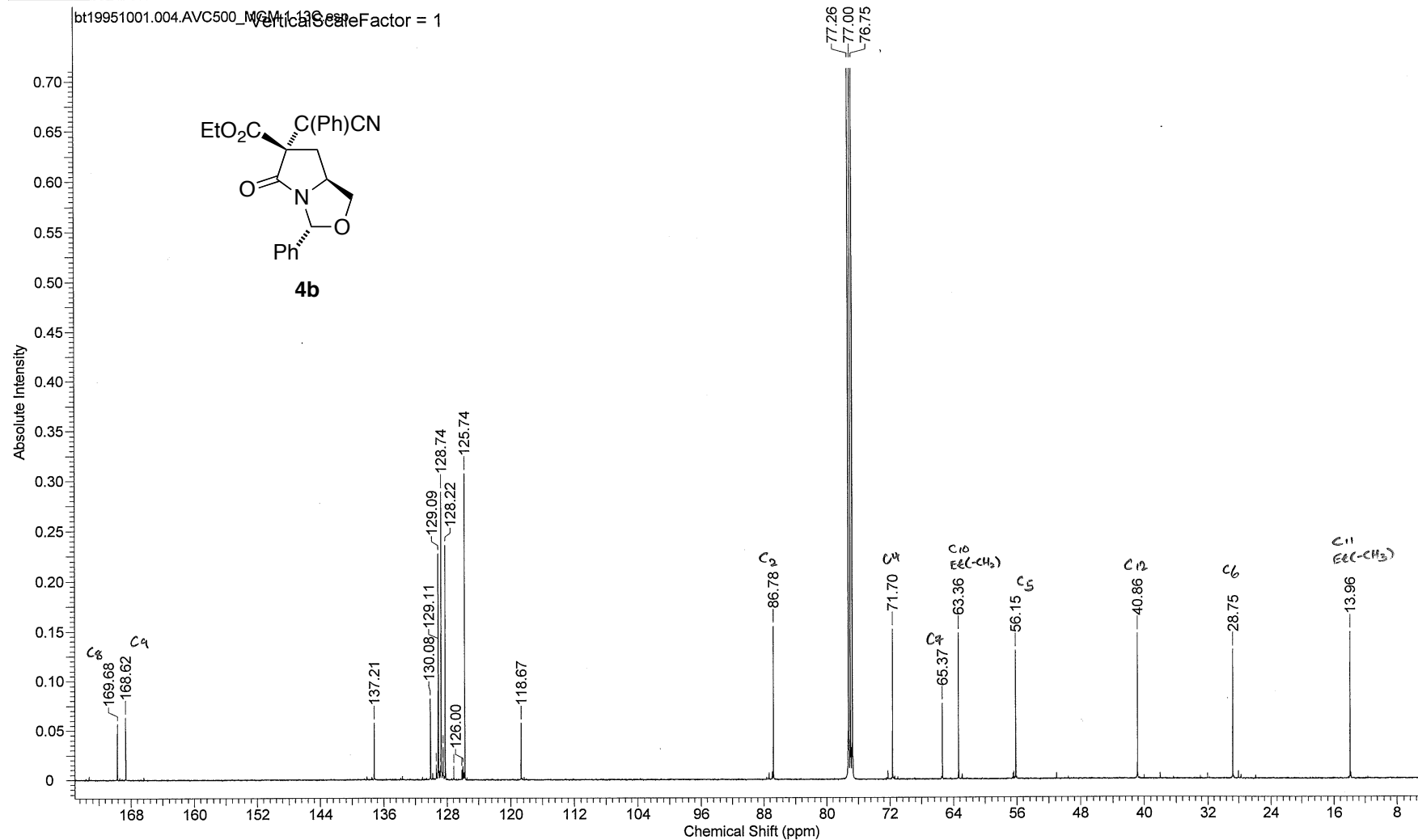Supplementary Information

Spirocyclic systems derived from pyroglutamic acid

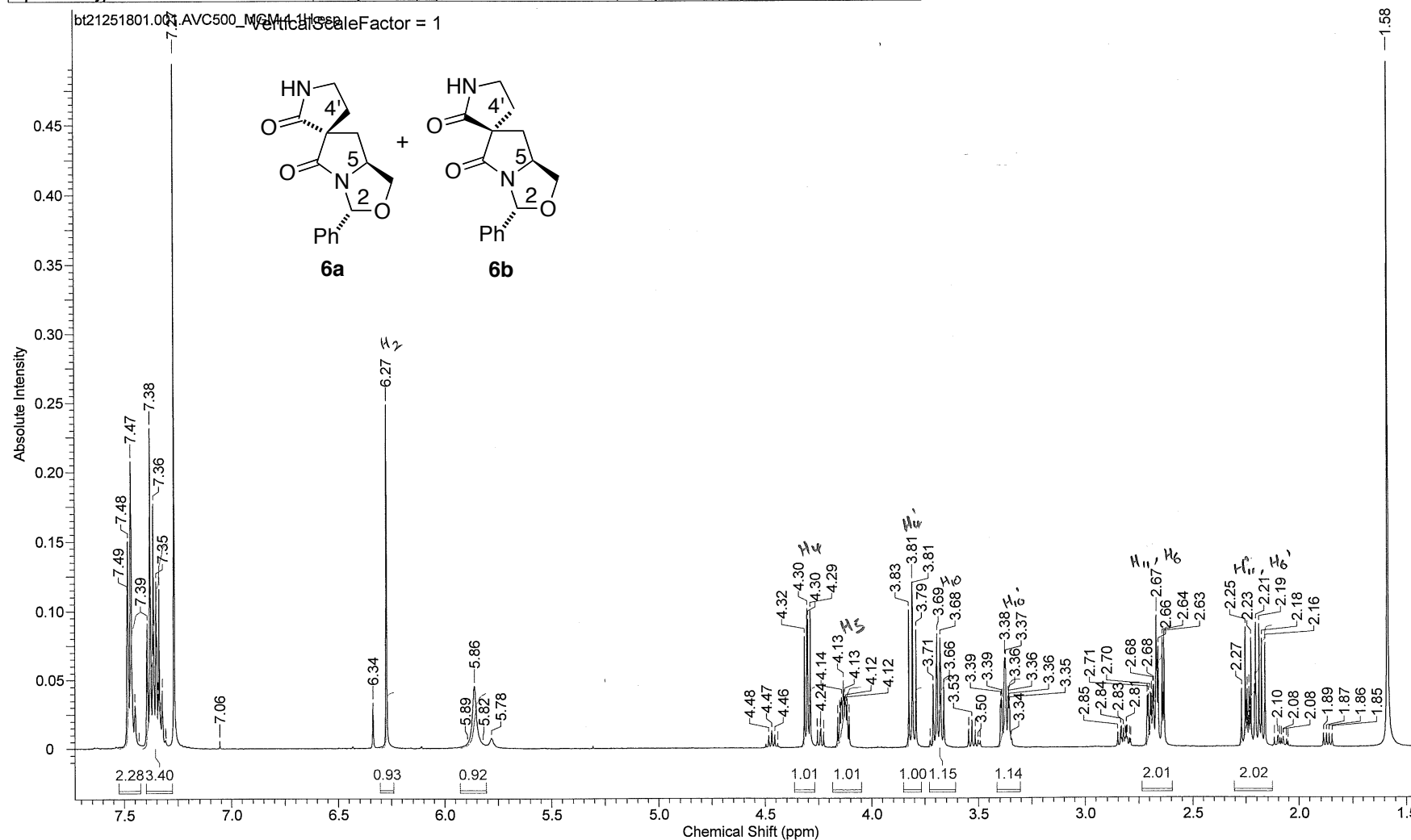Andrew R. Cowley, Thomas J. Hill, Petr Kocis, Mark G. Moloney, Robert D. Stevenson and Amber L. Thompson
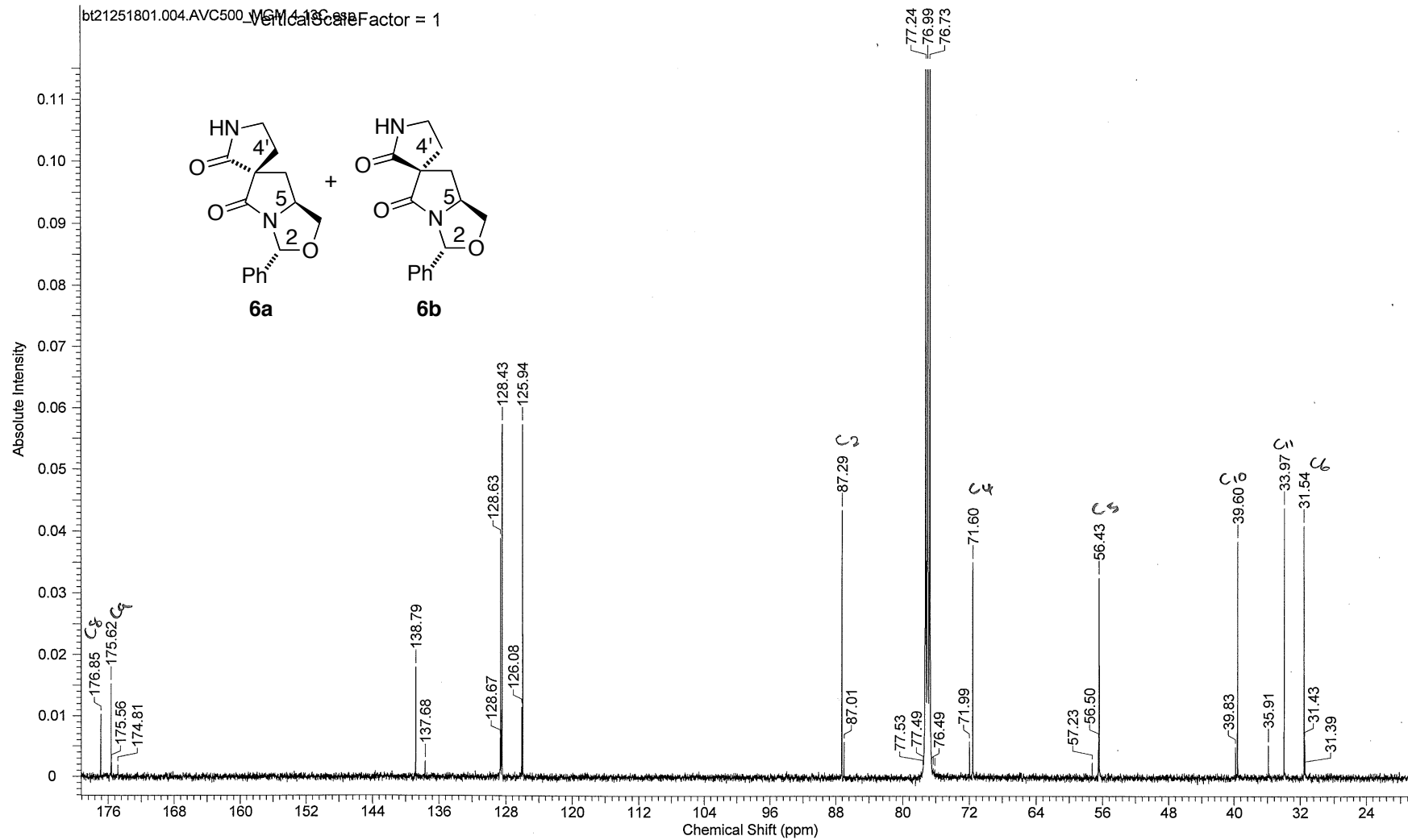
Acquisition Time (sec)	3.1719	Comment		Instrument AVC500 Group MGM 1995 Benjamin Tan 10/1/11		Date		11 Jan 2011 11:05:36
Date Stamp	11 Jan 2011 11:05:36					File Name		C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt19951001\1\pdata\1\1r
Frequency (MHz)	500.30	Nucleus	1H	Number of Transients	16	Origin		avc500
Original Points Count	32768	Owner	dp-nmrgroup	Points Count	32768	Pulse Sequence		zg30
Receiver Gain	4.00	SW(cyclical) (Hz)	10330.58	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)		3065.5417
Spectrum Type	STANDARD	Sweep Width (Hz)	10330.26	Temperature (degree C)	24.970			

bt19951001.001.AVC500_MGM 1 1H.esp VerticalScaleFactor = 1

4b

4b

Acquisition Time (sec)	1.0486	Comment		Instrument AVC500 Group MGM 1995 Benjamin Tan 10/1/11		Date	11 Jan 2011 12:16:00
Date Stamp	11 Jan 2011 12:16:00				File Name	C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt19951001\4\pdata\1\1r	
Frequency (MHz)	125.80	Nucleus	13C	Number of Transients	1024	Origin	avc500
Original Points Count	32768	Owner	dp-nmrgroup	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	1820.00	SW(cyclical) (Hz)	31250.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12571.3047
Spectrum Type	STANDARD	Sweep Width (Hz)	31249.05	Temperature (degree C)	24.970		

