

Supplementary data as an aid to the referees

Hydrogenation of aromatic ketones, aldehydes, and epoxides with hydrogen and Pd(0)EnCatTM 30NP.

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General: The compounds described in this paper were prepared according to the procedure discussed in the text by the authors. All starting materials were purchased from Sigma-Aldrich and used without further purification. All reaction products were identified by comparison with their ¹H NMR spectra versus authentic ¹H NMR obtained from Sigma-Aldrich database and/or the authentic sample. Conversions were calculated from the ¹H NMR spectrum based on the disappearance of the starting material. ¹H NMR spectra were recorded on a Bruker DPX300 300 MHz NMR spectrometer at room temperature. Chemical shifts are reported in ppm on the δ scale relative to the internal standard TMS.

Table (1)

4-Methoxybenzyl alcohol: ¹H NMR (CDCl₃): δ 7.28 (2H, m, Ar), 6.89 (2H, m, Ar), 4.61 (2H, s, CH₂), 3.81 (3H, s, CH₃), 1.71 (1H, broad s, OH). In agreement with Sigma Aldrich database
<http://www.sigmaaldrich.com/catalog/search/ProductDetail/ALDRICH/136905>

4-Methylanisole: ¹H NMR (CDCl₃): δ 7.01 (2H, m, Ar), 6.80 (2H, m, Ar), 3.78 (3H, s, CH₃), 2.27 (3H, s, CH₃). In agreement with Sigma Aldrich database
<http://www.sigmaaldrich.com/catalog/search/ProductDetail/FLUKA/61050>

4-Methoxy-alpha-methylbenzyl alcohol: ¹H NMR (CDCl₃): δ 7.30 (2H, m, Ar), 6.88 (2H, m, Ar), 4.86 (1H, q, J = 6.44 Hz, CH), 3.81 (3H, s, CH₃), 1.70 (1H, broad s, OH), 1.48 (3H, d, J = 6.44 Hz, CH₃). In agreement with commercially available sample.

Table (2)

2-Methoxy benzylalcohol: ¹H NMR (CDCl₃) δ 7.29-7.23 (2H, m, Ar), 6.96-6.86 (2H, m, Ar), 4.67 (2H, s, CH₂), 3.84 (3H, s, CH₃), 2.47 (1H, s, OH) in agreement with the Sigma Aldrich database.
<http://www.sigmaaldrich.com/catalog/search/ProductDetail/ALDRICH/M10808>

2,3-Methylenedioxy benzylalcohol: ^1H NMR (CDCl_3) δ 6.86-6.75 (3H, m, Ar), 5.95 (2H, s, CH_2), 4.66 (2H, s, CH_2), 2.16 (1H, bs, OH) in agreement with data published by Roesch KR, Larock RC, *J Org Chem* 2002, **67**: 86.

2,4-Bistrifluoromethyl benzylalcohol: ^1H NMR (CDCl_3) δ 7.96-7.84 (3H, m, Ar), 4.97 (2H, s, CH_2), 2.11 (1H, bs, 2H).

4-Fluorobenzaldehyde: ^1H NMR (CDCl_3) δ 7.27 (2H, m), 7.00 (2H, m), 4.58 (2H, s), 3.88 (1H, bs, OH) in agreement with the Sigma Aldrich database.

<http://www.sigmaaldrich.com/catalog/search/ProductDetail/FLUKA/46765>

4-Fluorobenzoic acid: ^1H NMR (CDCl_3) δ 8.05 (2H, m), 7.09 (2H, m) in agreement with the Sigma Aldrich database. <http://www.sigmaaldrich.com/catalog/search/ProductDetail/FLUKA/46600>

Table (3)

2-phenyl-1-phenylethanol: ^1H NMR (CDCl_3): δ 7.40-7.15 (10H, m, Ar), 4.89 (1H, m, CH), 3.10-2.90 (2H, m, CH_2), 1.95 (1H, broad s OH) In agreement with data published by Blake AJ, Cunningham A, Ford A, Teat SJ, Woodward S, *Chem Eur J* 2000, **6**:3586.

Dibenzyl: ^1H NMR (CDCl_3): δ 7.35-7.25 (10H, m, Ar), 2.92 (4H, s, $2\times\text{CH}_2$). In agreement with Sigma Aldrich database.

<http://www.sigmaaldrich.com/catalog/search/ProductDetail/FLUKA/14330>

Table (4)

2-Phenylethanol: ^1H NMR (CDCl_3) δ 7.40-7.21 (5H, m, Ar), 3.85 (2H, t, $J = 6.6$ Hz, CH_2), 2.86 (2H, t, $J = 6.6$ Hz, CH_2), 1.55 (1H, bs, OH) in agreement with data published by Ley, SV, Mitchell C, Pears D, Ramaro C, Yu J-Q, Zhou W, *Org Lett*, 2003, **5**:4665.

2-(4'-Fluorophenyl) ethanol: ^1H NMR (CDCl_3) δ 7.21-7.16 (2H, m, Ar), 7.03-6.96 (2H, m, Ar), 3.84 (2H, t, $J = 6.6$ Hz, CH_2), 2.84 (2H, t, $J = 6.6$ Hz, CH_2), 1.49 (1H, bs, OH) in agreement data published by Ley, SV, Mitchell C, Pears D, Ramaro C, Yu J-Q, Zhou W, *Org Lett*, 2003, **5**:4665.

1-Phenyl propan-2-ol: ^1H NMR (CDCl_3) δ 7.32-7.12 (5H, m, Ar), 4.04-3.93 (1H, m, CH), 2.78-2.64 (2H, m, CH_2), 1.88 (1H, bs, OH), 1.21 (3H, d, $J = 6.3$ Hz, CH_3) in agreement data published by Ley, SV, Mitchell C, Pears D, Ramaro C, Yu J-Q, Zhou W, *Org Lett*, 2003, **5**:4665.

3-Phenyl propane-1,2-diol: ^1H NMR (CDCl_3) δ 7.37-7.20 (5H, m, Ar), 3.96-3.88 (m, 1H, CHOH), 3.66 (1H, dd, $J = 11.1, 3.0$ Hz, CHH), 3.49 (1H, dd, $J = 11.1, 6.9$ Hz, CHH), 2.82-2.69 (2H, m, CH_2), 2.47 (2H, bs, $2\times\text{OH}$) in agreement data published by Ley, SV, Mitchell C, Pears D, Ramaro C, Yu J-Q, Zhou W, *Org Lett*, 2003, **5**:4665.

```
;zg30
;advance-version (02/05/31)
;ld sequence
;using 30 degree flip angle
```

```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power level for pulse (default
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

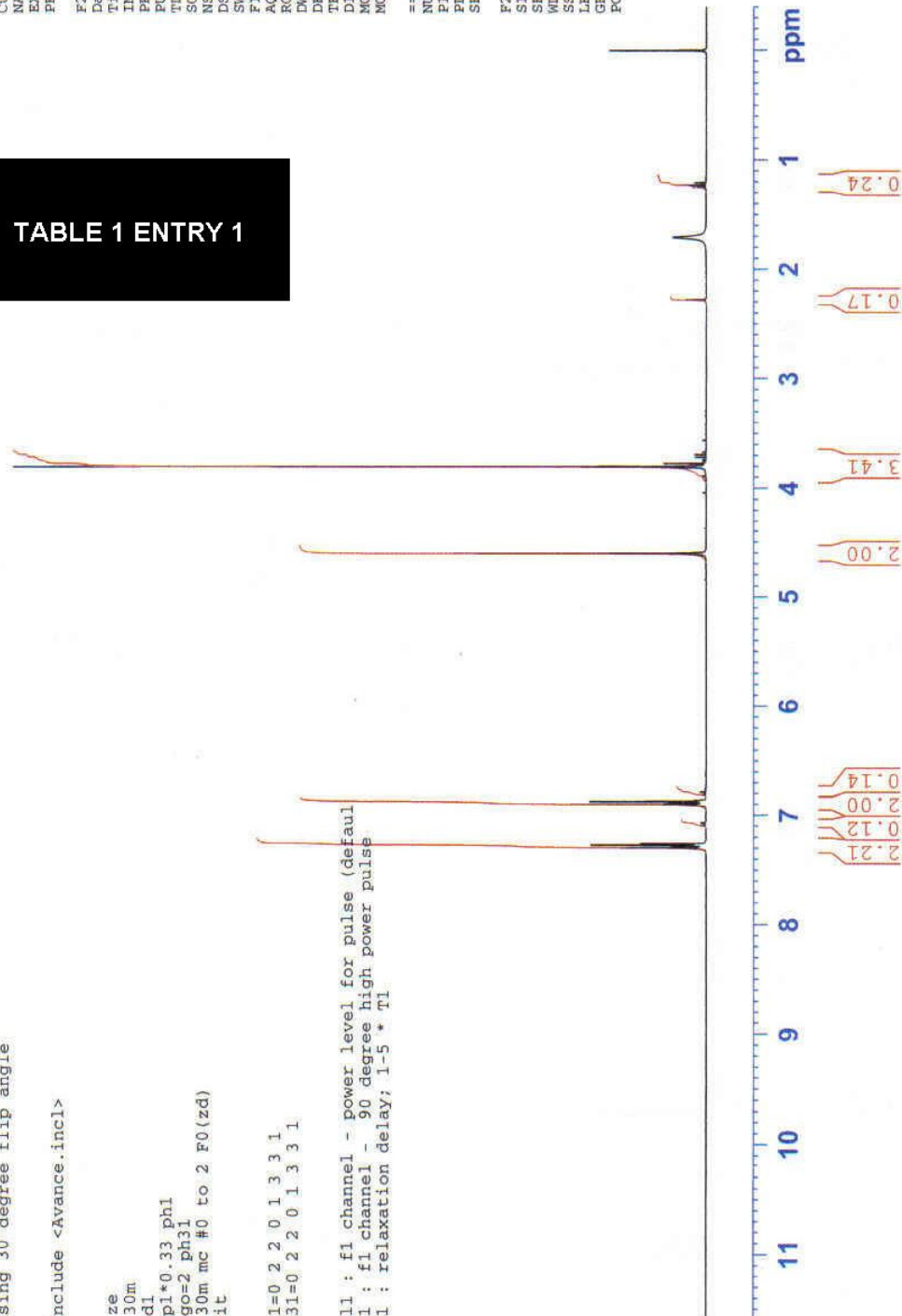
TABLE 1 ENTRY 1

```
Current Data Parameters
NAME 10375595
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051111
Time 15.37
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7181.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 322.5
DE 69.600 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.13300071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```



S.N 2
1111105

```
;zg30
;advance-version (02/05/31)
;ID sequence
;using 30 degree flip angle
```

```
#include <Advance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

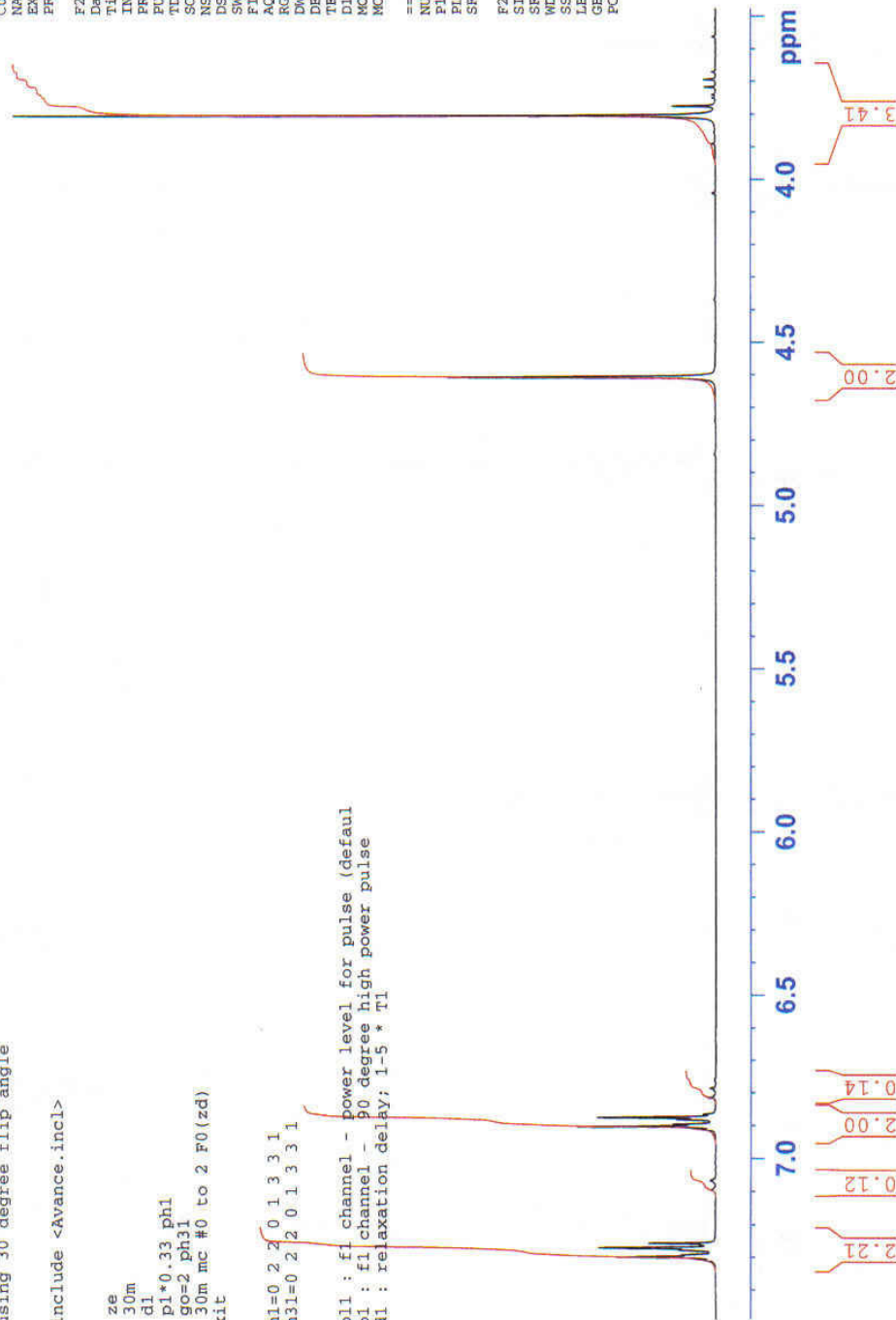
```
;p1 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay: 1-5 * T1
```

```
Current Data Parameters
NAME      10375595
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20051111
Time      15:37
INSTRUM   dpx300
PROBHD    5 mm QNP 1H/1
PULPROG   zg30
TD         48848
SOLVENT   CDCl3
NS         64
DS         2
SWH        7183.908 Hz
FIDRES     0.147067 Hz
AQ         3.3998709 sec
RG         322.5
DW         69.600 usec
DE         6.00 usec
TE         299.2 K
D1         6.59999990 sec
MCREST     0.00000000 sec
MCWRK     0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         9.40 usec
PL1        0.00 dB
SFO1       300.1330010 MHz

F2 - Processing parameters
SI         65536
SF         300.1300071 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         2.00
```



```
;zg30
;advance-version (02/05/31)
;ld sequence
;using 30 degree flip angle
```

```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p11 : f1 channel - power level for pulse (default
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

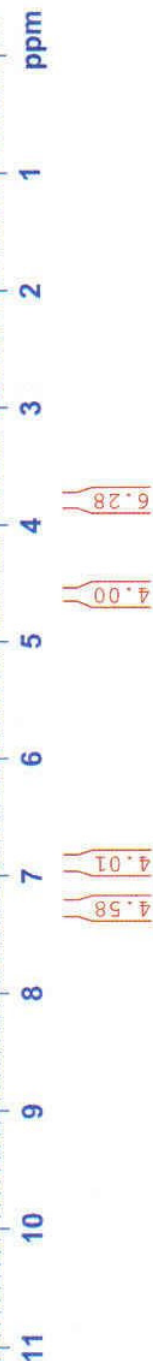
TABLE 1 ENTRY 2

```
Current Data Parameters
NAME 10376150
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051125
Time 19.10
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCL3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3988709 sec
RG 406.4
DE 69.600 usec
TE 299.2 K
DL 6.5999990 sec
MCREST 0.0000000 sec
MCWRR 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1330073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```



P. Dub
7/10/05

10376150, NBZ5781/10/4, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

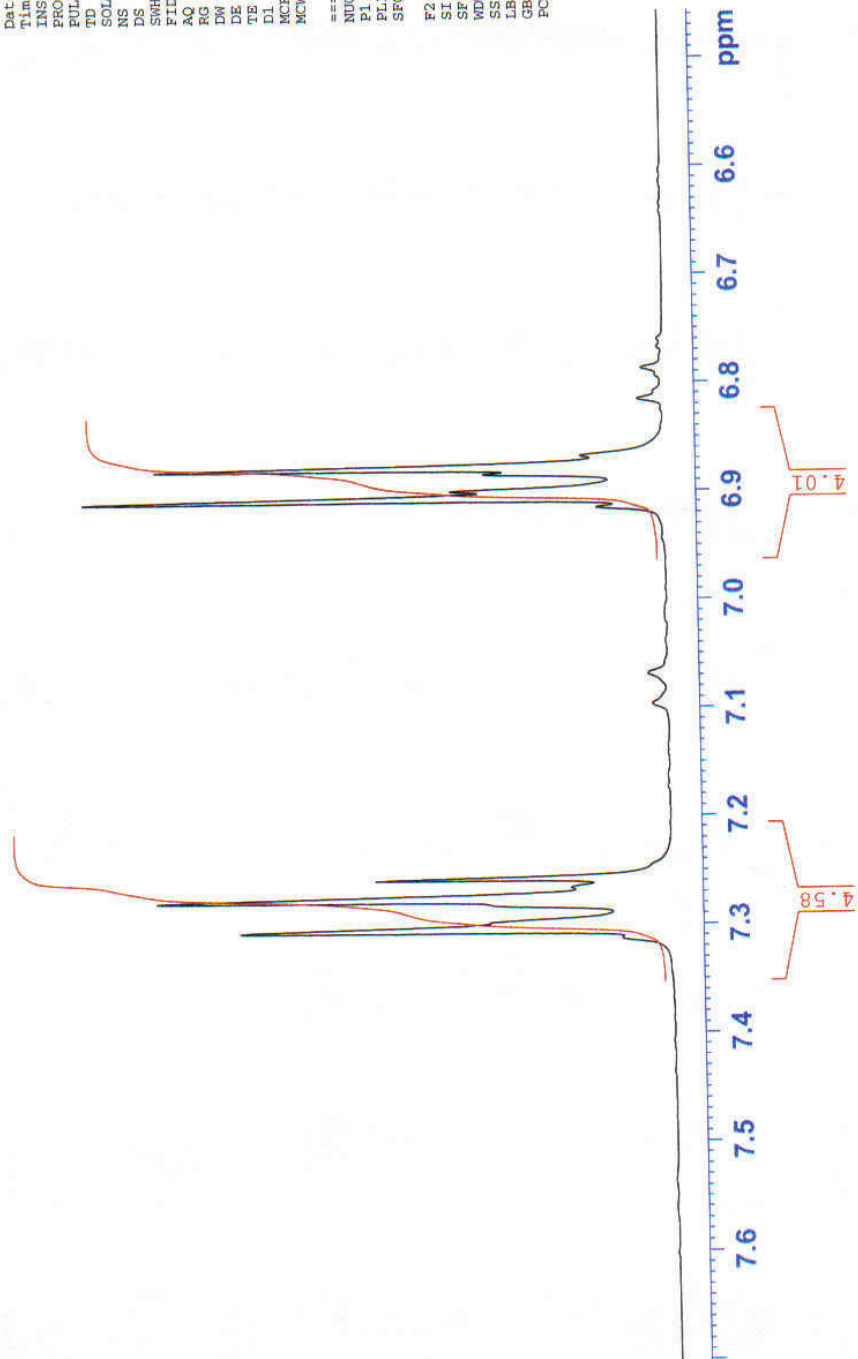
Intertek ASG

Current Data Parameters
NAME 10376150
EXNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051125
Time 19.10
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCL3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 406.4
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWREK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300073 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 2.00




```
;zg30
;advance-version (02/05/31)
;1d sequence
;using 30 degree flip angle
```

```
#include <Advance.incl>
```

```
1 ze
2 30m
  d1
  p1*0.33 ph1
  go=2 ph31
  30m mc #0 to 2 F0(zd)
  exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p11 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay: 1-5 * T1
```

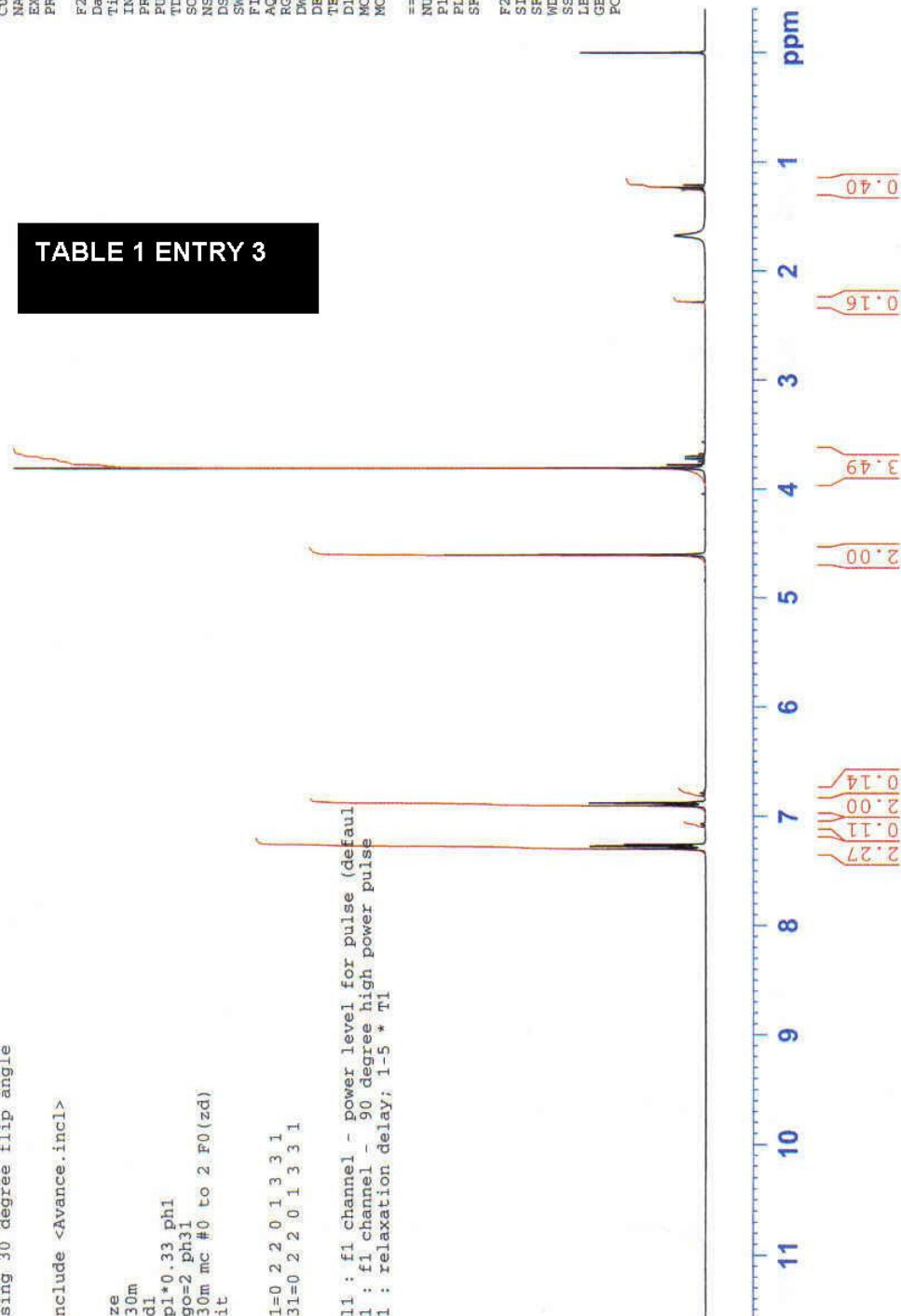
TABLE 1 ENTRY 3

```
Current Data Parameters
NAME      10375597
EXPNO     10
PROCNO     1

F2 - Acquisition Parameters
Date_      20051111
Time       16.03
INSTRUM    dpx300
PROBHD     5 mm QNP 1H/1
PULPROG    zg30
TD          48848
SOLVENT    CDCl3
NS          64
DS          2
SWH         7183.908 Hz
FIDRES      0.147067 Hz
AQ          3.3998709 sec
RG          362
DE          69.600 usec
TE          299.2 K
DL          6.5999990 sec
MCREST      0.0000000 sec
MCWRK      0.01500000 sec

