

SUPPORTING INFORMATION

Title: Efficient Copper(I)-Catalyzed C–S Cross Coupling of Thiols with Aryl Halides in Water

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(Diphenyl)sulfane:¹ Colorless liquid; yield 98%; ¹H NMR (CDCl₃, 400 MHz) δ 7.35-7.24 (m, 10H); ¹³C NMR (CDCl₃, 100 MHz) δ 131.25, 129.41, 127.71, 127.37.

(Phenyl)(2-tolyl)sulfane:² Colorless oil; yield 98%; ¹H NMR (CDCl₃, 400 MHz) δ 7.21-7.03 (m, 9H), 2.29 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) 140.15, 136.30, 133.92, 133.16, 130.79, 129.82, 129.32, 128.09, 126.91, 126.54, 20.80.

(Phenyl)(4-tolyl)sulfane:¹ Colorless oil; yield 99%; ¹H NMR (CDCl₃, 400 MHz) δ 7.30-7.25 (m, 6H), 7.20-7.12 (m, 3H), 2.31 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 137.80, 137.31, 132.48, 131.43, 130.26, 129.94, 129.24, 126.59, 21.34.

(4-Nitrophenyl)(phenyl)sulfane:¹ Yellow solid; yield 91%; m.p. 54 °C; ¹H NMR (CDCl₃, 400 MHz) δ 8.07 (dd, *J* = 8.8, 2.4 Hz, 2H), 7.55-7.53 (m, 2H), 7.47-7.45 (m, 3H), 7.16 (dd, *J* = 8.8, 2.8 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 148.74, 134.97, 130.59, 130.24, 129.89, 126.84, 124.24.

(2-Bromophenyl)(phenyl)sulfane:¹ Colorless oil; yield 96%; ¹H NMR (CDCl₃, 400 MHz) δ 7.56 (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), 6.91(d, *J* = 8 Hz, 1H); ¹³C NMR (CDCl₃, 100 MHz) 133.74, 133.23, 129.91, 129.86, 128.95, 128.70, 128.02, 127.89, 127.44.

(4-Bromophenyl)(phenyl)sulfane:¹ Colorless oil; yield 95%; ¹H NMR (CDCl₃, 400 MHz) δ 7.40 (dd, *J* = 6.8, 4.8 Hz, 2H), 7.36 -7.25 (m, 5H), 7.17 (dd, *J* = 6.8, 4.8 Hz, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 135.99, 132.74, 132.59, 132.06, 129.89, 128.08.

(4-Chlorophenyl)(phenyl)sulfane:² Colorless oil; yield 94%; ¹H NMR (CDCl₃, 400 MHz) δ 7.27 -7.13 (m, 9H); ¹³C NMR (CDCl₃, 100 MHz) δ 137.66, 134.82, 137.17, 132.20, 131.51, 130.44, 129.54, 129.52, 127.64.

(4-Methoxyphenyl)(phenyl)sulfane:¹ Colorless oil; yield 99%; ¹H NMR (CDCl₃, 400 MHz) δ 7.38 (dd, *J* = 8.8, 2.8 Hz, 2H), 7.2 3-7.12 (m, 5H), 6.86 (dd, *J* = 8.8, 2.4 Hz, 2H), 3.78 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) δ 159.99, 138.79, 135.56, 129.10, 128.32, 125.91, 124.41, 115.15, 55.52.

(Naphthalen-2-yl)(phenyl)sulfane:¹ Colorless solid, yield 99%; m.p. 49 °C; ¹H NMR (CDCl₃, 400 MHz) δ 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); ¹³C NMR (CDCl₃, 100 MHz) δ 131.14, 130.08, 129.44, 129.07, 128.95, 127.94, 127.62, 127.27, 126.80, 126.42.

Benzyl(phenyl)sulfane:¹ Colorless solid; yield 91%; m.p. 40°C; ¹H NMR (CDCl₃, 400 MHz) δ 7.31-7.23 (m, 10H), 4.12 (s, 2H); ¹³C NMR (CDCl₃, 100 MHz) δ 130.08, 129.05, 128.70, 127.38, 126.56, 39.28.

Butyl(phenyl)sulfane:¹ Colorless oil; yield 15%; ¹H NMR (CDCl₃, 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); ¹³C NMR (CDCl₃, 100 MHz) 137.55, 137.18, 130.32, 128.90, 127.53, 125.67, 33.28, 31.31, 22.08, 13.78.

(4-Nitrophenyl)(2-Tolyl)sulfane: Colorless oil; yield 98%; ¹H NMR (CDCl₃, 400 MHz) δ 8.05 (dd, *J* = 7.2 Hz, 2.0 Hz, 2H), 7.55 (d, *J* = 7.2 Hz, 1H), 7.41-7.39 (m, 2H), 7.29-7.26 (m, 1H), 7.08-7.05 (m, 2H), 2.37 (s, 3H); ¹³C NMR (CDCl₃, 100 MHz) 135.73, 131.59, 130.72, 128.16, 127.68, 126.00, 124.29, 20.87.

(4-Nitrophenyl)(4-tolyl)sulfane:³ Yellow needles; yield 98%; m.p. 83-85 °C; ¹H NMR (CDCl₃, 400 MHz) δ 7.98 (d, *J* = 9.2 Hz, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J*

= 8.8 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 149.59, 145.37, 140.48, 135.32, 131.10, 126.35, 124.21, 21.58.

bis(4-Nitrophenyl)sulfane:⁴ Yellow brown crystals; yield 94%; m.p. 152-155 °C; ^1H NMR (CDCl_3 , 400 MHz) δ 8.12-8.10 (m, 4H), 7.40 (dd, J = 8.8, 1.6 Hz, 4H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 147.36, 142.92, 131.36, 124.84,

(2-Bromophenyl)(4-nitrophenyl)sulfane: Yellow crystalline needles; yield 91%; m.p. 99-100 °C; ^1H NMR (CDCl_3 , 400 MHz) δ 8.04 (d, J = 8.4 Hz, 2H), 7.67 (d, J = 8.0 Hz, 1H), 7.50 (d, J = 7.6 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.25 (t, J = 7.6 Hz, 1H), 7.13 (d, J = 8.4 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) 146.18, 136.38, 134.38, 132.52, 131.21, 129.43, 128.87, 127.75, 124.43.

(4-Bromophenyl)(4-nitrophenyl)sulfane:⁵ Yellow needles; yield 99%; m.p. 94-96 °C; ^1H NMR (CDCl_3 , 400 MHz) δ 8.03 (dd, J = 7.6, 2.4 Hz, 2H), 7.52 -7.49 (m, 2H), 7.33 -7.31 (m, 2H), 7.18 (dd, J = 6.8, 4.8 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 159.41, 135.86, 133.13, 129.29, 126.99, 124.07.

(4-Chlorophenyl)(4-nitrophenyl)sulfane:⁵ Yellow solid; yield 98%; m.p. 84-85 °C; ^1H NMR (CDCl_3 , 400 MHz) δ 8.06 (d, J = 8.8 Hz, 2H), 7.45-7.38 (m, 4H), 7.16 (d, J = 8.8 Hz, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 147.79, 136.20, 136.02, 130.43, 129.28, 127.08, 124.30.

(4-Methoxyphenyl)(4-nitrophenyl)sulfane:⁵ Yellowish green solid; yield 99%; m.p. 61-62 °C; ^1H NMR (CDCl_3 , 400 MHz) δ 7.97 (dd, J = 8.8, 2.8 Hz, 2H), 7.41 (dd, J = 6.8, 2.0 Hz, 2H), 7.02 (dd, J = 6.4, 4.8 Hz, 2H), 6.92 (dd, J = 9.2, 7.2 Hz, 2H), 3.79 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 161.31, 150.28, 137.35, 125.75, 124.15, 120.31, 115.86, 55.67.

(Naphthalen-2yl)(4-nitrophenyl)sulfane: Yellow crystal; yield 97%; m.p. 115.5-106 °C; ^1H NMR (CDCl_3 , 400 MHz) δ 8.03-7.98 (m, 2H), 7.84-7.76 (m, 3H), 7.53-7.43 (m, 4H), 7.19-7.13 (m, 2H); ^{13}C NMR (CDCl_3 , 100 MHz) δ 148.59, 145.63, 134.83, 134.08, 133.55, 130.94, 130.09, 128.08, 127.71, 127.29, 127.06, 124.27.

Benzyl(4-nitrophenyl)sulfane:⁶ Yellow solid; yield 96%; m.p 122°C; ¹H NMR (CDCl₃, 400 MHz) δ 8.08 (d, *J* = 9.2 Hz, 2H), 7.34-7.29 (m, 7H), 4.22 (s, 2H); ¹³C NMR (CDCl₃, 400 MHz) δ 147.47, 145.79, 134.42, 129.06, 126.87, 124.15, 37.25.

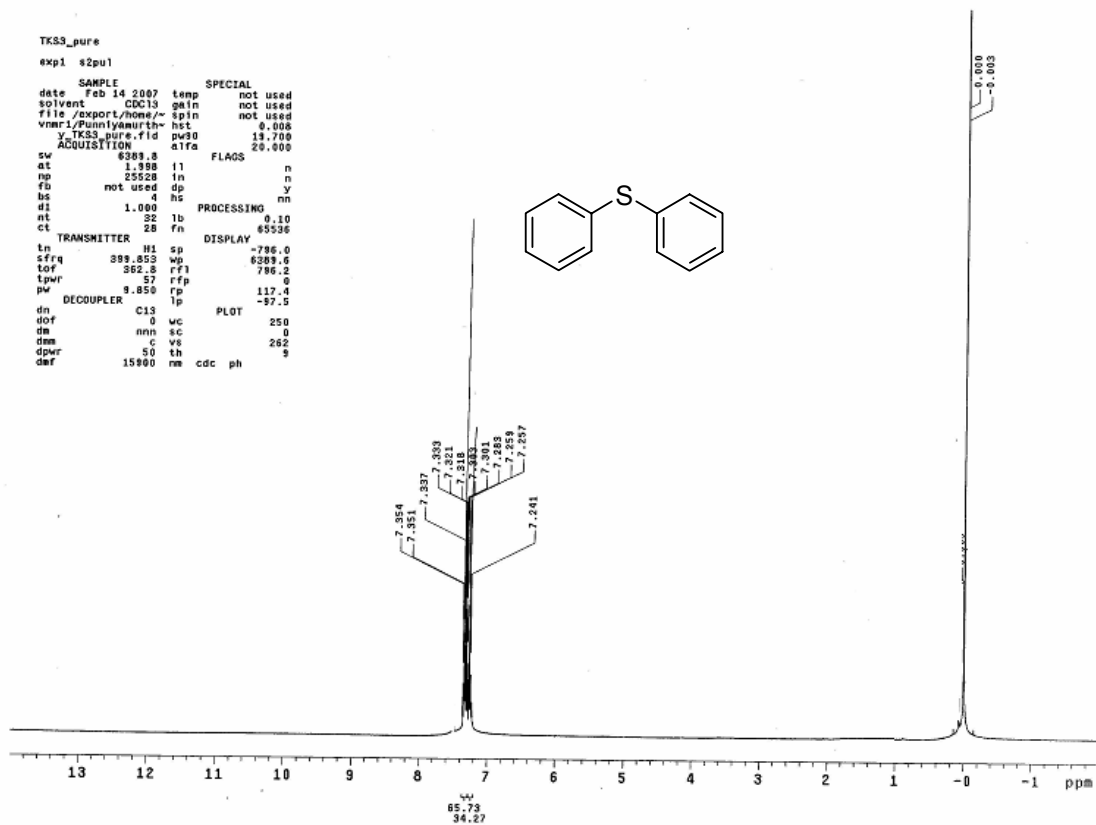
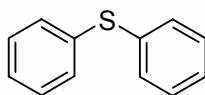
(2,4-Dimethylphenyl)(phenyl)sulfane: Colorless liquid; yield 85%; ¹H NMR (CDCl₃, 400 MHz) δ 7.22 (d, *J* = 8.0 Hz, 1H), 7.18-7.12 (m, 2H), 7.07-7.01 (m, 4H), 6.91 (d, *J* = 8.0 Hz, 1H), 2.24 (s, 6H); ¹³C NMR (CDCl₃, 400 MHz) δ 141.05, 138.77, 134.84, 131.80, 129.18, 127.78, 125.81, 21.30, 20.79.

