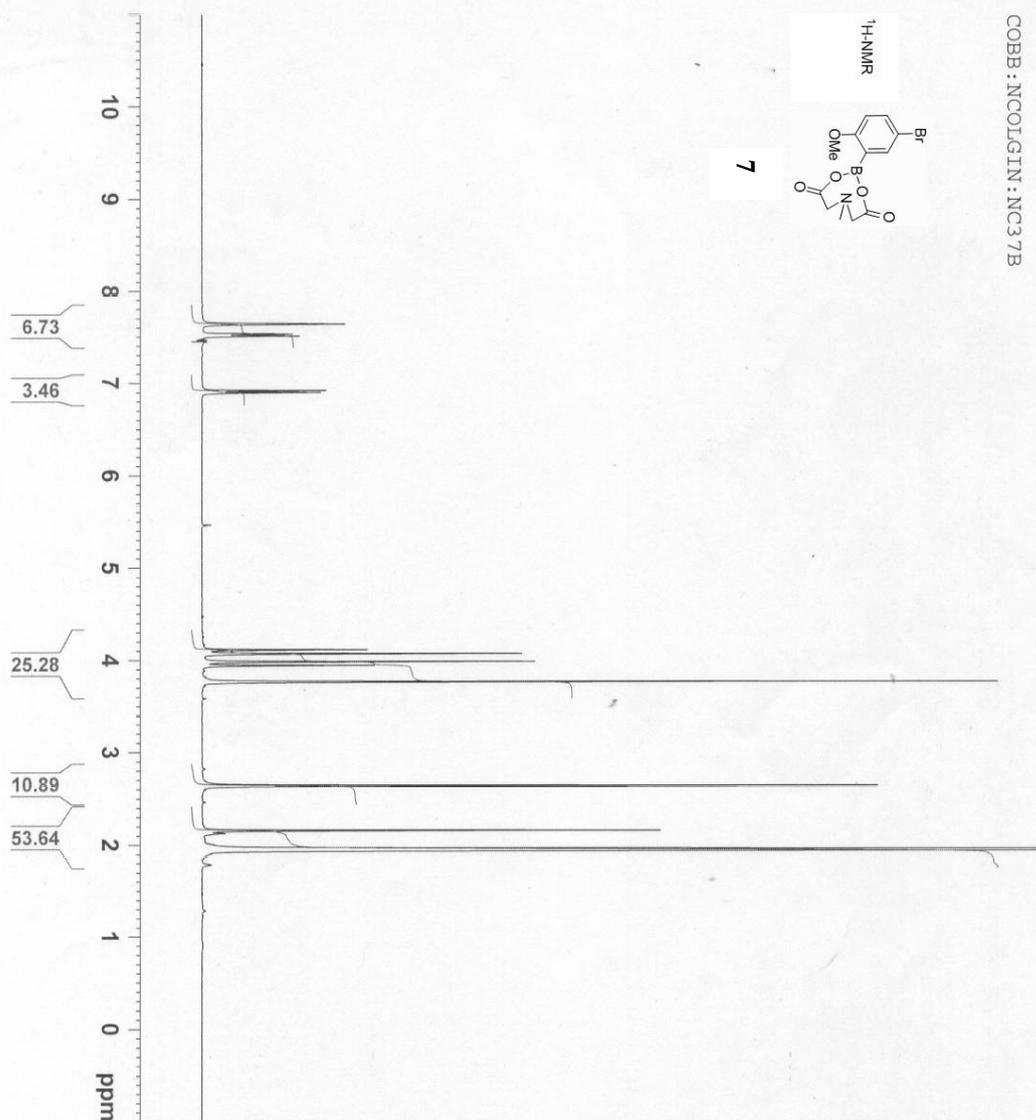**Supporting Information**

Synthesis and properties of MIDA boronate containing aromatic amino acids: New peptide building blocks[*]

Neil Colgin, Tony Flinn and Steven L Cobb*

(s.l.cobb@durham.ac.uk)

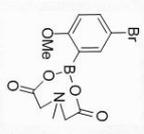**Part 1** ^{1}H and ^{13}C NMR Spectra

Part 2   Chiral HPLC Analysis for Compounds **9-11**

COBB:NCOLGIN:NC37B

13C-NMR

7

OMe

Br

Peaks:
168.21
161.17
136.50
133.03
116.99
112.55
112.26
63.23
54.78
46.99
0.62
0.56
0.41
0.36
0.21

BRUKER

Current Data Parameters
NAME   03154045
EXPNO   11
PROCNO   1
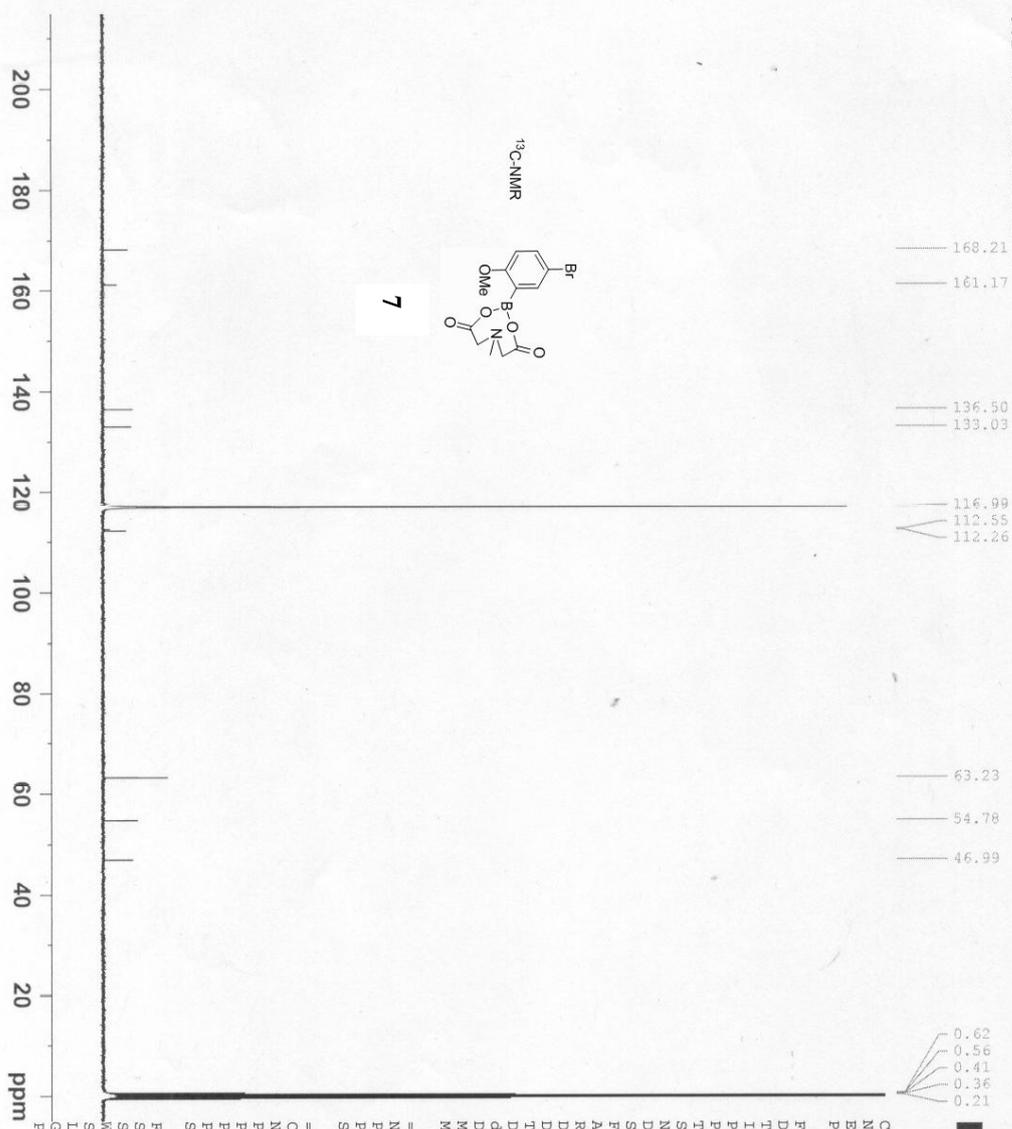
F2 - Acquisition Parameters
Date_   20100603
Time   19.04
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zgpg30
TD   65536
SOLVENT   CD3CN
NS   1024
DS   1
SWH   23980.814 Hz
FIDRES   0.365918 Hz
AQ   1.3664756 sec
RG   1149.4
DW   20.850 usec
DE   6.00 usec
TE   296.3 K
D1   2.00000000 sec
d11   0.03000000 sec
DELTA   1.89999998 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======== CHANNEL f1 ========
NUC1   13C
P1   7.80 usec
PL1   4.00 dB
SFO1   100.6027118 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   100.00 usec
PL2   7.00 dB
PL12   29.00 dB
PL13   29.00 dB
SFO2   400.0516002 MHz

F2 - Processing parameters
SI   65536
SF   100.5926856 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

^{13}C expansion: compound **7**
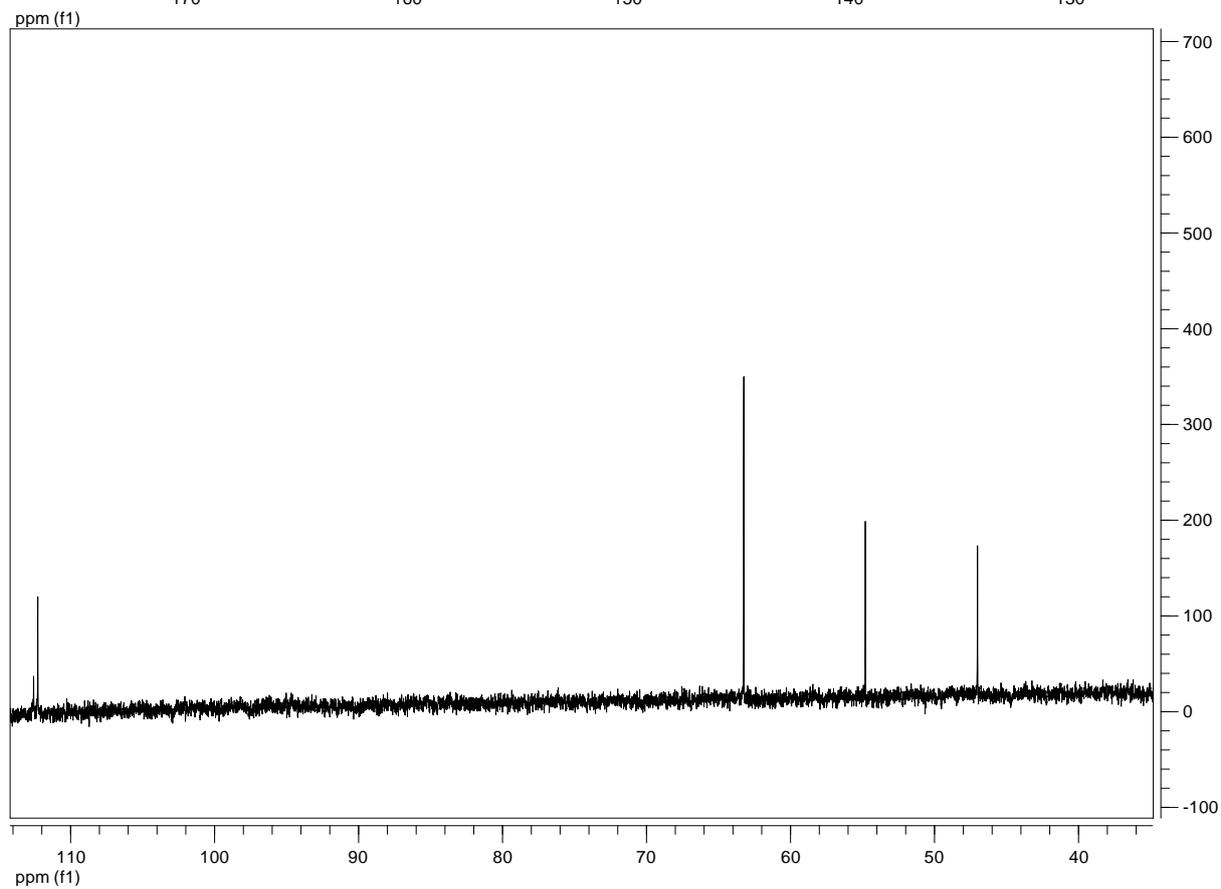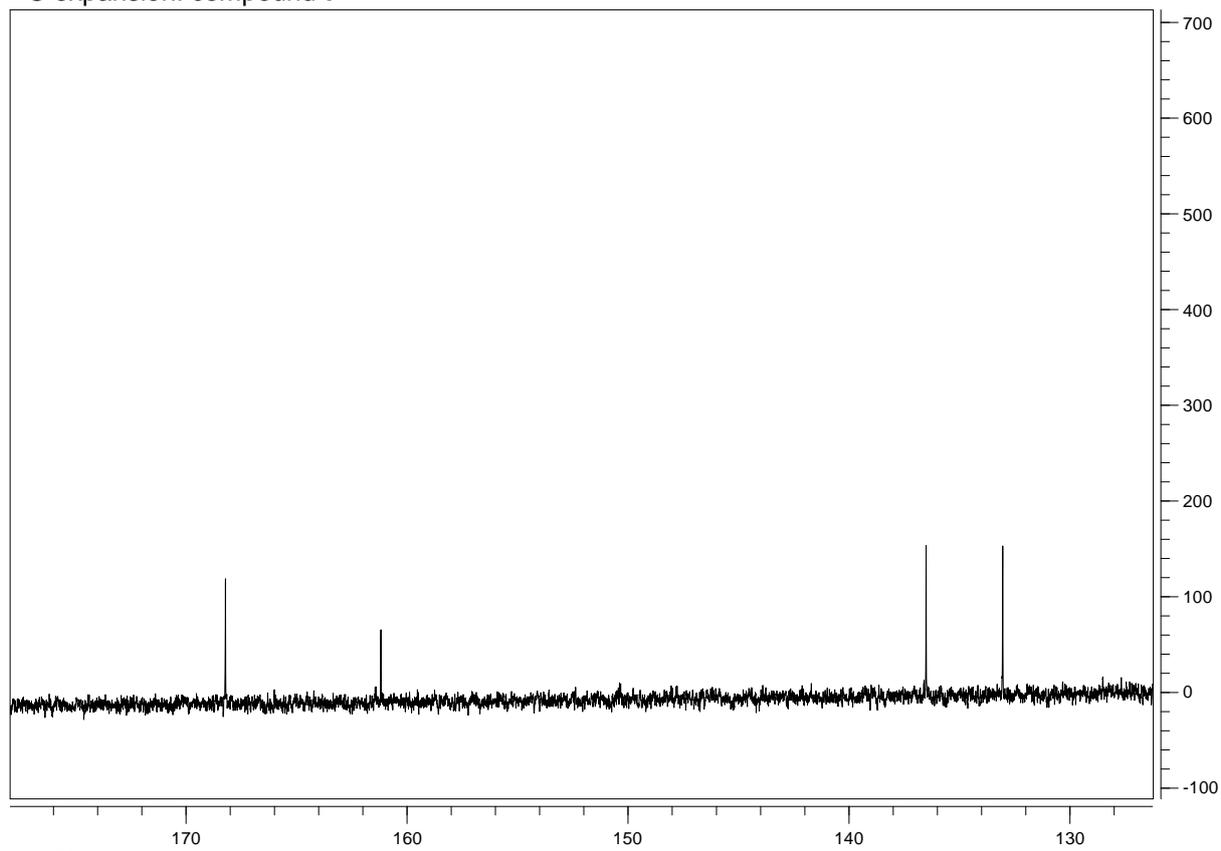
cobb:ncolgin:nc83