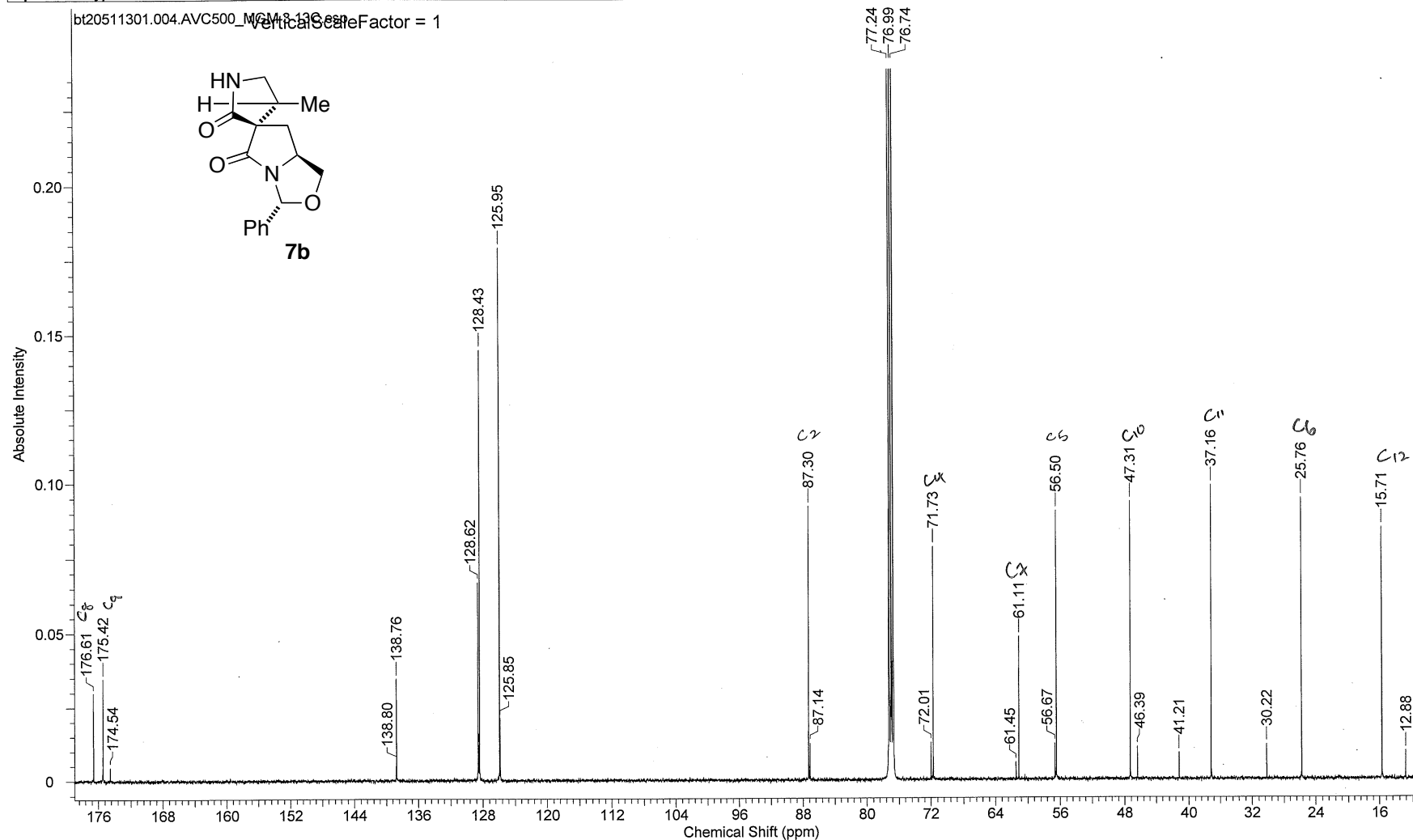| Acquisition Time (sec)	3.1719	Comment		Instrument AVC500 Group MGM 2125 Benjamin Tan 18/1/11		Date		20 Jan 2011 03:05:36
Date Stamp	20 Jan 2011 03:05:36			File Name		C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt21251801\1\pdata\1\1r		
Frequency (MHz)	500.30	Nucleus	1H	Number of Transients	16	Origin		avc500
Original Points Count	32768	Owner	dp-nmrgroup	Points Count	32768	Pulse Sequence		zg30
Receiver Gain	4.00	SW(cyclical) (Hz)	10330.58	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)		3065.5417
Spectrum Type	STANDARD	Sweep Width (Hz)	10330.26	Temperature (degree C)	24.970			

bt21251801.001.AVC500_MGM_1H.esp   VerticalScaleFactor = 1

Acquisition Time (sec)	1.0486	Comment		Instrument AVC500 Group MGM 2125 Benjamin Tan 18/1/11	Date	20 Jan 2011 04:16:00
Date Stamp	20 Jan 2011 04:16:00				File Name	C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt21251801\4\pdata\1\1r
Frequency (MHz)	125.80	Nucleus	13C		Number of Transients	1024	Origin	avc500
Original Points Count	32768	Owner	dp-nmrgroup		Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	812.00	SW(cyclical) (Hz)	31250.00		Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12571.3047
Spectrum Type	STANDARD	Sweep Width (Hz)	31249.05		Temperature (degree C)	24.970		

Acquisition Time (sec)	3.1719	Comment		Instrument AVC500 Group MGM 2051 Benjamin Tan 13/1/11		Date		15 Jan 2011 13:15:44
Date Stamp	15 Jan 2011 13:15:44				File Name		C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt20511301\1\pdata\1\1r	
Frequency (MHz)	500.30	Nucleus	1H		Number of Transients	16	Origin	avc500
Original Points Count	32768	Owner	dp-nmrgroup		Points Count	32768	Pulse Sequence	zg30
Receiver Gain	4.00	SW(cyclical) (Hz)	10330.58		Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	3065.5417
Spectrum Type	STANDARD	Sweep Width (Hz)	10330.26		Temperature (degree C)	24.970		

bt20511301.001.AVC500_MGM.3.1H.esp VerticalScaleFactor = 1

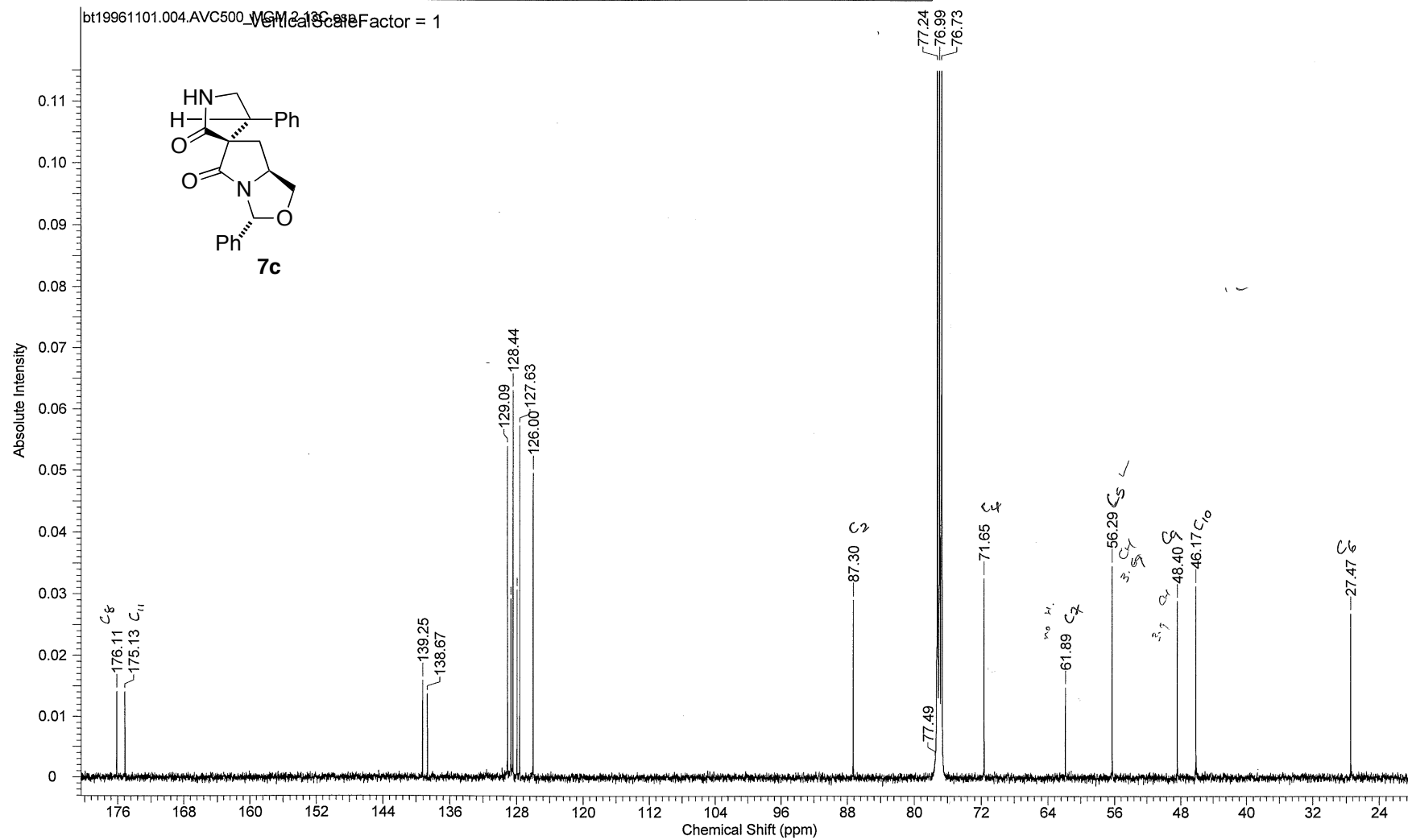| Acquisition Time (sec)	1.0486	Comment		Instrument AVC500 Group MGM 2051 Benjamin Tan 13/1/11		Date		15 Jan 2011 14:26:08
Date Stamp	15 Jan 2011 14:26:08				File Name		C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt20511301\4\pdata\1\1r	
Frequency (MHz)	125.80	Nucleus	13C	Number of Transients	1024	Origin		avc500
Original Points Count	32768	Owner	dp-nmrgroup	Points Count	32768	Pulse Sequence		zgpg30
Receiver Gain	1820.00	SW(cyclical) (Hz)	31250.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)		12571.3047
Spectrum Type	STANDARD	Sweep Width (Hz)	31249.05	Temperature (degree C)	24.970			

bt20511301.004.AVC500_MGM_8-13C.esp   VerticalScaleFactor = 1

Acquisition Time (sec)	1.0486	Comment		Instrument AVC500 Group MGM 1996 Benjamin Tan 11/1/11		Date	11 Jan 2011 22:26:08
Date Stamp	11 Jan 2011 22:26:08			File Name		C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt19961101\4\pdata\1\1r	
Frequency (MHz)	125.80	Nucleus	13C	Number of Transients	1024	Origin	avc500
Original Points Count	32768	Owner	dp-nmrgroup	Points Count	32768	Pulse Sequence	zgpg30
Receiver Gain	1820.00	SW(cyclical) (Hz)	31250.00	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	12571.3047
Spectrum Type	STANDARD	Sweep Width (Hz)	31249.05	Temperature (degree C)	24.970		

