m.p. 54 °C; ^1H NMR ($CDCl_3$, 400 MHz) d 8.00 (d, *J* = 8.8 Hz, 2H), 7.31-7.23 (m, 3H), 7.06 (d, *J* = 8.8 Hz, 2H), 6.72 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) d 158.94, 142.89, 136.24, 131.33, 125.91, 124.84, 115.15.

4-Bromophenyl phenyl sulfide (Table 4, entry 5).[3]

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz) d 7.41 -7.39 (dd, *J* = 6.8, 4.8 Hz, 2H), 7.36 -7.25 (m, 5H). 7.18 -7.16 (dd, *J* = 6.8, 4.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) d 135.99, 132.74, 132.59, 132.06, 129.89, 128.08.

2-Bromophenyl phenyl sulfide (Table 4, entry 6).[4]

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz) 7.57 -7.55 (d, *J* = 8 Hz, 1H), 7.49 -7.44 (m, 2H), 7.41-7.36 (m, 3H), 7.24 -7.23 (m, 1H), 7.16-7.12 (m, 1H), 7.05-7.01 (m, 1H), 6.92-6.90 (d, *J* = 8 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz) 133.74, 133.23, 129.91, 129.86, 128.95, 128.70, 128.02, 127.89, 127.44.

2-Naphthylphenyl sulfide (Table 4, entry 7).[3]

Colorless solid, m.p. 49 ^{o}C; ^{1}H NMR ($CDCl_3$, 400 MHz) d 7.83-7.76 (m, 2H), 7.74-7.70 (m, 2H), 7.48 -7.44 (m, 2H), 7.41-7.36 (m, 2H), 7.32 -7.23 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) d 131.14, 130.08, 129.44, 129.07, 128.95, 127.94, 127.62, 127.27, 126.80, 126.42.

Benzylphenyl sulfide (Table 4, entry 8).[5]

White solid, m.p. 40°C; ^{1}H NMR ($CDCl_3$, 400 MHz) d 7.31 -7.23 (m, 10H), 4.12 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) d 130.08, 129.05, 128.70, 127.38, 126.56, 39.28.

(*n*-Ethylthio)benzene (Table 5, entry 1).[6]

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33 -7.25 (m, 4H), 7.17-7.15 (m, 1H), 2.94 (m, 2H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) 136.79, 129.16, 129.0, 127.66, 127.32, 125.92, 27.78, 14.54.

(*n*-Butylthio)benzene (Table 5, entry 2).[7]

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.32 -7.24 (m, 4H), 7.16-7.14 (m, 1H), 2.88 (t, *J* = 7.6 Hz, 2H), 1.64-1.59 (m, 2H), 1.47-1.41 (m, 2H), 0.90 (t, *J* = 2.7 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) 137.55, 137.18, 130.32, 128.90, 127.53, 125.67, 33.28, 31.31, 22.08, 13.78.

(*n*-Hexylthio)benzene (Table 5, entry 3).[8]

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.31 -7.24 (m, 4H), 7.14-7.13 (m, 1H), 2.89 (t, *J* = 7.6 Hz, 2H); 1.65-1.59 (m, 2H), 1.42-1.39 (m, 2H), 1.37-1.25 (m, 2H), 0.85 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) 137.24, 128.93, 125.72, 33.68, 31.53, 29.26, 28.69, 22.70, 14.19.

(*n*-Octylthio)benzene(Table 5, entry 4).[9]

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.32 -7.25 (m, 4H), 7.17-7.15 (m, 1H), 2.91 (t, *J* = 7.6 Hz, 2H), 1.66-1.56 (m, 2H), 1.43-1.26 (m, 10H), 0.87 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) 137.63, 137.24, 130.39, 128.96, 125.74, 33.69, 31.98, 29.35, 29.31, 29.03, 22.83, 14.29.

(*n*-Decylthio)benzene (Table 5, entry 5).[10]

Colorless oil, ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.32 -7.59 (m, 4H), 7.17-7.15 (m, 1H), 2.91 (t, *J* = 7.6 Hz, 2H), 1.66-1.60 (m, 4H), 1.42-1.37 (m, 12H), 0.88 (t, *J* = 6 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) 137.43, 129.01, 125.81, 33.76, 32.12, 29.84, 29.55, 29.37, 29.06, 22.90, 14.33.

(*n*-Dodecylthio)benzene (Table 5, entry 6).[11]

Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.33 -7.26 (m, 4H), 7.25-7.13 (m, 1H), 2.91(t, *J* = 7.6 Hz, 2H), 1.66-1.56 (m, 4H), 1.43-1.25 (m, 12H), 0.88-0.86 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ137.43, 129.01, 125.80, 33.76, 32.12, 29.83, 29.55, 29.45, 29.37, 29.05, 28.74, 26.62, 23.73, 22.90,14.32.

1,4-Diphenyl butanethiol (Scheme 2).[12]

Colorless solid, m.p. 84 °C; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 7.29 -7.23 (m, 8H), 7.16 -7.14 (m, 2H), 2.90-2.87 (m, 4H), 1.76-1.73 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) 137.63, 129.44, 129.10, 33.47, 28.32.