1H-NMR

1a

BocHN

OBn

O

B

O

O

N

O

BRUKER

10   9   8   7   6   5   4   3   2   1   0 ppm

32.21

7.41
3.19

10.44

5.34

7.84

33.28

0.29

cobb:ncolgin:nc83

^{13}C-NMR

1a

^{13}Cexpansion:compound **1a**

cobb:ncolgin:nc67

1H-NMR

2a

31.95

7.42

3.33

11.52

5.75

8.64

31.39

10   9   8   7   6   5   4   3   2   1   0   ppm

BRUKER

Current Data Parameters
NAME   25135432
EXPNO   1C
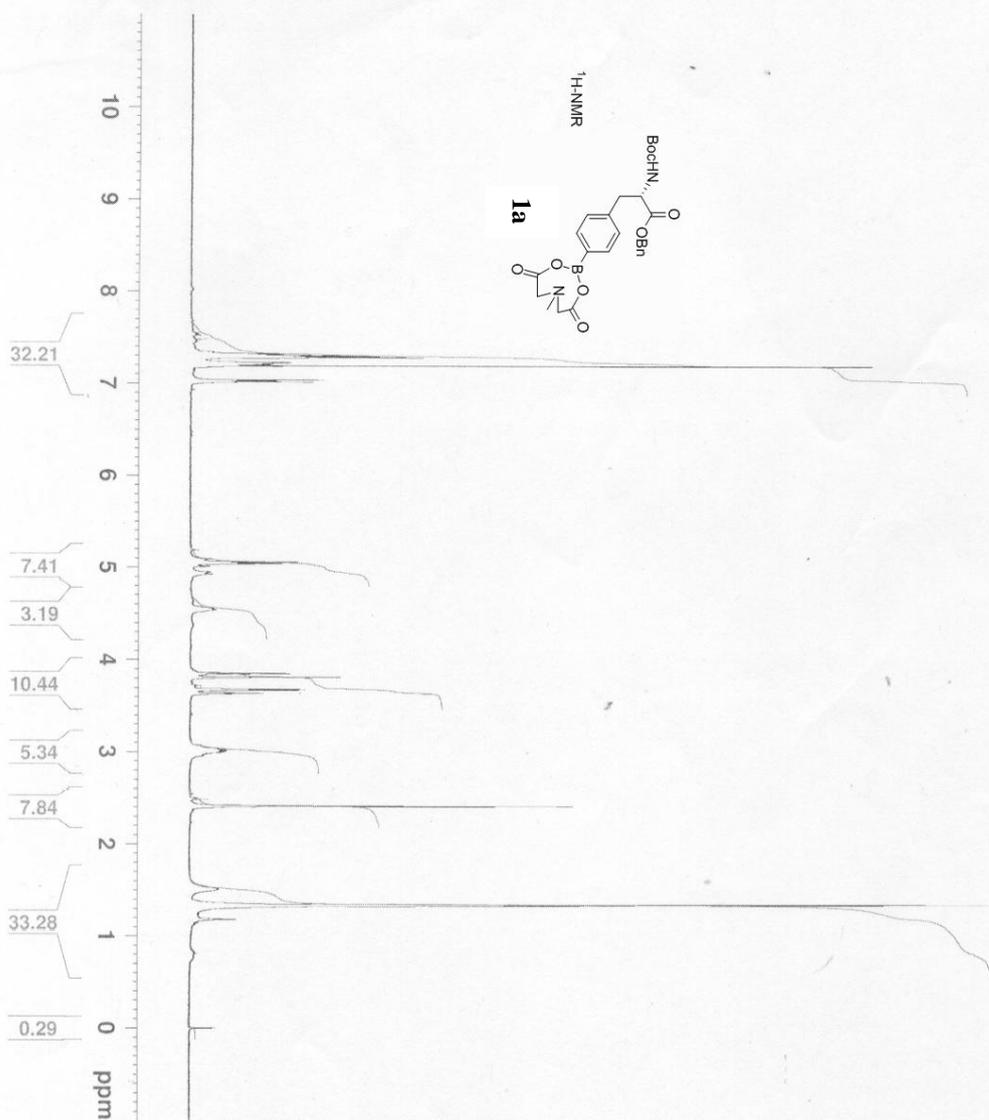PROCNO   1

F2 - Acquisition Parameters
Date_   20100415
Time   24.34
INSTRUM   av400
PROBEJ   5 mm 3B0 BB-1H
PULPROG   zg30
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8278.146 Hz
FIDRES   0.26314 Hz
AQ   3.9584243 sec
RG   406.4
DW   60.400 usec
DE   7.50 usec
TE   297.2 K
D1   1.00000000 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======== CHANNEL f1 ========
NUC1   1H
P1   9.50 usec
PL1   -1.00 dB
SFO1   400.1324700 MHz

F2 - Processing parameters
SI   32768
SF   400.1300357 MHz
WDW   EM
SSB   C
LB   0.30 Hz
GB   C
PC   1.00

COBB:NCOLGIN:NC67 3-MIDA ESTER

^{13}C-NMR

2a

171.9?
165.97

155.0?

135.3?
135.26
135.0?
133.??
132.0?
130.9?
130.75
126.62
128.45
128.36

80.37
79.85
77.46
77.34
77.14
76.82
67.08
61.89
55.99
54.81
53.50
47.71

32.30

29.67
26.29

200 180 160 140 120 100 80 60 40 20 0 ppm

BRUKER

Current Data Parameters
NAME   22113120
EXPNO   10
PROCNO   1

F2 - Acquisition Parameters
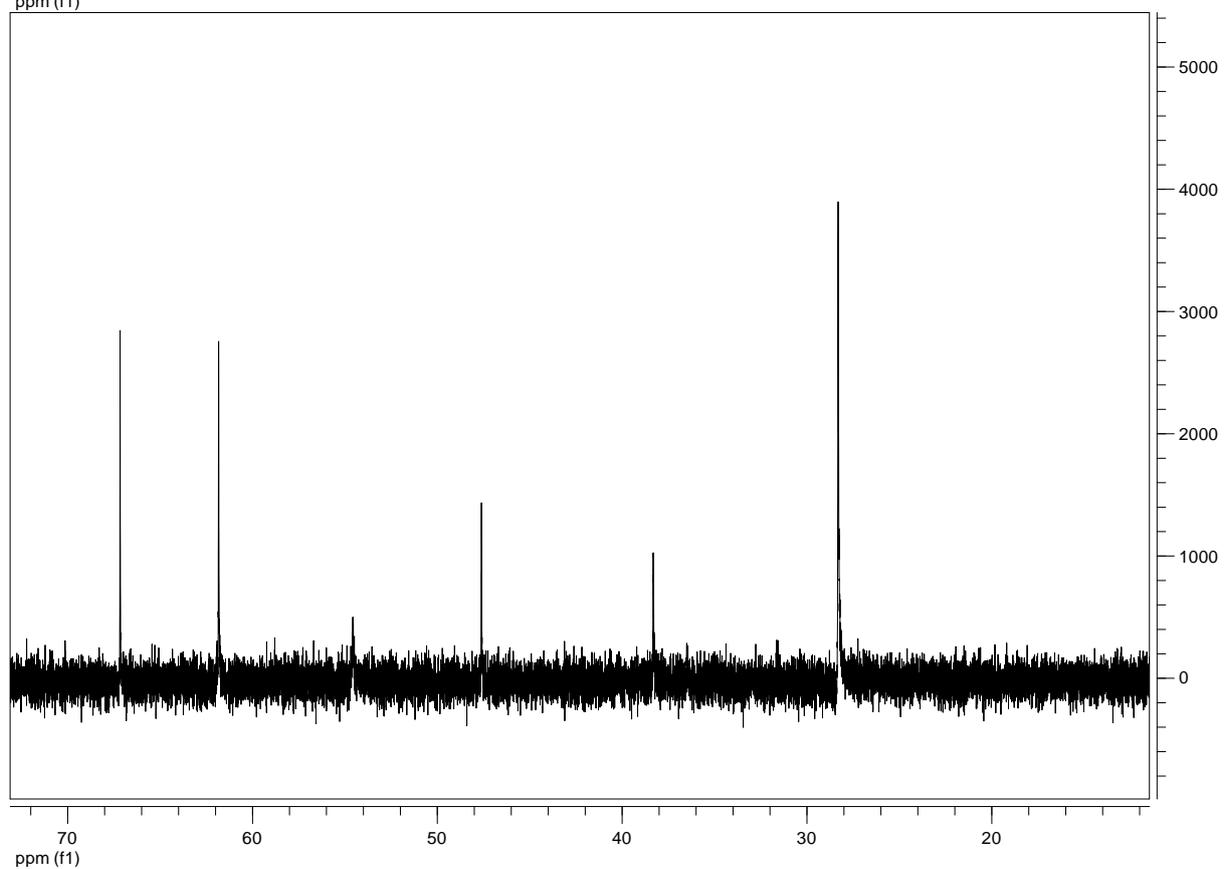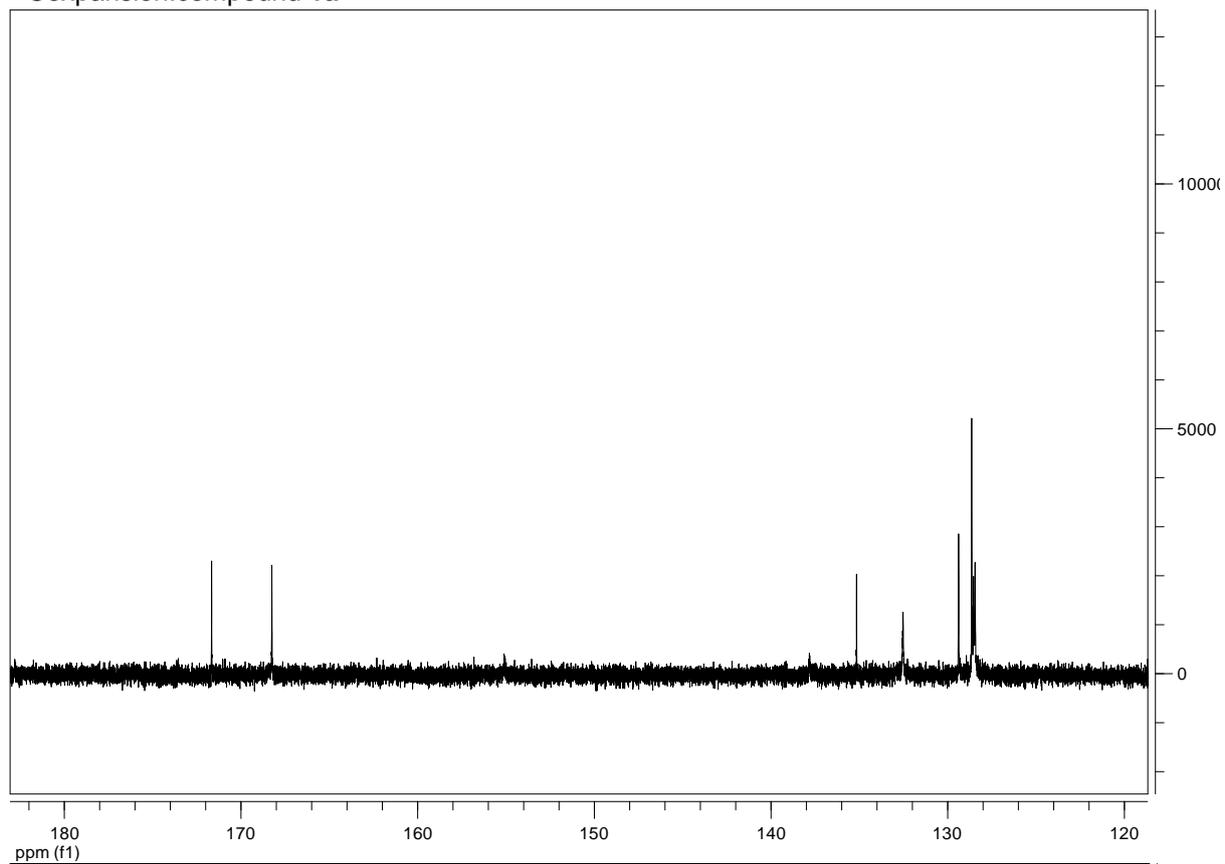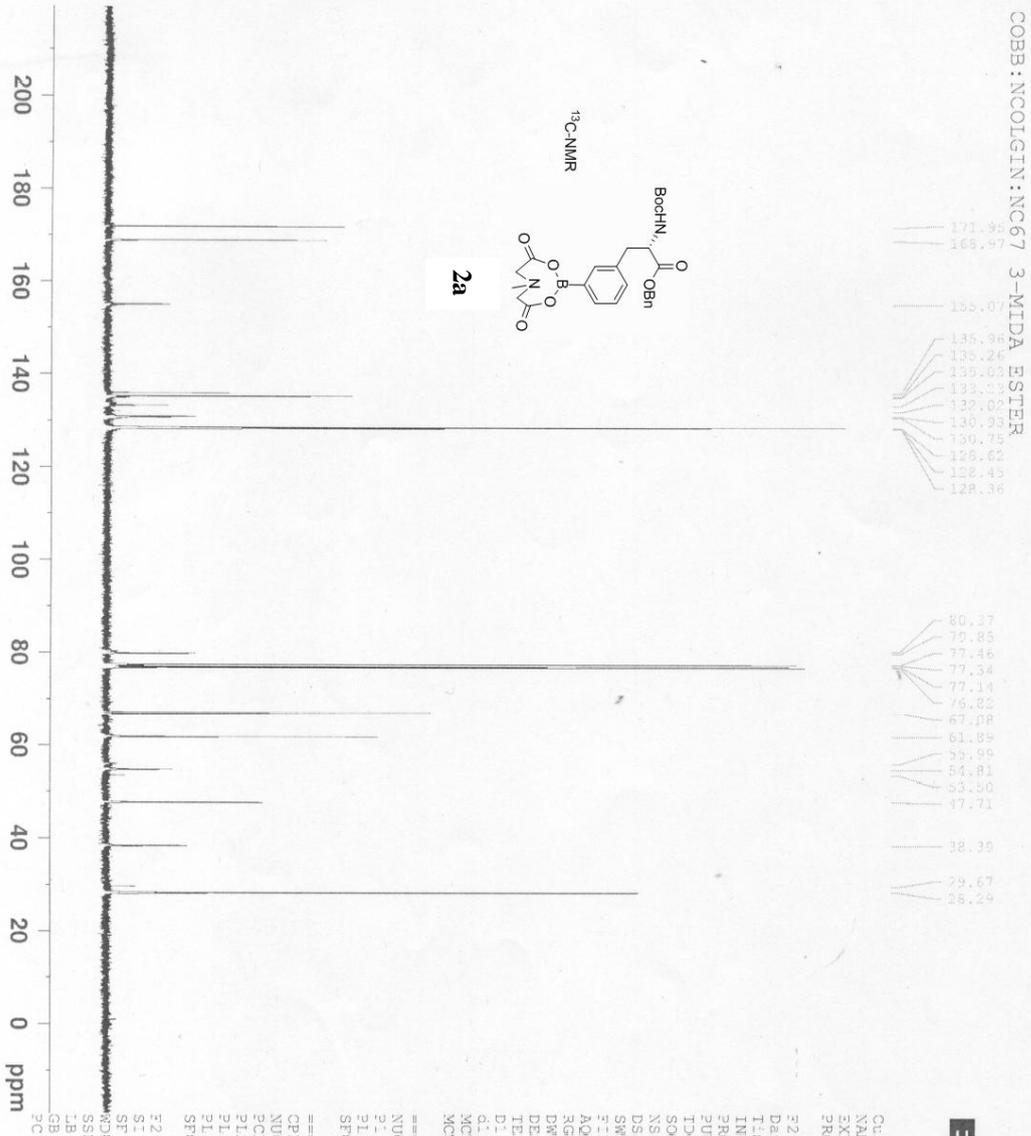Date_   20100122
Time   20.22
INSTRUM   av400
PROBHD   5 mm BBO BB-1H
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   1024
DS   4
SWH   23980.814 Hz
FIDRES   0.365918 Hz
AQ   1.3664756 sec
RG   9195.2
DW   20.850 usec
DE   7.50 usec
TE   299.2 K
D1   2.00000000 sec
d11   0.03000000 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======= CHANNEL f1 =======
NUC1   13C
P1   8.00 usec
PL1   -3.00 dB
SFO1   100.6228298 MHz