References

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- (5) Chandrasekaran, R.; Perumal, S.; Wilson, D. A. *Magnetic Resonance in Chemistry* **1987**, *25*, 1001
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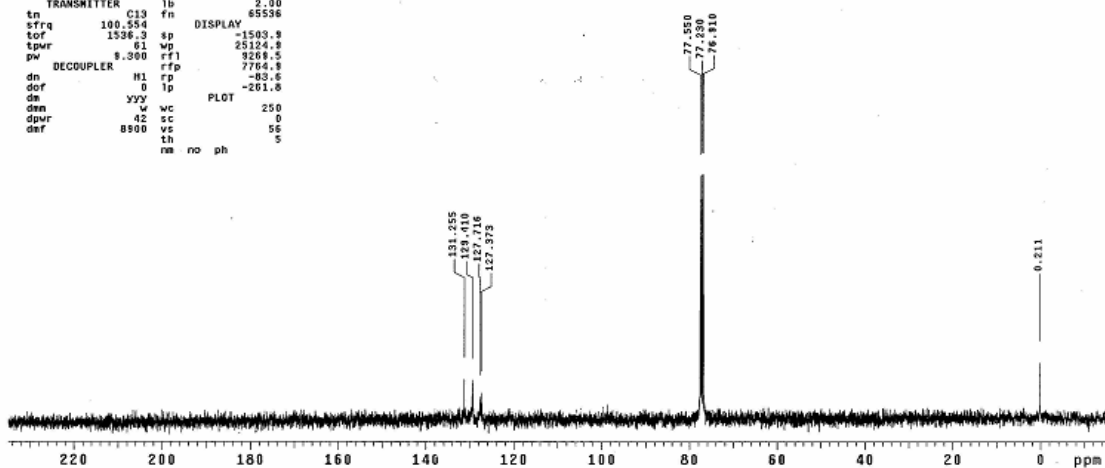
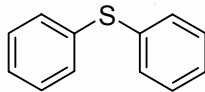
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TKS2_13C

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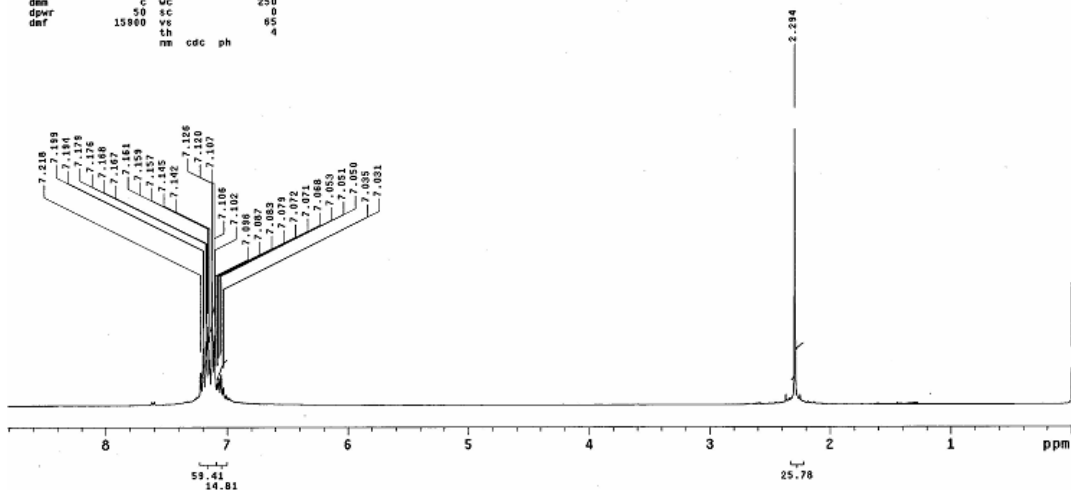
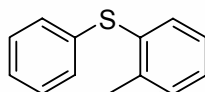
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L-2-me-sonic

expl s2pul

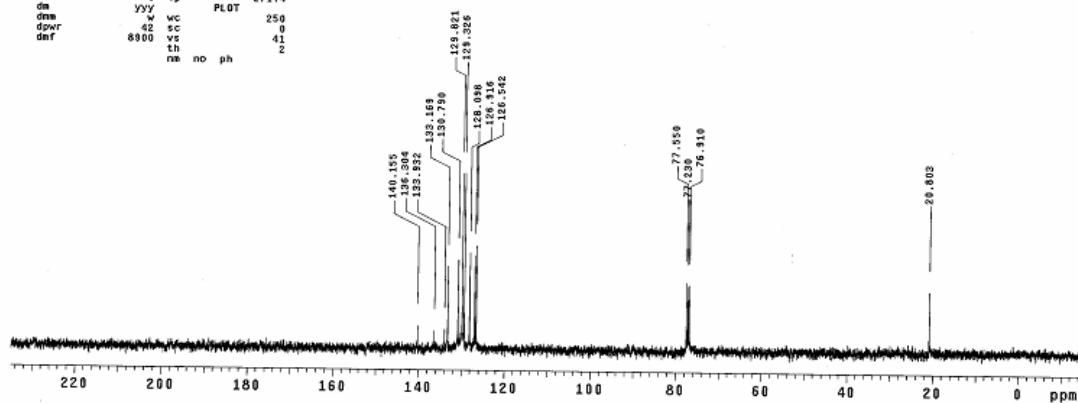
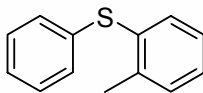
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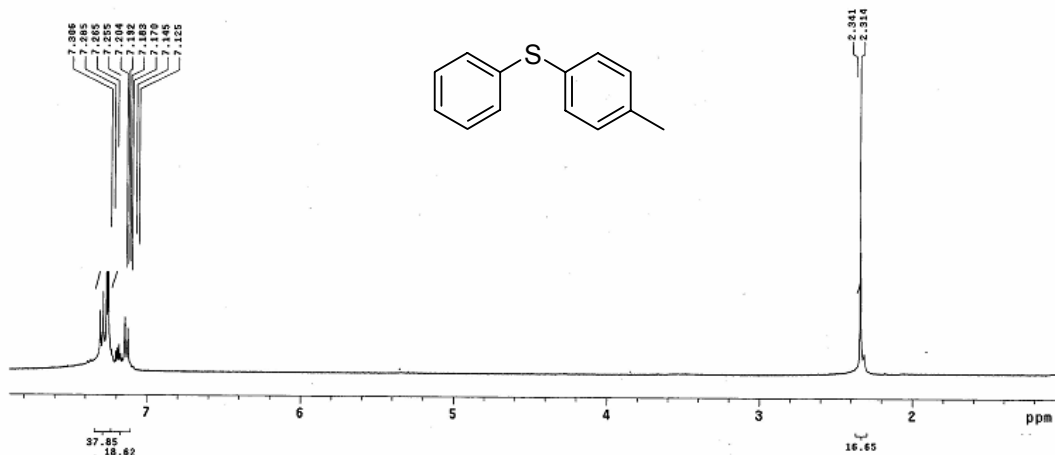
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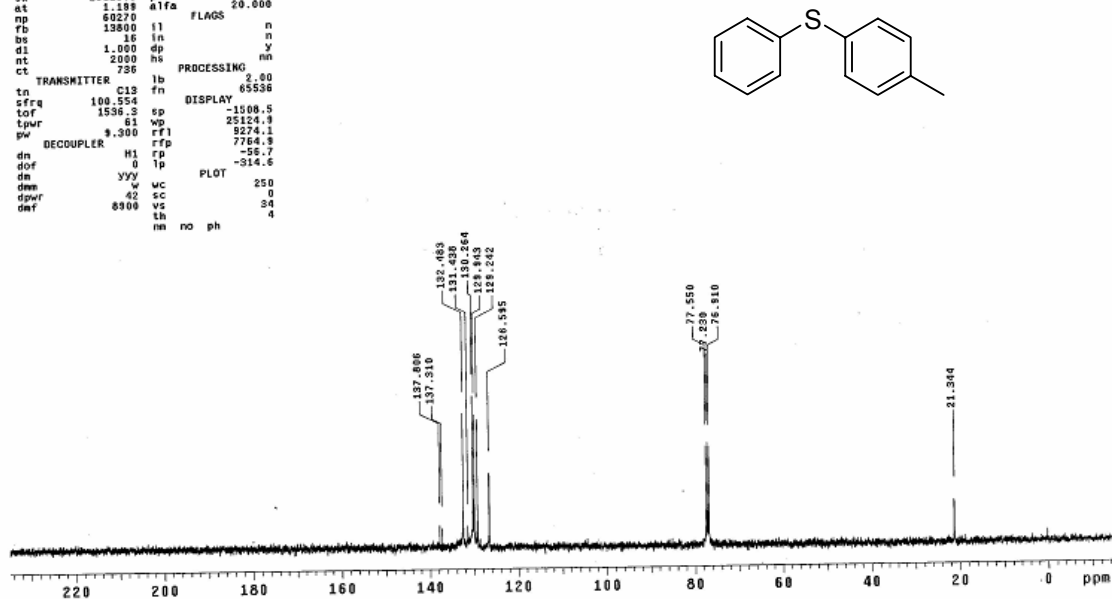
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TS5_13C

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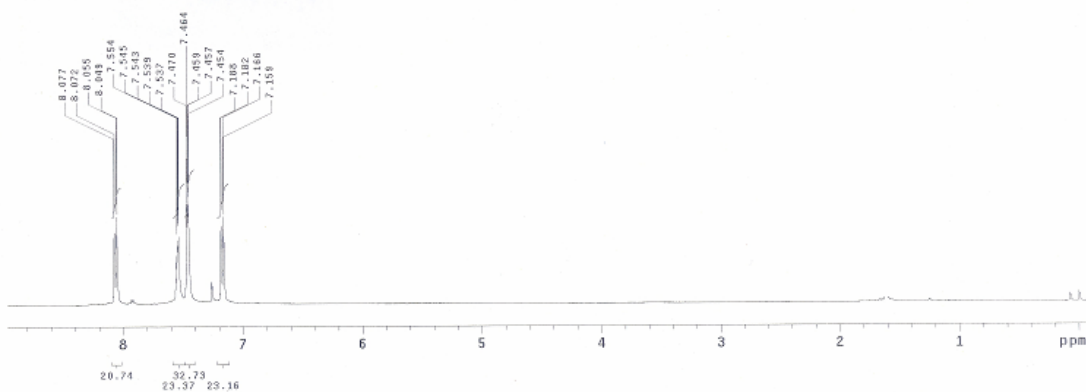
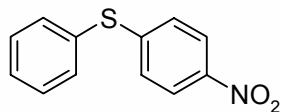
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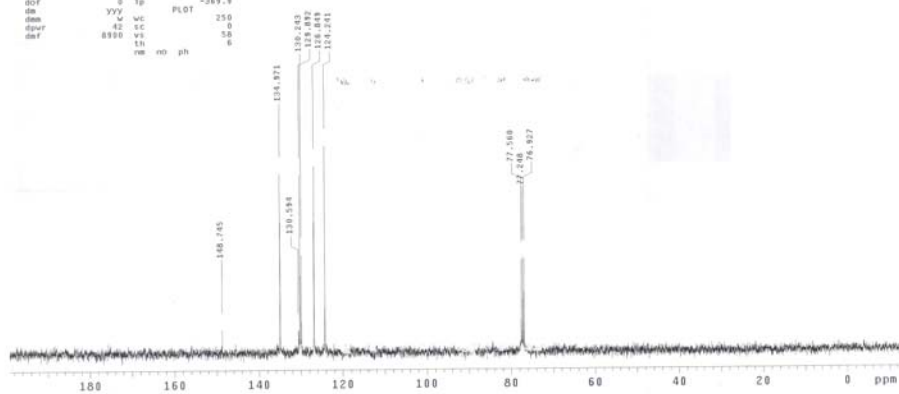
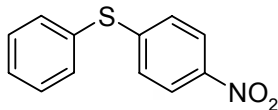
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53-15013C

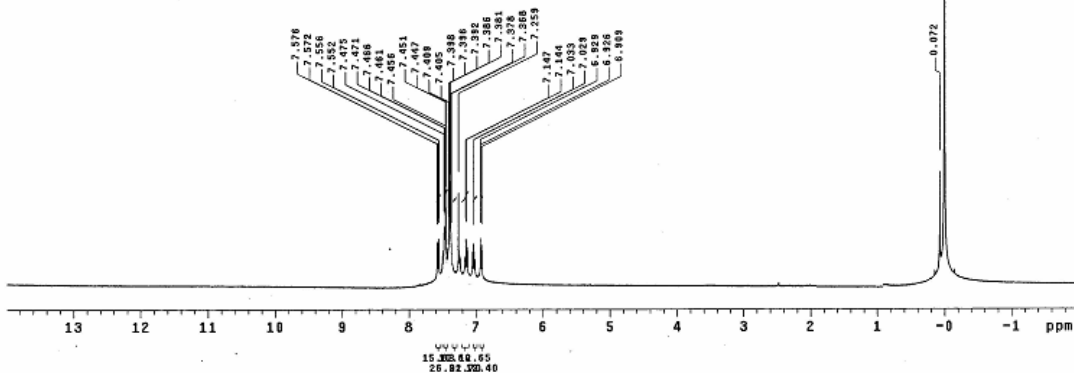
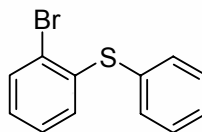
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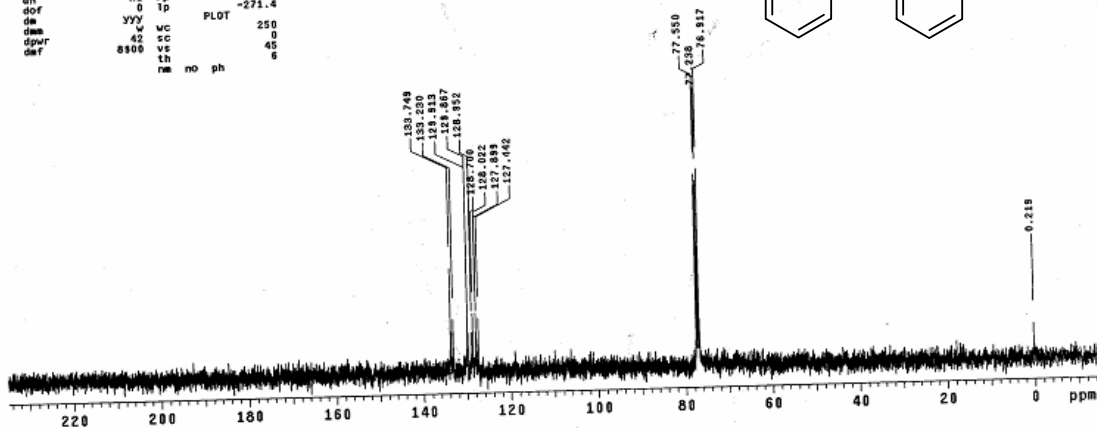
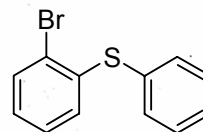
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TS-2Br
exp1 s2pu1

