

– Supporting Information (Part 2) –

Rationally Improved Chiral Brønsted Acid for Catalytic Enantio-selective Allylboration of Aldehydes with an Expanded Reagent Scope

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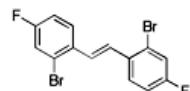
dennis.hall@ualberta.ca

15. Part 2: Reproductions of NMR spectra and HPLC chromatograms.....46 -

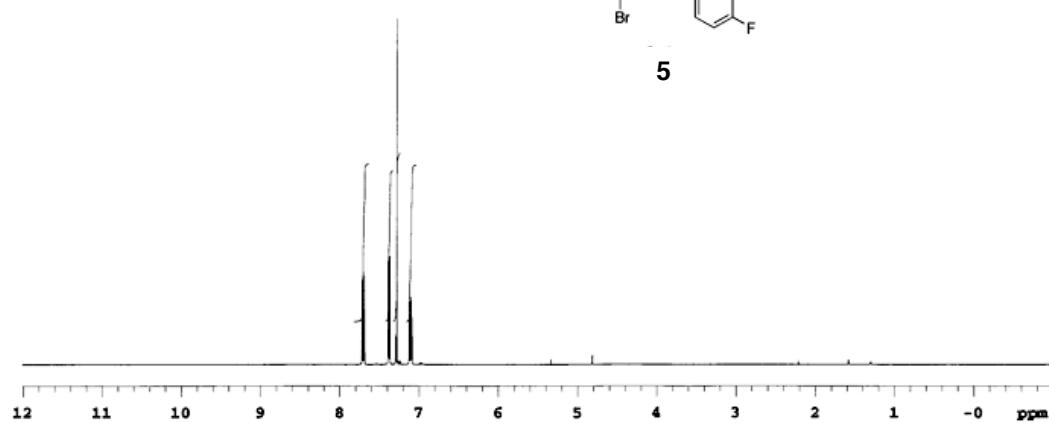
Vivek VRH-7-36A
499.821 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
Temp 26.1 C \rightarrow actual temp = 27.0 C, autondb probe

File: 2009.02.09.u5_VRH-7-36A_H1_1D
Pulse Sequence: s2pul

500 MHz, CDCl_3



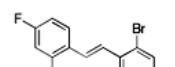
5



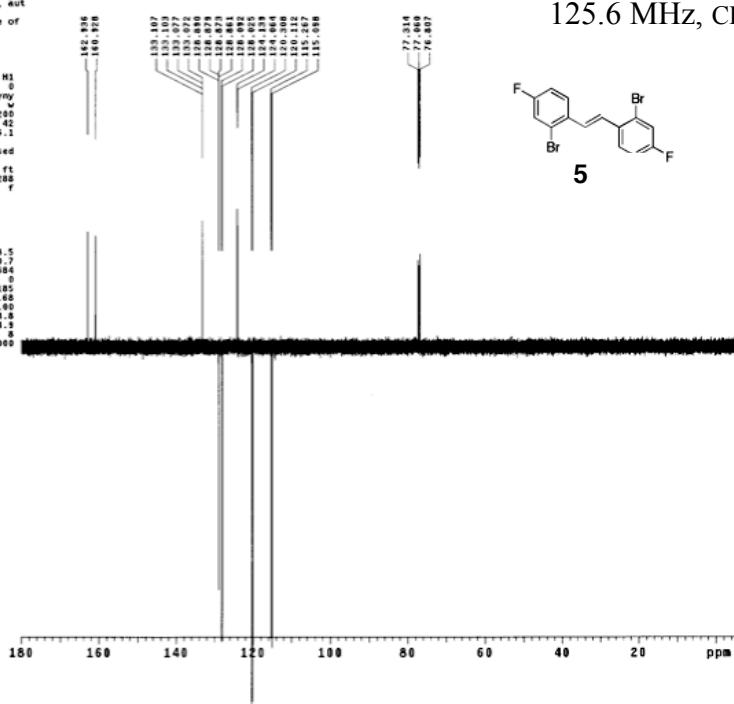
Vivek VRH-7-36A
499.821 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
Temp 26.1 C \rightarrow actual temp = 27.0 C, autondb probe
order CH & CH2 same, CH & CH3 opposite side of solvent signal

```
exp1 apt
SAMPLE          DEC. & VT
date  Feb 9 2009 dn      H1
solvent   cdcl3 dof      0
f1center,offset  7.26  7.26
e12/gnmmr/nordata-dmz
/HALL/VIVEK/2009.5-dmz
/DATA/2009.5-dmz
N-7-36A,CDCl3_apl.f1- temp 26.1
ACQUISITION      b  PROCESSING
sfrq  125.694 wfile not used
tn      125.694 wfile
c13    proc      rt
dt      2.000      524298
np      135136 math      r
tv      3378.0
td      100000 werr
bs      10000 wexp
tr      55 wint
tpwv      55 wint
pw      3.3 DISPLAY
p1      21.00 sp      122.5
d1      0.100 ws      23259.7
d2      0.007 vs      2684
d3      0.001 tc      0
tof      2500.0 vc      185
nt      100000 hzmn      125.68
ct      2500      510.00
clock      48 rfp      12164.8
gain      48 rfp      3684.5
t1      FLAGS      n ims      0
in      n ai      ph      100.000
in      n ai      ph      0
dp      y
ns      nn
```

125.6 MHz, CDCl_3

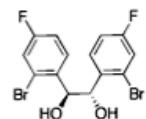


5



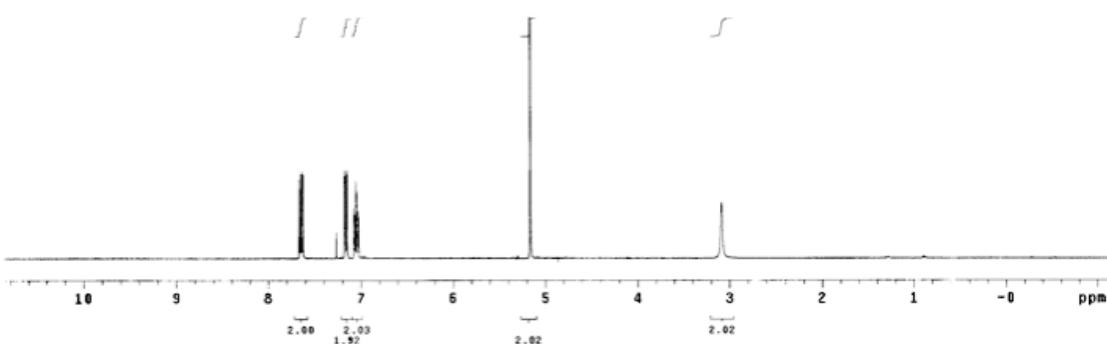
VRH-6-204-diol1-1

Pulse Sequence: s2pul



500 MHz, CDCl₃

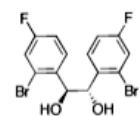
6



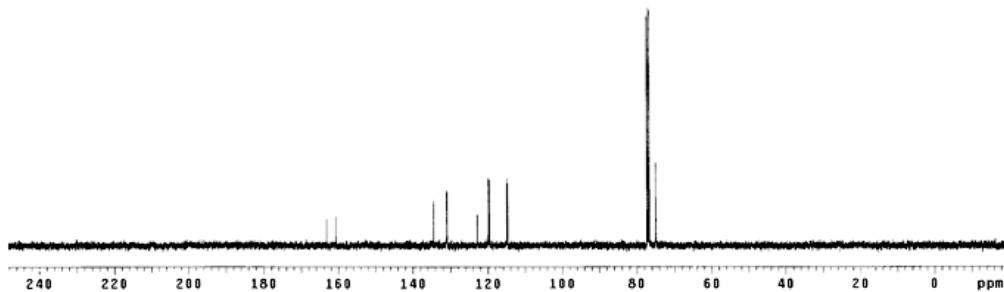
VRH-6-204-diol1-1-13C

Pulse Sequence: s2pul

125.7 MHz, CDCl₃



6



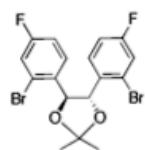
Pulse Sequence: s2pul

VRH-6-204-acetal

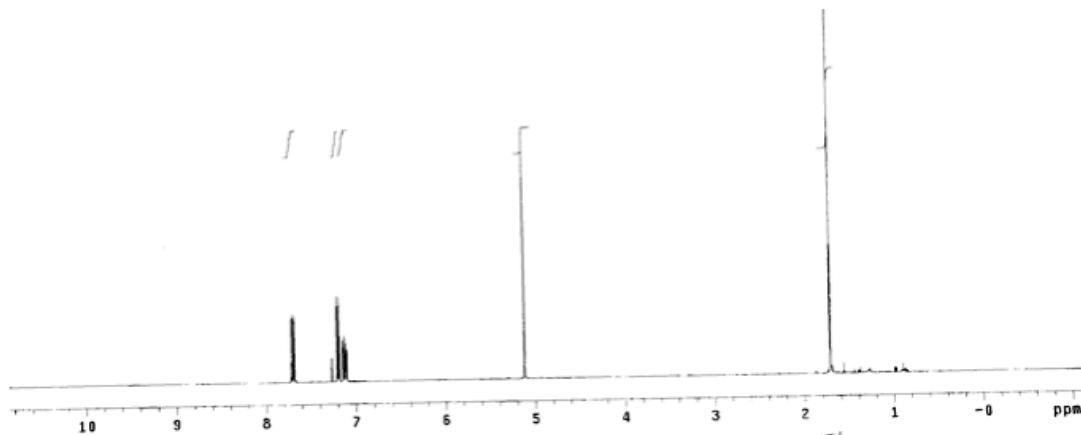
Solvent: CDCl_3
Temp: 26.5 °C / 293.6 K
Operator: Hallinan
INOVA-300 -1400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 4801.5 Hz
12 repetitions
OBSERVE H1 399.7923305 MHz
DATA PROCESSING
FT size 131072
Total time 1 hr, 25 min, 17 sec

400 MHz, CDCl_3



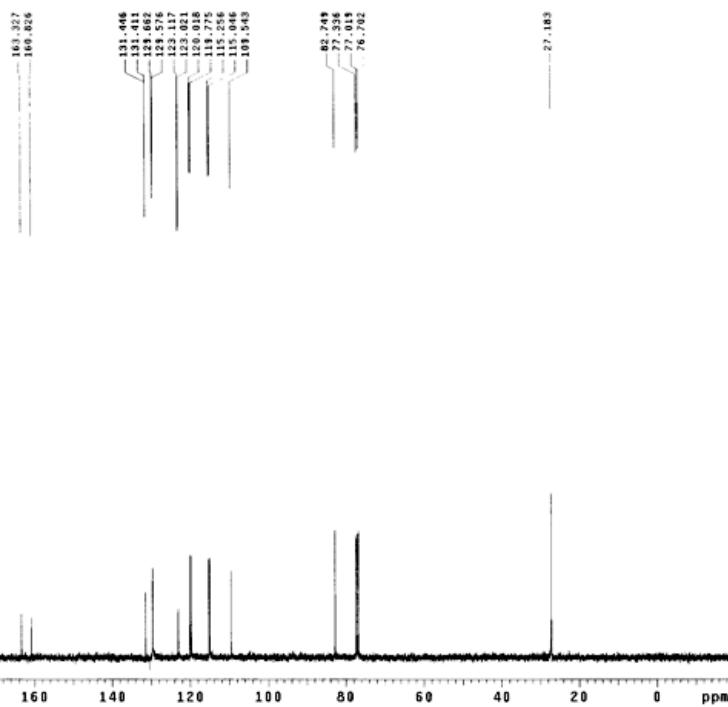
7

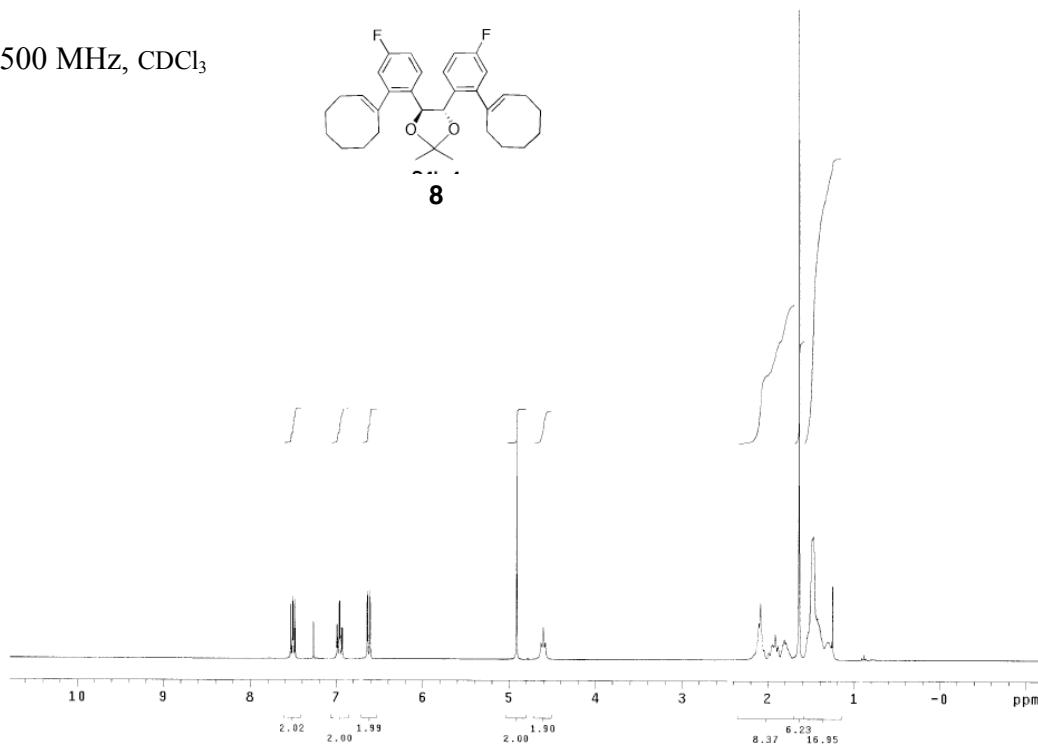
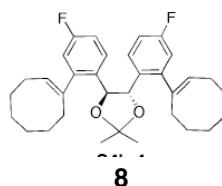


VRH-6-204-acetal

Pulse Sequence: s2pul

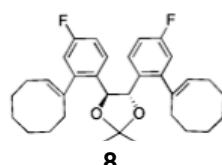
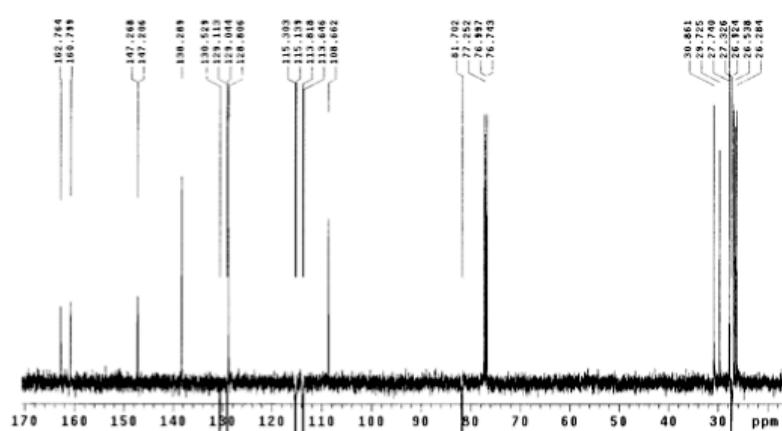
100.5 MHz, CDCl_3

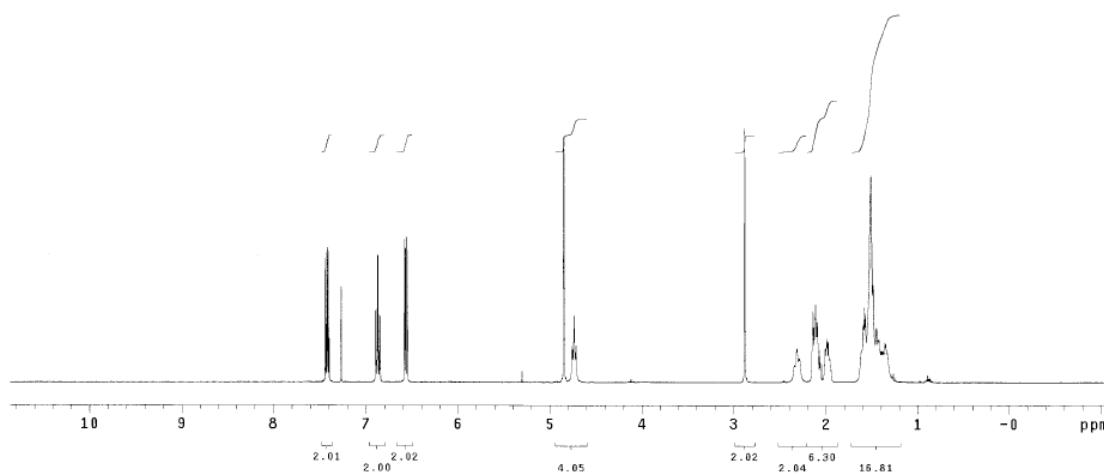
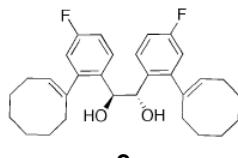


500 MHz, CDCl₃

Vines R., VRH-7-4IA
125 MHz APT in CDCl₃ (ref. to CDCl₃ @ 72.0 ppm), temp 26.1 C (\rightarrow actual temp = 27.0 C) and 2D probe
C & CH₂ same, CH & CH₃ opposite side of solvent signal

```
expli apt
SAMPLE           DEC. & VT
date Mar 25 2008 dn   H1
solvent  CDCl3 dpp   0
file /mnt/d800/home/dm  myy
e12/generat/madata: dms  w
/multiscan/2008  9391
3/2008.03.25  VR= dppr  42
H-7-4IA_C13_ap1.fl= temp 26.1
d      PROCESSING 26.1
ACQUISITION 1b      1.50
sfrq  125.694 wfile
tn    C13 proc   ft
at    2.00 tn   131972
rt    131136 with  7
sw   33783.8
tb   15000
ts   8
ss   8
tpur  54
pw   3.5
DISPLAY
pi   28.0 sp   2120.3
d1   0.100 w1  18307.5
d2   0.007 vs  12164
d3   0.001
t0f  2500.0 wc  180
nt   100000 hzem 107.26
et   200 r1  500.00
a1ock n   rfp  12164.1
gain  48 rfp  1877.3
FLAGS  n   th  14
i1   n   ph  180.000
in   n   a1 ph
dp   y
hs   nn
```

125 MHz, CDCl₃

500 MHz, CDCl₃

Vivek; VRH-7-41B
125.267 MHz C13[HI] apt in cdc13

exp11 apt

```

SAMPLE          DEC. & VT
date  Mar 27 2008 dn      H1
solvent   d600/hcore dof      0
f1inv/d600/hcore ds      ymy
e12/gemmr/mrdatas dms      w
/HALL/VIVEK/2008_0.dmt 10482
3/2008.03.27.15.15~ dpuv    49
H-7-41B_C13_apt.v1 temp   27.2
d      processing 1.50

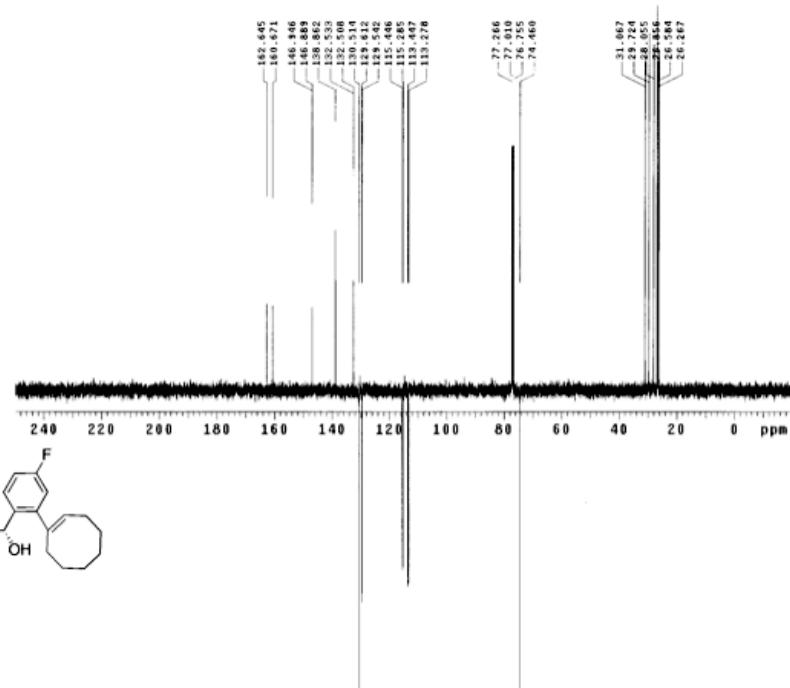
```

ACQUISITION 1.50

```

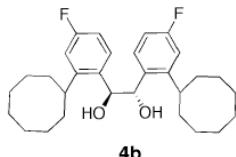
sfrq  125.267 urfile
tn      C13 proc      ft
at     1.996 fn      131072
np      135022 math      f
sw      33840
fb      not used werr
bs      8 wexp
ss      8 wbs
tpwrf  50 wnt
pw     4.1 DISPLAY
p1     24.4 sp      -2545.3
d1     0.116 ap      33826.1
d2     0.087 vs      3374
d3     0.001 vc      0
t0f    2500.0 wc      180
rt     1000.0 sec     187.32
ct     200 ts      500.00
alock   n rrf1    12131.3
gain   48 rfp    9845.5
fl     n ins      7
f1     n ins    100.000
in     n a1 ph
dp     y mn
hs     mn

```

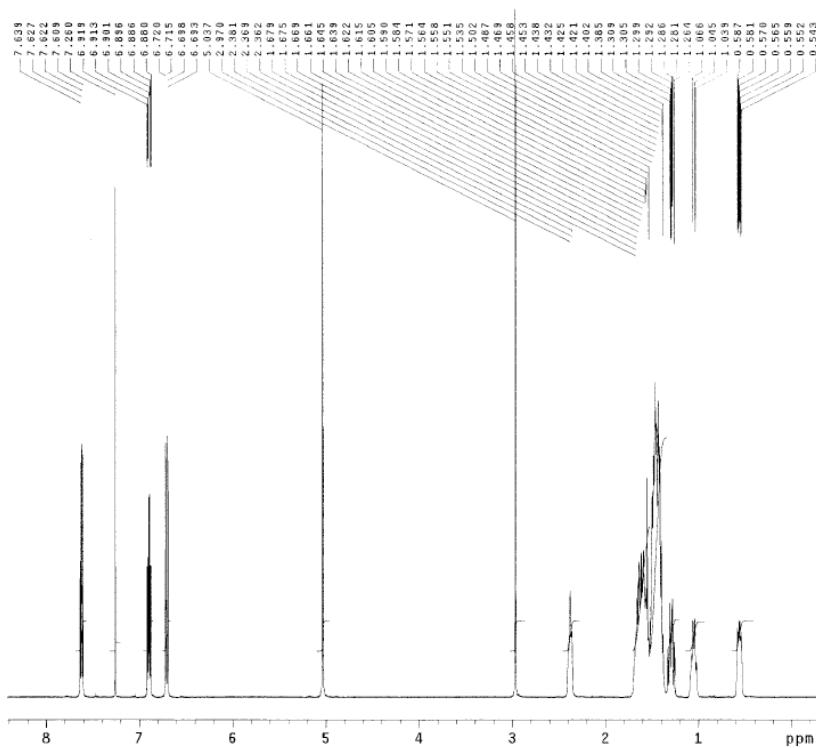
125 MHz, CDCl₃

Vivek, VRH-741C
499.823 MHz 1H in CDCl₃

```
exp10 Proton
SAMPLE SPECIAL
date Apr 8 2008 temp not used
solvent cdcl3 gain 26
file /mnt/d609/home/spin 18
size/genome 16000000 hst 0.006
JVAL/VIVEK/2008.04.08.u5.dpr 12.200
4/2008.04.08.u5.VR~ alfa 6.600
H-7-41C_H1_1D.T1d FLAGS
ACQUISITION 11 n
sw 10.4 in n
at 5.000 dp y
np 65104 hs mn
fb 4000 PROCESSING
bs 4 fn not used
d1 0.100 DISPLAY
nt 16 sp -148.7
ct 16 wpt 4357.1
TRANSMITTER 11 rfp 4153.5
tn H1 rfp 365.7
strg 499.822 rp -62.8
tof 249.8 lp -23.3
tpwr 61 PLOT
pw 4.067 wc 180
DECOUPLER sc 0
dn C13 vs 1576
dof 0 th
ds min a1 cdc ph
dmm c
dpwr 41
dmr 22400
```

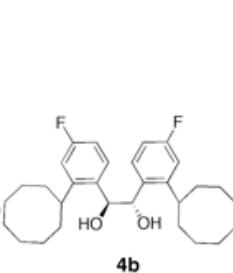


500 MHz, CDCl₃

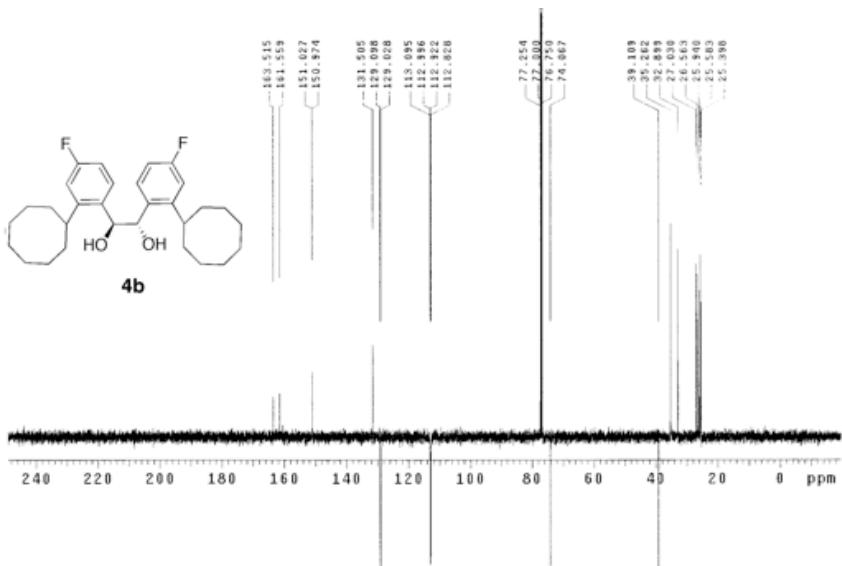


.0 ppm), temp 26.1 C -> actual temp = 27
0 C, autowdb probe
C & CH2 same, CH & CH3 opposite side of
solvent signal!

```
exp10 apt
SAMPLE DEC. & VT
date Apr 8 2008 dn H1
solvent cdcl3 dof 0
file /mnt/d609/home/ds yny
el2/generic/nmrdat=dss
JVAL/VIVEK/2008.04.08.u5.dpr 9380
4/2008.04.08.u5.VR~ dprf 42
H-7-41C_C13_ap1.f1= temp 26.1
d PROCESSING
ACQUISITION 16 1.56
sw 125.684 wtrfile
tn C13 proc ft
at 2.000 fn 131072
np 135136 math f
sw 33783.3
fb 15000 werr
bs 8 wexp
ts 8 wbs
tpwr 94 wnt
pw 3.2 DISPLAY
p1 20.0 sp -2482.7
d1 0.100 wpt 33783.3
d2 0.087 vs 15493
d3 0.000 tc 0
tof 2500.0 wc 180
nt 100000 hzmn 187.68
ct 1000 ls 500.00
alock n rfp 12161.7
gain 48 th 9678.4
FLAGS th 7
il n ins 100.000
in n a1 ph
dp y
hs nn
```