References

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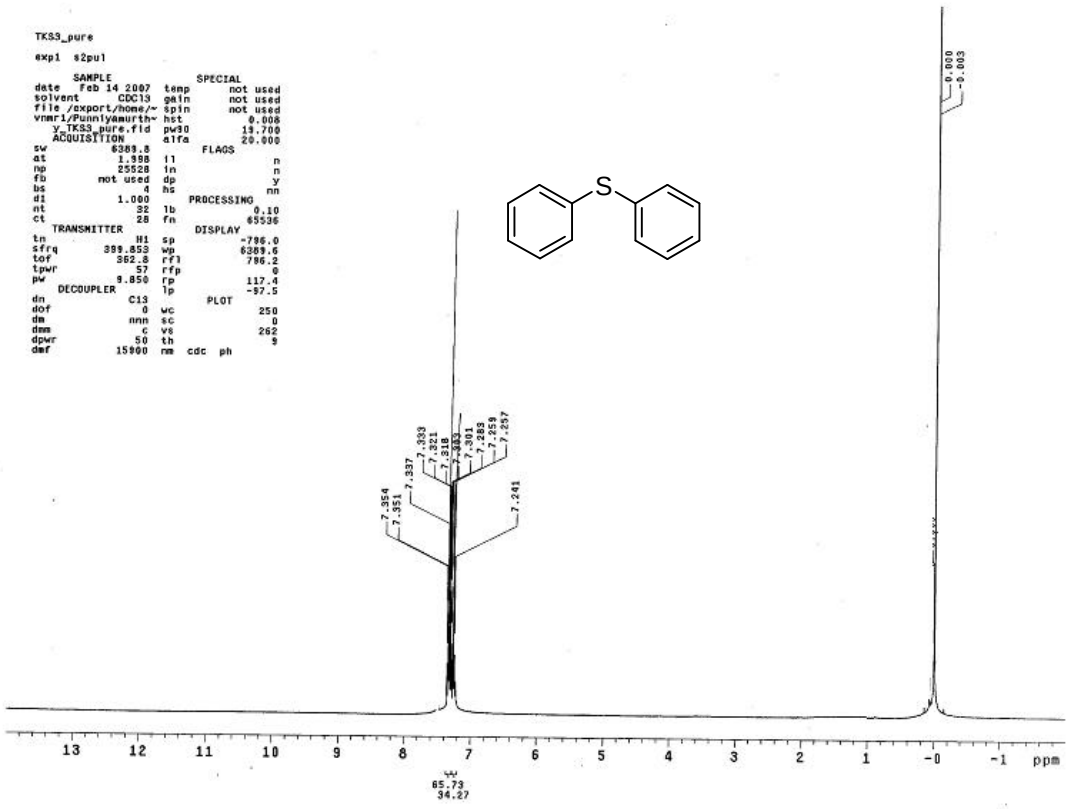
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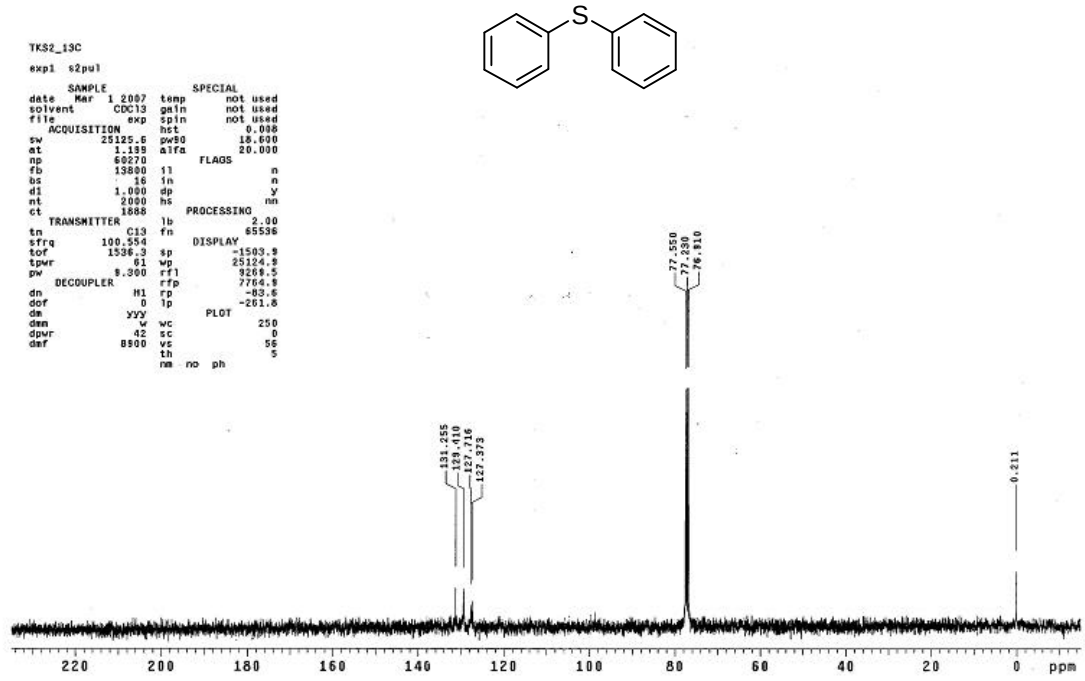
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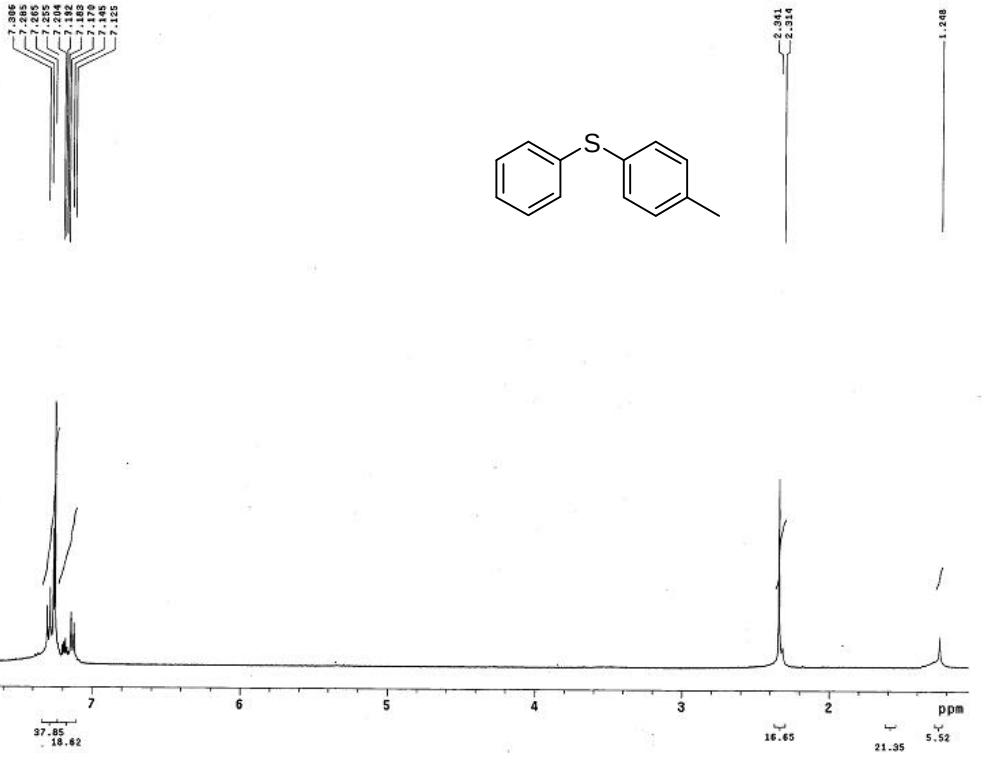
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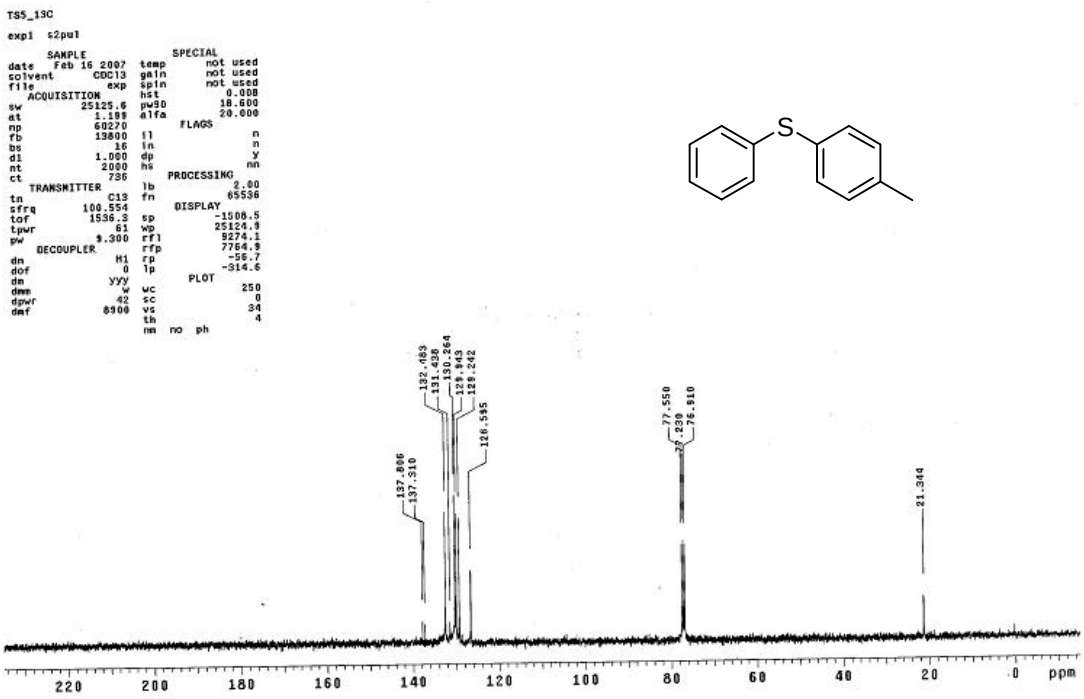
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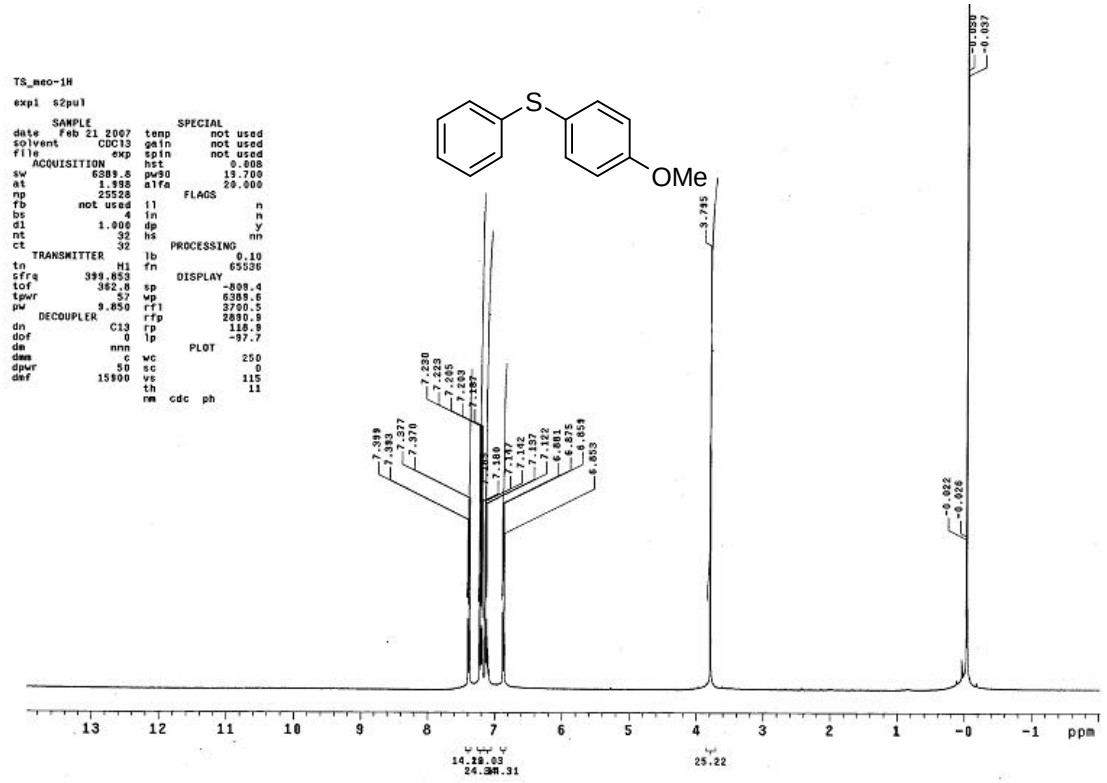