======= CHANNEL f2 =======
CPD2RG2   waltz16
NUC2   1H
CPD2   1H
PCPD2   80.00 usec
PL2   -1.00 dB
PL12   18.00 dB
PL13   18.00 dB
SFO2   400.1316005 MHz

F2 - Processing parameters
SI   32768
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

^{13}C expansion: compound **2a**

cobb:ncolgin:nc56

1H-NMR

3a

cobb:ncolgin:nc56

^{13}C-NMR

3a

BocHN

OBn

O

O

N

B

O

O

OMe

171.93
168.23

161.31
161.17
155.06

137.44
135.83
135.24
133.86
132.13
128.59
128.48
128.41

114.11
112.48
110.62

79.86
77.37
77.25
77.05
76.73
67.13
63.70
63.64
55.74
55.47
54.85
47.46

37.60

28.30

15.28

200 180 160 140 120 100 80 60 40 20 ppm

BRUKER

Current Data Parameters
NAME   04092630
EXPNO   10
PROCNO   1

F2 - Acquisition Parameters
Date_   20100504
Time   19.10
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   1024
DS   1
SWH   23980.814 Hz
FIDRES   0.365918 Hz
AQ   1.3664756 sec
RG   1149.4
DW   20.850 usec
DE   6.00 usec
TE   296.1 K
D1   2.00000000 sec
d11   0.03000000 sec
DELTA   1.89999998 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======== CHANNEL f1 ========
NUC1   13C
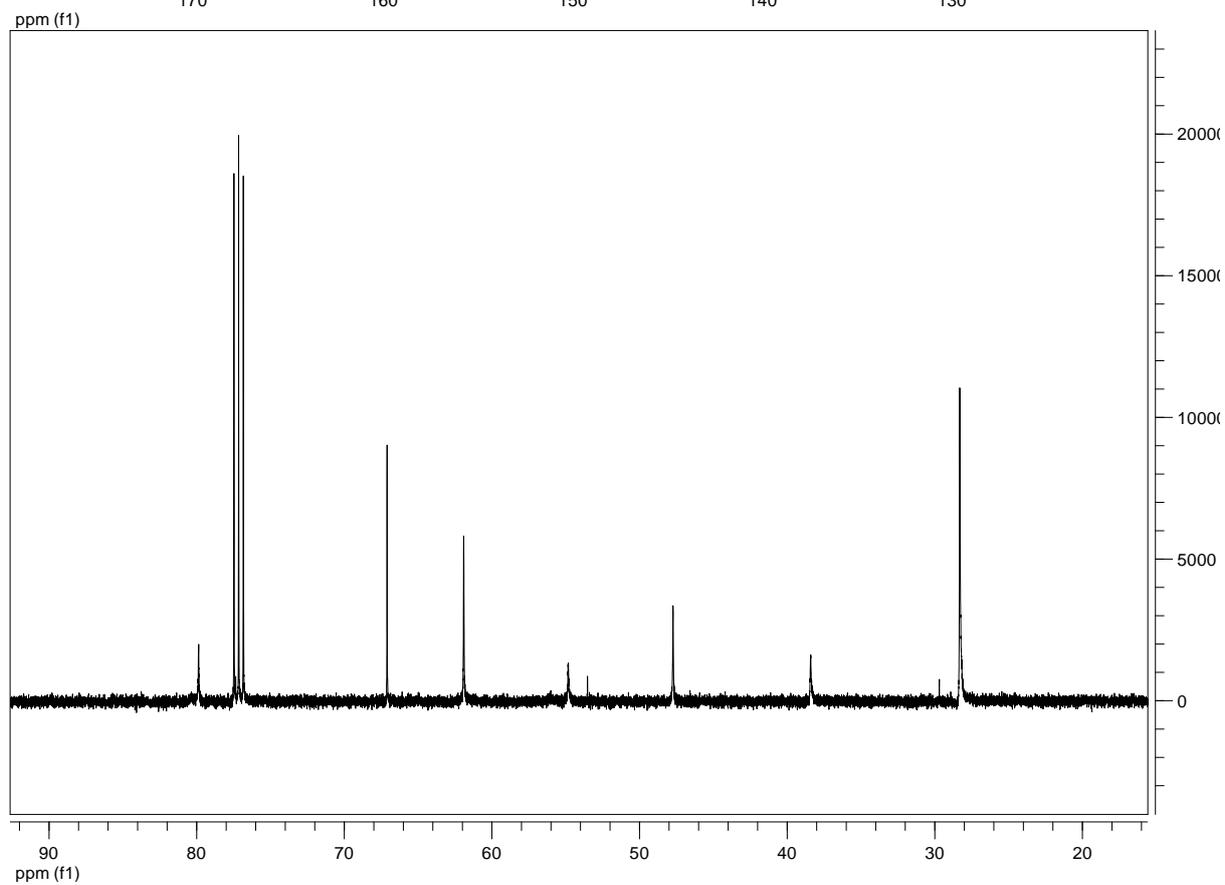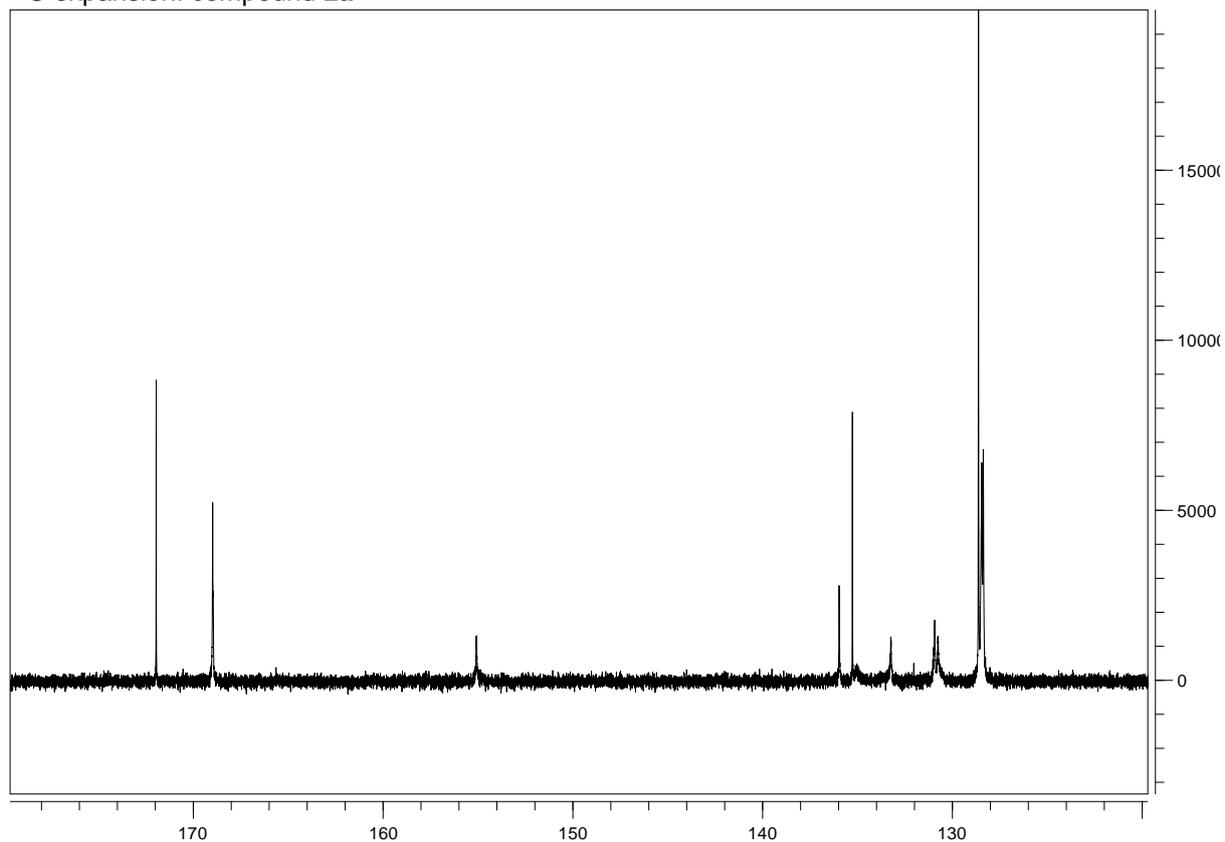P1   7.80 usec
PL1   4.00 dB
SFO1   100.6027118 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   100.00 usec
PL2   7.00 dB
PL12   29.00 dB
PL13   29.00 dB
SFO2   400.0516002 MHz

F2 - Processing parameters
SI   65536
SF   100.5926530 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

