

## Supporting Information

### TBOxCr<sup>III</sup>Cl-Catalyzed Enantioselective Synthesis of 1,3-dien-2-ylcarbinols

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#### General Procedures.

All non-aqueous reactions were carried out in flame-dried glassware under an atmosphere of argon or dry nitrogen and stirred via magnetic stir-plates. All reactions were monitored by analytical thin-layer chromatography using Merck pre-coated gel plates with F<sub>254</sub> indicator or Whatman pre-coated silica gel plates (0.25 mm) with F<sub>254</sub> indicator. Visualization was accomplished by UV light (256 nm), with combination of potassium permanganate and/or phosphomolibdic acid. Flash column chromatography was performed according to the method of Still using silica gel 60 (mesh 230-400) supplied by SILICYCLE. Yields refer to chromatographically and spectrographically pure compounds unless otherwise noted. All reactions were carried out with anhydrous solvents unless otherwise noted. Anhydrous THF, dichloromethane, diethyl ether and hexane were dried with a M BRAUN solvent purification system (A2 Alumina). Brine refers to a saturated aqueous solution of sodium chloride. Aldehydes were either distilled or chromatographed and refrigerated. Bromoallene **2**,<sup>1</sup> TBOxH ligand and TBOxCr<sup>III</sup>Cl complex<sup>2</sup> were prepared according to the previously reported procedures. All other reagents and starting materials, unless otherwise noted, were purchased from commercial vendors and used without further purification.

Infrared spectra were recorded as thin films on sodium chloride plates using Nicolet 20 SXB FTIR. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra were recorded on a Bruker Avance 400 (400 MHz <sup>1</sup>H, 100 MHz <sup>13</sup>C), or a Bruker Avance 500 (500 MHz <sup>1</sup>H, 125 MHz <sup>13</sup>C). Chemical shifts values (δ) are reported in ppm relative to the residual chloroform (δ 7.26 ppm for

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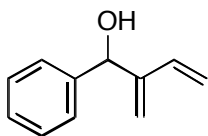
<sup>1</sup> Molander, G. A.; Cormier, E. P. *J. Org. Chem.* **2005**, *70*, 2622.

<sup>2</sup> Takenaka, N.; Xia, G.; Yamamoto, H. *J. Am. Chem. Soc.* **2004**, *126*, 13198.

$^1\text{H}$ ;  $\delta$  77.23 ppm for  $^{13}\text{C}$ ). The proton spectra are reported as follows:  $\delta$  (multiplicity, number of protons, coupling constant  $J$ ). Multiplicities are indicated by s (singlet), d (doublet), t (triplet), q (quartet), p (pentet), H (heptet), dd (doublet of doublet), dt (doublet of triplet), m (multiplet) and br (broad). High performance liquid chromatography (HPLC) was performed on a Varian ProStar Series equipped with a variable wavelength detector using chiral stationary columns (0.46 cm x 25 cm) equipped with guard columns from Daicel. Optical rotations were measured on a Jasco DIP-1000 digital polarimeter.

## General Experimental Procedure

A flame-dried test tube was charged with a magnetic stir bar,  $\text{TBOxCr}^{\text{III}}\text{Cl}$  (30 mg, 0.038 mmol, 10 mol%) and Mn powder 50-mesh (206 mg, 1.125 mmol) and flushed thoroughly with argon three times. To this mixture, anhydrous THF (3.8 mL) was added and the resulting yellow-brown mixture was stirred for 10 min. at room temperature. After 10 min., the catalyst solution was treated with bromoallene **2** (101 mg, 0.76 mmol) and the reaction mixture stirred for 20 min.. After that time, neat aldehyde (0.38 mmol) was added followed by the drop-wise addition of chlorotriethylsilane (62 mg, 69  $\mu\text{L}$ , 0.41 mmol). The reaction mixture was stirred vigorously at room temperature for 40 hours. After 40 hours, the reaction was quenched with saturated aq.  $\text{NaHCO}_3$  and filtered through a short pad of Celite®. After the removal of volatiles *in vacuo*, the remaining mixture was taken up in diethyl ether and washed with brine. Organic layer was dried over anhydrous  $\text{NaSO}_4$  and concentrated *in vacuo*. The crude reaction mixture was dissolved in THF (3.8 mL), treated with TBAF (380  $\mu\text{L}$ , 1.0 M solution in THF, 0.38 mmol) and stirred until the reaction is complete as judged by TLC. Upon the completion, the reaction is diluted with diethyl ether and washed with water and brine. Crude reaction mixture is purified by column chromatography on silica gel using hexane-ethyl acetate as eluent system.

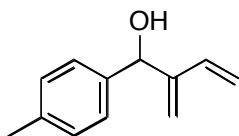


**(R)-2-Methylene-1-phenyl-but-3-en-1-ol<sup>3</sup>**:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , ppm): 7.41-7.29 (m, 5H), 6.31 (dd, 1H,  $J = 11.0$  Hz, 18 Hz), 5.49 (d, 1H,  $J = 4$  Hz), 5.42 (s, 1H), 5.34 (s, 1H), 5.23 (d, 1H,  $J = 18.0$  Hz), 5.05 (d, 1H,  $J = 11.0$  Hz), 1.93 (br, 1H). Enantiomeric excess determined by HPLC with a Chiracel OB-H column equipped with an OB-H

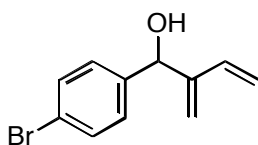
<sup>3</sup> (a) Soundararajan, R.; Li, G.; Brown, H. C. *J. Org. Chem.* **1996**, *61*, 100. (b) Yu, C.-M.; Lee, S.-J.; Jeon, M. *J. Chem. Soc., Perkin Trans. 1*, **1999**, 3557.