===== CHANNEL f1 =====
NUC1        1H
P1          9.40 usec
PL1         0.00 dB
SFO1        300.1330010 MHz

F2 - Processing parameters
SI          65536
SF          300.1300068 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          2.00
```



S.M. Z

111115

```
;zg30
;advance-version (02/05/31)
;1D sequence
;using 30 degree flip angle
```

```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0.2 2 0 1 3 3 1
ph31=0.2 2 0 1 3 3 1
```

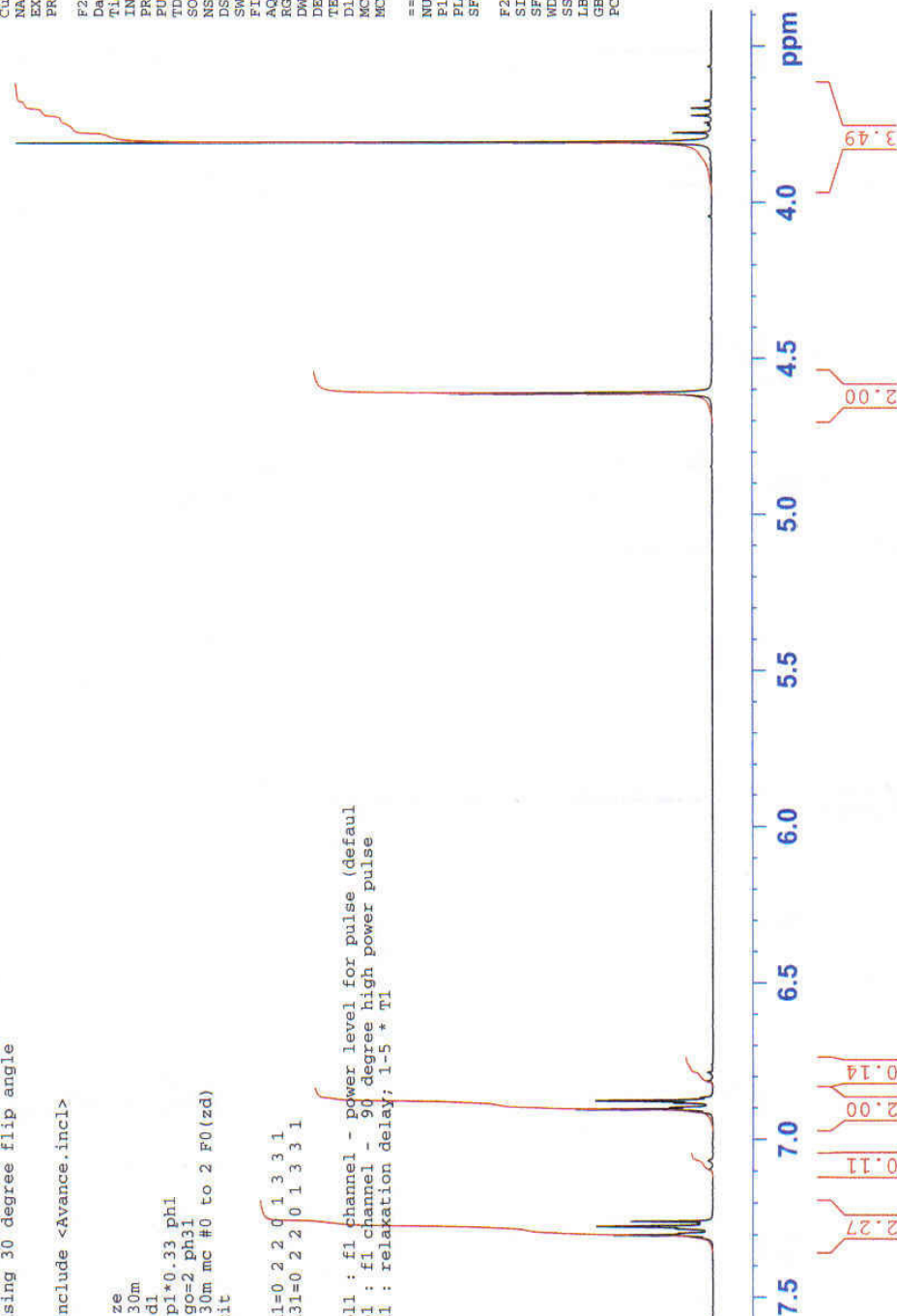
```
;p1 : f1 channel - power level for pulse (default
;p1 : f1 channel - 90 degree high power pulse
;di : relaxation delay; 1-5 * T1
```

```
Current Data Parameters
NAME 10375597
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051111
Time 16.03
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 4
SWH 7183.906 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 362
DE 69.600 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```



S.M.D
11/11/05


```
;zg30
;advance-version (02/05/31)
;1d sequence
;using 30 degree flip angle
```

```
#include <Avance.incl>
```

```
1 ze
2 30m
  d1
  p1*0.33 ph1
  go=2 ph31
  30m mc #0 to 2 F0(zd)
  exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p11 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

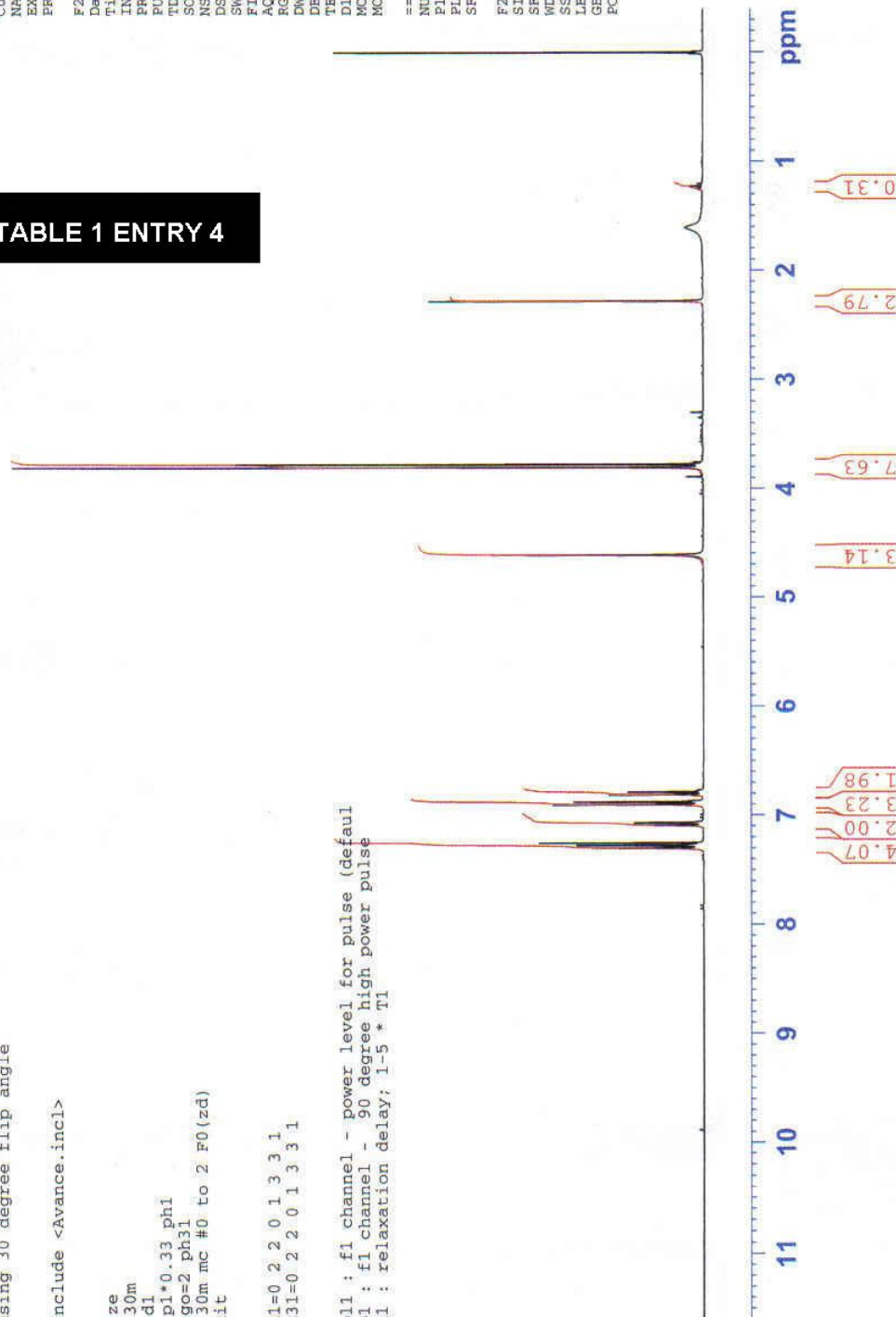
TABLE 1 ENTRY 4

```
Current Data Parameters
NAME      10376711
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20051207
Time      15.23
INSTRUM   dpx300
PROBHD    5 mm QNP 1H/1
PULPROG   zg30
TD        48848
SOLVENT   CDCL3
NS        64
DS        2
SWH        7183.908 Hz
FIDRES    0.147067 Hz
AQ        3.3998709 sec
RG        512
DE        69.600 usec
TE        299.2 K
D1        6.5999990 sec
MCREST    0.0000000 sec
MCWPRK    0.0150000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        9.40 usec
PL1       0.00 dB
SFO1      300.1330010 MHz

F2 - Processing parameters
SI        65536
SF        300.1330075 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        2.00
```



```

;zg30
;advance-version (02/05/31)
;ID sequence
;using 30 degree flip angle

```

```

#include <Avance.incl>

```

```

1 ze
2 30m
d1
p1+0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit

```

```

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

```

```

;p11 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1

```

```

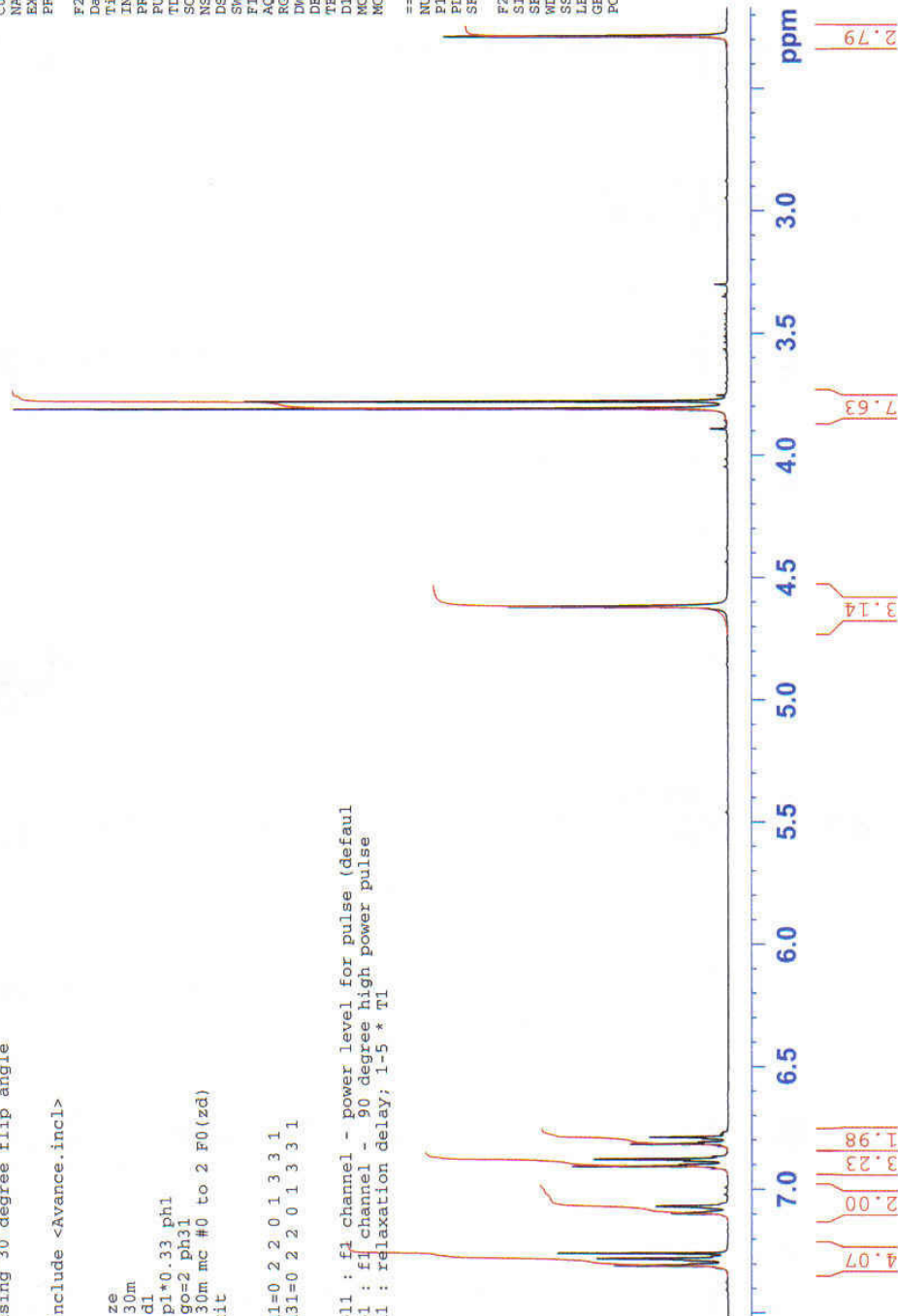
Current Data Parameters
NAME      10376711
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20051207
Time      15.23
INSTRUM   dpx300
PROBHD    5 mm QNP 1H/1
PULPROG   zg30
TD         48848
SOLVENT   CDCL3
NS         64
DS         2
SWH        7183.908 Hz
FIDRES     0.147067 Hz
AQ         3.3998709 sec
RG         512
DM         69.600 usec
DE         6.00 usec
TE         299.2 K
D1         6.59999990 sec
MCREST     0.00000000 sec
MCWK      0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         9.40 usec
PL1        0.00 dB
SFO1       300.1330010 MHz

F2 - Processing parameters
SI         65536
SF         300.1300075 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         2.00

```



```

;zg30
;advance-version (02/05/31)
;ld sequence
;using 30 degree flip angle

```

```

#include <Avance.incl>

```

```

1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit

```

```

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

```

```

;p11 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1

```

TABLE 1 ENTRY 5

```

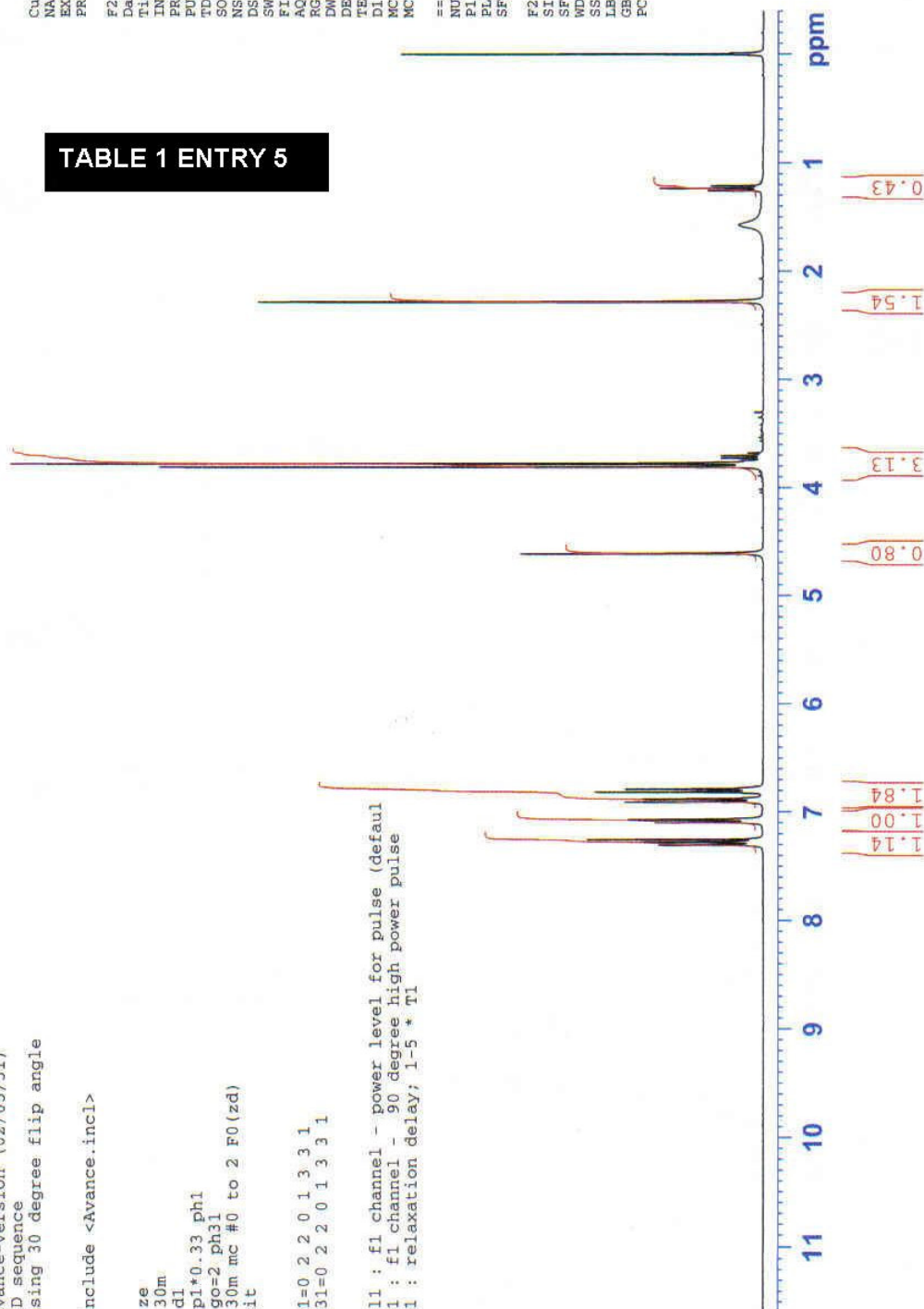
Current Data Parameters
NAME      10376147
EXPNO     10
PROCNO     1

F2 - Acquisition Parameters
Date_     20051125
Time      18.17
INSTRUM   dpx300
PROBHD    5 mm QNP 1H/1
PULPROG   zg30
TD        48848
SOLVENT   CDCL3
DS        64
NS        2
SHH       7183.908 Hz
FIDRES    0.147067 Hz
AQ        3.3998709 sec
RG        456.1
DW        69.600 usec
DE        6.00 usec
TE        299.2 K
D1        6.59999990 sec
MCREST    0.00000000 sec
MCWRK     0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        9.40 usec
PL1       0.00 dB
SFO1      300.1330010 MHz

F2 - Processing parameters
SI        65536
SF        300.1300077 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        2.00

```



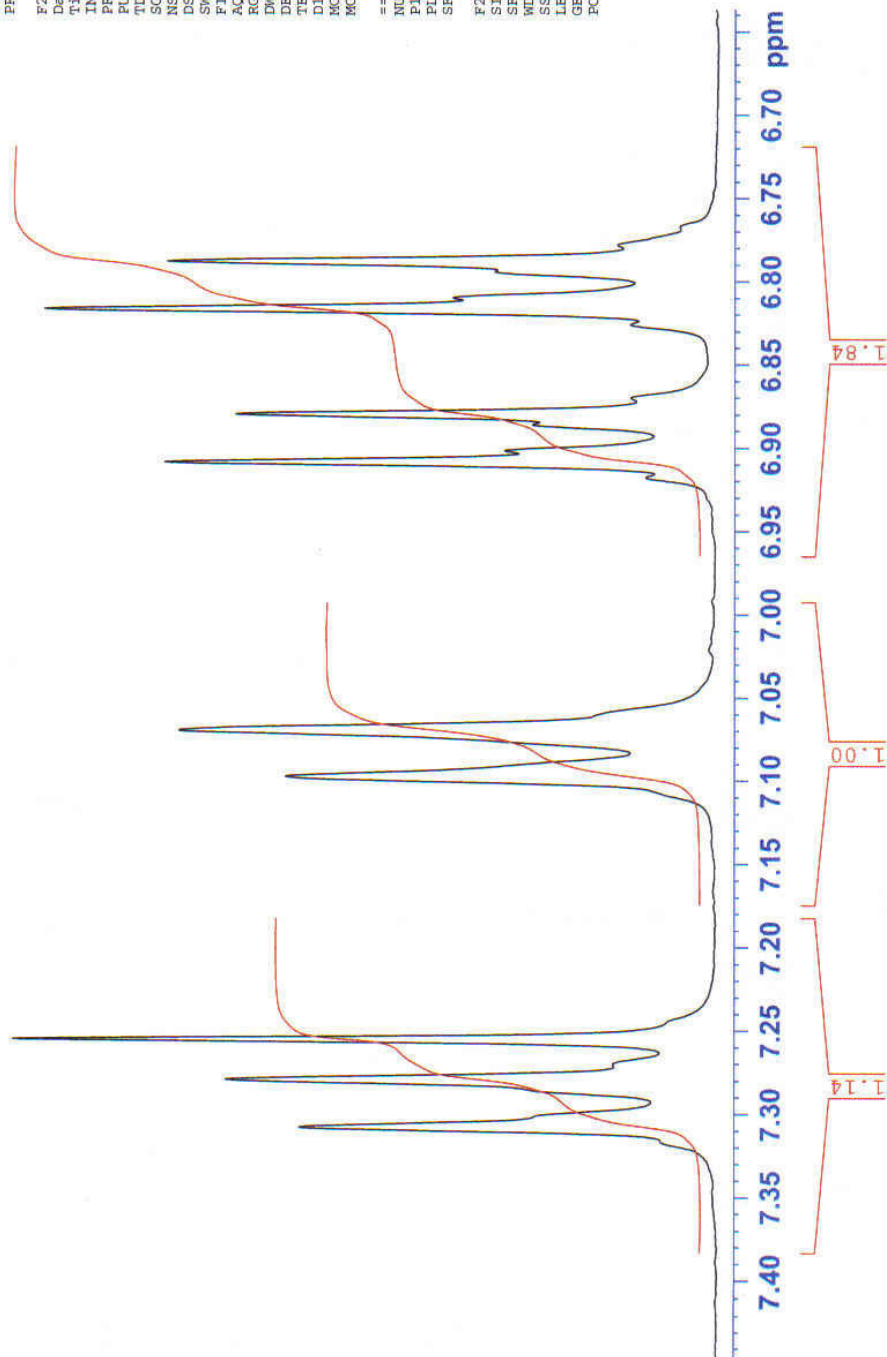
P. N. S. 2005/11/25

Current Data Parameters
NAME 10376147
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20051125
Time 18.17
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCL3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 456.1
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWFK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300077 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



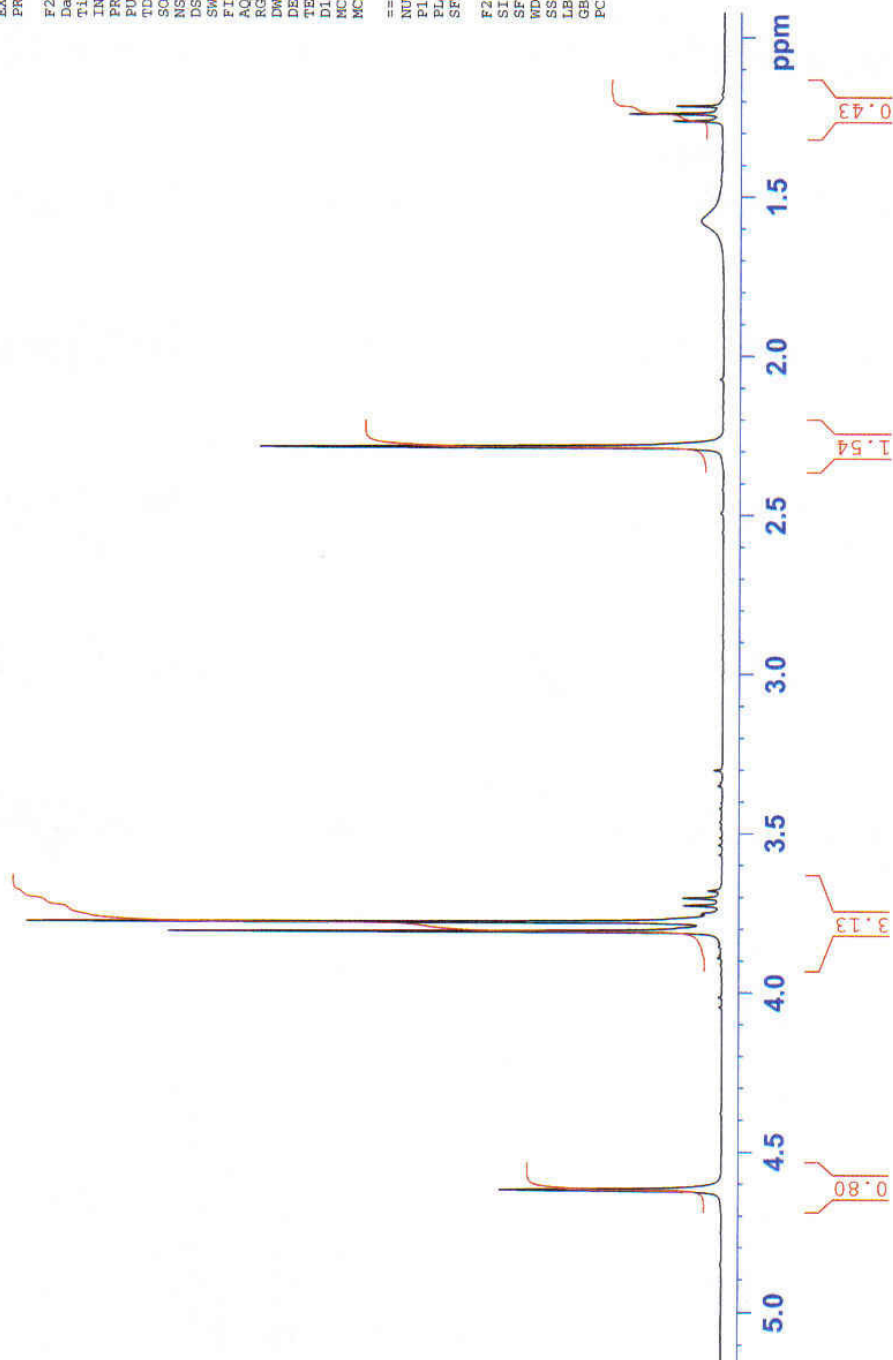
Q. N. 10/10/05

Current Data Parameters
 NAME 10376147
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20051125
 Time 18.17
 INSTRUM qpx300
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 48848
 SOLVENT CDCL3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.3998709 sec
 RG 456.1
 DW 69.600 usec
 DE 6.00 usec
 TE 299.2 K
 D1 6.59999990 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SF01 300.1330010 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1300077 MHz
 EM 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00



D. Nutt
 20/11/05