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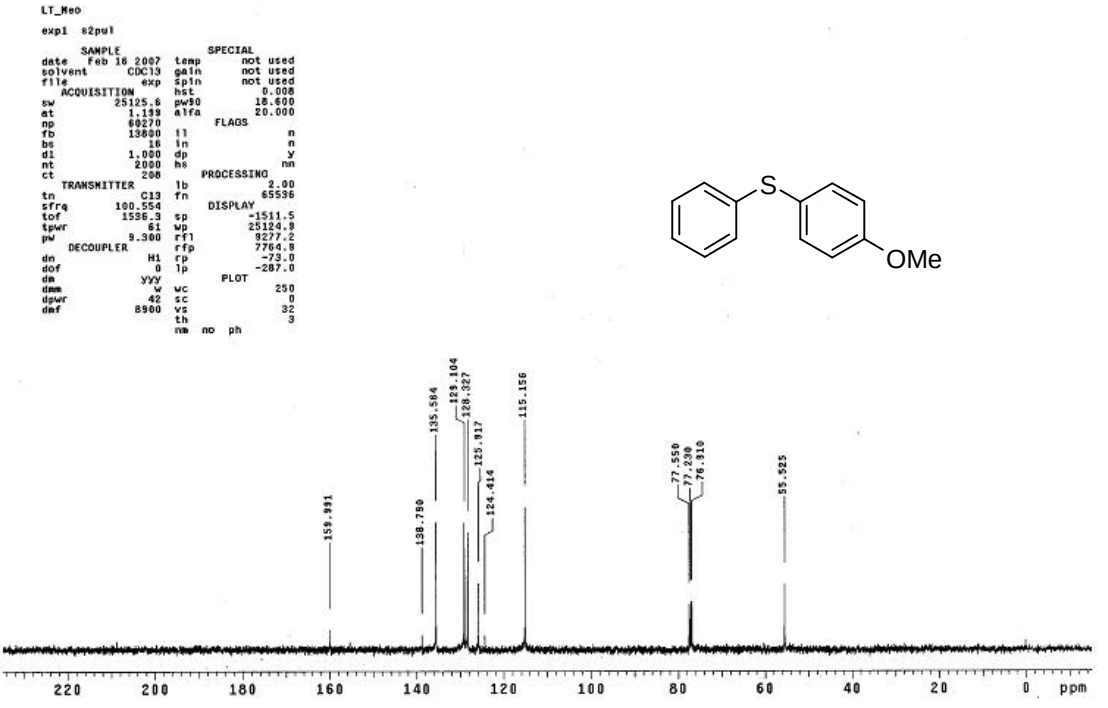
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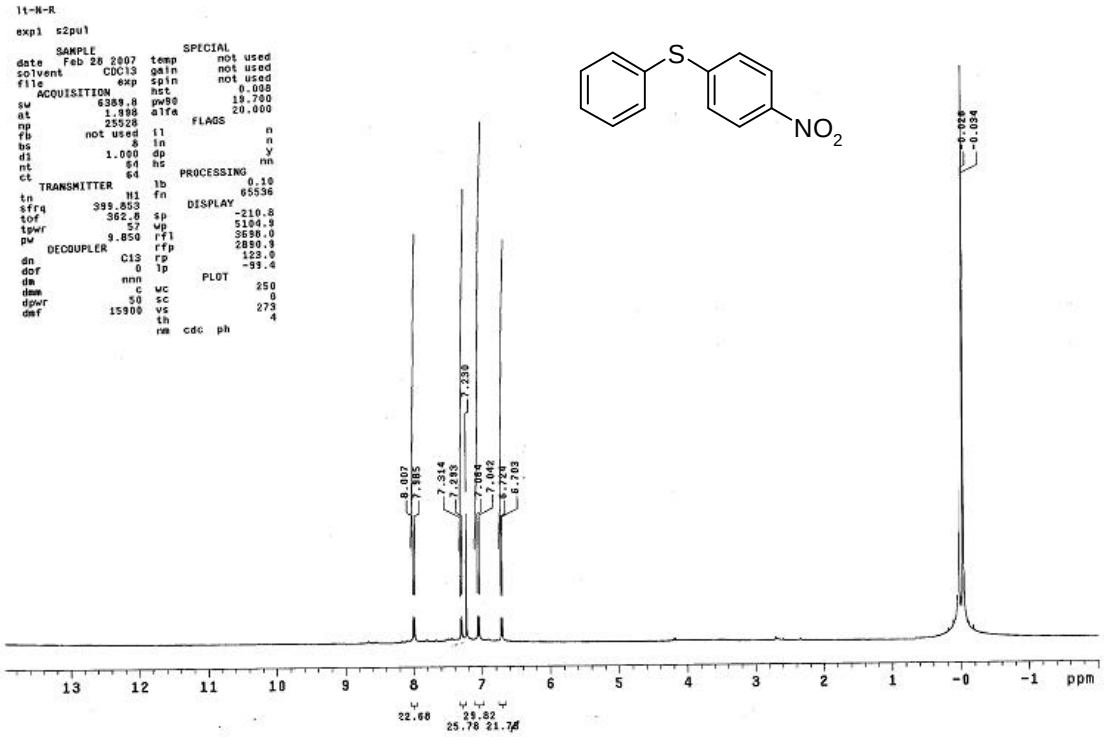
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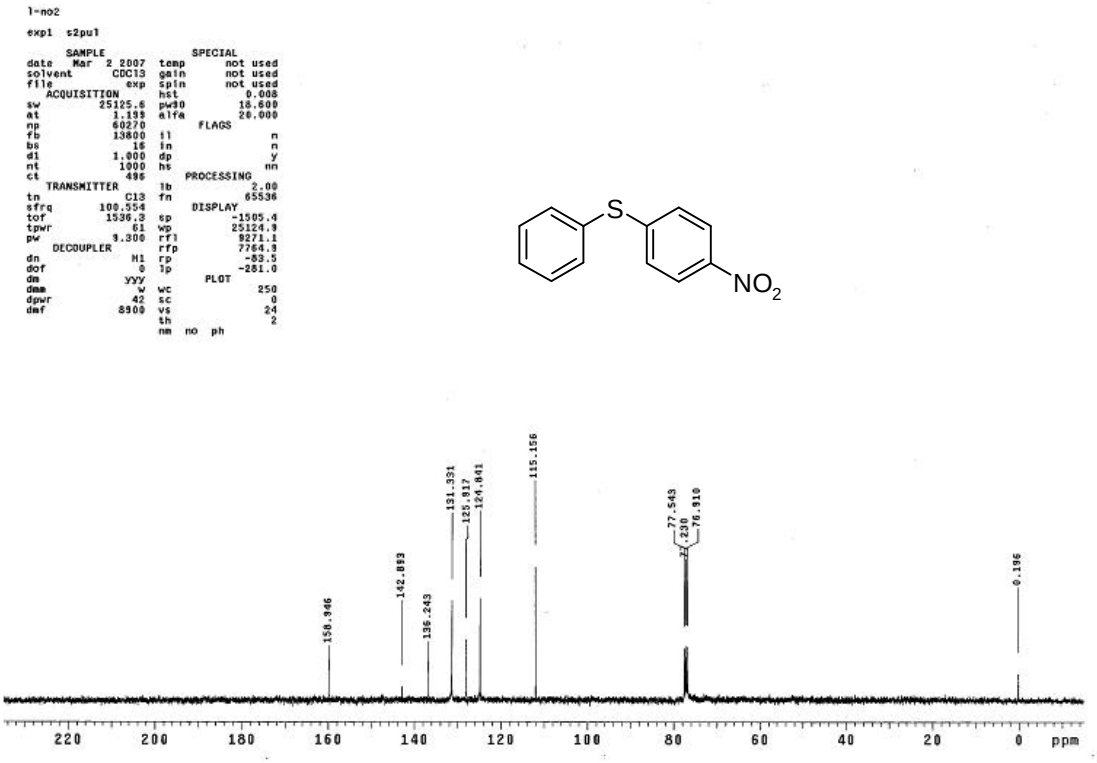
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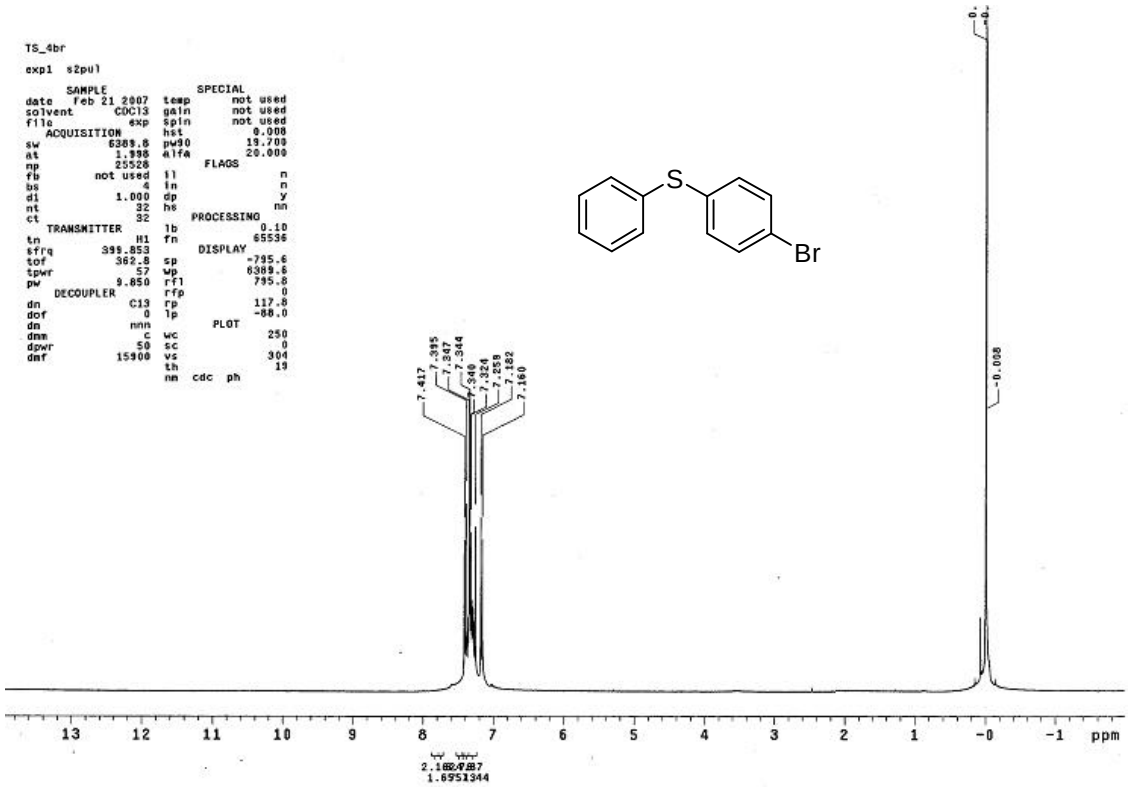