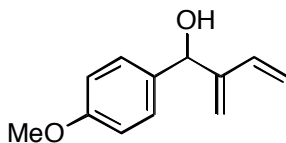
guard column (hexanes : 2-propanol = 99:1, flow rate = 1.0 mL/min)  $t_r$  (major) = 24.5 min.,  $t_r$  (minor) = 19.4 min.  $[\alpha]_D^{24} = +85.7$  ( $c = 1.1$ ,  $\text{CHCl}_3$ ). The reported value for S-enantiomer (98% ee) is  $[\alpha]_D^{20} = -93.2$  ( $c = 1.34$ ,  $\text{CHCl}_3$ ).<sup>3b</sup>



**(R)-2-Methylene-1-(4-methylphenyl)-but-3-en-1-ol:**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , ppm): 7.27-7.25 (d, 2H,  $J = 8$  Hz), 7.15-7.13 (d, 2H,  $J = 8$  Hz), 6.30 (dd, 1H,  $J = 11.5$  Hz, 18 Hz), 5.42 (s, 2H), 5.32 (s, 2H), 5.19 (d, 1H,  $J = 18$  Hz), 5.02 (d,  $J = 11.5$  Hz), 2.33 (s, 3H), 2.04 (br, 1H).  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm): 147.6, 139.1, 137.6, 135.9, 129.2, 126.8, 73.7. IR (neat on NaCl,  $\text{cm}^{-1}$ ): 3404.1, 3021.5, 2920.5, 1512.4, 1419.3, 1017.9. MS (EI): 174.1. Enantiomeric excess determined by HPLC with a Chiracel OB-H column equipped with an OB-H guard column (hexanes : 2-propanol = 99.5:0.5, flow rate = 1.0 mL/min.)  $t_r$  (major) = 35.8 min.,  $t_r$  (minor) = 20.3 min.  $[\alpha]_D^{24} = -69.2$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

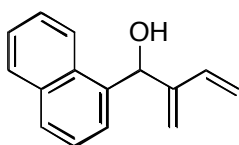


**(R)-1-(4-Bromophenyl)-2-methylenebut-3-en-1-ol<sup>4</sup>:**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , ppm): 7.48-7.45 (d, 2H,  $J = 10.5$  Hz), 7.29-7.26 (d, 2H,  $J = 10.5$  Hz), 6.29 (dd, 1H,  $J = 11.0$  Hz, 18 Hz), 5.44 (s, 1H), 5.37 (d, 1H), 5.33 (s, 1H), 5.22 (d, 1H,  $J = 18.0$  Hz), 5.06 (d, 1H,  $J = 11.0$  Hz), 1.99 (br, 1H). MS (EI): 238.9. Enantiomeric excess determined by HPLC with a Chiracel OB-H column equipped with an OB-H guard column (hexanes : 2-propanol = 99:1, flow rate = 1.0 mL/min)  $t_r$  (major) = 17.6 min.,  $t_r$  (minor) = 19.0 min.  $[\alpha]_D^{24} = -15.4$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).

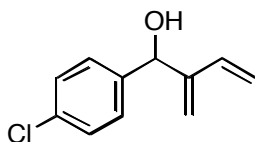


<sup>4</sup> Bloch, R.; Chaptal-Gardoz, N. *J. Org. Chem.* **1994**, *59*, 4162.

**(R)-1-(4-Methoxyphenyl)-2-methylene-but-3-en-1-ol**<sup>5</sup>: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, ppm): 7.28-7.26 (d, 2H, *J* = 8.0 Hz), 7.15-7.14 (d, 2H, *J* = 8.0 Hz), 6.30 (dd, 1H, *J* = 11.0 Hz, 18.0 Hz), 5.50 (s, 2H), 5.43 (s, 1H), 5.20 (d, 1H, *J* = 18.0 Hz), 5.03 (d, 1H, *J* = 18.0 Hz), 5.06 (d, 1H, *J* = 11.0 Hz), 3.78 (s, 3H), 2.02 (br, 1H). Enantiomeric excess determined by HPLC with a Chiracel OB-H column equipped with an OB-H guard column (hexanes : 2-propanol = 99:1, flow rate = 1.0 mL/min) *t*<sub>r</sub> (major) = 32.9 min., *t*<sub>r</sub> (minor) = 23.2 min. [ $\alpha$ ]<sub>D</sub><sup>24</sup> = -72.2 (c = 1.0, CHCl<sub>3</sub>).



**(R)-2-Methylene-1-(1-naphthyl)-but-3-en-1-ol**<sup>6</sup>: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, ppm): 8.11 (d, 2H, *J* = 9.0 Hz), 7.88 (d, 1H, *J* = 8.5 Hz), 7.82 (d, 1H, *J* = 8.0 Hz), 7.61 (d, 1H, *J* = 7.0 Hz), 7.53-7.46 (m, 3H), 6.43 (dd, 1H, *J* = 11.0, 17.5 Hz), 6.26 (s, 1H), 5.42 (s, 1H), 5.34 (d, 1H, *J* = 18.0 Hz), 5.23 (d, 1H, *J* = 18.0 Hz), 5.08 (d, 1H, *J* = 11.0 Hz), 2.06 (br, 1H). Enantiomeric excess determined by HPLC with a Chiracel OB-H column equipped with an OB-H guard column (hexanes : 2-propanol = 99:1, flow rate = 0.5 mL/min) *t*<sub>r</sub> (major) = 65.3 min., *t*<sub>r</sub> (minor) = 34.0 min. [ $\alpha$ ]<sub>D</sub><sup>24</sup> = -27.6 (c = 1.0, CHCl<sub>3</sub>).

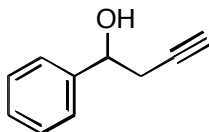


**(R)-1-(4-Chlorophenyl)-2-methylene-but-3-en-1-ol**: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>, ppm): 7.36-7.26 (m, 4H), 6.29 (dd, 1H, *J* = 11.0 Hz, 18.0 Hz), 5.45 (s, 1H), 5.38 (s, 1H), 5.33 (s, 1H), 5.21 (d, 1H, *J* = 18.0 Hz), 5.06 (d, 1H, *J* = 11.0 Hz), 2.05 (br, 1H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm): 147.4, 140.4, 135.5, 133.5, 128.6, 128.2, 73.4. IR (neat on NaCl, cm<sup>-1</sup>): 3363.5, 3090.4, 2917.5, 1594.8, 1489.8, 1407.3, 1091.2, 1014.0, 908.8, 825.1. MS(EI): 194.1. Enantiomeric excess determined by HPLC with a Chiracel OB-H column

<sup>5</sup> Lu, W.; Ma, J.; Yang, Y.; Chan, T. H. *Org. Lett.* **2000**, 2, 3469.

<sup>6</sup> Smulik, J. A.; Diver, S. T. *Org. Lett.* **2000**, 2, 2271.

equipped with an OB-H guard column (hexanes : 2-propanol = 99:1, flow rate = 0.5 mL/min)  $t_r(\text{major}) = 29.9$  min,  $t_r(\text{minor}) = 17.4$  min.  $[\alpha]_D^{24} = -27.7$  ( $c = 1.0$ ,  $\text{CHCl}_3$ ).



**1-Phenyl-but-3-yn-1-ol:**  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ , ppm): 7.41-7.29 (m, 5H), 4.88 (m, 1H), 2.65 (dd, 2H,  $J = 2.6$  Hz, 6.1 Hz), 2.37 (br, 1H), 2.08 (t, 1H,  $J = 2.6$  Hz, 5.2 Hz). Enantiomeric excess determined by HPLC with a Chiracel OD-H column equipped with an OD-H guard column (hexanes : 2-propanol = 95:5, flow rate = 0.5 mL/min)  $t_r$  (major) = 18.6 min.,  $t_r$  (minor) = 21.6 min.  $[\alpha]_D^{24} = +10.4$  ( $c = 1.0$ , MeOH). Reported value for *R*-enantiomer (93% ee) is  $[\alpha]_D^{28} = +11.18$  ( $c = 1.7$ , MeOH).<sup>7</sup>

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<sup>7</sup> Lai, C.; Soderquist, J. A. *Org. Lett.* **2005**, 7, 799.

