

Terms & Conditions

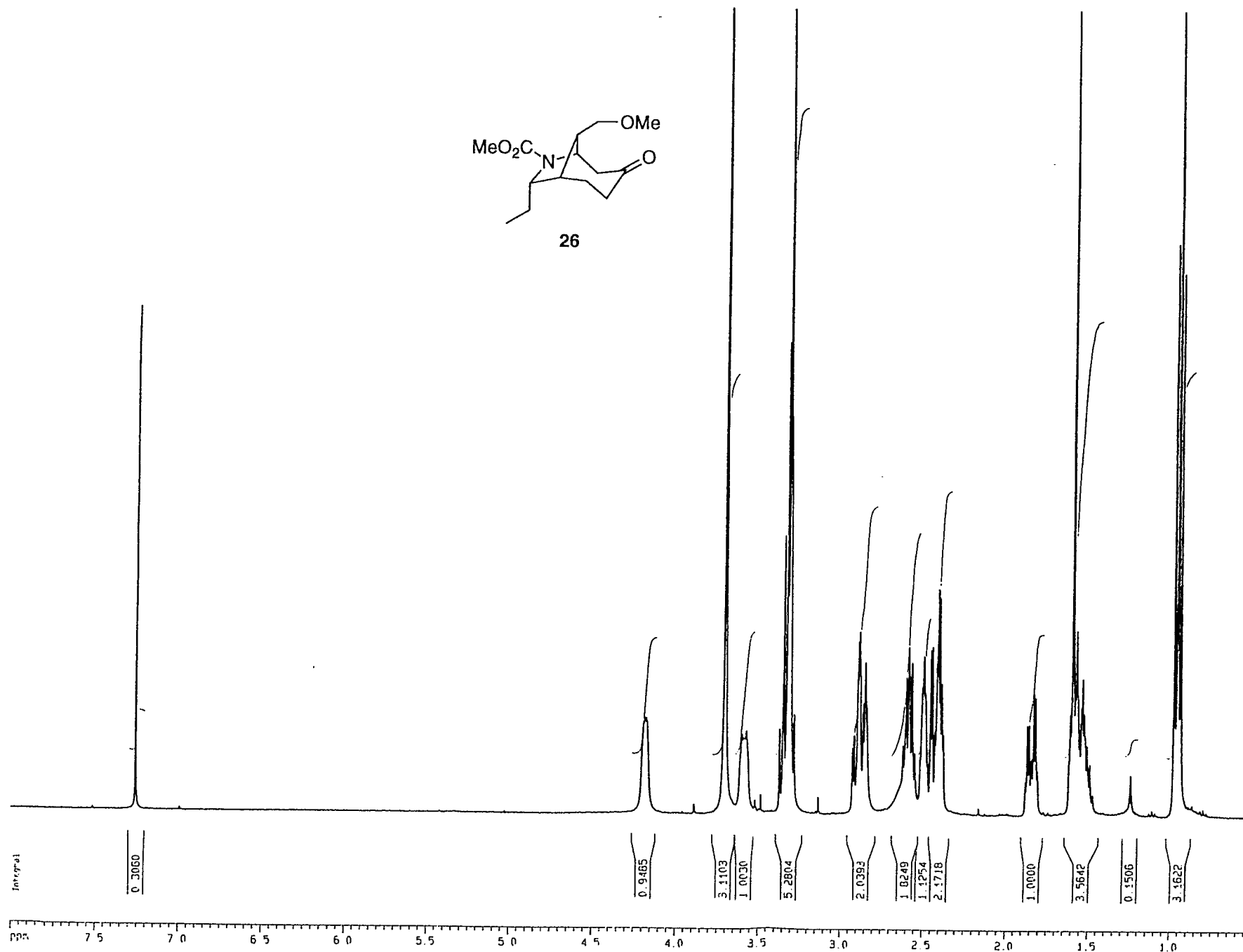
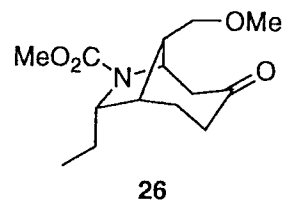
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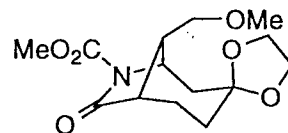


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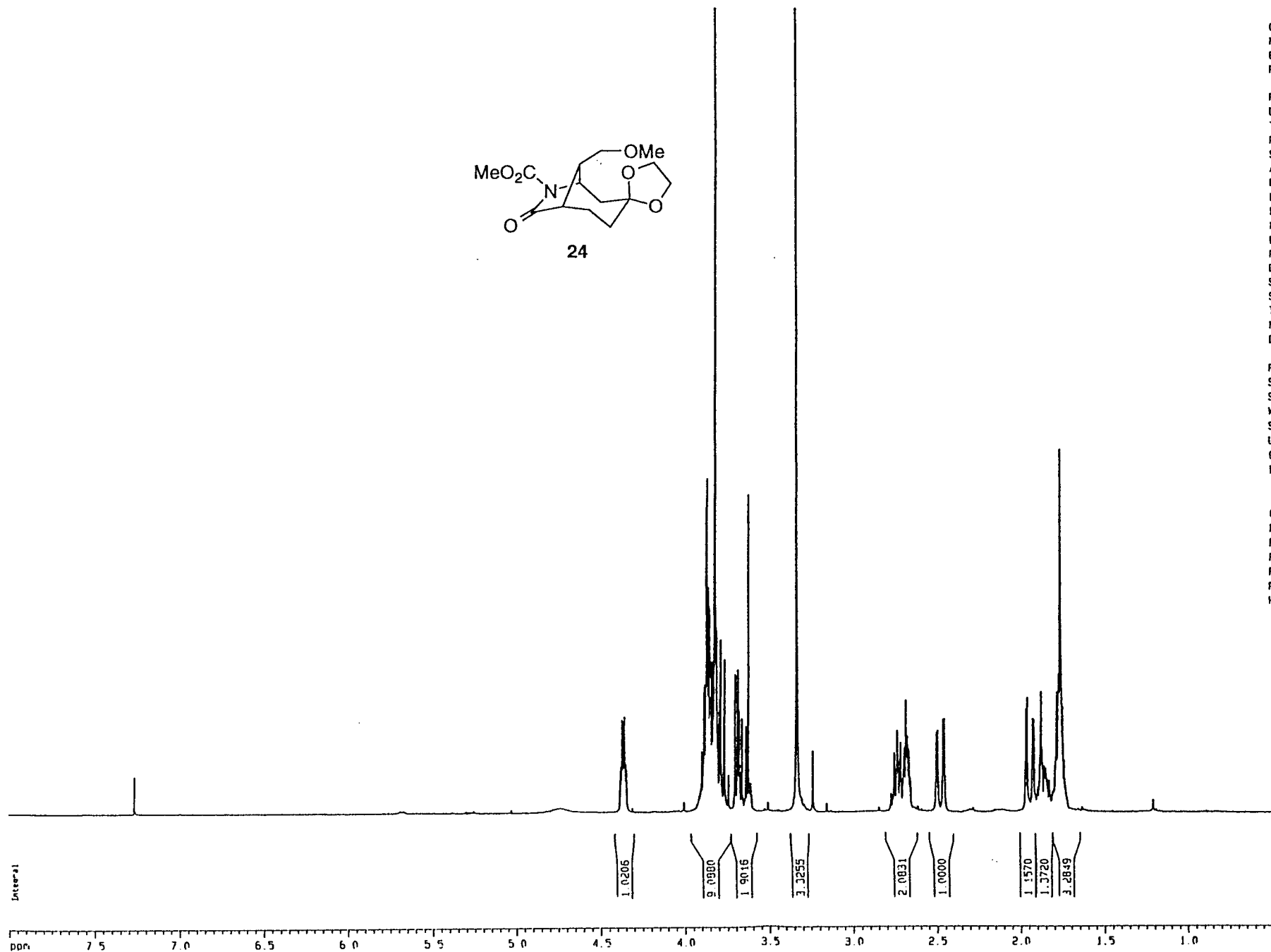
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1D NMR plot parameters
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 PPMCH 0.22590 ppm
 HZCH 90.39181 Hz



24

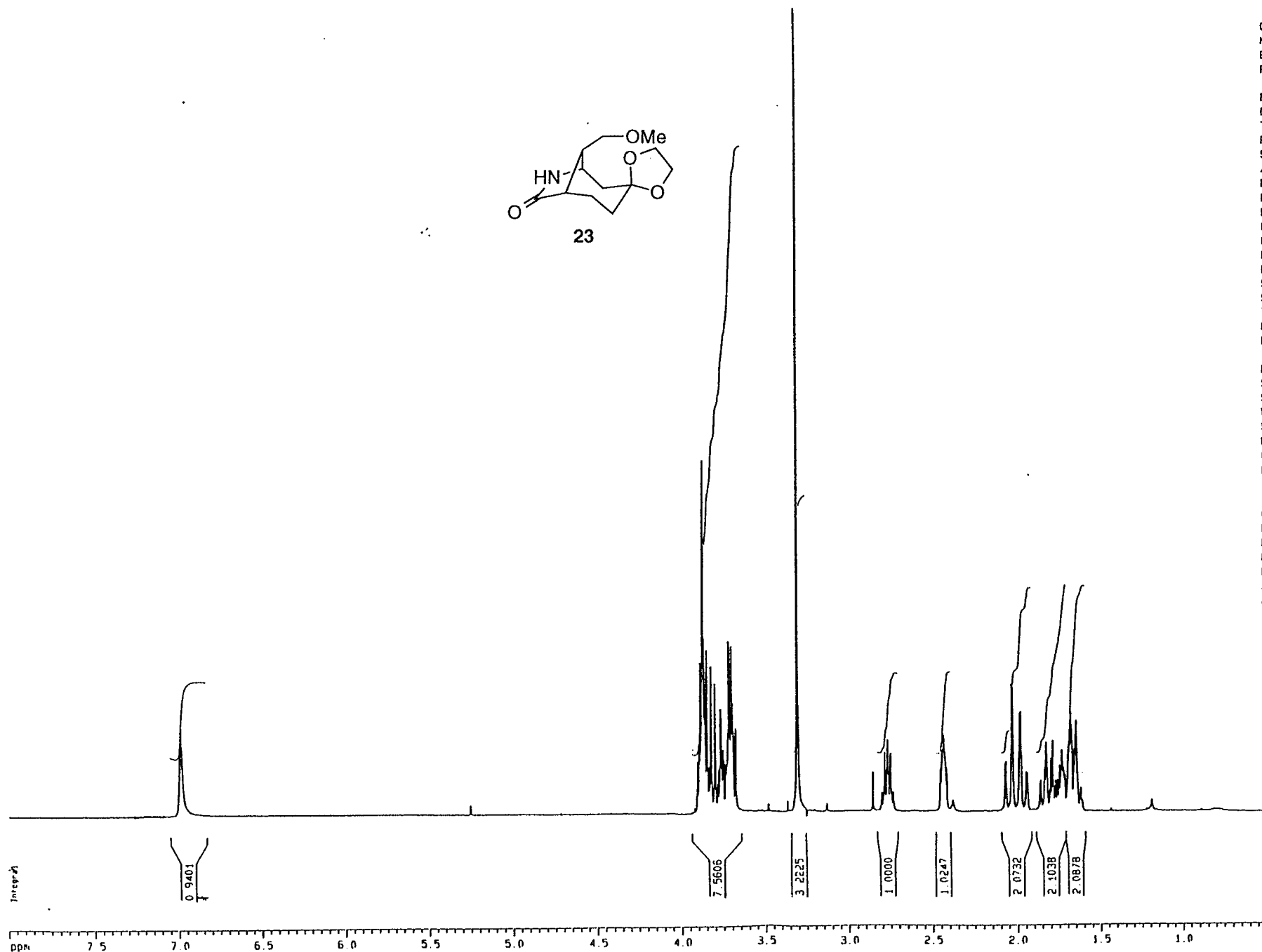
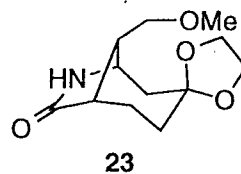


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LB 0.40 Hz
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F2 200.07 Hz
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HZCH 90.39181 Hz/

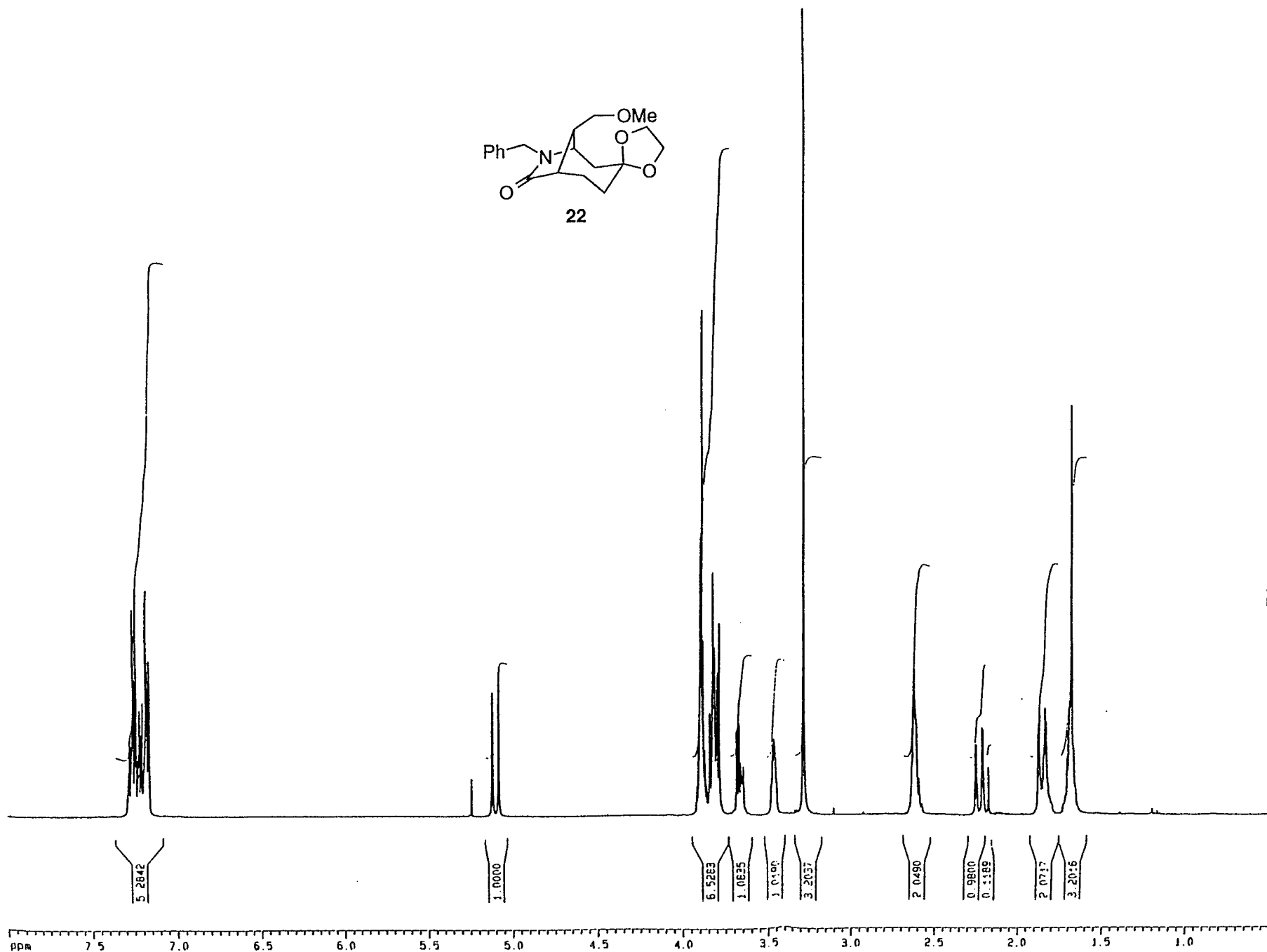
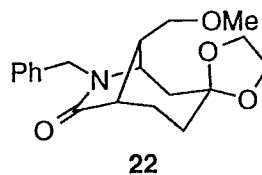


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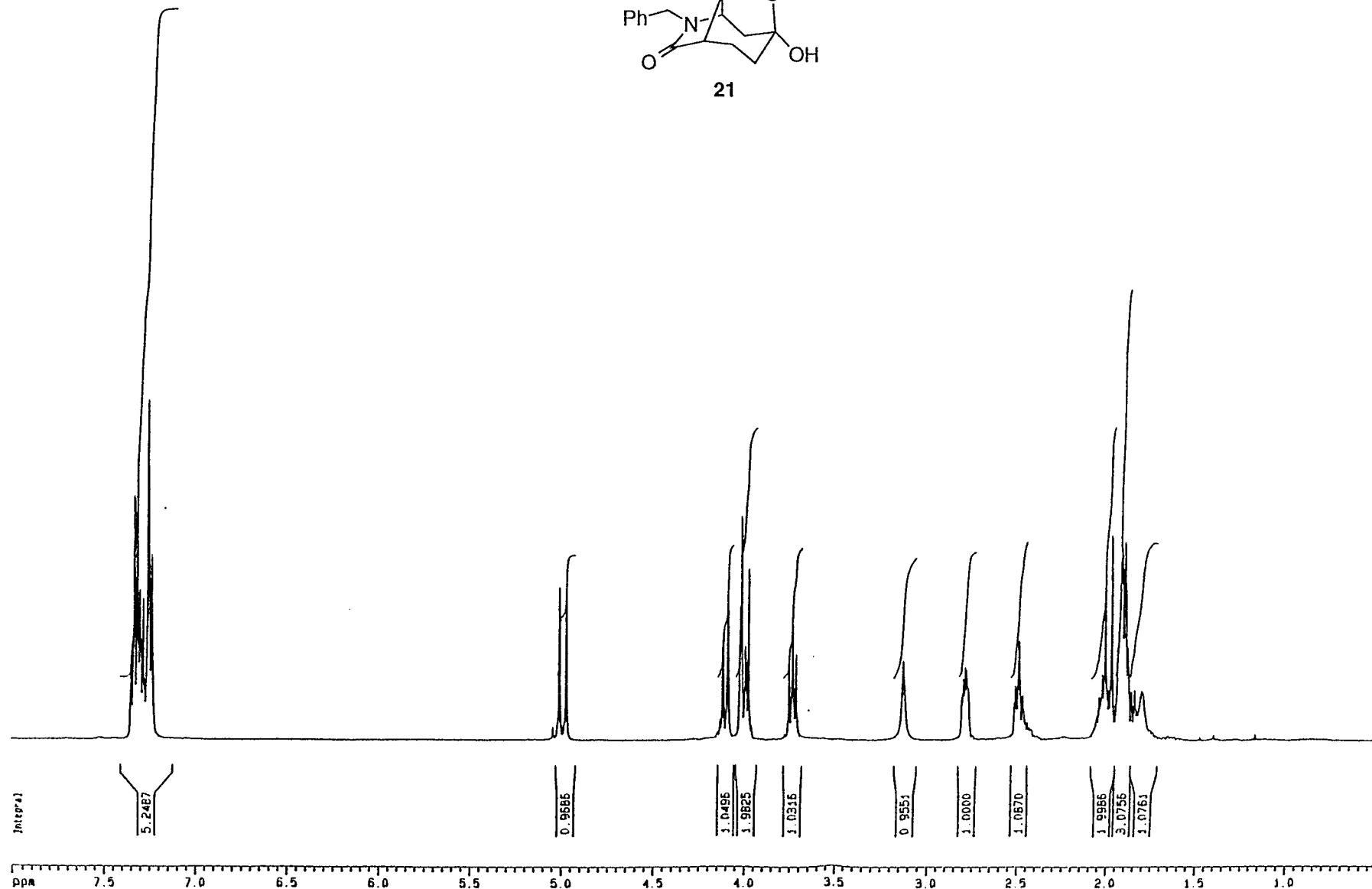
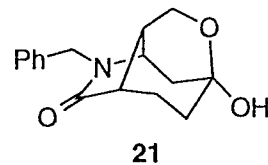
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TD 32768
NS 32
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1D 1H NMR plot parameters
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HZCM 90.39181

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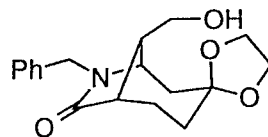
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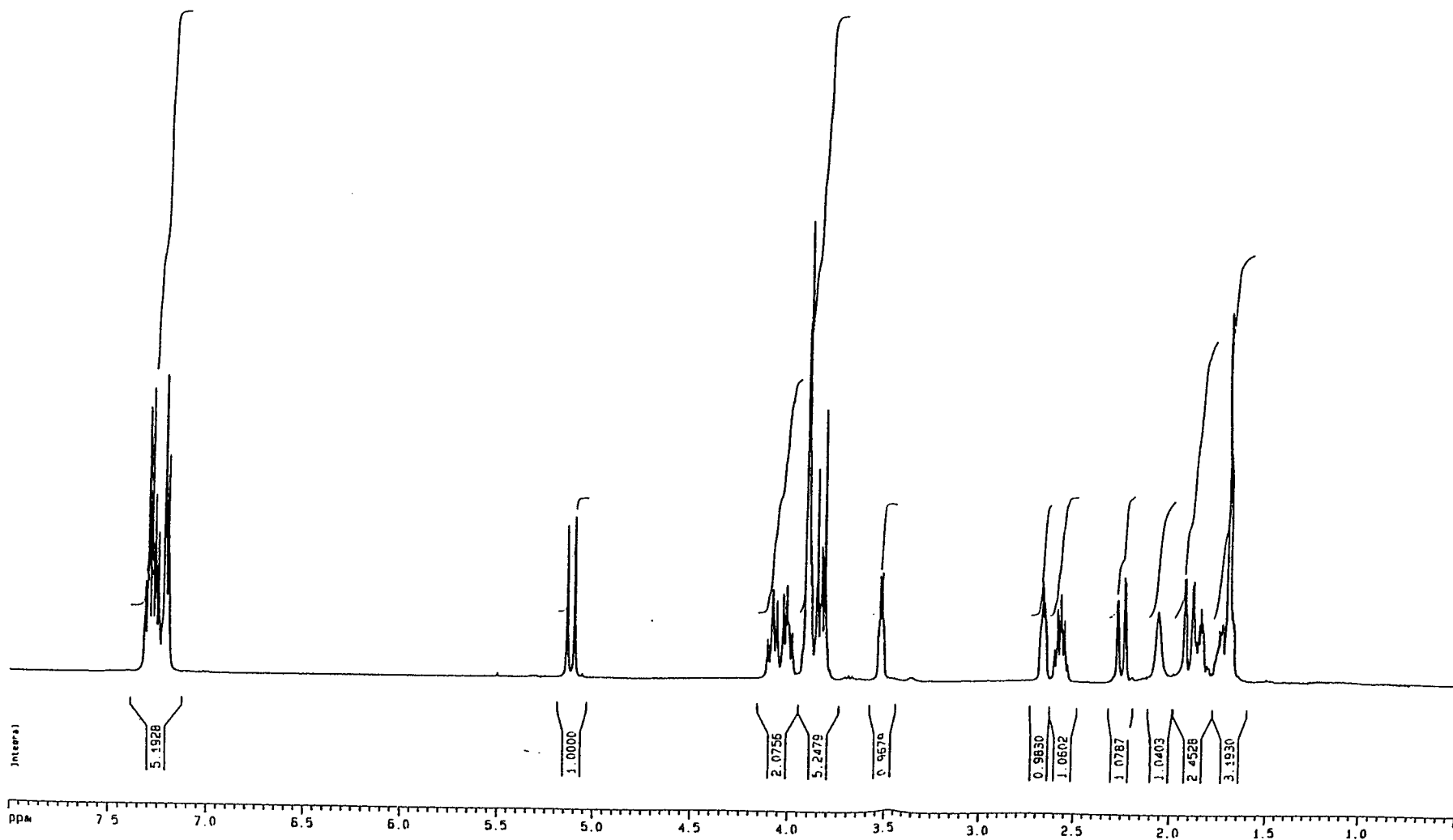
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20



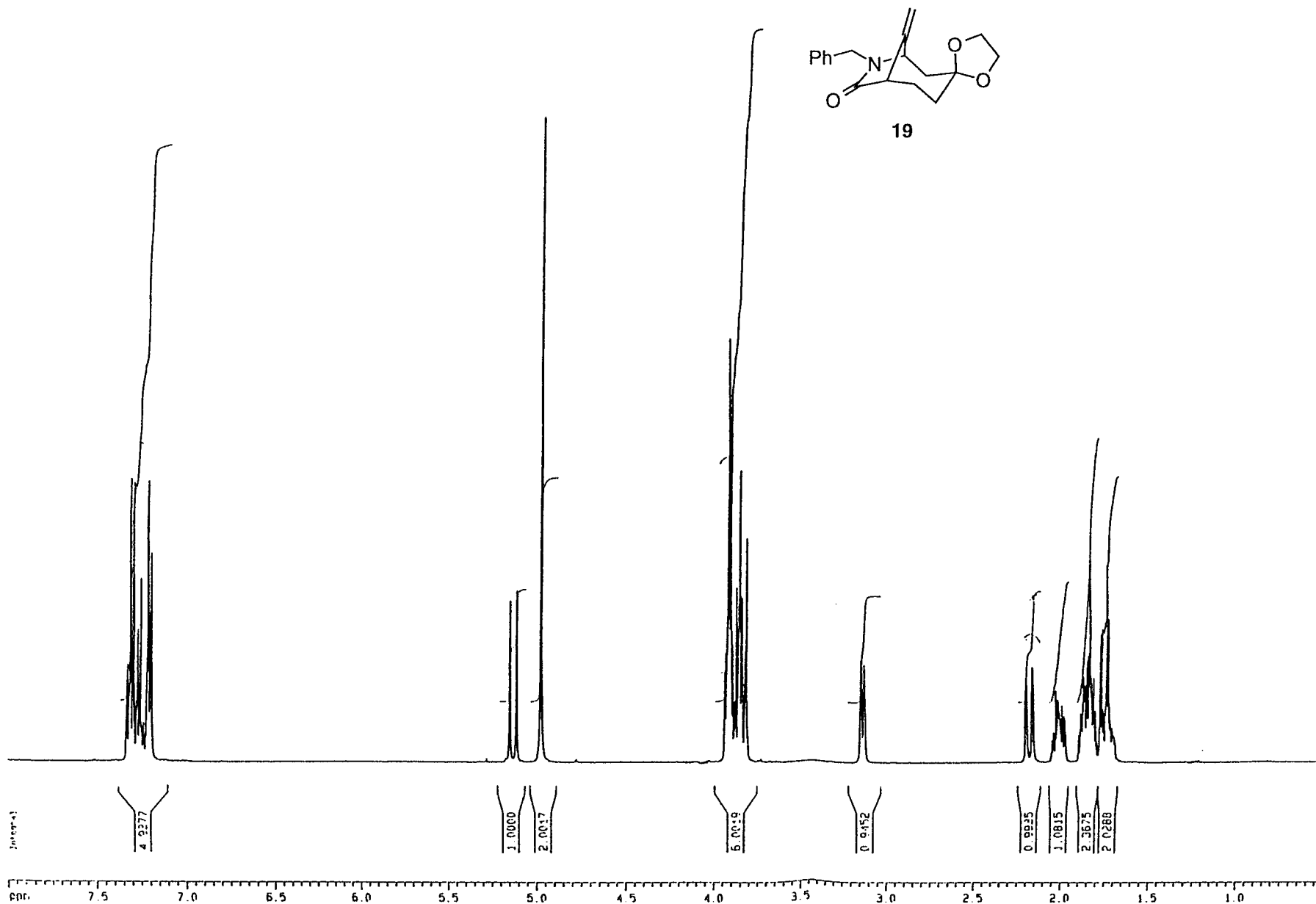
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DE
SFO1 400.1366
SWH 6410
TD 32
NS
DS

F2 - Processing parameters
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SF 400.1343
WDW
SSB
LB 0
GB
PC 1

1D NMR plot parameters
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F2P 0.5
F2 200
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HZCH 90.391

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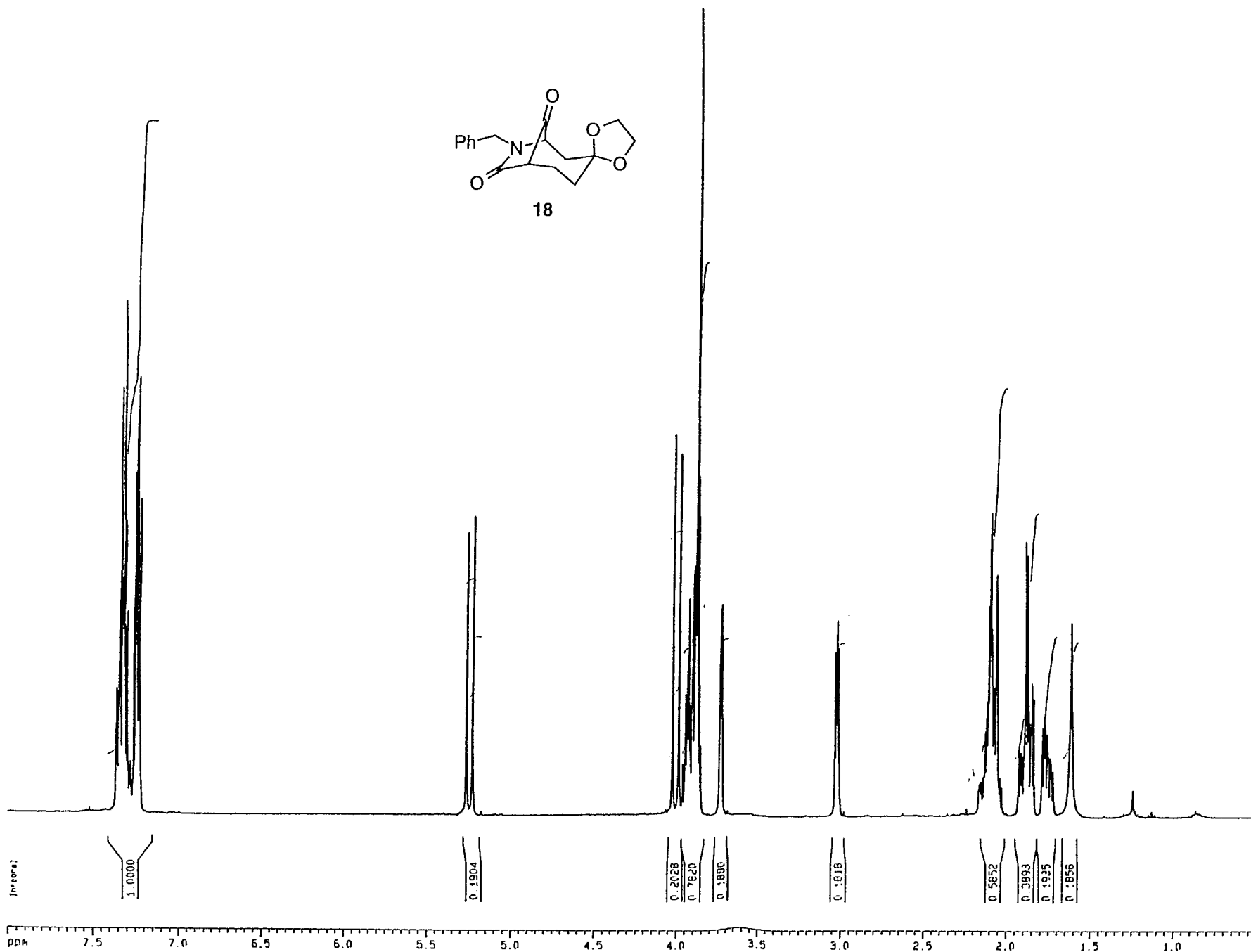
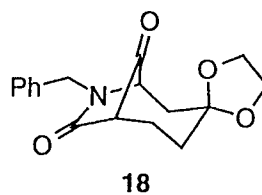
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 NUCLEUS 1H
 D1 1.0000000
 P1 10.4
 DE 97.5
 SF01 400.1368000
 SWH 6410.26
 TD 32768
 MS 32
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F2 - Processing parameters
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 SF 400.1343944
 WDW EM
 SSB 0
 LB 0.40
 GB 0
 PC 1.00

1D NMR plot parameters
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 F2P 0.500
 F2 200.07
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 HZCM 96.39181

POOR QUALITY ORIGINAL



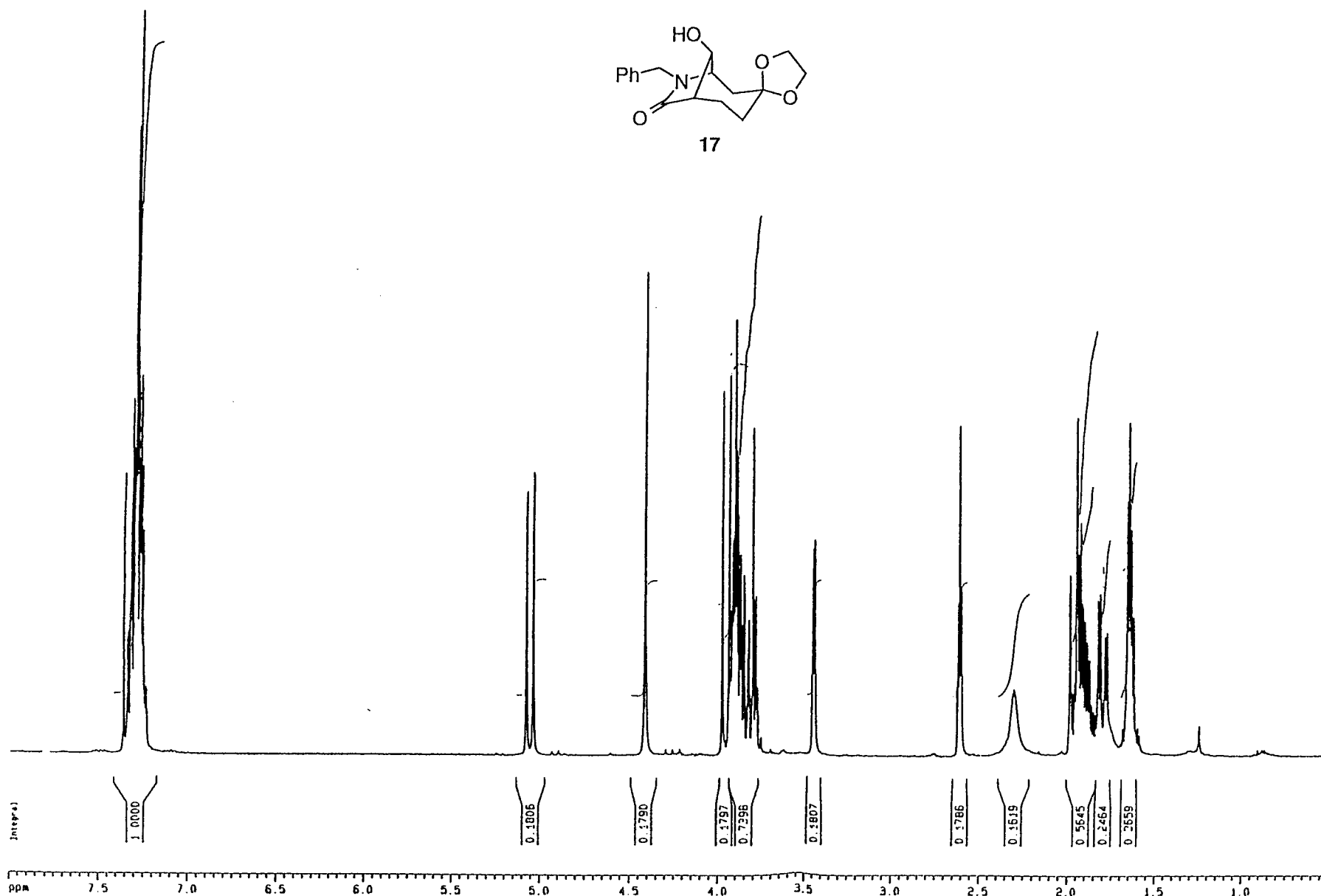
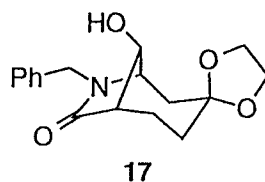
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FIDRES 0.19562
DM 78.
RG 102
NUCLEUS 1
D1 1.000000
P1 10.
DE 97.
SFO1 400.1368801
SWH 6410.21
TD 32761
NS 34
DS

F2 - Processing param
SI 32766
SF 400.1343944
WDW EM
SSB 0
LB 0.40
GB 0
PC 1.00

1D NMR plot parameters
CX 33.20
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F2P 0.500
F2 200.07
PPMCM 0.22590
HZCM 90.39181

POOR QUALITY ORIGINAL



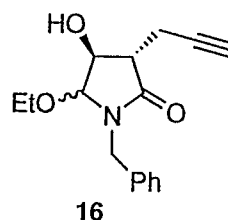
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 AG 715
 NUCLEUS 1H
 D1 1.0000000 s
 P1 10.4 u
 DE 97.5 u
 SFO1 400.1368800 MHz
 SMH 6410.26 Hz
 TD 32768
 NS 32
 DS 0

F2 - Processing parameters
 SI 32768
 SF 400.1343944 MHz
 WDM EM
 SSB 0
 LB 0.40 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 33.20 cm
 F1P 8.000 p
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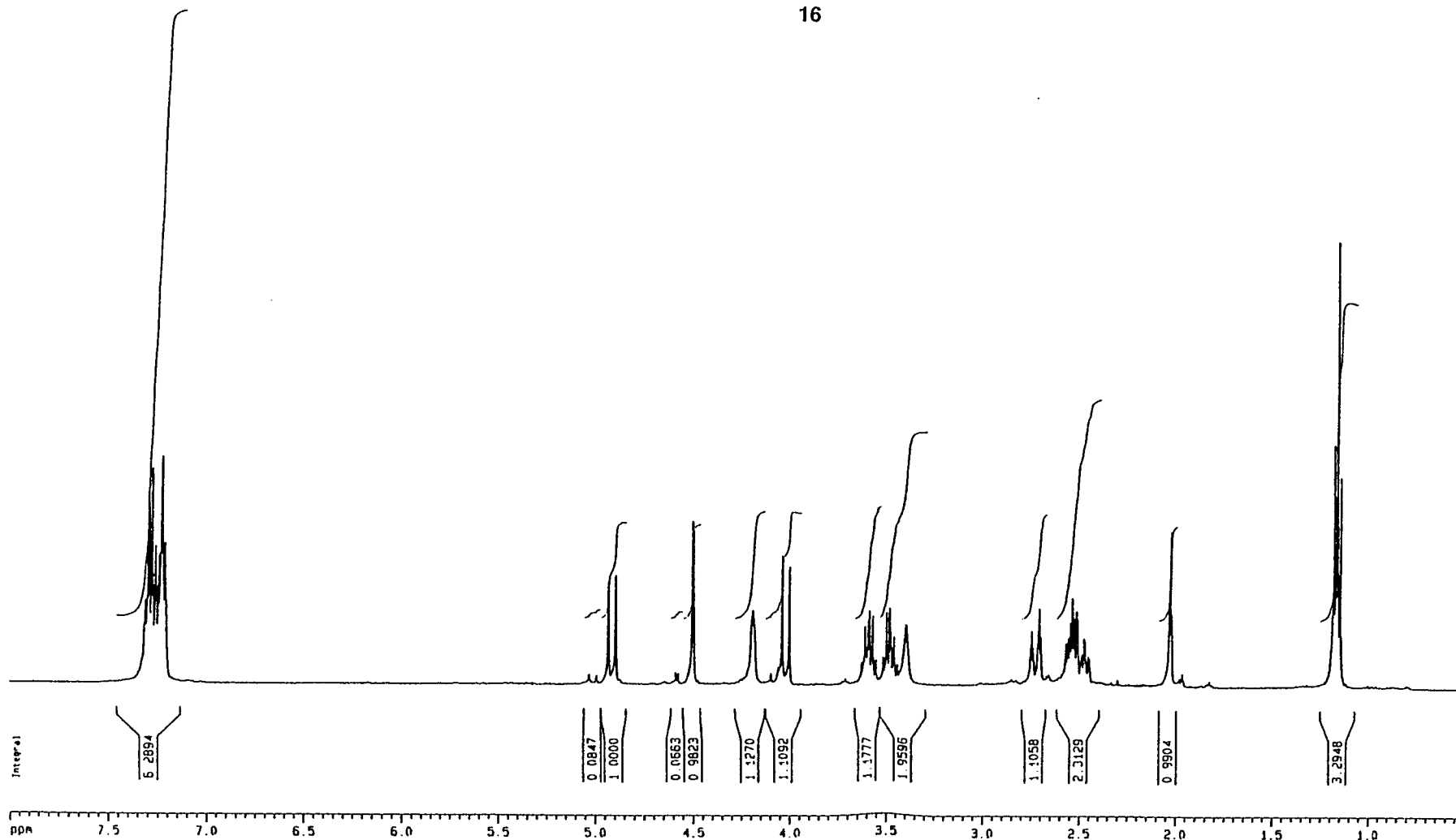


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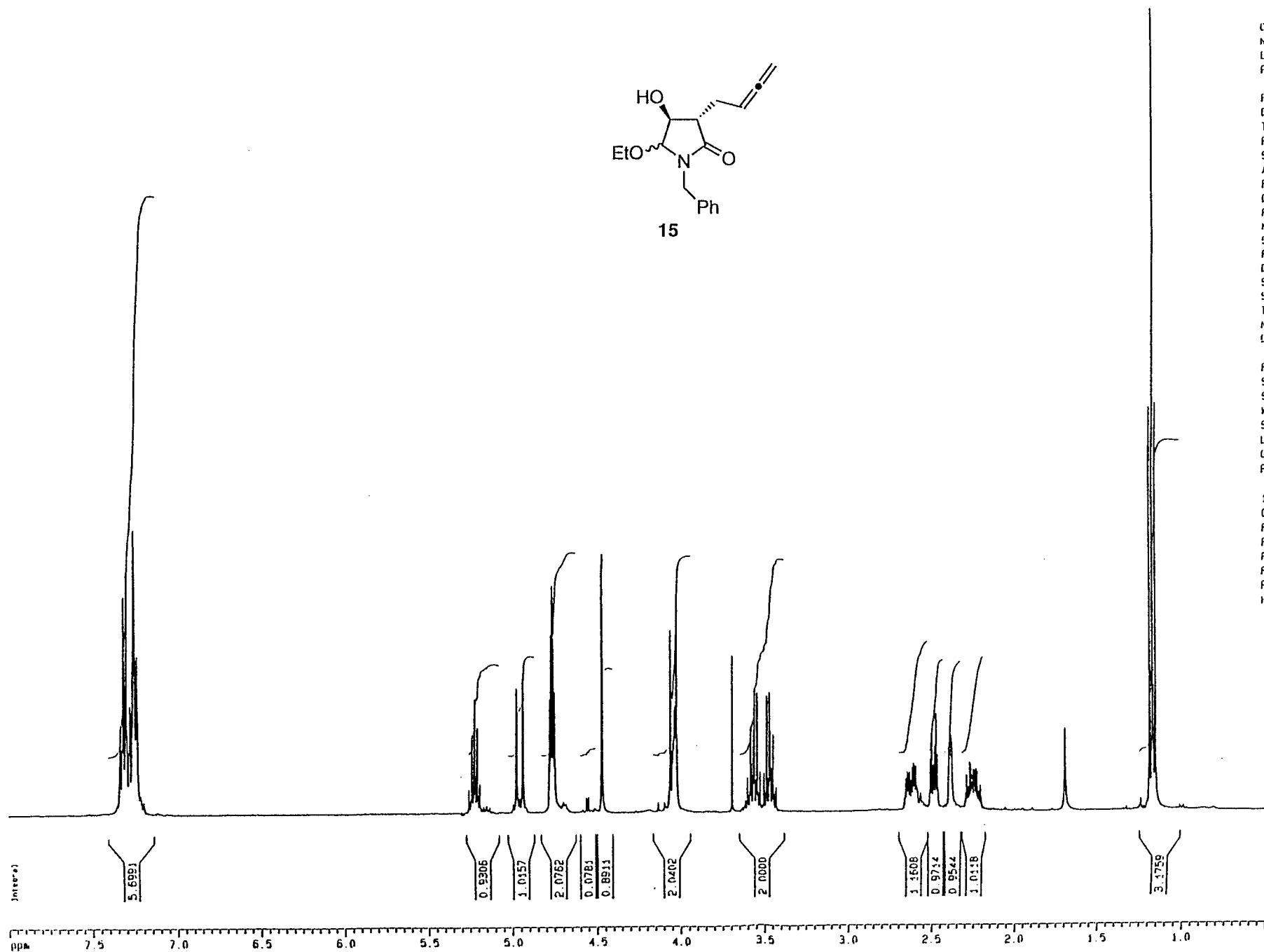
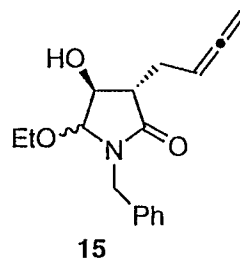
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 RG 360
 NUCLEUS 1H
 D1 1.0000000 sec
 P1 10.4 usec
 DE 97.5 usec
 SF01 400.1368000 MHz
 SMH 6410.26 Hz
 TD 32768
 NS 32
 DS 0

F2 - Processing parameters
 SI 32768
 SF 400.1343944 MHz
 WDW EM
 SSB 0
 LB 0.40 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 33.20 cm
 F1P 8.000 ppm
 F1 3201.08 Hz
 F2P 0.500 ppm
 F2 200.07 Hz
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 HZCH 90.39181 Hz/cm



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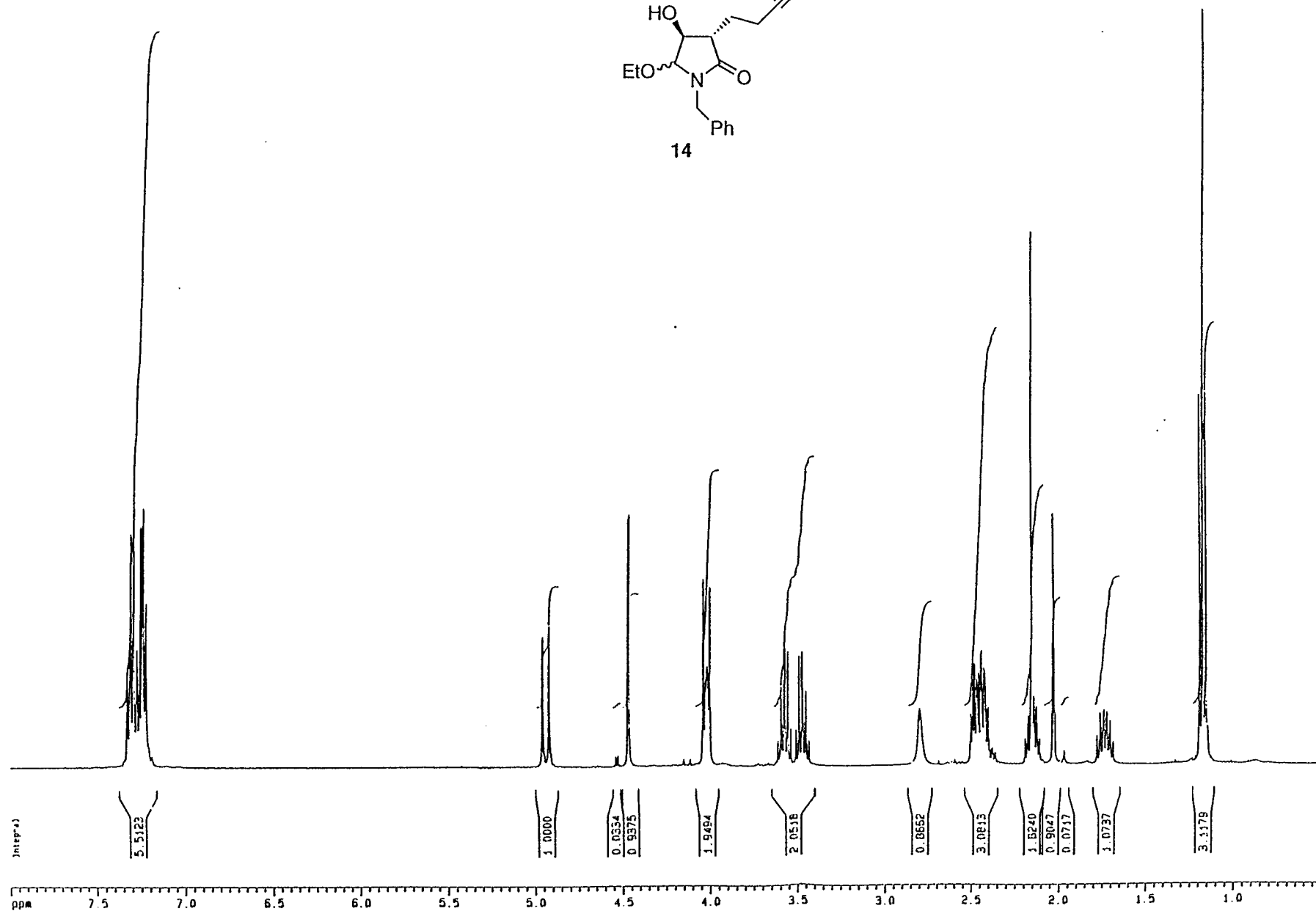
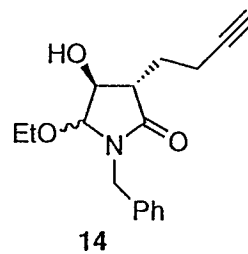
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FIDRES: 0.195
D1: 7
RG: 1
NUC1: EUS
D1: 1.0000
P1: 1
DE: 9
SF01: 400.1368
SMA: 6410
ID: 32
NS: 1
DS: 1

F2 - Processing parameters
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SF: 400.1343
WDW: 0
SSB: 0
LB: 0
GB: 1
PC: 1

1D NMR plot parameters
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F1P: 8
F1: 3201
F2: 0
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PP4CM: 0.22
HZCM: 90.39

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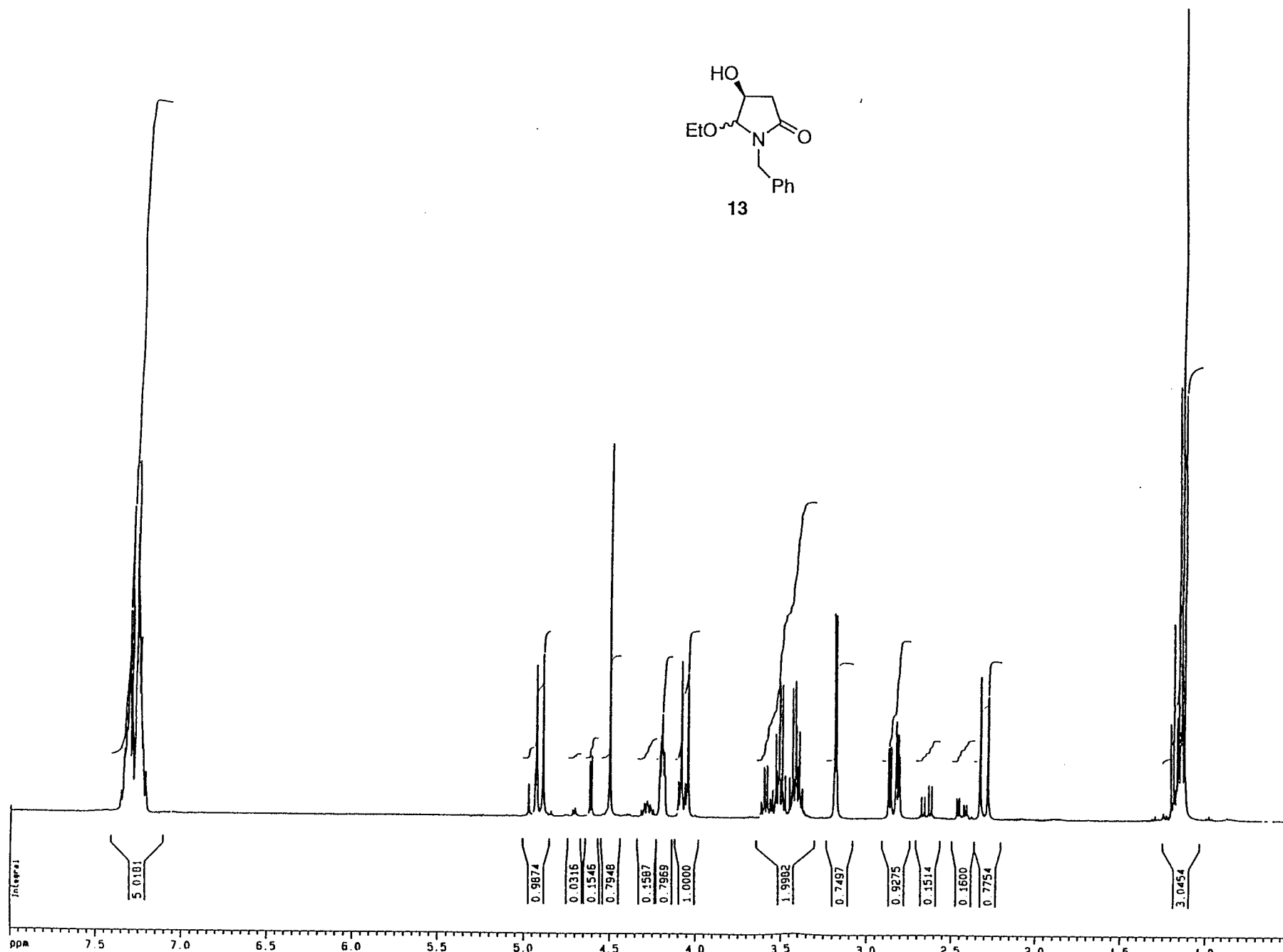
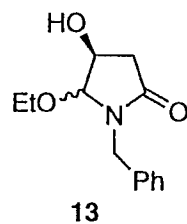
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NAME w.nfn
EXPNO
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RG 3
NUCLEUS
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P1 10
DE 97
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SH11 6410.1
TD 1271
NS
DS

F2 - Processing parameters
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WDW
SSB
LB 0.4
GB
PC 1.0

1D NMR plot parameters
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F1 3201.1
F2P 0.50
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H2CM 90.3911

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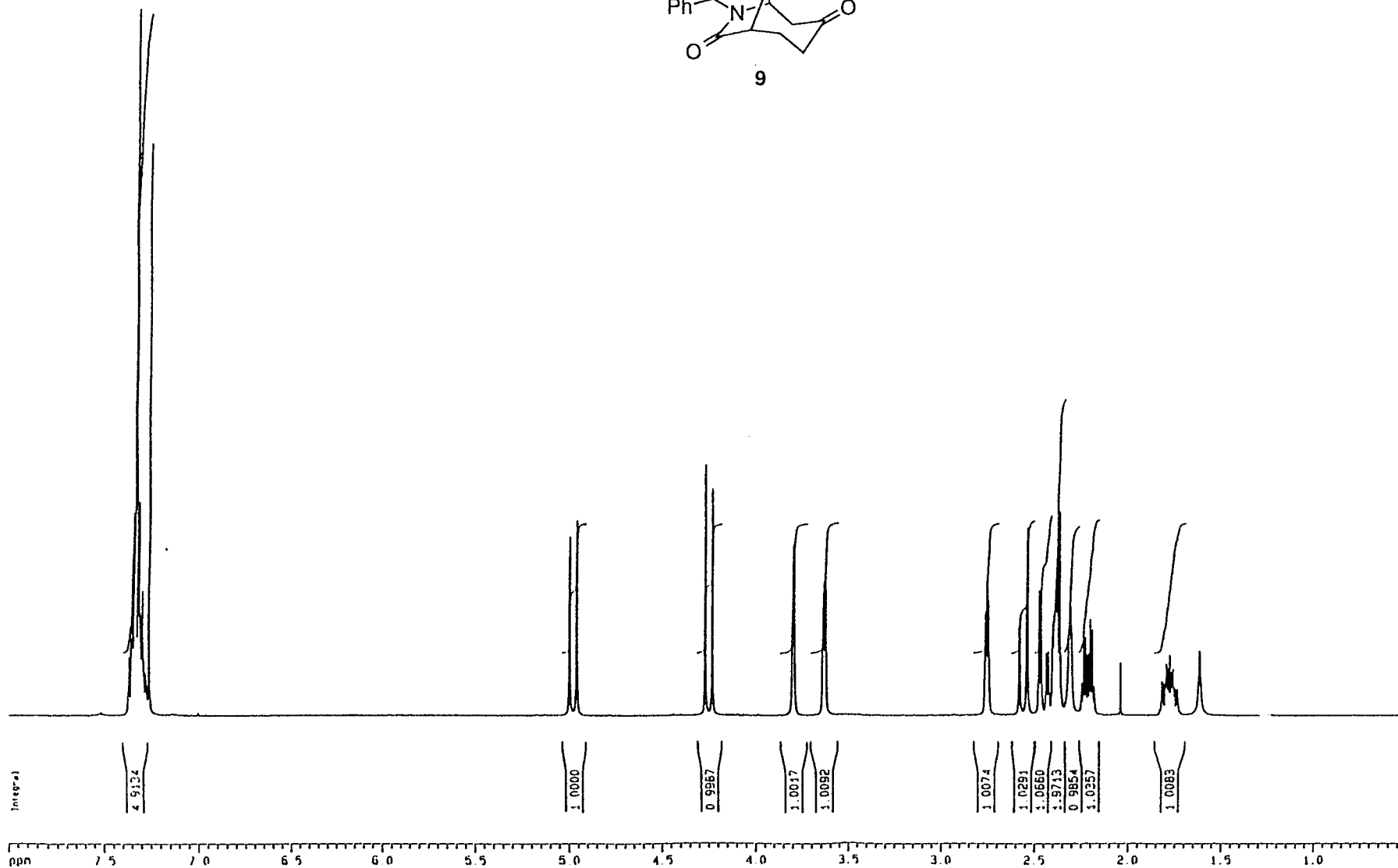
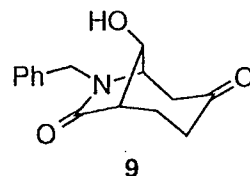
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RGRES: 0.105625 Hz
F4: 74.0 MHz
G6: 367
NUC1: 1H
D1: 1.000000 sec
F1: 1.000000 Hz
F2: 27.5 Hz
SI01: 100.1364000 MHz
CMA: 6410.2F Hz
TD: 32768
NS: 32
FS: 0

Processing parameters
SI: 32768
CF: 410.145944 MHz
VDM: EM
SFO: 0
LS: 40 Hz
CS: C
PC: 1.0

2D NMR plot parameters
CX: 33.20 Hz
FIP: 8.000 ppm
F1: 200.108 Hz
F2: 0.500 ppm
F2: 200.07 Hz
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HZCM: 80.39181 Hz/cm

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Current Data Parameters
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EXPNO: 1
PROCNO: 1

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Time 14.11
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P1 10.4
D2 97.5
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SFO2 5419.25
F0 32763
K5 32
D5 3

F2 - Processing parameters
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WDW EM
SSB 0
LB 0.4
GB 0
PC 1.00

1D NMR plot parameters
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ACQ 97.13191

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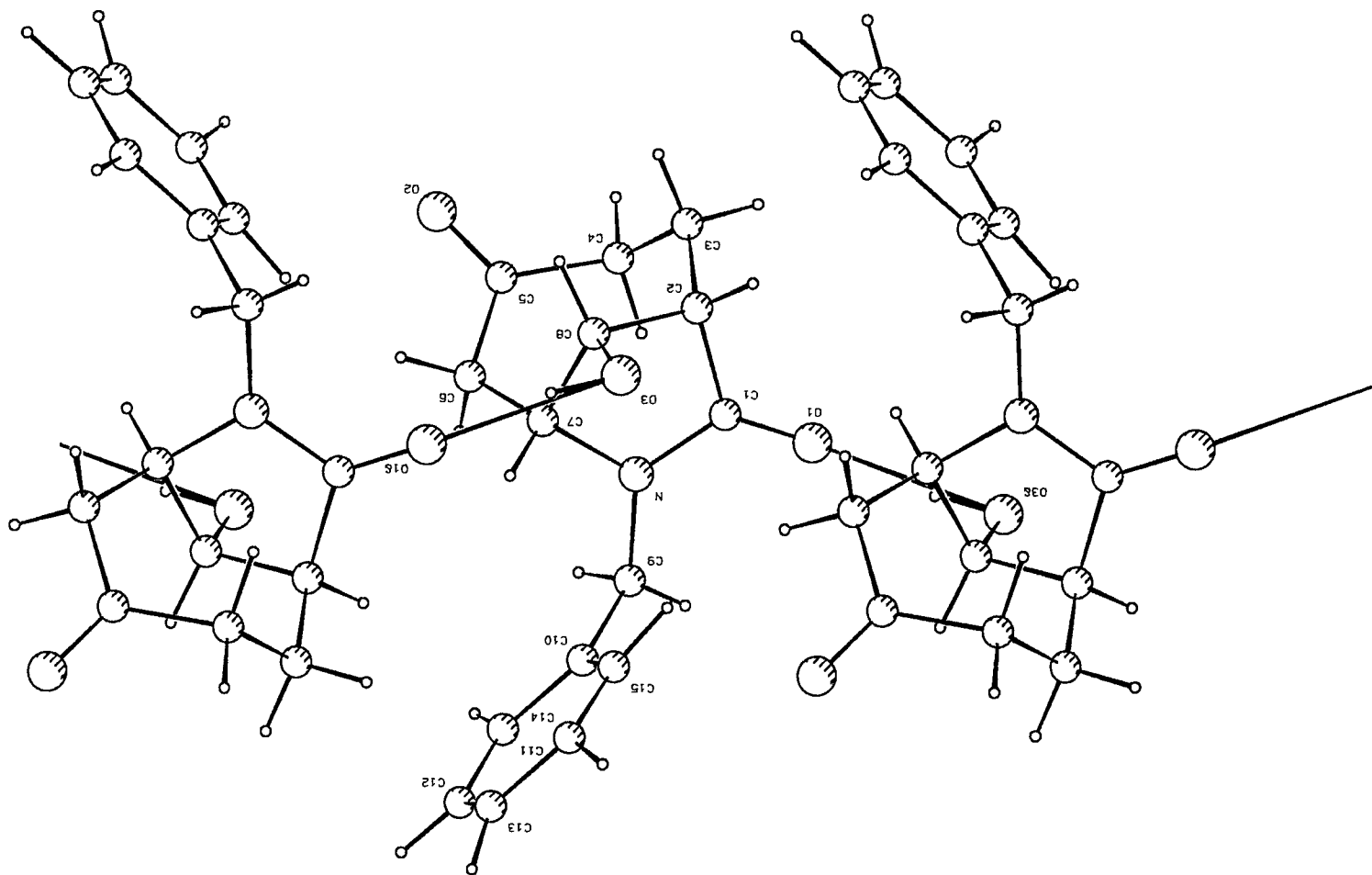
$C_{15}H_{17}NO_3$, $M_r=259.3$, monoclinic, $P2_1$, $a=7.0609(6)$, $b=9.7810(7)$, $c=9.758(1)$ Å, $V=667.3(1)$ Å³, $Z=2$, $D_x=1.29$ g cm⁻³, $\lambda(\text{CuK}\alpha)=1.5418$ Å, $\mu(\text{CuK}\alpha)=6.95$ cm⁻¹, $F(000)=276$, -20 °C. Final $R=0.042$ for 1297 observed reflections.

Experimental.

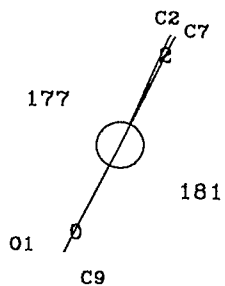
A crystal with dimensions 0.10 x 0.20 x 0.50 mm approximately was used for data collection on an Enraf-Nonius CAD-4 diffractometer with graphite-monochromated CuK α radiation and ω -2 θ scan. A total of 1449 unique reflections was measured within the range $-84 \leq h \leq 8, 0 \leq k \leq 12, 0 \leq l \leq 12$. Of these, 1297 were above the significance level of $2.5 \sigma(I)$. The range of $(\sin \theta)/\lambda$ was 0.052 - 0.625 Å⁻¹ ($4.64 \leq 2\theta \leq 74.6^\circ$). Two reference reflections ($\bar{1}01, 103$) were measured hourly and showed no decrease during the 32 h collecting time. Unit-cell parameters were refined by a least-squares fitting procedure using 23 reflections with $81 \leq 2\theta \leq 89^\circ$. Corrections for Lorentz and polarisation effects were applied. The structure was solved by Direct Methods. The hydrogen atoms were calculated. Full-matrix least-squares refinement on F , anisotropic for the non-hydrogen atoms and isotropic for the hydrogen atoms restraining the latter in such a way that the distance to their carrier remained constant at approximately 1.0 Å, converged to $R=0.042$, $R_w=0.040$, $(\Delta/\sigma)_{\max}=0.03$, $S=0.79$. A weighting scheme $w=[0.2 + 0.5*(\sigma(F_{\text{obs}}))^2 + 0.05/(\sigma(F_{\text{obs}}))]\text{ }^{-1}$ was used. The secondary isotropic extinction coefficient (Zachariasen 1967 ; Larson 1969) refined to $\text{Ext}=0.108(8)$. Attempts to refine the absolute structure parameter (Flack, 1983) with the aid of some 150 "Friedel" reflections failed, but the correct enantiomer has been determined by the reaction mechanism. A final difference Fourier map revealed a residual electron density between -0.17 and 0.16 e Å⁻³. Scattering factors were taken from Cromer and Mann (1968); *International Tables for X-ray Crystallography* (1974). All calculations were performed with XTAL3.4 (Hall, King and Stewart 1995), unless stated otherwise.

References

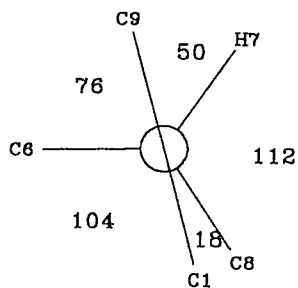
- Cromer, D.T. and Mann, J.B. (1968). *Acta Cryst.* A24, 321-324.
- International Tables for X-ray Crystallography* (1974). Vol. IV, p. 55. Birmingham : Kynoch Press.
- Flack, H.D. (1983). On enantiomorph-Polarity Estimation. *Acta Cryst.* A39 876.
- Hall, S.R., King, G.S.D. and Stewart, J.M. (1995). Eds. XTAL3.4 User's Manual. University of Western Australia : *Lamb, Perth*.
- Larson, A.C. (1969). The Inclusion of Secondary Extinction in Least-Squares Refinement of Crystal Structures. *Crystallographic Computing*. F.R. Ahmed, S.R. Hall, C.P. Huber eds. Munksgaard. Copenhagen: 291-294.
- Zachariasen, W.H. (1967). A General Theory of X-Ray Diffraction in Crystals *Acta Cryst.* A23, 558.
- Motherwell, W.D.S. and Clegg, W. (1978). *PLUTO*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.



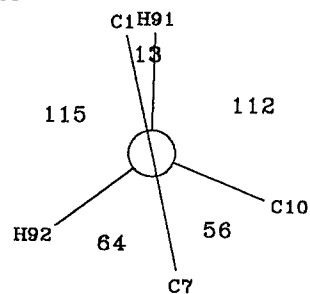
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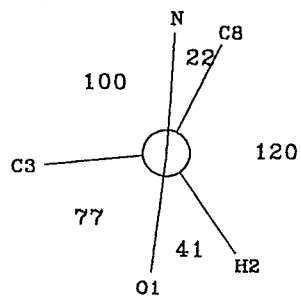
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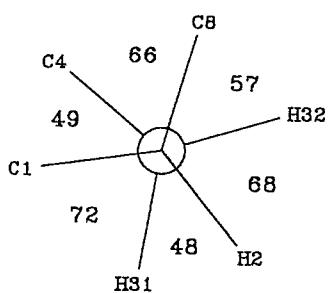
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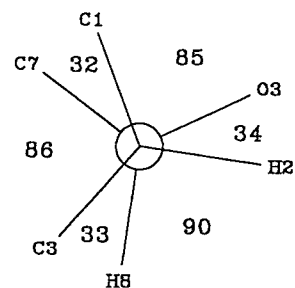
C1 — C2



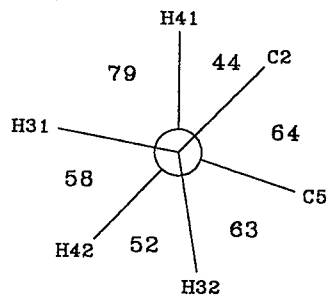
C2 — C3



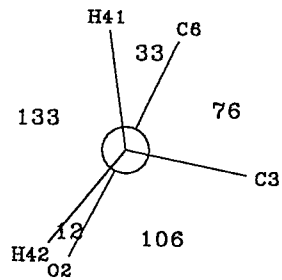
C2 — C8



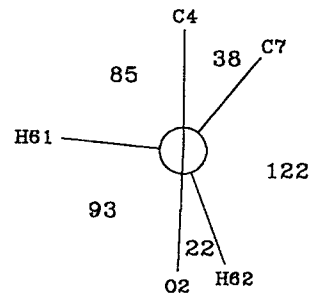
C3 — C4



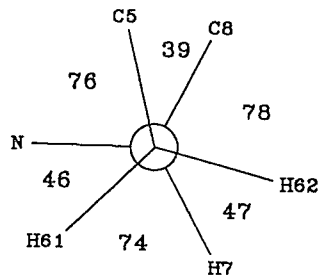
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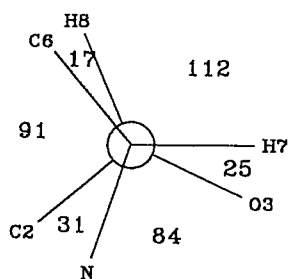
C5 — C6



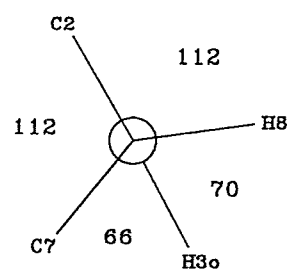
C6 — C7



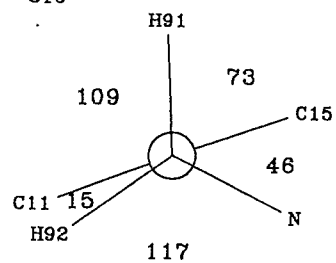
C7 — C8



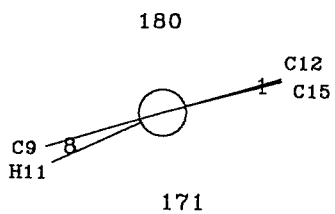
C8 — O3



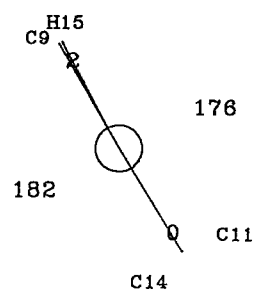
C9 — C10



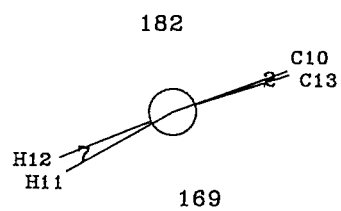
C10 — C11



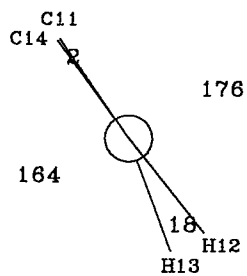
C10 — C15



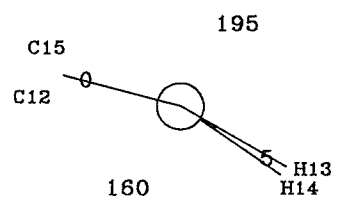
C11 — C12



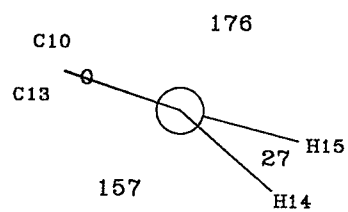
C12 — C13



C13 — C14



C14 — C15



De atomen zijn in de beschreven volgorde gesorteerd
De bijbehorende stralen zijn gebruikt voor de
berekening van de maximale bindingsafstand

	Atom	Radius	Afr.coor	Afr.u
1	C	0.9	AUTO ,	AUTO
2	N	0.9	AUTO ,	AUTO
3	O	0.9	AUTO ,	AUTO
4	H	0.5	AUTO ,	AUTO

Afrondingsfactor voor afstanden= 1.0E+001

Afrondingsfactor voor hoeken = 1.0E+001

De gelezen BDF heet m22bey.

Table 1

Fractional co-ordinates of the non-hydrogen atoms
and equivalent isotropic thermal parameters.

	X	Y	Z	Ueq
C(1)	-0.2266(5)	0.050(1)	-0.0612(4)	0.044(2)
C(2)	-0.1399(5)	0.088(1)	-0.1887(4)	0.044(2)
C(3)	-0.2976(6)	0.102(1)	-0.3124(4)	0.055(2)
C(4)	-0.4708(6)	0.191(1)	-0.2856(5)	0.062(3)
C(5)	-0.4190(6)	0.342(1)	-0.2547(4)	0.059(3)
C(6)	-0.3183(6)	0.381(1)	-0.1174(5)	0.051(2)
C(7)	-0.1624(5)	0.285(1)	-0.0453(4)	0.041(2)
C(8)	-0.0358(5)	0.221(1)	-0.1448(4)	0.042(2)
C(9)	-0.3245(6)	0.171(1)	0.1424(5)	0.055(3)
C(10)	-0.1898(5)	0.230(1)	0.2585(4)	0.047(2)
C(11)	-0.2497(7)	0.332(1)	0.3422(5)	0.067(3)
C(12)	-0.122(1)	0.387(1)	0.4492(6)	0.084(4)
C(13)	0.0639(9)	0.346(1)	0.4729(5)	0.083(4)
C(14)	0.1255(7)	0.246(1)	0.3903(5)	0.076(3)
C(15)	-0.0012(6)	0.190(1)	0.2858(4)	0.063(3)
N	-0.2405(4)	0.164(1)	0.0146(3)	0.044(2)
O(1)	-0.2845(4)	-0.065(1)	-0.0315(3)	0.061(2)
O(2)	-0.4669(6)	0.426(1)	-0.3436(4)	0.090(3)
O(3)	0.1468(3)	0.185(1)	-0.0727(3)	0.056(2)

Table 2

Fractional co-ordinates and isotropic thermal parameters
of the hydrogen atoms.

	X	Y	Z	U
H(2)	-0.050(4)	0.016(3)	-0.211(3)	0.039(9)
H(7)	-0.076(3)	0.327(3)	0.034(2)	0.029(8)
H(8)	-0.041(6)	0.266(4)	-0.237(2)	0.06(1)
H(11)	-0.380(3)	0.369(4)	0.309(4)	0.06(1)
H(12)	-0.154(8)	0.462(4)	0.511(5)	0.13(2)
H(13)	0.147(5)	0.370(5)	0.562(2)	0.07(1)
H(14)	0.246(5)	0.203(6)	0.436(5)	0.11(2)
H(15)	0.011(8)	0.122(5)	0.211(4)	0.11(2)
H(31)	-0.351(5)	0.010(2)	-0.343(4)	0.05(1)
H(32)	-0.253(6)	0.141(5)	-0.397(3)	0.08(2)
H(41)	-0.496(7)	0.159(5)	-0.192(3)	0.09(2)
H(42)	-0.565(4)	0.195(5)	-0.373(2)	0.05(1)
H(61)	-0.419(4)	0.393(5)	-0.057(4)	0.07(1)
H(62)	-0.261(5)	0.471(3)	-0.135(4)	0.06(1)
H(91)	-0.340(7)	0.099(5)	0.173(5)	0.08(2)
H(92)	-0.452(6)	0.237(5)	0.120(4)	0.08(1)
H(3o)	0.204	0.275	-0.044	0.1

Table 3

Anisotropic thermal parameters.

	U11	U22	U33	U12	U13	U23
C(1)	0.031(2)	0.043(2)	0.058(2)	-0.002(1)	0.003(1)	0.001(2)
C(2)	0.041(2)	0.042(2)	0.051(2)	0.002(2)	0.010(2)	-0.008(2)
C(3)	0.054(2)	0.056(3)	0.055(2)	-0.001(2)	0.005(2)	-0.009(2)
C(4)	0.049(2)	0.071(3)	0.063(3)	0.009(2)	-0.007(2)	-0.005(2)
C(5)	0.050(2)	0.065(3)	0.064(3)	0.021(2)	0.014(2)	0.010(2)
C(6)	0.045(2)	0.038(2)	0.074(3)	0.006(2)	0.018(2)	0.005(2)
C(7)	0.038(2)	0.033(2)	0.053(2)	-0.002(1)	0.010(2)	-0.002(2)
C(8)	0.037(2)	0.042(2)	0.050(2)	0.000(1)	0.011(1)	0.001(2)
C(9)	0.053(2)	0.063(3)	0.053(2)	-0.004(2)	0.017(2)	0.001(2)
C(10)	0.053(2)	0.045(2)	0.046(2)	0.000(2)	0.015(2)	0.005(2)
C(11)	0.076(3)	0.061(3)	0.071(3)	0.008(3)	0.031(2)	0.001(3)
C(12)	0.130(5)	0.067(3)	0.064(3)	-0.023(3)	0.038(3)	-0.015(3)
C(13)	0.108(4)	0.093(4)	0.049(3)	-0.041(4)	0.001(3)	0.013(3)
C(14)	0.080(3)	0.089(4)	0.055(3)	-0.001(3)	-0.009(2)	0.018(3)
C(15)	0.066(3)	0.061(3)	0.061(3)	0.013(2)	0.001(2)	0.004(2)
N	0.043(2)	0.041(2)	0.050(2)	-0.007(1)	0.013(1)	0.000(1)
O(1)	0.053(2)	0.034(1)	0.100(2)	-0.002(1)	0.020(2)	0.007(2)
O(2)	0.103(3)	0.081(3)	0.089(2)	0.041(2)	0.019(2)	0.022(2)
O(3)	0.034(1)	0.049(2)	0.084(2)	0.003(1)	0.007(1)	-0.007(1)

Table 4

Bond distances of the non-hydrogen atoms (Å)
with standard deviations in parentheses.

C(1)	-	C(2)	1.510(7)	C(7)	-	N	1.46(1)
C(1)	-	N	1.35(1)	C(8)	-	O(3)	1.423(6)
C(1)	-	O(1)	1.24(2)	C(9)	-	C(10)	1.492(8)
C(2)	-	C(3)	1.529(5)	C(9)	-	N	1.456(6)
C(2)	-	C(8)	1.52(1)	C(10)	-	C(11)	1.39(1)
C(3)	-	C(4)	1.55(1)	C(10)	-	C(15)	1.378(7)
C(4)	-	C(5)	1.54(2)	C(11)	-	C(12)	1.39(1)
C(5)	-	C(6)	1.476(7)	C(12)	-	C(13)	1.36(1)
C(5)	-	O(2)	1.21(1)	C(13)	-	C(14)	1.38(1)
C(6)	-	C(7)	1.54(1)	C(14)	-	C(15)	1.373(9)
C(7)	-	C(8)	1.542(9)				

Table 5

Bond distances of the hydrogen atoms (Å)
with standard deviations in parentheses

C(2)	-	H(2)	1.00(3)	C(9)	-	H(91)	0.78(5)
C(3)	-	H(31)	1.00(3)	C(9)	-	H(92)	1.11(5)
C(3)	-	H(32)	1.00(4)	C(11)	-	H(11)	1.00(3)
C(4)	-	H(41)	1.00(3)	C(12)	-	H(12)	1.00(5)
C(4)	-	H(42)	1.01(2)	C(13)	-	H(13)	1.01(3)
C(6)	-	H(61)	0.99(4)	C(14)	-	H(14)	1.00(4)
C(6)	-	H(62)	1.00(3)	C(15)	-	H(15)	1.00(4)
C(7)	-	H(7)	1.00(2)	O(3)	-	H(3o)	0.99(1)
C(8)	-	H(8)	1.00(3)				

Table 6

Bond angles of the non-hydrogen atoms
with standard deviations in parentheses.

C(2)	-	C(1)	-	N	108.2(9)
C(2)	-	C(1)	-	O(1)	127.1(9)
N	-	C(1)	-	O(1)	124.6(5)
C(1)	-	C(2)	-	C(3)	109.8(3)
C(1)	-	C(2)	-	C(8)	102.5(6)
C(3)	-	C(2)	-	C(8)	114.5(9)
C(2)	-	C(3)	-	C(4)	114.9(5)
C(3)	-	C(4)	-	C(5)	113.5(6)
C(4)	-	C(5)	-	C(6)	119.7(8)
C(4)	-	C(5)	-	O(2)	118.6(6)
C(6)	-	C(5)	-	O(2)	122(1)
C(5)	-	C(6)	-	C(7)	118.8(9)
C(6)	-	C(7)	-	C(8)	113.6(4)
C(6)	-	C(7)	-	N	112.9(4)
C(8)	-	C(7)	-	N	101.8(9)
C(2)	-	C(8)	-	C(7)	103.0(5)
C(2)	-	C(8)	-	O(3)	107.3(9)
C(7)	-	C(8)	-	O(3)	110.7(3)
C(10)	-	C(9)	-	N	112.0(5)
C(9)	-	C(10)	-	C(11)	120.8(5)
C(9)	-	C(10)	-	C(15)	122.1(8)
C(11)	-	C(10)	-	C(15)	117.1(6)
C(10)	-	C(11)	-	C(12)	119.8(6)
C(11)	-	C(12)	-	C(13)	121.9(9)
C(12)	-	C(13)	-	C(14)	118.9(7)
C(13)	-	C(14)	-	C(15)	119.5(6)
C(10)	-	C(15)	-	C(14)	122.7(9)
C(1)	-	N	-	C(7)	113.1(5)
C(1)	-	N	-	C(9)	125.2(9)
C(7)	-	N	-	C(9)	121.7(9)

Table 7

Bond angles of the hydrogen atoms
with standard deviations in parentheses.

C(1)	-	C(2)	-	H(2)	110(2)
C(3)	-	C(2)	-	H(2)	108(2)
C(8)	-	C(2)	-	H(2)	112(2)
C(2)	-	C(3)	-	H(31)	111(2)
C(2)	-	C(3)	-	H(32)	114(2)
C(4)	-	C(3)	-	H(31)	106(2)
C(4)	-	C(3)	-	H(32)	106(3)
H(31)	-	C(3)	-	H(32)	104(3)
C(3)	-	C(4)	-	H(41)	103(3)
C(3)	-	C(4)	-	H(42)	109(2)
C(5)	-	C(4)	-	H(41)	101(3)
C(5)	-	C(4)	-	H(42)	104(3)
H(41)	-	C(4)	-	H(42)	127(3)
C(5)	-	C(6)	-	H(61)	106(2)
C(5)	-	C(6)	-	H(62)	103(2)
C(7)	-	C(6)	-	H(61)	109(2)
C(7)	-	C(6)	-	H(62)	109(2)
H(61)	-	C(6)	-	H(62)	110(4)
C(6)	-	C(7)	-	H(7)	115(2)
C(8)	-	C(7)	-	H(7)	108(1)
N	-	C(7)	-	H(7)	104(2)
C(2)	-	C(8)	-	H(8)	100(2)
C(7)	-	C(8)	-	H(8)	116(2)
O(3)	-	C(8)	-	H(8)	118(2)
C(10)	-	C(9)	-	H(91)	100(3)
C(10)	-	C(9)	-	H(92)	110(2)
N	-	C(9)	-	H(91)	112(4)
N	-	C(9)	-	H(92)	106(2)
H(91)	-	C(9)	-	H(92)	117(4)
C(10)	-	C(11)	-	H(11)	114(2)
C(12)	-	C(11)	-	H(11)	125(3)
C(11)	-	C(12)	-	H(12)	124(3)
C(13)	-	C(12)	-	H(12)	114(3)
C(12)	-	C(13)	-	H(13)	121(2)
C(14)	-	C(13)	-	H(13)	119(2)
C(13)	-	C(14)	-	H(14)	111(3)
C(15)	-	C(14)	-	H(14)	126(3)
C(10)	-	C(15)	-	H(15)	103(3)
C(14)	-	C(15)	-	H(15)	134(3)
C(8)	-	O(3)	-	H(3o)	103.3(9)

>>> master file m22bey.aaa --> bdf m22bey.aal

 *** Begin SORTRF ***

Input m22bey.aal with file history... m22bey

STARTX	29-Nov96	09:30:33	ADDDTM	29-Nov96	09:30:43	CRYLSQ	29-Nov96	09:31:42
BONDLA	29-Nov96	09:31:46	CRYLSQ	29-Nov96	09:33:59	BONDLA	29-Nov96	09:34:03
REGWT	29-Nov96	10:31:38	CRYLSQ	29-Nov96	10:34:11	BONDLA	29-Nov96	10:34:16
REGWT	29-Nov96	10:50:18	CRYLSQ	29-Nov96	10:52:55	BONDLA	29-Nov96	10:53:00
ADDDTM	29-Nov96	10:54:08	REGWT	29-Nov96	10:54:10	CRYLSQ	29-Nov96	10:56:46
BONDLA	29-Nov96	10:56:51	REGWT	29-Nov96	10:58:38	CRYLSQ	29-Nov96	11:01:26
BONDLA	29-Nov96	11:01:31	REGWT	29-Nov96	11:01:56	CRYLSQ	29-Nov96	11:04:41
BONDLA	29-Nov96	11:04:47	ADDDTM	29-Nov96	11:05:07	CRYLSQ	29-Nov96	11:09:40
BONDLA	29-Nov96	11:09:47	REGWT	29-Nov96	11:11:40	CRYLSQ	29-Nov96	11:18:24
BONDLA	29-Nov96	11:18:32	REGWT	29-Nov96	11:19:17	CRYLSQ	29-Nov96	11:24:24
BONDLA	29-Nov96	11:24:31	ADDDTM	29-Nov96	11:47:34	REGWT	29-Nov96	11:47:37
CRYLSQ	29-Nov96	11:53:22	BONDLA	29-Nov96	11:53:38	ADDDTM	29-Nov96	12:52:32
REGWT	29-Nov96	12:52:34	CRYLSQ	29-Nov96	12:56:33	BONDLA	29-Nov96	12:56:40
ADDDTM	29-Nov96	13:23:19	REGWT	29-Nov96	13:23:21	CRYLSQ	29-Nov96	13:27:35
BONDLA	29-Nov96	13:27:43	CRYLSQ	29-Nov96	13:36:34	BONDLA	29-Nov96	13:36:42
BONDLA	29-Nov96	15:51:39	ADDDTM	10-Feb97	13:54:42	CRYLSQ	10-Feb97	13:59:03

SORTRF Control Parameters

 Sorting algorithm
 s/m/f ordering indices

1
 HKL

Reflections printed
 Reflections sorted

25
 1449

h	k	l
-8	0	1
-8	0	2
-8	0	3
-8	0	4
-8	0	5
-8	0	6
-8	1	1
-8	1	2
-8	1	3
-8	1	4
-8	1	5
-8	1	6
-8	2	1
-8	2	2
-8	2	3
-8	2	4
-8	2	5
-8	2	6
-8	3	1
-8	3	2
-8	3	3
-8	3	4
-8	3	5
-8	4	1
-8	4	2

Reflection packets output to archive 1449

Reflection statistics	h	k	l	theta
min	-8	0	0	4.58
max	8	12	12	74.64

Time	h m s	CPU secs	Total CPU secs	Memory words
	15:18:28	8.71000	8.80000	11211

>>>> ARCHIVE files interchanged. A in: m22bey.aa2 B out: m22bey.aa1

 *** Begin LISTFC ***

Input m22bey.aa2 with file history... m22bey

STARTX	29-Nov96	09:30:33	ADDATM	29-Nov96	09:30:43	CRYLSQ	29-Nov96	09:31:42
BONDLA	29-Nov96	09:31:46	CRYLSQ	29-Nov96	09:33:59	BONDLA	29-Nov96	09:34:03
REGWT	29-Nov96	10:31:38	CRYLSQ	29-Nov96	10:34:11	BONDLA	29-Nov96	10:34:16
REGWT	29-Nov96	10:50:18	CRYLSQ	29-Nov96	10:52:55	BONDLA	29-Nov96	10:53:00
ADDATM	29-Nov96	10:54:08	REGWT	29-Nov96	10:54:10	CRYLSQ	29-Nov96	10:56:46
BONDLA	29-Nov96	10:56:51	REGWT	29-Nov96	10:58:38	CRYLSQ	29-Nov96	11:01:26
BONDLA	29-Nov96	11:01:31	REGWT	29-Nov96	11:01:56	CRYLSQ	29-Nov96	11:04:41
BONDLA	29-Nov96	11:04:47	ADDATM	29-Nov96	11:05:07	CRYLSQ	29-Nov96	11:09:40
BONDLA	29-Nov96	11:09:47	REGWT	29-Nov96	11:11:40	CRYLSQ	29-Nov96	11:18:24
BONDLA	29-Nov96	11:18:32	REGWT	29-Nov96	11:19:17	CRYLSQ	29-Nov96	11:24:24
BONDLA	29-Nov96	11:24:31	ADDATM	29-Nov96	11:47:34	REGWT	29-Nov96	11:47:37
CRYLSQ	29-Nov96	11:53:22	BONDLA	29-Nov96	11:53:38	ADDATM	29-Nov96	12:52:32
REGWT	29-Nov96	12:52:34	CRYLSQ	29-Nov96	12:56:33	BONDLA	29-Nov96	12:56:40
ADDATM	29-Nov96	13:23:19	REGWT	29-Nov96	13:23:21	CRYLSQ	29-Nov96	13:27:35
BONDLA	29-Nov96	13:27:43	CRYLSQ	29-Nov96	13:36:34	BONDLA	29-Nov96	13:36:42
BONDLA	29-Nov96	15:51:39	ADDATM	10-Feb97	13:54:42	CRYLSQ	10-Feb97	13:59:03
SORTRF	11-Feb97	15:18:23						

LISTFC CONTROL PARAMETERS

ITEMS TO BE LISTED	1	1701	1800	1305
OUTPUT FORMATS ARE	I 4	F 6.1	F 6.1	F 4.1
ITEMS HAVE BEEN SCALED	1.00	1.00	1.00	1.00
CHARS/LINE LINES/PAGE	85	56		
FREL AND SIGF SCALE(S)	1	.1849		

				5	1.9	2.3	.1	5	3.7	4.1	.1
				6	1.1	1.3	.2	6	2.5	2.6	.1
				7	2.2	2.5	.1				
				8	1.9	2.3	.1				

								5	11.0	11.0	.1
								6	2.9	2.7	.1
								7	2.6	2.7	.1
1	4.6	4.5	.1	1	.6	.6	.2	8	1.6	1.5	.1
2	7.1	6.7	.1	2	1.0	.9	.2	9	1.9	1.9	.1
3	7.5	7.3	.1	3	1.5	1.3	.1	10	.5	.1	.2
4	6.4	6.0	.1	4	.9	1.0	.2				
5	5.0	5.2	.1	5	.8	.8	.2	-5,4,L			
6	3.0	2.9	.1								
7	1.3	1.3	.2	-5,0,L				1	5.5	5.2	.1
8	1.3	.7	.1					2	2.6	2.6	.1
9	1.6	1.6	.1	1	8.5	8.2	.1	3	3.9	3.6	.1
				2	.6	.0	.2	4	3.8	3.8	.1
-6,4,L				3	3.7	3.3	.1	5	7.7	7.7	.1
				4	10.5	10.0	.1	6	1.4	1.5	.2
1	2.1	2.4	.1	5	4.3	4.2	.1	7	3.7	3.9	.1
2	4.2	4.1	.1	6	11.6	12.1	.1	8	1.0	.7	.2
3	4.2	3.9	.1	7	2.7	2.8	.1	9	.6	.6	.2
4	7.8	7.9	.1	8	2.4	2.4	.1	10	1.4	1.5	.1
5	8.6	8.4	.1	9	1.0	1.5	.2				
6	4.3	4.2	.1	10	3.9	3.7	.1	-5,5,L			
7	1.4	1.5	.2								
8	1.1	.9	.2	-5,1,L				1	8.3	8.1	.1
9	2.3	2.3	.1					2	3.5	3.4	.1
				1	11.9	11.7	.1	3	11.4	11.4	.1
-6,5,L				2	8.7	8.4	.1	4	10.1	10.2	.1
				3	1.0	1.4	.2	5	4.6	4.5	.1
1	4.7	4.5	.1	4	6.1	6.1	.1	6	3.3	3.3	.1
2	1.6	2.1	.2	5	3.9	3.8	.1	7	4.1	4.0	.1
3	2.6	2.4	.1	6	3.7	3.5	.1	8	2.2	2.3	.1
4	2.3	2.6	.1	7	4.1	4.1	.1	9	1.2	1.2	.1
5	1.5	1.2	.2	8	1.4	1.6	.2				
6	1.5	1.5	.2	9	1.5	1.6	.1	-5,6,L			
7	2.2	2.1	.1	10	.5	.2	.2				
8	.6	.4	.2					1	4.4	4.2	.1
				-5,2,L				2	3.9	3.7	.1
-6,6,L								3	6.1	5.9	.1
				1	8.4	8.3	.1	4	4.7	4.9	.1
1	4.3	4.2	.1	2	13.2	13.0	.1	5	3.7	4.0	.1
2	1.1	1.1	.2	3	6.5	6.6	.1	6	.9	.5	.3
3	2.1	2.1	.1	4	6.4	6.1	.1	7	2.3	2.4	.1
4	1.5	1.5	.2	5	2.7	2.9	.1	8	1.5	1.3	.1
5	1.8	1.7	.1	6	6.8	6.6	.1				
6	1.2	1.1	.2	7	2.4	2.5	.1	-5,7,L			
7	4.2	4.5	.1	8	2.5	2.0	.1				
				9	1.5	1.2	.1	1	4.6	4.6	.1
-6,7,L				10	2.4	2.3	.1	2	3.0	3.1	.1
								3	2.6	2.4	.1
1	4.4	4.2	.1	-5,3,L				4	.7	1.1	.3
2	4.5	4.4	.1					5	.6	.2	.2
3	1.6	1.4	.1	1	10.0	10.0	.1	6	1.6	1.1	.1
4	.9	1.1	.2	2	3.7	3.4	.1	7	1.4	1.5	.1
5	2.8	3.2	.1	3	9.1	8.9	.1	8	.7	.8	.2
6	1.6	1.6	.1	4	5.3	5.3	.1				

				1	2.8	2.7	.1	1	8.2	8.2	.1
				2	12.0	12.3	.1	2	3.8	4.0	.1
				3	4.8	5.1	.1	3	5.0	4.8	.1
1	1.7	1.6	.1	4	14.9	14.8	.1	4	.7	.4	.3
2	2.4	2.5	.1	5	2.2	1.8	.1	5	4.4	4.2	.1
3	2.2	2.2	.1	6	3.5	3.7	.1	6	6.2	6.2	.1
4	.8	.9	.3	7	7.3	7.5	.1	7	3.5	4.2	.1
5	1.0	1.2	.2	8	1.5	1.2	.2	8	3.1	3.2	.1
6	2.5	2.5	.1	9	2.2	2.4	.1	9	1.0	1.0	.2
7	1.3	1.5	.1	10	.6	.7	.2				
				11	1.1	1.4	.1				
								</			

-3,0,L				-3,4,L				1	5.6	5.5	.1
3	27.8	28.2	.0	1	10.1	9.5	.1	2	6.6	6.3	.1
4	14.1	13.1	.0	2	4.7	4.3	.1	3	3.7	3.6	.1
5	12.9	13.2	.1	3	7.1	7.2	.1	4	1.5	1.1	.2
6	8.1	8.9	.1	4	3.3	3.6	.1	5	.6	.2	.3
7	7.8	7.9	.1	5	4.2	4.4	.1	6	2.3	2.4	.1
8	4.8	5.4	.1	6	2.0	2.5	.2	7	2.7	3.1	.1
9	7.1	8.0	.1	7	3.6	3.6	.1	8	2.5	2.4	.1
10	.6	.8	.2	8	3.0	2.8	.1	-3,9,L			
11	2.7	3.0	.1	9	2.6	2.6	.1	1	8.1	7.7	.1
-3,1,L				10	.9	.5	.3	2	3.0	3.1	.1
1	13.2	13.4	.0	11	1.6	1.6	.1	3	1.4	1.8	.2
2	5.4	5.0	.0	-3,5,L				4	2.6	2.6	.1
3	15.0	14.8	.0	1	3.6	3.1	.1	5	2.0	2.2	.1
4	21.3	21.3	.0	2	11.9	11.4	.1	6	1.5	1.6	.1
5	5.0	5.0	.1	3	8.7	8.1	.1	7	.5	.6	.2
6	2.5	2.7	.1	4	7.4	7.7	.1	-3,10,L			
7	9.7	10.1	.1	5	4.3	4.5	.1	1	5.3	5.2	.1
8	1.4	1.3	.2	6	13.3	13.6	.1	2	1.8	1.9	.1
9	3.4	3.7	.1	7	5.1	5.1	.1	3	1.5	1.5	.2
10	3.3	3.1	.1	8	1.6	1.9	.2	4	.5	.6	.2
11	.7	.5	.2	9	2.4	2.0	.1	5	1.3	1.1	.1
-3,2,L				10	2.9	2.8	.1	6	1.5	1.6	.1
1	23.5	22.5	.0	-3,6,L				-3,11,L			
2	7.1	6.8	.0	1	4.2	4.5	.1	1	3.1	2.9	.1
3	11.4	11.4	.0	2	6.5	6.4	.1	2	1.1	1.5	.2
4	11.8	11.9	.0	3	9.6	9.3	.1	3	1.2	1.3	.2
5	5.4	4.9	.1	4	4.5	4.0	.1	-2,0,L			
6	8.9	9.1	.1	5	6.3	6.3	.1	1	52.0	51.5	.1
7	6.5	6.9	.1	6	1.0	1.7	.3	2	27.3	27.5	.0
8	5.0	5.2	.1	7	3.2	3.3	.1	3	16.0	15.8	.0
9	5.2	5.2	.1	8	3.3	3.3	.1	4	22.3	22.2	.0
10	.9	.9	.2	9	2.0	1.8	.1	5	22.2	21.8	.0
11	.5	.6	.2	10	.5	.5	.2	6	5.4	5.3	.1
-3,3,L				-3,7,L				7	5.4	5.2	.1
1	4.6	4.2	.1	1	6.1	6.0	.1	8	4.2	4.5	.1
2	5.3	5.1	.1	2	6.7	6.2	.1	9	1.6	2.1	.2
3	1.2	1.5	.2	3	7.8	7.8	.1	10	.5	.4	.2
4	6.6	5.6	.1	4	6.5	6.3	.1	11	3.2	3.2	.1
5	7.0	7.1	.1	5	2.1	1.8	.1	12	3.2	3.2	.1
6	5.7	5.6	.1	6	5.7	6.4	.1	-2,1,L			
7	5.1	5.3	.1	7	2.8	3.3	.1	1	20.4	19.3	.0
8	2.4	2.5	.1	8	3.0	3.3	.1	2	27.6	26.6	.0
9	3.6	3.3	.1	9	3.0	3.0	.1	-3,8,L			
10	2.3	2.3	.1	-3,8,L							
11	.7	.8	.2								

				11	1.2	1.2	.1						
			-2,1,L						1	.8	.5	.3	
						-2,5,L			2	3.8	3.9	.1	
3	8.5	8.4	.0						3	6.6	6.4	.1	
4	21.1	21.7	.0	1	24.9	22.9	.0		4	5.0	4.9	.1	
5	15.9	16.2	.0	2	3.6	2.9	.1		5	3.1	3.6	.1	
6	8.0	8.3	.1	3	3.9	4.2	.1		6	1.3	1.1	.2	
7	2.8	2.8	.1	4	7.9	7.7	.1		7	1.6	1.6	.1	
8	5.8	5.9	.1	5	3.8	3.7	.1		8	1.5	1.5	.1	
9	5.6	5.9	.1	6	2.0	2.4	.2						
10	4.1	3.9	.1	7	1.2	1.4	.2			-2,10,L			
11	2.8	2.9	.1	8	2.6	2.4	.1						
12	1.7	1.4	.1	9	2.3	2.3	.1	1	3.7	3.5	.1		
				10	2.7	2.7	.1	2	2.7	2.5	.1		
			-2,2,L	11	1.2	1.0	.1	3	.7	.4	.3		
								4	2.4	2.8	.1		
1	20.4	19.7	.0			-2,6,L		5	1.2	1.3	.2		
2	10.7	10.4	.0					6	1.8	2.3	.1		
3	8.2	8.1	.0	1	5.8	5.4	.1						
4	18.6	17.9	.0	2	8.9	8.3	.1			-2,11,L			
5	14.2	14.1	.0	3	1.5	1.7	.2						
6	4.4	4.1	.1	4	8.4	8.9	.1	1	2.2	2.0	.1		
7	7.2	6.9	.1	5	7.6	7.6	.1	2	.7	.6	.3		
8	.6	.3	.3	6	11.7	12.3	.1	3	.9	1.0	.2		
9	1.6	1.3	.2	7	5.4	4.8	.1	4	3.0	3.3	.1		
10	3.2	3.1	.1	8	2.4	2.9	.1						
11	.8	.9	.2	9	1.6	1.4	.1			-1,0,L			
				10	2.0	1.9	.1						
			-2,3,L					1	17.3	17.3	.0		
						-2,7,L		2	34.4	34.4	.1		
1	14.3	13.6	.0					3	15.2	15.5	.0		
2	28.4	27.5	.0	1	4.8	4.9	.1	4	15.4	15.5	.0		
3	18.2	18.4	.0	2	5.4	5.2	.1	5	7.8	7.4	.0		
4	9.9	10.1	.0	3	4.9	4.8	.1	6	2.8	2.2	.1		
5	8.1	7.7	.1	4	3.6	3.1	.1	7	2.9	3.2	.1		
6	8.7	9.0	.1	5	5.5	5.3	.1	8	.6	1.3	.2		
7	4.8	4.6	.1	6	4.1	4.0	.1	9	6.7	6.6	.1		
8	3.0	2.9	.1	7	4.1	4.0	.1	10	.8	1.1	.3		
9	2.7	2.6	.1	8	1.8	1.5	.1	11	3.4	3.1	.1		
10	.8	1.1	.3	9	.7	.4	.2	12	3.3	3.0	.1		
11	1.6	1.5	.1										
						-2,8,L				-1,1,L			
			-2,4,L					1	42.4	41.3	.1		
1	26.1	23.9	.0	1	8.5	8.2	.1	2	66.3	65.5	.1		
2	25.2	24.3	.0										

				5	11.6	11.7	.1	7	.8	1.1	.2
	-1,1,L			6	3.3	3.2	.1	8	.7	.8	.2
				7	9.8	9.5	.1				
12	1.6	1.4	.1	8	7.0	7.2	.1		-1,10,L		
				9	5.5	5.5	.1				
	-1,2,L			10	2.0	2.1	.1	1	3.2	3.3	.1
				11	2.0	1.9	.1	2	1.2	1.4	.3
1	26.9	25.9	.0					3	2.9	2.9	.1
2	53.2	51.1	.2		-1,6,L			4	.8	1.4	.3
3	7.3	6.8	.0	1	12.6	11.9	.1	5	1.4	1.4	.2
4	23.5	23.2	.0	2	4.0	4.5	.1	6	1.2	1.1	.2
5	8.4	8.2	.0	3	4.5	4.7	.1	7	2.8	3.1	.1
6	3.3	3.5	.1	4	8.0	8.1	.1		-1,11,L		
7	3.5	3.3	.1	5	7.1	7.1	.1	1	.6	.5	.3
8	2.9	3.1	.1	6	3.2	3.6	.1	2	2.2	2.2	.1
9	6.7	6.7	.1	7	8.4	8.5	.1	3	1.6	1.8	.1
10	1.8	1.9	.1	8	3.1	3.2	.1	4	.9	.5	.2
11	.7	.7	.2	9	1.5	1.6	.2	5	1.2	.8	.1
12	1.6	1.4	.1	10	1.8	1.7	.1				
	-1,3,L										
					-1,7,L				-1,12,L		
1	7.2	6.6	.0	1	3.4	3.3	.1	1	2.0	1.9	.1
2	19.2	18.9	.0	2	5.7	5.5	.1	2	.5	1.9	.2
3	24.8	24.6	.0	3	5.0	4.8	.1				
4	17.8	17.5	.0	4	3.9	3.8	.1		0,0,L		
5	8.1	8.5	.1	5	7.3	7.2	.1	1	32.7	34.8	.1
6	9.7	9.7	.1	6	2.4	2.2	.1	2	2.3	2.6	.1
7	9.2	8.7	.1	7	.8	.9	.3	3	28.7	29.5	.0
8	10.6	10.5	.1	8	3.0	3.2	.1	4	6.7	7.0	.0
9	5.1	5.3	.1	9	1.2	1.2	.2	5	9.8	9.5	.0
10	5.9	5.3	.1	10	1.9	1.7	.1	6	4.6	4.5	.1
11	1.2	1.4	.2					7	4.3	4.4	.1
	-1,4,L				-1,8,L			8	.6	.3	.3
1	8.8	7.9	.0	1	3.0	3.1	.1	9	3.3	3.5	.1
2	23.4	22.7	.0	2	1.3	1.4	.2	10	4.0	3.7	.1
3	19.6	19.2	.0	3	6.3	6.4	.1	11	.5	.0	.2
4	7.0	6.9	.1	4	7.1	7.6	.1	12	.8	1.1	.2
5	12.1	12.3	.1	5	4.5	4.5	.1				
6	6.6	6.5	.1	6	.7	.8	.3		0,1,L		
7	5.5	5.4	.1	7	2.2	2.4	.1	1	12.7	13.9	.0
8	5.2	5.3	.1	8	2.1	1.9	.1	2	32.5	33.6	.1
9	.6	.4	.3	9	.5	.7	.2	3	10.6	11.5	.0
10	1.0	1.1	.2		-1,9,L			4	14.9	15.6	.0
11	1.9	1.7	.1					5	12.0	12.3	.0
	-1,5,L			1	8.6	8.2	.1	6	5.3	5.2	.1
				2	12.9	12.9	.1	7	9.4	10.0	.1
1	9.5	9.2	.0	3	4.1	4.1	.1	8	1.3	1.5	.2
2	18.3	17.7	.0	4	1.9	2.2	.2	9	6.1	6.0	.1
3	14.8	14.2	.1	5	1.0	.8	.3	10	2.3	2.1	.1
4	4.5	4.4	.1	6	1.4	.8	.2	11	1.8	1.7	.1

				4	2.5	2.5	.1	5	4.3	4.7	.1
		0,1,L		5	10.2	10.5	.1	6	4.1	4.0	.1
				6	2.4	1.8	.1	7	1.1	1.3	.2
12	1.5	1.2	.1	7	10.8	11.0	.1	8	1.1	.7	.1
				8	4.3	4.3	.1				
		0,2,L		9	1.9	1.5	.1		0,10,L		
				10	.8	.6	.2				
0	51.5	51.3	.1	11	.6	.8	.2	0	1.6	1.8	.2
1	31.5	32.1	.1					1	3.6	3.6	.1
2	25.1	26.0	.0			0,6,L		2	4.1	4.3	.1
3	2.6	2.5	.1					3	2.7	2.6	.1
4	2.2	2.5	.1	0	14.1	14.4	.1	4	2.2	1.9	.1
5	4.9	5.2	.1	1	2.1	2.3	.1	5	1.7	1.8	.1
6	6.6	6.8	.1	2	4.0	4.7	.1	6	.7	.3	.2
7	9.2	9.0	.1	3	9.0	9.1	.1				
8	6.8	7.1	.1	4	5.5	5.6	.1		0,11,L		
9	6.2	6.1	.1	5	8.6	8.8	.1				
10	4.5	4.2	.1	6	5.3	5.5	.1	1	2.8	3.2	.1
11	.6	.1	.2	7	2.8	2.8	.1	2	2.2	2.6	.1
				8	3.6	3.5	.1	3	3.3	3.5	.1
		0,3,L		9	1.7	1.7	.1	4	2.4	2.7	.1
				10	1.1	1.3	.2	5	1.0	1.3	.2
1	26.7	27.6	.2								
2	25.1	25.8	.0			0,7,L			0,12,L		
3	12.2	12.0	.0								
4	3.3	3.3	.1	1	2.6	3.2	.1	0	1.9	2.4	.1
5	11.9	12.0	.1	2	12.0	12.1	.1	1	1.4	1.4	.2
6	4.5	4.7	.1	3	3.2	3.0	.1	2	.7	1.4	.3
7	6.6	6.8	.1	4	1.3	1.6	.2				
8	8.1	7.6	.1	5	8.1	8.2	.1		1,0,L		
9	4.8	4.5	.1	6	1.1	1.5	.3				
10	2.3	2.3	.1	7	3.4	3.7	.1	0	22.4	22.8	.1
11	.5	.2	.2	8	3.6	3.2	.1	1	12.0	13.6	.0
				9	1.1	1.5	.2	2	19.3	20.4	.0
		0,4,L						3	27.8	29.0	.0
						0,8,L		4	.4	1.2	.2
0	37.0	36.1	.2					5	3.4	2.8	.1
1	15.5	15.3	.0	0	10.2	10.4	.1	6	9.5	9.0	.1
2	6.6	5.8	.0	1	10.6	11.4	.1	7	4.0	4.1	.1
3	11.4	11.1	.0	2	11.6	12.4	.1	8	4.1	3.8	.1
4	2.5	2.6	.1	3	8.5	9.2	.1	9	.6	.2	.3
5	4.1	4.0	.1	4	2.7	2.9	.1	10	.6	.6	.2
6	6.7	6.5	.1	5	2.7	2.8	.1	11	1.8	1.7	.1
7	8.0	8.1	.1	6	1.6	1.9	.2				
8	4.9	5.2	.1	7	.7	.8	.3		1,1,L		
9	5.3	5.0	.1	8	2.5	2.5	.1				
10	1.3	1.1	.2	9	1.6	1.8	.1	0	59.3	59.0	.1
11	1.4	1.3	.1					1	39.3	41.3	.1
						0,9,L		2	25.3	25.9	.0
		0,5,L		1	2.9	3.2	.1	3	28.2	29.4	.0
1	4.2	4.0	.1	2	2.6	2.8	.1	4	4.9	5.1	.0
2	2.7	2.7	.1	3	3.8	4.3	.1	5	11.0	10.9	.0
3	10.1	9.6	.1	4	5.0	5.5	.1	6	13.9	13.5	.1
								7	9.1	9.1	.1

								0	5.5	5.4	.1
		1,1,L		0	12.6	12.1	.0	1	9.2	9.4	.1
				1	13.9	13.3	.0	2	7.9	8.0	.1
8	6.3	6.2	.1	2	9.0	9.3	.1	3	1.3	1.5	.3
9	1.1	1.1	.2	3	9.7	9.4	.1	4	4.7	4.9	.1
10	.6	.6	.2	4	3.2	3.2	.1	5	4.2	4.4	.1
11	2.8	2.7	.1	5	1.7	1.8	.1	6	3.4	3.7	.1
				6	8.1	8.1	.1	7	1.4	1.4	.1
		1,2,L		7	4.4	4.5	.1				
				8	6.0	5.8	.1			1,10,L	
0	33.8	33.5	.1	9	2.7	2.5	.1				
1	28.3	29.7	.1	10	2.4	1.9	.1	0	2.2	2.2	.2
2	23.8	25.4	.0					1	1.7	1.8	.2
3	23.5	24.5	.0			1,6,L		2	1.7	1.6	.2
4	8.1	8.0	.0					3	4.3	4.8	.1
5	7.8	7.9	.1	0	7.1	6.5	.1	4	2.4	2.2	.1
6	2.7	2.5	.1	1	8.4	8.7	.1	5	2.4	2.3	.1
7	6.4	6.6	.1	2	12.1	12.2	.1	6	.8	.5	.2
8	4.0	4.3	.1	3	14.9	15.0	.1				
9	4.6	4.7	.1	4	6.7	7.0	.1			1,11,L	
10	1.5	1.4	.2	5	6.0	6.1	.1				
11	2.7	2.6	.1	6	7.6	7.5	.1	0	1.2	1.5	.2
				7	4.1	3.9	.1	1	1.6	1.1	.2
		1,3,L		8	1.1	.5	.2	2	1.9	1.7	.1
				9	1.3	1.0	.2	3	.5	.3	.2
0	21.8	21.8	.0	10	1.7	1.5	.1	4	.5	.4	.2
1	17.5	17.7	.0								
2	11.4	12.0	.0			1,7,L				1,12,L	
3	17.6	17.2	.0								
4	16.5	16.0	.0	0	6.6	6.6	.1	0	1.2	1.1	.2
5	6.0	6.0	.1	1	2.8	2.9	.1	1	.6	1.3	.3
6	5.9	6.4	.1	2	3.8	4.0	.1				
7	8.6	8.9	.1	3	11.0	11.3	.1			2,0,L	
8	1.2	1.0	.2	4	.7	1.2	.3				
9	4.9	4.7	.1	5	7.2	7.5	.1	0	24.1	24.1	.0
10	1.9	1.8	.1	6	3.6	3.8	.1	1	29.8	30.1	.2
11	1.6	1.7	.1	7	1.3	1.2	.2	2	37.1	38.7	.2
				8	1.1	.8	.2	3	18.3	18.5	.0
		1,4,L		9	1.7	1.5	.1	4	17.1	17.0	.0
								5	4.1	3.7	.1
0	15.3	14.5	.0			1,8,L		6	6.3	6.4	.1
1	18.7	18.8	.0					7	.7	.8	.3
2	12.4	12.1	.0	0	3.0	3.2	.1	8	1.1	1.1	.2
3	7.1	6.6	.1	1	5.5	6.0	.1	9	2.0	2.2	.1
4	6.2	5.9	.1	2	1.3	1.9	.3	10	.9	1.7	.3
5	5.7	5.2	.1	3	2.3	2.4	.1	11	.5	.6	.2
6	8.1	8.2	.1	4	1.0	1.0	.3				
7	4.1	4.1	.1	5	5.7	6.0	.1			2,1,L	
8	3.2	3.5	.1	6	5.1	5.3	.1				
9	2.9	2.7	.1	7	3.1	3.0	.1	0	17.9	18.0	.0
10	1.9	1.7	.1	8	2.3	1.9	.1	1	26.1	27.2	.0
11	1.3	1.4	.1					2	1.5	1.3	.1
						1,9,L		4	17.5	17.0	.0
		1,5,L						5	2.1	2.2	.1

				2,5,L				0	1.4	1.1	.3
2,1,L								1	7.7	7.9	.1
				0	17.4	16.8	.0	2	1.5	1.7	.2
6	6.4	6.2	.1	1	14.2	13.9	.1	3	.6	1.0	.3
7	5.7	5.2	.1	2	3.2	3.1	.1	4	.6	.7	.3
8	2.4	2.2	.1	3	5.1	5.3	.1	5	2.2	2.2	.1
9	5.0	4.9	.1	4	6.5	5.7	.1	6	.6	1.0	.2
10	.6	.9	.2	5	4.2	3.9	.1	7	.6	.3	.2
11	2.7	2.3	.1	6	4.8	4.5	.1	2,10,L			
2,2,L				7	6.2	6.1	.1				
				8	3.4	3.2	.1	0	3.5	3.3	.1
0	14.6	14.4	.0	9	2.6	2.7	.1	1	4.1	4.0	.1
1	12.2	12.1	.0	10	2.3	2.2	.1	2	.9	.9	.3
2	15.8	15.6	.0	2,6,L				3	5.8	5.8	.1
3	16.4	16.2	.0					4	2.5	2.4	.1
4	9.5	9.3	.0	0	6.9	6.7	.1	5	.5	1.1	.2
5	2.5	2.8	.1	1	3.4	3.7	.1	6	3.0	3.1	.1
6	3.9	3.4	.1	2	3.7	3.7	.1	2,11,L			
7	3.2	3.8	.1	3	5.2	4.9	.1	0	1.8	1.8	.1
8	3.5	3.5	.1	4	8.1	8.1	.1	1	4.5	4.8	.1
9	5.5	5.0	.1	5	5.5	5.9	.1	2	1.0	.9	.2
10	1.3	.8	.2	6	3.5	3.3	.1	3	.9	1.5	.2
11	1.9	1.6	.1	7	1.9	2.0	.1	4	1.6	2.2	.1
2,3,L				8	.6	.7	.2				
				9	4.1	3.7	.1	3,0,L			
				2,7,L				0	13.3	13.0	.0
0	6.8	6.8	.0					1	14.0	14.0	.0
1	14.5	14.2	.0	0	7.0	6.7	.1	2	3.7	3.4	.1
2	6.0	6.6	.0	1	4.7	4.7	.1	3	1.9	1.6	.1
3	5.7	5.4	.1	2	4.7	4.8	.1	4	1.3	1.3	.1
4	5.3	5.8	.1	3	7.4	7.8	.1	5	1.0	1.3	.2
5	9.6	9.4	.1	4	5.4	5.7	.1	6	8.0	7.7	.1
6	5.0	4.9	.1	5	1.6	1.6	.2	7	8.3	8.3	.1
7	4.7	4.4	.1	6	.7	.6	.3	8	1.7	1.9	.2
8	6.7	6.9	.1	7	2.8	2.3	.1	9	.5	.8	.2
9	3.9	4.1	.1	8	.8	1.1	.2	10	1.6	1.1	.1
10	3.2	2.7	.1	9	1.1	.8	.1	3,1,L			
11	2.4	2.2	.1	2,8,L				0	20.4	20.4	.0
2,4,L								1	16.8	16.5	.0
				0	4.7	4.7	.1	2	26.9	27.7	.0
0	8.3	8.9	.0	1	10.3	10.3	.1	3	18.1	18.6	.0
1	5.4	5.4	.1	2	11.3	10.8	.1	4	8.1	7.9	.1
2	11.7	11.7	.0	3	3.2	3.4	.1	5	7.1	6.9	.1
3	17.4	17.1	.1	4	5.4	5.9	.1	6	4.4	4.5	.1
4	8.5	8.3	.1	5	3.9	3.9	.1	7	3.5	3.6	.1
5	2.6	2.3	.1	6	1.5	1.5	.2	8	1.9	1.9	.1
6	6.9	6.7	.1	7	1.6	1.5	.1	9	1.6	1.7	.2
7	5.0	5.3	.1	8	2.2	1.9	.1	10	2.5	2.2	.1
8	5.7	5.4	.1	2,9,L							
9	3.9	3.9	.1								
10	1.9	1.3	.1								

				9	3.5	3.5	.1	4	1.1	1.0	.2
3,2,L								5	2.3	2.5	.1
				3,6,L				3,11,L			
0	11.7	11.3	.0	0	3.8	3.2	.1				
1	18.9	19.3	.0	1	7.2	7.1	.1	0	1.5	1.2	.1
2	17.1	16.9	.0	2	3.6	3.7	.1	1	2.3	2.6	.1
3	13.1	13.0	.1	3	1.9	2.1	.2	2	3.1	3.0	.1
4	9.4	9.0	.1	4	4.7	4.9	.1	4,0,L			
5	5.2	4.7	.1	5	1.4	1.2	.2				
6	6.5	6.1	.1	6	3.4	3.7	.1	0	8.5	8.8	.1
7	2.7	2.9	.1	7	2.8	2.8	.1	1	.5	1.5	.2
8	4.7	4.7	.1	8	.6	.8	.2	2	5.6	5.5	.1
9	.6	.5	.2	9	2.5	2.2	.1	3	8.3	8.6	.1
10	2.6	2.3	.1	3,7,L				4	5.0	4.9	.1
3,3,L				0	3.8	3.9	.1	5	3.0	3.7	.1
0	6.3	6.5	.1	1	12.1	12.2	.1	6	7.2	7.8	.1
1	19.2	19.6	.0	2	8.5	7.9	.1	7	4.0	4.3	.1
2	5.7	5.9	.1	3	1.6	1.8	.2	8	2.6	2.2	.1
3	5.7	5.7	.1	4	5.4	5.4	.1	9	.5	.1	.2
4	11.3	11.0	.1	5	3.6	3.5	.1	10	1.0	.7	.1
5	9.3	9.4	.1	6	2.4	2.5	.1	4,1,L			
6	7.2	7.8	.1	7	3.7	3.2	.1				
7	.8	.4	.3	8	2.1	1.9	.1	0	10.8	10.6	.0
8	2.9	2.9	.1	3,8,L				1	3.9	3.7	.1
9	1.5	1.4	.1	0	3.9	4.2	.1	2	5.0	5.4	.1
10	1.4	1.5	.1	1	4.6	4.6	.1	3	9.3	9.1	.1
3,4,L				2	4.0	4.1	.1	4	18.7	18.5	.1
0	8.3	8.2	.1	3	4.8	4.4	.1	5	6.7	6.6	.1
1	11.5	11.4	.1	4	3.2	2.9	.1	6	2.4	2.4	.1
2	3.4	3.7	.1	5	4.9	5.0	.1	7	1.2	1.2	.2
3	6.3	6.4	.1	6	2.6	2.8	.1	8	.5	.7	.2
4	3.4	3.2	.1	7	.9	1.2	.2	9	2.3	1.8	.1
5	7.6	7.5	.1	3,9,L				4,2,L			
6	5.4	5.2	.1	0	5.2	5.3	.1	0	4.4	4.8	.1
7	2.0	1.6	.1	1	10.3	10.5	.1	1	8.6	8.2	.1
8	2.7	3.2	.1	2	4.1	4.0	.1	2	12.6	12.5	.1
9	2.4	2.2	.1	3	1.7	1.5	.1	3	8.0	7.6	.1
10	1.6	1.3	.1	4	3.1	3.4	.1	4	5.3	4.7	.1
3,5,L				5	1.8	1.7	.1	5	2.5	2.8	.1
0	8.7	8.3	.1	6	.6	.4	.2	6	5.4	5.4	.1
1	11.0	11.0	.1	3,10,L				7	7.1	7.1	.1
2	7.4	7.5	.1	0	1.4	1.5	.2	8	2.8	2.1	.1
3	3.0	2.5	.1	1	.9	.7	.3	9	.6	.7	.2
4	9.5	9.8	.1	2	4.4	5.2	.1	4,3,L			
5	2.7	2.5	.1	3	.8	.8	.2	0	6.4	6.6	.1
6	5.7	5.7	.1					1	5.9	5.9	.1
7	3.0	2.4	.1					2	8.3	8.2	.1
8	2.1	2.2	.1								

				4	2.5	2.6	.1				
		4,3,L		5	3.1	3.0	.1			5,2,L	
				6	2.6	2.7	.1				
3	8.5	8.4	.1	7	1.1	1.3	.1	0	5.9	5.7	.1
4	9.3	9.5	.1					1	.7	1.0	.3
5	7.3	7.0	.1			4,8,L		2	7.2	7.0	.1
6	3.9	3.8	.1					3	6.4	6.4	.1
7	3.9	3.7	.1	0	4.3	4.5	.1	4	7.4	7.7	.1
8	1.7	1.2	.1	1	5.0	5.3	.1	5	1.5	1.4	.2
9	.6	.3	.2	2	1.0	1.1	.3	6	5.6	5.0	.1
		4,4,L		3	3.4	3.3	.1	7	3.0	2.8	.1
				4	3.9	3.7	.1	8	.6	.4	.2
				5	2.0	2.0	.1				
0	7.6	7.8	.1	6	1.9	1.8	.1			5,3,L	
1	.6	.4	.3								
2	11.6	11.7	.1			4,9,L		0	8.1	8.6	.1
3	3.2	2.9	.1					1	2.5	2.6	.1
4	5.6	5.6	.1	0	2.6	2.5	.1	2	8.5	8.4	.1
5	3.1	3.3	.1	1	1.3	1.2	.2	3	6.1	6.1	.1
6	1.3	1.5	.2	2	3.1	3.3	.1	4	4.1	3.8	.1
7	5.6	5.4	.1	3	2.1	1.8	.1	5	7.7	7.5	.1
8	2.3	2.1	.1	4	.5	.4	.2	6	1.6	1.2	.2
9	1.5	1.4	.1	5	1.4	1.5	.1	7	2.0	2.0	.1
		4,5,L				4,10,L		8	.8	.9	.2
										5,4,L	
0	8.8	8.7	.1	0	3.8	4.0	.1				
1	8.2	8.7	.1	1	4.0	4.1	.1	0	8.1	7.7	.1
2	2.9	3.3	.1	2	3.1	3.2	.1	1	11.9	12.2	.1
3	6.8	6.9	.1	3	.8	.5	.2	2	7.3	7.7	.1
4	8.4	8.5	.1					3	4.2	4.3	.1
5	3.5	2.9	.1			5,0,L		4	1.5	1.6	.2
6	1.8	1.8	.1					5	2.1	1.7	.1
7	.6	.6	.2	0	4.3	4.5	.1	6	2.5	2.0	.1
8	1.6	1.4	.1	1	5.1	5.3	.1	7	.6	.4	.2
		4,6,L		2	6.7	6.8	.1	8	1.1	1.1	.1
				3	.7	.9	.3				
				4	1.9	1.9	.2			5,5,L	
0	1.8	1.8	.2	5	2.7	2.7	.1				
1	3.3	3.5	.1	6	1.1	1.5	.2	0	6.0	6.0	.1
2	4.4	4.5	.1	7	.9	.3	.2	1	4.4	4.6	.1
3	2.8	3.1	.1	8	1.0	.8	.2	2	2.0	2.1	.2
4	3.0	3.0	.1					3	1.5	1.6	.2
5	3.7	3.6	.1			5,1,L		4	2.0	2.3	.1
6	1.8	1.6	.1					5	1.6	2.1	.2
7	1.7	1.3	.1	0	9.2	9.7	.1	6	2.6	2.2	.1
8	2.6	2.3	.1	1	3.6	3.8	.1	7	1.3	.8	.1
		4,7,L		2	11.1	11.6	.1				
				3	12.7	12.8	.1			5,6,L	
				4	4.9	5.0	.1				
0	4.4	4.3	.1	5	4.6	4.4	.1	0	4.0	4.2	.1
1	2.9	3.5	.1	6	2.5	2.4	.1	1	2.6	2.7	.1
2	7.3	7.4	.1	7	2.2	1.5	.1	2	5.5	5.6	.1
3	6.5	6.4	.1	8	1.7	1.3	.1	3	3.6	3.5	.1