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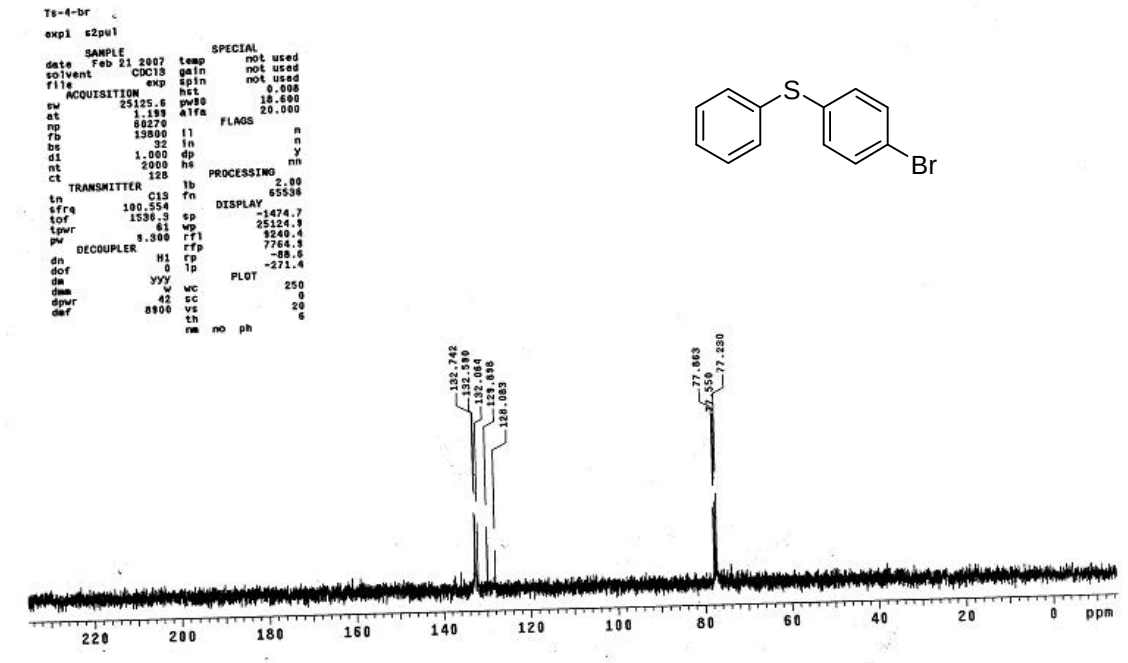
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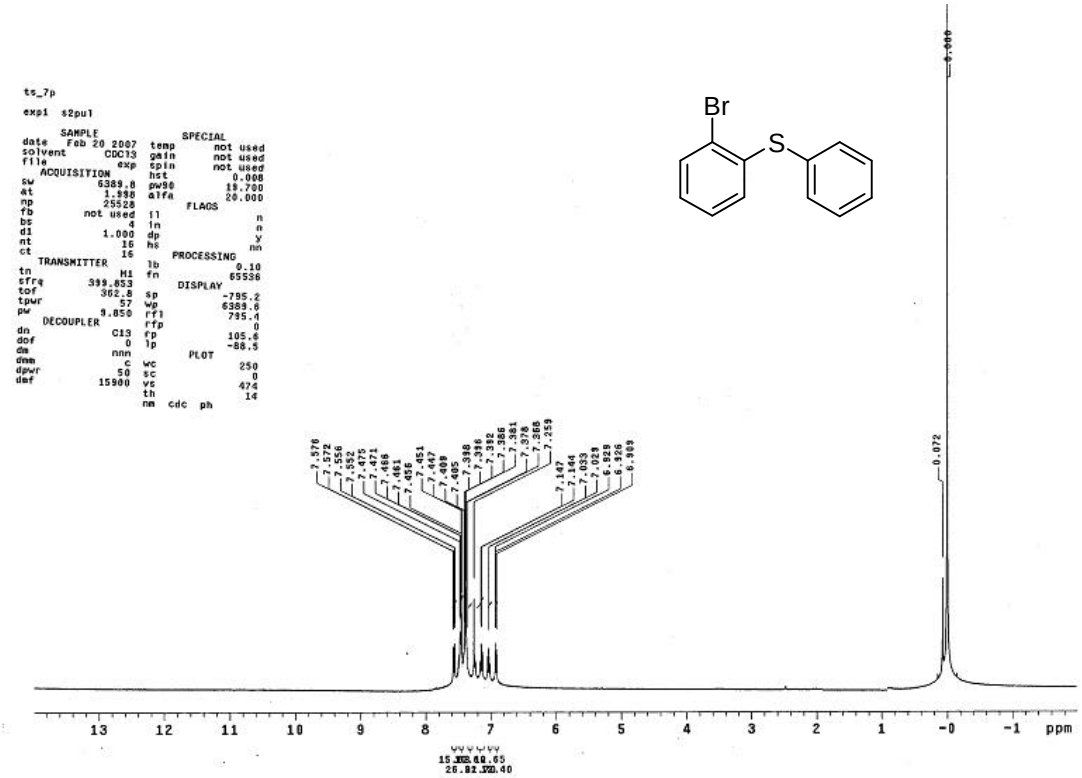
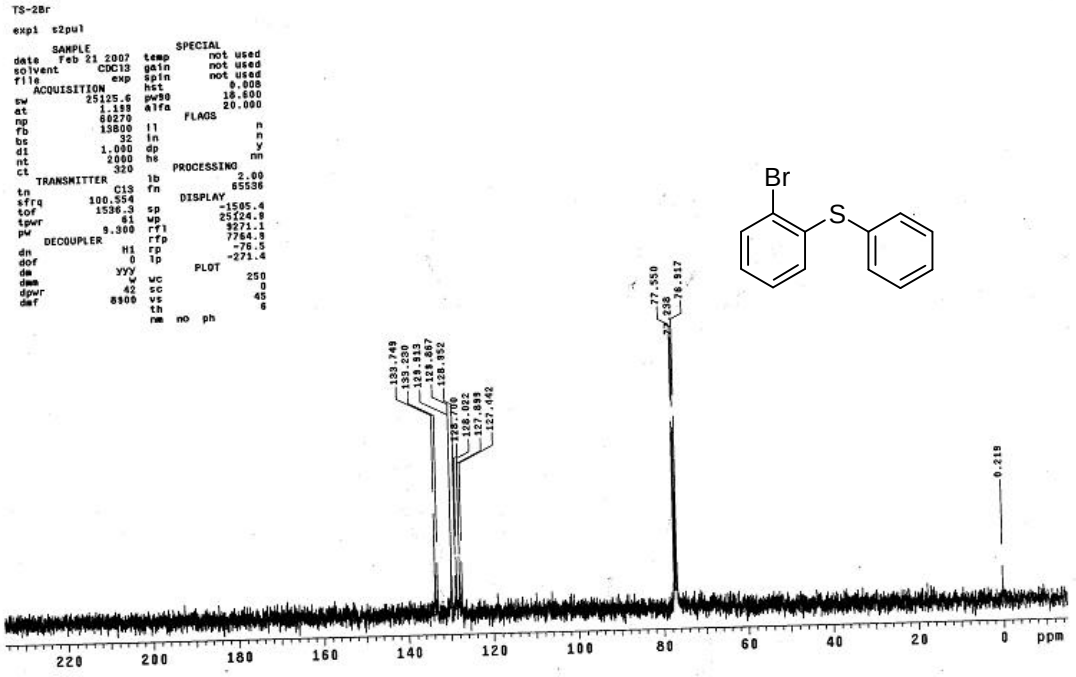
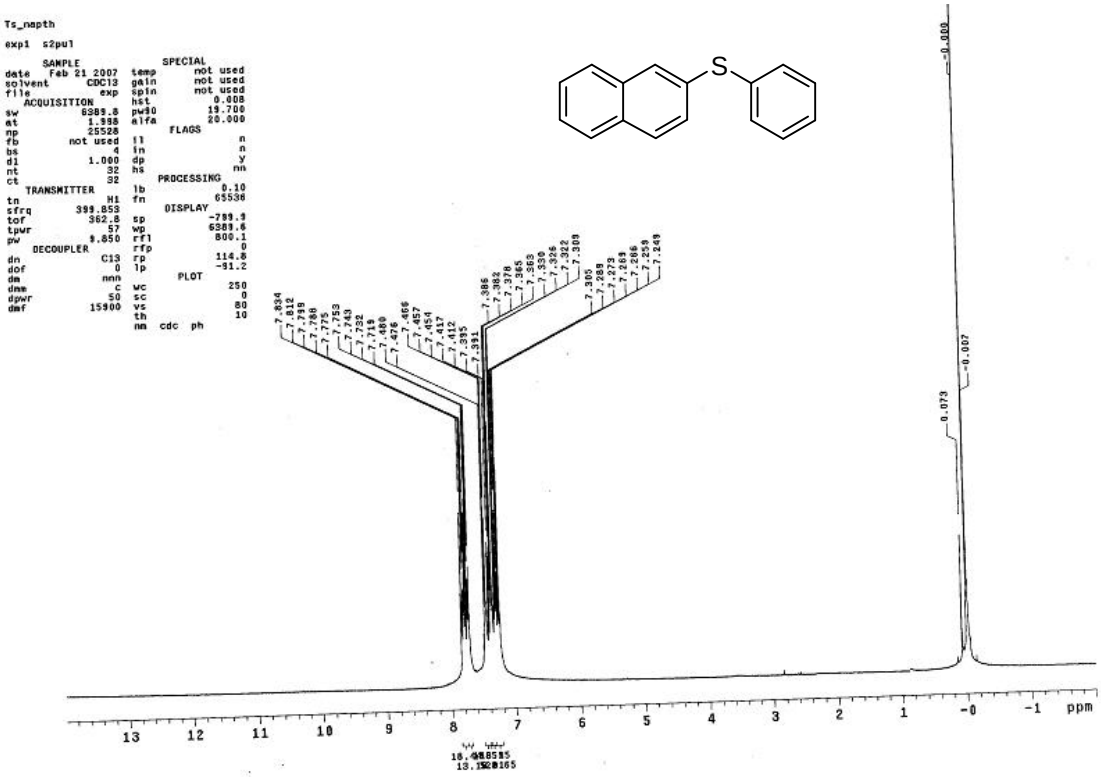
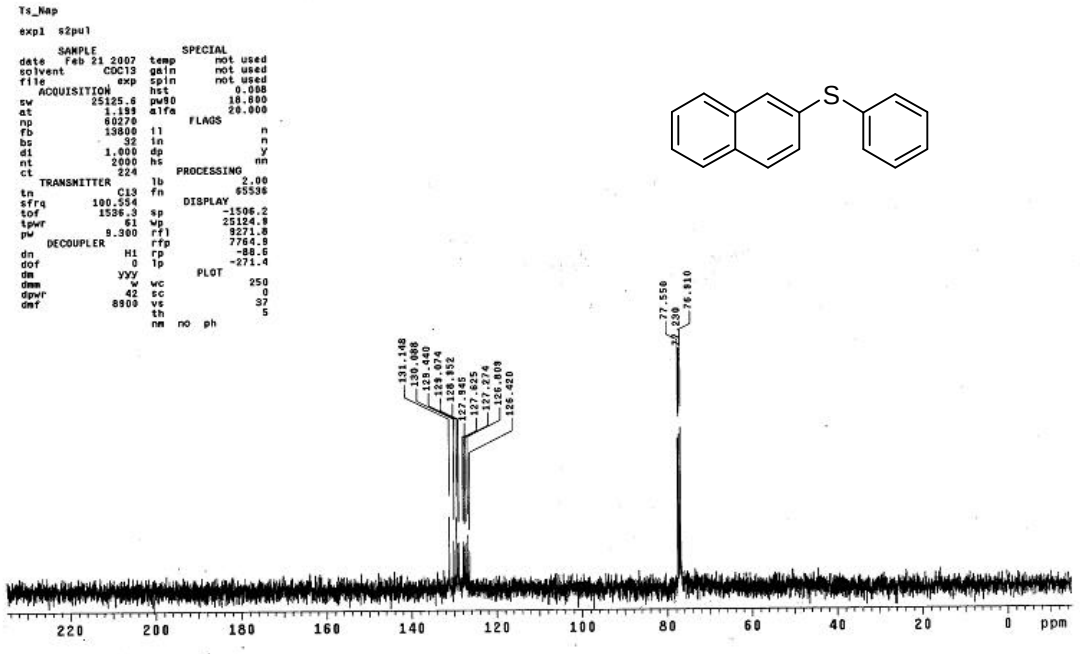
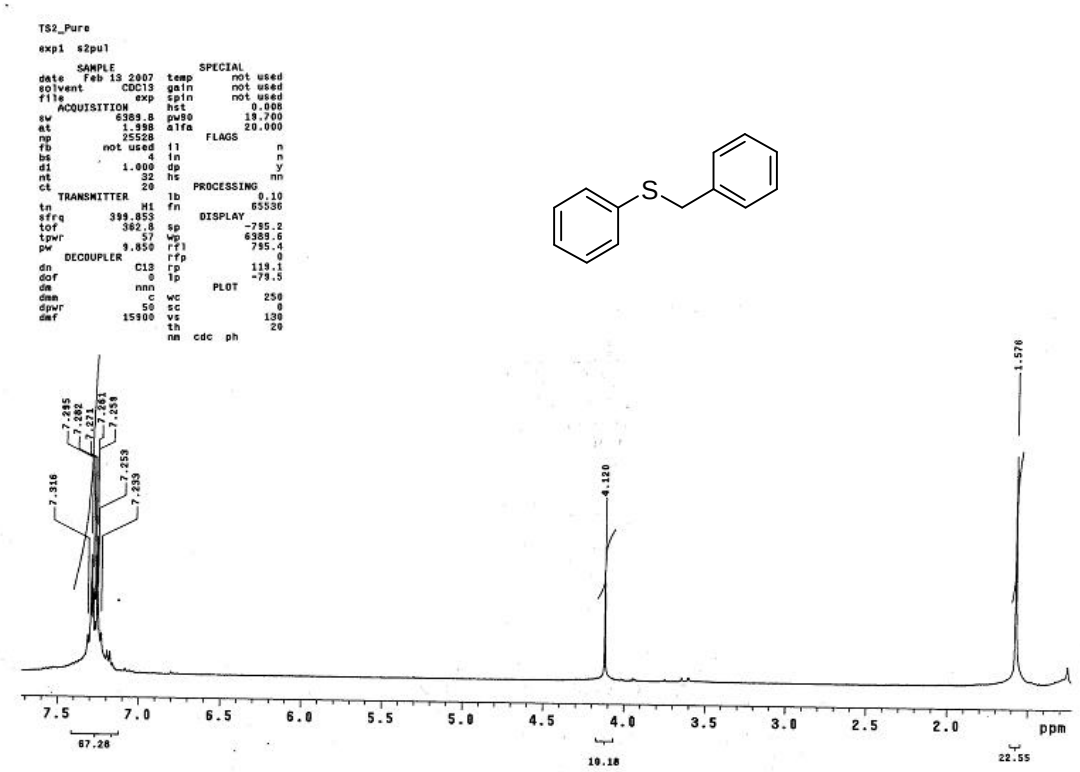
vs 20
th 6
nm no ph
S
Br
132.742
132.590
132.064
129.698
128.083
77.663
77.550
77.280
220 200 180 160 140 120 100 80 60 40 20 0 ppm

