

# Rhenium Catalyzed 1,3-Isomerization of Allylic Alcohols: Scope and Chirality Transfer

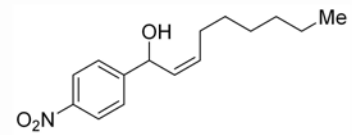
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Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, 1200 E. California Blvd.,  
Pasadena, CA 91125.

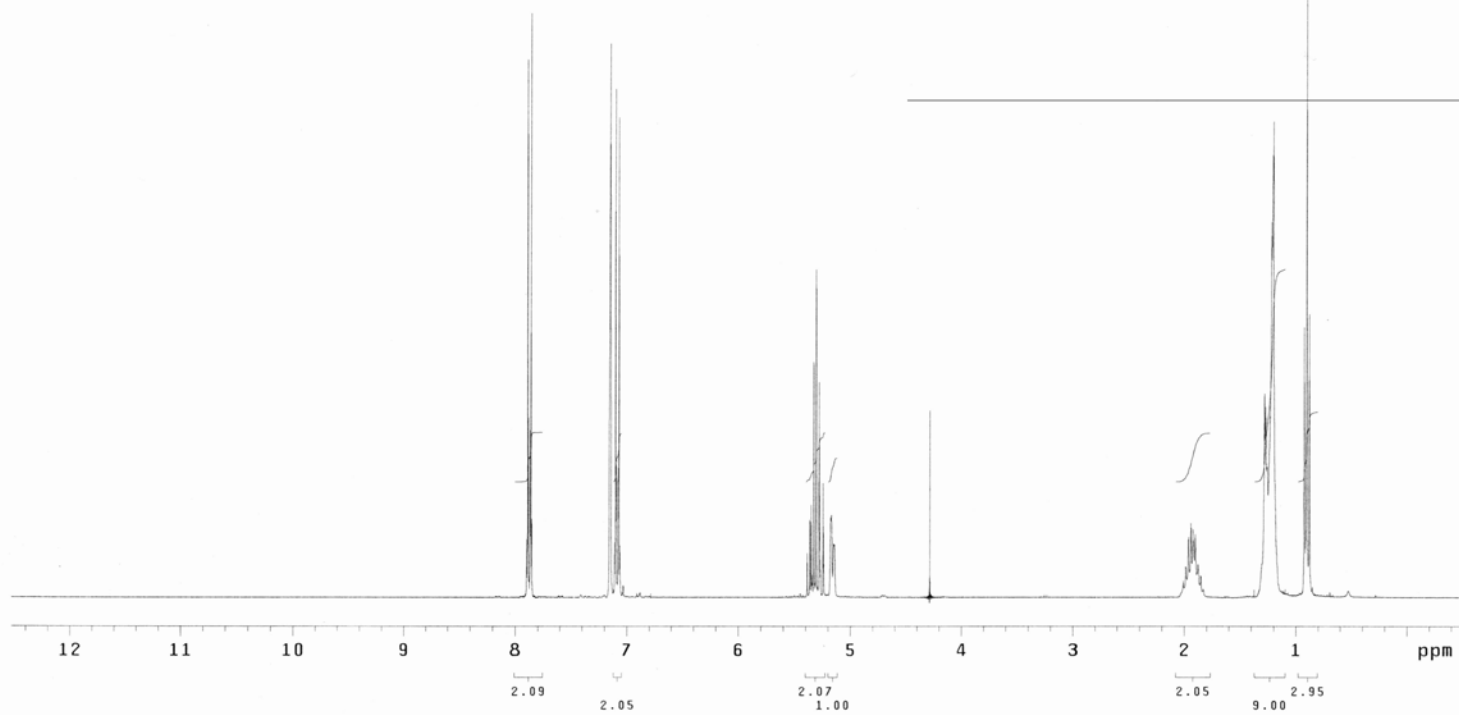
## Contents:

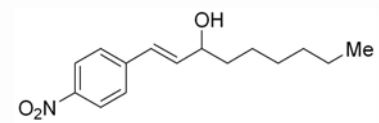
1. $^1\text{H}$ NMR spectra of compounds .....	S36
2. $^{13}\text{C}$ NMR spectra of compounds .....	S68

The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on an Oxford NMR spectrometer running Varian VNMR software. Chemical shifts are reported in parts per million (ppm) downfield from tetramethylsilane (TMS) with reference to the internal solvent. Multiplicities are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), quintet (quint), multiplet (m), and broad (br). The reported  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR data refer to the major alkene isomer (which is identified) except when otherwise noted. Assignment of the *E/Z* stereochemistry for the disubstituted alkenes was based upon the coupling constants of their vinylic protons, and that for the trisubstituted alkenes was based upon NOE experiments.

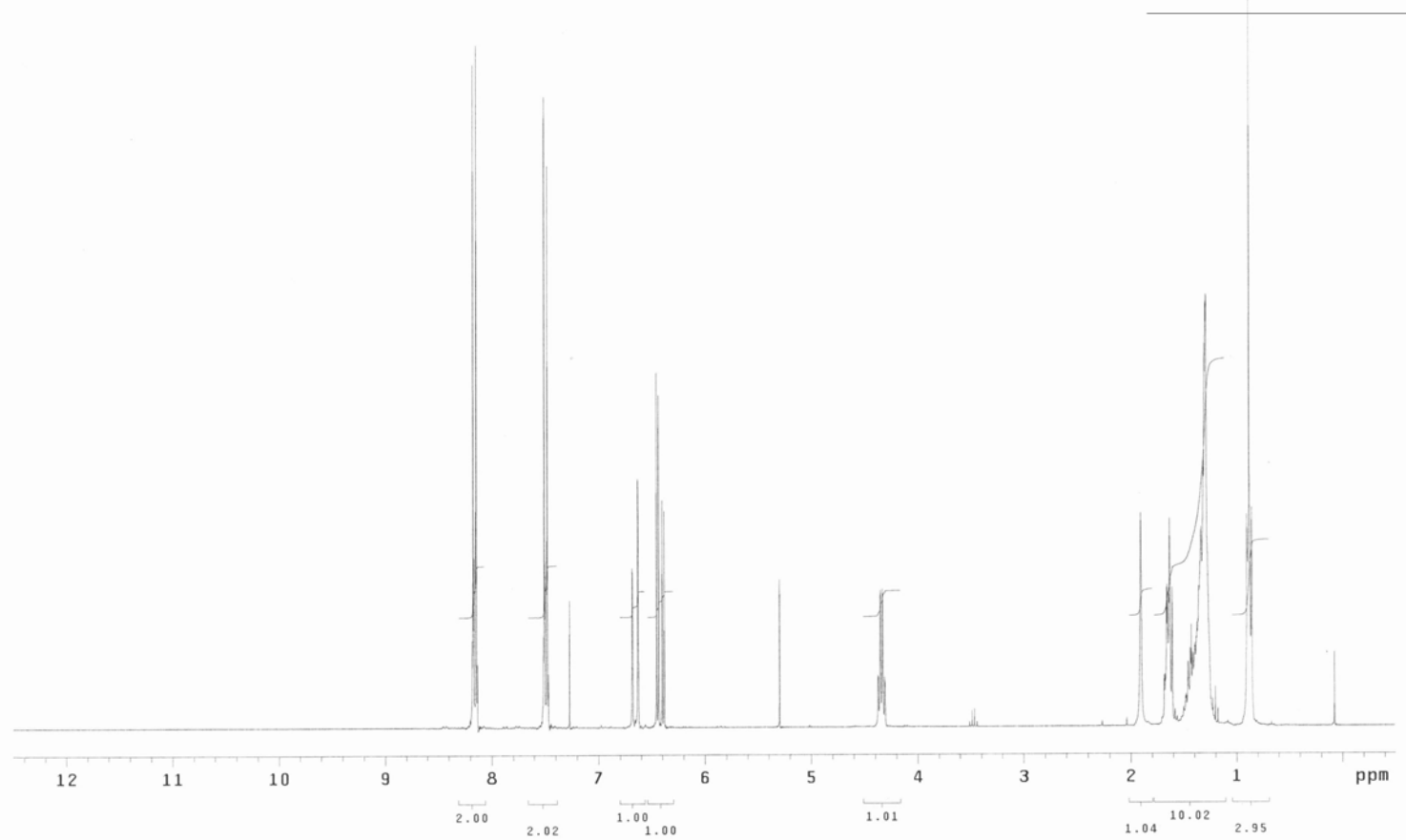


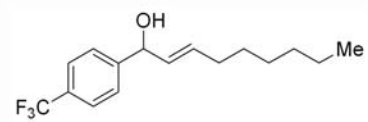
compound (Z)-18b



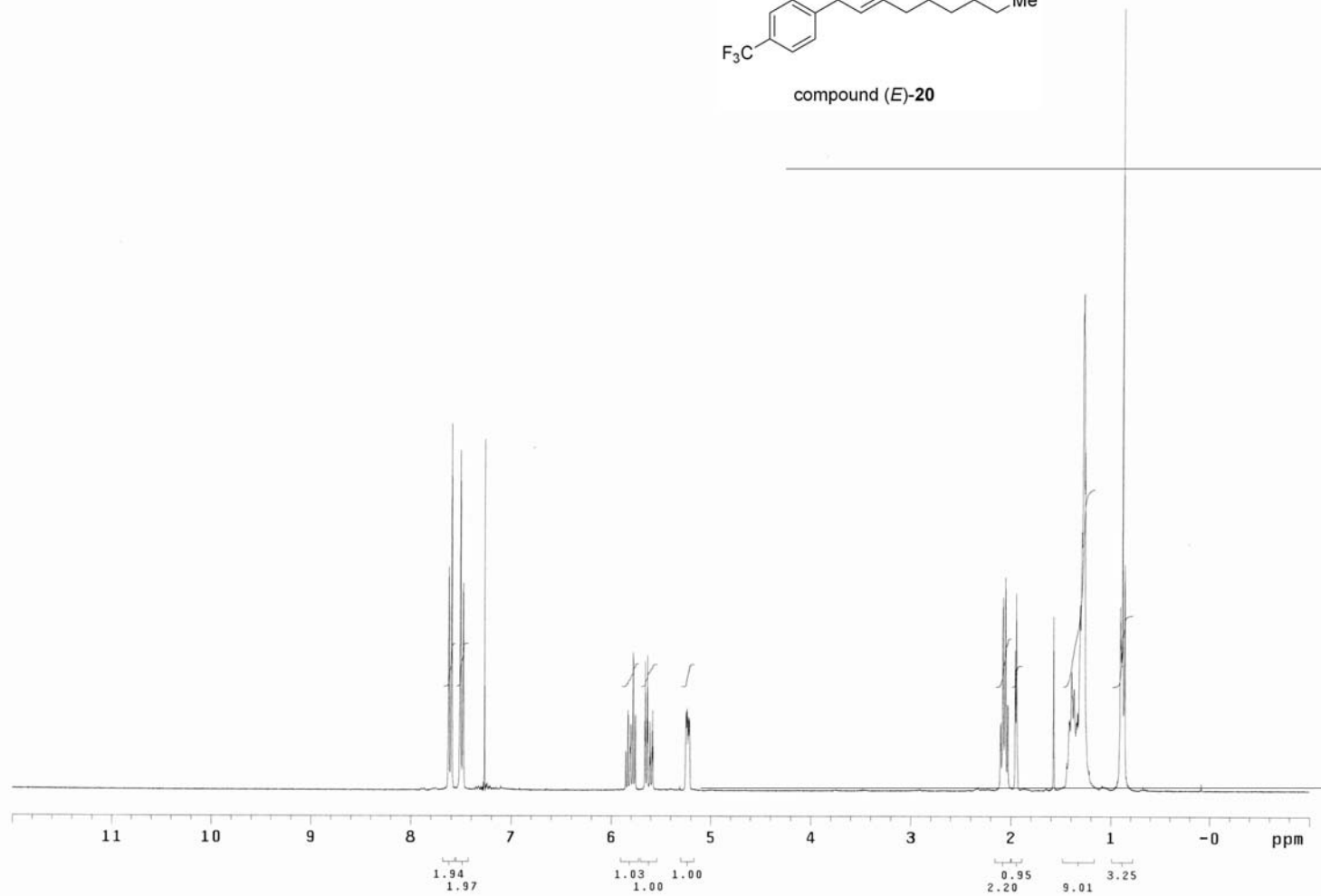


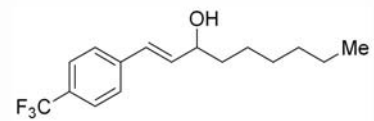
compound (E)-19b



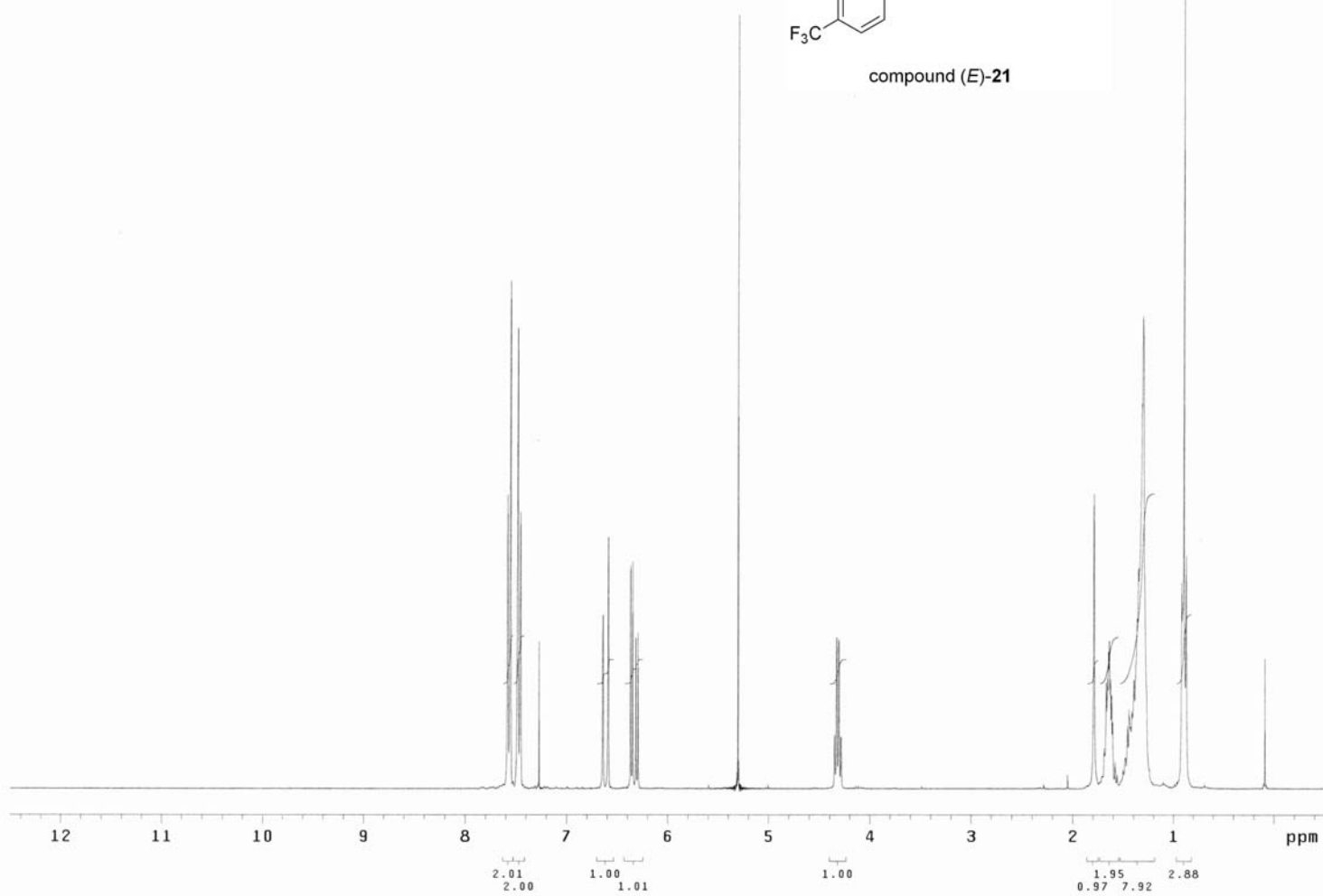


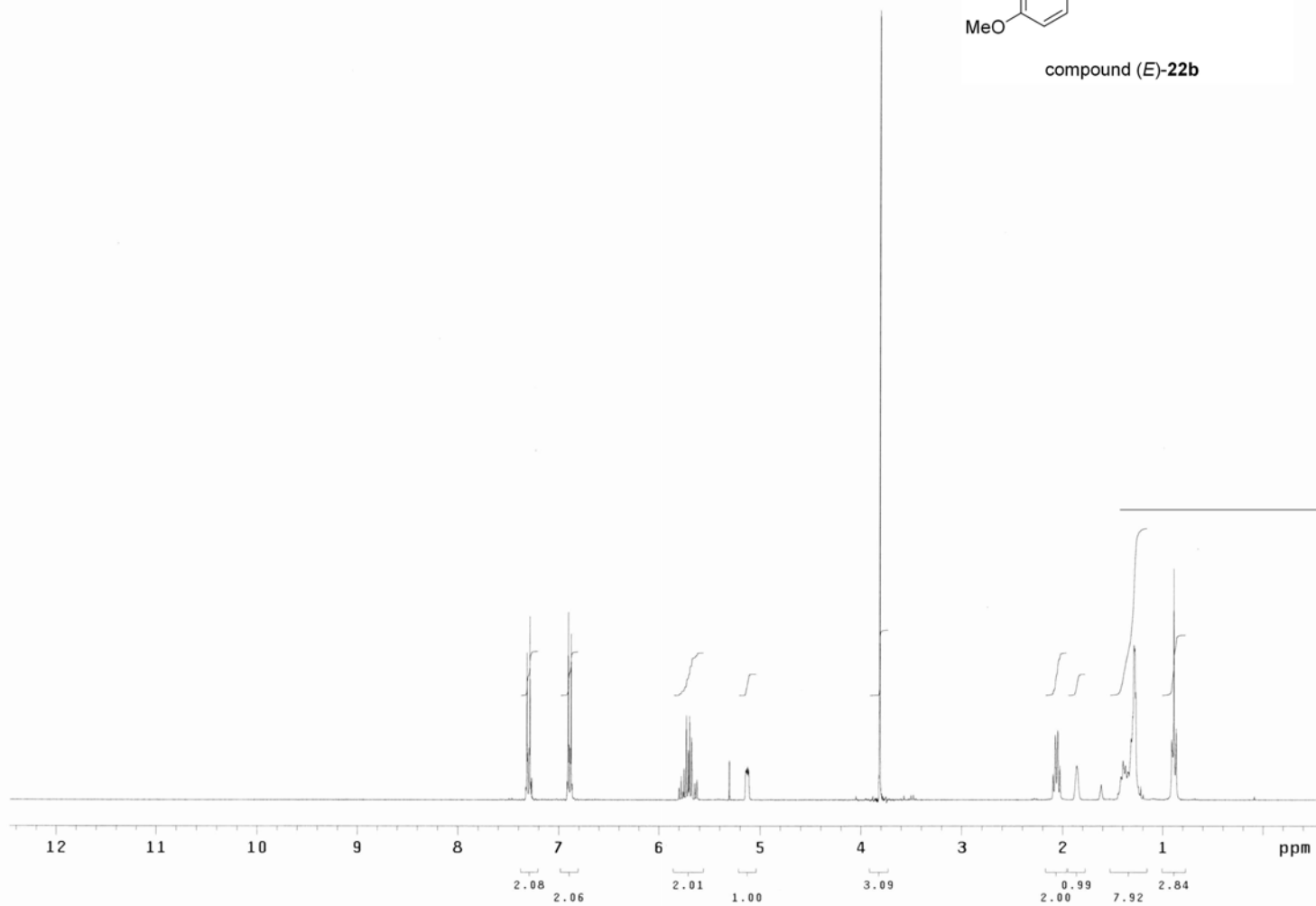
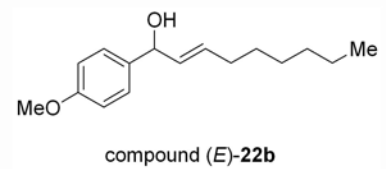
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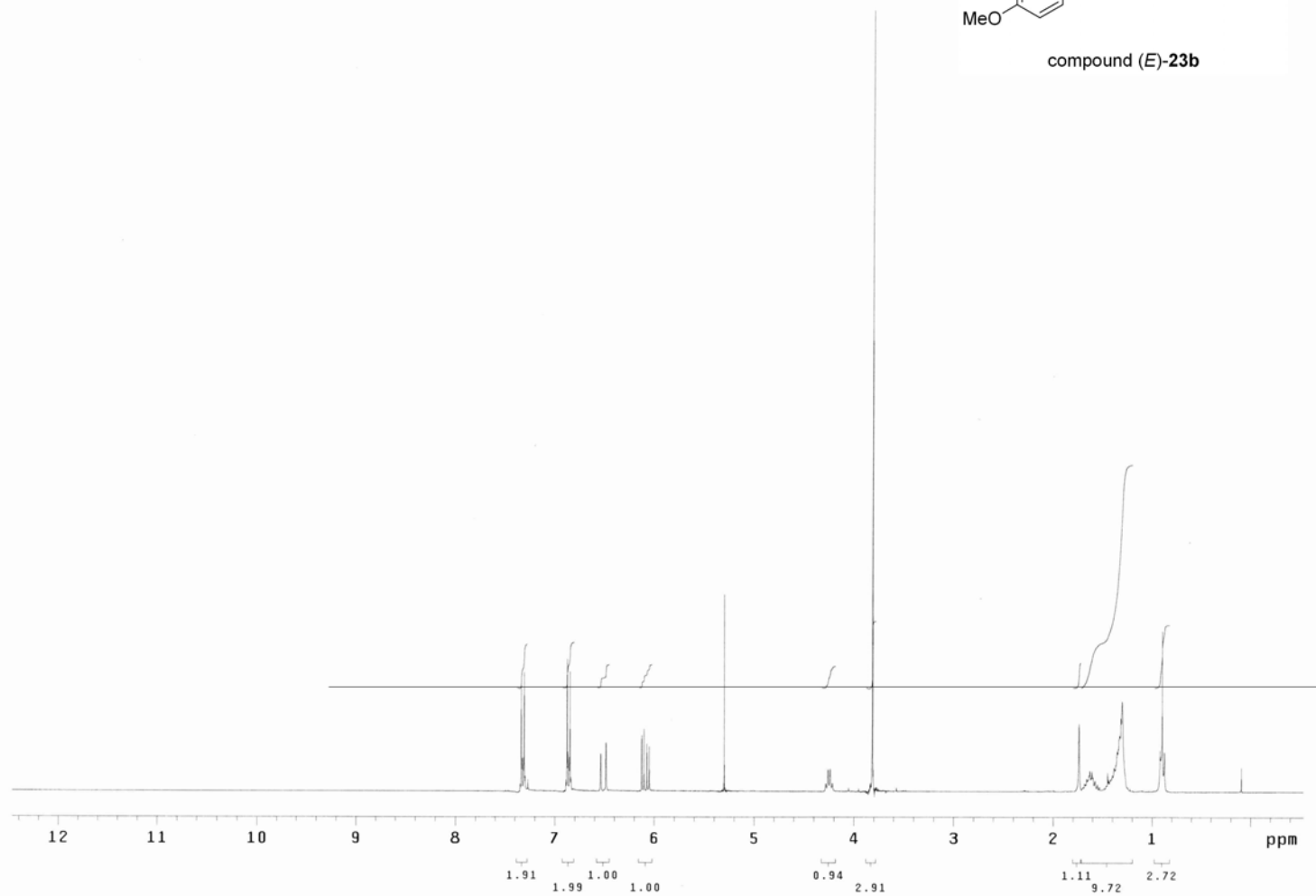
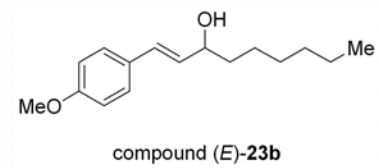




compound (E)-21



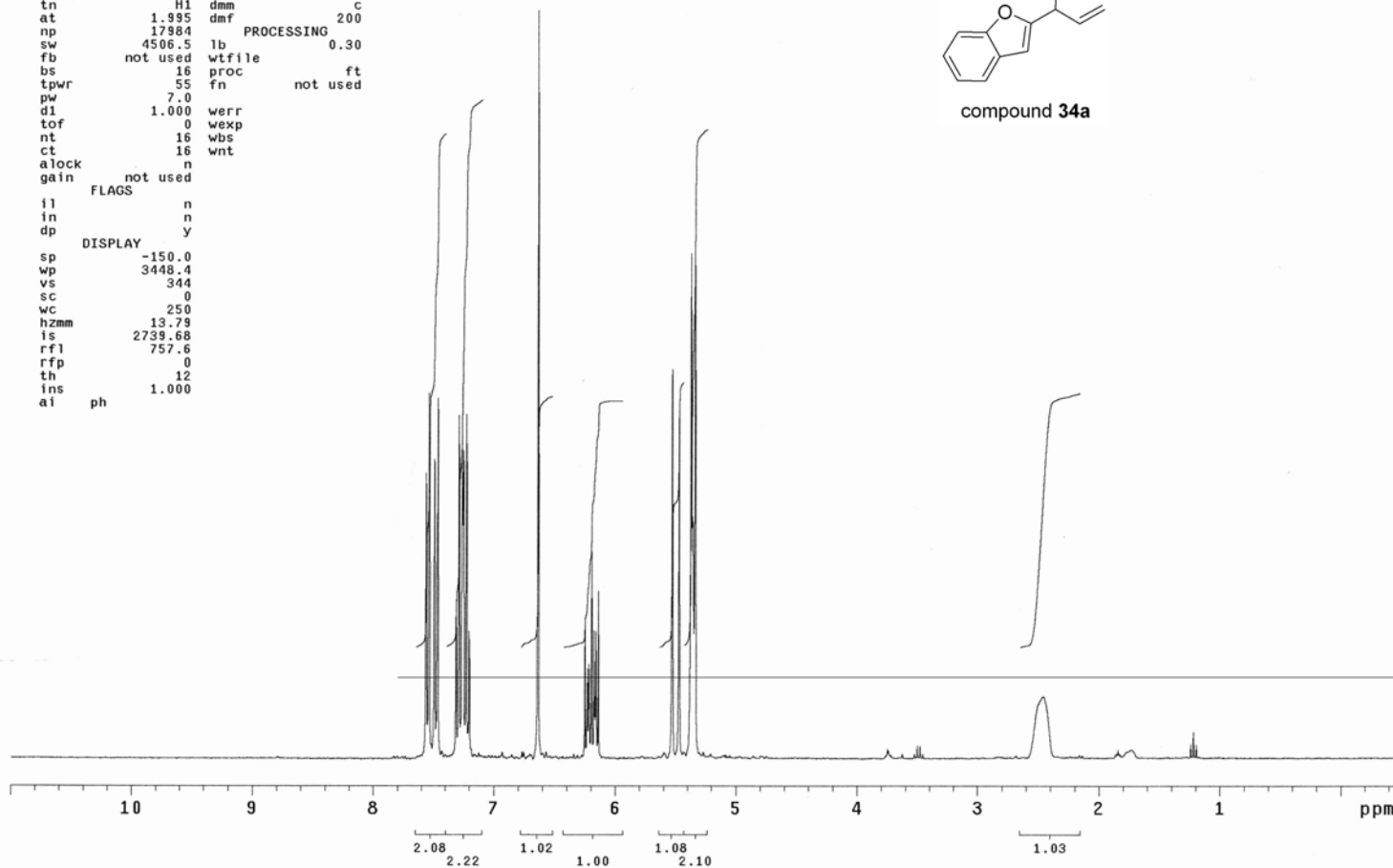
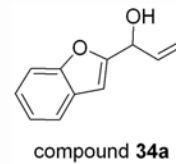




GB464F

exp3 std1h

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date	Oct 3 2005	dfrq	299.868
solvent	CDC13	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	299.868	da	nnn
tn	H1	dmm	c
at	1.995	dmf	200
np	17984	PROCESSING	
sw	4506.5	lb	0.30
fb	not used	wtfile	
bs	16	proc	ft
tpwr	55	fn	not used
pw	7.0		
d1	1.000	werr	
tof	0	wexp	
nt	16	wbs	
ct	16	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-150.0		
wp	3448.4		
vs	344		
sc	0		
wc	250		
hzmm	13.79		
is	2739.68		
rfl	757.6		
rfp	0		
th	12		
ins	1.000		
al	ph		