Acquisition Time (sec)	3.1719	Comment		Instrument AVC500 Group MGM 1996 Benjamin Tan 11/1/11		Date		11 Jan 2011 21:15:44
Date Stamp	11 Jan 2011 21:15:44				File Name		C:\Documents and Settings\mgmgroup.CHEM\Desktop\bt19961101\1\pdata\1\1r	
Frequency (MHz)	500.30	Nucleus	1H	Number of Transients	16	Origin		avc500
Original Points Count	32768	Owner	dp-nmrgroup	Points Count	32768	Pulse Sequence		zg30
Receiver Gain	4.00	SW(cyclical) (Hz)	10330.58	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)		3065.5417
Spectrum Type	STANDARD	Sweep Width (Hz)	10330.26	Temperature (degree C)	24.970			

bt19961101.001.AVC500_MGM-2-1H.esp VerticalScaleFactor = 1

7c

Instrument DPX200
Chemist RDS
Group MGM
RS01–5
h1acq.au CDCl3 u mgmgrp 40

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5a

8.97 (1H, d, J=2.35 CH(C(NO₂))₂)

8.45 (1H, dd, J=8, 2.54 CH C(NO₃))

7.72 (1H, d, J=8.61 NO₂ C CHC H₆)

7.37-7.58 (5H, m Ar-H)

6.43 (1H, s, N(2))

4.41 (1H, d, J=5.87 H₄ exo)

4.24 (2H, q, J=7.24 CH₃CH₂O)

4.02-4.16 (1H, m, H₅)

3.93 (1H, t, J=8.61 H₄ endo)

3.48 (1H, d, d, J=14.67, 4.90 H₆ endo)

2.57 (1H, dd, J=7.63, 14.67 H₆ exo)

1.23 (3H, t, J=7.04 CH₃CH₂O)

Instrument DQX400
Chemist RDS
Group MGM
RS01-5(1SPOT)
c13acq.au CDCl3 e:\\ mgmgrp 55

5a

Instrument DQX400
Chemist RDS
Group MGM
RS01-9(TS)
h1acq.au CDCl3 e:\\ mgmgrp 11

NMR@CHEM.OX

5b

7.36 — 7.47 (3H, m PhH)

7.49 — 7.53 (2H, m, PhH)

7.36 (1H, d, J=2.65) (CH (CNH₂NO₂))

6.40 (1H, s, H₂)

6.71 (1H, d, J= 265, 8.46) (H₂NCCH)

7.11 (1H, d, J= 8.46) (NH₂CCHCH)

4.18–4.23 (2H, m, CH₃CH₂O)

4.33 (1H, q, J= 6.06, 7.96) (H₄ EXO)

4.4H (2H NH₂)

4.02–4.09 (1H, m, H₅)

3.86 (1H, "t", J=8.3) H₄ ENDO

3.375 (1H, t, J= 5.6, 14.3) H₅ ENDO

2.53 (1H, dd, J= 7.71, 14.3) H₆ EXO

1.22 (3H, t, J= 7.1 CH₃CH₂O)

| 10.5 | 10.0 | 9.5 | 9.0 | 8.5 | 8.0 | 7.5 | 7.0 | 6.5 | 6.0 | 5.5 | 5.0 | 4.5 | 4.0 | 3.5 | 3.0 | 2.5 | 2.0 | 1.5 | 1.0 | 0.5 | 0.0 | ppm |

25.69   3.35 3.33   28.47   0.38   20.54   18.25

Instrument DQX400
Chemist RDS
Group MGM
RS01-9(TS) 7
c13acq.au CDCl3 e:\\ mgmgrp 11

NMR@CHEM.OX

173.64
169.52
148.07
147.40
138.27
130.21
128.96
128.75
128.65
128.06
126.06
123.08
119.45
111.77
87.67
77.40
77.28
77.08
76.76
71.79
66.52
62.66
56.37
37.37
29.69
13.89
1.79
1.15
1.04

Ph C
128.9 128.6 (2xC)
126.0 (2xC)

NH₂

O₂N

EtO₂C

O

N

O

Ph

5b

NH₂CCHCH (2)
130.1

Ar C
123

NH₂CCH
119.4

ArC
148.0 147.3
138.2

111.7
(CH CNH₂
CHO₂)

Carbonyls
173.6
169.4

87.6
(7)

(3)

C(7)
66.43

62.6
CH₃CH₂O

71.7
C(4)

C(5)
56.3

C(6)
37.3

13.8
CH₃CH₂O

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Current Data Parameters
NAME   Nov20-2006-11
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20061121
Time   17.57
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   256
DS   4
SWH   26178.010 Hz
FIDRES   0.399445 Hz
AQ   1.2517875 sec
RG   32768
DW   19.100 usec
DE   7.50 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   9.50 usec
PL1   0.00 dB
SFO1   100.6403931 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   0.00 dB
PL12   19.00 dB
PL13   25.00 dB
SFO2   400.2016008 MHz

F2 - Processing parameters
SI   32768
SF   100.6303718 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
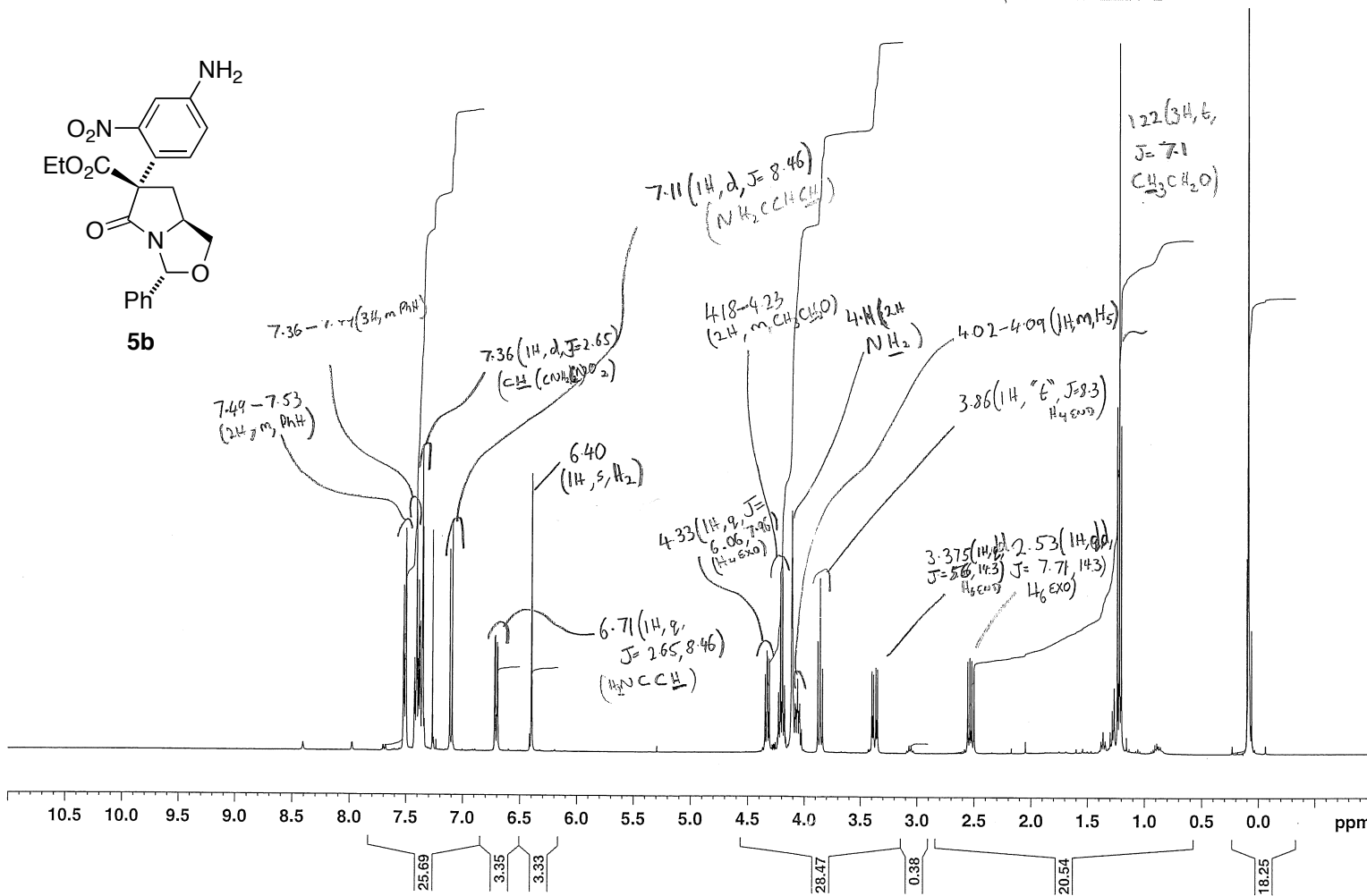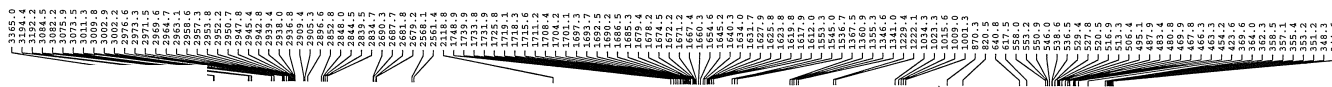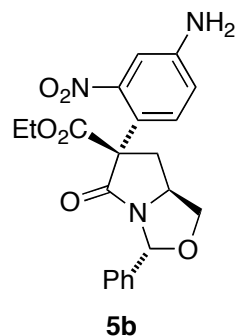PC   1.40
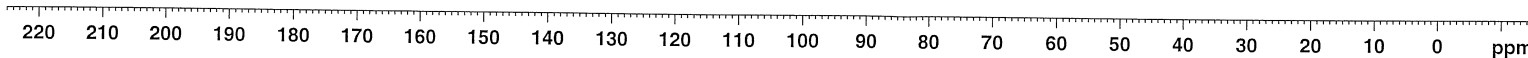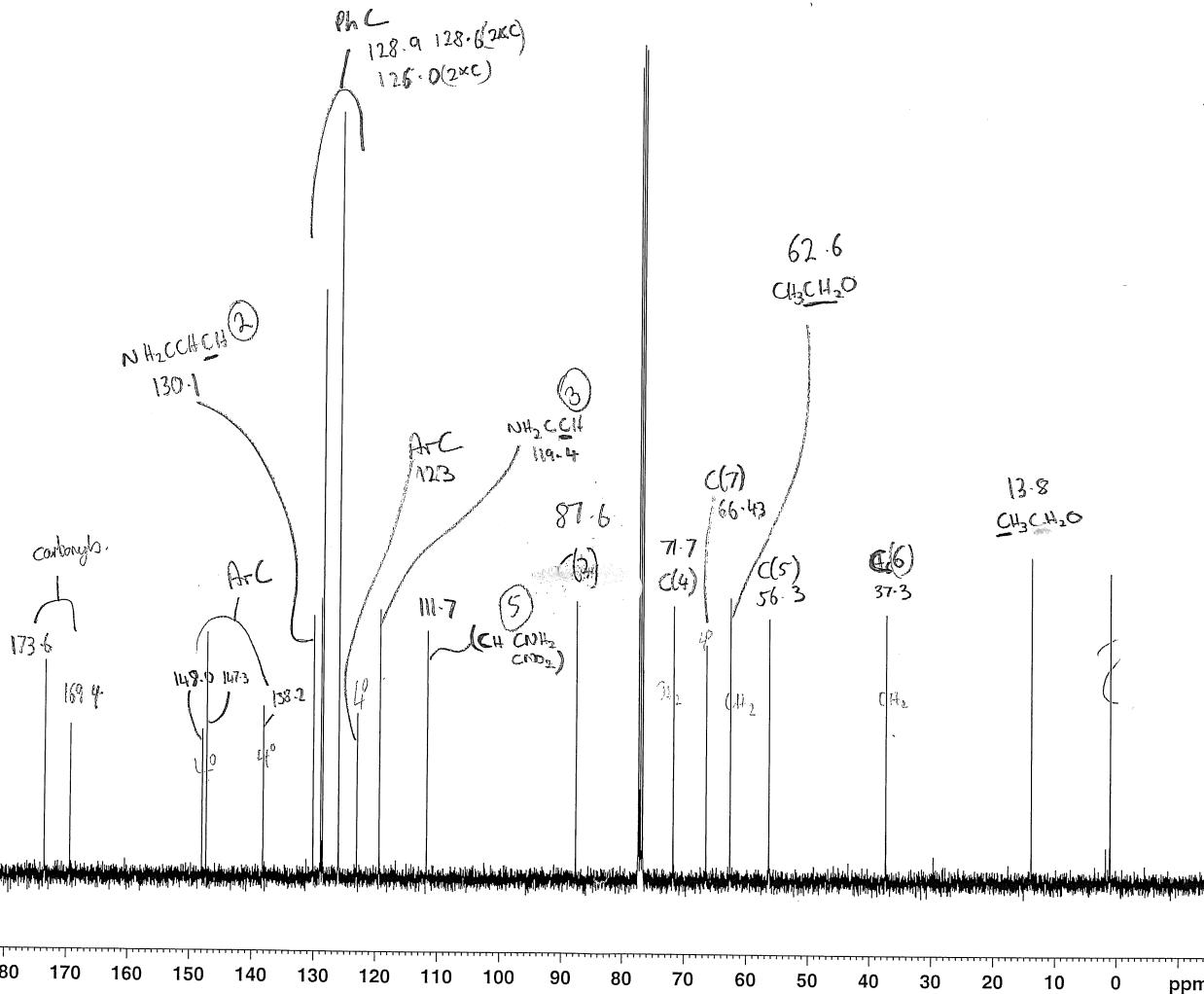
Instrument DQX400
Chemist RDS
Group MGM
RSByCy
h1acq.au CDCl3 e:\\ mgmgrp 54