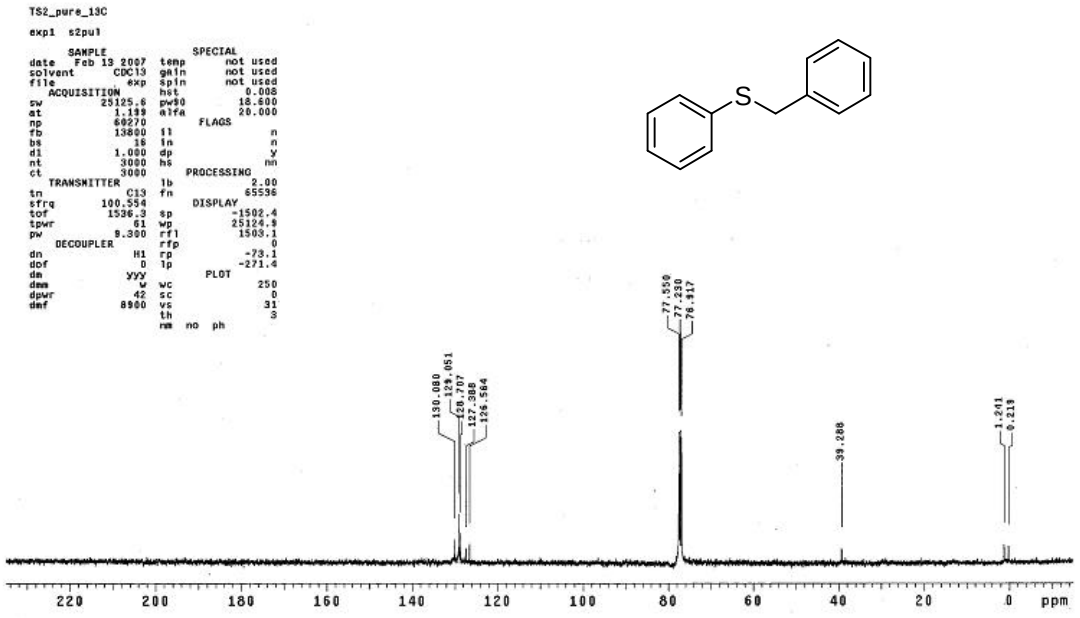

ts_7p
expl s2pul
SAMPLE
date Feb 20 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 16
ct 16
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -795.2
wp 6389.6
rfl 795.4
rfp 0
rp 105.6
lp -88.5
PLOT
wc 250
sc 0
vs 474
th 14
nm cdc ph
Br
S
7.576
7.572
7.556
7.552
7.475
7.471
7.466
7.461
7.456
7.451
7.447
7.409
7.405
7.398
7.392
7.386
7.381
7.378
7.368
7.259
7.147
7.144
7.033
7.029
6.929
6.326
6.309
0.000
0.072
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

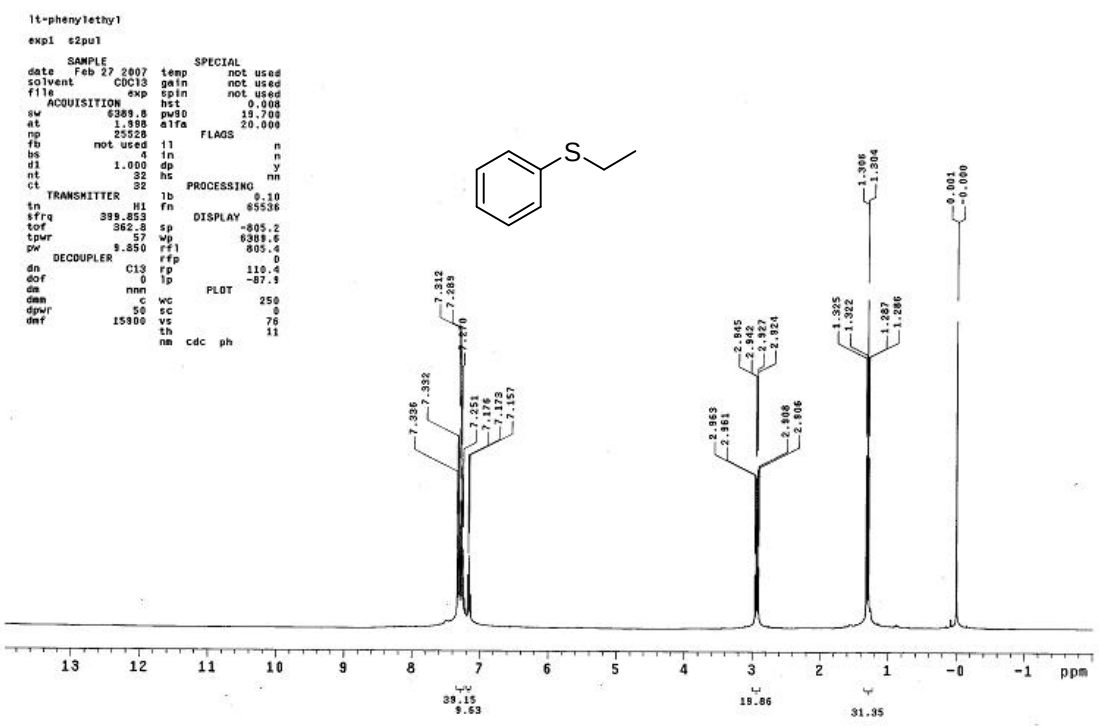

TS-2Br
expl s2pul
SAMPLE
date Feb 21 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.189
np 60270
fb 13800
bs 32
d1 1.000
nt 2000
ct 320
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1505.4
wp 25124.9
rfl 9271.1
rfp 7764.8
rp -76.5
lp -271.4
PLOT
wc 250
sc 0
vs 45
th 6
nm no ph
Br
S
133.749
133.239
131.113
129.867
128.952
128.700
128.022
127.899
127.442
77.550
77.238
76.917
0.219
220 200 180 160 140 120 100 80 60 40 20 0 ppm

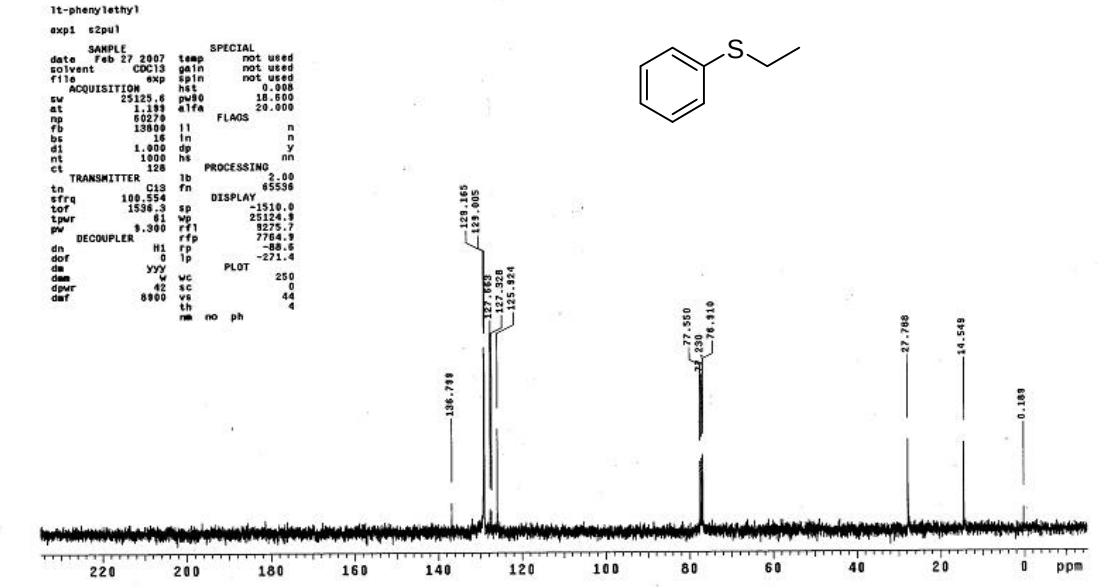

Ts_napth
exp1 s2pul
SAMPLE
date Feb 21 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -799.8
wp 6389.6
rfl 800.1
rfp 0
rp 114.8
lp -91.2
PLOT
wc 250
sc 0
vs 80
th 10
nm cdc ph
7.834
7.812
7.798
7.788
7.775
7.753
7.743
7.732
7.719
7.480
7.475
7.466
7.457
7.454
7.417
7.412
7.395
7.391
7.386
7.382
7.376
7.365
7.363
7.330
7.326
7.322
7.309
7.305
7.289
7.273
7.269
7.265
7.255
7.249
0.073
-0.000
-0.007
S
13
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm

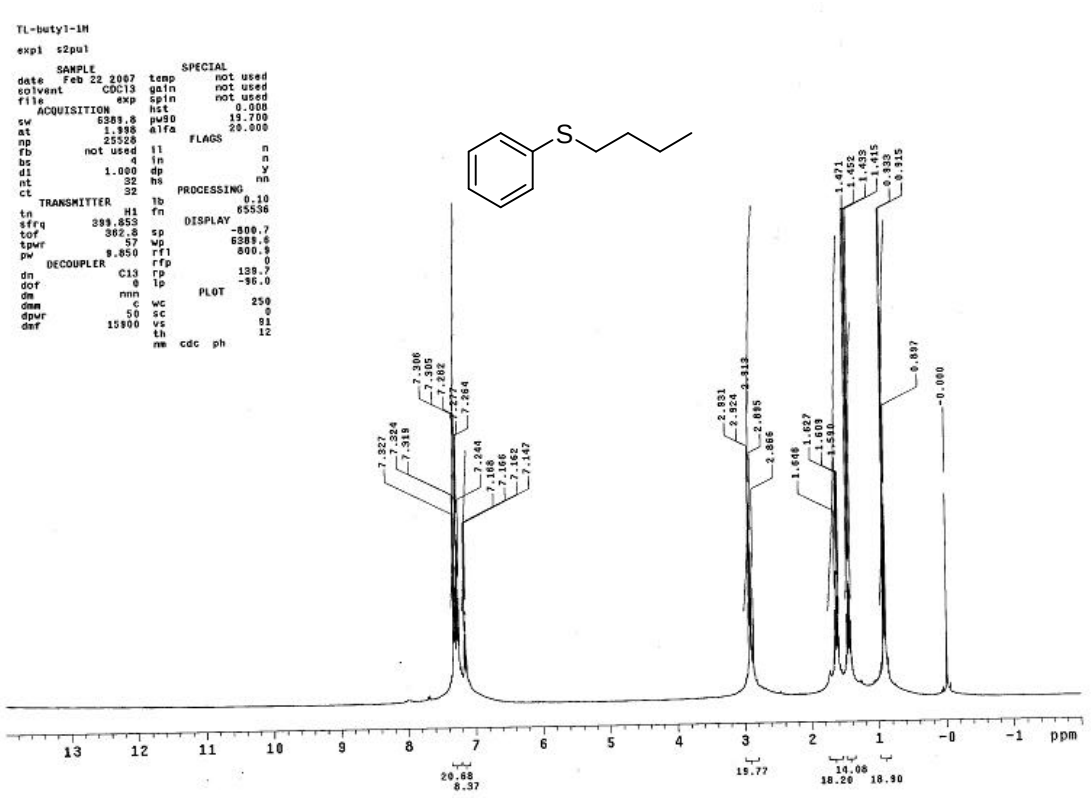

Ts_Nap
exp1 s2pul
SAMPLE
date Feb 21 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.195
np 60270
fb 13800
bs 32
d1 1.000
nt 2000
ct 224
TRANSMITTER
tn C13
sfrq 100.554
tof 1538.3
tpwr 61
pw 8.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 10.800
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1506.2
wp 25124.8
rfl 9271.8
rfp 7764.8
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 37
th 5
nm no ph
131.148
130.688
129.440
129.074
128.852
127.945
127.825
127.774
126.809
126.420
77.550
77.230
76.910
S
220
200
180
160
140
120
100
80
60
40
20
0
ppm