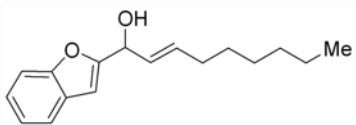




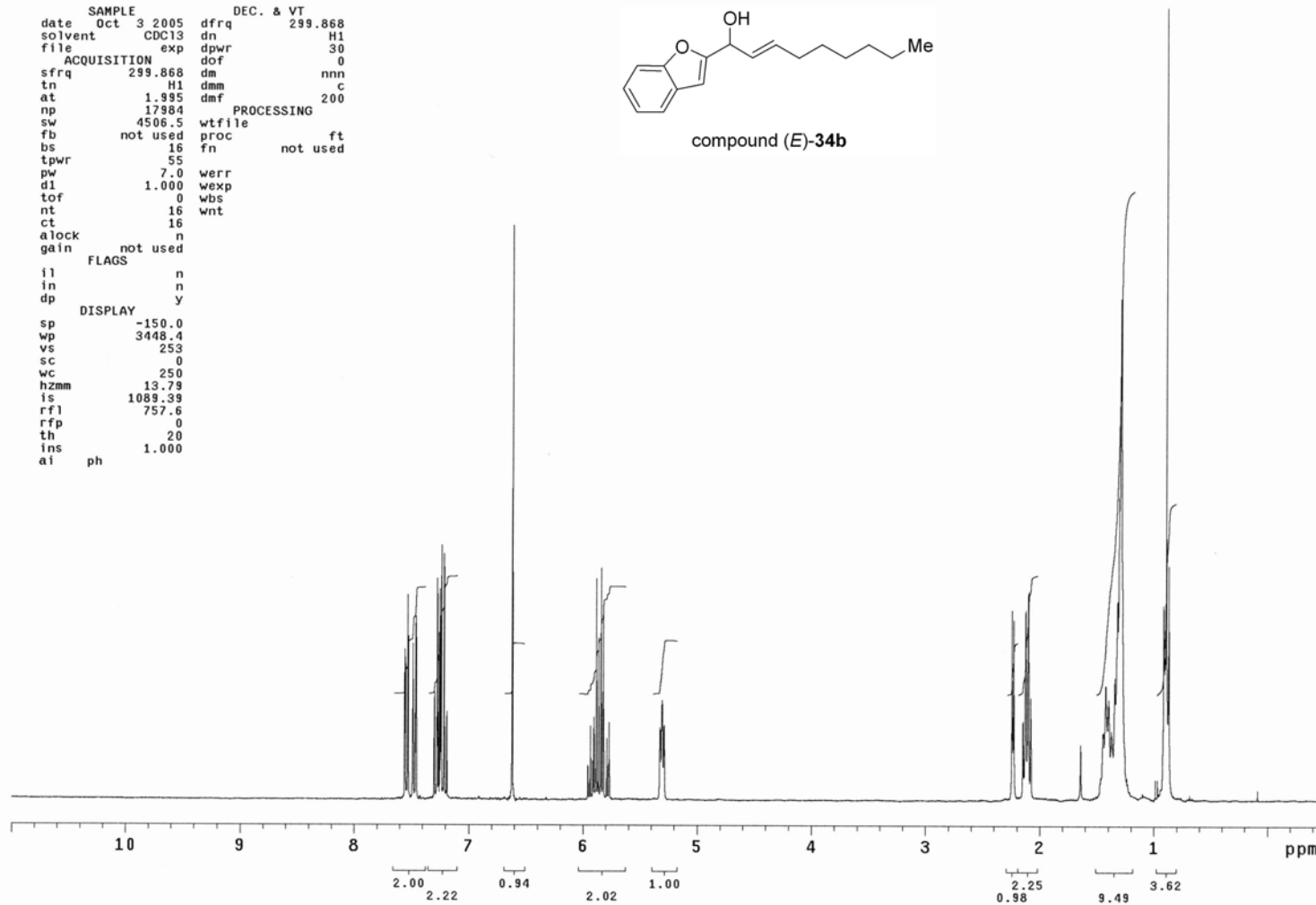
GB447F

exp3 stdih

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file     exp       dpwr    30
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sfrq     299.868  dm      nnn
tn       H1       dmm     c
at       1.995    dmf     200
np       17984
sw       4506.5   wtfile
fb       not used proc     ft
bs       16      fn      not used
tpwr     55
pw       7.0     werr
d1       1.000   wexp
tof      0       wbs
nt       16     wnt
ct       16
alock    not used
gain
  FLAGS
  il     n
  in     n
  dp     y
  DISPLAY
  sp     -150.0
  wp     3448.4
  vs     253
  sc     0
  wc     250
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  rfl    757.6
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  th     20
  ins    1.000
  al     ph
```



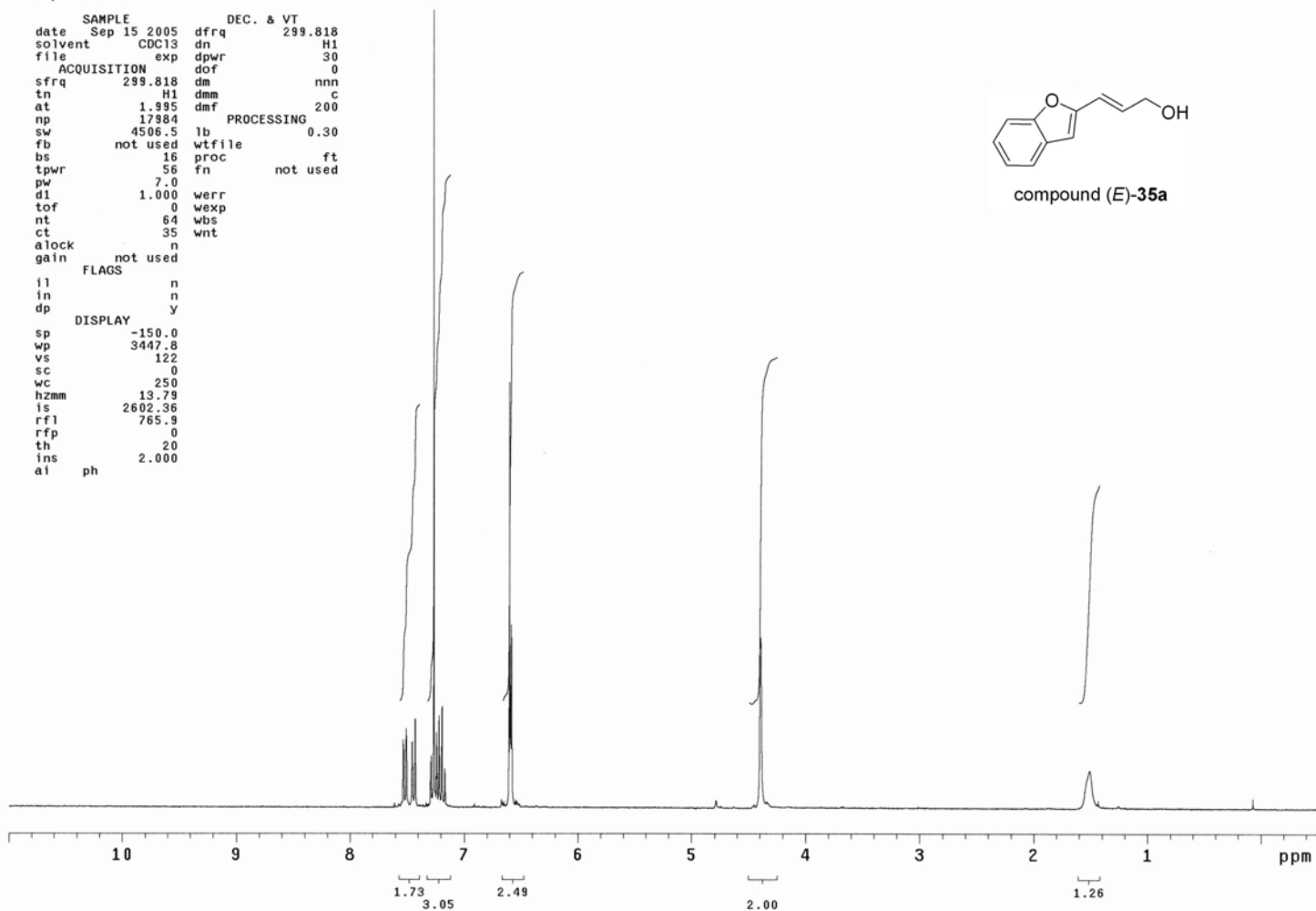
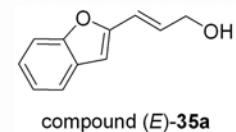
compound (E)-34b



GB459F

exp3 std1h

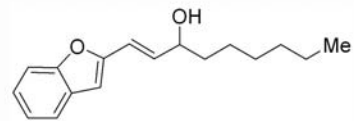
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solvent CDC13      dn          H1
file      exp      dpwr         30
ACQUISITION exp      dof         0
sfrq      299.818  dm          nnn
tn         H1      dmm          C
at         1.995   dmf          200
np         17984   PROCESSING
sw         4506.5 lb          0.30
fb         not used wfile
bs         16     proc         ft
tpwr       56     fn          not used
pw         7.0
d1         1.000  werr
tof        0     wexp
nt         64    wbs
ct         35    wnt
alock      n
gain       not used
FLAGS
il         n
in         n
dp         y
DISPLAY
sp        -150.0
wp        3447.8
vs         122
sc         0
wc         250
hzm       13.79
is        2602.36
rf1       765.9
rfp        0
th         20
ins       2.000
ai        ph
```



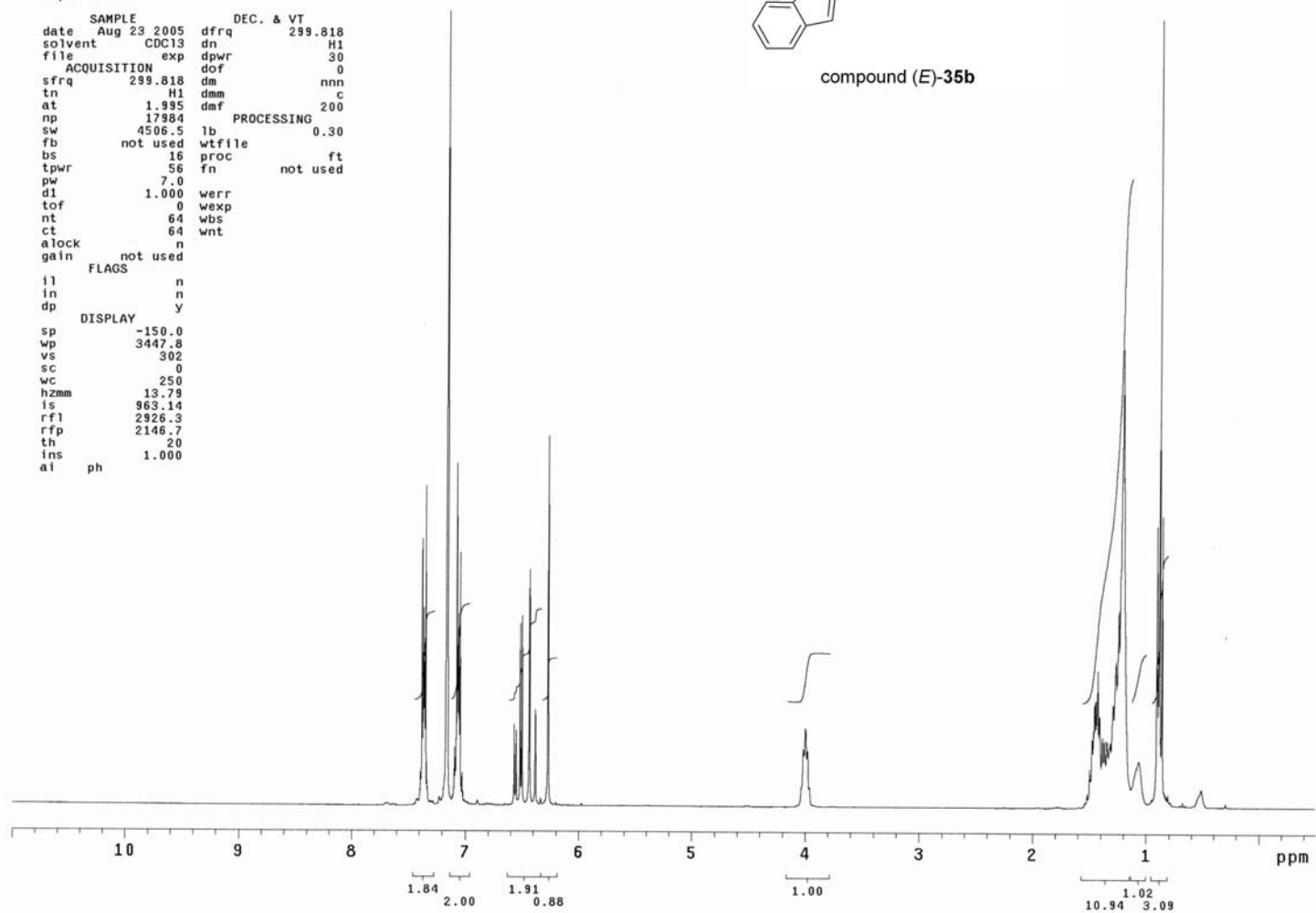
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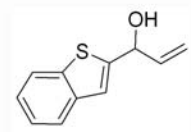
exp2 std1h