Current Data Parameters
NAME   Apr03-2007-54
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20070404
Time   16.06
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zg60
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8278.146 Hz
FIDRES   0.126314 Hz
AQ   3.9584243 sec
RG   362
DW   60.400 usec
DE   7.50 usec
TE   294.5 K
D1   1.00000000 sec

======== CHANNEL f1 ========
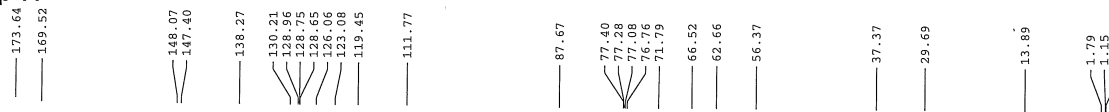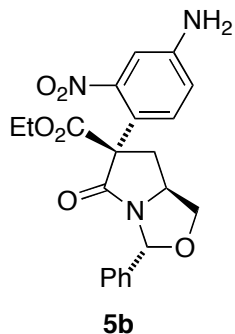NUC1   1H
P1   9.00 usec
PL1   0.00 dB
SFO1   400.2024714 MHz

F2 - Processing parameters
SI   32768
SF   400.2000028 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

Instrument DQX400
Chemist RDS
Group MGM
RSByCy
c13dept135.au CDCl3 e:\\ mgmgrp 54

NMR@CHEM.OX

128.72
128.52
125.98
123.48
108.96
97.90
87.26
71.94
56.91
33.63

9
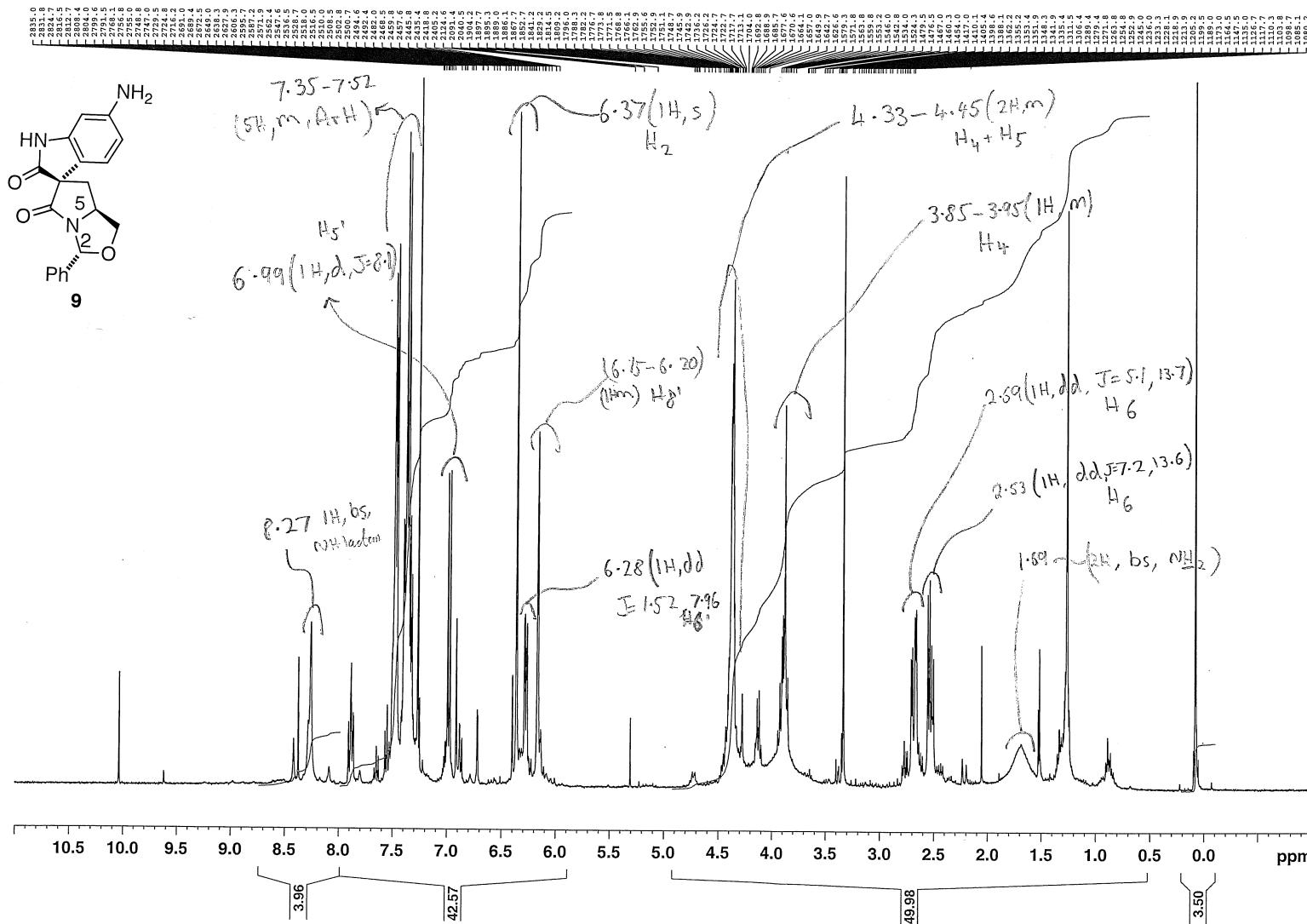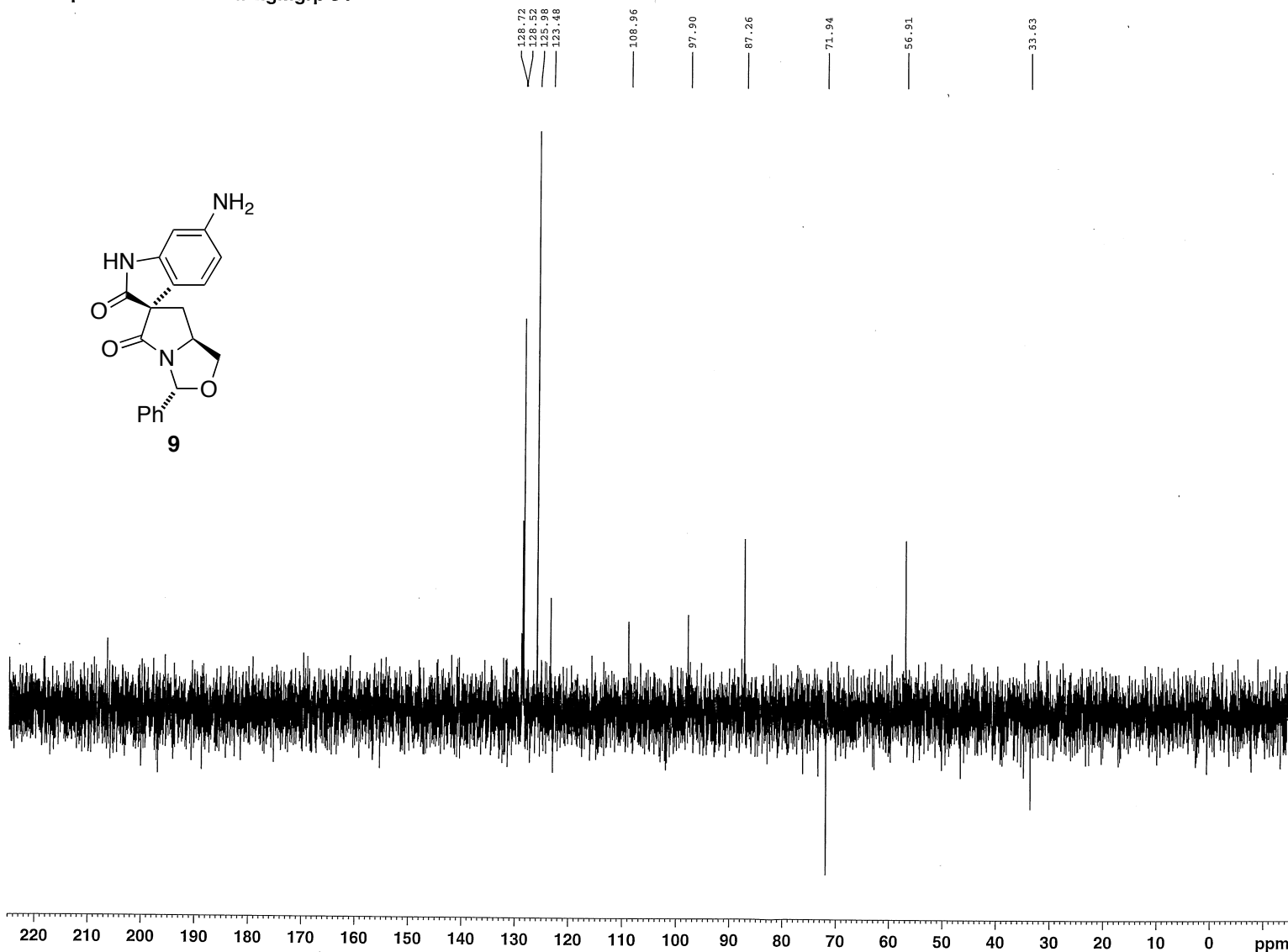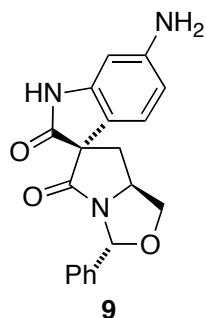
Current Data Parameters
NAME   Apr03-2007-54
EXPNO   3
PROCNO   1