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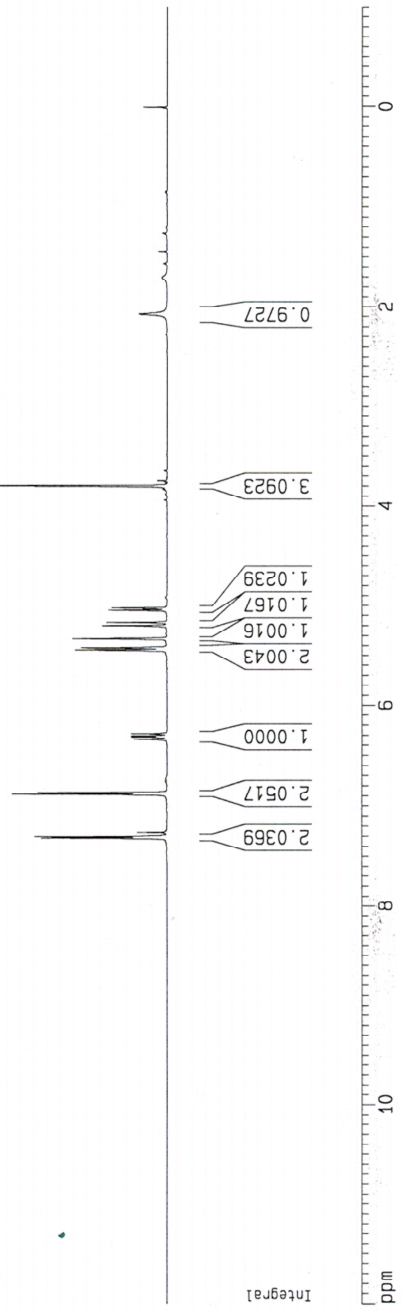
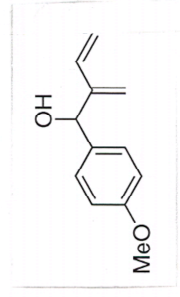
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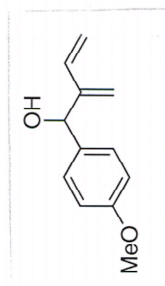