125 MHz, CDCl₃

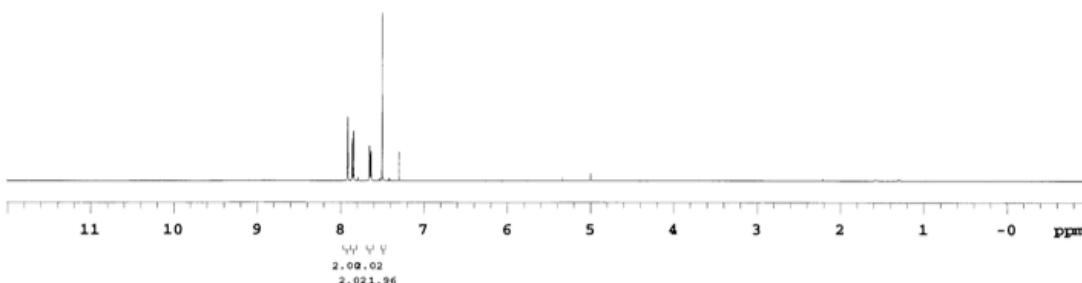
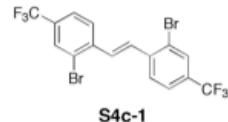


Vivek VRM-CF3-Stillbene
499.821 MHz H1 ID in cdcl3 (ref. to CDCl3 @ 7.26 ppm)
Temp 26.1 C -> actual temp = 27.0 C, autoxdB probe

File: 2009.02.09.u5_VRM-CF3-Stillbene_H1_ID

Pulse Sequence: s2pul

500 MHz, CDCl₃

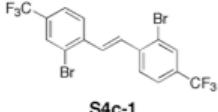
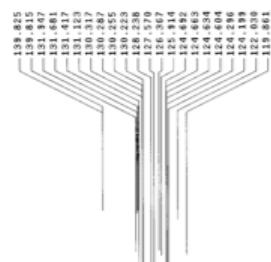


Vivek VRM-CF3-Stillbene
125.693 MHz CD₃[H1] apt in cdcl3 (ref. to CDCl3 @ 77.06 ppm)
Temp 26.1 C -> actual temp = 27.0 C, aut
oxdB probe
C & CH2 same, CH & CH3 opposite side of
solvent signal

5 Hz/cm

exp2 apt

```
SAMPLE           DEC. & VT
date Feb 9 2009 dn   H1
solvent   cdcl3  d0f    5
file /mnt/d600/hcmv/dm      ymy
e12/gemmr/mrdatav  dms
/HALL/VIVEK/2009.0  dat  8260
2/2009.0 00:00:00  dtr  45.0
H-CF3-Stillbene_C13> temp 26.1
          apt.fid  PROCESSING
ACQUISITION          1b          0.50
sfrq  125.694 wtitle
tn      C13 proc      rt
at     2.000 fn      524288
rt     135.36 math      f
sw    33783.8
fb    15000 werr
bs      6 wexp
si      8 Wht
tpwrf 55 wint
pw     5.5 DISPLAY
p1     2.00 sp      -628.5
d1     0.100 wp      23259.7
d2     0.007 vs      4420
d3     0.001 tc
tof    2500.0 wc      185
nt    100000 hzmn  125.68
et     240 ls      510.00
alock   n rf      12150.1
gain   48 rfp      1664.9
        th      3
il      n ins  100.000
in      n at  ph
dp      y
hs      nn
```



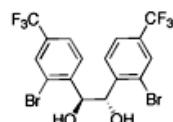
125 MHz, CDCl₃



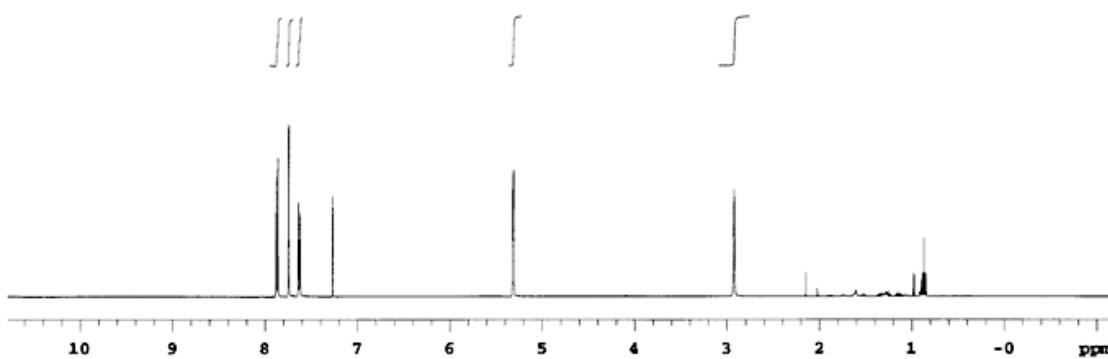
Vivek VRM-CF3-DIOL
499.821 MHz H1 1D in CDCl_3 (ref. to CDCl_3 at 7.26 ppm)
Temp 26.1 C \rightarrow actual temp = 27.0 C, autoweb probe

Pulse Sequence: s2pul

500 MHz, CDCl_3



S4c-2



Vivek VRM-CF3-DIOL
125.653 MHz, $\text{C}_13[\text{H}1]$ apt in CDCl_3 (ref. t
to CDCl_3 at 7.26 ppm)
Temp 26.1 C \rightarrow actual temp = 27.0 C, aut
oxdb probe
C & CH2 same, CH & CH3 opposite side of
solvent signal

exp2 apt

SAMPLE DEC. & VT
date Feb 10 2009 dn H1
 solvent CDCl3 dpr 0
 f1 125.653 MHz dppf 0
 f12/2emar/mrdatav dsw 0
 /HALL/VIVEK/2009.0- dse 8200
 2/2009.02.19.05.CF- dpr 42
 3-Br-Diol, CDCl_3 , dppf temp 26.1

fid

PROCESSING 1b 0.28

acquisition 1b 0.28

sfreq 125.654 MHz profile

tn C13 proc ft

at 2.000 fn 524288

rt 133.000 math r

sw 33783.6

fb 15000 werr

bs 8 wexp

ss 8 bsize

tpwr 55 wint

pw 3.3 DISPLAY

gt 25.0 SP -628.5

d1 0.100 w1 23250.7

d2 0.087 v5 4722

d3 0.087 v5 4722

tof 2500.0 uc 185

nt 100000 hzmn 9.16

sc 400 ts 500.00

clock n 11 125.653

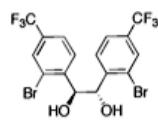
gain 48 rfp 3864.5

11 F1AOS th 4

in n 1ms 100.000

dp y ph

hs nn



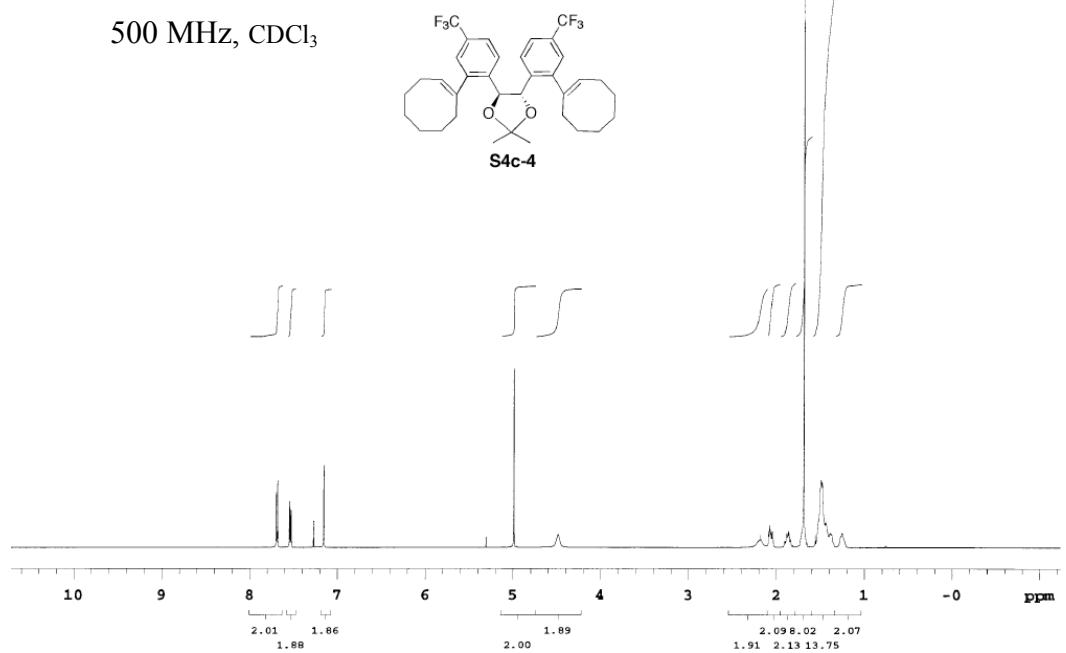
S4c-2

125 MHz, CDCl_3



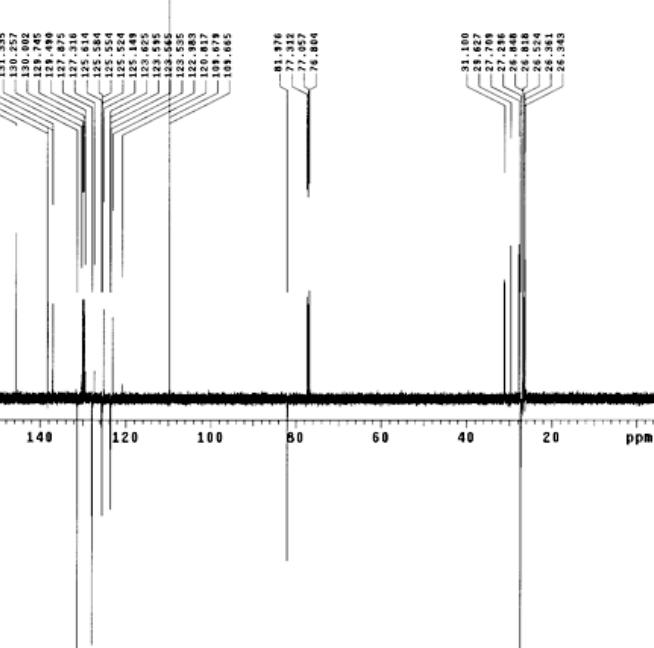
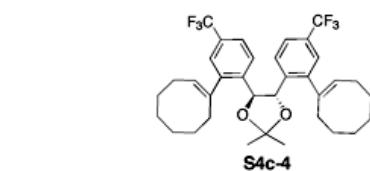
Vivek VRH-CF3-Cycloalkene-acetal
499.821 MHz H1 1D in CDCl₃ (ref. to CDCl₃ at 7.26 ppm)
Temp 26.1 °C → actual temp = 27.0 °C, autoxdb probe

Pulse Sequence: s2pul



Vivek VRH-CF3-Cycloalkene-acetal
125.633 MHz C13[1H] apt in CDCl₃ (ref. t o CDCl₃ at 77.06 ppm)
Temp 26.1 °C → actual temp = 27.0 °C, aut oxdb probe
C & CH2 same, CH & CH3 opposite side of solvent signal

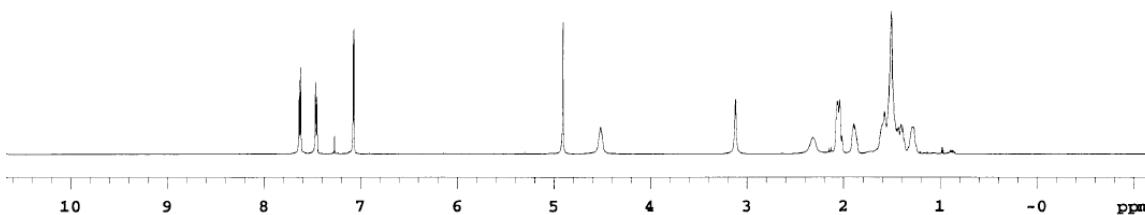
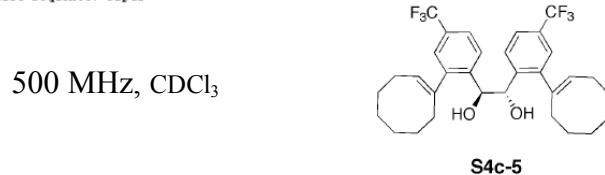
exp2 appt
SAMPLE dn DEC. & VT
date Feb 16 2009 dn H1
solvent cdcl3 dof 0
file /mnt/d680/home/dm_ymy/
el2d_125.633.appt doff v
/HAL/VIVEK/2009.0- dprf 8240
2/2009.02.10.us.vh- dppr 42
H-CF3-Cycloalkene-- temp 26.1
acqtime 1.000 sec fid 1.000 sec
ACQUISITION 1b PROCESSING 0.20
sfreq 125.634 wfile
tr 1.000 proc ft
at 2.000 n 524200
np 135136 math f
sw 33783.8
fb 15080 warr
bs 8 wexp
ss 8 wbs
tpwr 55 wnt
pw 3.3 DISPLAY -628.5
p1 20.0 sp 23250.7
d1 0.100 wp 500.0
d2 0.001 sc 322.0
d3 0.001 sc 0
t0f 2500.0 wc 185
nt 160000 hzmn 13.84
ct 300.0 s 500.0
clock 48 rrf1 12162.2
gain 48 rfp 9684.9
11 flags 1 ins 3
in 1 n 100.000
in 1 n 100.000
dp y ph
hs nm



125 MHz, CDCl₃

Vivek VRH-CF₃-Cycloalkene-diol
499.821 MHz H1 1D in CDCl₃ (ref. to CDCl₃ @ 7.26 ppm)
Temp 26.1 C -> actual temp = 27.0 C, autoxdB probe

Pulse Sequence: s2pul



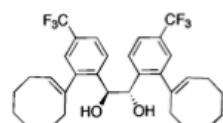
Vivek VRH-CF₃-Cycloalkene-diol
125 MHz, CDCl₃] apt in CDCl₃ (ref. t
o CDCl₃ @ 7.26 ppm)
Temp 26.1 C -> actual temp = 27.0 C, aut
oxdB probe
Q = CH₂ same, CH & CH₃ opposite side of
solvent signal

exp2 apt

SAMPLE	DEC. & VT		
date	Feb 10 2009	dn	H1
solvent	CDCl ₃	dpf	0
file	/mnt/ds00/bcm	dm	yiny
e12/gemini/mrdatc	dmw	dw	w
nh	1000	spw	8200
z/2009.02.10.05.05.vpr	dprv	temp	42
H-CF ₃ -Cycloalkene-diol	temp	26.1	
diol.C13apt.fid			

ACQUISITION

sfrq	125.694	vtfile	0.28
tn	C13	proc	ft
rt	2	ppm	5242.6
np	155136	math	f
sw	33783.8		
fb	1500	verr	
bs	8	versp	
ss	8	vbs	
tpur	55	vnt	
pw	3.3	DISPLAY	
p1	20.0	sp	-628.5
di	0.100	wp	23259.7
d2	0.010	vs	589.7
d3	0.001	sc	0
tof	2500.0	vc	185
nt	10000	thres	0.00
ct	100	is	500.00
alock	n	r1f	12162.2
gain	48	rfp	9884.5
FLAQ5	n	is	
11	n	ins	100.000
in	n	at	
dp	y	ph	
hs	nn		



S4c-5

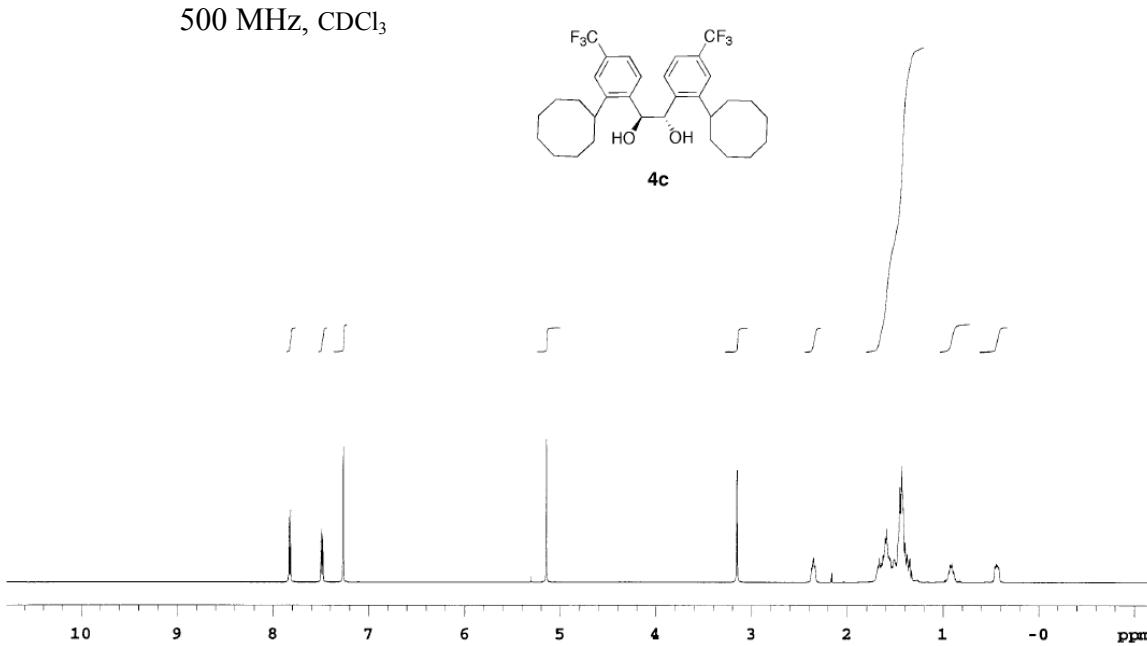
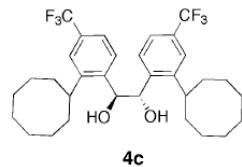
125 MHz, CDCl₃



499.821 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
 Temp 26.1 C -> actual temp = 27.0 C, autoxdb probe

Pulse Sequence: s2pul

500 MHz, CDCl_3

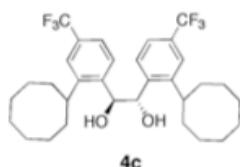
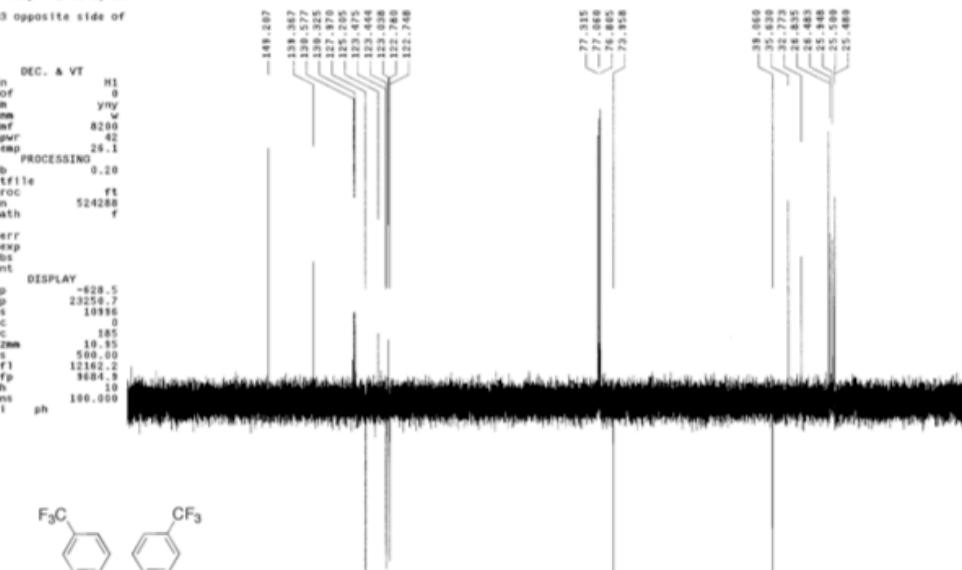


Vivek_VFC3-VIVOL
 125 MHz, CDCl_3 (ref. CDCl_3)
 o CDCl_3 @ 77.05 ppm
 Temp 26.1 C -> actual temp = 27.0 C, aut
 oxdb probe
 C & CH2 same, CH & CH3 opposite side of
 solvent signal

exp2 apt

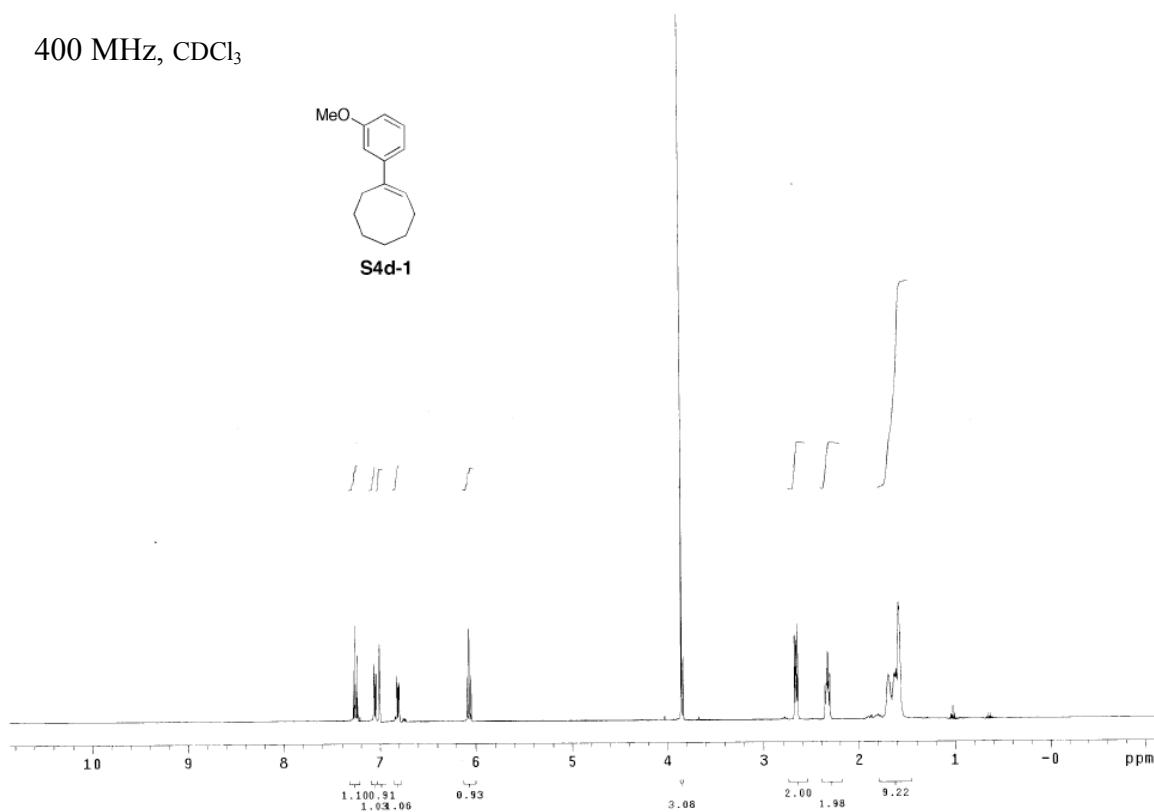
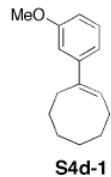
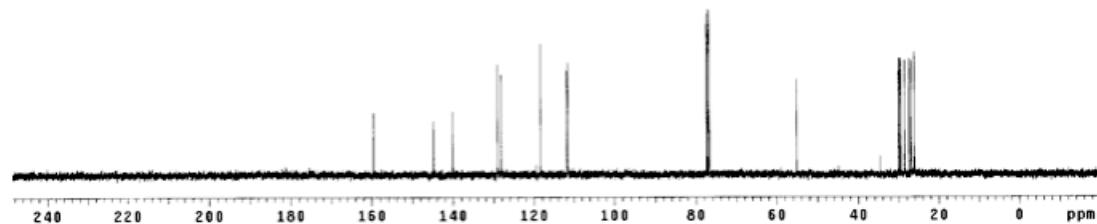
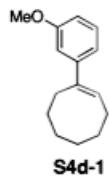
SAMPLE DEC. & VT
 date Feb 10 2009 dn H1
 solvent CDCl_3 dof 0
 file /mnt/s600/home/dm ymy
 #12/proc/dec2009.d
 #/H20/VIVEK/2009.d
 2/2009.02.10.u5.VK-
 dpwr 42
 H-CF3-VIVOL_C13.ap- temp 26.1
 t.fid PROCESSING

ACQUISITION 1b 0.20
 sfr4 125.694 wtfille
 tn C13 proc rt
 at 2.089 fn 524288
 np 128.000 math f
 sw 33783.8
 fb 15000 werr
 bs 8 wexp
 ss 8 wbs
 tppr 50 wnt
 pw 3.3 wnt
 pi 29.0 sp -628.5
 d1 9.109 wp 23256.7
 d2 0.444 v1 10398
 d3 0.001 v2 0
 tof 2500.0 wc 185
 nt 100000 hzmn 10.95
 ct 280 ls 500.00
 aclock 12180.2
 gain 48 rfp 3884.9
 flags th 10
 i1 n ins 100.000
 in n at ph
 dp mm
 hs nn



