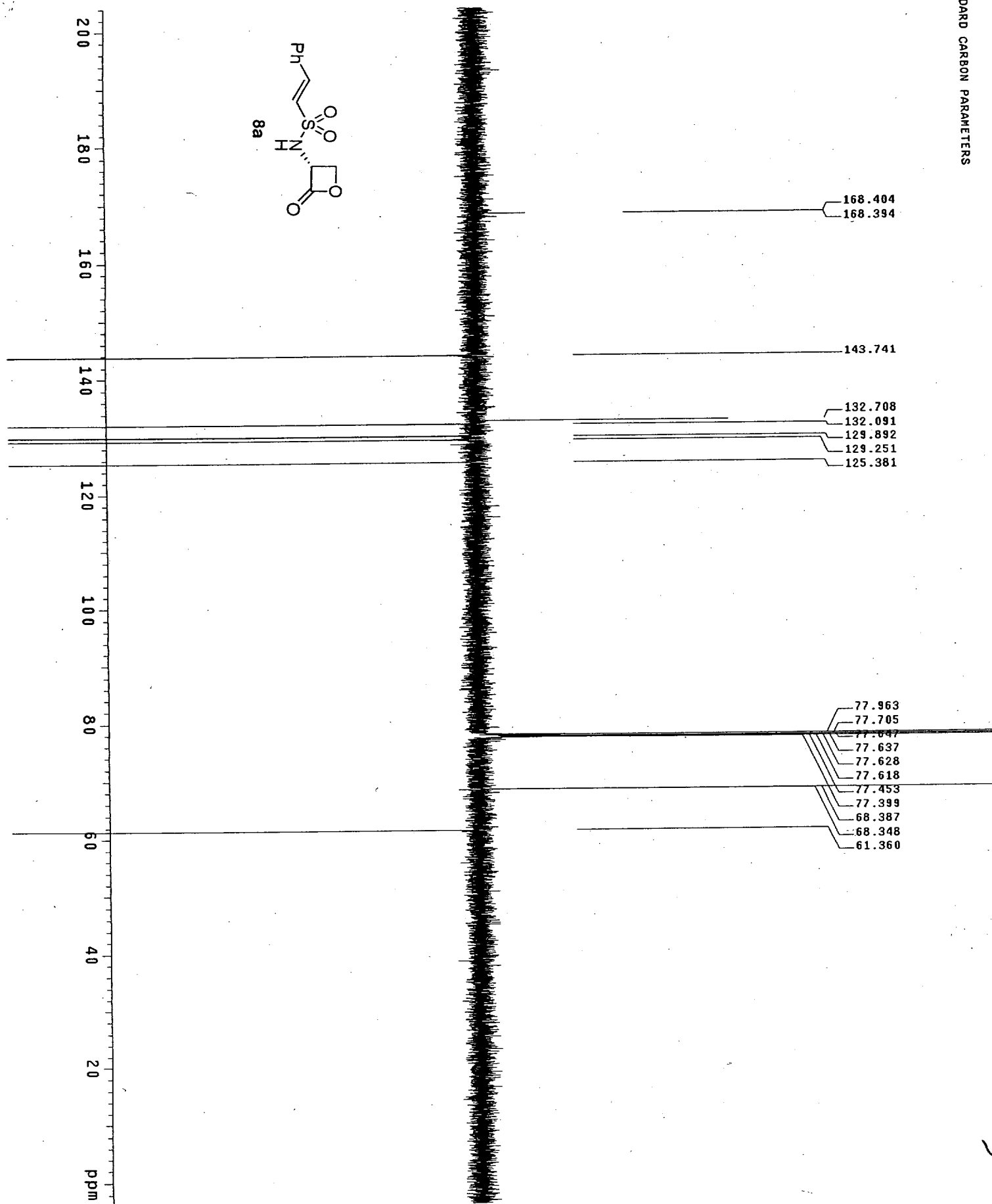
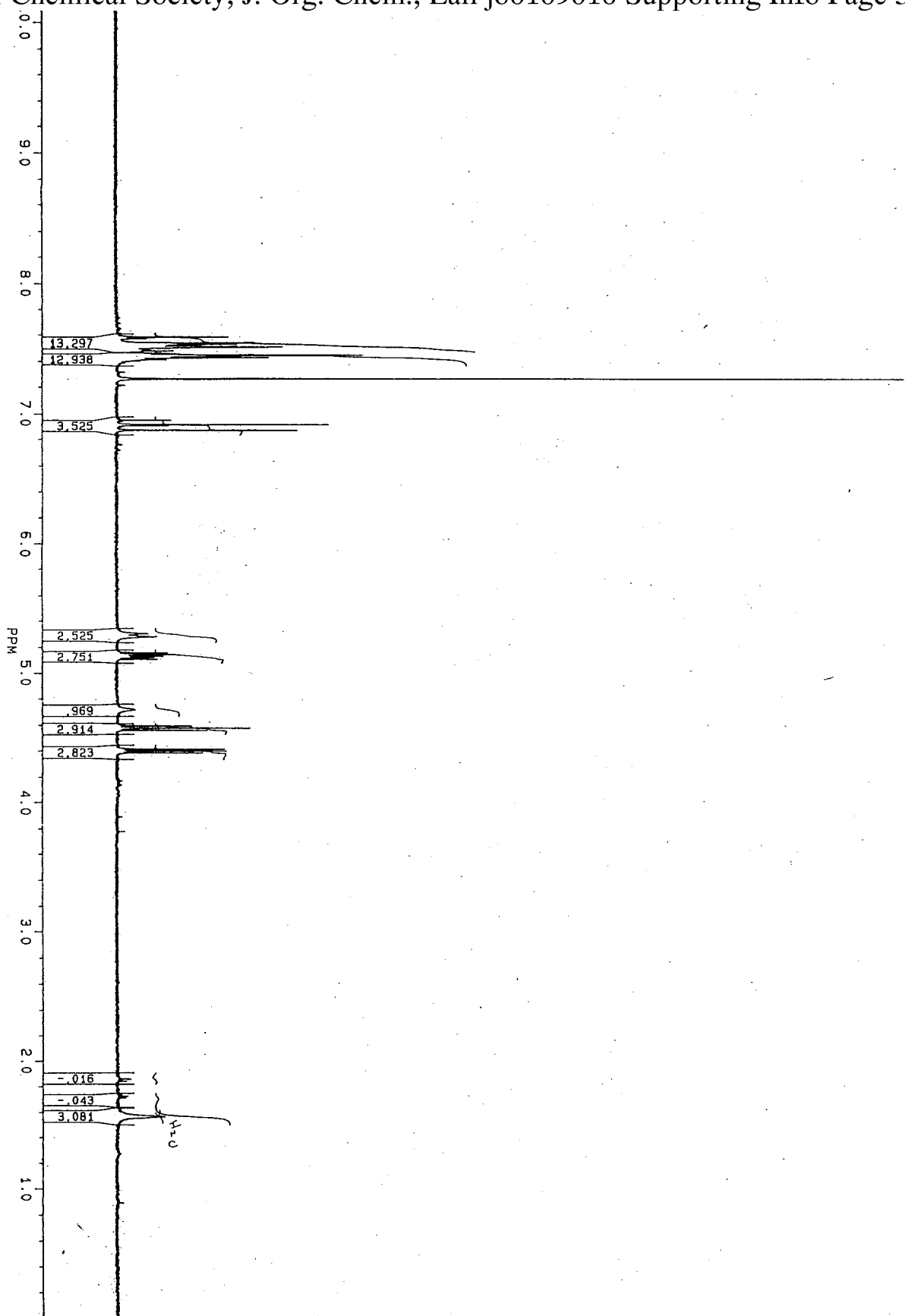
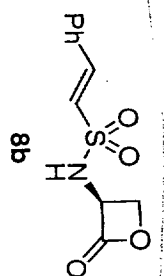


RM104141.001
 DATE: 20-4-99
 TIME: 10:29
 SF 360.134
 SY 120.0
 O1 5800.000
 S1 32768
 I1 32768
 SM 6024.086
 HZ/PT .368
 PW 3.0
 RD 0.0
