Electronic Supplementary Material (ESI) for Chemical Communications

Chiral Brønsted Acid Catalyzed Enantioselective Allenylation of Aldehydes

Leleti Rajender Reddy,*

Chemical and Analytical Development, Novartis Pharmaceutical Corporation, East Hanover, New Jersey 07936, USA

General Information. All the reactions were performed under nitrogen gas in glassware's (screw-cap test tubes) that was flame-dried and equipped with a magnetic stirring bar. Thin-layer chromatography (TLC) was performed using silica gel 60 F254 pre-coated plates (0.25 mm). Flash chromatography was performed using silica gel (40 µm particle size). All compounds were judged pure by TLC analysis (single spot/ two solvent systems) using a UV lamp or PMA for detection purposes. ^{1}H and ^{13}C NMR spectra were recorded on a FT-NMR spectrometer at 500 and 125 MHz, respectively. High-resolution mass spectroscopy (HRMS) was carried out in electro spray mode. Enantiomeric excess (ee) was determined using a Waters HPLC a 996 photodiode array detector. The (*R*)-TRIP-PA (**4**) was purchased from Aldrich. All solvents were purchased from Aldrich and used without further purification. The propargyl borolane (**2**) was prepared according to literature procedures.[1] Unless indicated otherwise, the reaction temperatures refer to external reaction temperatures. All the compounds were known compounds and were characterized by comparing their ^{1}H NMR and ^{13}C NMR values to the reported values.

General procedure for the asymmetric propargylation of aldehydes (GP1):

A screw-cap reaction tube with a stir bar was evacuated, flame-dried, and back-filled with nitrogen. To this tube was added the (*R*)-TRIP-PA catalyst **4** (5 mol %), aldehyde **1** (1.0 mmol) and cyclohexane (10.0 mL). The reaction mixture was then cooled to 0 °C followed by the addition of propargyl borolane **2** (1.2 mmol), drop wise (10 min). The mixture was stirred at this temperature 12 h. The reaction mixture was washed with saturated $NaHSO_3$ solution (10 mL) and water (10 mL) and purified by flash chromatography using ethyl acetate and heptanes (2: 8). The pure silyl alcohol was dissolved in THF (5 mL) and was added commercially available tetrabutylammonium fluoride (2 mL, 2.0 mmol, 1.0 M solution in THF, dried over 4 Å molecular sieves for 48 h) at −78 °C. After stirring the reaction mixture for 4 h at −78 °C , it was quenched

with saturated NaCl solution (10mL) at the same temperature and the reaction mixture was allowed to room temperature. The reaction mixture was extracted with ethyl acetate (2 X 10 mL). The combined organic layers was washed with water (10 mL) and concentrated to dryness to obtain crude product. This was purified by flash chromatography using ethyl acetate and heptanes (2: 8) to obtain pure alcohol **3**.

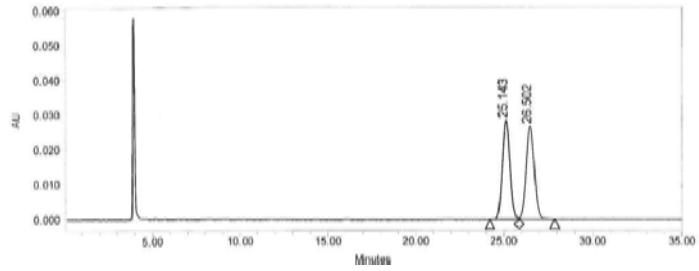
General procedure for the asymmetric propargylation of aldehydes (GP2):

A screw-cap reaction tube with a stir bar was evacuated, flame-dried, and back-filled with nitrogen. To this tube was added the (*R*)-TRIP-PA catalyst **4** (5 mol %), aldehyde **1** (1.0 mmol) and cyclohexane (10.0 mL). The reaction mixture was then cooled to 0 °C followed by the addition of propargyl borolane **2** (1.2 mmol), drop wise (10 min). The mixture was stirred at this temperature 12 h. After comlition of the reaction, it was diluted with THF (5 mL) and was added commercially available tetrabutylammonium fluoride (2 mL, 2.0 mmol, 1.0 M solution in THF, dried over 4 Å molecular sieves for 48 h) at −78 °C. After stirring the reaction mixture for 4 h at −78 °C, it was quenched with saturated NaCl solution (10mL) at the same temperature and the reaction mixture was allowed to room temperature. The reaction mixture was extracted with ethyl acetate (2 X 10 mL). The combined organic layers was washed with water (10 mL) and concentrated to dryness to obtain crude product. This was purified by flash chromatography using ethyl acetate and heptanes (2: 8) to obtain pure alcohol **3**.

(*R*)-1-(4-chlorophenyl)buta-2,3-dien-1-ol (3a):

Following the general procedure (GP1), the reaction of adehyde **1a** (140 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3a** as viscous oil (170 mg, 94%) with 95% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (2% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 25.03 min, t_{minor} = 26.40 min. $[\alpha]^{20}_{D}$ = −56.2 (c 0.8, $CHCl_3$), [literature[2] for *R*-enantiomer with 76% ee. $[\alpha]^{20}_{D}$ = –45.2 (c 1.0, $CHCl_3$)]. ^{1}H NMR (400 MHz, *CDCl*$_3$) δ ppm 7.32 (s, 4 H), 5.39 (q, *J*=6.48 Hz, 1 H), 5.23 (dd, *J*=4.17, 2.40 Hz, 1 H), 4.86 - 5.00 (m, 2 H), 2.34 (s, 1 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.1, 141.2, 133.4, 128.6, 127.5, 94.9, 78.4, 71.3.

Following the general procedure (GP2), the reaction of adehyde **1a** (141 mg, 1.0 mmol) with boronate **2** (286 mg, 1.2 mmol) afforded alcohol **3a** as viscous oil (160 mg, 88%) with 95% ee.



Peak Results

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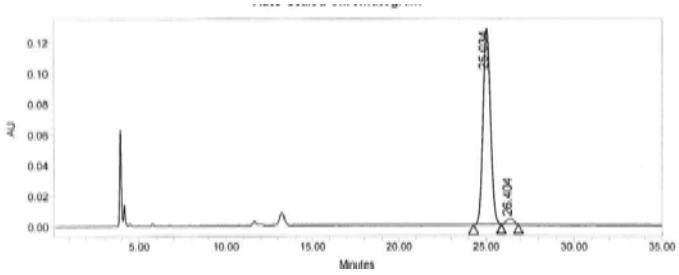

Peak Results

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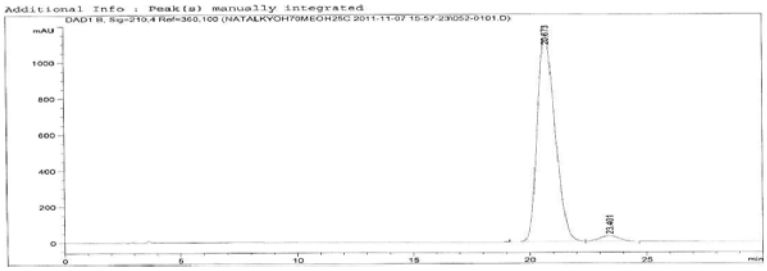
1		25.034	3808103	127432	97.30
2		26.404	105653	3842	2.70

(*R*)-1-(4-bromophenyl)buta-2,3-dien-1-ol (3b):

Following the general procedure (GP1), the reaction of adehyde **1b** (185 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3b** as viscous oil (200 mg, 90%) with 95% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (2% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 20.88 min, t_{minor} = 23.35 min. $[\alpha]^{20}_{D} = -52.2$ (c 1.1, $CHCl_3$). ^{1}H NMR (400 MHz, *CDCl*$_3$) δ ppm 7.26 - 7.37 (m, 2 H), 7.11 (d, *J*=8.34 Hz, 2 H), 5.23 (q, *J*=6.57 Hz, 1 H), 5.01 - 5.09 (m, 1 H), 4.68 - 4.84 (m, 2 H), 2.30 (br. s., 1 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 206.9, 141.5, 131.2, 127.6, 121.3, 94.6, 78.2, 71.1.



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1	20.673	BB	0.8287	6.02536e4	1141.66907	97.2409
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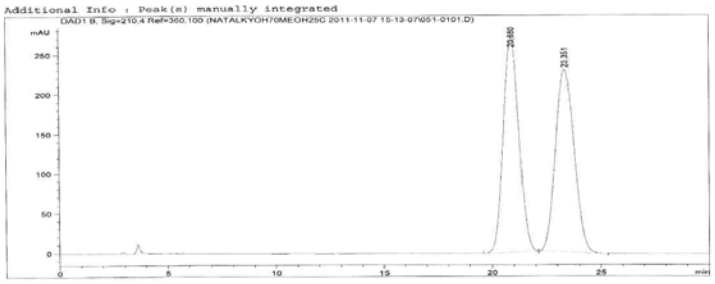

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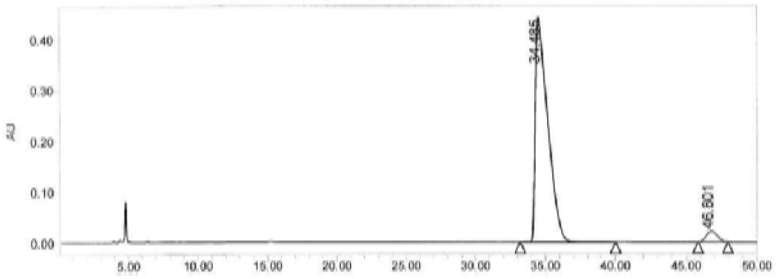
1	20.880	BB	0.7823	1.34776e4	270.03278	50.0167
2	23.351	BB	0.9235	1.34686e4	229.90001	49.9833

(*R*)-1-phenylbuta-2,3-dien-1-ol (3c):

Following the general procedure (GP1), the reaction of adehyde **1c** (108 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3c** as viscous oil (132 mg, 93%) with 91% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column equipped with an OJ-H guard column (3% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 34.22 min, t_{minor} = 46.19 min. $[\alpha]^{20}_{D} = -33.2$ (c 1.0, $CHCl_3$). [literature[3] for *R*-enantiomer with 99% ee. $[\alpha]^{20}_{D} = -34.1$ (c 1.2, $CHCl_3$)]. ^{1}H NMR (400 MHz, *CDCl*$_3$) δ ppm 7.15 - 7.45 (m, 5 H), 5.44 (q, *J*=6.57 Hz, 1 H), 5.26 (d, *J*=6.32 Hz, 1 H), 4.83 - 5.01 (m, 2 H), 2.25 (s, 1 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.1, 142.8, 128.5, 127.8, 126.1, 95.2, 78.2, 72.0.



Peak Results

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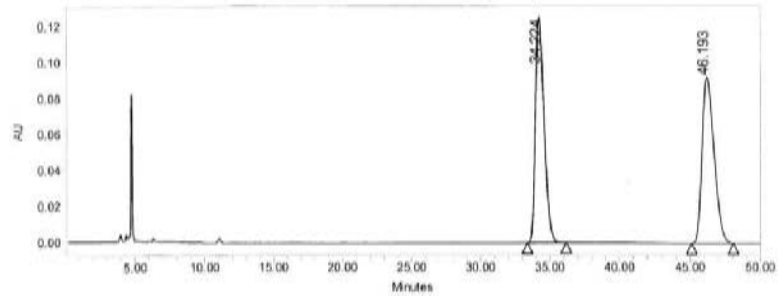
1		34.485	27341299	442860	95.87
2		46.801	1178920	21199	4.13

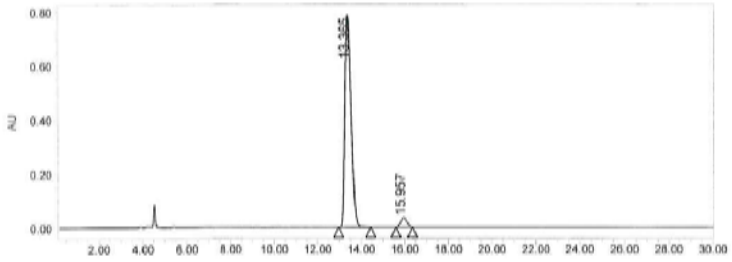


Peak Results

	Name	RT	Area	Height	% Area
1		34.224	5436131	125504	49.97
2		46.193	5441675	92323	50.03

(*R*)-1-(*o*-tolyl)buta-2,3-dien-1-ol (3d):

Following the general procedure (GP1), the reaction of adehyde **1d** (120 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3d** as viscous oil (144 mg, 90%) with 91% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (2.5% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 13.42 min, t_{minor} = 15.85 min. (The silyl intermediate was isolated 202 mg, 92% yield). $[\alpha]^{20}_{D}$ = −46.2 (c 1.3, $CHCl_3$). ^{1}H NMR (400 MHz, *CDCl*$_3$) δ 7.28 - 7.39 (m, 1 H), 6.93 - 7.15 (m, 3 H), 5.31 - 5.38 (m, 1 H), 5.25 (q, *J*=6.48 Hz, 1 H), 4.64 - 4.82 (m, 2 H), 2.21 (s, 3 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.0, 140.5, 134.9, 130.2, 127.3, 126.0, 125.1, 94.1, 77.7, 68.8, 24.4, 18.8.