125 MHz, CDCl_3

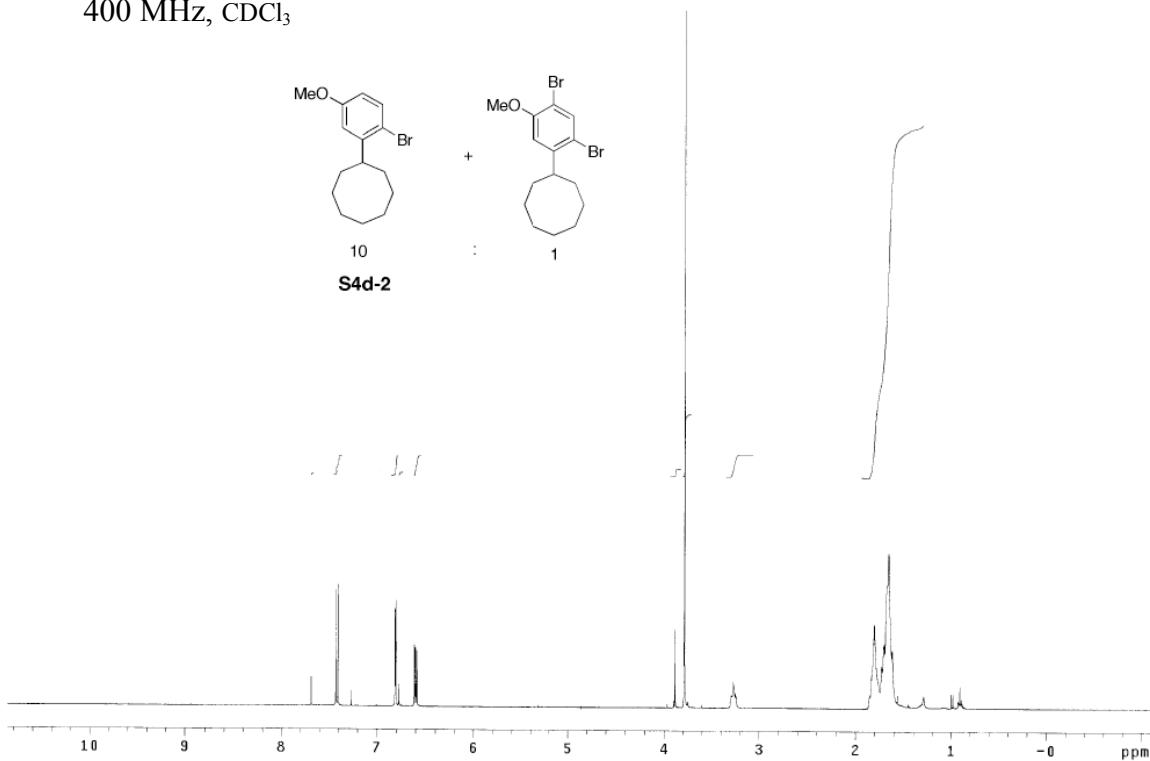
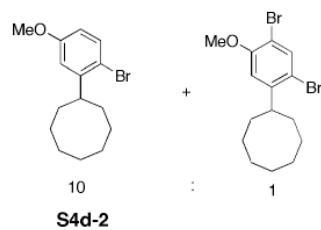


400 MHz, CDCl₃100.5 MHz, CDCl₃

VRH-8-100-4-bromoalkane

Pulse Sequence: s2pul

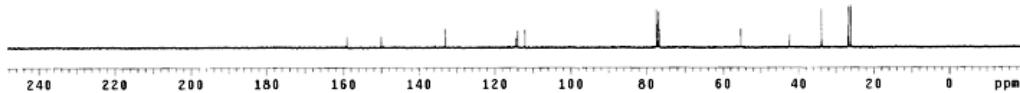
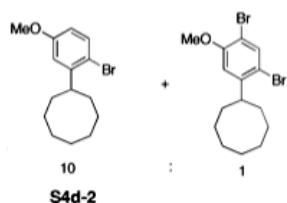
400 MHz, CDCl₃



VRH-8-100-4-bromo-cycloalkane

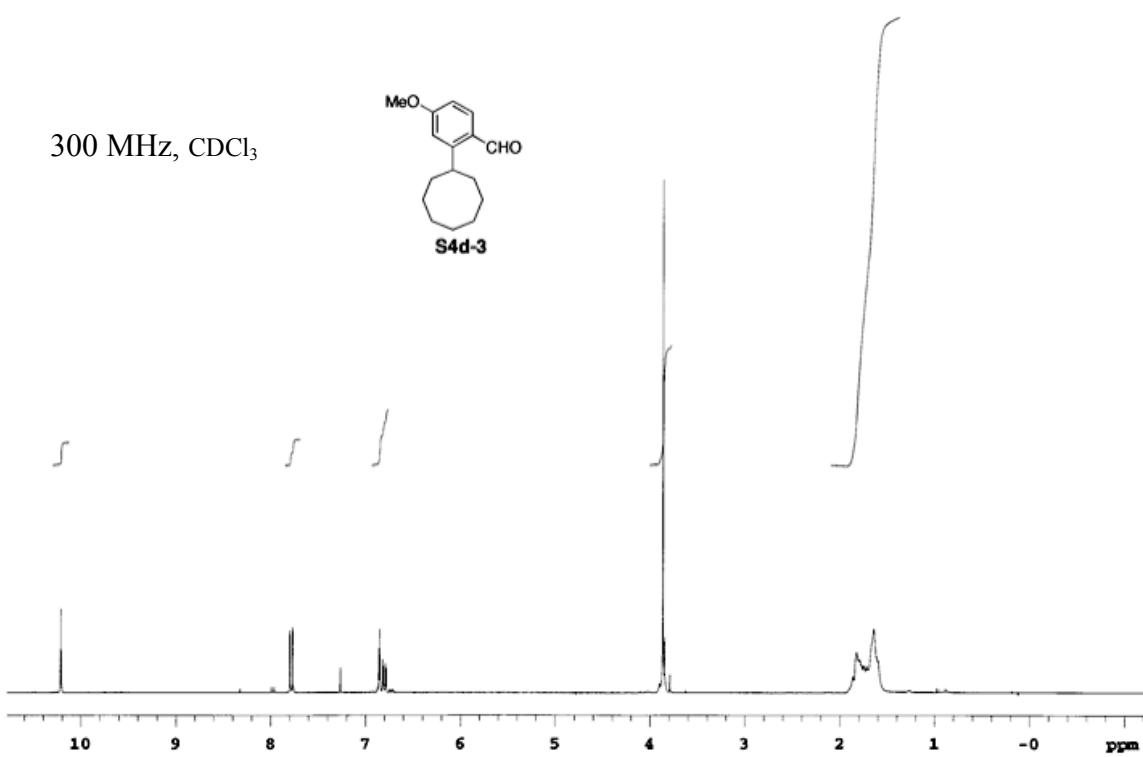
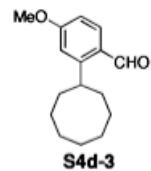
Pulse Sequence: s2pul

100.5 MHz, CDCl₃



VRH-8-102-aldehyde
Pulse Sequence: s2pul

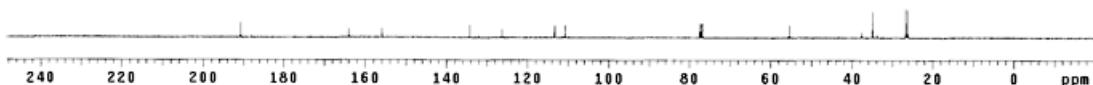
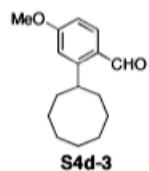
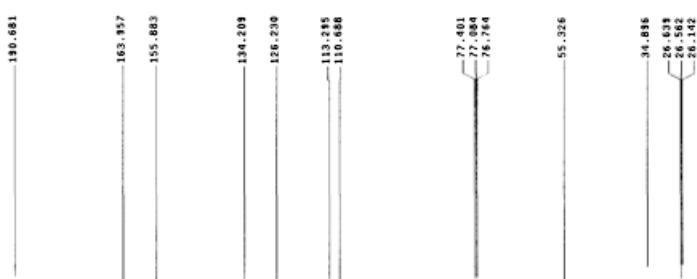
300 MHz, CDCl₃



VRH-8-101-aldehyde

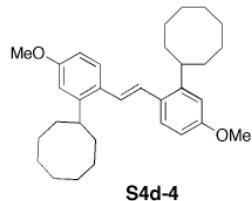
Pulse Sequence: s2pul

100.5 MHz
CDCl₃

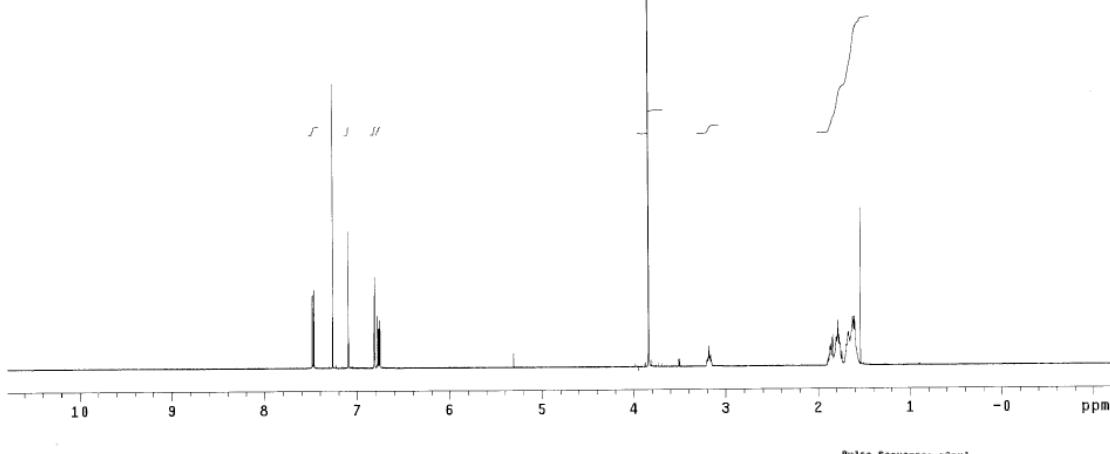


499.821 MHz HI 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm), temp 26.1 C -> actual temp = 27.0 C, autoxdb probe
Pulse Sequence: s2pul

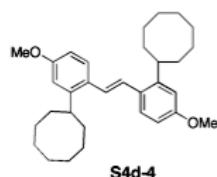
500 MHz, CDCl_3



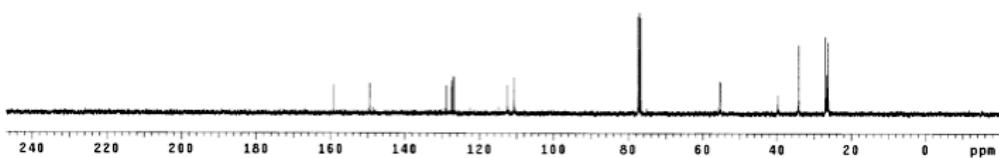
S4d-4



100.5 MHz,
 CDCl_3



S4d-4

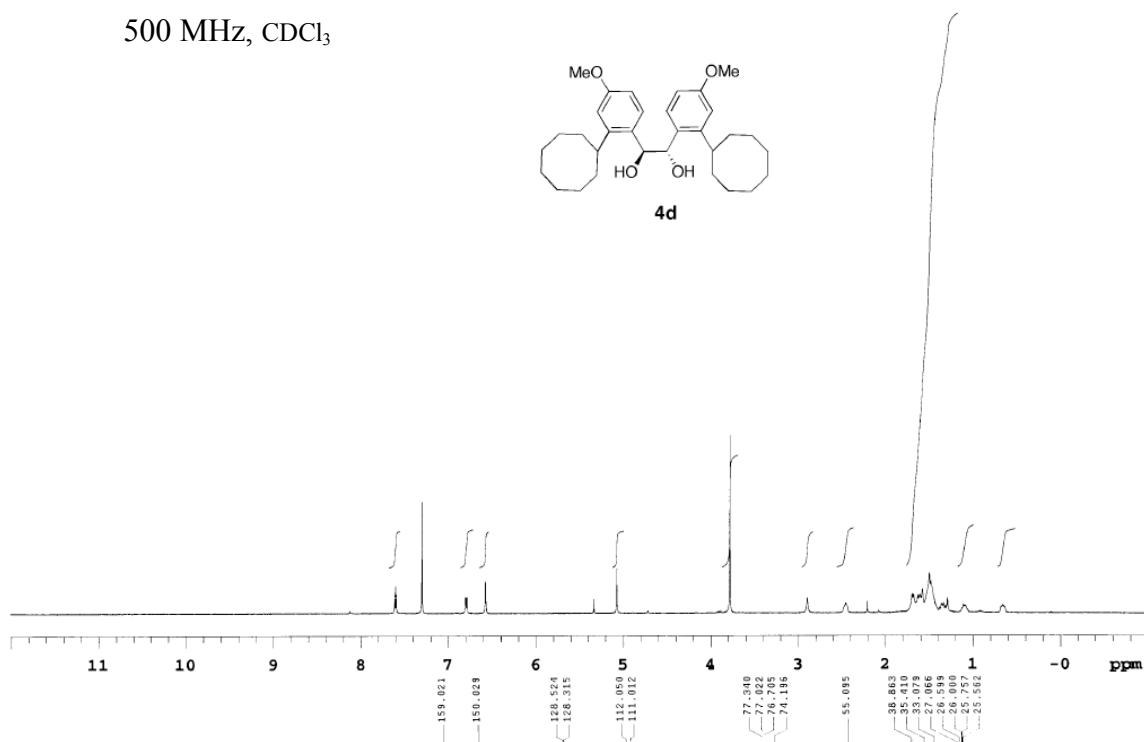
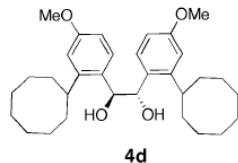


Vivek VRH-4-MeO-VIVOL
499.821 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm)
Temp 26.1 C -> actual temp = 27.0 C, autoddb probe

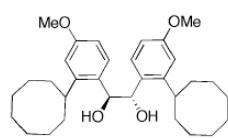
File: 2009.02.09.u5_VRH-4-MeO-VIVOL_H1_1D

Pulse Sequence: s2pul

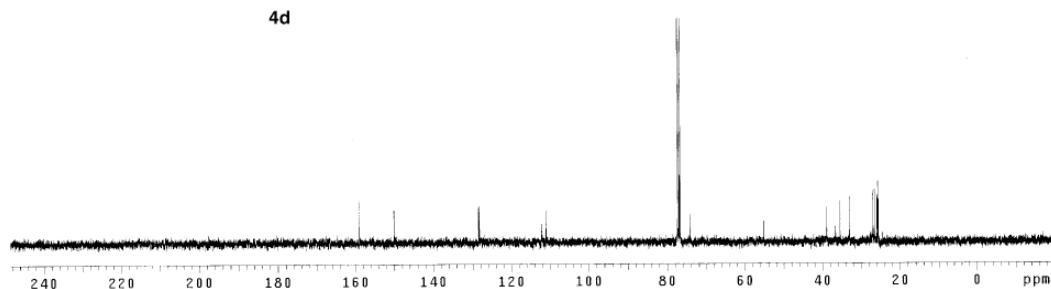
500 MHz, CDCl_3



100.5 MHz, CDCl_3



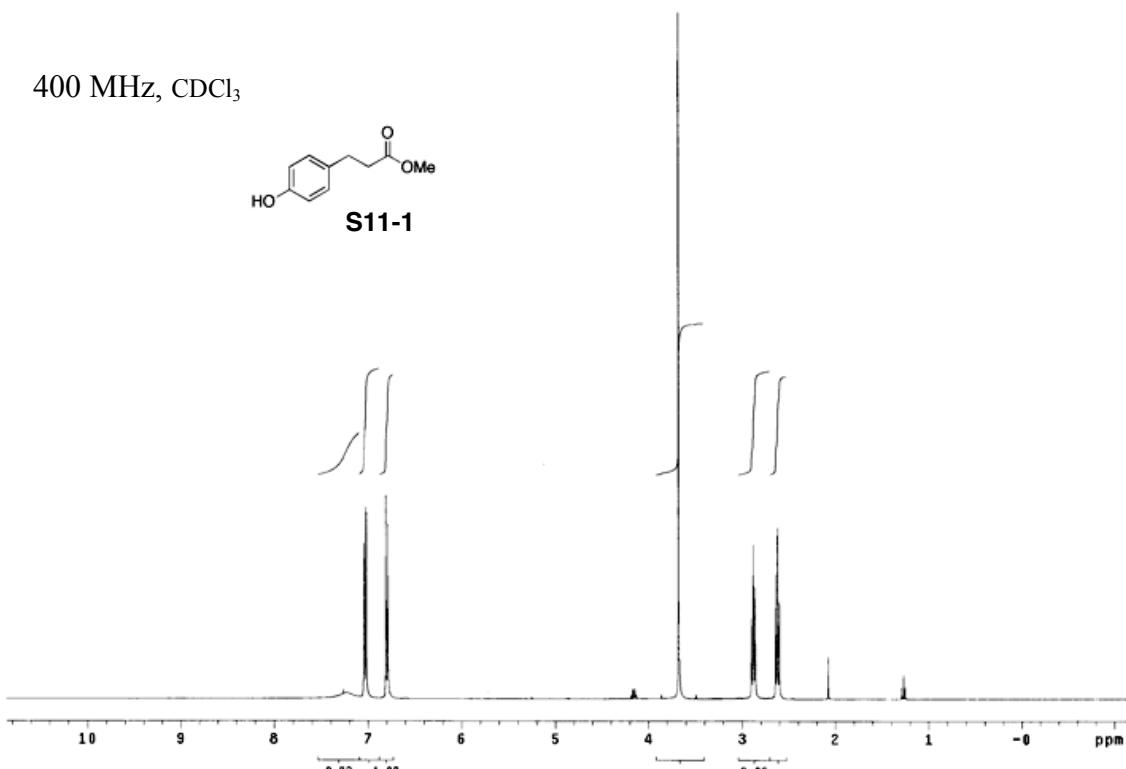
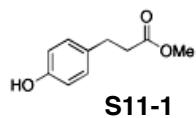
4d



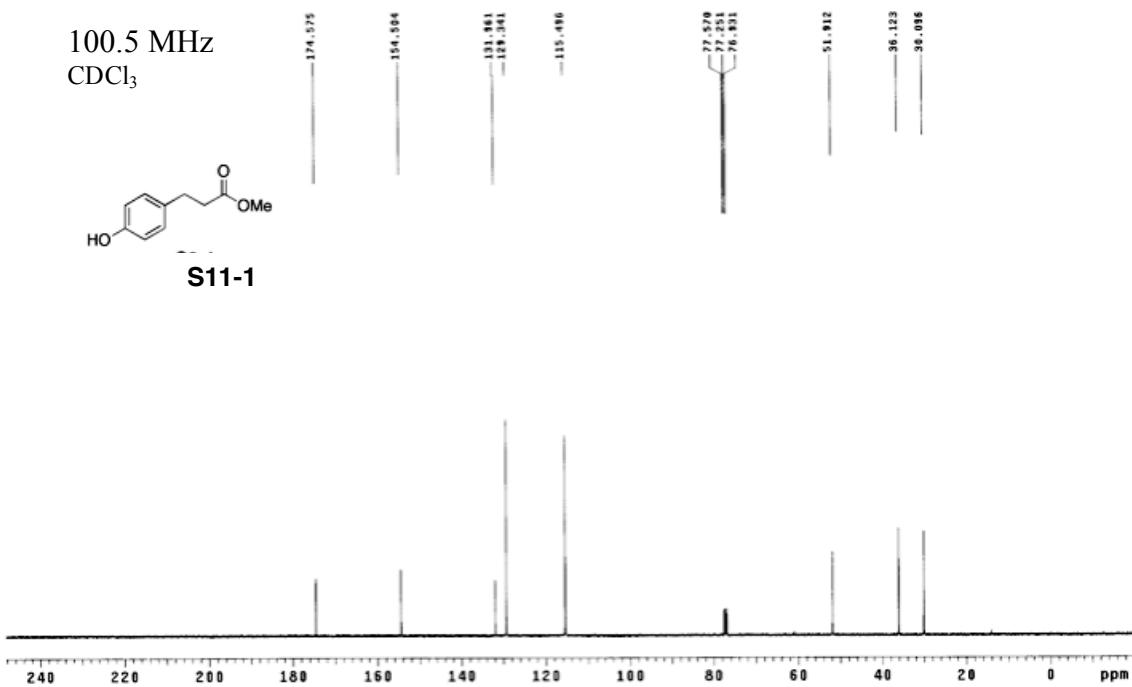
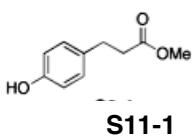
VRH-7-136A

Pulse Sequence: s2pul

400 MHz, CDCl₃

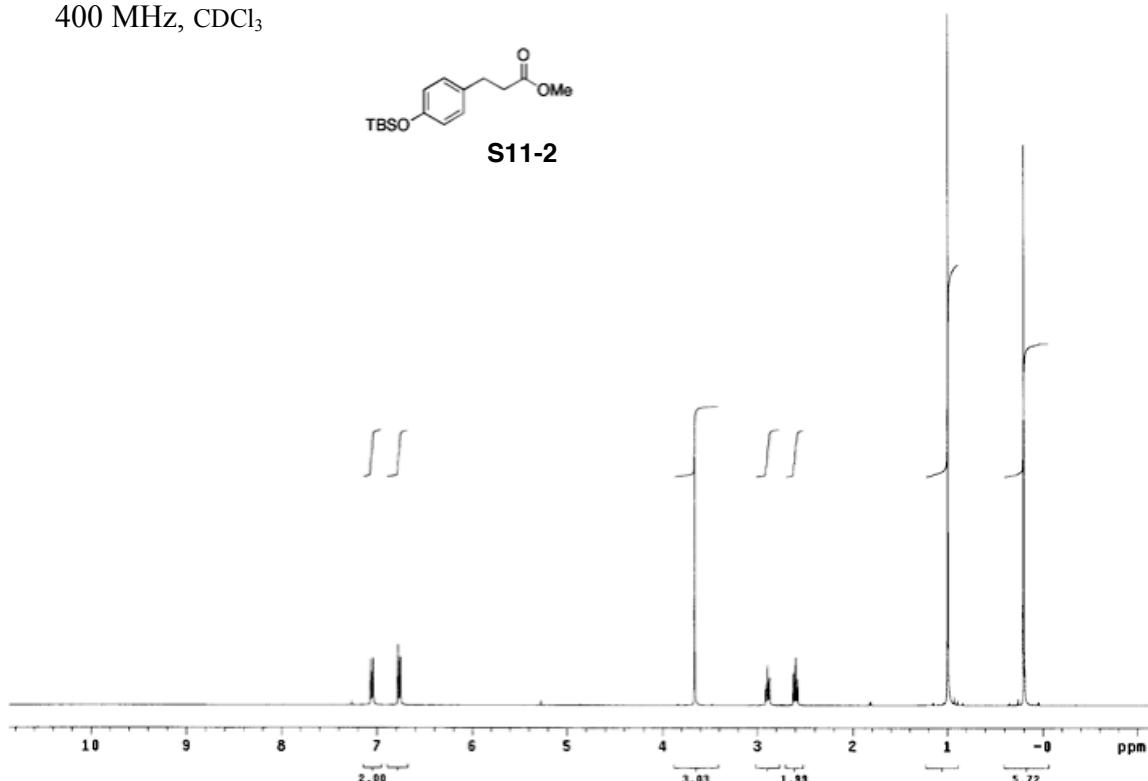
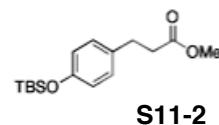


100.5 MHz
CDCl₃



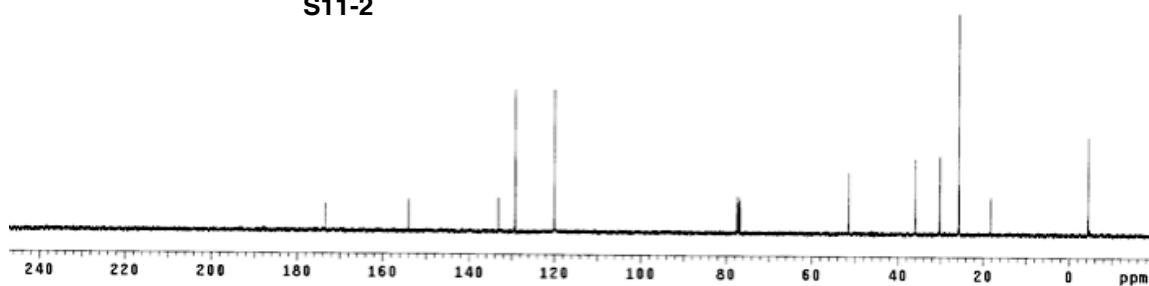
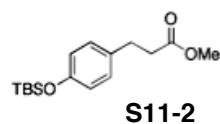
VRH-7-137A