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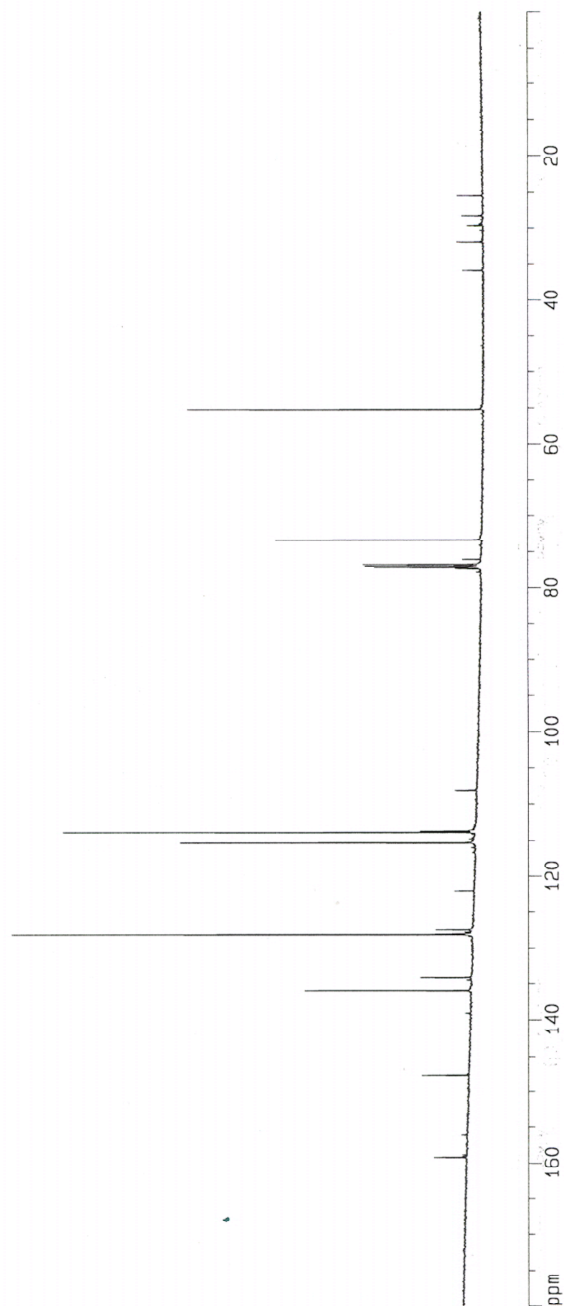
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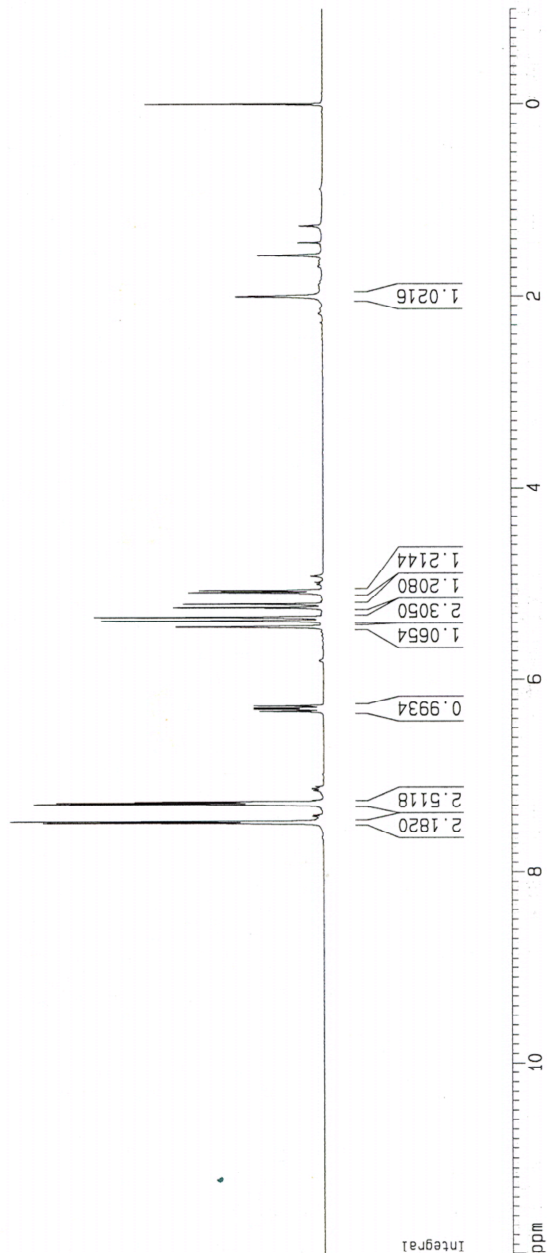
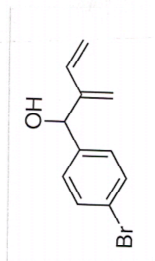
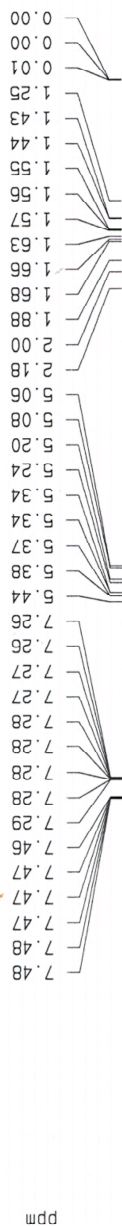
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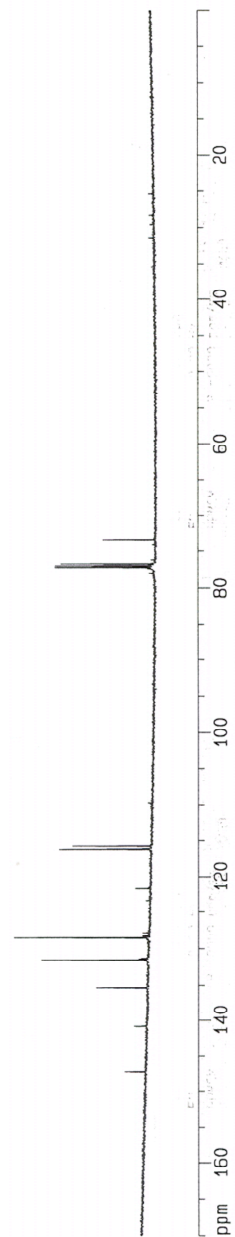
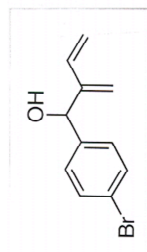
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1D NMR plot parameters  
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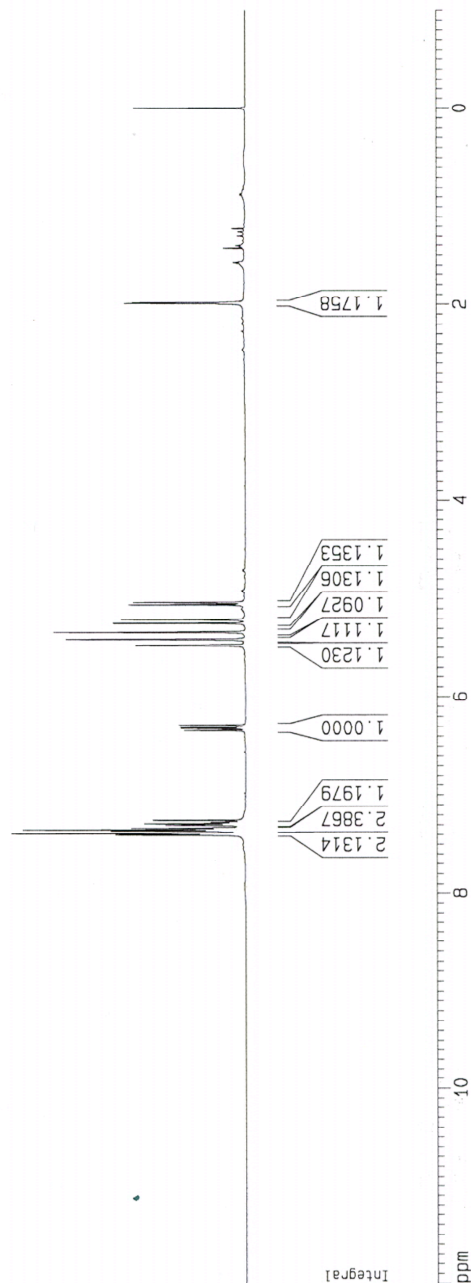
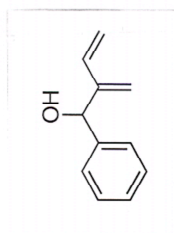
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P1 16.00 usec  
PL1 -3.00 dB  
SF01 125.7049314 MHz

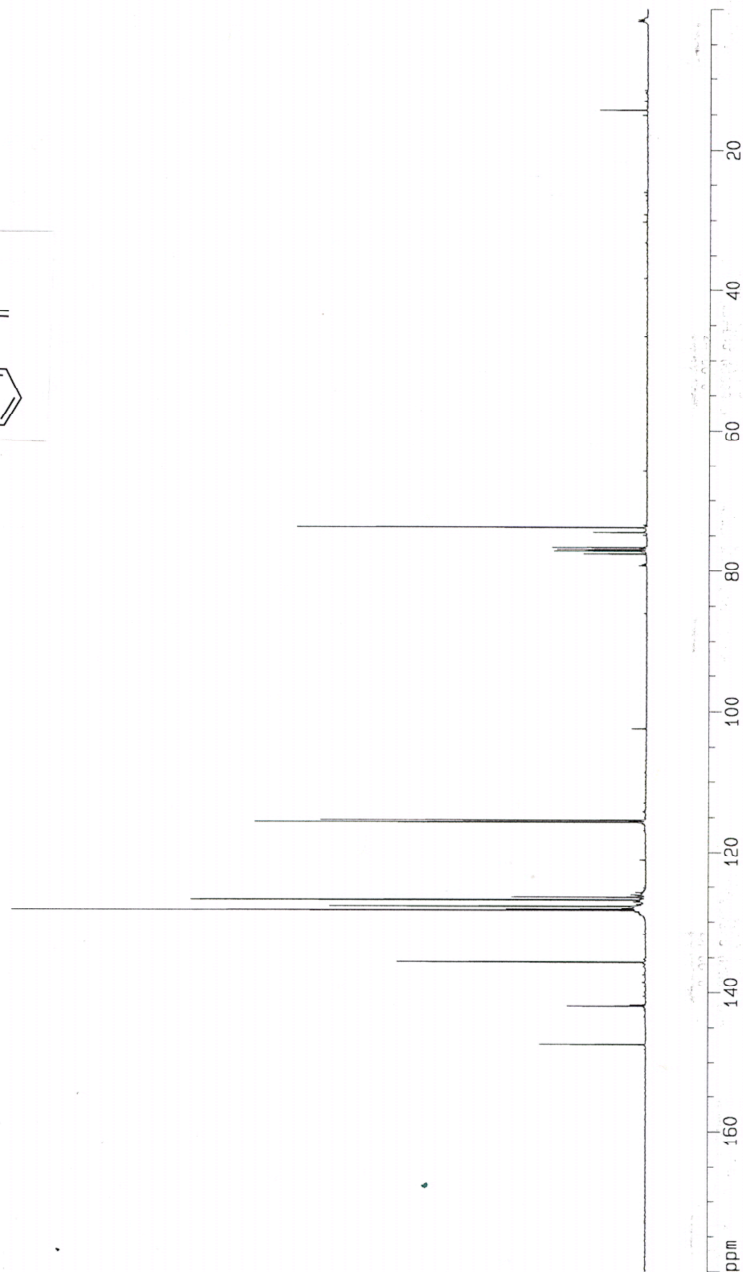
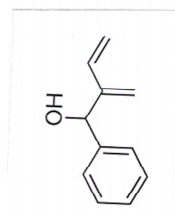
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 100.00 usec  
PL2 120.00 dB  
PL12 28.00 dB  
SF02 499.8772000 MHz