Peak Results

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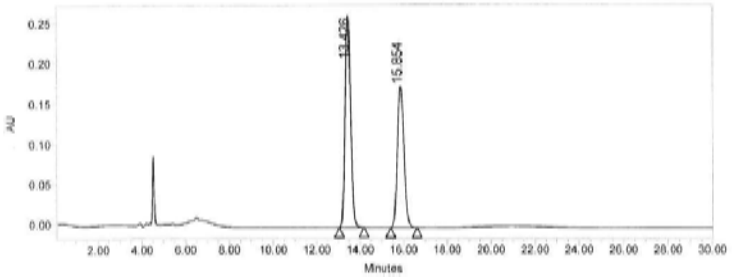
1		13.365	15468272	787563	95.58
2		15.957	718699	35771	4.42



Peak Results

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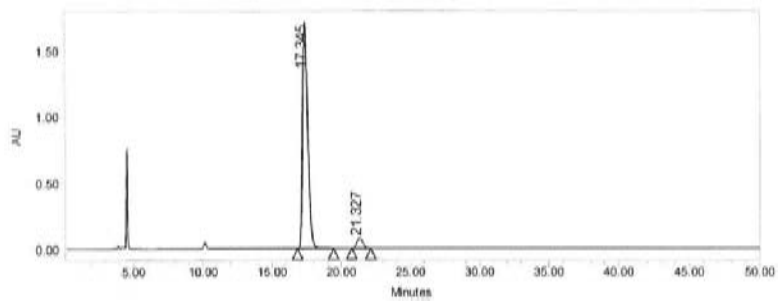
1		13.426	4655892	263467	55.78
2		15.854	3690670	175780	44.22

(*R*)-1-(*p*-tolyl)buta-2,3-dien-1-ol (3e):

Following the general procedure (GP1), the reaction of adehyde **1e** (120 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3e** as viscous oil (148 mg, 93%) with 91% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (5% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 17.34 min, t_{minor} = 21.32 min. $[\alpha]^{20}_{D} = -52.5$ (c 0.9, $CHCl_3$). ^{1}H NMR (400 MHz, *CDCl*$_3$) δ 7.28 (d, *J*=8.08 Hz, 2 H), 7.16 (d, *J*=7.83 Hz, 2 H), 5.42 (q, *J*=6.57 Hz, 1 H), 5.18 - 5.29 (m, 1 H), 4.84 - 4.98 (m, 2 H), 2.34 (s, 3 H), 2.13 (br. s., 1 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.1, 139.9, 137.5, 129.2, 126.0, 95.2, 78.1, 71.8, 21.1.



Peak Results

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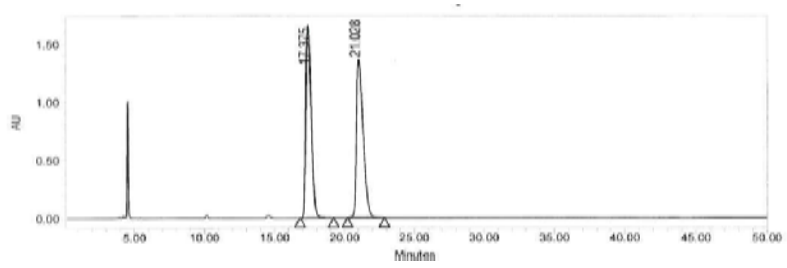
1		17.345	45365362	1710374	95.28
2		21.327	2245944	76827	4.72

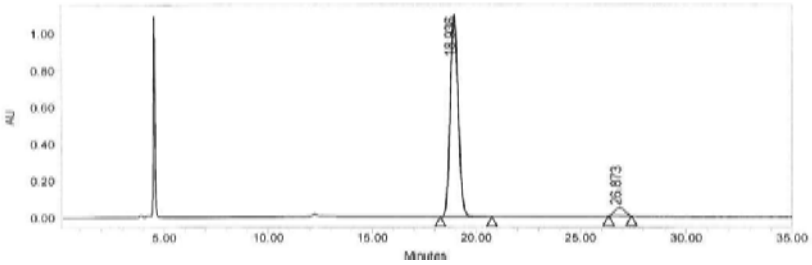


Peak Results

	Name	RT	Area	Height	% Area
1		17.375	44115631	1657882	49.33
2		21.028	45317201	1363009	50.67

(*R*)-1-(*p*-Methoxyphenyl)buta-2,3-dien-1-ol (3f):

Following the general procedure (GP1), the reaction of adehyde **1f** (136 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3f** as viscous oil (163 mg, 93%) with 90% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (2.5% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 18.93 min, t_{minor} = 26.87 min. $[\alpha]^{20}_{D} = -53.1$ (c 0.8, $CHCl_3$). ^{1}H NMR (400 MHz, *CDCl*$_3$) δ 77.24 - 7.39 (m, 2 H), 6.85 - 6.96 (m, 2 H), 5.21 (t, *J*=2.91 Hz, 1 H), 4.71 (dd, *J*=4.93, 3.16 Hz, 2 H), 3.75 - 3.89 (m, 4 H), 1.91 (s, 1 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.8, 160.4, 136.3, 129.4, 114.7, 102.6, 85.1, 74.1, 73.4, 56.4, 25.8.



Peak Results

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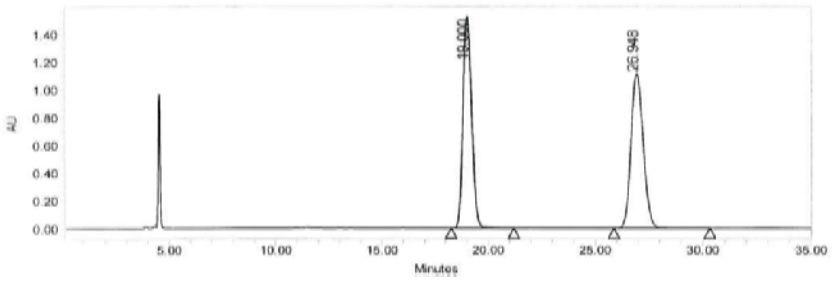
1		18.936	29808915	1098263	95.01
2		26.873	1566343	46129	4.99

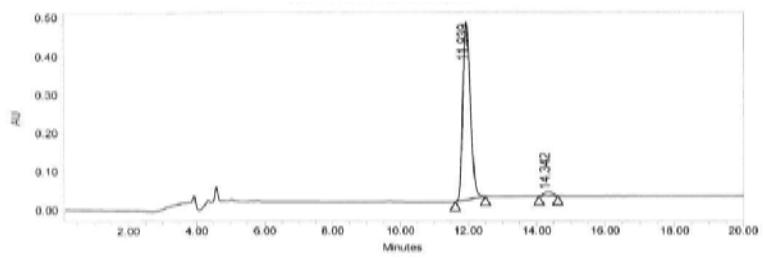


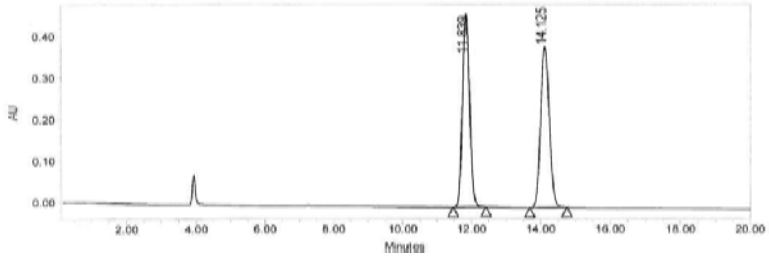
Peak Results

	Name	RT	Area	Height	% Area
1		19.000	43745538	1522072	49.40
2		26.948	44801759	1110865	50.60

(*R*)-1-(thiophen-2-yl)buta-2,3-dien-1-ol (3g):

Following the general procedure (GP1), the reaction of adehyde **1g** (112 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3g** as viscous oil (135 mg, 89%) with 95% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (5% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 11.93 min, t_{minor} = 14.34 min. $[\alpha]^{20}_{D} = -42.3$ (c 1.2, $CHCl_3$). ^{1}H NMR (400 MHz, *CDCl*$_3$) δ 7.10 - 7.18 (m, 1 H), 6.77 - 6.95 (m, 2 H), 5.26 - 5.50 (m, 2 H), 4.70 - 4.94 (m, 2 H), 2.27 (d, *J*=3.79 Hz, 11 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.1, 146.9, 126.7, 125.2, 124.3, 94.8, 78.8, 68.0.



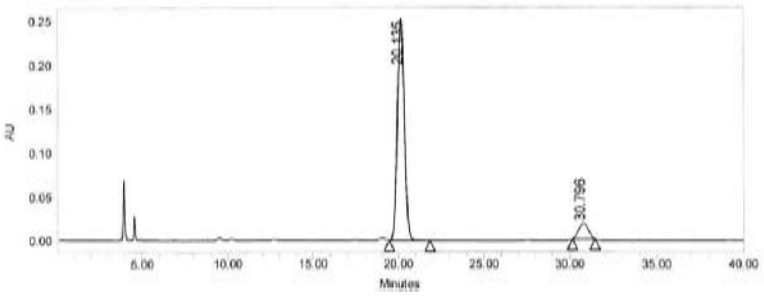


Peak Results

	Name	RT	Area	Height	% Area
1		11.839	6644911	466049	49.94
2		14.125	6660333	387159	50.06

(*S,E*)-1-phenylhexa-1,4,5-trien-3-ol (3h):[4]

Following the general procedure (GP1), the reaction of adehyde **1h** (132 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3h** as viscous oil (158 mg, 92%) with 82% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (5% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 20.13 min, t_{minor} = 30.79 min. $[\alpha]^{20}_{D}$ = +51.5 (c 0.6, $CHCl_3$). ^{1}H NMR (400 MHz, *CDCl*$_3$) δ 7.35 - 7.42 (m, 2 H), 7.27 - 7.35 (m, 2 H), 7.19 - 7.27 (m, 1 H), 6.63 (d, *J*=15.66 Hz, 1 H), 6.27 (dd, *J*=15.92, 6.32 Hz, 1 H), 5.36 (q, *J*=6.32 Hz, 1 H), 4.92 (dd, *J*=6.57, 2.53 Hz, 2 H), 4.80 - 4.89 (m, 1 H), 2.13 (br. s., 1 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.3, 136.5, 130.7, 130.4, 128.6, 127.8, 126.6, 98.8, 78.2, 70.4.



Peak Results

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1		20.135	7112260	252763	91.07
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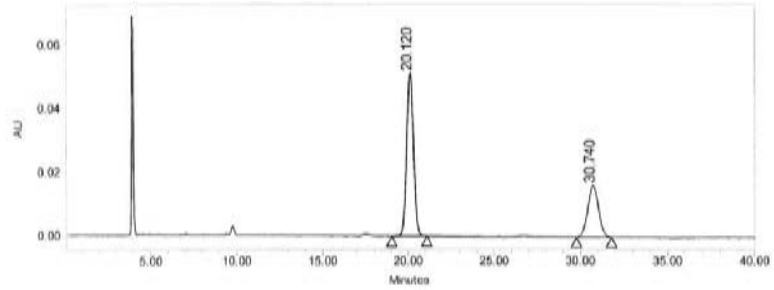
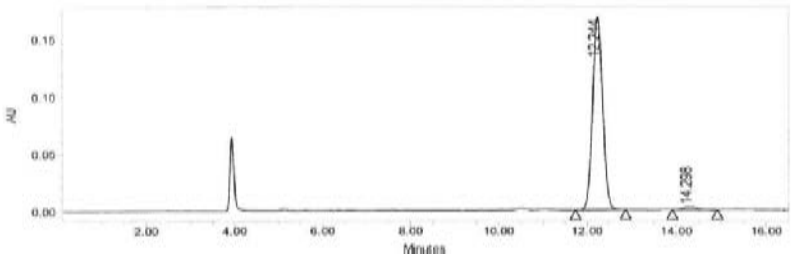


Peak Results

	Name	RT	Area	Height	% Area
1		20.120	1440060	51204	66.67
2		30.740	720054	16277	33.33

(*S*)-1-phenylhexa-4,5-dien-3-ol (3i):

Following the general procedure (GP1), the reaction of adehyde **1i** (134 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3i** as viscous oil (156 mg, 90%) with 96% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OD-H column equipped with an OD-H guard column (8% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 12.24 min, t_{minor} = 14.29 min. $[\alpha]^{20}_{D}$ = +14.3 (c 1.1, $CHCl_3$). [literature[4] for *S*-enantiomer with 88% ee. $[\alpha]^{20}_{D}$ = +11.8 (c 1.0, $CHCl_3$)]. ^{1}H NMR (400 MHz, *CDCl*$_3$) δ 7.09 - 7.37 (m, 5 H), 5.28 (q, *J*=6.57 Hz, 1 H), 4.88 (dd, *J*=6.69, 2.40 Hz, 2 H), 4.12 - 4.25 (m, 1 H), 2.61 - 2.86 (m, 2 H), 1.82 - 2.00 (m, 2 H), 1.71 (br. s., 1 H). ^{13}C NMR (125 MHz, *CDCl*$_3$) δ ppm 207.0, 141.8, 128.4, 125.8, 94.7, 77.8, 68.9, 39.0, 31.7.