 AG 2.720
 RG 800
 NS 32
 TE 297
 FW 7800
 O2 0.0
 DP 40L P0
 LB 0.0
 GB 0.0
 CC 36.00
 CY 0.0
 F1 10.501P
 F2 105.024
 PPM/CM .292
 SR 3983.30



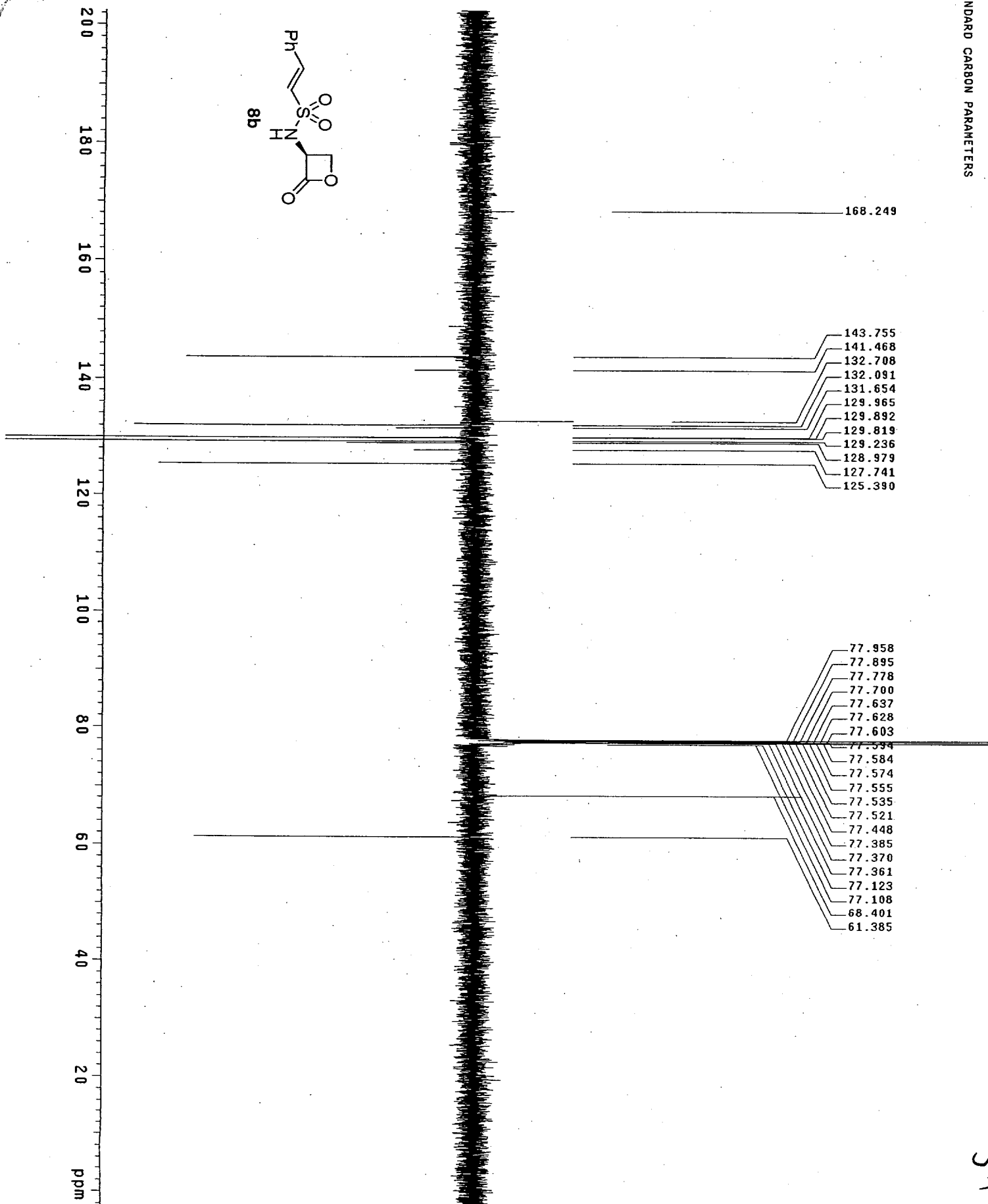
S1



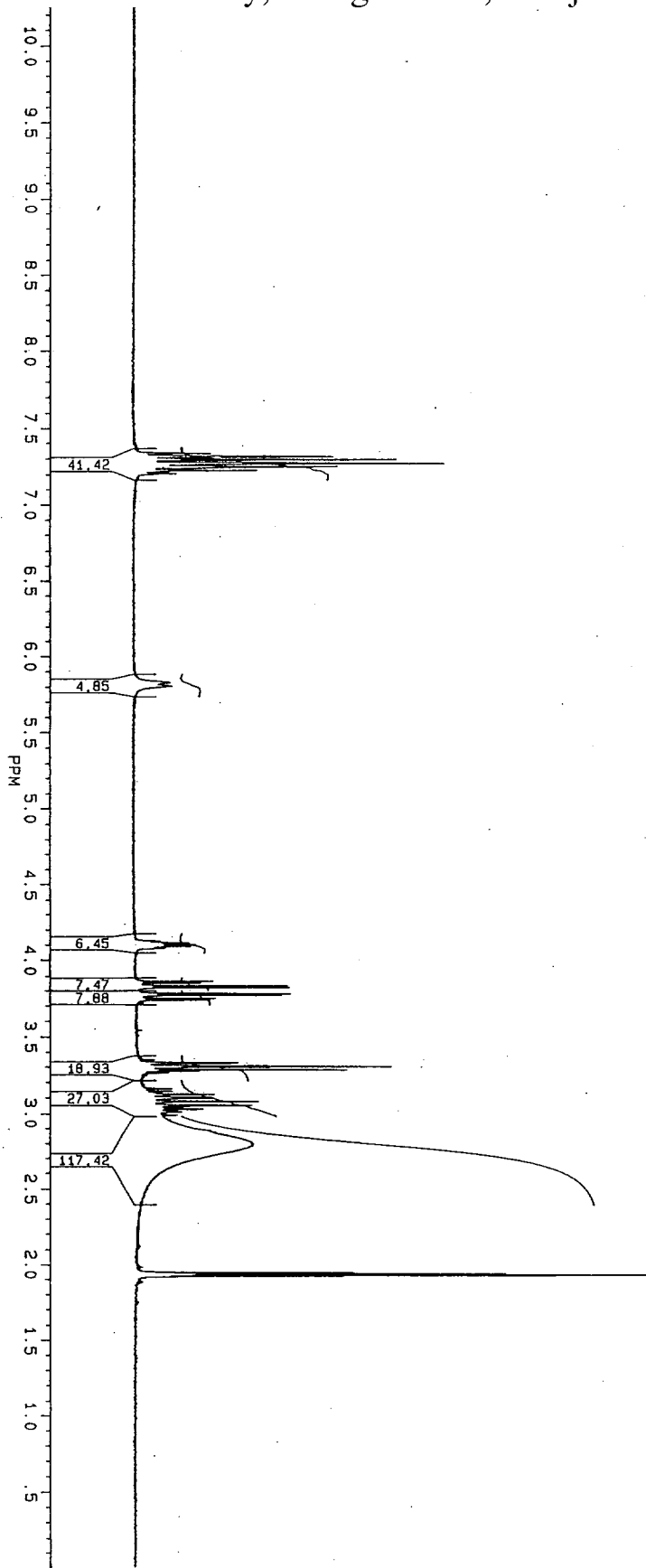
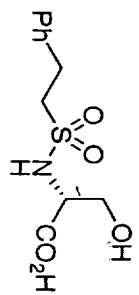


