

Rh-Catalyzed Highly Enantioselective Formation of Functionalized Cyclopentanes and Cyclopentanones

Fei Liu^a, Qiang Liu^a, Minsheng He^b, Xumu Zhang^{*a,b} and Aiwen Lei^{*a,b}

^a *College of Chemistry and Molecular Sciences, Wuhan University, Wuhan, 430072, P. R. China*

^b *Department of Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania 16802*

Supporting Information

Millennium Results Report
Report Method: Jason_Report
Channel Descr: 254

Printed: February 4, 2002
Version: 2.00

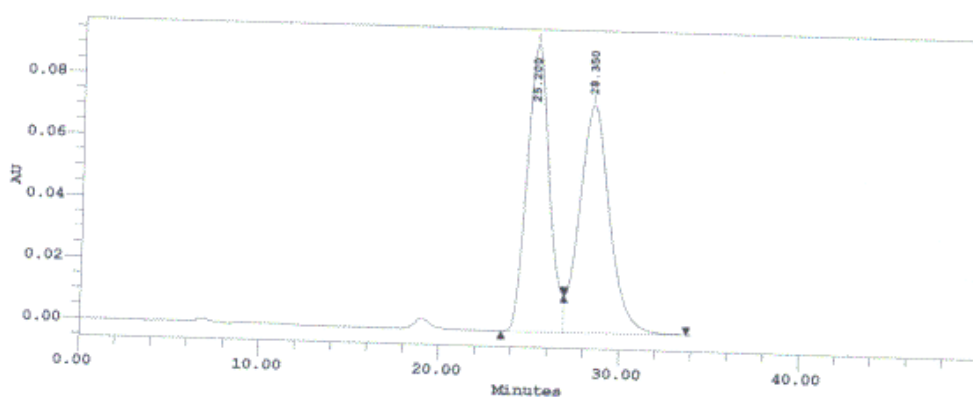
Page: 1 of 1

Millennium Sample Information

Project Name: Aiwon Lei
Sample Name: La8-9a
Date Acquired: 02/04/02 05:04 PM
Acq Meth Set: Jason_MS
Processing Method: Jason_PM

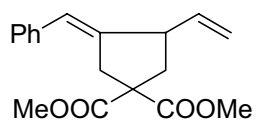
Volume: 10.00
Run Time: 50.0 min
Date Processed: 02/04/02 05:41 PM
SolventPercent: 97/3
Column name: 05

0.5 mL/min



Peak Results

#	Name	Ret Time (min)	Area (uV*sec)	Height (uV)	% Area
1		25.200	8040559	93205	48.26
2		28.350	8621657	73766	51.74



4b

Millennium Results Report
Report Method: Jason_Report
Channel Descr: 254

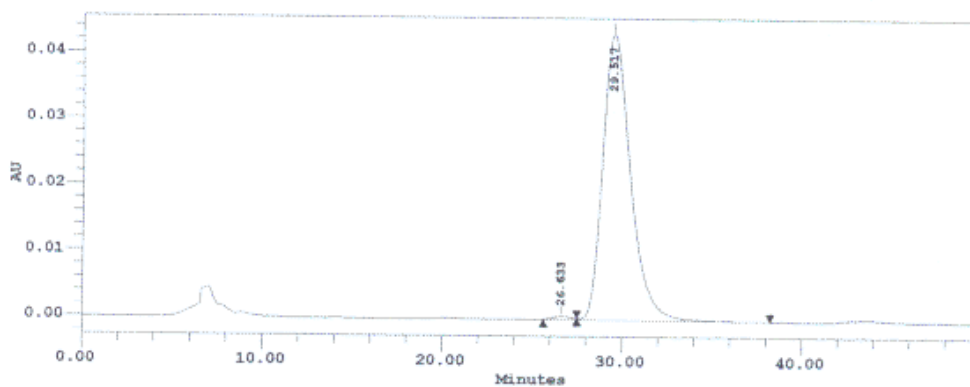
Printed: February 4, 2006
Version: 2.00

Page: 1 of 1

Millennium Sample Information

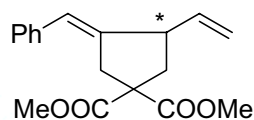
Project Name: Alwen_Lei
Sample Name: La9-9b
Date Acquired: 02/04/02 05:39 PM
Acq Meth Set: Jason_MS
Processing Method: Jason_EM

Volume: 10.00
Run Time: 50.0 min
Date Processed: 02/04/02 07:21 PM
SolventPercent H₂O: 20/propyl = 80/20
Column_name 0J

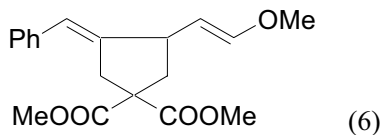


Peak Results

#	Name	Ret Time (min)	Area (uV*sec)	Height (uV)	% Area
1		26.633	37444	534	0.79
2		29.517	4689210	43464	99.21



4b



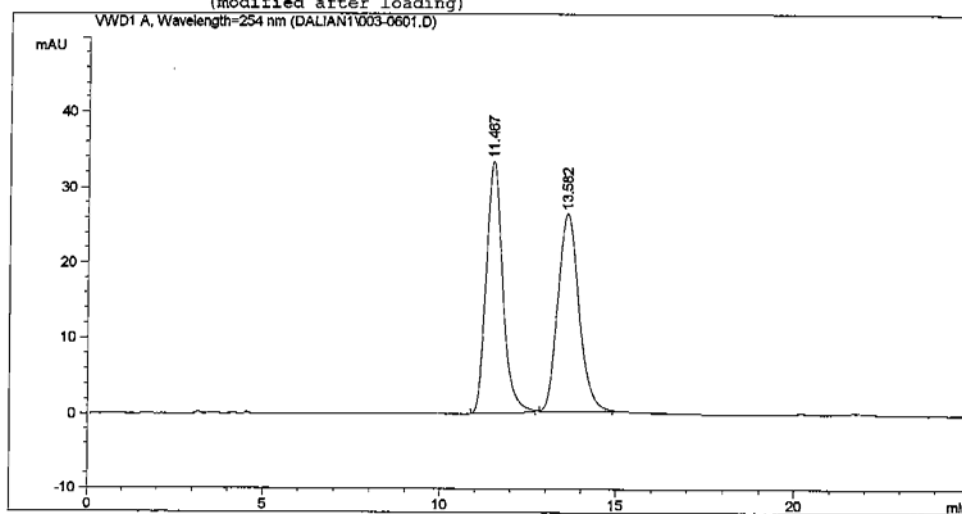
Data File C:\HPCHEM\2\DATA\DALIAN1\003-0601.D

Sample Name: La9-70a

racemic sample, OJ-H, 90:10, 254 nm, 1 ml/min

```
=====
Injection Date   : 7/30/2002 8:18:48 PM      Seq. Line   :    6
Sample Name      : La9-70a                  Location    : Vial 3
Acq. Operator    : CQ                      Inj         :    1
                                           Inj Volume  : 1 µl

Acq. Method      : C:\HPCHEM\2\METHODS\C90-25.M
Last changed     : 7/30/2002 5:38:54 PM by CQ
Analysis Method  : C:\HPCHEM\2\METHODS\C90-10.M
Last changed     : 7/31/2002 11:59:06 AM by CQ
                  (modified after loading)
=====
```



Area Percent Report

```
Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
```

6

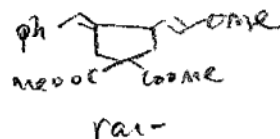
Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]
1	11.467	BB	0.4972	1092.72473	49.8088	33.36107
2	13.582	BB	0.6464	1101.11267	50.1912	26.34020

Totals : 2193.83740 59.70127

Results obtained with enhanced integrator!

*** End of Report ***



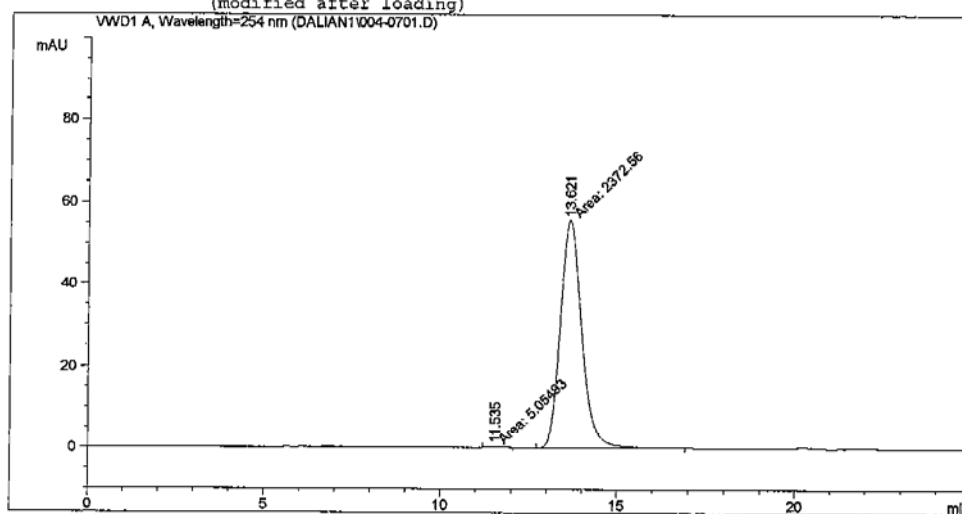
Data File C:\HPCHEM\2\DATA\DALIAN1\004-0701.D

Sample Name: La9-70b

S-Binap, OJ-H, 90:10, 254 nm, 1 ml/min

```
=====
Injection Date   : 7/30/2002 8:44:43 PM      Seq. Line :    7
Sample Name      : La9-70b                  Location  : Vial 4
Acq. Operator    : CQ                       Inj       :    1
                                           Inj Volume: 1 µl

Acq. Method      : C:\HPCHEM\2\METHODS\C90-25.M
Last changed     : 7/30/2002 5:38:54 PM by CQ
Analysis Method  : C:\HPCHEM\2\METHODS\C90-10.M
Last changed     : 7/31/2002 12:01:06 PM by CQ
                  (modified after loading)
=====
```



Area Percent Report

```
=====
Sorted By       : Signal
Multiplier      : 1.0000
Dilution        : 1.0000
=====
```

Signal 1: VWD1 A, Wavelength=254 nm

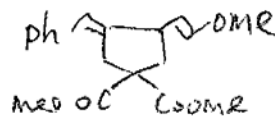
Peak #	RetTime [min]	Type	Width [min]	Area mAU	Area %	Height [mAU]	Area %
1	11.535	MM	0.4345	5.05493	0.2126	1.93881e-1	0.2126
2	13.621	MM	0.7094	2372.55542	99.7874	55.73927	99.7874

Totals : 2377.61035 55.93315

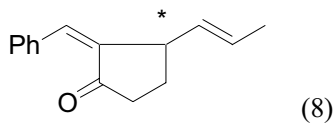
Results obtained with enhanced integrator!

*** End of Report ***

6



From S-BINAP



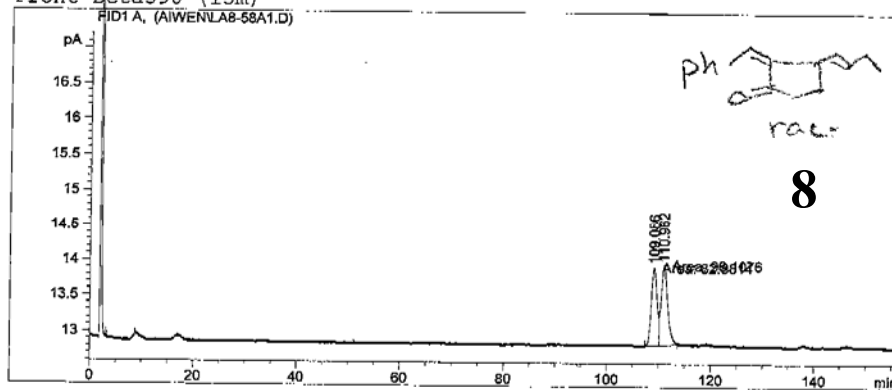
Data File C:\HPCHEM\1\DATA\AIWEN\LA8-58A1.D

Sample Name: LA8-58A

DL-3-33-3, CHIRASIL III, 170C

```

=====
Injection Date   : 3/7/02 5:24:32 PM
Sample Name     : LA8-58A
Acq. Operator   : AIWEN
Method          : C:\HPCHEM\1\METHODS\FRONT.M
Last changed    : 3/7/02 5:21:54 PM by AIWEN
                  (modified after loading)
Vial            : 1
Inj            : 1
Inj Volume     : Manually
Front Beta390 (15m)
  
```



Data File C:\HPCHEM\1\DATA\AIWEN\LA8-58B0.D

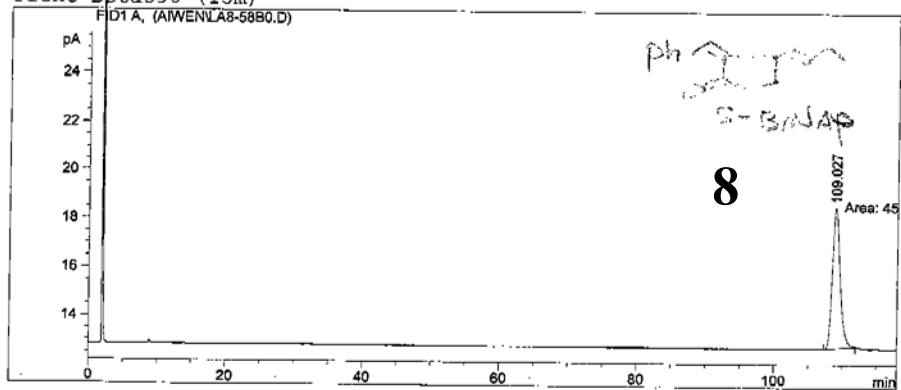
Sample Name: LA8-58B

DL-3-33-3, CHIRASIL III, 170C

=====

Injection Date	: 3/7/02 8:02:41 PM	
Sample Name	: LA8-58B	Vial : 1
Acq. Operator	: AIWEN	Inj : 1
		Inj Volume : Manually
Acq. Method	: C:\HPCHEM\1\METHODS\FRONT.M	
Last changed	: 3/7/02 5:21:54 PM by AIWEN	
	(modified after loading)	
Analysis Method	: C:\HPCHEM\1\METHODS\FRONT.M	
Last changed	: 3/7/02 10:11:59 PM by AIWEN	
	(modified after loading)	