Peak Results

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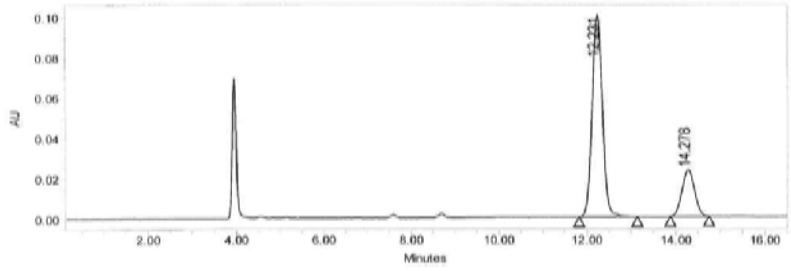

Peak Results

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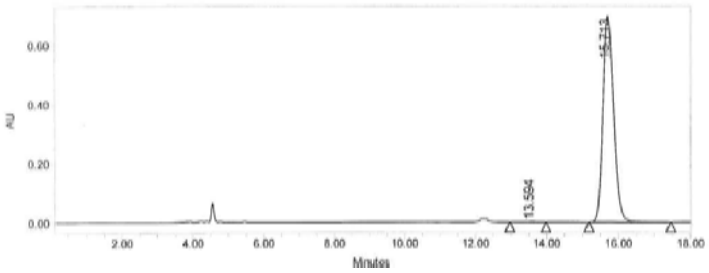
1		12.231	1614107	100039	78.20
2		14.278	450008	23163	21.80

(*S*)-1-cyclohexylbuta-2,3-dien-1-ol (3j):

Following the general procedure (GP1), the reaction of adehyde **1j** (112 mg, 1.0 mmol) with boronate **2** (285 mg, 1.2 mmol) afforded alcohol **3j** as viscous oil (142 mg, 94%) with 99% ee. Enantiomeric excess was determined by HPLC with a Chiralcel OJ-H column equipped with an OJ-H guard column (1% IPA in hexane, flow rate = 0.8 mL/min), t_{major} = 15.71 min, t_{minor} = 13.59 min. $[\alpha]^{20}_{D}$ = +16.8 (c 1.0, Benzene). [literature[4] for *S*-enantiomer with 90% ee. $[\alpha]^{20}_{D}$ = +14.2 (c 1.1, Benzene)]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.09 (q, *J*=6.57 Hz, 1 H), 4.71 (dd, *J*=6.57, 2.27 Hz, 2 H), 3.72 - 3.86 (m, 1 H), 1.46 - 1.79 (m, 6 H), 1.23 - 1.40 (m, 1 H), 0.77 - 1.23 (m, 5 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ ppm 207.0, 93.0, 73.8, 43.9, 28.4, 28.0, 26.2, 25.8, 25.8, 24.4.



Peak Results

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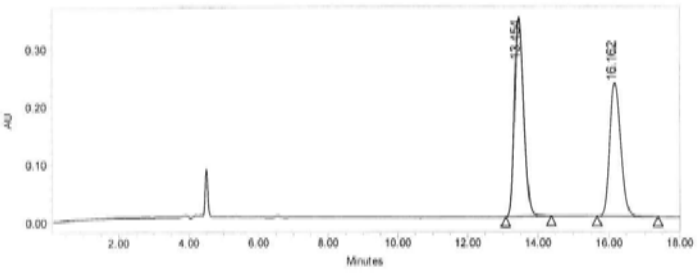
2		15.713	14271321	695433	99.83



[1] R. W.Hoffmann, H. Brinkmann, G. Frenking, *Chemische Berichte* **1990**, *123*, 2387.

[2] Y. Wang, K. Zheng, R. Hong. *J. Am. Chem. Soc*. **2012**, *134*, 4096.

[3] M. Yoshida, Y. Shoji, K. Shishido. *Tetrahedron* **2010**, *66*, 5053.

[3] E. J. Corey, M. L. Chan, H. Duck. *J. Am. Chem. Soc*. **1990**, *112*, 878.

[4] G. Xia, H. Yamamoto. *J. Am. Chem. Soc*. **2007**, *129*, 496.

5/16/2012 3:54:14 PM

Acquisition Time (sec)	3.9584	***Comment***	Chloro-allenyl-p	***Date***	18 Apr 2012 23:10:56		
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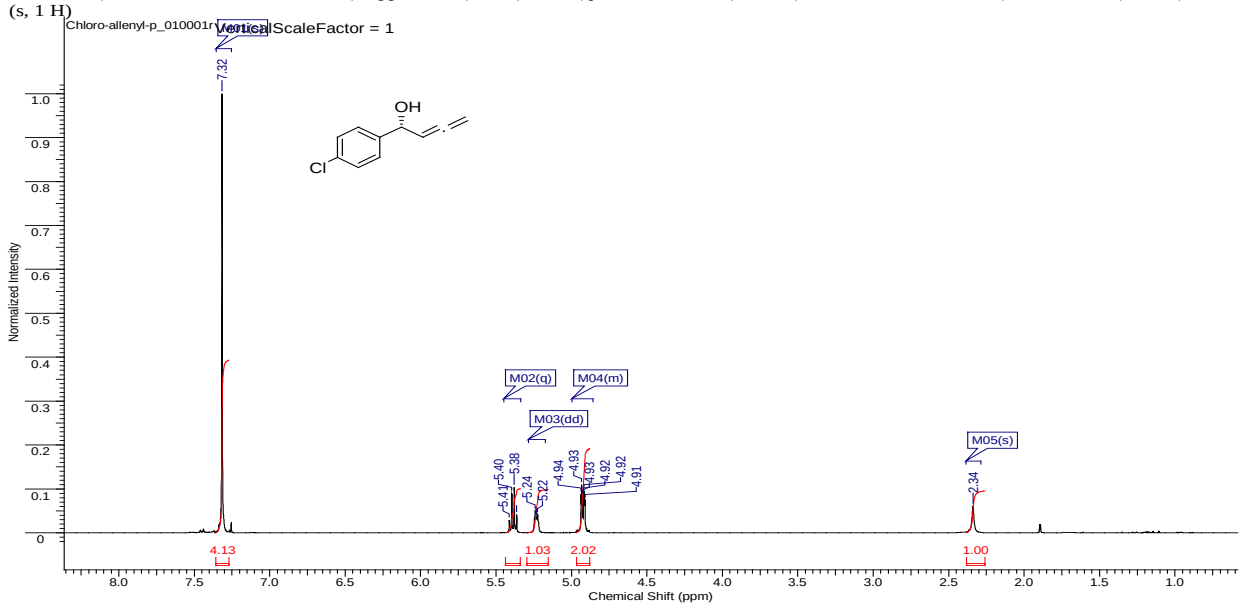
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	128.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2455.5339
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.32 (s, 4 H), 5.39 (q, *J*=6.48 Hz, 1 H), 5.23 (dd, *J*=4.17, 2.40 Hz, 1 H), 4.86 - 5.00 (m, 2 H), 2.34 (s, 1 H)



5/16/2012 3:57:46 PM

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Date Stamp	19 Apr 2012 05:41:20						
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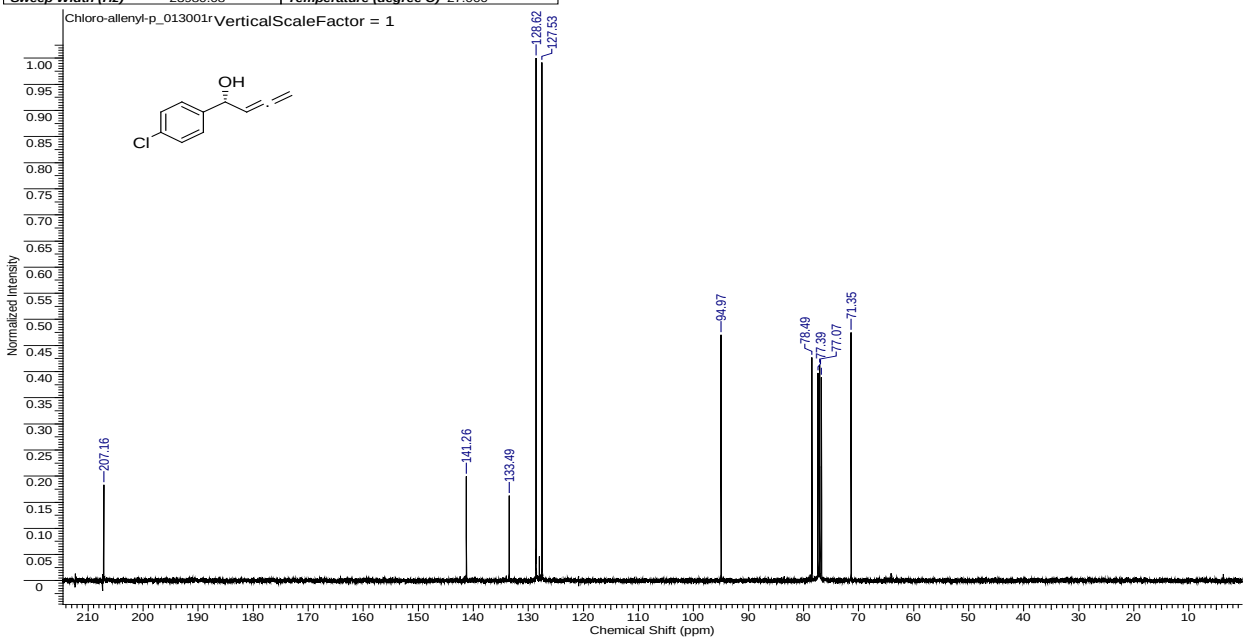
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	14596.50
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 4:26:29 PM

Acquisition Time (sec)	3.9584	***Comment***	P-Br-all-2	***Date***	06 May 2012 00:00:00		
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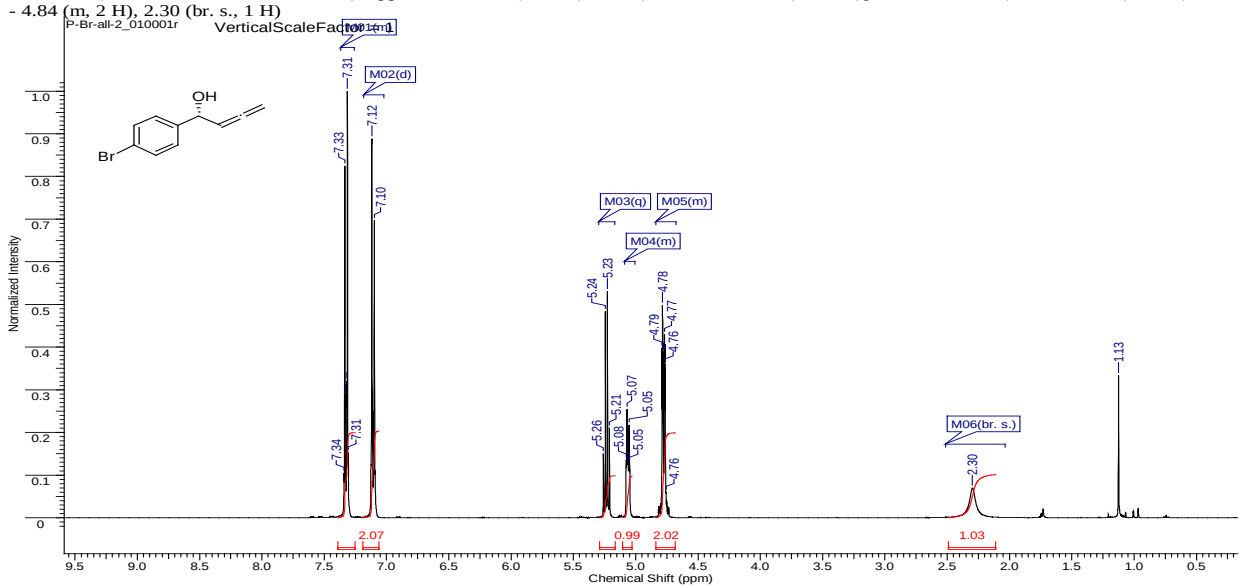
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	90.50
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2400.6772
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.26 - 7.37 (m, 2 H), 7.11 (d, *J*=8.34 Hz, 2 H), 5.23 (q, *J*=6.57 Hz, 1 H), 5.01 - 5.09 (m, 1 H), 4.68 - 4.84 (m, 2 H), 2.30 (br. s., 1 H)



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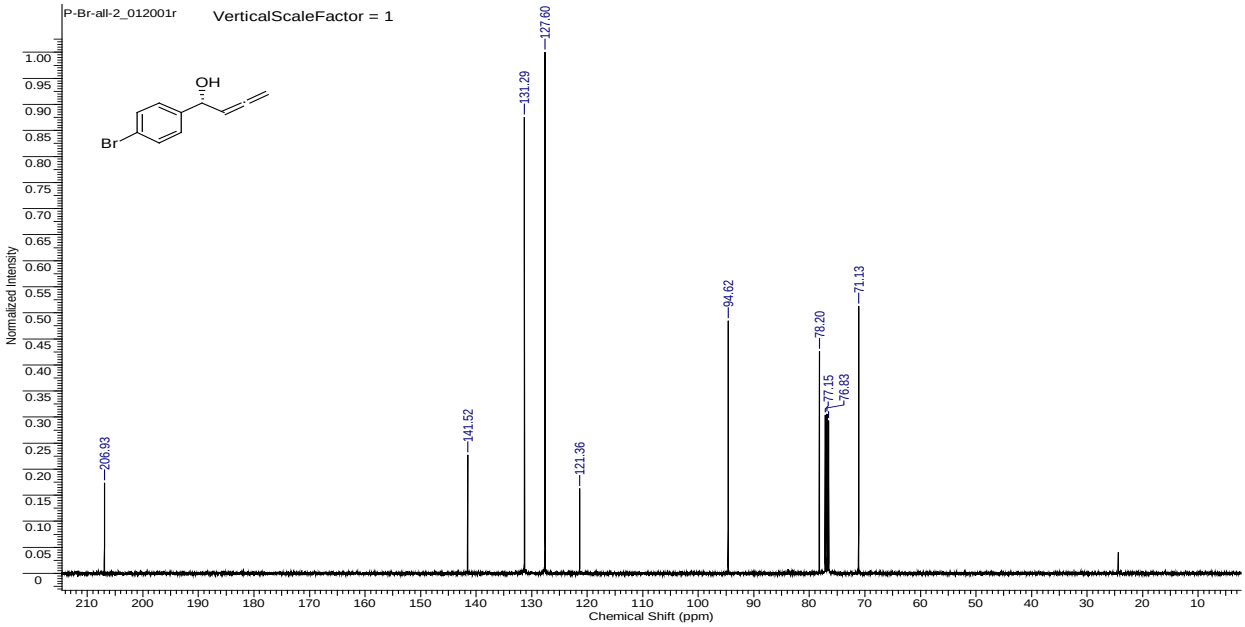
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10035.1045
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