F2 - Processing parameters  
SI 32768  
SF 125.6936874 MHz  
WDW EN  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR plot parameters  
CX 20.00 cm  
CY 10.00 cm  
F1P 180.000 ppm  
F1 22624.86 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCM 9.000000 ppm/cm  
HZCM 1131.24316 Hz/cm

77.251  
76.997  
76.743  
73.844

147.484  
141.891  
135.758  
128.406  
128.244  
127.735  
126.843  
126.478  
115.648  
115.375



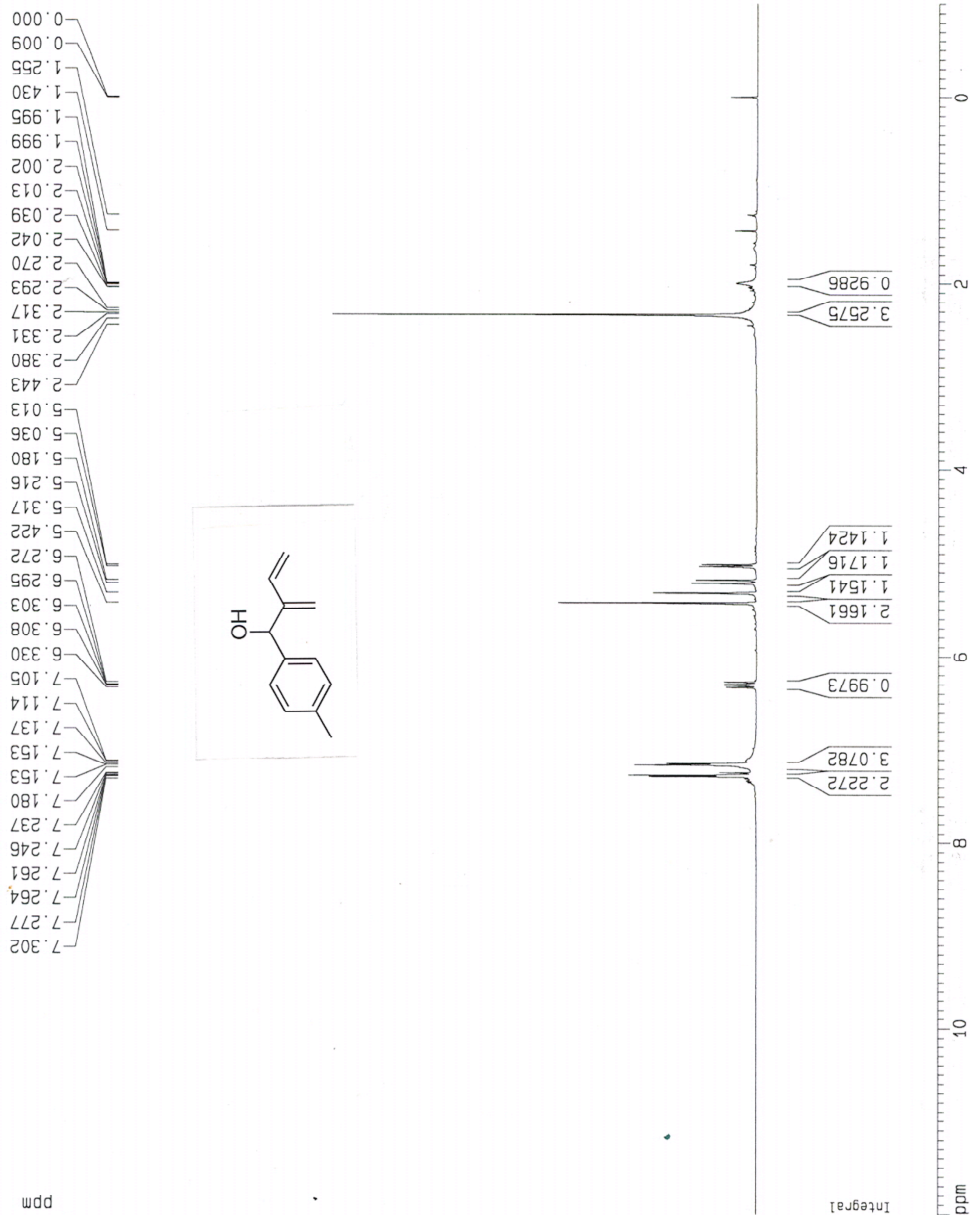
Current Data Parameters  
NAME mn8\_122.r9p  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080429  
Time 11.00  
INSTRUM spect  
PROBHD 5 mm QNP 1H  
PULPROG zg  
TD 48076  
SOLVENT CDCl3  
NS 4  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.156670 Hz  
AQ 2.9999924 sec  
RG 32  
DW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 3.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.50 usec  
PL1 0.00 dB  
SF01 500.1325006 MHz

F2 - Processing parameters  
SI 55536  
SF 500.1300253 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 12.000 ppm  
F1 6001.56 Hz  
F2P -1.000 ppm  
F2 -500.13 Hz  
PPHMM 0.65000 ppm/cm  
HZCM 325.08453 Hz/cm



Current Data Parameters  
NAME mm8\_126.4We  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080503  
Time 15.57  
INSTRUM spect  
PROBHD 5 mm QNP 1H  
PULPROG zgdc  
TD 75184  
SOLVENT CDCl3  
NS 2000  
DS 0  
SWH 37593.984 Hz  
FIDRES 0.500026 Hz  
AQ 0.9999972 sec  
RG 1024  
EW 13.300 usec  
DE 7.50 usec  
TE 300.0 K  
D1 0.10000000 sec  
d11 0.03000000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 4.60 usec  
PL1 0.00 dB  
SF01 125.7690572 MHz