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solvent CDC13      dn       H1
file      exp      dpwr     30
ACQUISITION     dof       0
sfrq      299.818  dm       nnn
tn         H1       dmm     c
at         1.995   dmf     200
np         17984   PROCESSING 0.30
sw         4506.5  lb
fb         not used wtfile
bs         16     proc     ft
tpwr       56     fn       not used
pw         7.0
d1         1.000  werr
tof        0     wexp
nt         64    wbs
ct         64    wnt
alock      n
gain       not used
FLAGS      n
il         n
in         n
dp         y
DISPLAY
sp         -150.0
wp         3447.8
vs         302
sc         0
wc         250
hzmm       13.79
is         963.14
rf1        2926.3
rfp        2146.7
th         20
ins        1.000
al ph
```

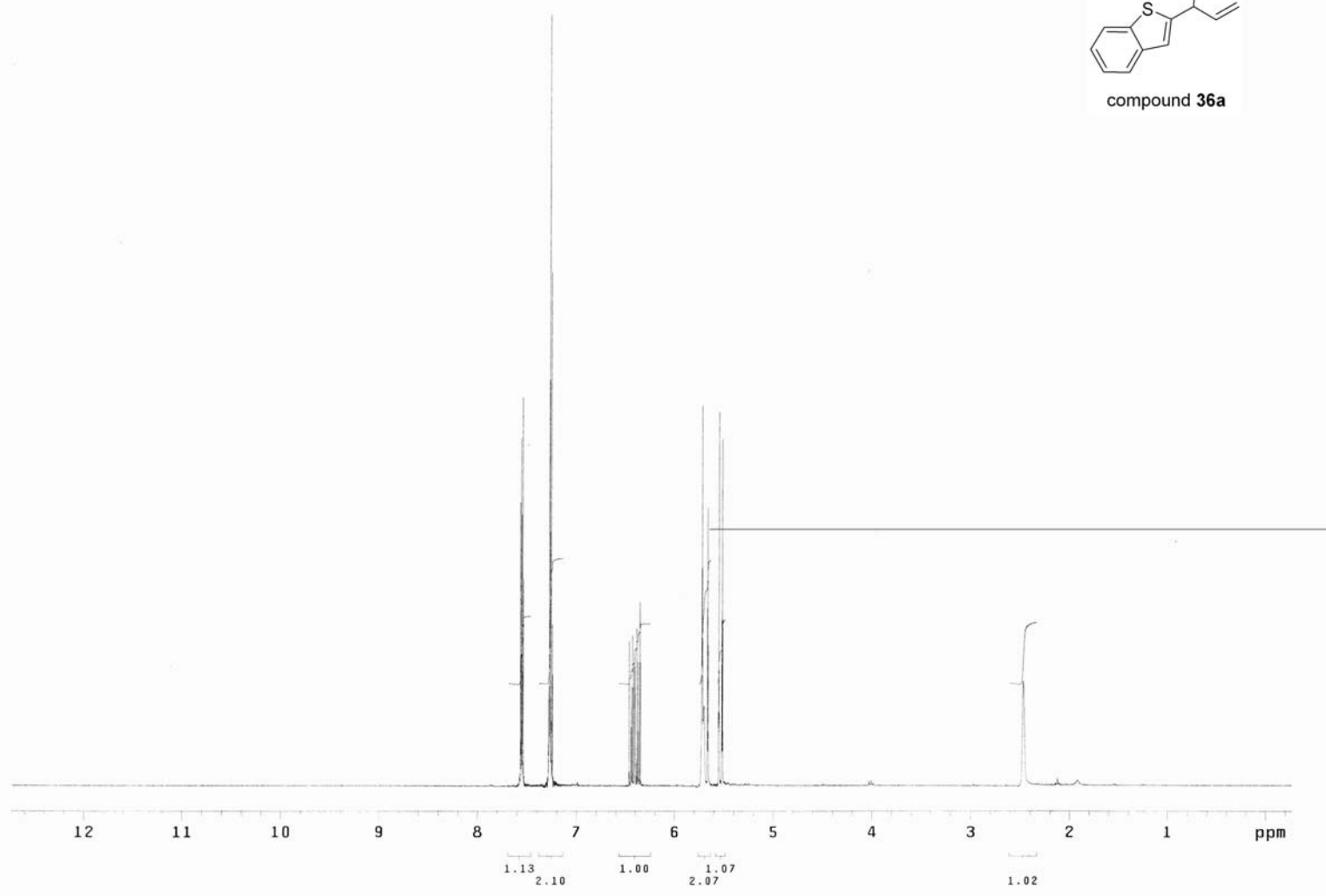


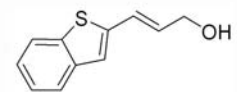
compound (E)-35b



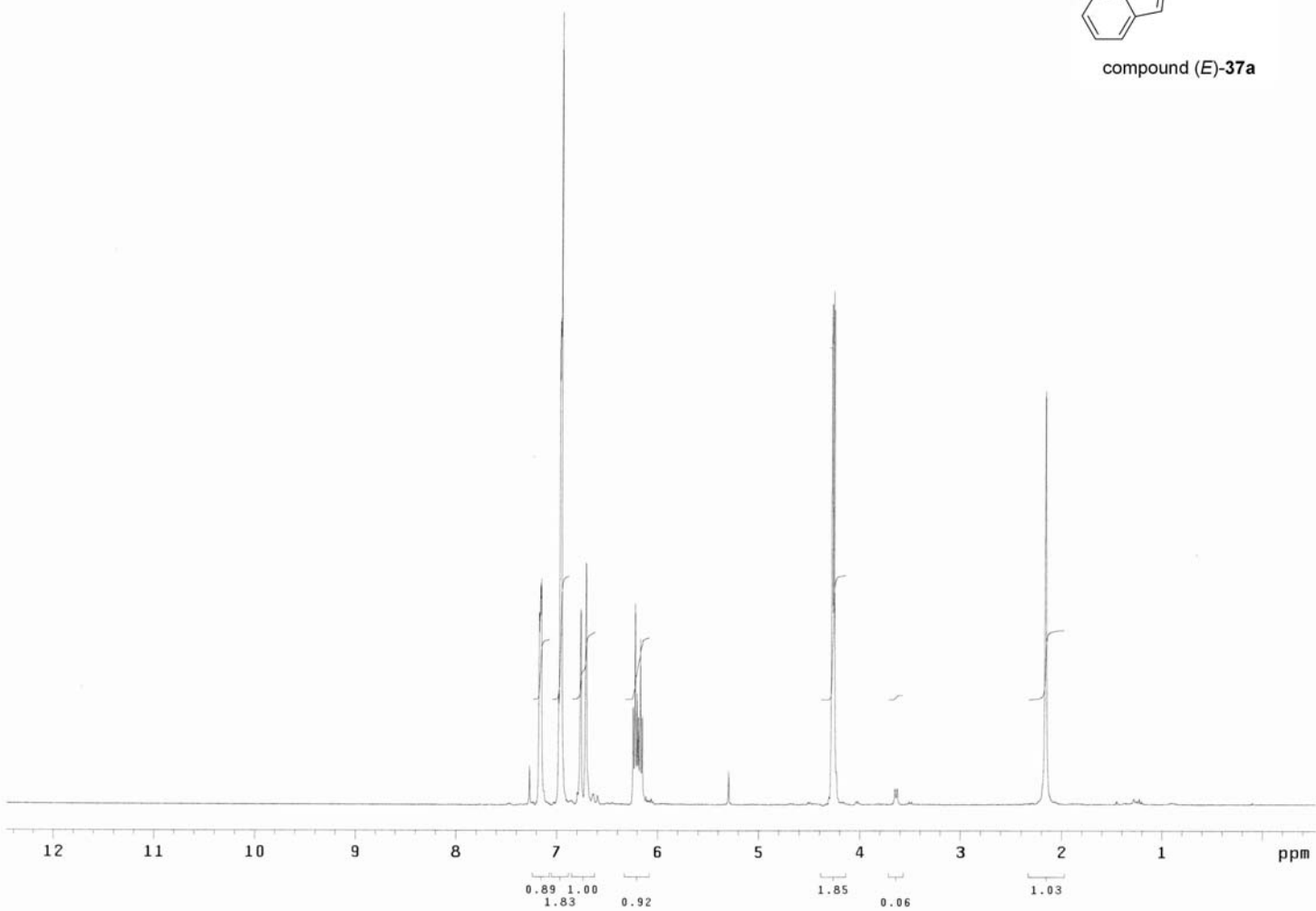


compound 36a





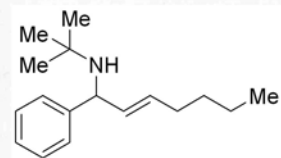
compound (E)-37a



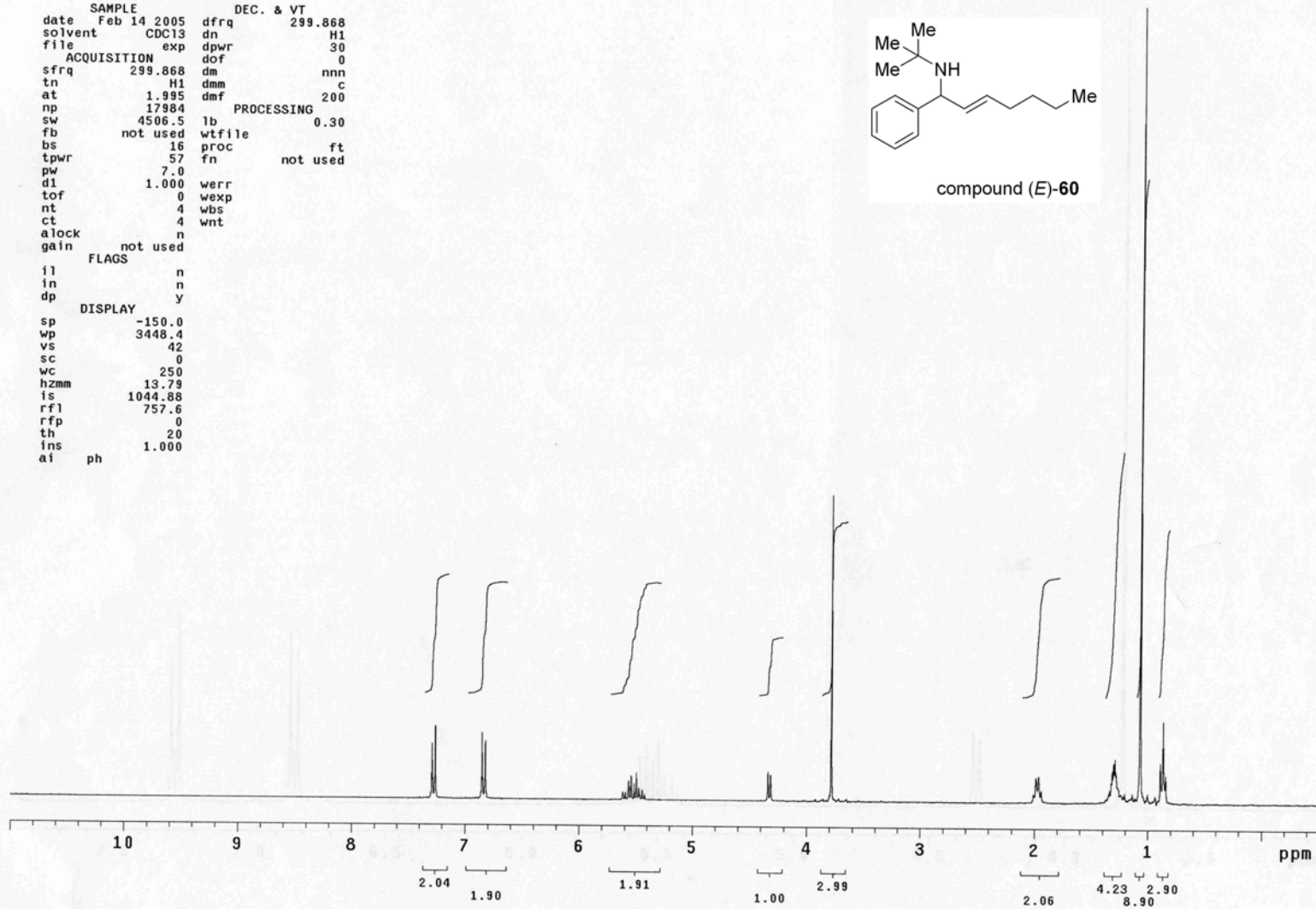
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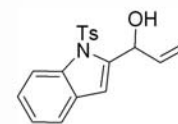
exp1 std1h

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file	exp	dpwr	30
ACQUISITION		PROCESSING	
sfrq	299.868	dm	nnn
tn	H1	dmm	c
at	1.995	dmf	200
np	17984	lb	0.30
sw	4506.5	wtfile	
fb	not used	proc	ft
bs	16	fn	not used
tpwr	57		
pw	7.0		
d1	1.000	werr	
tof	0	wexp	
nt	4	wbs	
ct	4	wnt	
alock	not used		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-150.0		
wp	3448.4		
vs	42		
sc	0		
wc	250		
hzmm	13.79		
is	1044.88		
rfl	757.6		
rfp	0		
th	20		
ins	1.000		
ai	ph		

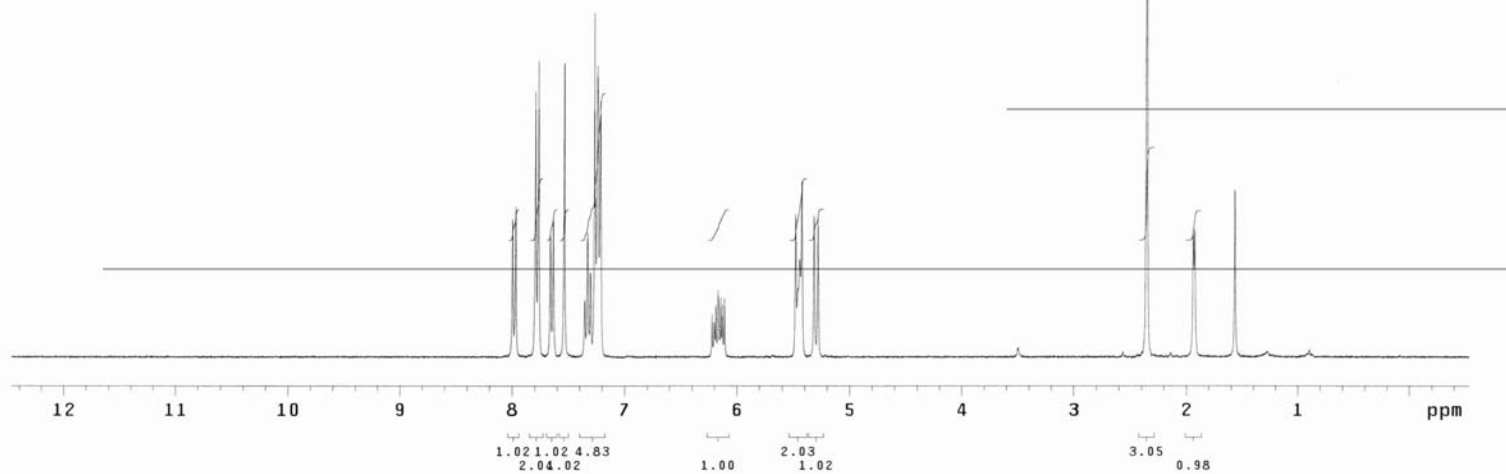


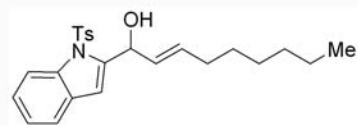
compound (E)-60



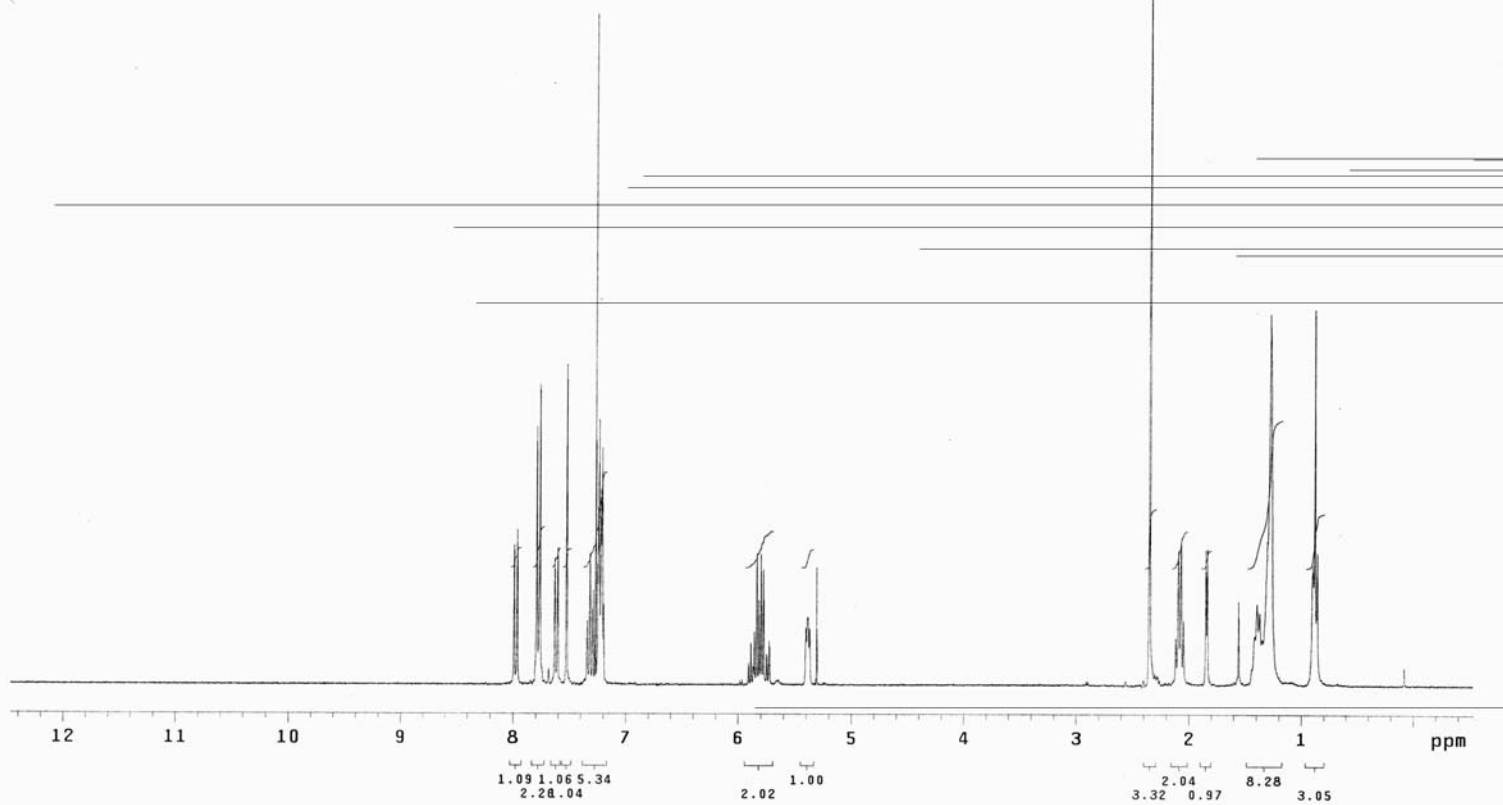


compound 38a

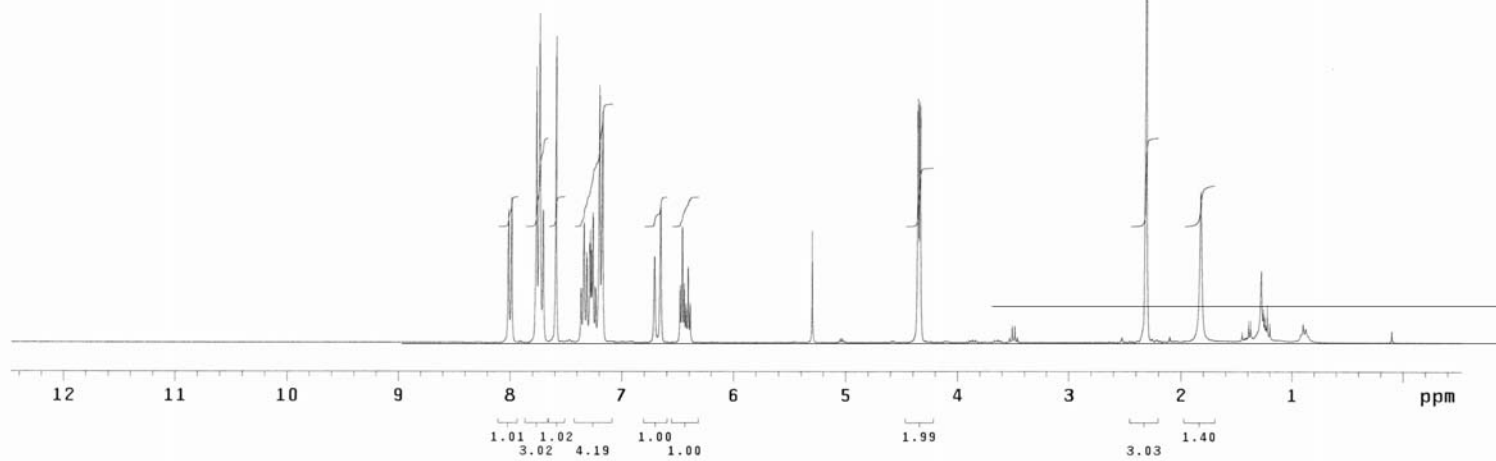
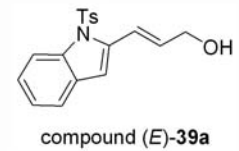


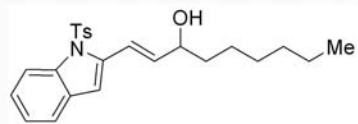


compound (E)-38b

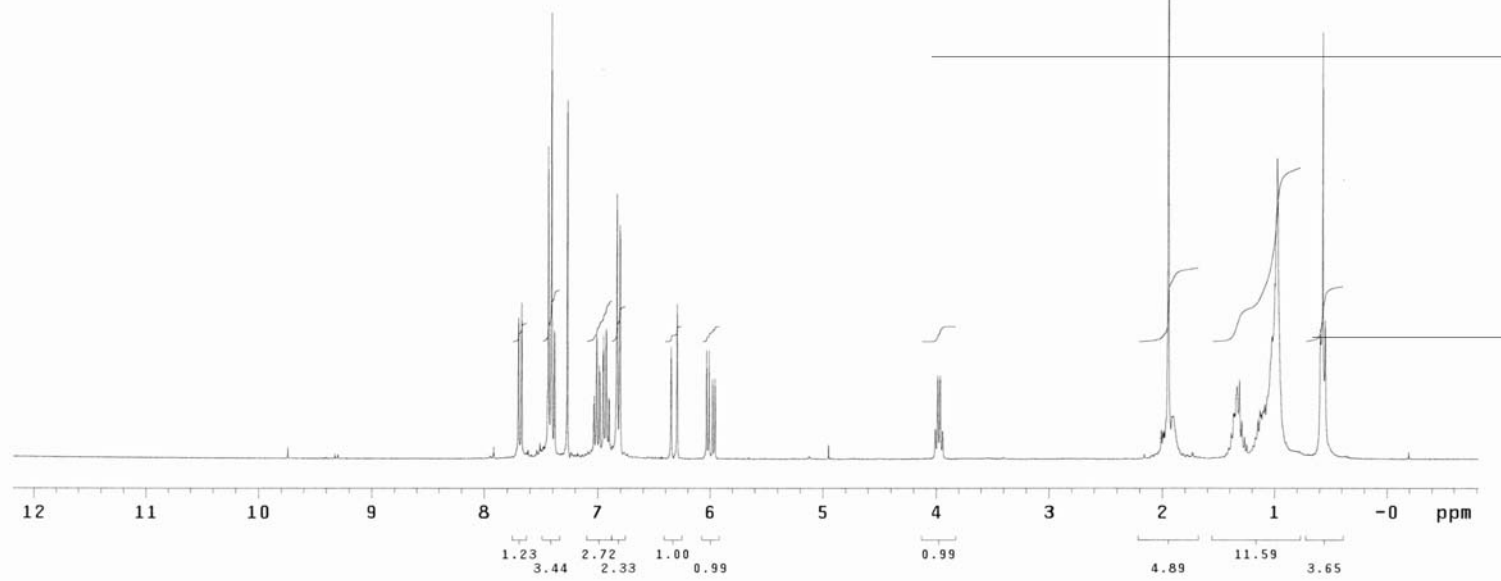








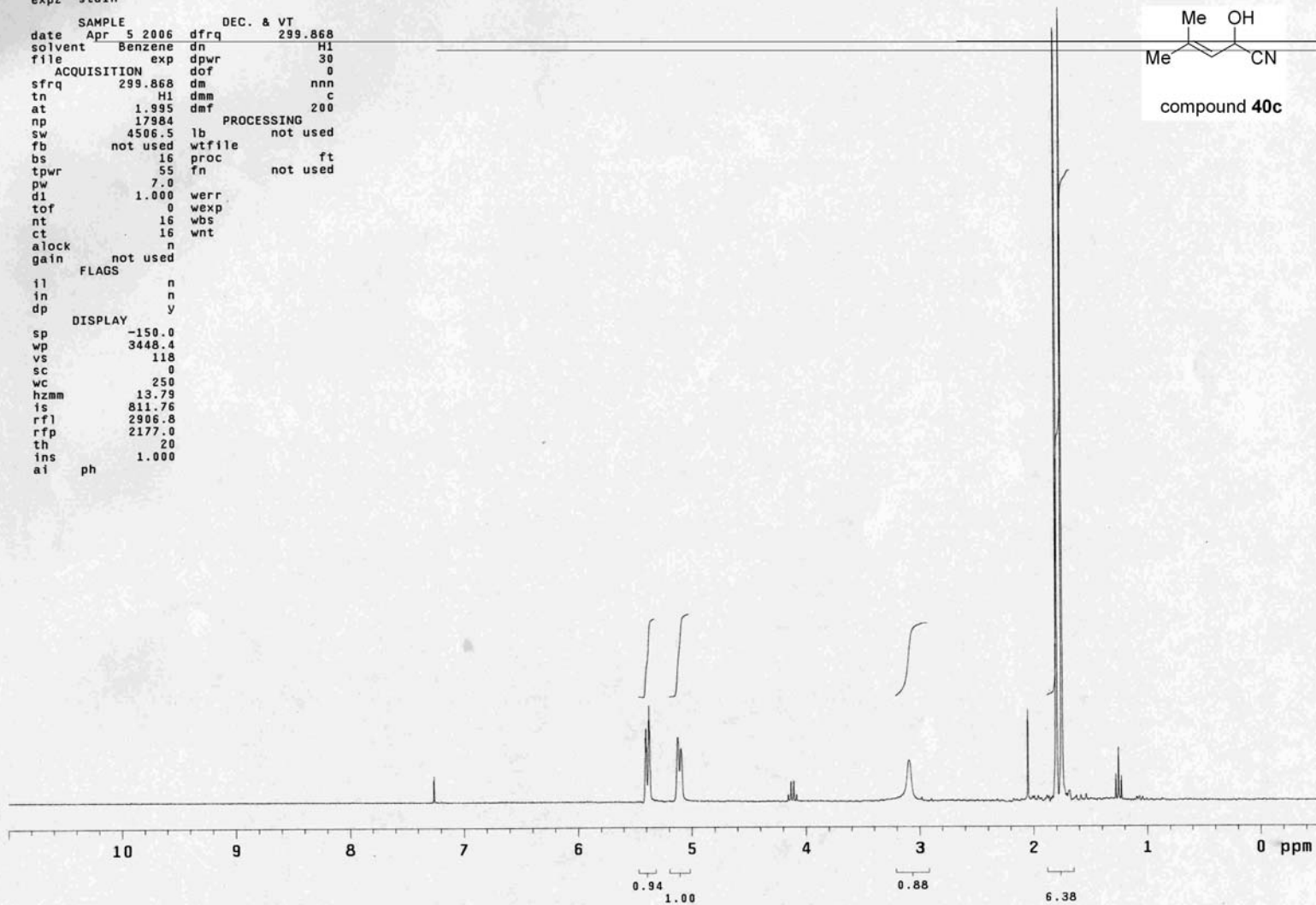
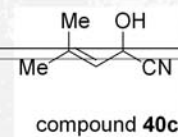
compound (*E*)-39b



GB573F

exp2 std1h

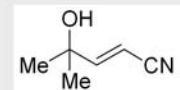
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solvent Benzene dn HI  
file exp dpwr 30  
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sfrq 299.868 dm nnn  
tn HI dmm c  
at 1.995 dmf 200  
np 17984 PROCESSING  
sw 4506.5 lb not used  
fb not used wtfile  
bs 16 proc ft  
tpwr 55 fn not used  
pw 7.0  
d1 1.000 werr  
tof 0 wexp  
nt 16 wbs  
ct 16 wnt  
alock n  
gain not used  
FLAGS  
il n  
in n  
dp y  
DISPLAY  
sp -150.0  
wp 3448.4  
vs 118  
sc 0  
wc 250  
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rfl 2906.8  
rfp 2177.0  
th 20  
ins 1.000  
ai ph



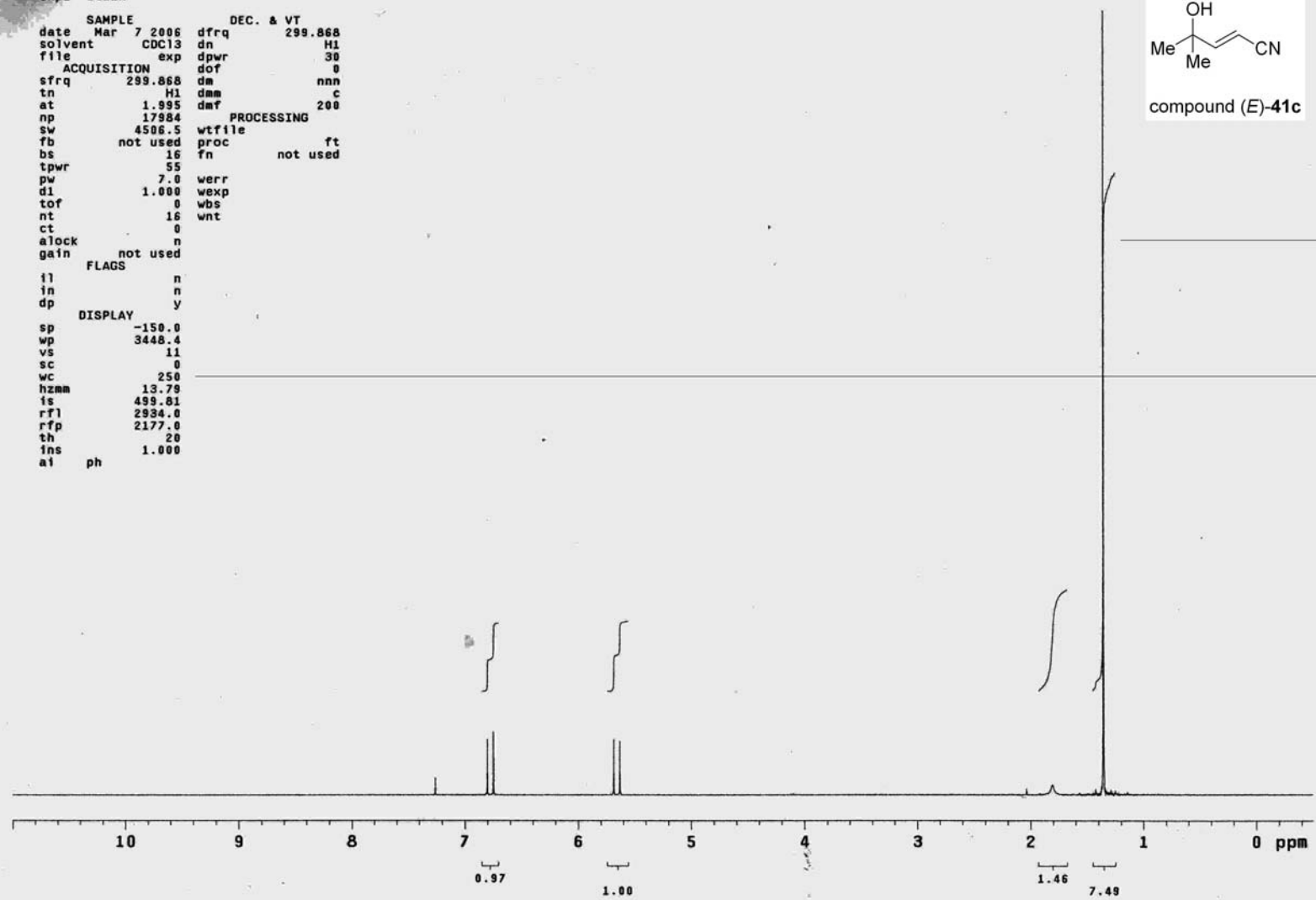
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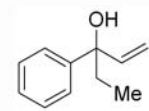
expl std1h

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ACQUISITION				
sfrq	299.868	dm		nnn
tn	H1	dmm		c
at	1.995	dmf		200
np	17984	PROCESSING		
sw	4508.5	wtfile		
fb	not used	proc		ft
bs	16	fn		not used
tpwr	55			
pw	7.0	werr		
d1	1.000	wexp		
tof	0	wbs		
nt	16	wnt		
ct	0			
alock	n			
gain	not used			
FLAGS				
il	n			
in	n			
dp	y			
DISPLAY				
sp	-150.0			
wp	3448.4			
vs	11			
sc	0			
wc	250			
hzmm	13.79			
fs	499.61			
rfl	2934.0			
rfp	2177.0			
th	20			
ins	1.000			
al	ph			

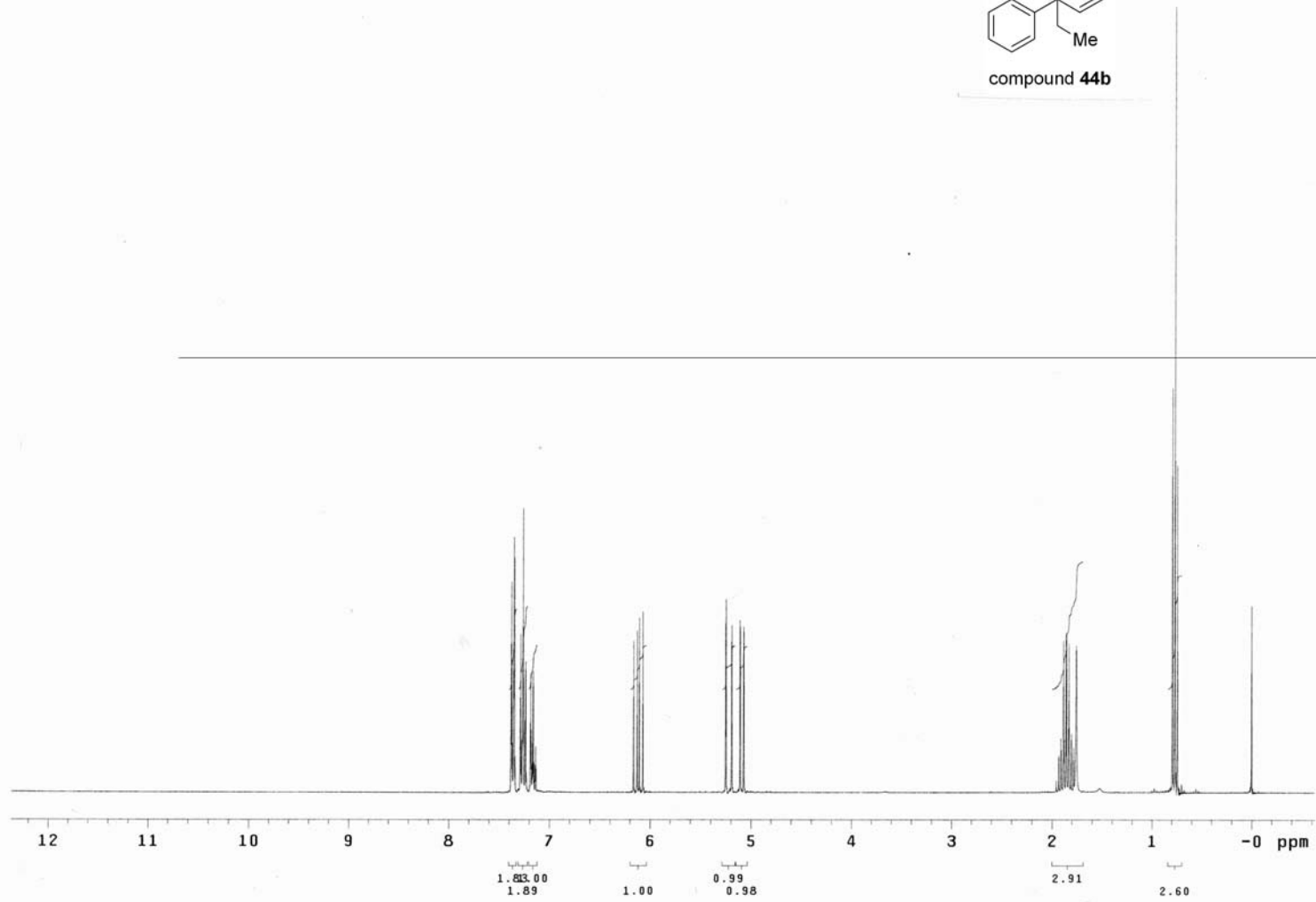


compound (E)-41c

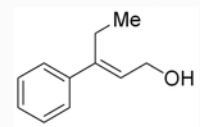




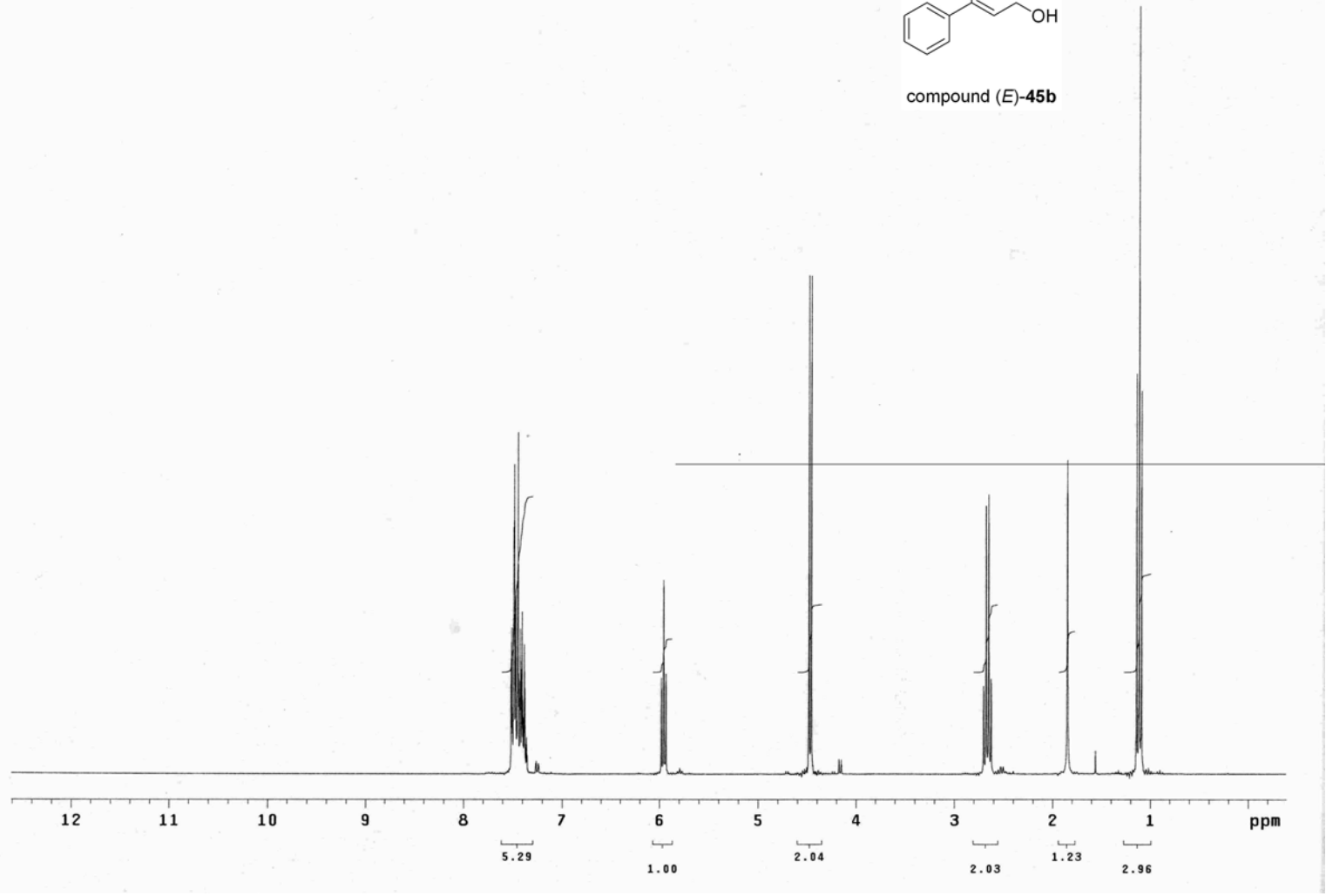
compound **44b**

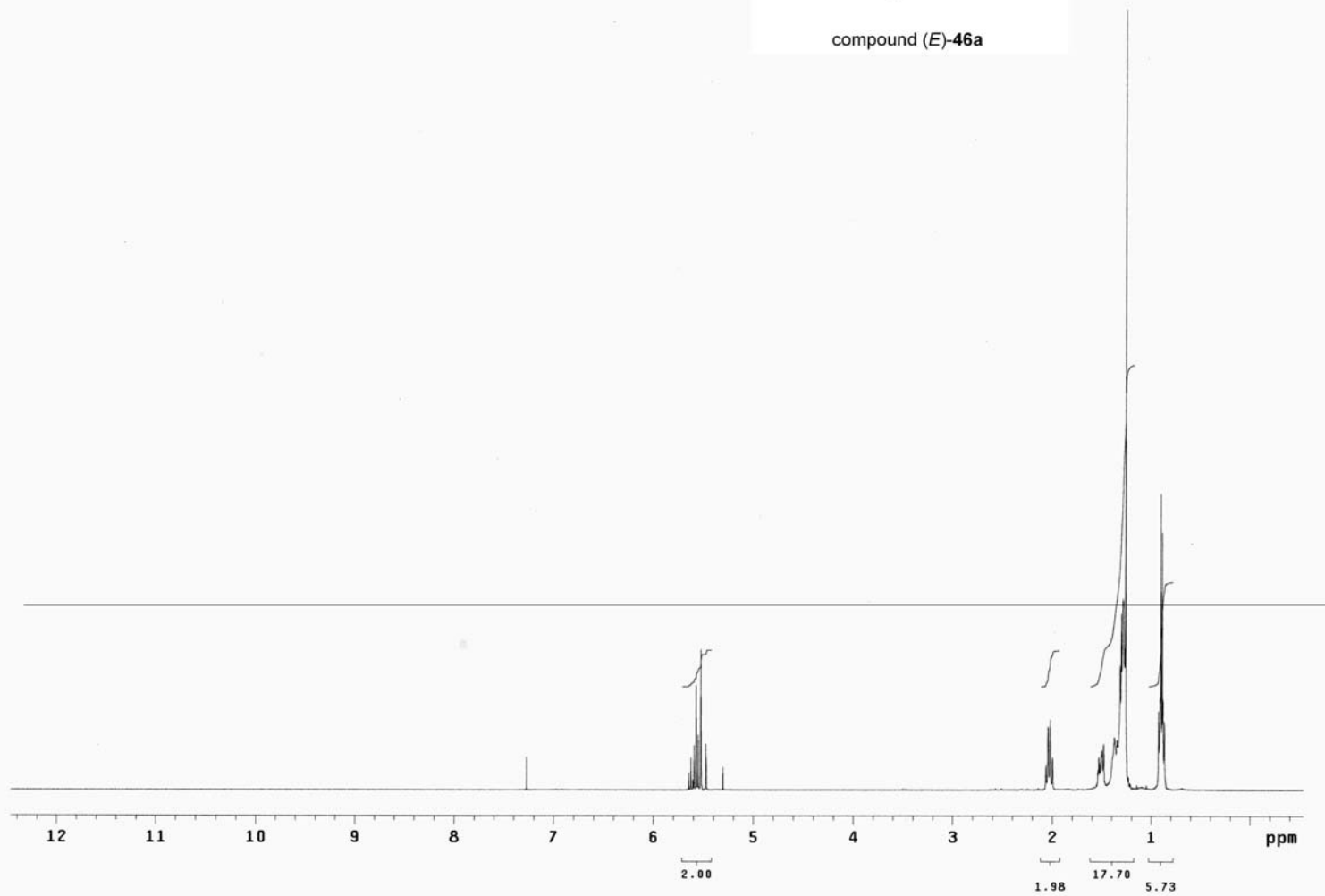
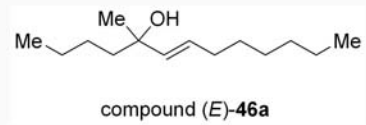


30 01 2010



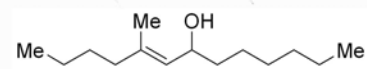
compound (E)-45b



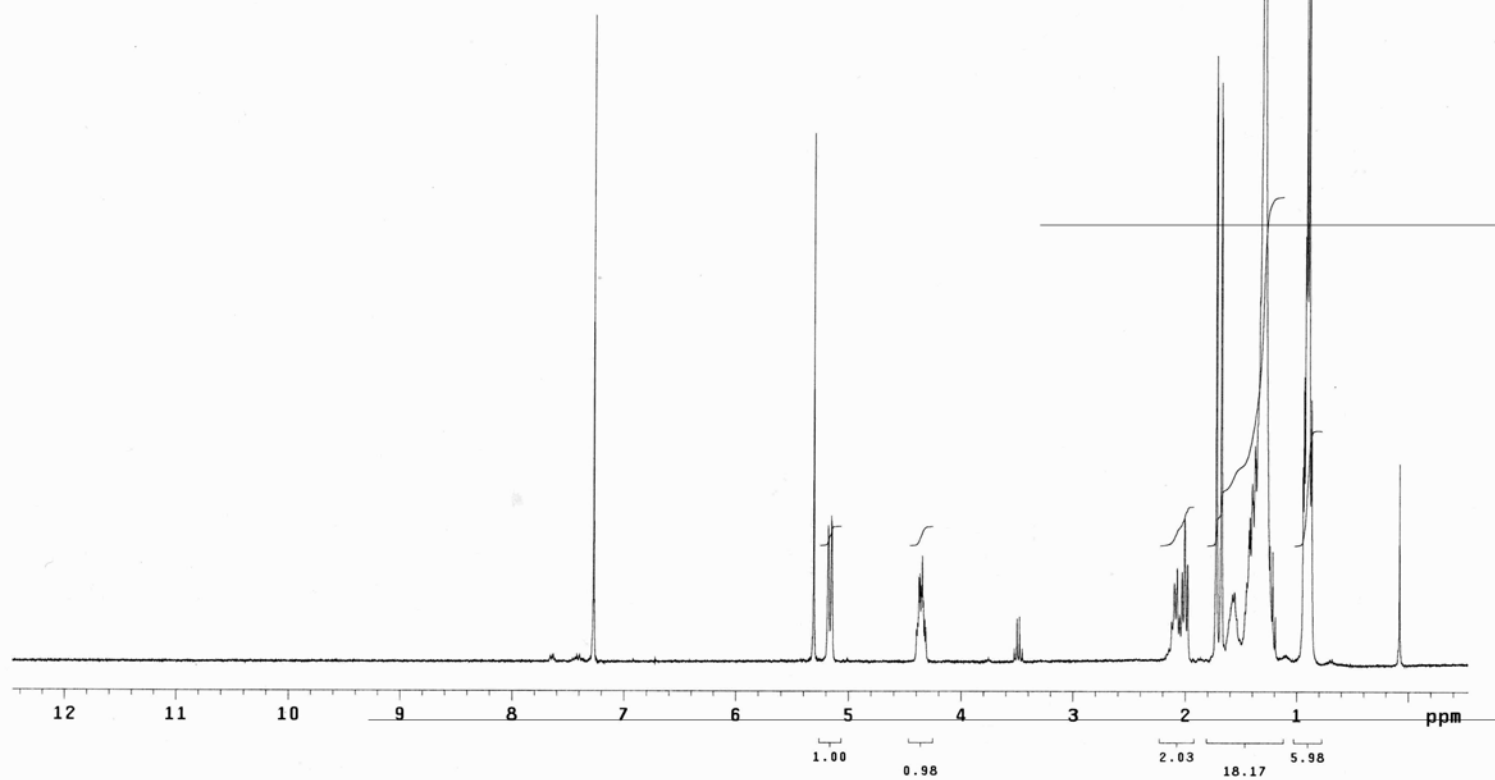


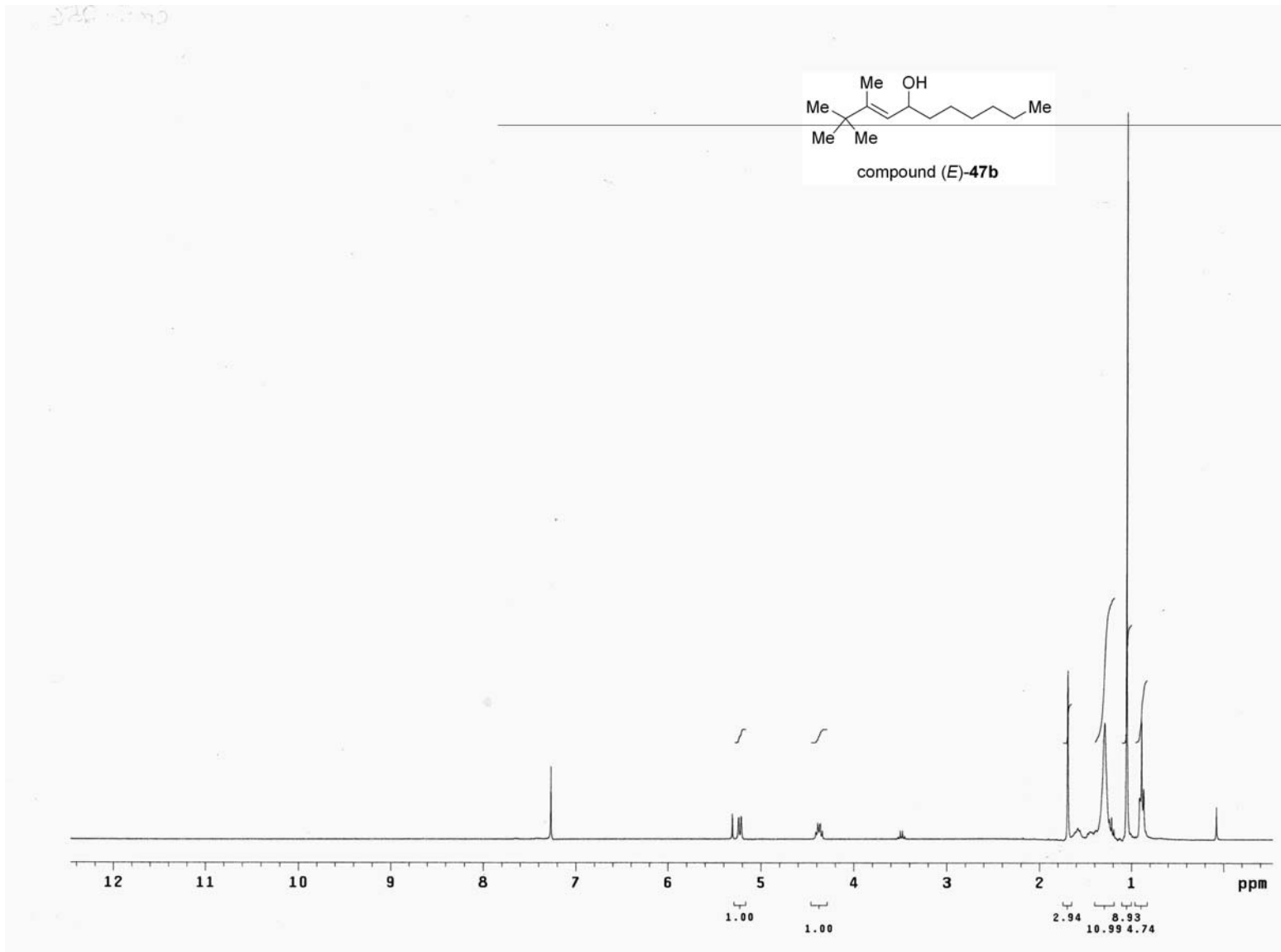


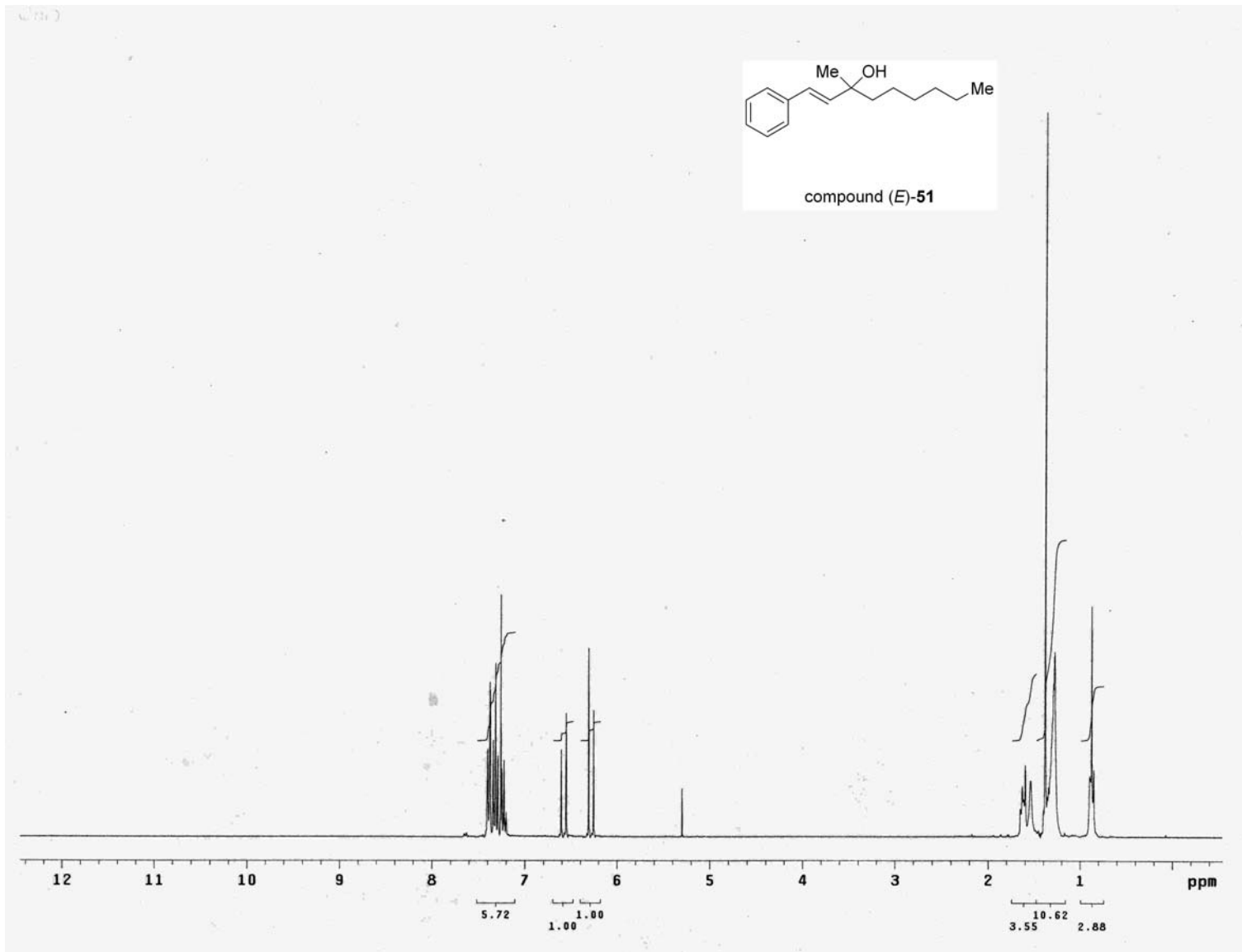


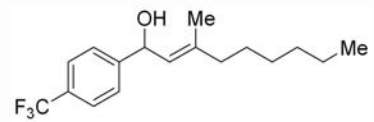


compound (E)-47a

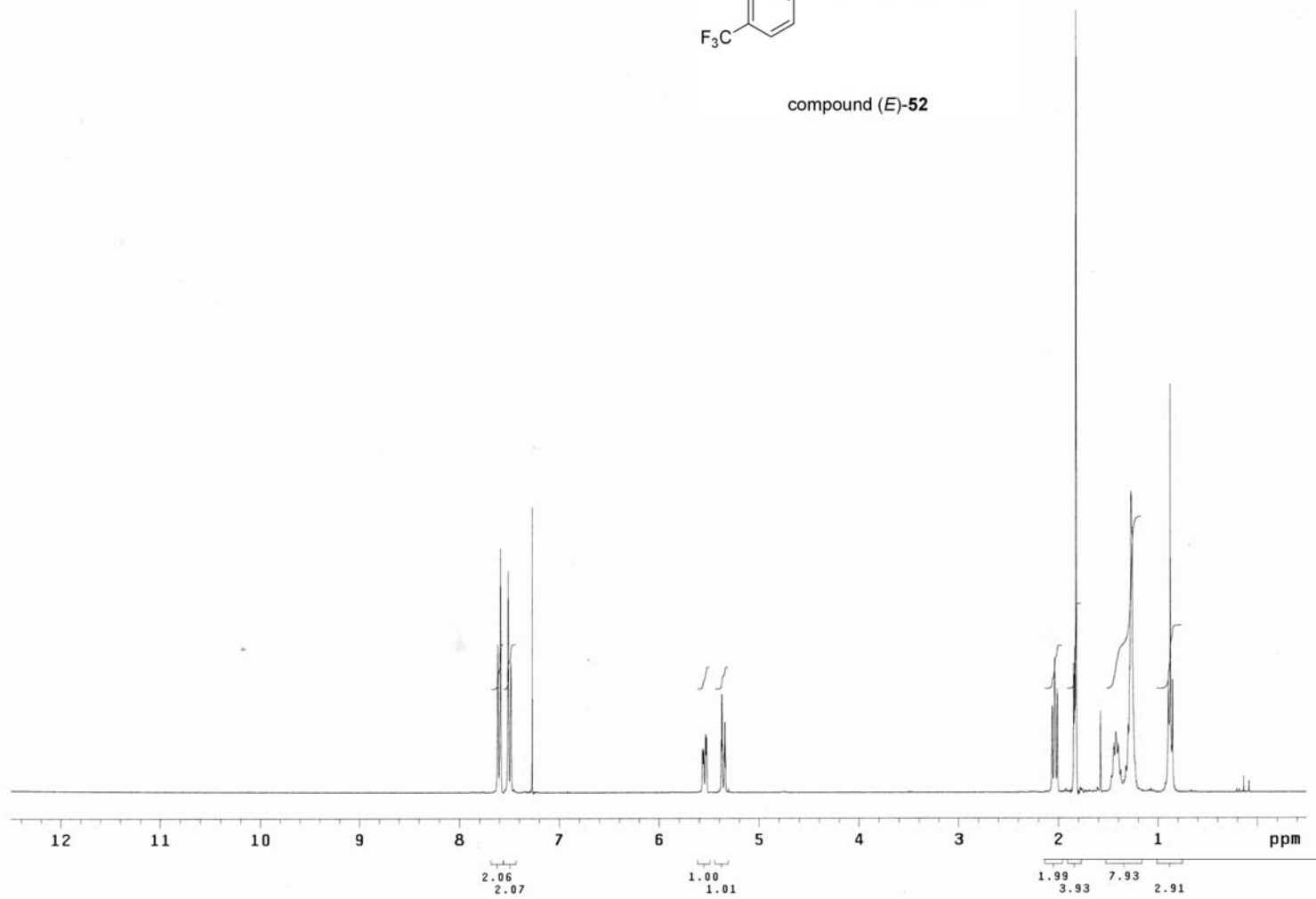


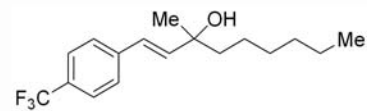




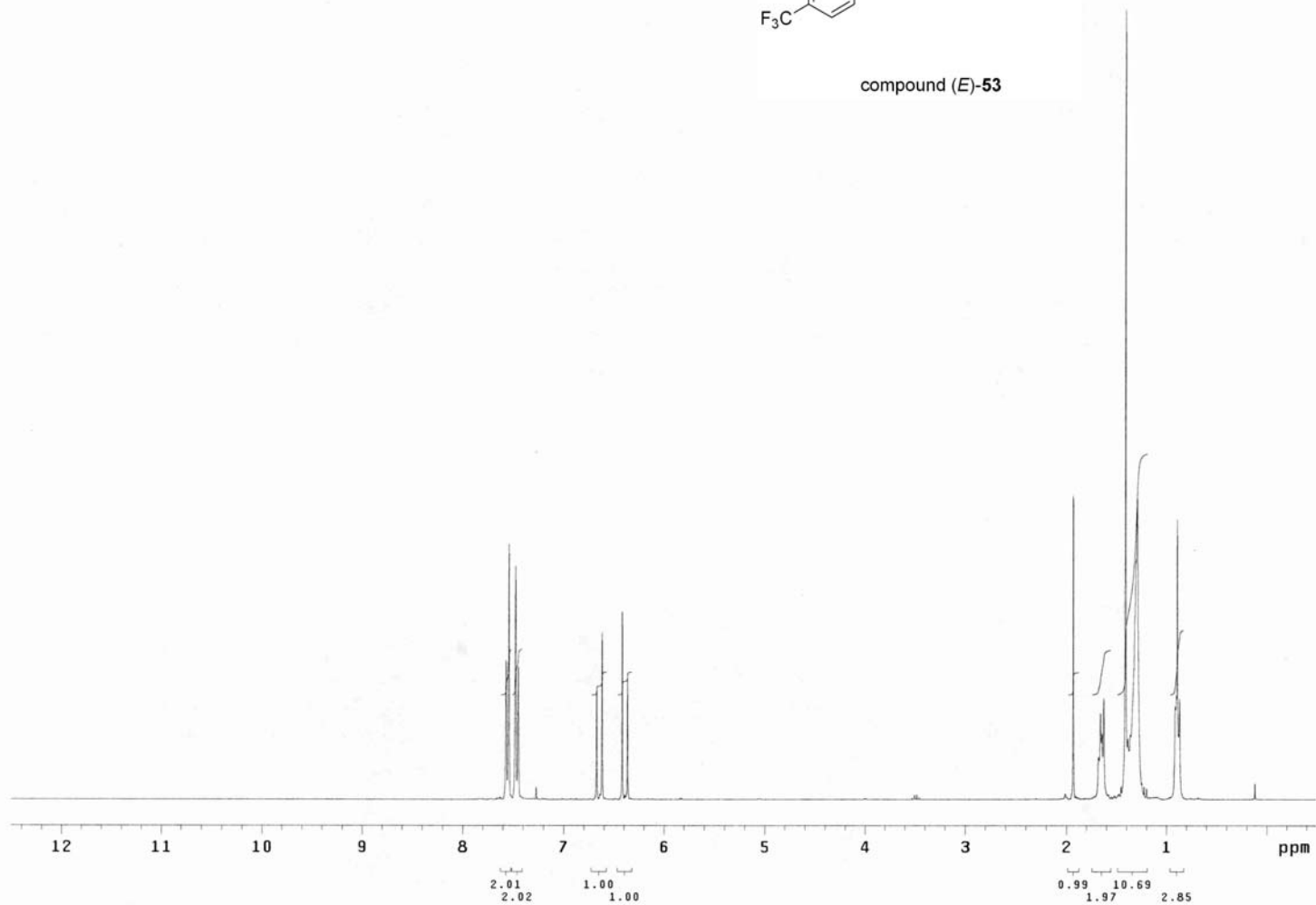


compound (E)-52





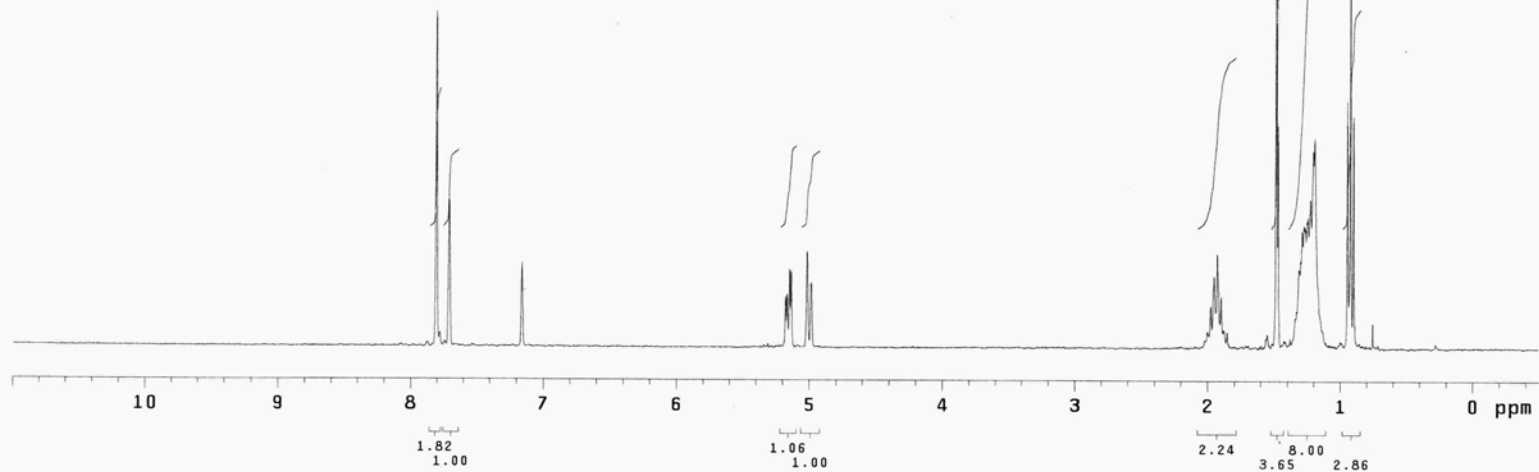
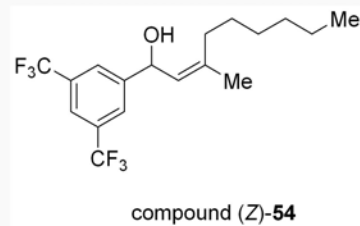
compound (E)-53



GB560HPLC

exp1 std1h

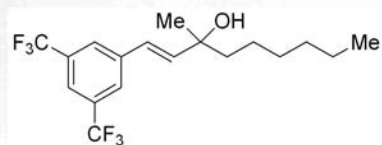
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solvent Benzene dn H1
file exp dpwr 30
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sfrq 299.868 dm nnn
tn H1 dmm c
at 1.995 dmf 200
np 17984 PROCESSING
sw 4506.5 lb not used
fb not used wtfile
bs 16 proc ft
tpwr 55 fn not used
pw 7.0
d1 1.000 werr
tof 0 wexp
nt 16 wbs
ct 16 wnt
alock n
gain not used
FLAGS
ll n
ln n
dp y
DISPLAY
sp -150.0
wp 3448.4
vs 166
sc 0
wc 250
hzmm 13.79
is 1102.09
rfl 2891.1
rfp 2147.0
th 20
ins 1.000
ai cdc ph
```