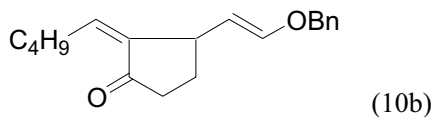
Front Beta390 (15m)



HP 6890 3/7/02 10:12:13 PM AIWEN

Page 2 of 3

F90/8102



Data File C:\HPCHEM\2\DATA\DALIAN1\007-0801.D

Sample Name: La9-60a

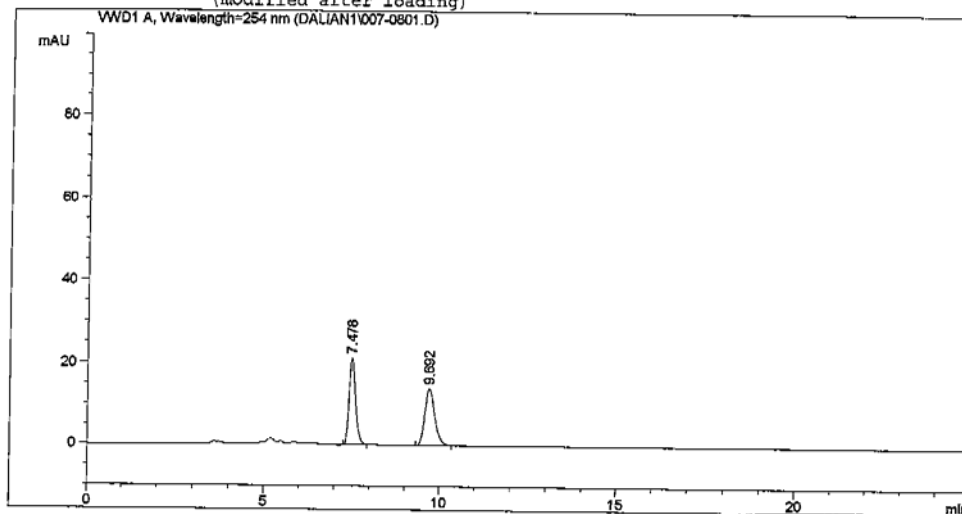
racemic sample, OJ-H, 90:10, 254 nm, 1 ml/min

```

=====
Injection Date   : 7/30/2002 9:10:36 PM      Seq. Line :    8
Sample Name     : La9-60a                  Location  : Vial 7
Acq. Operator   : CQ                      Inj       :    1
                                           Inj Volume: 1 µl

Acq. Method     : C:\HPCHEM\2\METHODS\C90-25.M
Last changed    : 7/30/2002 5:38:54 PM by CQ
Analysis Method : C:\HPCHEM\2\METHODS\C90-10.M
Last changed    : 7/31/2002 12:01:06 PM by CQ
                  (modified after loading)
=====

```



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000

```

Signal 1: WVD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU	Height [mAU]	Area %
1	7.478	PB	0.1954	273.86392	21.26752	49.5806
2	9.692	BB	0.3052	278.49734	14.06742	50.4194

Totals : 552.36127 35.33494

Results obtained with enhanced integrator!

*** End of Report ***

10b



rac

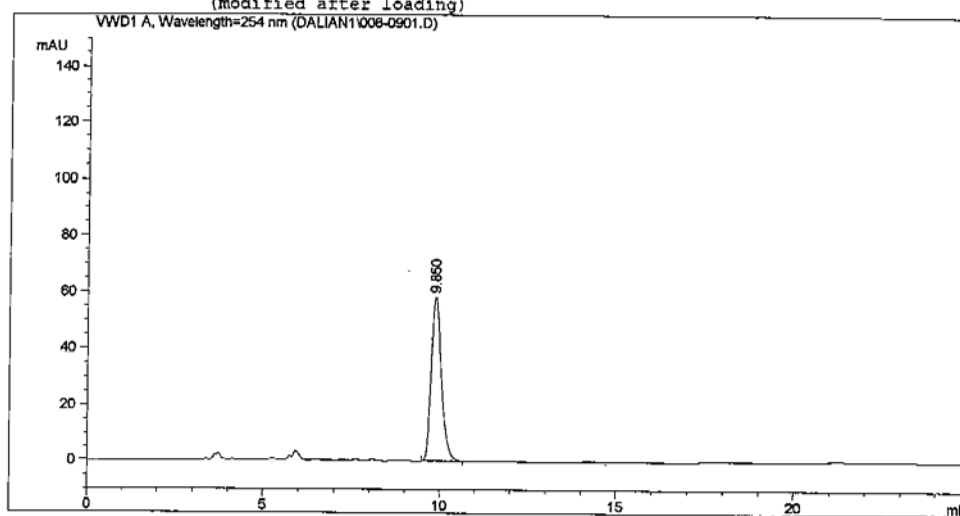
Data File C:\HPCHEM\2\DATA\DALIAN1\008-0901.D

Sample Name: La9-60b

S-Binap, OJ-H, 90:10, 254 nm, 1 ml/min

```
=====
Injection Date : 7/30/2002 9:36:30 PM      Seq. Line : 9
Sample Name    : La9-60b                  Location  : Vial 8
Acq. Operator  : CQ                      Inj      : 1
                                           Inj Volume: 1 µl

Acq. Method    : C:\HPCHEM\2\METHODS\C90-25.M
Last changed   : 7/30/2002 5:38:54 PM by CQ
Analysis Method: C:\HPCHEM\2\METHODS\C90-10.M
Last changed   : 7/31/2002 12:09:32 PM by CQ
                  (modified after loading)
=====
```



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: VWD1 A, Wavelength=254 nm

Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	9.850	BB	0.3096	1177.74792	58.38401	100.0000

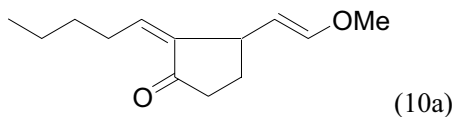
Totals : 1177.74792 58.38401

Results obtained with enhanced integrator!

=====
*** End of Report ***

10b

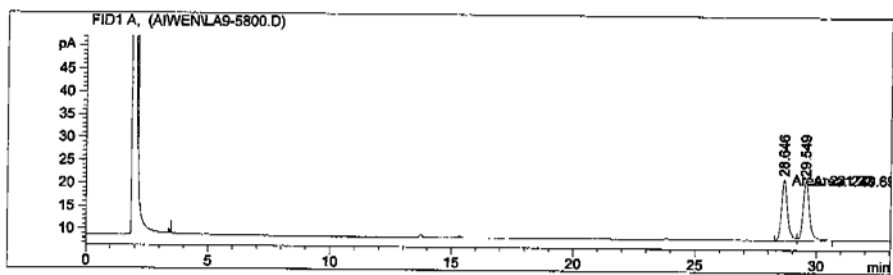
Cc1ccc(cc1)[C@H]2C[C@@H](c3ccccc3)C[C@H]2C OBn
S-BINAP



026/054

Data File C:\HPCHEM\1\DATA\AIWEN\LA9-5800.D Sample Name: LA9-58A
LA9-58a, RACMIX SAMPLE, CHIRASELECT 1000, 1.5 ML/MIN; 1
500C

=====
Injection Date : 6/23/02 7:47:47 PM
Sample Name : LA9-58A Vial : 1
Acq. Operator : AIWEN Inj : 1
Inj Volume : Manually
Acq. Method : C:\HPCHEM\1\METHODS\FRONT.M
Last changed : 6/23/02 7:59:29 PM by AIWEN
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\FRONT.M
Last changed : 6/23/02 8:23:51 PM by AIWEN
(modified after loading)
Front Beta390 (15m)
=====



=====
Area Percent Report
=====

Sorted By : Retention Time
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: FID1 A,

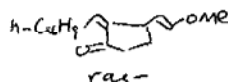
Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	28.646	1	MF	231.23030	13.18893	48.99724
2	29.549	1	FM	240.69489	13.07718	51.00276

Totals : 471.92519 26.26612

Results obtained with standard integrator!

*** End of Report ***

10a

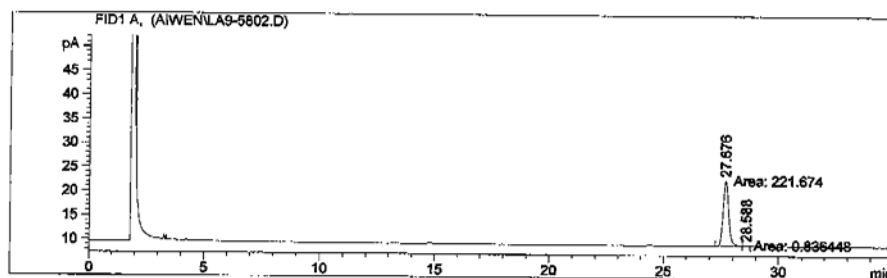


Data File C:\HPCHEM\1\DATA\AIWEN\LA9-5802.D
 LA9-58b, s-binap, CHIRASELECT 1000, 1.5 ML/MIN; 1500C

Sample Name: LA9-58b

```
=====
Injection Date   : 6/23/02 9:58:50 PM
Sample Name      : LA9-58b
Acq. Operator    : AIWEN
Vial             : 1
Inj              : 1
Inj Volume       : Manually

Acq. Method      : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 6/23/02 9:57:51 PM by AIWEN
                  (modified after loading)
Analysis Method  : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 6/24/02 12:17:00 AM by AIWEN
                  (modified after loading)
Front Beta390 (15m)
=====
```



Area Percent Report

```
Sorted By      : Retention Time
Multiplier     : 1.0000
Dilution       : 1.0000
```

Signal 1: FID1 A,

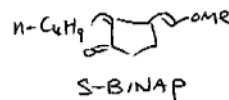
Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	27.676	1	MM	221.67352	13.47112	99.62408
2	28.588	1	MM	8.36448e-1	8.52030e-2	0.37592

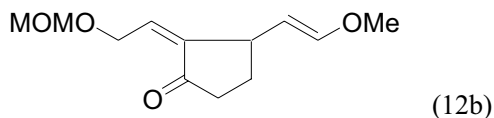
Totals : 222.50997 13.55633

Results obtained with standard integrator!

*** End of Report ***

10a

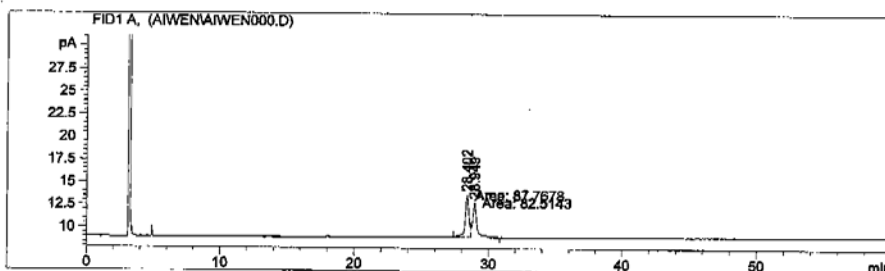




1a9-87a, racmic sample, chiralselect 1000, 180oC, 1.5 m
l/min

```
=====
Injection Date   : 7/14/02 11:27:52 AM
Sample Name      : 1a9-87a
Acq. Operator    : aiwen
Vial             : 1
Inj              : 1
Inj Volume       : Manually

Acq. Method      : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 7/14/02 11:25:06 AM by WANG
                  (modified after loading)
Analysis Method  : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 7/14/02 6:17:03 PM by aiwen
                  (modified after loading)
Front Beta390 (15m)
=====
```



Area Percent Report

```
=====
Sorted By       : Retention Time
Multiplier      : 1.0000
Dilution        : 1.0000
=====
```

Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	28.402	1	MF	87.76783	4.63988	51.54259
2	28.949	1	FM	82.51431	3.78118	48.45741

Totals : 170.28214 8.42106

Results obtained with standard integrator!

*** End of Report ***



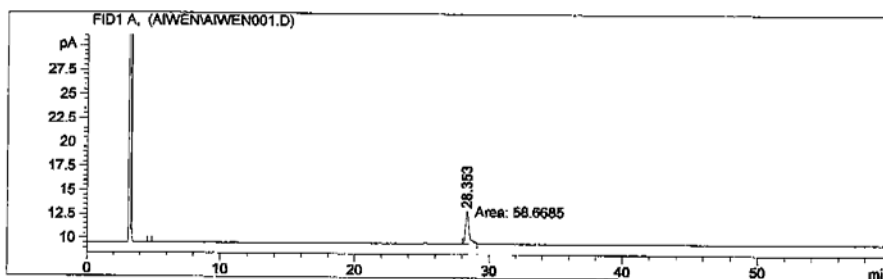
12b

1a9-8/b, chiraiselect 1000, 180oC, 1.5 ml/min

=====

Injection Date	: 7/14/02 1:52:39 PM	
Sample Name	: 1a9-87b	Vial : 1
Acq. Operator	: aiwen	Inj : 1
		Inj Volume : Manually
Acq. Method	: C:\HPCHEM\1\METHODS\FRONT.M	
Last changed	: 7/14/02 11:25:06 AM by WANG	
	(modified after loading)	
Analysis Method	: C:\HPCHEM\1\METHODS\FRONT.M	
Last changed	: 7/14/02 6:17:03 PM by aiwen	
	(modified after loading)	
Front Beta390	(15m)	

=====



=====
Area Percent Report
=====

Sorted By : Retention Time
Multiplier : 1.0000
Dilution : 1.0000

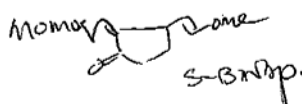
Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	28.353	1	MM	58.66851	3.31897	1.000e2

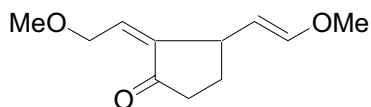
Totals : 58.66851 3.31897

Results obtained with standard integrator!

*** End of Report ***



12b

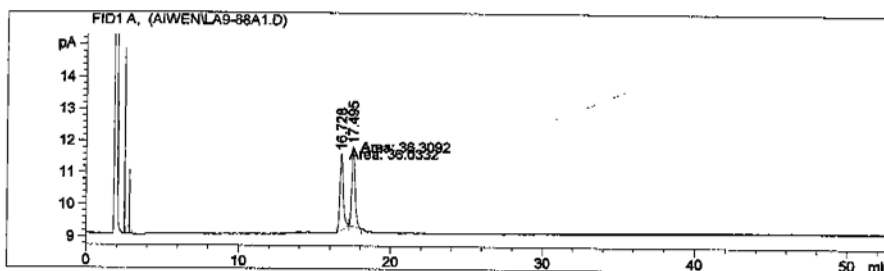


(12a)

Data File C:\HPCHEM\1\DATA\AIWEN\LA9-88A1.D Sample Name: la9-88a
 la9-88a, racemic sample, CHIRAL SELECT 1000, 150oC, 1.5
 ml/min