```
;zg30
;advance-version (02/05/31)
;ID sequence
;using 30 degree flip angle
```

```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p11 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

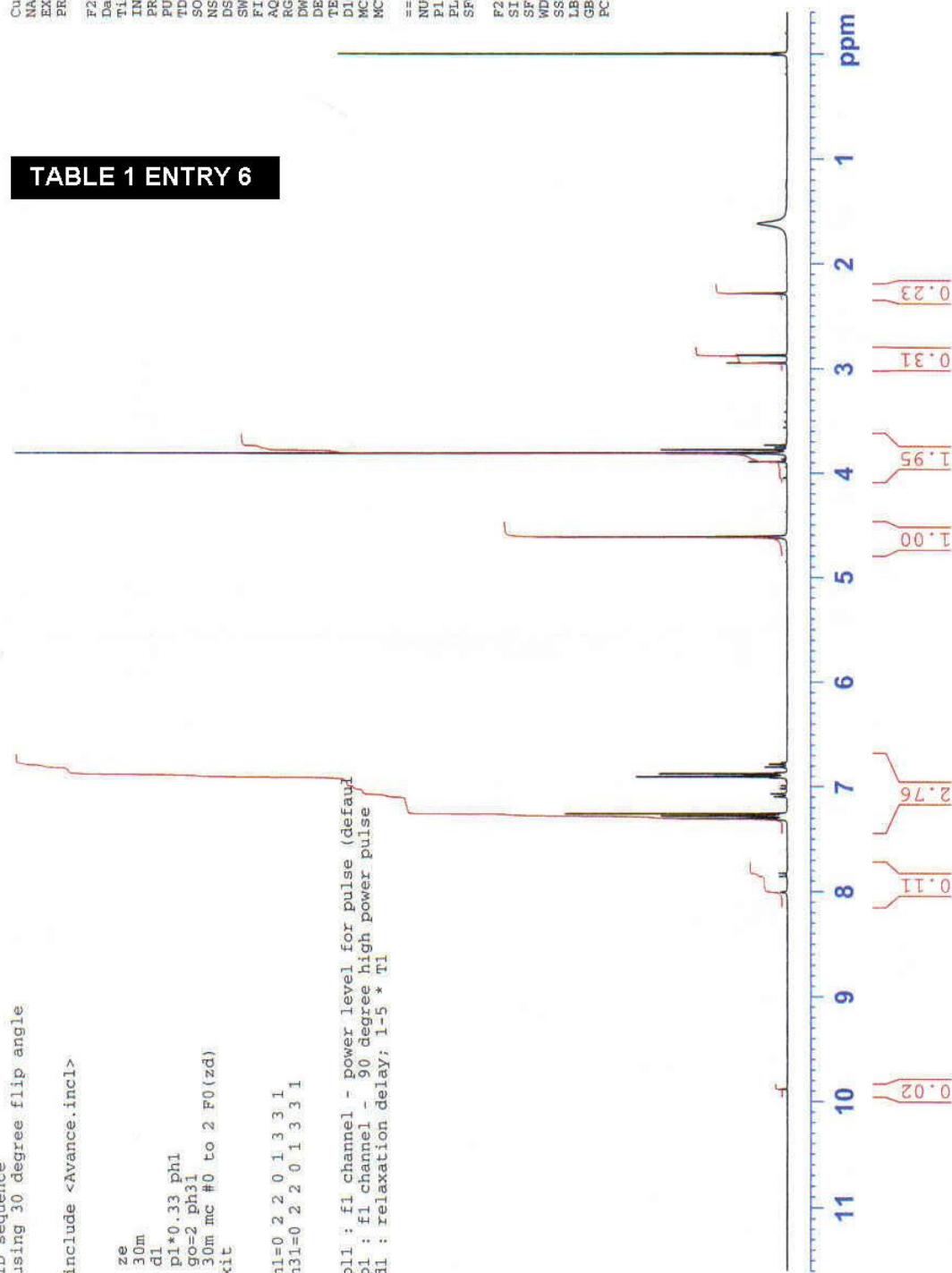
TABLE 1 ENTRY 6

```
Current Data Parameters
NAME      10371786
EXPNO     10
PROCNO     1

F2 - Acquisition Parameters
Date_      20050819
Time       18.34
INSTRUM    dpx300
PROBHD     5 mm QNP 1H/1
PULPROG    zg30
TD          48848
SOLVENT    CDCL3
NS          64
DS          2
SWH         7183.908 Hz
FIDRES     0.147067 Hz
AQ          3.3998709 sec
RG          645.1
DW          69.600 usec
DE          6.00 usec
TE          299.2 K
D1          6.59999990 sec
MCREST     0.00000000 sec
MCWRK      0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1          9.40 usec
PL1         0.00 dB
SFO1       300.1330010 MHz

F2 - Processing parameters
SI          65536
SF          300.13300064 MHz
WDW         EM
SSB         0
LB          0.30 Hz
GB          0
PC          2.00
```



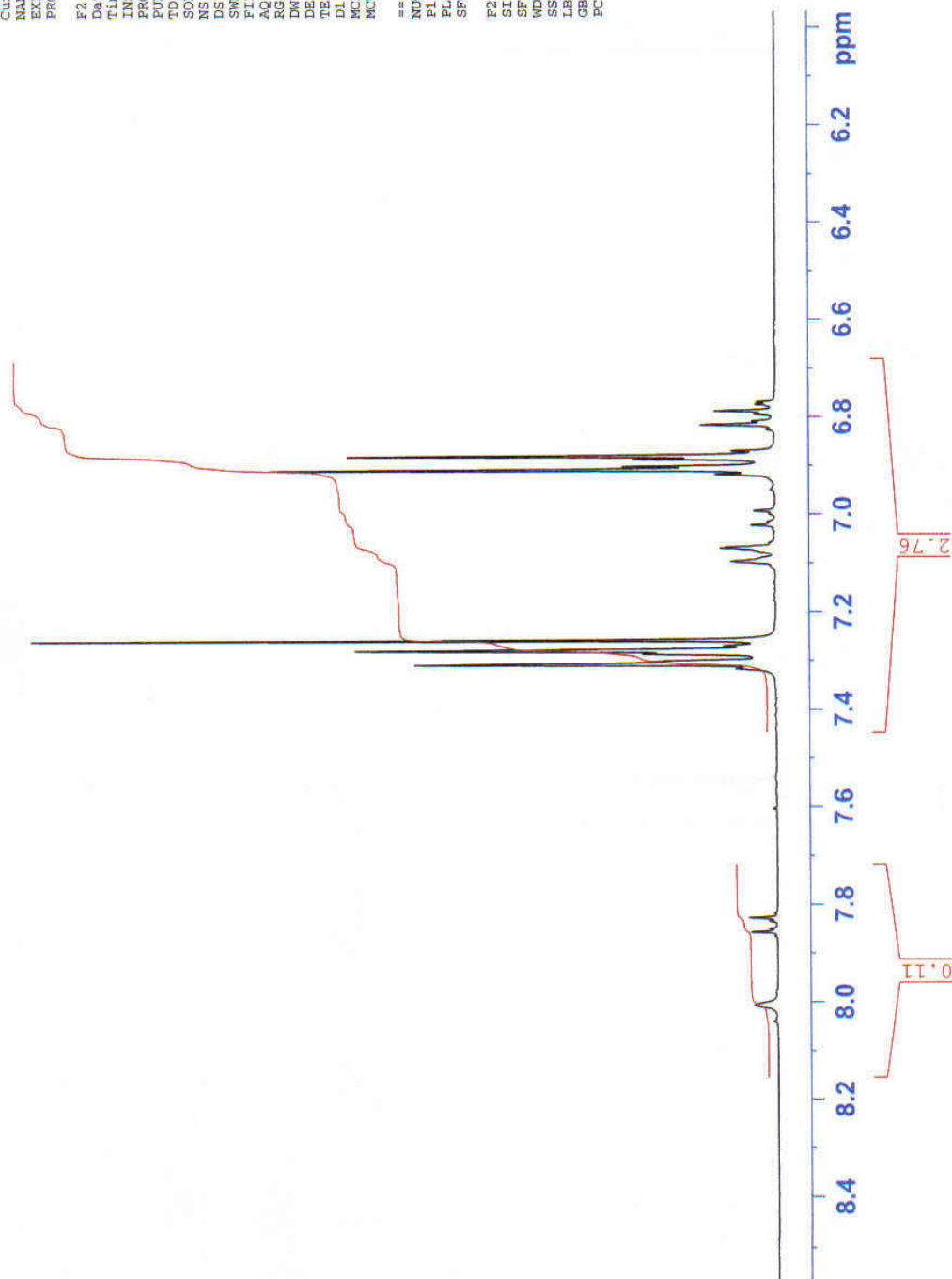
J. Nut
22/8/05

Current Data Parameters
 NAME 10371786
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050819
 Time 18.34
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H/1
 PULPROG zgpg30
 TD 65536
 ID 48848
 SOLVENT CDCL3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.3998709 sec
 RG 645.1
 DW 69.600 usec
 DE 6.00 usec
 TE 299.2 K
 D1 6.59999990 sec
 MCREST 0.00000000 sec
 MCWPK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SFO1 300.1330010 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1300064 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00



D. N. N. N.
 22/8/05



```
;zg30
;advance-version (02/05/31)
;1d sequence
;using 30 degree flip angle
```

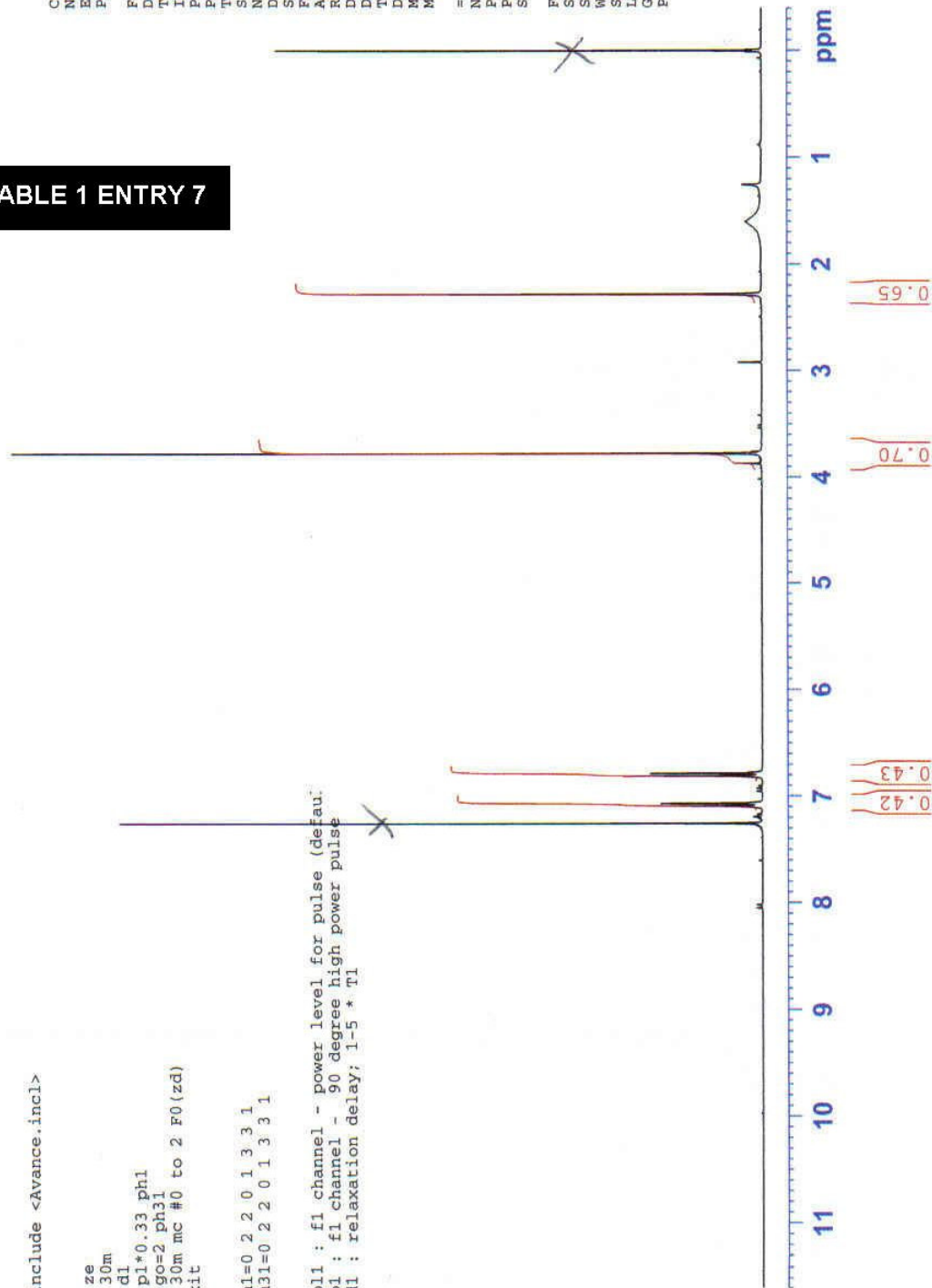
```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p11 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

TABLE 1 ENTRY 7



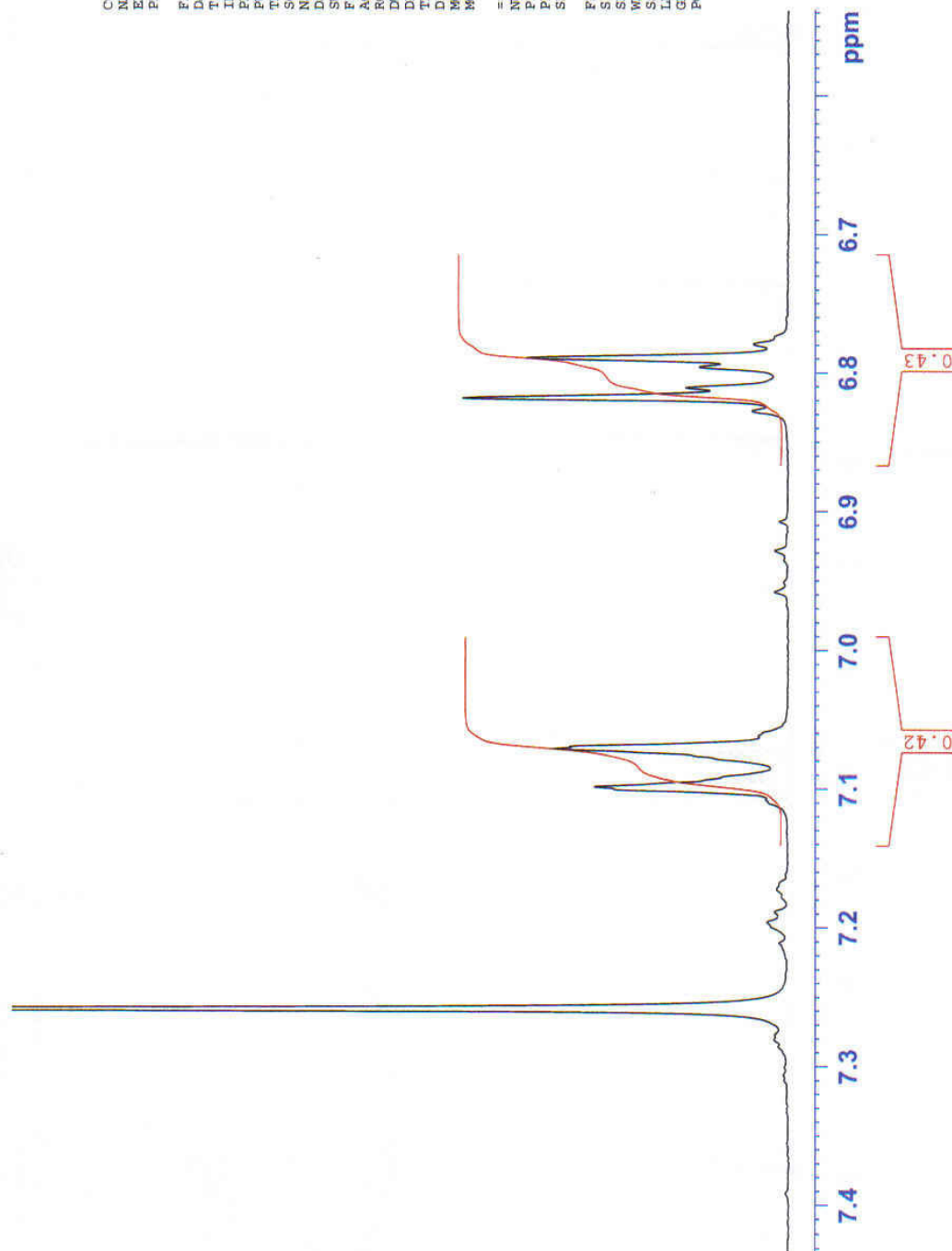
```
Current Data Parameters
NAME 10368723
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050609
Time 14.46
INSTRUM qnp300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCL3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3988709 sec
RG 1290.2
DE 63.600 usec
TE 299.2 K
DI 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```

D. Mout
10/6/05



Current Data Parameters
NAME 10368723
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050609
Time 14.46
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCl₃
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 1290.2
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

J. N. N. N.
10/6/05

```

;zg30
;advance-version (02/05/31)
;1d sequence
;using 30 degree flip angle

```

```

#include <h1vance.incl>

```

```

1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit

```

```

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

```

```

;p1 : f1 channel - power level for pulse (default)
;pl : f1 channel - 90 degree high power pulse
;dl : relaxation delay; 1-5 * T1

```

TABLE 1 ENTRY 8

```

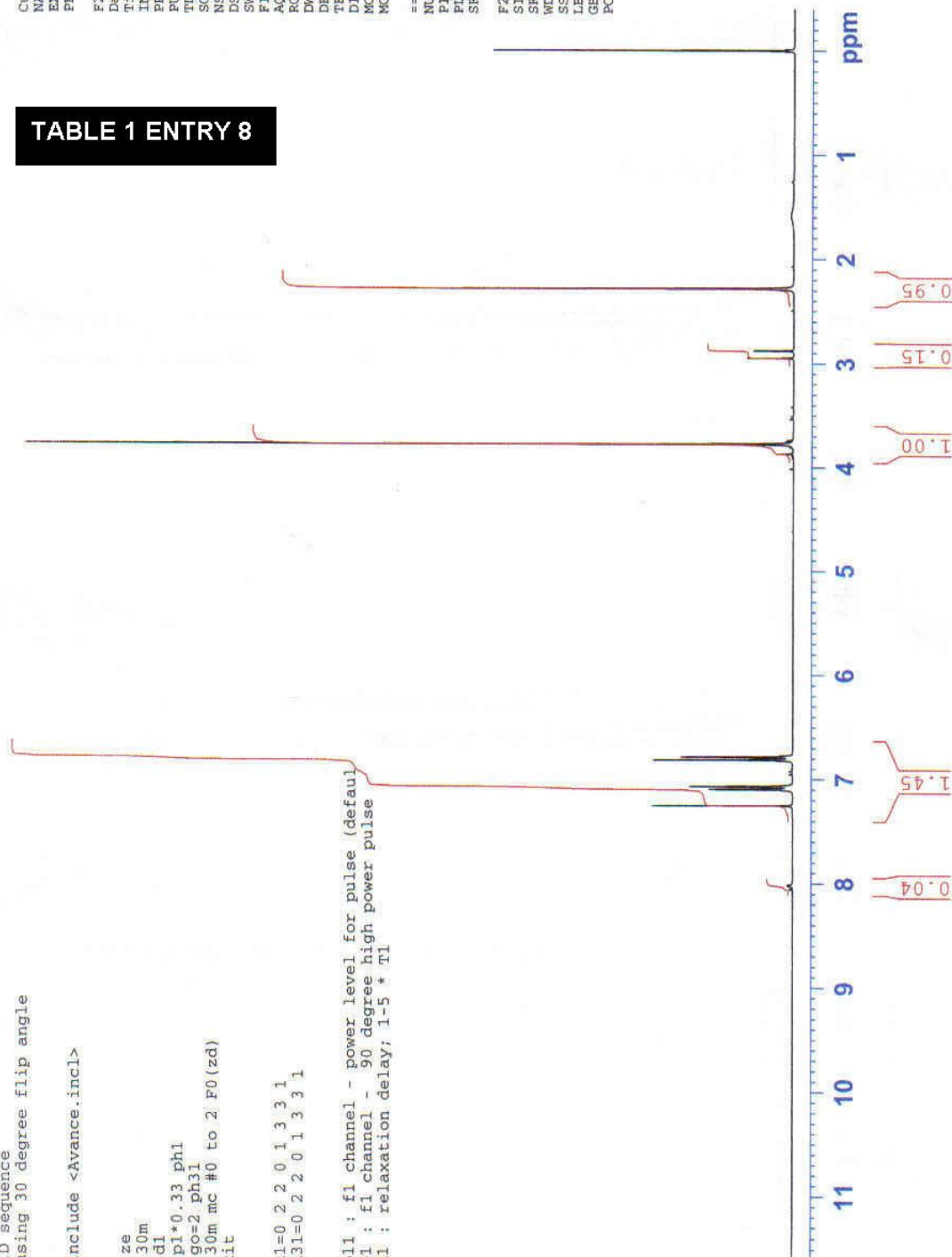
Current Data Parameters
NAME      10371787
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20050819
Time      18:51
INSTRUM   gpx300
PROBHD    5 mm QNP 1H/1
PULPROG   zg30
TD         48848
SOLVENT   CDCl3
NS         64
DS         2
SWH        7183.908 Hz
FIDRES     0.147067 Hz
AQ         3.3998709 sec
RG         512
DE         69.600 usec
TE         299.2 K
D1         6.59999990 sec
MCPRST     0.00000000 sec
MCWRK     0.01500000 sec

===== CHANNEL f1 =====
NUC1       1H
P1         9.40 usec
PL1        0.00 dB
SFO1       300.1330010 MHz

F2 - Processing parameters
SI         65536
SF         300.1300078 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         2.00