0X2143
 DATE 0-4-99
 TIME 23:05
 SF 360.134
 SY 120.0
 O1 5800.000
 SI 32768
 TD 32768
 SW 6024.096
 HZ/PT .358
 PW 3.0
 RD 0.0
 AQ 2.720
 RG 800
 NS 32
 TE 297
 FW 7600
 O2 0.0
 DP 40L P0
 LB 0.0
 GB 0.0
 CX 36.00
 CY 0.0
 F1 10.501P
 F2 0.022P
 HZ/CN 105.024
 PPM/CN 292
 SR 3983.30





LD3CN
1H IN ACETONE-D6

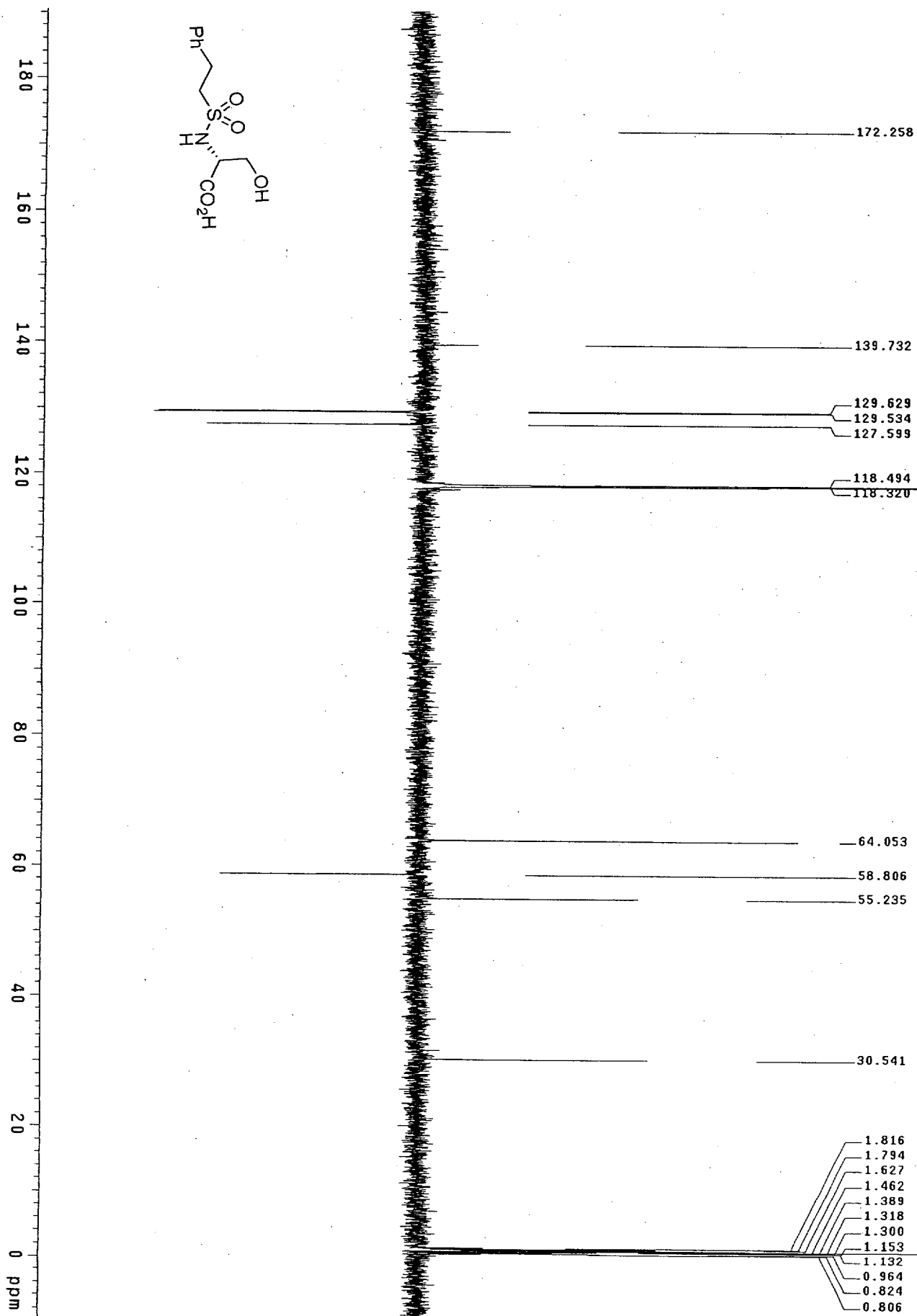


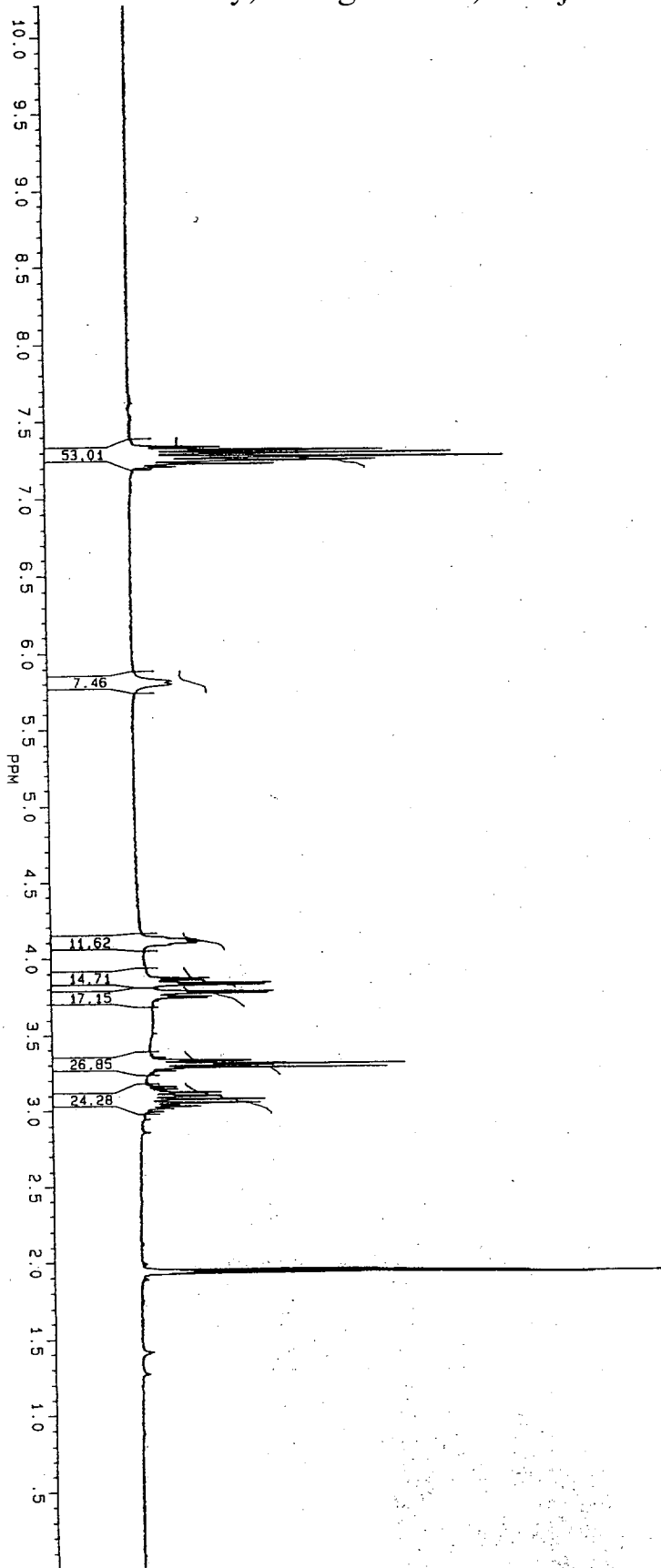
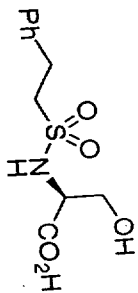
VY948B.001
DATE 20-4-99
TIME 15:22
SF 360.136
O1 8100.000
SI 32768
TD 32768