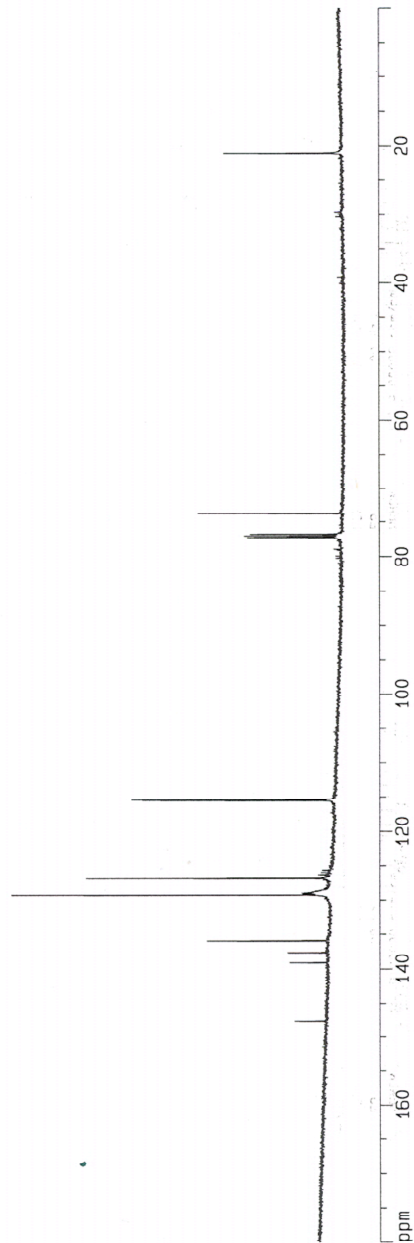
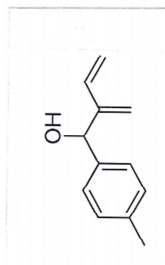
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 120.00 dB  
PL12 19.00 dB  
SF02 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7577963 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR plot parameters  
CX 20.00 cm  
F1P 180.000 ppm  
F1 22636.40 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCK 9.00000 ppm/cm  
HZCM 1131.82019 Hz/cm

77.26  
77.00  
76.75  
73.74

147.61  
139.06  
137.58  
135.91  
129.20  
129.10  
128.93  
126.85  
115.45  
115.33



Current Data Parameters  
NAME mm8\_126\_Napht  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080503  
Time 19.01  
INSTRUM spect  
PROBHD 5 mm QNP 1H  
PULPROG zg  
TD 48076  
SOLVENT CDCl3  
NS 8  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.166670 Hz  
AQ 2.9999924 sec  
RG 128  
DW 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 3.00000000 sec

===== CHANNEL f1 =====

NUC1 1H  
P1 9.50 usec  
PL1 0.00 dB  
SF01 500.1325006 MHz

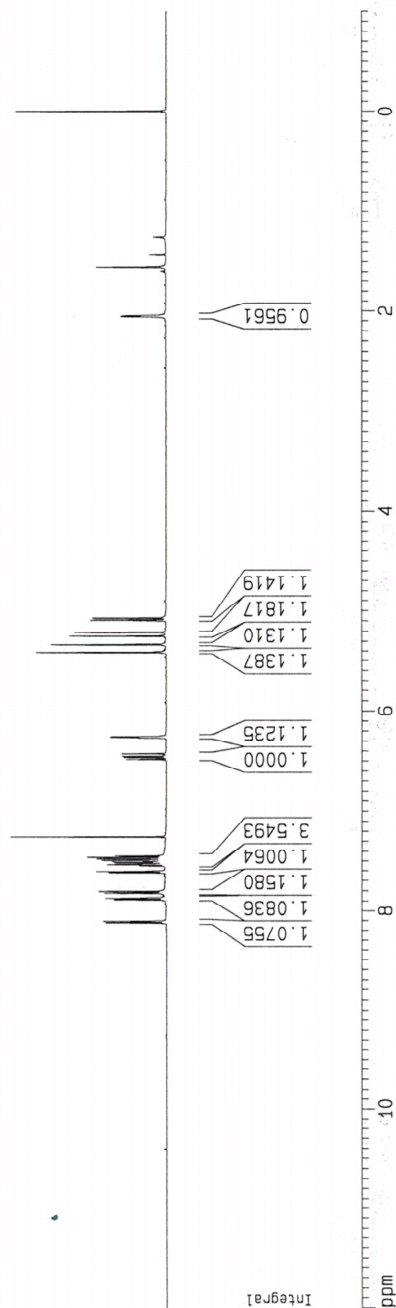
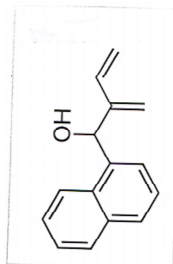
F2 - Processing parameters  
SI 65536  
SF 500.1300168 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 12.000 ppm  
F1 6001.56 Hz  
F2P -1.000 ppm  
F2 -500.13 Hz  
PPMCM 0.65000 ppm/cm  
HZCM 325.08450 Hz/cm

0.01  
0.00  
0.01

1.25  
1.43  
1.55  
1.60  
2.05  
2.06

5.07  
5.09  
5.21  
5.25  
5.34  
5.34  
5.41  
5.42  
5.42  
6.26  
6.26  
7.25  
7.46  
7.48  
7.50  
7.51  
7.52  
7.53  
7.60  
7.62  
7.62  
7.81  
7.82  
7.82  
7.87  
7.87  
7.89  
8.11  
8.12



Current Data Parameters  
 NAME mmB\_125.Npht  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080503  
 Time 19.36

INSTRUM spect  
 PROBHD 5 mm QNP 1H  
 PULPROG zgpg  
 TO 75184  
 SOLVENT CDCl3  
 NS 4000  
 DS 0  
 SWH 37593.984 Hz  
 FIDRES 0.500026 Hz  
 AQ 0.9999972 sec  
 RG 1024  
 DW 13.300 usec  
 DE 7.50 usec  
 TE 300.0 K  
 D1 0.10000000 sec  
 d11 0.03000000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.60 usec  
 PL1 0.00 dB  
 SF01 125.7690572 MHz