```



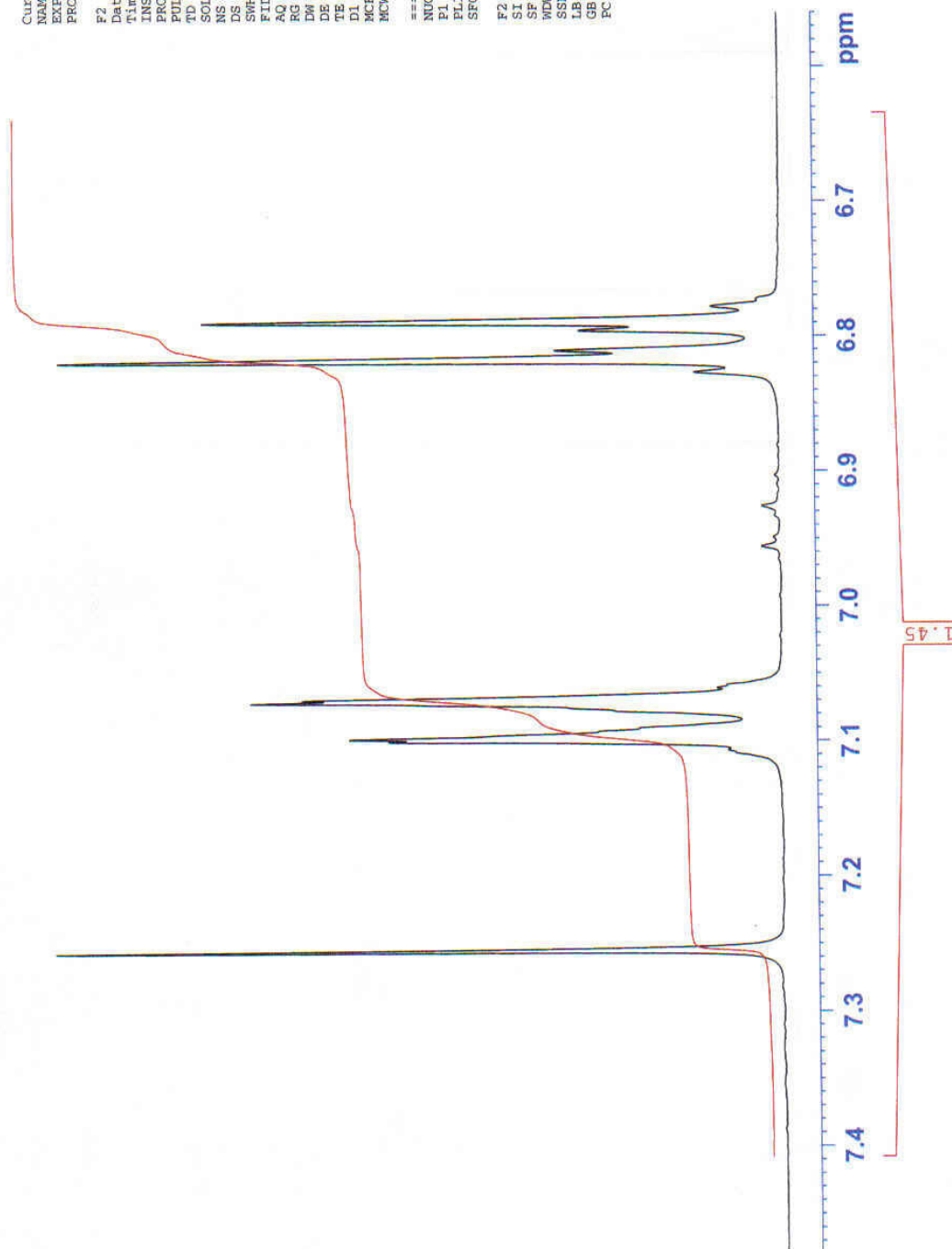
P. Nut
22/8/05

Current Data Parameters
 NAME 10371787
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20050819
 Time_ 18:51
 INSTRUM dpx300
 PROBD 5 mm QNP 1H/1
 PULPROG zg30
 TD 48848
 SOLVENT CDCL3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.3998709 sec
 RG 32
 DE 69.600 usec
 TE 299.2 K
 DI 6.5999990 sec
 MCREST 0.0000000 sec
 MCWRR 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SFO1 300.1330010 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1300078 MHz
 EX
 WDW 0
 SSB 0.30 Hz
 LB 0
 GB 0
 PC 2.00



P. N. N. N.
 22/8/07



```
;zg30
;advance-version (02/05/31)
;1D sequence
;using 30 degree flip angle
```

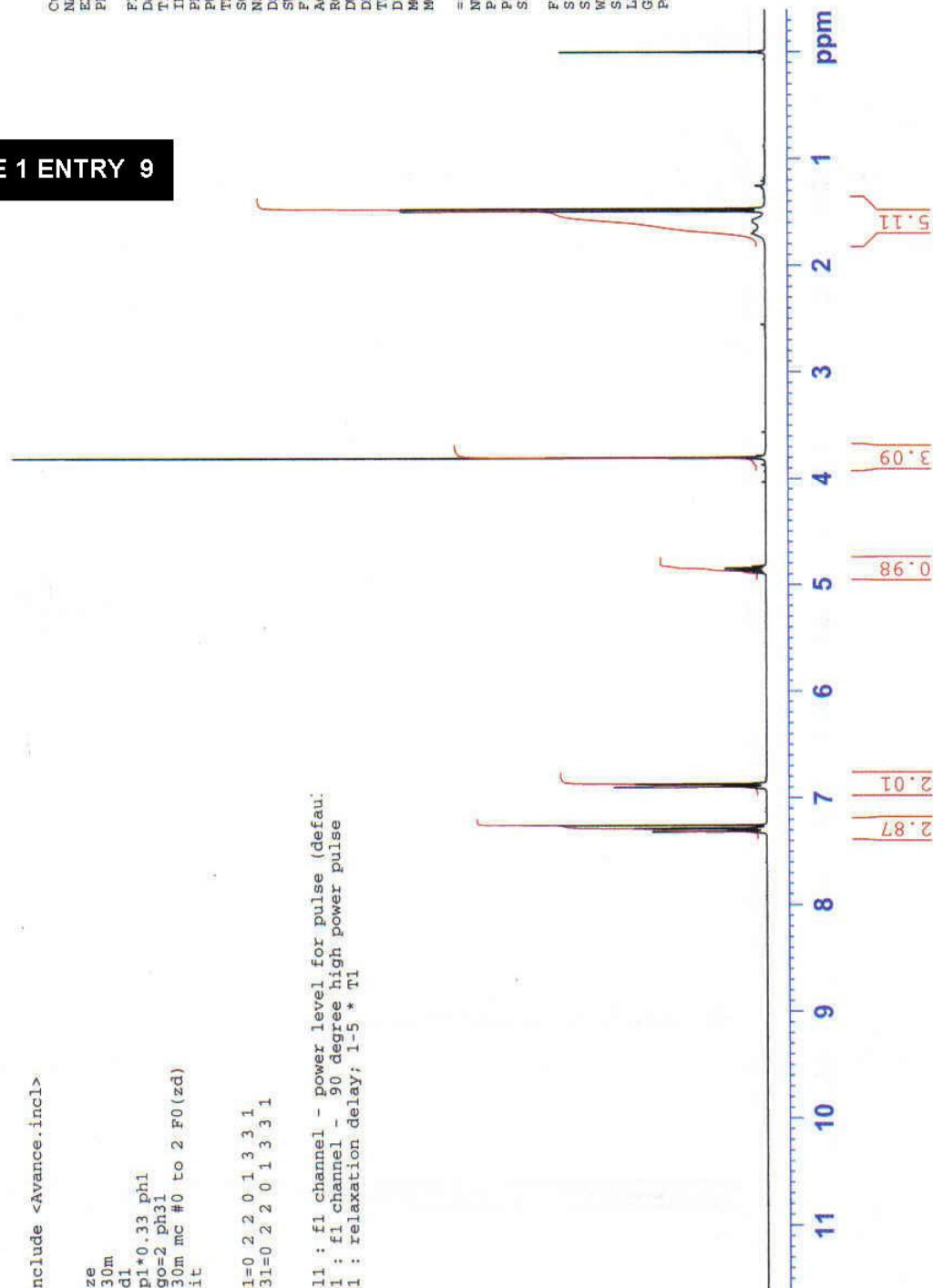
```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

TABLE 1 ENTRY 9



```
Current Data Parameters
NAME 10368721
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050609
Time 14.12
INSTRUM qnp300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
AQ 0.147067 Hz
RG 3.3998709 sec
FIDRES 724.1
DE 69.600 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```

D. Nurb
10/6/05



10383512, RX0002/40A, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:- CDCl3/TMS

```
;zg30
;avance-version (02/05/31)
;1d sequence
;using 30 degree flip angle
```

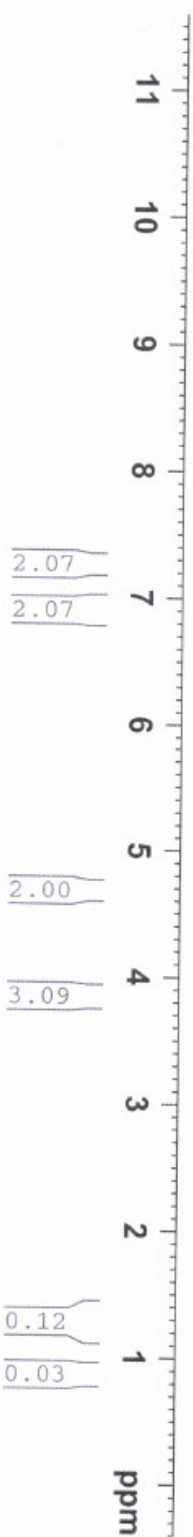
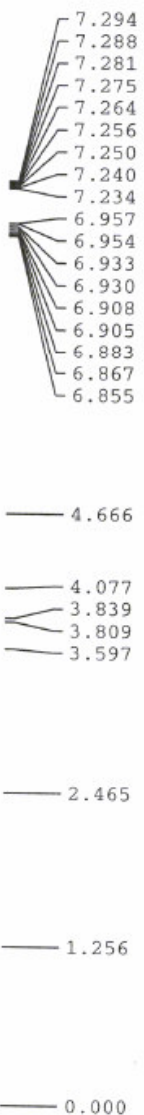
```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power leve
;p1 : f1 channel - 90 degree
;dl : relaxation delay; 1-5 *
```

TABLE 2 ENTRY 1



Intertek ASG

Current Data Parameters
NAME 10383512
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060713
Time 12.01
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 101.6
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz
F2 - Processing Parameters
SI 65536
SF 300.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 300.00

S.N. 131710e

10383512, RX0002/40A, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:- CDCl3/TMS

```

;zg30
;advance-version (02/05/31)
;1D sequence
;using 30 degree flip angle
7.294
7.288
7.281
7.275
7.264
7.256
7.250
7.240
7.234
9.957
9.954
9.933
9.930
9.908
9.905
9.883
9.867
9.855

```

#include <Avance.incl>

```

1 ze
2 30m
d1
p1*0.33 p1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit

```

```

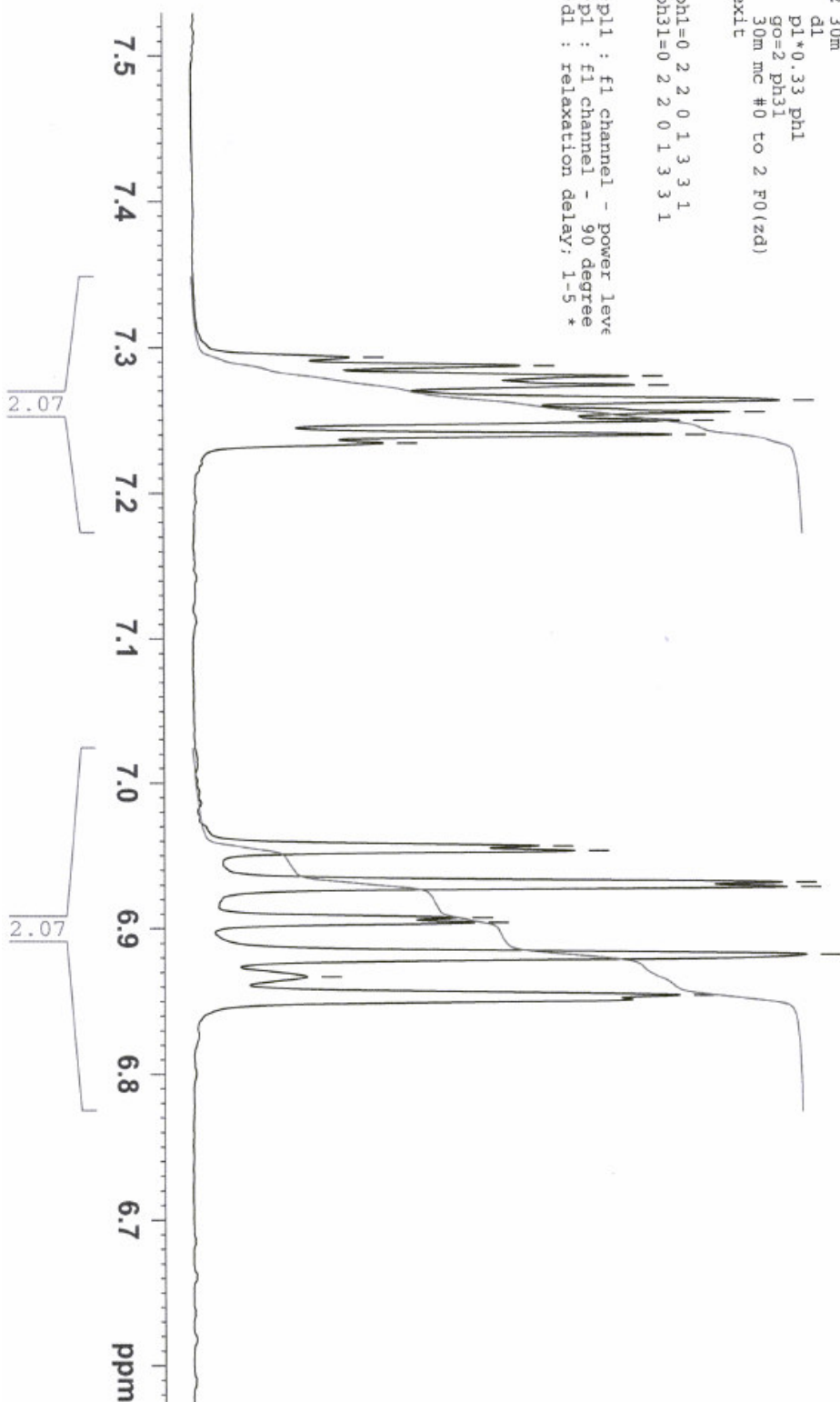
p1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

```

```

;p1 : f1 channel - power level
;p1 : f1 channel - 90 degree
;dl : relaxation delay; 1-5 *

```



Intertek ASG

Current Data Parameters
NAME 10383512
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060713
Time 12.01

INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64

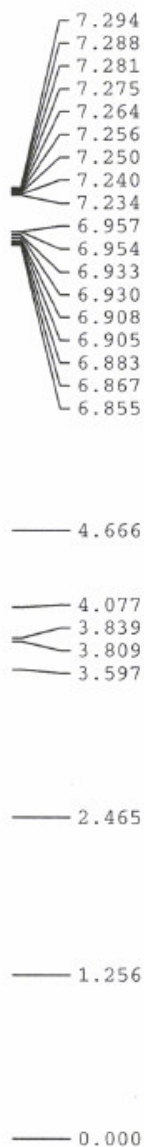
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 101.6
DM 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing Parameters
SI 65536
SF 300.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 300.00

S. 131710a

10383512, RX0002/40A, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV;- CDCl3/TMS

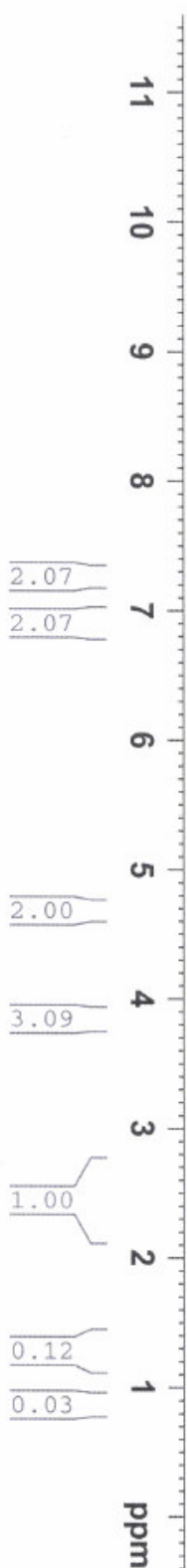


#include <Avance.incl>

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power leve
;p1 : f1 channel - 90 degree
;d1 : relaxation delay; 1-5 *
```



Intertek ASG

Current Data Parameters
NAME 10383512
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060713
Time 12.01
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 101.6
DM 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz
F2 - Processing parameters
SI 65536
SF 300.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 300.00

Handwritten signature and date:
20/7/06

Intertek ASG

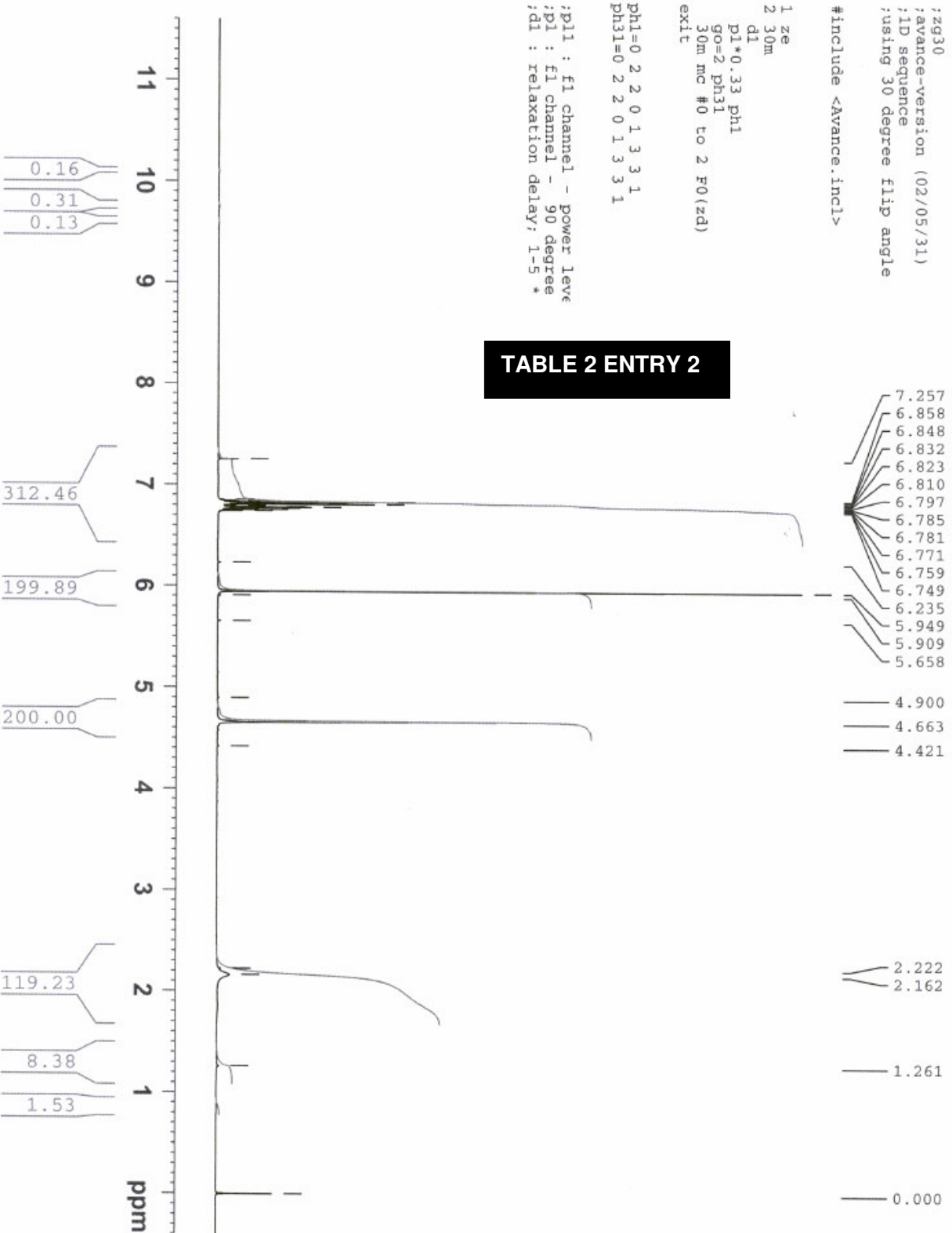
```
;zg30
;avance-version (02/05/31)
;ID sequence
;using 30 degree flip angle
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power leve
;p1 : f1 channel - 90 degree
;d1 : relaxation delay; 1-5 *
```

TABLE 2 ENTRY 2



Current Data Parameters
NAME 10383516
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060713
Time 12.54
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDC13
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 128
DM 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz
F2 - Processing parameters
SI 65536
SF 300.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 100.00

S.v
1317/100

10383614, RX0002/42A, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

Intertek ASG

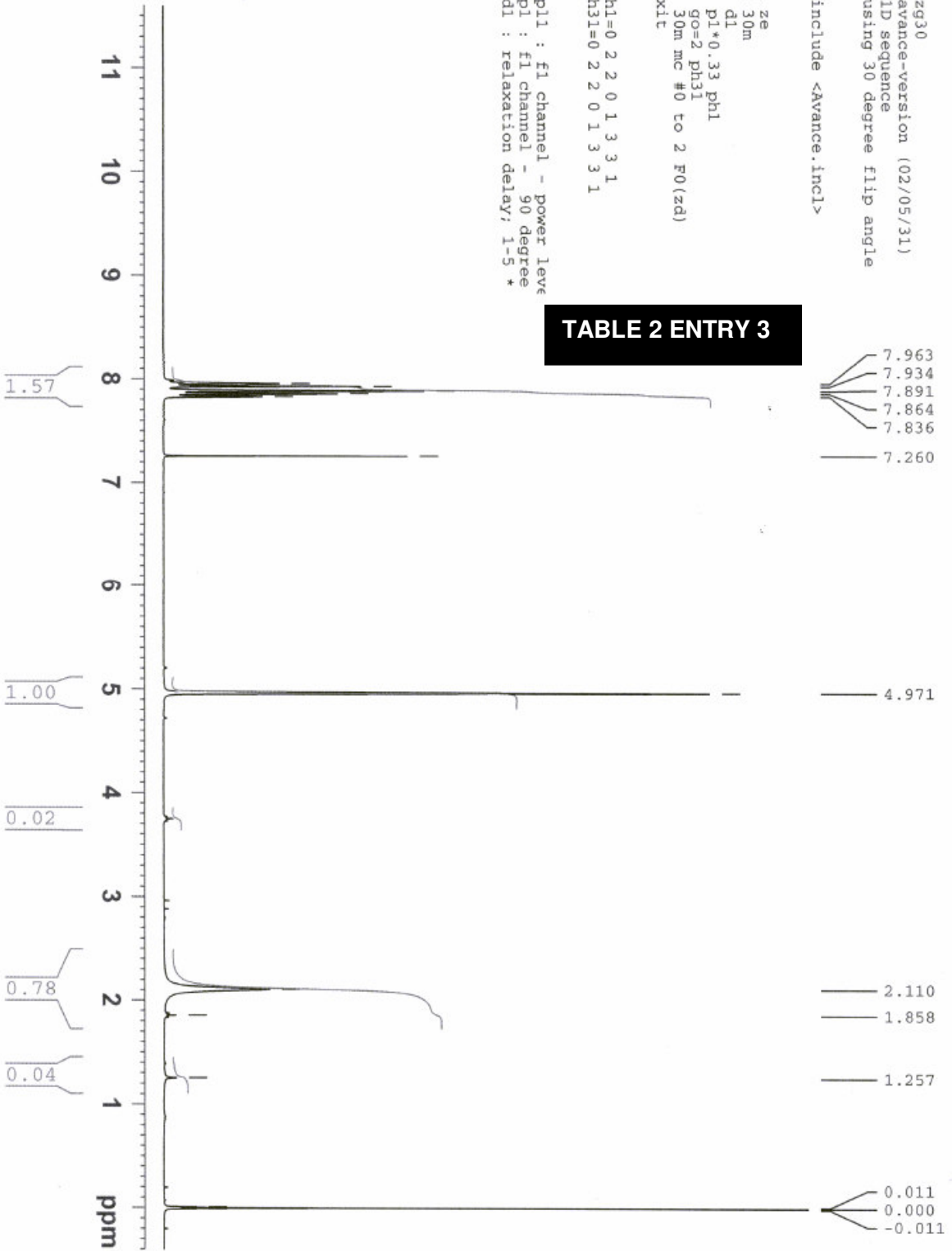
```
;zg30
;advance-version (02/05/31)
;ID sequence
;using 30 degree flip angle
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power leve
;p1 : f1 channel - 90 degree
;dl : relaxation delay; 1-5 *
```

TABLE 2 ENTRY 3



Current Data Parameters
NAME 10383614
EXPNO 10
PROCNO 1

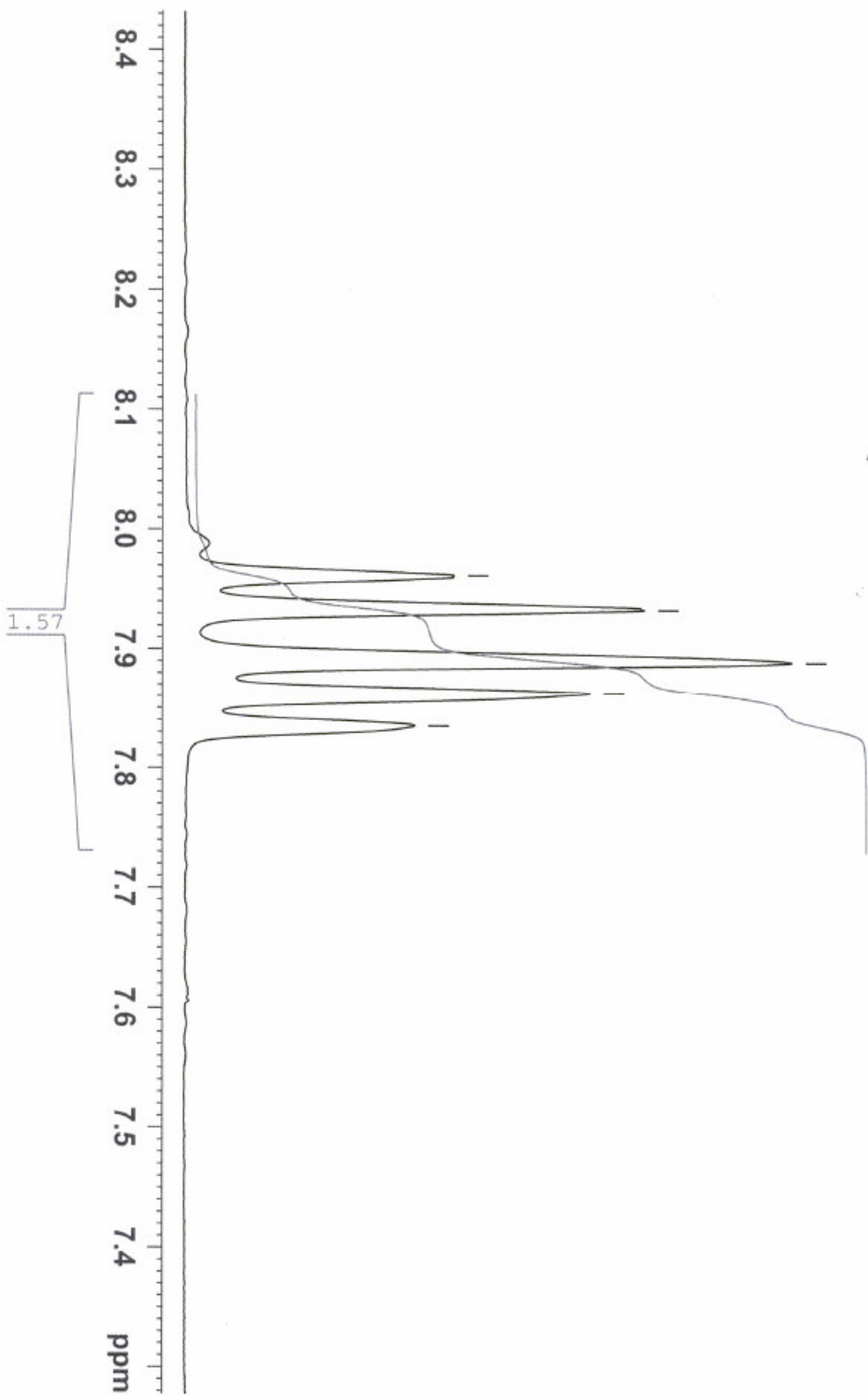
F2 - Acquisition Parameters
Date_ 20060717
Time 12.53
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 724.1
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCNRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz
F2 - Processing parameters
SI 65536
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

D. H. A.
18/7/06

10383614, RX0002/42A, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

7.963
7.934
7.891
7.864
7.836



Intertek **ASG**

Current Data Parameters
NAME 10383614
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060717
Time 12.53
INSTRUM gpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3989709 sec
RG 724.1
RW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCPRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing Parameters
SI 65536
SF 300.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

0.166

10383515, RX0002/40C, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:- CDCl3/TMS