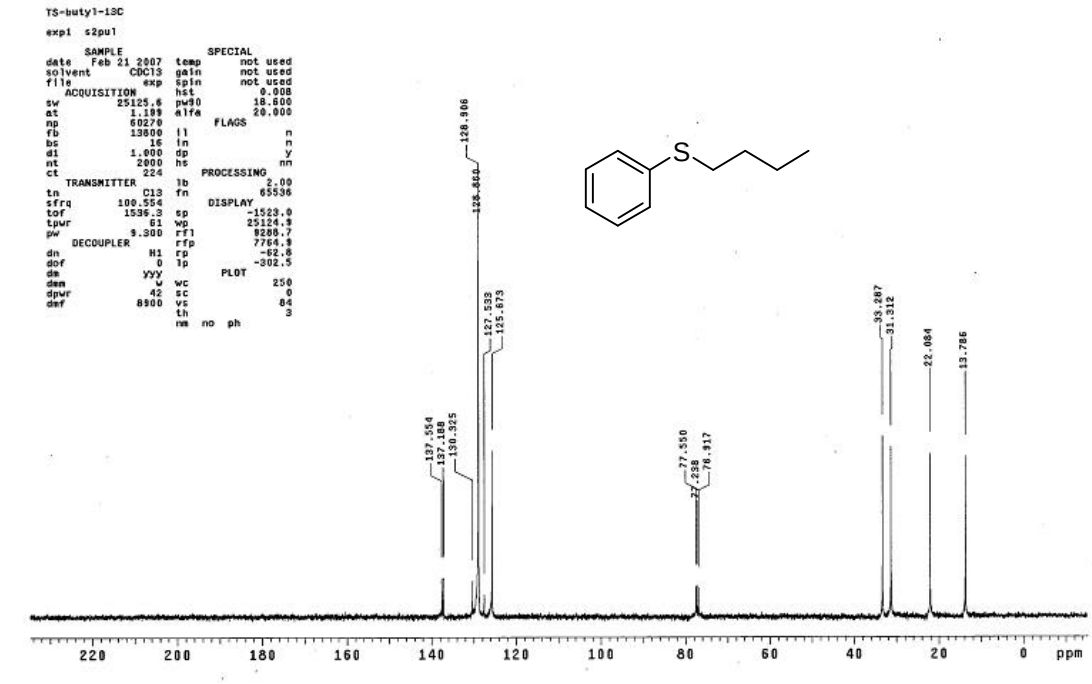

TS2_Pure
exp1 s2pul
SAMPLE
date Feb 13 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 20
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -785.2
wp 6389.6
rf1 795.4
rfp 0
rp 119.1
lp -79.5
PLOT
wc 250
sc 0
vs 130
th 20
nm cdc ph
7.295
7.282
7.271
7.261
7.259
7.316
7.259
7.239
4.120
1.578
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
67.28
10.18
22.55

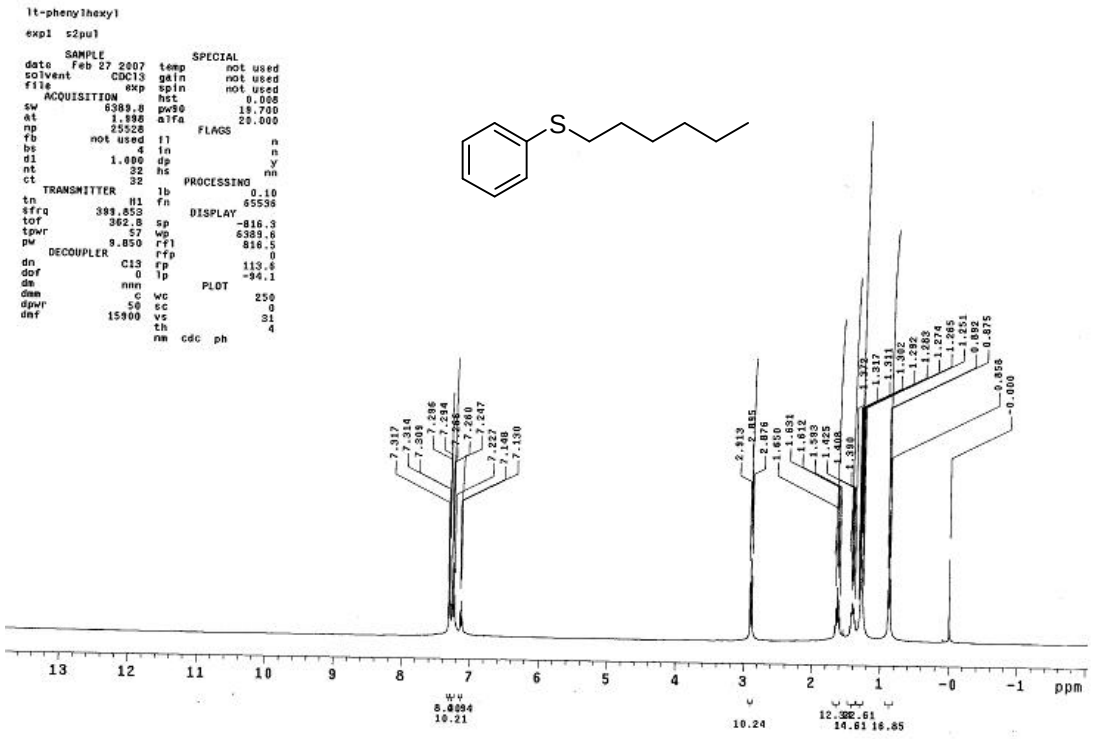

TS2_pure_13C
exp1 s2pul
SAMPLE
date Feb 13 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 3080
ct 3080
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8980
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1502.4
wp 25124.9
rf1 1503.1
rfp 0
rp -73.1
lp -271.4
PLOT
wc 250
sc 0
vs 31
th 3
nm no ph
130.080
129.051
128.707
127.388
126.564
77.550
77.230
76.917
39.288
1.241
0.218
220
200
180
160
140
120
100
80
60
40
20
0
ppm

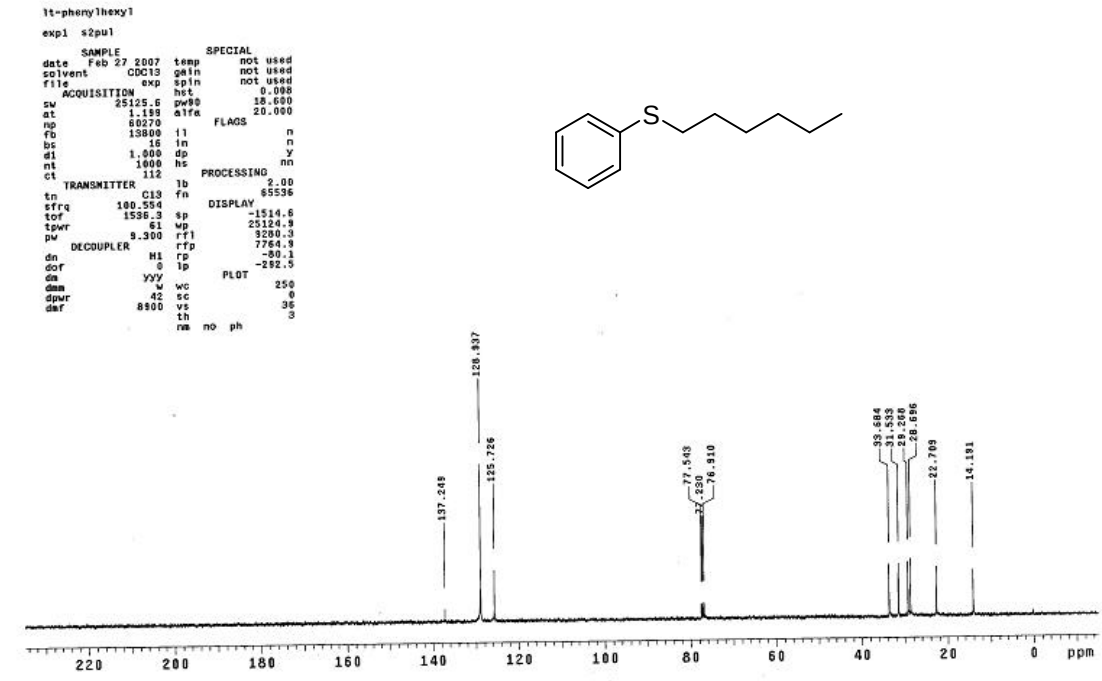

1t-phenylethyl
exp1 s2pul
SAMPLE
date Feb 27 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.988
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -805.2
wp 6388.6
rfl 805.4
rfp 0
rp 110.4
lp -87.9
PLOT
wc 250
sc 0
vs 76
th 11
nm cdc ph
7.312
7.289
7.270
7.336
7.332
7.251
7.176
7.173
7.157
2.945
2.942
2.927
2.924
2.863
2.861
2.908
2.906
1.325
1.322
1.287
1.286
1.306
1.304
0.001
0.000
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
39.15
9.63
18.86
31.35

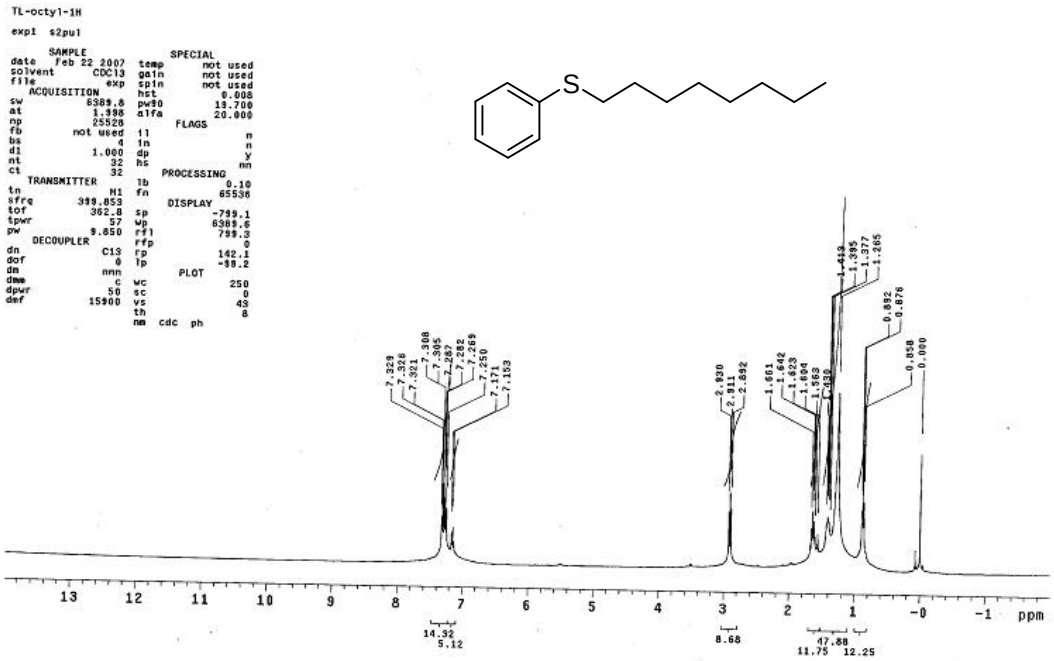

1t-phenylethyl
exp1 s2pul
SAMPLE
date Feb 27 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.189
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 128
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1510.0
wp 25124.9
rfl 9275.7
rfp 7764.9
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 44
th 4
nm no ph
128.165
128.005
127.669
127.328
125.924
77.550
77.230
76.910
27.788
14.549
0.188
220 200 180 160 140 120 100 80 60 40 20 0 ppm