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Acquisition Time (sec)	3.9584	***Comment***	Chloro-allenyl-p	***Date***	18 Apr 2012 23:10:56		
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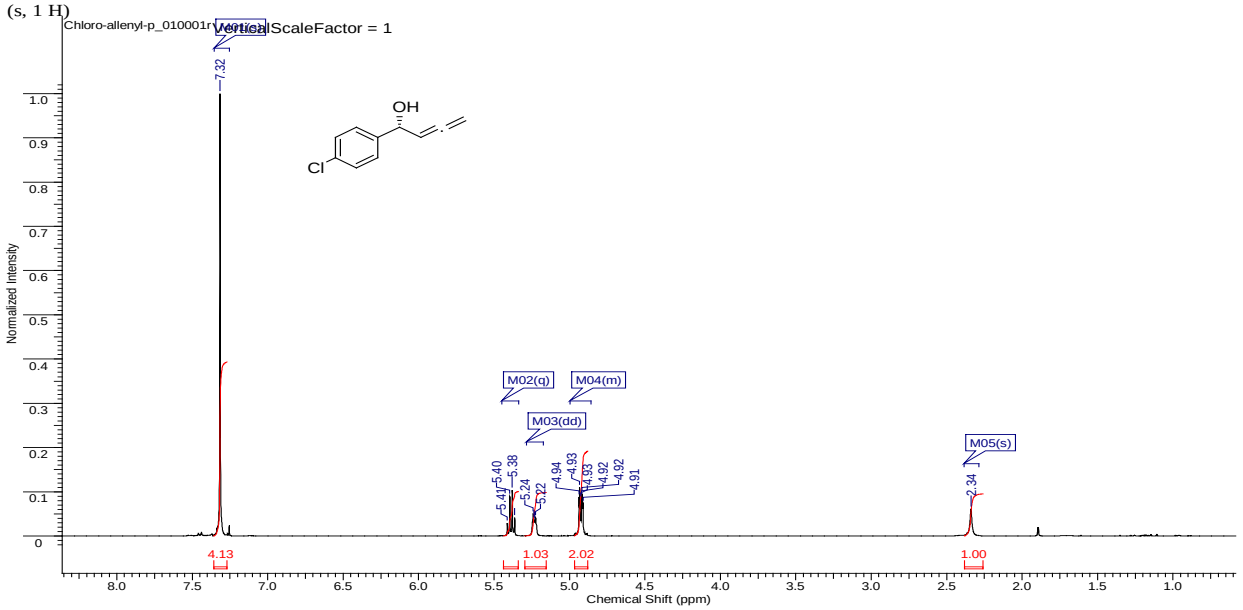
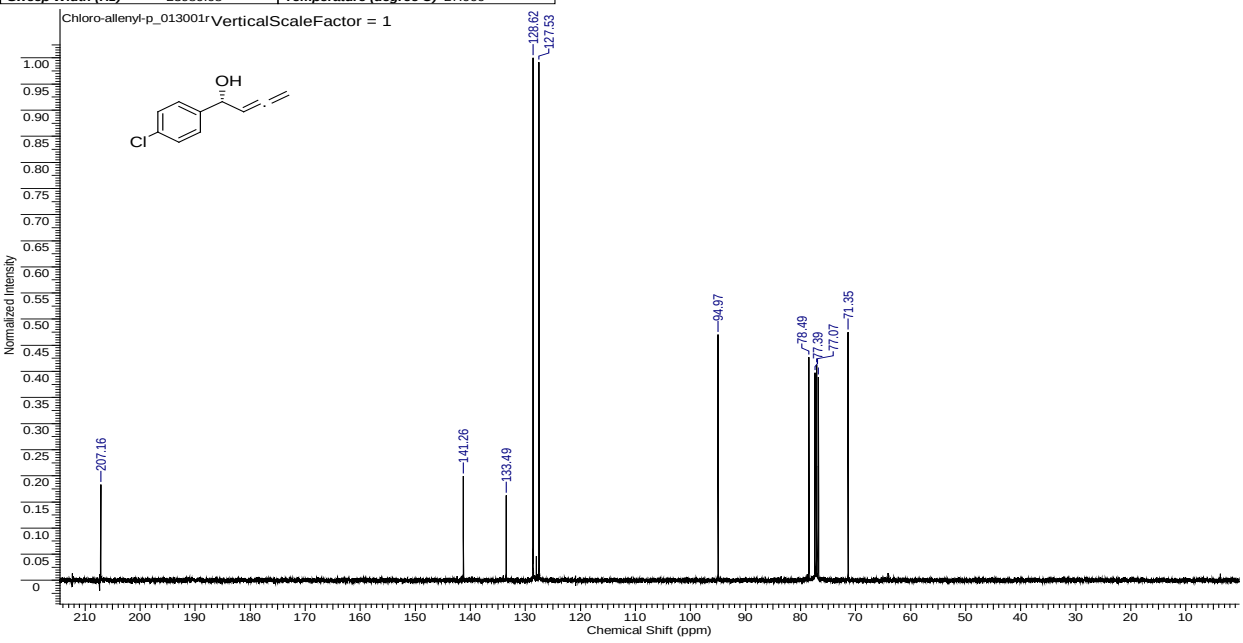
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Chloro-allenyl-p_010001r					***Frequency (MHz)***	400.19
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	128.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2455.5339
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.32 (s, 4 H), 5.39 (q, *J*=6.48 Hz, 1 H), 5.23 (dd, *J*=4.17, 2.40 Hz, 1 H), 4.86 - 5.00 (m, 2 H), 2.34 (s, 1 H)



5/16/2012 3:57:46 PM

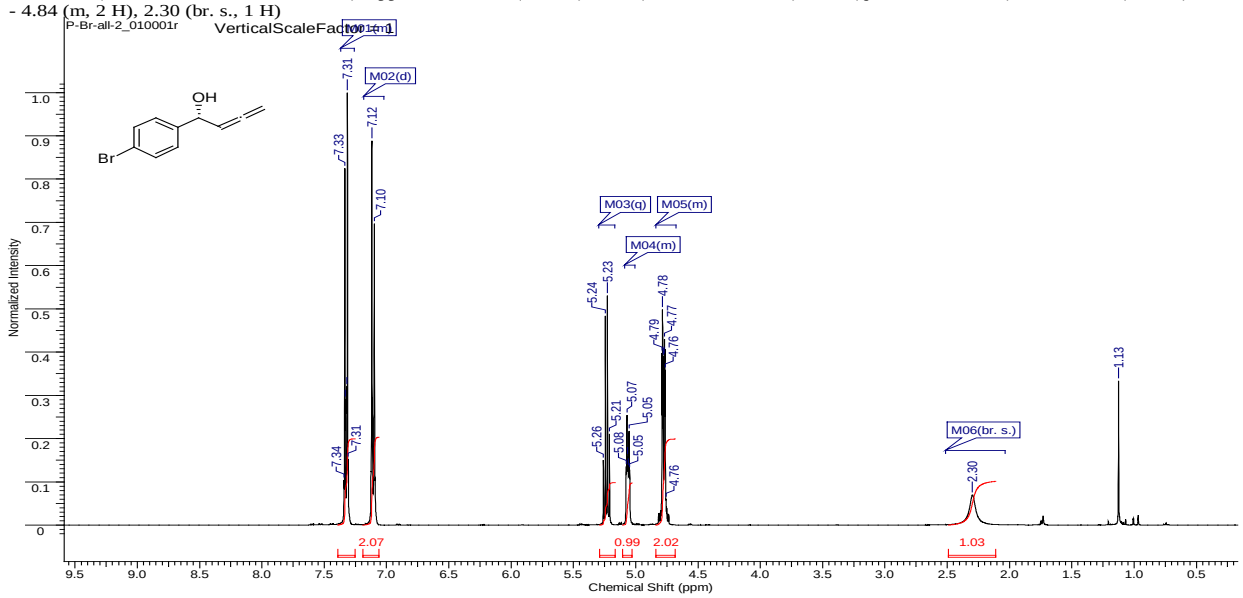
Acquisition Time (sec)	1.3664	***Comment***	Chloro-allenyl-p	***Date***	19 Apr 2012 05:41:20		
Date Stamp	19 Apr 2012 05:41:20						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Chloro-allenyl-p_013001r					***Frequency (MHz)***	100.63
Nucleus	13C	***Number of Transients***	2048	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	14596.50
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 4:26:29 PM

Acquisition Time (sec)	3.9584	***Comment***	P-Br-all-2	***Date***	06 May 2012 00:00:00		
Date Stamp	06 May 2012 00:00:00						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\P-Br-all-2_010001r					***Frequency (MHz)***	400.19
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	90.50
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2400.6772
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.26 - 7.37 (m, 2 H), 7.11 (d, *J*=8.34 Hz, 2 H), 5.23 (q, *J*=6.57 Hz, 1 H), 5.01 - 5.09 (m, 1 H), 4.68 - 4.84 (m, 2 H), 2.30 (br. s., 1 H)



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Acquisition Time (sec)	1.3664	***Comment***	P-Br-all-2	***Date***	06 May 2012 01:16:48		
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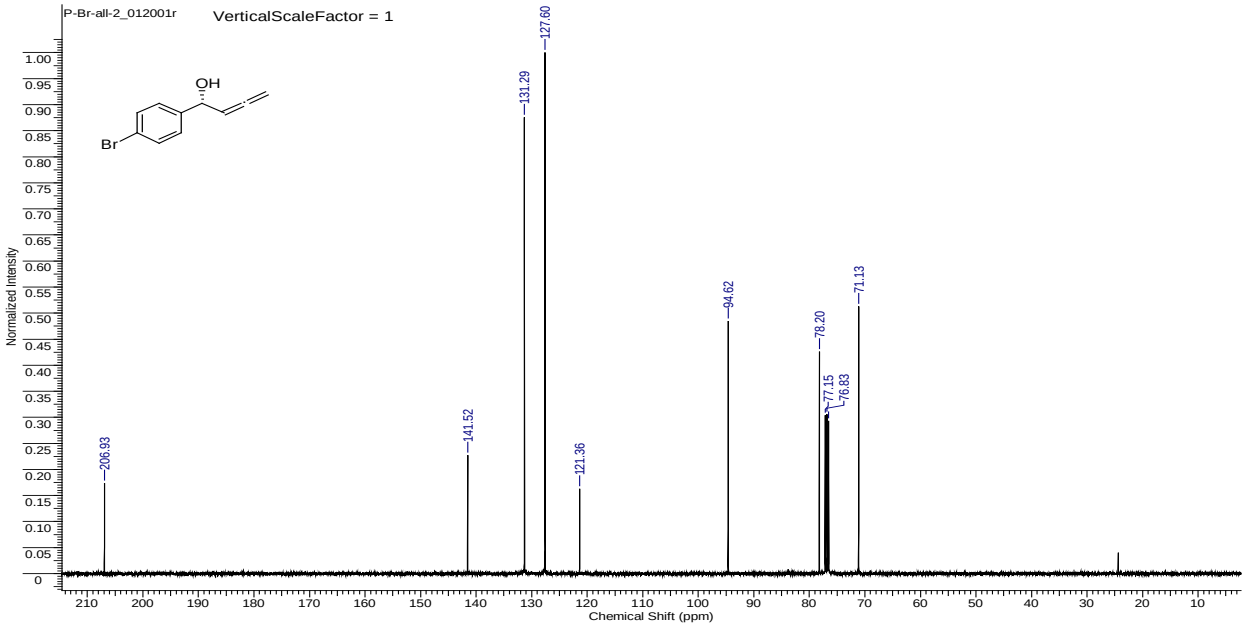
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10035.1045
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