```
;zg30
;advance-version (02/05/11)
;1d sequence
;using 30 degree flip angle
```

0.067
0.059
0.049
0.037
0.026
0.019
7.293
7.286
7.275
7.264
7.253
7.246
7.123
7.116
7.094
7.065
7.038
7.029
7.021
7.007
7.000
6.992
6.977
6.970
6.961

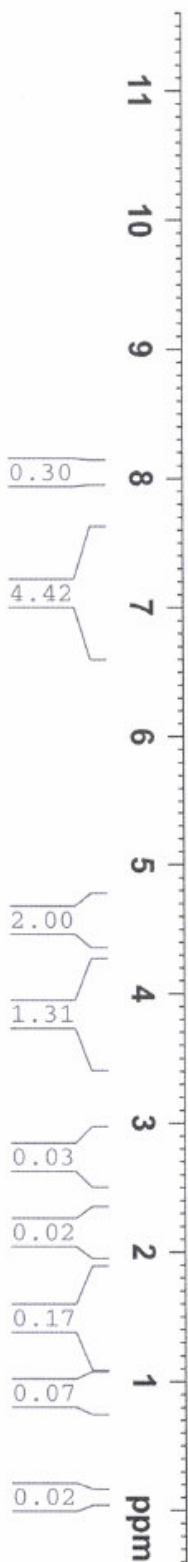
```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power leve
;p1 : f1 channel - 90 degree
;d1 : relaxation delay: 1-5 *
```

TABLE 2 ENTRY 4



Intertek ASG

Current Data Parameters
NAME 10383515
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060713
Time 13.12
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 71.8
DM 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
ICREST 0.00000000 sec
MCMRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz
F2 - Processing parameters
SI 65536
SF 300.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 250.00

S.A.
1317100

10383515, RX0002/40C, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:- CDCl3/TMS

```
;zg30
;adv-verse 102.05/31)
;1d sequence
;using 30 degree flip angle
```

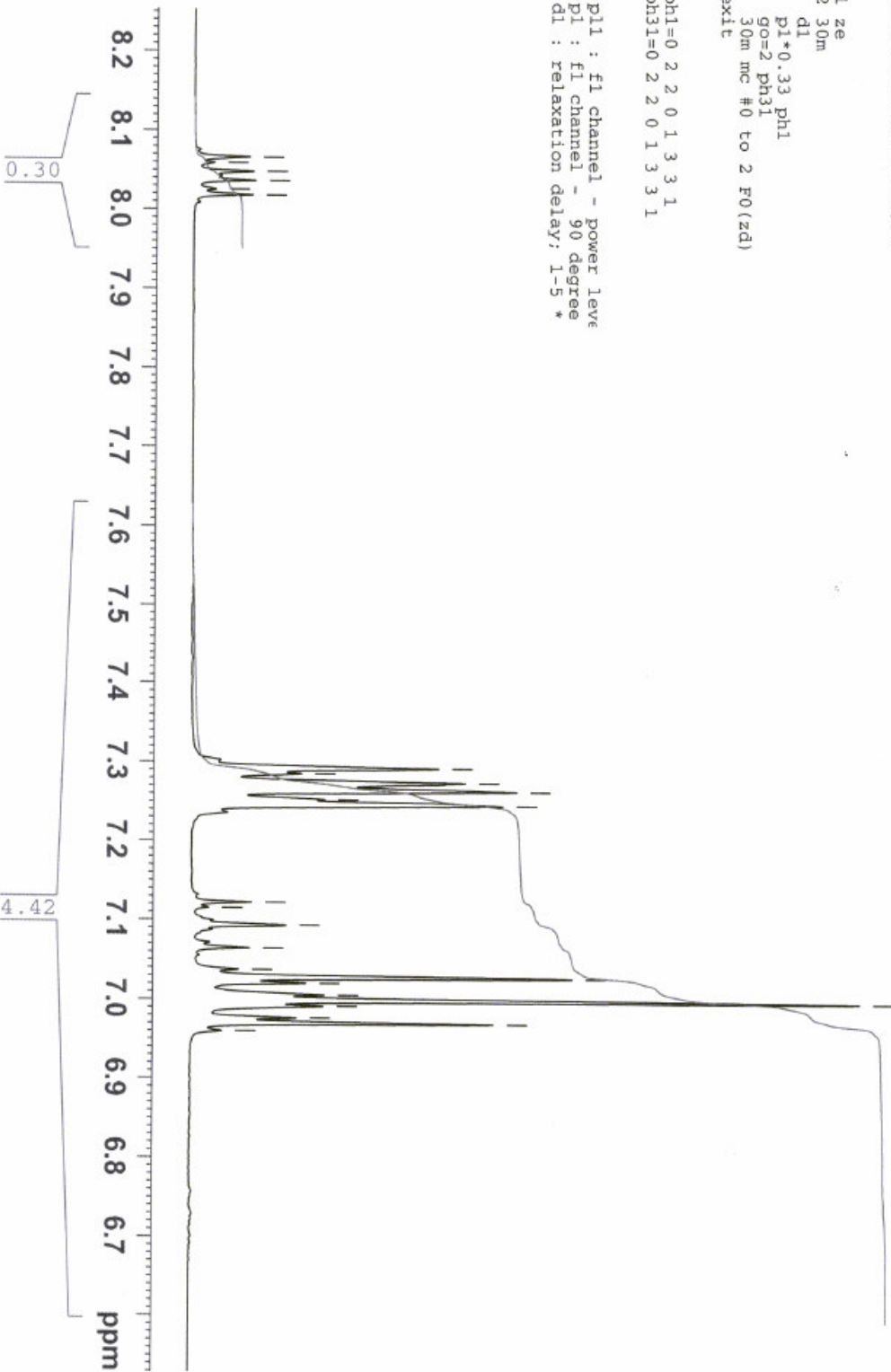
7.293
7.286
7.275
7.264
7.253
7.246
7.123
7.116
7.094
7.065
7.038
7.029
7.021
7.007
7.000
6.992
6.977
6.970
6.961

```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power leve
;p1 : f1 channel - 90 degree
;d1 : relaxation delay; 1-5 *
```



Intertek ASG

Current Data Parameters
NAME 10383515
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060713
Time 13.12
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 71.8
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59899990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing Parameters
SI 65536
SF 300.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 250.00

5.1710e

```
;zg30
;advance-version (02/05/31)
;1d sequence
;using 30 degree flip angle
```

```
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p11 : f1 channel - power level for pulse (defau
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

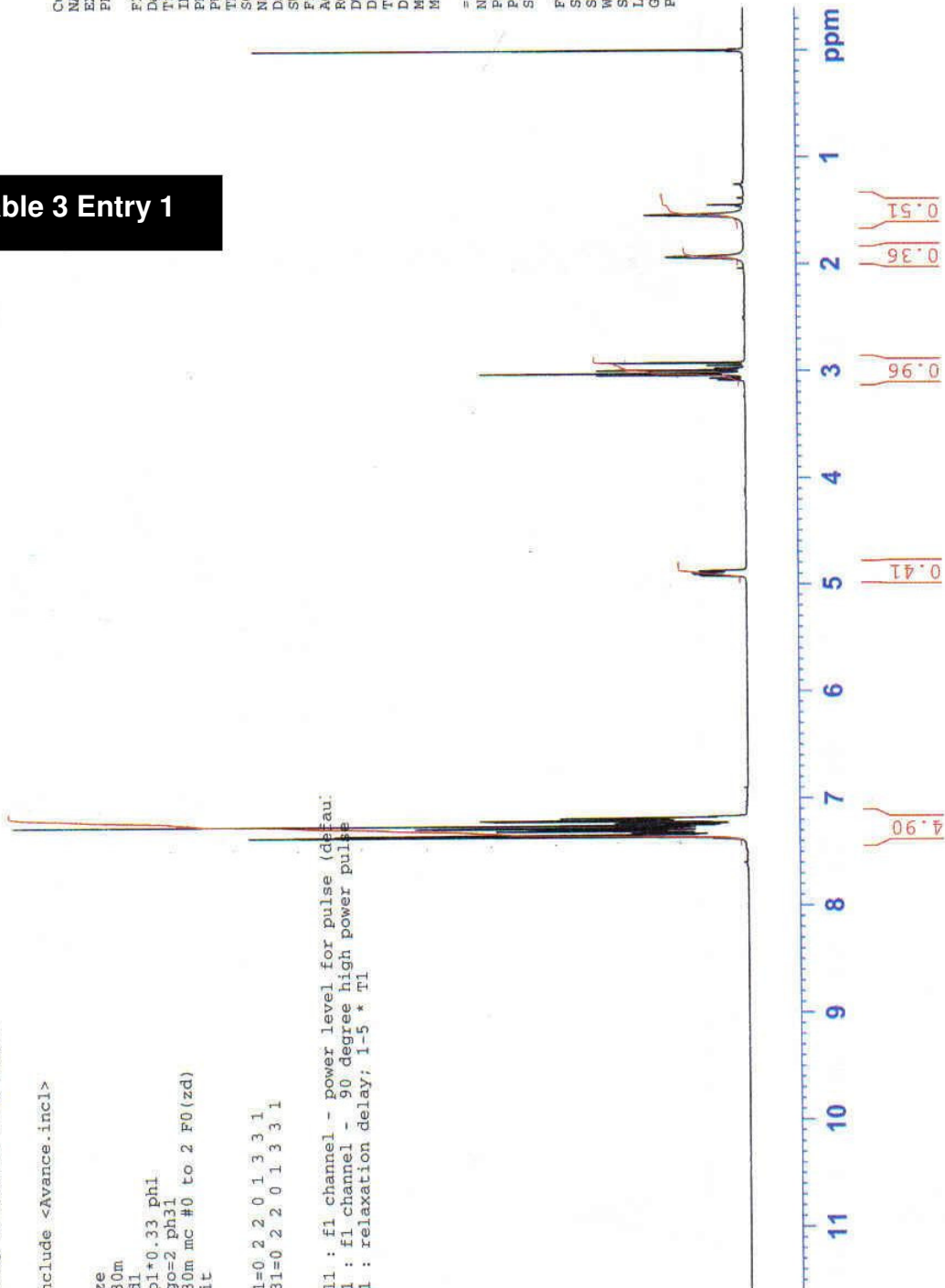
Table 3 Entry 1

```
Current Data Parameters
NAME 10368288
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050526
Time 21.12
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCL3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 724.1
DE 69.600 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

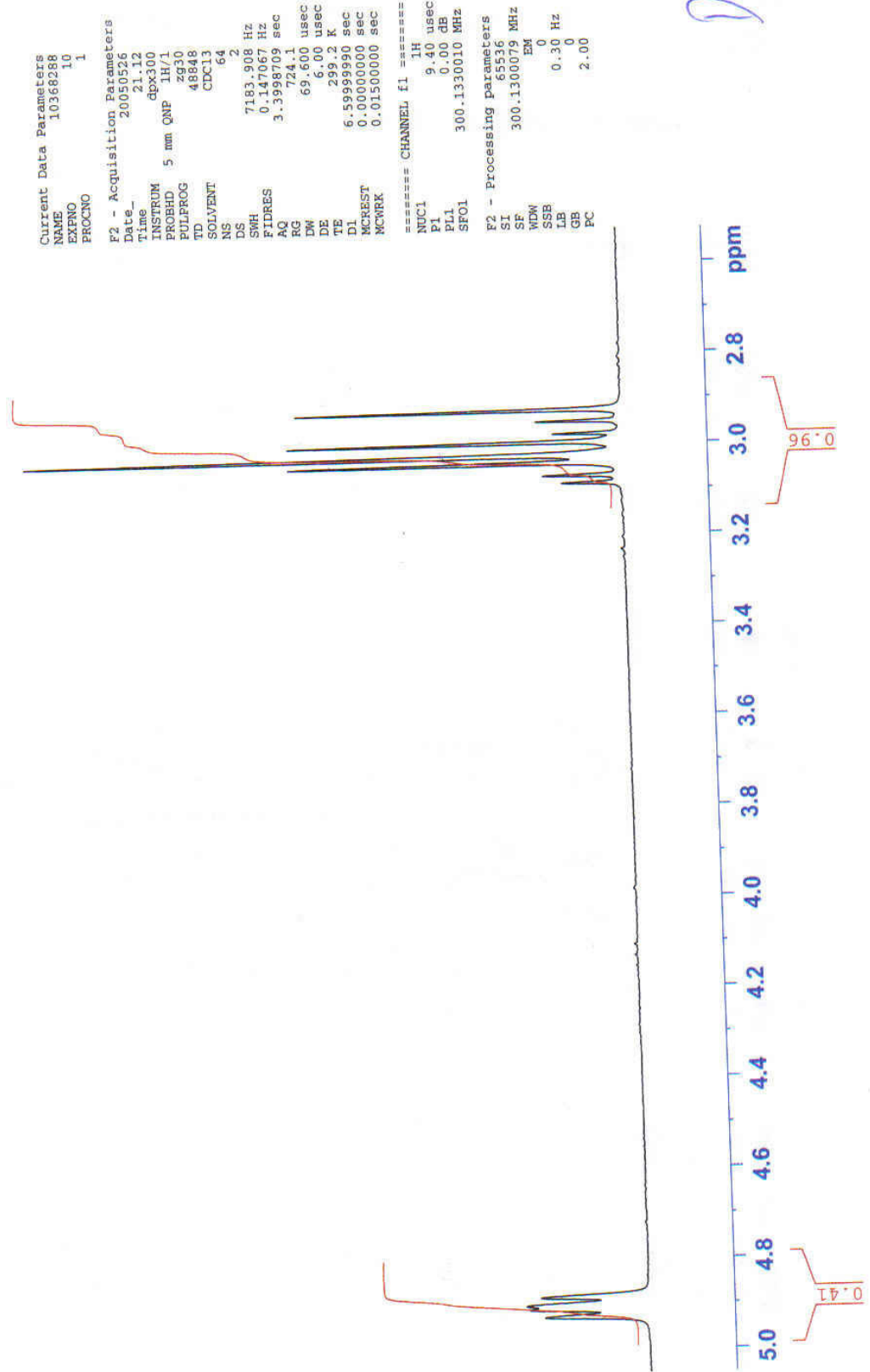
===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```



D. North
27/5/05

10368288, NBZ5769/1/8, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:- CDCL3/TMS



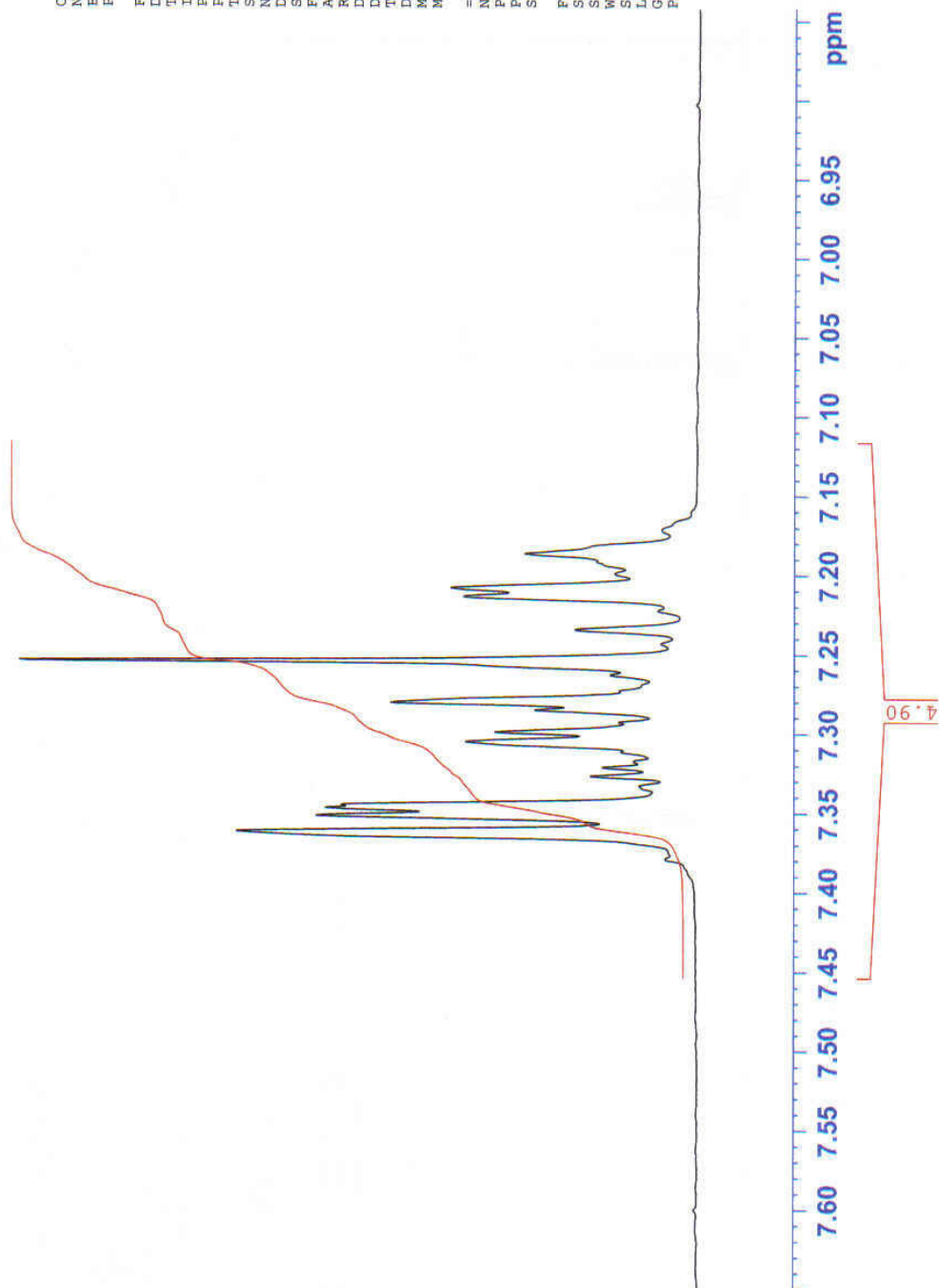
D. M. G.
 27/5/05

Current Data Parameters
NAME 10368288
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050526
Time 21.12
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCL3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 724.1
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300079 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00



D-164
27/5/05


```

;zg30
;advance-version (02/05/31)
;ld sequence
;using 30 degree flip angle

```

```

#include <Avance.incl>

```

```

1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit

```

```

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

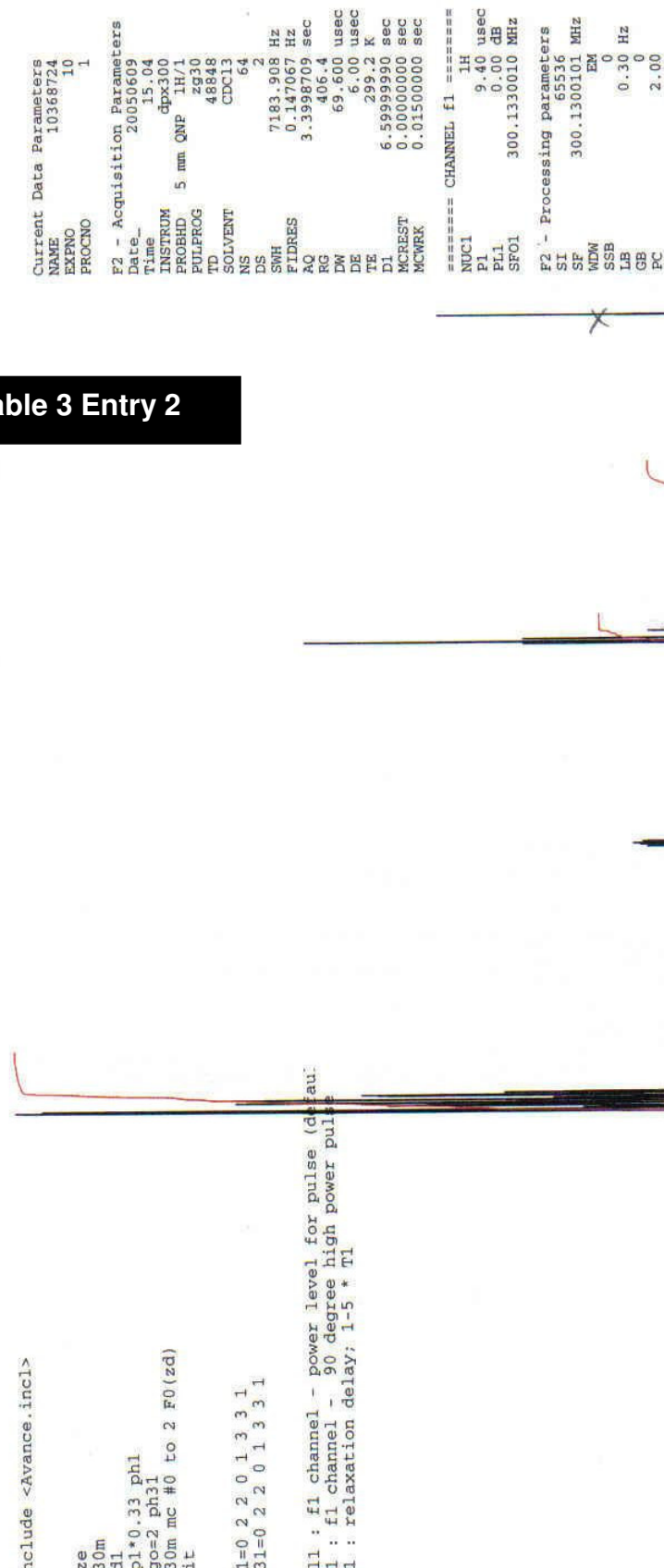
```

```

;p11 : f1 channel - power level for pulse (default)
;pi : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1