```
=====
Injection Date   : 7/13/02 1:00:01 PM
Sample Name      : la9-88a
Acq. Operator    : aiwen
Vial :           1
Inj :            1
Inj Volume : Manually

Acq. Method      : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 7/13/02 12:59:09 PM by aiwen
                  (modified after loading)
Analysis Method  : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 7/13/02 1:55:30 PM by aiwen
                  (modified after loading)
Front Beta390 (15m)
=====
```



Area Percent Report

```
Sorted By      : Retention Time
Multiplier     : 1.0000
Dilution       : 1.0000
```

Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	16.728	1	MM	36.03318	2.39289	49.80924
2	17.495	1	MM	36.30917	2.47868	50.19076

Totals : 72.34235 4.87156

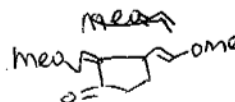
Results obtained with standard integrator!

*** End of Report ***

12a

HP 6890 7/13/02 1:55:49 PM aiwen

rac-

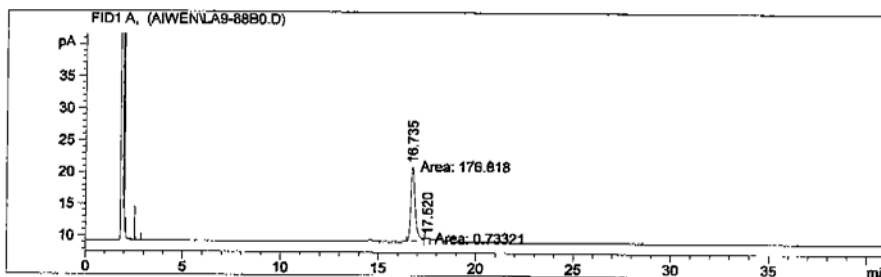


Page 1 of 1

Data File C:\HPCHEM\1\DATA\AIWEN\LA9-88B.D Sample Name: la9-88b
 la9-88b, S-BINAP, CHIRAL SELECT 1000, 150oC, 1.5 ml/min

```
=====
Injection Date   : 7/13/02 1:54:40 PM
Sample Name      : la9-88b
Acq. Operator    : aiwen
Vial             : 1
Inj              : 1
Inj Volume       : Manually

Acq. Method      : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 7/13/02 1:55:30 PM by aiwen
                  (modified after loading)
Analysis Method  : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 7/14/02 11:25:06 AM by WANG
                  (modified after loading)
Front Beta390 (15m)
=====
```



Area Percent Report

```
Sorted By      : Retention Time
Multiplier     : 1.0000
Dilution       : 1.0000
```

Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	16.735	1	MM	176.81850	11.70209	99.58704
2	17.520	1	MM	7.33210e-1	1.02605e-1	0.41296

Totals : 177.55171 11.80470

Results obtained with standard integrator!

*** End of Report ***

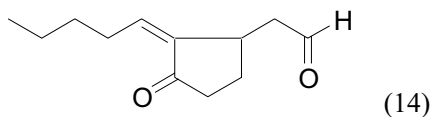
mean zone

S-BINAP

12a

HP 6890 7/14/02 11:25:13 AM WANG

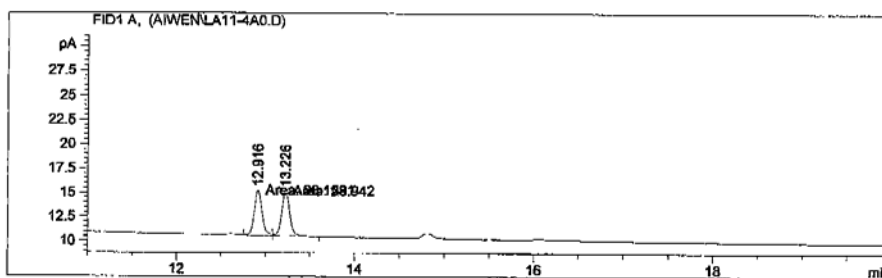
Page 1 of 1



LA11-4A, RACMIC SAMPLE, GAMA 225, 1.5 ML/MIN, 170C

```
=====
Injection Date   : 9/25/02 9:33:52 PM
Sample Name      : LA11-4A
Acq. Operator    : AIWEN
Vial             : 1
Inj              : 1
Inj Volume       : Manually

Acq. Method      : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 9/25/02 9:31:22 PM by TANG
                  (modified after loading)
Analysis Method  : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 9/25/02 11:14:51 PM by AIWEN
                  (modified after loading)
Front Beta390 (15m)
=====
```



Area Percent Report

```
=====
Sorted By       : Retention Time
Multiplier      : 1.0000
Dilution        : 1.0000
=====
```

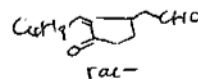
Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	12.916	1	MF	28.15913	4.68690	49.31445
2	13.226	1	FM	28.94205	4.66257	50.68555

Totals : 57.10118 9.34946

Results obtained with standard integrator!

*** End of Report ***



14

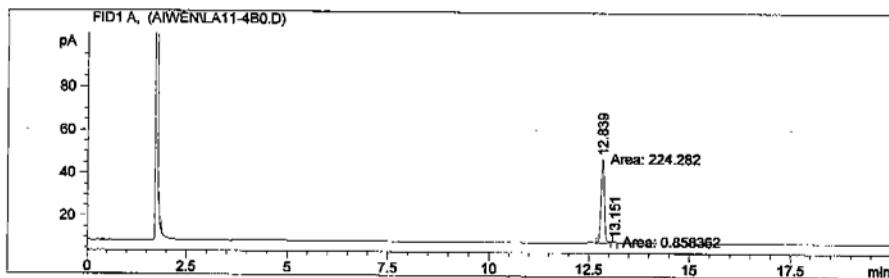
LA11-4D, S-BINAP, GAMA 225, 1.5 ML/MIN, 170C

=====

Injection Date	: 9/25/02 10:47:06 PM	Vial	: 1
Sample Name	: LA11-4b	Inj	: 1
Acq. Operator	: AIWEN	Inj Volume	: Manually

Acq. Method : C:\HPCHEM\1\METHODS\FRONT.M
Last changed : 9/25/02 9:31:22 PM by TANG
(modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\FRONT.M
Last changed : 9/25/02 11:18:33 PM by AIWEN
(modified after loading)
Front Beta390 (15m)

=====



=====
Area Percent Report
=====

Sorted By : Retention Time
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	12.839	1	MM	224.28206	39.31352	99.61874
2	13.151	1	MM	8.58362e-1	2.07797e-1	0.38126

Totals : 225.14042 39.52132

Results obtained with standard integrator!

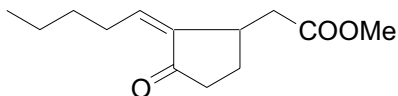
*** End of Report ***

14 Cc1ccc(cc1)C(=O)O
R-BINAP

HP 6890 9/25/02 11:21:19 PM AIWEN

Page 1 of 1

190/0100



052/054

Data File C:\HPCHEM\1\DATA\WU\WU393005.D
 WU-3-93-9 CHIRALSELECT 1000, ~~180°C, 1mL/min~~
 180°C 2 mL/min

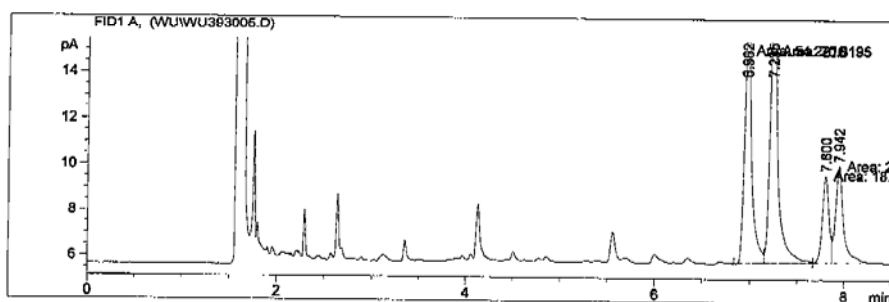
Sample Name: WU-3-93-9

Injection Date : 10/26/02 8:47:47 PM
 Sample Name : WU-3-93-9
 Acq. Operator : WU

Vial : 1
 Inj : 1

Inj Volume : Manually

Method : C:\HPCHEM\1\METHODS\FRONT.M
 Last changed : 10/26/02 8:49:02 PM by WU
 (modified after loading)
 Front Beta390 (15m)



Area Percent Report

Sorted By : Retention Time
 Multiplier : 1.0000
 Dilution : 1.0000

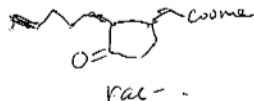
Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	6.962	1	MF	54.22163	10.99227	32.32964
2	7.235	1	MF	70.81948	13.47830	42.22610
3	7.800	1	MF	18.13536	3.80147	10.81321
4	7.942	1	FM	24.53846	4.20792	14.63105

Totals : 167.71494 32.47997

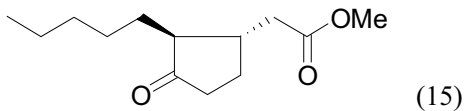
Results obtained with standard integrator!

*** End of Report ***



HP 6890 10/26/02 8:58:37 PM WU

Page 1 of 1



053/054

Data File C:\HPCHEM\1\DATA\WU\WU393011.D
~~WU-3-93-9 CHIRALSELECT 1000, 100C, 1ML/MIN~~

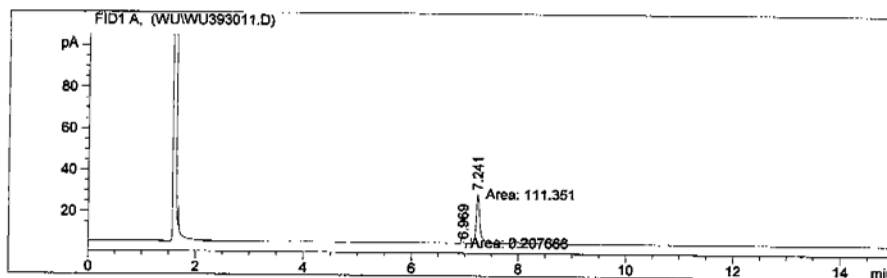
Sample Name: WU-3-93-9

150°C 2ml/min

```

=====
Injection Date   : 10/26/02 9:57:43 PM
Sample Name      : WU-3-93-9
Acq. Operator    : WU
Vial             : 1
Inj              : 1
Inj Volume       : Manually

Acq. Method      : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 10/26/02 9:59:27 PM by WU
                  (modified after loading)
Analysis Method  : C:\HPCHEM\1\METHODS\FRONT.M
Last changed     : 10/26/02 11:03:08 PM by WU
                  (modified after loading)
Front Beta390 (15m)
=====
  
```



Area Percent Report