^{13}C expansion: compound **3a**

COBB:NCOLGIN:NC148

1H-NMR

BocHN

OH

O

B

O

O

N

O

O

12

14.01

85.99

10 9 8 7 6 5 4 3 2 1 0 ppm

BRUKER

Current Data Parameters
NAME   0816063Z
EXPNO   10
PROCNO   1

F2 - Acquisition Parameters
Date_   2010060B
Time   16.20
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   16
DS   2
SWH   8278.146 Hz
FIDRES   0.126314 Hz
AQ   3.9584243 sec
RG   101.6
DW   60.400 usec
DE   6.00 usec
TE   295.3 K
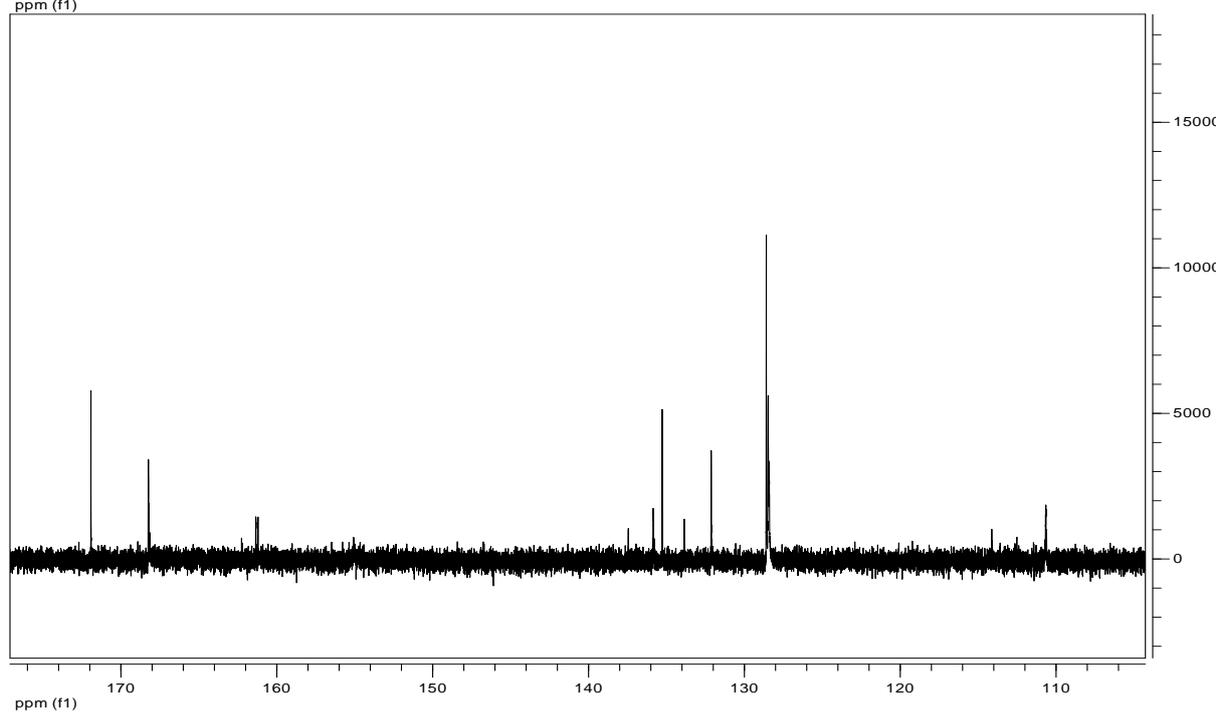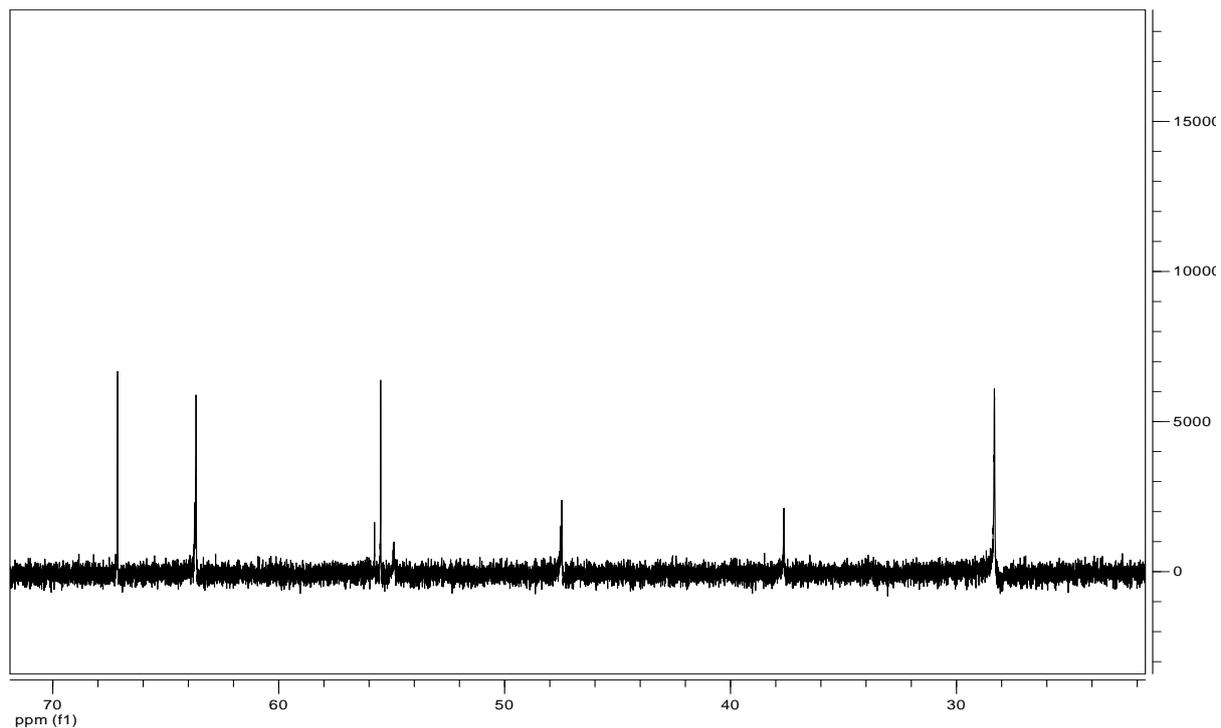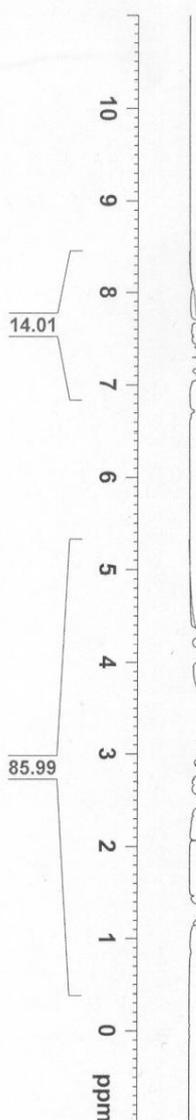D1   1.00000000 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======== CHANNEL f1 ========
NUC1   1H
P1   8.00 usec
PL1   7.00 dB
SFO1   400.0524705 MHz

F2 - Processing parameters
SI   131072
SF   400.0500000 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

COBB:NCOLGIN:NC148

13C-NMR

12

BocHN

OH

O

B

O

N

O

O

Current Data Parameters
NAME   08160632
EXPNO   11
PROCNO   1

F2 - Acquisition Parameters
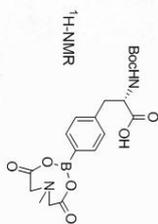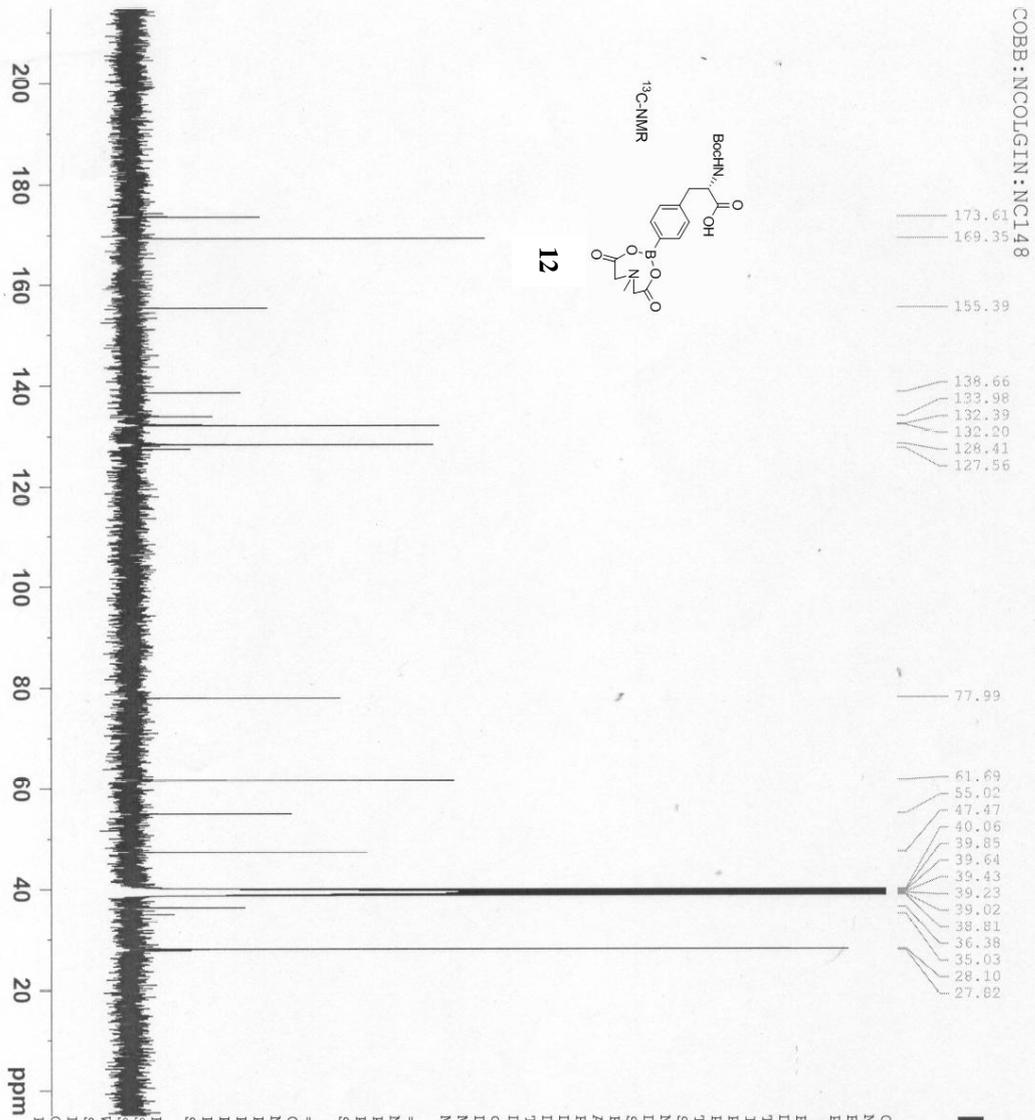Date_   20100608
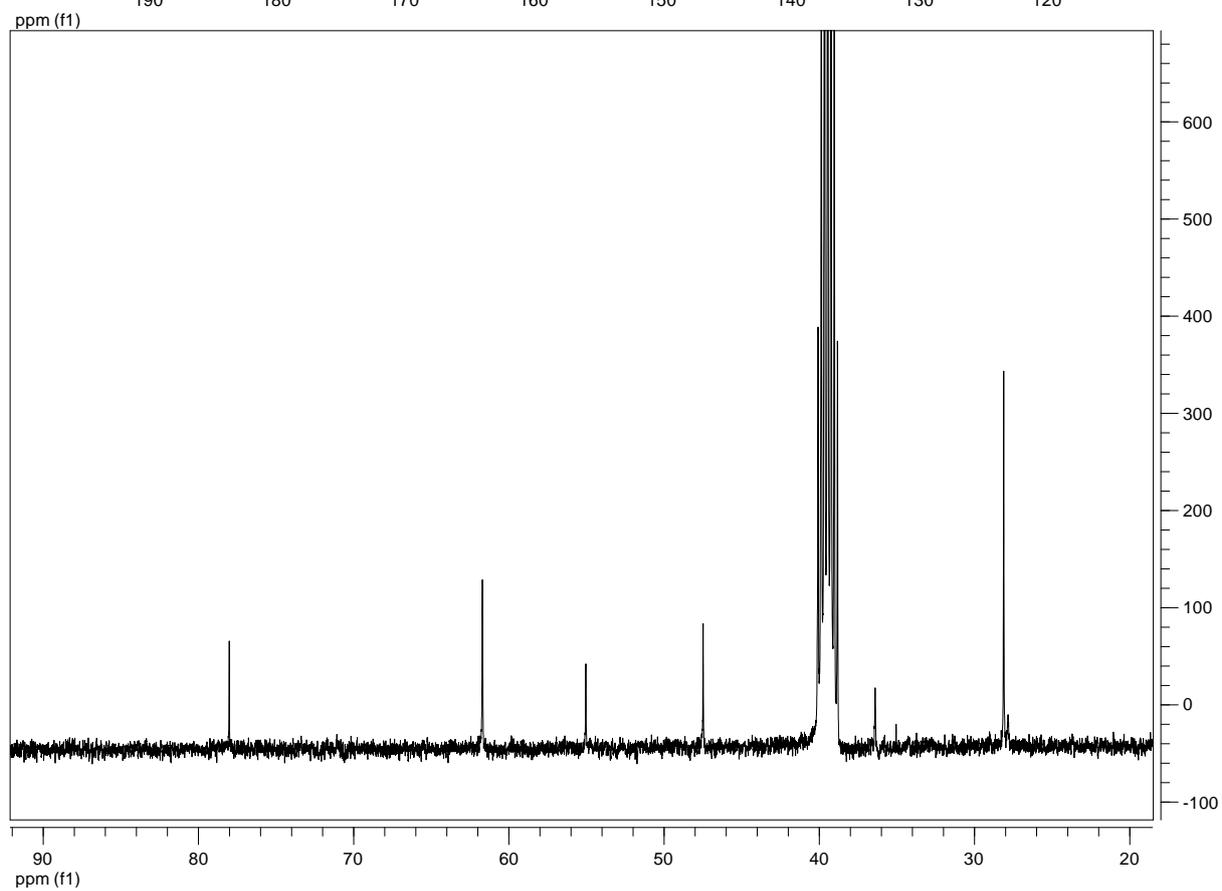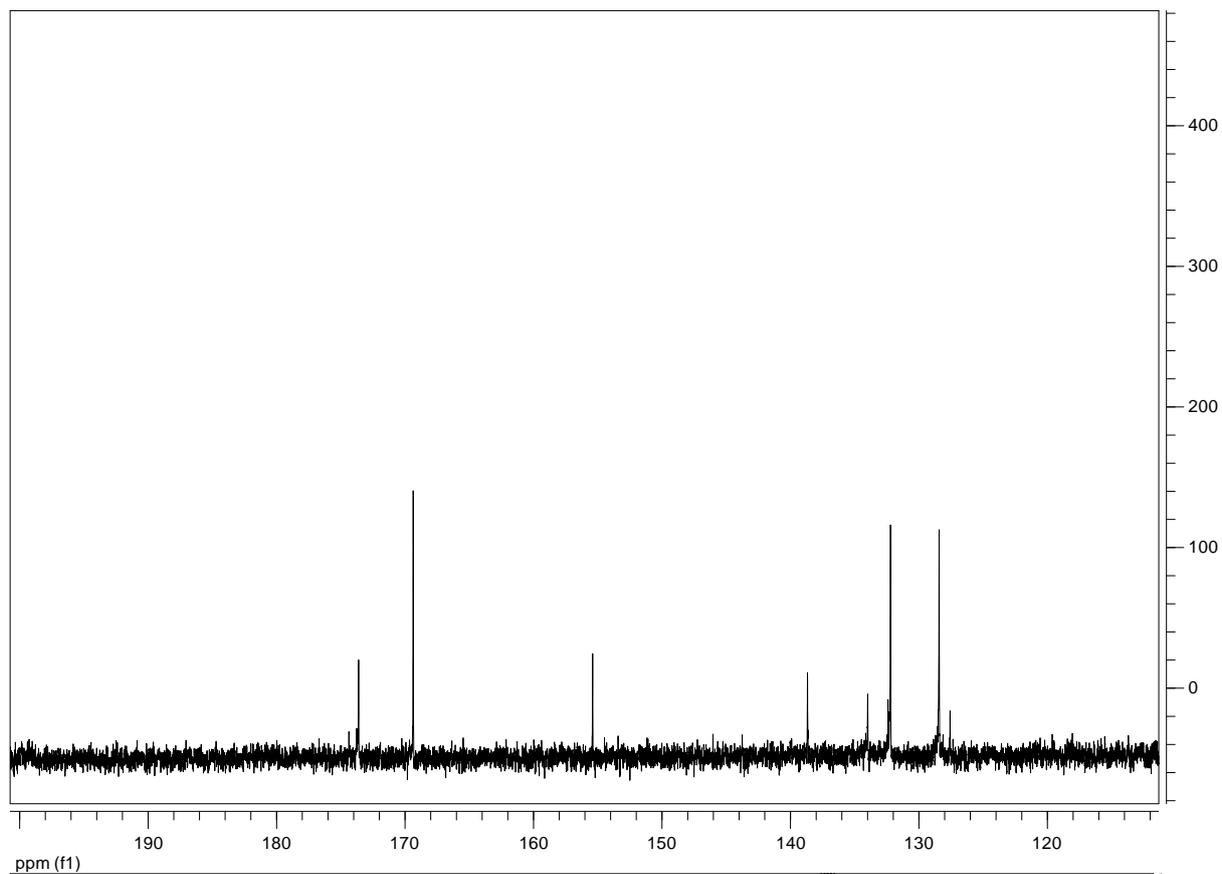Time_   23.55
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   1024
DS   1
SWH   23980.814 Hz
FIDRES   0.365918 Hz
AQ   1.3664756 sec
RG   1290.2
DW   20.850 usec
DE   6.00 usec
TE   296.0 K
D1   2.00000000 sec
d11   0.03000000 sec
DELTA   1.89999998 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======== CHANNEL f1 ========
NUC1   13C
P1   7.80 usec
PL1   4.00 dB
SFO1   100.6027118 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   100.00 usec
PL2   7.00 dB
PL12   29.00 dB
PL13   29.00 dB
SFO2   400.0516002 MHz