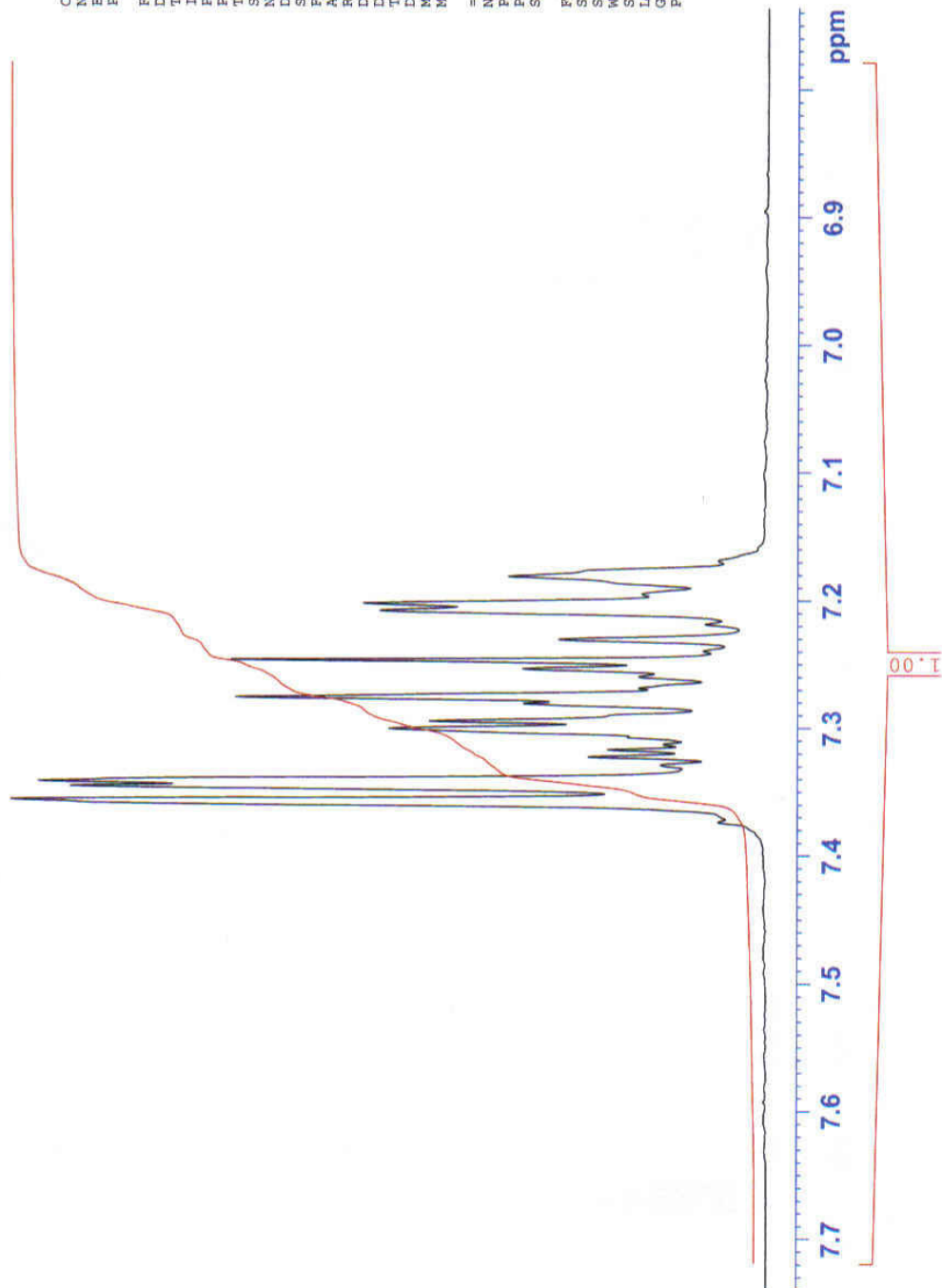
```

Table 3 Entry 2



J. N. N. N.
10/6/05

10368724, NBZ5769-9-4, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV: CDCL3/TMS



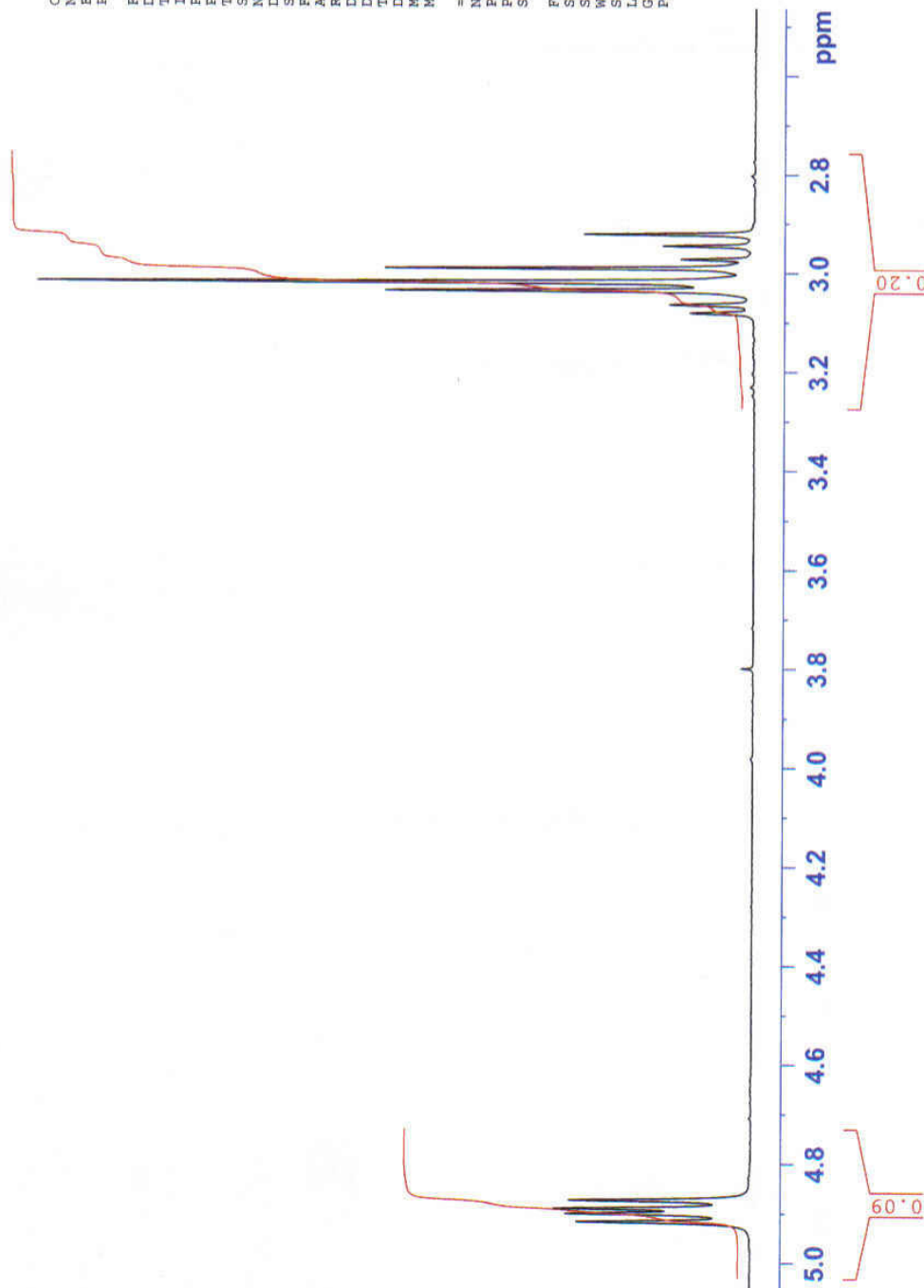
Current Data Parameters
NAME 10368724
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050609
Time 15.04
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 406.4
DM 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

J. New
10/6/05



D. N. M. H.
10/6/05

```

;zg30
;advance-version (02/05/31)
;1D sequence
;using 30 degree flip angle

```

```

#include <Advance.incl>

```

```

1 ze
2 30m
d1
  pl*0.33 ph1
  go=2 ph31
  30m mc #0 to 2 F0(zd)
exit

```

```

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

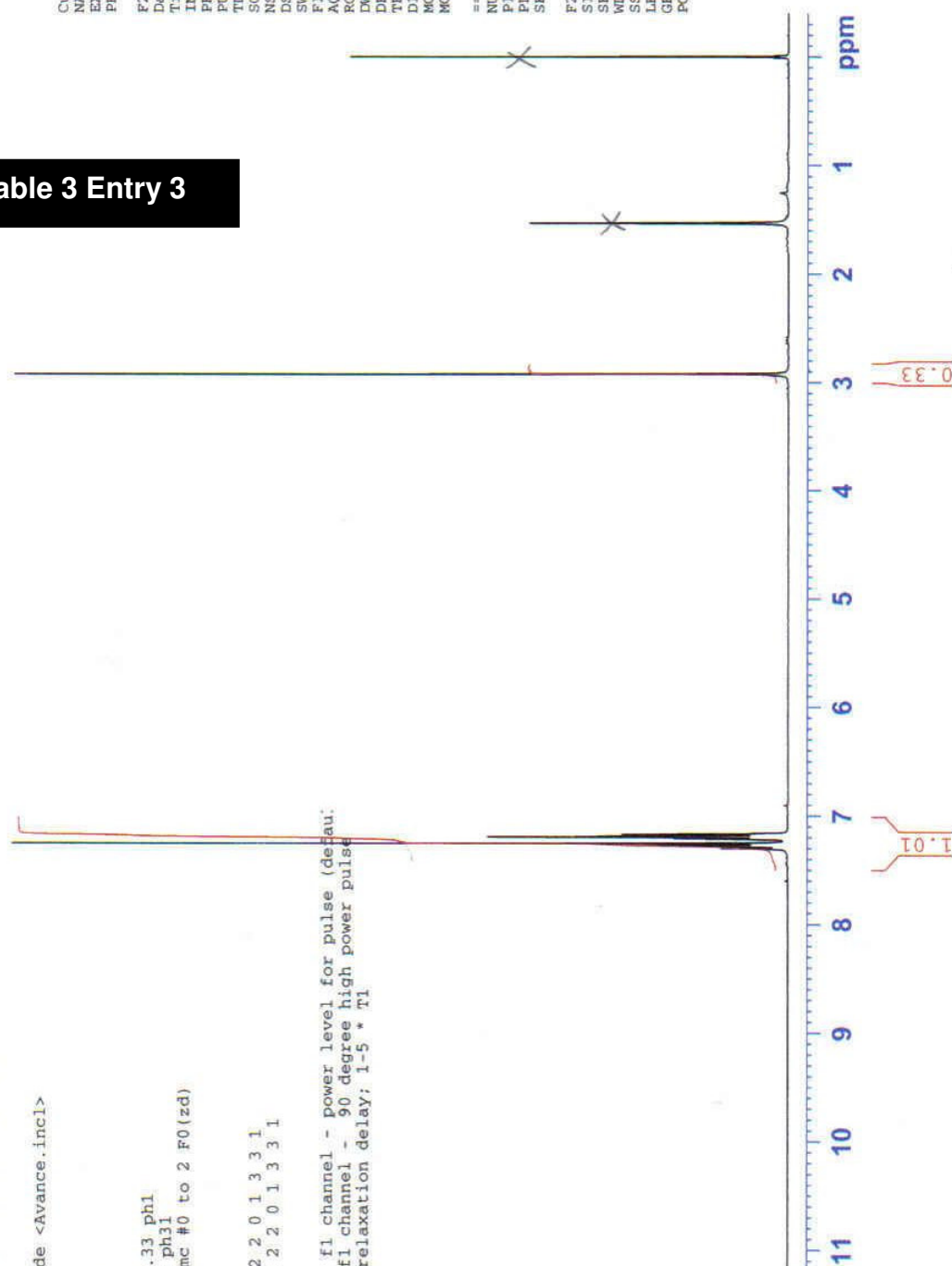
```

```

;pl1 : f1 channel - power level for pulse (default)
;pl : f1 channel - 90 degree high power pulse
;d1 : relaxation delay: 1-5 * T1

```

Table 3 Entry 3



```

Current Data Parameters
NAME 10368725
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050609
Time 15.21
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 1290.2
DE 69.600 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRRK 0.01500000 sec

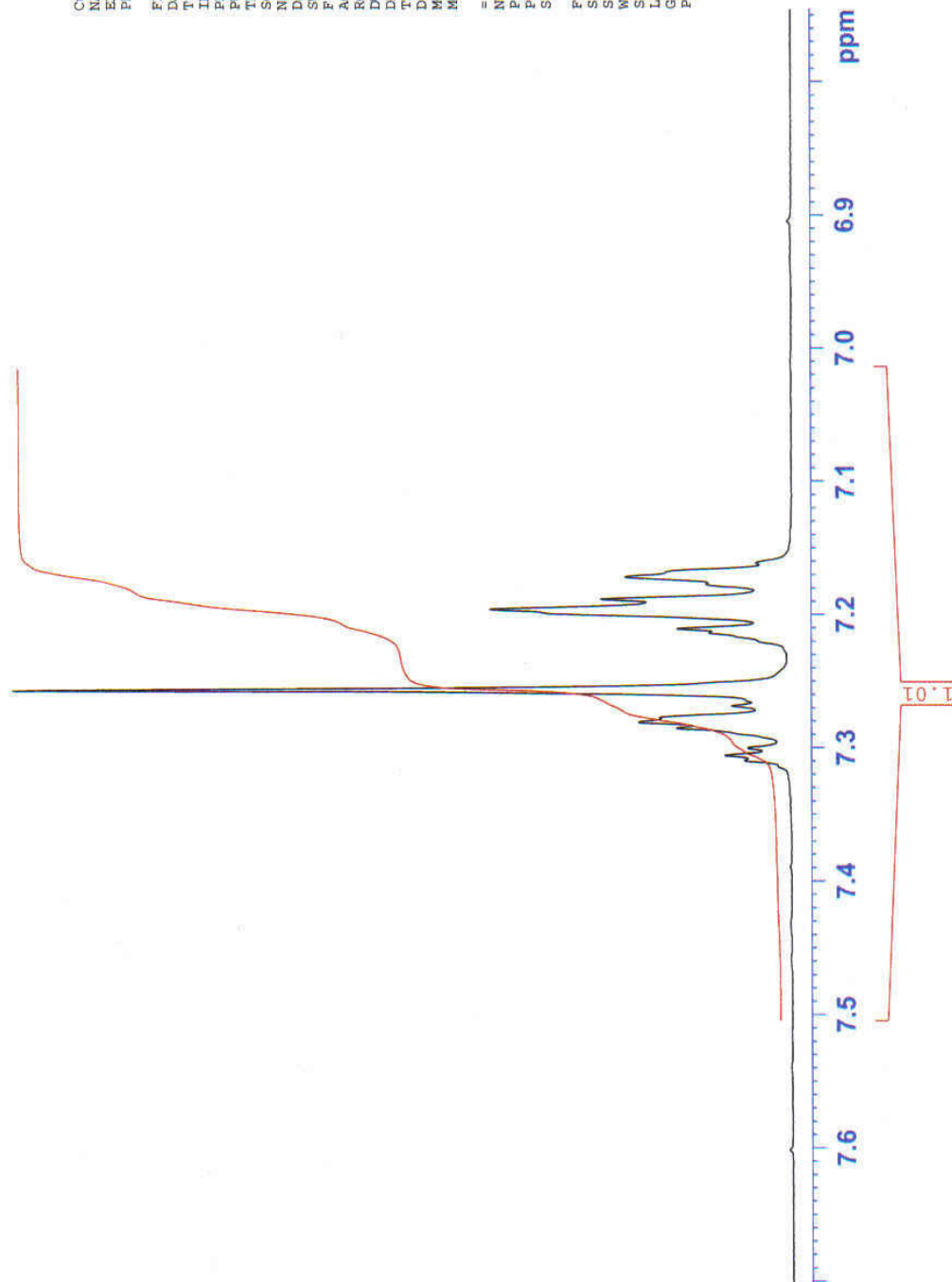
===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

```

D. N. N. N.
10/6/05

10368725, NBZ5769-9-5, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV: CDCL3/TMS



Current Data Parameters
NAME 10368725
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050609
Time 15.21
INSTRUM qnp300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCL3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 1290.2
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

D. West
10/6/05


```
;zg30
;advance-version (02/05/31)
;1D sequence
;using 30 degree flip angle
```

```
#include <Advance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power level for pulse (default)
;p1 : f1 channel - 90 degree high power pulse
;d1 : relaxation delay; 1-5 * T1
```

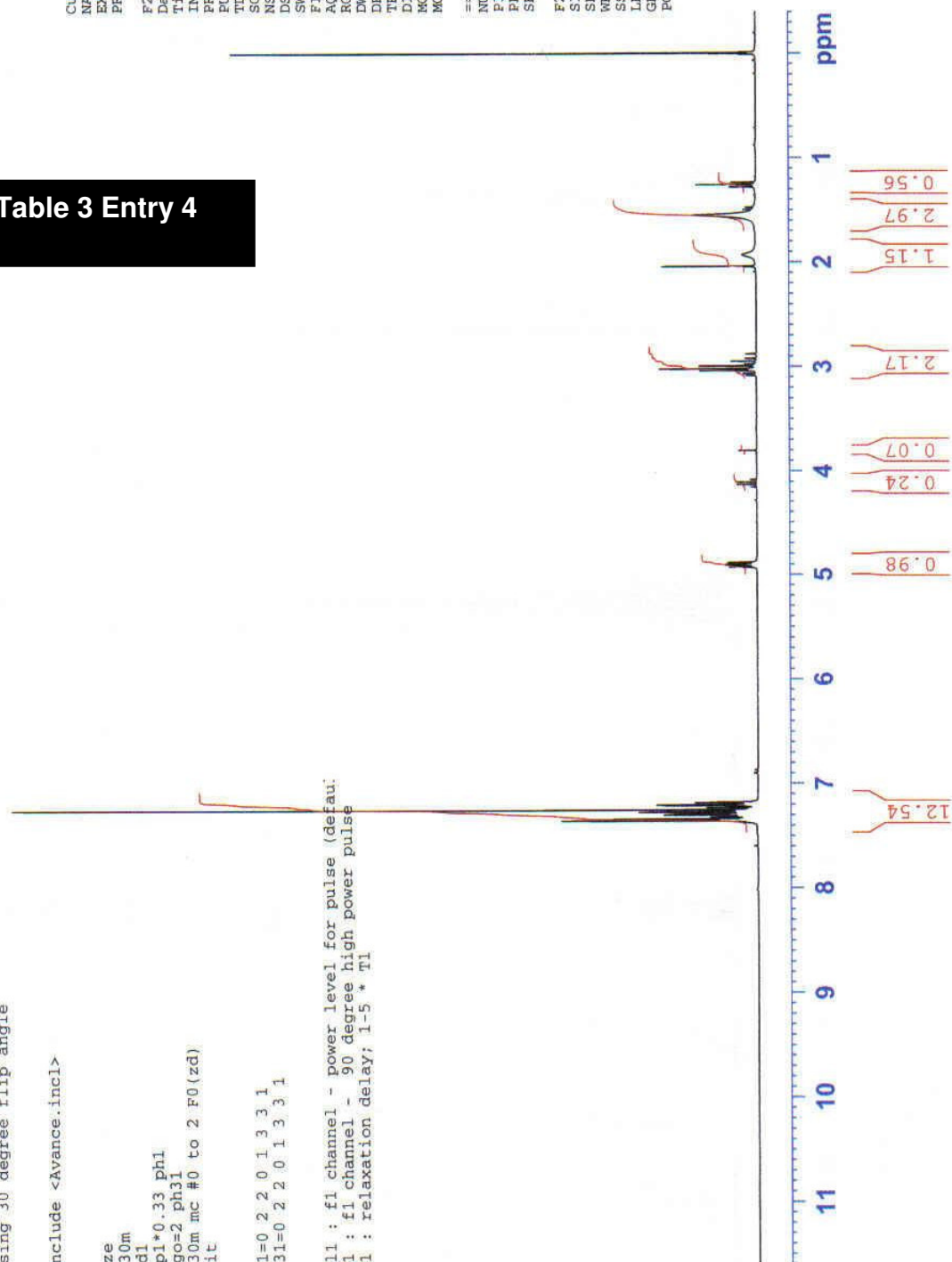
Table 3 Entry 4

```
Current Data Parameters
NAME 10368961
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20050615
Time 12.27
INSTRUM dpx300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 1290.2
DE 69.600 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.0000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```