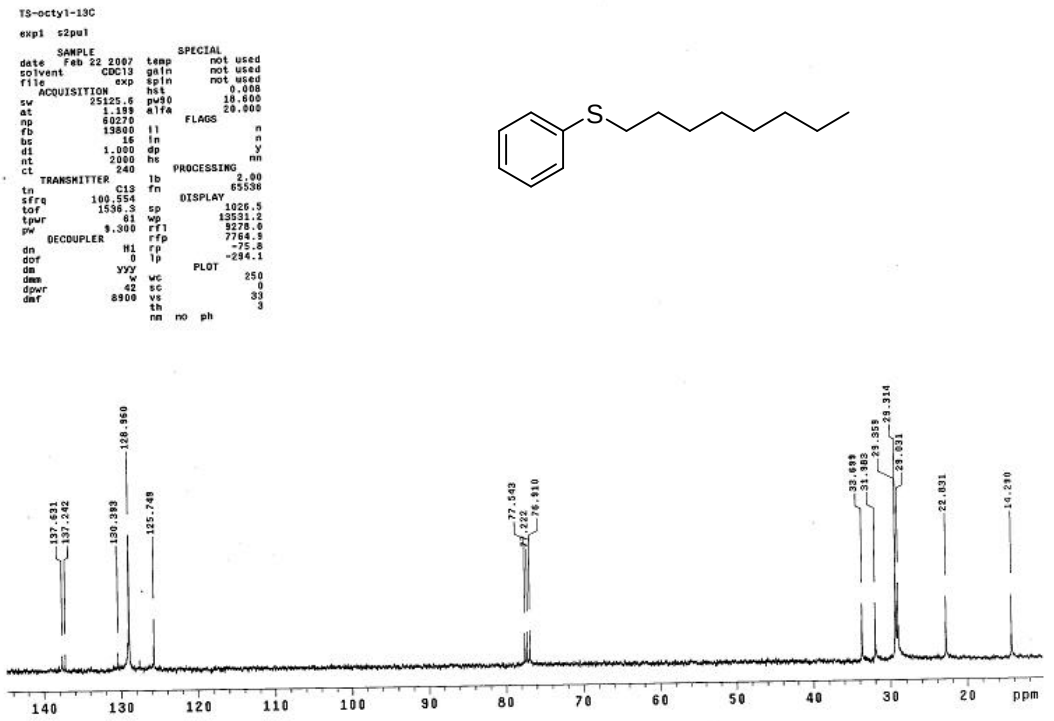

TL-butyl-1H
expl s2pul
SAMPLE
date Feb 22 2007
solvent CDCl3
file exp
ACQUISITION
sw 6388.8
at 1.998
np 25528
fb not used
bs 4
dl 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
pw90 19.700
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -800.7
wp 6389.6
rfl 800.0
rfp 0
rp 138.7
lp -96.0
PLOT
wc 250
sc 0
vs 91
th 12
nm cdc ph
S
7.327
7.324
7.319
7.306
7.305
7.262
7.260
7.244
7.168
7.166
7.162
7.147
2.931
2.924
2.913
2.885
2.866
1.646
1.627
1.609
1.590
1.471
1.452
1.433
1.415
0.933
0.915
0.897
-0.060
ppm
20.68
8.37
19.77
14.08
18.20
18.90

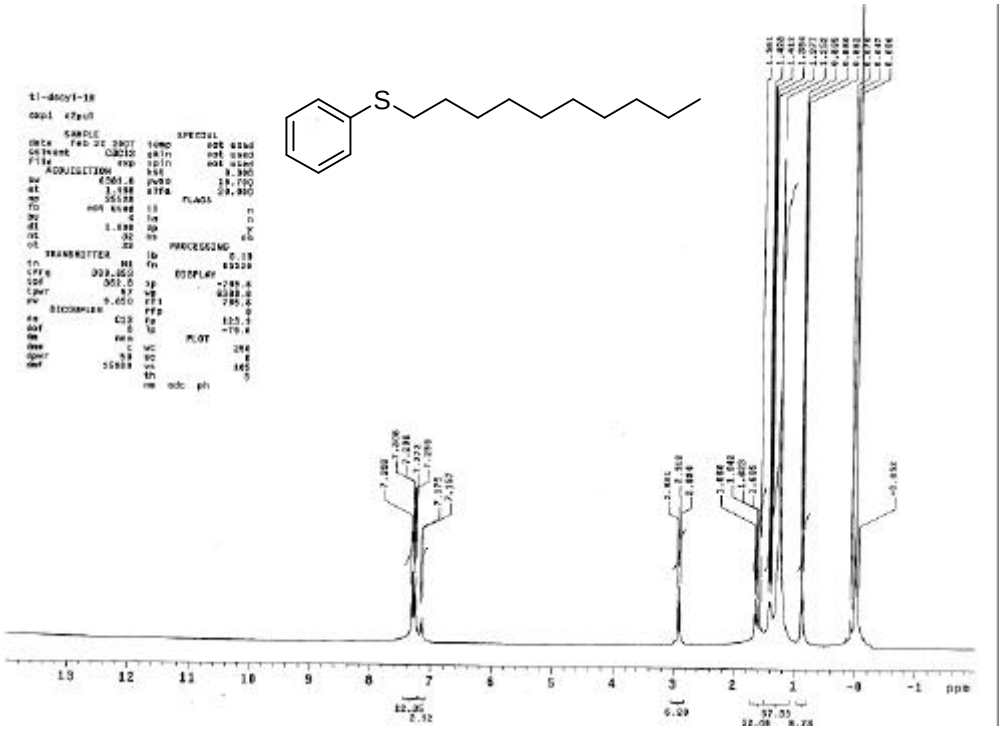

TS-butyl-13C
expl s2pul
SAMPLE
date Feb 21 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
dl 1.000
nt 2000
ct 224
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1523.0
wp 25124.9
rfl 9288.7
rfp 7764.9
rp -62.8
lp -302.5
PLOT
wc 250
sc 0
vs 84
th 3
nm no ph
S
128.906
128.664
127.533
125.673
137.554
137.188
130.365
77.550
77.238
76.917
33.287
31.312
22.084
13.786
ppm

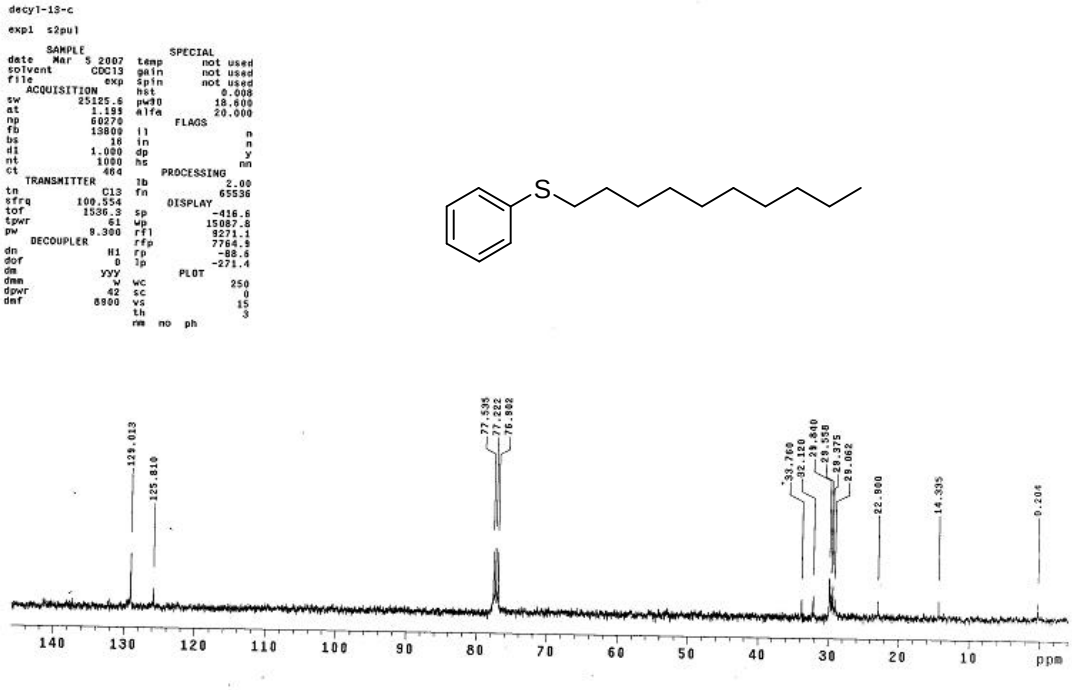

lt-phenylhexyl
expl s2pul
SAMPLE
date Feb 27 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.068
pw90 18.700
alfa 20.000
FLAGS
fl n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -816.3
wp 6389.6
rfl 816.5
rfp 0
fp 113.6
lp -94.1
PLOT
wc 250
sc 0
vs 31
th 4
nm cdc ph
7.317
7.314
7.309
7.286
7.284
7.280
7.247
7.227
7.148
7.130
2.913
2.876
2.855
1.650
1.631
1.612
1.583
1.425
1.408
1.398
1.379
1.347
1.311
1.302
1.292
1.283
1.274
1.265
1.251
0.892
0.875
0.858
-0.000
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
8.0894
10.21
10.24
12.322.61
14.61 16.85

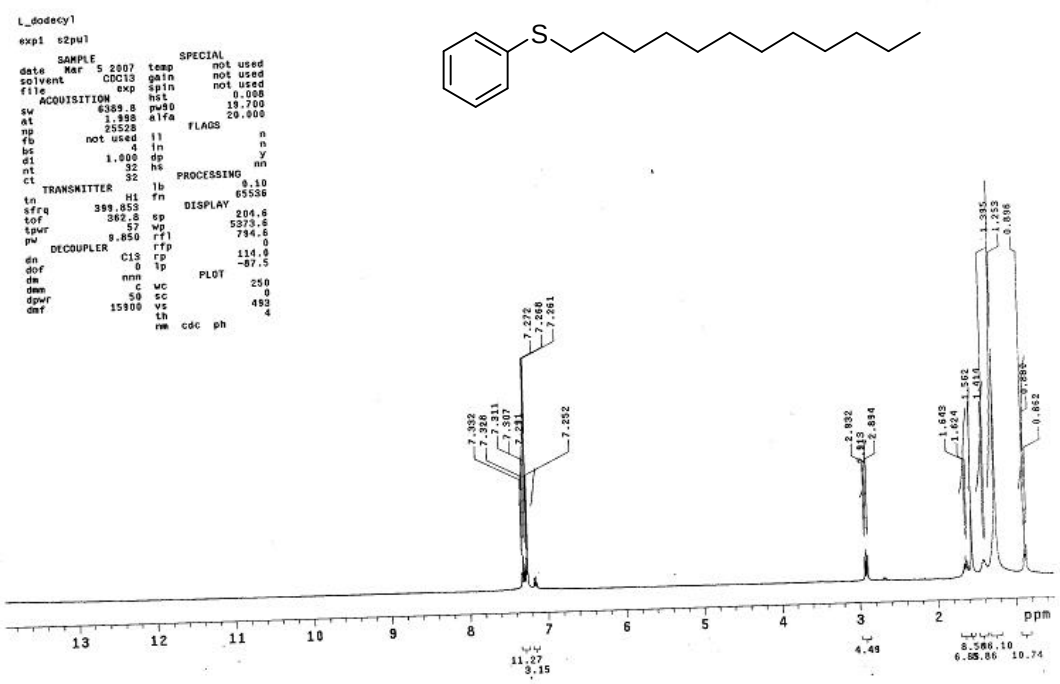

lt-phenylhexyl
expl s2pul
SAMPLE
date Feb 27 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.198
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 112
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
fl n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1514.6
wp 25124.9
rfl 3280.3
rfp 7764.9
rp -80.1
lp -292.5
PLOT
wc 250
sc 0
vs 35
th 3
nm no ph
137.248
126.837
125.726
77.543
77.230
76.910
30.684
31.553
29.260
28.686
22.709
14.181
220 200 180 160 140 120 100 80 60 40 20 0 ppm