```

Sorted By      : Retention Time
Multiplier     : 1.0000
Dilution       : 1.0000
  
```

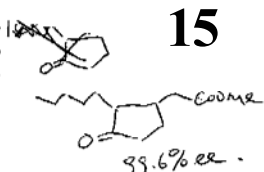
Signal 1: FID1 A,

Peak #	RetTime [min]	Sig	Type	Area [pA*s]	Height [pA]	Area %
1	6.969	1	MM	2.07666e-1	9.70385e-2	0.18615
2	7.241	1	MM	111.35127	23.45995	99.81385

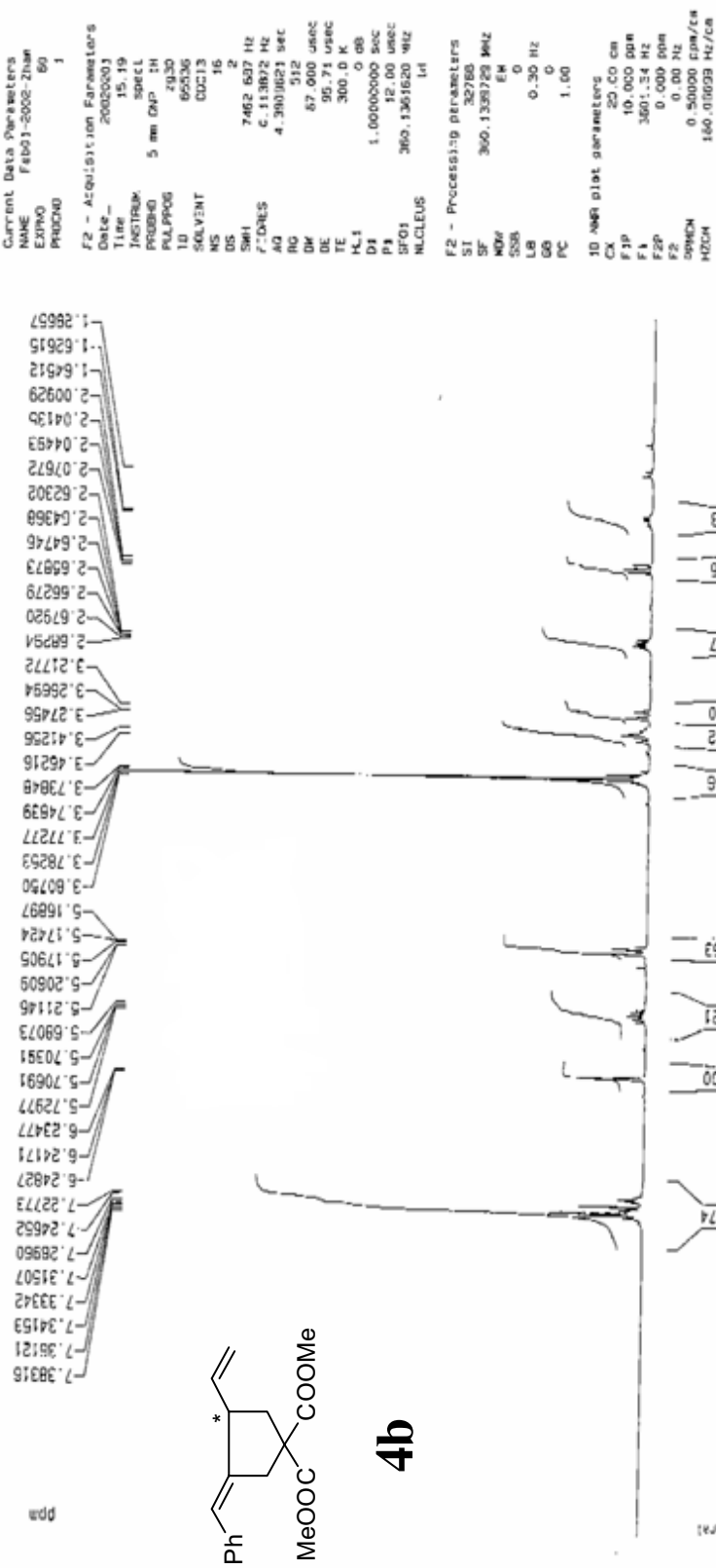
Totals : 111.55894 23.55699

Results obtained with standard integrator!

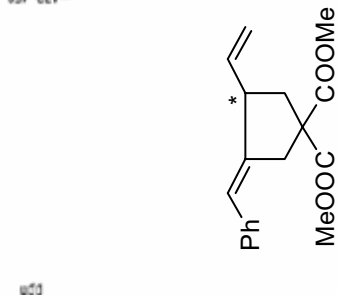
*** End of Report ***



Lab-06



LoB-9b



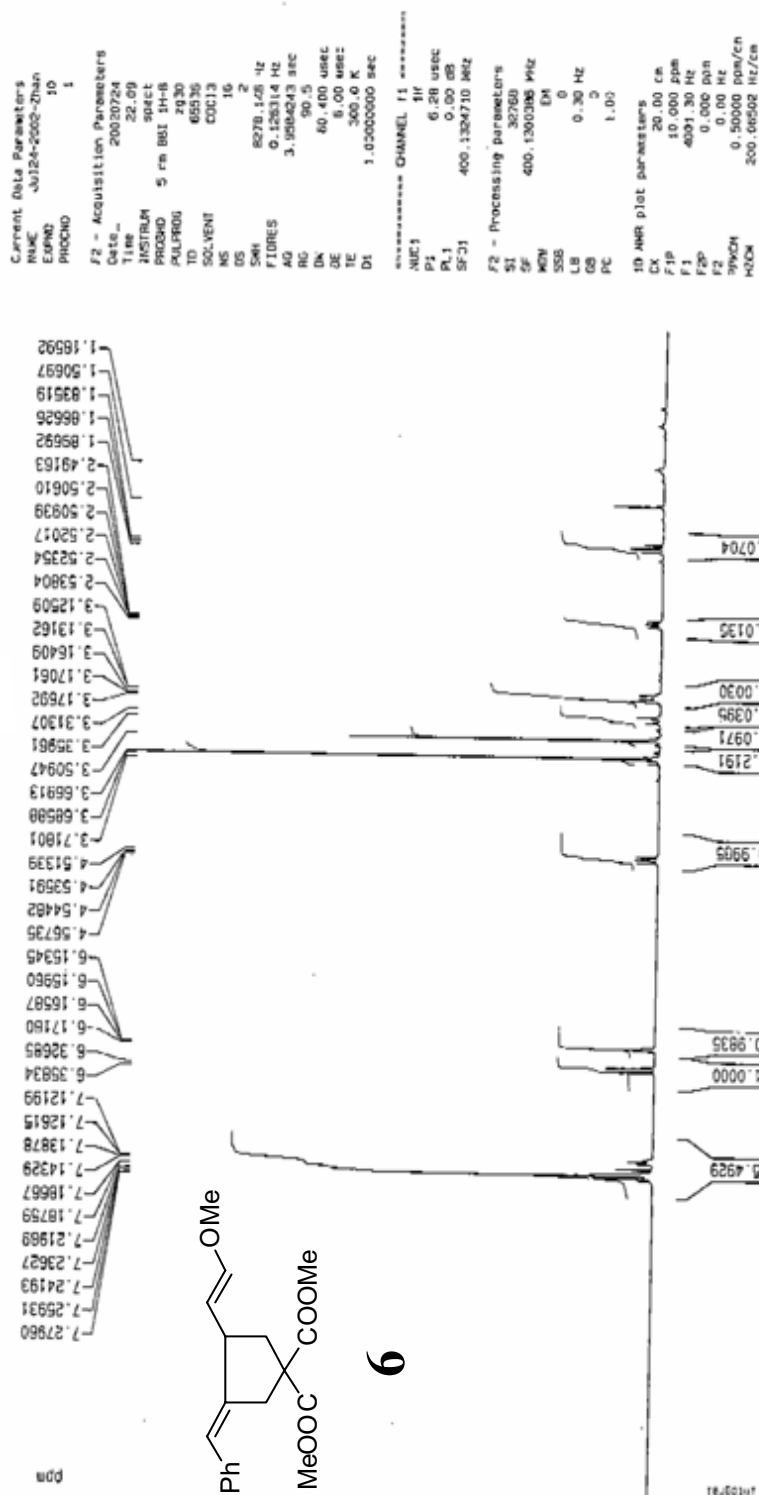
77.777
77.424
77.072
59.776
53.326
53.274
50.136
40.136
39.224

172.460
172.361
143.601
139.653
138.078
128.676
126.818
124.446
117.254

Current Data Parameters
NAME / 8001-2002-Zhen
EXPNO 61
PROCNO 1
F2 - Acquisition Parameters
Date_ 20030203
Time 15.35
INSTRUM spect
PROBHD 5 mm QNP 1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
AQ 7.26
RG 327.68
SH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 3.4418420 sec
RG 327.68
DE 22.000 usec
DC 31.43 usec
TE 300.0 K
NUC1 13C
NUC2 1H
D1 2.0000000 sec
DPRG10 waltz16
P31 100.00 usec
S4 30 dB
O11 0.0200000 sec
S2 30 dB
P1 7.90 usec
PCPD1 90.5658983 MHz
NOCLEUS 13C
F2 - Processing parameters
SI 32768
SF 90.1967236 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 3.40
ID Refl p10L parameters
CX 20.00 cm
FLP 237.816 ppm
F1 21535.63 Hz
F2P -13.59 ppm
Z 1181.84 Hz
PCPD1 90.5658983 MHz
PCPD2 90.5658983 MHz

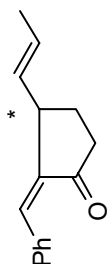


La9-70a





Lab-50a



8

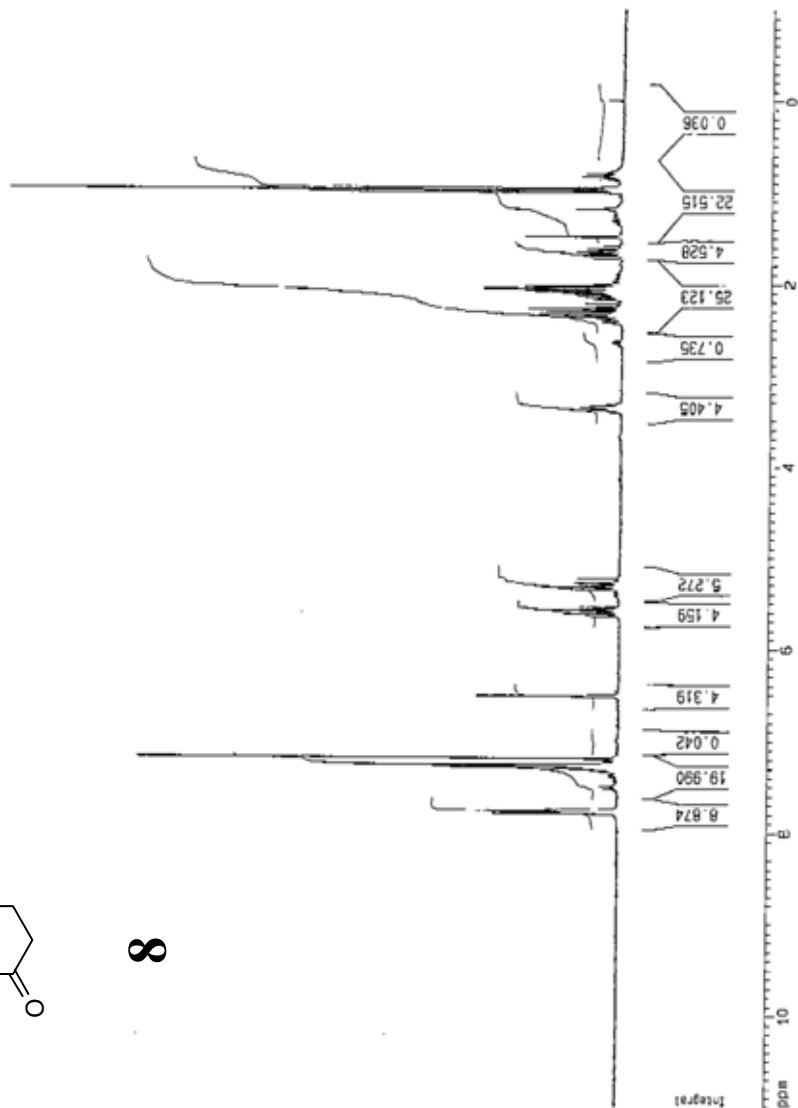
Current Data Parameters
 NAME Mr00-2002-Zhan
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20020306
 Time 22.25
 INSTRUM spect
 PROBHD 5 mm Auto line
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.875 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084560 sec
 RG 912.3
 EM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00200000 sec

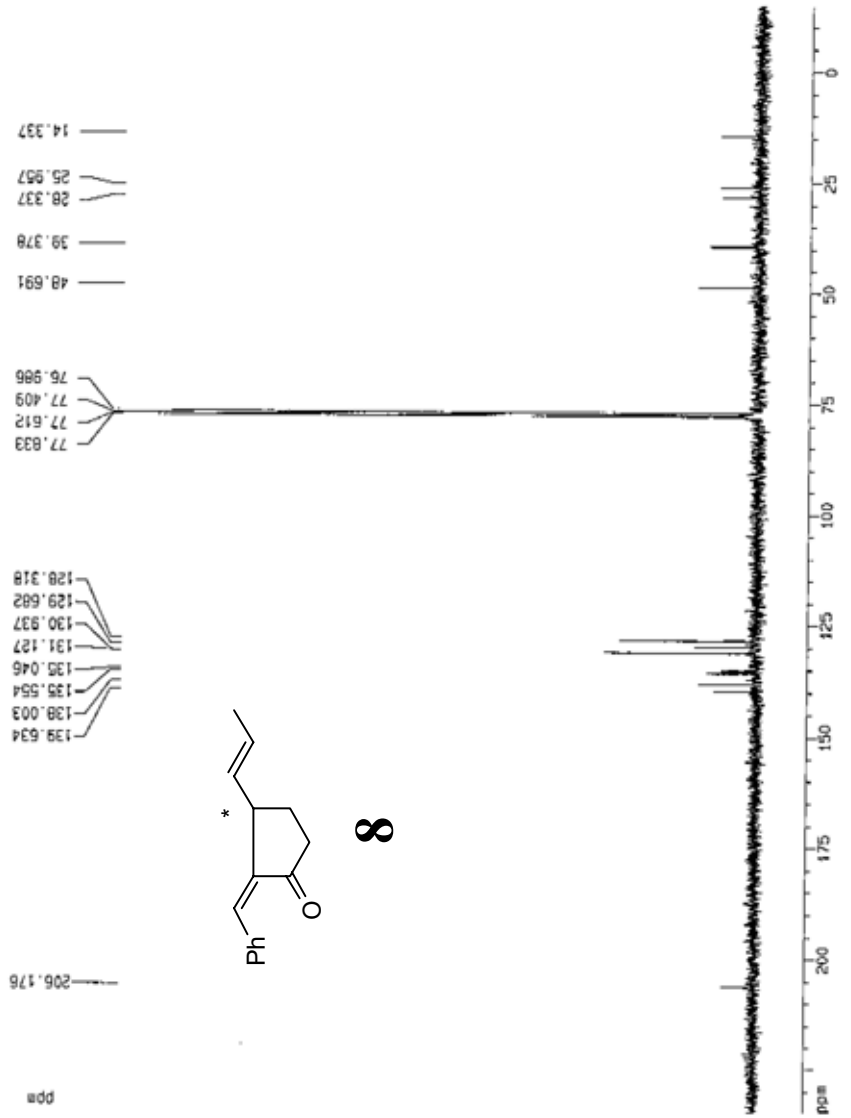
===== CHANNEL f1 =====
 NUC1 1H
 P1 9.80 usec
 PL1 -6.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300270 MHz
 MDN EN
 SSB 0
 LB 0.30 Hz
 DB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cr
 F1P 11.000 gpc
 F1 3301.43 Hz
 F2P -1.000 gpc
 F2 -300.13 Hz
 RFMDM 0.60000 gpc/cc
 MDN 180.07802 Hz/cm



1a8-569



Current Date Parameters
NAME Mu-76-2002-7mm
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020308
Time 23.02
INSTRUM spect
PROBHD 5 mm N1H/1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 16832.303 Hz
FIDRES 0.587360 Hz
AQ 1.7400368 sec
RG 13004
DM 25.500 uSAC
DE 6.00 uSAC
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
d12 0.3000000 sec

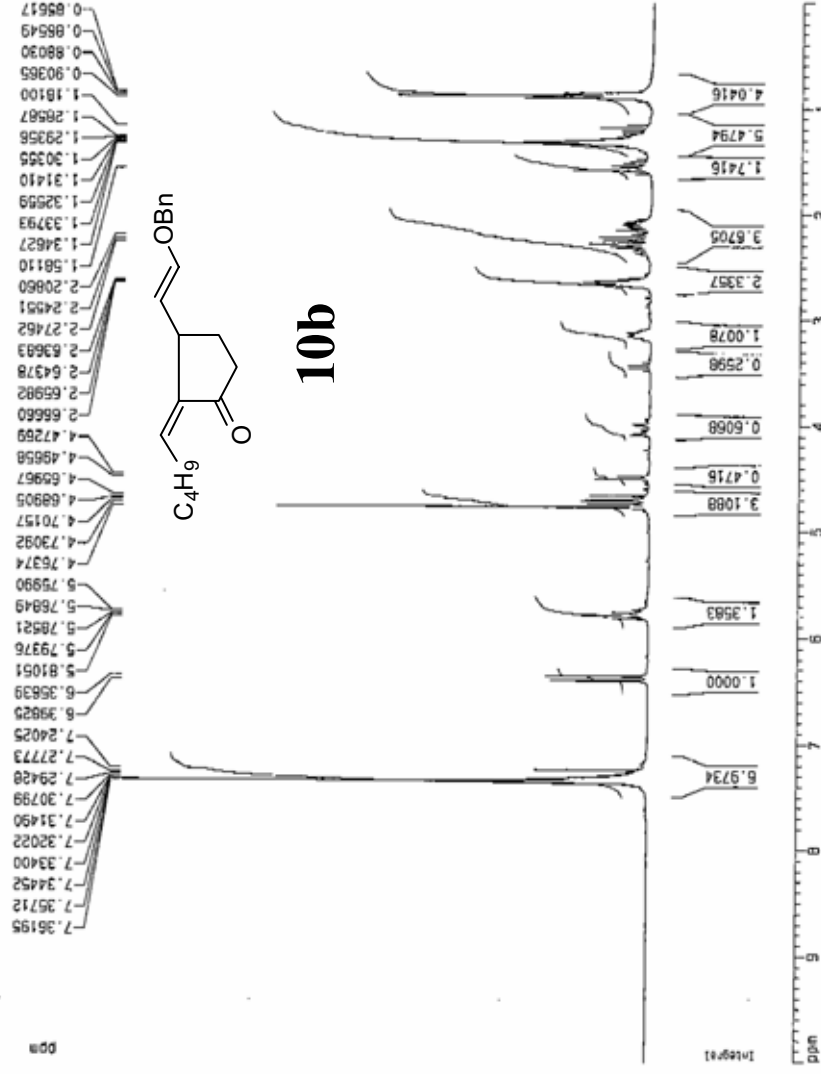
===== CHANNEL f1 =====
NUC1 1H
P1 5.50 uSAC
PL1 -2
SFO1 75.476300 MHz

===== CHANNEL f2 =====
XPRP22 N111210
VOC2 1H
PCPD2 114.00 uSAC
PL2 -8.00 dB
PL12 18.00 dB
PL13 18.00 dB
SFO2 300.131005 MHz

