

Copies of NMR Spectra
For

Synthesis and anticancer activity studies of α -aminoalkylated conjugated nitroalkenes

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Table of Contents

	Page
1 Figure S1. ¹ H NMR Spectrum of 3a	3
2 Figure S2. ¹³ C NMR Spectrum of 3a	4
3 Figure S3. ¹ H- ¹ H NOESY Spectrum of 3a	5
4 Figure S4. ¹ H- ¹ H COSY Spectrum of 3a	6
5 Figure S5. ¹ H NMR Spectrum of 3b	7
6 Figure S6. ¹³ C NMR Spectrum of 3b	8
7 Figure S7. ¹³ C NMR Spectrum of 3b (Expansion)	9
8 Figure S8. ¹ H NMR Spectrum of 3c	10
9 Figure S9. ¹³ C NMR Spectrum of 3c	11
10 Figure S10. ¹ H NMR Spectrum of 3d	12
11 Figure S11. ¹³ C NMR Spectrum of 3d	13
12 Figure S12. ¹³ C NMR Spectrum of 3d (Expansion)	14
11 Figure S13. ¹ H NMR Spectrum of 3e	15
12 Figure S14. ¹³ C NMR Spectrum of 3e	16
13 Figure S15. ¹ H NMR Spectrum of 3f	17
14 Figure S16. ¹³ C NMR Spectrum of 3f	18
15 Figure S17. ¹ H NMR Spectrum of 3g	19
16 Figure S18. ¹³ C NMR Spectrum of 3g	20
17 Figure S19. ¹ H NMR Spectrum of 3h	21

18	Figure S20. ^{13}C NMR Spectrum of 3h	22
19	Figure S21. ^1H NMR Spectrum of 3i	23
20	Figure S22. ^{13}C NMR Spectrum of 3i	24
21	Figure S23. ^1H NMR Spectrum of 3j	25
22	Figure S24. ^{13}C NMR Spectrum of 3j	26
23	Figure S25. ^{13}C NMR Spectrum of 3j (Expansion)	27
24	Figure S26. ^1H NMR Spectrum of 3k	28
25	Figure S27. ^{13}C NMR Spectrum of 3k	29

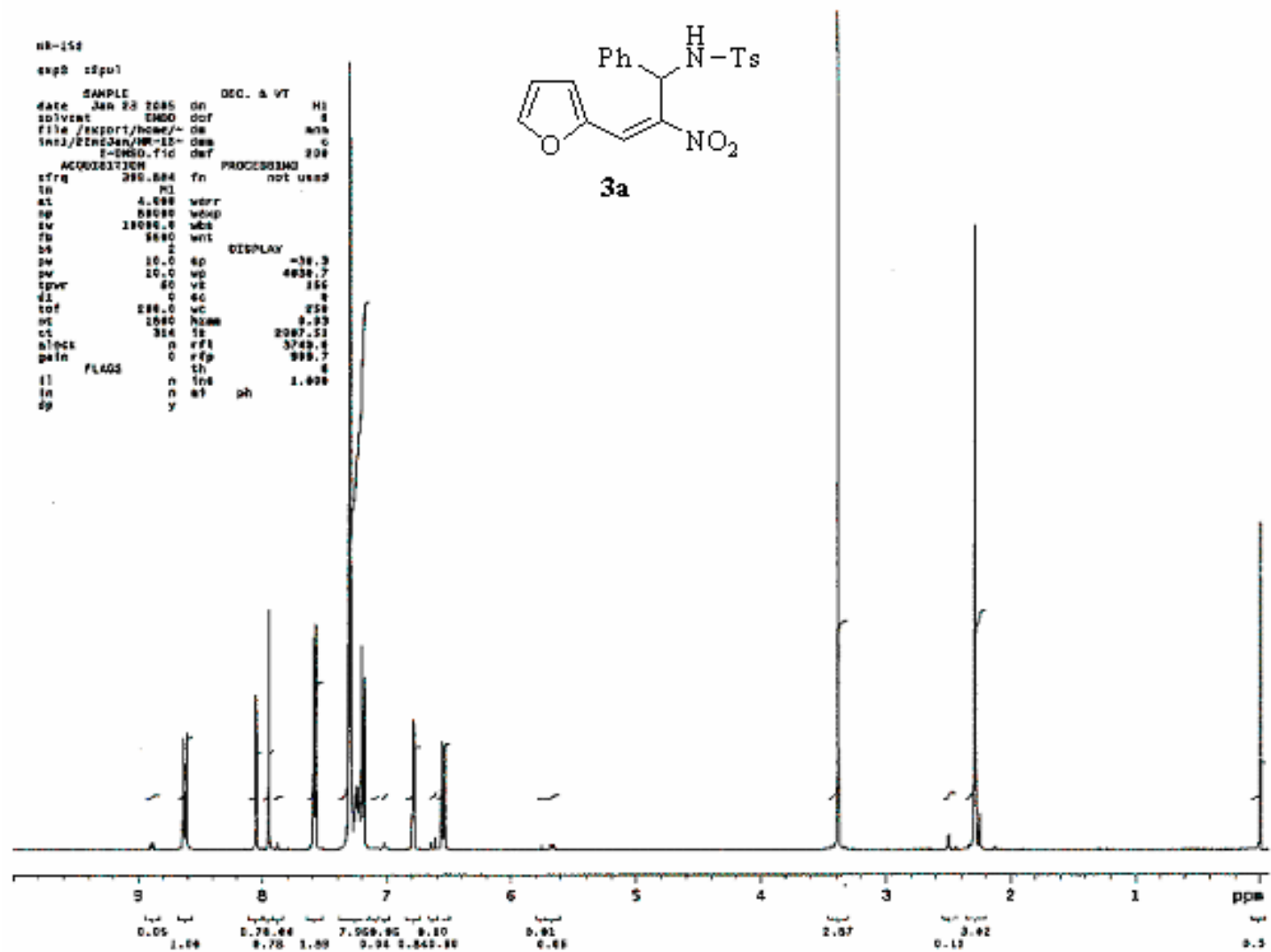


Figure S1. ¹H NMR Spectrum of 3a

NR-152

cp2 CARBON

date	Jan 31 2005	temp	not used
solvent	DMSO	gain	not used
file /export/ROSA/		spin	not used
quest/internal/24H-		hst	0.000
-25/31-dm/INM-ME-		pv20	14.000
152-de-C13.fid		alfa	20.000
ACQUISITION			
sv	25125.6	fl	n
as	1.130	in	n
sp	40270	ep	n
rb	13000	hs	y
bc	4	PROCESSED	on
dl	1.000	to	1.00
nt	2400	fn	not used
ct	2191	DISPLAY	
TRANSMITTER			
tn	C13	vg	-261.7
sfrq	100.622	rft	14474.6
tof	1554.3	rff	5020.0
tpwr	36	rp	3971.7
pw	7.000	lp	-281.6
DECOUPLER			
dn	H1	vc	250
dof	0	sc	0
dm	VVV	vb	121
dms	w	th	11
dpwr	41	at	ph
def	11900		

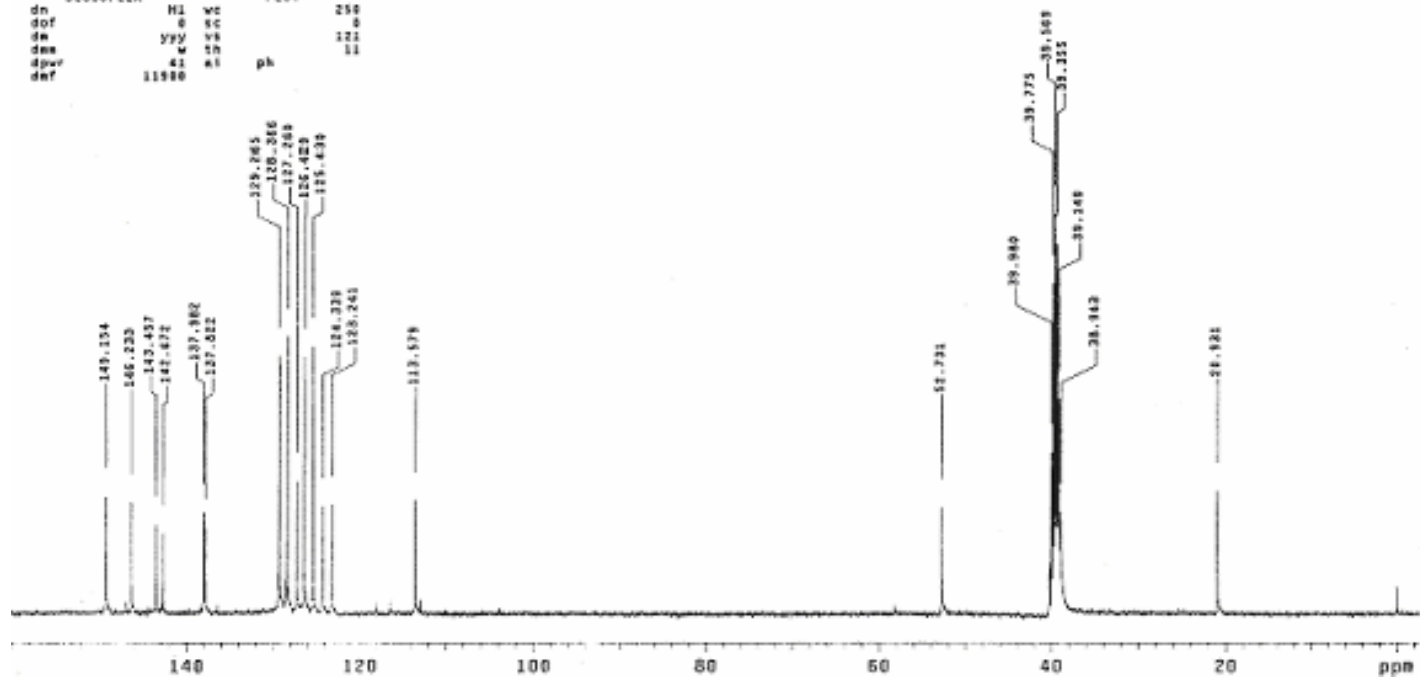
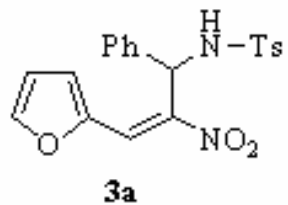


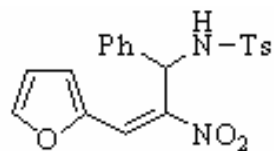
Figure S2. ¹³C NMR Spectrum of 3a

4R-152-NOESY

Data Collected on: iitbchemmercury400
Archive directory: /export/home/iitb/vmr/sys/data
Sample directory: iitb_2005-11-16-125524
File: NOESY

Pulse Sequence: NOESY
Solvent: DMSO
Temp: 20.5 C / 293.4 K

Relax. delay 1.098 sec
Mixing 0.719 sec
Acq. time 3.150 sec
Width 4345.5 Hz
F2 Width 4345.5 Hz
8 repetitions
2 x 128 increments
OBSERVE F1: 399.8821678 MHz
DATA PROCESSING
Gauss apodization 0.363 sec
F1 DATA PROCESSING
Gauss apodization 0.164 sec
FT size 2540 x 2540
Total time 1 hr, 7 min



3a

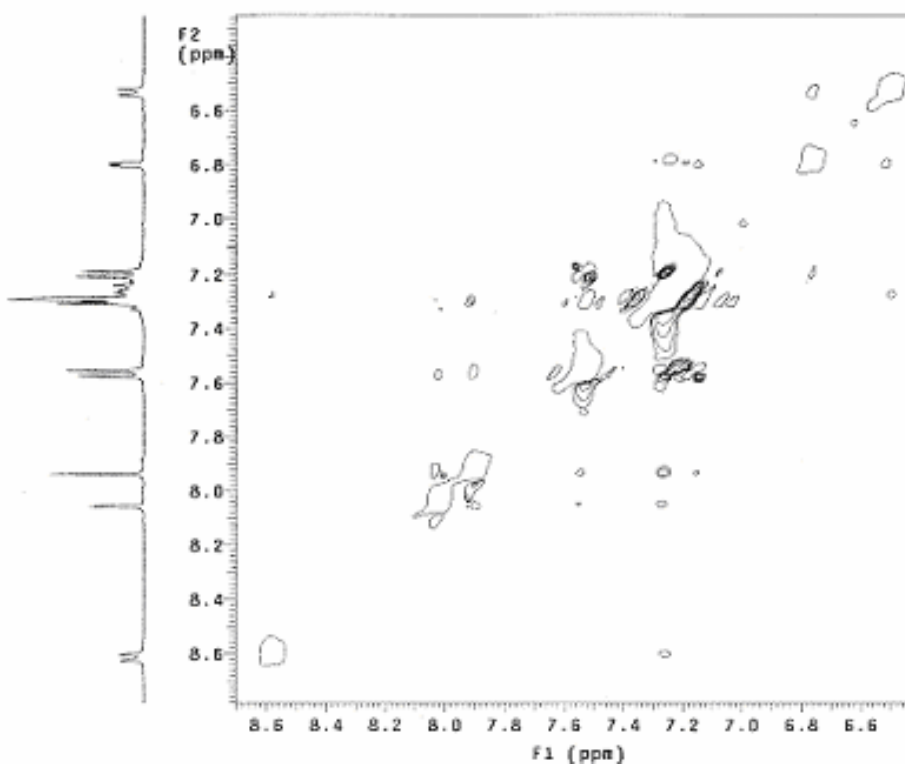
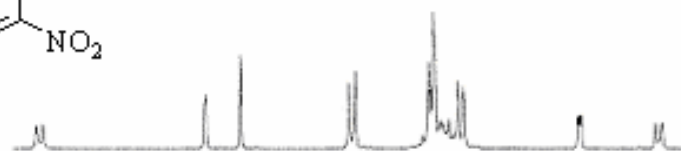
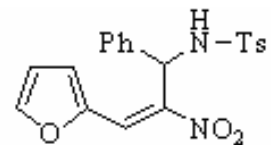