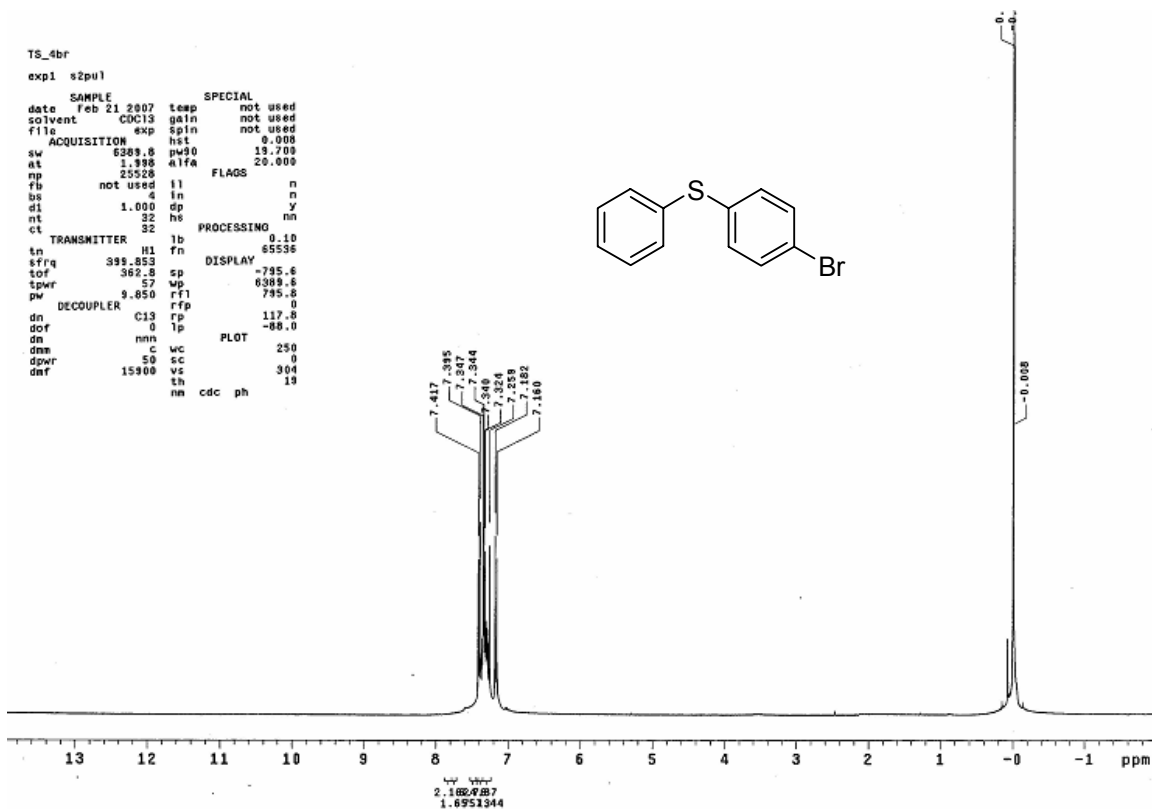
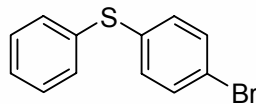
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date	Feb 21 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		ht	0.008
sw	25125.6	pw90	18.490
at	1.188	alpha	20.000
mp	60270	FLAGS	
fb	15800	ll	n
bs	32	in	n
d1	1.090	dp	y
nt	2080	hs	nn
ct	320		
TRANSMITTER		PROCESSING	
tn	C13	lb	2.00
cfra	100.554	fn	65536
tof	1536.3	sp	-1505.4
tpur	61	wp	25124.8
pw	9.300	rfl	9271.1
DECOUPLER		rtp	7764.8
dn	H1	rp	-78.5
dof	0	lp	-271.4
dm	yyy	PLOT	
dpr	42	vc	250
daf	8900	cc	45
		th	6
		nm	no ph



TS_4br

exp1 s2pu1

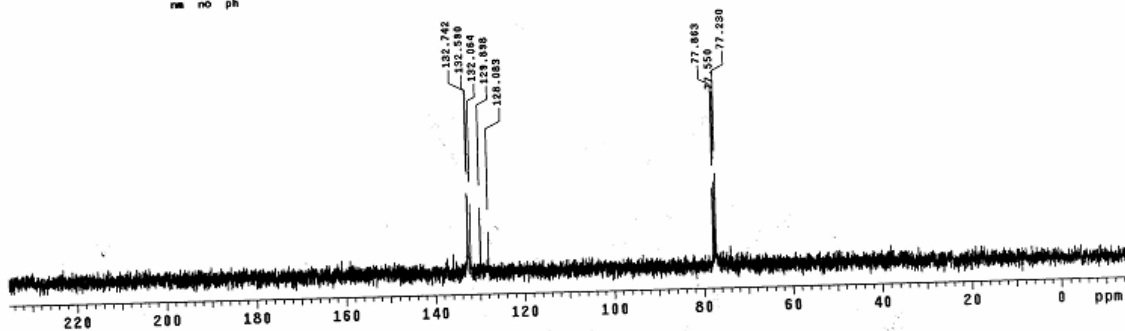
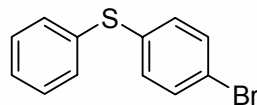
SAMPLE		SPECIAL	
date	Feb 21 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	6388.8	pw90	19.709
at	1.988	alpha	20.000
np	25528	FLAGS	
fb	not used	l1	n
bs	4	in	n
dl	1.000	dp	y
nt	32	hv	no
ct	32	PROCESSING	
tn	H1	lb	0.10
tfreq	399.853	fn	65536
tof	362.8	sp	-795.6
tpwr	57	wp	6389.6
pw	9.850	rf1	795.6
DECOUPLER		rfp	0
dn	C13	rp	117.6
dof	0	lp	-86.0
dm	nnn	PLOT	
dma	c	vc	250
dpwr	50	sc	0
dmf	15900	vs	304
	th	nm	13
	nm	cdc	ph



TS-4-br

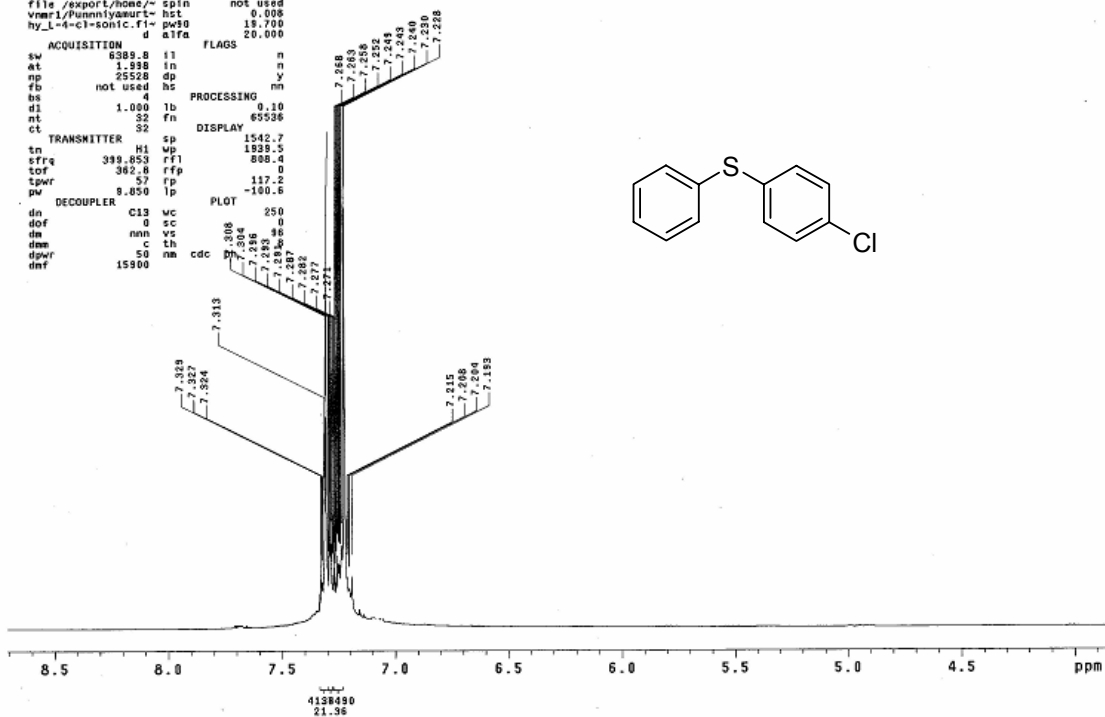
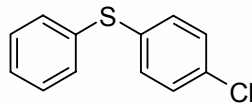
exp1 s2pu1

SAMPLE		SPECIAL	
date	Feb 21 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	25125.6	pw90	15.600
at	1.198	alpha	20.000
np	60270	FLAGS	
fb	13800	l1	n
bs	32	in	n
dl	1.000	dp	y
nt	2000	hs	nm
ct	128	PROCESSING	
tn	C13	lb	2.80
tfreq	100.554	fn	65536
tof	1536.3	sp	-1474.7
tpwr	61	wp	25124.9
pw	9.800	rf1	9249.4
DECOUPLER		rfp	7764.9
dn	H1	rp	-86.6
dof	0	lp	-271.4
dm	yyy	PLOT	
dma	w	vc	250
dpwr	42	sc	0
dmf	8900	vs	20
	th	nm	6
	nm	no	ph



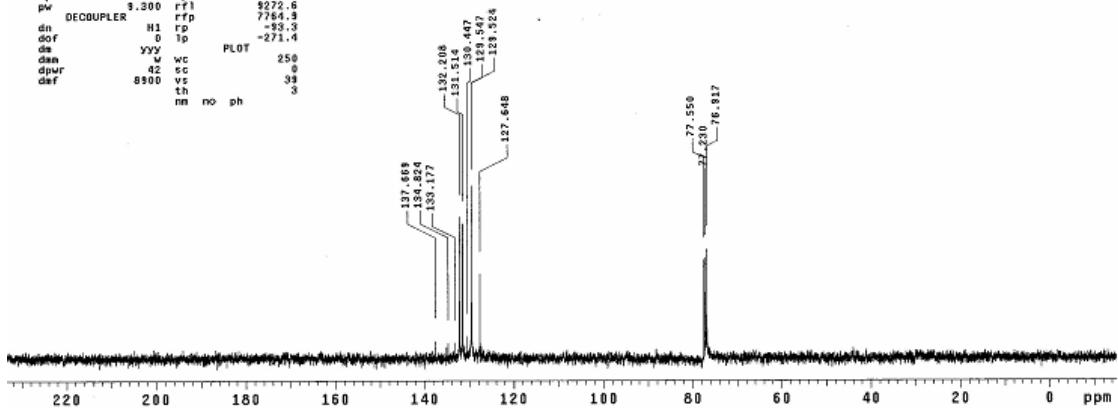
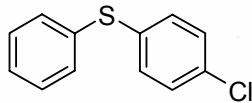
1-4-cl-sonic
exp1 s2pu1

SAMPLE		SPECIAL	
date	Jun 11 2007	temp	not used
solvent	CDCl3	gain	not used
file	/export/boas/-	spin	not used
nmr1/Punniyawurt-	hst	0.008	
hy_L-4-cl-sonic.fl	pw90	18.700	
	d	20.000	
ACQUISITION		FLAGS	
sw	6389.8	il	n
at	1.898	in	n
np	25528	dp	y
fb	not used	hs	nm
bs	4		
d1	1.000	lb	0.10
nt	32	fn	65536
ct	32		
TRANSMITTER		PROCESSING	
tn	H1	sp	1542.7
tfre	399.853	rf1	1939.5
tof	362.8	rpf	888.4
tpwr	57	rp	137.2
pw	8.050	lp	-100.6
DECOUPLER		PLOT	
dn	C13	wc	250
dof	0	sc	0
dm	nm	vs	98
dmc	c	th	7.304
dpwr	50	nm	7.287
dmf	15900		7.282