F2 - Processing parameters
SI 32768
SF 75.4037190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR peak parameters
CX 20.00 cm
FSP 234.251 ppm
F1 17756.12 Hz
F2 -14.793 ppm
F2 -1116.27 Hz
PPH2 12.47742 ppm/cm
H2CN 941.61823 Hz/cm

1a9-60a



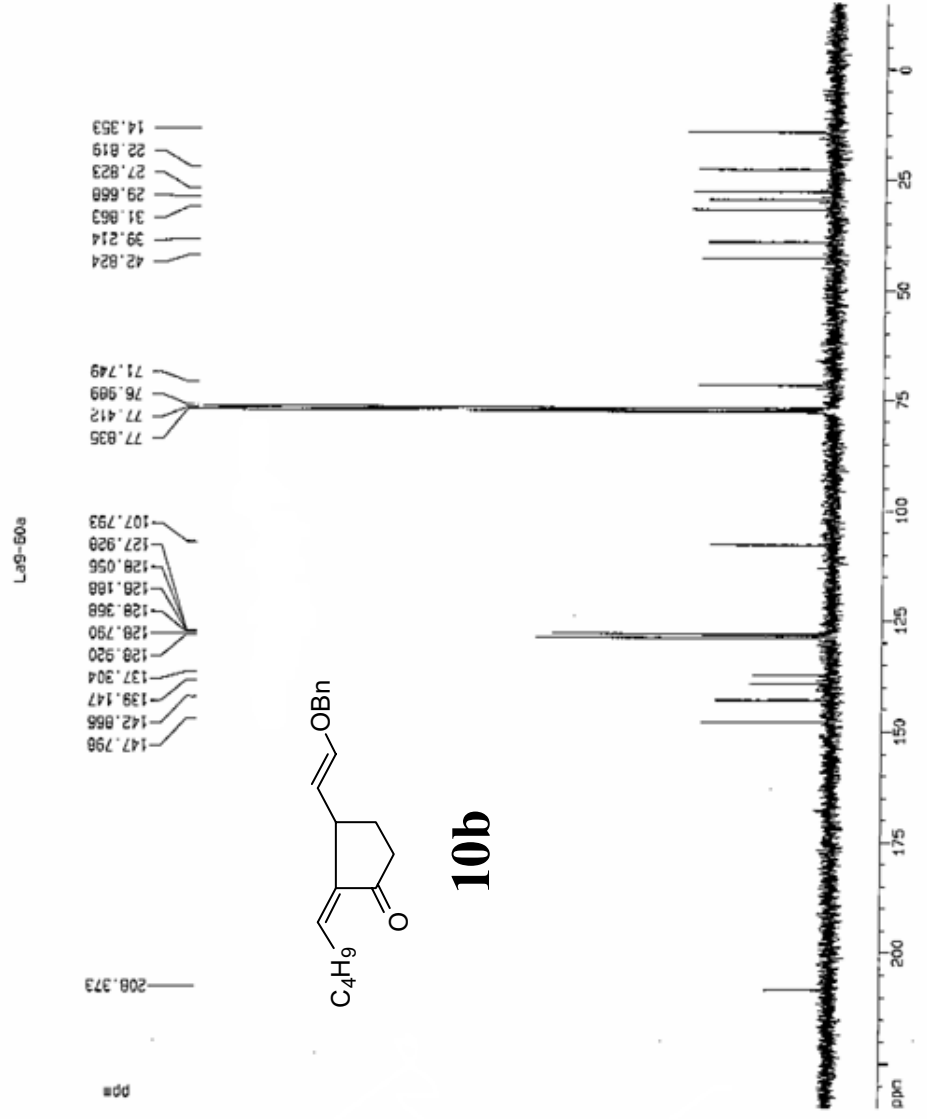
Current Data Parameters
 NAME: 1a9-60a-2002-Zhan
 EXPNO: 20
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20020724
 Time: 22.01
 INSTRUM: spect
 PROBRG: 5 ne Multinu
 PULPROG: zg30
 TD: 65535
 SOLVENT: CDCl3
 NS: 16
 DS: 2
 SWH: 6172.879 Hz
 FIDRES: 0.094190 Hz
 AQ: 5.5084660 sec
 RG: 302.5
 DM: 81.000 ussec
 DE: 6.00 ussec
 TE: 300.0 K
 D1: 1.00000000 sec

===== CHANNEL f1 =====
 NUC1: ¹H
 P1: 9.80 ussec
 PL1: -5.00 dB
 SFO1: 300.1318534 MHz

F2 - Processing parameters
 SI: 32768
 SF: 300.1300120 MHz
 KDN: EM
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 1.00

ID NMR plot parameters
 CX: 20.00 cm
 FID: 10.000 ppm
 F1: 3001.30 Hz
 F2: 0.000 ppm
 F3: 0.00 Hz
 FREQH: 0.00000 ppm/cg
 MZCM: 150.00000 Hz/cm



Current Data Parameters
NAME Jul24-2002-Zhan
EXPNO 21
PROCNO 1

F2 - Acquisition Parameters
Date_ 20020724
Time 22.21

PROBHD 5 mm Multinu
PULPROG zgpg30
TO 209130
DELTA 0.000000
SOLVENT CDCl3
NS 896
DS 4
SFO1 14032.353 Hz
FIDRES 0.287360 Hz
AQ 1.7460308 sec
RG 15384
DM 78.550 uSAC
DE 5.00 uSAC
TE 300.0 K
D1 2.00000000 sec
D11 0.00000000 sec
D12 0.60000000 sec

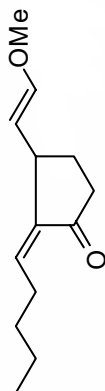
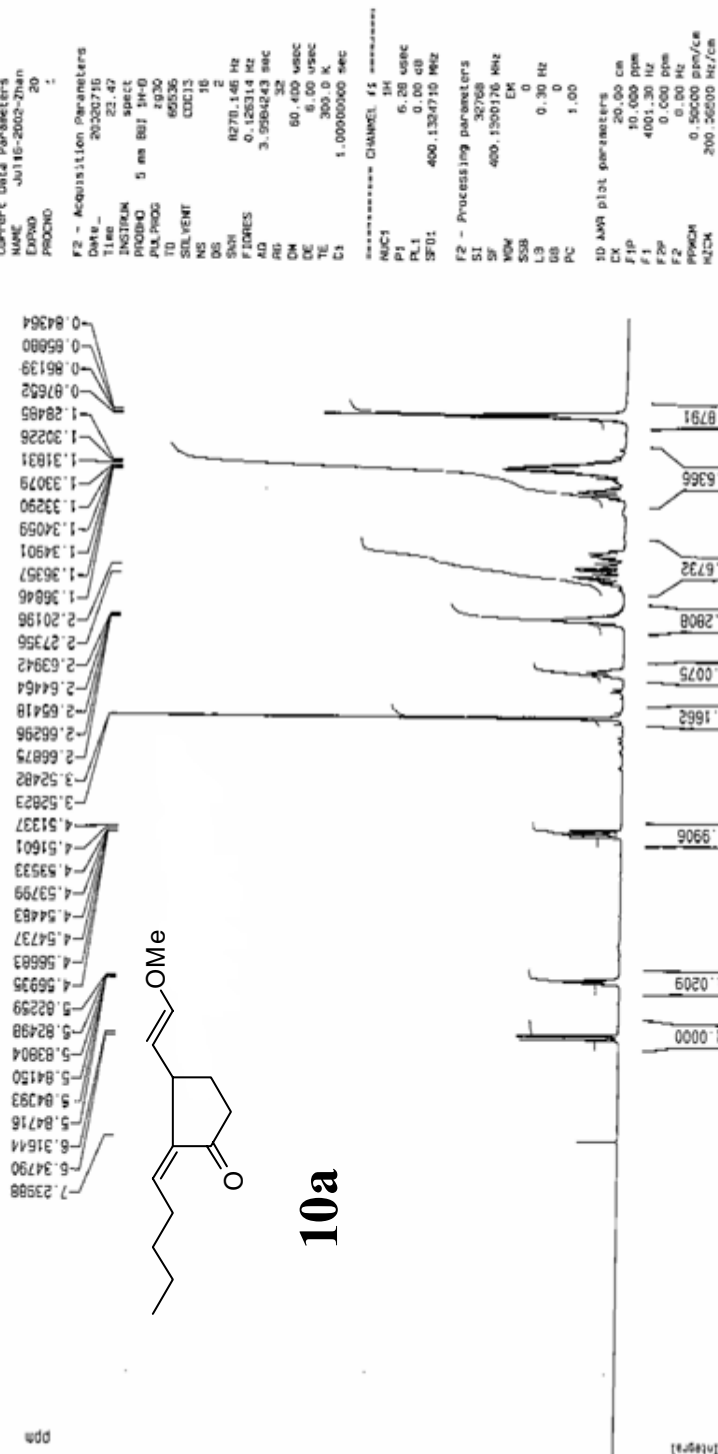
***** CHANNEL f1 *****
NUC1 13C
P1 5.00 uSAC
PL1 -5.00 dB
SF01 75.476000 MHz

***** CHANNEL f2 *****
CPUPRG2 M11210
NUC2 1H
PCPD2 194.00 uSAC
PL2 -5.00 dB
PL12 18.00 dB
PL13 18.00 dB
SF02 300.131000 MHz

F2 - Processing parameters
SI 32768
SF 75.4677100 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

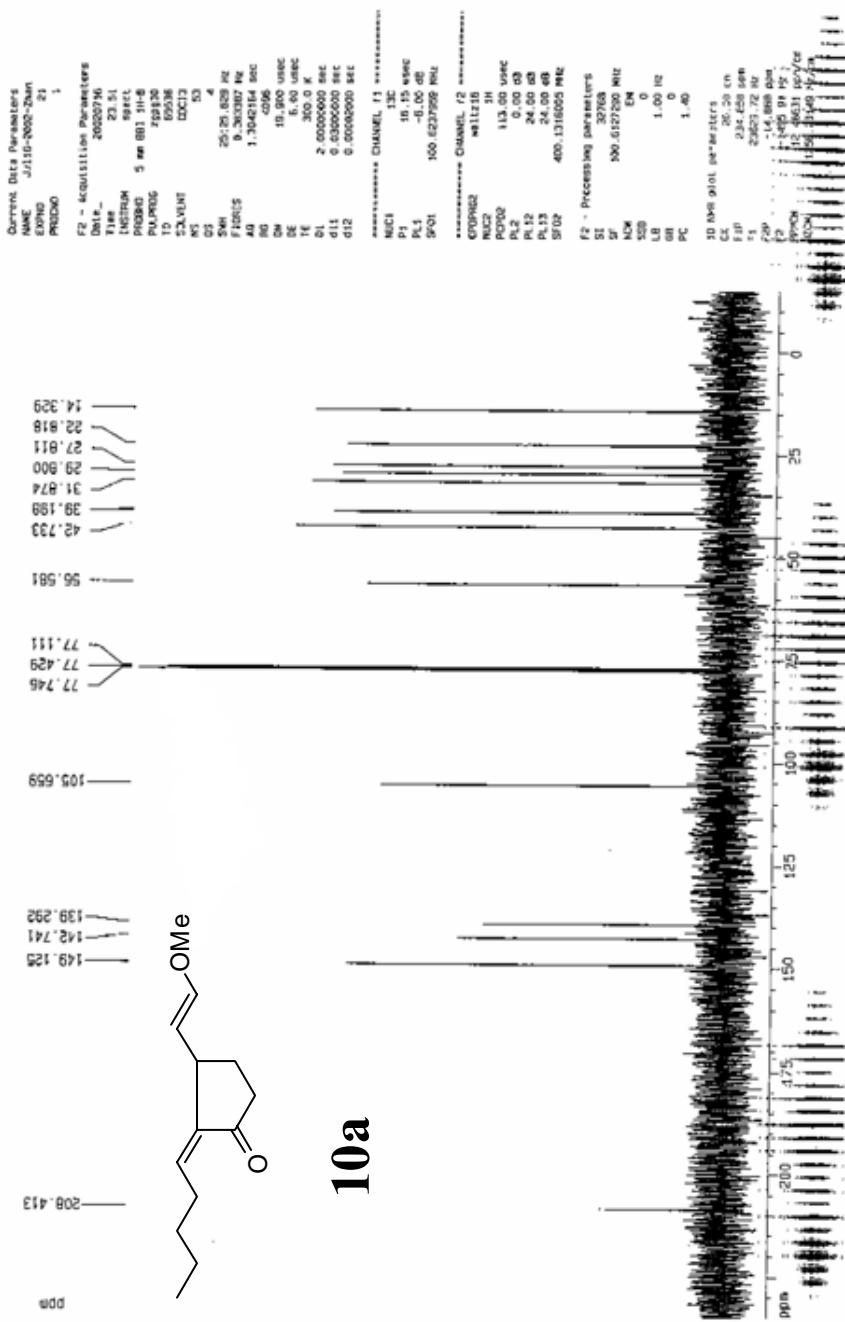
1D NMR d1c1 parameters
CX 20.00 cm
FAP 234.751 ppm
F1 17716.12 Hz
F2P -14.781 ppm
F2 -1116.27 Hz
FREQH 12-47712 ppm/cm
HZCM 941.61951 Hz/cm

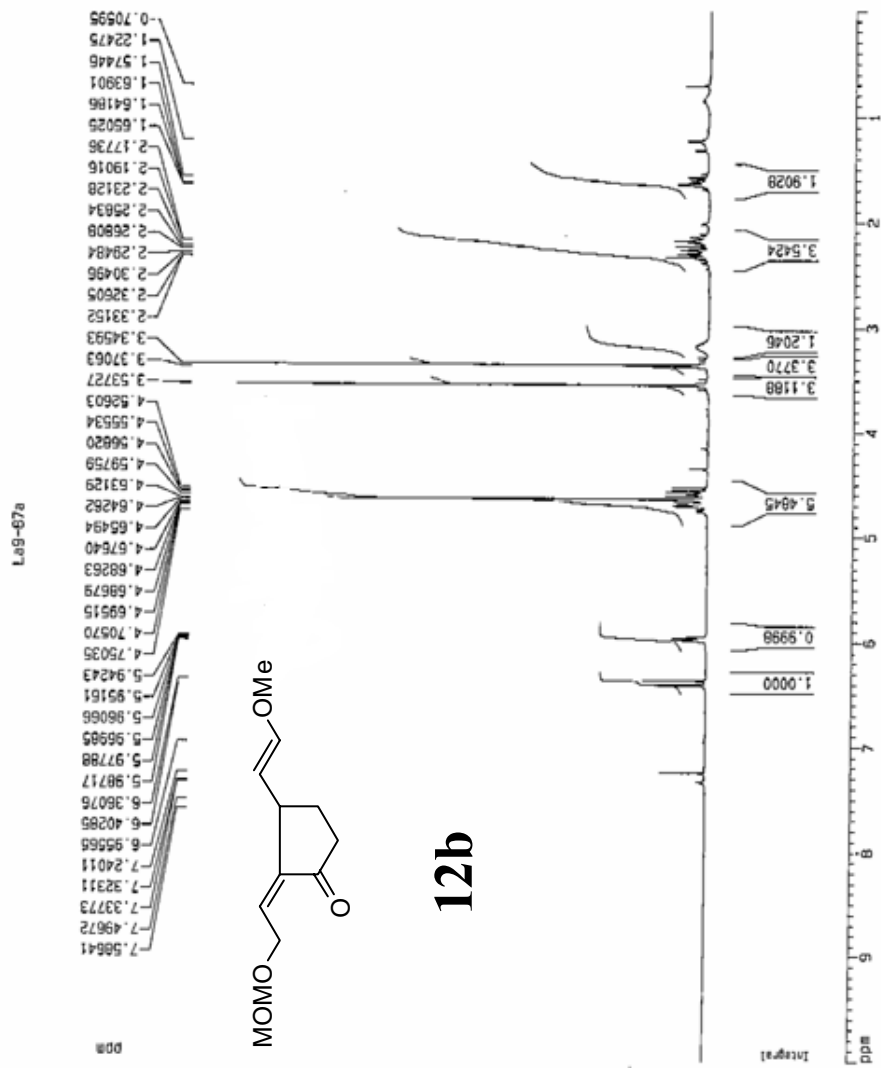
La10-2



10a

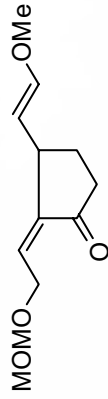
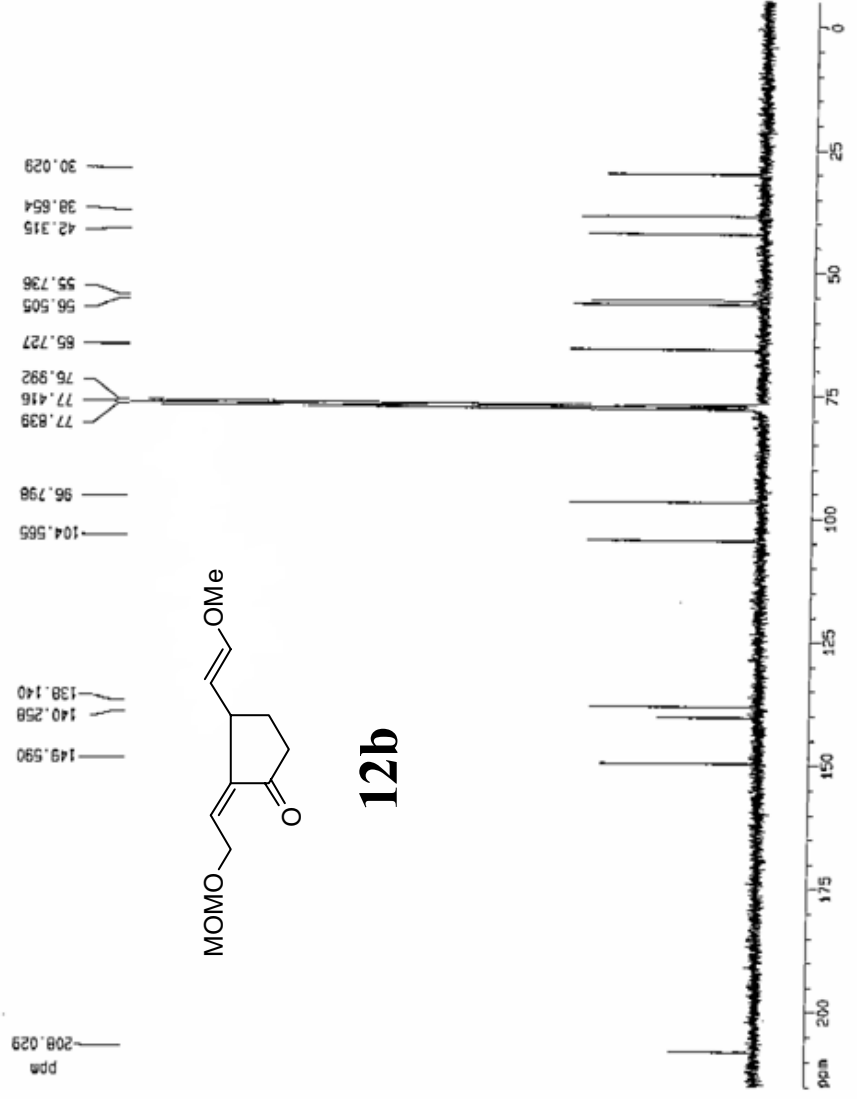
La10-2





Current Data Parameters
 NAME Jul20-2000-Zhan
 EXPNO 20
 PROCNO 1
 F2 - Acquisition Parameters
 DATE_ 20000720
 TIME 22.32
 INSTRUM spect
 PULPROG 5 mm Muicnu
 TD 7830
 ID 66535
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 5172.839 Hz
 FIDRES 0.004195 Hz
 AQ 5.3054659 sec
 RG 326.5
 DQ 81.000 usec
 DE 8.00 usec
 TE 300.0 K
 TC 1.00000000 sec
 D1 1.00000000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 9.00 usec
 PL1 -5.00 dB
 SFO1 300.1318534 MHz
 F2 - Processing parameters
 SI 32768
 SF 300.1300120 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00
 SD NMR plot parameters
 CX 20.00 cm
 ZF1 40.000 MHz
 F1 300.130 MHz
 F2 0.000 MHz
 F3 0.000 MHz
 PRONM 0.55000 ppm/cm
 HZDN 150.08500 Hz/cm

109-07a



12b