F2 - Acquisition Parameters
Date_   20070404
Time   16.36
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   dept135
TD   65536
SOLVENT   CDCl3
NS   256
DS   4
SWH   26178.010 Hz
FIDRES   0.399445 Hz
AQ   1.2517875 sec
RG   32768
DW   19.100 usec
DE   7.50 usec
TE   295.0 K
CNST2   145.0000000
D1   2.00000000 sec
d2   0.00344828 sec
d12   0.00002000 sec
DELTA   0.00001210 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======== CHANNEL f1 ========
NUC1   13C
P1   9.50 usec
p2   19.00 usec
PL1   0.00 dB
SFO1   100.6403931 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
P3   9.00 usec
p4   18.00 usec
PCPD2   80.00 usec
PL2   0.00 dB
PL12   19.00 dB
SFO2   400.2016008 MHz

F2 - Processing parameters
SI   32768
SF   100.6303718 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Instrument DQX400
Chemist RDS
Group MGM
RS01-10b
h1acq.au CDCl3 e:\\ mgmgrp 18
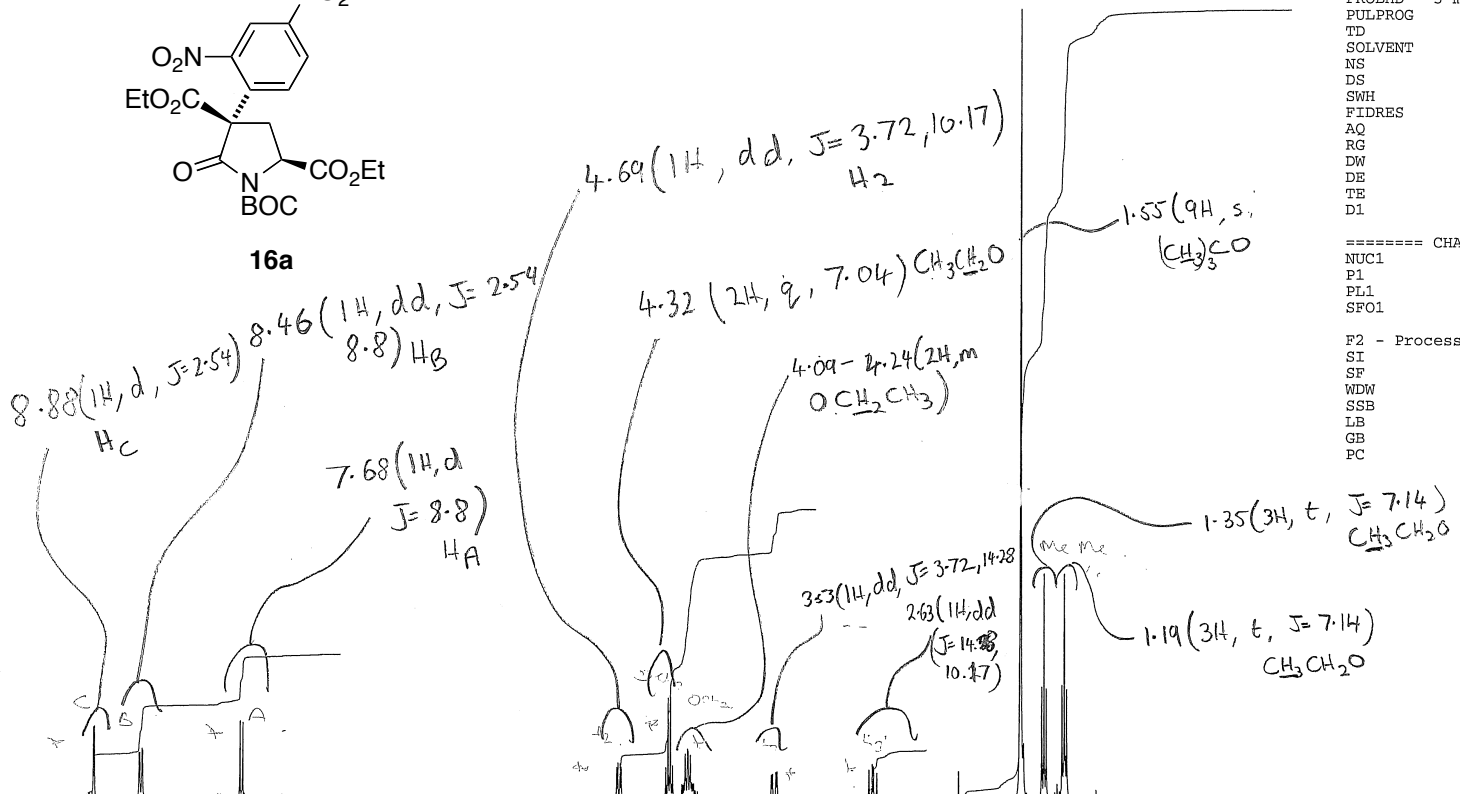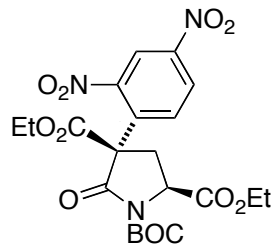
$\alpha_D^{22} = -38.4 \quad c = 1 \text{ in DCM}$

16a

8.88 (1H, d, J=2.54) H_C

8.46 (1H, dd, J= 2.54 8.8) H_B

7.68 (1H, d J= 8.8) H_A

4.69 (1H, dd, J= 3.72, 10.17) H_2

4.32 (2H, q, 7.04) CH_3CH_2O

4.09 – 4.24 (2H, m OCH_2CH_3)

3.53 (1H, dd, J= 3.72, 14.28)

2.63 (1H, dd J= 14.28, 10.17)

1.55 (9H, s $(CH_3)_3CO$)

1.35 (3H, t, J= 7.14) CH_3CH_2O

1.19 (3H, t, J= 7.14) CH_3CH_2O

Me Me

11.21   22.78   4.07   61.95

Instrument DQX400
Chemist RDS
Group MGM
RS01-10
c13acq.au CDCl3 e:\\ mgmgrp 18

16a

NMR@CHEM.OX

Current Data Parameters
NAME   Dec12-2006-18
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20061213
Time   17.40
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   256
DS   4
SWH   26178.010 Hz
FIDRES   0.399445 Hz
AQ   1.2517875 sec
RG   32768
DW   19.100 usec
DE   7.50 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   9.50 usec
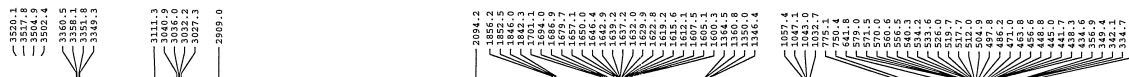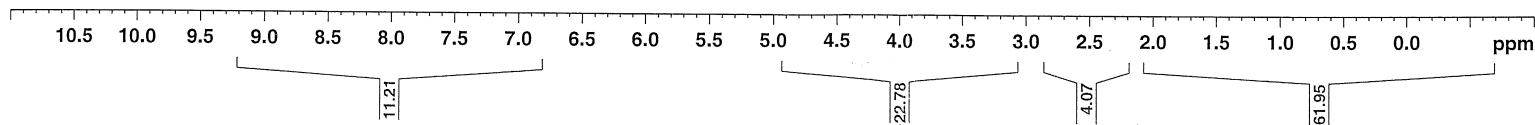PL1   0.00 dB
SFO1   100.6403931 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   0.00 dB
PL12   19.00 dB
PL13   25.00 dB
SFO2   400.2016008 MHz
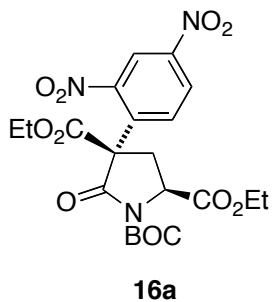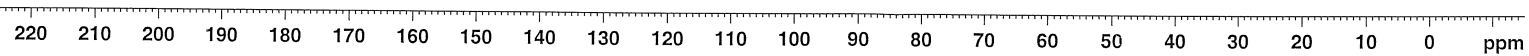
F2 - Processing parameters
SI   32768
SF   100.6303718 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

Instrument DQX400
Chemist RDS
Group MGM
RS01-11B   21
h1acq.au CDCl3 e:\\ mgmgrp 13