Pulse Sequence: s2pul

400 MHz, CDCl₃

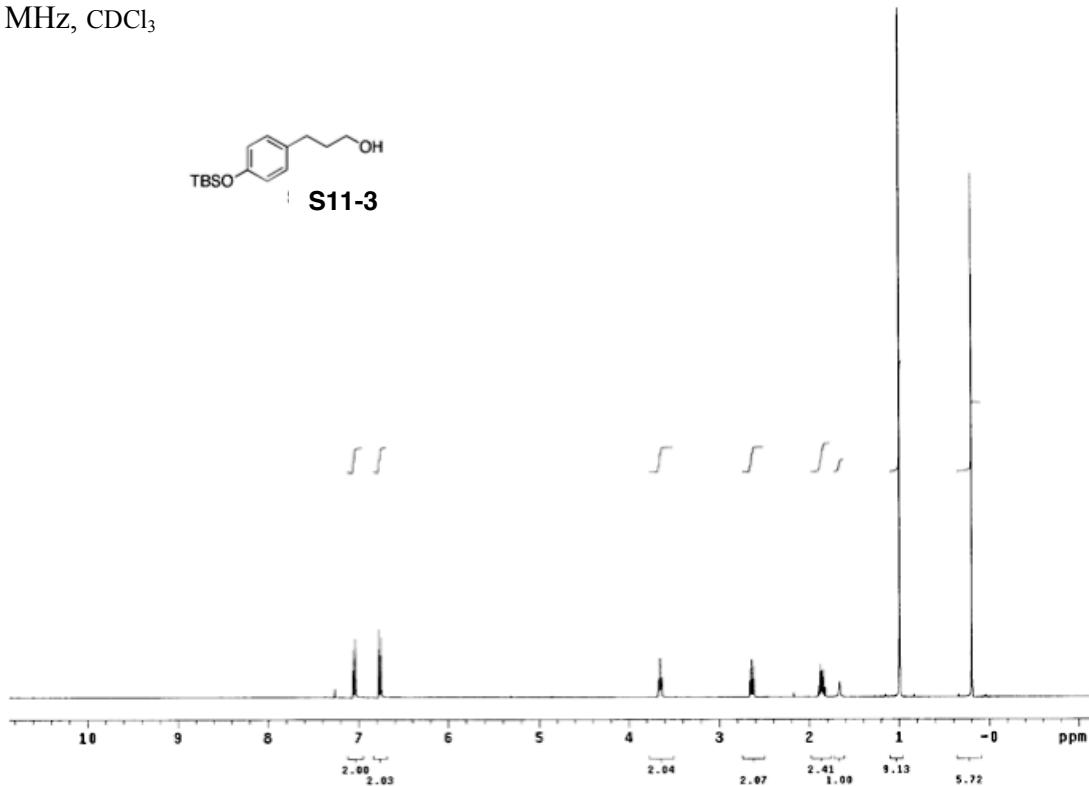
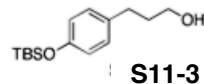
VRH-7-137A

Pulse Sequence: s2pul

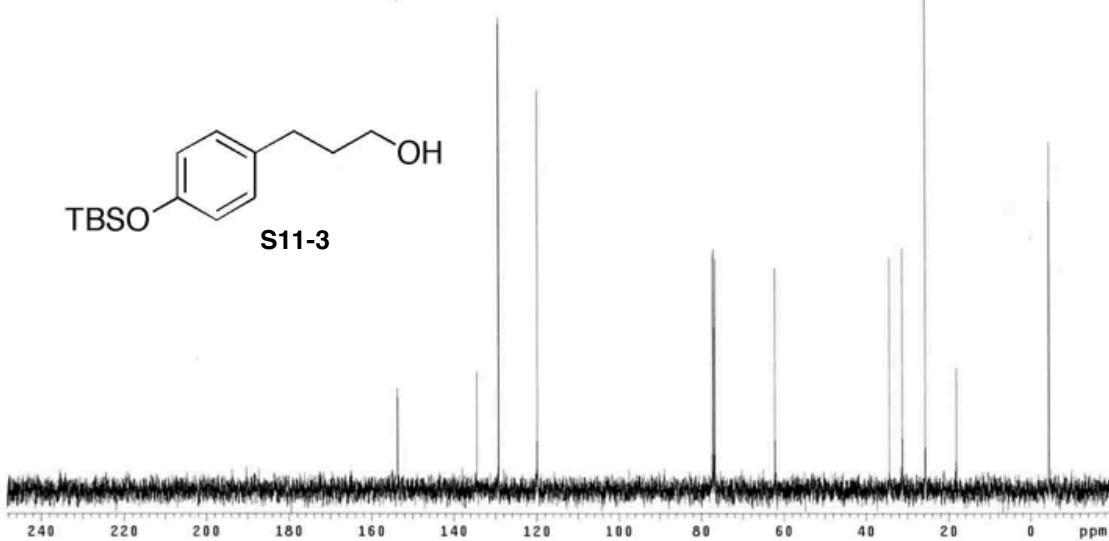
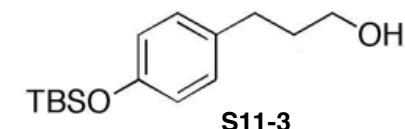
100.5 MHz,
CDCl₃

VRH-7-1378

Pulse Sequence: s2pul

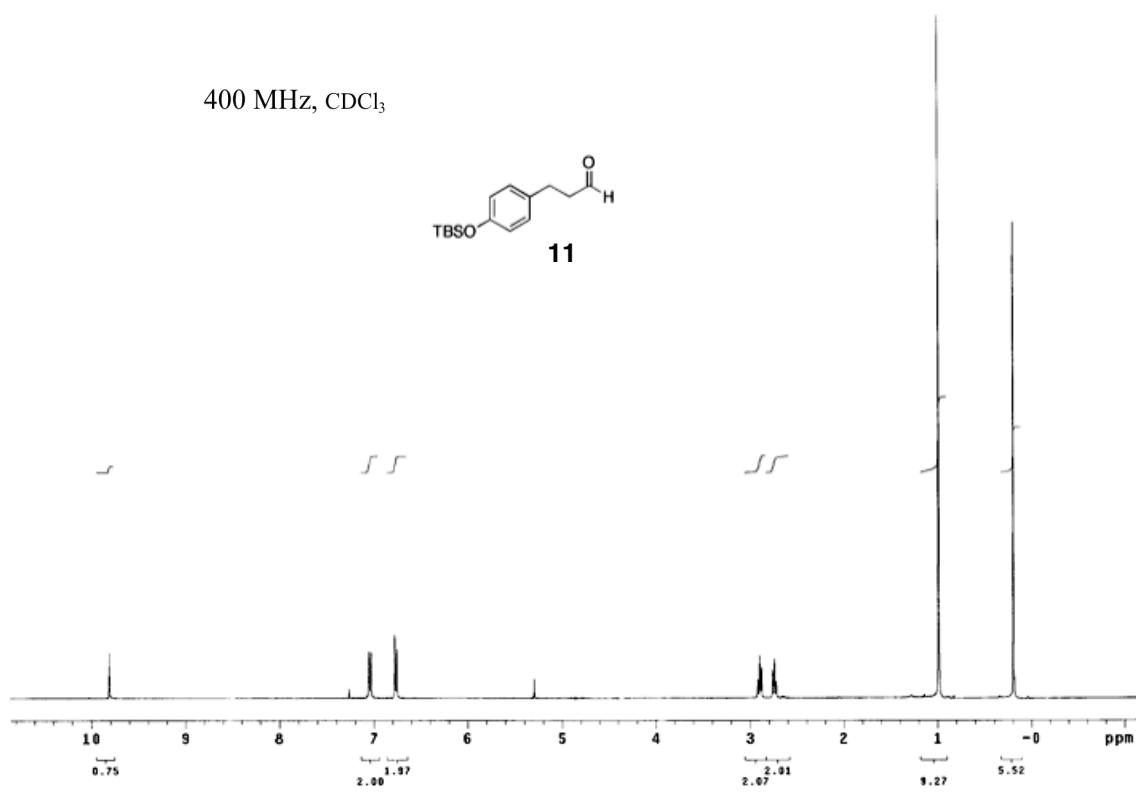
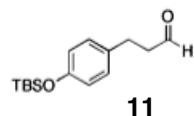
400 MHz, CDCl₃

VRH-7-1378

100.5 MHz, CDCl₃

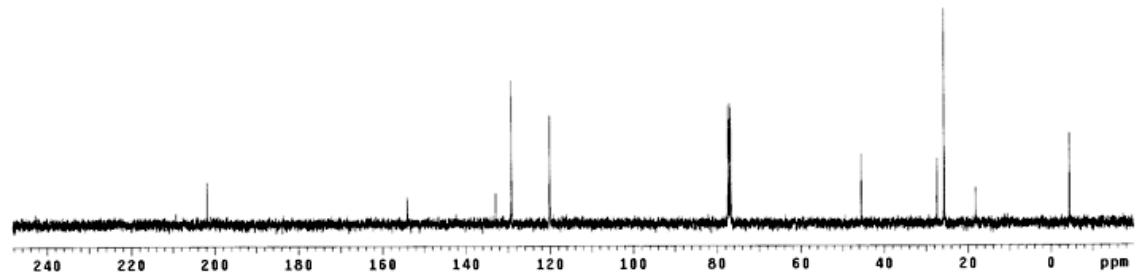
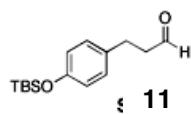
VRH-7-141A

Pulse Sequence: s2pul

400 MHz, CDCl₃

VRH-7-141A

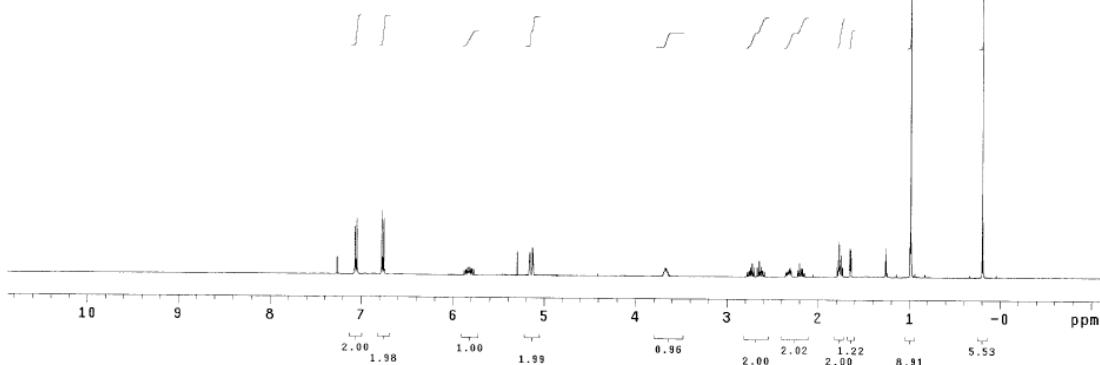
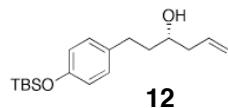
Pulse Sequence: s2pul

100.5 MHz, CDCl₃

VRH-7-141B

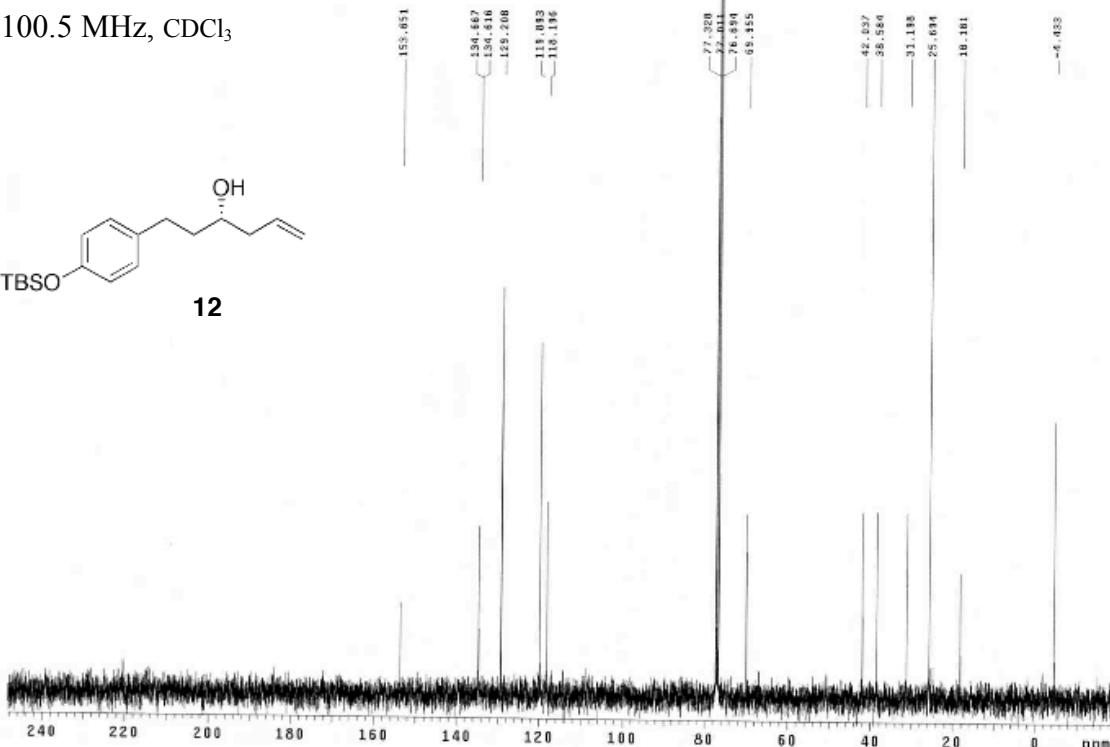
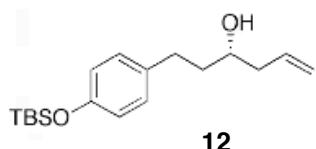
Pulse Sequence: s2pul

Solvent: CDCl_3
 Temp. 26.5 C / 299.6 K
 Operator: hellmr
 INOVA-400 "1400"
 Relax. delay 0.100 sec
 Pulse 45.0 degrees
 Acq. time 4.98 sec
 VNA 400.0 Hz
 16 repetitions
 OBSERVE H1, 399.7923305 MHz
 DATA PROCESSING
 FT size 131072
 Total time 1 min, 31 sec

400 MHz, CDCl_3 

100.537 MHz C^{13}H_1 1D in CDCl_3 [ref. to CDCl_3 at 77.06 ppm], Temp 26.5 C \rightarrow actual temp = 27.0 C, autoxdb probe

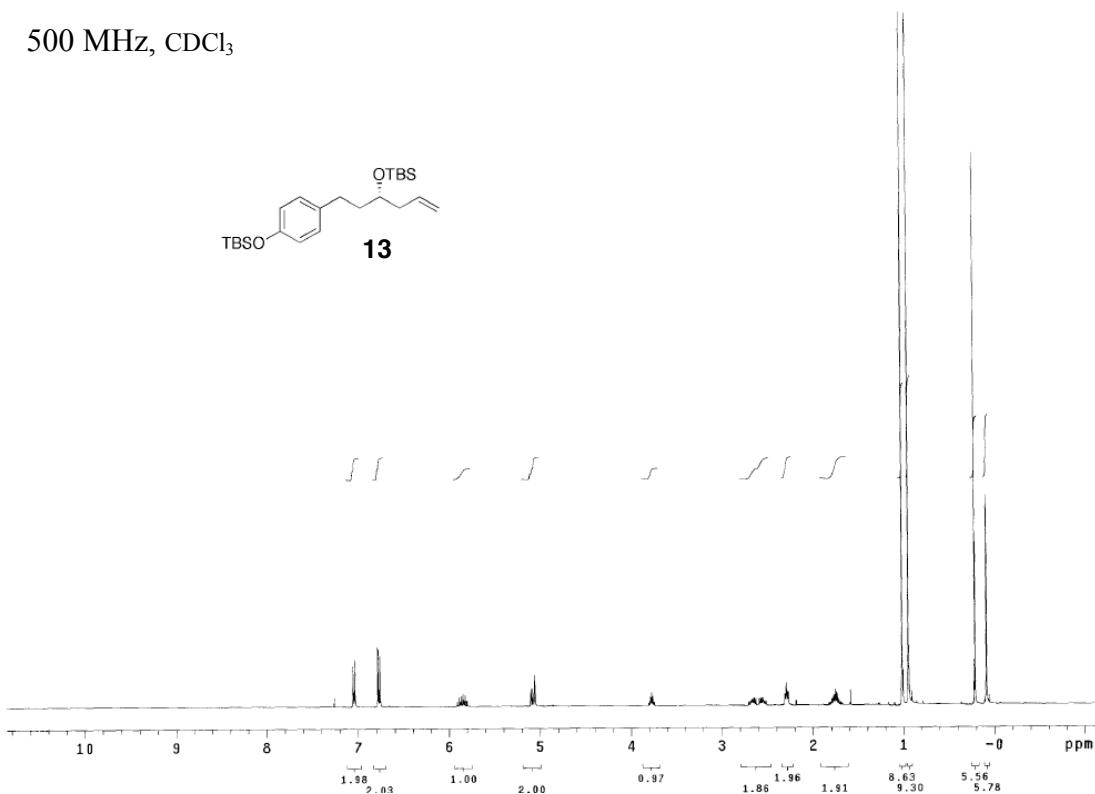
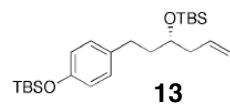
Pulse Sequence: s2pul

100.5 MHz, CDCl_3 

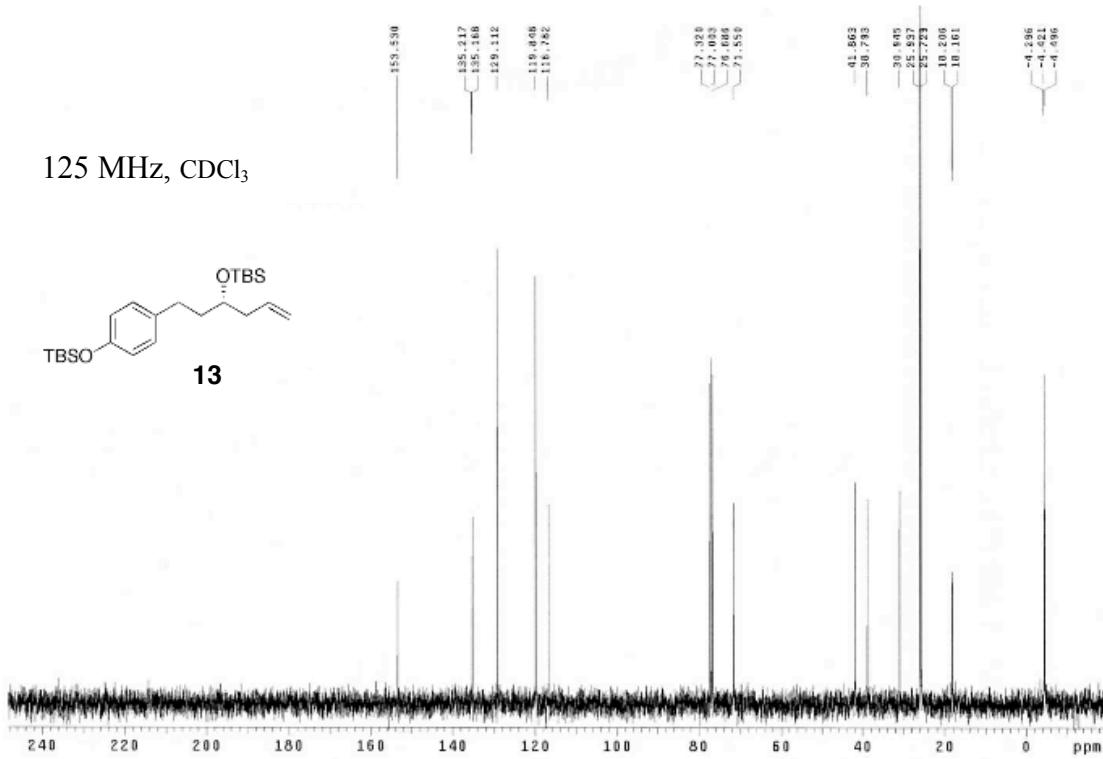
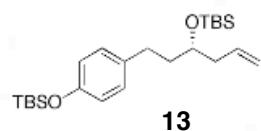
Pulse Sequence: s2pul

VRH-7-142

500 MHz, CDCl₃



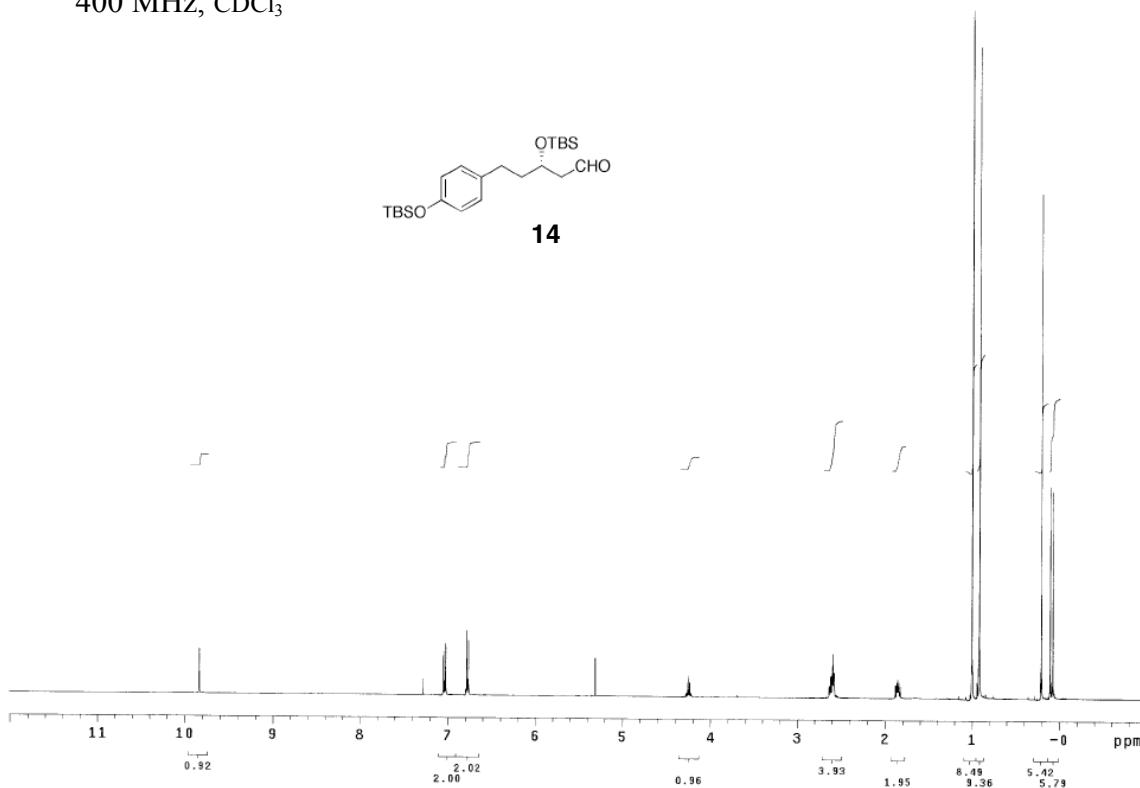
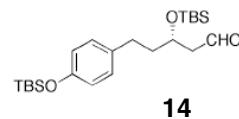
125 MHz, CDCl₃



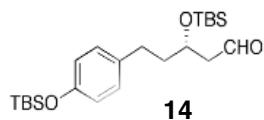
VRH-7-143C-after-flash

Pulse Sequence: s2pul

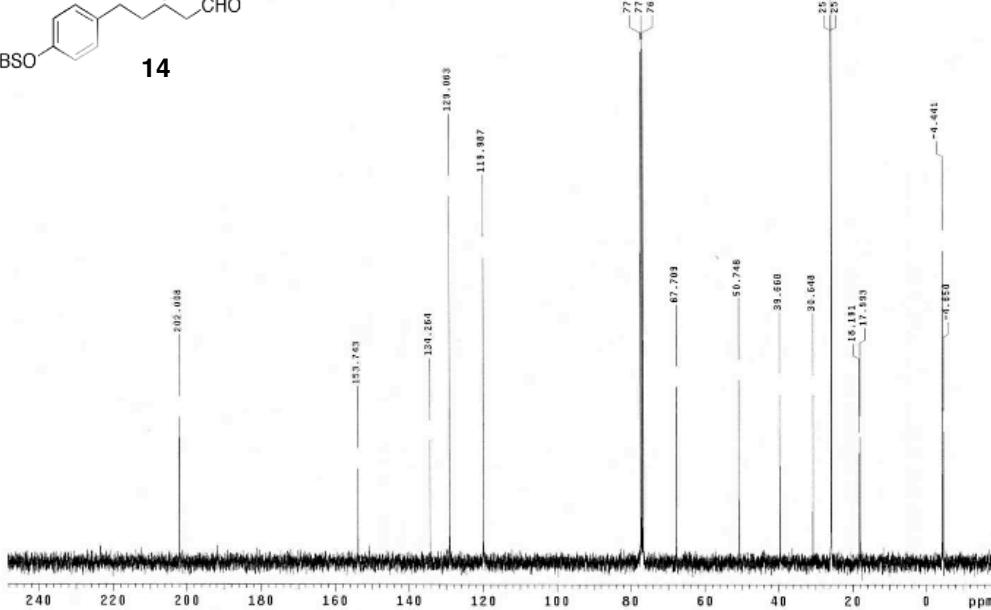
400 MHz, CDCl₃



125 MHz, CDCl₃

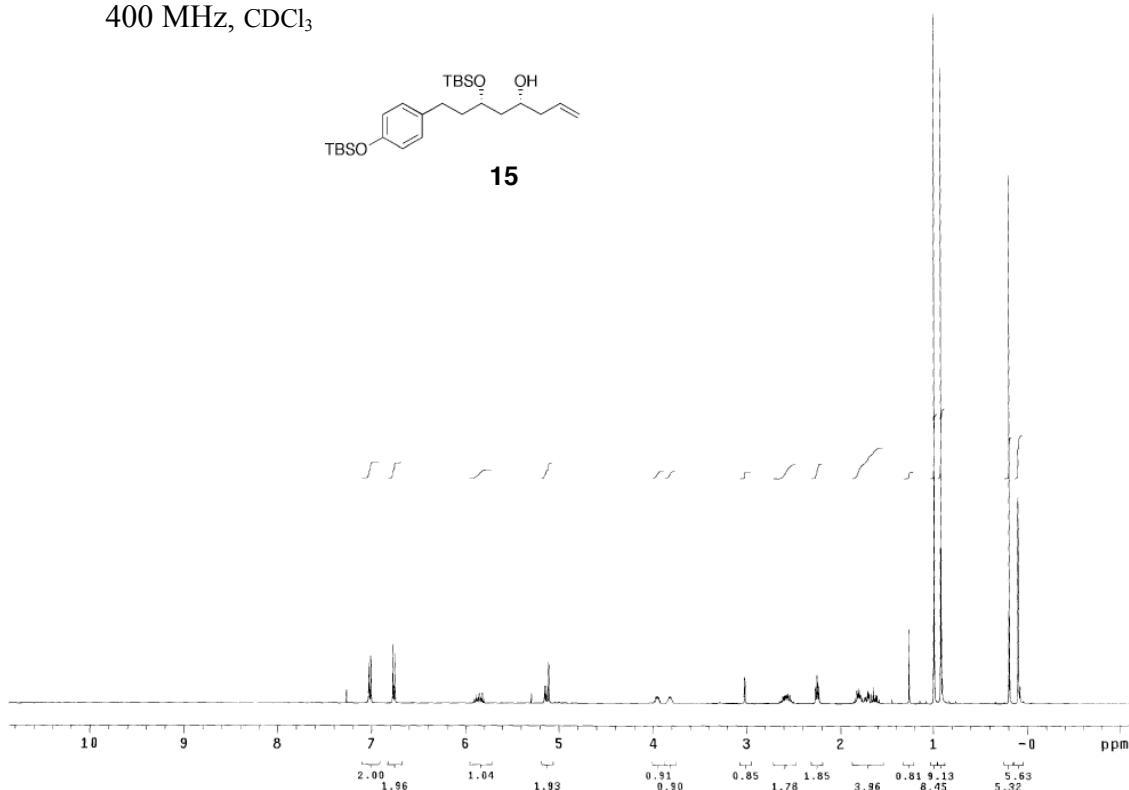
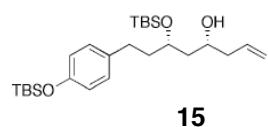