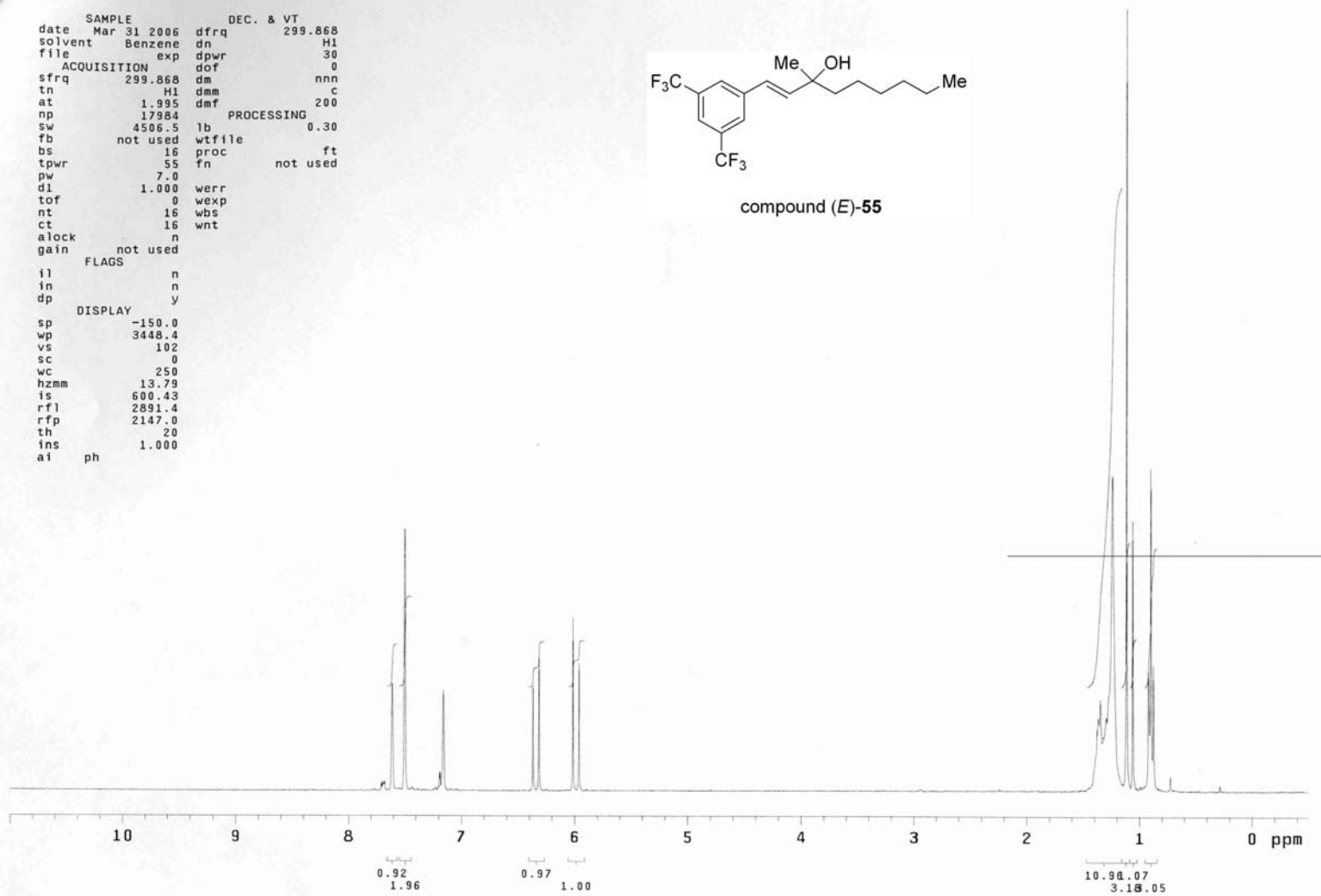
GB568F

exp4 std1h

```
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solvent Benzene  dn        H1
file      exp   dpwr      30
ACQUISITION exp   dof      0
sfrq     299.868 dm        nnn
tn       H1    dmm        c
at       1.995 dmf       PROCESSING 200
np       17984 lb         wtfile  0.30
sw       4506.5 not used
fb       not used
bs       16    proc      ft
tpwr     55    fn        not used
pw       7.0
d1       1.000 werr
tof      0    wexp
nt       16   wbs
ct       16   wnt
alock    n
gain     not used
FLAGS
il        n
in        n
dp        y
DISPLAY
sp        -150.0
wp        3448.4
vs        102
sc        0
wc        250
hzmm     13.79
is        600.43
rf1       2891.4
rfp       2147.0
th        20
ins       1.000
ai        ph
```



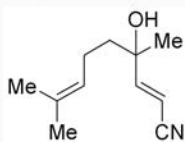
compound (E)-55



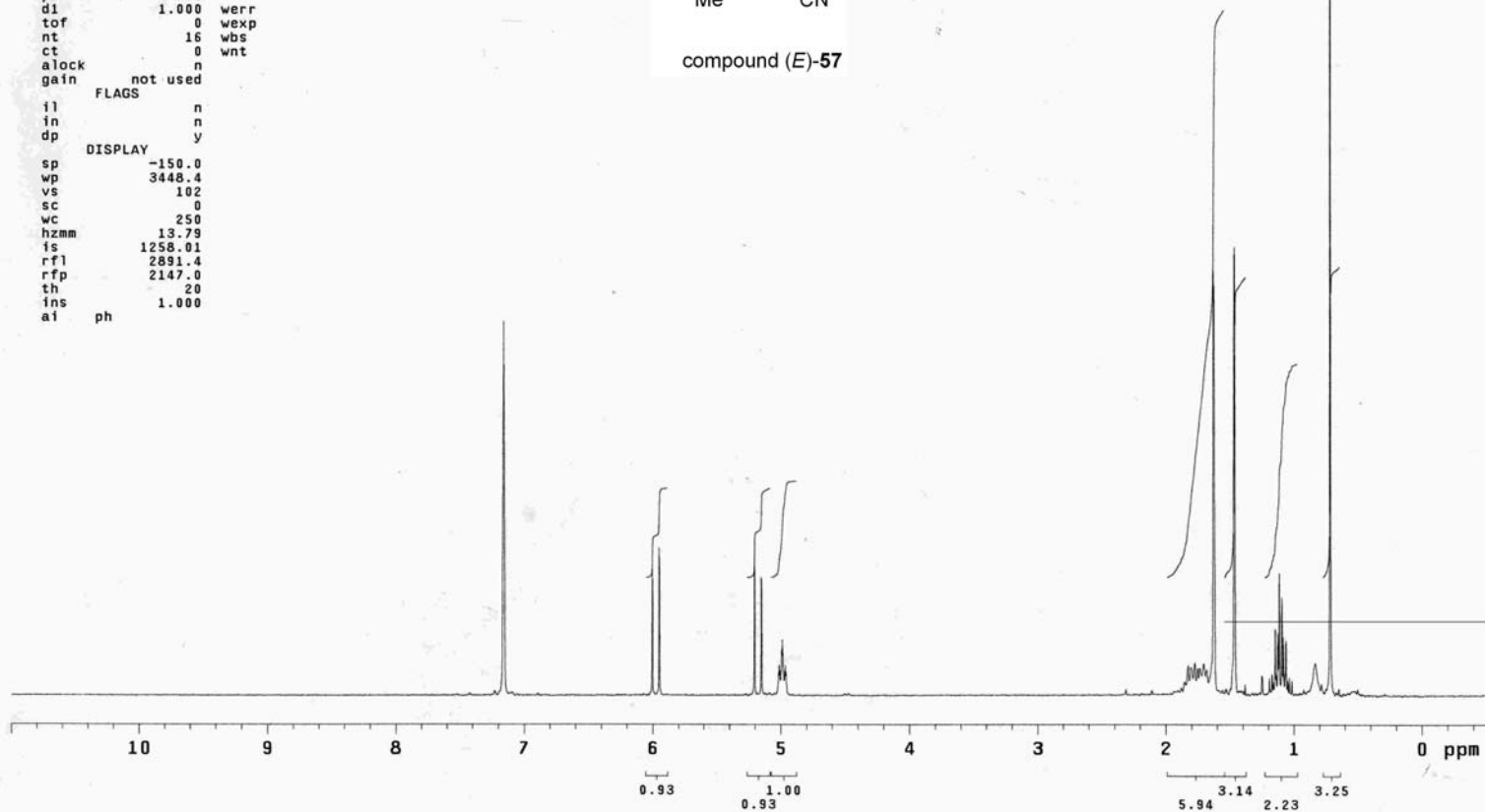
GB549F

exp2 stdih

```
SAMPLE DEC. & VT
date Mar 8 2006 dfrq 299.868
solvent Benzene dn H1
file exp dpwr 30
ACQUISITION dof 0
sfrq 299.868 dm nnn
tn H1 dmm c
at 1.995 dmf 200
np 17984 PROCESSING
sw 4506.5 lb 0.30
fb not used wtfile
bs 16 proc ft
tpwr 55 fn not used
pw 7.0
d1 1.000 verr
tof 0 wexp
nt 16 wbs
ct 0 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -150.0
wp 3448.4
vs 102
sc 0
wc 250
hzmm 13.79
fs 1258.01
rf1 2891.4
rfp 2147.0
th 20
ins 1.000
al ph
```