F2 - Processing parameters
SI   65536
SF   100.5927033 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

BRUKER

173.61
169.35

155.39

138.66
133.98
132.39
132.20
128.41
127.56

77.99

61.69
55.02
47.47
40.06
39.85
39.64
39.43
39.23
39.02
38.81
36.38
35.03
28.10
27.82

200 180 160 140 120 100 80 60 40 20 ppm

^{13}C expansion: compound **12**

SC02-031(2)
Automation directory: /export/home/vnmr1/automation/Wed2401_auto
File : /data/151011/24163604-01

Pulse Sequence: s2pul

Solvent: CD3CN
Ambient temperature
Sample #8,
File: 151011/24163604-01
Experiment run on Nov 24 2010
INOVA-500 "flume"

Pulse 45.0 degrees
Acq. time 4.100 sec
Width 7996.0 Hz
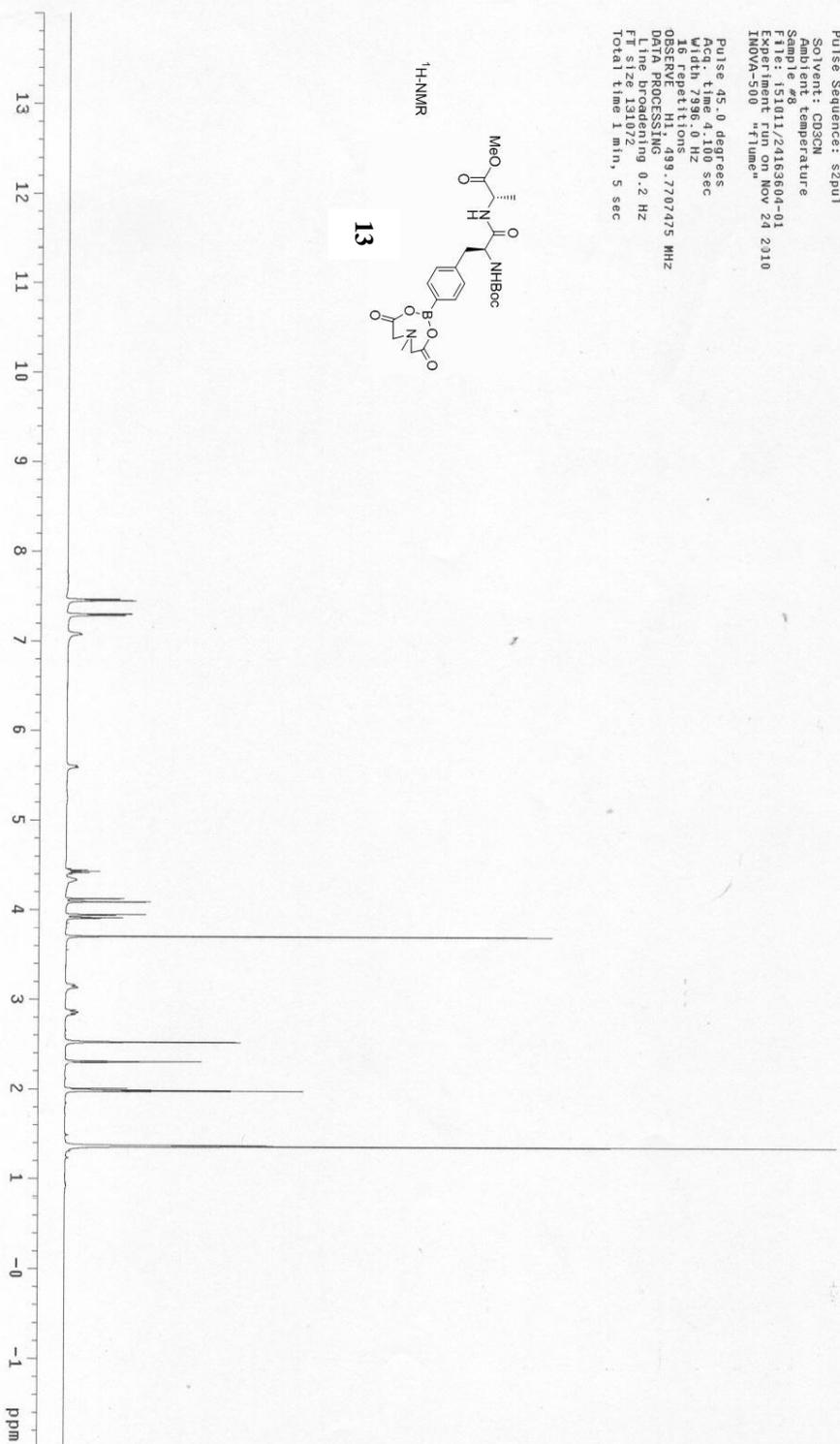16 repetitions
OBSERVE H1, 499.7707475 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 131072
Total time 1 min, 5 sec

13

¹H-NMR

13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

SC02-031(2)

Automation directory: /export/home/vnmr1/automation/Wed2401_auto
File : /data/i51011/24163604-02

Pulse Sequence: s2pul

Solvent: CD3CN
Ambient temperature
Sample #8, user 1-14-87
File: i51011/24163604-02
Experiment run on Nov 24 2010
INOVA-500 "rflume"

Relax. delay 3.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 31421.8 Hz
1024 repetitions
OBSERVE C13, 125.6674244 MHz
DECOUPLE H1, 499.7732465 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 1 hr, 13 min, 51 sec

13

^{13}C-NMR

^{13}C expansion: compound **13**

NC163

Sample Name:
    service
Data Collected on:
    huple-vnmrs700
Archive directory:
    /data/d71012
Sample directory:
    Nov3015234
FidFile: PROTON_01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Dec 1 2010

Temp. 25.0 C / 298.1 K
Sample #43, Operator: service

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.910 sec
Width 11261.3 Hz
4 repetitions
OBSERVE   H1, 699.7350702 MHz
DATA PROCESSING
FT size 65536
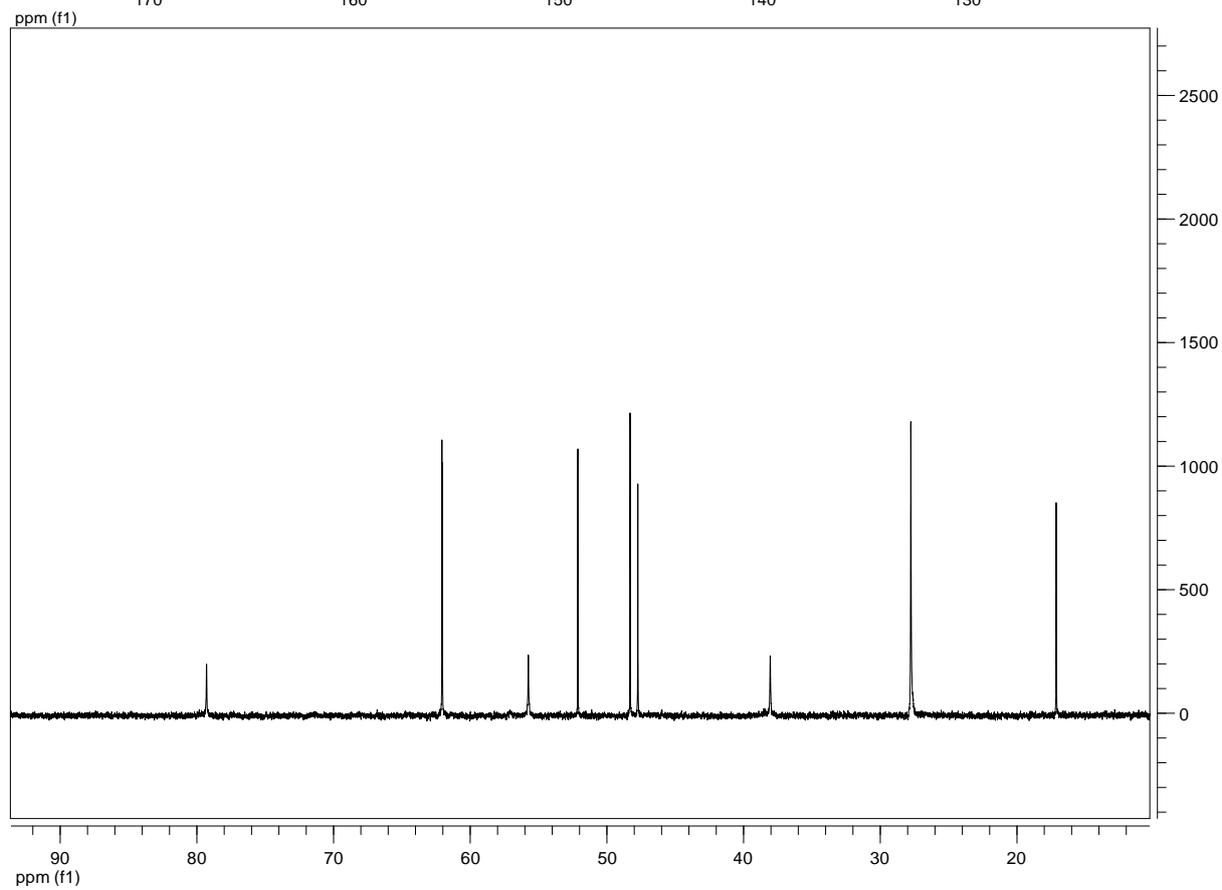Total time 0 min 16 sec

1H-NMR

15

VARIAN

20.30

0.17

1.84

4.56

2.20

10.94

4.52

29.88

25.39

0.19

9   8   7   6   5   4   3   2   1   ppm

NC163

Sample Name:
  service
Data Collected on:
  huple-vnmrs700
Archive directory:
  /data/d71012
Sample directory:
  Nov3015234
FidFile: CARBON_01

Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: Dec 1 2010

Sample #43, Operator: service
Temp. 25.0 C / 298.1 K

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.468 sec
Width 44642.9 Hz
5000 repetitions
OBSERVE C13, 175.9485234 MHz
DECOUPLE H1, 699.7385689 MHz
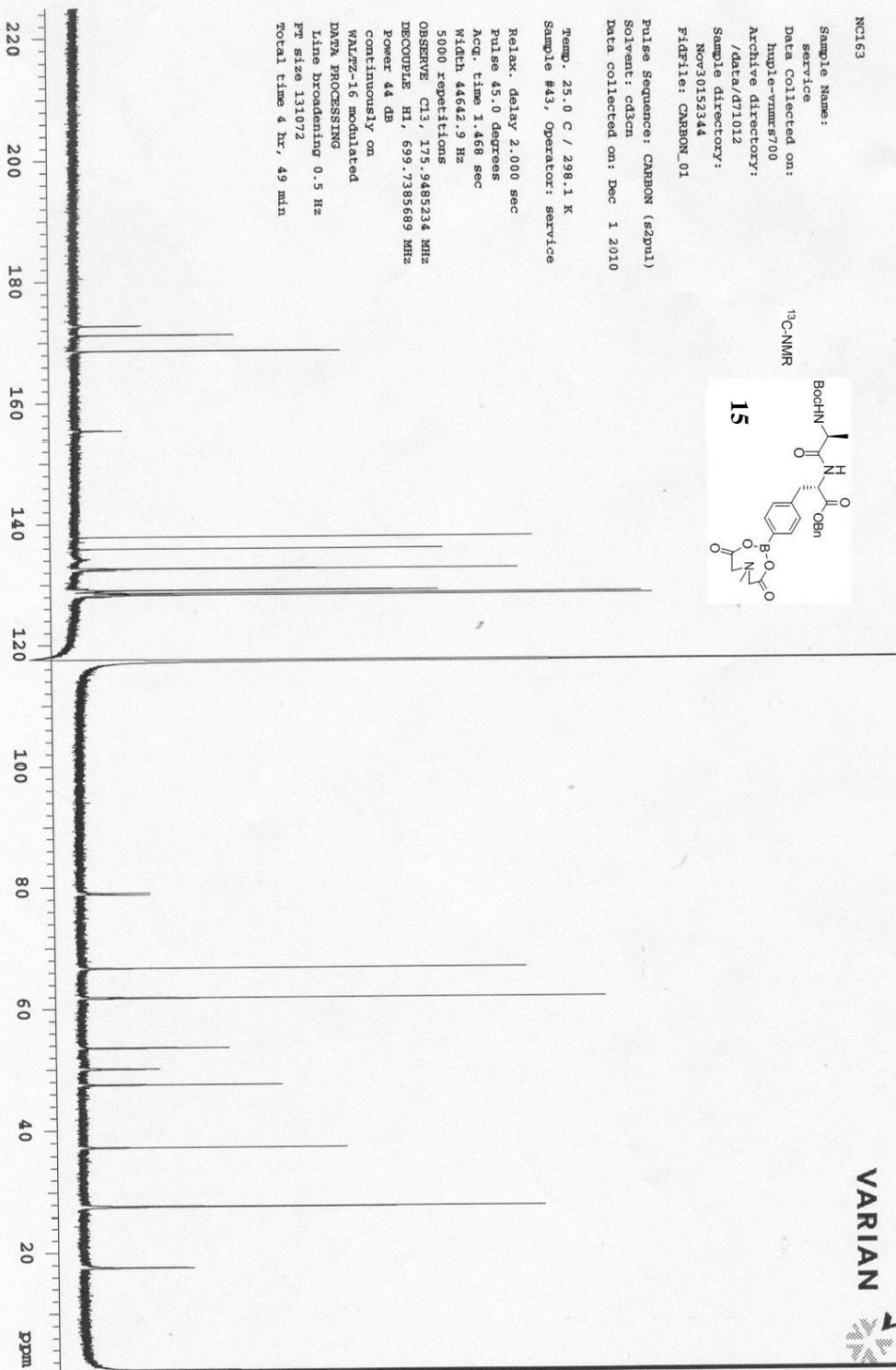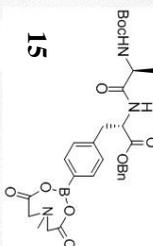Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
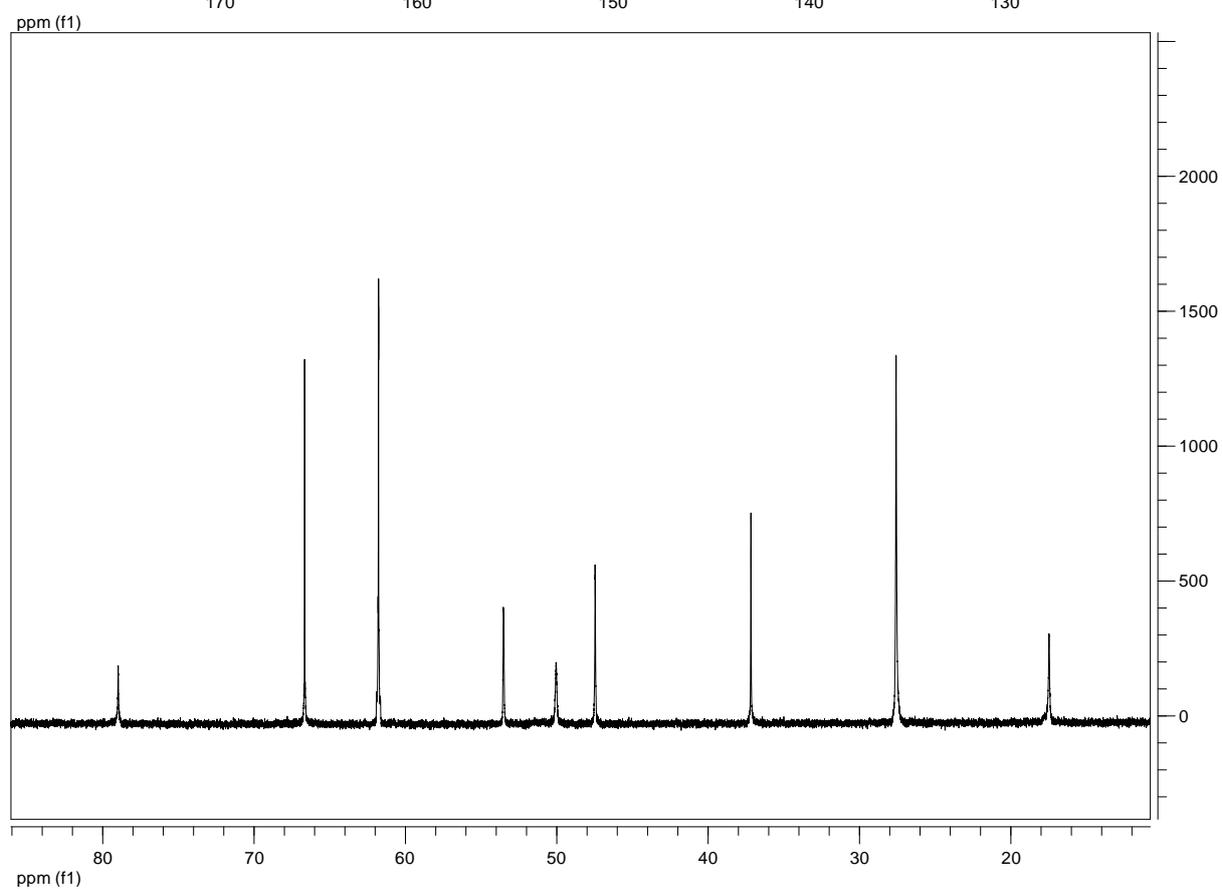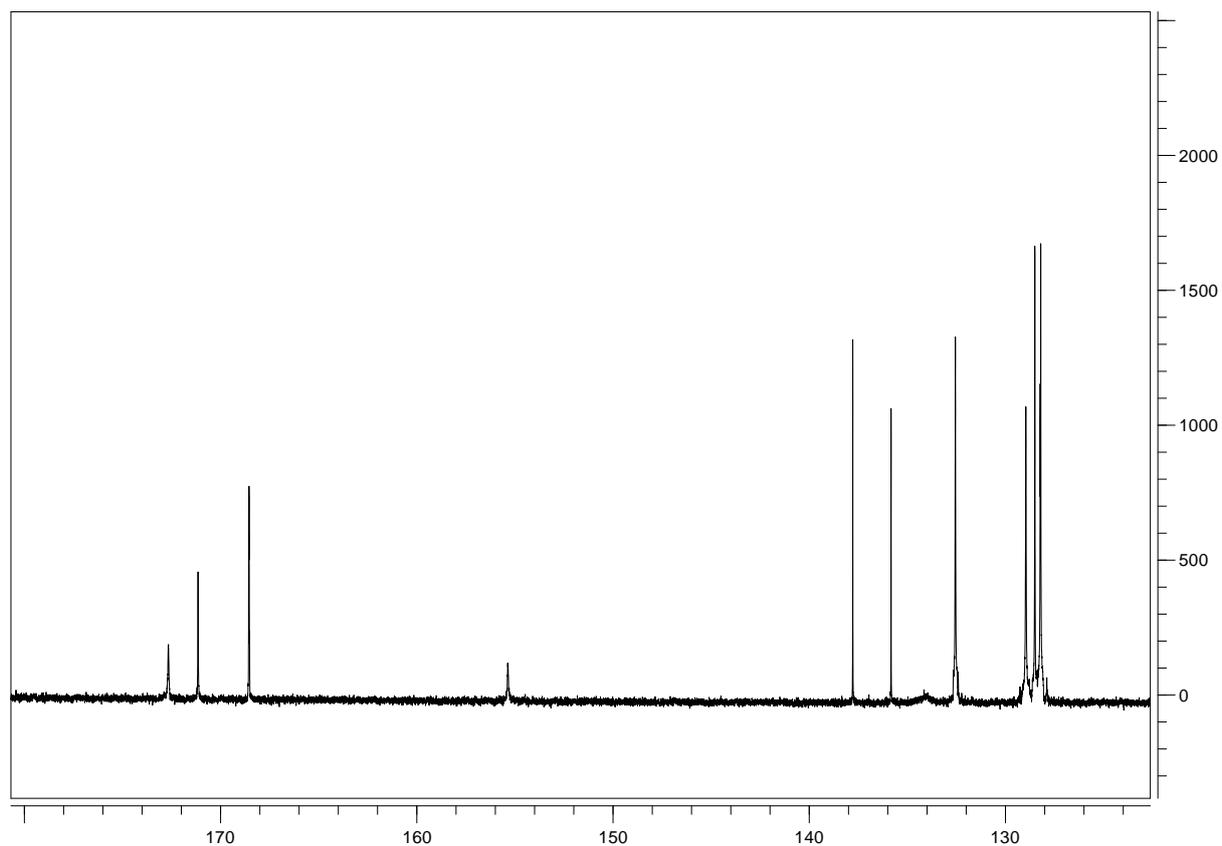Line broadening 0.5 Hz
FT size 131072
Total time 4 hr, 49 min

^{13}C-NMR

15

VARIAN

^{13}C expansion: compound **15**

Part 2   Chiral HPLC Analysis for Compounds 9-11

```
Data File C:\CHEM32\2\DATA\ONY_0510\170510000023.D
Sample Name: NC REF 4

==================================================================
Acq. Operator   : Katie Poole              Seq. Line :    2
Acq. Instrument : AS_LC3                    Location`: Vial 12
Injection Date  : 17/05/2010 17:28:35       Inj       :    2
                                            Inj Volume : 10 µl
Different Inj Volume from Sequence !    Actual Inj Volume : 5 µl
Acq. Method     : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 17/05/2010 16:22:47  by Katie Poole
Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 18/05/2010 09:39:07  by Katie Poole
                  (modified after loading)
Method Info     : Chiral purity by HPLC

                  Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)

Sample Info     : NC131 + NC137

                  Chrialpak IA 250 x 150
```

Chiral HPLC Test mix for **9a** and **9b**


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

Sorted By             :      Signal
Calib. Data Modified  :      18/05/2010 09:39:08
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=220 nm

Peak RetTime  Type   Width     Area        Area      Name
  #   [min]         [min]    mAU   *s        %
----|-------|------|-------|----------|--------|----------------------
  1   5.276  MM    0.1759  1.84702e4   78.6343  (R)-Enantiomer
  2   6.254  MM    0.2074  5018.54932  21.3657  (S)-Enantiomer

Totals :                    2.34888e4
```

```
Data File C:\CHEM32\2\DATA\ONY_0510\170510000025.D
 Sample Name: NC131

    =====================================================================
    Acq. Operator   : Katie Poole              Seq. Line :   3
    Acq. Instrument : AS_LC3                    Location : Vial 13
    Injection Date  : 17/05/2010 18:00:47           Inj :   2
                                             Inj Volume : 10 μl
    Different Inj Volume from Sequence !   Actual Inj Volume : 5 μl
    Acq. Method     : C:\CHEM32\2\METHODS\MIDA60.M
    Last changed    : 17/05/2010 16:22:47  by Katie Poole
    Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
    Last changed    : 18/05/2010 09:39:07  by Katie Poole
                      (modified after loading)
    Method Info     : Chiral purity by HPLC

                      Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)