Pulse Sequence: s2pul

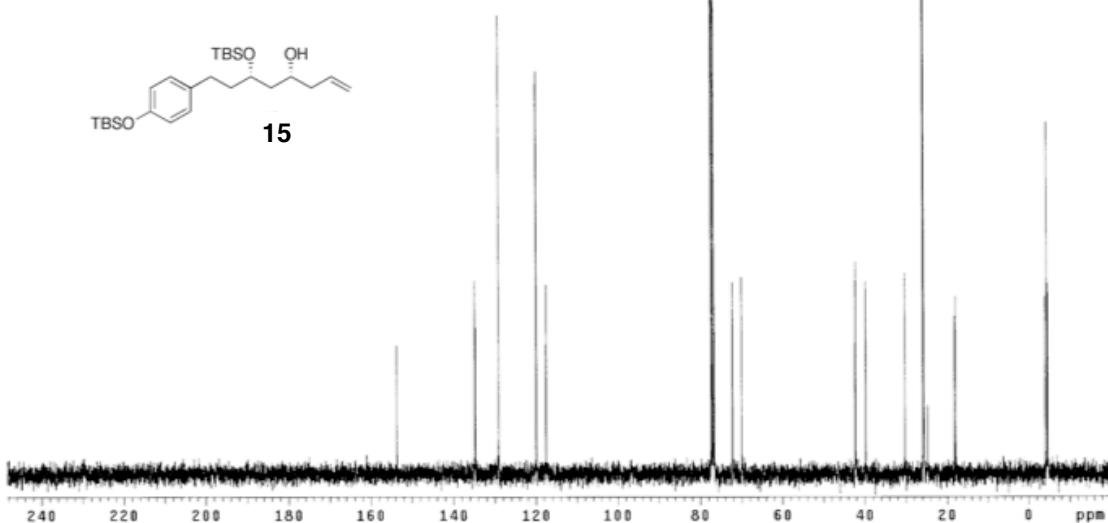
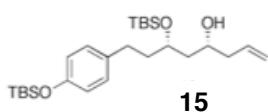


VRH-7-145

Pulse Sequence: s2pul

400 MHz, CDCl₃

Pulse Sequence: s2pul

125 MHz, CDCl₃

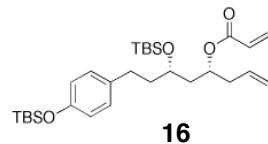
VRH-7-148

Pulse Sequence: s2pul

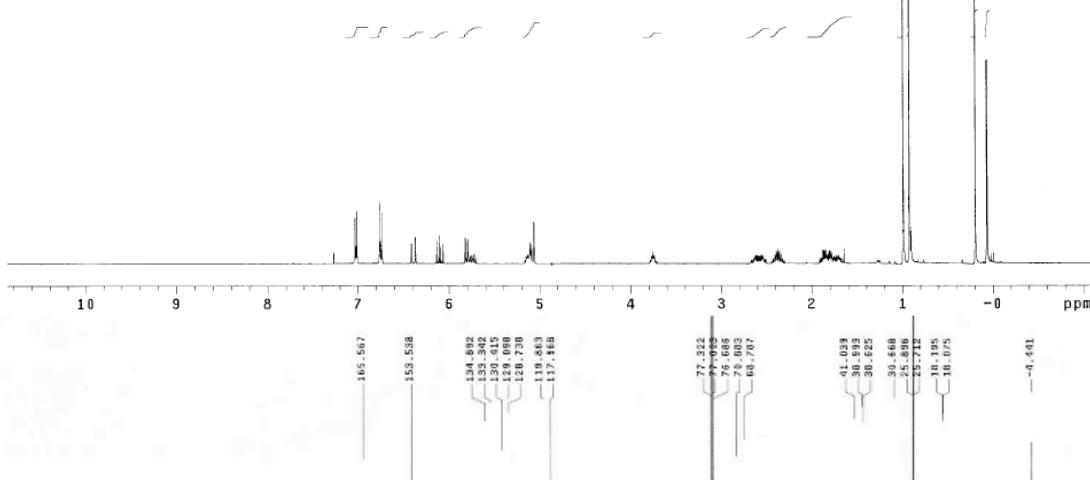
Solvent: *cdcl*3
Temp: 26.5 C / 299.6 K
Operator: hal1
INNOVA-400 "1400"

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 4.998 sec
Width 480.0 Hz
16 repetitions
OBSERVE H1, 399.7923305 MHz
DATA PROCESSING
FT size 131072
Total time 1 min, 31 sec

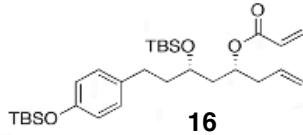
400 MHz, *CDCl*3



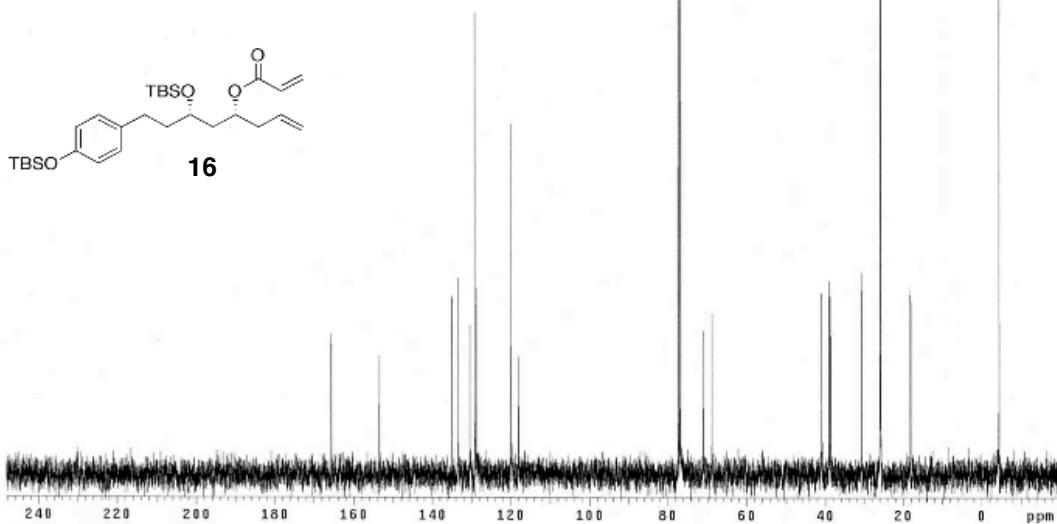
16

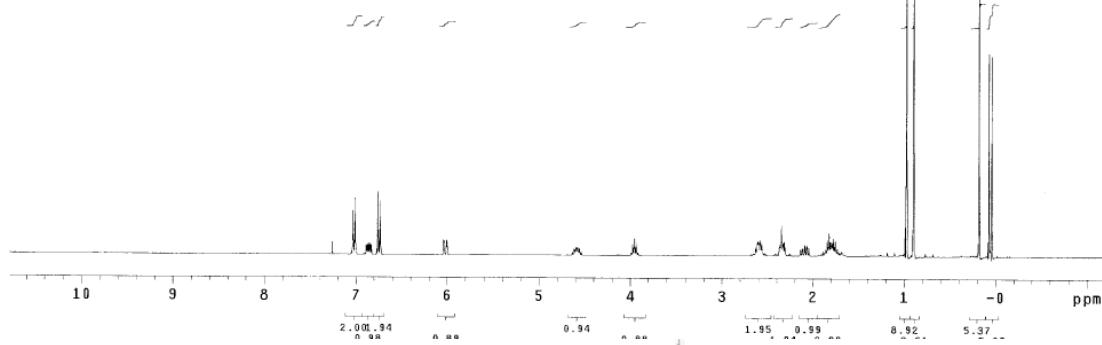
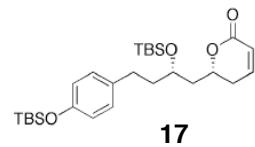
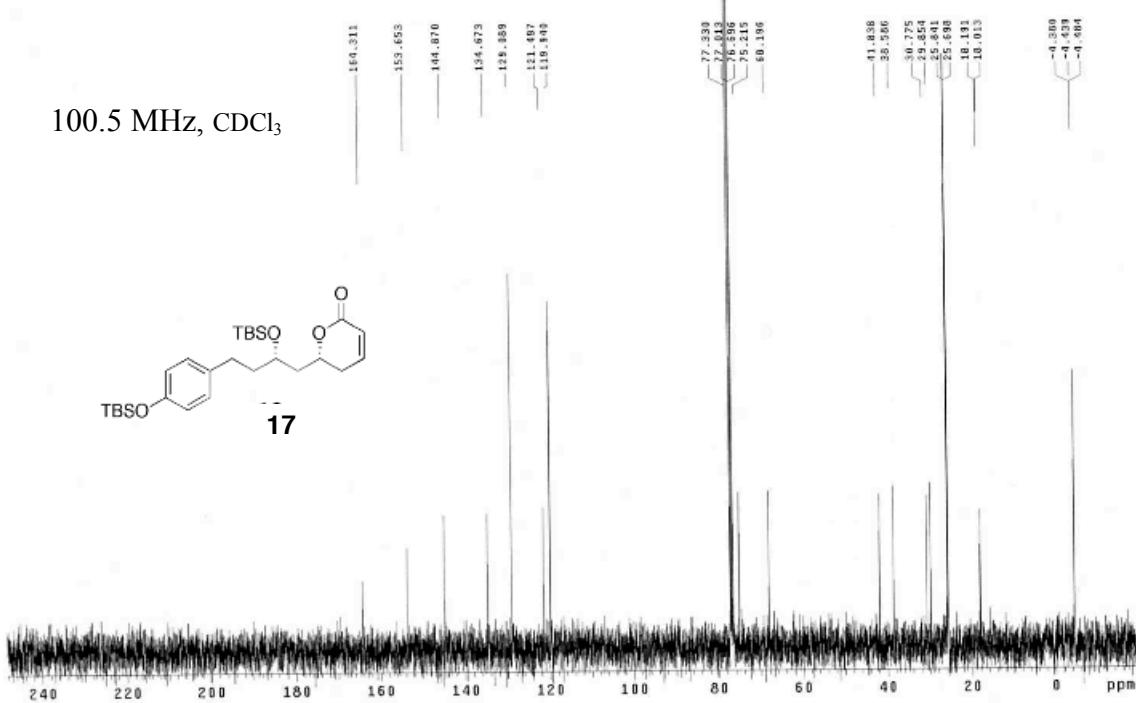
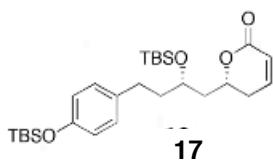


125 MHz, *CDCl*3



16

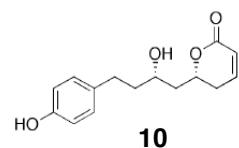


400 MHz, CDCl₃100.5 MHz, CDCl₃

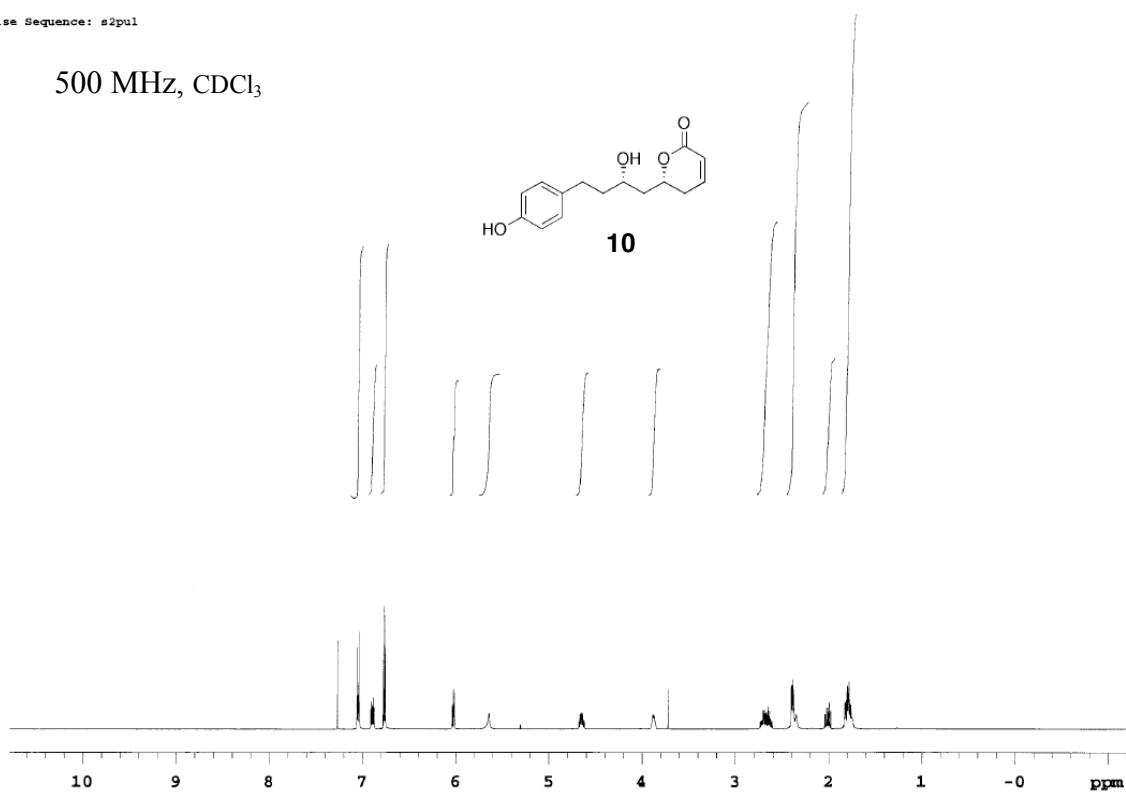
499.821 MHz H1 1D in cdcl3 (ref. to CDCl3 @ 7.26 ppm), temp 26.1 C -> actual temp = 27.0 C, autoxdp probe

Pulse Sequence: s2pul

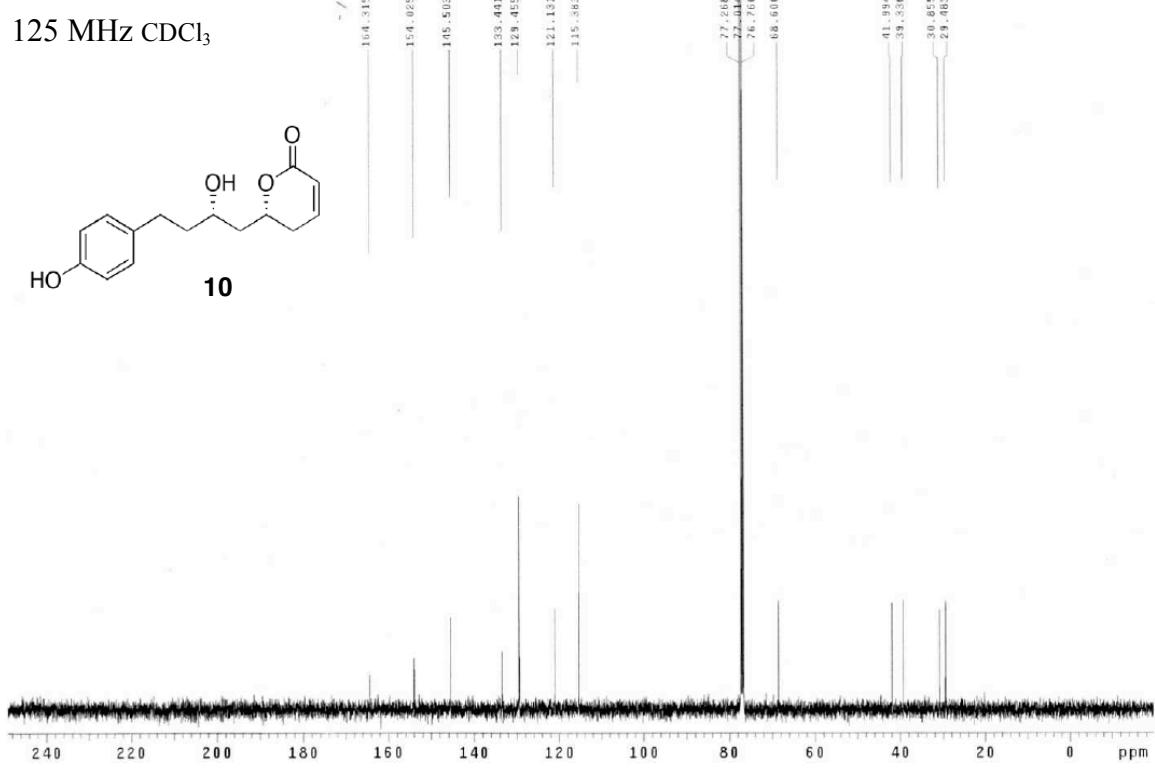
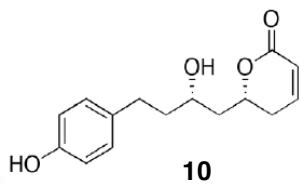
500 MHz, CDCl₃



10



125 MHz CDCl₃



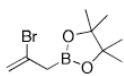
VRH-7-155-after-distillation

Pulse Sequence: s2pul

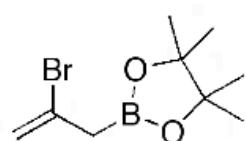
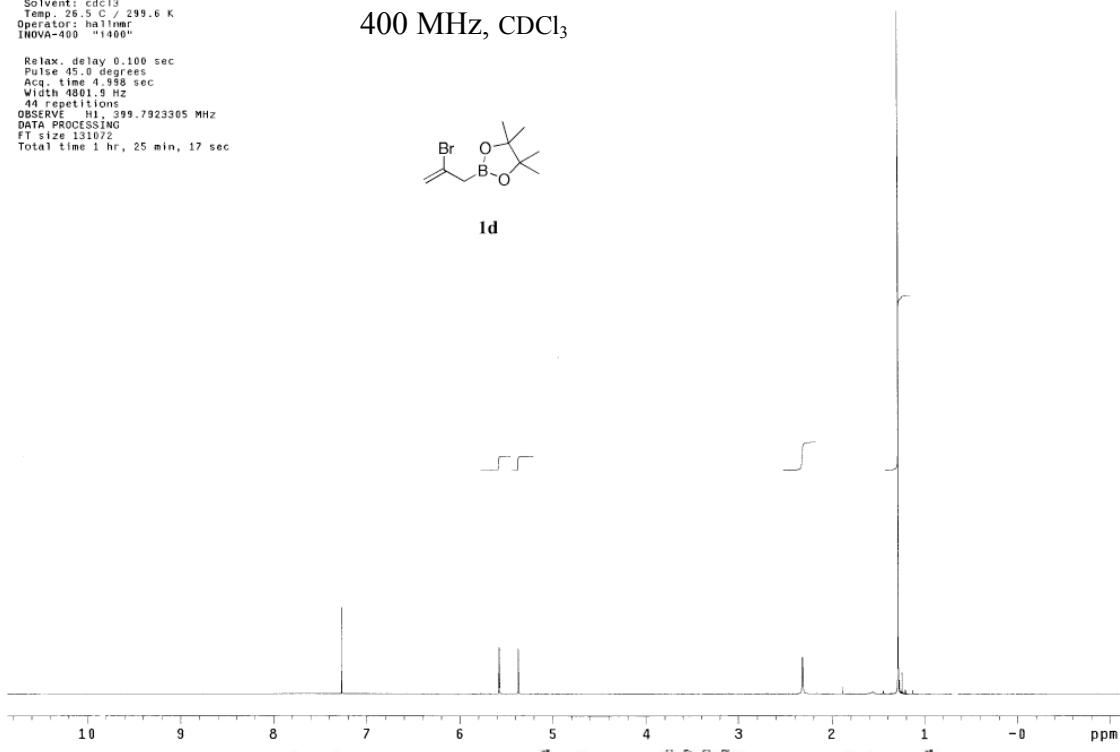
Solvent: CDCl₃
Temp.: 23.0 °C / 299.6 K
Operator: hallmar
INNOVA-400 "1400"

Relax. delay 0.100 sec
Pulse 15.0 degrees
Acc. time 0.006 sec
Width 4801.5 Hz
44 repetitions
OBSERVE: H1 399.7923305 MHz
DATA PROCESSING
FT size 131072
Total time 1 hr, 25 min, 17 sec

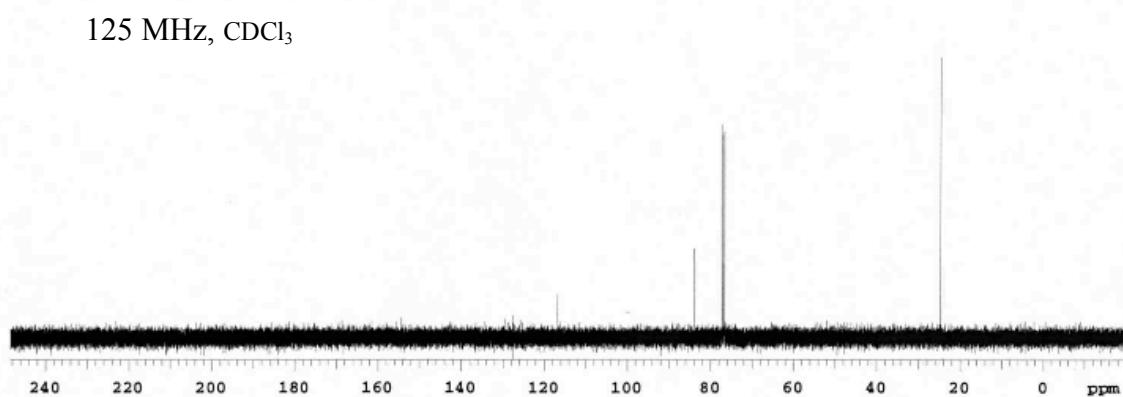
400 MHz, CDCl₃

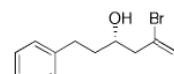
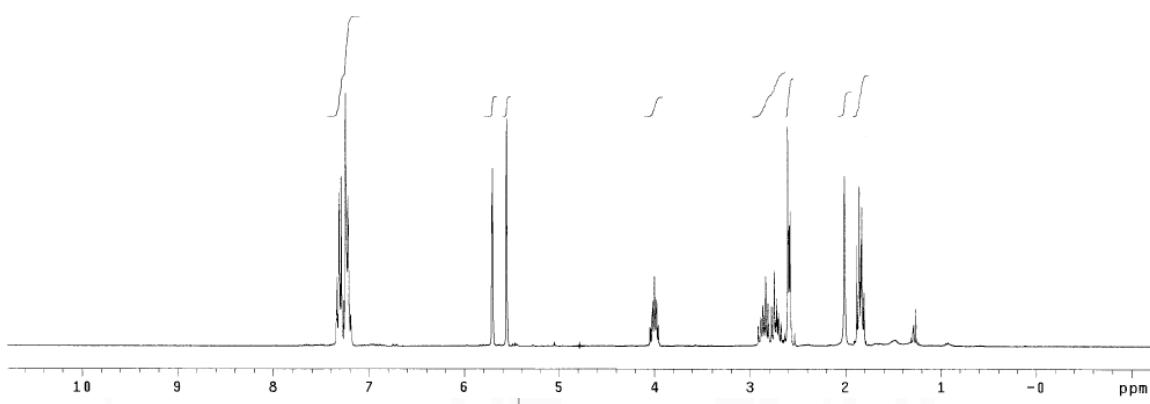
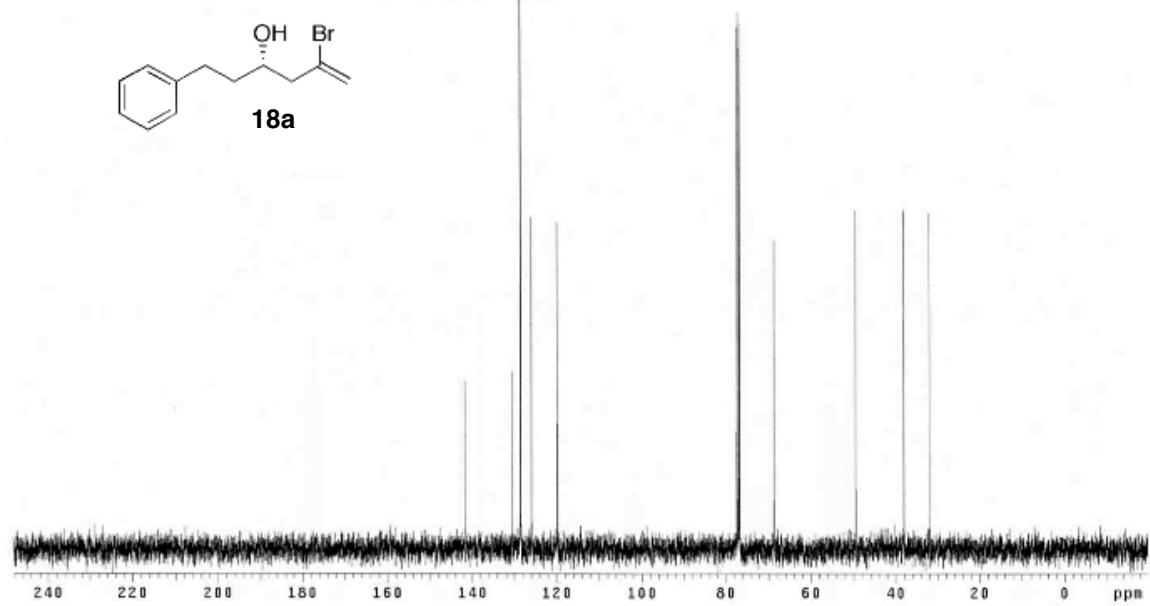
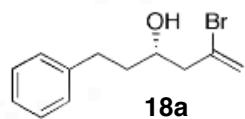