compound (E)-57

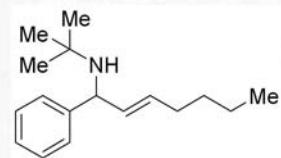




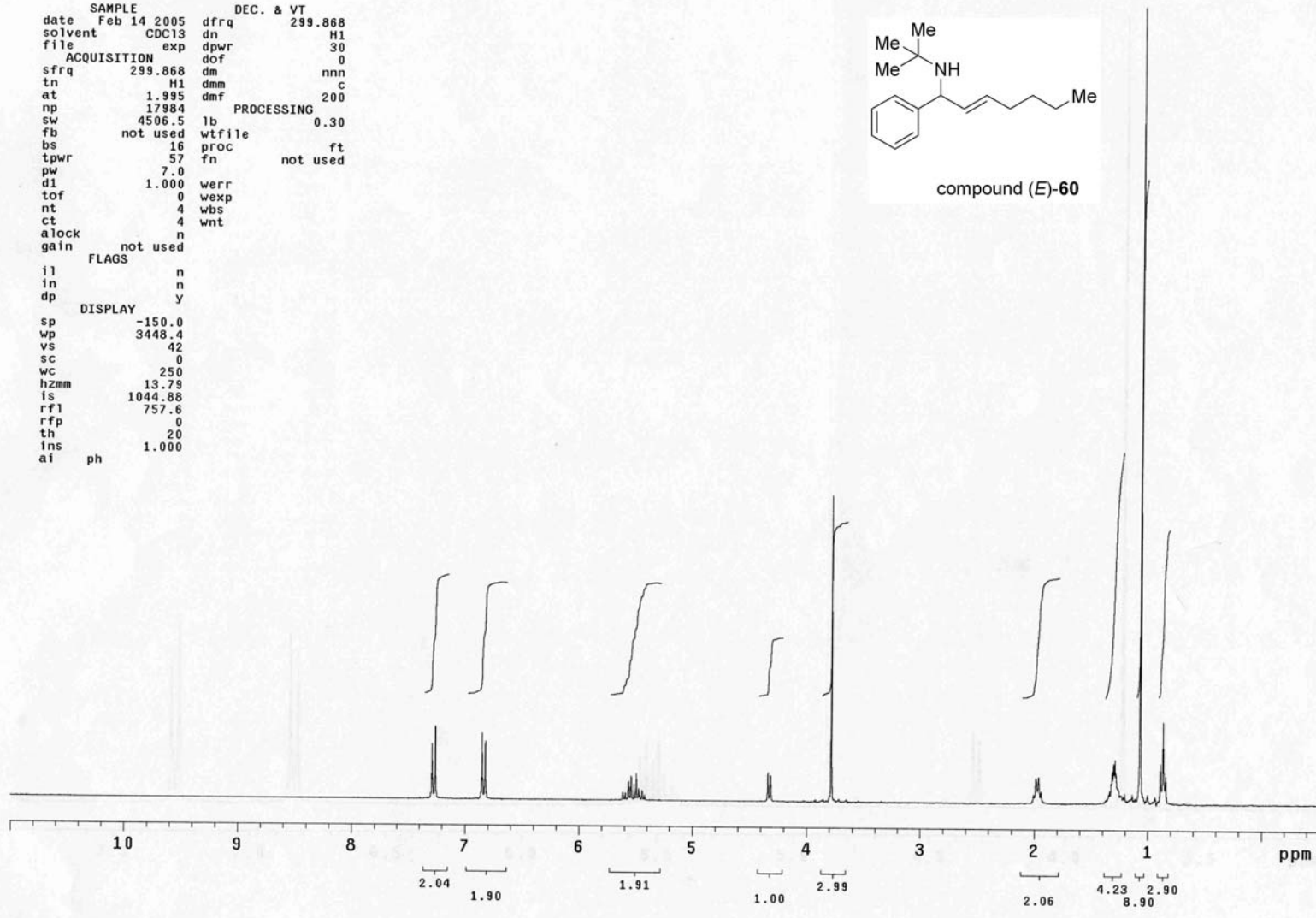
GB298FA

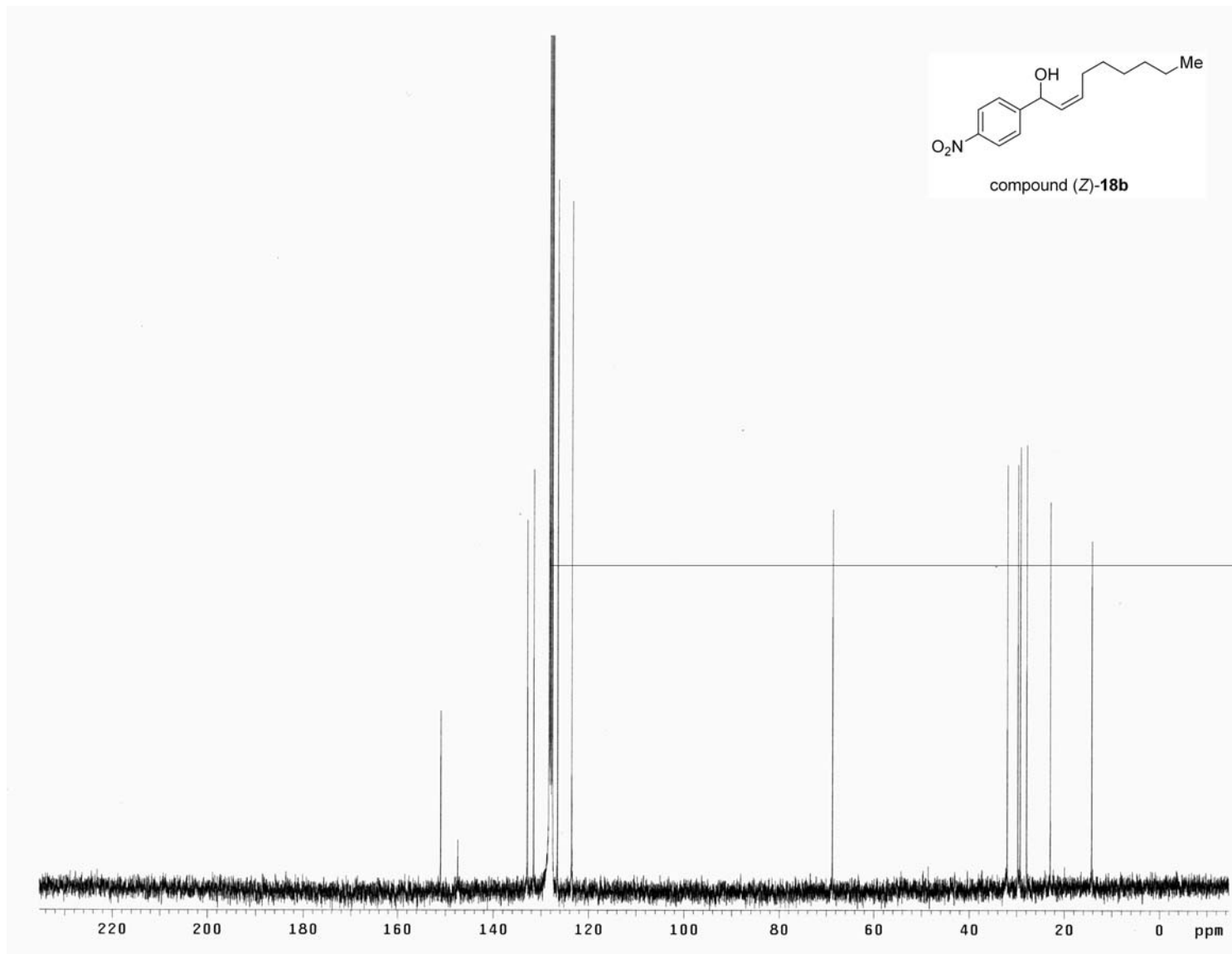
exp1 std1h

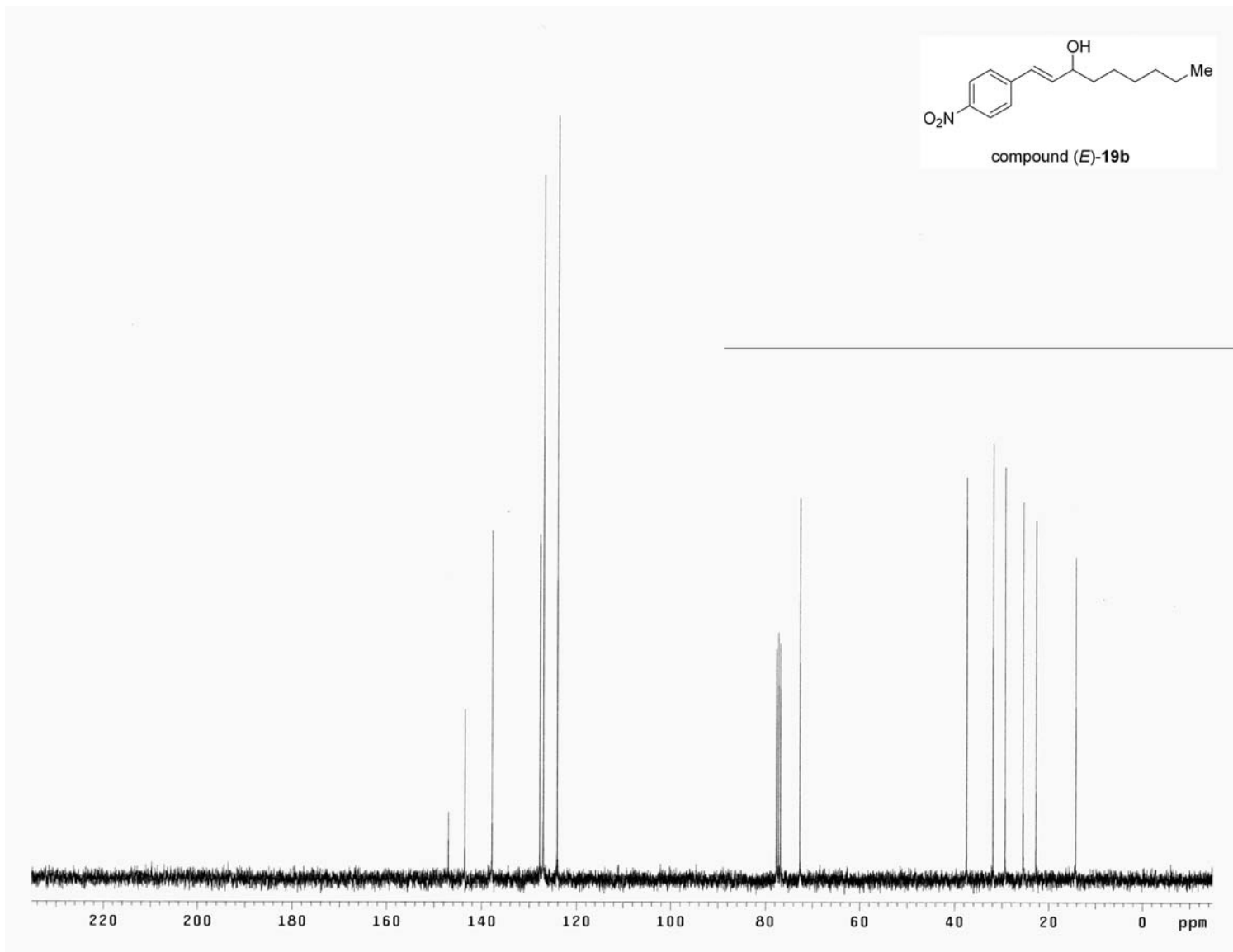
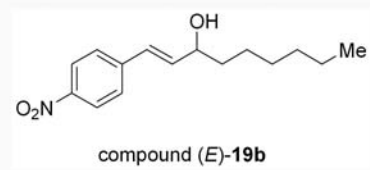
SAMPLE		DEC. & VT	
date	Feb 14 2005	dfrq	299.868
solvent	CDC13	dn	H1
file	exp	dpwr	30
ACQUISITION		dof	0
sfrq	299.868	dm	nnn
tn	H1	dmm	c
at	1.995	dmf	200
np	17984	PROCESSING	
sw	4506.5	lb	0.30
fb	not used	wtfile	
bs	not used	proc	ft
tpwr	57	fn	not used
pw	7.0		
d1	1.000	werr	
tof	0	wexp	
nt	4	wbs	
ct	4	wnt	
alock	not used		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-150.0		
wp	3448.4		
vs	42		
sc	0		
wc	250		
hzmm	13.79		
is	1044.88		
rf1	757.6		
rfp	0		
th	20		
ins	1.000		
ai	ph		

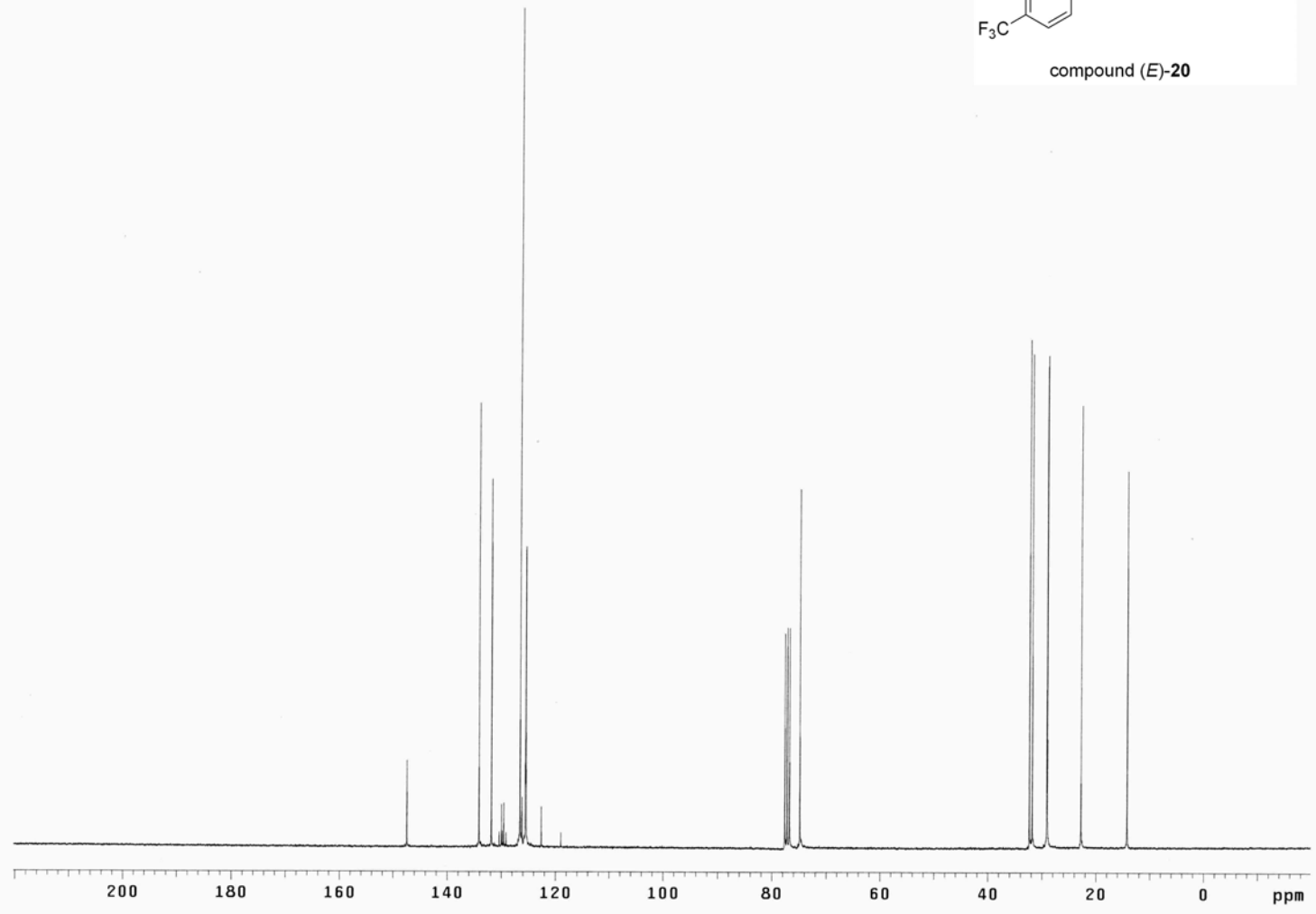
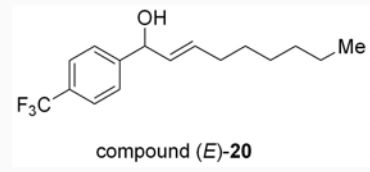


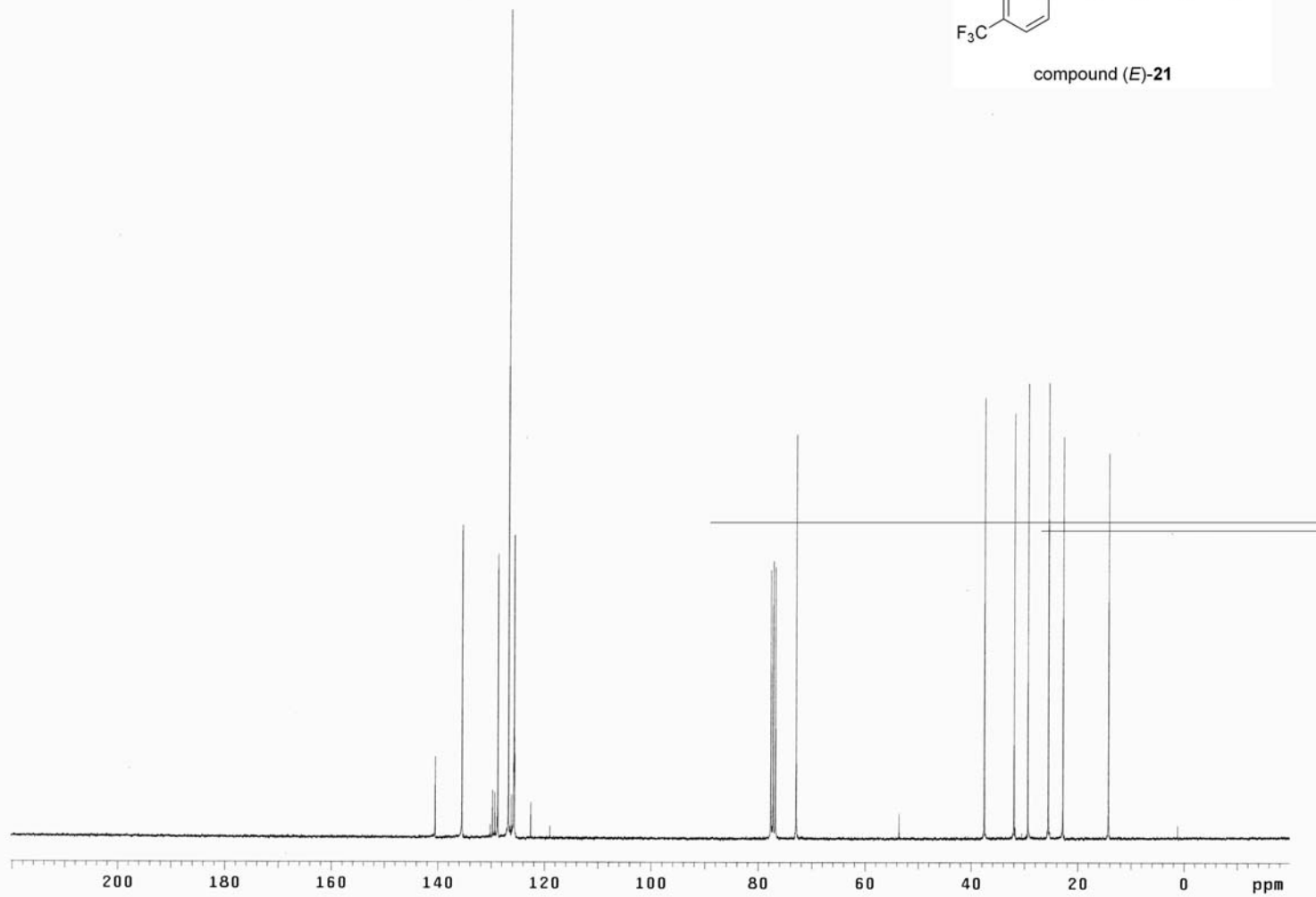
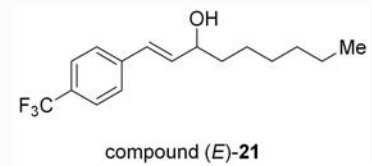
compound (E)-60

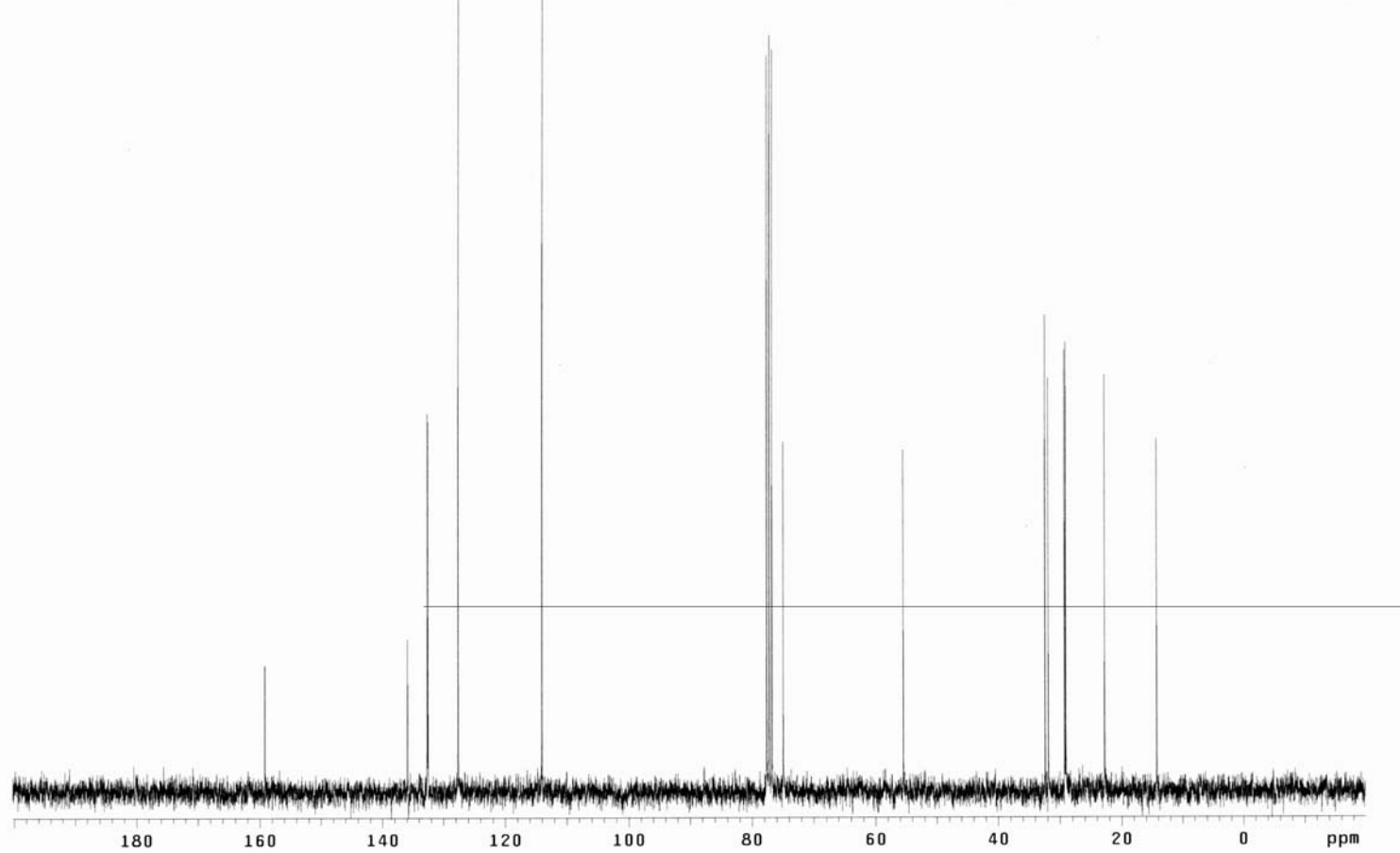
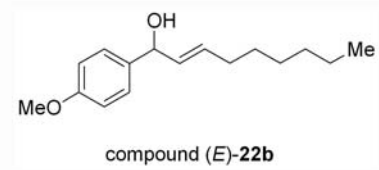


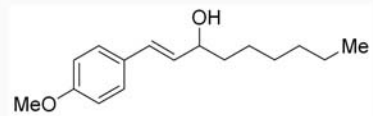




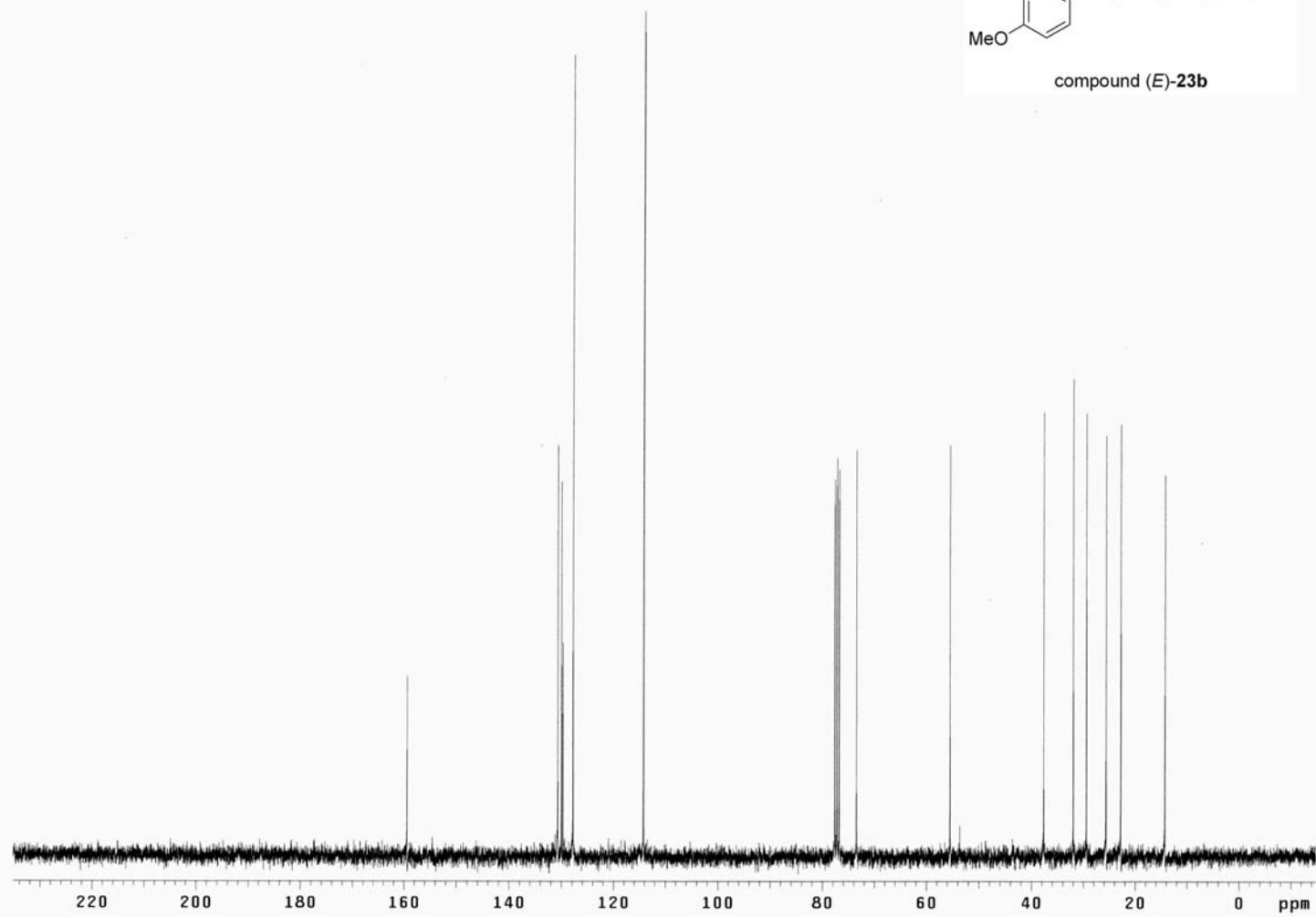








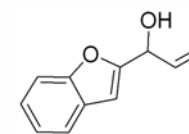
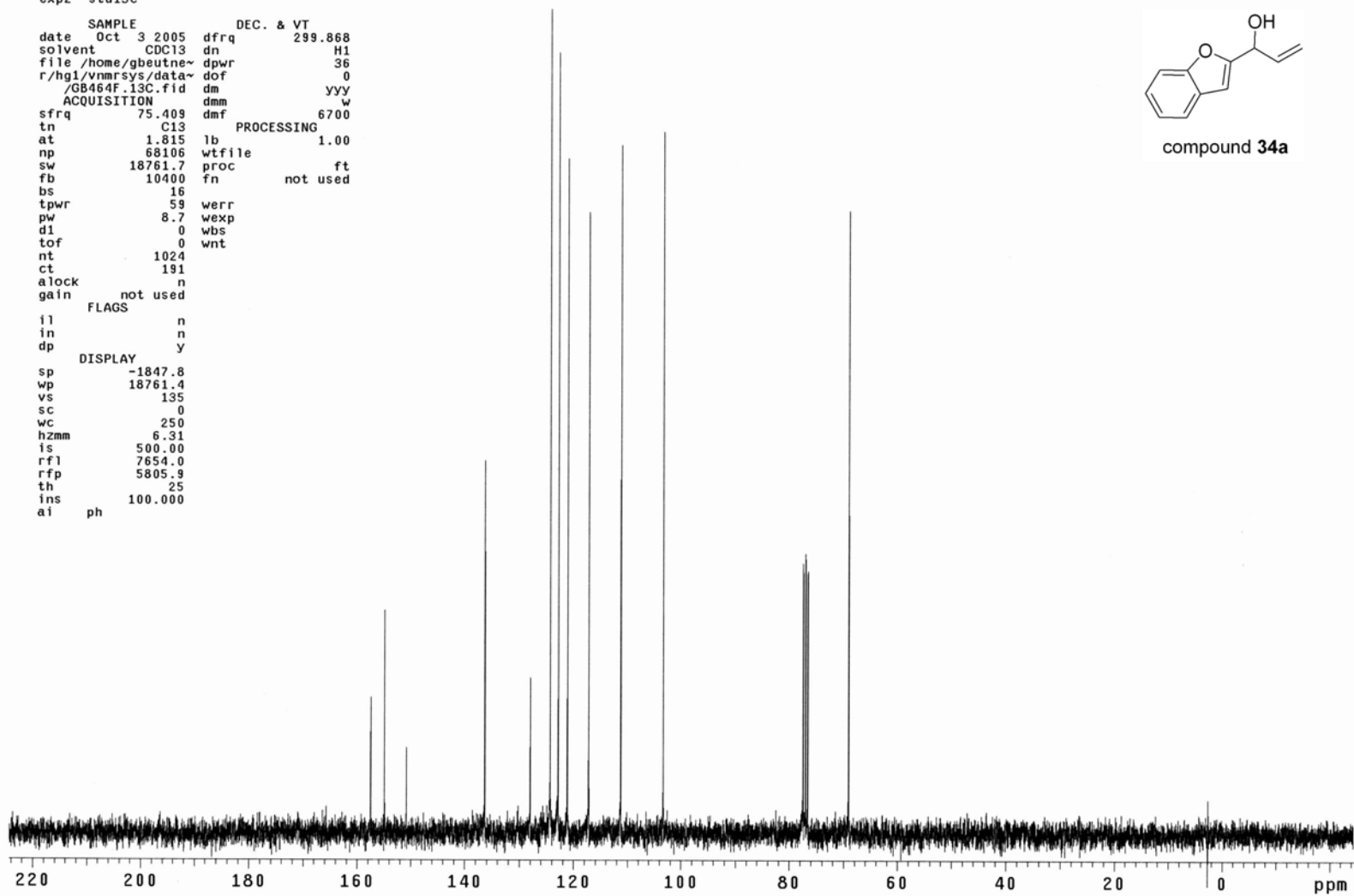
compound (*E*)-23b



GB464F.13C

exp2 std13c

```
SAMPLE          DEC. & VT
date   Oct 3 2005  dfrq      299.868
solvent CDC13      dn        H1
file   /home/gbeutne~ dpwr     36
r/hg1/vnmrsys/data~ dof      0
/GB464F.13C.fid   dm        yyy
ACQUISITION      dmm        w
sfrq      75.409  dmf      6700
tn         C13      PROCESSING
at         1.815    lb        1.00
np         68106    wtfile
sw         18761.7  proc      ft
fb         10400    fn        not used
bs         16
tpwr       59      werr
pw         8.7     wexp
d1         0       wbs
tof        0       wnt
nt         1024
ct         191
alock      n
gain       not used
          FLAGS
il         n
in         n
dp         y
          DISPLAY
sp         -1847.8
wp         18761.4
vs         135
sc         0
wc         250
hzmm       6.31
is         500.00
rfl        7654.0
rfp        5805.9
th         25
ins        100.000
ai         ph
```



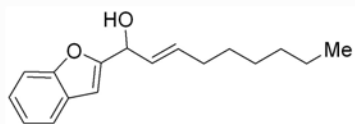
compound 34a



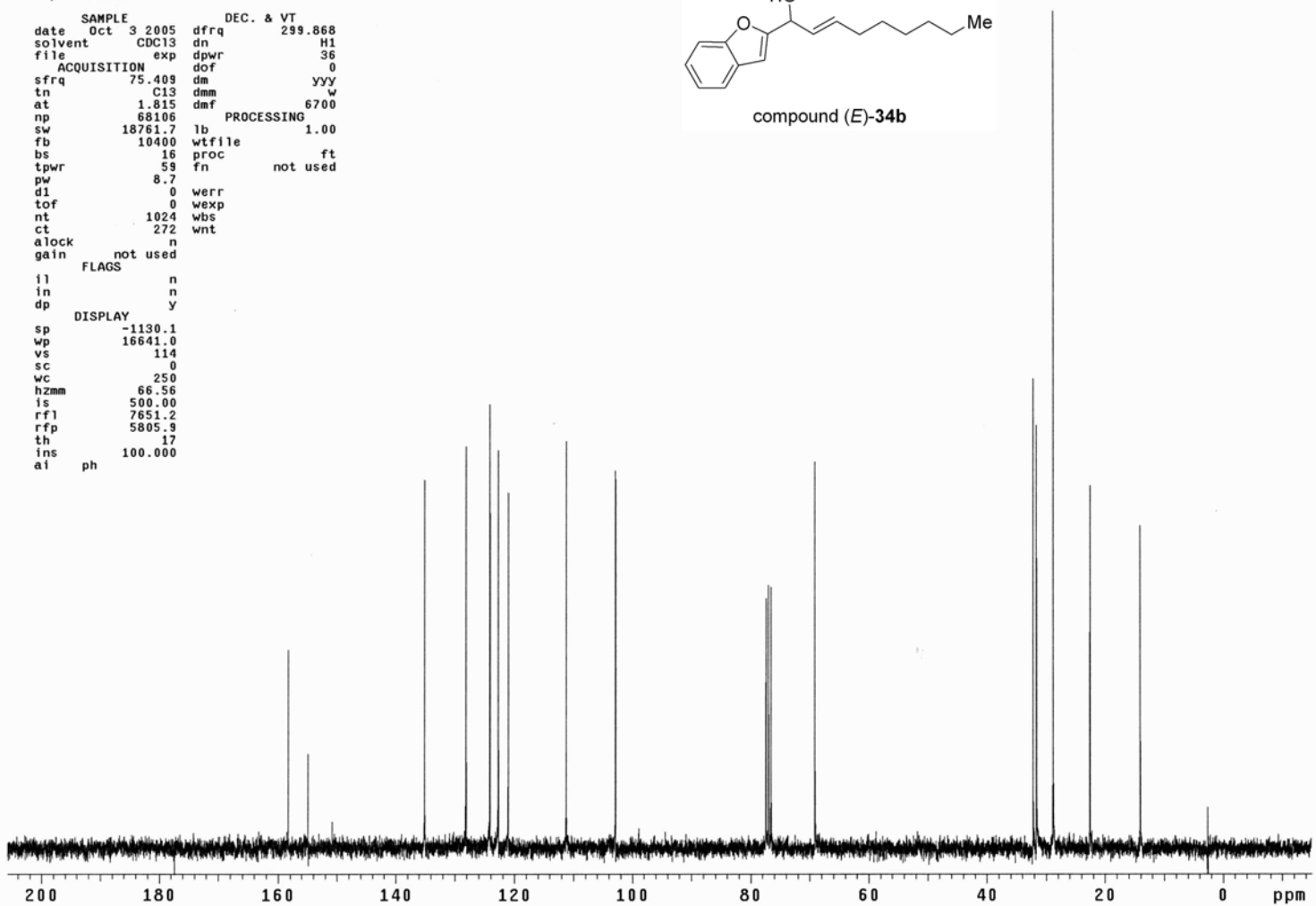
13C OBSERVE

exp2 std13c

SAMPLE		DEC. & VT	
date	Oct 3 2005	dfrq	299.868
solvent	CDC13	dn	H1
file	exp	dpwr	36
ACQUISITION		dof	0
sfrq	75.409	dm	yyy
tn	C13	dmm	w
at	1.815	dmf	6700
np	68106	PROCESSING	
sw	18761.7	lb	1.00
fb	10400	wtfile	
bs	16	proc	ft
tpwr	59	fn	not used
pw	8.7		
d1	0	werr	
tof	0	wexp	
nt	1024	wbs	
ct	272	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-1130.1		
wp	16641.0		
vs	114		
sc	0		
wc	250		
hzmm	66.56		
is	500.00		
rfl	7651.2		
rfp	5805.9		
th	17		
ins	100.000		
al	ph		