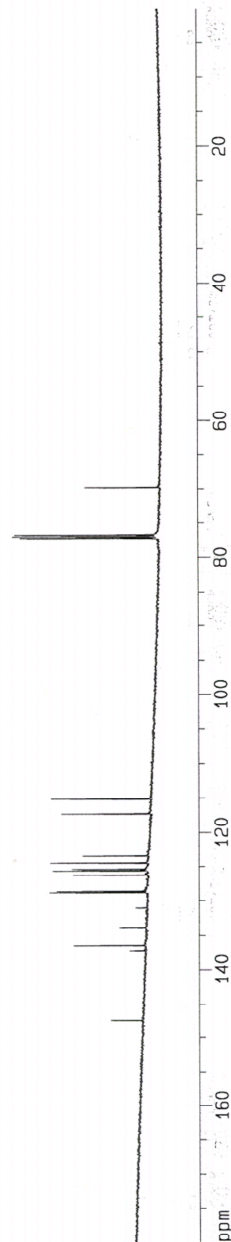
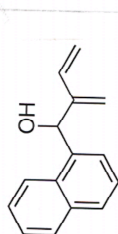
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 120.00 dB  
 PL12 19.00 dB  
 SF02 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7577929 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 F1P 179.908 ppm  
 F1 22624.81 Hz  
 F2P 0.082 ppm  
 F2 10.33 Hz  
 PPMCM 8.99128 ppm/cm  
 HZCM 1130.72400 Hz/cm

77.25  
 77.00  
 76.75  
 69.77

147.37  
 136.45  
 133.90  
 128.81  
 128.62  
 126.32  
 125.65  
 125.40  
 124.48  
 123.42  
 117.26  
 115.12



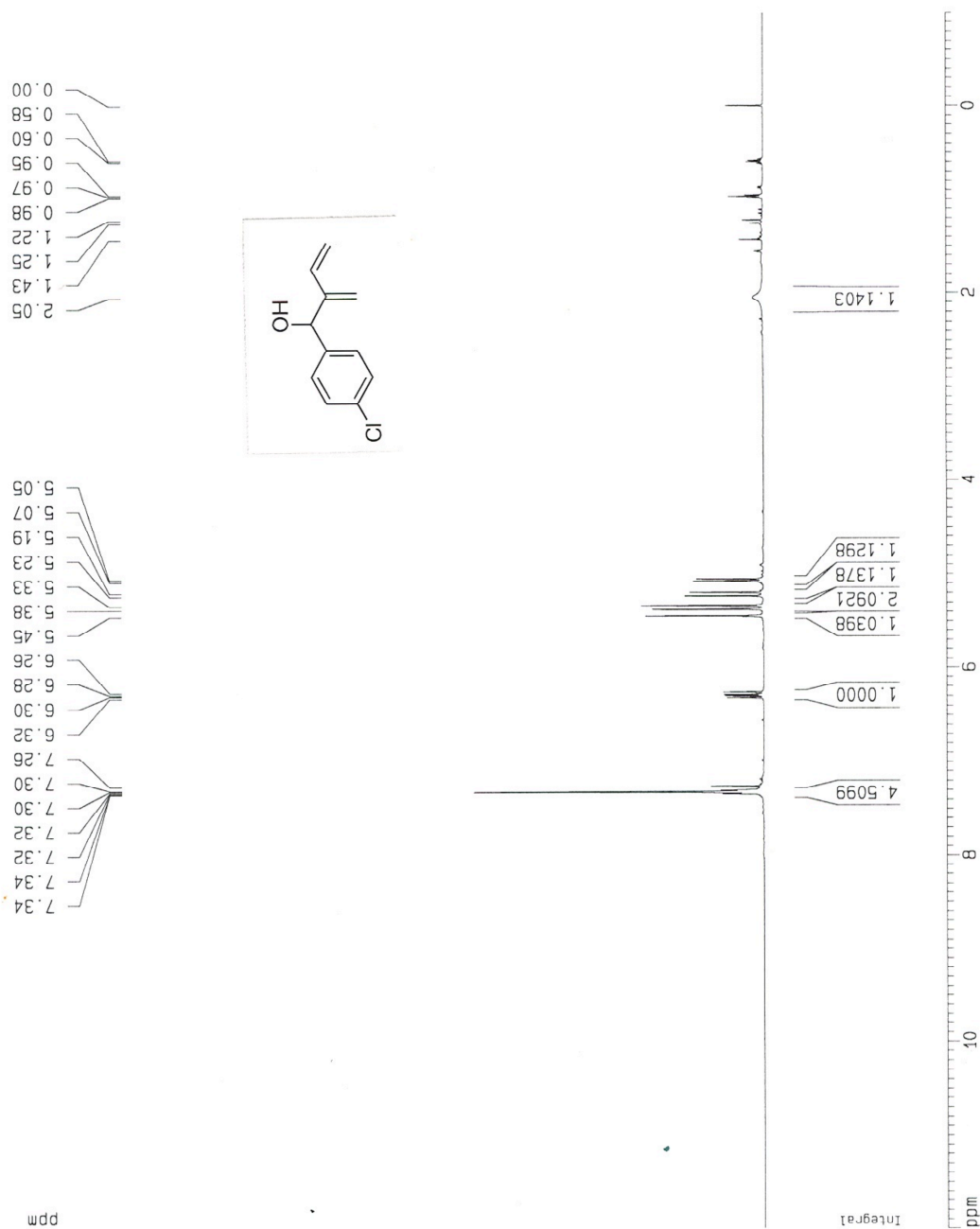
Current Data Parameters  
NAME mm8\_126.pC1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080504  
Time 13:07  
INSTRUM spect  
PROBHD 5 mm GNP 1H  
PULPROG zg  
TD 48076  
SOLVENT CCCl3  
NS 8  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.166670 Hz  
AQ 2.999924 sec  
RG 64  
DM 62.400 usec  
DE 4.50 usec  
TE 300.0 K  
D1 3.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.50 usec  
PL1 0.00 dB  
SF01 500.1325006 MHz

F2 - Processing parameters  
SI 65536  
SF 500.1300158 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
F1P 12.000 ppm  
F1 6001.56 Hz  
F2P -1.000 ppm  
F2 -500.13 Hz  
PPMCM 0.65000 ppm/cm  
HZCM 325.08450 Hz/cm





Current Data Parameters  
NAME mm8\_126.pCl  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080504  
Time 13.50  
INSTRUM spect  
PROBHD 5 mm QNP 1H  
PULPROG zgpg  
TD 75184  
SOLVENT CDCl3  
NS 4000  
DS 0  
SWH 37593.984 Hz  
FIDRES 0.500026 Hz  
AQ 0.9999972 sec  
RG 1024  
DM 13.300 usec  
DE 7.50 usec  
TE 300.0 K  
D1 0.10000000 sec  
d11 0.03000000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 4.60 usec  
PL1 0.00 dB  
SF01 125.7690572 MHz