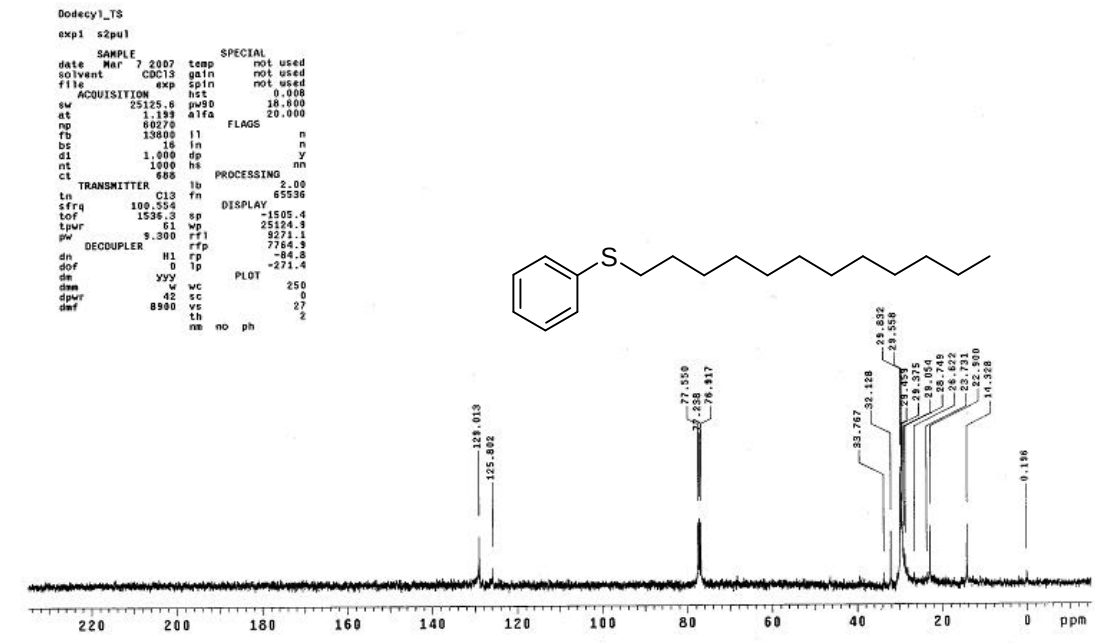

TL-octyl-1H
expl s2pul
SAMPLE
date Feb 22 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
di 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 13.700
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -799.1
wp 6389.6
rfl 799.3
rfp 0
rp 142.1
lp -88.2
PLOT
wc 250
sc 0
vs 48
th 8
nm cdc ph
S
7.329
7.328
7.311
7.308
7.305
7.287
7.282
7.269
7.250
7.171
7.153
2.830
2.811
2.892
1.661
1.642
1.623
1.604
1.568
1.438
1.413
1.395
1.377
1.265
0.892
0.876
0.858
0.000
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
14.32
5.12
8.68
47.88
11.75
12.25

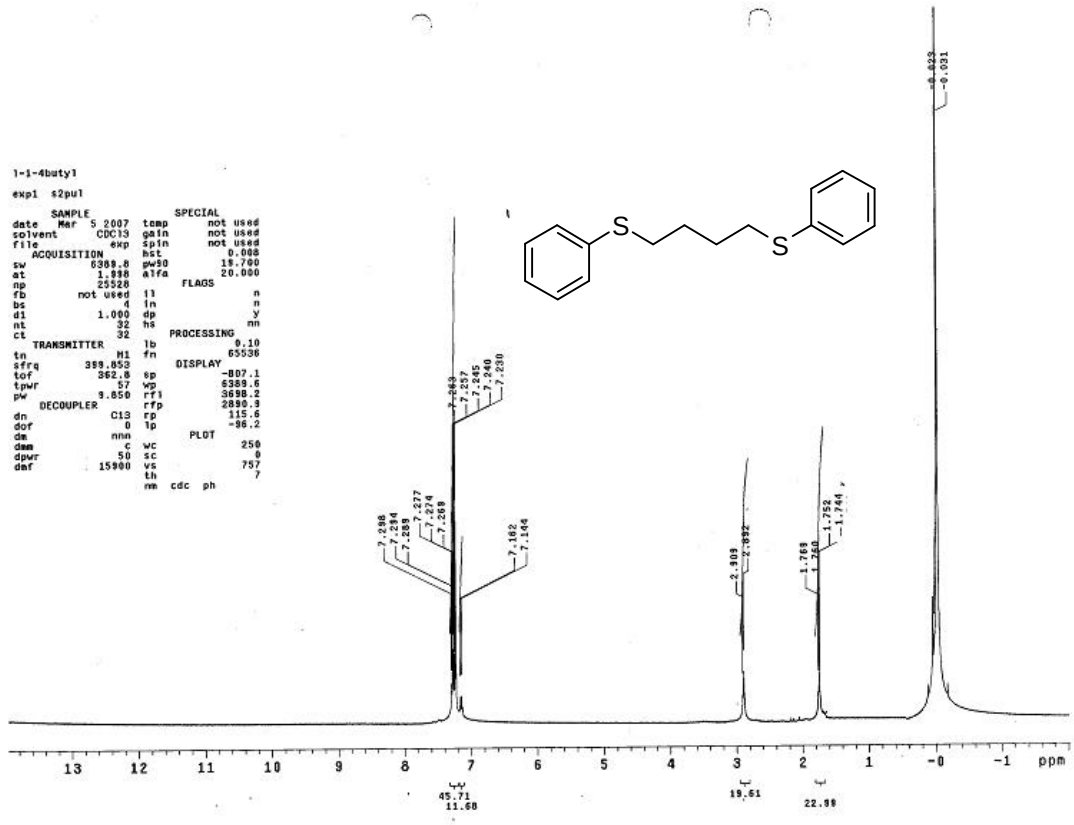

TS-octyl-13C
expl s2pul
SAMPLE
date Feb 22 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
di 1.000
nt 2000
ct 240
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp 1026.5
wp 13531.2
rfl 9278.9
rfp 7764.9
rp -75.8
lp -294.1
PLOT
wc 250
sc 0
vs 33
th 3
nm no ph
S
137.631
137.242
130.393
128.360
125.749
77.543
77.222
76.910
33.699
31.983
29.358
29.314
29.031
22.831
14.240
140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

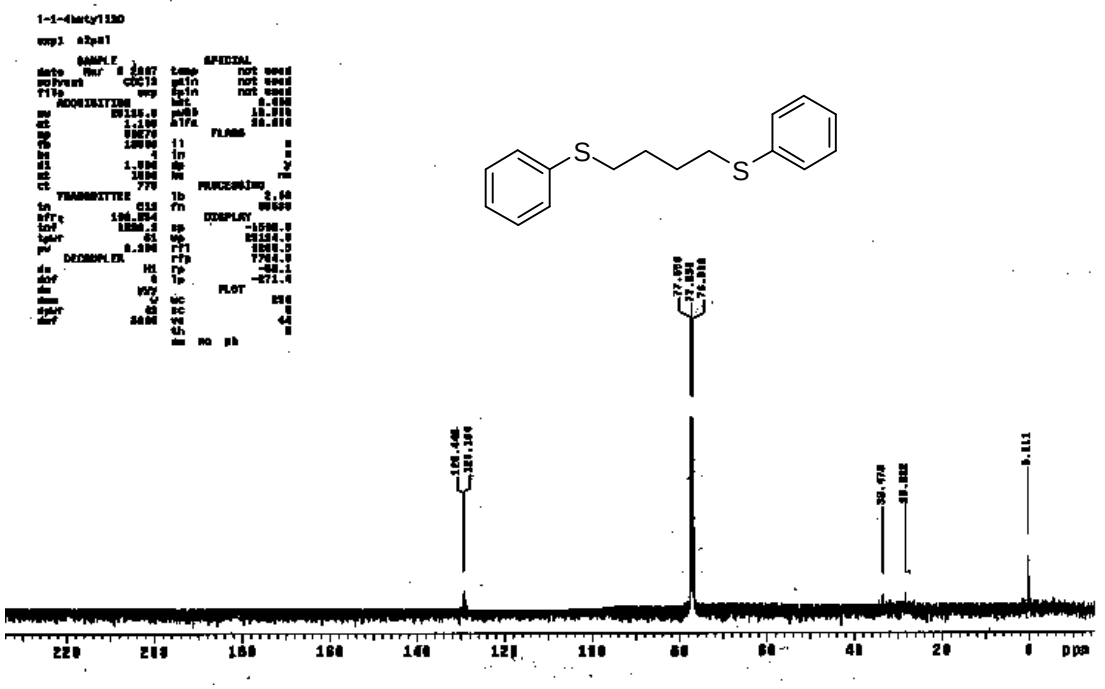

S
ppm


S
ppm


L_dodecyl
exp1 s2pul
SAMPLE
date Mar 5 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
dl 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 204.6
wp 5373.6
rfl 794.6
rfp 0
rp 114.0
lp -87.5
PLOT
wc 250
sc 0
vs 493
th 4
nm cdc ph
S
7.332
7.328
7.311
7.307
7.291
7.272
7.268
7.261
7.252
2.932
2.913
2.894
1.649
1.562
1.414
1.395
1.253
0.898
0.862
ppm
11.27
3.15
4.49
8.58
6.65
8.10
6.86
10.74


Dodecyl_TS
exp1 s2pul
SAMPLE
date Mar 7 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
dl 1.000
nt 1000
ct 688
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.800
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1505.4
wp 25124.9
rf1 9271.1
rfp 7764.9
rp -84.8
lp -271.4
PLOT
wc 250
sc 0
vs 27
th 2
nm no ph
S
128.013
125.892
77.550
77.238
76.917
33.767
32.128
29.832
29.558
29.453
29.375
29.054
28.874
28.822
28.731
22.900
14.328
0.156
ppm


1-1-4butyl
exp1 s2pul
SAMPLE
date Mar 5 2007
solvent CDCl3
file exp
ACQUISITION
sw 6388.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.852
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 15.700
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -807.1
wp 6389.6
rf1 3698.2
rfp 2890.8
rp 115.6
lp -96.2
PLOT
wc 250
sc 0
vs 757
th 7
nm cdc ph
7.298
7.284
7.269
7.277
7.274
7.268
7.162
7.144
7.269
7.257
7.245
7.240
7.230
2.909
2.892
1.768
1.760
1.752
1.744
0.022
0.031
S
S
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm
45.71
11.68
19.61
22.98


1-1-4butyl13D
exp1 s2pul
S
S
77.059
77.259
76.858
139.446
139.164
30.478
29.852
8.111
220 200 180 160 140 120 100 80 60 40 20 0 ppm