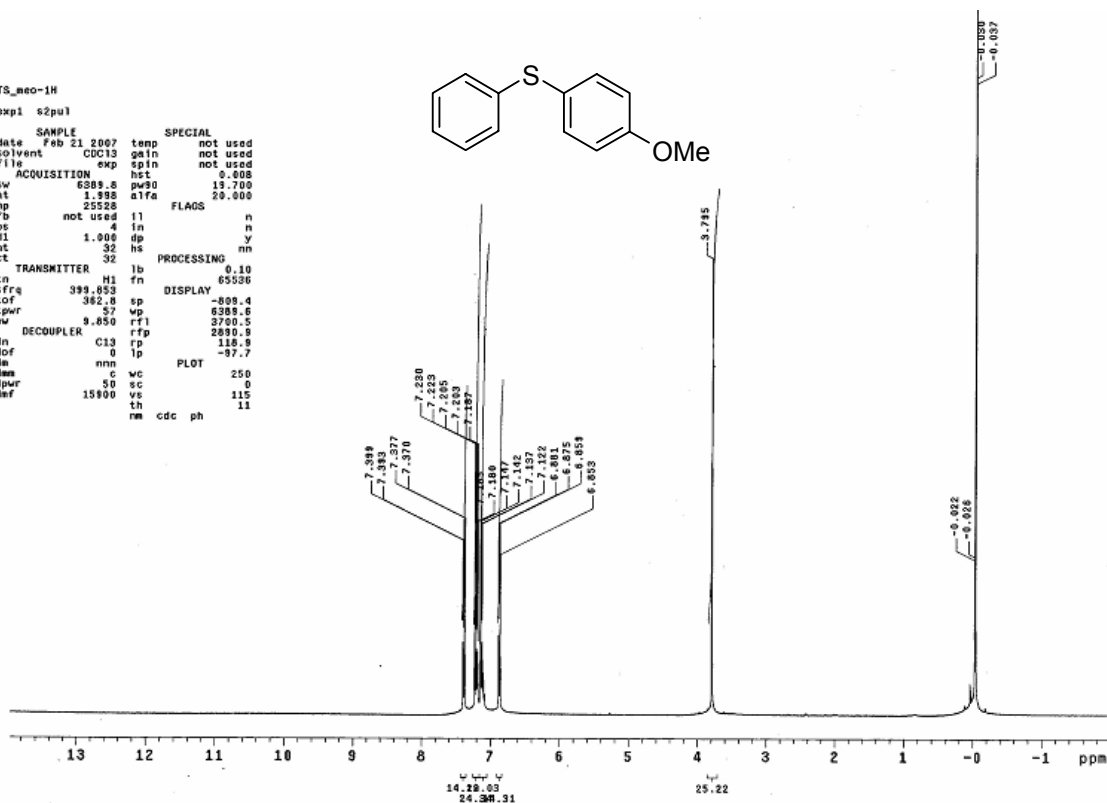
1-4-cl-13c-sonic
exp1 s2pu1

SAMPLE		SPECIAL	
date	Jun 11 2007	temp	not used
solvent	CDCl3	gain	not used
file	/export/boas/-	spin	not used
nmr1/Punniyawurt-	hst	0.008	
hy_L-4-cl-sonic.fl	pw90	18.600	
	d	20.000	
ACQUISITION		FLAGS	
sw	25125.6	il	n
at	1.199	in	n
np	60276	dp	y
fb	13800	hs	nm
bs	16		
d1	1.000	lb	2.00
nt	1000	fn	65536
ct	352		
TRANSMITTER		PROCESSING	
tn	C13	sp	-1506.9
tfre	100.554	rf1	25124.9
tof	1536.3	rpf	9272.6
tpwr	61	rp	7764.9
pw	3.300	lp	-93.3
DECOUPLER		PLOT	
dn	H1	wc	250
dof	0	sc	0
dmc	nm	vs	39
dpwr	8900	th	3
dmf		nm	no ph



TS_meo-1H
expt s2pul

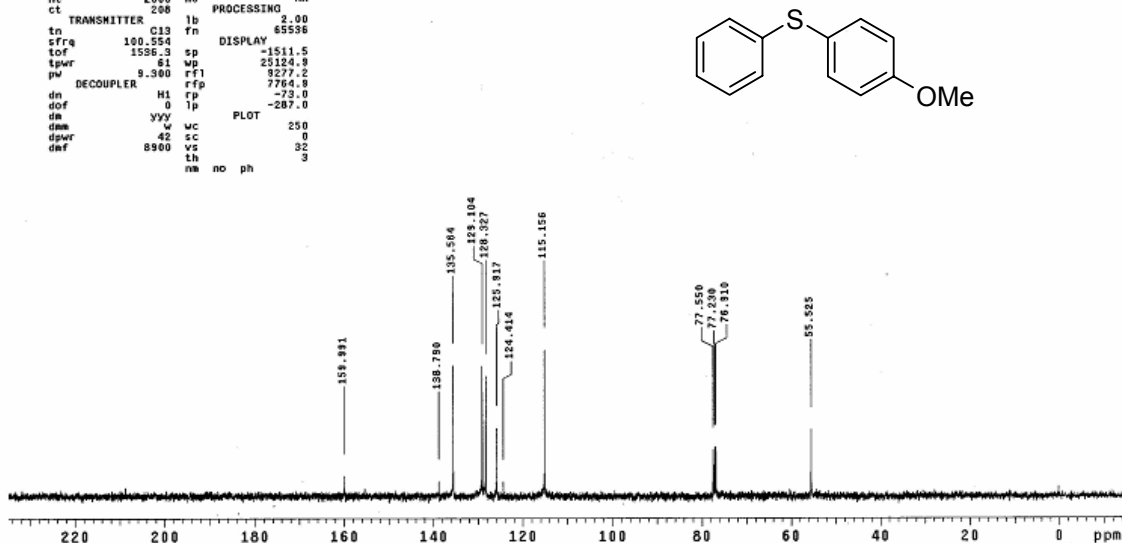
SAMPLE		SPECIAL	
date	Feb 21 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		SPECIAL	
sw	6389.6	hst	0.008
at	1.998	pw90	19.700
np	25528	atfa	20.000
fb	not used	il	n
bs	4	in	n
d1	1.000	dp	y
nt	32	hs	nm
ct	32		
TRANSMITTER		PROCESSING	
tn	H1	fb	0.10
sfreq	399.853	fn	65536
tof	362.0	sp	-808.4
tpwr	57	wp	6389.6
pw	9.850	rf1	3700.5
dn	DECOUPLER	rfp	2890.9
dof	C13	rp	115.9
da	nm	lp	-97.7
dma	c	wc	250
dpwr	50	sc	0
daf	15900	vs	115
	th	nm	cdc ph
			11



LT_Meo

expt s2pul

SAMPLE		SPECIAL	
date	Feb 18 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		SPECIAL	
sw	25125.6	hst	0.008
at	1.189	pw90	18.600
np	60270	atfa	20.000
fb	13600	il	n
bs	16	in	n
d1	1.000	dp	y
nt	2000	hs	nm
ct	208		
TRANSMITTER		PROCESSING	
tn	C13	fb	2.00
sfreq	100.554	fn	65536
tof	1536.3	sp	-1511.5
tpwr	61	wp	25124.9
pw	9.300	rf1	9277.2
dn	DECOUPLER	rfp	7764.9
dof	H1	rp	-73.0
da	YVY	lp	-287.0
dma	w	wc	250
dpwr	42	sc	0
daf	8900	vs	32
	th	nm	no ph
			3

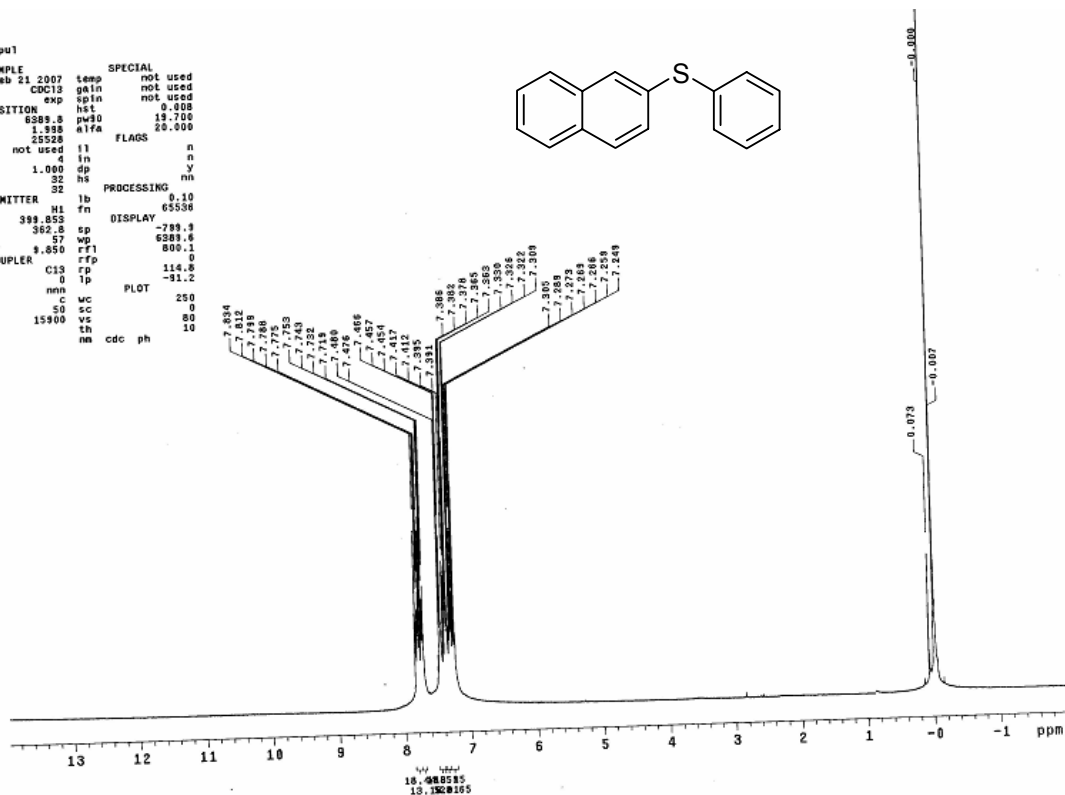
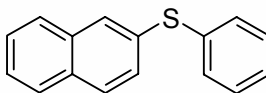


Ts_napth

exp1 s2pu1

SAMPLE SPECIAL
date Feb 21 2007 temp not used
solvent CDCl3 gain not used
file exp sp in not used
ACQUISITION hst 0.008
sw 6389.8 pw40 19.700
at 1.998 alfa 20.000
np 25528
fb not used il n
bs 4 in n
dl 1.000 dp y
nt 32 hs nn
ct 32

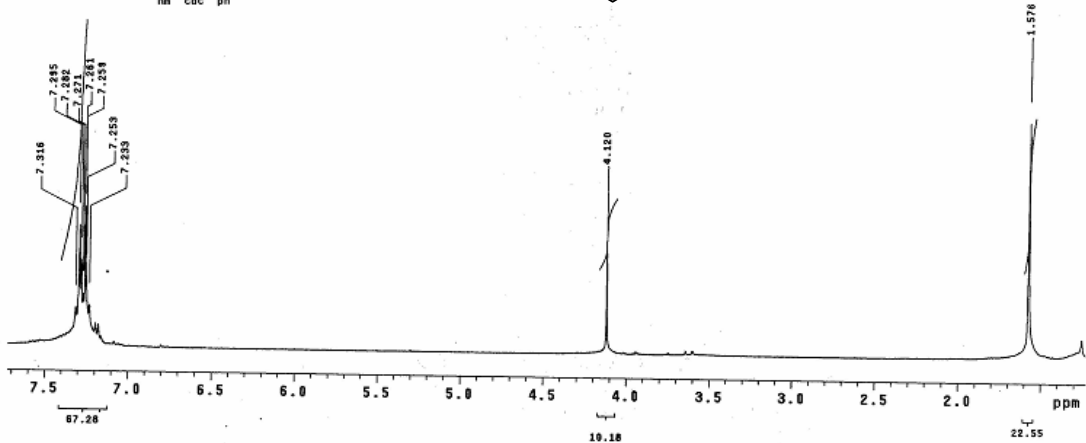
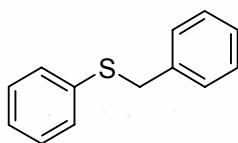
TRANSMITTER lb 0.10
tn H1 fn 65536
sfrq 399.853 DISPLAY
tof 362.8 sp -789.3
tpwr 57 wp 6389.6
pw 1.850 rfi 800.1
DECOUPLER C13 rp 114.8
dn 0 lp -81.2
dm nnn
dme 50
dpr 50
dmf 15900 vs 250
th 80
nm cdc ph 10



TS2_Pure

exp1 s2pu1

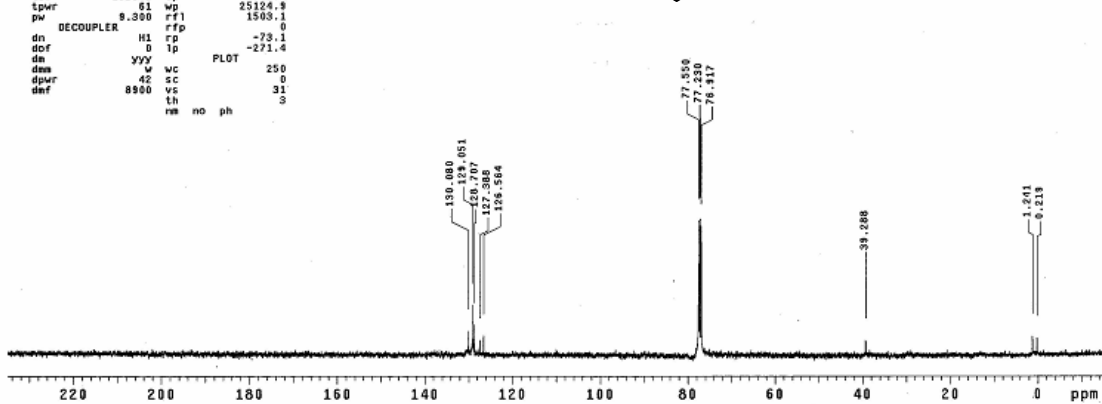
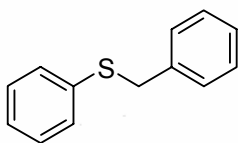
SAMPLE		SPECIAL	
date	Feb 13 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sv	6389.6	pu0	19.700
at	1.998	alfa	20.000
np	25528	FLAGS	
fb	not used	l1	n
bs	4	ln	n
d1	1.000	dp	y
nt	32	hs	nn
ct	20	PROCESSING	
TRANSMITTER		l1	fn
tn	H1	65536	
sfreq	399.853	DISPLAY	-785.2
tof	362.8	sp	6389.6
tpwr	57	wp	795.4
pw	9.850	rf1	0
DECOUPLER		rfp	119.1
dn	C13	lp	-79.5
dof	0	PLOT	
da	nnn	wc	250
dma	c	sc	0
dprf	50	vs	130
daf	15100	th	20
	na	cdc	ph