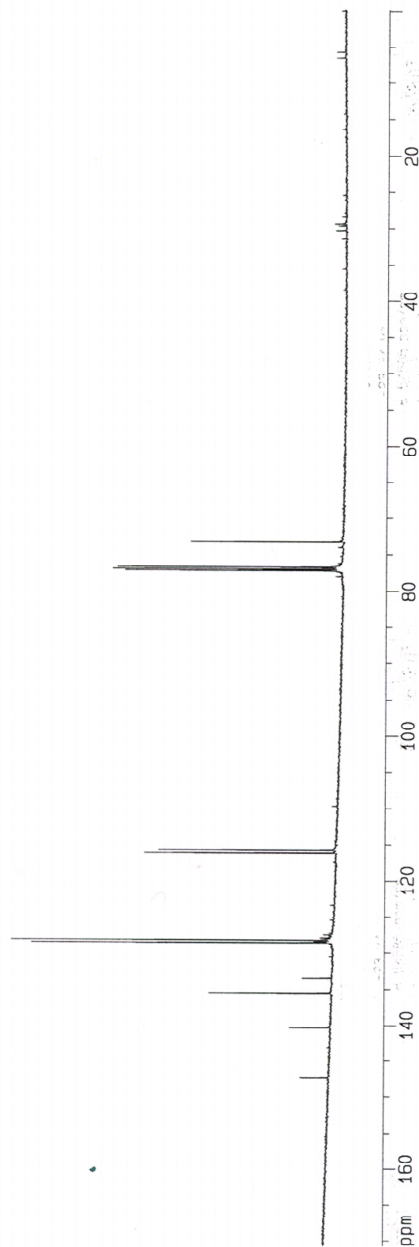
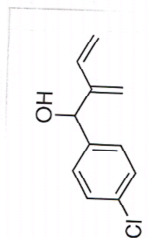
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 120.00 dB  
PL12 19.00 dB  
SF02 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7577941 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR plot parameters  
CX 20.00 cm  
F1P 170.731 ppm  
F1 21470.79 Hz  
F2P -0.186 ppm  
F2 -23.34 Hz  
PPMCM 8.54585 ppm/cm  
HZCM 1074.70667 Hz/cm

77.25  
77.00  
76.75  
73.37

147.36  
140.36  
135.51  
133.54  
128.62  
128.46  
128.24  
116.13  
115.73



Current Data Parameters  
 NAME mm8\_hp  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080706  
 Time 15.05  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-BB  
 PULPROG zg  
 TO 450.44  
 SOLVENT CDCl3  
 NS 8  
 DS 0  
 SWH 7507.507 Hz  
 FIDRES 0.166671 Hz  
 AQ 2.9999804 sec  
 RG 22.6  
 DW 66.600 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 1.00000000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 5.80 usec  
 PL1 0.00 dB  
 SF01 499.8779993 MHz

F2 - Processing parameters  
 SI 32768  
 SF 499.8750197 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

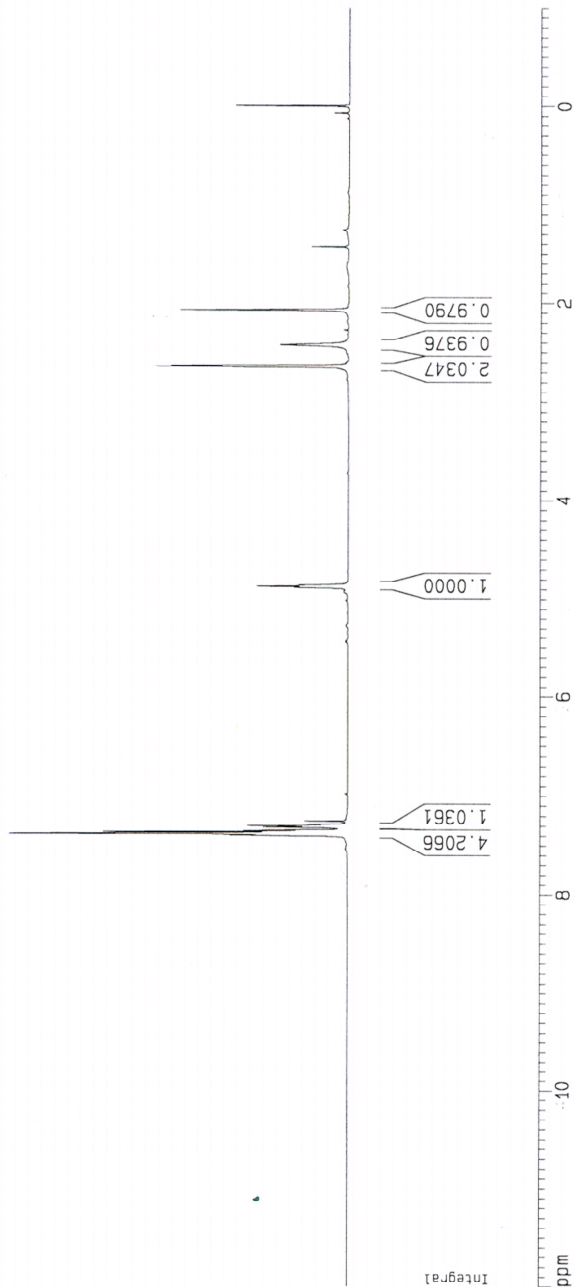
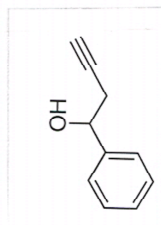
1D NMR plot parameters  
 CX 20.00 cm  
 CY 3.00 cm  
 F1P 12.000 ppm  
 F1 5998.50 Hz  
 F2P -1.000 ppm  
 F2 -499.88 Hz  
 PPMCM 0.65000 ppm/cm  
 HZCM 324.91876 Hz/cm

0.0718  
0.0001

2.6475  
2.6434  
2.6352  
2.6258  
2.0707  
1.4300

4.8812  
4.8693  
4.8576

7.3943  
7.3804  
7.3737  
7.3588  
7.3435  
7.3125  
7.2985  
7.2852  
7.2498





Current Data Parameters  
 NAME mmB\_hjo  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080705  
 Time\_ 15.53  
 INSTRUM spect  
 PROBHD 5 mm BEI 1H-BB  
 PULPROG zgpg  
 TD 181814  
 SOLVENT CDCl3  
 NS 755  
 DS 0  
 SWH 30303.031 Hz  
 FIDRES 0.166671 Hz  
 AQ 2.9999809 sec  
 RG 9195.2  
 DM 16.500 usec  
 DE 4.50 usec  
 TE 300.0 K  
 D1 3.00000000 sec  
 d11 0.03000000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.00 usec  
 PL1 -3.00 dB  
 SF01 125.7049314 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCH02 100.00 usec  
 PL2 120.00 dB  
 PL12 28.00 dB  
 SF02 499.8772000 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.6936781 MHz  
 WDW EN  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1P 180.000 ppm  
 F1 22624.86 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 9.00000 ppm/cm  
 HZCM 1131.24316 Hz/cm