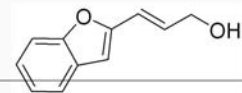
compound (E)-34b



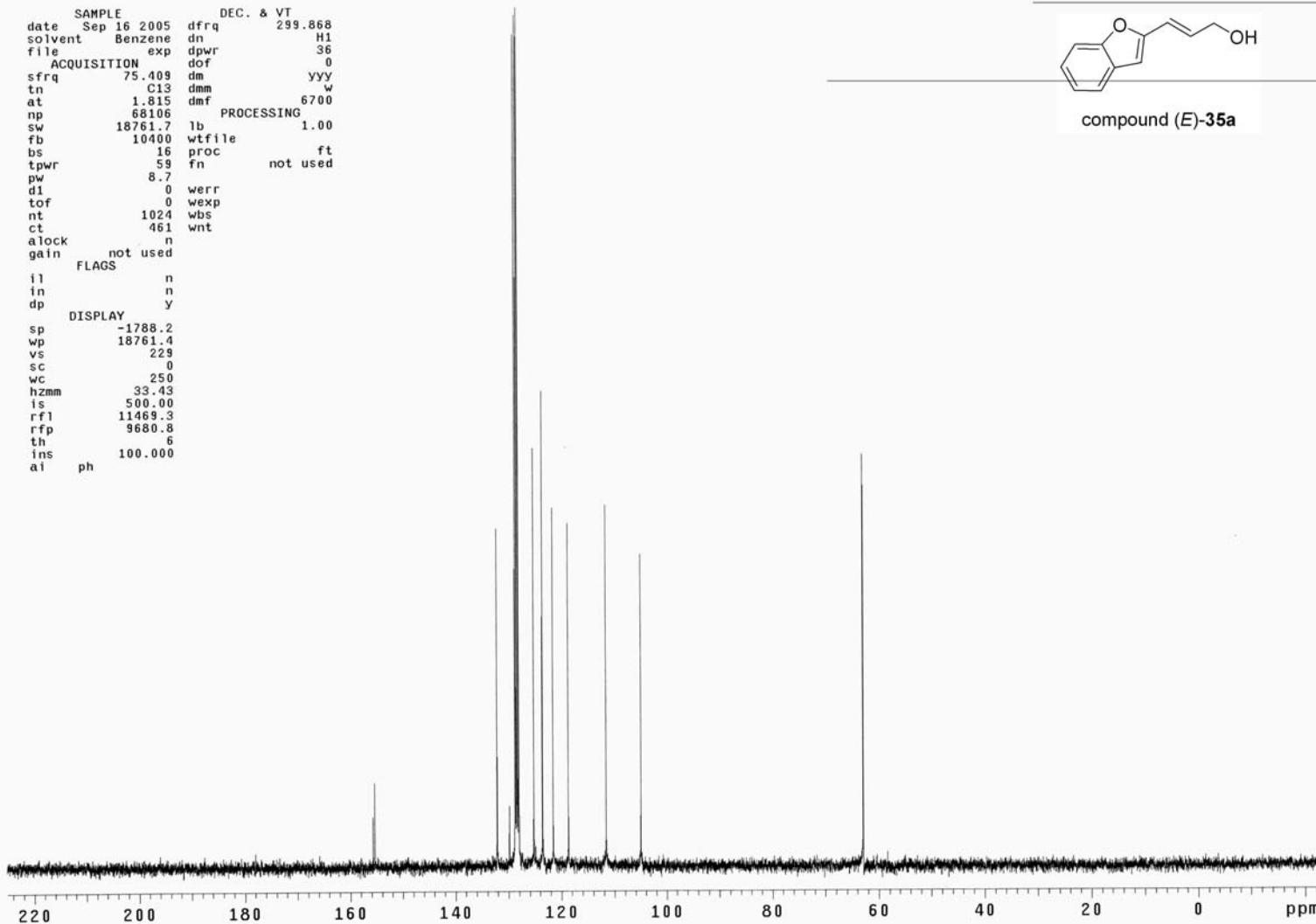
GB459F.13C

exp2 std13c

```
SAMPLE          DEC. & VT
date   Sep 16 2005  dfrq      299.868
solvent Benzene     dn        H1
file   exp         dpwr      36
          ACQUISITION  dof        0
sfrq   75.409     dm         yy
tn      C13       dmm        w
at      1.815     dmf       6700
np      68106
sw      18761.7   lb         1.00
fb      10400    wtfile
bs      16       proc        ft
tpwr    59       fn         not used
pw      8.7
d1      0        werr
tof     0        wexp
nt      1024    wbs
ct      461     wnt
alock   not used
gain    not used
          FLAGS
il      n
in      n
dp      Y
          DISPLAY
sp      -1788.2
wp      18761.4
vs      229
sc      0
wc      250
hzmm    33.43
is      500.00
rfl     11469.3
rfp     9680.8
th      6
ins     100.000
ai      ph
```



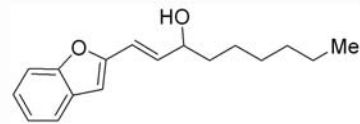
compound (E)-35a



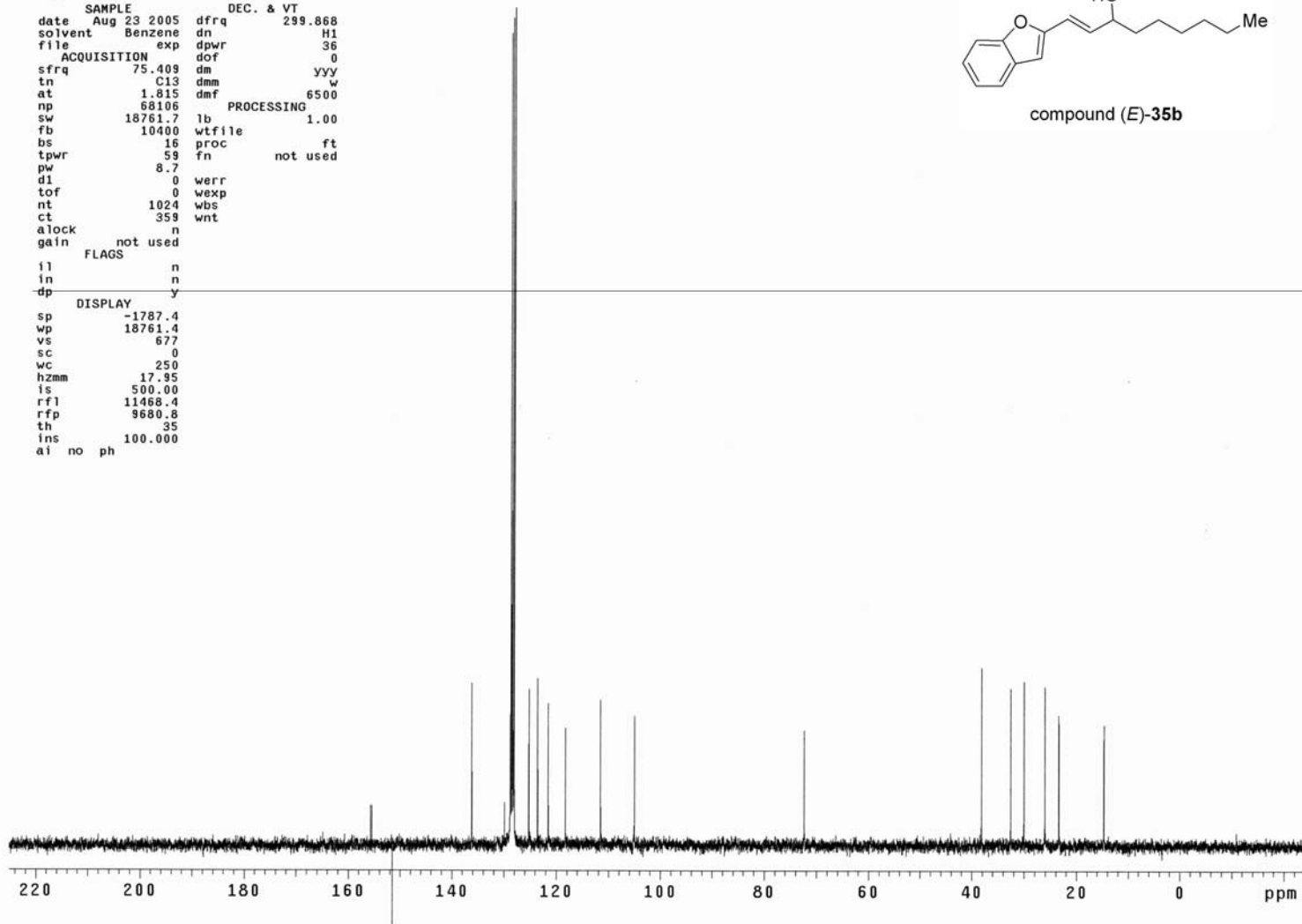
GB450F.13C

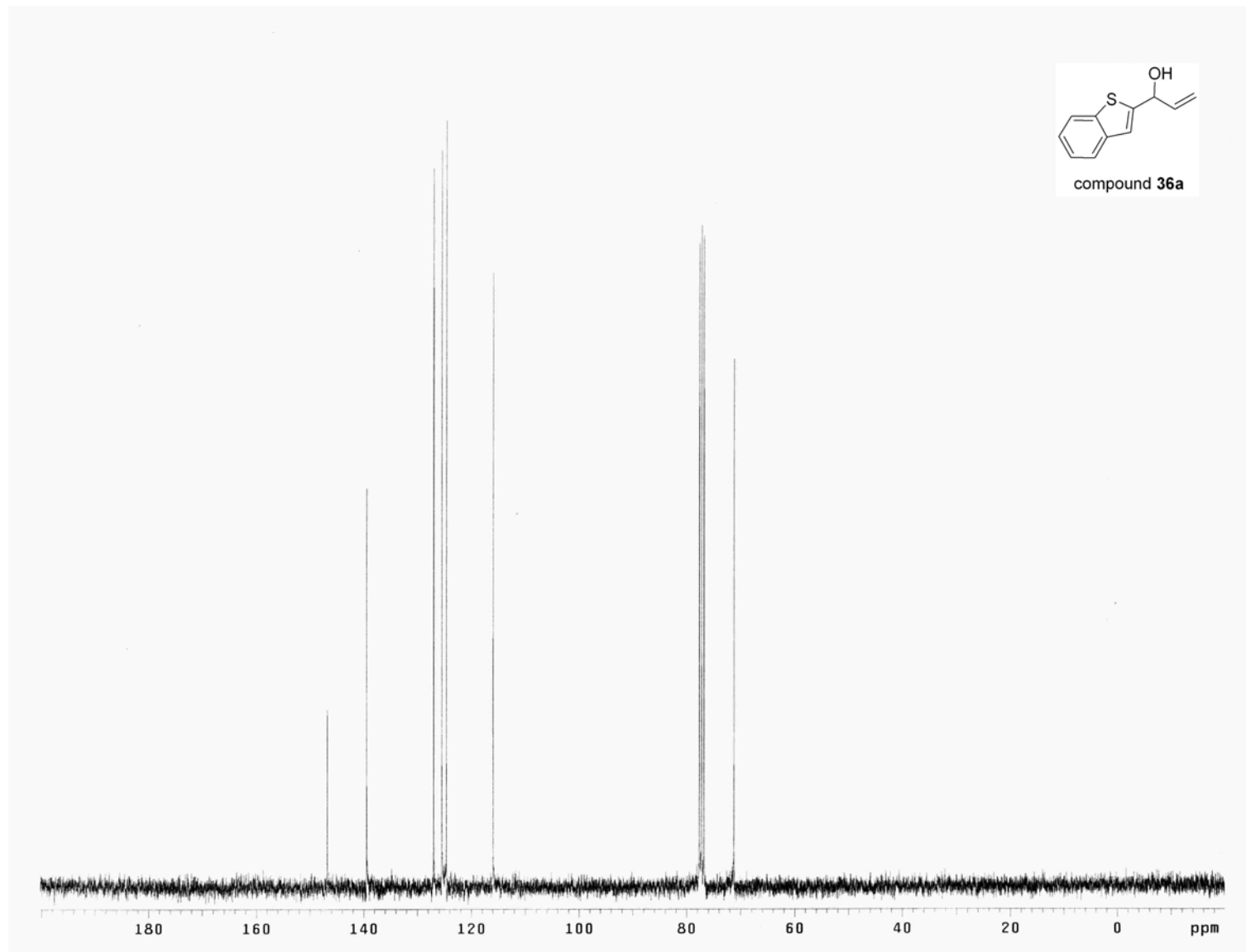
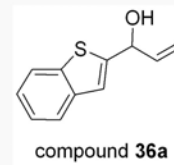
exp2 std13c

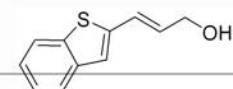
```
SAMPLE          DEC. & VT
date Aug 23 2005 dfrq      299.868
solvent Benzene  dn        H1
file          exp dpwr      36
ACQUISITION    dof        0
sfrq      75.409 dm         yyy
tn         C13 dmm         w
at         1.815 dmf        6500
np         68106 PROCESSING
sw         18761.7 lb        1.00
fb         10400 wtfile
bs         16 proc         ft
tpwr      59 fn           not used
pw         8.7
d1         0 werr
tof        0 wexp
nt         1024 wbs
ct         359 wnt
alock      n
gain       not used
FLAGS
il         n
in         n
dp         y
DISPLAY
sp        -1787.4
wp        18761.4
vs         677
sc         0
wc         250
h2mm      17.35
ls         500.00
rf1       11468.4
rfp       9680.8
th         35
ins       100.000
ai no ph
```



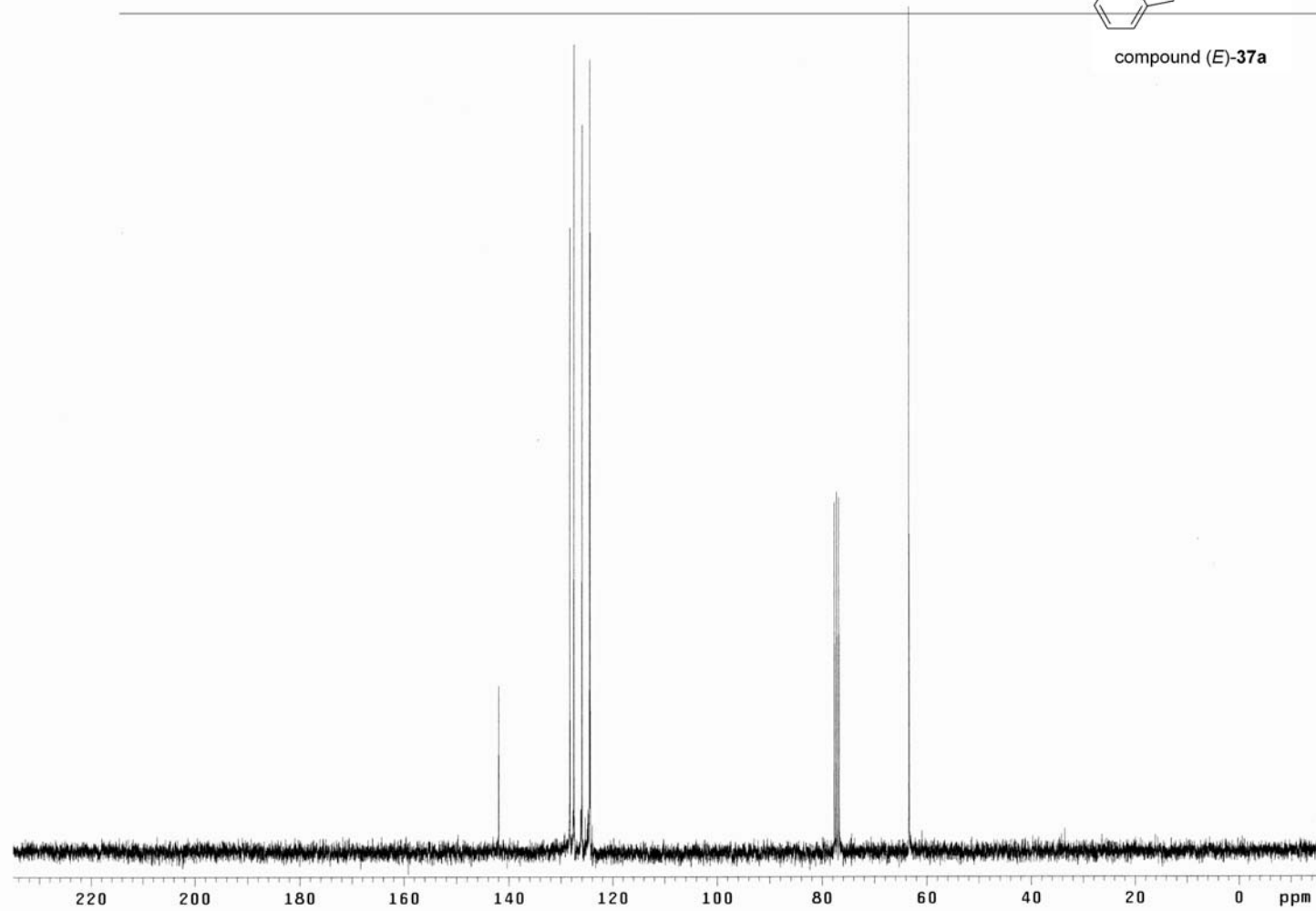
compound (E)-35b

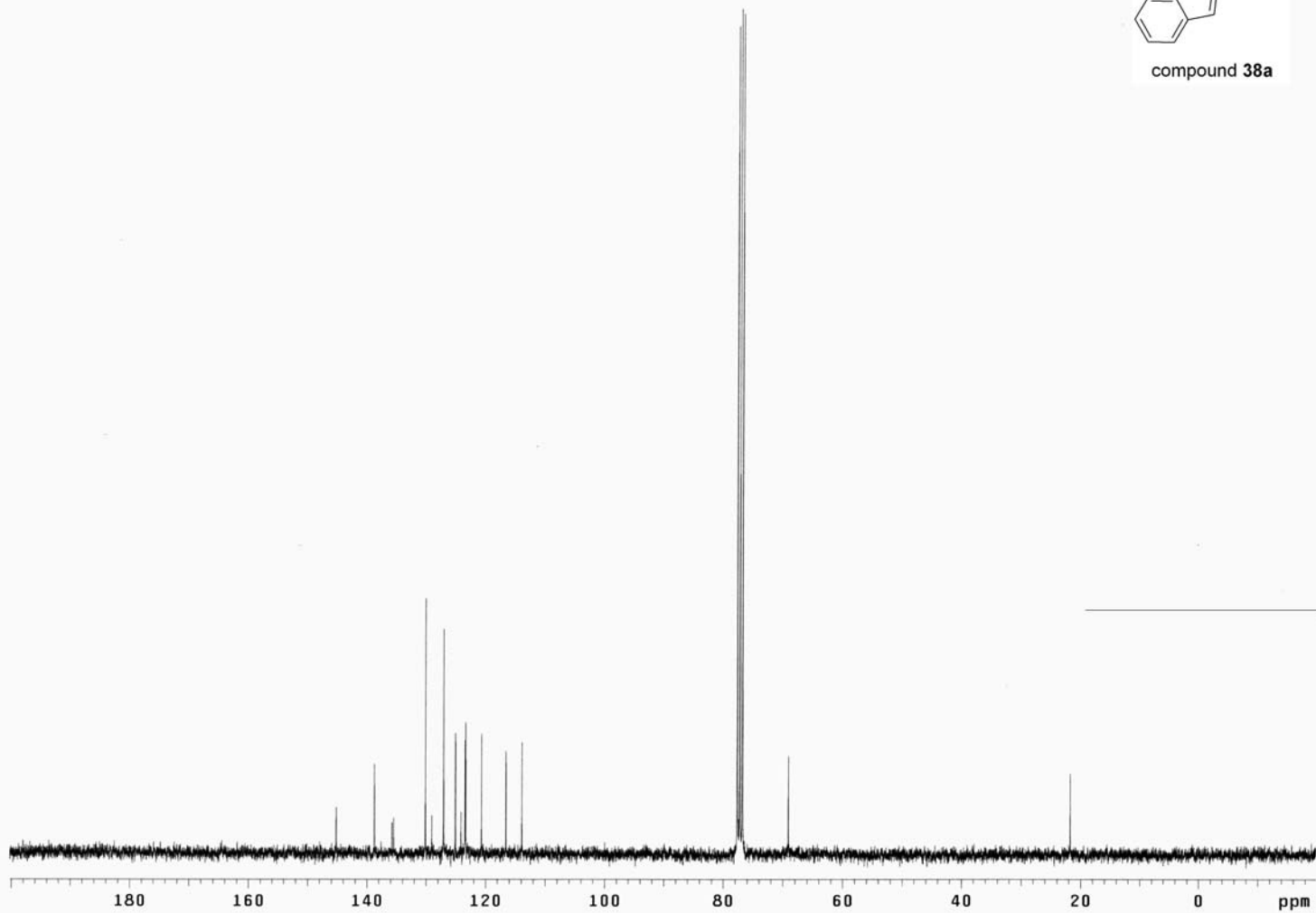
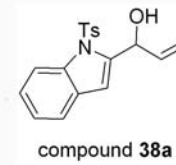


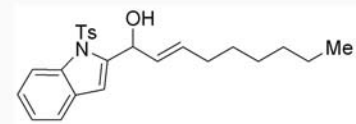




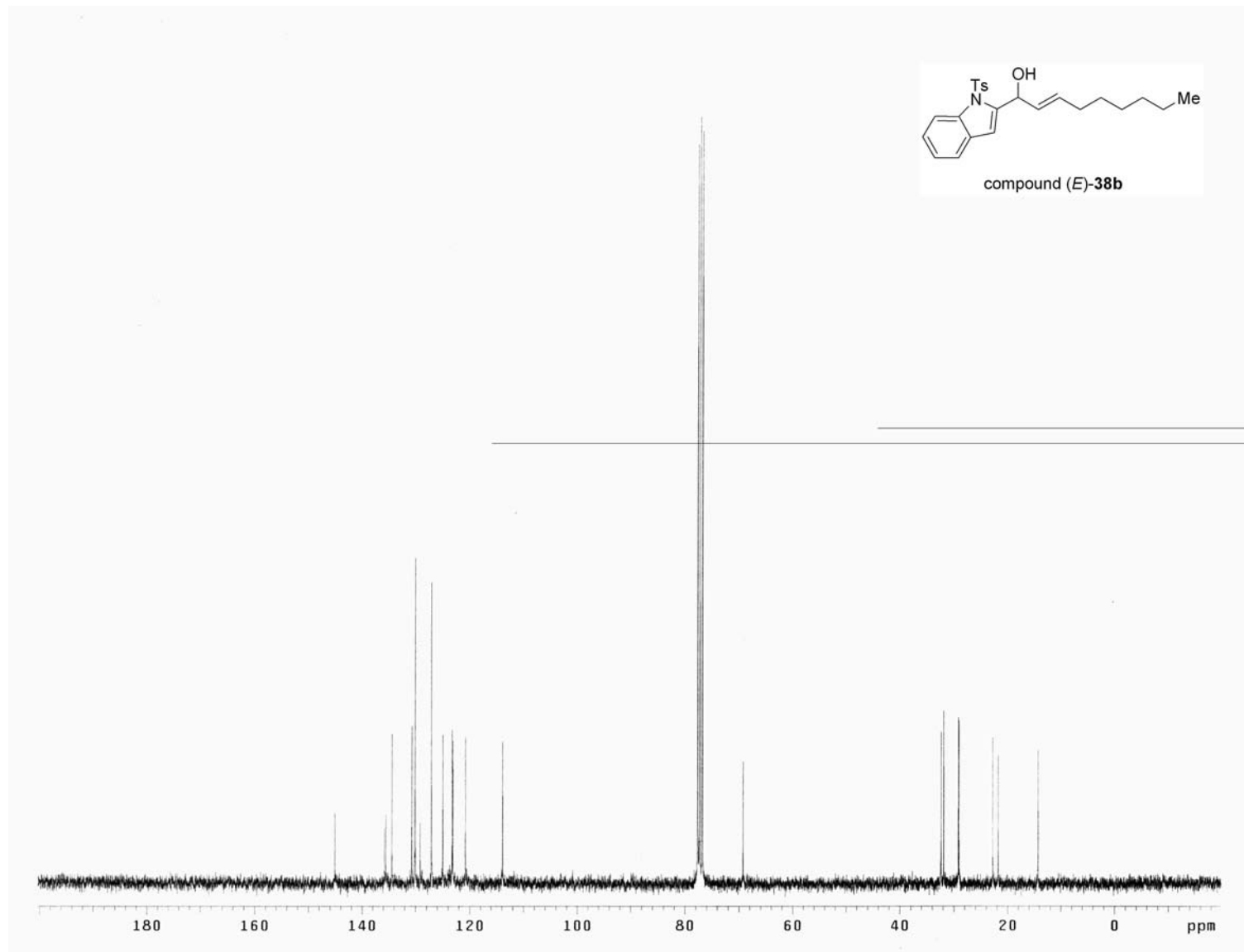
compound (E)-37a

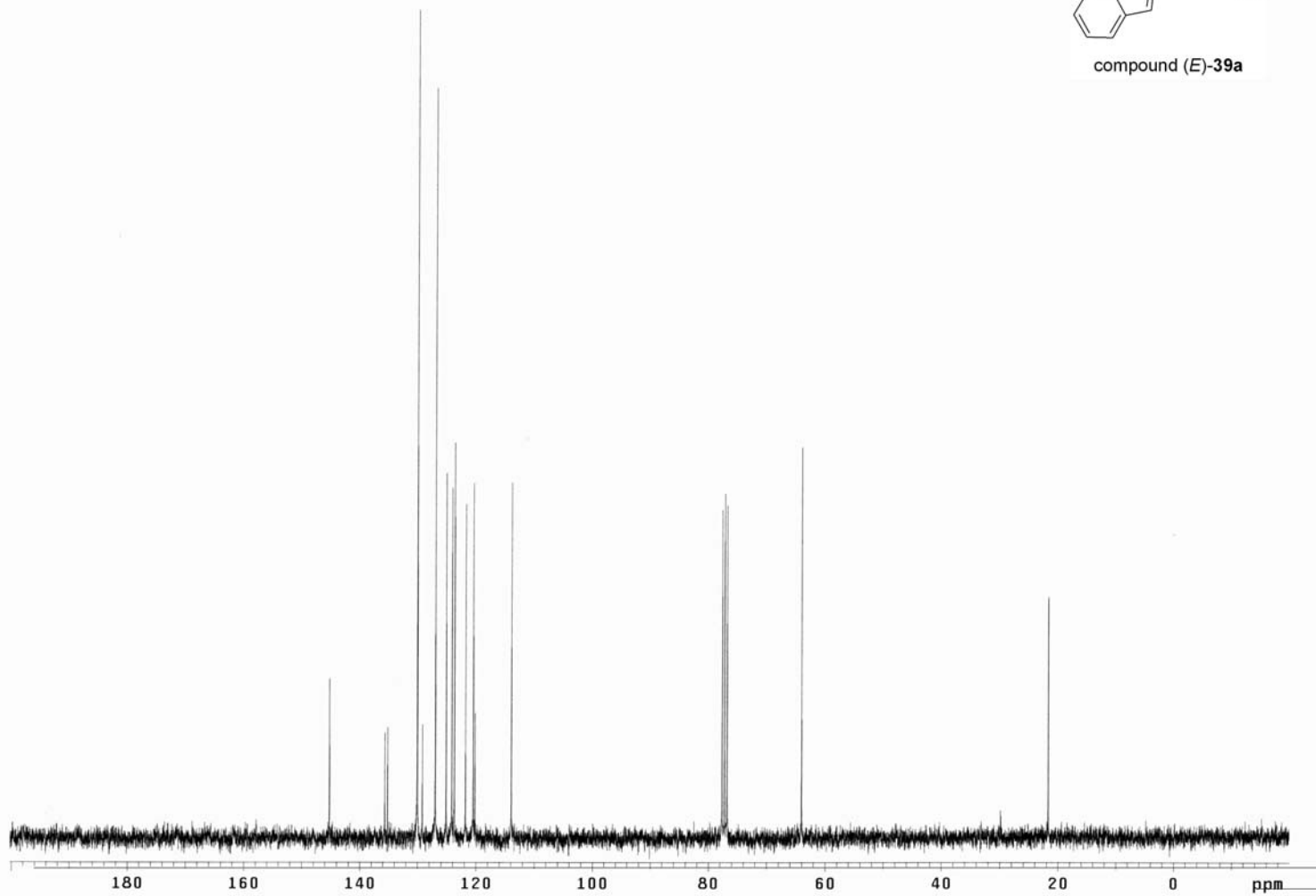
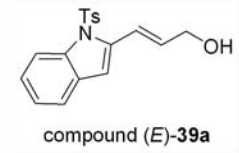