    Sample Info     : (S)-Enantiomer
```
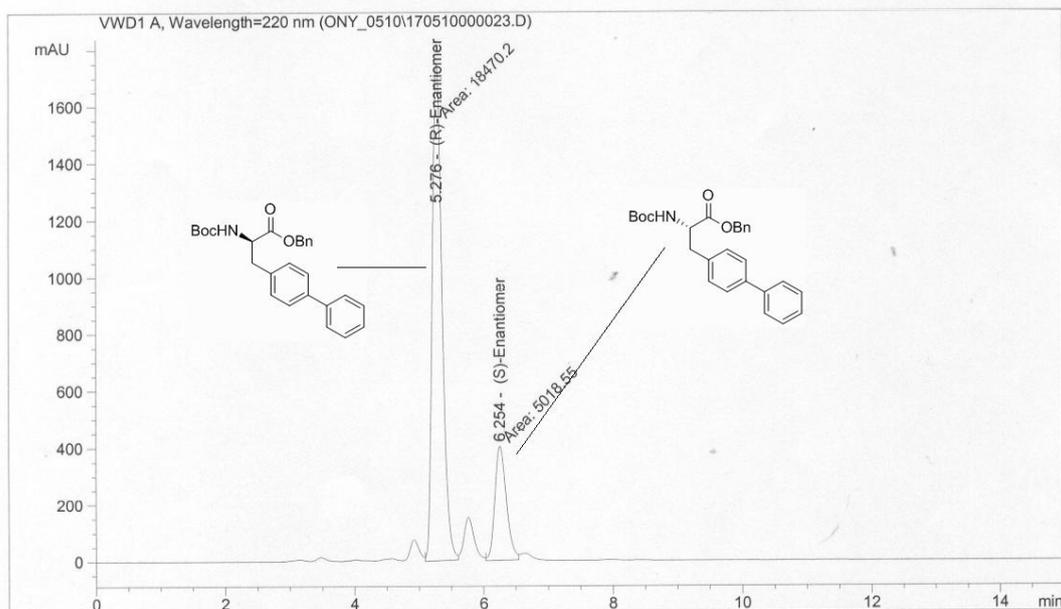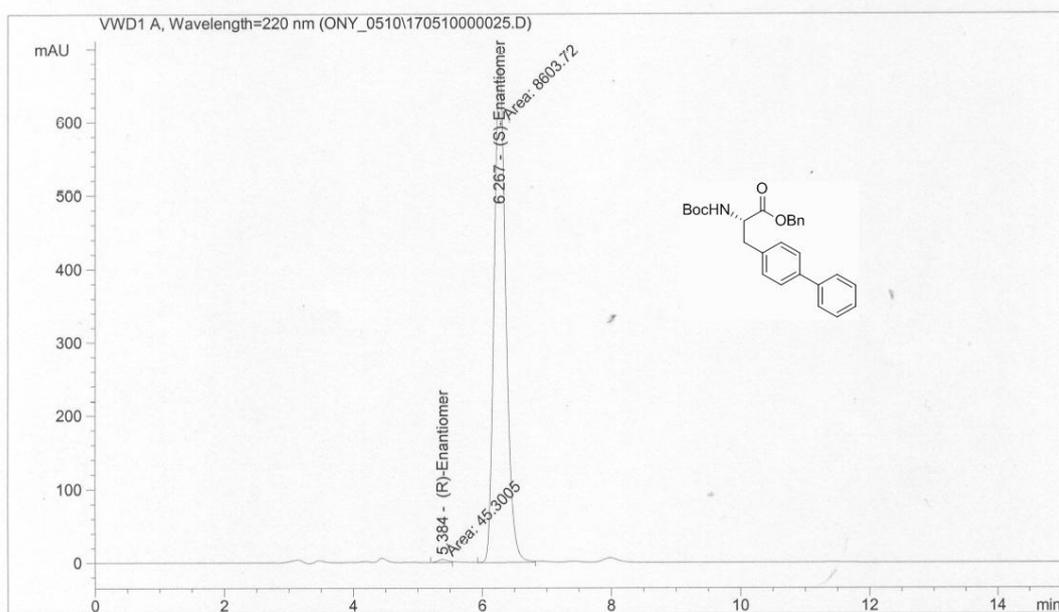


```
    =====================================================================
                         Area Percent Report
    =====================================================================

    Sorted By          :      Signal
    Calib. Data Modified :    18/05/2010 09:39:08
    Multiplier         :      1.0000
    Dilution           :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: VWD1 A, Wavelength=220 nm

    Peak RetTime Type   Width     Area       Area     Name
     #   [min]         [min]    mAU   *s       %
    ----|-------|------|-------|----------|--------|--------------------
       1  5.384 MM     0.1797   45.30048   0.5238 (R)-Enantiomer
       2  6.267 MM     0.2116 8603.71582  99.4762 (S)-Enantiomer

    Totals :                  8649.01630


    1 Warnings or Errors :
```
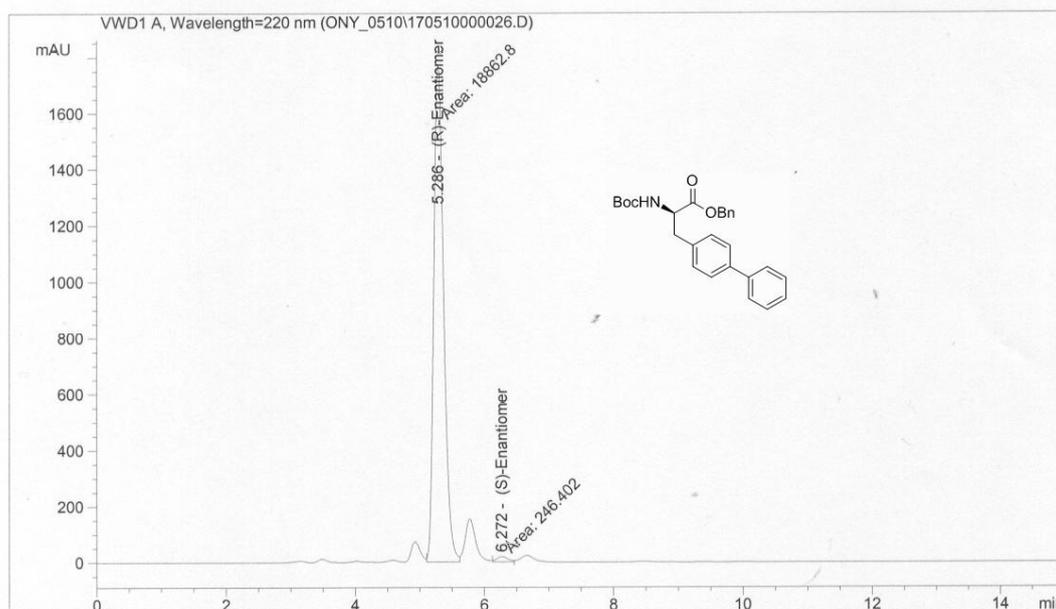
Data File C:\CHEM32\2\DATA\ONY_0510\170510000026.D
Sample Name: NC137

```
=================================================================
Acq. Operator   : Katie Poole              Seq. Line :   4
Acq. Instrument : AS_LC3                    Location : Vial 14
Injection Date  : 17/05/2010 18:16:51            Inj :   1
                                        Inj Volume : 10 μl
Different Inj Volume from Sequence !    Actual Inj Volume : 5 μl
Acq. Method     : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 17/05/2010 16:22:47  by Katie Poole
Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 18/05/2010 09:39:07  by Katie Poole
                  (modified after loading)
Method Info     : Chiral purity by HPLC

                  Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)

Sample Info     : (R)-Enantiomer
```



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

Sorted By              :       Signal
Calib. Data Modified   :       18/05/2010 09:39:08
Multiplier             :       1.0000
Dilution               :       1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=220 nm

Peak RetTime Type   Width     Area       Area      Name
 #   [min]        [min]   mAU   *s       %
----|-------|------|-------|----------|--------|--------------------
  1   5.286 FM    0.1773 1.88628e4   98.7106 (R)-Enantiomer
  2   6.272 FM    0.2088  246.40179   1.2894 (S)-Enantiomer

Totals :                  1.91093e4


1 Warnings or Errors :
```

Data File C:\CHEM32\2\DATA\ONY_0510\170510000028.D
Sample Name: NC REF 5

```
========================================================================
Acq. Operator   : Katie Poole                    Seq. Line :   5
Acq. Instrument : AS_LC3                          Location : Vial 15
Injection Date  : 17/05/2010 18:49:04             Inj :    1
                                                  Inj Volume : 10 μl
Different Inj Volume from Sequence !    Actual Inj Volume : 5 μl
Acq. Method     : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 17/05/2010 16:22:47  by Katie Poole
Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 18/05/2010 09:42:08  by Katie Poole
                  (modified after loading)
Method Info     : Chiral purity by HPLC

                  Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)

Sample Info     : NC133 + NC138

                  Chrialpak IA 250 x 150
```
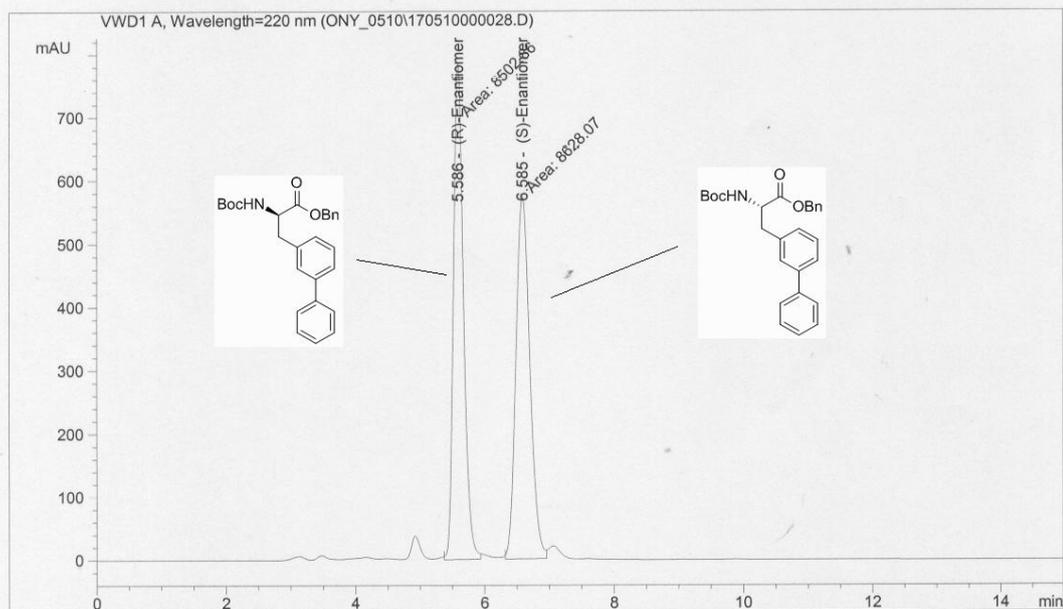
Chiral HPLC Test mix for **10a** and **10b**


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

Sorted By            :      Signal
Calib. Data Modified :      18/05/2010 09:42:08
Multiplier           :      1.0000
Dilution             :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=220 nm

Peak RetTime  Type    Width      Area        Area      Name
  #   [min]           [min]    mAU *s         %
----|-------|------|-------|----------|--------|---------------------
  1   5.586  MM    0.1801  8502.86426  49.6346  (R)-Enantiomer
  2   6.585  MM    0.2506  8628.07422  50.3654  (S)-Enantiomer

Totals :                    1.71309e4
```

AS_LC3 18/05/2010 09:42:32 Katie Poole   Page   1 of 2

```
Data File C:\CHEM32\2\DATA\ONY_0510\170510000031.D
 Sample Name: NC133
```

```
====================================================================
 Acq. Operator   : Katie Poole                Seq. Line :    6
 Acq. Instrument : AS_LC3                      Location : Vial 16
 Injection Date  : 17/05/2010 19:37:24              Inj :    2
                                            Inj Volume : 10 μl
 Different Inj Volume from Sequence !    Actual Inj Volume : 5 μl
 Acq. Method       : C:\CHEM32\2\METHODS\MIDA60.M
 Last changed      : 17/05/2010 16:22:47  by Katie Poole
 Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
 Last changed      : 18/05/2010 11:46:05  by Katie Poole
                     (modified after loading)
 Method Info       : Chiral purity by HPLC

                     Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)


 Sample Info       : (S)-Enantiomer
```
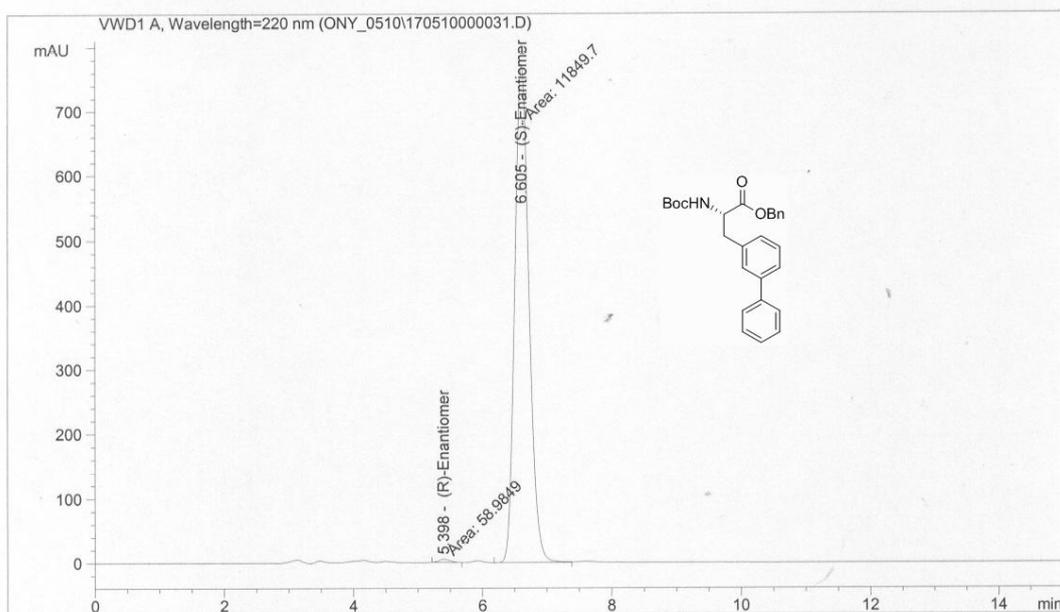


```
====================================================================
                      Area Percent Report
====================================================================

 Sorted By              :       Signal
 Calib. Data Modified   :       18/05/2010 11:46:05
 Multiplier             :       1.0000
 Dilution               :       1.0000
 Use Multiplier & Dilution Factor with ISTDs


 Signal 1: VWD1 A, Wavelength=220 nm

 Peak RetTime Type  Width     Area        Area      Name
  #   [min]         [min]   mAU   *s        %
 ----|-------|------|-------|----------|--------|--------------------
   1   5.398 MM     0.1895    58.98486   0.4953 (R)-Enantiomer
   2   6.605 MM     0.2561  1.18497e4   99.5047 (S)-Enantiomer