TS2_pure_13C

exp1 s2pu1

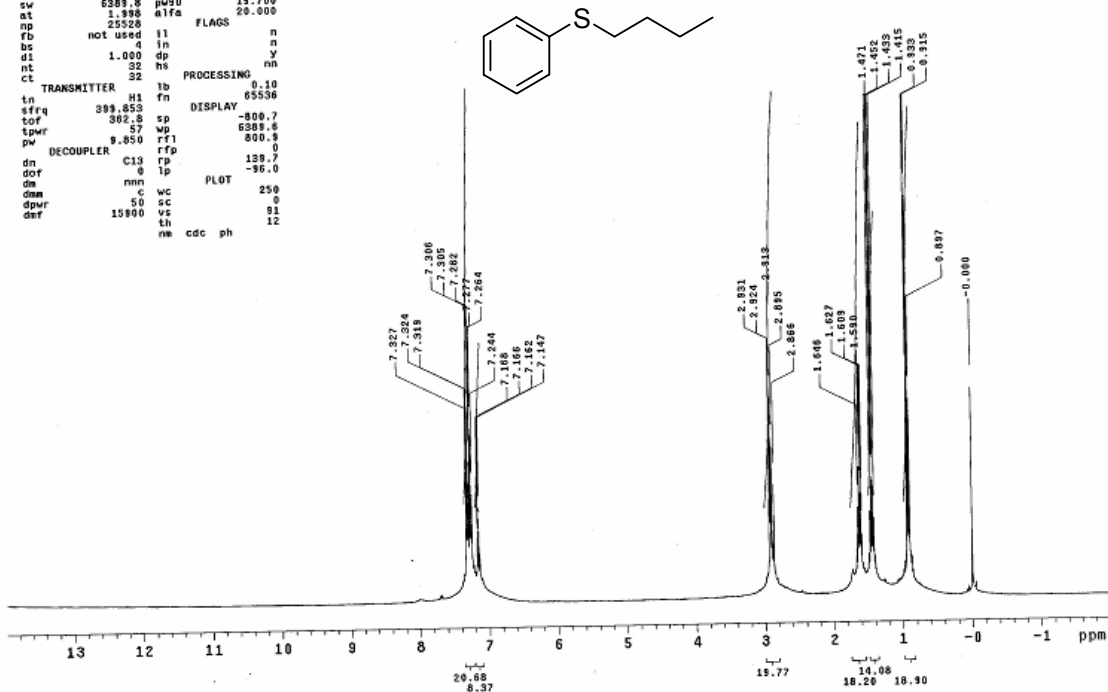
SAMPLE		SPECIAL	
date	Feb 13 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sv	25125.6	pu0	18.600
at	1.199	alfa	20.000
np	68270	FLAGS	
fb	13800	l1	n
bs	18	ln	n
d1	1.000	dp	y
nt	3000	hs	nn
ct	3000	PROCESSING	
TRANSMITTER		l1	fn
tn	C13	65536	
sfreq	100.534	DISPLAY	-1502.4
tof	1536.3	sp	25124.9
tpwr	61	wp	1503.1
pw	9.300	rf1	0
DECOUPLER		rfp	-73.1
dn	H1	lp	-271.4
dof	0	PLOT	
da	yyy	wc	250
dma	w	sc	0
dprf	42	vs	31
daf	8900	th	3
	rm	no	ph



YL-buty1-1H

expi s2pul

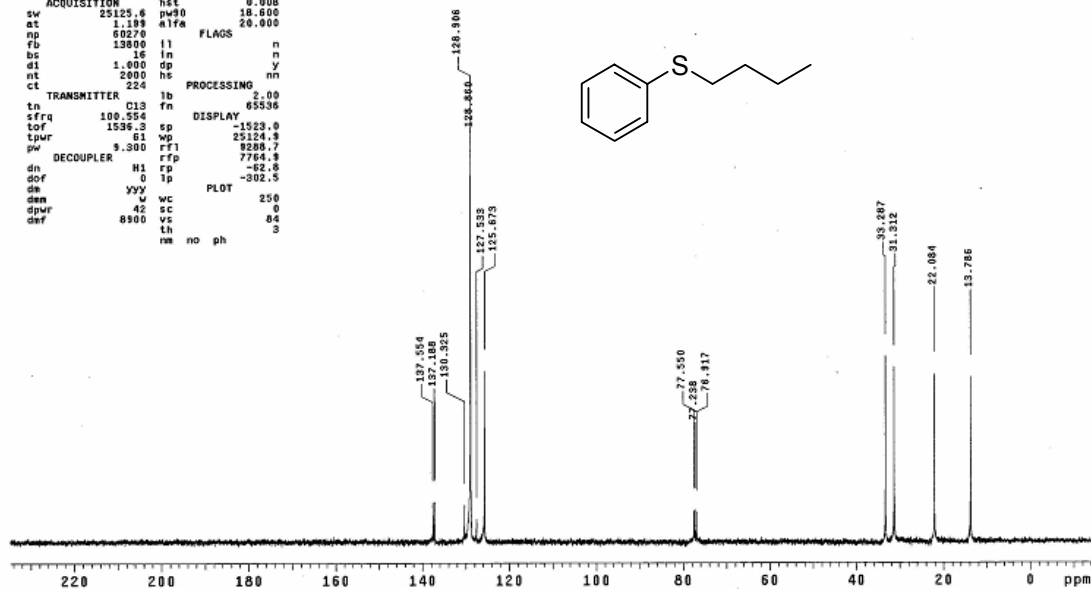
SAMPLE		SPECIAL	
date	Feb 22 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	6389.8	pw90	15.700
at	1.998	alfa	20.000
np	25528	FLAGS	
fb	not used	il	n
bs	1.000	dp	y
di	32	hs	nn
nt	32		
ct	32		
TRANSMITTER		lb	0.10
tn	H1	fn	65536
sfrq	399.853	sp	-800.7
tofr	302.8	wp	6389.8
tpwr	9.850	rfl	800.8
pw		rpf	0
DECOUPLER		rp	129.7
dn	C13	lp	-36.0
dof	0		
dm	nnn	wc	250
dme	50	sc	0
dpar	15900	vs	91
dof		th	12
		ne	cdc ph



TS-buty1-13C

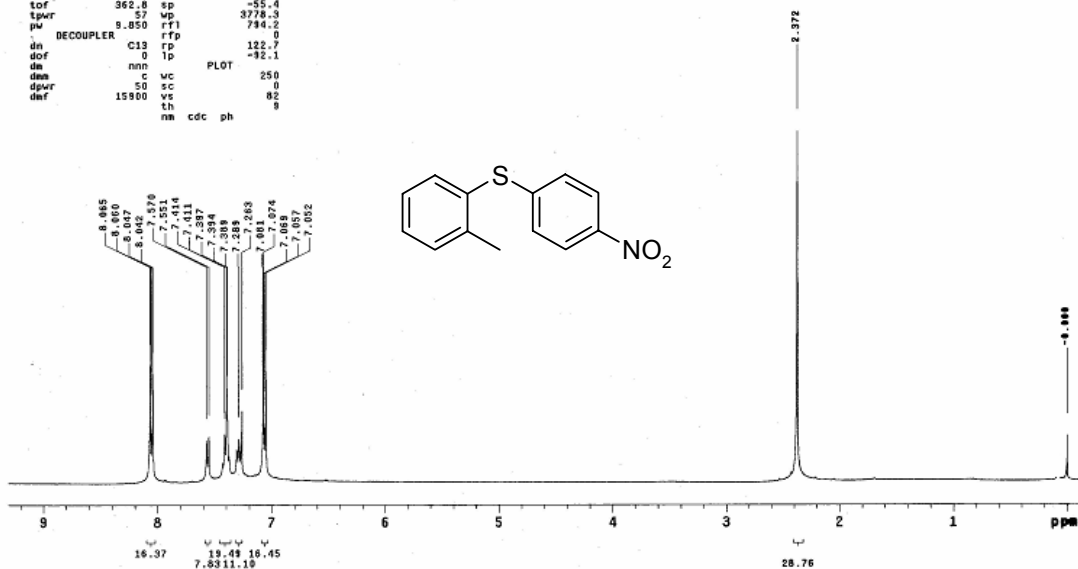
expi s2pul

SAMPLE		SPECIAL	
date	Feb 21 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	25125.6	pw90	18.800
at	1.189	alfa	20.000
np	60220	FLAGS	
fb	13000	il	n
bs	16	in	n
di	1.000	dp	y
nt	2000	hs	nn
ct	224		
TRANSMITTER		lb	2.00
tn	C13	fn	65536
sfrq	100.554	sp	-1523.0
tofr	1536.3	wp	25124.9
tpwr	61	rfl	8286.7
pw	9.300	rpf	7764.9
DECOUPLER		rp	-62.6
dn	H1	lp	-302.5
dof	0		
dm	YYY	wc	250
dme	42	sc	0
dpar	8900	vs	84
dof		th	0
		ne	no ph



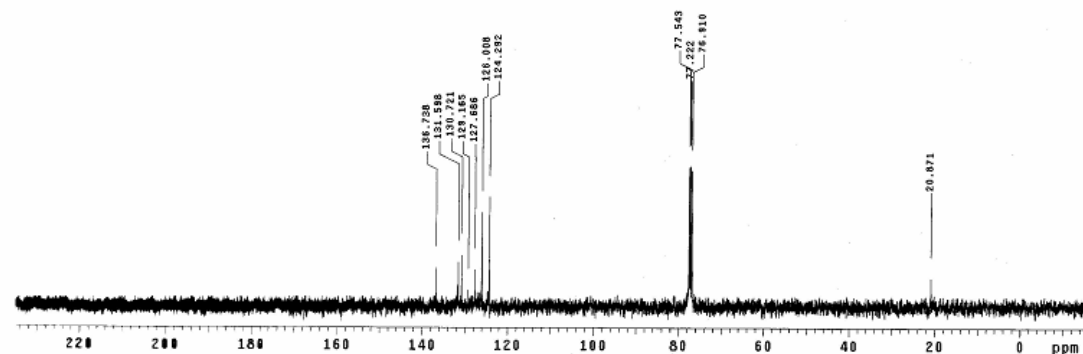
ps-2-mtb-no2
exp1 s2pul

SAMPLE		SPECIAL	
date	Jul 26 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	
sw	6389.8	pw90	0.008
at	1.358	a1fa	15.700
np	25528	flags	20.000
fb	not used	l1	n
bs	4	in	n
d1	1.000	dp	y
nt	32	hs	nn
ct	32	PROCESSING	
tn	TRANSMITTER	l1	0.10
sfre	399.053	fn	65536
tof	362.8	sp	-55.4
tpwr	57	wp	3778.3
pw	9.850	rf1	794.2
dn	DECOUPLER	rfp	0
dof	C13	rp	122.7
dm	nmh	lp	-92.1
dpr	50	vc	250
daf	15900	vs	82
		th	8
		nm	cdc ph



ps-2-mtb-no2
exp1 s2pul

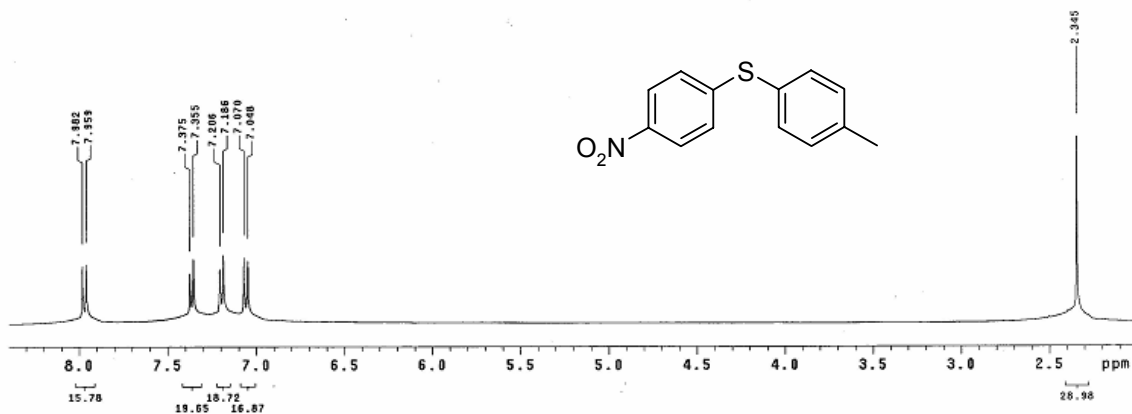
SAMPLE		SPECIAL	
date	Jul 26 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	
sw	25125.6	pw90	18.600
at	1.199	a1fa	20.000
np	68270	flags	
fb	13800	l1	n
bs	16	in	n
d1	1.000	dp	y
nt	2080	hs	nn
ct	432	PROCESSING	
tn	TRANSMITTER	l1	2.00
sfre	100.554	fn	65536
tof	1536.3	sp	-1506.2
tpwr	61	wp	25124.8
pw	9.300	rf1	8271.8
dn	DECOUPLER	rfp	7764.3
dof	0	lp	-86.4
dm	yyv	vc	-271.4
dpr	42	vs	250
daf	8100	th	32
		nm	no ph



TS-Tolyl-4-N02I

expl s2pul

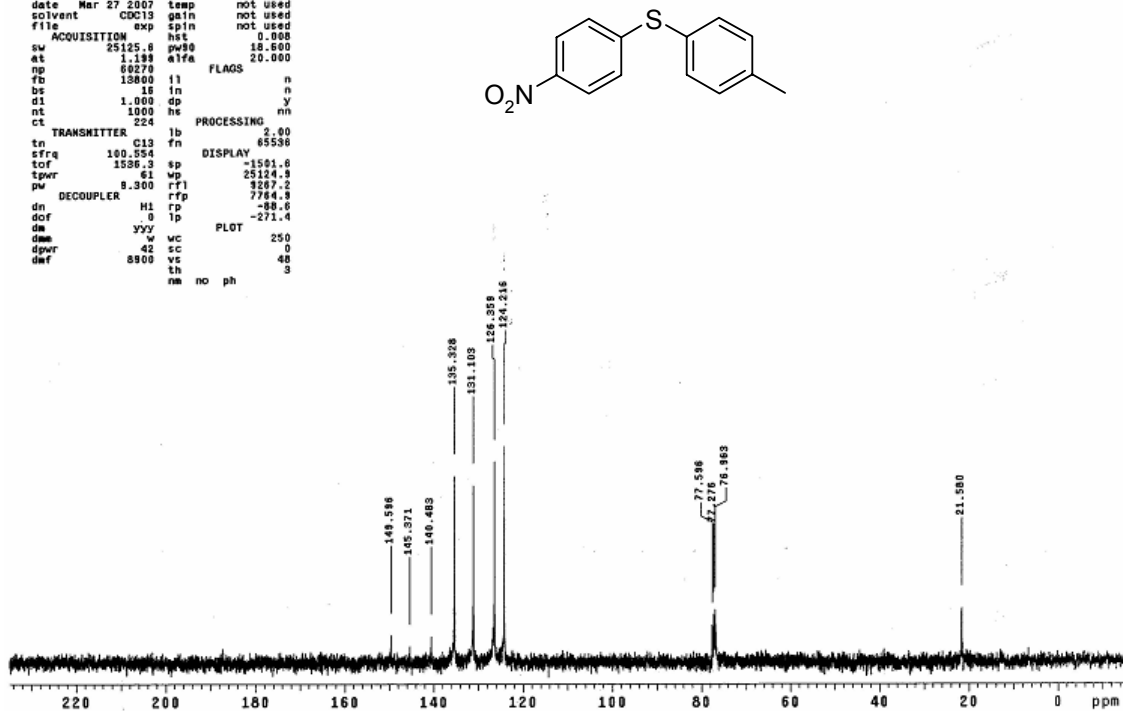
SAMPLE		SPECIAL	
date	Mar 27 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	8389.8	pw90	19.700
at	1.998	alpha	20.000
np	25528	FLAGS	
fb	not used	l1	n
bs	4	ln	n
d1	1.000	dp	y
nt	32	hs	nn
ct	32	PROCESSING	0.10
TRANSMITTER		lb	85536
tn	H1	fn	
sfrq	399.853	DISPLAY	805.5
tof	362.8	sp	2552.4
tpwr	57	wp	823.5
pw	8.850	rfl	0
DECOUPLER		rfl	0
dn	C13	rp	125.8
dof	0	lp	-111.4
dm	nnn	PLOT	250
dpr	50	sc	0
dwf	15900	vs	41
		th	8
	nm	cdc	ph



TS-Tolul-4N02I-13C

expl s2pul

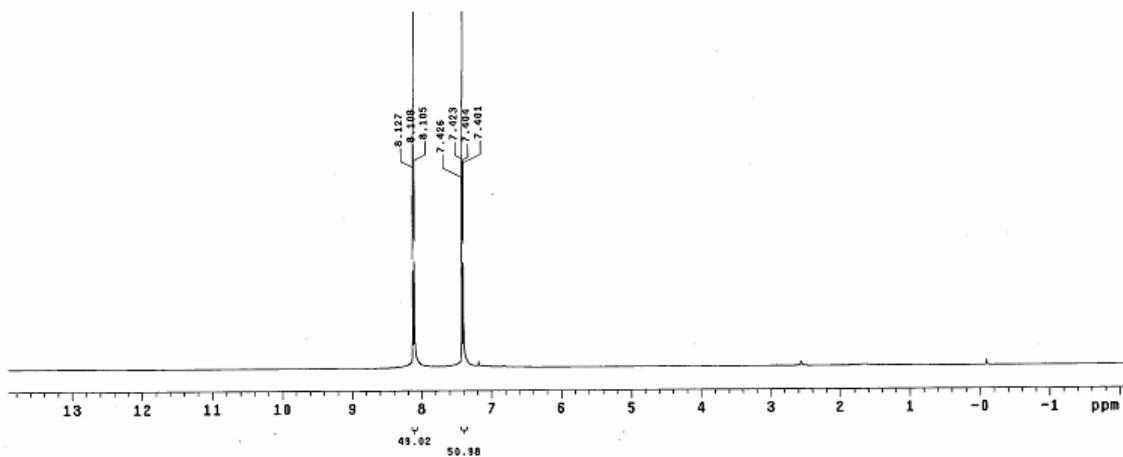
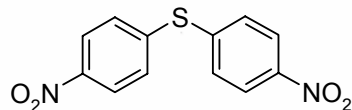
SAMPLE		SPECIAL	
date	Mar 27 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	25125.8	pw90	18.600
at	1.198	alpha	20.000
np	66270	FLAGS	
fb	13800	l1	n
bs	16	ln	n
d1	1.000	dp	y
nt	1000	hs	nn
ct	224	PROCESSING	2.00
TRANSMITTER		lb	65536
tn	C13	fn	
sfrq	100.624	DISPLAY	-1501.6
tof	1536.3	sp	25124.9
tpwr	61	wp	9287.2
pw	8.300	rfl	7764.9
DECOUPLER		rfl	-88.6
dn	H1	rp	-271.4
dof	0	lp	
dm	yyy	PLOT	250
dpr	42	sc	0
dwf	8900	vs	48
		th	3
	nm	no	ph



TS-4-NO2-NO2

exp1 s2pul

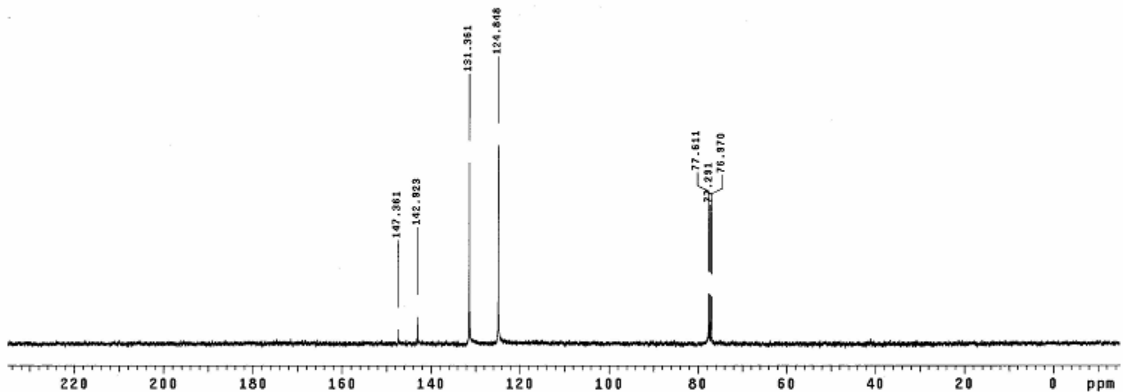
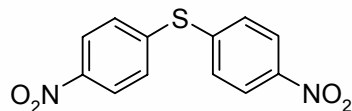
SAMPLE		SPECIAL	
date	Apr 1 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		ht	0.008
sw	6389.8	pu90	18.700
at	1.998	alpha	20.000
np	25528	FLAGS	
rb	not used	l1	n
bs	4	ln	n
d1	1.000	dp	y
nt	32	hs	nn
ct	32	PROCESSING	
TRANSMITTER		lb	0.10
tn	H1	fn	65536
sfrq	389.853	sp	-825.6
tof	362.8	wp	6389.6
tpwr	57	rft	825.6
pw	9.850	rft	0
DECOUPLER		rp	124.7
dn	C13	lp	-105.6
dof	0	pl	
da	nnn	PLOT	
dma	c	wc	250
dpar	50	sc	0
daf	15900	vs	24
	th	ph	6



TS-4NO2-4NO2-13C

exp1 s2pul

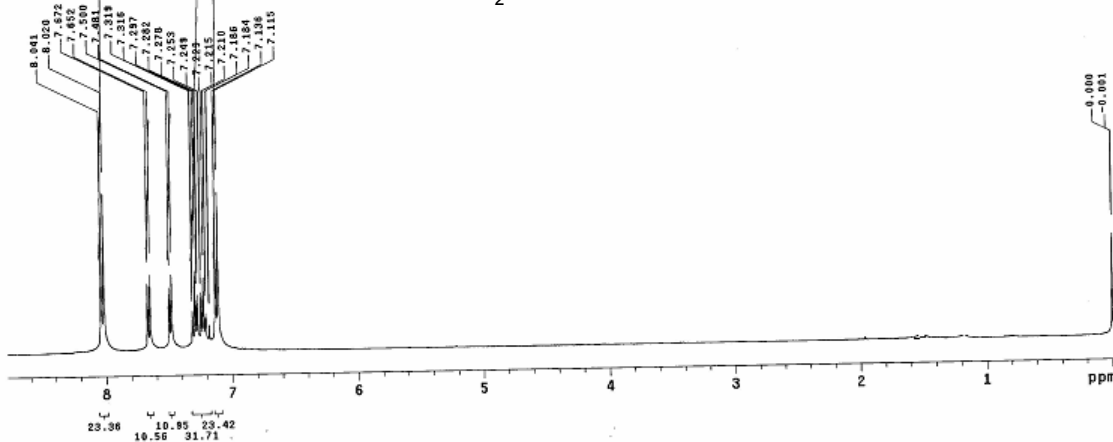
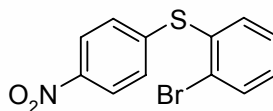
SAMPLE		SPECIAL	
date	Apr 1 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		ht	0.008
sw	25125.6	pu90	18.600
at	1.199	alpha	20.000
np	80278	FLAGS	
rb	13800	l1	n
bs	32	ln	n
d1	1.000	dp	y
nt	1000	hs	nn
ct	576	PROCESSING	
TRANSMITTER		lb	2.00
tn	C13	fn	65536
sfrq	100.624	sp	-1502.4
tof	1536.3	wp	25124.9
tpwr	61	rft	1503.1
pw	9.300	rft	0
DECOUPLER		rp	-5.5
dn	H1	lp	-440.7
dof	0	pl	
da	yzy	PLOT	
dma	w	wc	250
dpar	42	sc	0
daf	8800	vs	44
	th	ph	2



TS-2Br-NO2

expl s2pu1

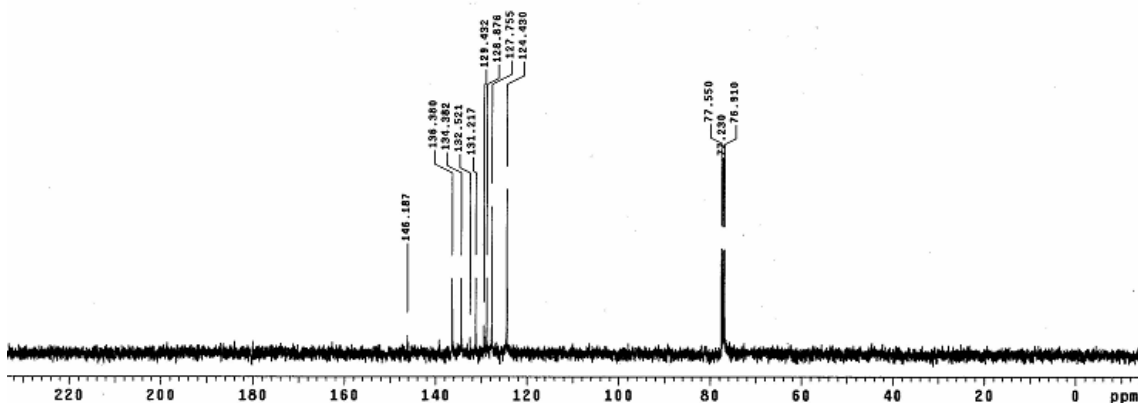
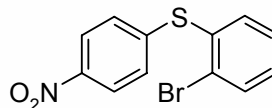
SAMPLE		SPECIAL	
date	Apr 1 2007	temp	not used
solvent	CDCl3	gain	not used
file		exp	not used
ACQUISITION		SPECIAL	
sw	538.8	pw90	19.700
at	1.998	alpha	20.000
np	25528	flags	
fb	not used	l1	n
bs	4	in	n
dl	1.000	dp	y
nt	32	hs	nn
ct	32	hs	
TRANSMITTER		PROCESSING	
tn	H1	fb	9.10
sfrq	399.853	fn	65536
tof	362.8	sp	-25.4
tpwr	57	wp	3537.3
pw	9.850	rfl	825.8
DECOUPLER		PLOT	
dn	C13	rp	129.2
dof	0	lp	-100.1
dm	nnn	wc	250
dpr	50	sc	0
def	15900	vs	36
		th	6
		nm	
		cac	ph



TS-Br-NO2

expl s2pu1

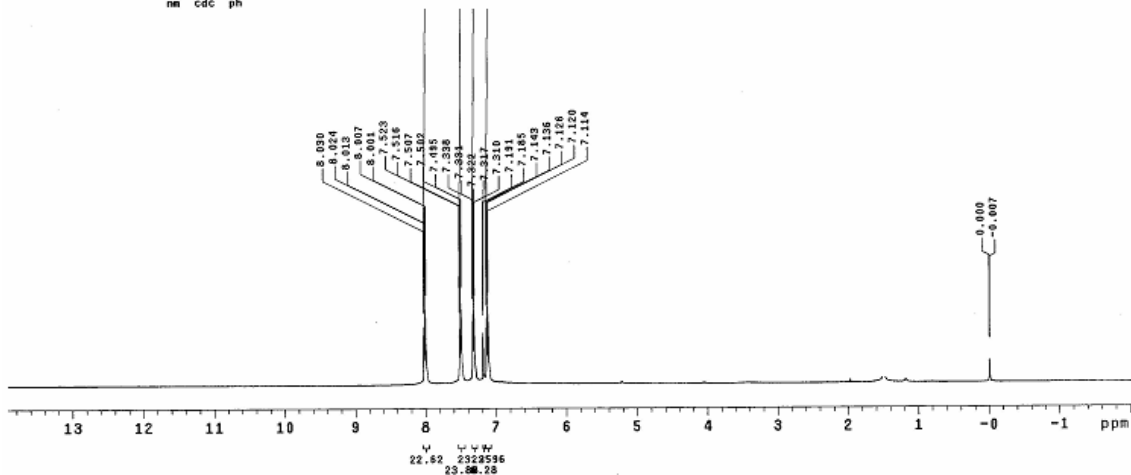
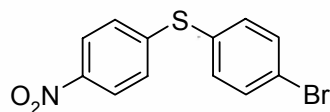
SAMPLE		SPECIAL	
date	Apr 1 2007	temp	not used
solvent	CDCl3	gain	not used
file		exp	not used
ACQUISITION		SPECIAL	
sw	25125.6	pw90	18.600
at	1.189	alpha	20.000
np	66270	flags	
fb	13800	l1	n
bs	32	in	n
dl	1.000	dp	y
nt	1000	hs	nn
ct	320	hs	
TRANSMITTER		PROCESSING	
tn	C13	fb	2.00
sfrq	100.554	fn	65536
tof	1536.3	sp	-1505.4
tpwr	61	wp	25124.3
pw	9.300	rfl	1506.2
DECOUPLER		PLOT	
dn	H1	rp	-82.8
dof	0	lp	-271.4
dm	yyy	wc	250
dpr	42	sc	0
def	8900	vs	36
		th	3
		nm	no ph



TS-Br-4NO2I

exp1 s2pu1

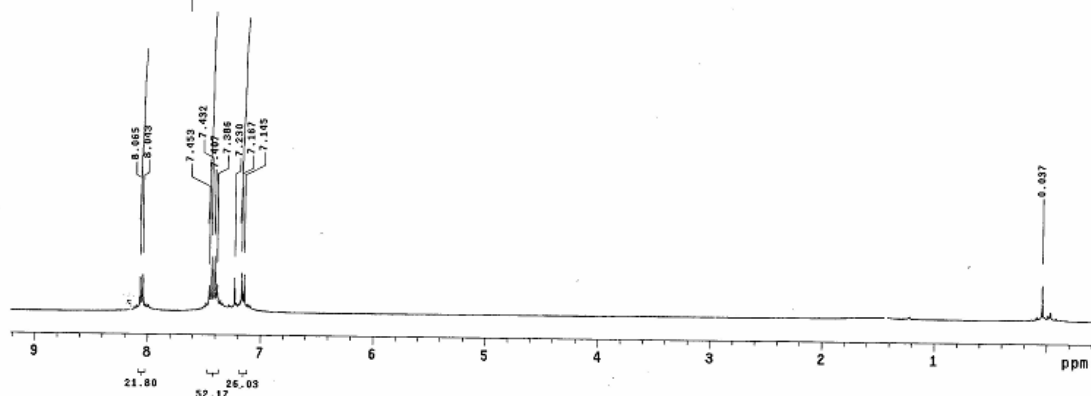
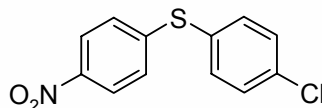
SAMPLE		SPECIAL	
date	Mar 27 2007	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		SPECIAL	
sw	8398.8	hst	0.008
at	1.998	pw	19.700
np	25528	alpha	20.000
fb	not used	flags	n
bs	4	in	n
dl	1.000	dp	y
nt	32	hs	nn
ct	32		
TRANSMITTER		PROCESSING	
tn	H1	fb	8.10
sfreq	399.853	fn	65536
tof	362.8	sp	-822.1
tpwr	57	up	6389.6
pw	9.850	rfl	822.3
DECOUPLER		PLOT	
dn	C13	rfp	0
dof	0	lp	-90.0
dm	nnn	wc	250
dma	50	sc	0
dpwr	15900	vs	24
dmf		th	4
		nm	cdc ph



4-cl-no2

exp1 s2pu1

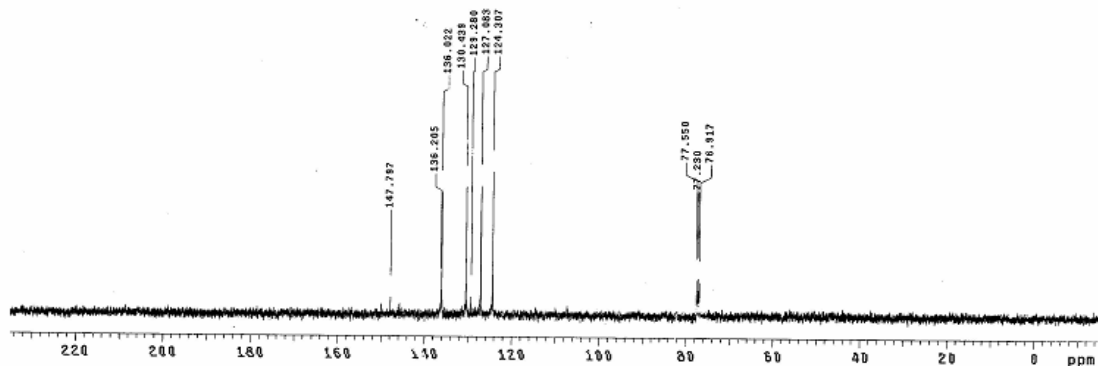
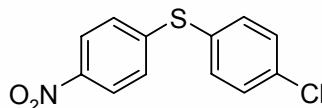
SAMPLE		SPECIAL	
date	Apr 19 2007	temp	not used
solvent	CDCl3	gain	not used
file		spin	not used
ACQUISITION		SPECIAL	
sw	6389.8	hst	0.000
at	1.998	pw90	15.700
np	25528	alpha	20.000
fb	not used	ll	n
bs	4	in	n
d1	1.000	dp	y
nt	32	hs	nm
ct	32		
TRANSMITTER		PROCESSING	
tn	h1	lb	0.10
sfrq	399.853	fn	65536
tor	362.8	sp	-169.0
tpwr	57	wp	3853.0
pw	9.850	rfl	3838.0
deCOUPLER	C13	rtp	2830.0
dn	0	rp	138.6
dof	0	lp	-100.3
da	nnn		
dma	c	vc	250
dpwr	50	sc	0
daf	15900	vs	24
		th	5
		nm	cdc ph



TS28-130

exp1 s2pu1

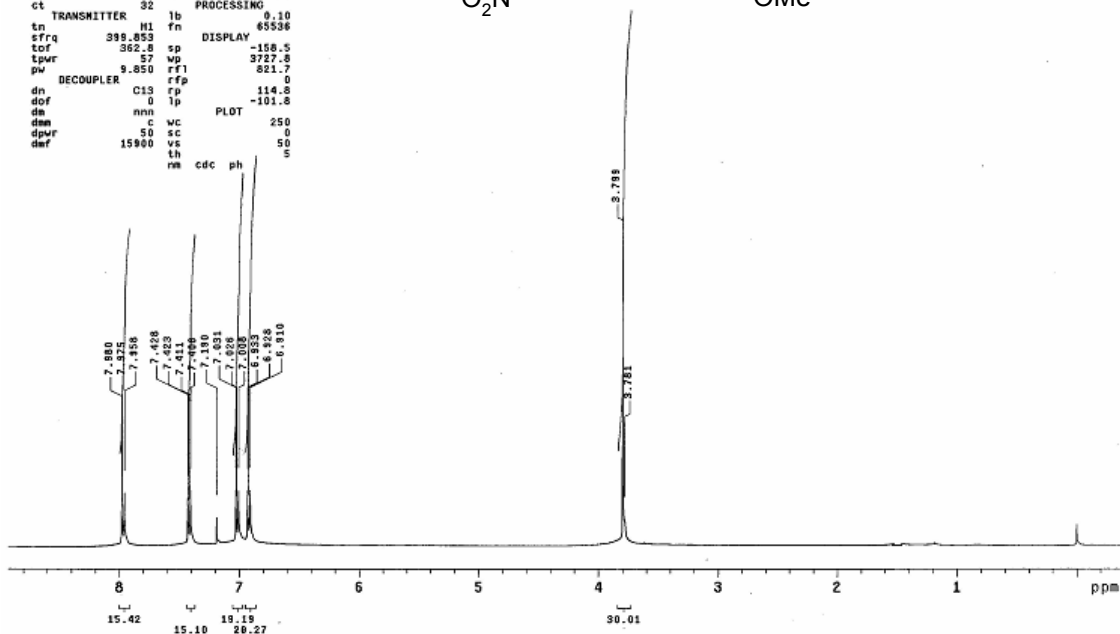
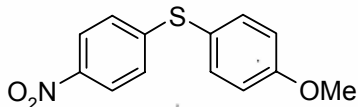
SAMPLE		SPECIAL	
date	Apr 12 2007	temp	not used
solvent	CDCl3	gain	not used
file		spin	not used
ACQUISITION		SPECIAL	
sw	25125.6	hst	0.000
at	1.189	pw90	18.600
np	60270	alpha	20.000
fb	13800	ll	n
bs	16	in	n
d1	1.000	dp	y
nt	2000	hs	nm
ct	200		
TRANSMITTER		PROCESSING	
tn	C13	lb	2.00
sfrq	100.625	fn	65536
tor	1536.8	sp	-1518.0
tpwr	61	wp	25124.3
pw	9.300	rfl	3275.7
deCOUPLER	H1	rtp	7764.3
dn	0	rp	-88.6
dof	0	lp	-271.4
da	yyy		
dma	w	vc	250
dpwr	42	sc	0
daf	8900	vs	33
		th	3
		nm	no ph



TS-Anisyl-4NO2I

exp1 s2pul

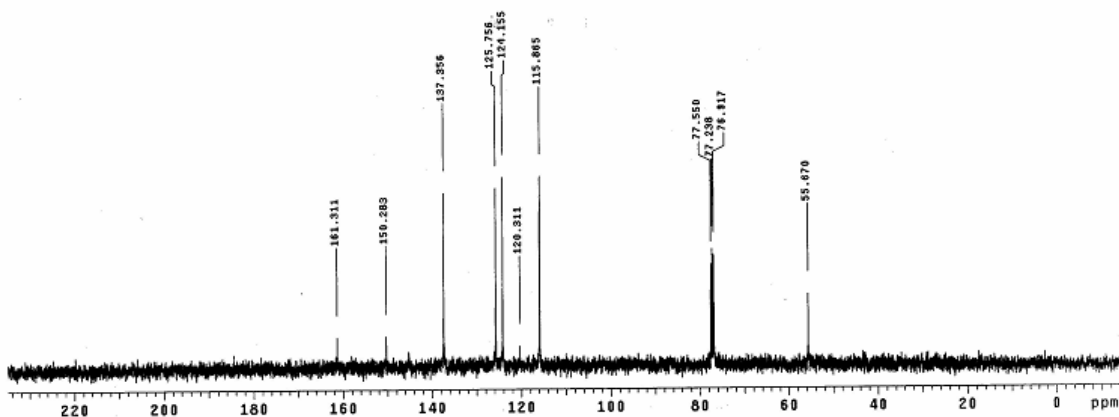
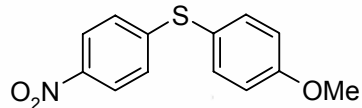
SAMPLE		SPECIAL	
date	Mar 27 2007	temp	not used
solvent	CDC13	gain	not used
file	exp	spin	not used
ACQUISITION		SPECIAL	
sw	6389.8	hst	0.088
at	1.998	atfa	19.760
np	25528	flags	20.000
fb	not used	l1	n
bs	4	ln	n
d1	1.000	dp	y
nt	32	hs	nn
ct	32		
TRANSMITTER		PROCESSING	
tn	H1	fb	0.10
sfreq	399.853	fn	65536
tof	362.8	sp	DISPLAY
tpwr	57	wp	-158.5
pw	9.850	rf1	3727.8
		rfp	821.7
DECOUPLER		PLOT	
dn	C13	fp	114.8
dof	0	lp	-101.8
dm	nn	wc	250
dpr	50	sc	0
daf	15900	vs	50
	th	nm	5
	cdc	ph	



TS-Anisyl-4-NO2I-13C

exp1 s2pul

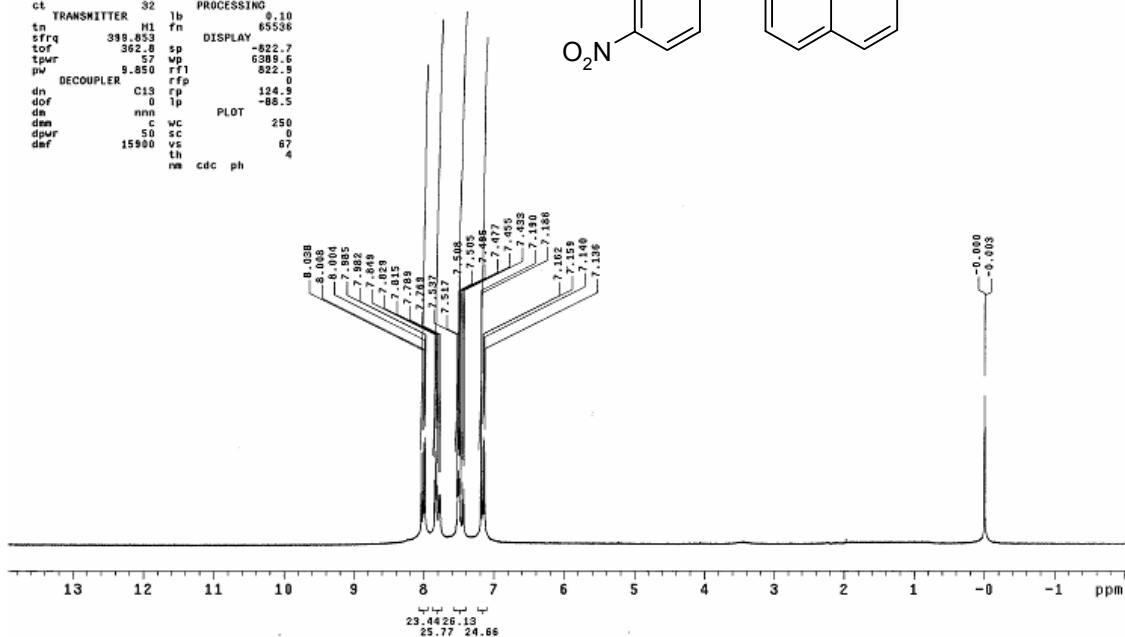
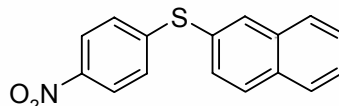
SAMPLE		SPECIAL	
date	Mar 27 2007	temp	not used
solvent	CDC13	gain	not used
file	exp	spin	not used
ACQUISITION		SPECIAL	
sw	25125.6	hst	0.088
at	1.198	atfa	19.760
np	80270	flags	20.000
fb	13800	l1	n
bs	32	ln	n
d1	1.000	dp	y
nt	1000	hs	nn
ct	280		
TRANSMITTER		PROCESSING	
tn	C13	fb	2.00
sfreq	100.624	fn	65536
tof	1536.3	sp	DISPLAY
tpwr	61	wp	-1504.6
pw	9.300	rf1	25124.9
		rfp	8270.3
DECOUPLER		PLOT	
dn	H1	fp	7764.9
dof	0	lp	-70.0
dm	yyy	wc	-304.3
dpr	42	sc	250
daf	8900	vs	0
	th	nm	42
	no	ph	4



exp1 s2pu1

SAMPLE

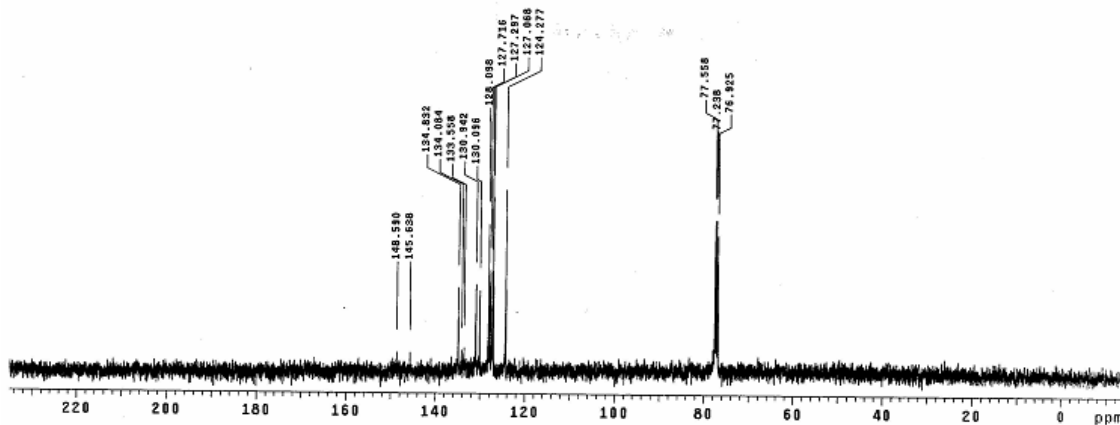
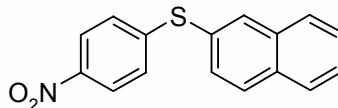
date	Mar 27 2007	temp	not used
solvent	CDCl3	gain	not used
1	1	spin	not used
ACQUISITION		hst	0.008
sv	6389.8	psv50	18.700
at	1198	1194	20.000
nb	25528		
fl			FLAOS
fp		11	n
bs	4	1n	n
d1	1.000	dp	y
ns	32	hs	n
ac	32		
TRANSMITTER			PROCESSING
h1	fb		0.010
tr			65536
sn	398.853		
rf	362.8	sp	-822.7
wp		wp	6398.5
pw	9.850	rf1	822.9
DECOUPLER		rpf	
c13			124.9
dof		0 1p	-88.5
nm	nmn		
wc			PLOT
50	50	sc	250
vs			0
th			67
nm	cdc	ph	



TS-Naph-4-NO2Y

exp1 s2pu1

SAMPLE			SPECIAL		
date	Mar 27	2007	temp	not used	
solvent	CDCl3	gain	exp	not used	
file		spin	spin	not used	
ACQUISITION			PROC		
sv	25125.6	int	pw90	18.600	
at	1.139	acq	af1a	0.000	
ft	600.0	res		20.000	
fb	13580.0	f1		FLAGS	
sw	32	in		n	n
pr	1.000	dp		y	m
nt	1000	hs			
ct	352	lb			
TRANSMITTER			PROCESSING		
tx	C13	fn		2.00	
srfrq	100.554			85538	
pc	1586.3	wp		-1504.6	
tpwr	81	rf		25124.9	
tf	8.300	rfl		8270.3	
		rpf		7764.9	
DECOUPLER			PLOT		
dn	H1	rp		-364.2	
df	0	lp			
dm	yyf	wc			
dpwr	42	vs		250	0
daf	8900	th			40
		nm		no	ph



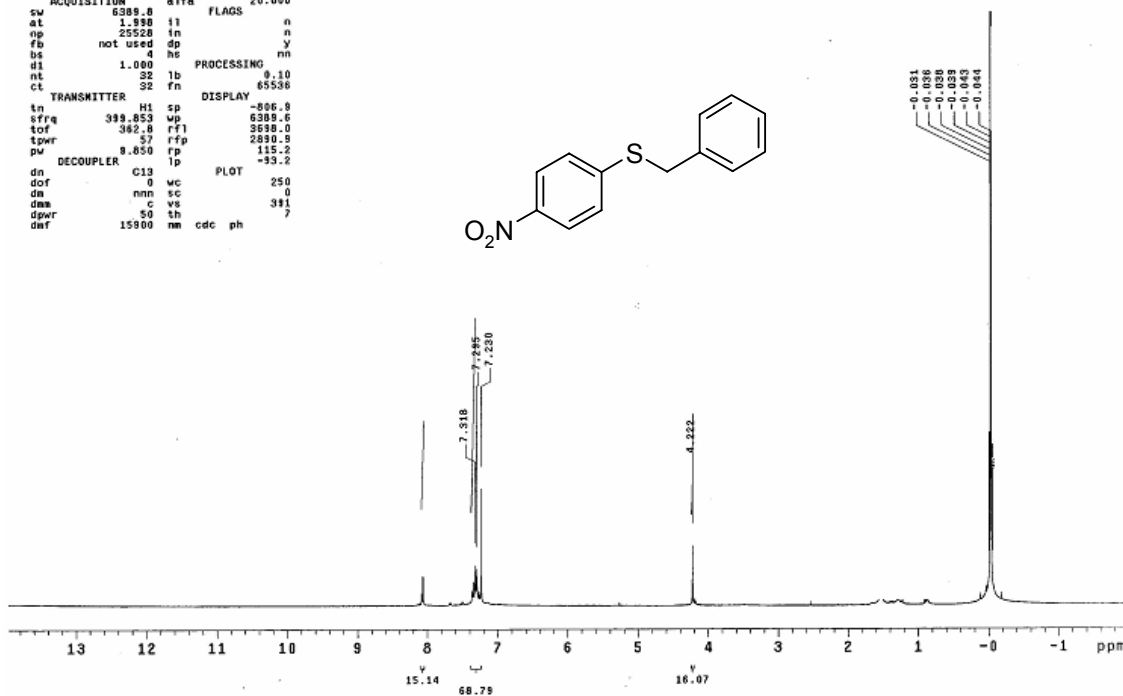
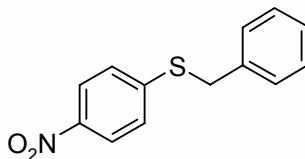
TS_16b_M
 expl s2pu1

SAMPLE		SPECIAL	
date	Mar 16 2007	temp	not used
solvent	CDCl3	gain	not used
file	/export/home/~	spin	not used
view1	Pannayamurthi	het	0.008
y_TS_16b_M.fid	pw90	15.700	
ACQUISITION	alpha	20.000	

ACQUISITION		FLAGS	
sw	6389.8	il	n
at	1.998	in	n
np	25528	dp	y
fb	not used	hs	nn
bs	4	hs	nn
dl	1.000	lb	0.10
nt	32	fn	65536
ct	32	fn	65536

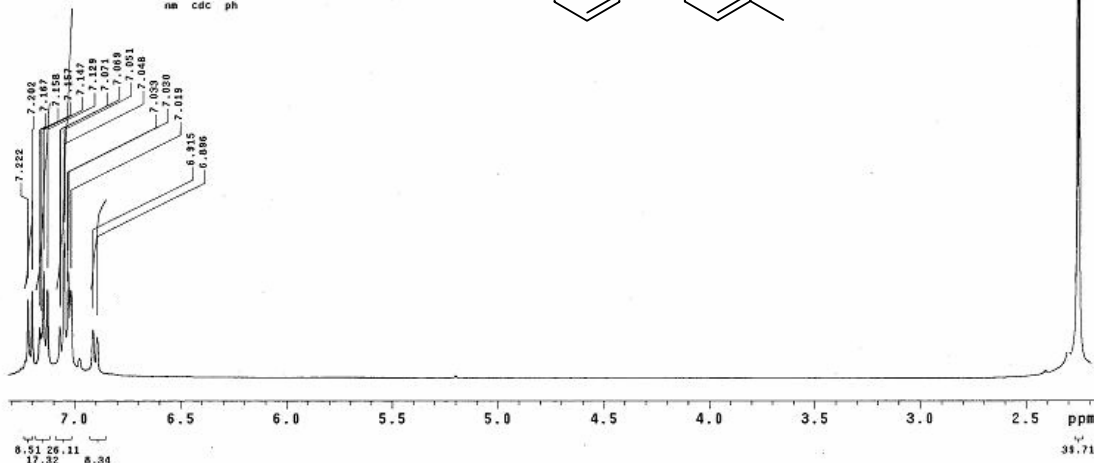
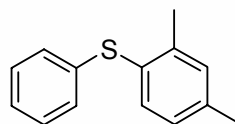
TRANSMITTER		DISPLAY	
tn	H1	sp	-806.8
sfrq	399.853	wp	6389.6
tof	362.6	rfl	3898.0
tpwr	5	rfl	2890.9
pw	9.850	rp	115.2
DECOUPLER	C13	lp	-93.2

PLOT	
dn	0
dof	0
dm	nn
dma	sc
dpwr	50
dnt	15900
na	cdc ph
7	



L-124dmib
 exp1 s2pul

SAMPLE		SPECIAL	
date	Jun 25 2007	temp	not used
solvent	CDC13	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	8384.8	pw90	18.700
at	1.998	alpha	20.000
np	25528	FLAGS	
fb	not used	l1	n
bs	4	in	n
d1	1.000	dp	y
nt	32	hs	nn
ct	32	PROCESSING	
tn	TRANSMITTER	lb	0.10
tfre	399.853	fn	65536
tof	362.8	sp	858.8
tpwr	57	wp	2085.4
pw	9.850	rfl	838.9
dn	DECOUPLER	rfl	0
dof	C13	rp	121.6
dm	nnn	lp	-91.0
dpr	50	vc	250
dpr	50	sc	0
dpr	15900	vs	111
dpr	nm	th	8
dpr	nm	cdc ph	



1-124-dmib
 exp1 s2pul

SAMPLE		SPECIAL	
date	Jun 26 2007	temp	not used
solvent	CDC13	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.008
sw	25125.8	pw90	18.600
at	1.199	alpha	20.000
np	60270	FLAGS	
fb	13800	l1	n
bs	18	in	n
d1	1.000	dp	y
nt	1800	hs	nn
ct	112	PROCESSING	
tn	TRANSMITTER	lb	2.00
tfre	C13	fn	65536
tof	100.504	sp	-1506.3
tpwr	1536.3	wp	25124.9
pw	01	rfl	9272.8
dn	DECOUPLER	rfl	7784.3
dof	H1	rp	-88.6
dm	0	lp	-271.4
dpr	yyv	vc	250
dpr	42	sc	0
dpr	8900	vs	14
dpr	th	th	2
dpr	nm	no ph	