16b

NMR@CHEM.OX

Current Data Parameters
NAME   Jan29-2007-13
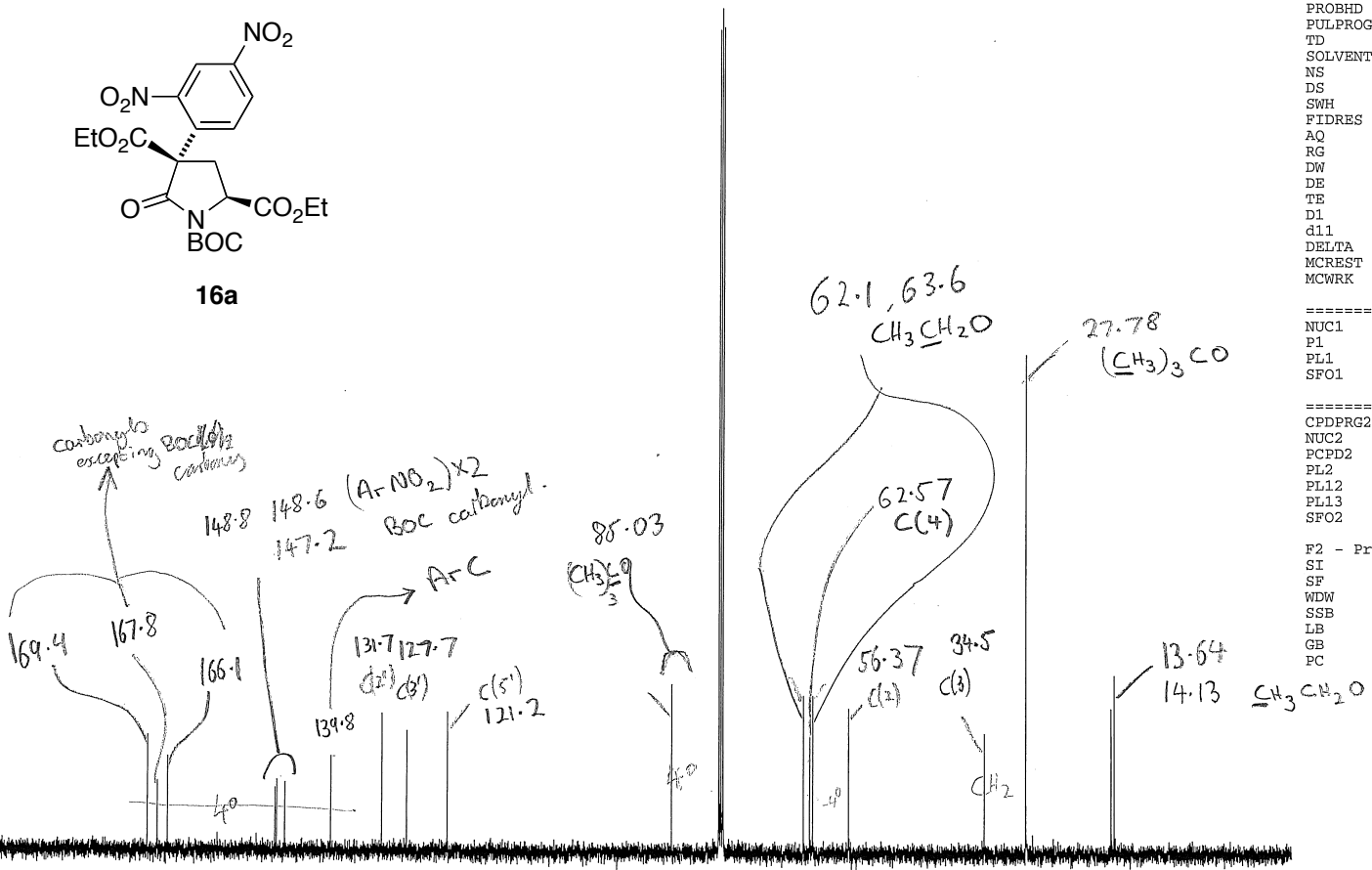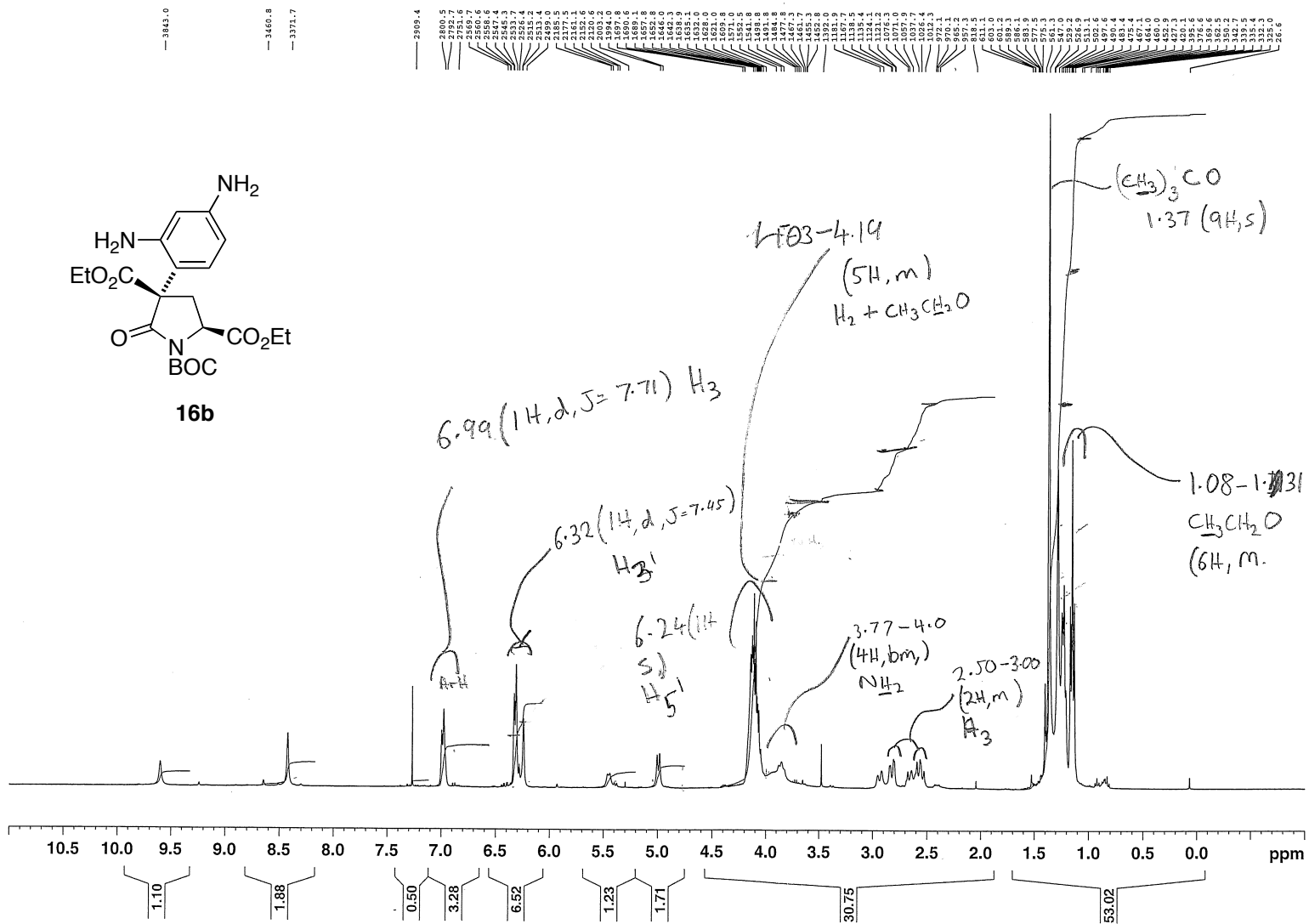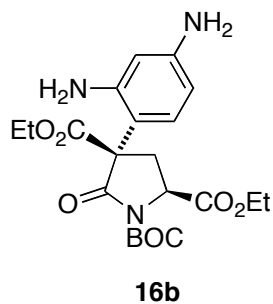EXPNO   1
PROCNO   1
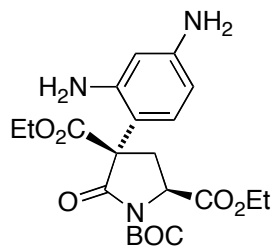
F2 - Acquisition Parameters
Date_   20070129
Time   15.14
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zg60
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8278.146 Hz
FIDRES   0.126314 Hz
AQ   3.9584243 sec
RG   90.5
DW   60.400 usec
DE   7.50 usec
TE   295.3 K
D1   1.00000000 sec

======== CHANNEL f1 ========
NUC1   1H
P1   9.00 usec
PL1   0.00 dB
SFO1   400.2024714 MHz

F2 - Processing parameters
SI   32768
SF   400.2000028 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

$(CH_3)_3CO$
1.37 (9H,s)

1.03-4.14
(5H,m)
$H_2 + CH_3CH_2O$

6.99 (1H, d, J= 7.71) H_3

6.32 (1H, d, J=7.45)
H_3'

6.24 (1H,
s)
H_5'

3.77-4.0
(4H,bm,)
NH_2

2.50-3.00
(2H,m)
H_3

1.08-1.031
CH_3CH_2O
(6H, m.

ArH

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

1.10   1.88   0.50 3.28   6.52   1.23 1.71   30.75   53.02

Instrument DQX400
Chemist RDS
Group MGM
RS01-11B
c13acq.au CDCl3 e:\\ mgmgrp 13

16b

Instrument DQX400
Chemist RDS
Group MGM
RS01-14TS
h1acq.au CDCl3 e:\\ mgmgrp 55

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DCM

18a

Structure: EtO$_2$C (wedge), CH$_2$CN, ring with O=, N-BOC, CO$_2$Et

2.8 (1H, d, J=17.02)

3.23 (1H, d, J=17.02)

CH$_2$CN

3.03 (1H, dd, J= 9.0, 13.9) H$_3$

1.5 (9H, s,) (CH$_3$)$_3$CO

CH$_3$CH$_2$O

1.32 (6H, 6J=7.04) CH$_3$CH$_2$O

4.73 (1H, dd J=6.26, 9.0) H$_2$

H$_3$'
2.12 (1H, dd J=(6.26, 14.09))