```

Current Date Parameters
      39120-2602-Zhen
      21
      1
PRDNO

F2 - Acquisition Parameters
Date= 20020729
Time= 23.52
INSTR= spect
PROB= 5 mm MSL10mm
PULPROG= zgpg30
TD= 65536
SOLVENT= CDCl3
AQ= 1200
RG= 4
SFO1= 400.1303 MHz
FIDRES= 0.38776 Hz
AQ= 0.38776 Hz
RG= 1.7469308 sec
F2= 11585.2 Hz
DM= 38.550 uSec
DE= 6.00 uSec
TE= 300.00 K
D1= 2.00000000 sec
g1= 0.63000000 sec
g12= 6.00000000 sec

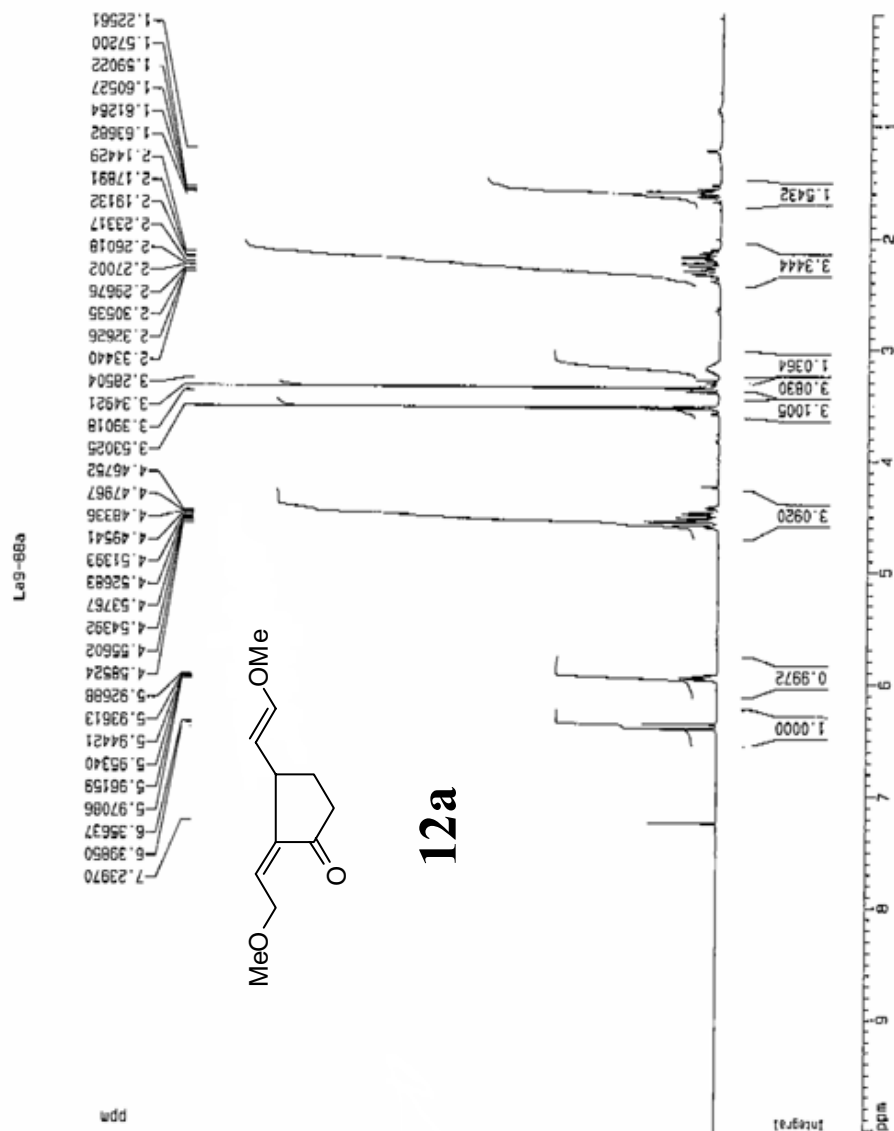
***** CHANNEL F1 *****
NUC1= 13C
P1= 5.00 uSec
PL1= -0.00 dB
SFO1= 75.470300 MHz

***** CHANNEL F2 *****
CPDPRG2= MSL1218
NUC2= 1H
P2= 114.00 uSec
PL2= -6.00 dB
PL12= 18.90 dB
PL13= 18.00 dB
PL14= 18.00 dB
SFO2= 300.1313005 MHz

F2 - Processing parameters
F1= 37.708 MHz
F2= 75.4677100 MHz
EN= En
SFO= 1.60 Hz
L6= 0
SFO= 0
SC= 1.40