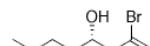
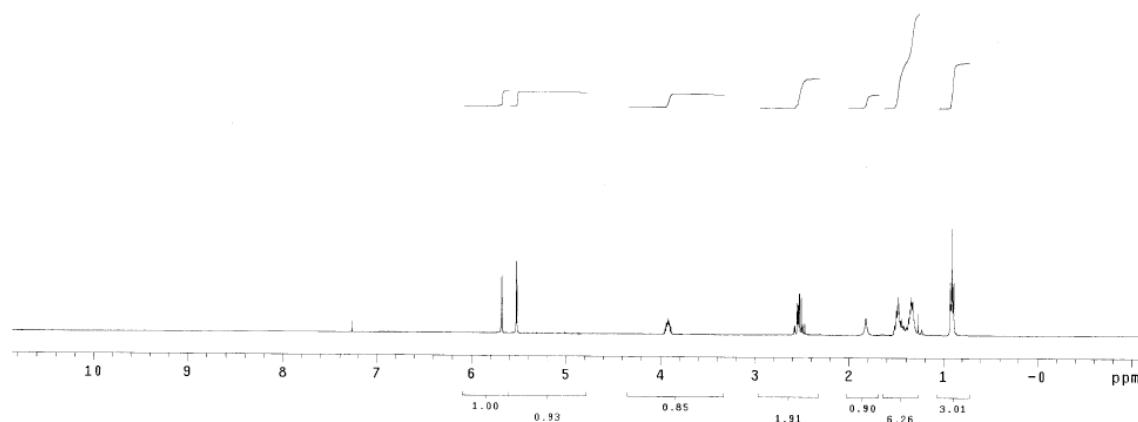
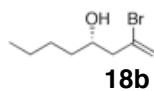
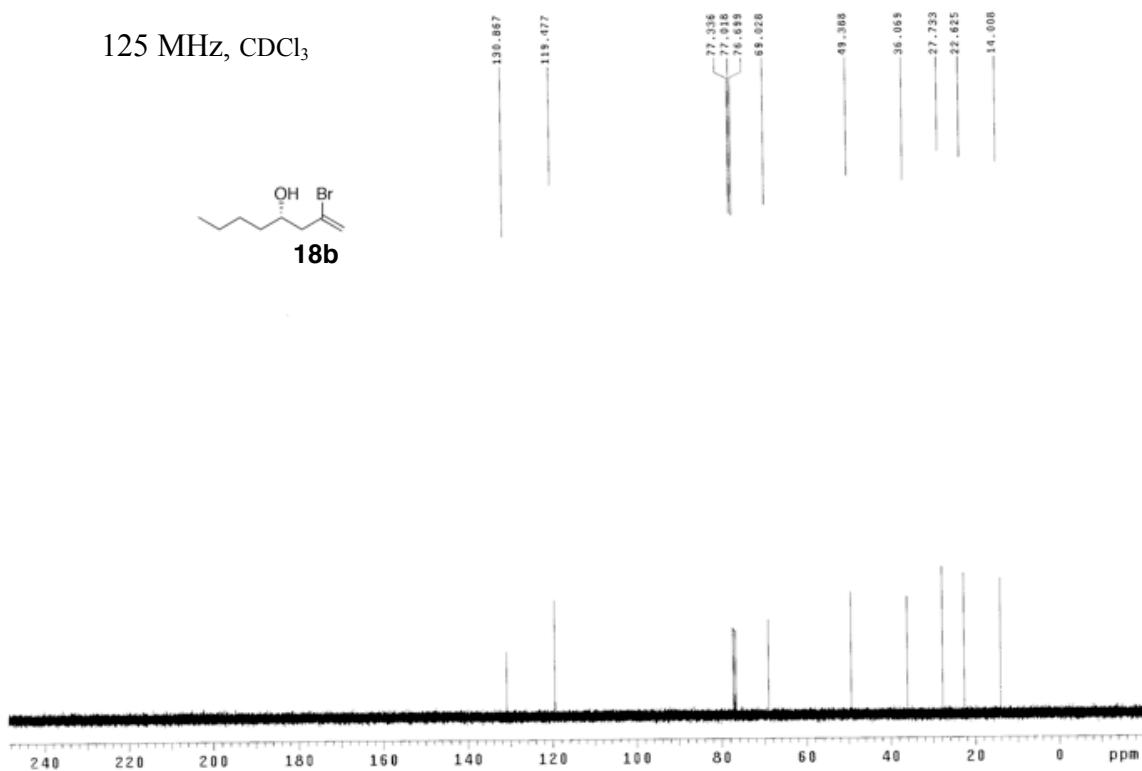
1d



1d

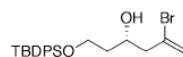


400 MHz, CDCl₃**18a**125 MHz, CDCl₃

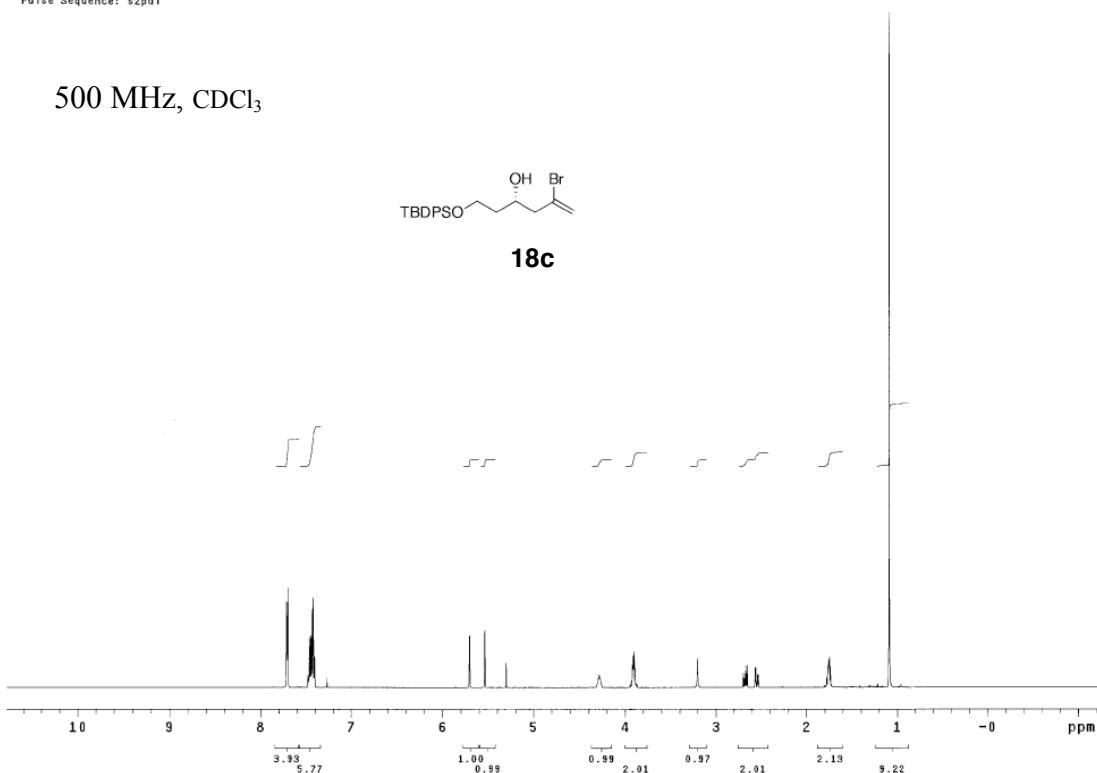
400 MHz, CDCl₃**18b**125 MHz, CDCl₃**18b**

499.821 MHz H1 1D in CDCl_3 (ref. to CDCl_3 @ 7.26 ppm), temp 26.1 C \rightarrow actual temp = 27.0 C, autoxdp probe
Pulse Sequence: s2put

500 MHz, CDCl_3

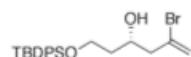


18c

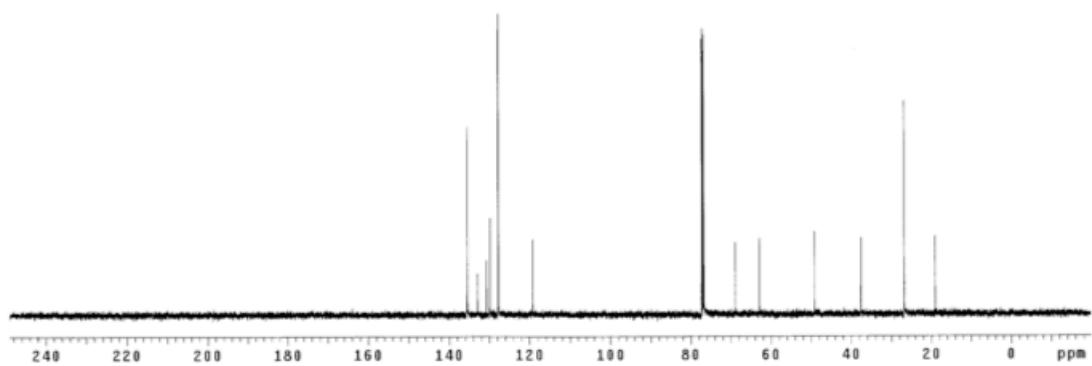
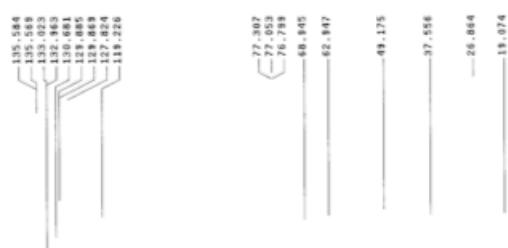


125.691 MHz C13[H1] 1D in CDCl_3 (ref. to CDCl_3 @ 77.06 ppm), temp 26.1 C \rightarrow actual temp = 27.8 C, autoxdp probe
Pulse Sequence: s2put

125 MHz, CDCl_3

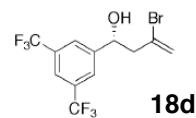


18c

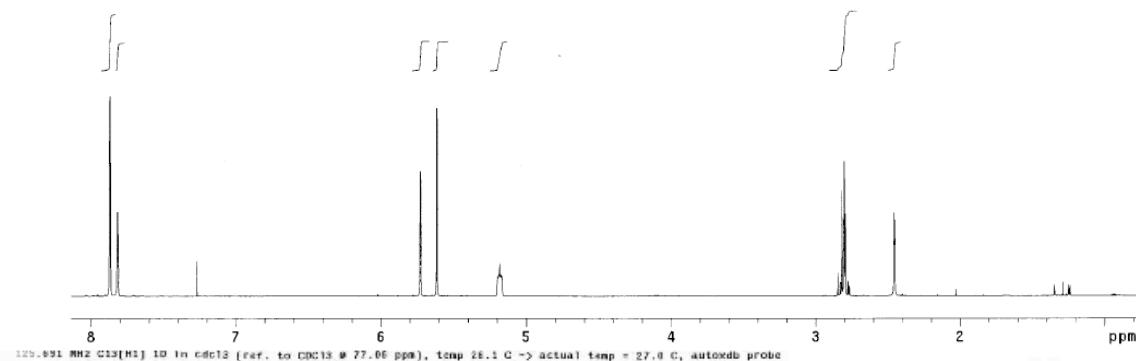


VRH-8-95A-1H
Pulse Sequence: s2pul

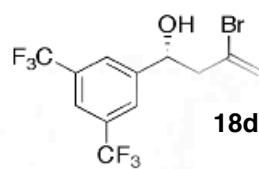
500 MHz, CDCl₃



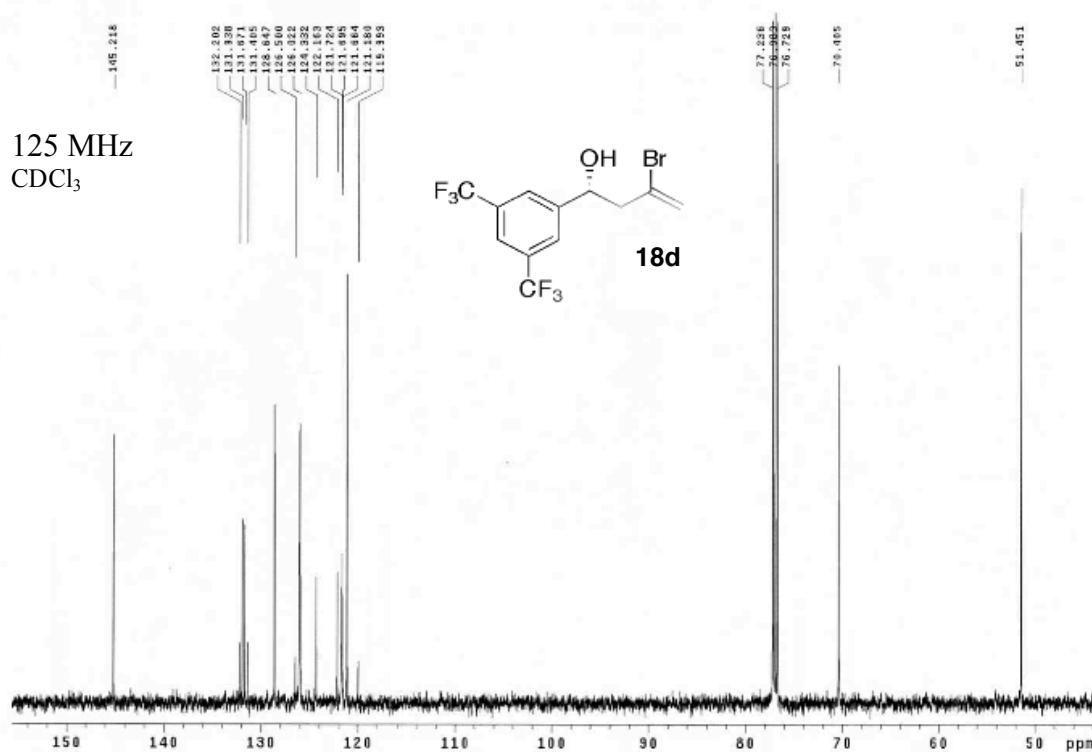
18d



125 MHz
CDCl₃



18d

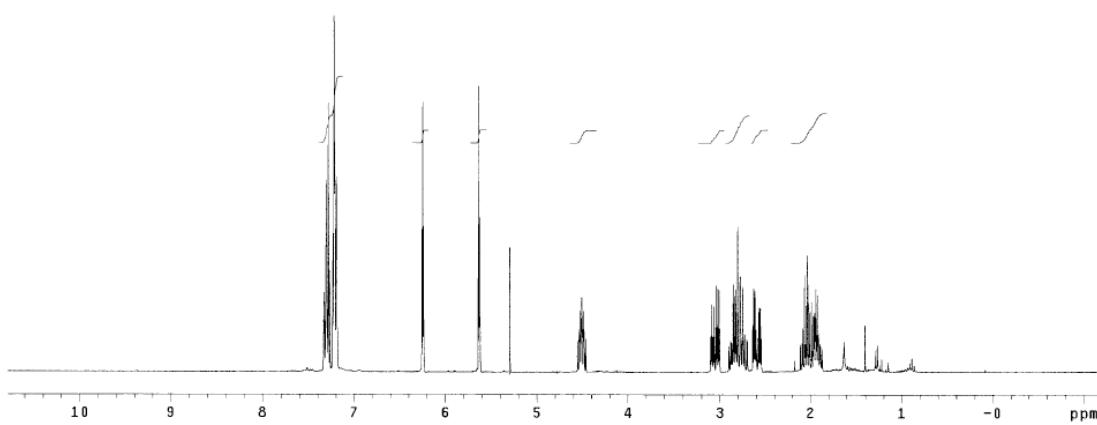
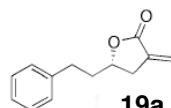
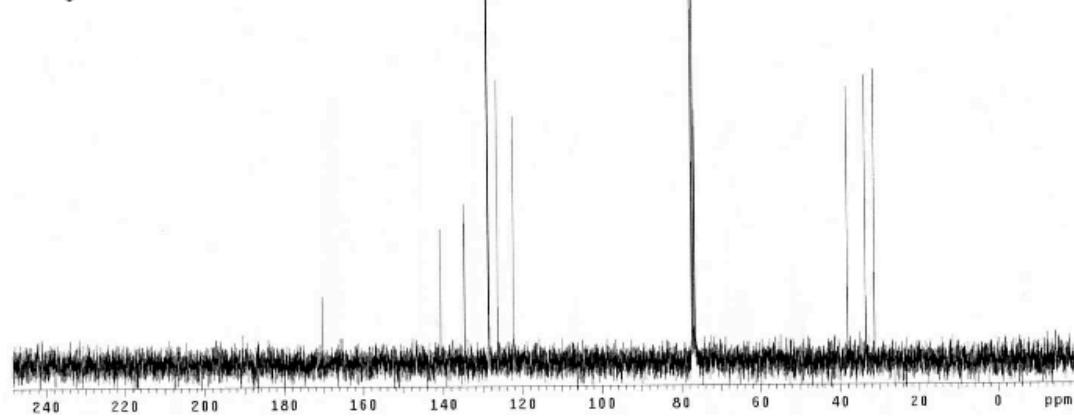
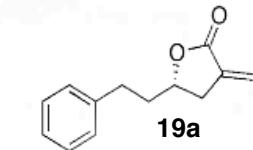


VRH-7-162

Pulse Sequence: s2pul

Solvent: *cdcl*3
 Temp: 27.5 °C / 300.6 K
 Operator: vrlm11mr
 File: vrh-7-162
 INOVA-400 "1400"

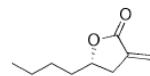
Relax delay 0.100 sec
 Pulse 90.4 degrees
 Acq. time 4.00 sec
 Width 3600.7 Hz
 28 repetitions
 OBSERVE FREQ 299.9696605 MHz
 DATA PROCESSING
 Gauss Window 0.500 sec
 center at 0.400 sec
 FT size 131072
 Total time 1 hr, 25 min, 18 sec

400 MHz, *CDCl*₃125 MHz, *CDCl*₃

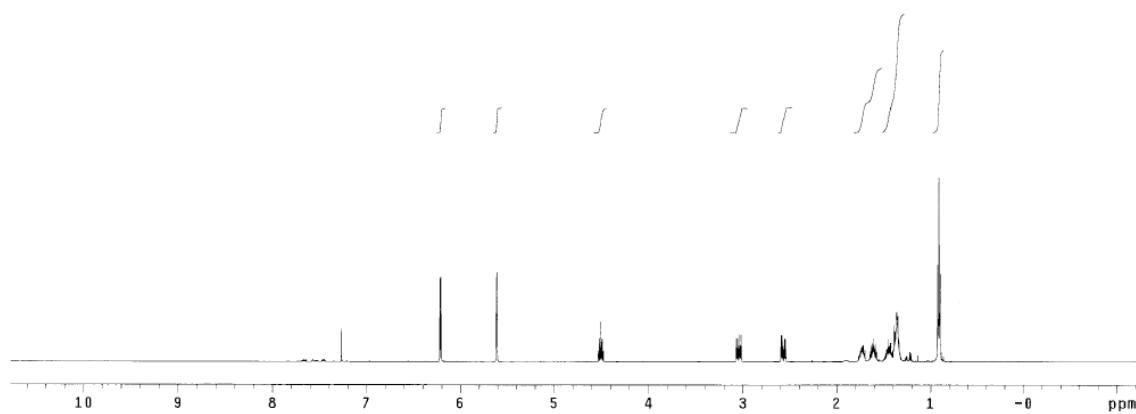
VRH-7-165

Pulse Sequence: s2pul

300 MHz, CDCl₃



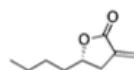
19b



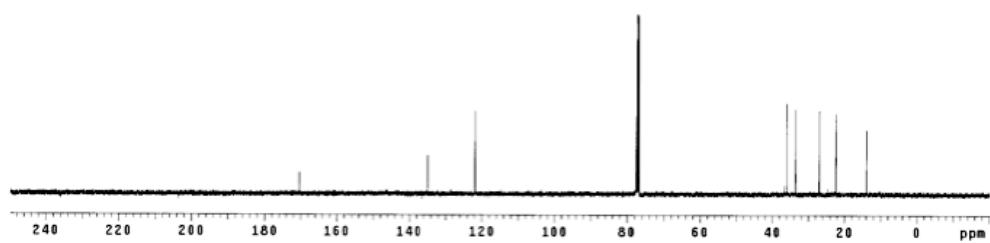
VRH-7-165

Pulse Sequence: s2pul

125 MHz, CDCl₃



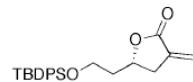
19b



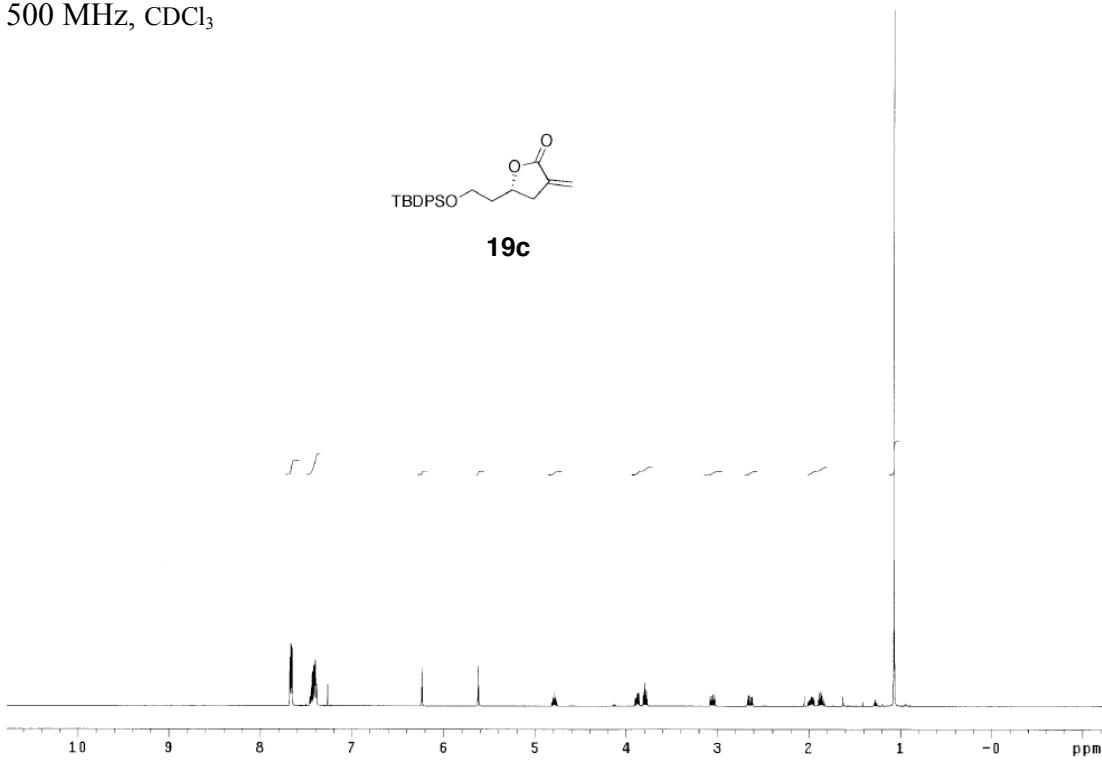
VRH-8-103A

Pulse Sequence: s2pul

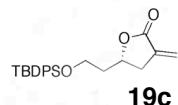
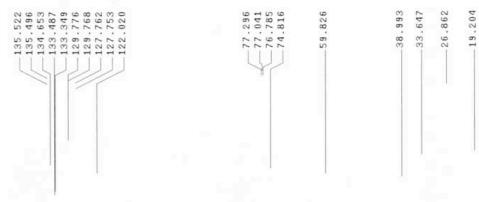
500 MHz, CDCl₃