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

3.34   96.66

Instrument DQX400
Chemist RDS
Group MGM
RSCN1
h1acq.au CDCl3 e:\\ mgmgrp 25

NMR@CHEM.OX

c = 0.5 in DCM

$\alpha_D^{22} = +8.0$

Current Data Parameters
NAME   Apr03-2007-25
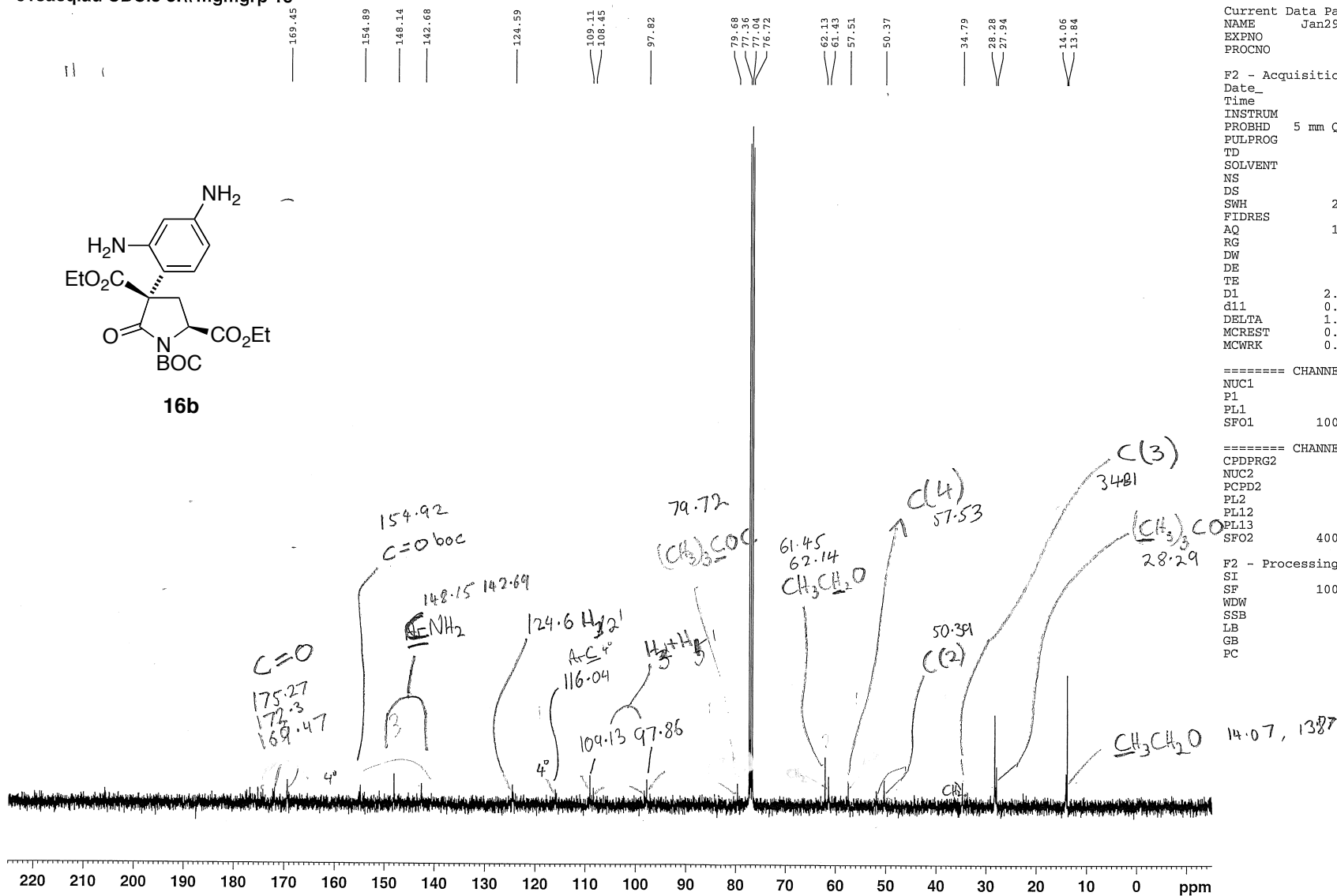EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20070405
Time   10.06
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zg60
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8278.146 Hz
FIDRES   0.126314 Hz
AQ   3.9584243 sec
RG   143.7
DW   60.400 usec
DE   7.50 usec
TE   295.1 K
D1   1.00000000 sec

======== CHANNEL f1 ========
NUC1   1H
P1   9.00 usec
PL1   0.00 dB
SFO1   400.2024714 MHz

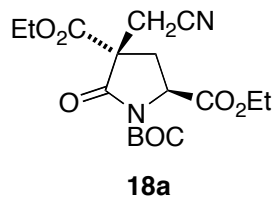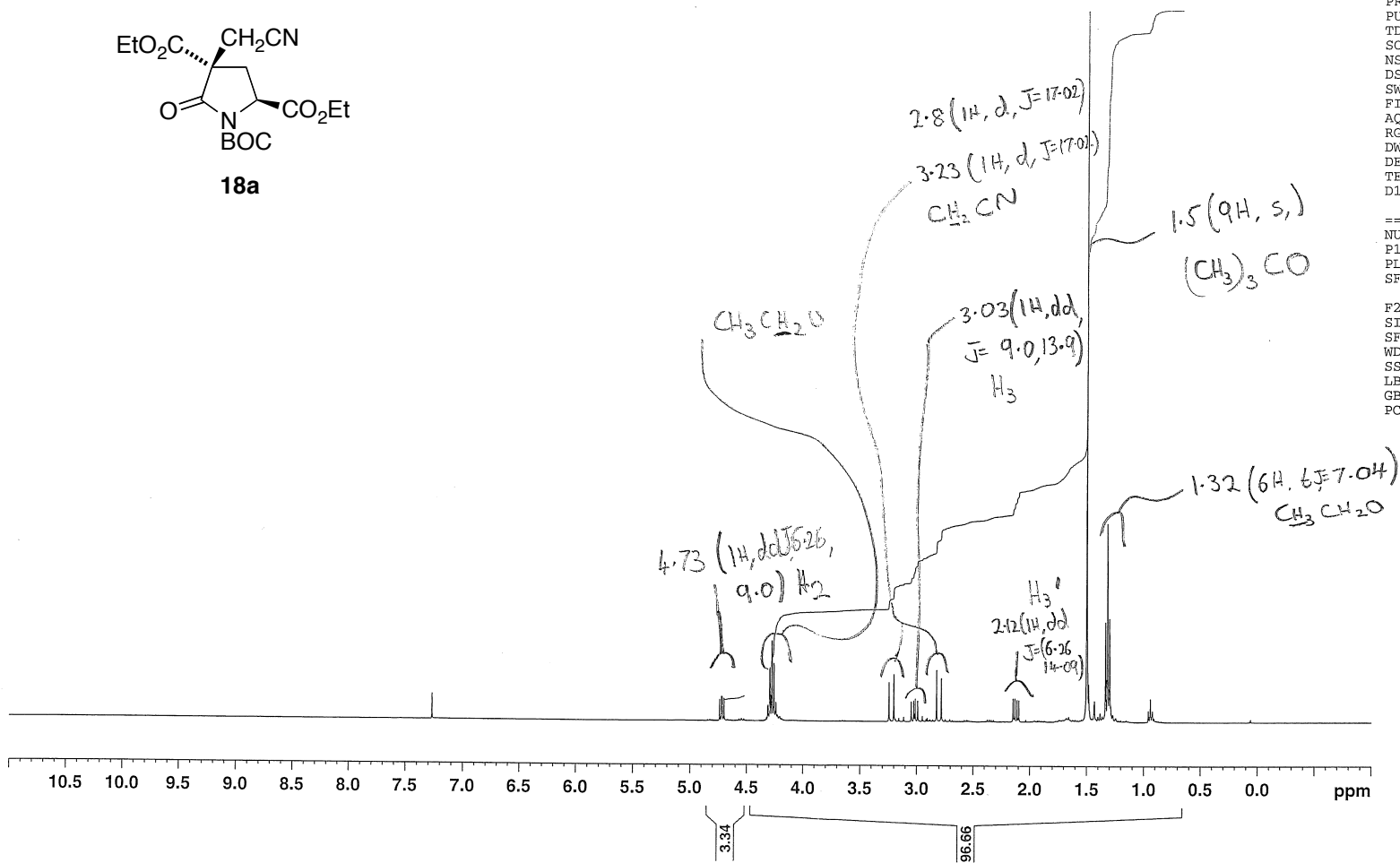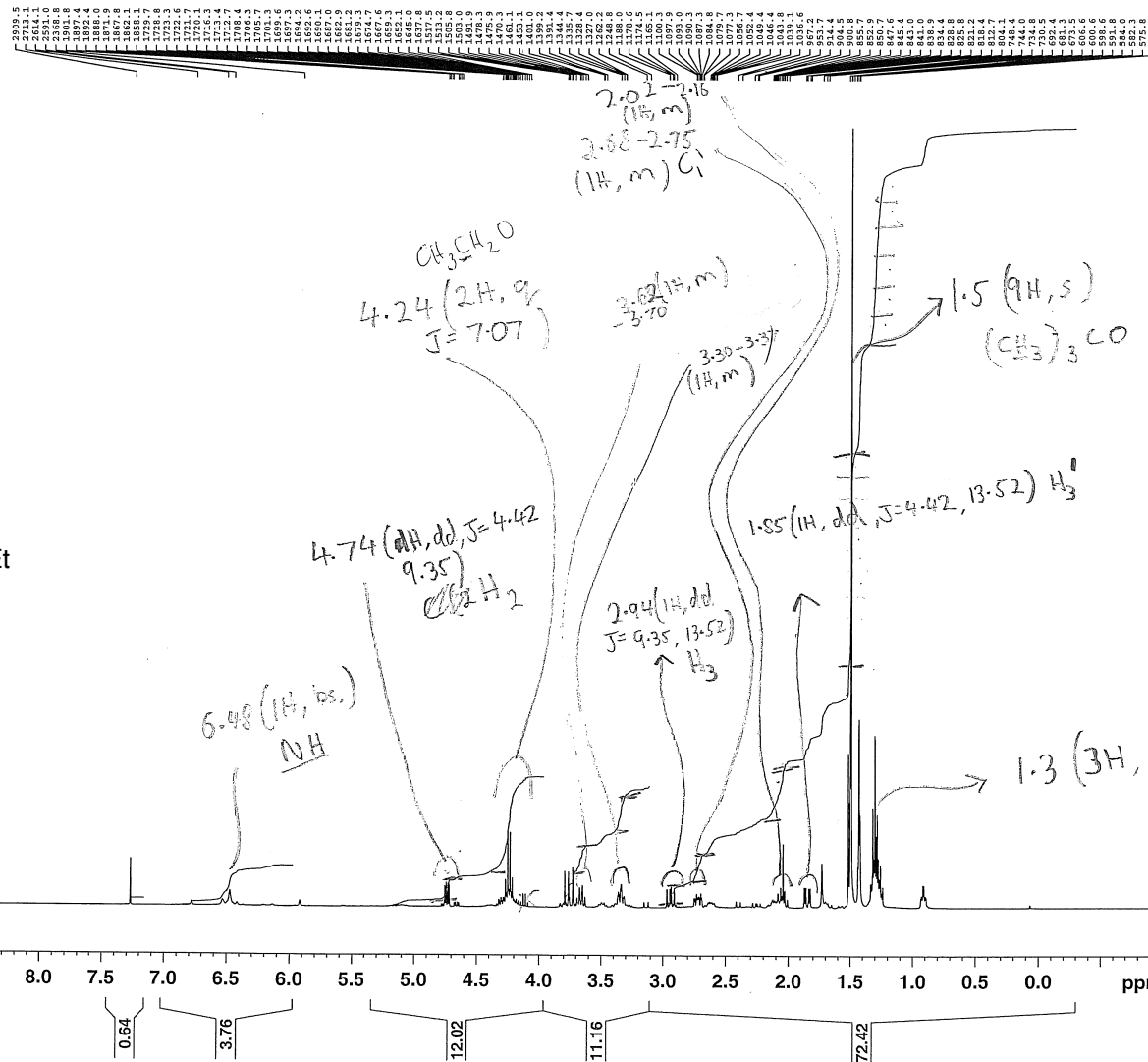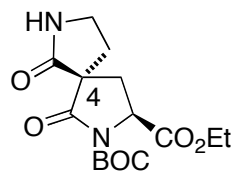F2 - Processing parameters
SI   32768
SF   400.2000028 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

19

2.02–2.16 (15, m)

2.68–2.75 (1H, m) C1

CH_3CH_2O
4.24 (2H, q, J = 7.07)

3.62 (1H, m)
3.70

3.30–3.37 (1H, m)

1.5 (9H, s)
$(CH_3)_3CO$

4.74 (1H, dd, J = 4.42, 9.35) CH, H2

1.85 (1H, dd, J = 4.42, 13.52) H3'

2.94 (1H, dd, J = 9.35, 13.52) H3

6.48 (1H, bs) NH

1.3 (3H, t, J = 7.07)

0.64   3.76   12.02   11.16   72.42

10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

Instrument DQX400
Chemist RDS
Group MGM
RSCN1
c13acq.au CDCl3 e:\\ mgmgrp 25

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174.91
172.12
171.49

149.00

84.10

77.35
77.03
76.71

61.78

56.97
53.85
53.64

39.67

32.85
31.40
28.27
27.83
27.74
25.27

14.13
13.98

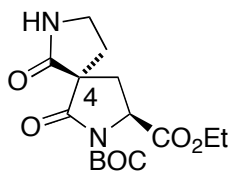Current Data Parameters
NAME   Apr03-2007-25
EXPNO   2
PROCNO   1