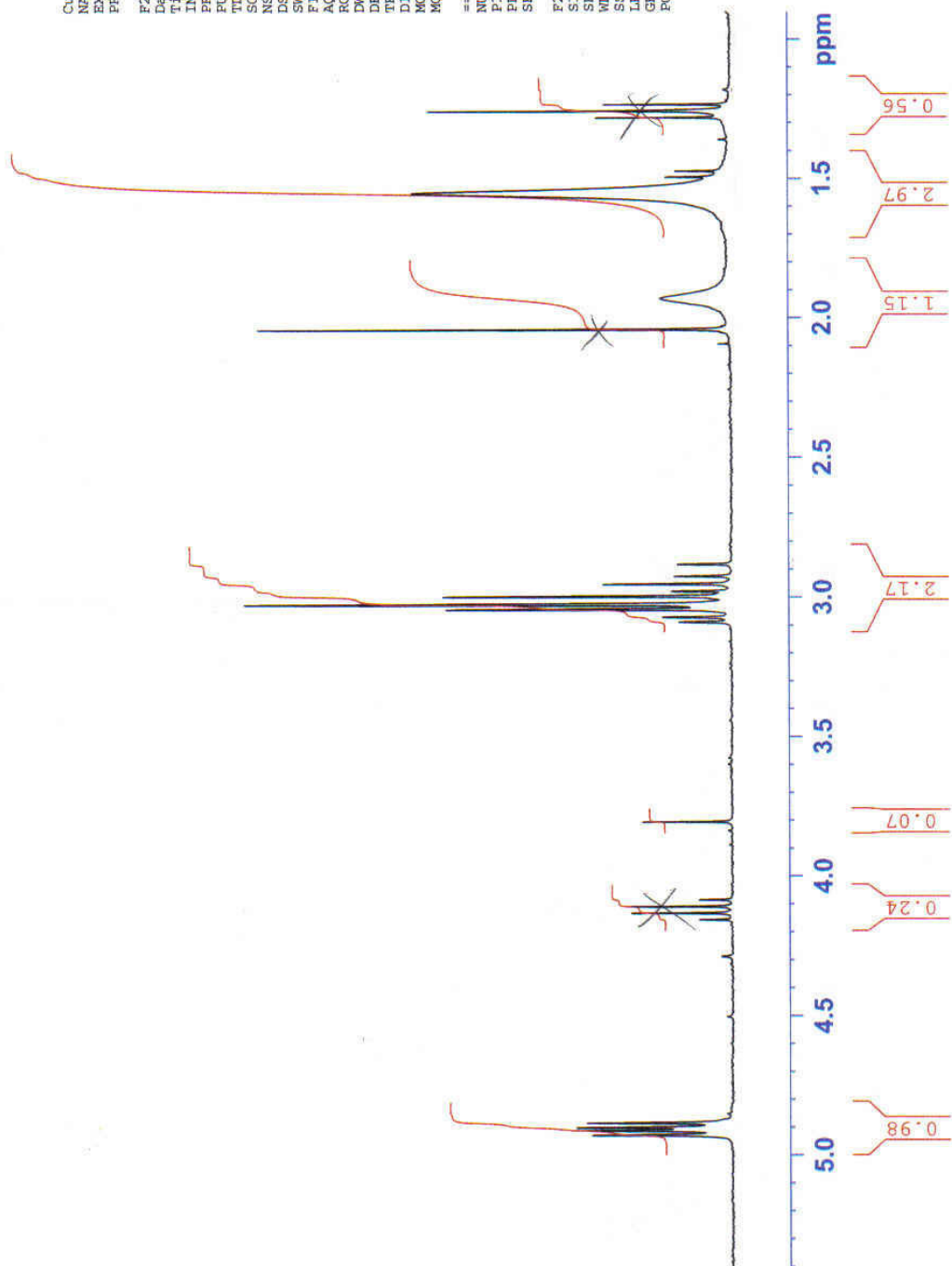
P. Nut
16/6/05

Current Data Parameters
 NAME 10368961
 EXPNO 10
 PROCNO 1

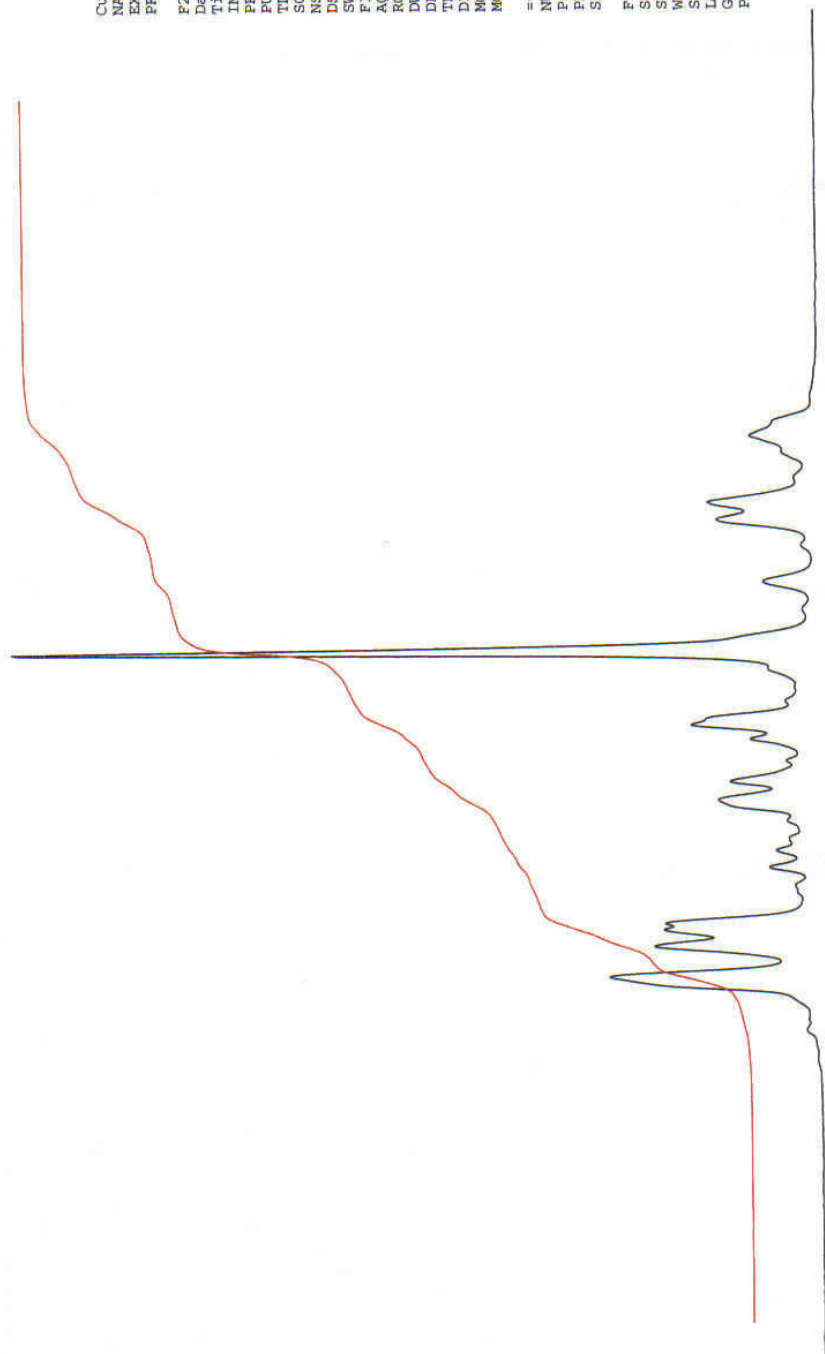
F2 - Acquisition Parameters
 Date_ 20050615
 Time 12.27
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 48848
 SOLVENT CDCL3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.3998709 sec
 RG 1290.2
 DW 69.600 usec
 DE 6.00 usec
 TE 299.2 K
 D1 6.5999990 sec
 MCREST 0.0000000 sec
 MCWCK 0.0150000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SF01 300.1330010 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1300068 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00



J. Dut
 16/6/05



7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 ppm

12.54

Current Data Parameters
 NAME 10368961
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20050615
 Time 12.27
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 48848
 SOLVENT CDCL3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.3998709 sec
 RG 1290.2
 DW 69.600 usec
 DE 6.00 usec
 TE 299.2 K
 D1 6.59999990 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SFO1 300.1330010 MHz
 F2 - Processing parameters
 SI 65536
 SF 300.1300068 MHz
 EM 0
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

D. Dub

16/6/05

Signature

```

;zg30
;avance-version (06/05/31)
;1d sequence
;using 30 degree flip angle
#include <Avance.incl>

```

7.395
7.372
7.348
7.338
7.332
7.317
7.313
7.309
7.303
7.290
7.248
7.237
7.226
7.212

3.874
3.852
3.830
3.685
3.677

2.886
2.864
2.842

1.553
1.251
1.228

0.000

```

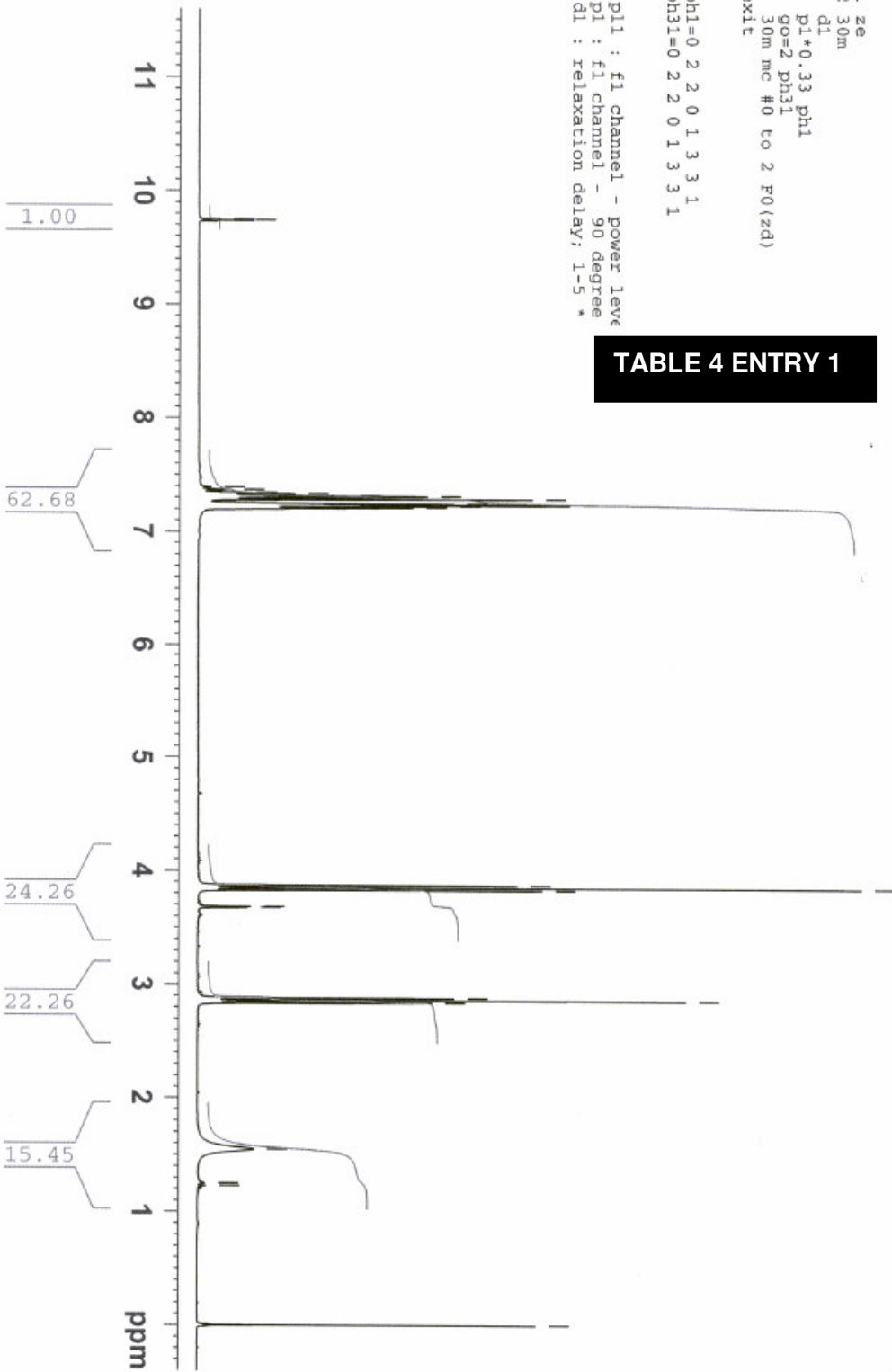
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit

ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

;p1: f1 channel - power leve
;pl: f1 channel - 90 degree
;dl: relaxation delay; 1-5 *

```

TABLE 4 ENTRY 1



Intertek ASG

Signature

```

Current Data Parameters
NAME 10383689
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060719
Time 12.00
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 322.5
DM 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1350010 MHz

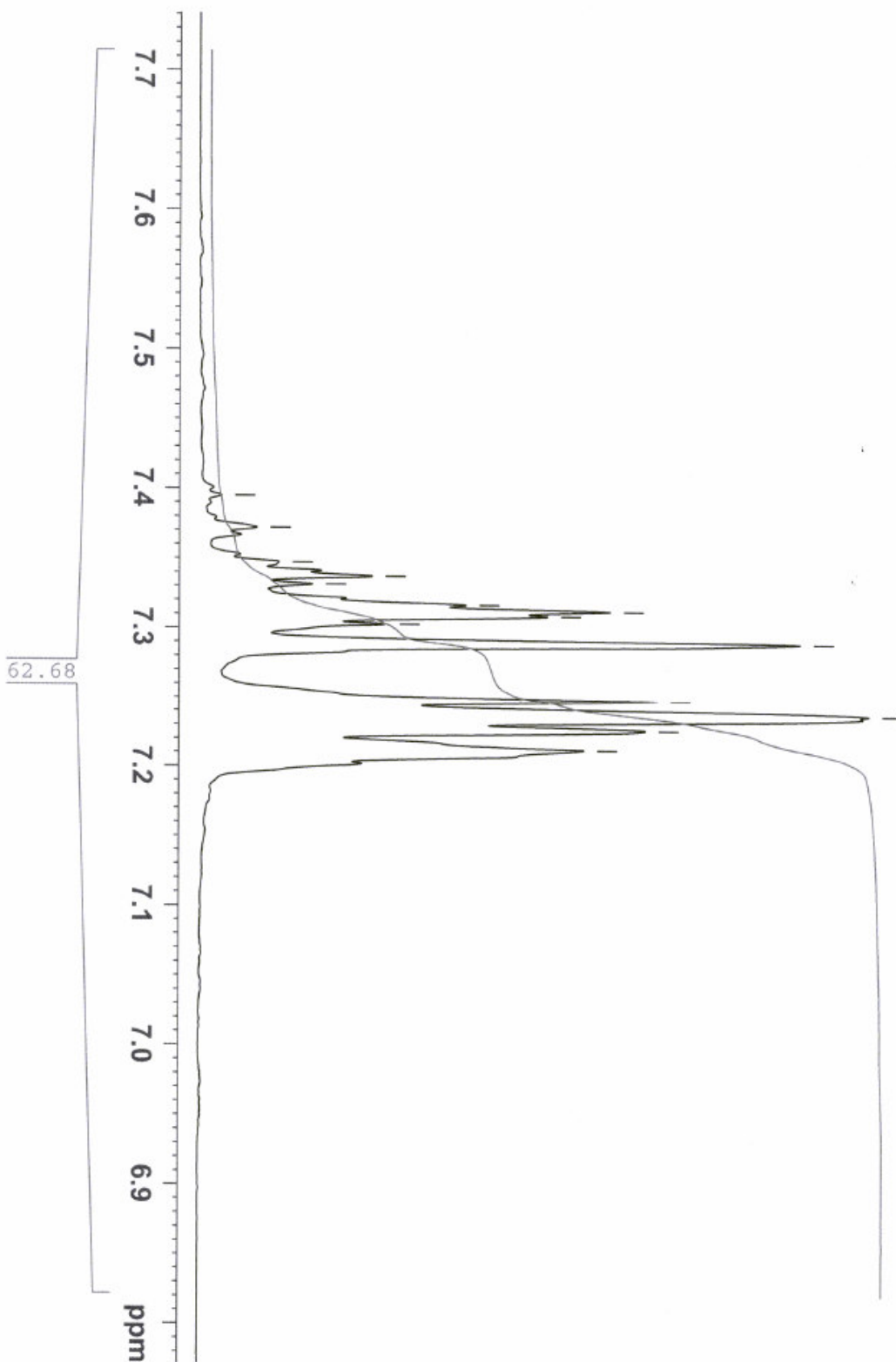
F2 - Processing parameters
SI 65536
SF 300.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 20.00

```

P. West
1917106

10383689, RX0002/44A, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCl3/TMS

7.395
7.372
7.348
7.338
7.332
7.317
7.313
7.309
7.303
7.290
7.248
7.237
7.226
7.212



Intertek ASG

Current Data Parameters
NAME 10383689
EXPNO 10
PROCNO 1

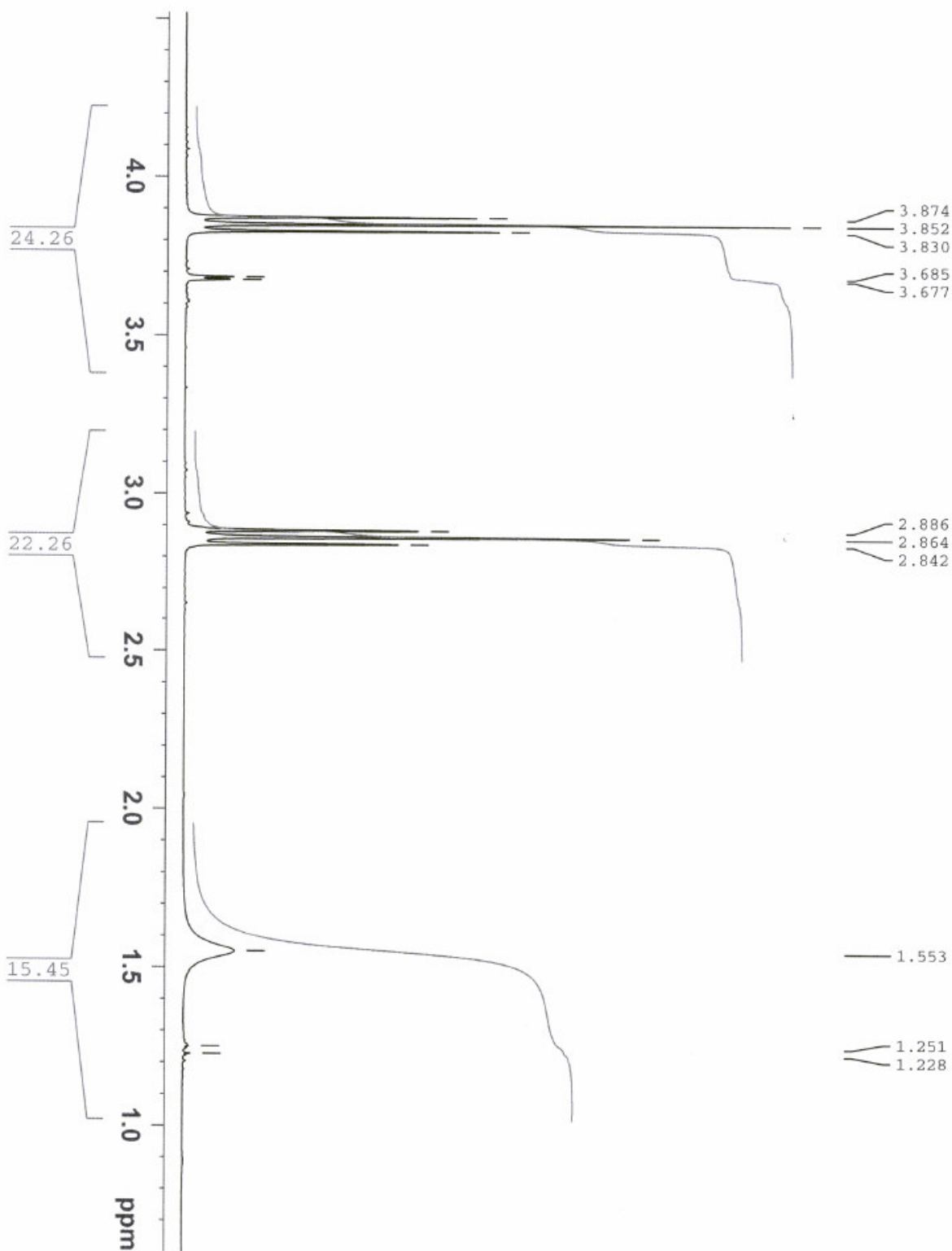
F2 - Acquisition Parameters
Date_ 20060719
Time 12.00
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 322.5
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing Parameters
SI 65536
SF 300.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 20.00

D. Nutt
1/17/06

10383689, RX0002/44A, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCl3/TMS

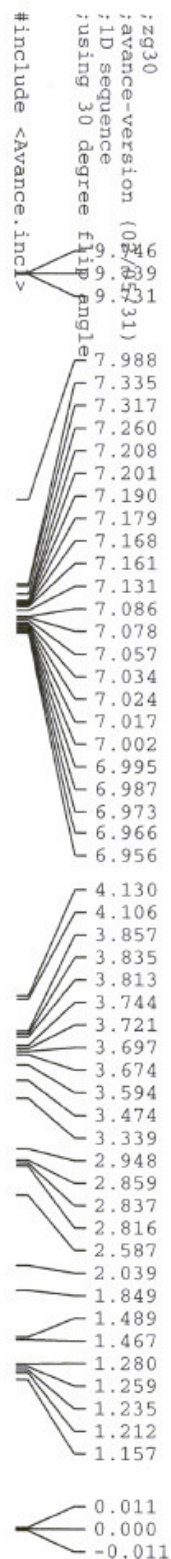


Intertek ASG

Current Data Parameters
 NAME 10383689
 EXPNO 10
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20060719
 Time 12.00
 INSTRUM dpx300
 PROBD 5 mm QNP 1H/13
 PULPROG zg30
 TD 48848
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.3998709 sec
 RG 322.5
 DW 69.600 usec
 DE 6.00 usec
 TE 299.2 K
 D1 6.59999990 sec
 MCREST 0.00000000 sec
 MCPRK 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SFO1 300.1330010 MHz
 F2 - Processing parameters
 SI 65536
 SF 300.1300095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 20.00

P. Hunt
 19/7/06

10383690, RX0002/44B, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

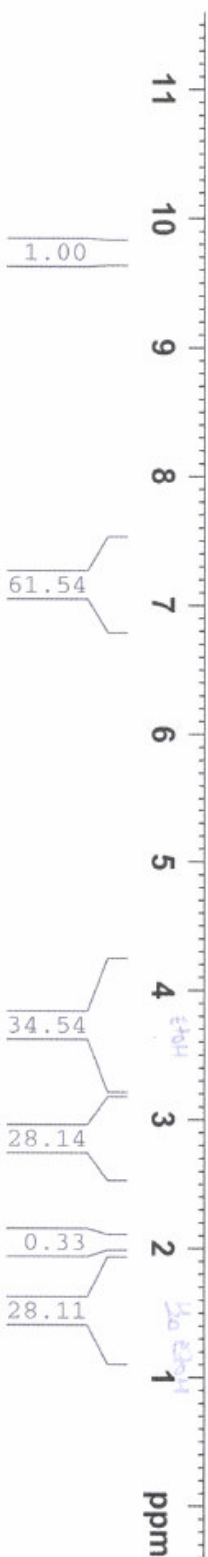


```

1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
; p1 : f1 channel - power leve
; p1 : f1 channel - 90 degree
; d1 : relaxation delay: 1-5 *

```

TABLE 4 ENTRY 2



Intertek ASG

Current Data Parameters
NAME 10383690
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060719
Time 12.18
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDC13
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 322.5
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWPRK 0.01500000 sec

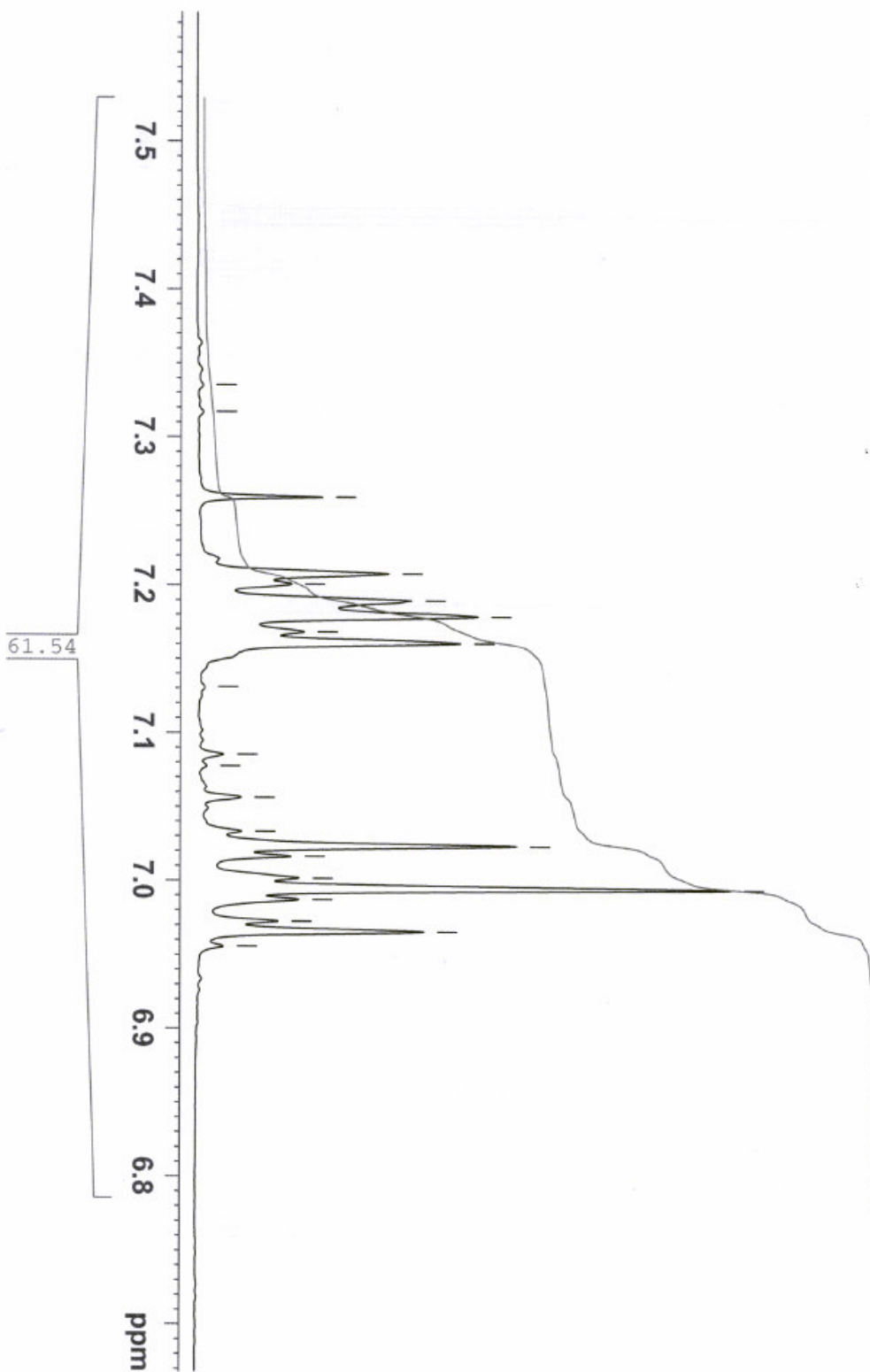
===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