 Totals :                   1.19087e4


 1 Warnings or Errors :
```
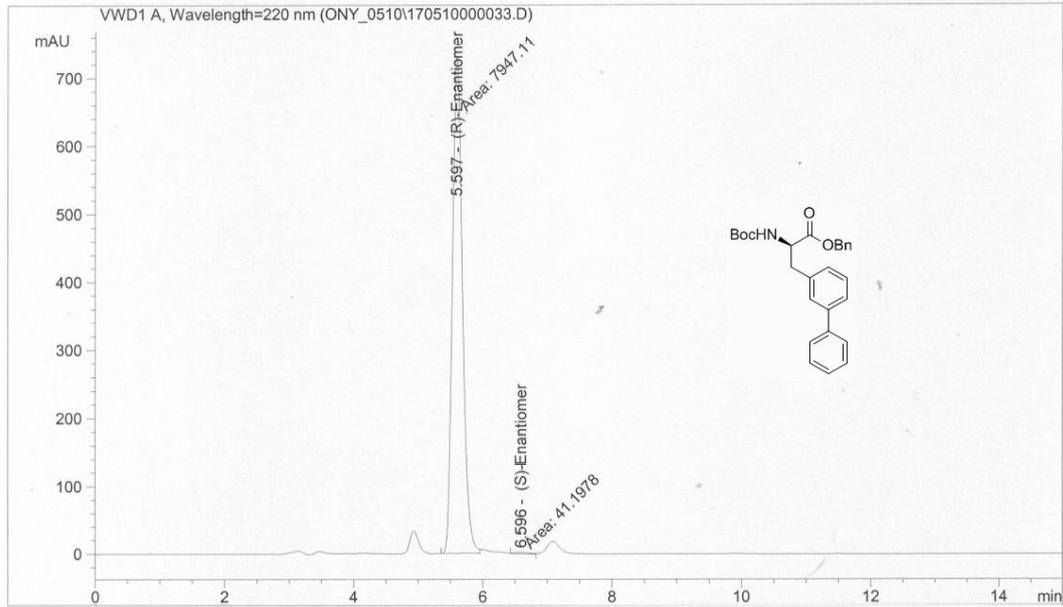
```
Data File C:\CHEM32\2\DATA\ONY_0510\170510000033.D
Sample Name: NC138

=================================================================
Acq. Operator   : Katie Poole                Seq. Line :    7
Acq. Instrument : AS_LC3                      Location : Vial 17
Injection Date  : 17/05/2010 20:09:33             Inj :    2
                                         Inj Volume : 10 µl
Different Inj Volume from Sequence !    Actual Inj Volume : 5 µl
Acq. Method     : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 17/05/2010 16:22:47  by Katie Poole
Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 18/05/2010 11:47:40  by Katie Poole
                  (modified after loading)
Method Info     : Chiral purity by HPLC

                  Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)

Sample Info     : (R)-Enantiomer
```



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

Sorted By            :      Signal
Calib. Data Modified :      18/05/2010 11:47:40
Multiplier           :      1.0000
Dilution             :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=220 nm

Peak RetTime Type   Width     Area        Area     Name
 #   [min]        [min]  mAU  *s        %
----|-------|------|-------|----------|--------|--------------------
   1   5.597 MM   0.1812 7947.11475  99.4843 (R)-Enantiomer
   2   6.596 MM   0.2636   41.19783   0.5157 (S)-Enantiomer

Totals :                  7988.31257


1 Warnings or Errors :
```

AS_LC3 18/05/2010 11:47:59 Katie Poole   Page   1 of 2

```
Data File C:\CHEM32\2\DATA\ONY_0510\170510000035.D
 Sample Name: NC REF 6

   ================================================================
   Acq. Operator   : Katie Poole              Seq. Line :   8
   Acq. Instrument : AS_LC3                    Location : Vial 18
   Injection Date  : 17/05/2010 20:41:40           Inj :   2
                                             Inj Volume : 10 µl
   Different Inj Volume from Sequence !   Actual Inj Volume : 5 µl
   Acq. Method      : C:\CHEM32\2\METHODS\MIDA60.M
   Last changed    : 17/05/2010 16:22:47  by Katie Poole
   Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
   Last changed    : 18/05/2010 11:48:29  by Katie Poole
                     (modified after loading)
   Method Info     : Chiral purity by HPLC

                     Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)

   Sample Info     : NC136 + NC139

                     Chrialpak IA 250 x 150
```
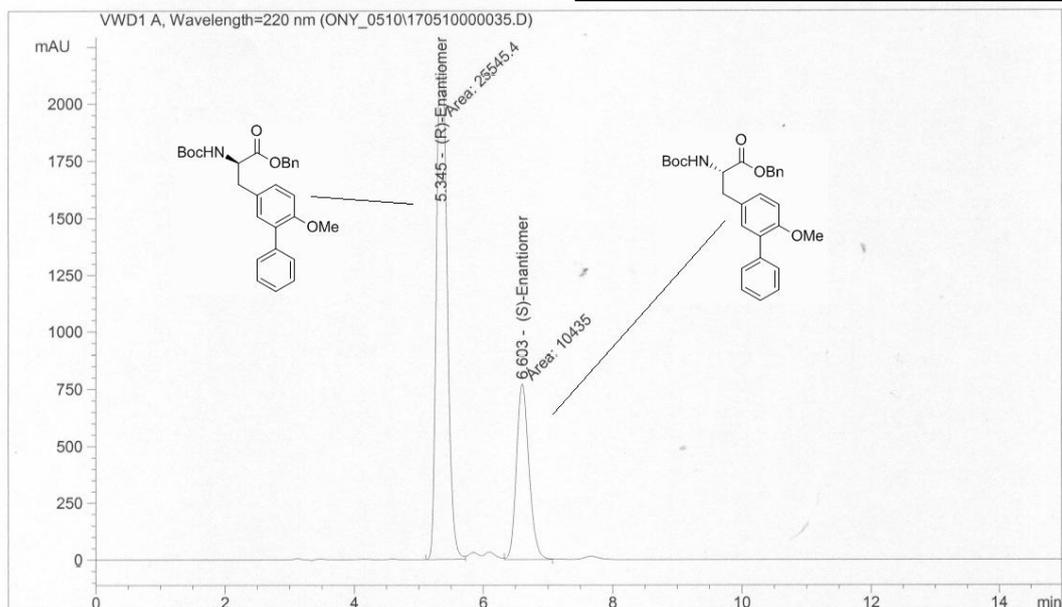

Chiral HPLC Test mix for **11a** and **11b**

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

   Sorted By              :      Signal
   Calib. Data Modified   :      18/05/2010 11:48:29
   Multiplier             :      1.0000
   Dilution               :      1.0000
   Use Multiplier & Dilution Factor with ISTDs


   Signal 1: VWD1 A, Wavelength=220 nm

   Peak RetTime Type   Width     Area        Area     Name
    #   [min]         [min]   mAU   *s        %
   ----|-------|------|-------|----------|--------|--------------------
    1   5.345 MM       0.1951 2.55454e4    70.9981 (R)-Enantiomer
    2   6.603 MM       0.2255 1.04350e4    29.0019 (S)-Enantiomer

   Totals :                   3.59803e4
```

AS_LC3 18/05/2010 11:49:03 Katie Poole

```
Data File C:\CHEM32\2\DATA\ONY_0510\170510000037.D
Sample Name: NC136
```

```
==================================================================
Acq. Operator   : Katie Poole              Seq. Line :    9
Acq. Instrument : AS_LC3                    Location : Vial 19
Injection Date  : 17/05/2010 21:13:51           Inj :    2
                                         Inj Volume : 10 μl
Different Inj Volume from Sequence !   Actual Inj Volume : 5 μl
Acq. Method     : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 17/05/2010 16:22:47  by Katie Poole
Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
Last changed    : 18/05/2010 11:48:29  by Katie Poole
                  (modified after loading)
Method Info     : Chiral purity by HPLC

                  Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)

Sample Info     : (S)-Enantiomer
```
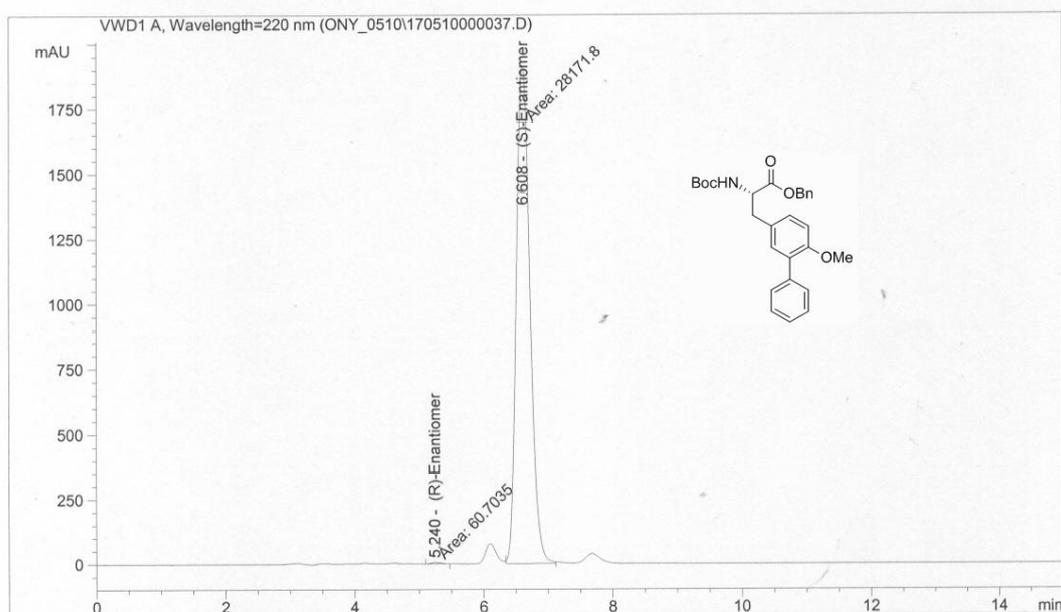


```
==================================================================
                    Area Percent Report
==================================================================

Sorted By          :      Signal
Calib. Data Modified :    18/05/2010 11:48:29
Multiplier         :      1.0000
Dilution           :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=220 nm

Peak RetTime  Type   Width      Area       Area      Name
 #   [min]          [min]   mAU  *s         %
----|-------|------|-------|-----------|---------|--------------------
  1   5.240  MM    0.1708    60.70354   0.2150  (R)-Enantiomer
  2   6.608  MM    0.2455  2.81718e4   99.7850  (S)-Enantiomer

Totals :                   2.82325e4


1 Warnings or Errors :
```

AS_LC3 18/05/2010 11:49:47 Katie Poole

```
Data File C:\CHEM32\2\DATA\ONY_0510\170510000039.D
Sample Name: NC139

=====================================================================
Acq. Operator   : Katie Poole                Seq. Line :   10
Acq. Instrument : AS_LC3                      Location : Vial 20
Injection Date  : 17/05/2010 21:46:03         Inj :    2
                                              Inj Volume : 10 µl
Different Inj Volume from Sequence !    Actual Inj Volume : 5 µl
Acq. Method       : C:\CHEM32\2\METHODS\MIDA60.M
Last changed      : 17/05/2010 16:22:47  by Katie Poole
Analysis Method : C:\CHEM32\2\METHODS\MIDA60.M
Last changed      : 18/05/2010 11:48:29  by Katie Poole
                    (modified after loading)
Method Info       : Chiral purity by HPLC

                    Chiralcel IA 250 x 4.6mm, 5um PS (Daicel; #80325)

Sample Info       : (R)-Enantiomer
```
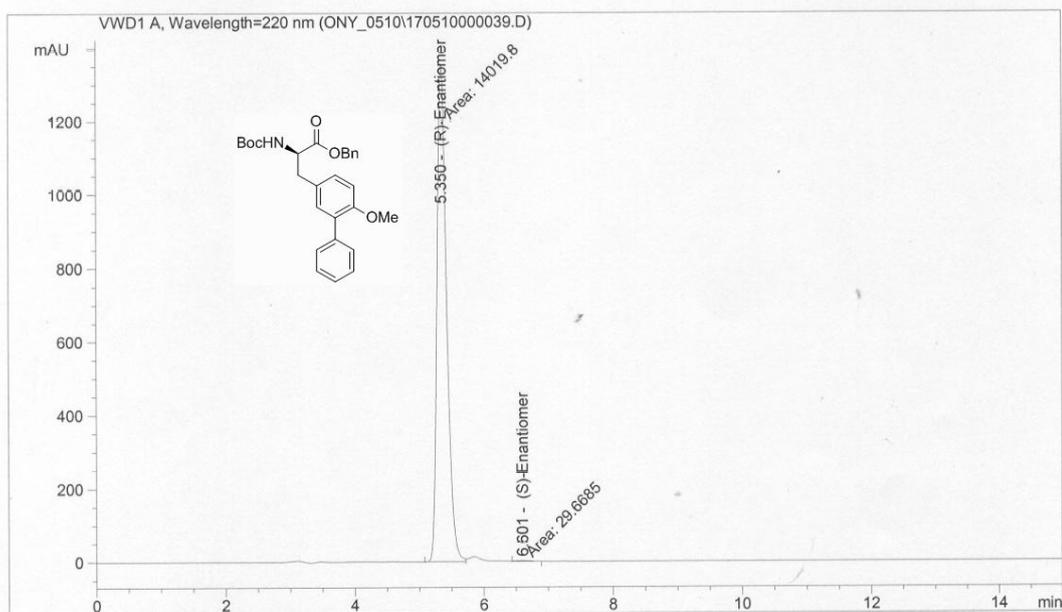


```
=====================================================================
                       Area Percent Report
=====================================================================

Sorted By               :       Signal
Calib. Data Modified    :       18/05/2010 11:48:29
Multiplier              :       1.0000
Dilution                :       1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=220 nm

Peak RetTime  Type   Width     Area        Area     Name
  #   [min]          [min]   mAU    *s       %
----|-------|-------|-------|----------|--------|--------------------
   1    5.350  MF    0.1724  1.40198e4   99.7888  (R)-Enantiomer
   2    6.601  MM    0.2500  29.66854     0.2112  (S)-Enantiomer

Totals :                     1.40495e4


1 Warnings or Errors :
```