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Date Stamp	23 Apr 2012 18:52:48						
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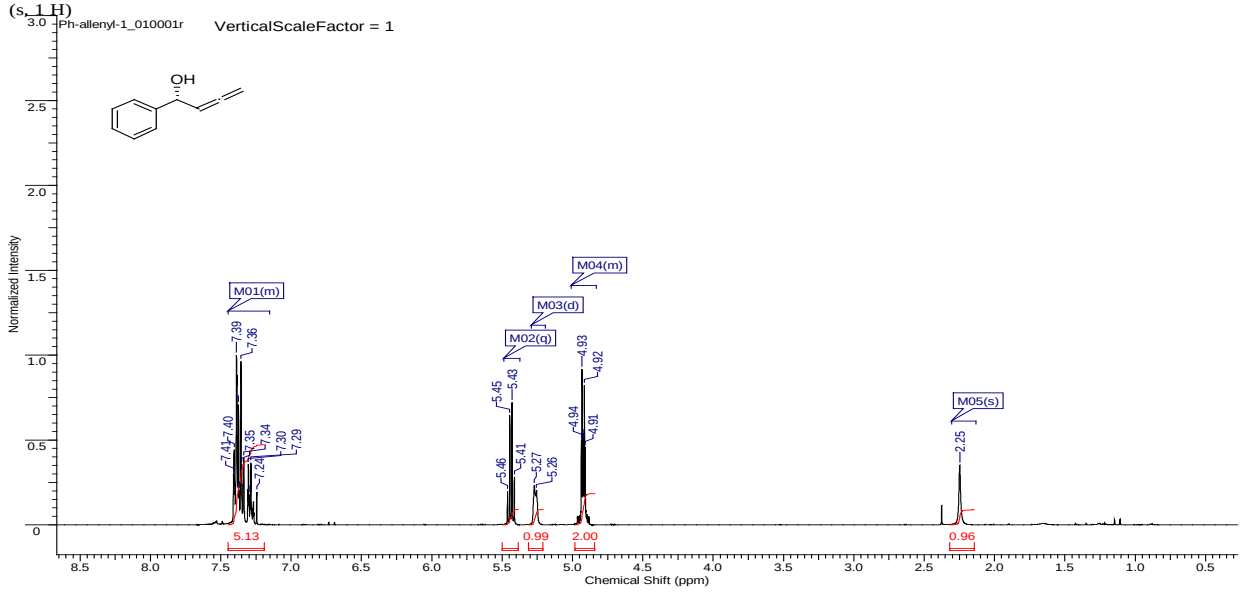
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	128.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2451.4324
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.15 - 7.45 (m, 5 H), 5.44 (q, *J*=6.57 Hz, 1 H), 5.26 (d, *J*=6.32 Hz, 1 H), 4.83 - 5.01 (m, 2 H), 2.25 (s, 1 H)



5/16/2012 5:15:21 PM

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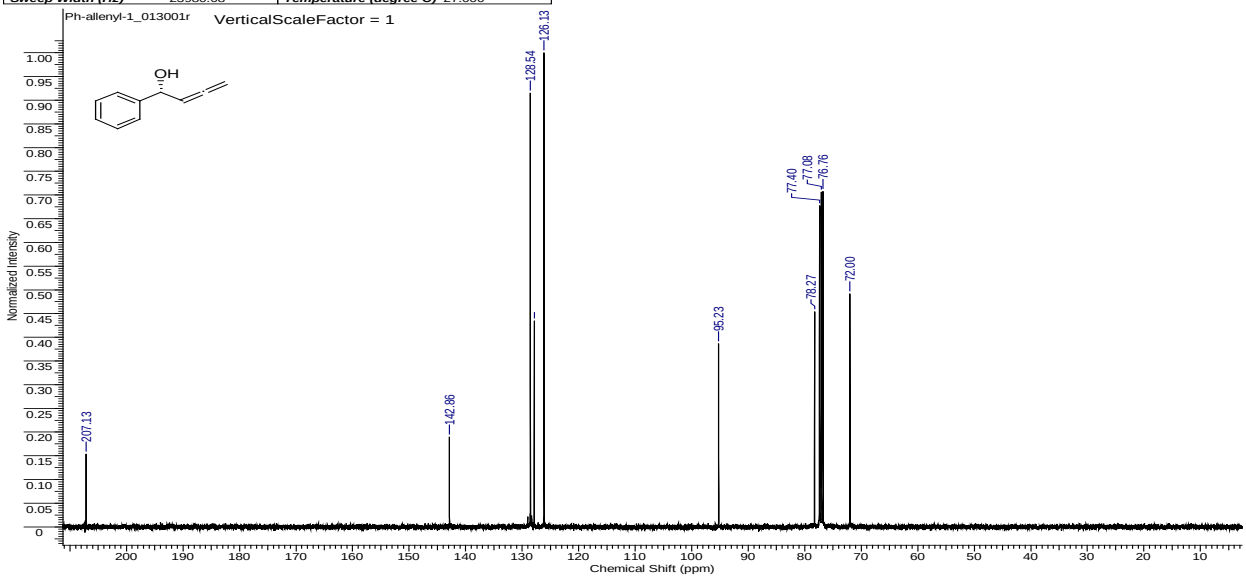
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 5:36:23 PM

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Date Stamp	04 May 2012 23:47:12						
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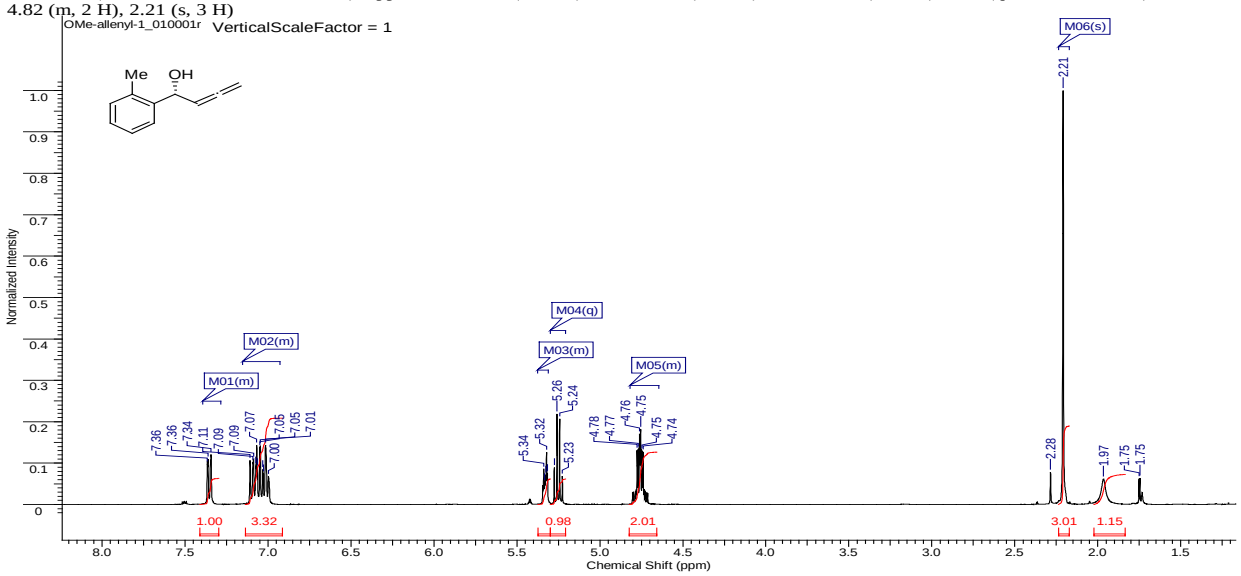
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	128.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2396.3875
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.28 - 7.39 (m, 1 H), 6.93 - 7.15 (m, 3 H), 5.31 - 5.38 (m, 1 H), 5.25 (q, *J*=6.48 Hz, 1 H), 4.64 - 4.82 (m, 2 H), 2.21 (s, 3 H)



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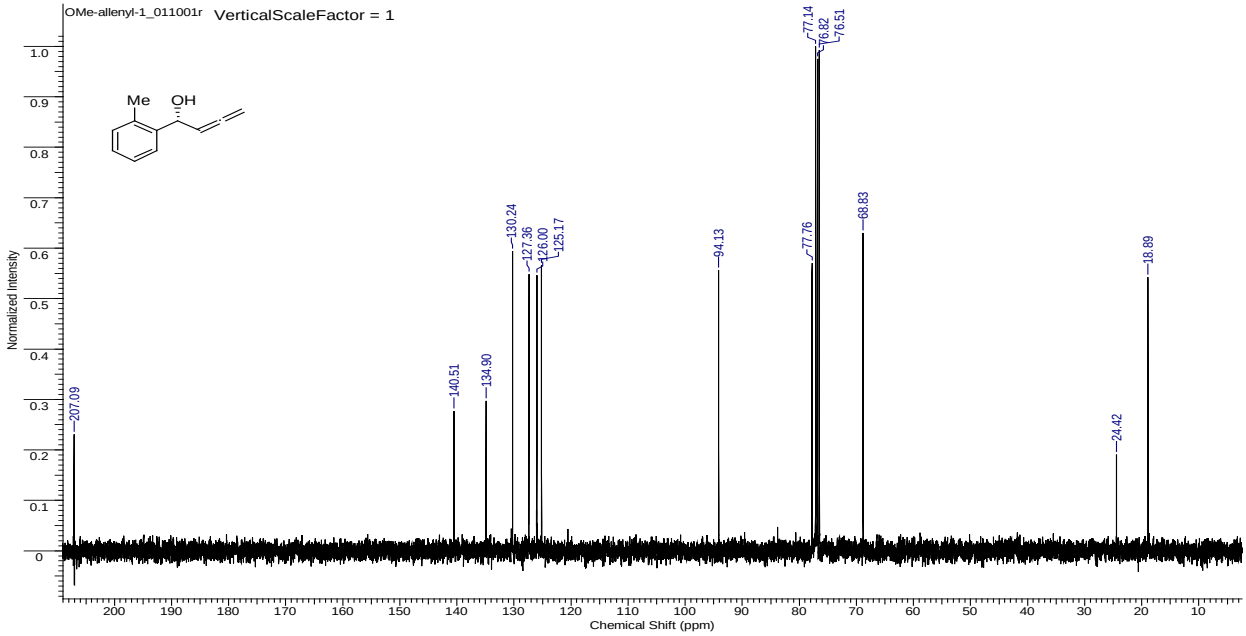
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11042.7217
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



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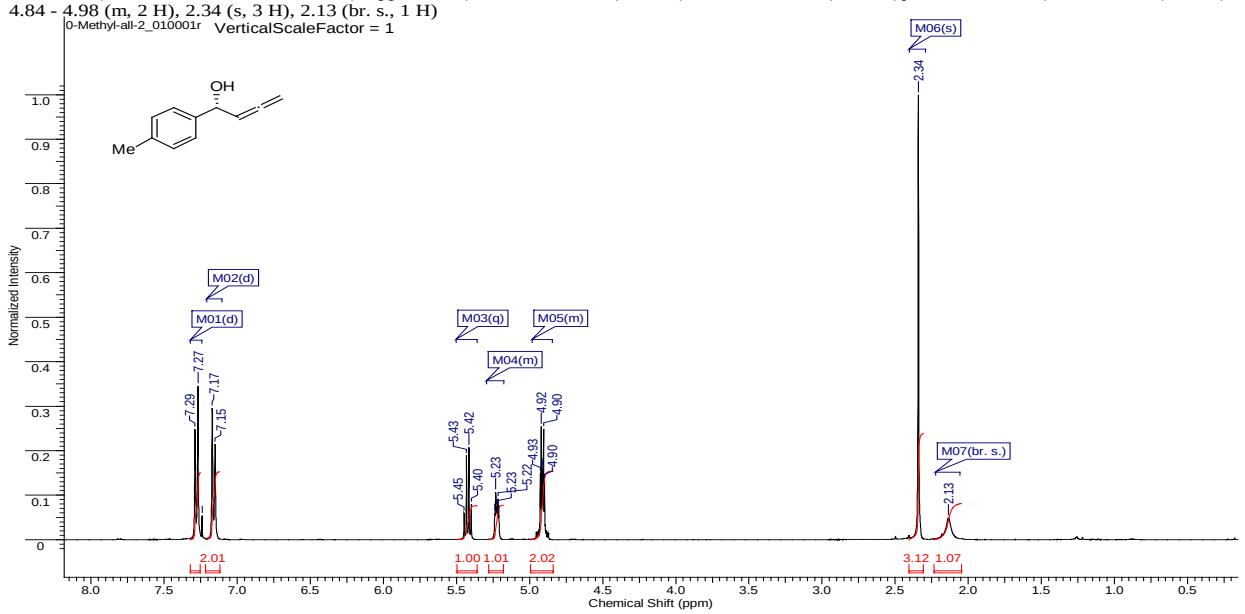
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	101.60
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2449.8203
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.28 (d, *J*=8.08 Hz, 2 H), 7.16 (d, *J*=7.83 Hz, 2 H), 5.42 (q, *J*=6.57 Hz, 1 H), 5.18 - 5.29 (m, 1 H), 4.84 - 4.98 (m, 2 H), 2.34 (s, 3 H), 2.13 (br. s., 1 H)



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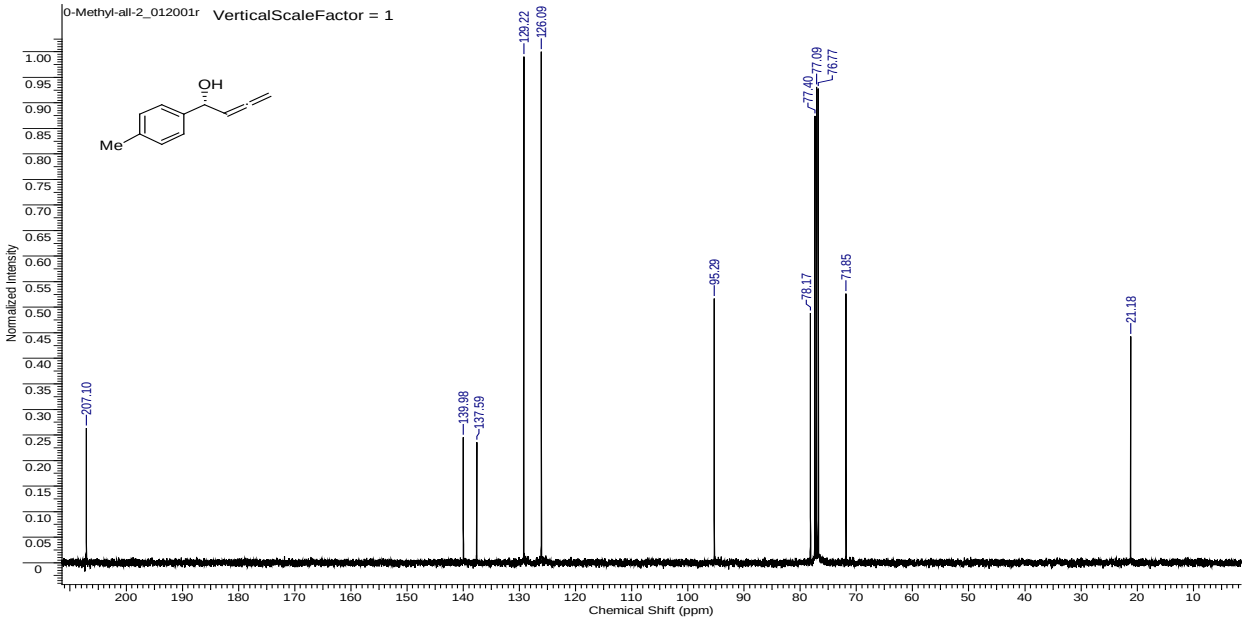
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	13004.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 6:30:09 PM