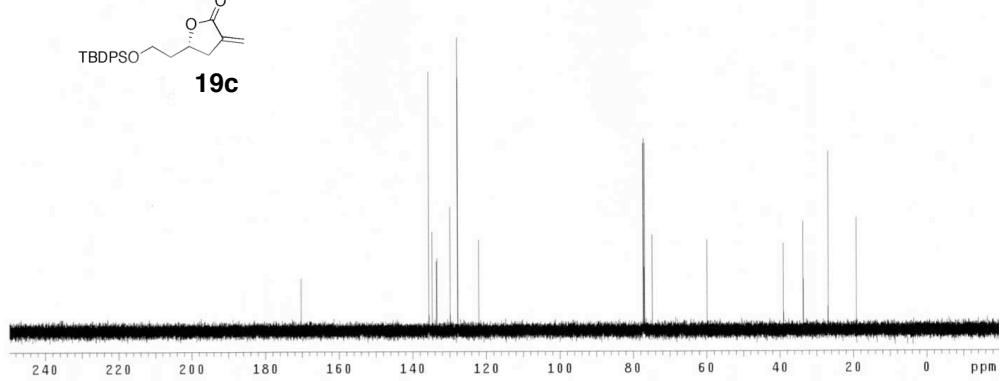
19c

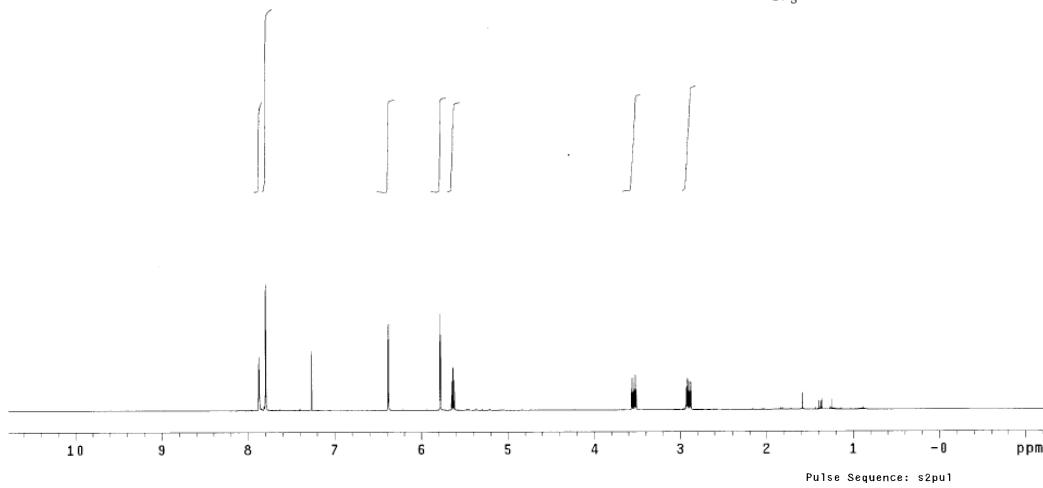
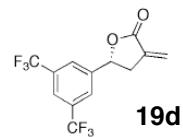
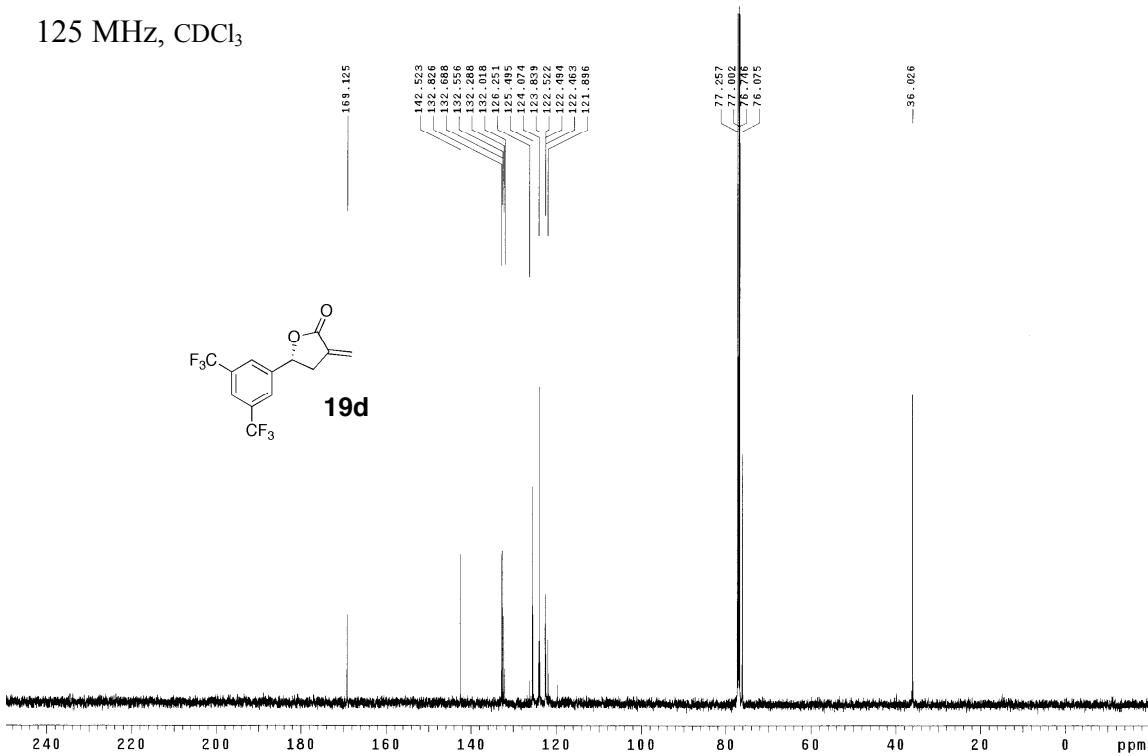


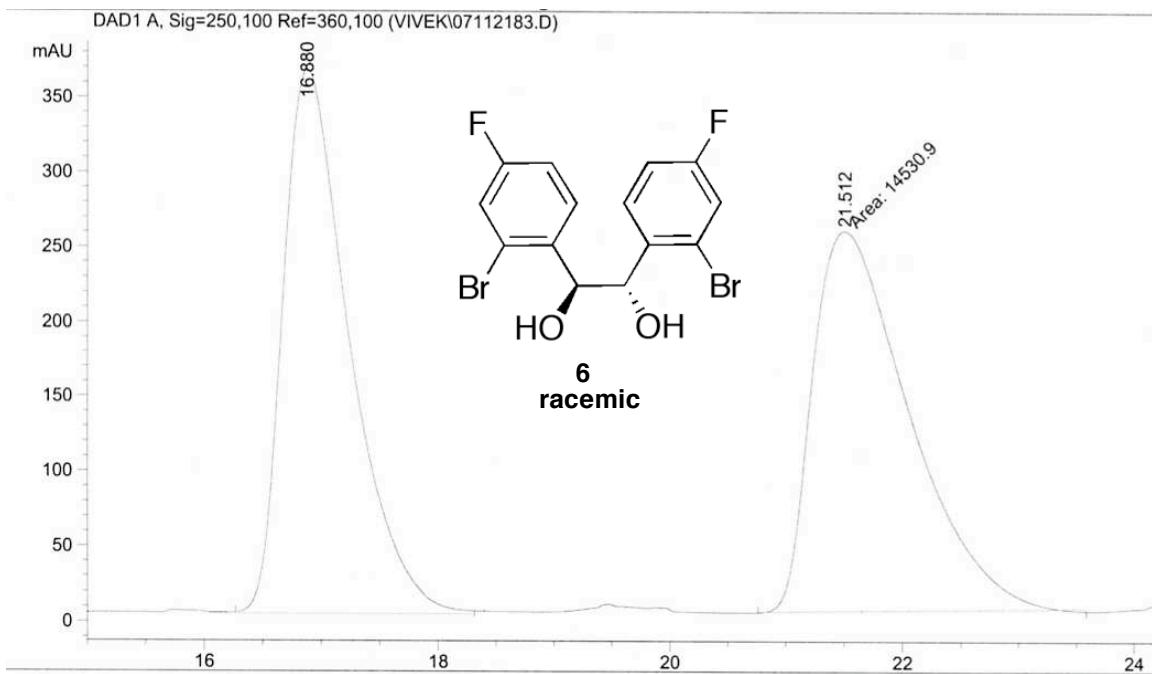
125 MHz, CDCl₃



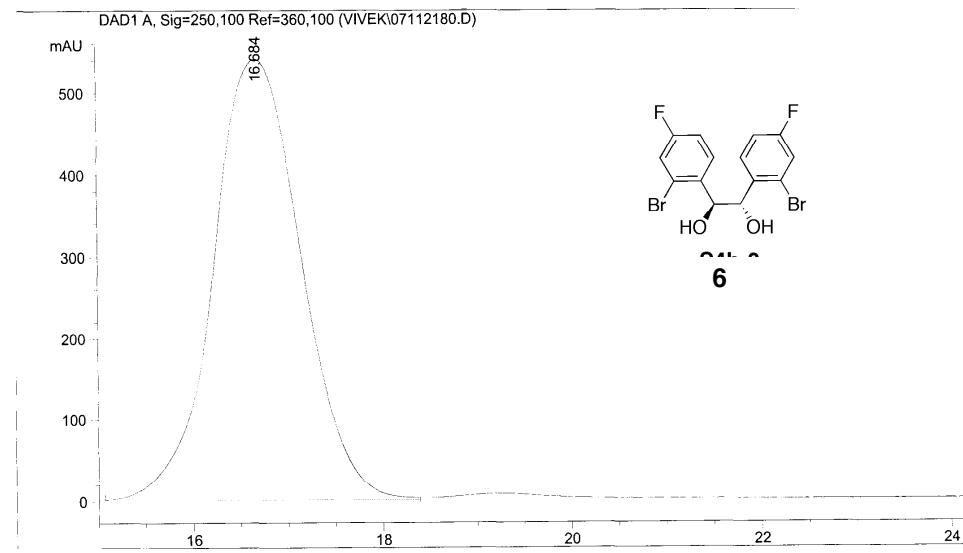
19c



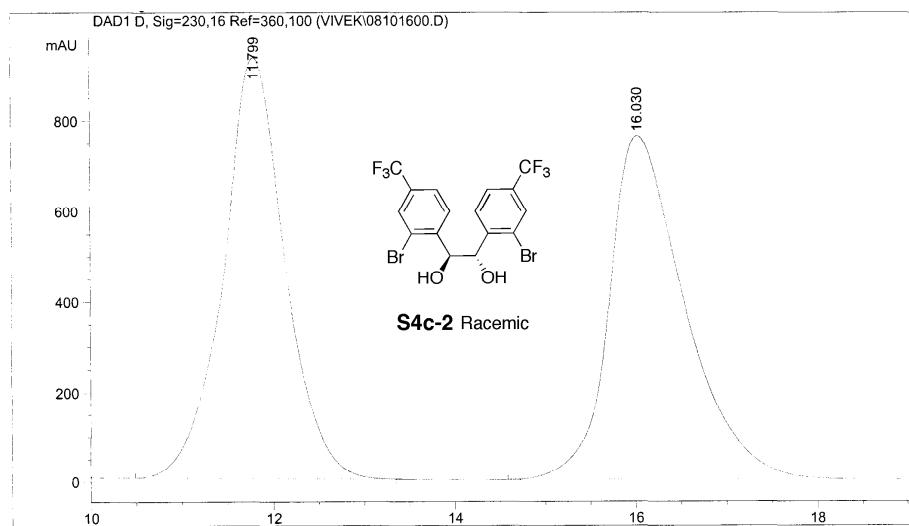
500 MHz, CDCl₃125 MHz, CDCl₃



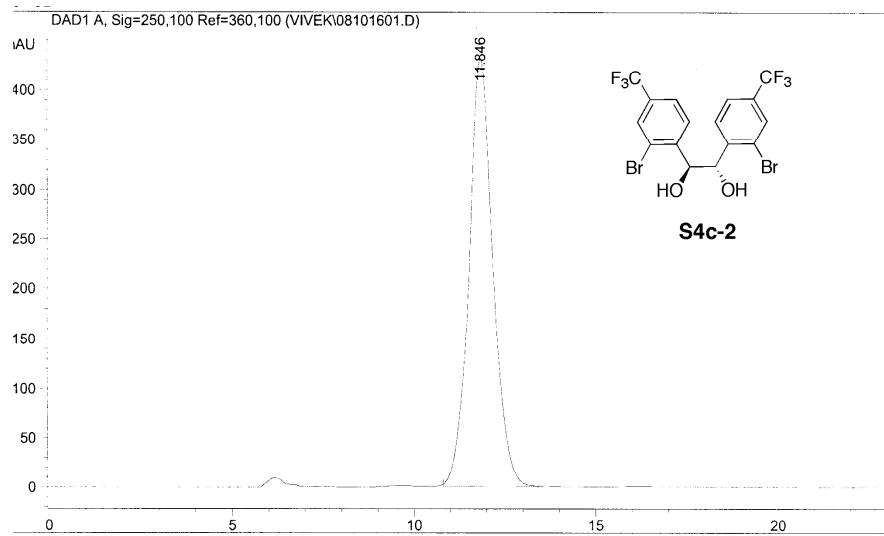
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.880	HH	0.5925	1.42880e4	363.55612	49.5785
2	21.512	MM	0.9549	1.45309e4	253.61821	50.4215



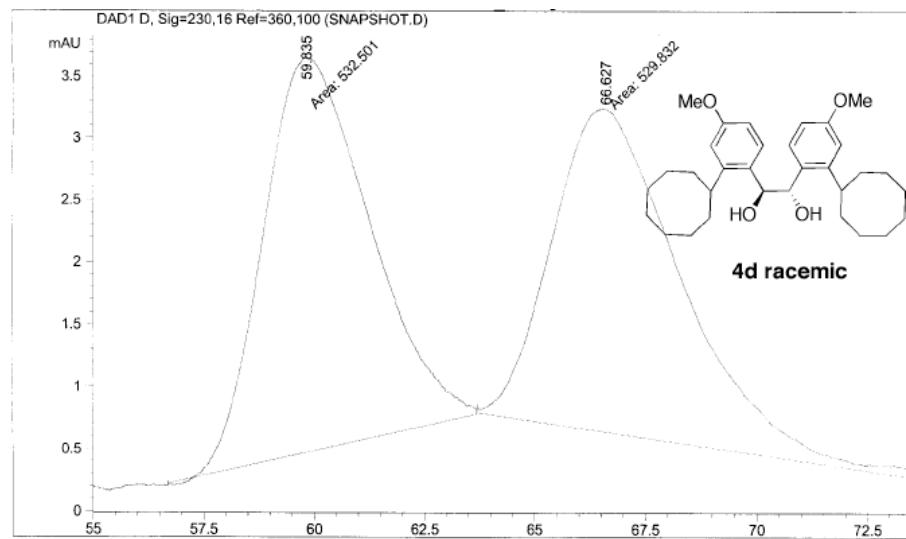
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.684	HH	0.8288	3.46918e4	540.52716	100.0000



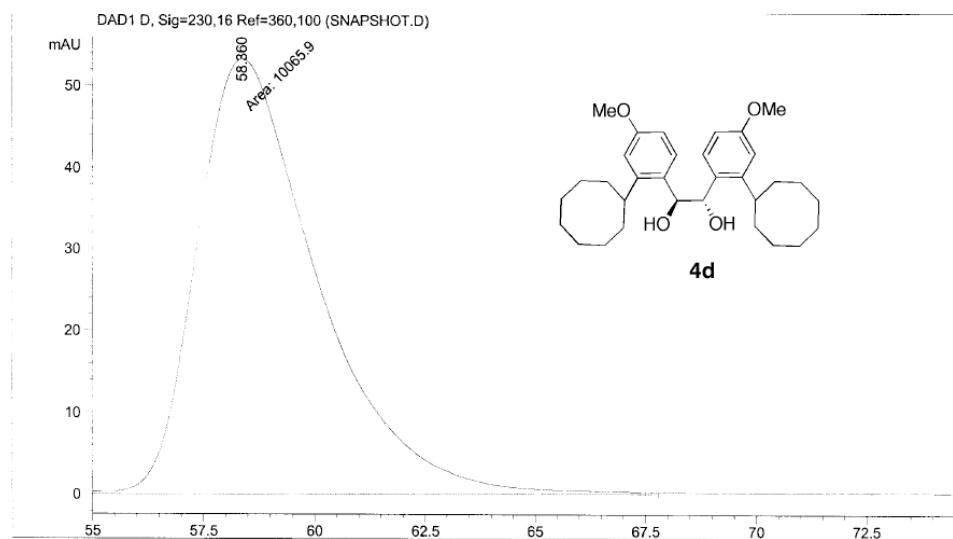
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.799	BB	0.6955	4.39238e4	932.61749	49.7726
2	16.030	BB	0.8714	4.43253e4	763.37067	50.2274



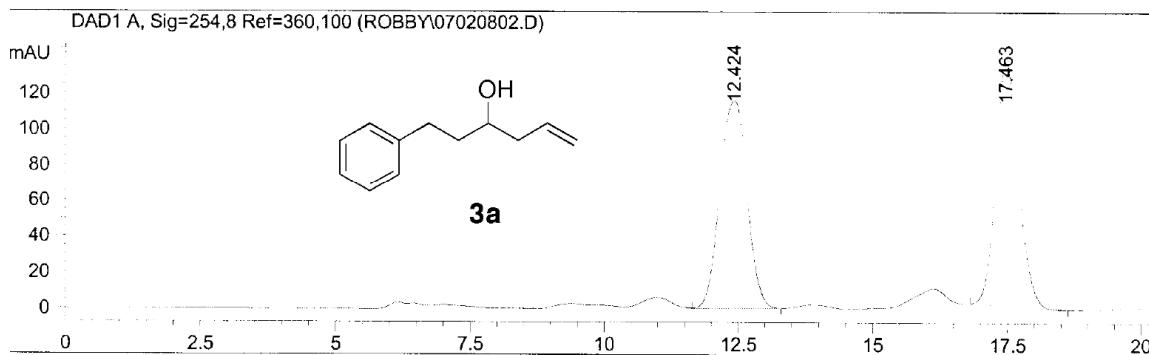
RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
11.846	BB	0.6890	1.98583e4	431.39435	100.0000



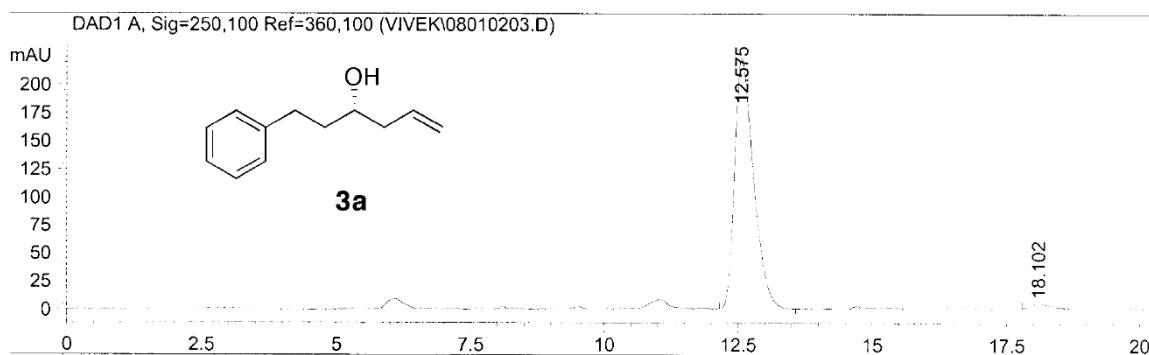
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	59.835	MM	2.7869	532.50055	3.18460	50.1256
2	66.627	MM	3.3910	529.83240	2.60409	49.8744



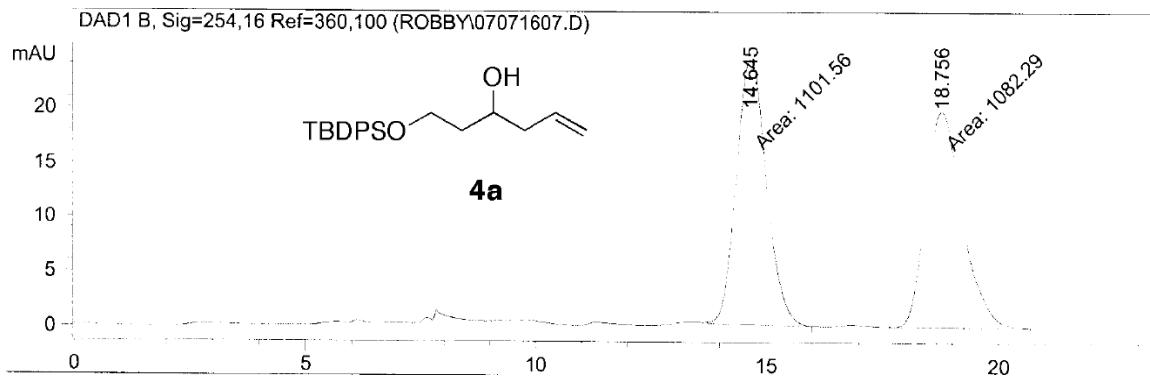
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	58.360	MM	3.1493	1.00659e4	53.27106	100.0000



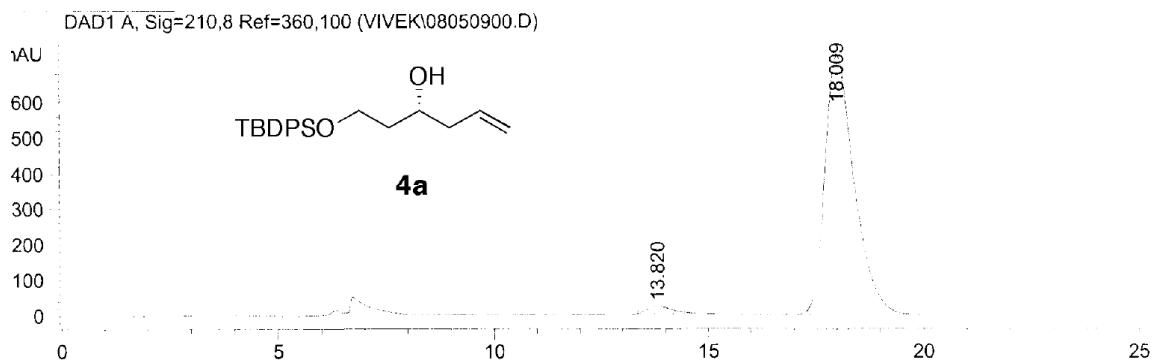
k	RetTime	Type	Width	Area	Height	Area
	[min]		[min]	[mAU*s]	[mAU]	%
1	12.424	VBA	0.5623	4075.71582	115.89481	50.6680
2	17.463	BP	0.4339	3968.24341	138.64215	49.3320



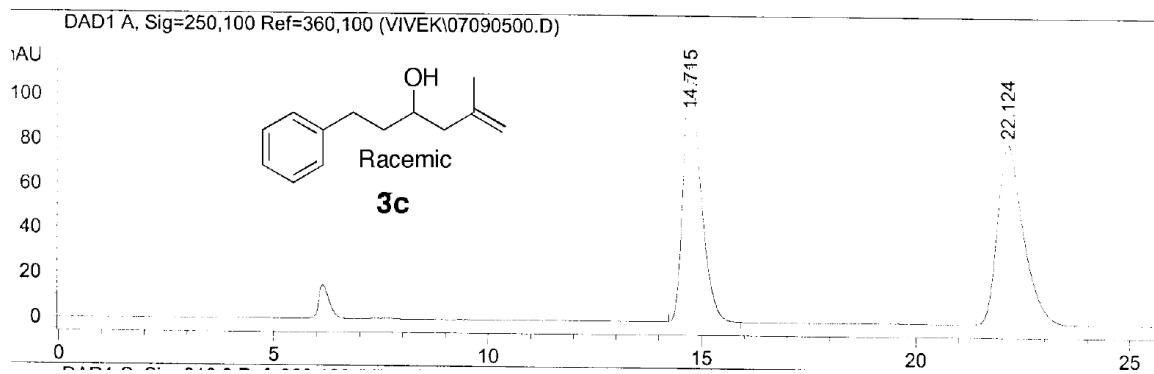
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.575	BB	0.3771	5488.06543	223.00400	98.2760
2	18.102	BBA	0.3656	96.27657	3.67493	1.7240



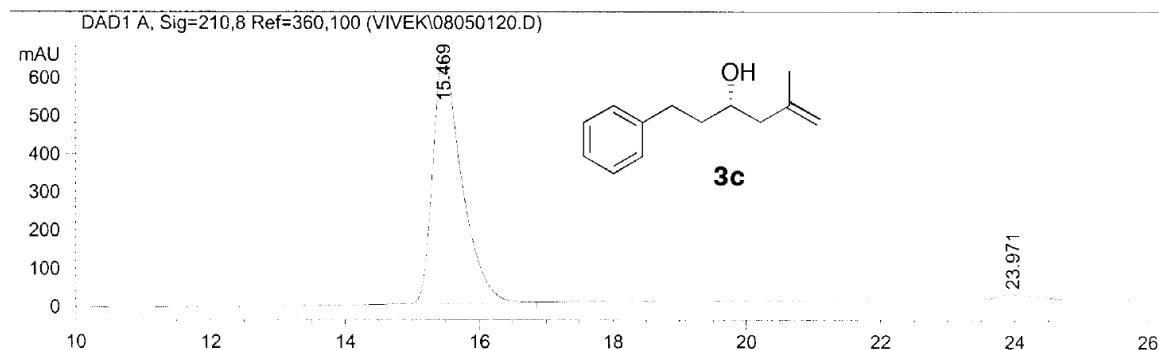
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.645	MM	0.7576	1101.56250	24.23255	50.4412
2	18.756	MM	0.9102	1082.29102	19.81870	49.5588



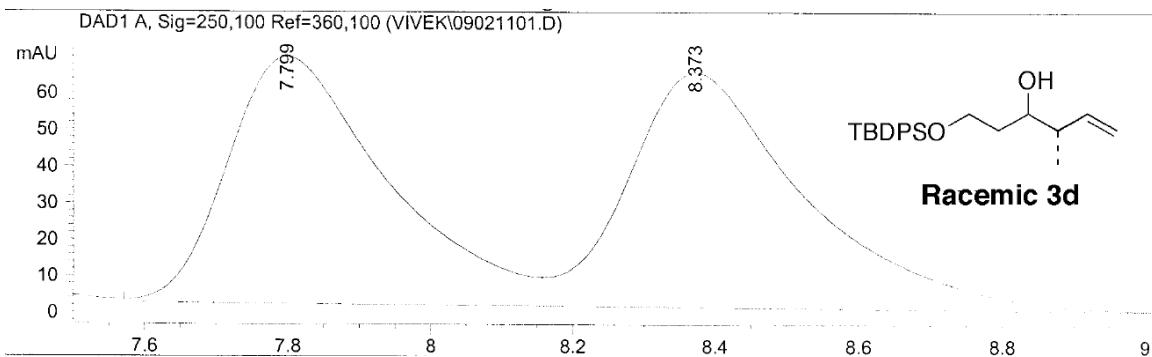
<	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.820	BBA	0.6002	819.63556	21.14736	2.3348
2	18.009	BB	0.7178	3.42852e4	727.57269	97.6652



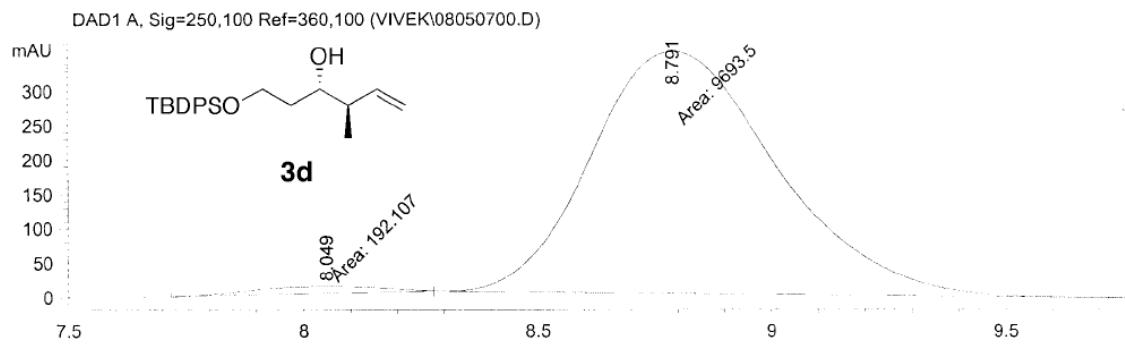
RetTime	Type	Width	Area	Height	Area
[min]		[min]	[mAU*s]	[mAU]	%
14.715	BB	0.4256	3282.81909	116.18489	49.3926
22.124	BB	0.6139	3363.56348	80.76607	50.6074