10 Wt plot parameters
ID= 20.00 cm
F1P= 235.000 ppm
F1= 18.000 Hz
F2P= -5.000 Hz
F2= -377.34 Hz
P1= 11.00000000 Hz/cm
P1CM= 030.14400 Hz/cm

```



Current Data Parameters
 NAME j1115-2002-Zhan
 EXPNO 10
 PROCNO 1

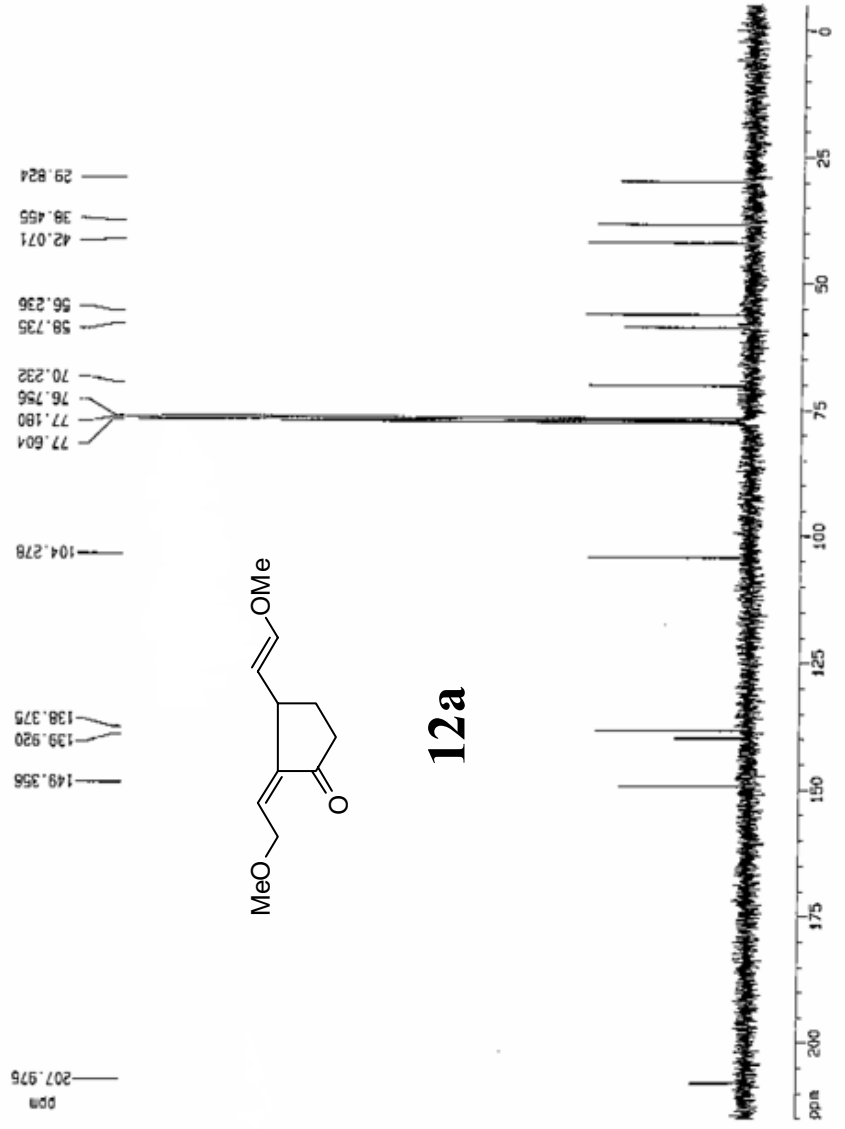
F2 - Acquisition Parameters
 Date_ 20020716
 Time 9.43
 INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TO 69536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.636 Hz
 FIDRES 0.094190 Hz
 AQ 5.3004650 sec
 RG 237.4
 DM 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.00000000 sec

===== CHANNEL f1 =====
 NUC1 1-1
 P1 11.70 usec
 PL1 6.00 dB
 SF01 259.8716518 MHz

F2 - Processing parameters
 S1 32768
 SF 259.8700161 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 F1P 10.000 ppm
 F1 2598.70 Hz
 F2P 0.000 ppm
 F2 0.00 Hz
 PH0K 0.50050 ppm/cm
 HZCM 149.93521 Hz/cm

La9-059a



Current Data Parameters
 NAME J0116-2662-2hab
 EXPNO 11
 PROCNO 1

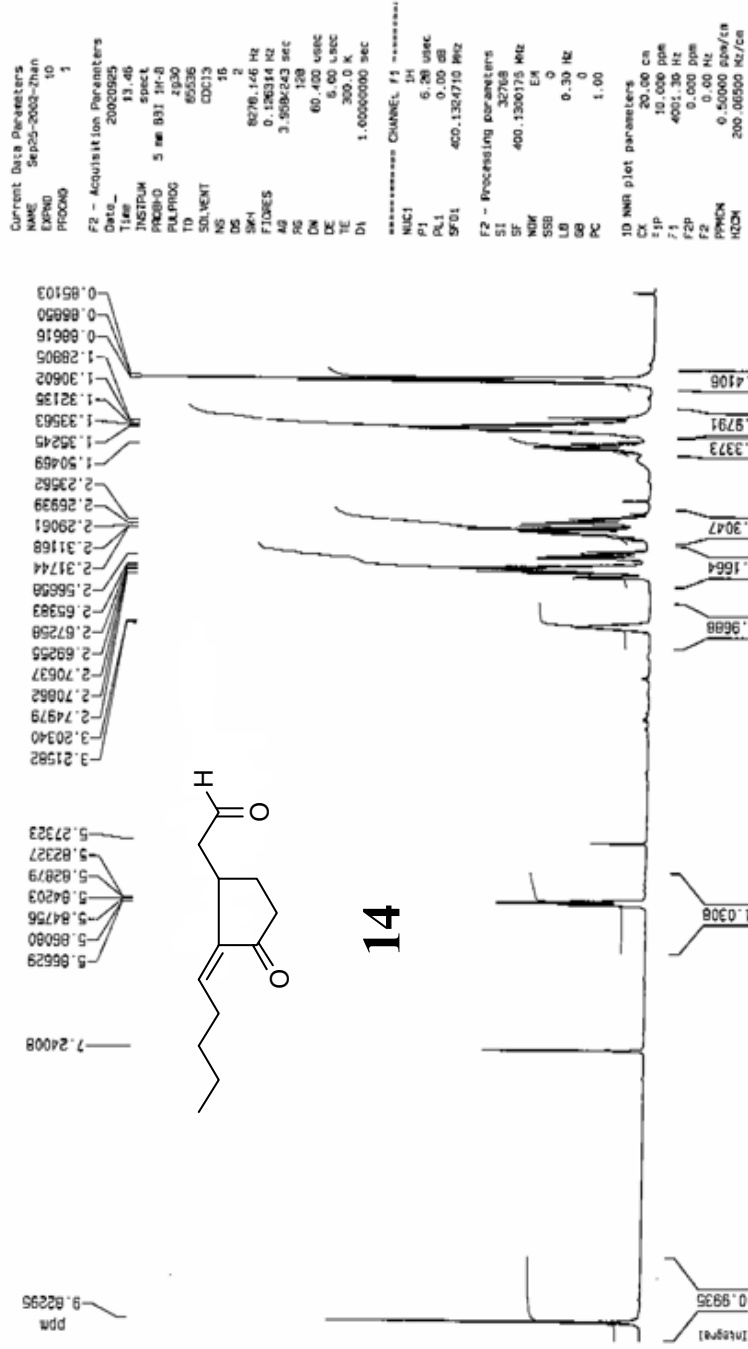
F2 - Acquisition Parameters
 Date_ 20200715
 Time 10.01
 INSTRUM spect
 PULPROG 5 ms GNP INV1
 TO 09430
 SOLVENT CDCl₃
 NS 245
 DS 4
 SWH 18795.902 Hz
 FIDRES 0.206819 Hz
 AQ 1.7433078 sec
 RG 320
 CM 25.000 USEC
 DE 300.6 K
 TE 300.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 D12 0.00000000 sec

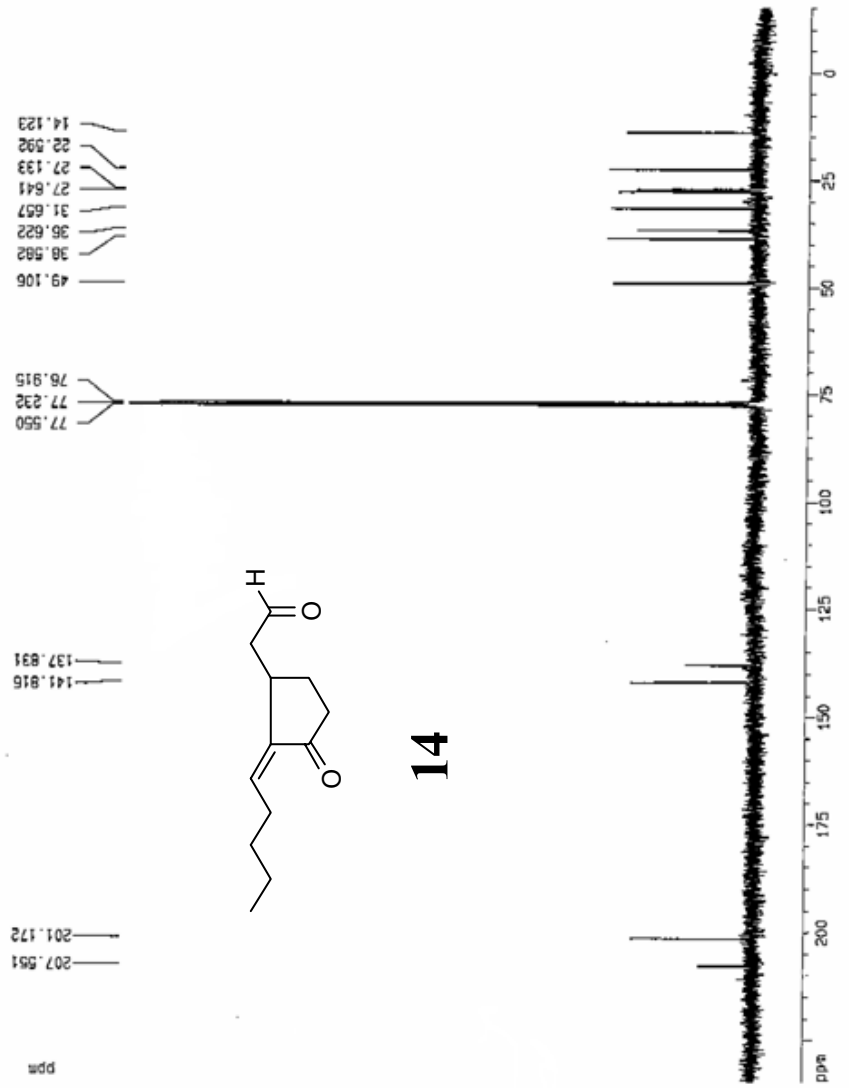
===== CHANNEL f1 =====
 NUC1 13C
 P1 5.48 USEC
 PL1 -8.00 DB
 SF01 75.4156357 MHz

===== CHANNEL f2 =====
 DROPOUT 1H
 NUC2 1H
 P2 115.00 USEC
 PL2 0.00 DB
 PL12 20.00 dB
 PL13 20.00 dB
 SF02 299.6711995 MHz

F2 - Processing parameters
 S1 32768
 SF 75.4023001 MHz
 WHW 6M
 SFO 16211.51 Hz
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 30.00 Hz
 F1F 215.000 ppm
 F1 16211.51 Hz
 F2 -5.000 ppm
 F2 -377.01 Hz
 PRON 11.00000 ppm/cm
 RCON 829.40250 Hz/cm





Current Data Parameters
NAME Sap25-2002-ZnH
EXPNO 11
PROCNO 1

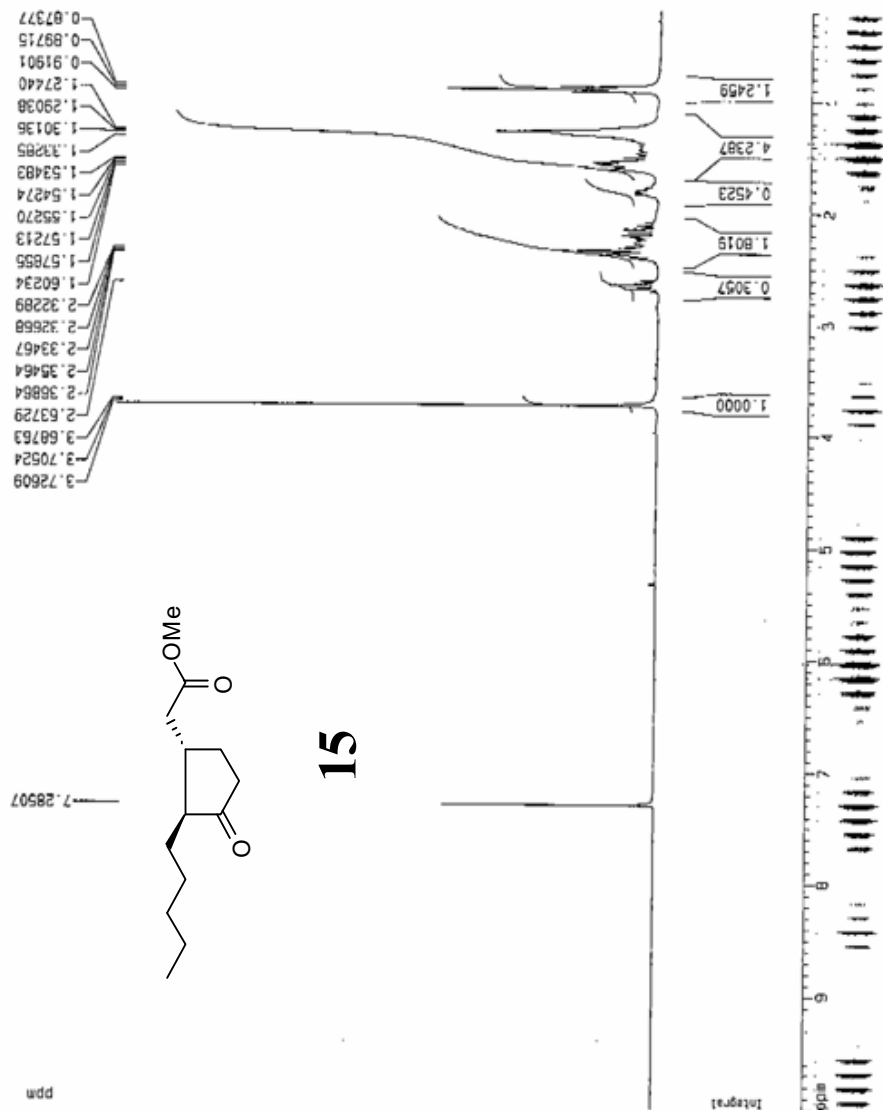
F2 - Acquisition Parameters
Date_ 20030825
Time 14.00
PROBHD 5 mm BBI 1H-B
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 595
DS 4
SWH 25425.638 Hz
FIDRES 0.383317 Hz
AQ 1.3042164 sec
RG 4836
DM 19.920 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00600000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 18.15 usec
PL1 -5.00 dB
SFO1 100.6277559 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P2 113.60 usec
PL2 0.00 dB
PL12 24.00 dB
PL13 24.00 dB
SFO2 400.1310003 MHz

F2 - Processing parameters
SI 32768
SF 100.6127759 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR file parameters
CK 20.00 cm
F1P 234.658 ppm
F1 23609.56 Hz
F2P -10.000 ppm
F2 -1516.67 Hz
PCNA 32.48830 per/cm
NDCN 125.88137 Hz/cm