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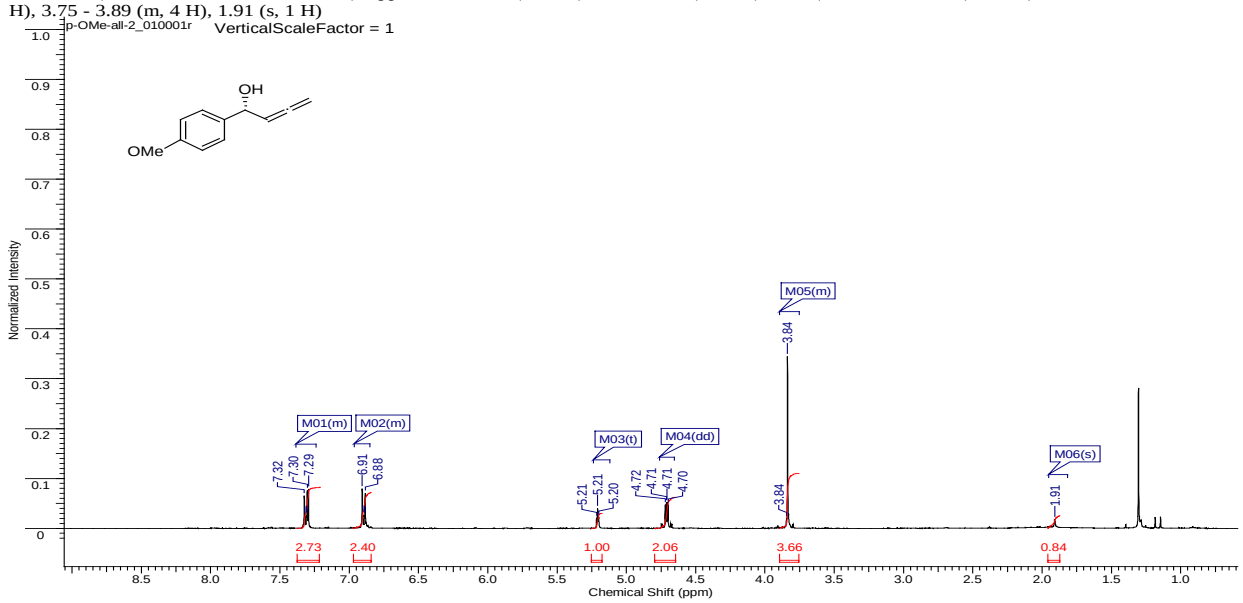
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	181.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2471.1260
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.24 - 7.39 (m, 2 H), 6.85 - 6.96 (m, 2 H), 5.21 (t, *J*=2.91 Hz, 1 H), 4.71 (dd, *J*=4.93, 3.16 Hz, 2 H), 3.75 - 3.89 (m, 4 H), 1.91 (s, 1 H)



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Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
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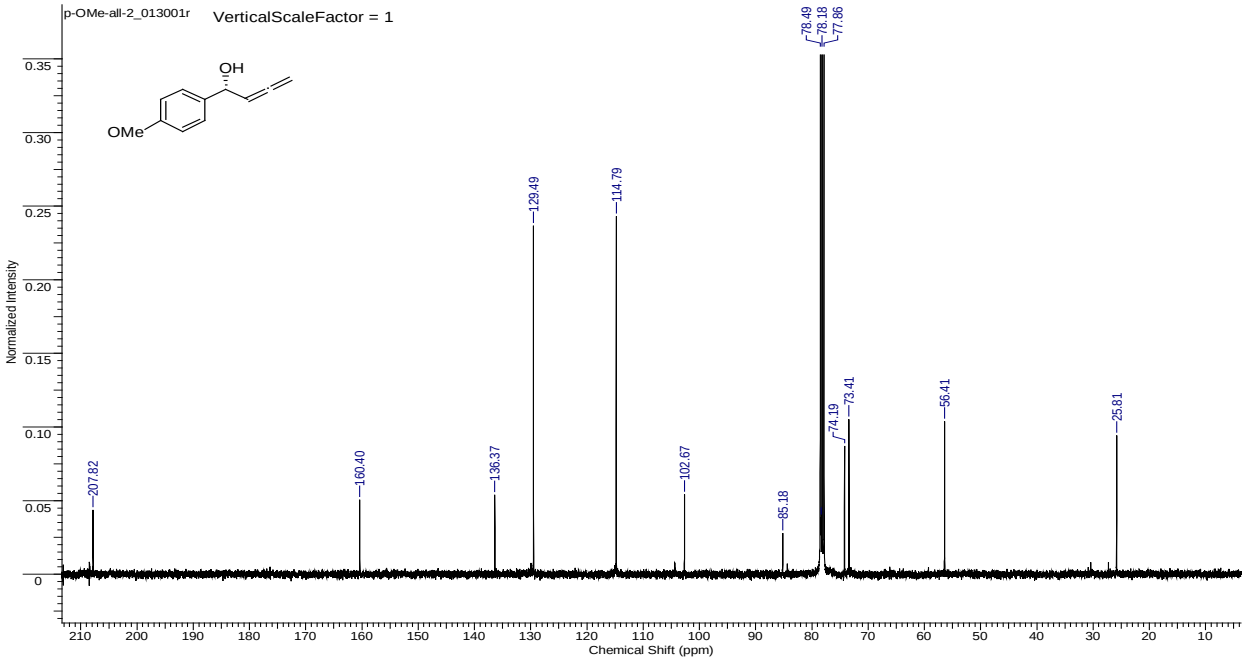

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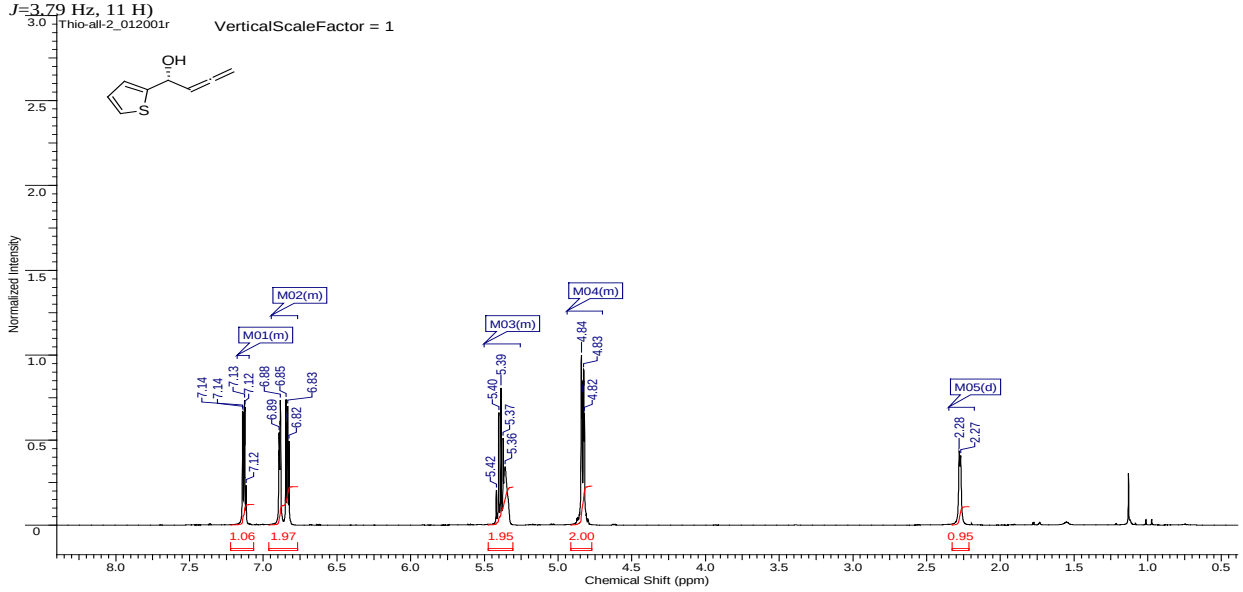
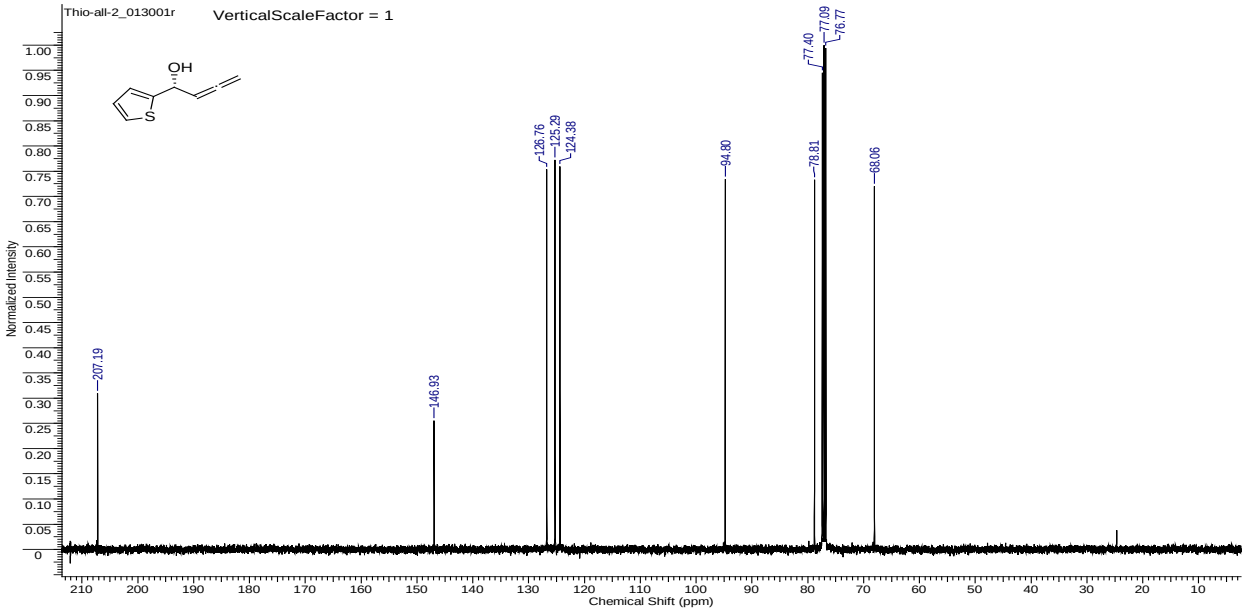
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	128.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2399.9490
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.10 - 7.18 (m, 1 H), 6.77 - 6.95 (m, 2 H), 5.26 - 5.50 (m, 2 H), 4.70 - 4.94 (m, 2 H), 2.27 (d, *J*=3.79 Hz, 11 H)



5/16/2012 7:52:22 PM

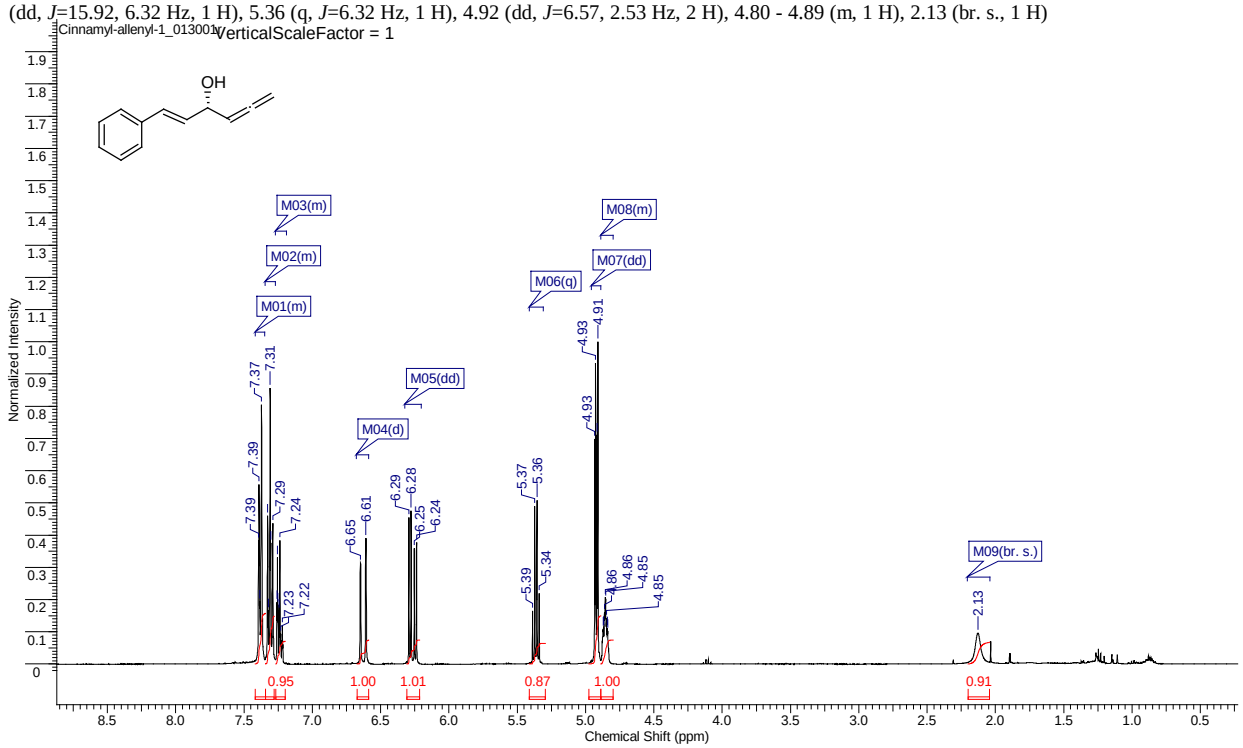
Acquisition Time (sec)	1.3664	***Comment***	Thio-all-2	***Date***	07 May 2012 03:14:08		
Date Stamp	07 May 2012 03:14:08						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Thio-all-2_013001r					***Frequency (MHz)***	100.63
Nucleus	13C	***Number of Transients***	2048	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 10:31:21 PM