SM 6024.096
HZ/PT 368
PM 3.0
RD 0.0
AG 2.720
RG 100
NS 32
TE 297
FW 7600
DP 40L P0
LB 0.0
GB 0.0
CX 36.00
CY 0.0
F1 10.500P
H2/CM 105.024
PPM/CM .292
SR 5901.12



55

125 MHz APT in CDCl₃ (ref. to CDCl₃ @ 77.0 ppm), temp. = 30.6 °C → actual temp = 27.0 °C
CH, CH3 positive; C, CH2 negative





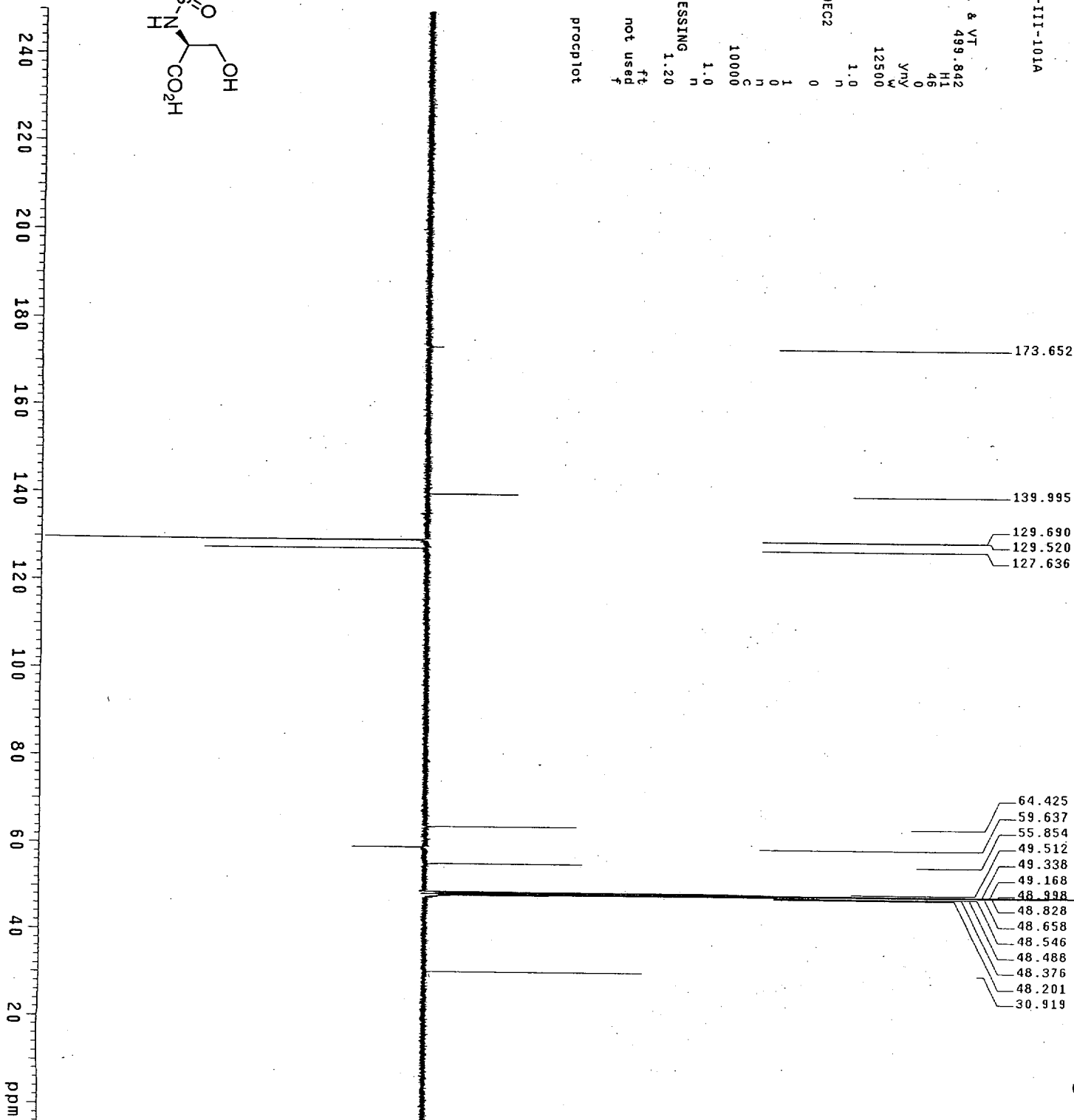
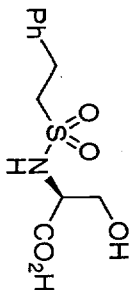
FID3
 DATE 1-4-99
 TIME 16:44
 SF 360.136
 SY 120.000
 GI 8100.000
 SI 32788
 TD 32768
 SW 6024.096
 HZ/PT .368
 PM 3.0
 RD 0.0
 AG 2.720
 RG 160
 NS 35