```

Current Data Parameters
NAME      Oct26-2005-27.m
EXPNO     10
PROCNO    3

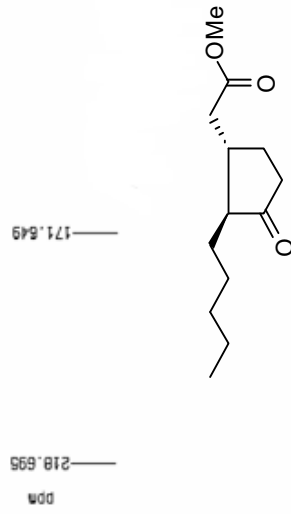
F2 - Acquisition Parameters
Date_     20051026
Time      23.36
INSTRUM   spect
PROBHD    5 mm BBO 1H/1
PULPROG   zg30
TO        49.30
RG         655.36
CQ1C3     0.013
SOLVENT   CDCl3
NS         2
DS         16
SWH        6172.809 Kz
FIDRES     0.054199 Hz
AQ         5.3044660 sec
RG         382
DE         81.000 usec
TE         6.00 usec
D1         300.0 K
O1         1.00000000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         11.70 usec
PL1        0.00 dB
SFO1       299.6718518 MHz

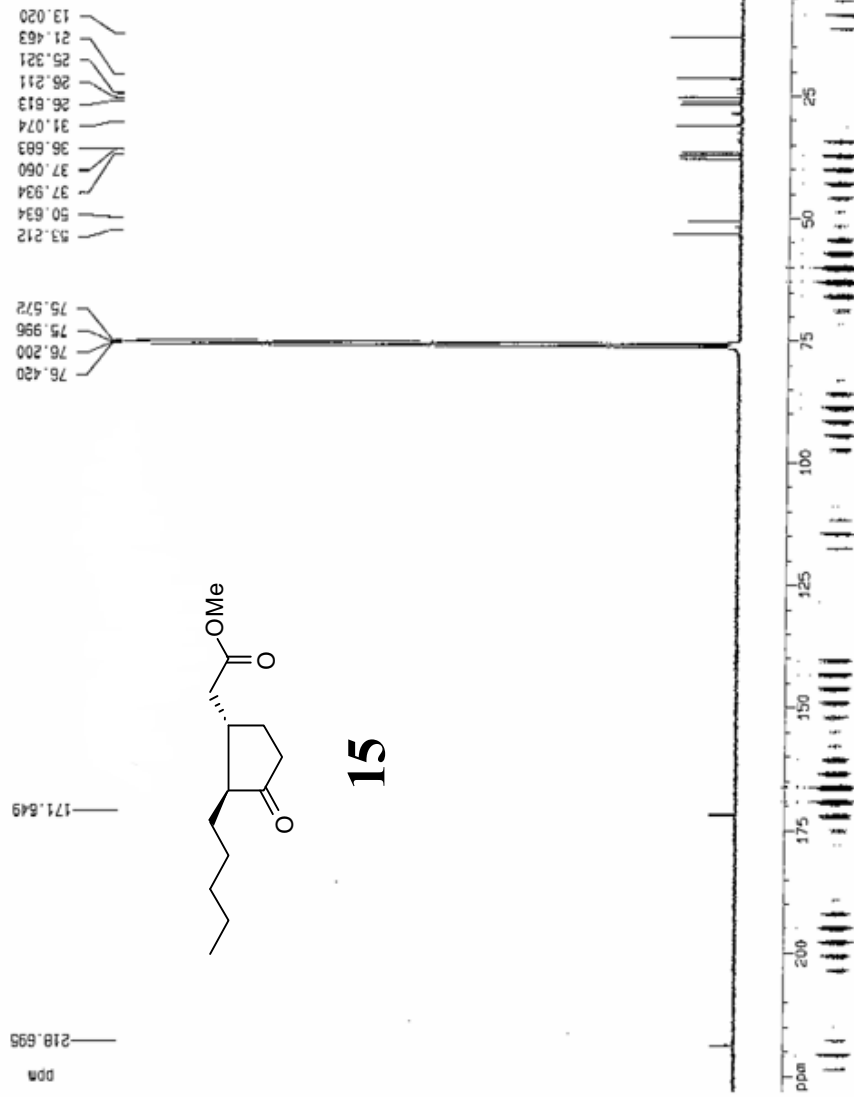
F2 - Processing parameters
SI         32768
SF          299.6700025 MHz
EN         EN
GB         0
GB2        0
GB3        0
GB4        0
GB5        0
GB6        0
GB7        0
GB8        0
GB9        0
GB10       0
GB11       0
GB12       0
GB13       0
GB14       0
GB15       0
GB16       0
GB17       0
GB18       0
GB19       0
GB20       0
GB21       0
GB22       0
GB23       0
GB24       0
GB25       0
GB26       0
GB27       0
GB28       0
GB29       0
GB30       0
GB31       0
GB32       0
GB33       0
GB34       0
GB35       0
GB36       0
GB37       0
GB38       0
GB39       0
GB40       0
GB41       0
GB42       0
GB43       0
GB44       0
GB45       0
GB46       0
GB47       0
GB48       0
GB49       0
GB50       0
GB51       0
GB52       0
GB53       0
GB54       0
GB55       0
GB56       0
GB57       0
GB58       0
GB59       0
GB60       0
GB61       0
GB62       0
GB63       0
GB64       0
GB65       0
GB66       0
GB67       0
GB68       0
GB69       0
GB70       0
GB71       0
GB72       0
GB73       0
GB74       0
GB75       0
GB76       0
GB77       0
GB78       0
GB79       0
GB80       0
GB81       0
GB82       0
GB83       0
GB84       0
GB85       0
GB86       0
GB87       0
GB88       0
GB89       0
GB90       0
GB91       0
GB92       0
GB93       0
GB94       0
GB95       0
GB96       0
GB97       0
GB98       0
GB99       0
GB100      0
GB101      0
GB102      0
GB103      0
GB104      0
GB105      0
GB106      0
GB107      0
GB108      0
GB109      0
GB110      0
GB111      0
GB112      0
GB113      0
GB114      0
GB115      0
GB116      0
GB117      0
GB118      0
GB119      0
GB120      0
GB121      0
GB122      0
GB123      0
GB124      0
GB125      0
GB126      0
GB127      0
GB128      0
GB129      0
GB130      0
GB131      0
GB132      0
GB133      0
GB134      0
GB135      0
GB136      0
GB137      0
GB138      0
GB139      0
GB140      0
GB141      0
GB142      0
GB143      0
GB144      0
GB145      0
GB146      0
GB147      0
GB148      0
GB149      0
GB150      0
GB151      0
GB152      0
GB153      0
GB154      0
GB155      0
GB156      0
GB157      0
GB158      0
GB159      0
GB160      0
GB161      0
GB162      0
GB163      0
GB164      0
GB165      0
GB166      0
GB167      0
GB168      0
GB169      0
GB170      0
GB171      0
GB172      0
GB173      0
GB174      0
GB175      0
GB176      0
GB177      0
GB178      0
GB179      0
GB180      0
GB181      0
GB182      0
GB183      0
GB184      0
GB185      0
GB186      0
GB187      0
GB188      0
GB189      0
GB190      0
GB191      0
GB192      0
GB193      0
GB194      0
GB195      0
GB196      0
GB197      0
GB198      0
GB199      0
GB200      0
GB201      0
GB202      0
GB203      0
GB204      0
GB205      0
GB206      0
GB207      0
GB208      0
GB209      0
GB210      0
GB211      0
GB212      0
GB213      0
GB214      0
GB215      0
GB216      0
GB217      0
GB218      0
GB219      0
GB220      0
GB221      0
GB222      0
GB223      0
GB224      0
GB225      0
GB226      0
GB227      0
GB228      0
GB229      0
GB230      0
GB231      0
GB232      0
GB233      0
GB234      0
GB235      0
GB236      0
GB237      0
GB238      0
GB239      0
GB240      0
GB241      0
GB242      0
GB243      0
GB244      0
GB245      0
GB246      0
GB247      0
GB248      0
GB249      0
GB250      0
GB251      0
GB252      0
GB253      0
GB254      0
GB255      0
GB256      0
GB257      0
GB258      0
GB259      0
GB260      0
GB261      0
GB262      0
GB263      0
GB264      0
GB265      0
GB266      0
GB267      0
GB268      0
GB269      0
GB270      0
GB271      0
GB272      0
GB273      0
GB274      0
GB275      0
GB276      0
GB277      0
GB278      0
GB279      0
GB280      0
GB281      0
GB282      0
GB283      0
GB284      0
GB285      0
GB286      0
GB287      0
GB288      0
GB289      0
GB290      0
GB291      0
GB292      0
GB293      0
GB294      0
GB295      0
GB296      0
GB297      0
GB298      0
GB299      0
GB300      0
GB301      0
GB302      0
GB303      0
GB304      0
GB305      0
GB306      0
GB307      0
GB308      0
GB309      0
GB310      0
GB311      0
GB312      0
GB313      0
GB314      0
GB315      0
GB316      0
GB317      0
GB318      0
GB319      0
GB320      0
GB321      0
GB322      0
GB323      0
GB324      0
GB325      0
GB326      0
GB327      0
GB328      0
GB329      0
GB330      0
GB331      0
GB332      0
GB333      0
GB334      0
GB335      0
GB336      0
GB337      0
GB338      0
GB339      0
GB340      0
GB341      0
GB342      0
GB343      0
GB344      0
GB345      0
GB346      0
GB347      0
GB348      0
GB349      0
GB350      0
GB351      0
GB352      0
GB353      0
GB354      0
GB355      0
GB356      0
GB357      0
GB358      0
GB359      0
GB360      0
GB361      0
GB362      0
GB363      0
GB364      0
GB365      0
GB366      0
GB367      0
GB368      0
GB369      0
GB370      0
GB371      0
GB372      0
GB373      0
GB374      0
GB375      0
GB376      0
GB377      0
GB378      0
GB379      0
GB380      0
GB381      0
GB382      0
GB383      0
GB384      0
GB385      0
GB386      0
GB387      0
GB388      0
GB389      0
GB390      0
GB391      0
GB392      0
GB393      0
GB394      0
GB395      0
GB396      0
GB397      0
GB398      0
GB399      0
GB400      0
GB401      0
GB402      0
GB403      0
GB404      0
GB405      0
GB406      0
GB407      0
GB408      0
GB409      0
GB410      0
GB411      0
GB412      0
GB413      0
GB414      0
GB415      0
GB416      0
GB417      0
GB418      0
GB419      0
GB420      0
GB421      0
GB422      0
GB423      0
GB424      0
GB425      0
GB426      0
GB427      0
GB428      0
GB429      0
GB430      0
GB431      0
GB432      0
GB433      0
GB434      0
GB435      0
GB436      0
GB437      0
GB438      0
GB439      0
GB440      0
GB441      0
GB442      0
GB443      0
GB444      0
GB445      0
GB446      0
GB447      0
GB448      0
GB449      0
GB450      0
GB451      0
GB452      0
GB453      0
GB454      0
GB455      0
GB456      0
GB457      0
GB458      0
GB459      0
GB460      0
GB461      0
GB462      0
GB463      0
GB464      0
GB465      0
GB466      0
GB467      0
GB468      0
GB469      0
GB470      0
GB471      0
GB472      0
GB473      0
GB474      0
GB475      0
GB476      0
GB477      0
GB478      0
GB479      0
GB480      0
GB481      0
GB482      0
GB483      0
GB484      0

```

(+)-Methyl Dihydrojasmonate



15



```

Current Data Parameters
NAME      05120-2002-Zhen
EXPNO     11
PROCNO    1
F2 - Acquisition Parameters
Date_     20021027
Time      8.47
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         5567
DS         4
SWH        10756.952 Hz
FIDRES     6.2865919 Hz
AQ         1.7433076 sec
RG          2048
XY         20.800 usec
YF          5.00 usec
ZD          200.0 K
ZG          2.0000000 sec
ZS          0.0000000 sec
ZC          0.0000000 sec
ZD          0.0000000 sec
===== CHANNEL f1 =====
NUC1       13C
P1          13C
PL1         5.40 usec
RF1         -6.00 dB
===== CHANNEL f2 =====
CONTCENT   wait 36
NUC2        13C
P2          13C
PL2         5.00 usec
RF2         0.00 dB
PL12        20.00 dB
PL13        20.00 dB
SF02        200.071935 MHz
F2 - Processing parameters
SI          32768
SF          75.4024885 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
=====
1D NMR pict parameters
EX          20.00 usec
F-SP        227.025 ps
F1          17186.07 Hz
F2          4.765 usec
F3          255.36 usec
F4          11.15781 usec
F5          0.4113507 usec
=====

```