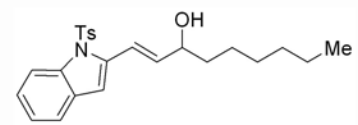


compound (E)-38b

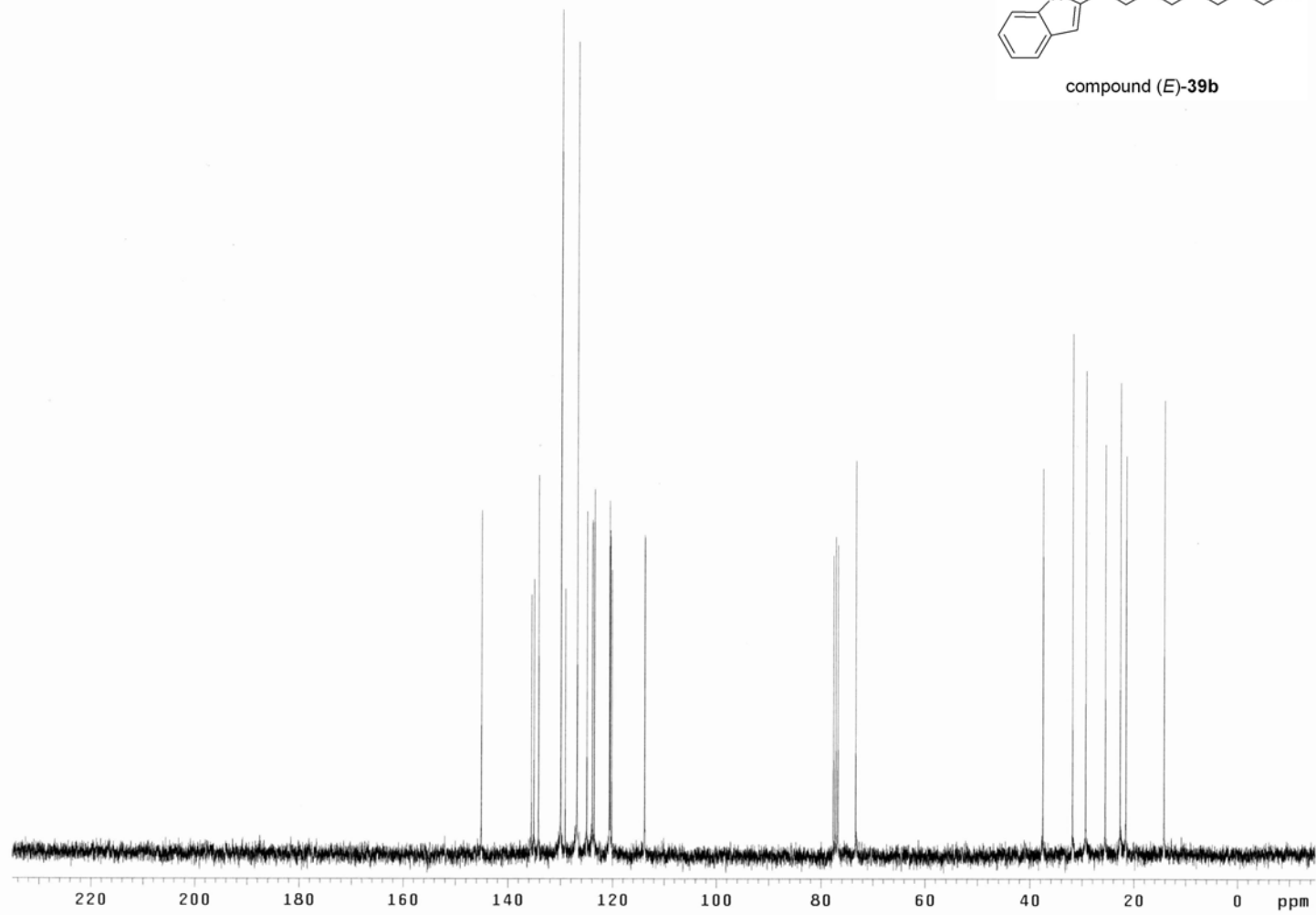








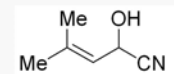
compound (*E*)-**39b**



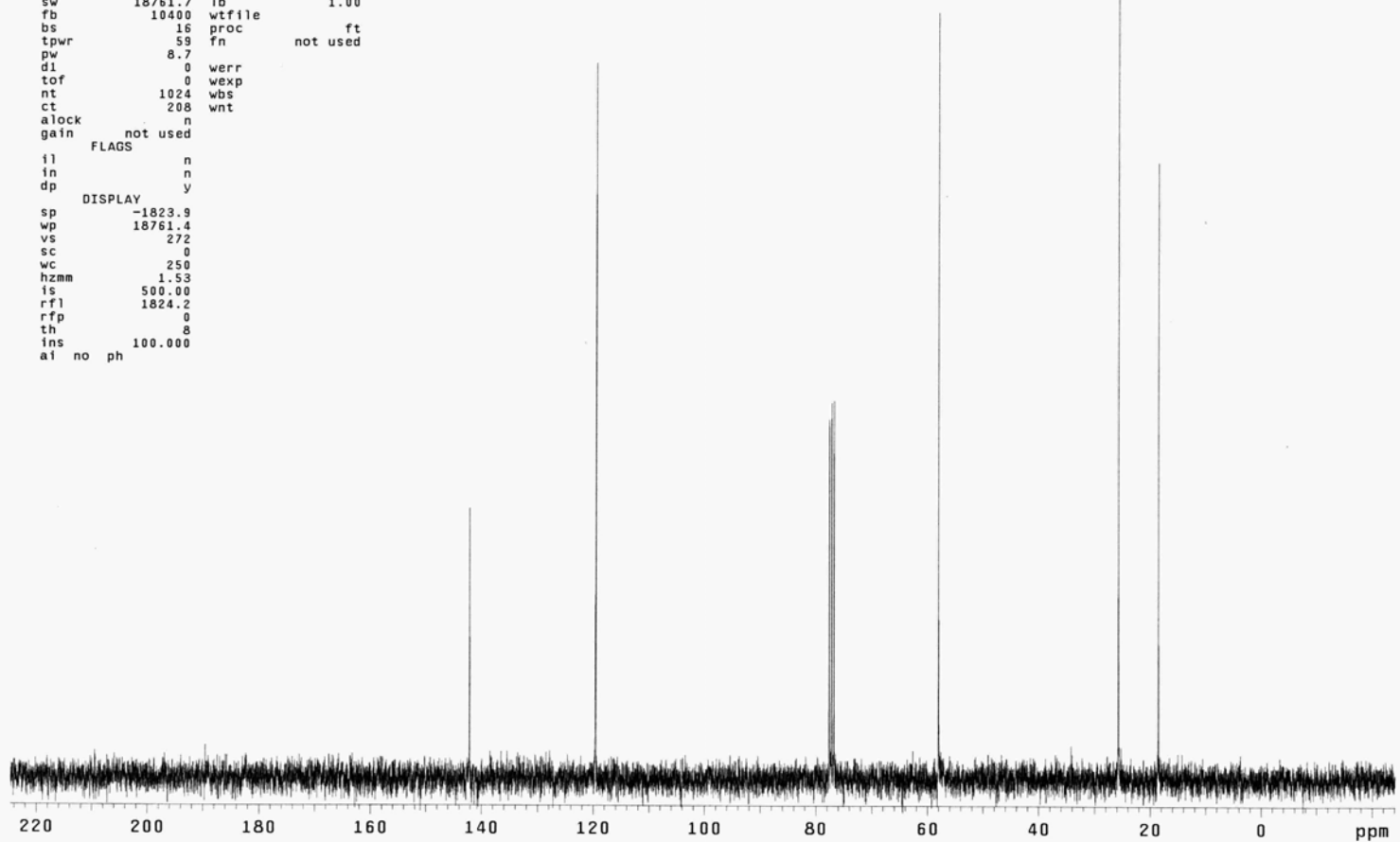
GB573F.13C

exp3 std13c

```
SAMPLE          DEC. & VT
date Apr 5 2006  dfrq      299.868
solvent Benzene  dn        H1
file exp dpwr      36
ACQUISITION     dof      0
sfrq 75.409 dm       yyy
tn C13 dmm        w
at 1.815 dmf      6500
np 68106 PROCESSING
sw 18761.7 lb      1.00
fb 10400 wtfile
bs 16 proc      ft
tpwr 59 fn      not used
pw 8.7
d1 0 werr
tof 0 wexp
nt 1024 wbs
ct 208 wnt
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1823.9
wp 18761.4
vs 272
sc 0
wc 250
hzmm 1.53
is 500.00
rfl 1824.2
rfl 0
th 8
ins 100.000
ai no ph
```



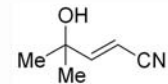
compound 40c



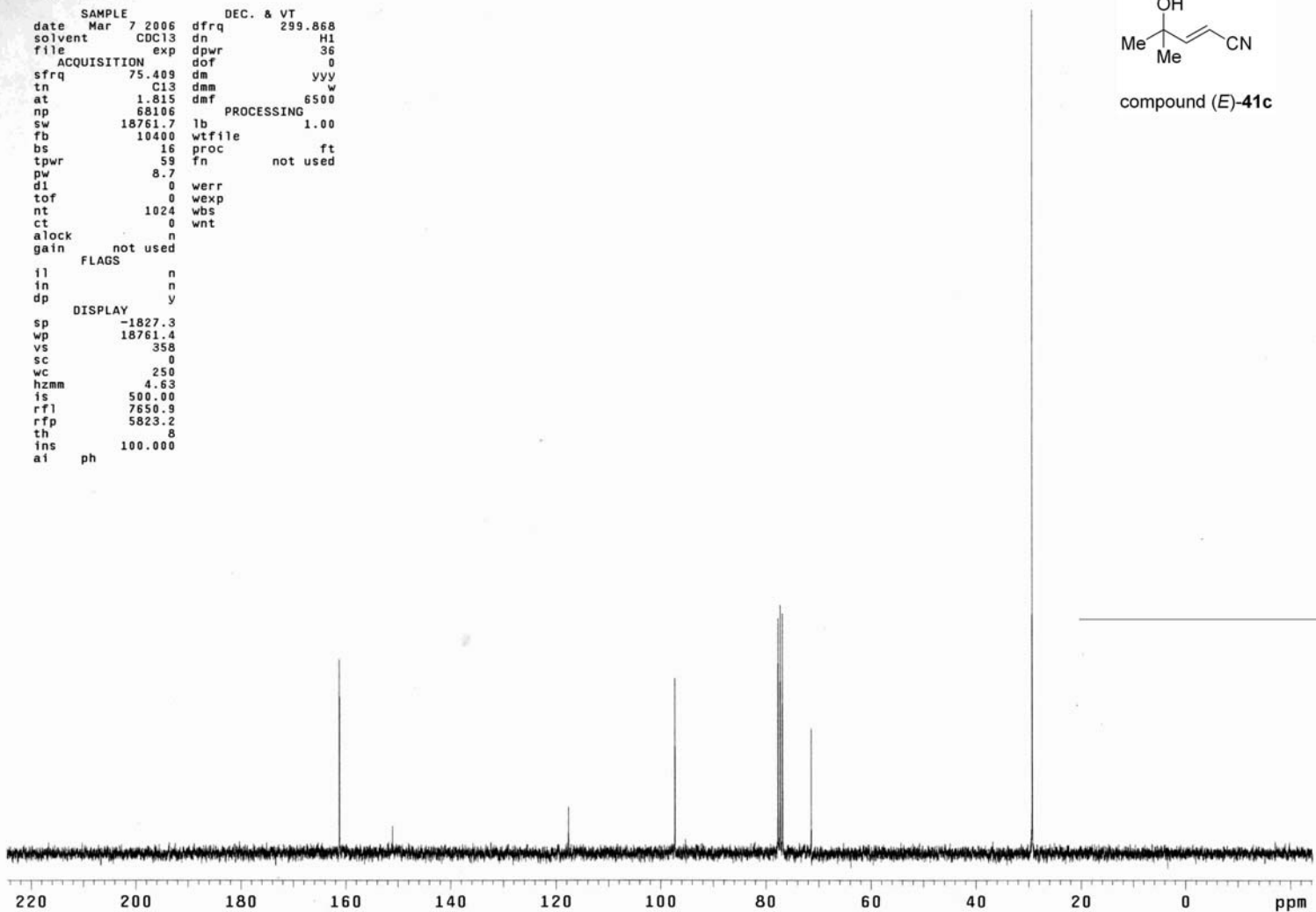
GB545F.13C

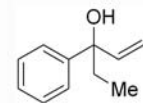
exp2 std13c

```
SAMPLE          DEC. & VT
date    Mar 7 2006  dfrq    299.868
solvent  CDC13      dn      H1
file     exp       dpwr    36
ACQUISITION      dof      0
sfrq     75.409   dm      yyy
tn       C13      dmm     w
at       1.815   dmf    6500
np       68106   PROCESSING
sw       18761.7 lb      1.00
fb       10400  wtfile
bs       16     proc     ft
tpwr     59     fn      not used
pw       8.7
d1       0     werr
tof      0     wexp
nt       1024  wbs
ct       0     wnt
alock    n
gain     not used
FLAGS
jl       n
in       n
dp       y
DISPLAY
sp      -1827.3
wp      18761.4
vs      358
sc      0
wc      250
hzmm    4.63
is      500.00
rfl     7650.9
rfp     5823.2
th      8
ins     100.000
ai      ph
```

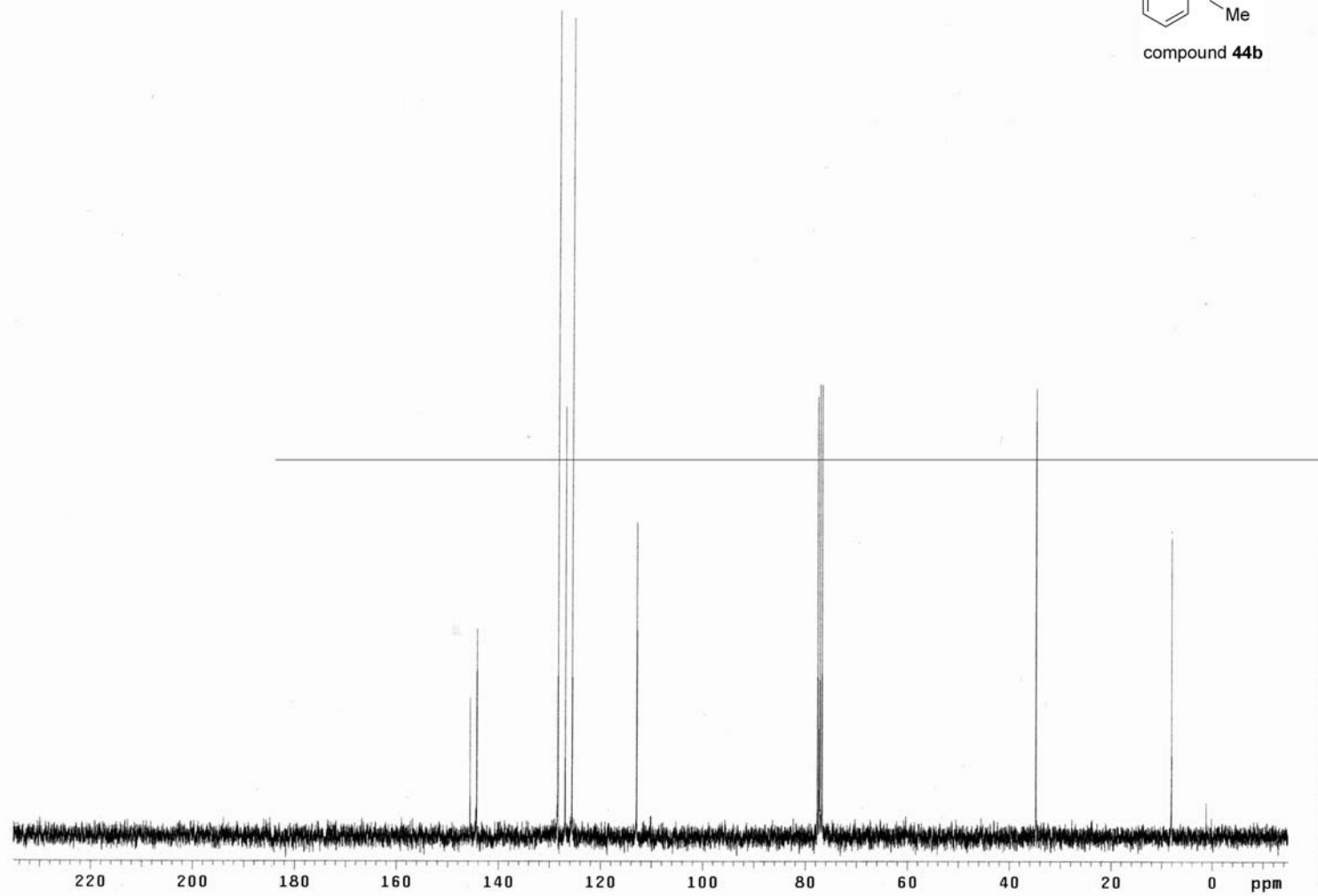


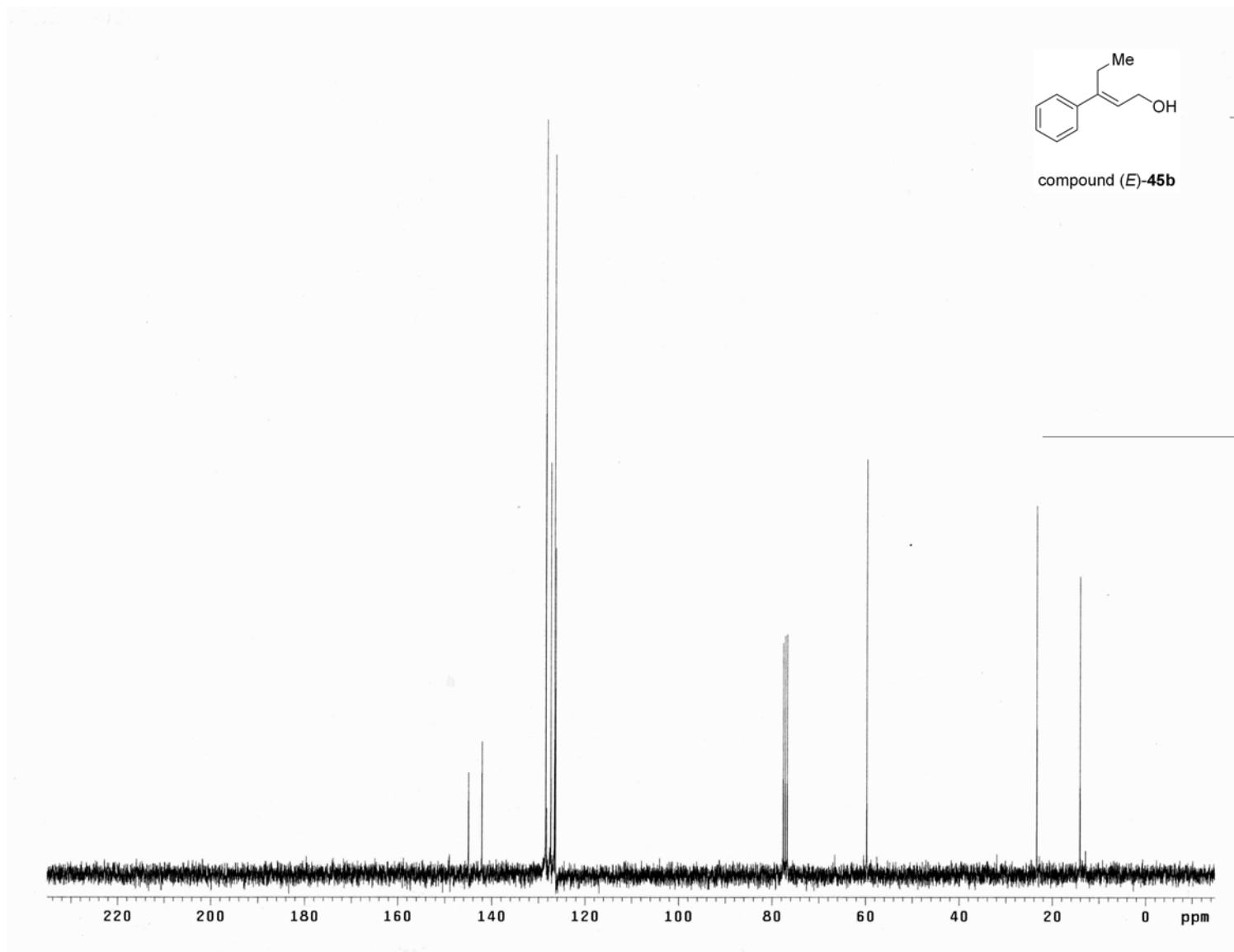
compound (E)-41c

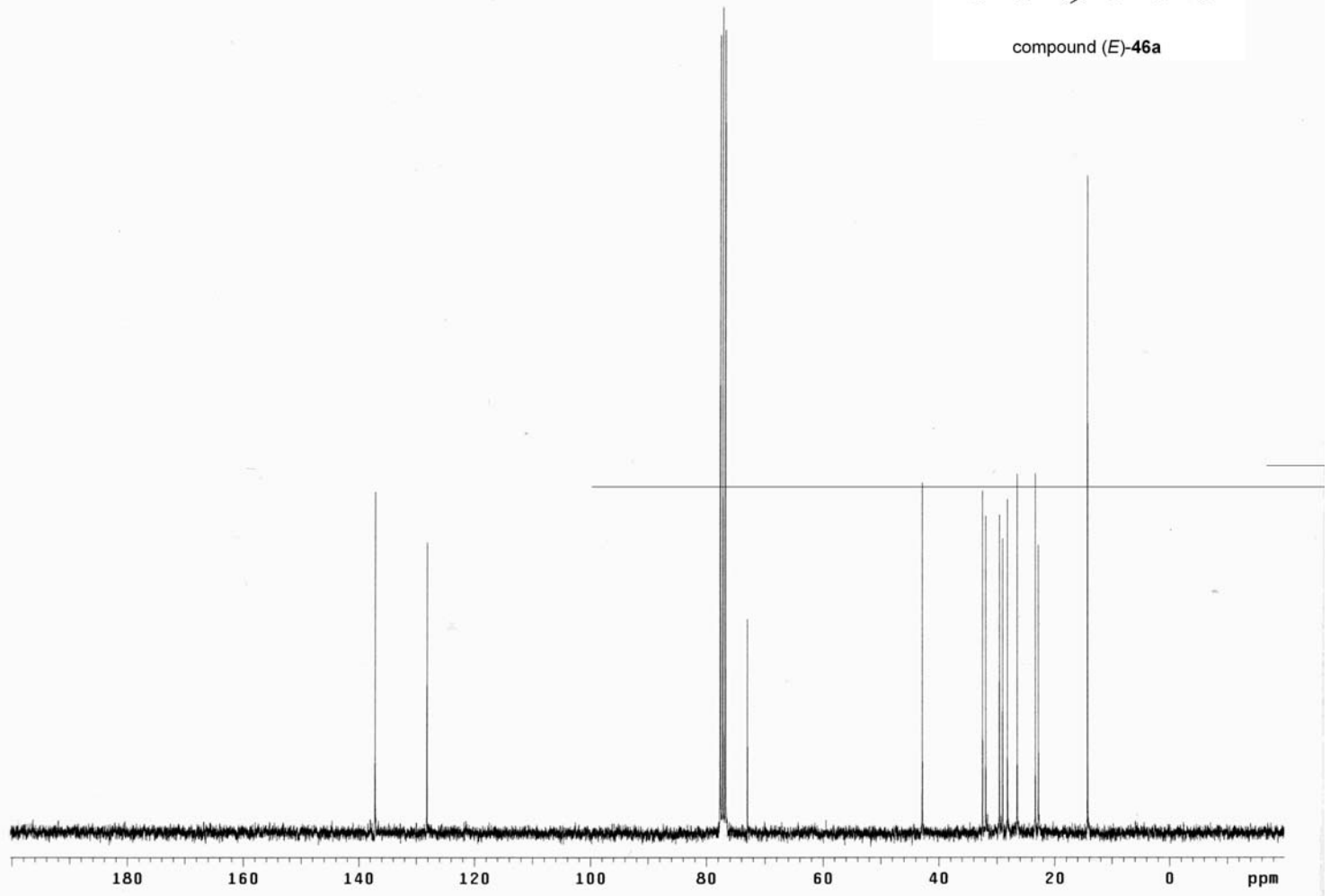
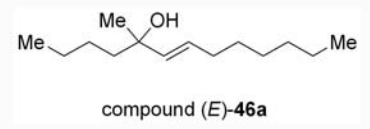