J. Webb
19/12/06

10383690, RX0002/44B, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

7.335
7.317
7.260
7.208
7.201
7.190
7.179
7.168
7.161
7.131
7.086
7.078
7.057
7.034
7.024
7.017
7.002
6.995
6.987
6.973
6.966
6.956



Intertek ASG

Current Data Parameters
NAME 10383690
EXPNO 10
PROCNO 1

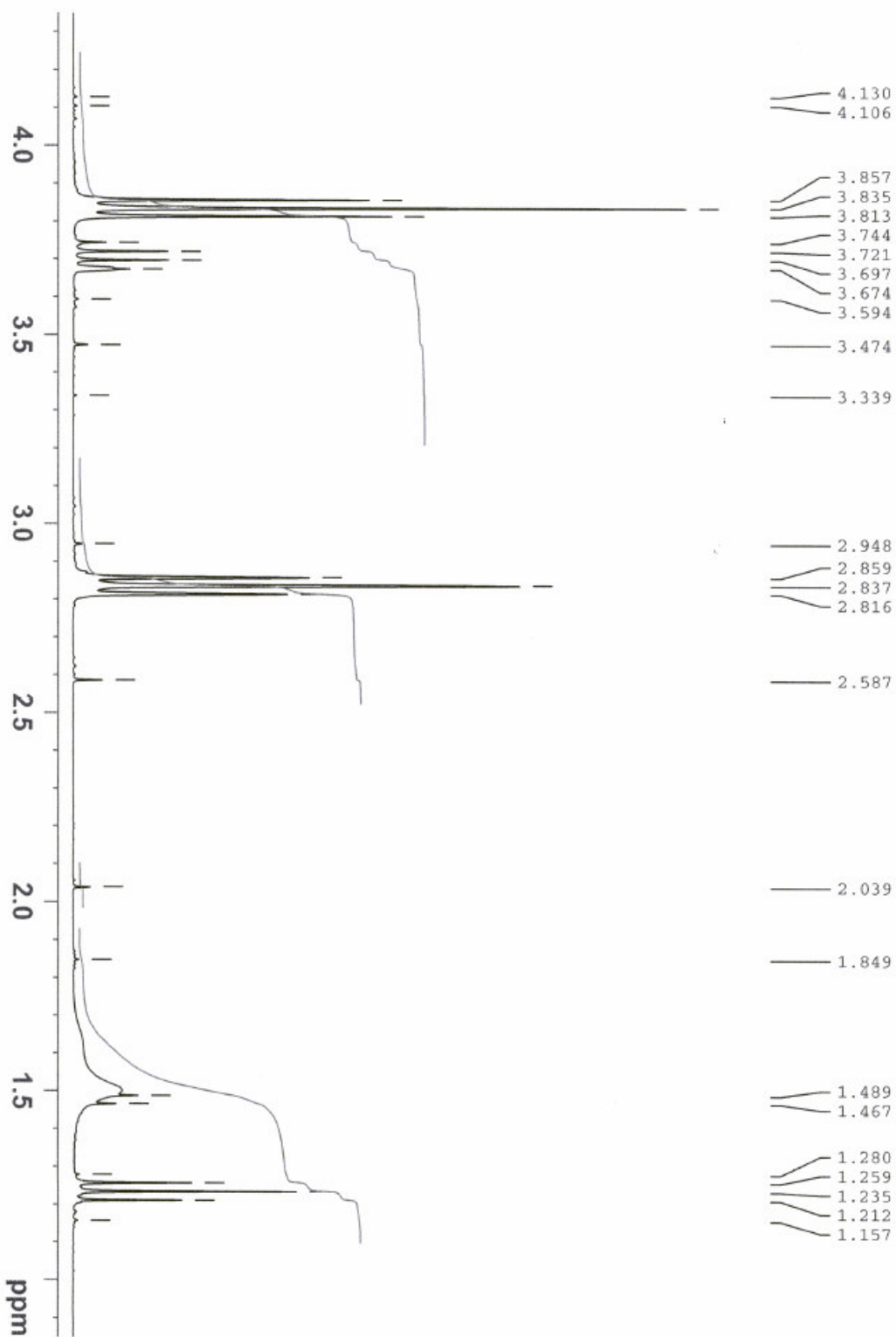
F2 - Acquisition Parameters
Date_ 20060719
Time 12.18
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 322.5
DW 69.600 usec
DE 6.00 usec
TE 289.2 K
D1 6.5999990 sec
MCREST 0.0000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing Parameters
SI 65536
SF 300.130062 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

D. M. A.
19n1c

10383690, RX0002/44B, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS



Intertek ASG

Current Data Parameters
 NAME 10383690
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060719
 Time 12.18
 INSTRUM dpx300
 PROBD 5 mm QNP 1H/13
 PULPROG zg30
 TD 48848
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.398709 sec
 RG 322.5
 DW 69.600 usec
 DE 6.00 usec
 TE 299.2 K
 DL 6.59999990 sec
 MCOREST 0.00000000 sec
 MCWRRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SFO1 300.1330010 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1300062 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

~ 1.1.17

10383450, RX0002/38/3, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

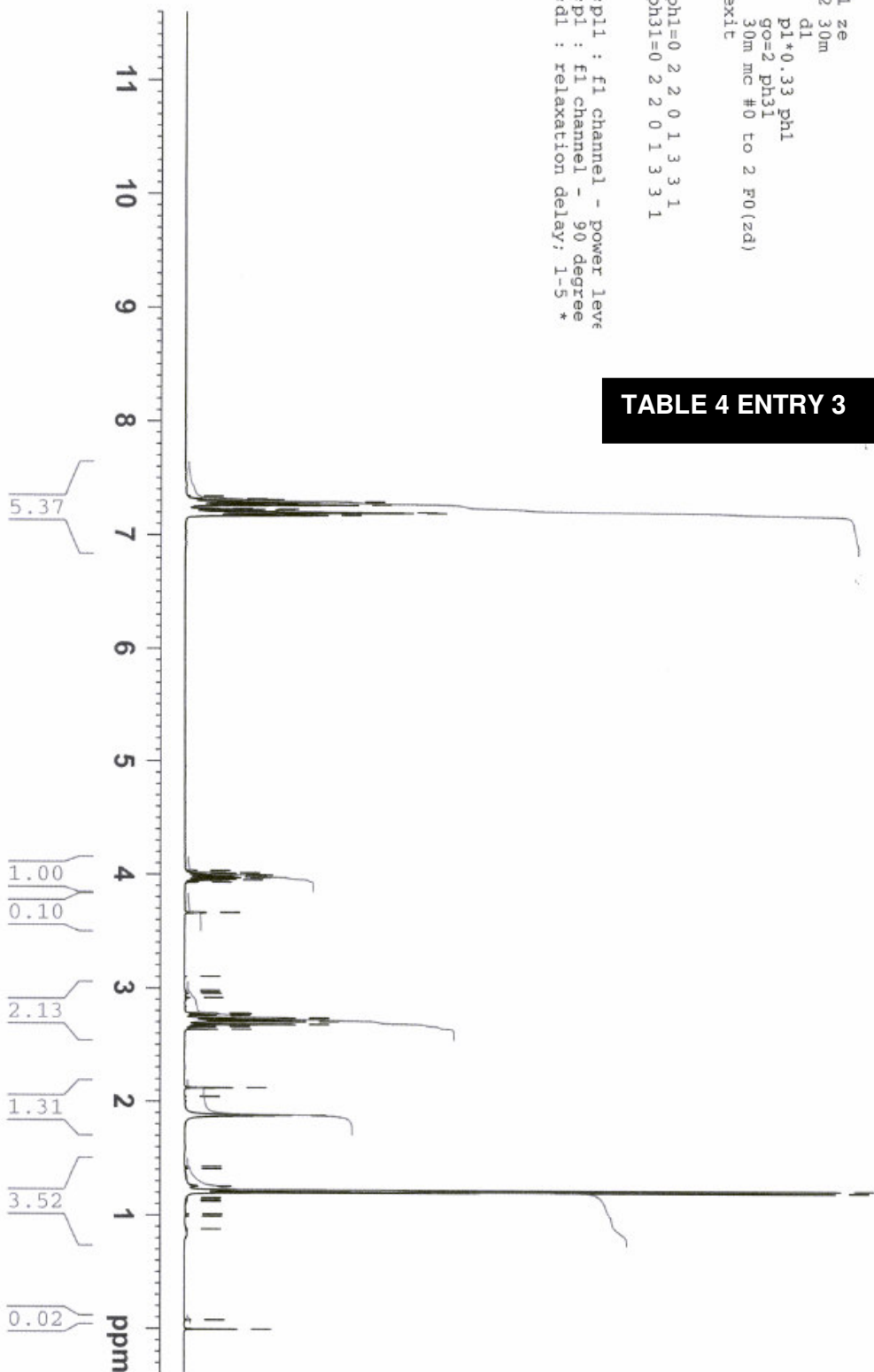
```
;zg30
;avance-version (02/05/31)
;1d sequence
;using 30 degree flip angle
#include <Avance.incl>
```

```
1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
```

```
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;p1 : f1 channel - power level
;p1 : f1 channel - 90 degree
;dl : relaxation delay: 1-5 *
```

TABLE 4 ENTRY 3



Intertek **ASG**

```
Current Data Parameters
NAME 10383450
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060712
Time 12.45
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 64
DE 69.600 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1350010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300146 MHz
WDW EN
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
```


10383450, RX0002/38/3, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

7.345
7.322
7.317
7.312
7.301
7.295
7.283
7.275
7.270
7.238
7.233
7.228
7.205
7.199
7.190
7.184
7.178

5.37

7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 ppm

Intertek ASG

Current Data Parameters
NAME 10383450
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060712
Time 12.45
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2
SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.398709 sec
RG 64
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.5999990 sec
MCREST 0.0000000 sec
MCMRK 0.01500000 sec

==== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

P. Hest

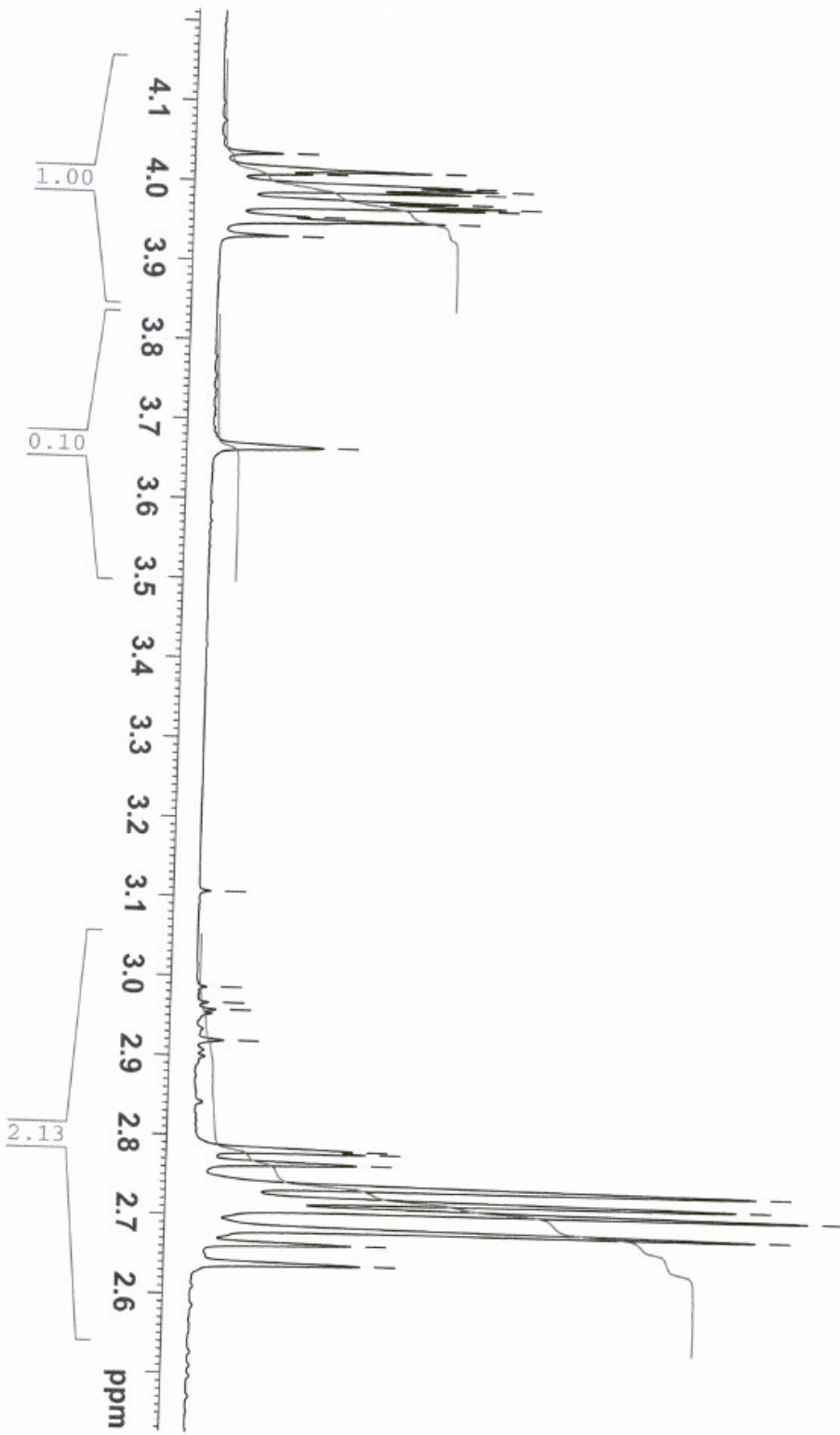
LV303420, FX0002/38/3, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCl3/TMS

4.037
4.016
4.011
3.998
3.995
3.991
3.978
3.973
3.970
3.957
3.953
3.932

3.667

3.107
2.987
2.968
2.959
2.921

2.784
2.781
2.767
2.739
2.722
2.711
2.685
2.666
2.640



Intertek ASG

Current Data Parameters
NAME 10383450
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060712

Time 12.45
INSTRUM dpX300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2

SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 64

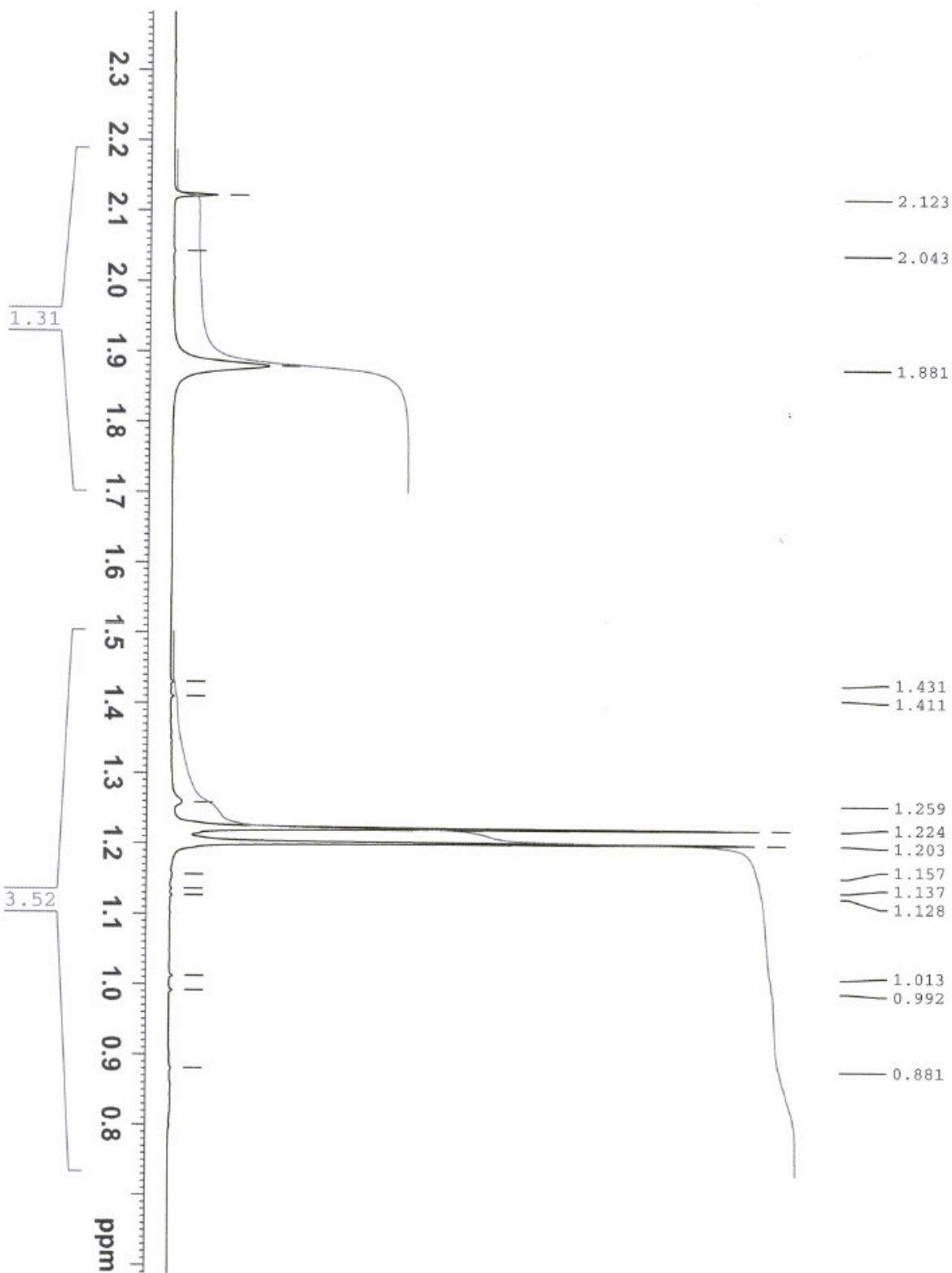
DM 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCNRR 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300146 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

D. Nord

10383450, RX0002/38/3, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS



Intertek **ASG**

Current Data Parameters
 NAME 10383450
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20060712
 Time 12.45
 INSTRUM dpx300
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 48848
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 7183.908 Hz
 FIDRES 0.147067 Hz
 AQ 3.3998709 sec
 RG 64
 DW 69.600 usec
 DE 6.00 usec
 TE 299.2 K
 D1 6.59999990 sec
 MCREST 0.00000000 sec
 MCWK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.40 usec
 PL1 0.00 dB
 SFO1 300.1330010 MHz

F2 - Processing parameters
 SI 65536
 SF 300.1300146 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 2.00

P. West

10383691, RX0002/44C, BRUKER DPX300, QNP, H1 SPECTRUM, SOLV:-CDCL3/TMS

1-04

Intertek ASG

```

;zg30          50.41
;advance-version (02/05/91) 7.329
;1d sequence   7.324
;using 30 degree flip angle 7.314
                                     7.308
                                     7.296
                                     7.287
                                     7.283
                                     7.255
                                     7.250
                                     7.245
                                     7.223
                                     7.217
                                     7.201
                                     7.196
                                     4.841
                                     4.824
                                     4.269
                                     3.960
                                     3.950
                                     3.936
                                     3.930
                                     3.925
                                     3.916
                                     3.911
                                     3.906
                                     3.901
                                     3.892
                                     3.882
                                     3.795
                                     3.727
                                     3.715
                                     3.704
                                     3.682
                                     3.672
                                     3.657
                                     3.645
                                     3.634
                                     3.517
                                     3.494
                                     3.480
                                     3.457
                                     2.939
                                     2.862
                                     2.815
                                     2.795
                                     2.769
                                     2.760
                                     2.750
                                     2.735
                                     2.714
                                     2.689
                                     2.469
                                     1.316
                                     1.309
#include <Advance.incl>

```

```

1 ze
2 30m
d1
p1*0.33 ph1
go=2 ph31
30m mc #0 to 2 F0(zd)
exit
ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1

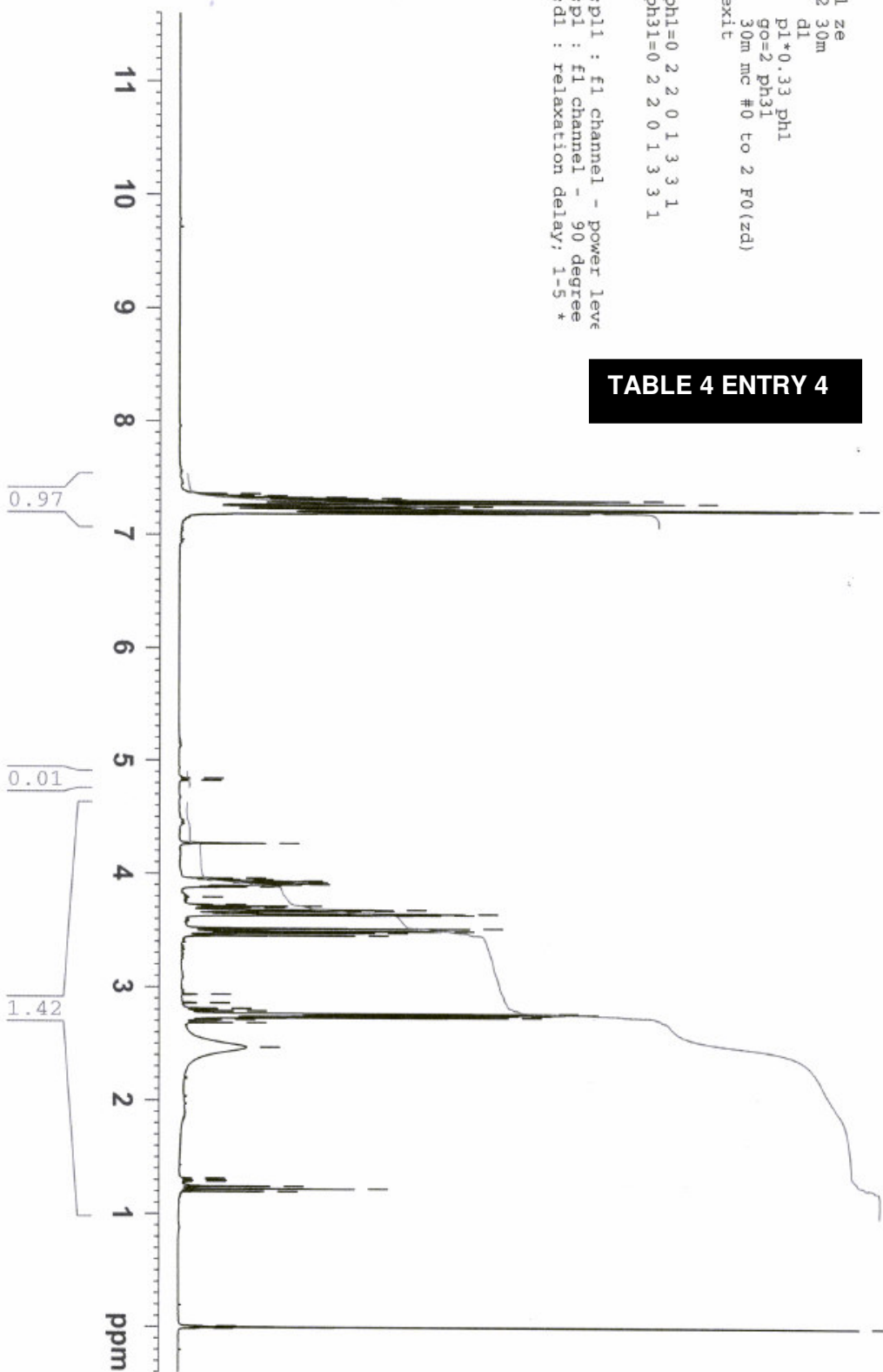
```

```

;p11 : f1 channel - power leve
;p1 : f1 channel - 90 degree
;d1 : relaxation delay; 1-5 *

```

TABLE 4 ENTRY 4



Current Data Parameters
NAME 10383691
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060719
Time 12.35
INSTRUM dpx300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 48848
SOLVENT CDCl3
NS 64
DS 2

SWH 7183.908 Hz
FIDRES 0.147067 Hz
AQ 3.3998709 sec
RG 322.5
DW 69.600 usec
DE 6.00 usec
TE 299.2 K
D1 6.59999990 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 usec
PL1 0.00 dB
SFO1 300.1330010 MHz

F2 - Processing parameters
SI 65536
SF 300.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00

D. N. V. K.
19/7/06