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.469	BB	0.4452	1.96508e4	649.03888	97.7181
2	23.971	BBA	0.5864	458.88187	12.10097	2.2819



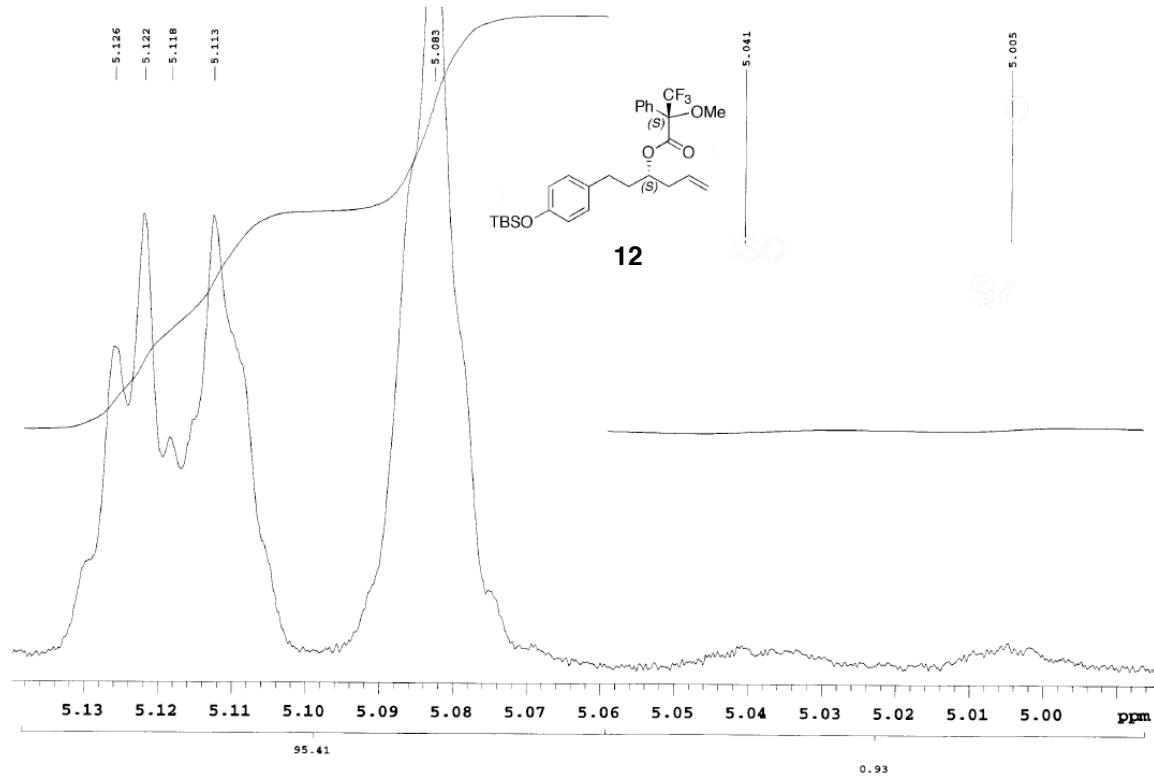
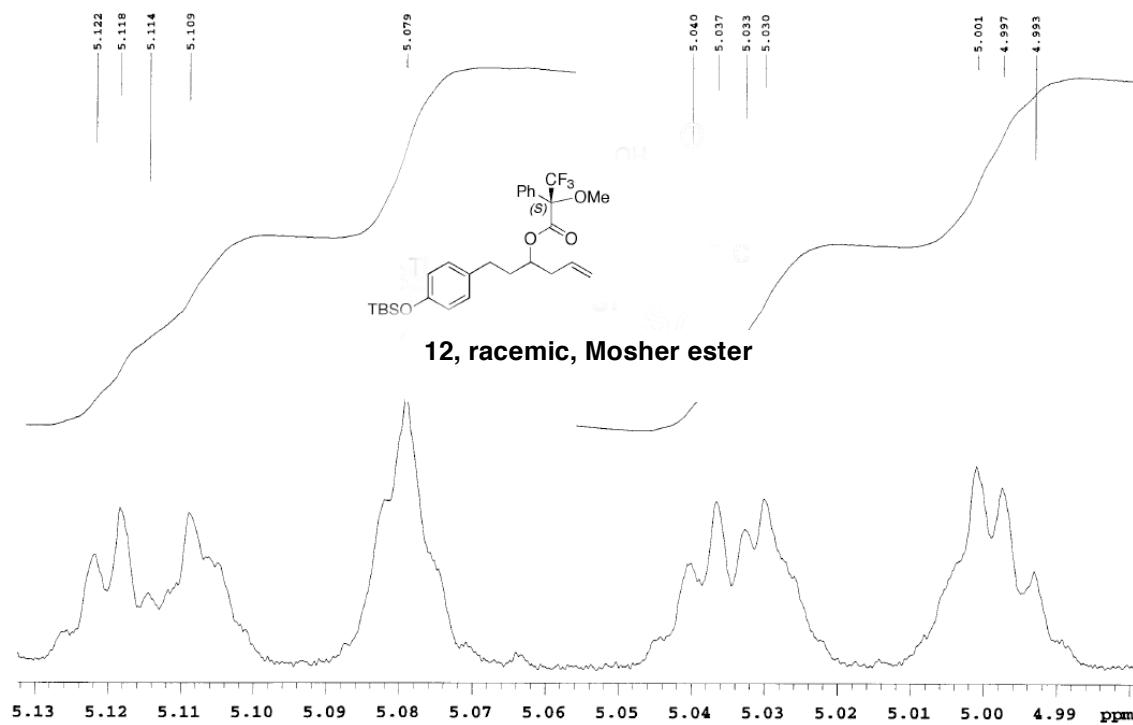
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.799	VV	0.2298	1057.54297	67.84789	48.7791
2	8.373	VB	0.2491	1110.48364	64.42460	51.2209

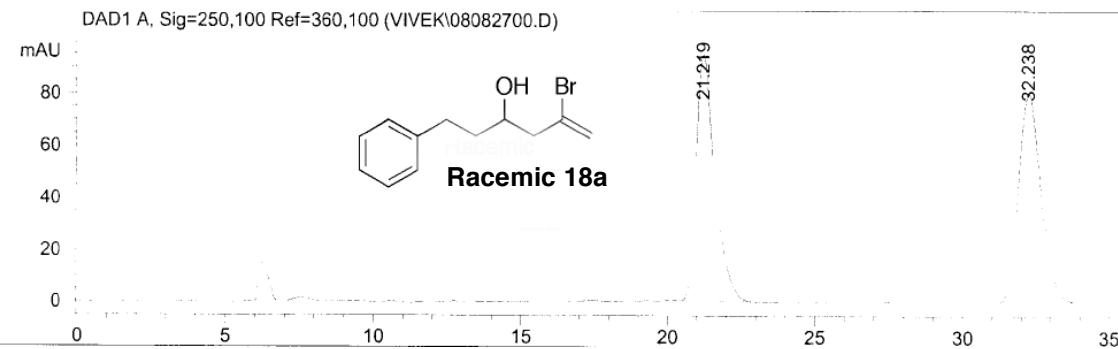


Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.049	MM	0.3167	192.10703	10.10999	1.9433
2	8.791	MM	0.4582	9693.49902	352.60538	98.0567

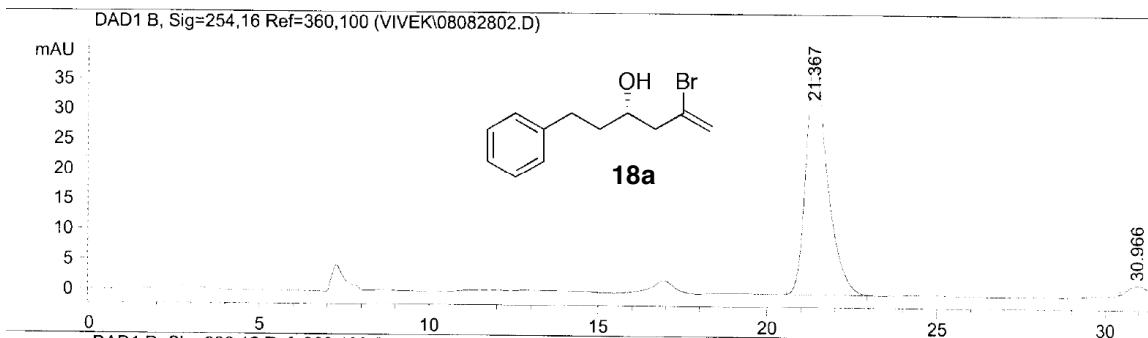
VRH-7-141B-R-Mosher-ester-Racemic

Pulse Sequence: s2pul

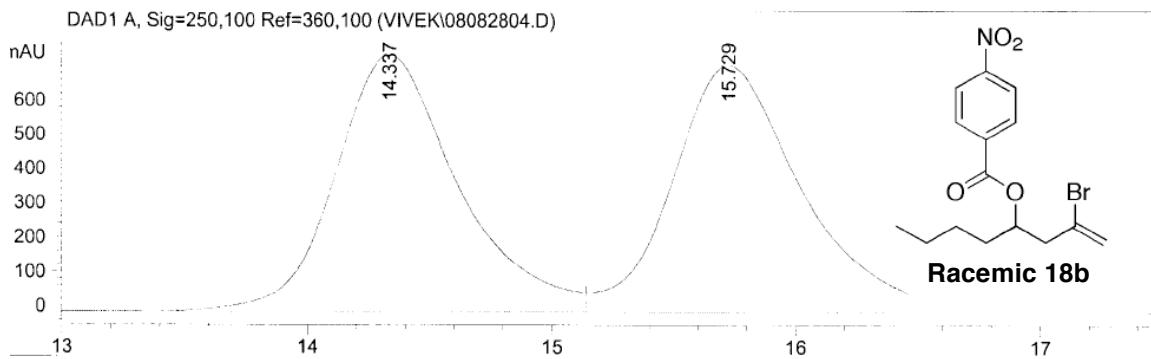




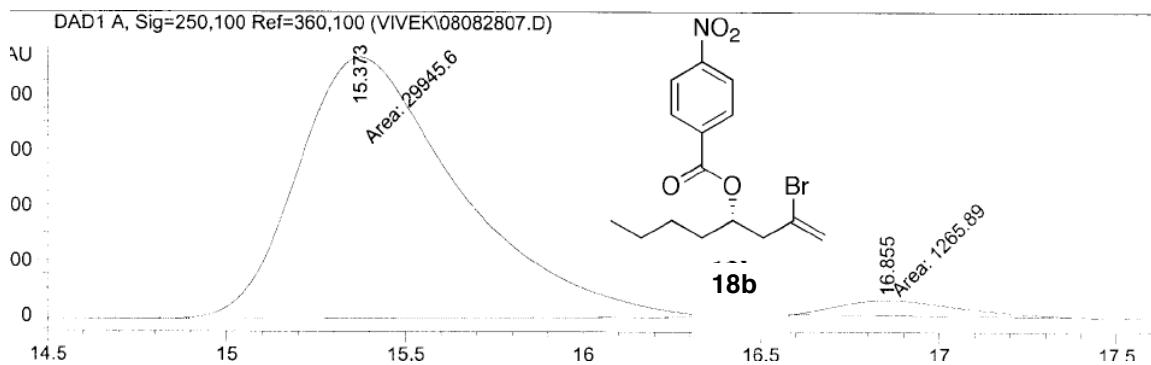
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.219	PB	0.6684	4238.57910	94.65417	49.9276
2	32.238	BB	0.8144	4250.86523	79.94146	50.0724



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.367	BB	0.6330	1715.52869	39.47300	96.5278
2	30.966	BBA	0.4750	61.70845	1.55483	3.4722



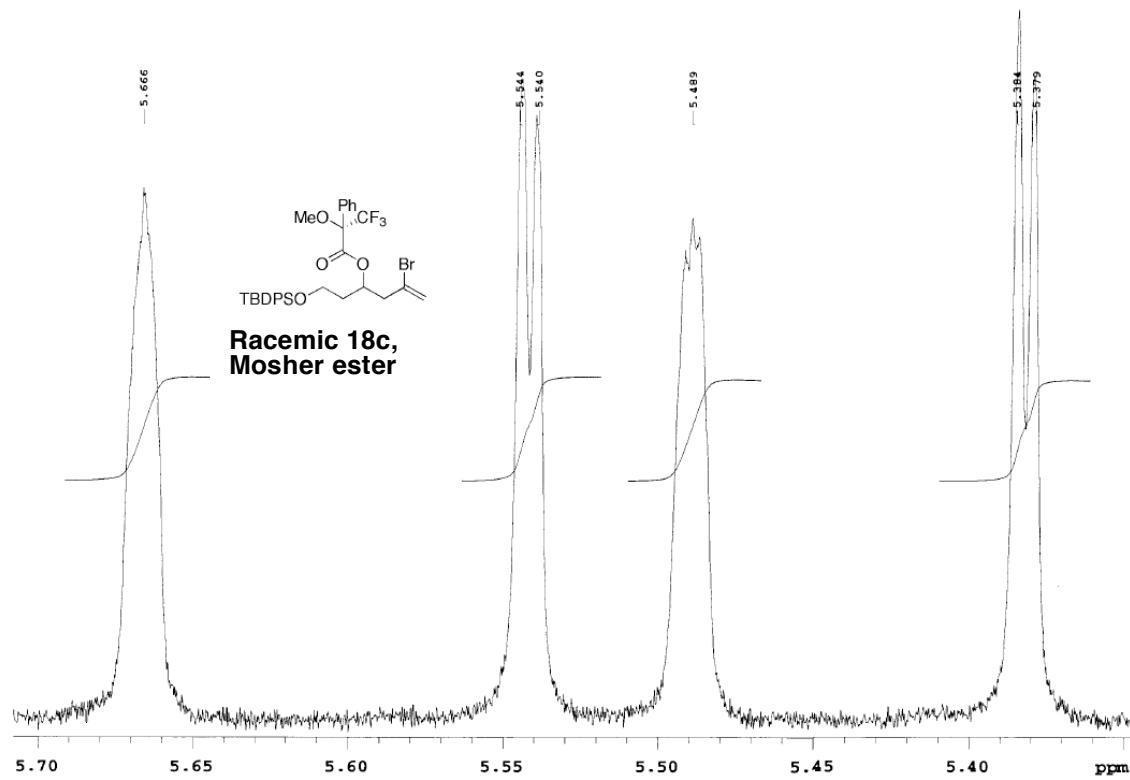
RetTime	Type	Width	Area	Height	Area
[min]		[min]	[mAU*s]	[mAU]	%
14.337	BV	0.5277	2.62381e4	750.78644	50.0036
15.729	VBA	0.5515	2.62343e4	722.75531	49.9964



RetTime	Type	Width	Area	Height	Area
[min]		[min]	[mAU*s]	[mAU]	%
15.373	MM	0.5268	2.99456e4	947.35559	95.9441
16.855	MM	0.3957	1265.89136	53.32430	4.0559

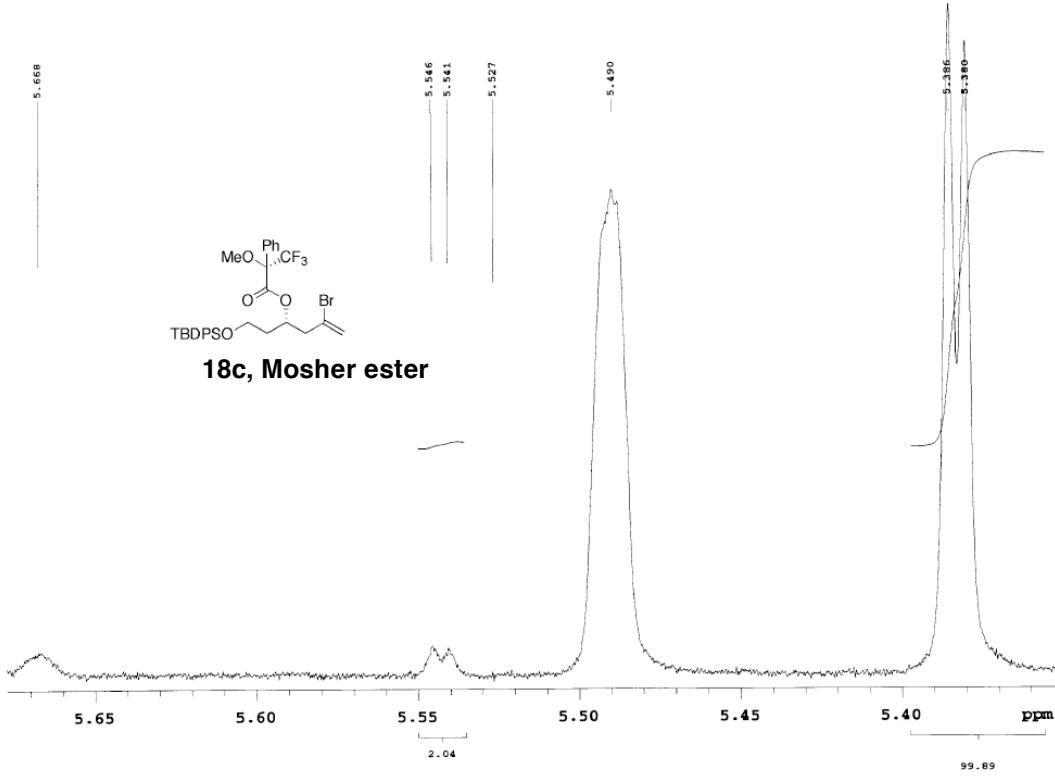
VRH-8-95A-S-Mosher-RACEMIC

Pulse Sequence: s2pul

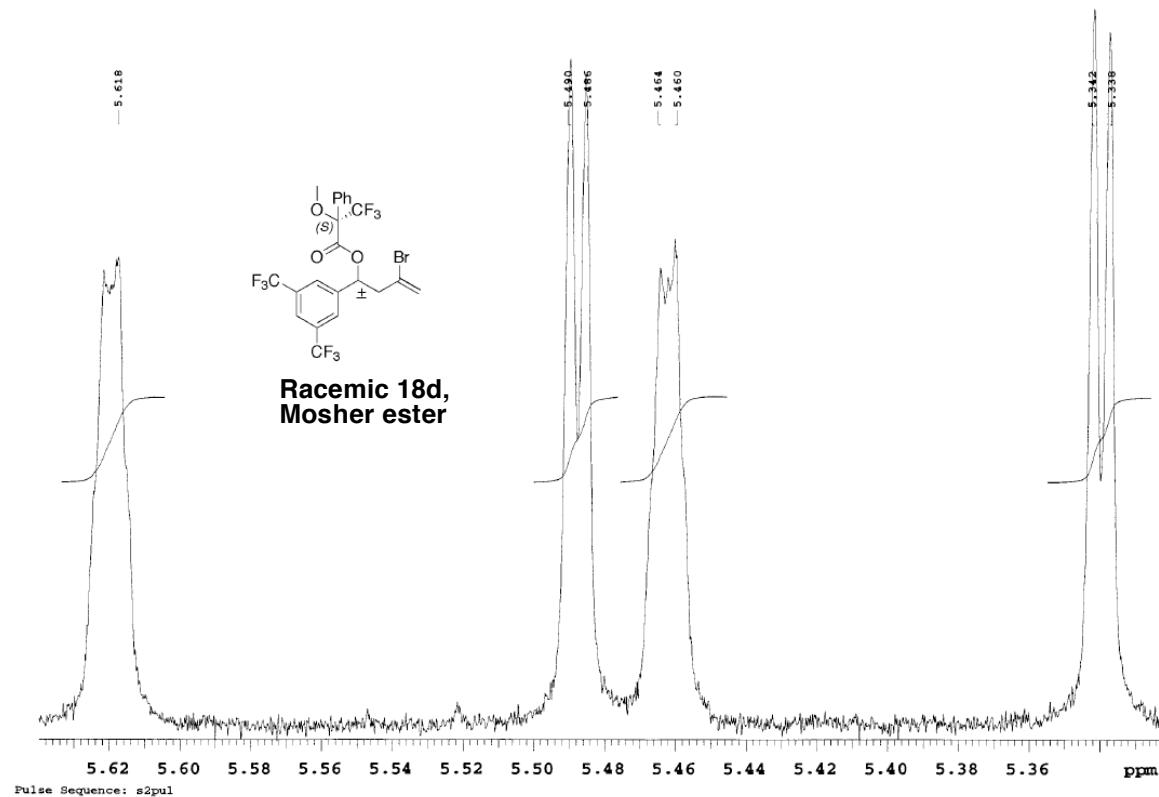


VRH-8-95-Chiral-1H-S-Mosher

Pulse Sequence: s2pul

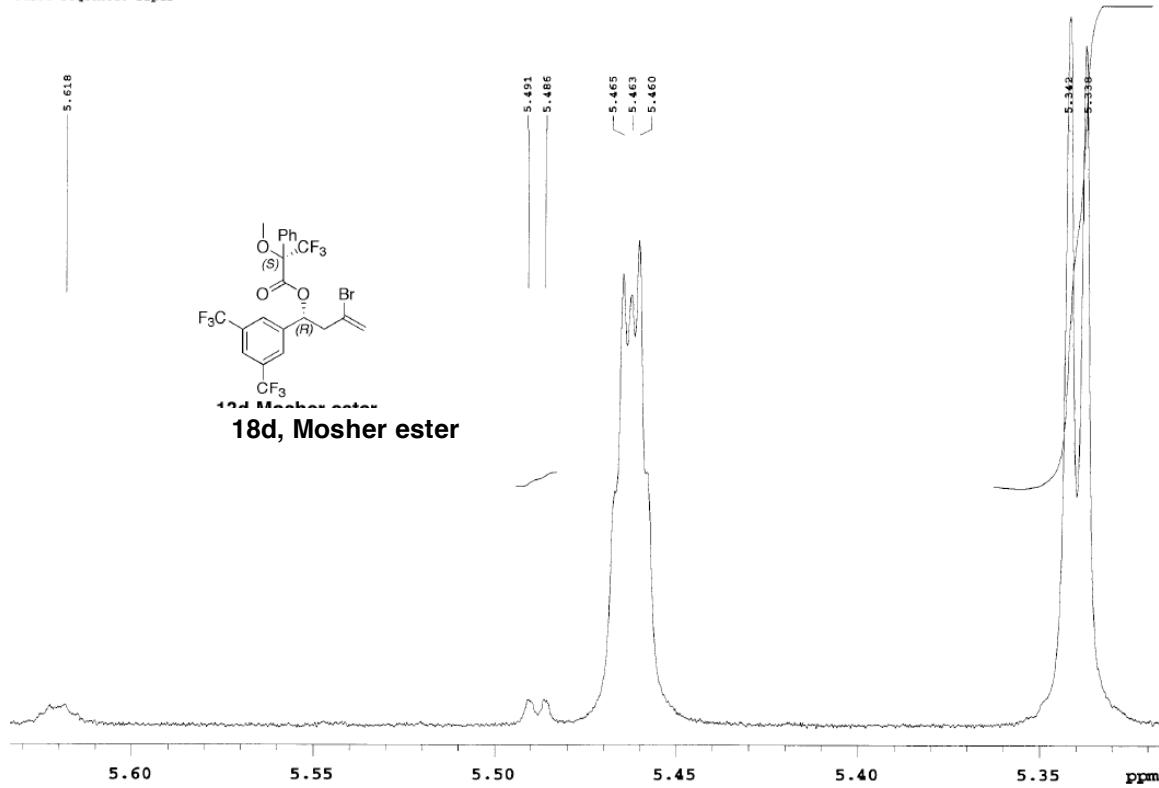


Pulse Sequence: s2pul

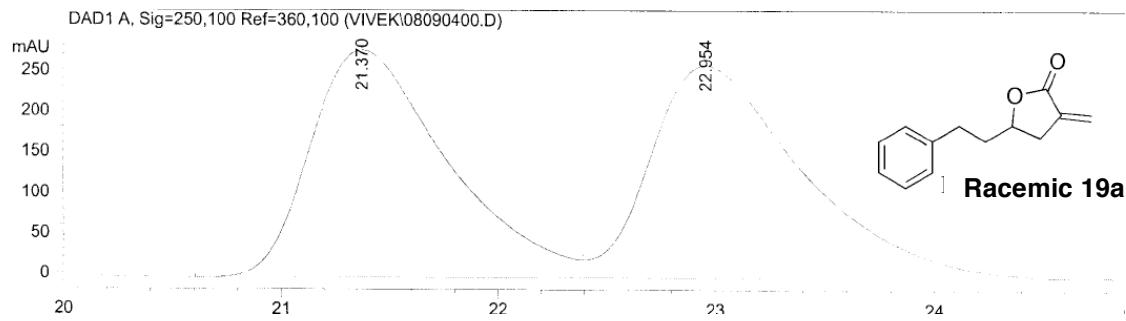


Racemic 18d,
Mosher ester

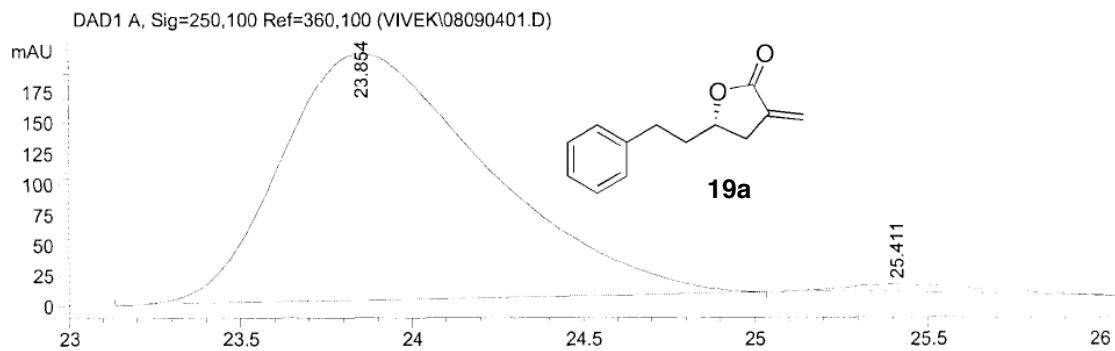
Pulse Sequence: s2pul



18d, Mosher ester



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.370	VV	0.6544	1.22958e4	281.05505	49.3313
2	22.954	VB	0.7210	1.26292e4	261.72470	50.6687



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	23.854	PBA	0.6346	8494.29199	201.98326	97.9461
2	25.411	BBA	0.4265	178.11966	6.36471	2.0539