F2 - Acquisition Parameters
Date_   20070405
Time   10.21
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zgpg30
TD   65536
SOLVENT   CDCl3
NS   256
DS   4
SWH   26178.010 Hz
FIDRES   0.399445 Hz
AQ   1.2517875 sec
RG   32768
DW   19.100 usec
DE   7.50 usec
TE   295.0 K
D1   2.00000000 sec
d11   0.03000000 sec
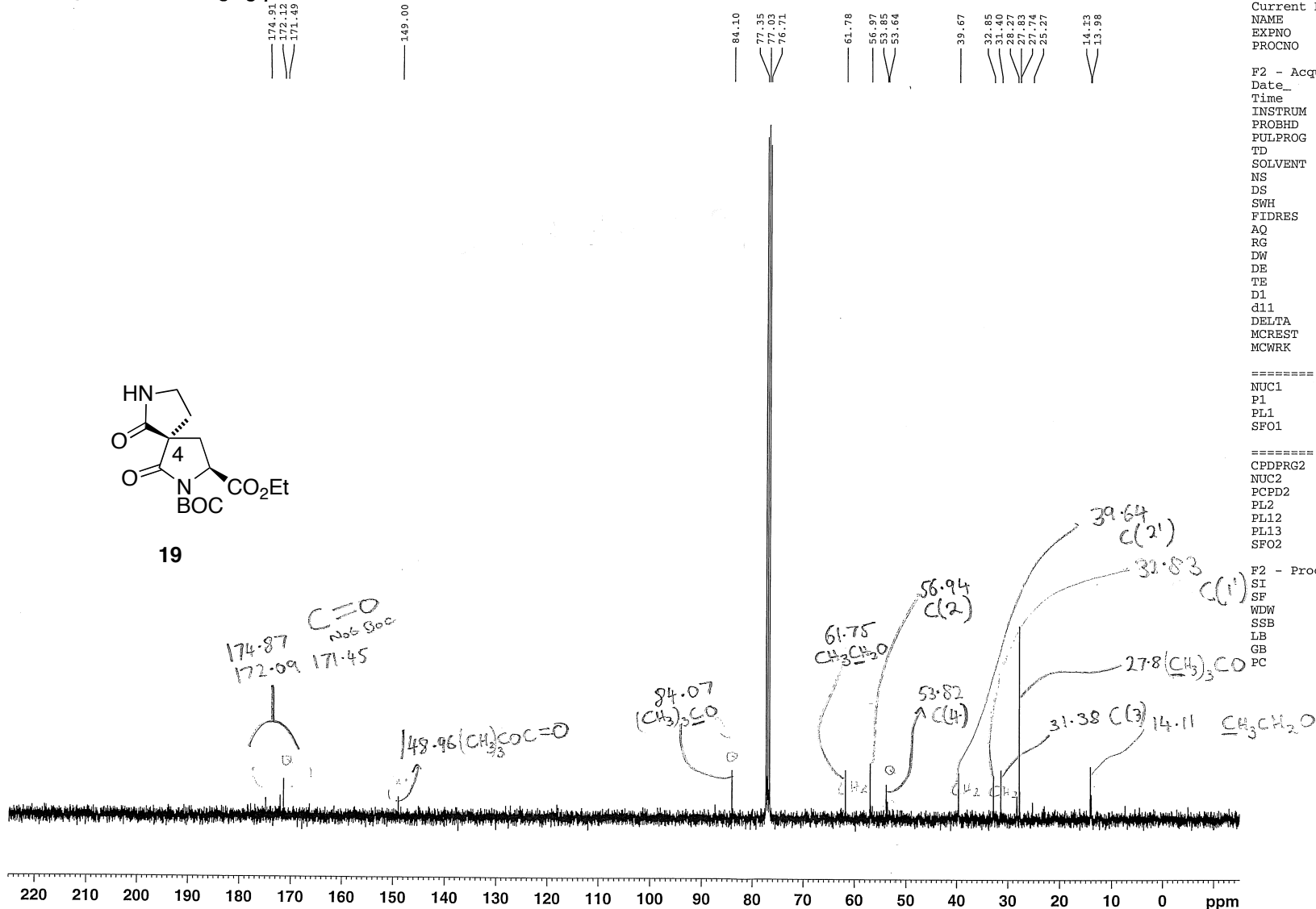DELTA   1.89999998 sec
MCREST   0.00000000 sec
MCWRK   0.01500000 sec

======== CHANNEL f1 ========
NUC1   13C
P1   9.50 usec
PL1   0.00 dB
SFO1   100.6403931 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   80.00 usec
PL2   0.00 dB
PL12   19.00 dB
PL13   25.00 dB
SFO2   400.2016008 MHz

F2 - Processing parameters
SI   32768
SF   100.6303718 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

19

HN

O

4

O

N
BOC

CO₂Et

174·87 C=O
172·09 171·45 Not Boc

148·96(CH₃)₃COC=O

84·07
(CH₃)₃CO

61·75
CH₃CH₂O

56·94
C(2)

39·64
C(2')

31·83 C(1')

53·82
C(4)

27·8(CH₃)₃CO

31·38 C(3) 14·11 CH₃CH₂O

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Instrument DQX400
Chemist RDS
Group MGM
RS01-15-2nd   22.
h1acq.au CDCl3 e:\\ mgmgrp 51

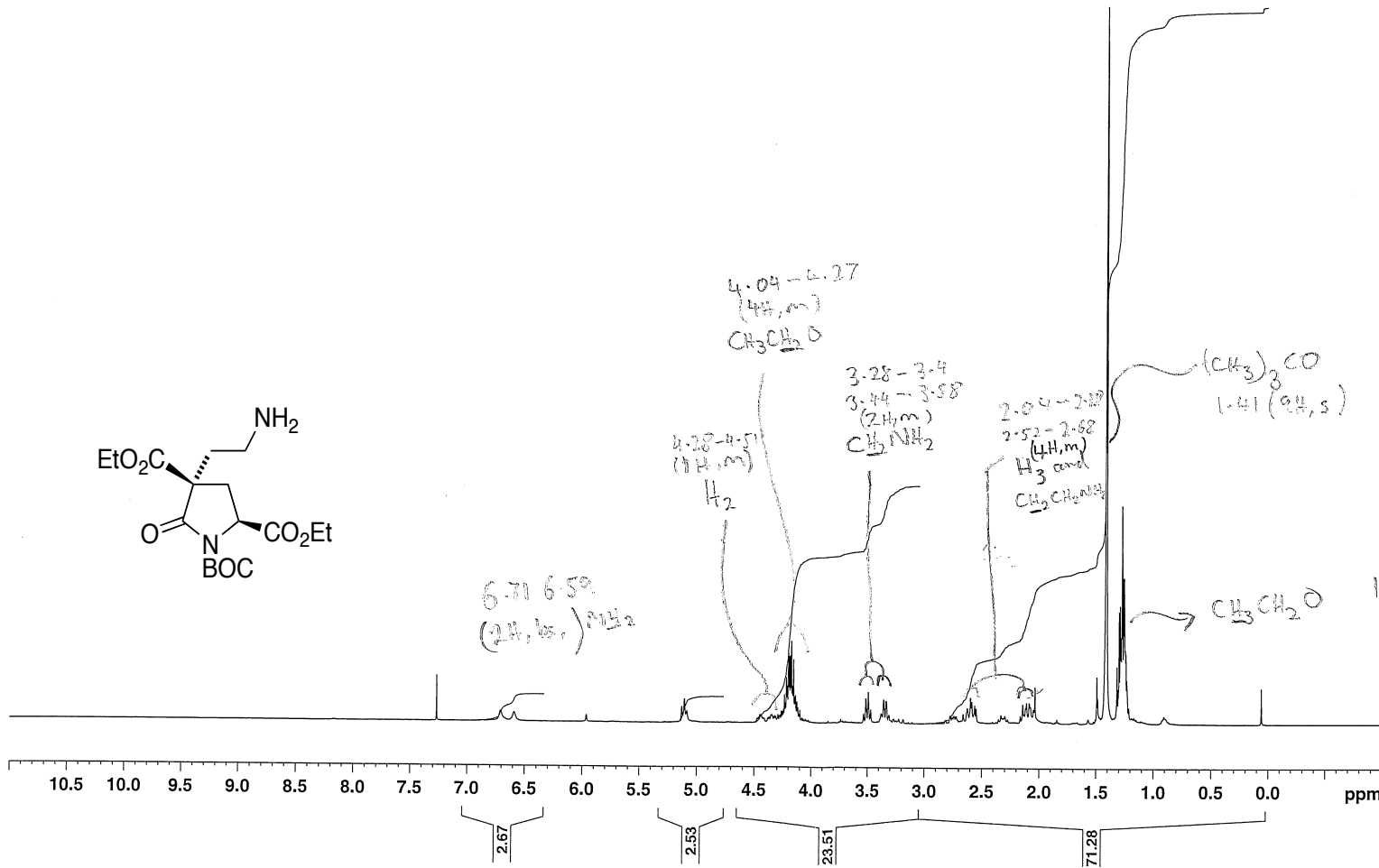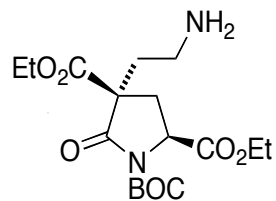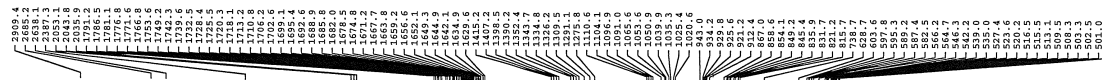NMR@CHEM.OX

Current Data Parameters
NAME   Mar23-2007-51
EXPNO   1
PROCNO   1

F2 - Acquisition Parameters
Date_   20070324
Time   22.36
INSTRUM   av400
PROBHD   5 mm QNP 1H/13
PULPROG   zg60
TD   65536
SOLVENT   CDCl3
NS   16
DS   2
SWH   8278.146 Hz
FIDRES   0.126314 Hz
AQ   3.9584243 sec
RG   90.5
DW   60.400 usec
DE   7.50 usec
TE   294.9 K
D1   1.00000000 sec

======== CHANNEL f1 ========
NUC1   1H
P1   9.00 usec
PL1   0.00 dB
SFO1   400.2024714 MHz

F2 - Processing parameters
SI   32768
SF   400.2000028 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

Instrument DQX400
Chemist RDS
Group MGM
RS01-15-2nd
c13acq.au CDCl3 e:\\ mgmgrp 51

172.14
155.25
79.98 77.35 77.03 76.72
61.95 61.55
53.26 50.70
39.99 35.99
28.26
14.06 13.97

61.92 $C\underline{H_3}CH_2O$

61.52 $CH_3\underline{C}H_2O$

53.23 C(4)

50.67 C(2)

39.96 $\underline{C}H_2NH_2$

35.96 $\underline{C}H_2CH_2NH_2$

34.94 C(3)

28.24 $(\underline{C}H_3)_3C$

14.04
13.95 $\underline{C}H_3CH_2O$

79.95 $(CH_3)_3\underline{C}$

30.96

29.29

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm