

# SUPPORTING INFORMATION

## Highly Chemoselective Addition of Amines to Epoxides in Water

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### Experimental Section

**General.** All chemicals were purchased and used without any further purification. NMR spectra were recorded at 500 MHz for proton and at 125.7 MHz for carbon nuclei in (CDCl<sub>3</sub> + CCl<sub>4</sub>) or (C<sub>6</sub>D<sub>6</sub> + CCl<sub>4</sub>). The products were purified by column chromatography carried out on silica gel (230-400 mesh), and by using ethyl acetate/ petroleum ether mixtures. Reactions were carried out room temperature, all the epoxides used are known and all amines employed are commercially available. All β-amino alcohols obtained are known compound.

### **General procedure for the synthesis of $\beta$ -amino alcohols:**

In the test tube equipped were introduces 5 mmol epoxides and 2 ml of water. The amine (6mmol) was added in one portion and the test tube was kept at 0 °C and warmed to room temperature under vigorous stirring for 14 h for styrene oxides (Table 1) and 5-24 h for other epoxides (Table 2). If no participation occurred, water (2 ml) was added and the aqueous mixture was extracted with 10 ml of diethyl ether or ethyl acetate and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>, and solvent was removed under reduce pressure to give the  $\beta$ -amino alcohols in the pure state. The crude product was analyzed by <sup>1</sup>H and <sup>13</sup>C NMR. For the compound Table 1, Entry 3, 6, 8 and Table 2 entry 23, 25, further purification was carried out by short column chromatography on silica gel (ethyl acetate/petroleum ether). All compounds were characterized on the basis of their spectroscopic data (IR, NMR) and by comparison with those reported in the literature.<sup>1-11</sup>

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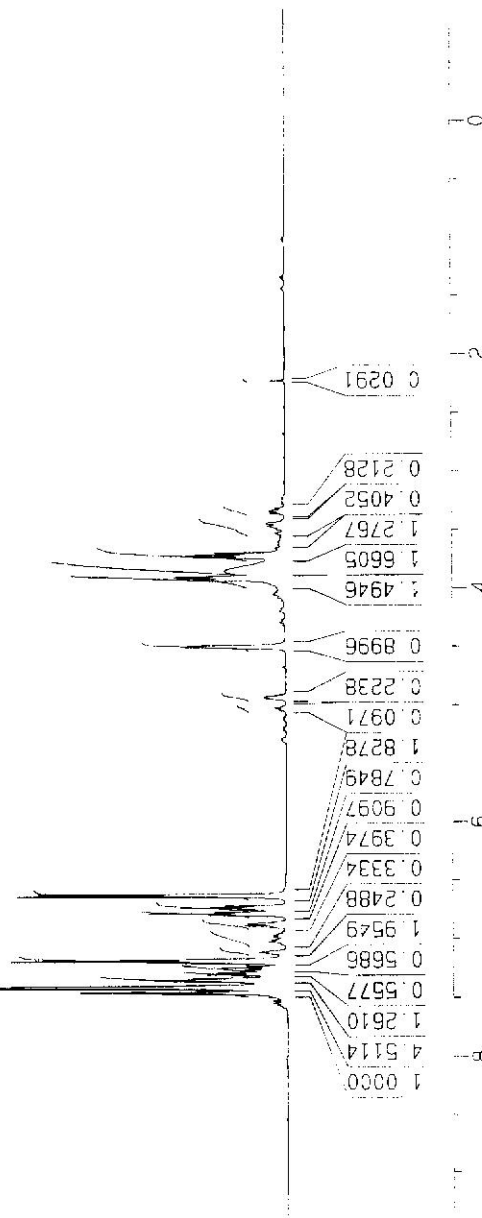
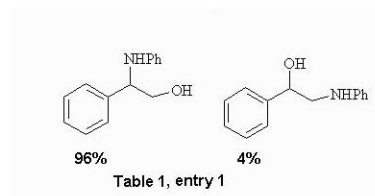
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 DS 2  
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 FIDRES 0.315264 Hz  
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 DE 5.50 usec  
 TE 300.0 K  
 D1 5.0000000 sec

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 WDW EM  
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 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
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 CY 11.00 cm  
 F1P 10.706 ppm  
 F1 5354.41 Hz  
 F2P -0.962 ppm  
 F2 -480.90 Hz  
 PPMQCM 6.64820 ppm/cm  
 HZCM 324.18417 Hz/cm

7.46387  
7.45587  
7.41672  
7.40824  
7.36412  
7.35588  
7.34718  
7.33938  
7.30367  
7.20481  
7.18844  
7.17359  
6.80057  
6.78637  
6.77201  
6.73461  
6.63937  
6.62388  
4.51157  
4.50375  
4.49765  
4.48996  
3.93117  
3.92482  
3.90913  
3.90303  
3.73584  
3.72051  
3.71419  
3.44544



ph.

5 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298K 83/01/24

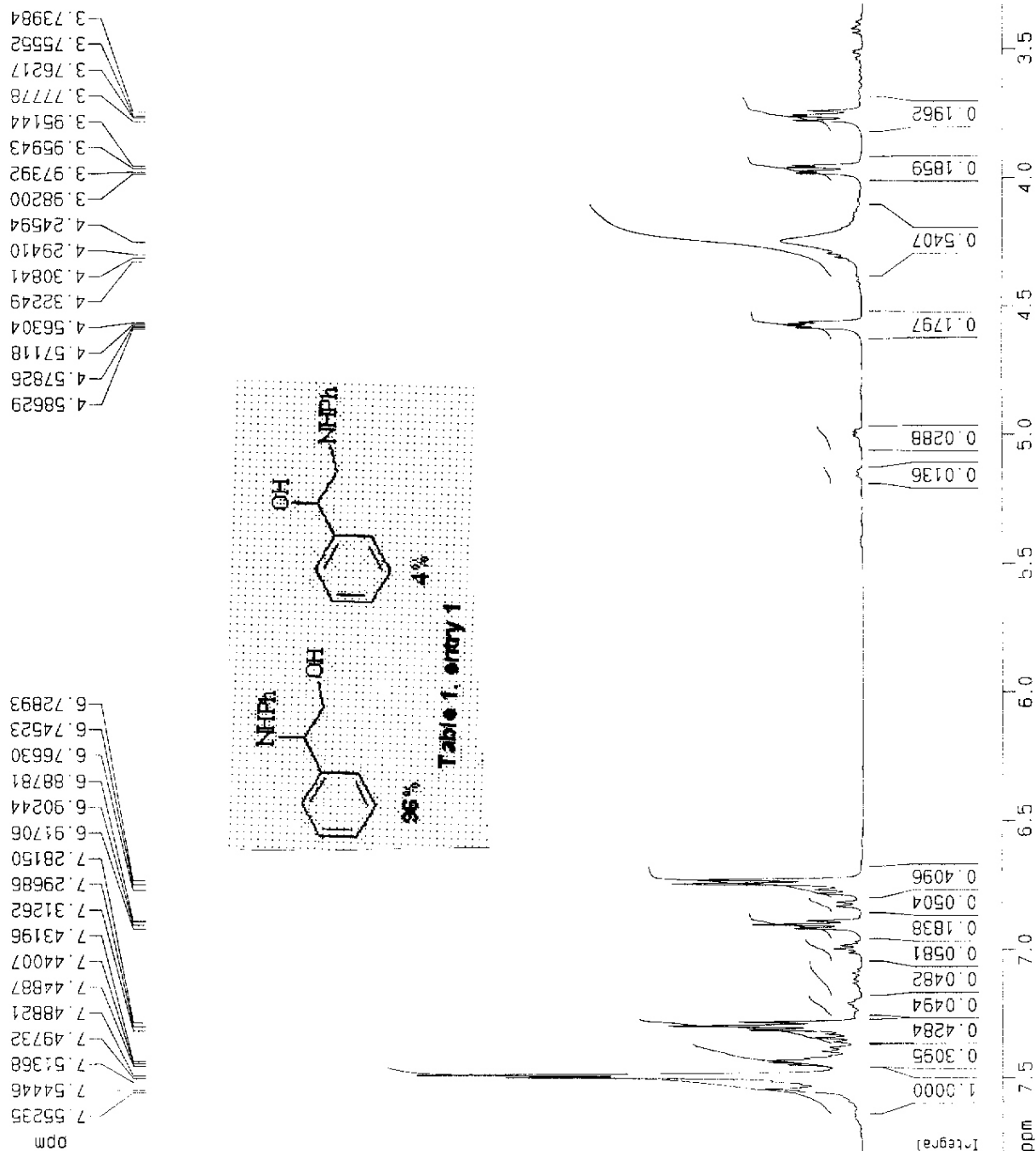
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 TO 32768  
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 NS 8  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
 RG 12.7  
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 TE 300.0 K  
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 GB 0  
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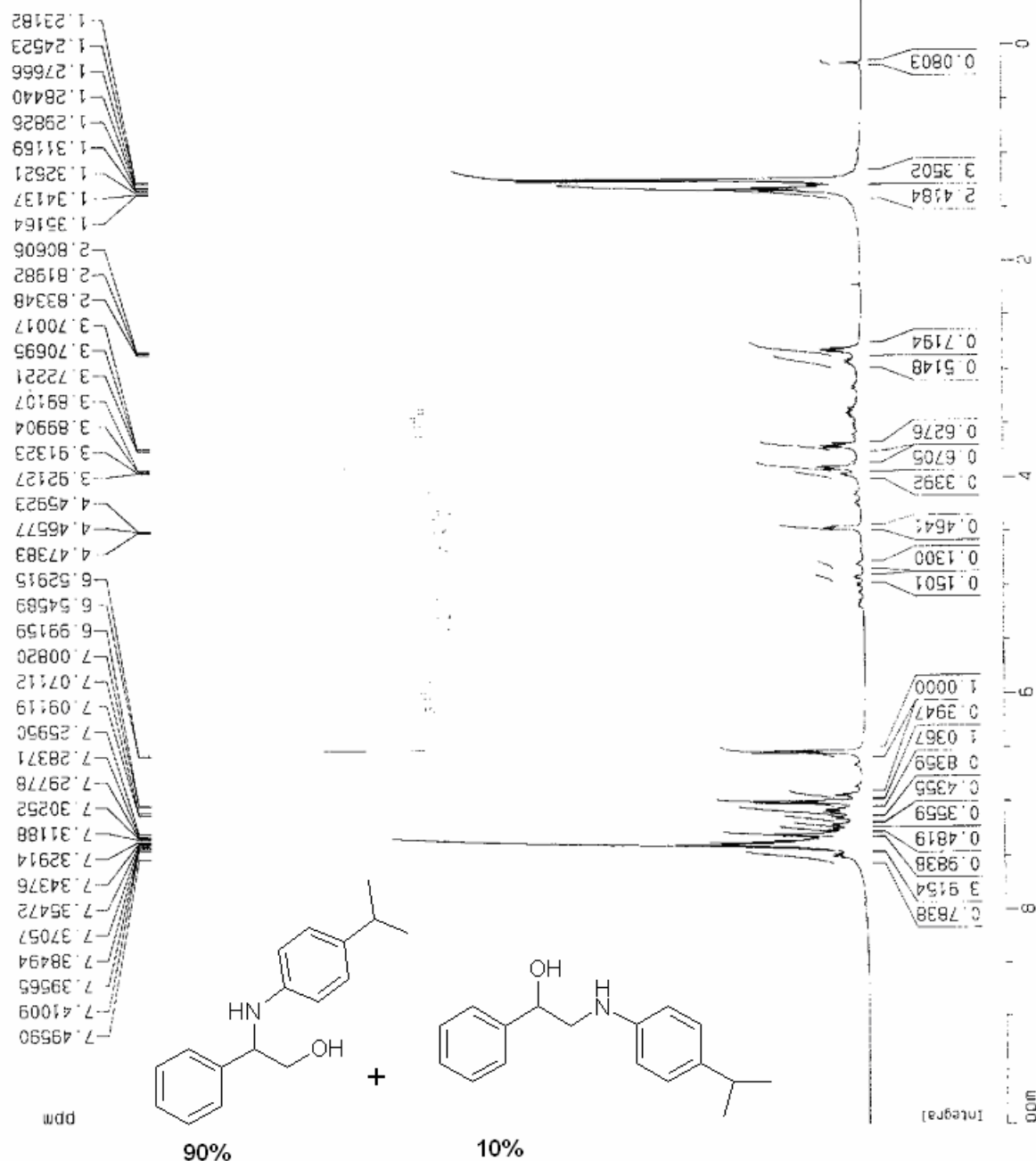
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CC(C)C1=CC=C(C=C1)NC(CO)Cc2ccccc2 + CC(C)C1=CC=C(C=C1)NC(CO)Cc2ccccc2 + CC(C)C1=CC=C(C=C1)NC(CO)Cc2ccccc2

P-8 1H NMR in CDCl3 at 298K 83/03/26



Current Data Parameters  
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 PROCNO 1  
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 Time 11.13  
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 PULPROG zg30  
 TO 32768  
 SOLVENT CDCl3  
 NS 6  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
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 DE 6.50 usec  
 TE 300.0 K  
 D1 5.00000000 sec  
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 PL1 3.00 dB  
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 F2 - Processing parameters  
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 SF 500.1330000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00  
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 CY 5.50 cm  
 F1P 10.000 ppm  
 F1 5001.30 Hz  
 F2P -0.500 ppm  
 F2 250.07 Hz  
 PPMCM 0.58333 ppm/cm  
 HZCM 291.74249 Hz/cm

Table 1, Entry 2

AD-1

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 EXPNO 367  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20040528  
 Time 11.14  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 71  
 DS 2  
 SWH 40000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8192625 sec  
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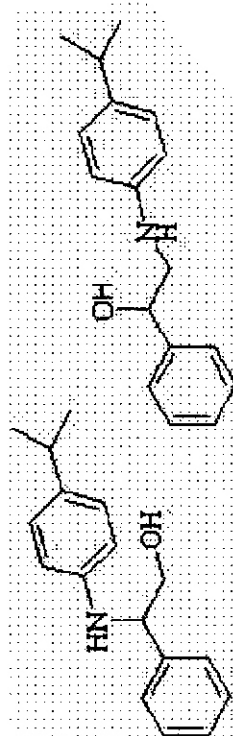
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 PCPD2 80.00 usec  
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 PL12 22.00 dB  
 PL13 22.00 dB  
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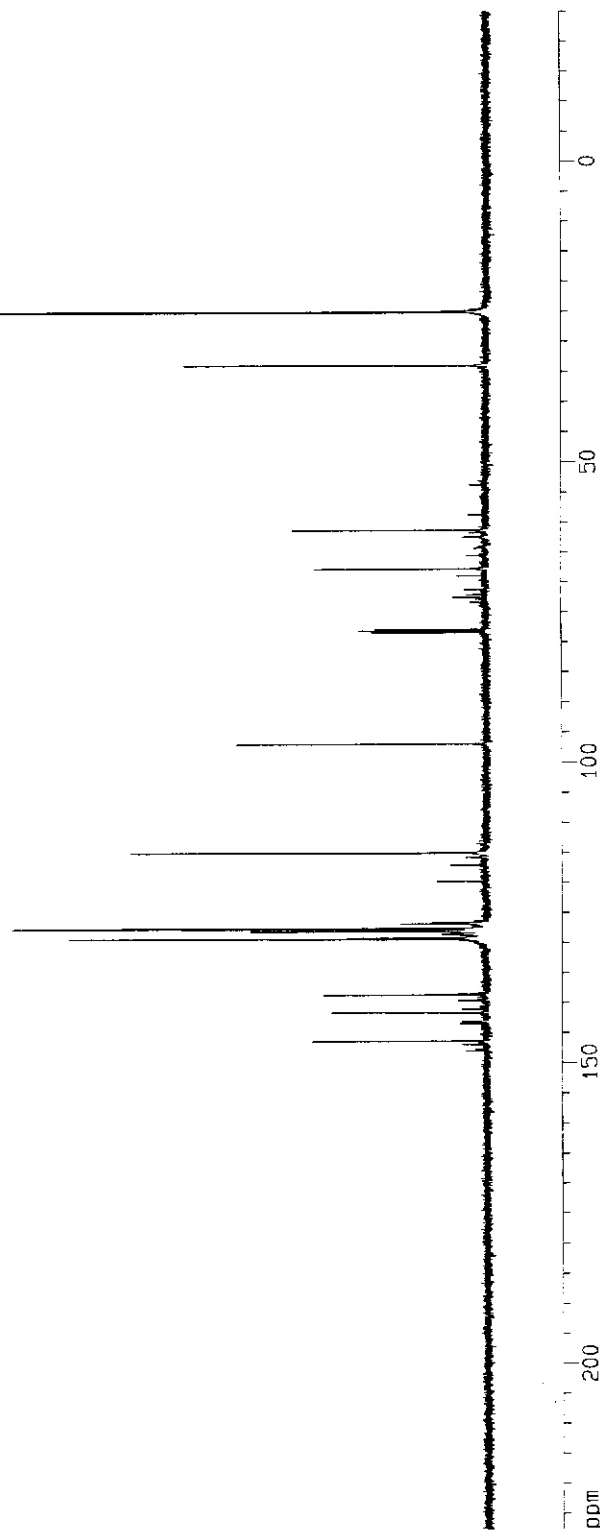
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 CY 10.96 cm  
 F1P 227.585 ppm  
 F1 28620.75 Hz  
 F2P -25.064 ppm  
 F2 -3151.98 Hz  
 PPMCM 12.63251 ppm/cm  
 HZCM 1588.63647 Hz/cm

146.377  
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 141.623  
 139.599  
 138.723  
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 128.639  
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 127.967  
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 78.165  
 77.911  
 72.588  
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 69.019  
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 24.761



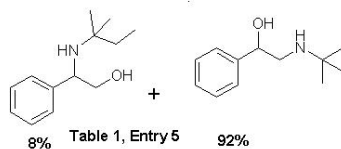
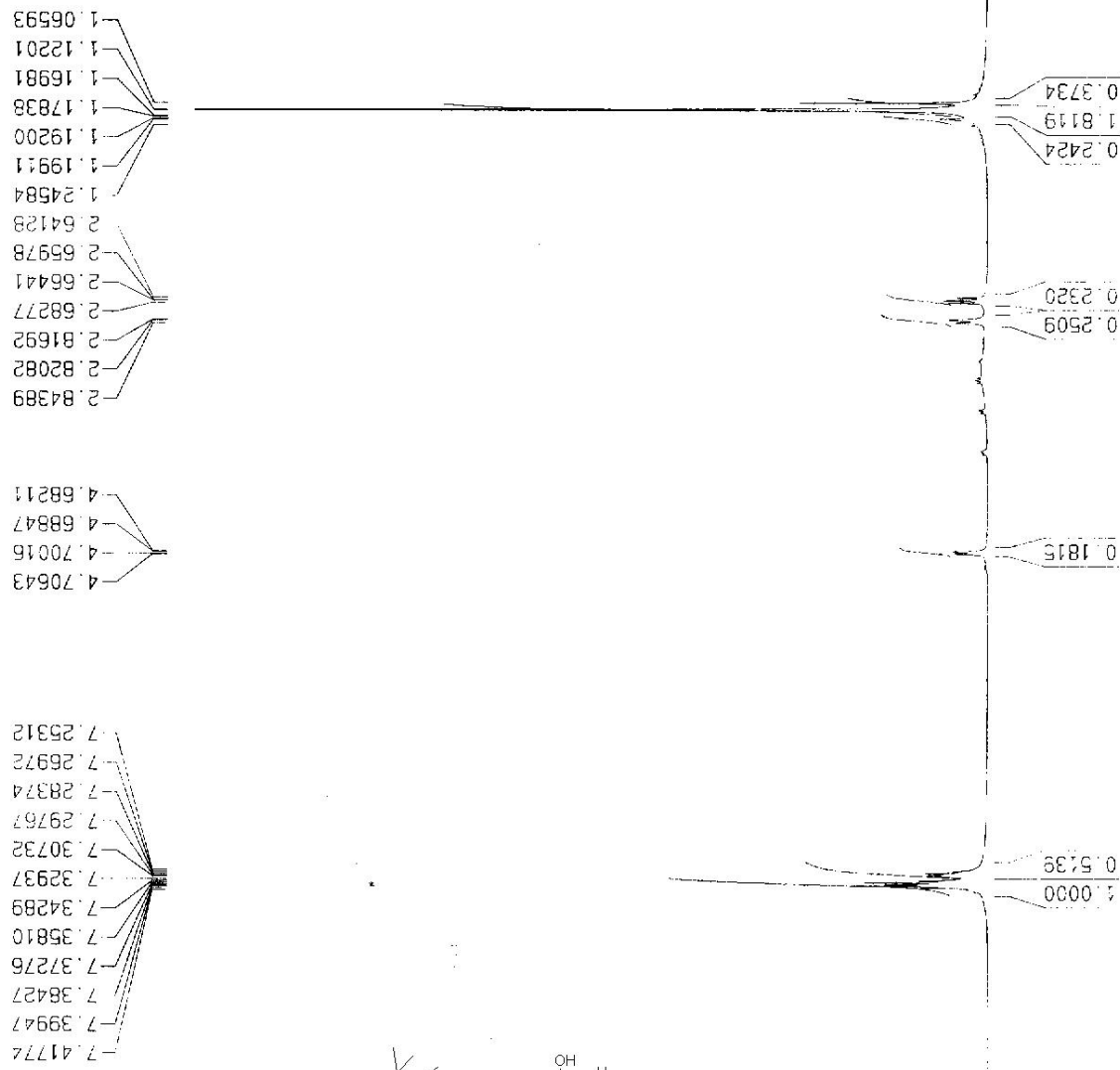
30% Table 1, entry 2 10%





P-6 1H NMR in CDCl3 at 298K 03/03/26

92-1



Current Data Parameters

NAME Poorhasan

EXPNO 20

PROCNO 1

F2 - Acquisition Parameters

Date\_ 20040615

Time 10.50

INSTRUM spect

PROBHD 5 mm BBI 1H-

PULPROG zg30

TO 32768

SOLVENT CDCl3

NS 8

DS 2

SWH 10330.578 Hz

FIDRES 0.315264 Hz

AQ 1.5860696 sec

RG 18

DW 48.400 usec

DE 6.50 usec

TE 300.0 K

D1 5.00000000 sec

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

NUC1 1H

P1 9.30 usec

PL1 3.00 dB

SF01 500.1330885 MHz

F2 - Processing parameters

SI 32768

SF 500.1300000 MHz

WDW EM

SSB 0

LB 0.30 Hz

GB 0

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1D NMR plot parameters

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CY 11.00 cm

FID 10.000 ppb

F1 5001.30 Hz

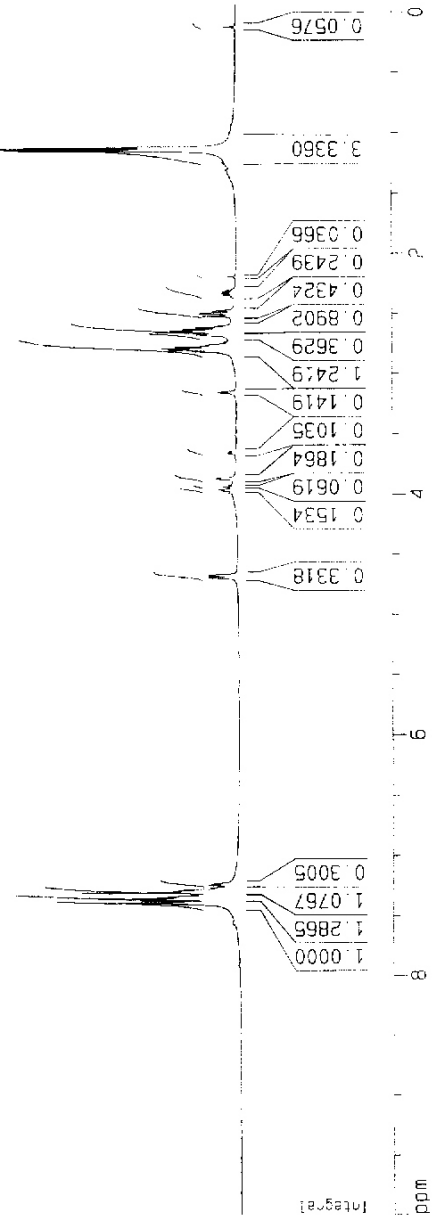
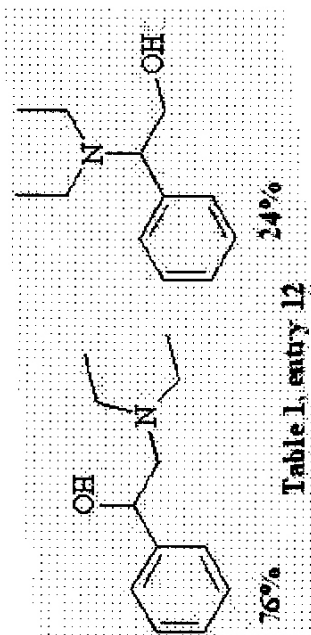
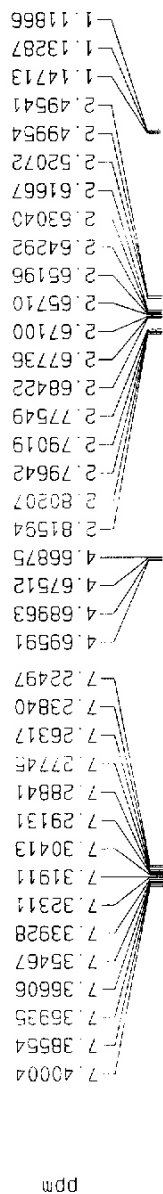
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PHASE 0.58333 ppm/cm

WZCM 291.74249 Hz/cm

93

P 9 1H NMR in CDCl3 at 298K 83/03/26



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EXPNO 23  
PROCNO 1

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Date\_ 20040615  
Time 11:22  
INSTRUM spect  
PROBHD 5 mm BBI 1H-  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 8  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.9860696 sec  
RG 35.9  
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DE 6.50 usec  
TE 300.0 K  
D1 2.00000000 sec

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PL1 3.00 dB  
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F2 - Processing parameters  
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WDW FM  
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LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 18.00 cm  
CY 5.50 cm  
F1P 10.000 ppm  
F1 5001.30 Hz  
F2P -0.500 ppm  
F2 -250.07 Hz  
PPMCM 0.58333 ppm/cm  
HZCM 291.74249 Hz/cm

Current Data Parameters  
 NAME AZ121  
 EXPNO 368  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20040628  
 Time 11:52  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-  
 PULPROG zgpg30  
 TO 65536  
 SOLVENT CDCl3  
 NS 38  
 DS 2  
 SMH 40000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8192625 sec  
 RG 456.1  
 DM 12.500 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 10.00000000 sec  
 d11 0.03000000 sec  
 d12 0.0002000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.80 usec  
 PL1 0.00 dB  
 SF01 125.7703143 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 3.00 dB  
 PL12 22.00 dB  
 PL13 22.00 dB  
 SF02 500.1320005 MHz

F2 - Processing parameters  
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 EM  
 NDM 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
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 CY 10.96 cm  
 F1P 227.586 ppm  
 F1 28620.75 Hz  
 F2P -25.064 ppm  
 F2 -3151.98 Hz  
 PPMCM 12.63251 ppm/cm  
 HZCM 1586.63647 Hz/cm

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 125.806  
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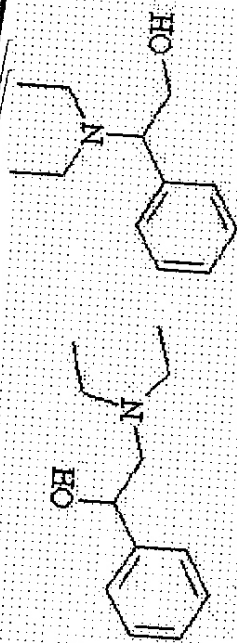
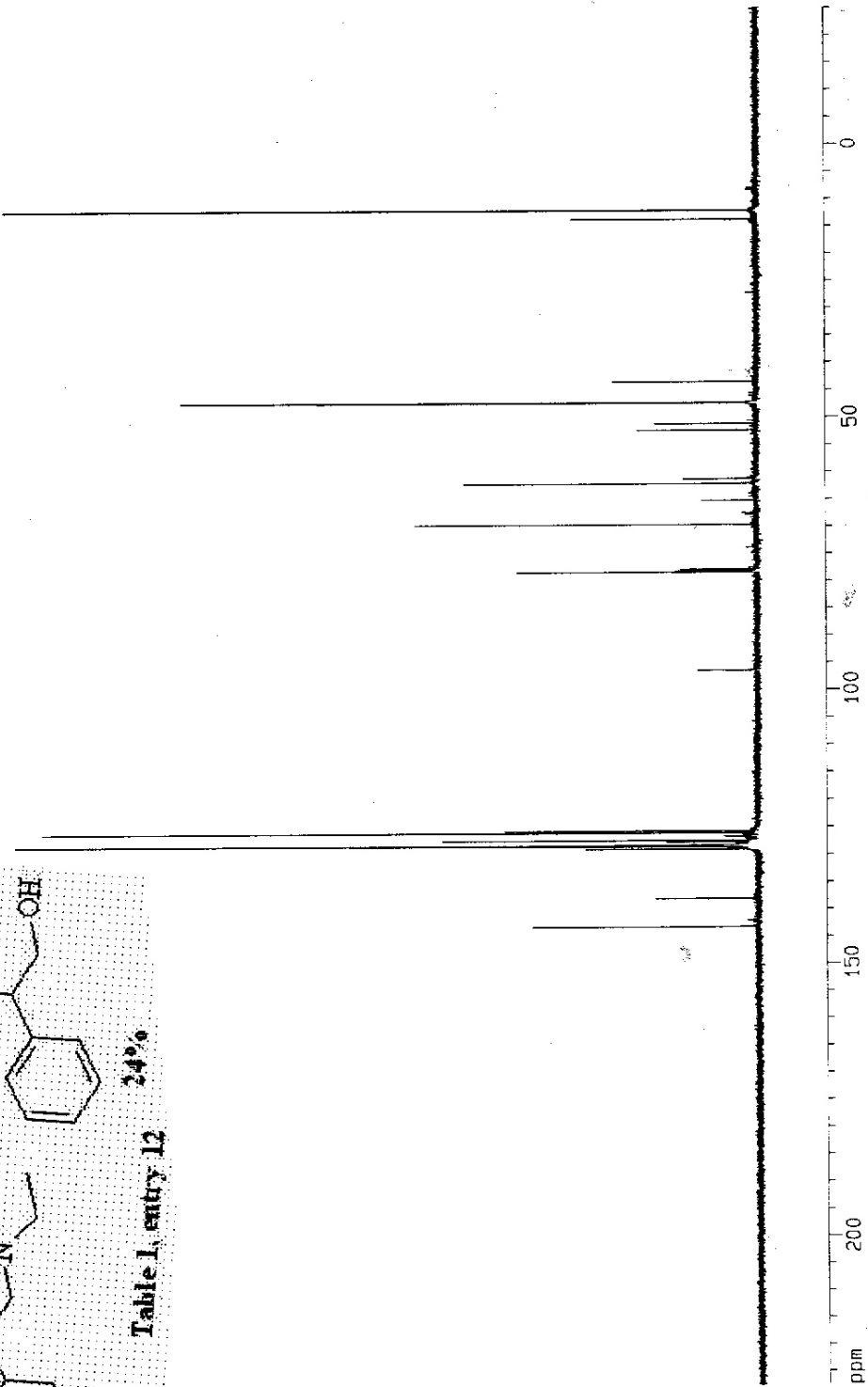


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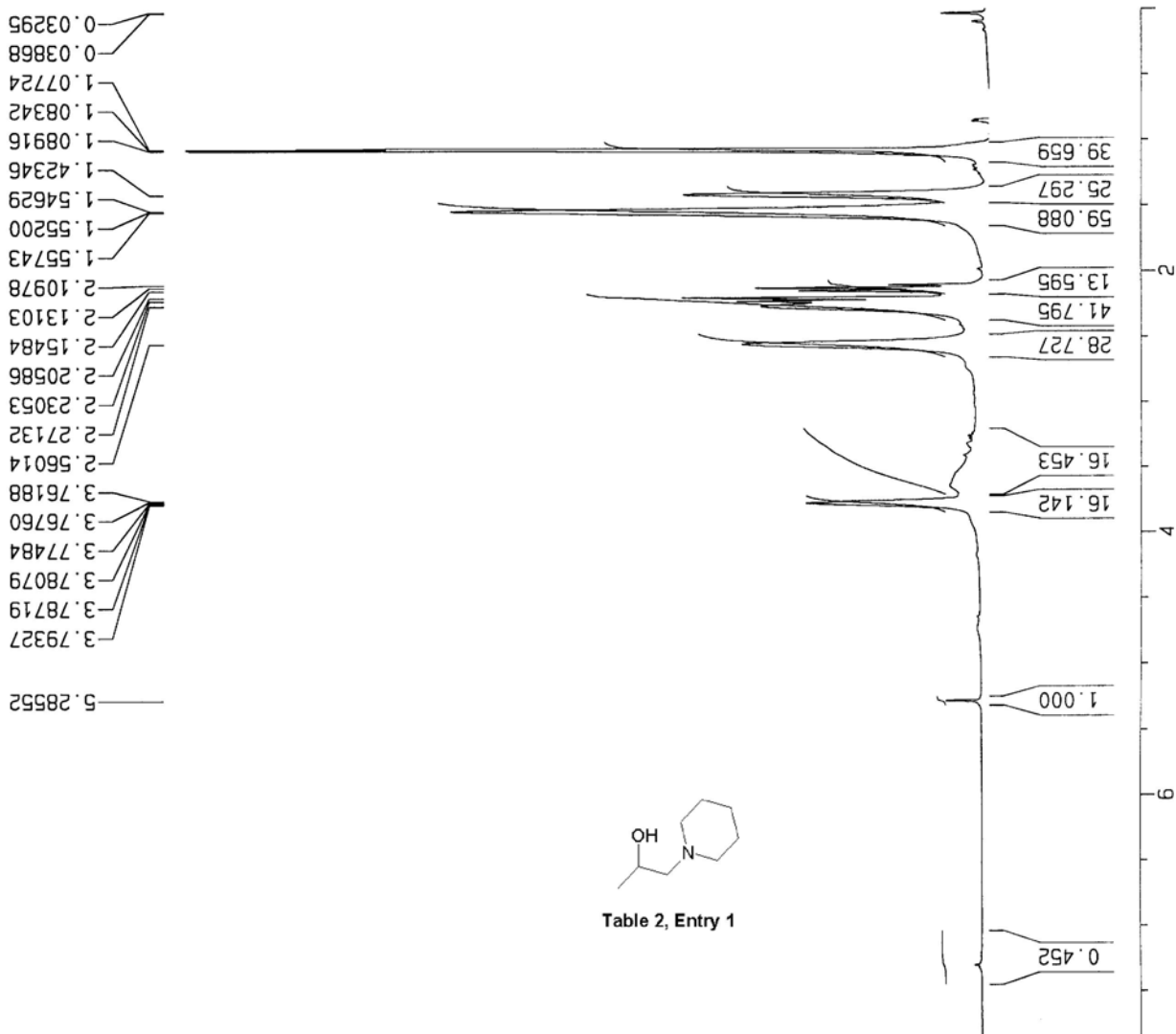
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PROCNO 1

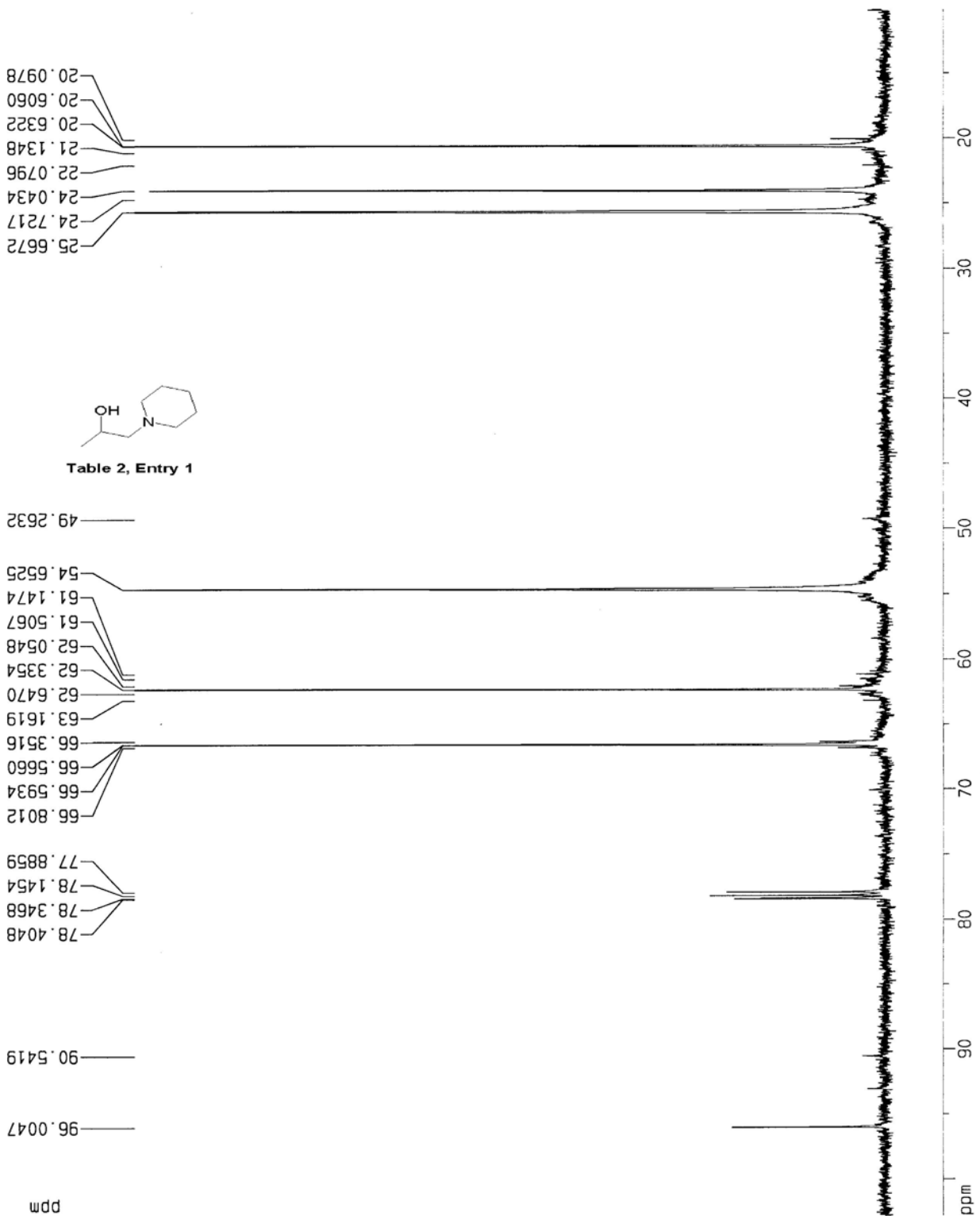
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SOLVENT CDCl3  
NS 4  
DS 0  
SMH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 35.9  
DW 48.400 usec  
DE 6.50 usec  
TE 295.0 K  
D1 10.0000000 sec

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PL1 3.00 dB  
SF01 500.1330885 MHz

F2 - Processing parameters  
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SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
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CY 11.00 cm  
F1P 10.000 ppm  
F1 5001.30 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCM 0.55556 ppm/cm  
HZCM 277.85001 Hz/cm





Current Data Parameters

NAME Az121

EXPNO 407

PROCNO 1

F2 - Acquisition Parameters

Date\_ 20040904

Time 14.37

INSTRUM spect

PROBHD 5 mm BBI 4H-

PULPROG zgpg30

TD 65536

SOLVENT CDCl3

NS 69

DS 2

SWH 40000.000 Hz

FIDRES 0.610352 Hz

AQ 0.8192625 sec

RG 32000

DW 12.500 usec

DE 6.50 usec

TE 300.0 K

D1 5.00000000 sec

d11 0.03000000 sec

d12 0.0002000 sec

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

NUC1 13C

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PL1 0.00 dB

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===== CHANNEL f2 =====

CPDPRG2 waltz16

NUC2 1H

PCPD2 80.00 usec

PL2 3.00 dB

PL12 22.00 dB

PL13 22.00 dB

SFO2 500.1320005 MHz

F2 - Processing parameters

SF 32768

SF 125.7577390 MHz

WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

1D NMR plot parameters

CX 20.00 cm

CY 21.64 cm

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F2P 10.091 ppm

F2 1268.99 Hz

PPMCM 4.63855 ppm/cm

HZCM 583.33331 Hz/cm

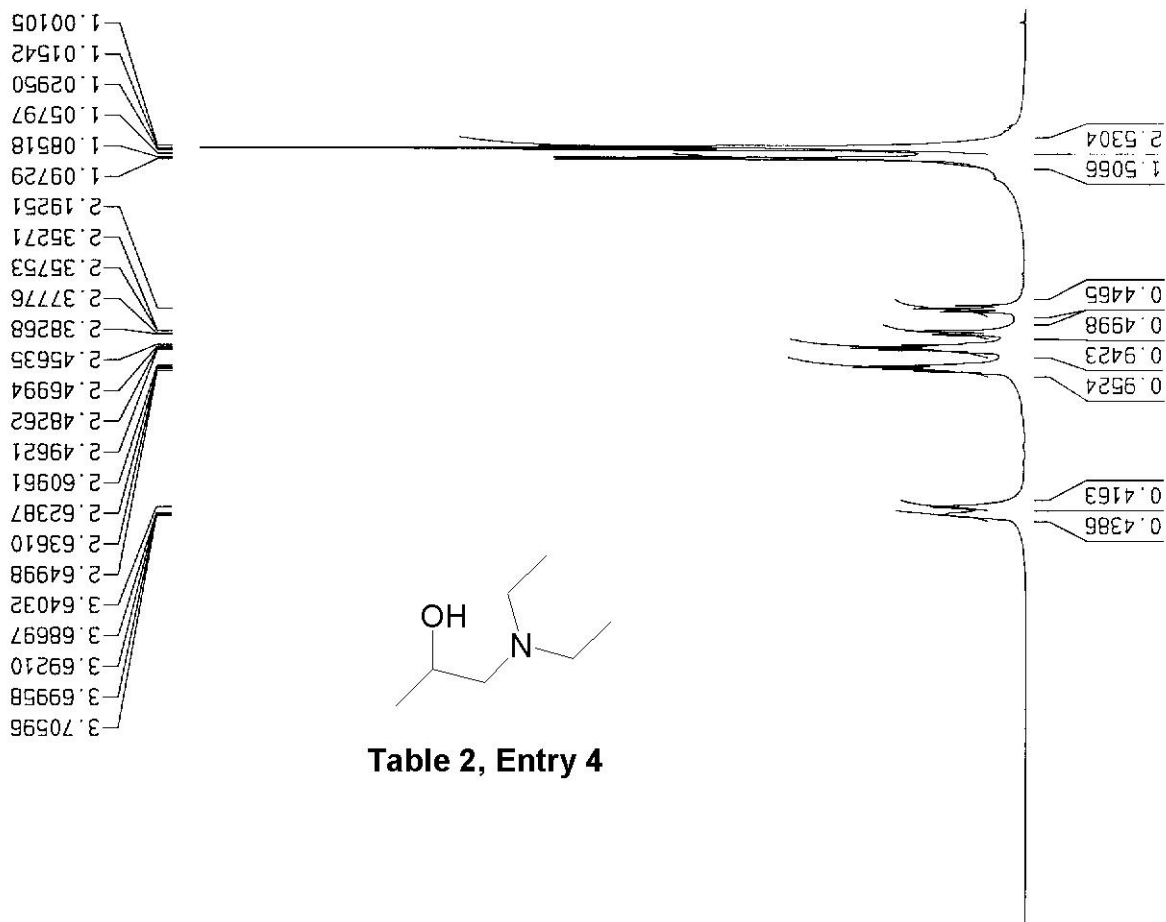
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 PULPROG zg30  
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 SOLVENT CDCl3  
 NS 4  
 DS 0  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
 RG 35.9  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 295.0 K  
 D1 10.0000000 sec

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 PL1 3.00 dB  
 SF01 500.1330895 MHz

F2 - Processing parameters  
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 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
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 CY 10.96 cm  
 F1P 10.000 ppm  
 F1 5001.30 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 0.55556 ppm/cm  
 HZCM 277.85001 Hz/cm





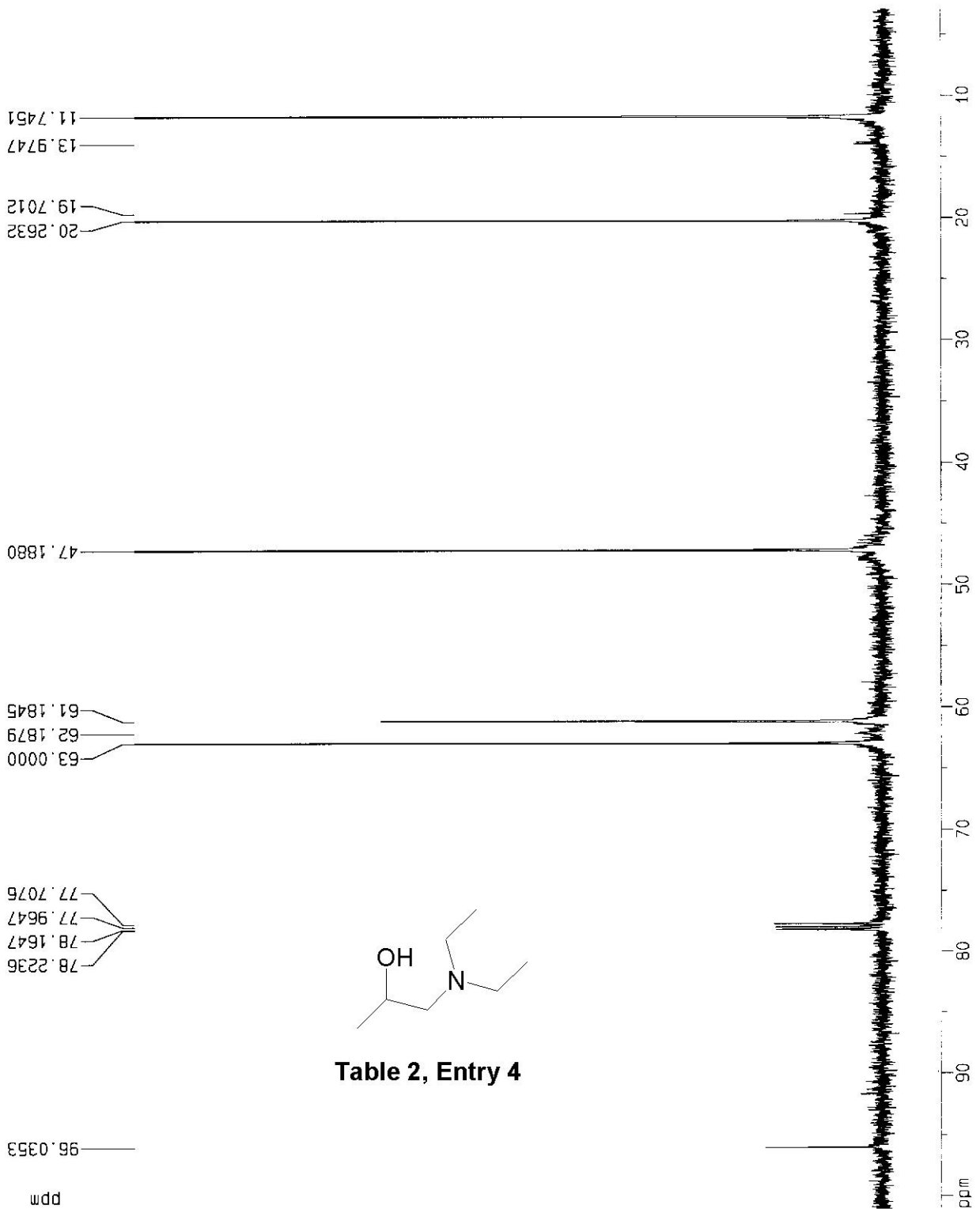


Table 2, Entry 4

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PROCNO 1

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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 20  
DS 2  
SWH 40000.000 Hz  
FIDRES 0.610352 Hz  
AQ 0.6192625 sec  
RG 32000  
DW 12.500 usec  
DE 6.50 usec  
TE 300.0 K  
d1 5.00000000 sec  
d11 0.03000000 sec  
d12 0.00002000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 10.80 usec  
PL1 0.00 dB  
SF01 125.7703143 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 3.00 dB  
PL12 22.00 dB  
PL13 22.00 dB  
SF02 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7577350 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR plot parameters  
CX 20.00 cm  
CY 26.41 cm  
F1P 101.071 ppm  
F1 12710.43 Hz  
F2P 2.927 ppm  
F2 368.09 Hz  
SFOCM 4.90719 ppm/cm  
HZCM 617.1113 Hz/cm

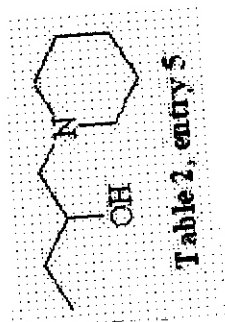
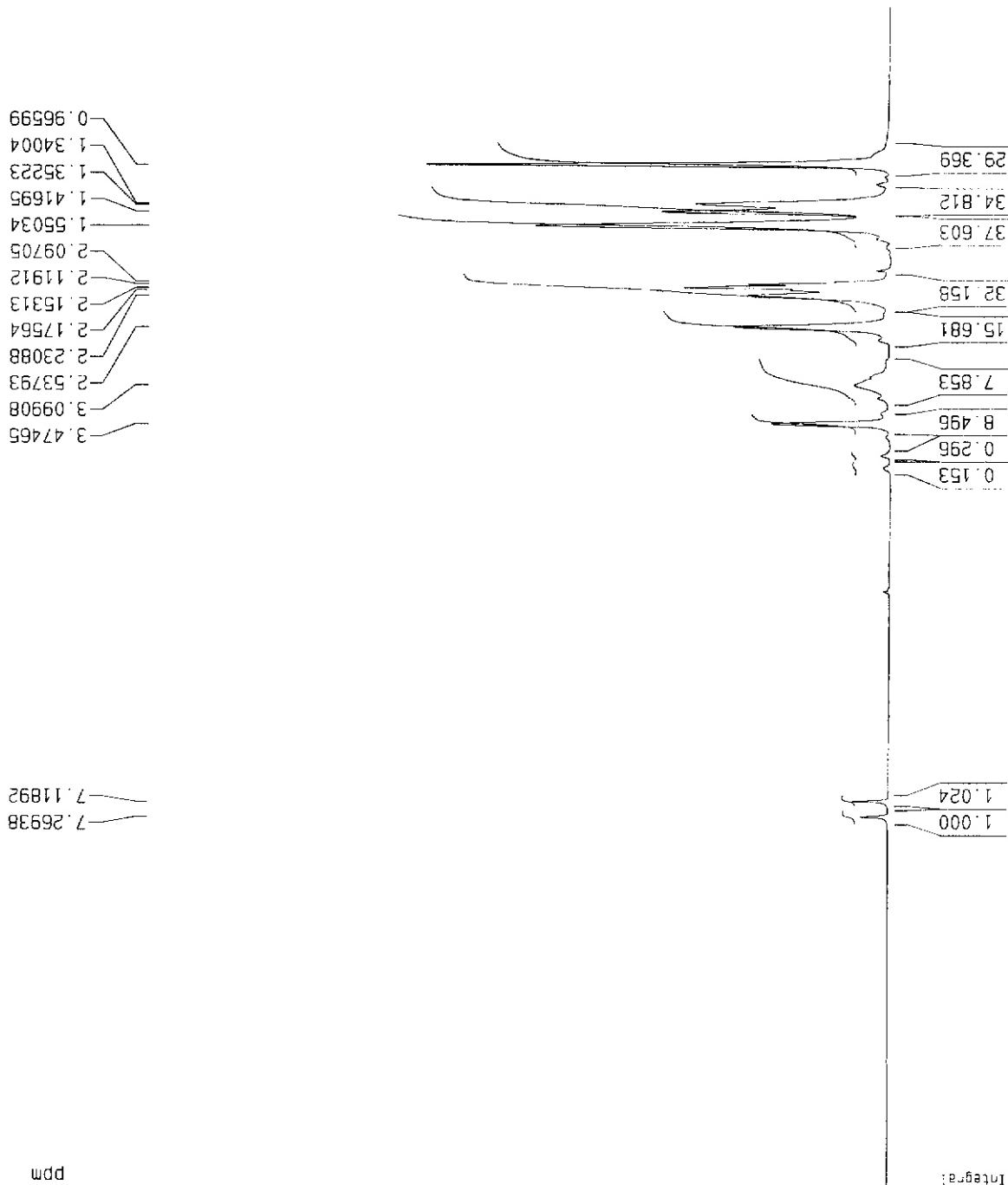


Table 2, entry 5

59 <sup>1</sup>HMR in CDCl<sub>3</sub> at 298K 83/02/28



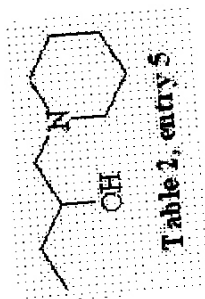
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PULPROG zg30  
TD 32768  
SOLVENT C6D6  
NS 8  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 143.7  
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DE 6.50 usec  
TE 300.0 K  
D1 5.0000000 sec

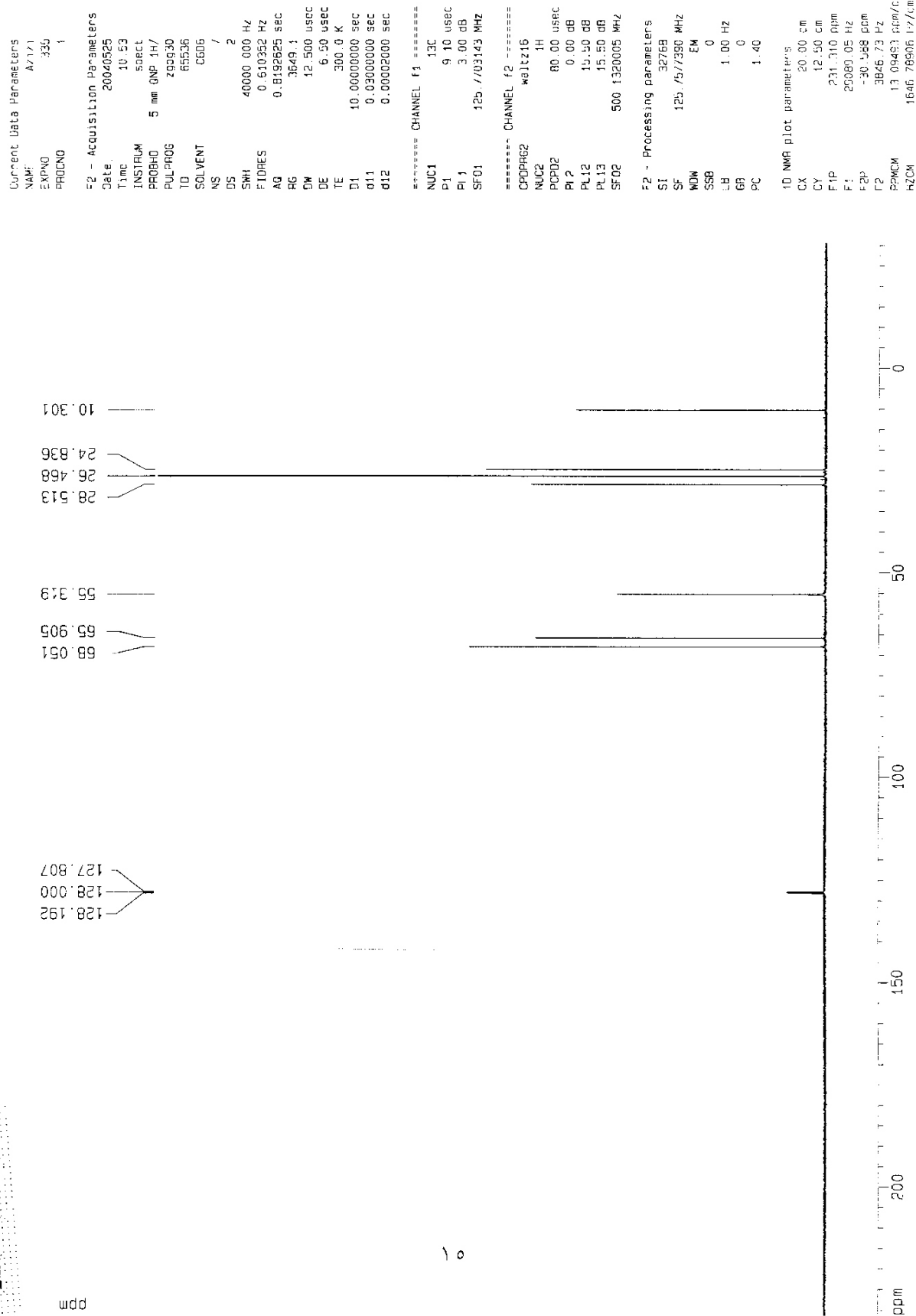
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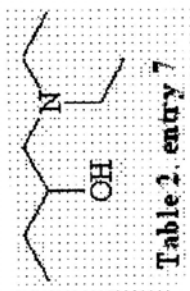
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LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 18.00 cm  
CY 7.06 cm  
F1P 10.864 ppm  
F1 5433.28 Hz  
F2P -0.551 ppm  
F2 -275.73 Hz  
PPMCM 0.63417 ppm/cm  
H7CM 317.16690 Hz/cm



59 <sup>13</sup>CNMR in C6D6 at 298K 83/03/05





29 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298K 82/09/26

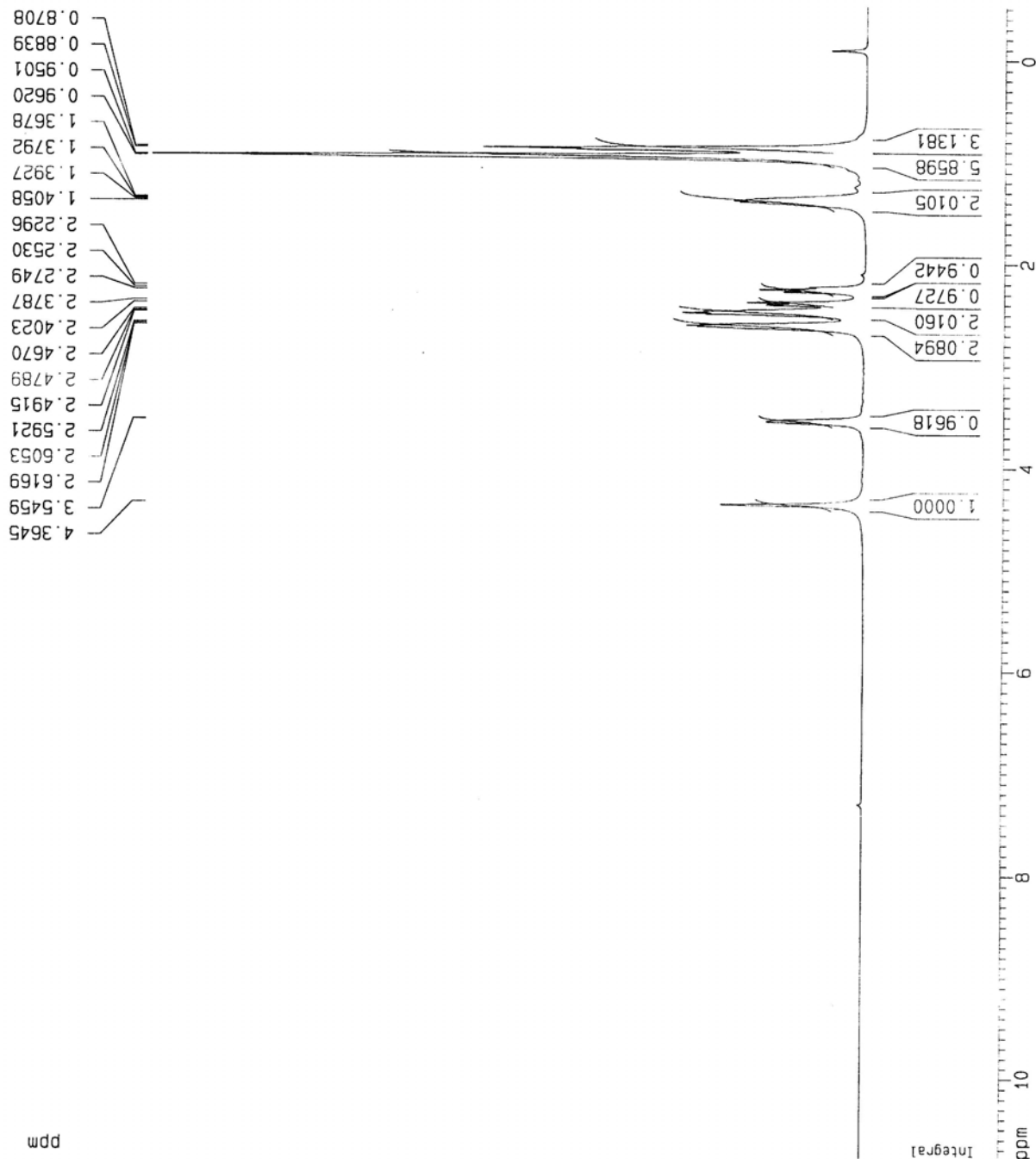
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 PROCNO 1

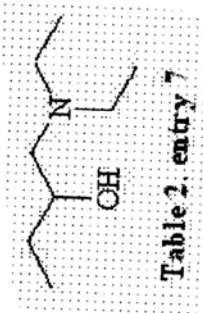
F2 - Acquisition Parameters  
 Date\_ 20031217  
 Time 15.38  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-BB  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 8  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
 RG 25.4  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 5.00000000 sec

===== CHANNEL f1 =====  
 NUC1 <sup>1</sup>H  
 P1 9.30 usec  
 PL1 3.00 dB  
 SF01 500.1330885 MHz

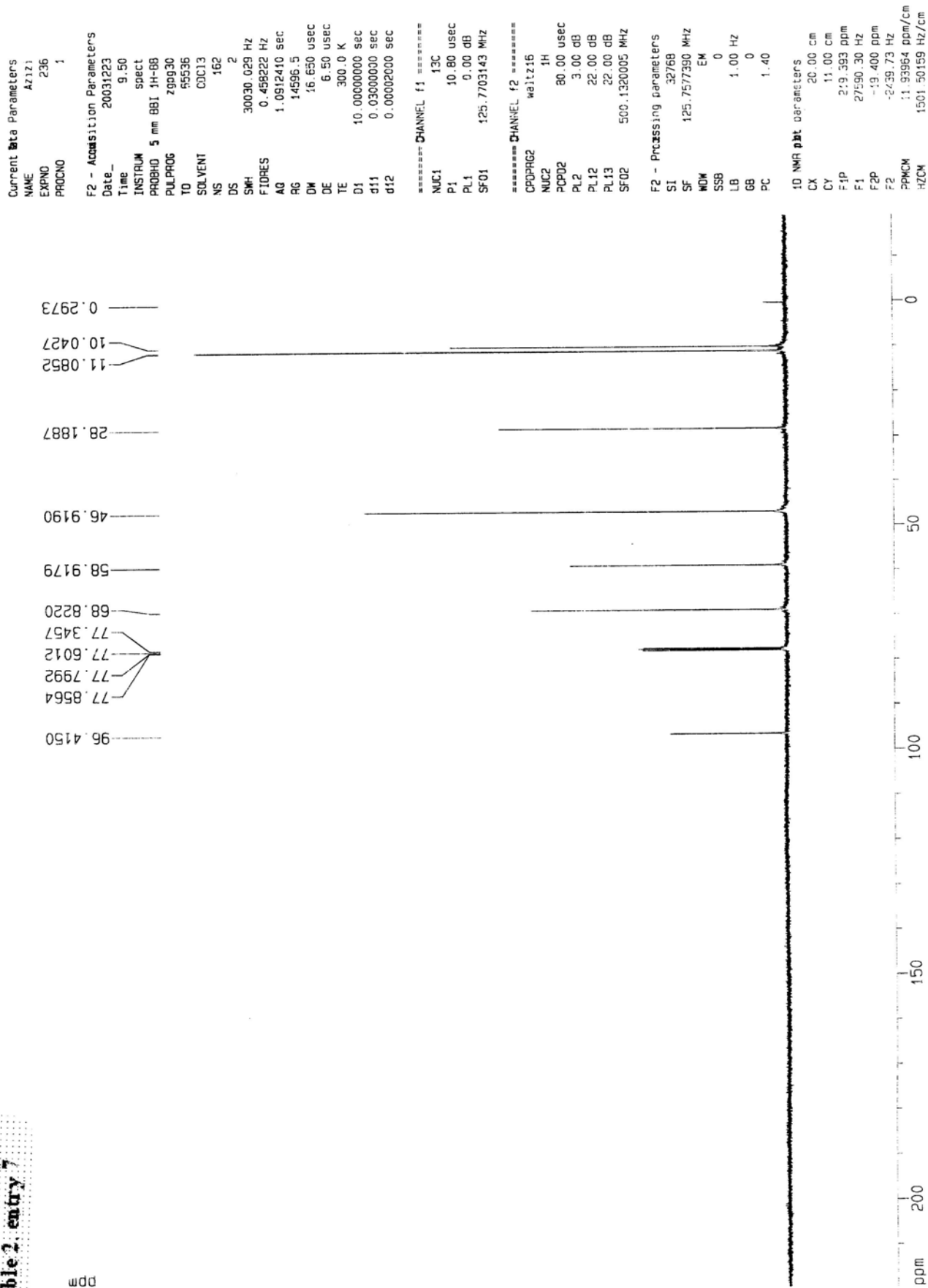
F2 - Processing parameters  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 18.00 cm  
 CY 11.24 cm  
 F1P 10.781 ppm  
 F1 5391.95 Hz  
 F2P -0.524 ppm  
 F2 -261.95 Hz  
 PPMCM 0.62805 ppm/cm  
 HZCM 314.10544 Hz/cm



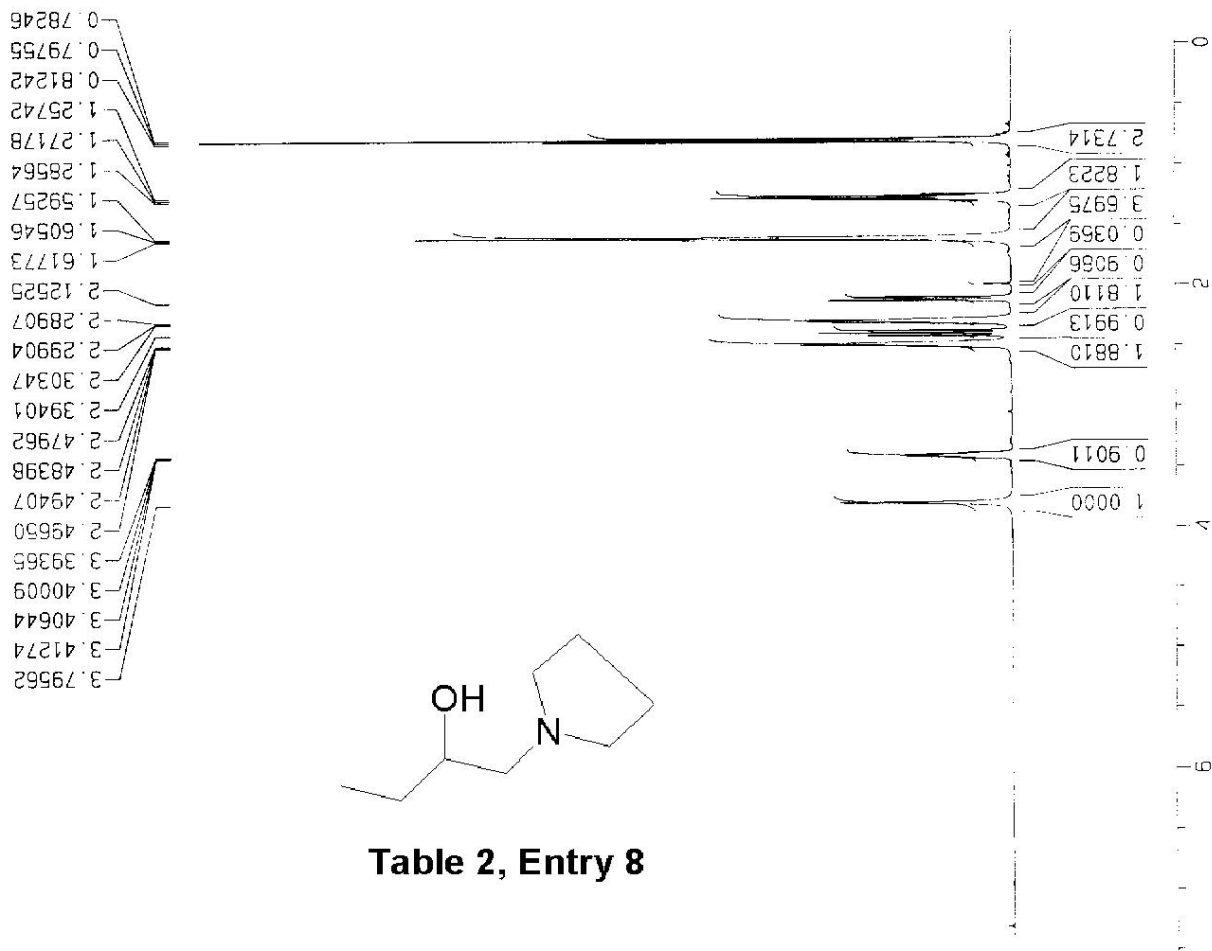


29 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298K 82/10/02



9.0

55-1 1H NMR in CDCl3 at 298K 83/03/05



Current Data Parameters  
 NAME A7171  
 EXPNO 334  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20040525  
 Time 10.40  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 8  
 DS 2  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
 RG 10.1  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 5.0000000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.50 usec  
 PL1 -3.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 18.00 cm  
 CY 11.00 cm  
 FI 10.747 ppm  
 F1 5374.98 Hz  
 F2 0.362 ppm  
 F2 -181.26 Hz  
 PPMCM 0.61720 ppm/cm  
 HZCM 308.67999 Hz/cm

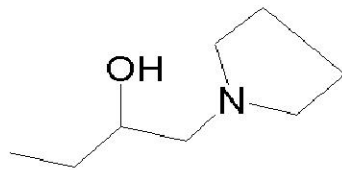
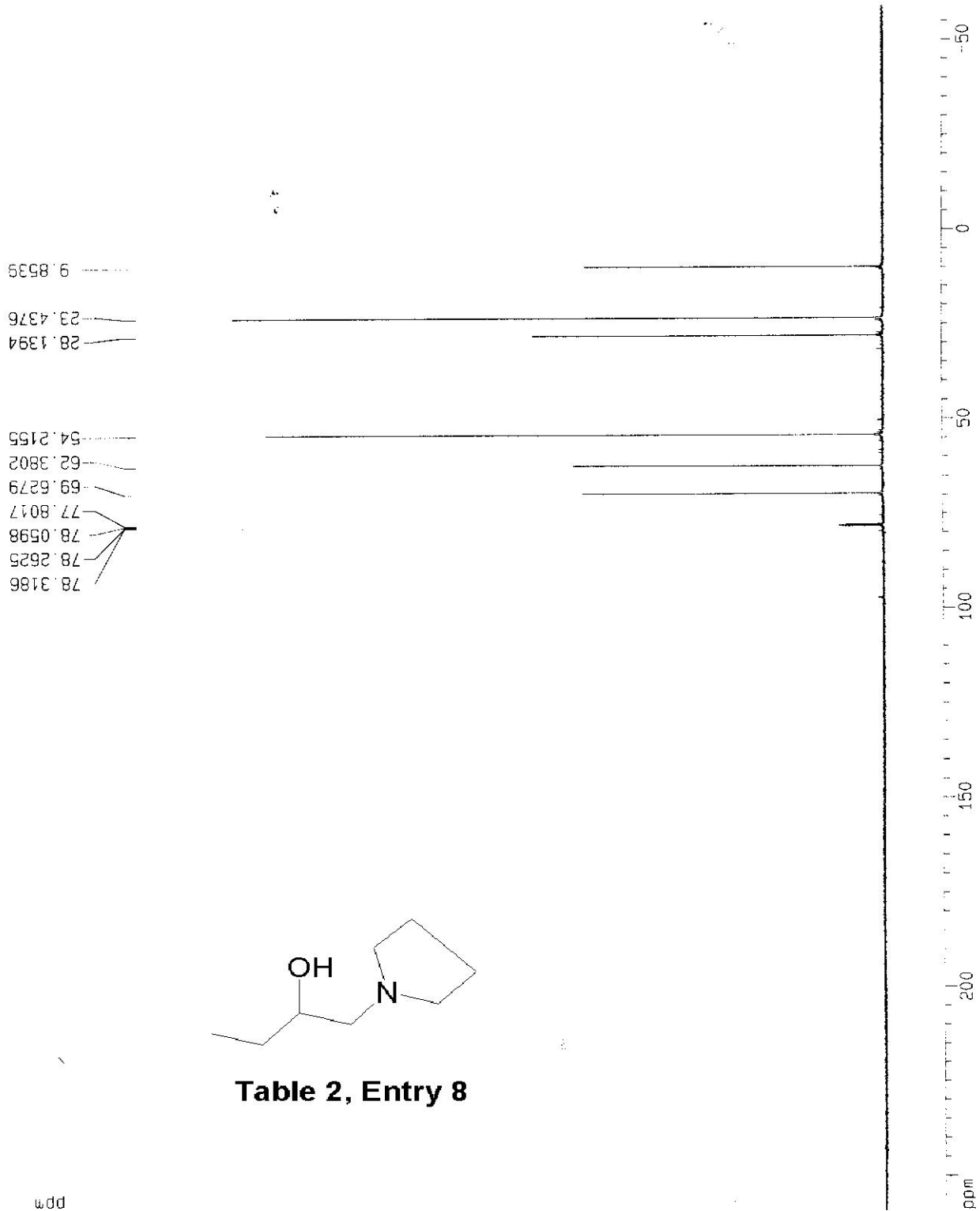


Table 2, Entry 8



Current Data Parameters  
 NAME A712  
 EXPNO 339  
 PROCNO 1

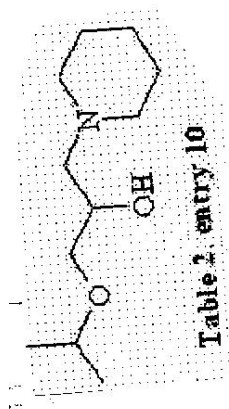
F2 - Acquisition Parameters  
 Date\_ 20070601  
 Time 9.35  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 37  
 DS 2  
 SWH 40000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.8192625 sec  
 RG 2896.3  
 DW 12.500 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 10.00000000 sec  
 d11 0.03000000 sec  
 d12 0.00002000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 10.60 usec  
 PL1 0.00 dB  
 SF01 125.763143 MHz

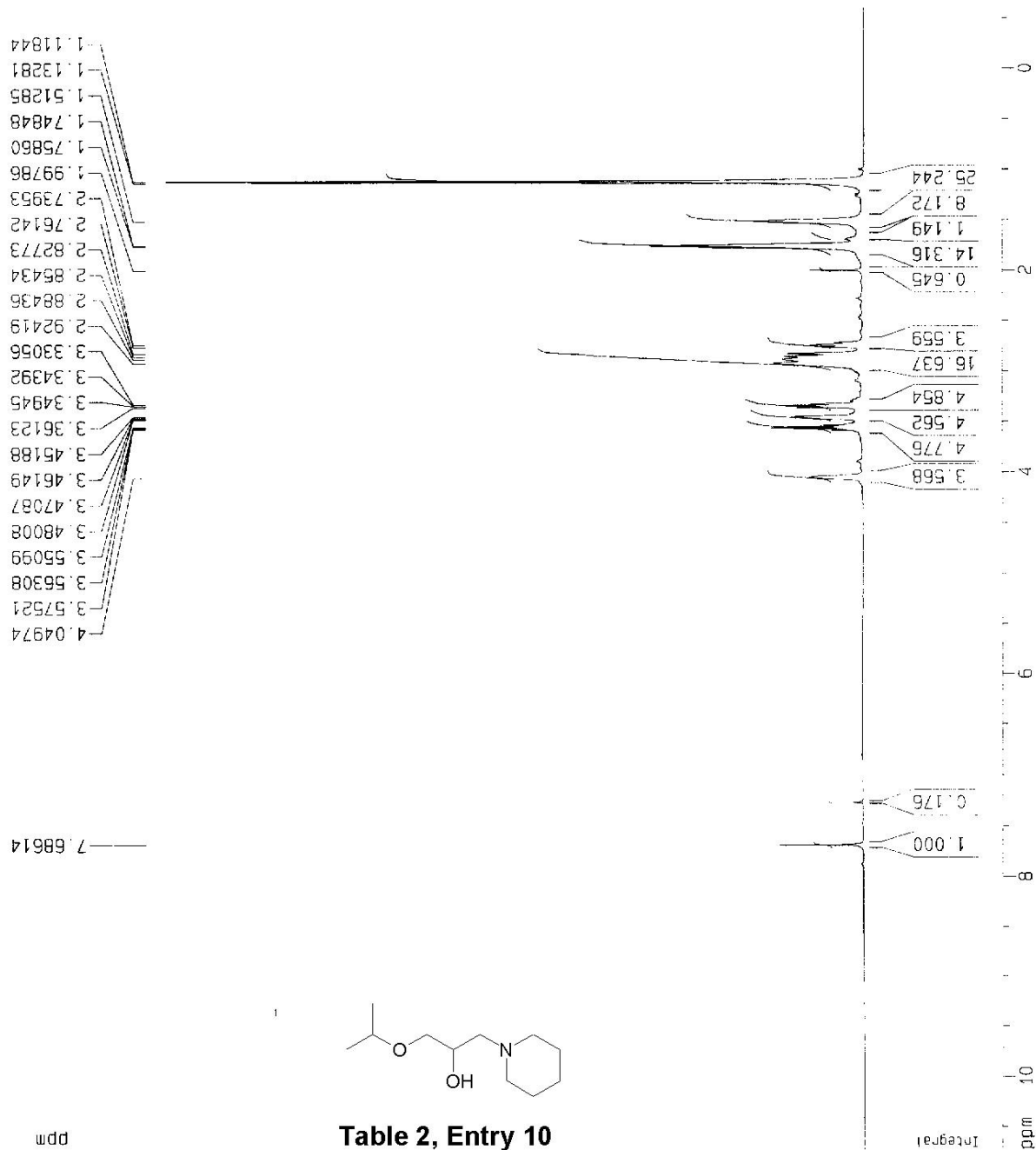
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 3.00 dB  
 PL12 22.00 dB  
 PL13 22.00 dB  
 SF02 500.1320003 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.757390 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX PC OC cm  
 CY 10.66 cm  
 FIP 259.032 ppm  
 F1 32575.29 Hz  
 F2H -55.040 ppm  
 F2 -1454.71 Hz  
 PCMC 15.30309 ppm/cm  
 -ZCM 1999.99995 Hz/cm



P-4 1H-NMR in C6D6 at 298K 83/03/17



Current Data Parameters  
NAME Poorhassan  
EXPNO 19  
PROCNO 1

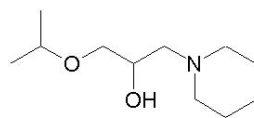
F2 - Acquisition Parameters  
Date\_ 20040606  
Time 10.08  
INSTRUM spect  
PROBHD 5 mm BBI 1H-  
PULPROG zg30  
TD 32768  
SOLVENT C6D6  
NS 8  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 18  
DW 48.400 usec  
DE 5.50 usec  
TE 300.0 K  
D1 5.00000000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.30 usec  
PL1 3.00 dB  
SF01 500.1300885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 18.00 cm  
CY 11.00 cm  
F1P 10.725 ppm  
F1 5363.69 Hz  
F2P -0.611 ppm  
F2 -305.63 Hz  
PPMCM 0.62978 ppm/cm  
HZCM 314.97333 Hz/cm

Table 2, Entry 10





91 13CNMR in C6D6 at 298K 83/03/20

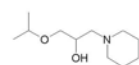
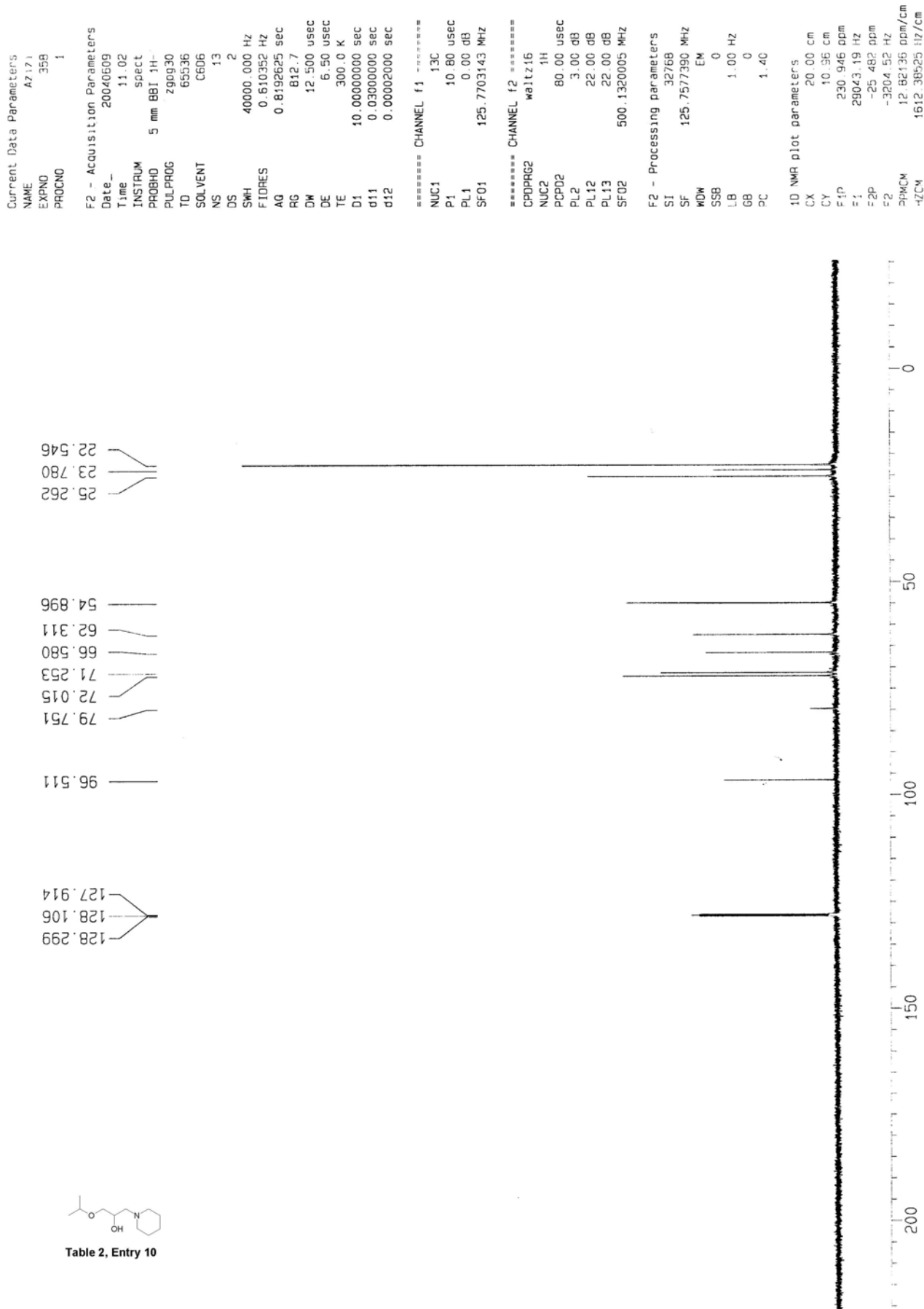


Table 2, Entry 10



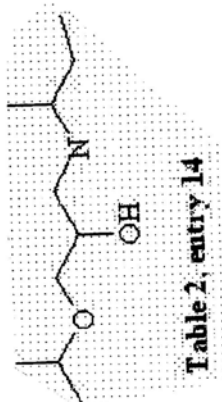
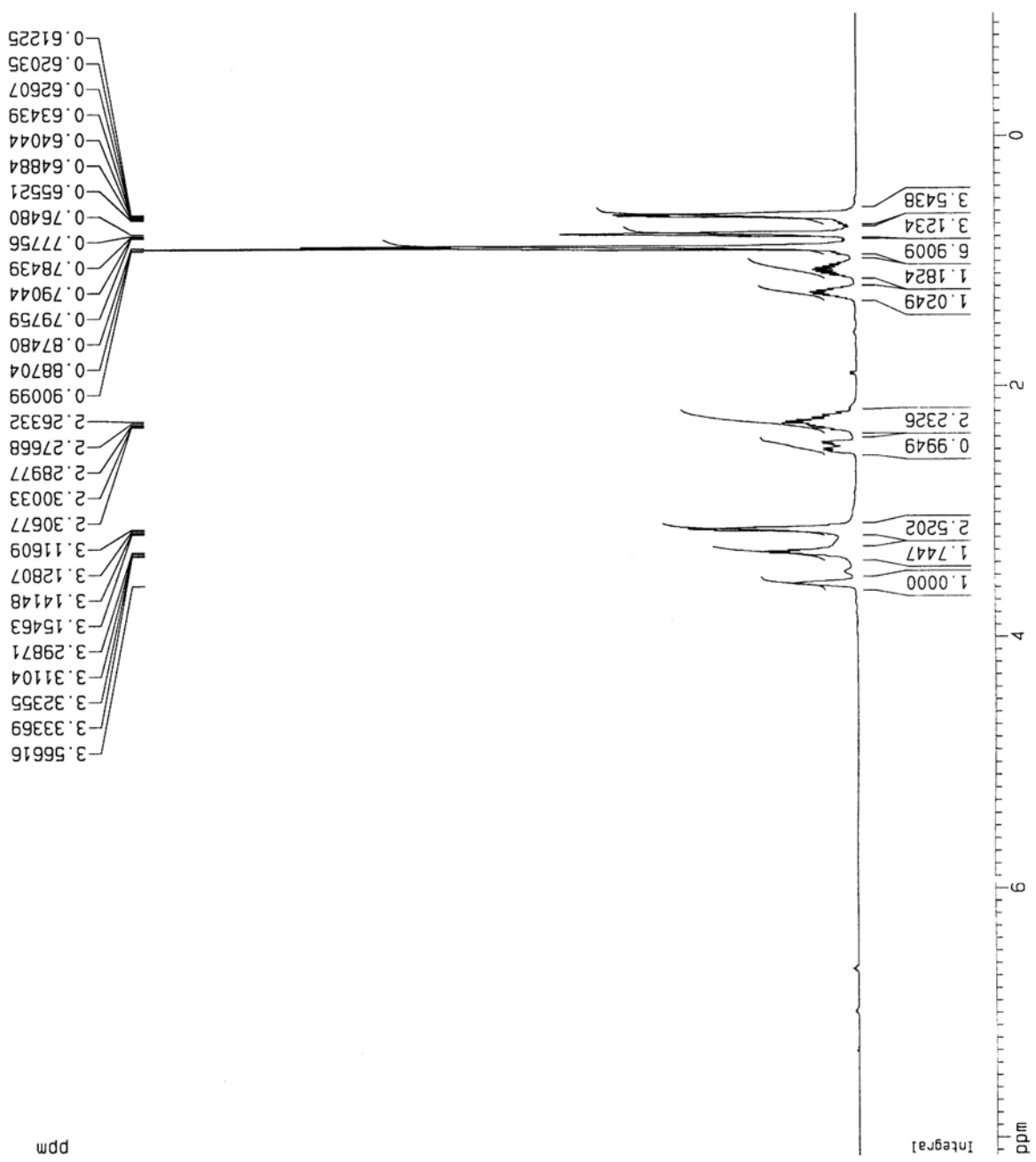


Table 2, entry 14

sample 15 1H NMR in CDCl3 83/10/6



Current Data Parameters  
NAME Azizi  
EXPNO 26  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20041226  
Time 14.57  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 4  
DS 1  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 28.5  
DM 48.400 usec  
DE 6.50 usec  
TE 0.0 K  
D1 5.0000000 sec  
MCREST 0.0000000 sec  
MCMRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.30 usec  
PL1 3.00 dB  
SF01 500.130885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 18.00 cm  
CY 11.43 cm  
F1P 8.140 ppm  
F1 4071.28 Hz  
F2P -0.976 ppm  
F2 -488.34 Hz  
PPMCM 0.50649 ppm/cm  
HZCM 253.31247 Hz/cm

#1 1H NMR in CDCl3 at 298K 83/07/22

Current Data Parameters  
 NAME AZIZI  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20041212  
 Time 12.41  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-BB  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
 RG 11.3  
 DW 48.400 usec  
 DE 6.50 usec  
 TE 0.0 K  
 D1 5.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 9.30 usec  
 PL1 3.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 18.00 cm  
 CY 11.32 cm  
 F1P 8.369 ppm  
 F1 4185.56 Hz  
 F2P 0.623 ppm  
 F2 311.59 Hz  
 PPMCM 0.43033 ppm/cm  
 HZCM 215.22038 Hz/cm

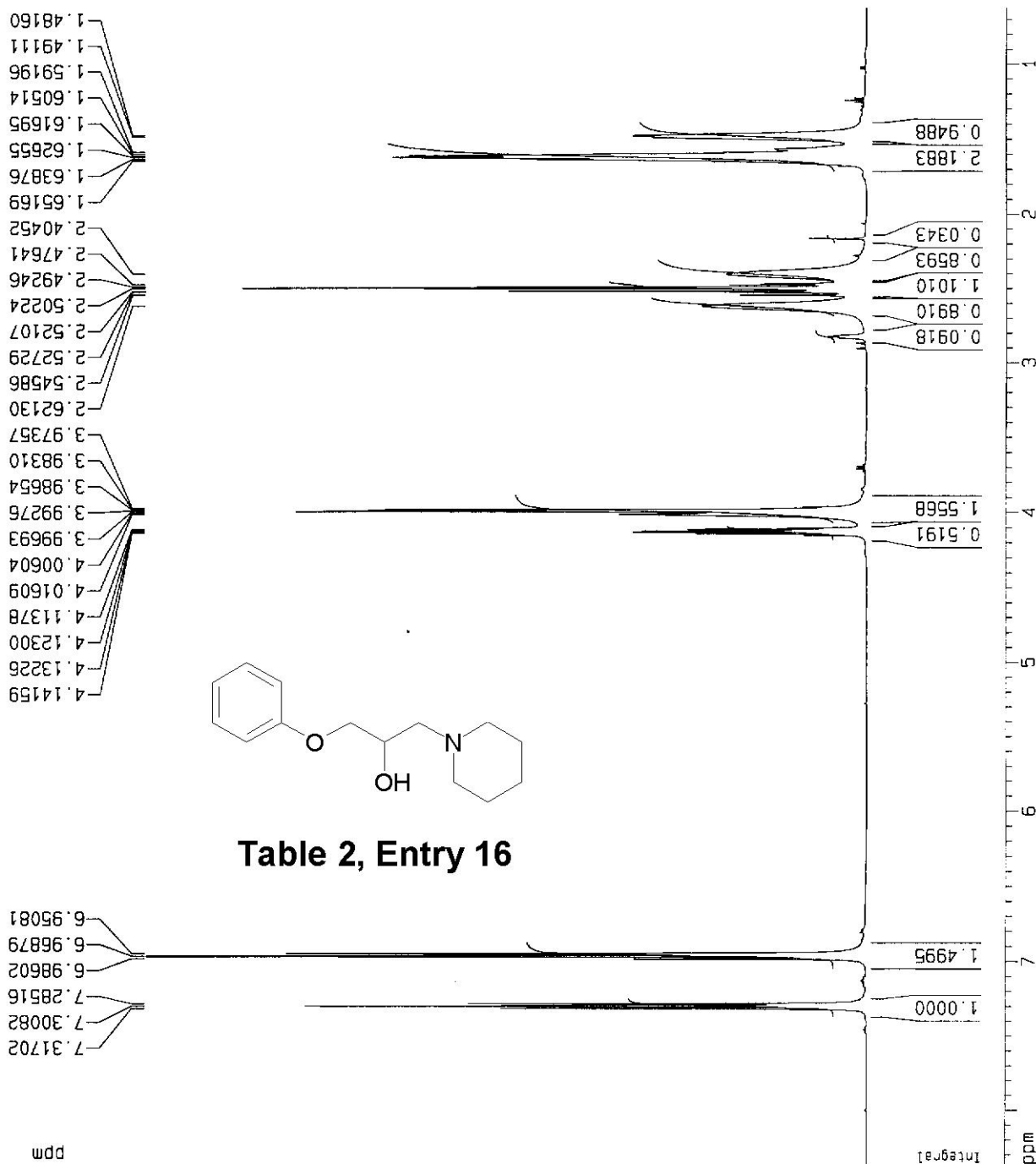


Table 2, Entry 16

Current Data Parameters  
 NAME Az11  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20041212  
 Time 12.42  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-BB  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 7  
 DS 2  
 SWH 40000.000 Hz  
 FIDRES 0.610352 Hz  
 AQ 0.6192525 sec  
 RG 32000  
 DE 12.500 usec  
 TE 0.0 K  
 D1 5.00000000 sec  
 d11 0.03000000 sec  
 DELTA 4.90000010 sec  
 MCREST 0.00000000 sec  
 MCWPK 0.01500000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 10.80 usec  
 PL1 0.00 dB  
 SF01 125.7703143 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 3.00 dB  
 PL12 22.00 dB  
 PL13 22.00 dB  
 SF02 500.1320005 MHz

F2 - Processing parameters  
 SI 32768  
 SF 125.7571397 MHz  
 NDM FM  
 SS0 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

1D NMR plot parameters  
 CX 20.00 cm  
 CY 20.78 cm  
 F1P 196.392 ppm  
 F1 23440.08 Hz  
 F2P 10.466 ppm  
 F2 1316.18 Hz  
 PPMCM 8.75628 ppm/cm  
 HZCM 1106.19470 Hz/cm

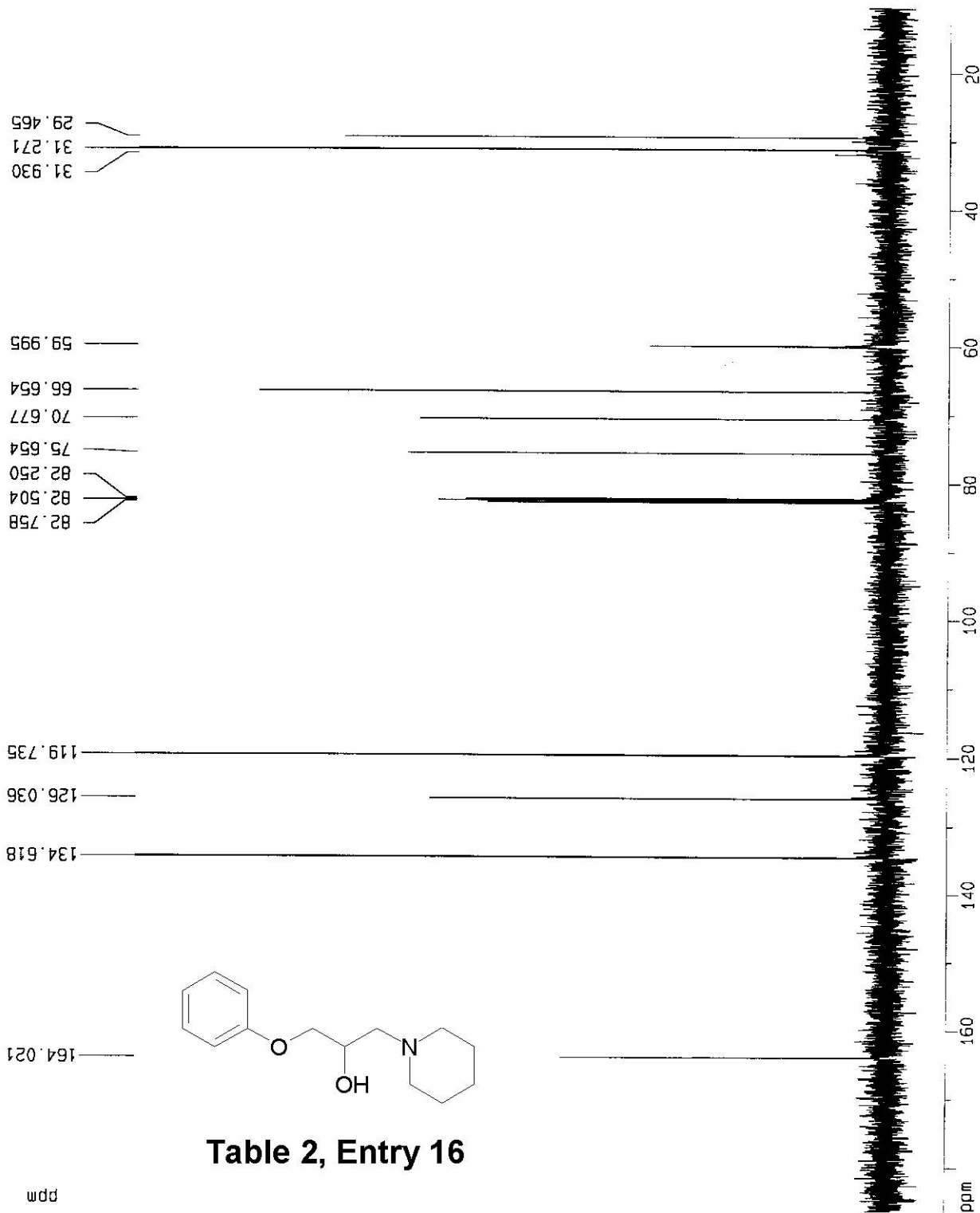
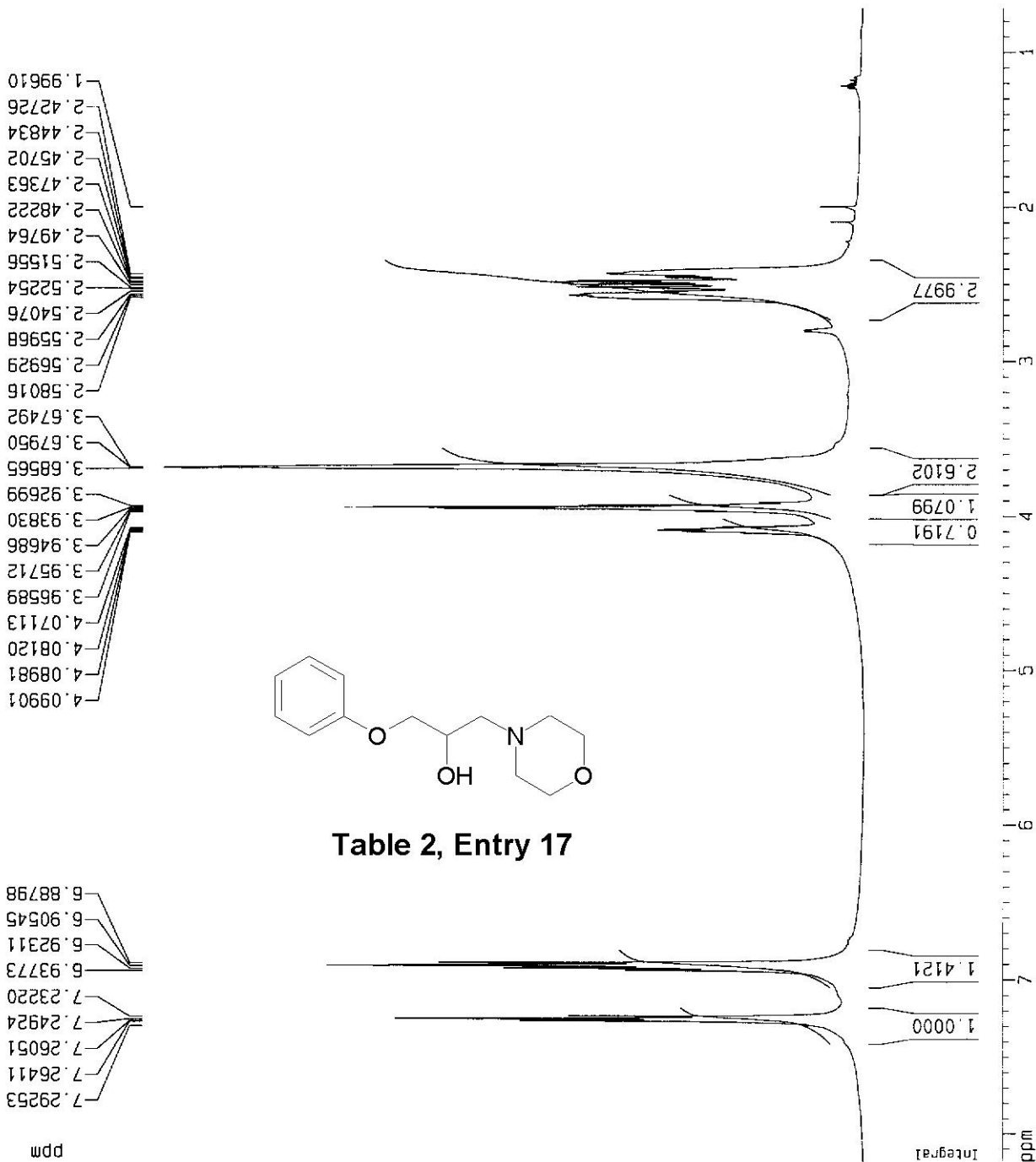


Table 2, Entry 16



Current Data Parameters

NAME Azizi  
EXPNO 16  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20041219  
Time 13.05  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 4  
DS 1  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 8  
DM 48.400 usec  
DE 6.50 usec  
TE 0.0 K  
D1 5.00000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

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

NUC1 <sup>1</sup>H  
P1 9.30 usec  
PL1 3.00 dB  
SF01 500.1330885 MHz

F2 - Processing parameters

SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters

CX 16.00 cm  
CY 11.00 cm  
F1p 8.186 ppm  
F1 4094.14 Hz  
F2p 0.714 ppm  
F2 357.30 Hz  
PQCM 0.41510 ppm/cm  
HZCM 207.60197 Hz/cm

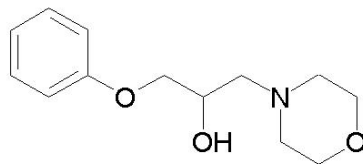
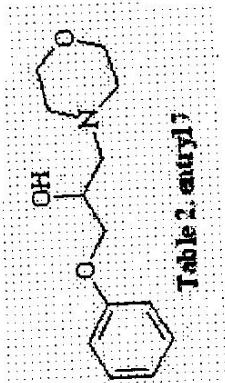
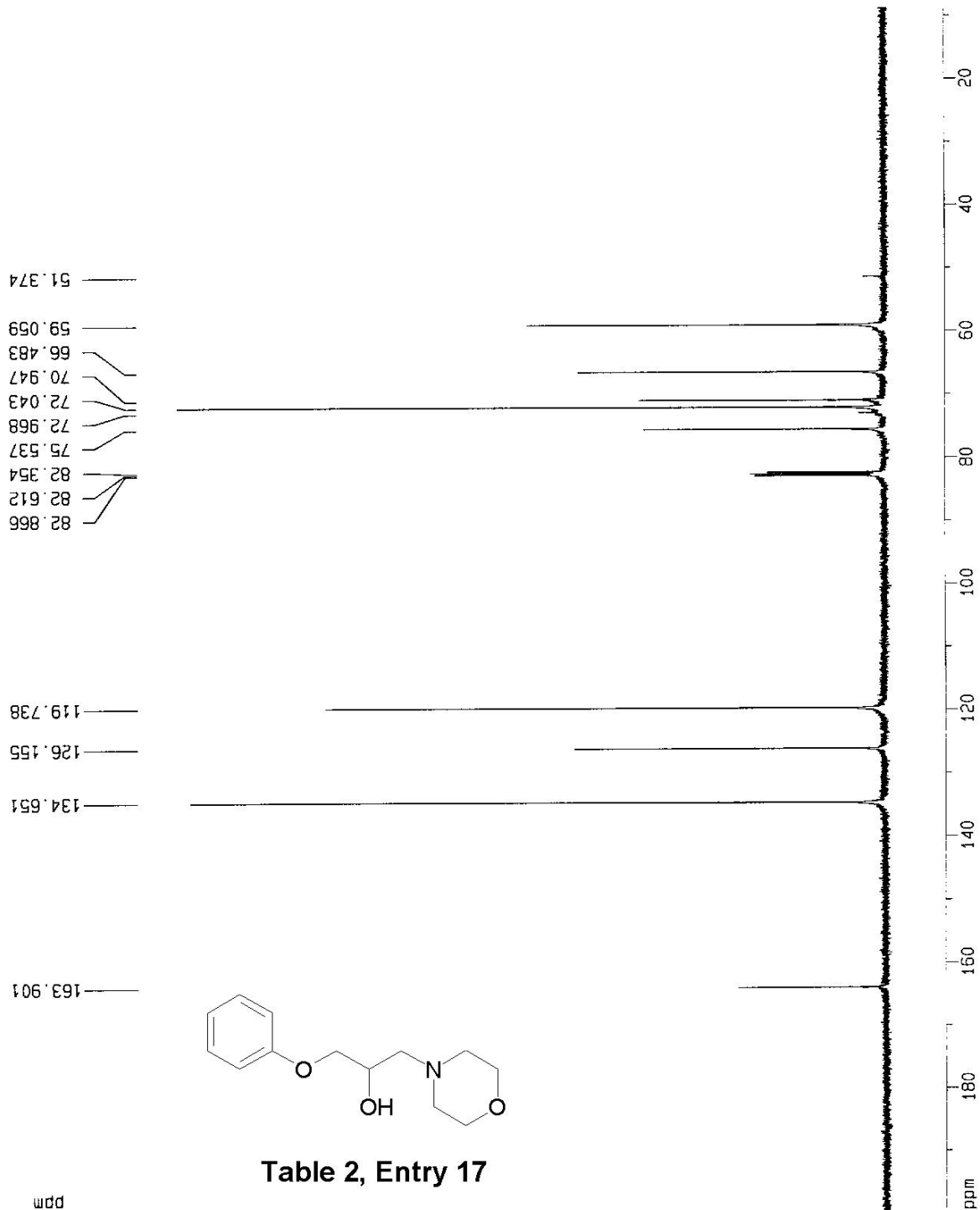


Table 2, Entry 17

4 <sup>13</sup>C NMR in CDCl<sub>3</sub> at 298K 03/07/29



Current Data Parameters  
NAME Az171  
EXPNO 17  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20041219  
Time 13.16  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 100  
DS 2  
SWH 40000.000 Hz  
FIDRES 0.610352 Hz  
AQ 0.8192626 sec  
RG 5792.16  
DM 12.500 usec  
DE 6.50 usec  
TE 0.0 K  
D1 5.0000000 sec  
d11 0.0300000 sec  
DELTA 4.90000010 sec  
MCPRST 0.0000000 sec  
MCWPK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 <sup>13</sup>C  
P1 10.80 usec  
PL1 0.00 dB  
SF01 125.7703143 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 <sup>1</sup>H  
PCPD2 90.00 usec  
PL2 3.00 dB  
PL12 22.00 dB  
PL13 22.00 dB  
SF02 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7571397 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR plot parameters  
CX 20.00 cm  
CY 12.15 cm  
F1P 199.410 ppm  
F1 25077.25 Hz  
F2P 8.707 ppm  
F2 1094.95 Hz  
PPMCH 9.53516 ppm/cm  
HZCM 1199.11499 Hz/cm

Current Data Parameters  
NAME Az121  
EXPNO 18  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20041219  
Time 13.25  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 4  
DS 1  
SWH 10330.576 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 8  
DM 48.400 usec  
DE 6.50 usec  
TE 0.0 K  
D1 5.00000000 sec  
MCREST 0.00000000 sec  
MCWPK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.30 usec  
PL1 3.00 dB  
SF01 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00  
1D NMR plot parameters  
CX 18.00 cm  
CY 11.82 cm  
F1P 8.255 ppm  
F1 4126.42 Hz  
F2P 0.006 ppm  
F2 3.05 Hz  
PPMCM 0.45626 ppm/cm  
HZCM 229.18748 Hz/cm

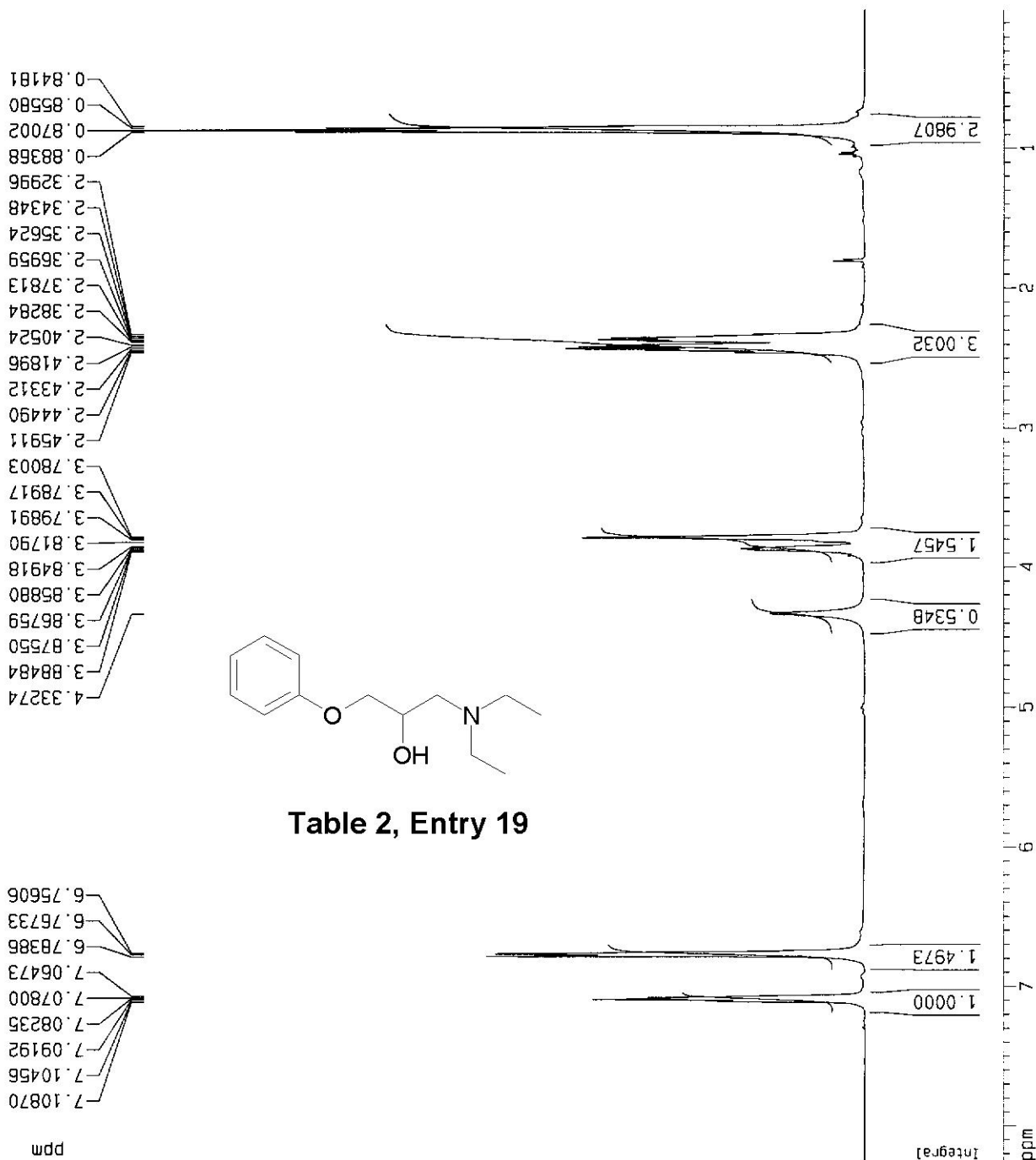


Table 2, Entry 19

## Current Data Parameters

NAME Az121  
EXPNO 19  
PROCNO 1

## F2 - Acquisition Parameters

Date\_ 20041219  
Time 13.28  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 18  
DS 2  
SWH 40000.000 Hz  
FIDRES 0.610352 Hz  
AQ 0.5192625 sec  
RG 5792.5  
DM 12.500 usec  
DE 6.50 usec  
TE 0.0 K  
D1 5.0000000 sec  
d11 0.0300000 sec  
DELTA 4.9000010 sec  
MCREST 0.0000000 sec  
MCMRK 0.0150000 sec

## ===== CHANNEL f1 =====

NUC1 13C  
P1 10.80 usec  
PL1 0.00 dB  
SF01 125.7703143 MHz

## ===== CHANNEL f2 =====

CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 3.00 dB  
PL12 22.00 dB  
PL13 22.00 dB  
SF02 500.1320005 MHz

## F2 - Processing parameters

SI 32768  
SF 125.7571397 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40  
1D NMR plot parameters  
CX 20.00 cm  
CY 12.15 cm  
F1P 200.466 ppm  
F1 25209.99 Hz  
F2P 2.022 ppm  
F2 254.24 Hz  
PPMCM 9.92220 ppm/cm  
HZCM 1247.78750 Hz/cm

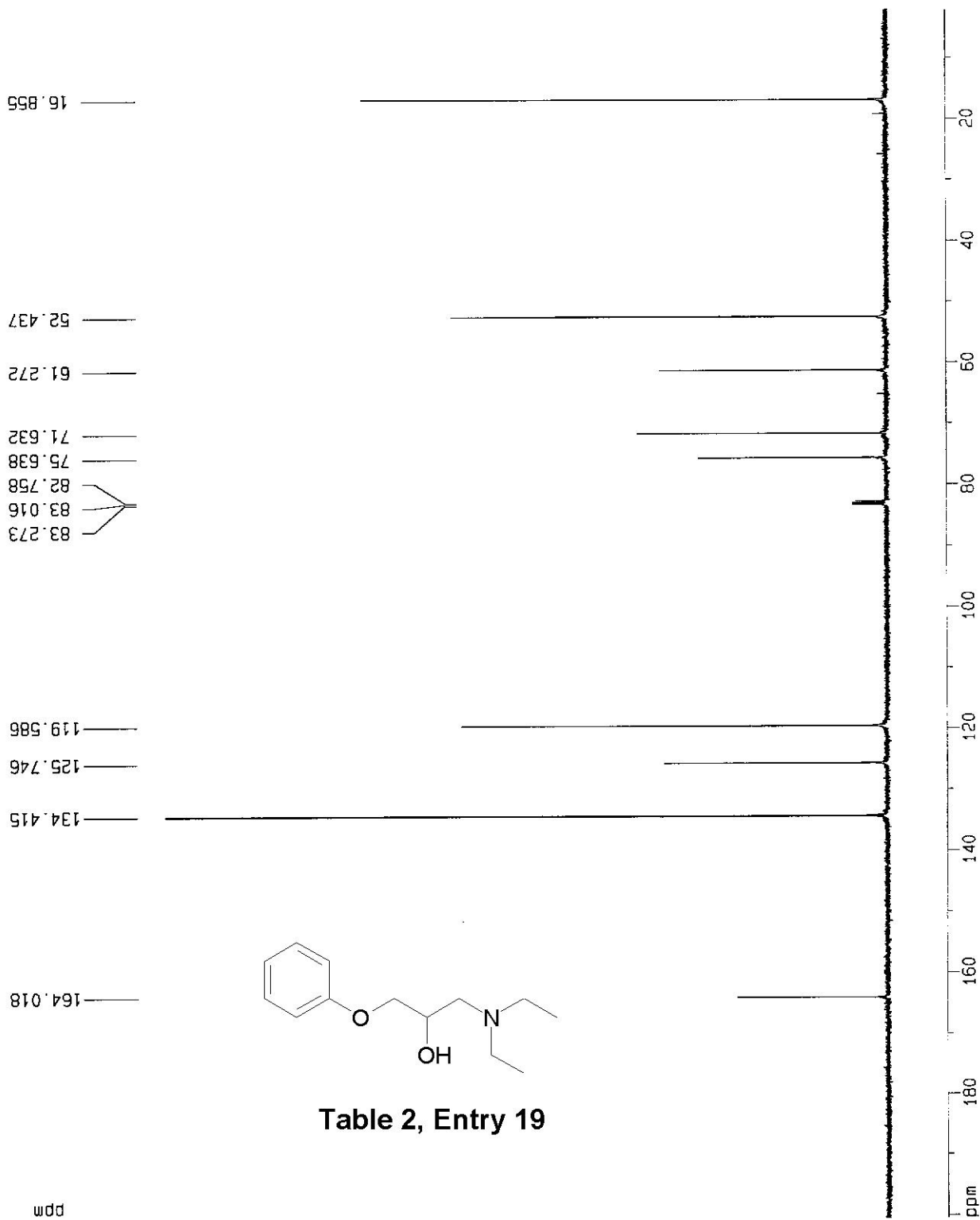


Table 2, Entry 19



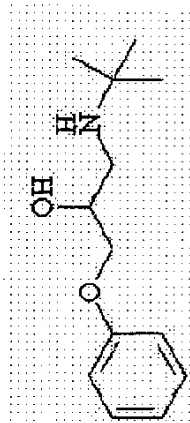
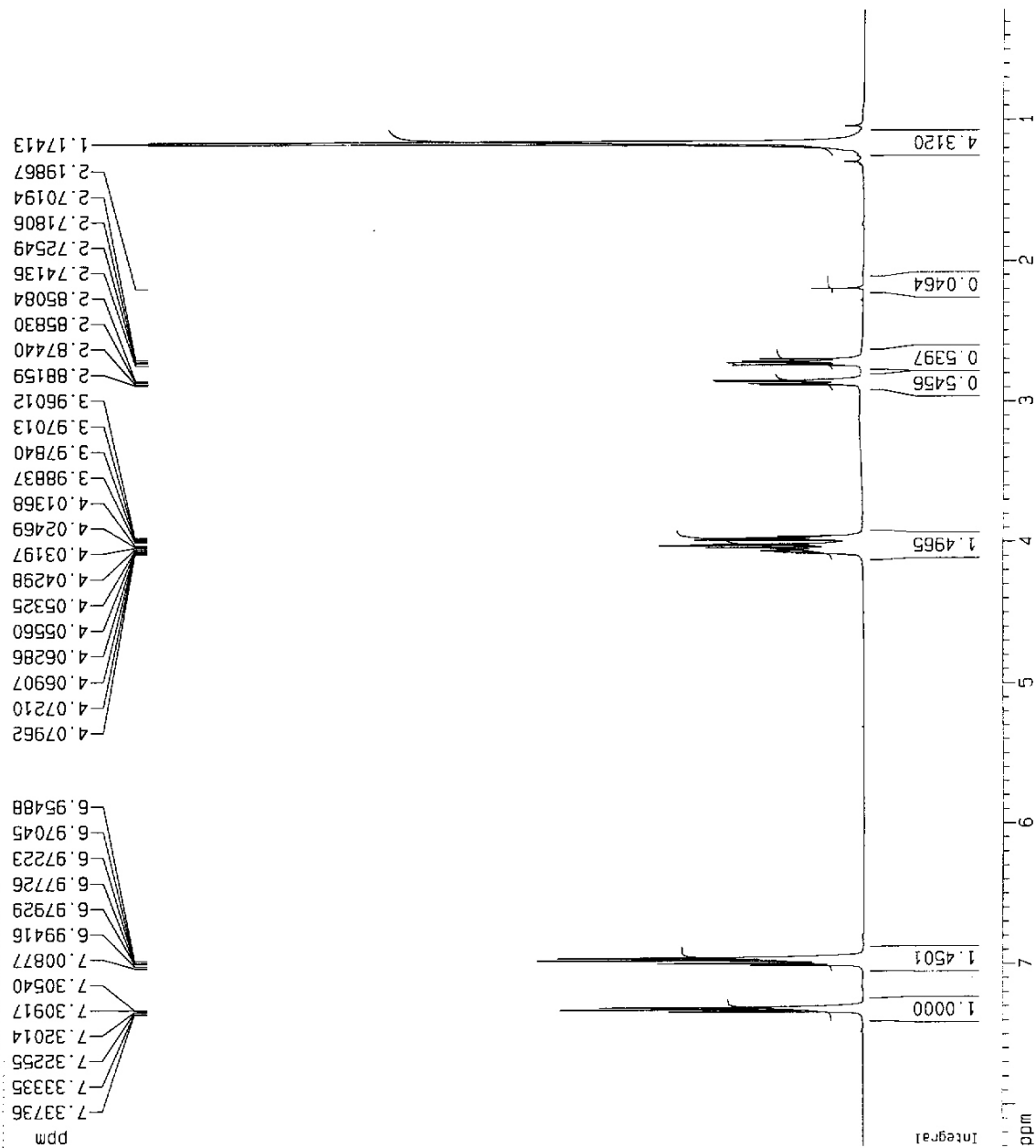


Table 2, entry 20

<sup>1</sup>H NMR in CDCl<sub>3</sub> at 298K 83/07/29



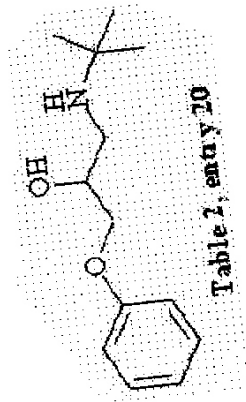
Current Data Parameters  
NAME Az121  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20041219  
Time 12.34  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zg30  
TD 32768  
SOLVENT DMSO  
NS 4  
DS 1  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 11.3  
DM 48.400 usec  
DE 5.50 usec  
TE 0.0 K  
D1 5.00000000 sec  
MCHST 0.00000000 sec  
MCWRK 0.01500000 sec

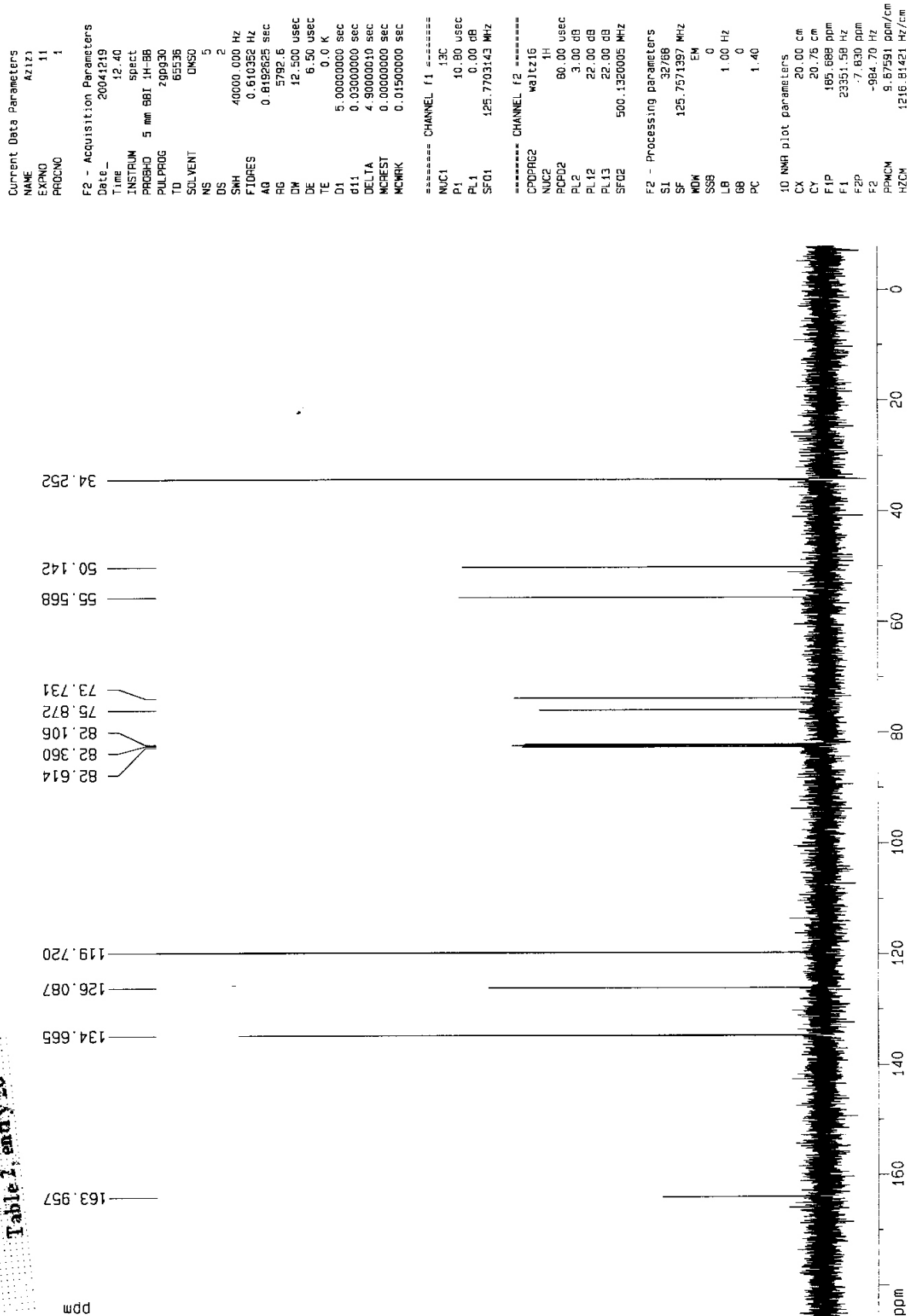
===== CHANNEL f1 =====  
NUC1 1H  
P1 9.30 usec  
PL1 3.00 dB  
SF01 500.1330865 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 18.00 cm  
CY 33.34 cm  
F1P 8.300 ppm  
F1 4151.28 Hz  
F2 0.212 ppm  
F2 105.89 Hz  
PPMCM 0.44537 ppm/cm  
HZCM 224.74339 Hz/cm



1 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298K 83/07/29



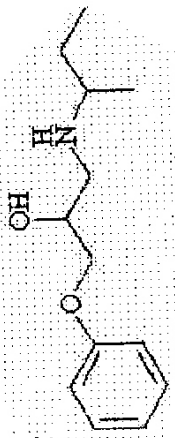
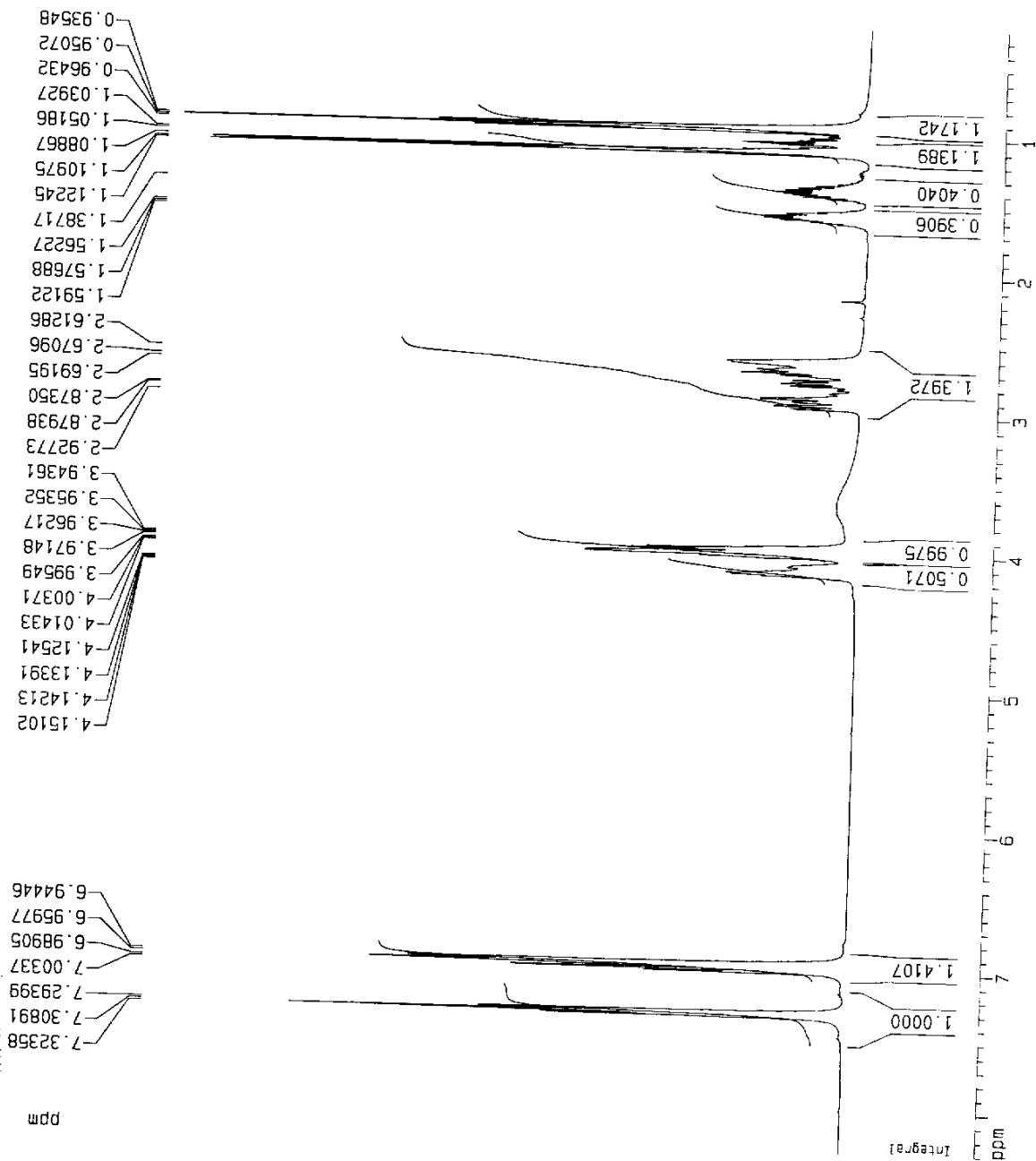


Table 2, entry 21

#2 1H NMR in CDCl<sub>3</sub> at 298K 83/07/22



Current Data Parameters  
NAME Az121  
EXPNO 8  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20041212  
Time 12.50  
INSTRUM spect  
PROBHD 5 mm BBI 4H-BB  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 4  
DS 1  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 11.3  
DM 48.400 usec  
DE 6.50 usec  
TE 0.0 K  
D1 5.0000000 sec  
MCREST 0.0000000 sec  
MCWRK 0.0150000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 9.30 usec  
PL1 3.00 dB  
SF01 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 18.00 cm  
CY 11.09 cm  
F1P 8.300 ppm  
F1 4151.28 Hz  
F2P 0.212 ppm  
F2 105.89 Hz  
PPMCM 0.44937 ppm/cm  
HZCM 224.74339 Hz/cm

Current Data Parameters  
 NAME Azizi  
 EXPNO 12  
 PROCNO 1

F2 - Acquisition Parameters

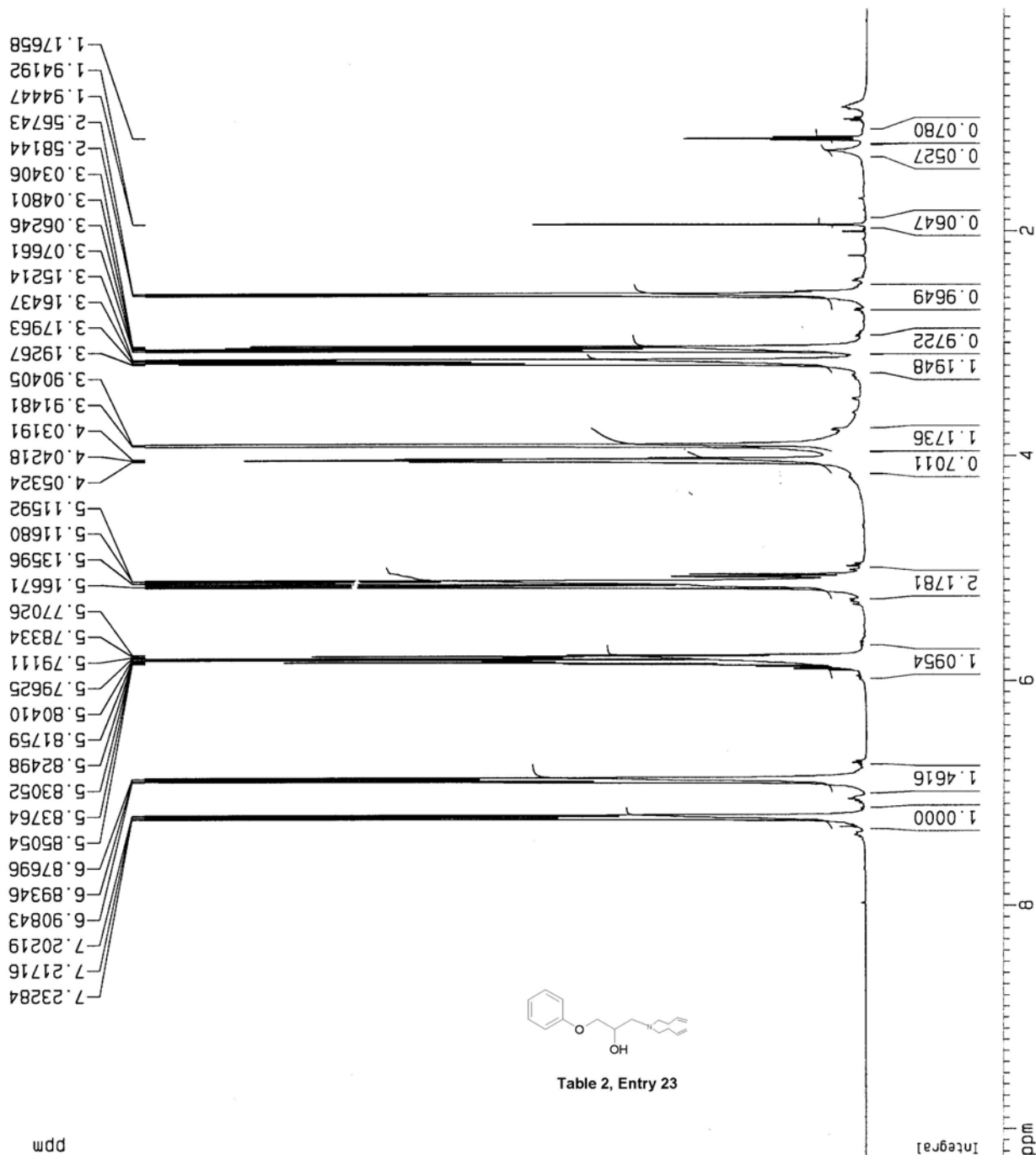
Date\_ 20041219  
 Time 12.47  
 INSTRUM spect  
 PROBHD 5 mm BBI 1H-BB  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 4  
 DS 1  
 SWH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
 RG 8  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 0.0 K  
 D1 5.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

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

NUC1 1H  
 P1 9.30 usec  
 PL1 3.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters

SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00  
 1D NMR plot parameters  
 CX 18.00 cm  
 CY 33.34 cm  
 F1P 10.243 ppm  
 F1 5122.62 Hz  
 F2P 0.029 ppm  
 F2 14.47 Hz  
 PPMCM 0.56742 ppm/cm  
 HZCM 283.78619 Hz/cm



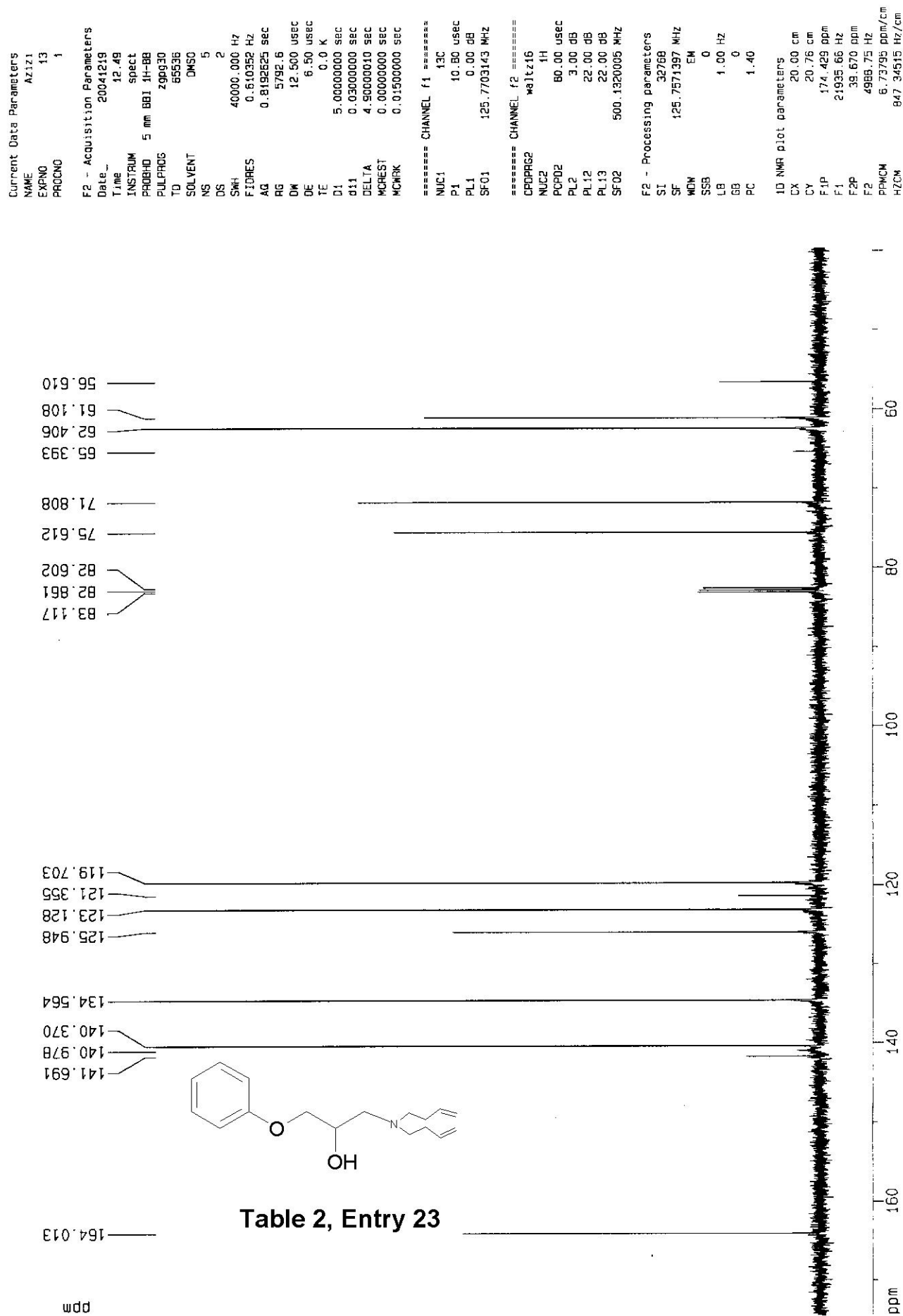
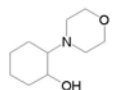
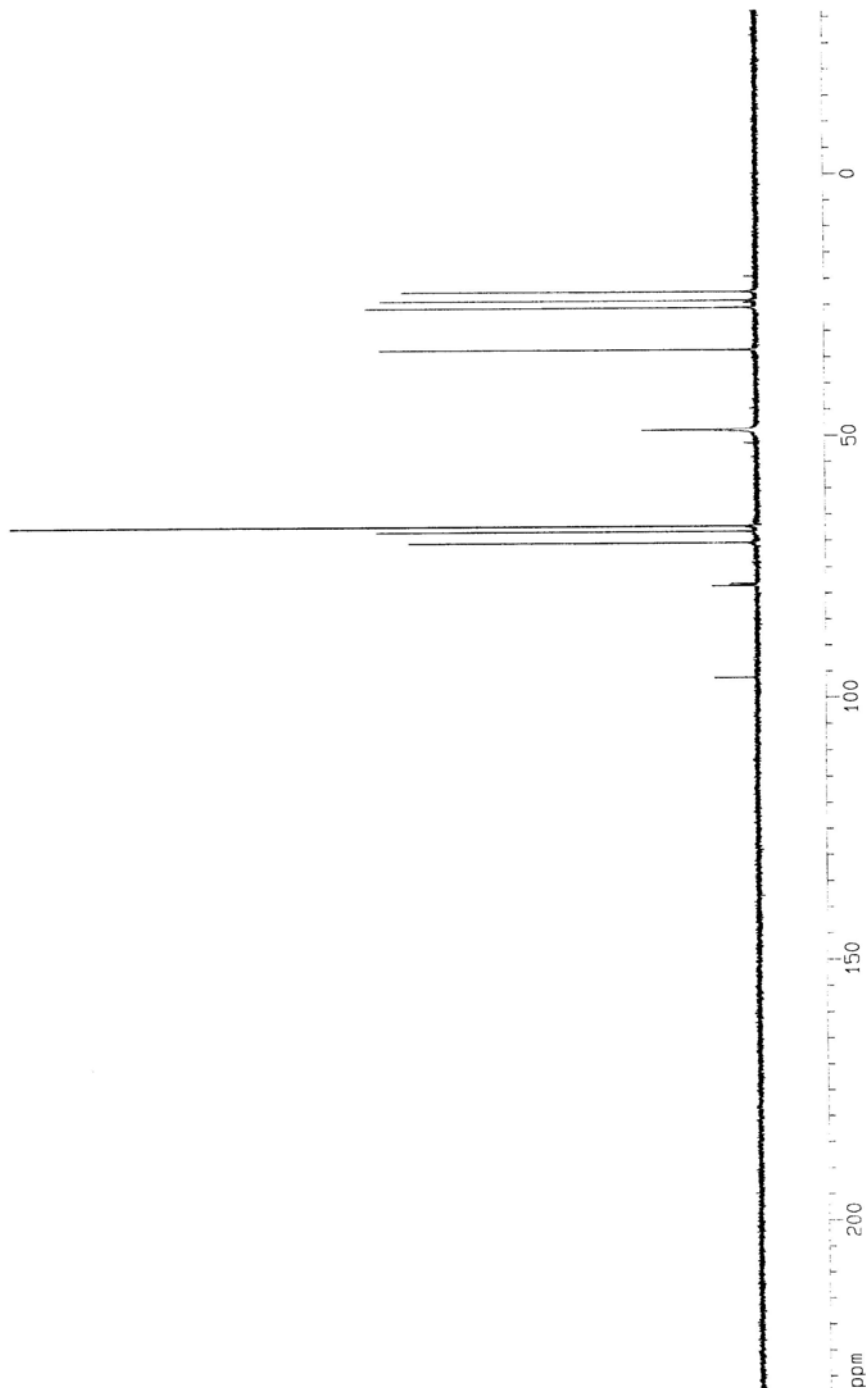


Table 2, Entry 27

106 <sup>13</sup>CNMR in CDCl<sub>3</sub> at 298K 83/03/26



96.0837  
78.5275  
78.4609  
78.2667  
78.0084  
70.3599  
68.2241  
67.1985  
51.3085  
48.8224  
33.4948  
25.4672  
24.4739  
24.0707  
22.3512  
19.4652



Current Data Parameters  
NAME AZ171  
EXPNO 360  
PROCNO 1

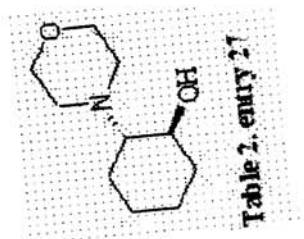
F2 - Acquisition Parameters  
Date\_ 20040615  
Time 8.32  
INSTRUM spect  
PROBHD 5 mm BBI 1H-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 11  
DS 2  
SWH 40000.000 Hz  
FIDRES 0.610392 Hz  
AQ 0.8192625 sec  
RG 4597.6  
DW 12.500 usec  
DE 6.50 usec  
TE 300.0 K  
D1 10.0000000 sec  
d11 0.0300000 sec  
d12 0.0000200 sec

===== CHANNEL f1 =====  
NUC1 <sup>13</sup>C  
P1 10.80 usec  
PL1 0.00 dB  
SF01 125.7703143 MHz

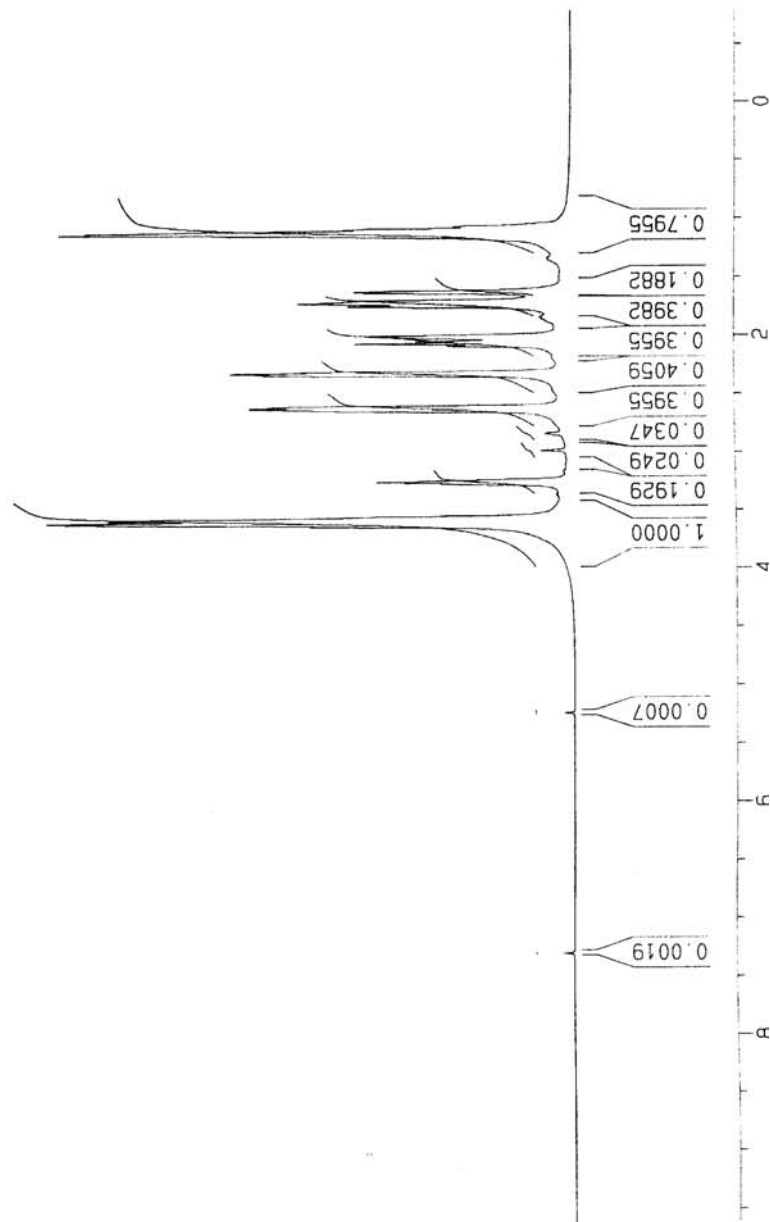
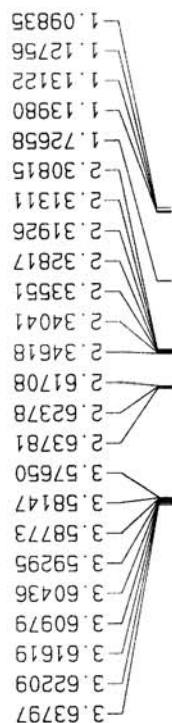
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 <sup>1</sup>H  
PCPD2 80.00 usec  
PL2 3.00 dB  
PL12 22.00 dB  
PL13 22.00 dB  
SF02 500.1320005 MHz

F2 - Processing parameters  
SI 32768  
SF 125.7577390 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

1D NMR plot parameters  
CX 20.00 cm  
CY 10.96 cm  
FIP 232.405 ppm  
F1 29226.67 Hz  
F2 -31.318 ppm  
F2 -3938.47 Hz  
OPCM 13.18612 ppm/cm  
HZCM 1658.25684 Hz/cm



37 <sup>1</sup>HNMR in CDCl<sub>3</sub> at 298K 83/02/12



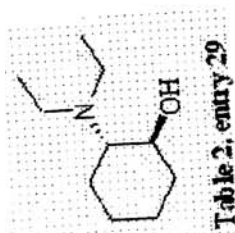
Current Data Parameters  
NAME Az121  
EXPNO 313  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20040501  
Time 11.10  
INSTRUM spect  
PROBHD 5 mm BBI 1H-BB  
PULPROG zg30  
TD 32768  
SOLVENT CDCl<sub>3</sub>  
NS 8  
DS 2  
SWH 10330.578 Hz  
FIDRES 0.315264 Hz  
AQ 1.5860696 sec  
RG 18  
DW 48.400 usec  
DE 6.50 usec  
TE 300.0 K  
D1 5.0000000 sec

===== CHANNEL f1 =====  
NUC1 <sup>1</sup>H  
P1 9.30 usec  
PL1 3.00 dB  
SF01 500.1330885 MHz

F2 - Processing parameters  
SI 32768  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 18.00 cm  
CY 7.06 cm  
F1P 10.768 ppm  
F1 5385.46 Hz  
F2P -0.794 ppm  
F2 -396.92 Hz  
PPMCM 0.64232 ppm/cm  
HZCM 321.24341 Hz/cm



20 <sup>1</sup>H NMR in CDCl<sub>3</sub> at 298K 82/09/23

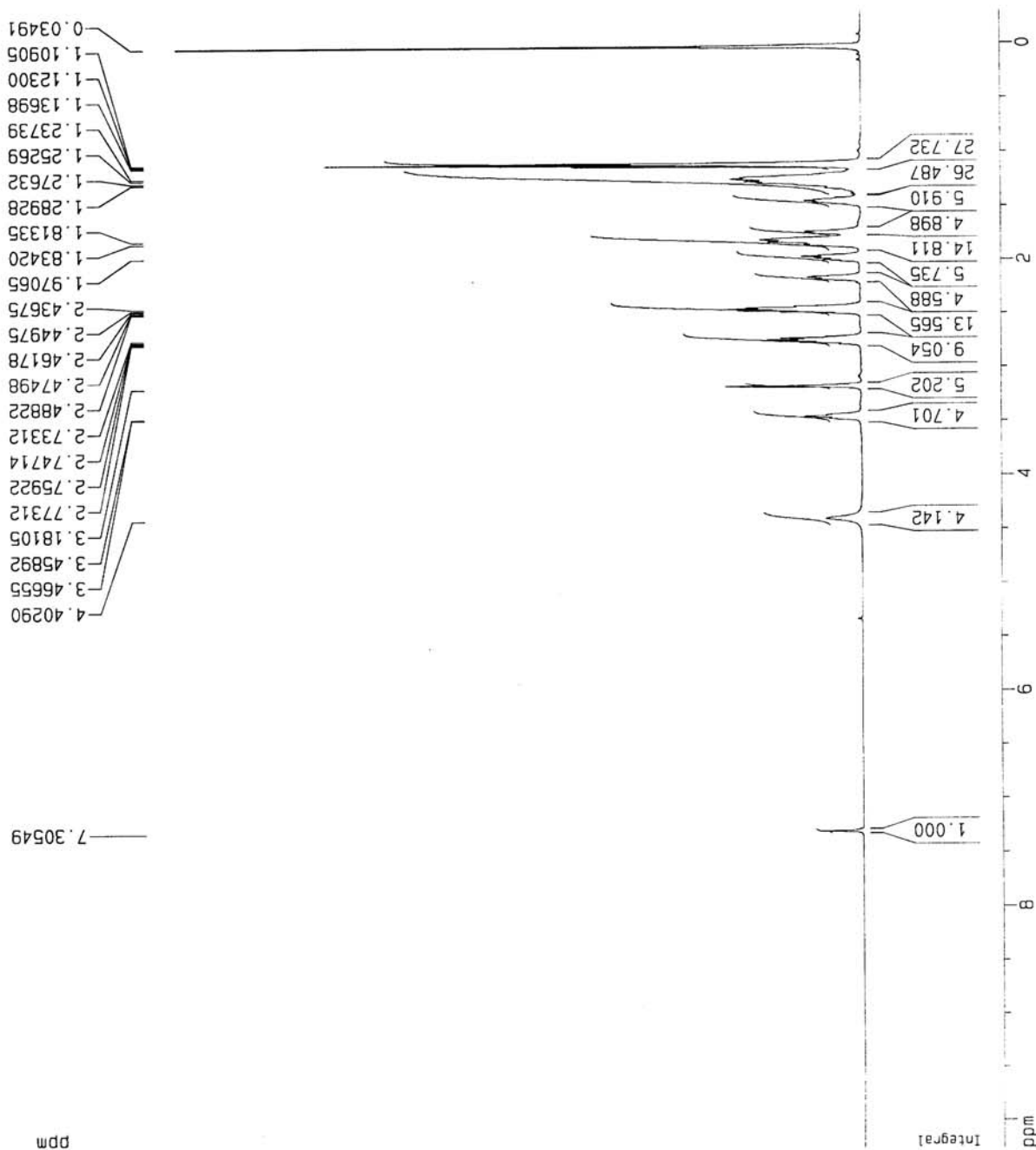
Current Data Parameters  
 NAME AZ121  
 EXPNO 217  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20031214  
 Time 9.42  
 INSTRUM spect  
 PROBHD 5 mm BB1 1H-BB  
 PULPROG zg30  
 TD 32768  
 SOLVENT CDCl<sub>3</sub>  
 NS 16  
 DS 2  
 SMH 10330.578 Hz  
 FIDRES 0.315264 Hz  
 AQ 1.5860696 sec  
 RG 64  
 DM 48.400 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 5.0000000 sec

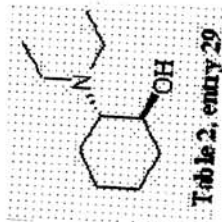
===== CHANNEL f1 =====  
 NUC1 1H  
 P1 9.30 usec  
 PL1 3.00 dB  
 SF01 500.1330885 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.1300000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

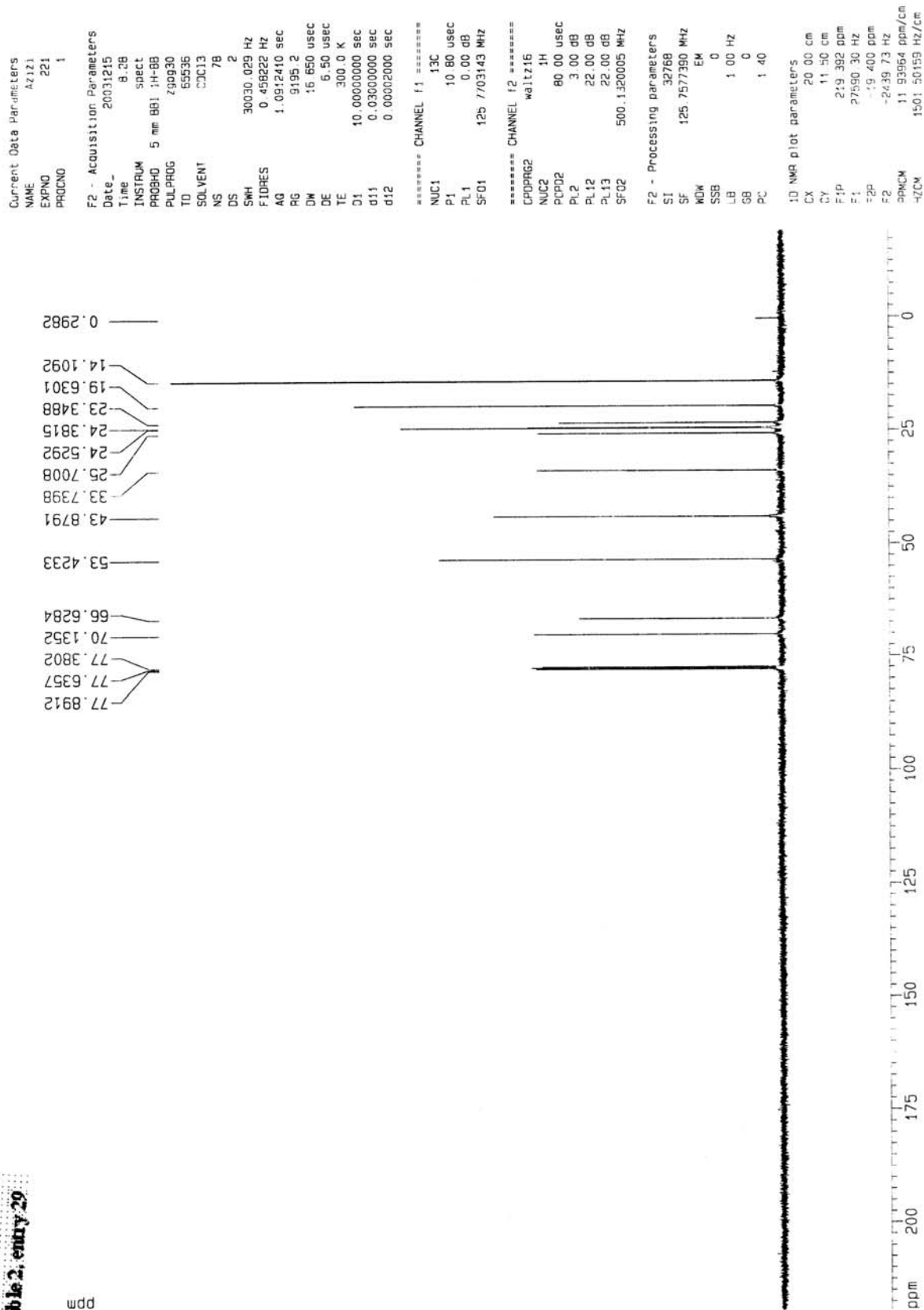
1D NMR plot parameters  
 CX 18.00 cm  
 CY 10.79 cm  
 F1P 10.272 ppm  
 F1 5137.24 Hz  
 F2P -0.304 ppm  
 F2 -152.22 Hz  
 PPMCM 0.58756 ppm/cm  
 HZCM 293.85861 Hz/cm







Sample (20) 13C NMR in CDCl3 at 298K 82/09/240



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