Figure S3. ^1H - ^1H NOESY Spectrum of 3a



3a

INH-152-COSY

Data Collected on: 5/13/2004 10:00:00
 Archive directory: /exp04/004/10/1/5/5/152/004
 Sample directory: 004_2895-01-20
 File: 004-152-COSY

Pulse Sequence: COSY
 Solvent: DMSO

Relax. delay: 1.000 sec
 Acq. time: 0.150 sec
 VPROB: zgpg30
 CD VialID: 4745.0 Hz
 4 repetitions
 200 increments
 OBSERVE: 1H, 399.8823483 MHz
 DATA PROCESSING:
 S1: time 0:11 8.875 sec
 F1: DATA PROCESSING
 S1: time 0:11 8.882 sec
 F1: time 0:14 2.248 sec
 Total time: 17 min

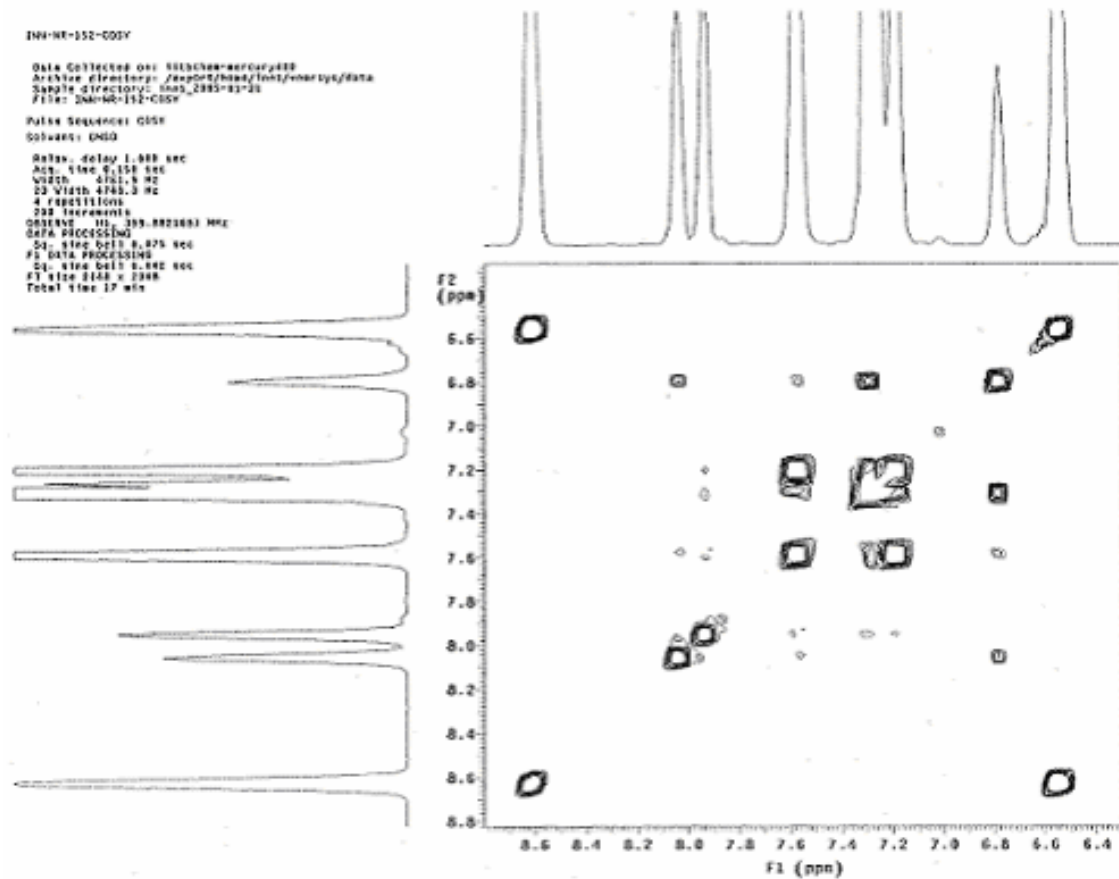


Figure S4. ¹H-¹H COSY Spectrum of 3a

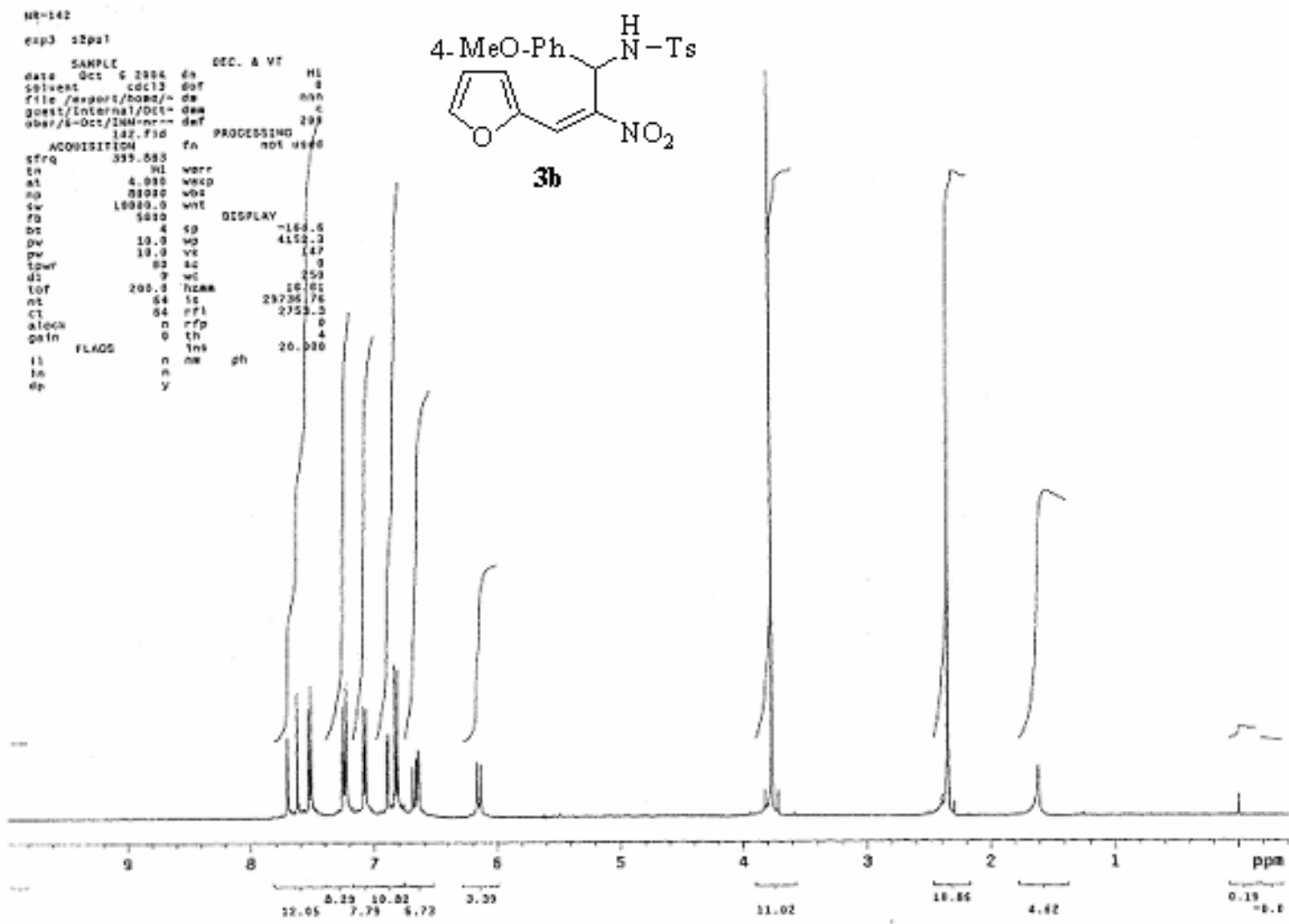


Figure S5. ¹H NMR Spectrum of **3b**

```

NR-142
exp3 s2p1
SAMPLE          SPECIAL
date  Jun 8 2004  comp  not used
solvent  CDCl3  gain  10
file          exp  spin  not used
ACQUISITION    hst  2.000
sw  25000.0  pwr0  9.500
st  1.200  s1fa  10.000
rp  64000  FLAG  h
f0  10000  f1  h
b0  6  f0  h
d1  3.000  d0  7
nt  3200  h0  h
CL  172  PROCESSING  1.00
TRANSMITTER    lb  not used
in  C13  fn  DISPLAY
sfreq  75.438  sp  -3.2
tot  746.8  wp  10000.0
tpwr  55  rft  10000.0
pw  4.750  rfp  2015.4
DECOUPLER      H1  fp  -134.9
d0  0  fp  -300.0
cm  yyy  PLOT
dsw  w  wc  250
sper  35  sc  0
dat  10000  vl  82
sh  h  6
nm  cdc ph  6

```

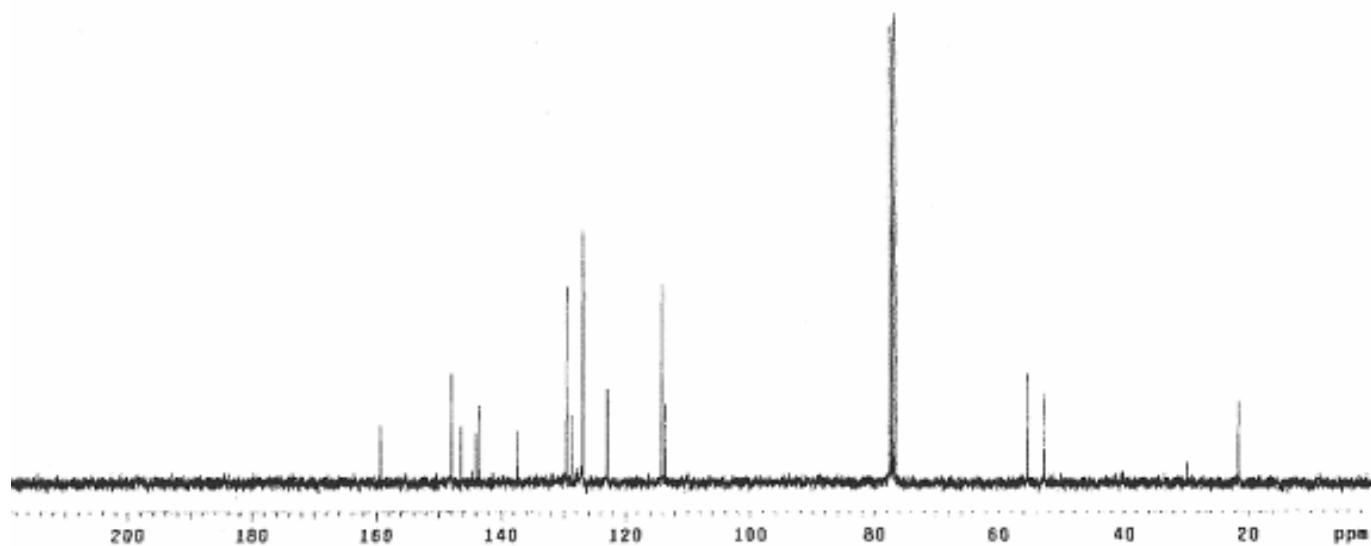
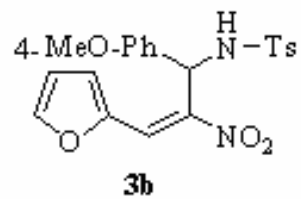


Figure S6. ¹³C NMR Spectrum of **3b**

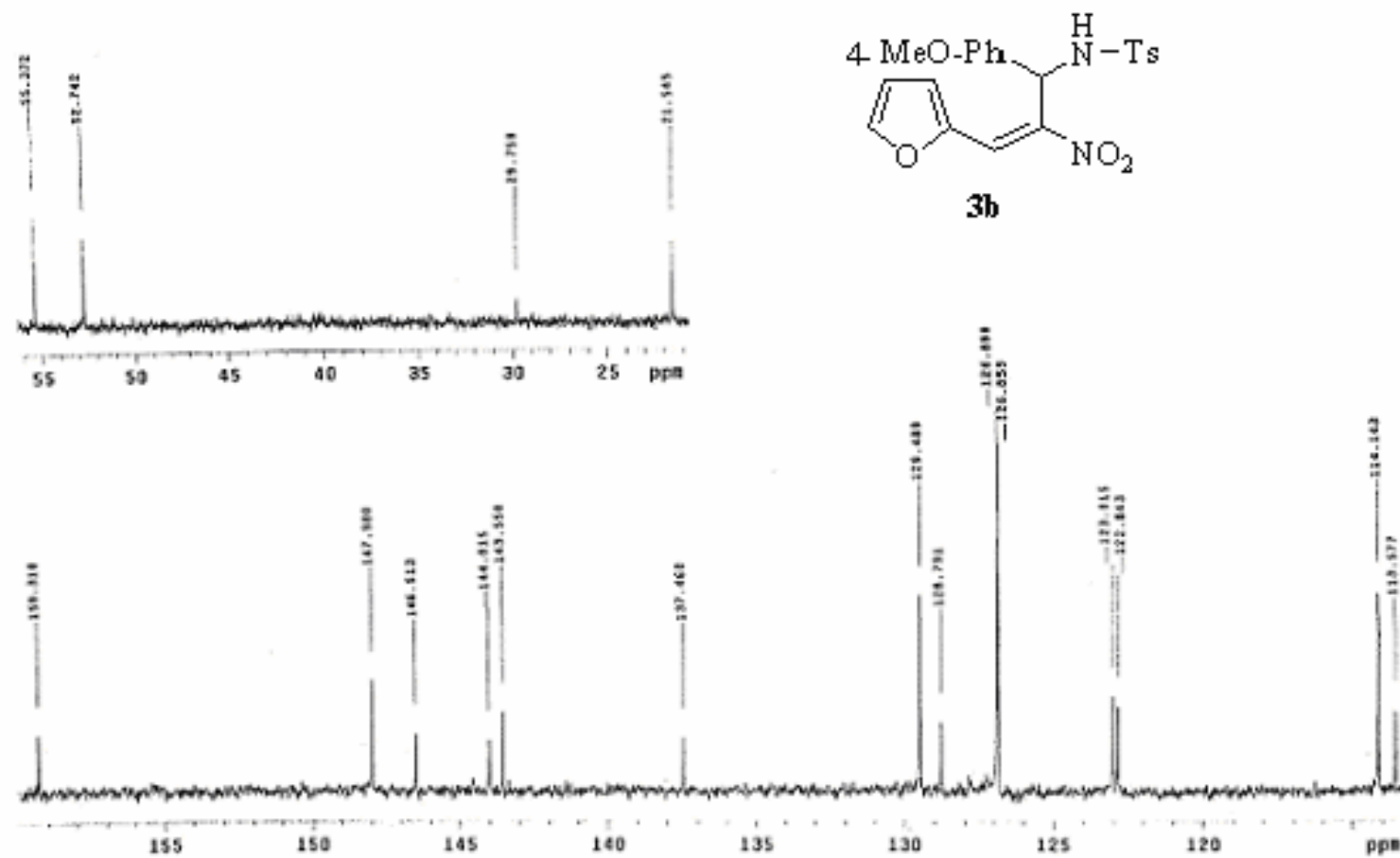


Figure S7. ¹³C NMR Spectrum of **3b** (Expansion)

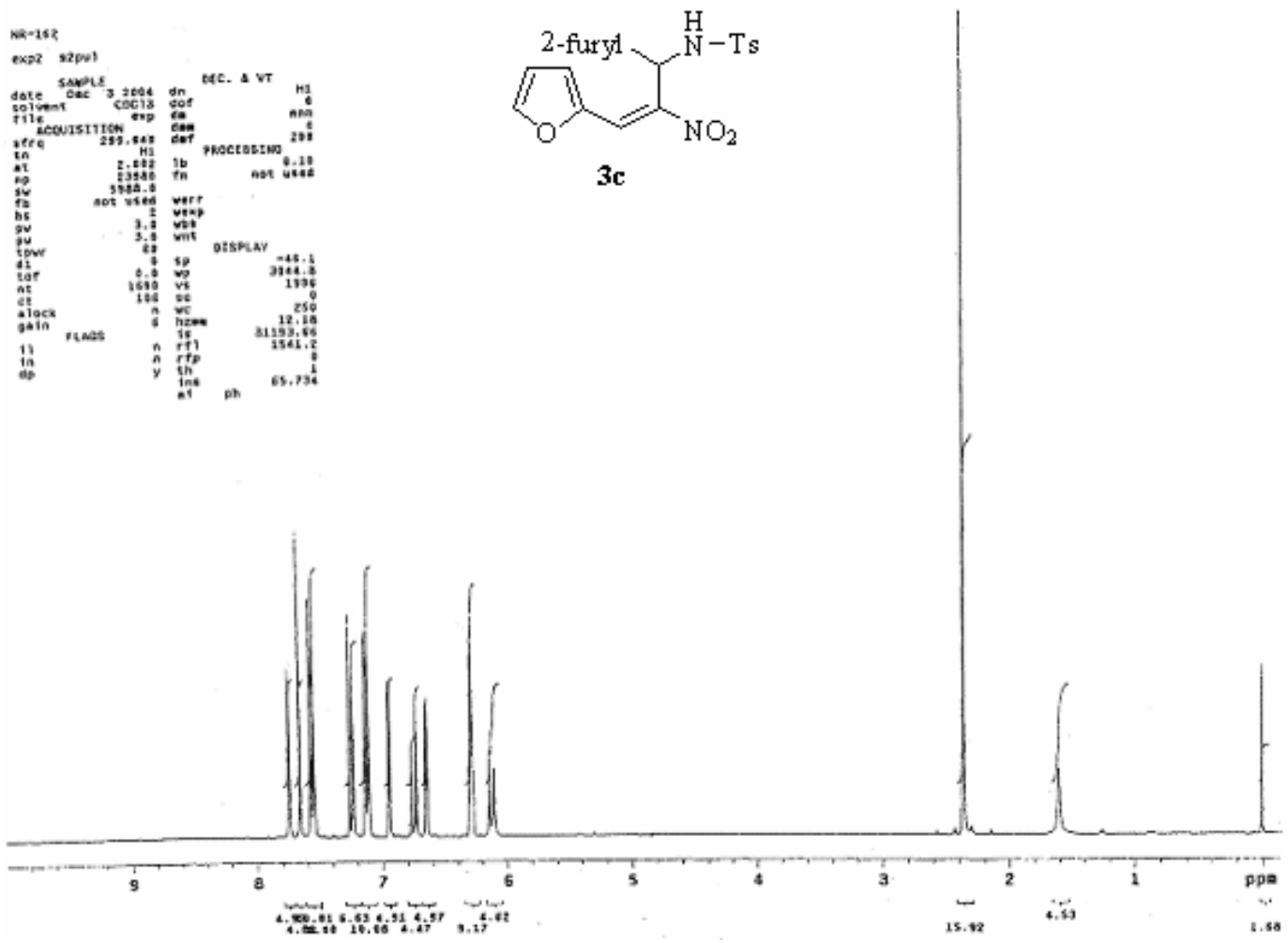


Figure S8. ¹H NMR Spectrum of **3c**

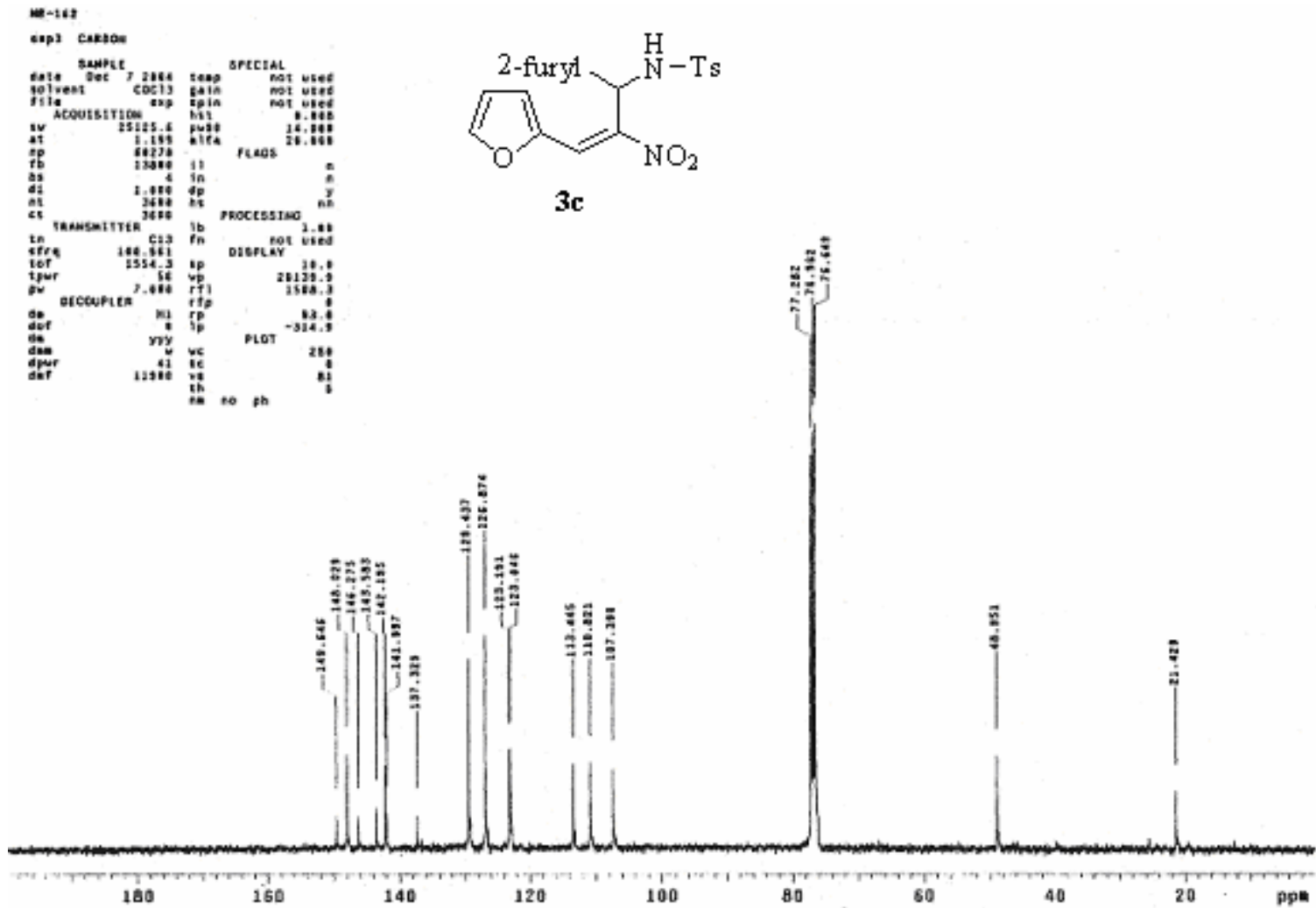


Figure S9. ^{13}C NMR Spectrum of **3c**

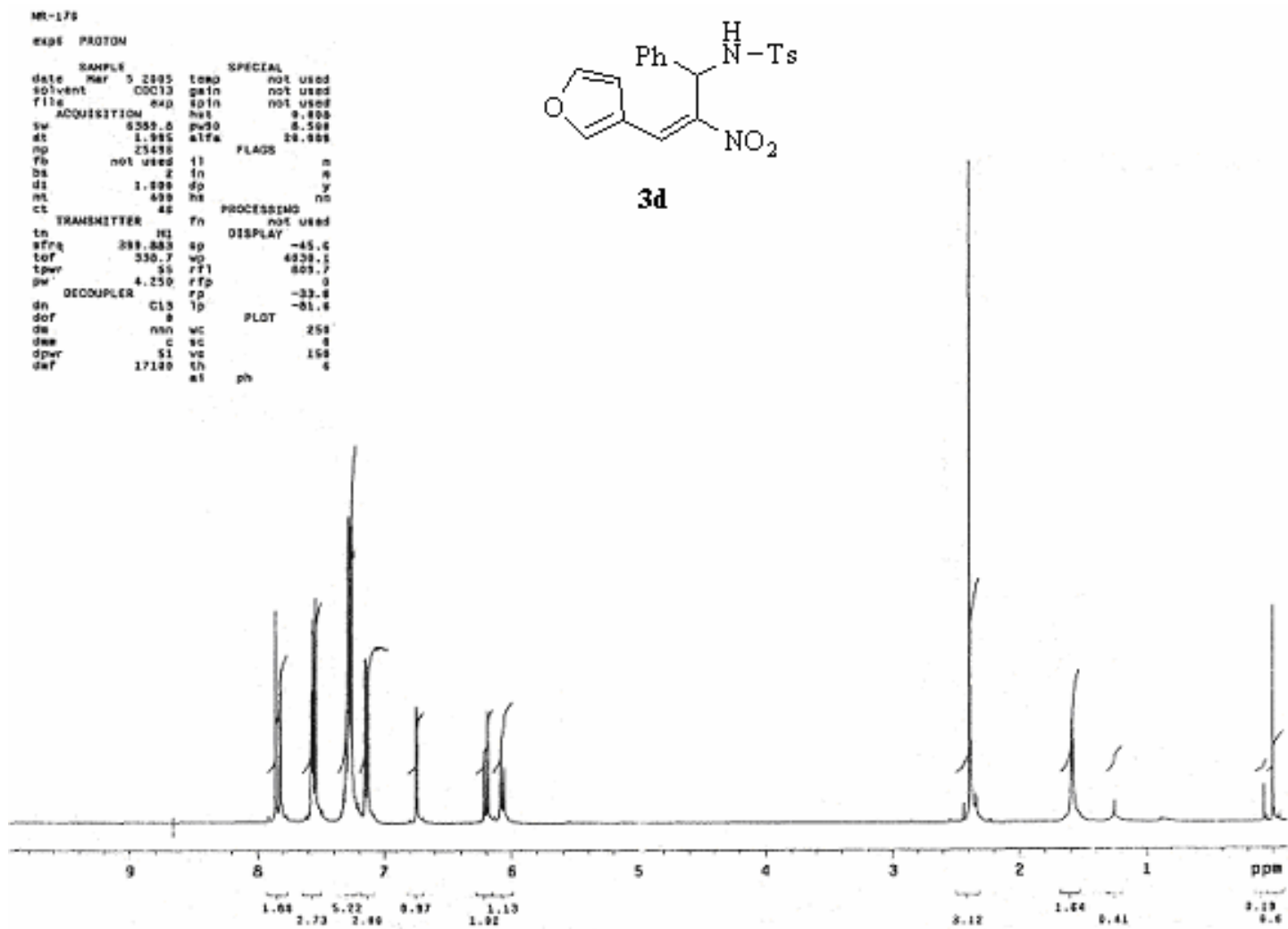


Figure S10. ¹H NMR Spectrum of **3d**

```

NR-176-130
exp3 s2pu1
SAMPLE
date Mar 9 2005 temp not used
solvent COCl2 gain 18
file exp spin not used
ADQUISITION
sw 25000.0 hst 0.000
at 1.015 pws 11.500
f0 10752.0 rfa 20.000
f1 FLAGE f1 0
f2 4 f2 m
d0 3.000 dp 3
d1 1680 h0
d2 124
ct PROCESSING
lb 2.00
tm C13 fa not used
sfreq 75.438 display
tof 748.9 sp -540.0
tpwr 55 wp 15801.2
pv 4.750 rfs 10034.0
DECOUPLER rfg 5815.0
hl rf -175.0
dof 4 lp -370.0
de 333 w PLOT
dca 30 wc 256
dpr 30 sc 0
sar 11300 ve 66
rh th 0
ph

```

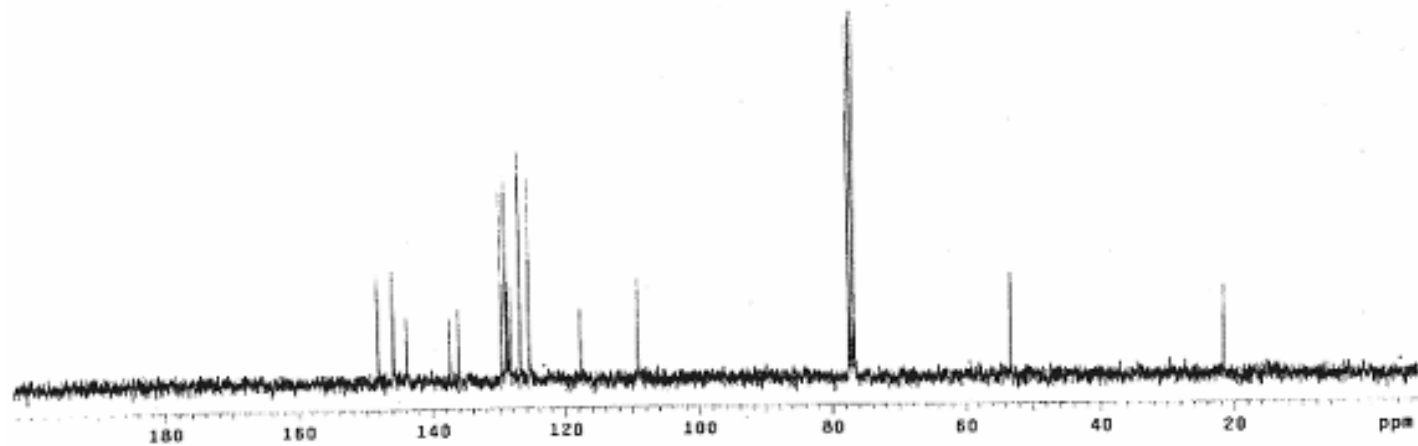
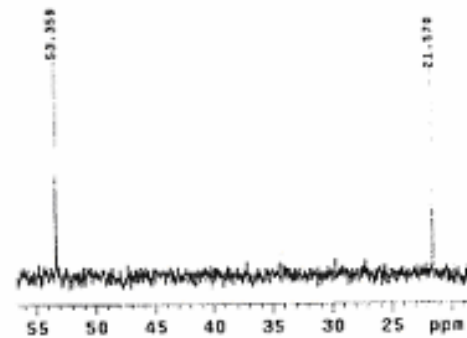
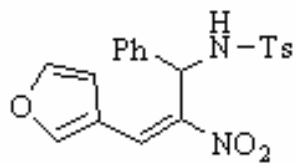
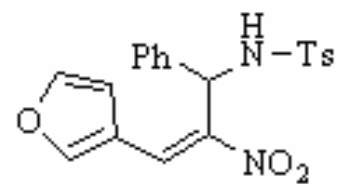


Figure S11. ¹³C NMR Spectrum of 3d



3d

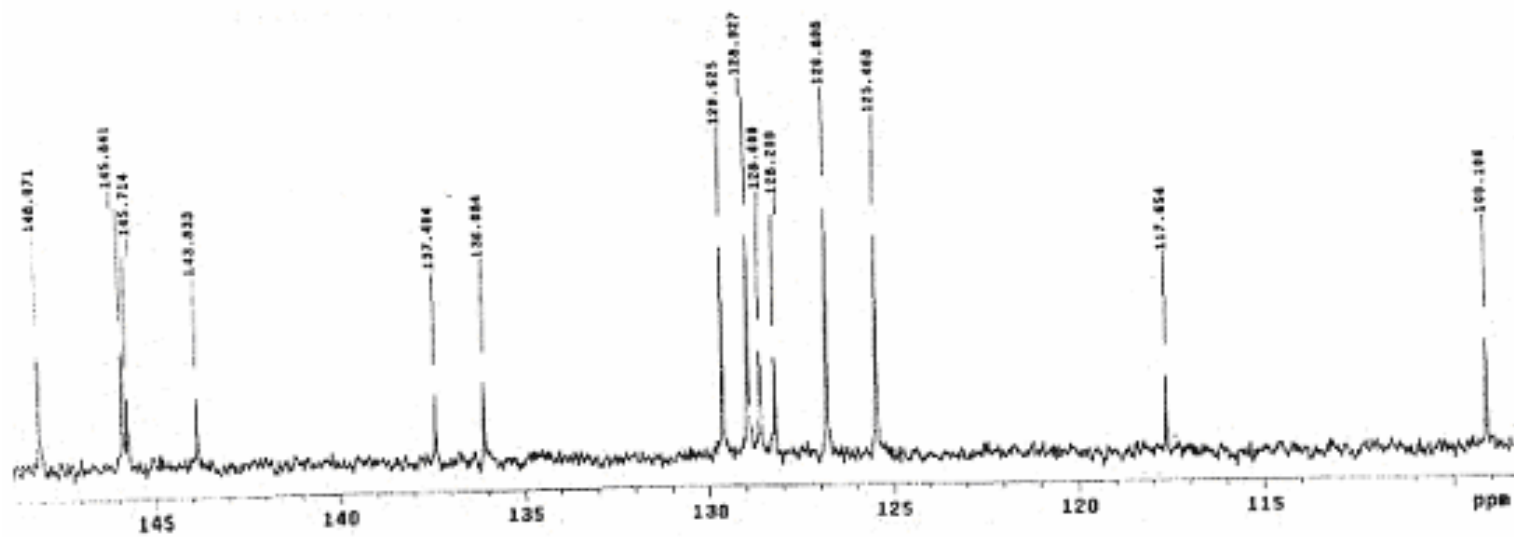


Figure S12. ¹³C NMR Spectrum of **3d** (Expansion)

```

NR-184
exp#  PROTON
SAMPLE
date   Mar 11 2005  temp  not used
solvent CDC13      gain  not used
file    exp        cp1m  not used
ACQUISITION  h1    1.000
sw      5200.0     p000  4.500
at      1.595     w17a  20.000
ap      25400     FLAG
fb      not used  f1    n
bs      2         fa    m
dl      1.000     dp    y
nt      400      h0
ct      0         PROCESSING  nh
TRANSMITTER  f0  not used
ch      H1      DISPLAY
cfrq    300.000  sp      -45.0
tot     330.7   wd      4030.7
tprw    15      r11    000.7
pw      4.250   r1p    -30.0
DECOUPLER  C13  ip      -85.0
dof     0       PLOT
ds      non     wd      250
das     0       sc      0
dpar    51      vs      241
dnt     17100  th      10
          at    ph

```

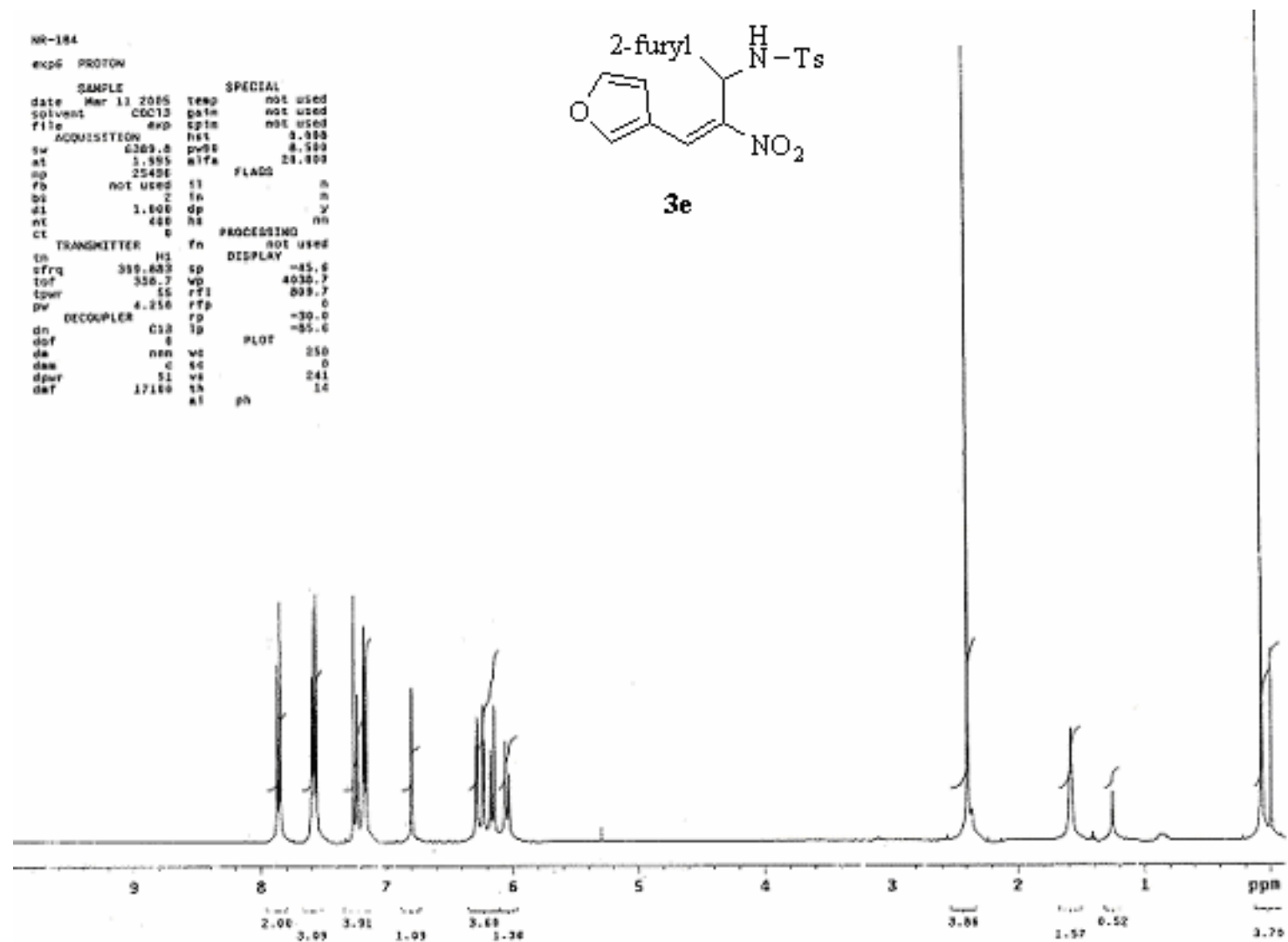
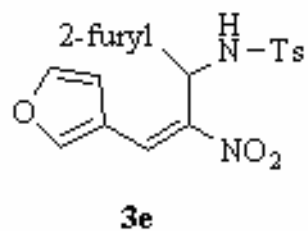
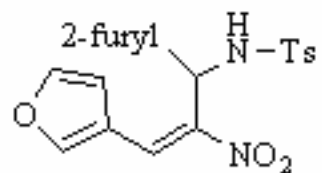


Figure S13. ¹H NMR Spectrum of **3e**

NR-184

exp6 CARBON

SAMPLE		SPECIAL	
date	Mar 13 2015	time	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	0.000
sv	25125.0	pw90	14.000
at	1.199	altm	20.000
np	80273	FLAGS	
fb	12000	fl	n
bs	4	sn	n
d1	1.400	dp	y
nt	1800	ns	ns
ct	0	PROCESSING	
TRANSMITTER		lb	1.00
tn	CL3	fn	not used
strq	180.561	DISPLAY	
tof	1554.3	sp	-55.0
tpwr	50	wp	10158.5
pv	7.000	rfl	9253.7
DECOUPLER		rff	7782.5
ca	HL	rp	48.5
cof	0	lp	-331.2
ca	yyy	PLOT	
cam	w	wc	250
davr	41	sc	0
dat	11300	va	40
		th	2
at	no	ph	2



3e

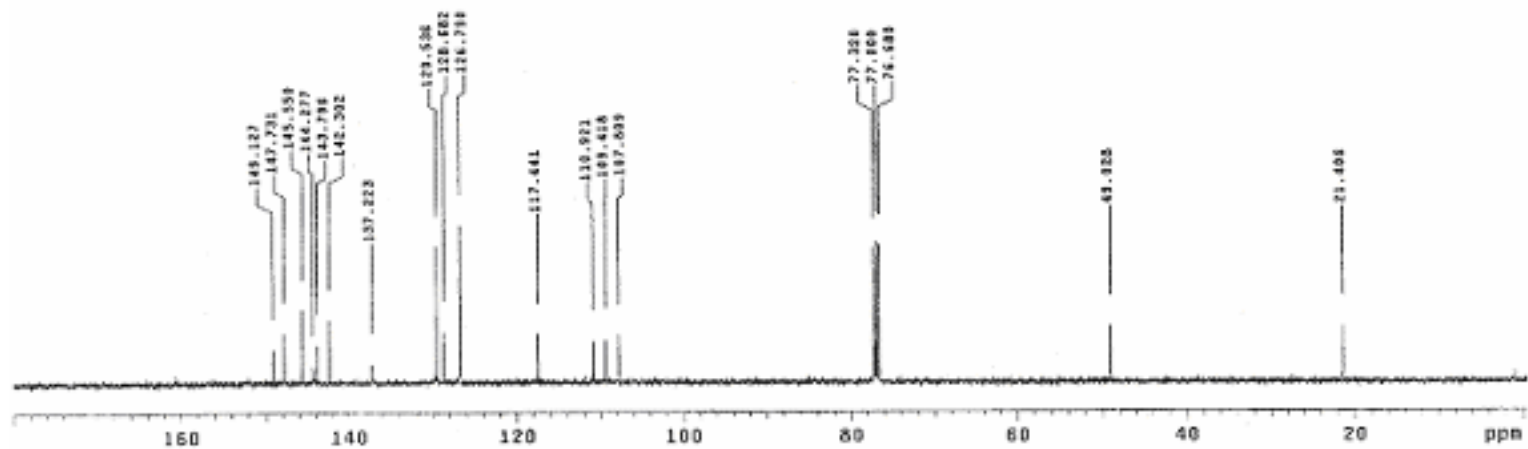


Figure S14. ¹³C NMR Spectrum of 3e


```

MR-178
exp# PROTON
SAMPLE
date Mar 3 2005 TEMP not used
solvent CDCl3 gain not used
file exp gain not used
ACQUISITION hst 0.000
sw 6000.0 pws 8.500
at 1.885 aifa 20.000
ap 25.000 FLAQ n
fb not used ii n
gc 4 in n
gl 1.000 op y
ht 64 hs nh
ct TRANSMITTER 64 PROCESSING not used
ln hl DISPLAY
frc 359.863 sp -79.2
tof 338.7 wd 4167.5
tpwr 55 rfi 889.3
pw 4.259 rfp 8
dc DECOUPLER c13 rpd -35.4
dd 0 tp -74.3
ddt 0 PLOT 250
da nnn wc 0
dss c 60 51
dpr 51 ve 51
dnt 17100 lb 10
at ph 4

```

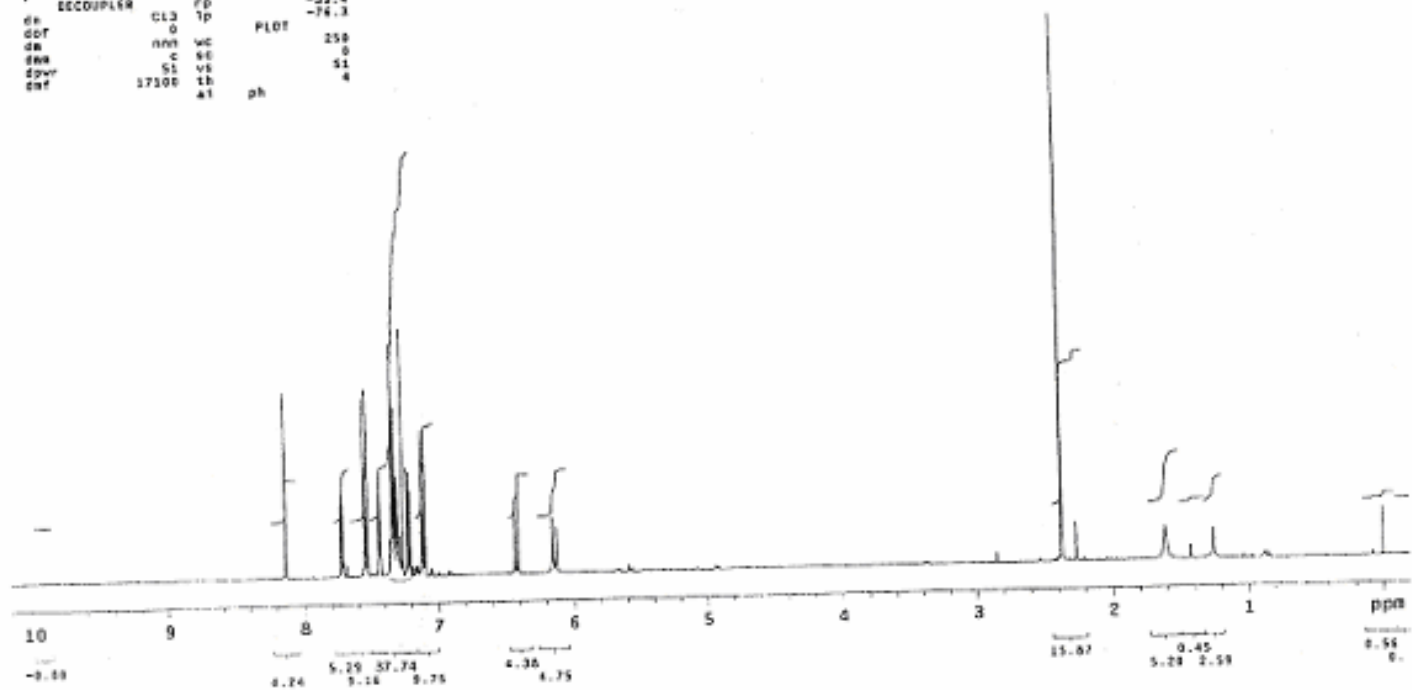
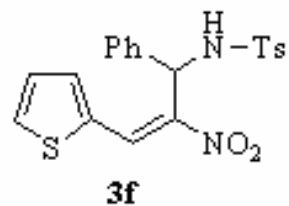


Figure S15. ¹H NMR Spectrum of 3f

NR-17B

exp3 CARBON

SAMPLE		SPECIAL	
date	Oct 5 2005	temp	not used
solvent	CDCl3	gain	not used
file	/export/home/~	spin	not used
inn1	october/3thoc	hst	0.000
t/NR-17B-C13.f3d	pv93	14.000	
ACQUISITION		atfa	20.000

sw		25125.0	FLAGS
st	1.100	sl	n
sp	80270	ln	n
fb	13000	dp	y
bc	4	hs	n
dl	1.000	PROCESSING	nt
nt	50000	lb	2.00
ct	584	fn	not used
TRANSMITTER		DISPLAY	
tn	C13	sp	5.4
xfrq	100.621	wp	20100.0
top	1534.3	rft	0155.0
tpwr	56	rfd	7742.3
pv	7.000	rp	67.0
DECOUPLER		lp	-324.0

dn		hl	PL0T
dof	0	wc	250
da	yyy	sc	8
daw	w	vs	51
dpvr	41	th	4
daf	11300	al	no ph

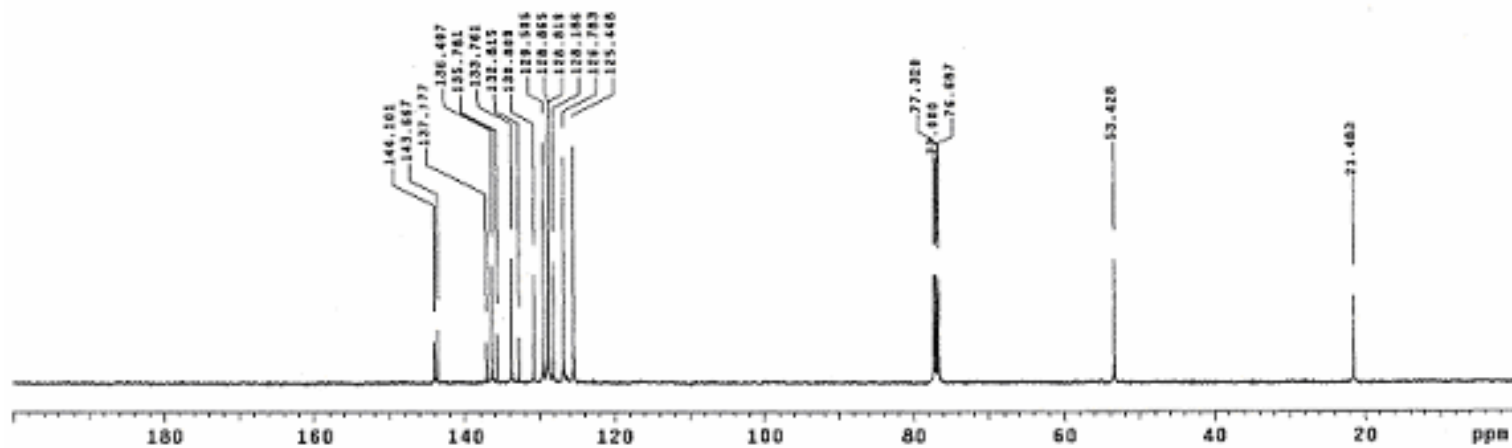
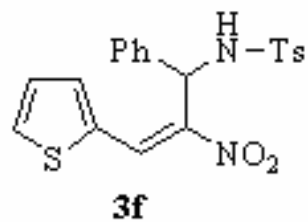


Figure S16. ¹³C NMR Spectrum of **3f**

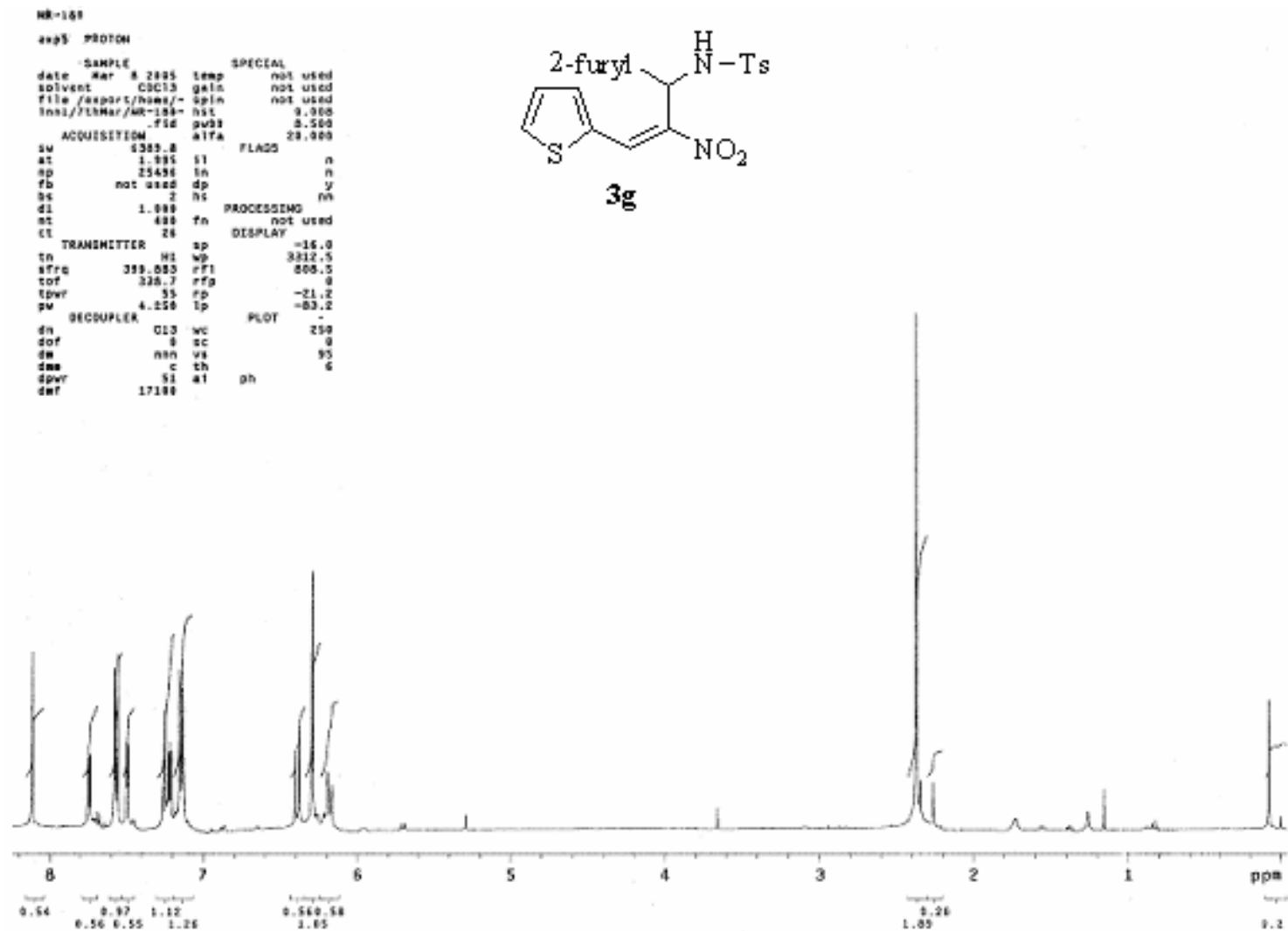


Figure S17. ¹H NMR Spectrum of **3g**

```

NR-180
exp# CARBON
SAMPLE
date Mar 5 2005
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
sp 86270
fo 13000
bs 4
dl 1.000
nt 1000
ct 980
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
puls 14.000
alpha 20.000
FLAGS
i1 n
in n
dp y
hc an
PROCESSING
f2 1.00
f3 800
f4 4500
f5 1310.7
f6 21427.4
f7 9250.9
f8 7742.3
f9 64.7
f10 -874.7
PLOT
w 250
sc 8
vs 100
th 4
al no ph
TRANSMITTER
tn C13
afreq 100.621
tof 1554.3
tpwr 50
pw 7.000
DECOUPLER
dn HI
sot 0
dm yyy
dnn w
dpr 41
dmf 11010

```

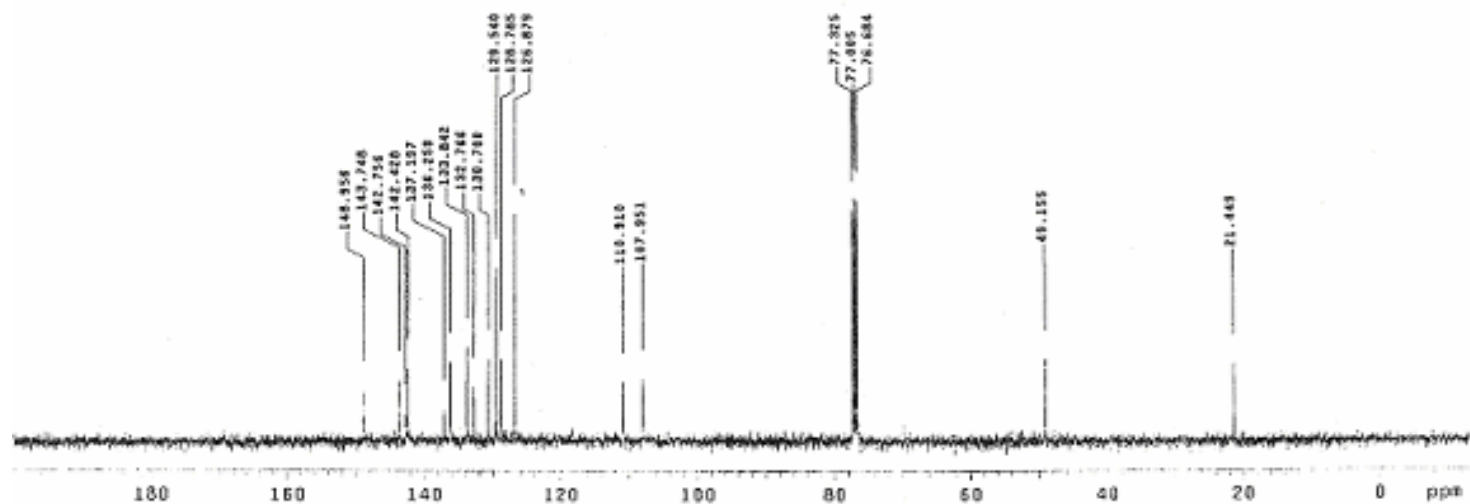
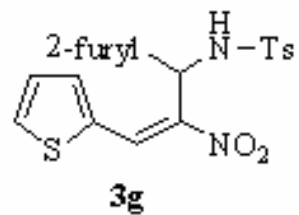


Figure S18. ¹³C NMR Spectrum of 3g

MR-179

Exp1 PROTON

PARAMETER	VALUE	UNIT	DESCRIPTION
DATE	FEB 25 1985		
TIME	12:15		
PROG	CDCL3		
INSTR	FT/MS		
PROB	5MM		
NUC1	1H		
NUC2	13C		
FLAGS	29.000		
ACQUISITION			
SI	3200.0	Hz	
ST	1.000	s	
SP	15.000	Hz	
TD	65536		
SB	1		
AL	1.000		
HT	400	Hz	
CT	02		
TRANSMITTER			
LS	H1		
RF1	299.820	MHz	
RF2	320.7	MHz	
CPUR	50	Hz	
PR	4.250	Hz	
RECEIVER			
SI	C13		
ST	2		
SP	15.000	Hz	
TD	65536		
SB	1		
AL	1.000		
HT	400	Hz	
CT	02		

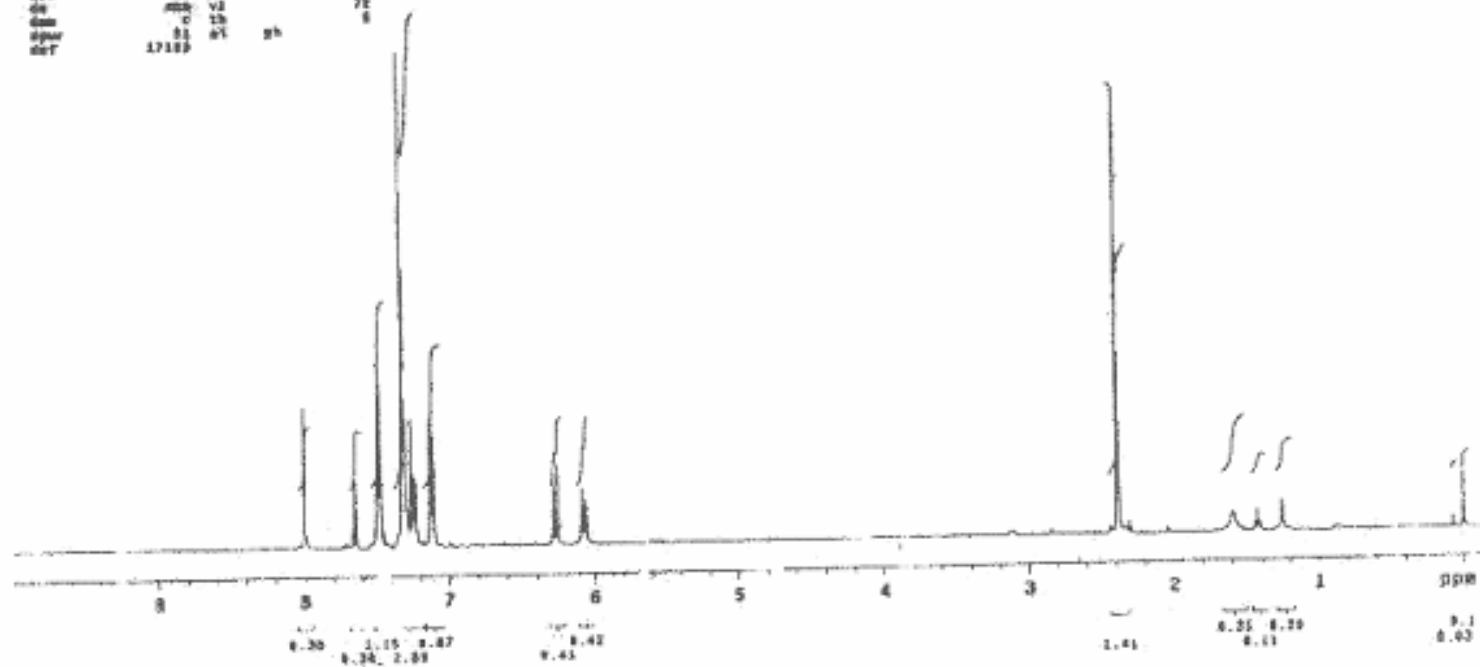
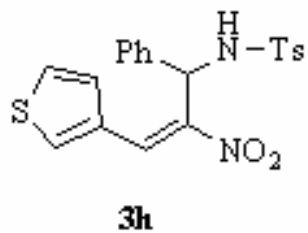


Figure S19. ¹H NMR Spectrum of **3h**

NR-175

exp6 CARBON

SAMPLE		SPECIAL	
date	Mar 27 2003	temp	not used
solvent	CDCl3	gain	not used
file	exp	spin	not used
ACQUISITION		hst	8.888
sv	29125.6	pr99	14.888
at	1.188	at7a	28.888
nd	8079	FLAGS	
fb	13889	fl	n
bc	4	in	m
dl	1.888	ep	y
nt	1888	hs	ns
cl	1788	PROCESSING	
TRANSMITTER		td	1.98
tr	C13	fa	not used
sfrq	100.621	DISPLAY	
tot	1554.3	ep	5.4
tpwr	55	vd	16125.5
pr	7.888	rt1	8255.2
DECOUPLER		rt2	7742.3
dn	H1	rp	48.8
dot	8	lp	-328.3
sw	20V	PLOT	
dsw	w	wd	258
cpwr	41	sc	8
dwt	11888	vs	38
		th	2
		rm	80 ph

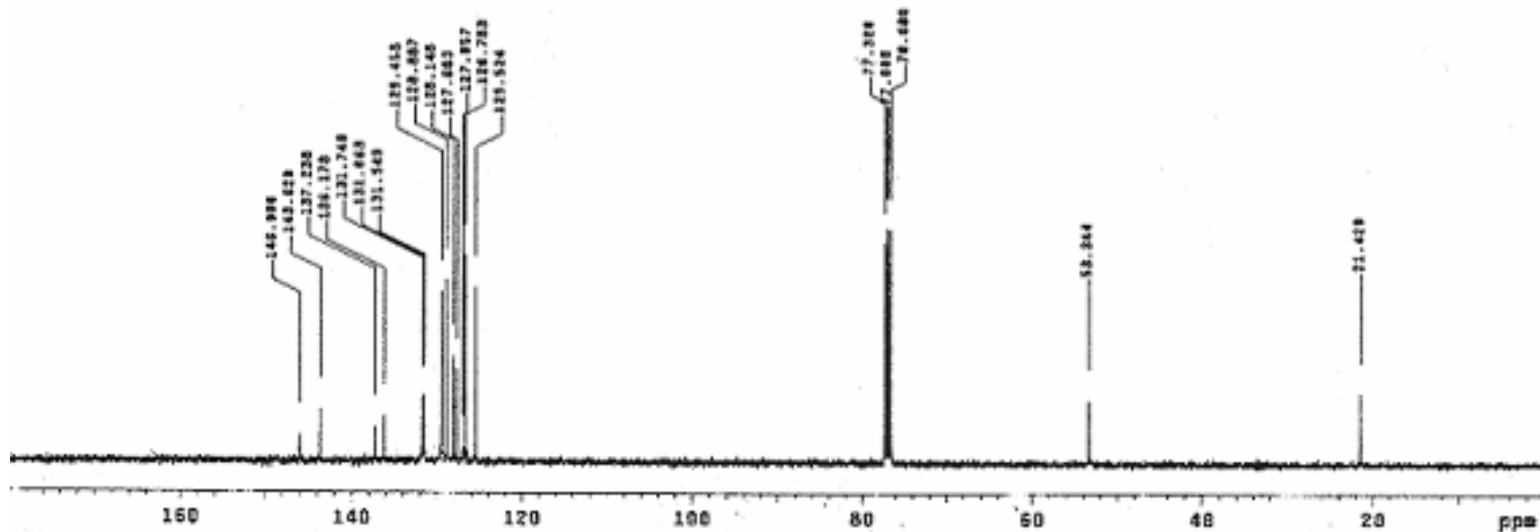
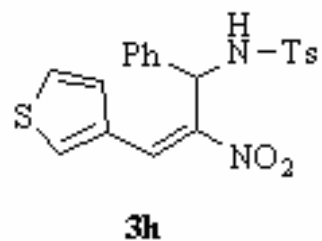


Figure S20. ¹³C NMR Spectrum of 3h

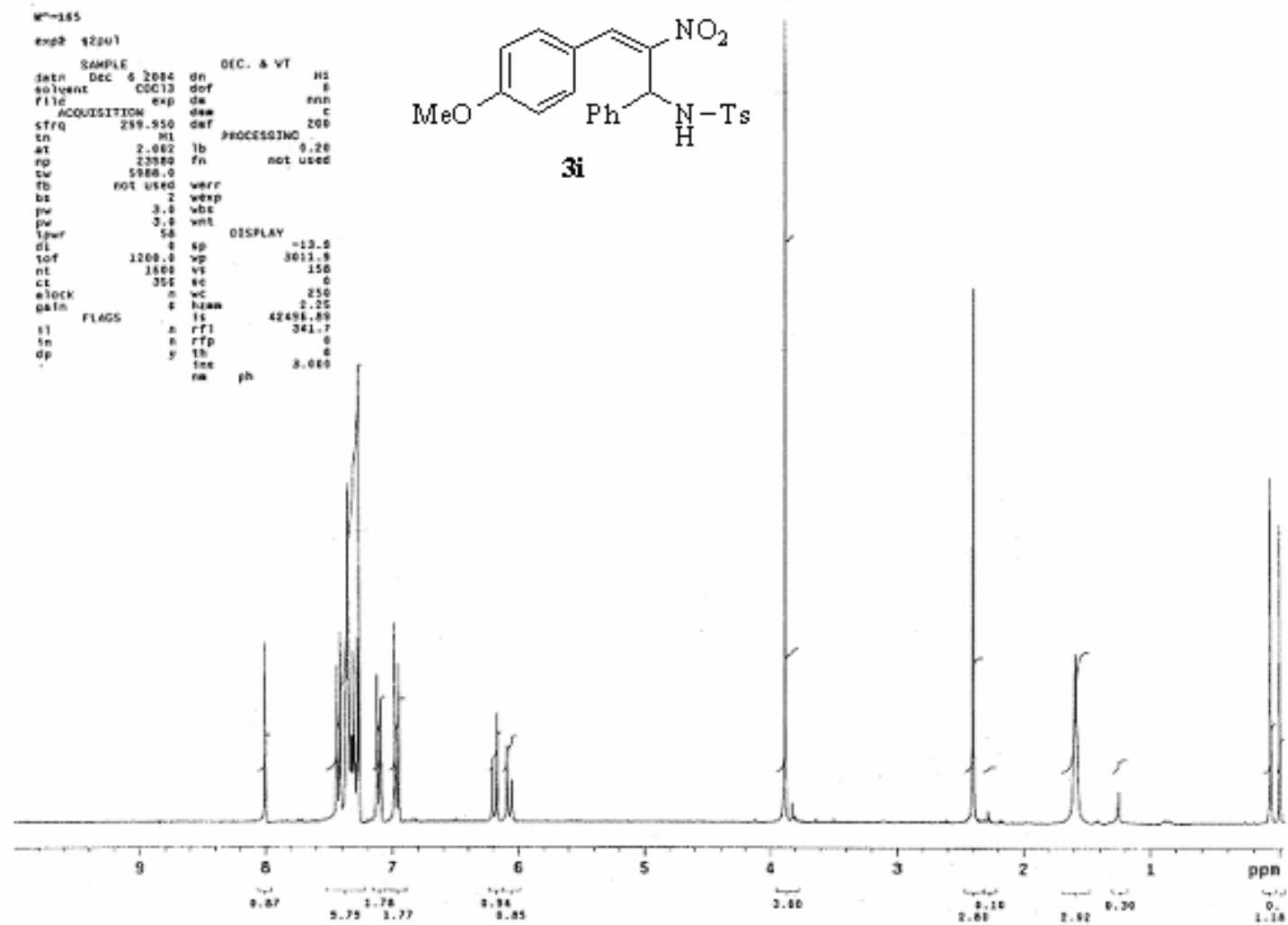


Figure S21. ¹H NMR Spectrum of **3i**

```

NR-165-C13
exp4 CARBON
SAMPLE
date Sep 28 2005 temp not used
solvent CDCl3 gain not used
file /export/home/ spin not used
fn3/September/201- not
h/NR-165-C13.f16 pw90 14.800
ACQUISITION alfa 20.000
sw 25125.6 FLAS
at 1.199 t1 n
ap 80276 tn n
fb 13800 dp y
ss 4 hs
cl 1.000 PROCESSING
ct 5000 tb 2.00
ct 716 tn not used
TRANSMITTER DISPLAY
tn C13 cp -25.3
strq 199.561 vp 23172.9
tof 1554.3 rft 9252.8
tpwr 56 rfp 7742.3
pw 7.000 rp 74.7
DECOUPLER lp -325.7
dn H1 PLOT
dof 0 vc 250
dw 22V tc 8
dwm v vs 84
dpwr 41 th 4
dwt 11900 at no ph

```

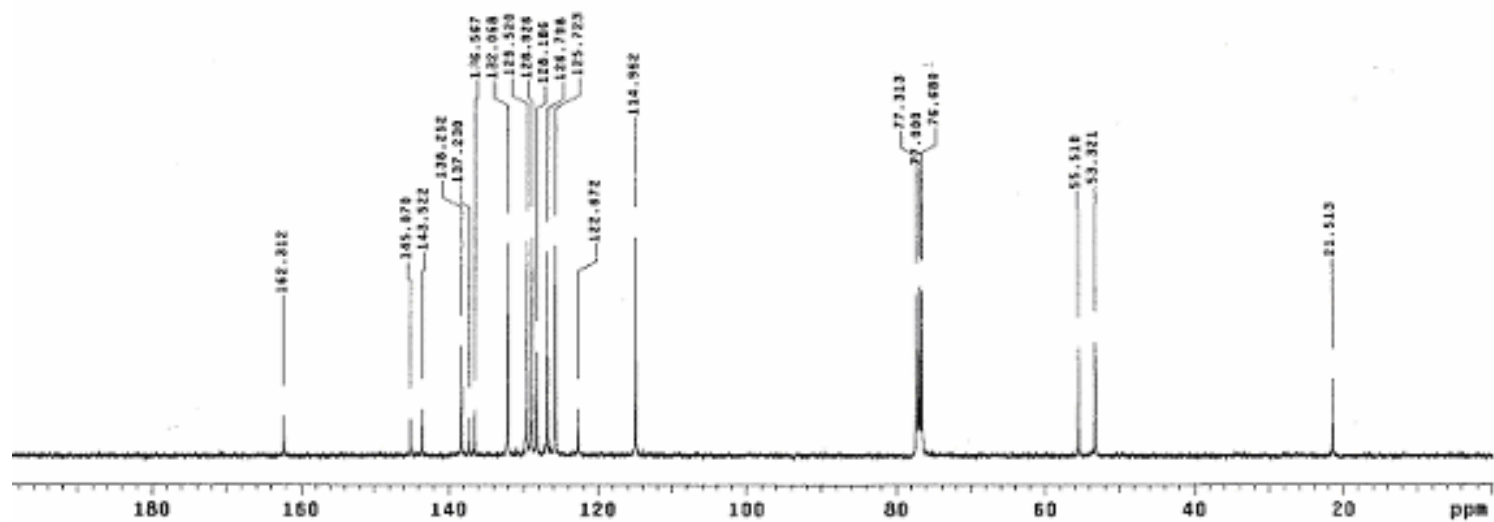
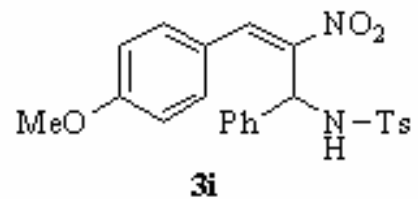


Figure S22. ¹³C NMR Spectrum of **3i**

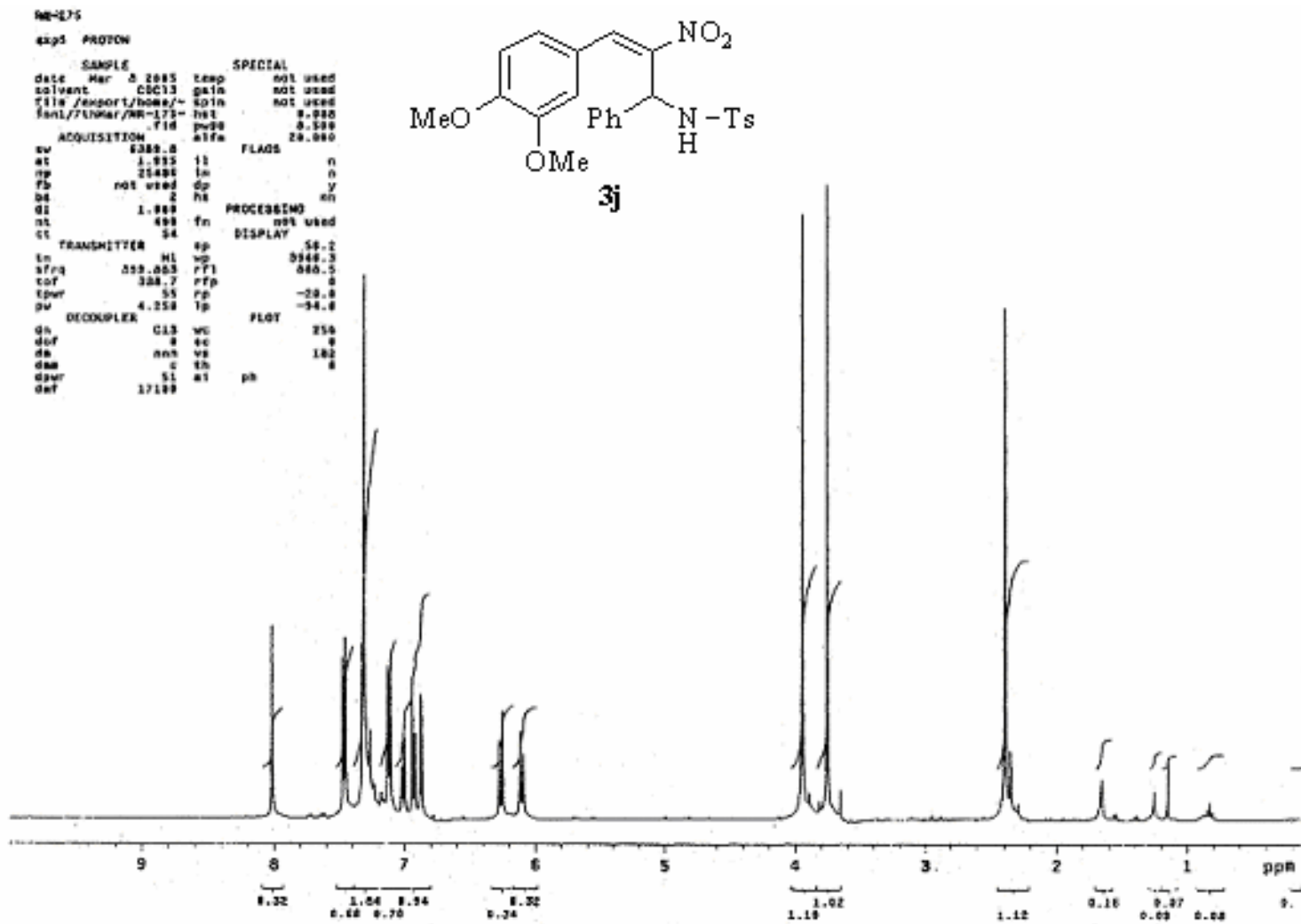


Figure S23. ¹H NMR Spectrum of **3j**

MR-175

exp3 s2pu1

SAMPLE		SPECIAL	
date	Feb 28 2005	temp	not used
solvent	CDCl3	gain	16
Title	exp	spin	not used
ACQUISITION		ns1	0.000
sw	25000.0	sw90	11.500
at	1.015	alt0	20.000
rg	10752	FLAG	
rb	15000	l1	n
rb	4	l2	n
ds	3.000	dp	y
nt	1000	ns	nn
ct	200	PROCESSING	
TRANSMITTER		tb	2.00
ta	Cl3	fn	not used
ifrq	75.430	DISPLAY	
tof	740.0	sp	40.7
lqwr	50	vs	1500.0
pv	4.750	rfl	10000.0
DECOUPLER		rfp	500.0
dn	H1	rp	100.0
dof	0	lp	-324.0
ds	VVV	PLOT	
sm	w	uc	250
zpw	30	sc	0
gat	11000	vs	104
		th	10
		re	ph

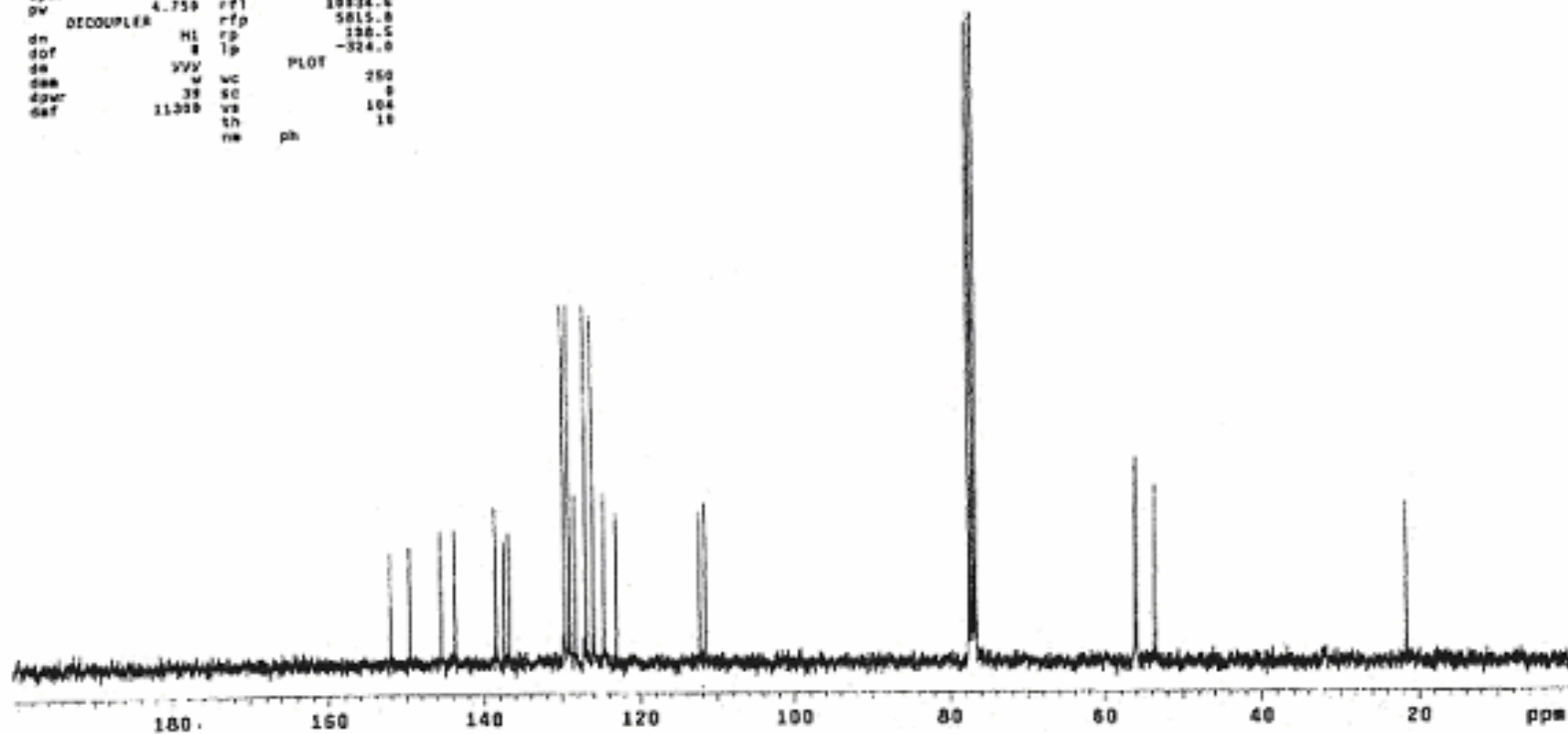
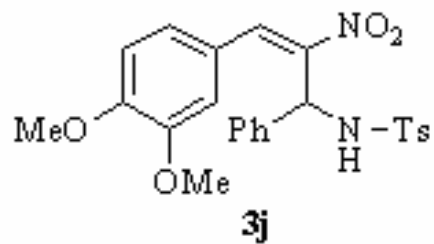


Figure S24. ¹³C NMR Spectrum of **3j**

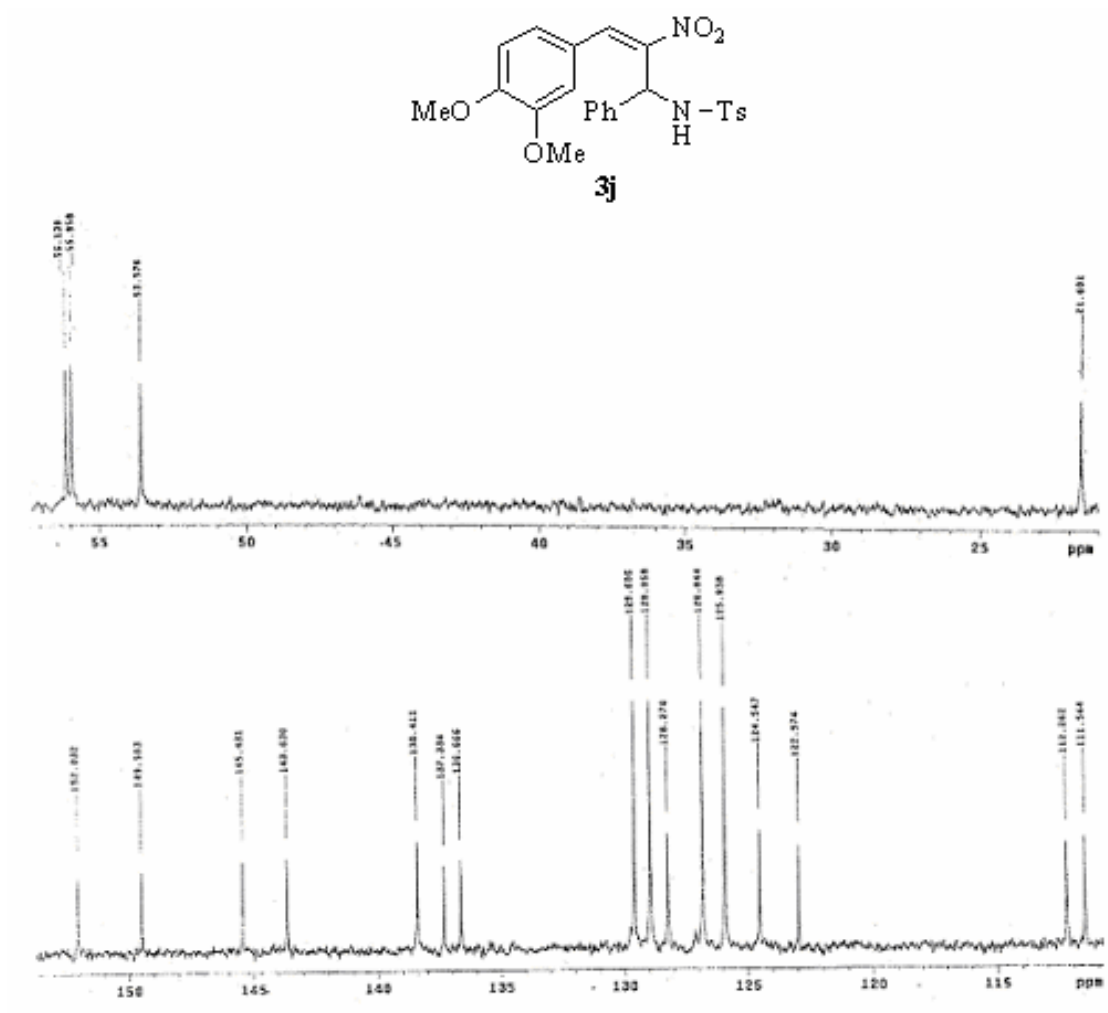


Figure S25. ¹³C NMR Spectrum of **3j** (Expansion)

```

NR-177
exp5  PROTON
SAMPLE
date   Oct 25 2005 1940 SPECIAL not used
solvent CDCL3 gain not used
file   /export/home/ q21n not used
Invt/October/25th/- hit 0.000
NR-177.f16 pv99 8.500
ACQUISITION
sw 10010.0 Hz FLAGS n
at 1.593 s1 m
no 38902 in m
fo not used 69 y
ba 2 hz nn
ol 1.000 PROCESSING
oc 400 F0 not used
ct 40 DISPLAY
TRANSMITTER
tn H1 M0 -34.5
sfrq 355.883 r71 4024.0
tof 200.0 rfp 2757.1
tpr 55 rp 17.3
pw 4.250 tp -124.9
DECOUPLER
dn C13 wc 250
dof 0 sc 0
dm nnn vs 22
dca C th 4
dpr 51 w1 ph
dof 17100

```

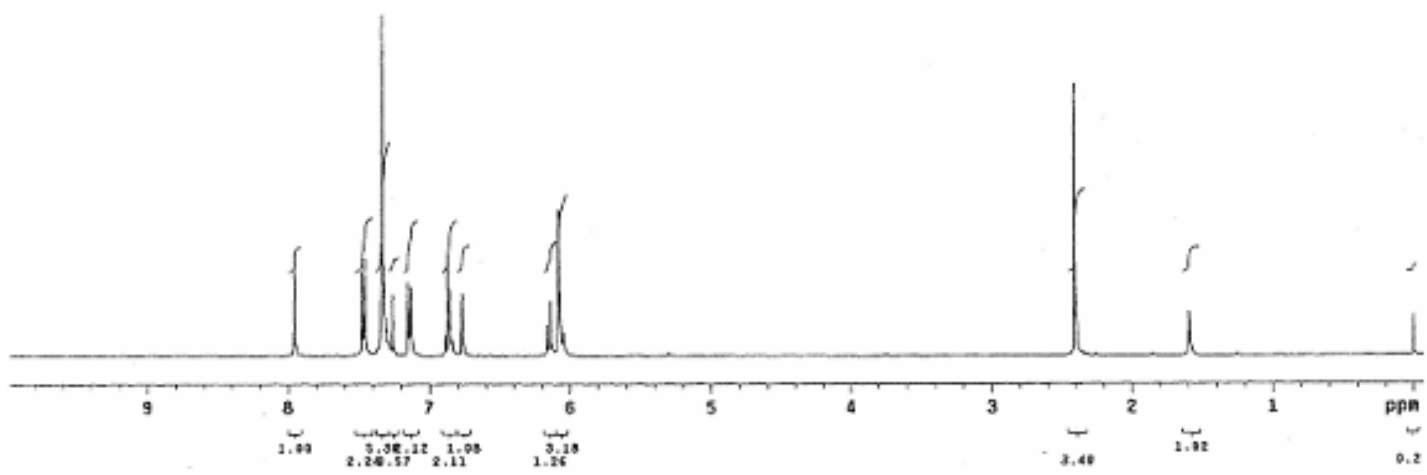
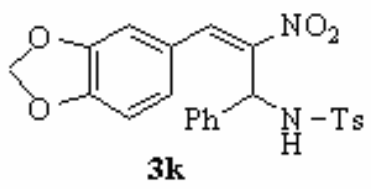


Figure S26. ¹H NMR Spectrum of 3k

NR-177

exp6 CARBON

SAMPLE		SPECIAL	
date	NOV 2 1995	temp	not used
solvent	CDCl3	gain	not used
File	exp	spin	not used
ACQUISITION		int	0.000
sv	25125.6	pw90	14.000
at	1.100	ctfa	20.000
np	60270	FLAGS	
fb	13500	f1	n
bs	4	fm	n
ds	1.000	dp	y
nl	50000	hs	wn
ct	204	PROCESSING	
TRANSMITTER	CL3	fb	1.00
tn	CL3	fn	not used
sfrq	100.621	DISPLAY	
tof	1554.8	ep	42.2
tpwr	50	vp	10017.3
pm	7.000	rf1	3251.4
DECOUPLER		rfp	3742.3
dn	HL	ty	71.5
dof	0	lp	-347.8
dm	yyv	PLOT	
dms	w	vc	250
edw	41	ec	0
dwt	11500	vs	30
		th	5
		al	na ph

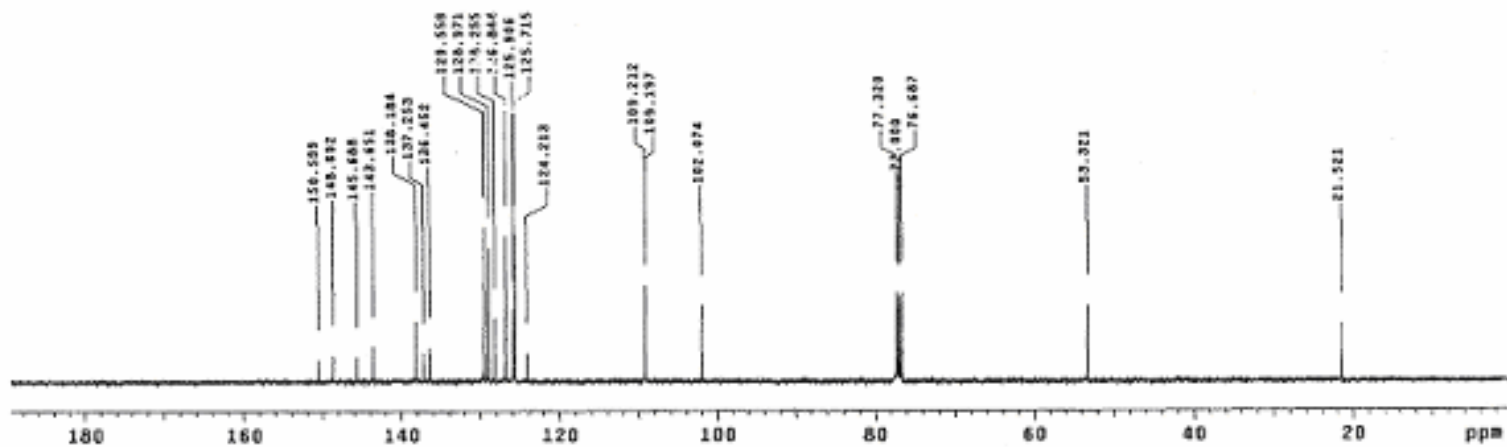
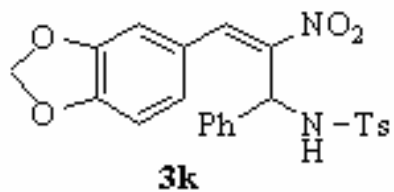


Figure S27. ¹³C NMR Spectrum of **3k**