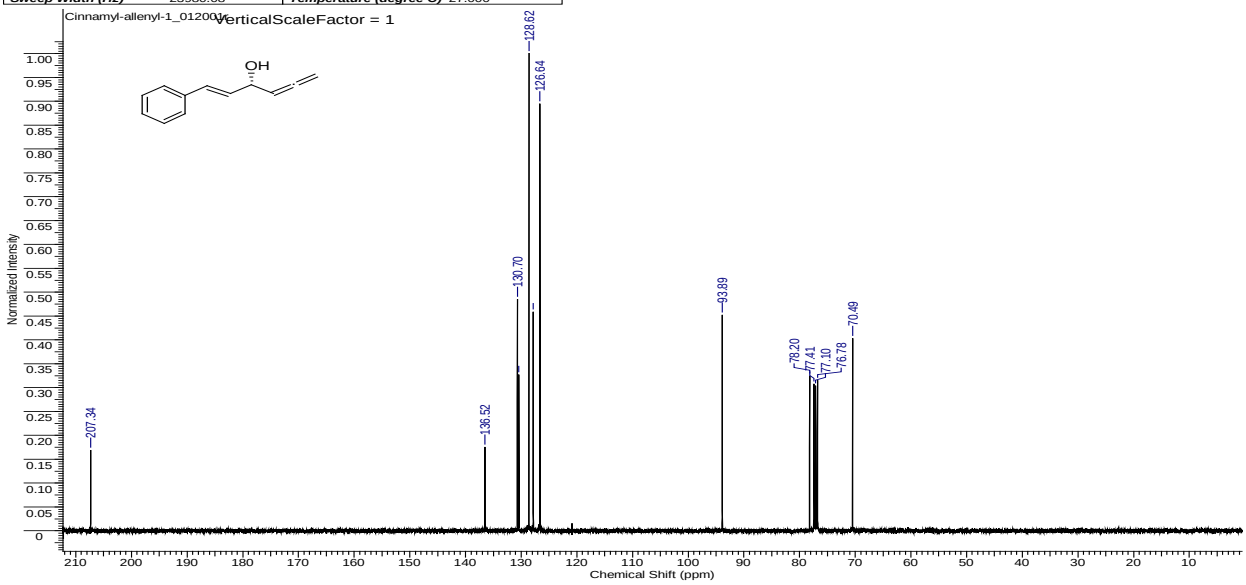
Acquisition Time (sec)	3.9584	***Comment***	Cinnamyl-allenyl-1			***Date***	25 Apr 2012 05:41:20
Date Stamp	25 Apr 2012 05:41:20						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Cinnamyl-allenyl-1_013001r					***Frequency (MHz)***	400.19
Nucleus	1H	***Number of Transients***	1024	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	114.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2450.5845
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.35 - 7.42 (m, 2 H), 7.27 - 7.35 (m, 2 H), 7.19 - 7.27 (m, 1 H), 6.63 (d, *J*=15.66 Hz, 1 H), 6.27 (dd, *J*=15.92, 6.32 Hz, 1 H), 5.36 (q, *J*=6.32 Hz, 1 H), 4.92 (dd, *J*=6.57, 2.53 Hz, 2 H), 4.80 - 4.89 (m, 1 H), 2.13 (br. s., 1 H)



5/16/2012 10:35:54 PM

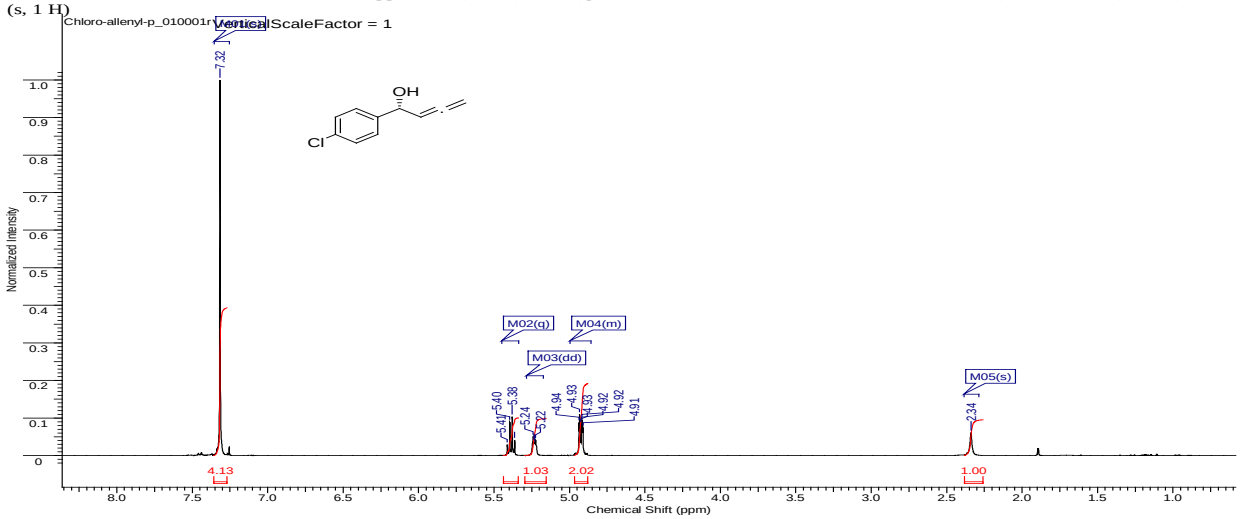
Acquisition Time (sec)	1.3664	***Comment***	Cinnamyl-allenyl-1			***Date***	25 Apr 2012 04:16:00
Date Stamp	25 Apr 2012 04:16:00						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Cinnamyl-allenyl-1_012001r					***Frequency (MHz)***	100.63
Nucleus	13C	***Number of Transients***	2048	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	16384.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 3:54:14 PM

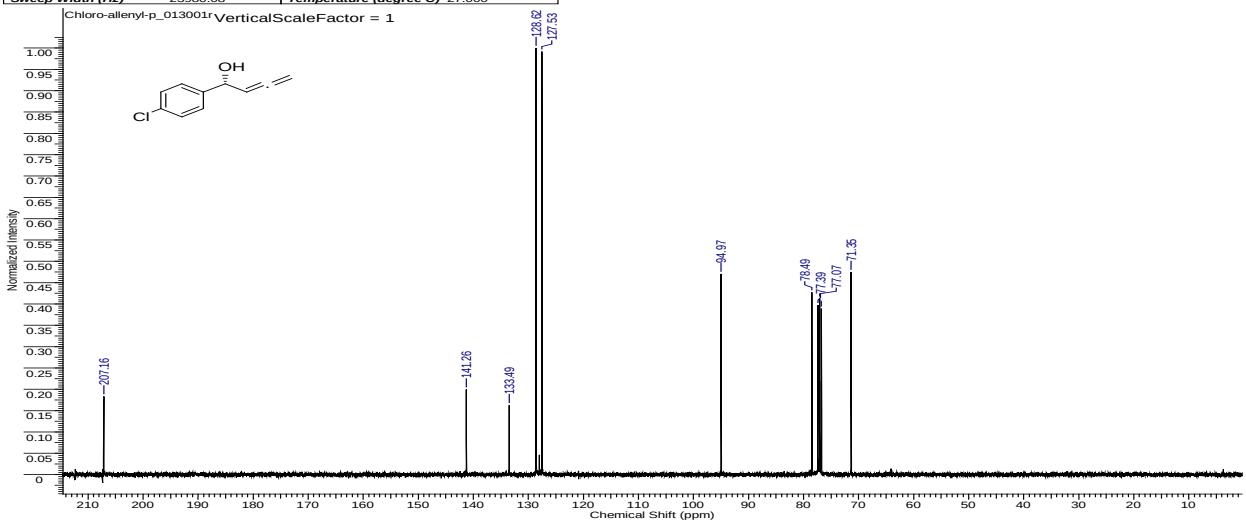
Acquisition Time (sec)	3.9584	***Comment***	Chloro-allenyl-p	***Date***	18 Apr 2012 23:10:56		
Date Stamp	18 Apr 2012 23:10:56						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Chloro-allenyl-p_010001r					***Frequency (MHz)***	400.19
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	128.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2455.5339
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.32 (s, 4 H), 5.39 (q, *J*=6.48 Hz, 1 H), 5.23 (dd, *J*=4.17, 2.40 Hz, 1 H), 4.86 - 5.00 (m, 2 H), 2.34 (s, 1 H)



5/16/2012 3:57:46 PM

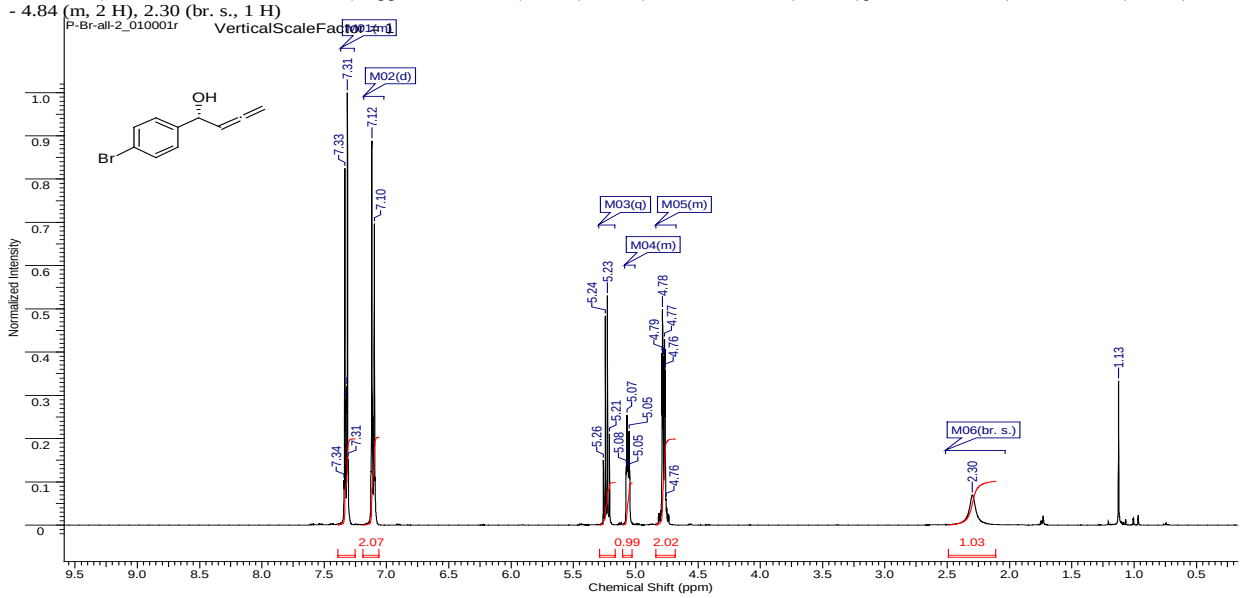
Acquisition Time (sec)	1.3664	***Comment***	Chloro-allenyl-p	***Date***	19 Apr 2012 05:41:20		
Date Stamp	19 Apr 2012 05:41:20						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Chloro-allenyl-p_013001r					***Frequency (MHz)***	100.63
Nucleus	13C	***Number of Transients***	2048	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	14596.50
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 4:26:29 PM