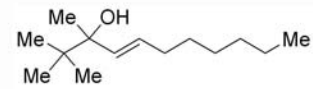


compound 44b

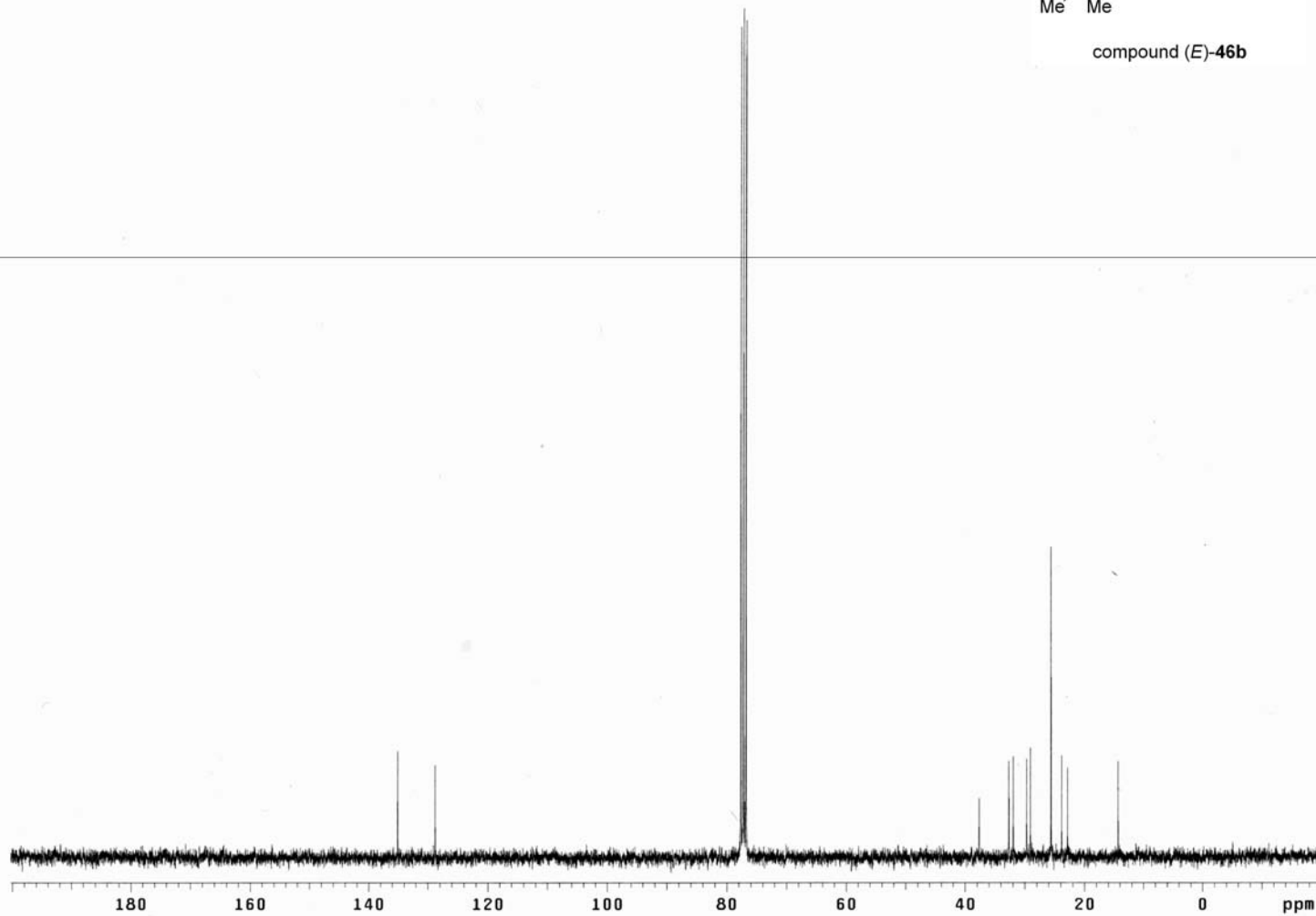


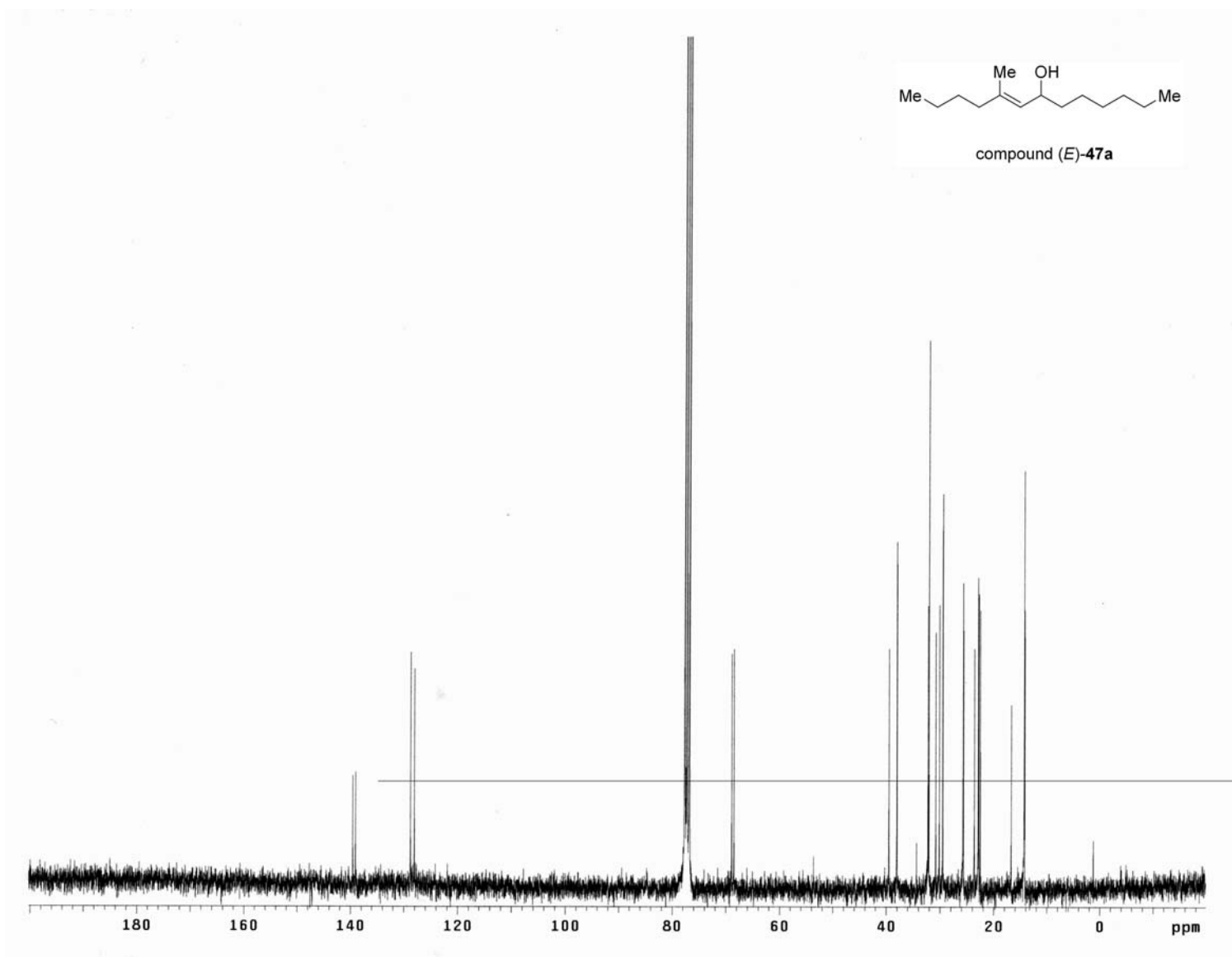




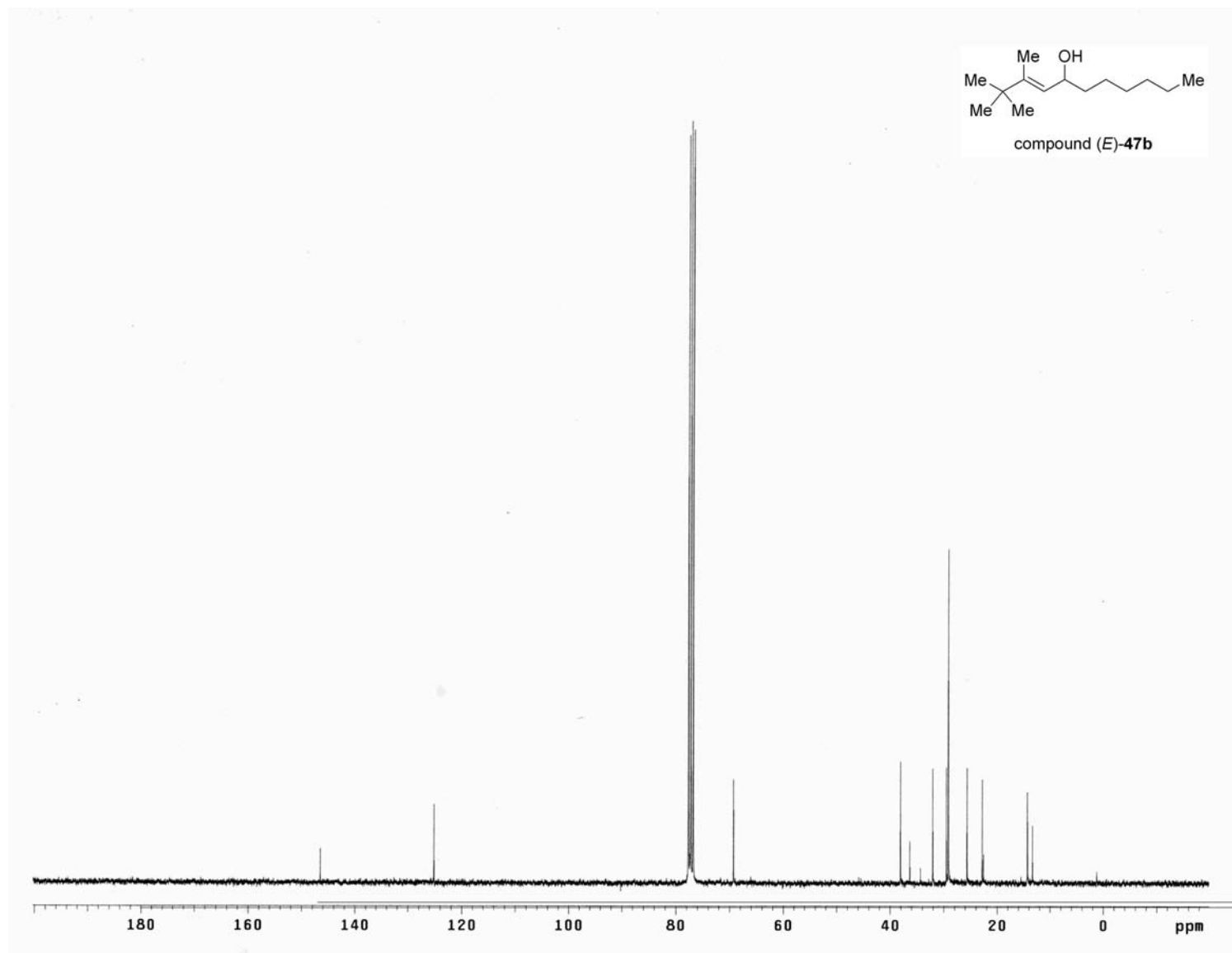


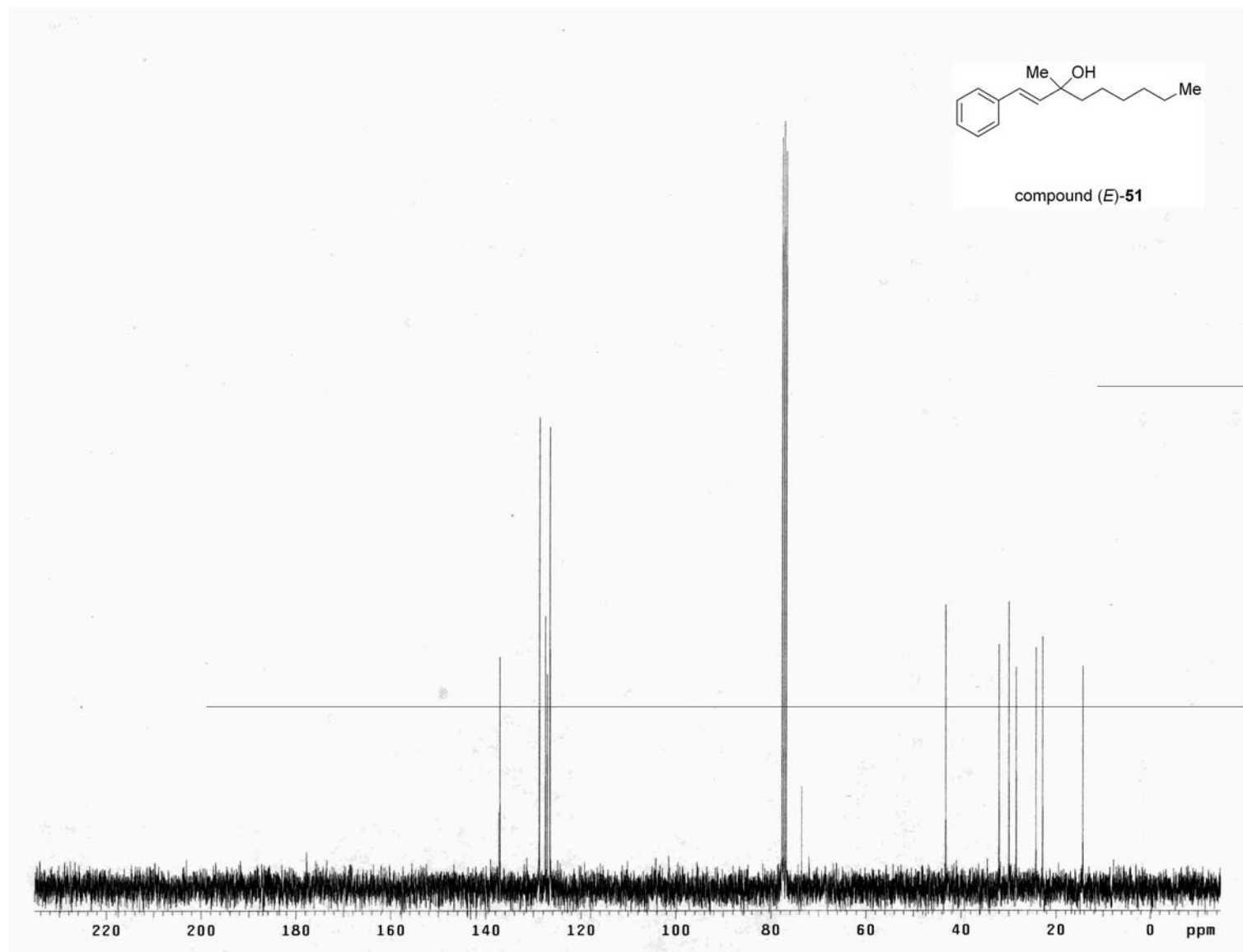
compound (E)-46b

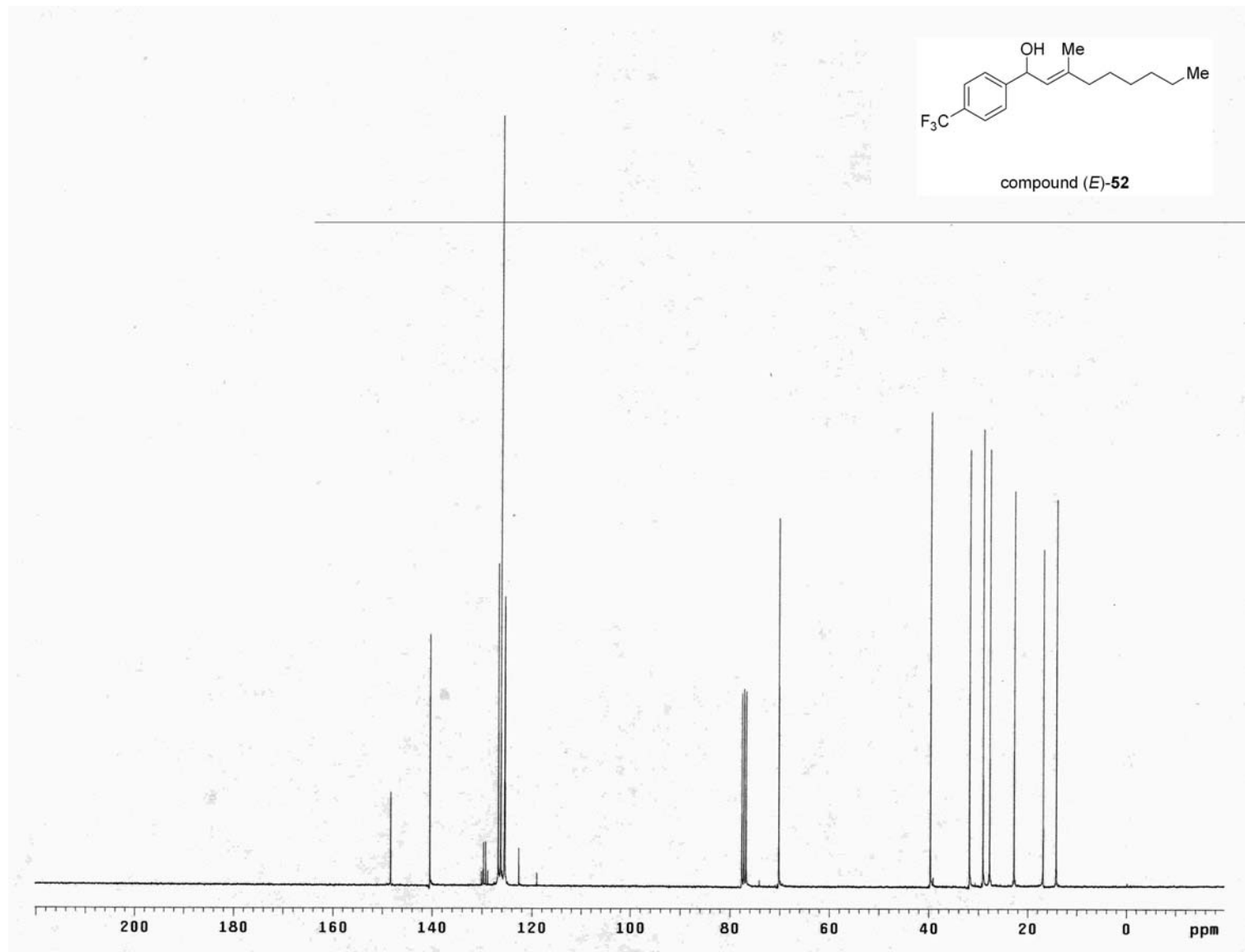
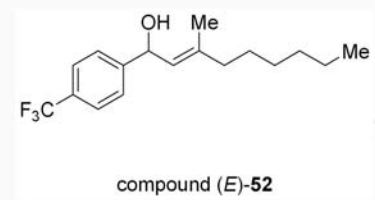


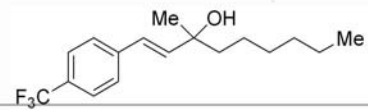




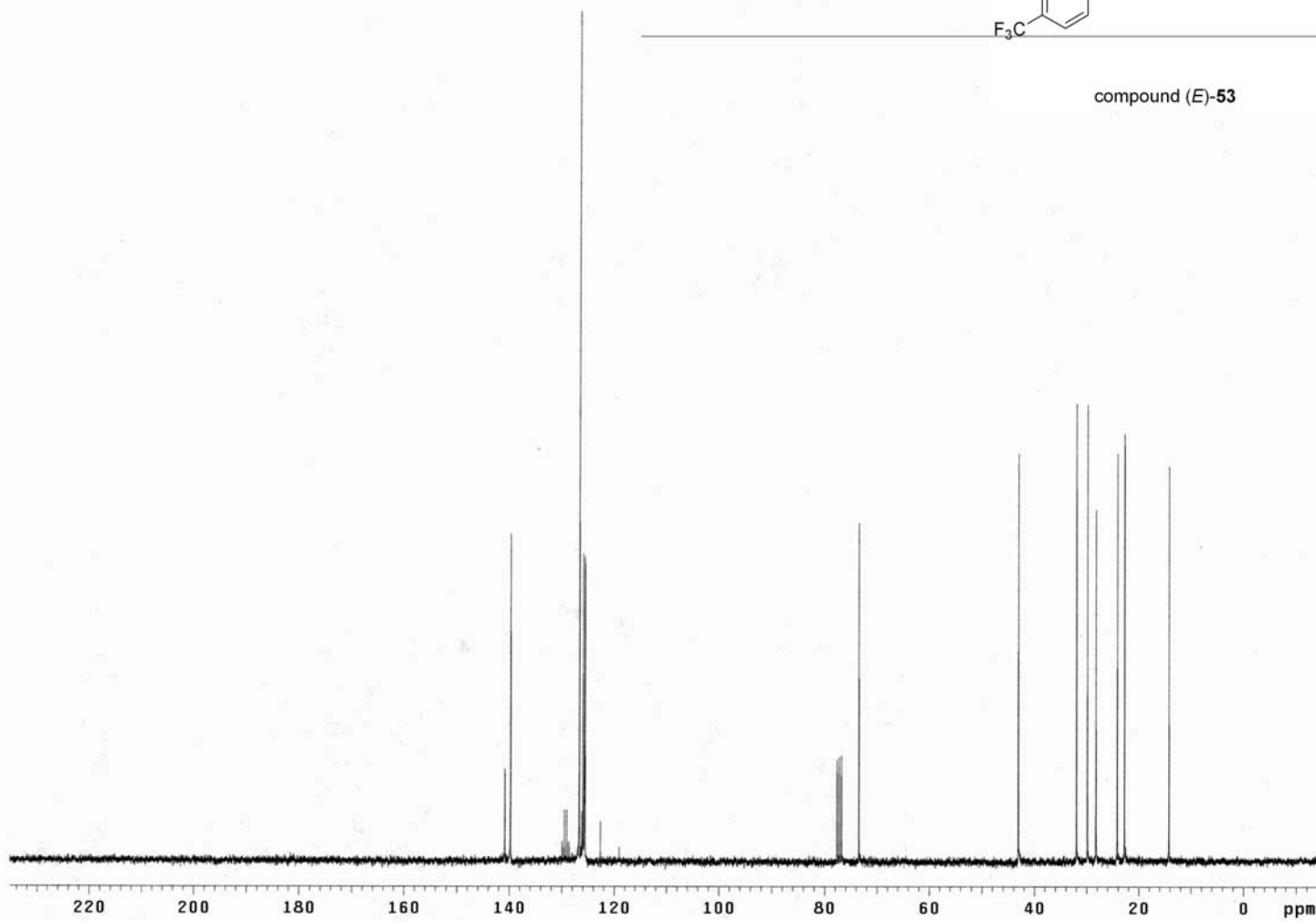








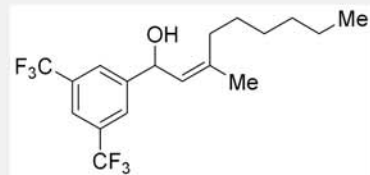
compound (E)-53



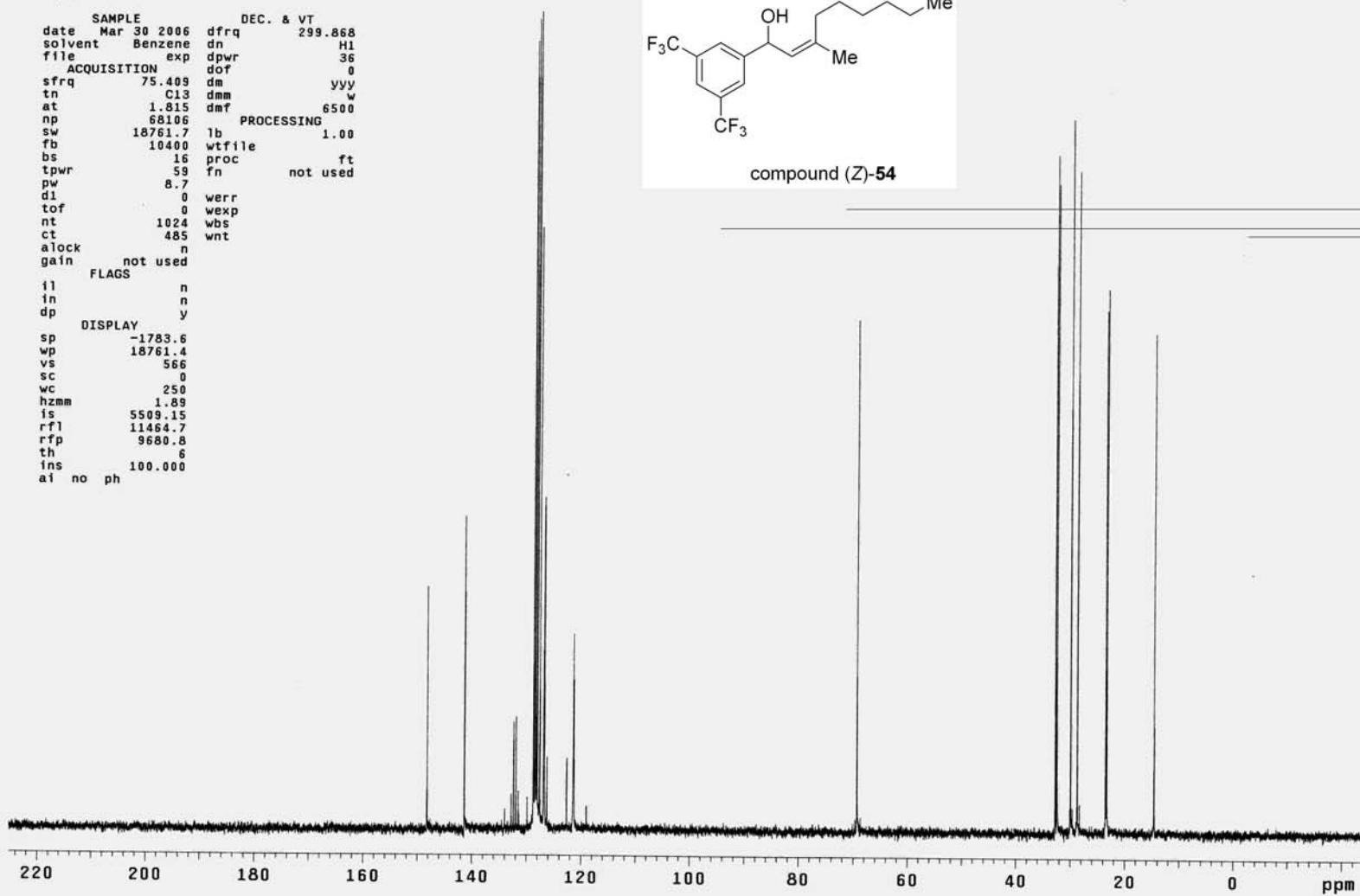
GB560HPLC.13C

exp2 std13c

SAMPLE DEC. & VT  
date Mar 30 2006 dfrq 299.868  
solvent Benzene dn H1  
file exp dpwr 36  
ACQUISITION dof 0  
sfrq 75.409 dm yyy  
tn C13 dmm w  
at 1.815 dmf 6500  
np 68106 PROCESSING  
sw 18761.7 lb 1.00  
fb 10400 wtfile  
bs 16 proc ft  
tpwr 59 fn not used  
pw 8.7  
d1 0 verr  
tof 0 wexp  
nt 1024 wbs  
ct 485 wnt  
alock n  
gain not used  
FLAGS  
il n  
in n  
dp y  
DISPLAY  
sp -1783.6  
wp 18761.4  
vs 566  
sc 0  
wc 250  
hzmm 1.89  
is 5509.15  
rfl 11464.7  
rfp 9680.8  
th 6  
ins 100.000  
ai no ph



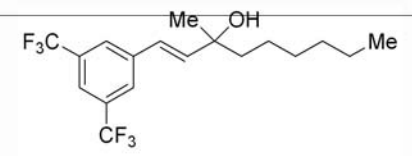
compound (Z)-54



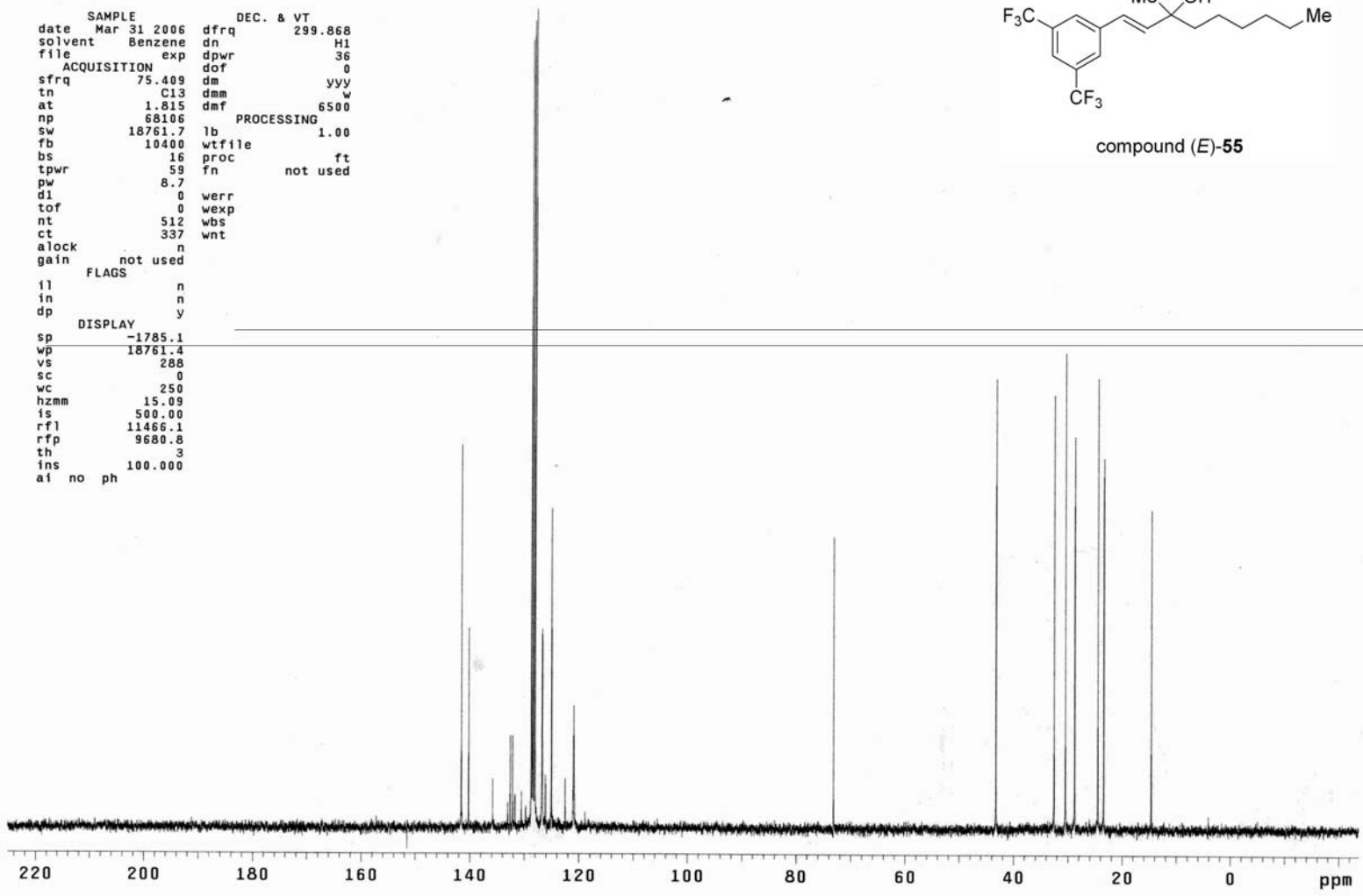
GB568F.13C

expl std13c

SAMPLE		DEC. & VT	
date	Mar 31 2006	dfrq	299.868
solvent	Benzene	dn	H1
file	exp	dpwr	36
ACQUISITION			
sfrq	75.409	dm	yyy
tn	C13	dmm	w
at	1.815	dmf	6500
np	68106	PROCESSING	
sw	18761.7	lb	1.00
fb	10400	wtfile	
bs	16	proc	ft
tpwr	59	fn	not used
pw	8.7		
d1	0	werr	
tof	0	wexp	
nt	512	wbs	
ct	337	wnt	
alock	n		
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-1785.1		
wp	18761.4		
vs	288		
sc	0		
wc	250		
hzmm	15.09		
is	500.00		
rfl	11466.1		
rfp	9680.8		
th	3		
ins	100.000		
ai	no	ph	

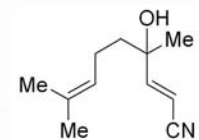


compound (E)-55

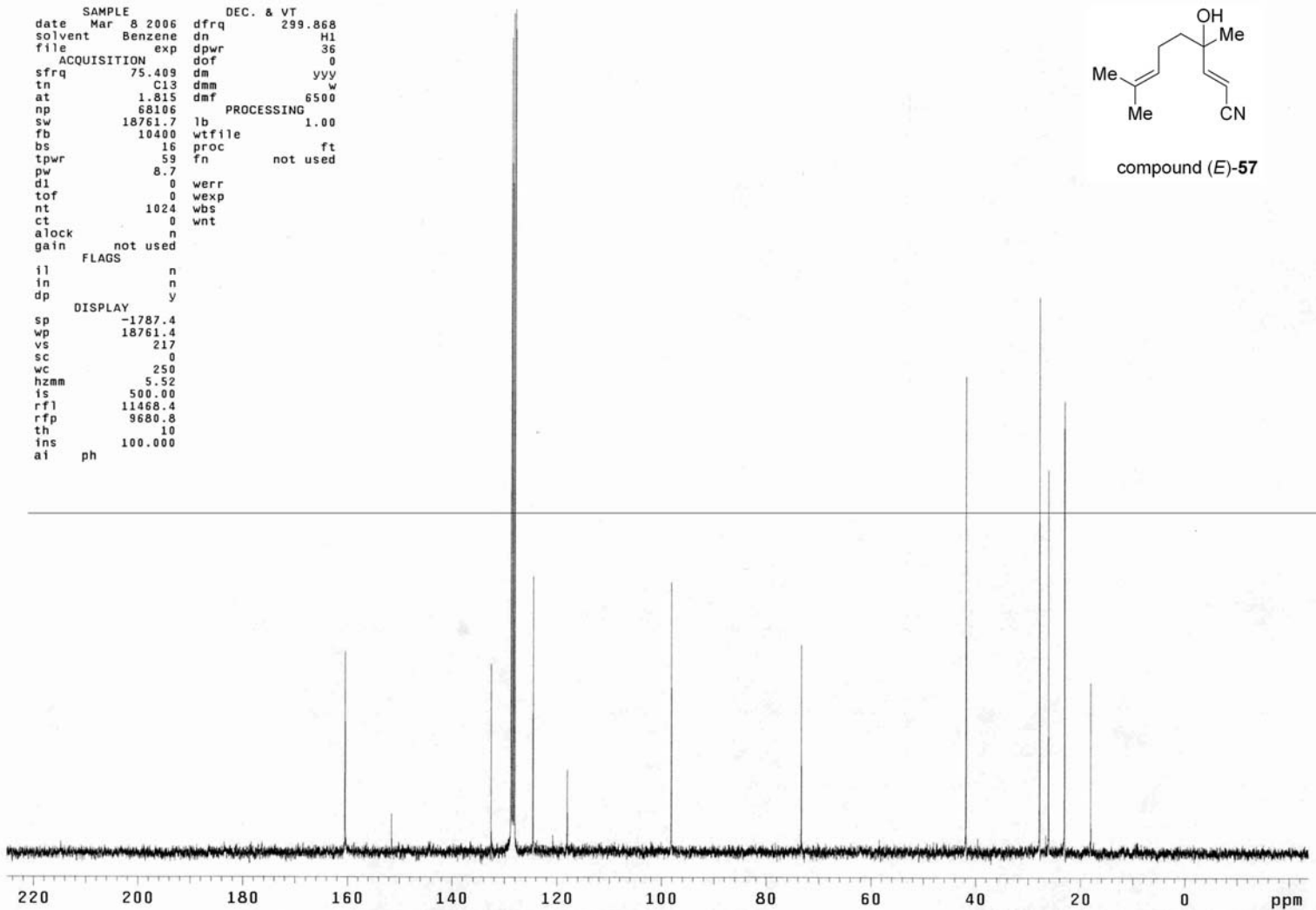


GB549F.13C  
exp3 std13c

```
SAMPLE          DEC. & VT
date   Mar  8 2006  dfrq      299.868
solvent Benzene    dn        H1
file   exp        dpwr       36
ACQUISITION      dof        0
sfrq   75.409    dm         yyy
tn     C13       dmm        w
at     1.815     dmf       6500
np     68106     PROCESSING
sw     18761.7   lb         1.00
fb     10400    wtfile
bs     16       proc        ft
tpwr   59      fn        not used
pw     8.7
d1     0       werr
tof    0       wexp
nt     1024    wbs
ct     0       wnt
alock  not used
gain  not used
FLAGS
il     n
in     n
dp     y
DISPLAY
sp     -1787.4
wp     18761.4
vs     217
sc     0
wc     250
hzmm   5.52
is     500.00
rf1    11468.4
rfp    9680.8
th     10
ins    100.000
a1     ph
```



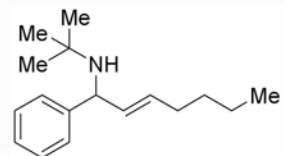
compound (E)-57



GB298FA.13C

exp3 std13c

SAMPLE		DEC. & VT	
date	Feb 14 2005	dfrq	299.868
solvent	CDC13	dn	H1
file	exp	dpwr	37
ACQUISITION		PROCESSING	
sfrq	75.409	dm	yyy
tn	C13	dmm	w
at	1.815	dmf	6700
np	88106	lb	1.00
sw	18761.7	wtfile	
fb	10400	proc	ft
bs	16	fn	not used
tpwr	59	werr	
pw	8.7	wexp	
d1	0	wbs	
tof	0	wnt	
nt	1024		
ct	151		
alock			
gain	not used		
FLAGS			
il	n		
in	n		
dp	y		
DISPLAY			
sp	-1843.8		
wp	18761.4		
vs	185		
sc	0		
wc	250		
hzmm	4.14		
is	500.00		
rfl	7650.0		
rfp	5805.9		
th	14		
ins	100.000		
al	no ph		



compound (E)-60