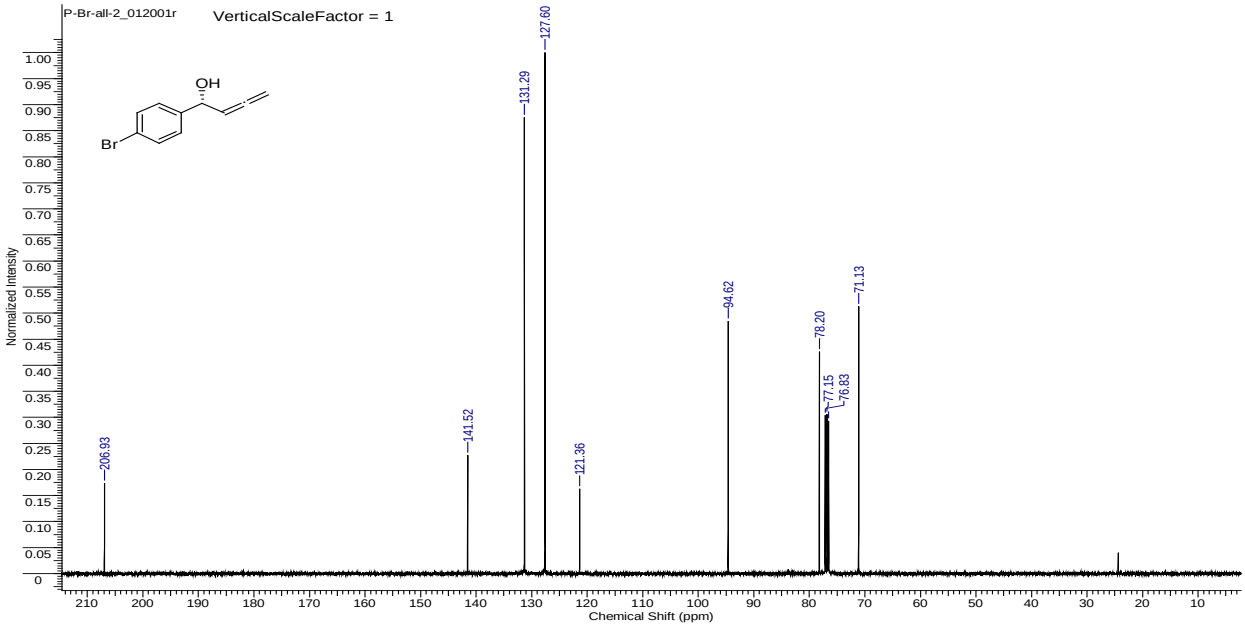
Acquisition Time (sec)	3.9584	***Comment***	P-Br-all-2	***Date***	06 May 2012 00:00:00		
Date Stamp	06 May 2012 00:00:00						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\P-Br-all-2_010001r					***Frequency (MHz)***	400.19
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	90.50
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2400.6772
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.26 - 7.37 (m, 2 H), 7.11 (d, *J*=8.34 Hz, 2 H), 5.23 (q, *J*=6.57 Hz, 1 H), 5.01 - 5.09 (m, 1 H), 4.68 - 4.84 (m, 2 H), 2.30 (br. s., 1 H)



5/16/2012 4:29:03 PM

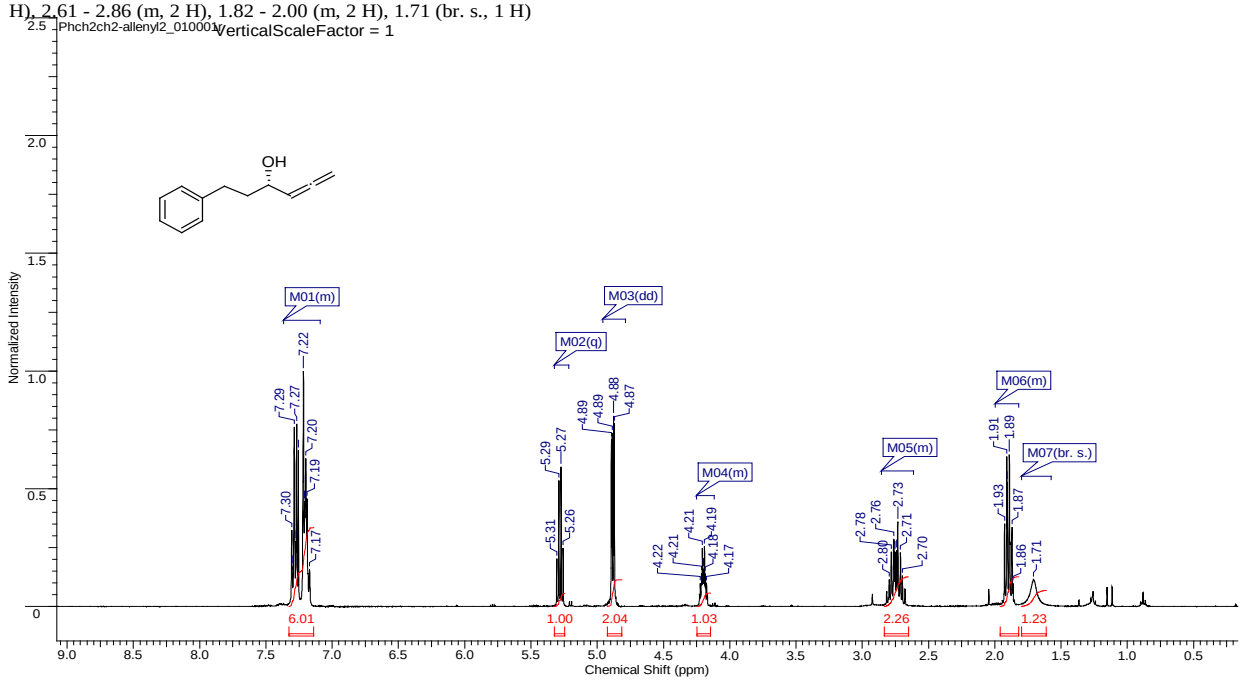
Acquisition Time (sec)	1.3664	***Comment***	P-Br-all-2	***Date***	06 May 2012 01:16:48		
Date Stamp	06 May 2012 01:16:48						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\P-Br-all-2_012001r					***Frequency (MHz)***	100.63
Nucleus	13C	***Number of Transients***	2048	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10035.1045
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 11:00:43 PM

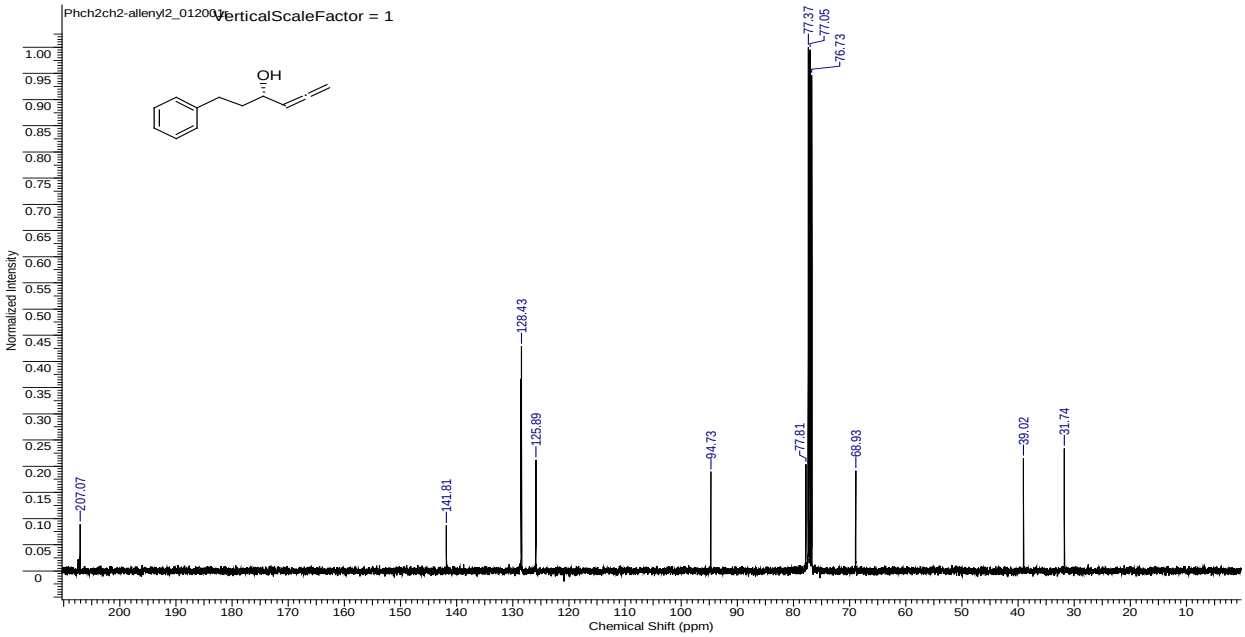
Acquisition Time (sec)	3.9584	***Comment***	Phch2ch2-allenyl2			***Date***	27 Apr 2012 18:46:24
Date Stamp	27 Apr 2012 18:46:24						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Phch2ch2-allenyl2_010001r					***Frequency (MHz)***	400.19
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	256.00
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2455.4819
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 7.09 - 7.37 (m, 5 H), 5.28 (q, *J*=6.57 Hz, 1 H), 4.88 (dd, *J*=6.69, 2.40 Hz, 2 H), 4.12 - 4.25 (m, 1 H), 2.61 - 2.86 (m, 2 H), 1.82 - 2.00 (m, 2 H), 1.71 (br. s., 1 H)



5/16/2012 11:03:52 PM

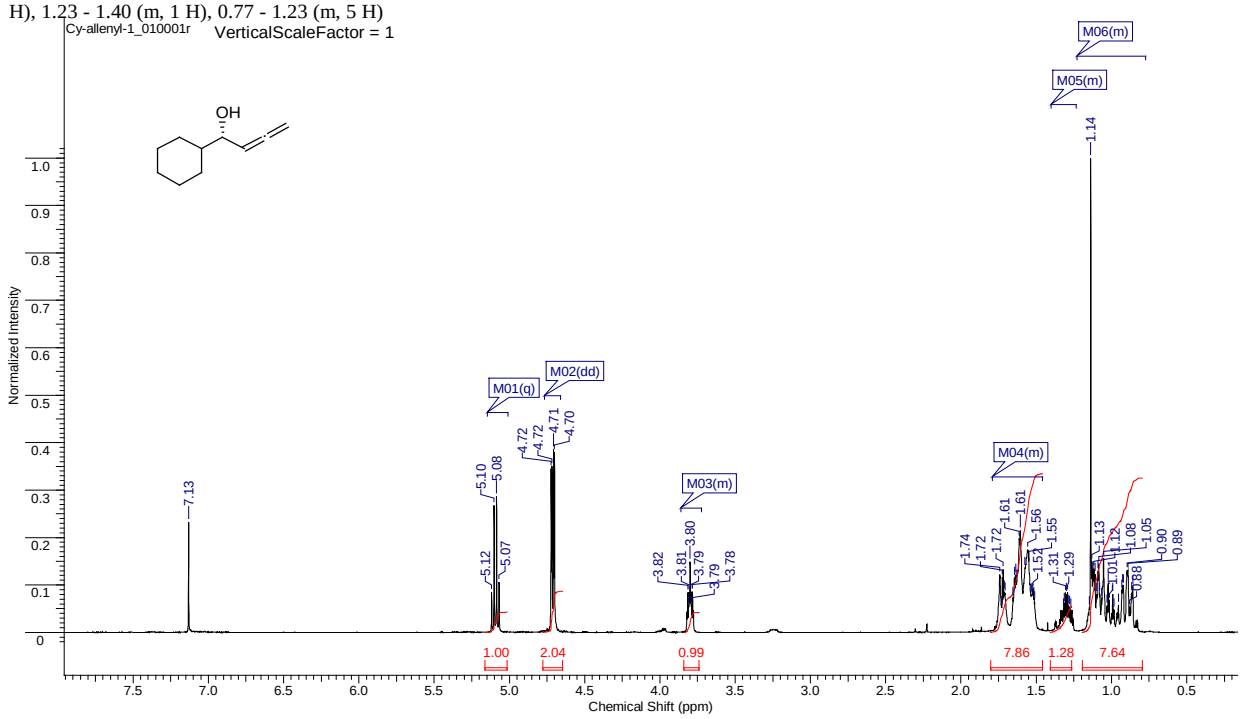
Acquisition Time (sec)	1.3664	***Comment***	Phch2ch2-allenyl2			***Date***	28 Apr 2012 04:16:00
Date Stamp	28 Apr 2012 04:16:00						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Phch2ch2-allenyl2_012001r					***Frequency (MHz)***	100.63
Nucleus	13C	***Number of Transients***	2048	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10062.3271
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000				



5/16/2012 11:30:04 PM

Acquisition Time (sec)	3.9584	***Comment***	Cy-allenyl-1	***Date***	04 May 2012 23:57:52		
Date Stamp	04 May 2012 23:57:52						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Cy-allenyl-1_010001r					***Frequency (MHz)***	400.19
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	143.70
SW(cyclical) (Hz)	8278.15	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2405.8555
Sweep Width (Hz)	8277.89	***Temperature (degree C)***	27.000				

1H NMR (400 MHz, CHLOROFORM-*d*) δ ppm 5.09 (q, *J*=6.57 Hz, 1 H), 4.71 (dd, *J*=6.57, 2.27 Hz, 2 H), 3.72 - 3.86 (m, 1 H), 1.46 - 1.79 (m, 6 H), 1.23 - 1.40 (m, 1 H), 0.77 - 1.23 (m, 5 H)



5/16/2012 11:34:32 PM

Acquisition Time (sec)	1.3664	***Comment***	Cy-allenyl-1	***Date***	05 May 2012 00:06:24		
Date Stamp	05 May 2012 00:06:24						
File Name	C:\Documents and Settings\leletra1\Desktop\Old_Desktop\paper12\NMRs\Cy-allenyl-1_011001r					***Frequency (MHz)***	100.63
Nucleus	13C	***Number of Transients***	256	***Origin***	spect	***Original Points Count***	32768
Owner	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	8192.00
SW(cyclical) (Hz)	23980.81	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11045.6777
Sweep Width (Hz)	23980.08	***Temperature (degree C)***	27.000