 TE 297
 FM 7600
 DP 0.0
 40L PD
 LB 0.0
 GB 0.0
 CX 36.00
 CY 0.0
 F1 10.300P
 F2 105.024
 HZ/CM 292
 PPM/CM 105.024
 SR 15901.12



57

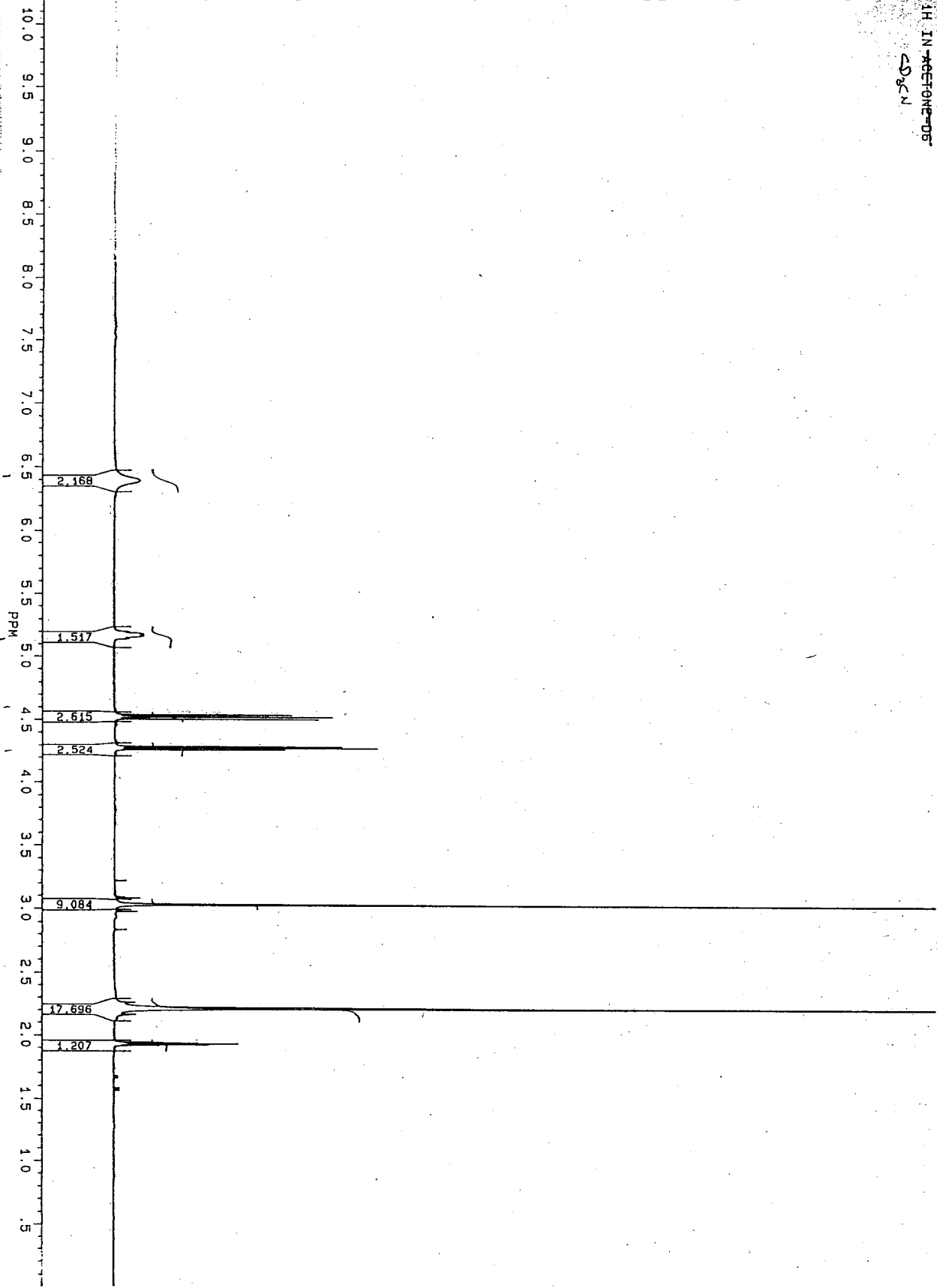
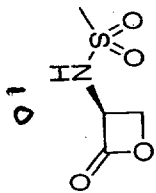
STANDARD CARBON PARAMETERS
Manj Lall apt on sample MSL-III-101A

expt	apt	date	APR 28 99	DEC. & VT	499.842
		solvent	cdcl3	dn	H1
		file	/export/home/~	dpwr	46
		nmr1/fids/	apr2851-	dot	0
		4c		ymv	W
ACQUISITION					
sfreq	125.697	dm		12500	
tn	C13	dmm			
at	1.300	dmsq			
np	104000	dres	1.0		
sw	40000.0	homo	n		
fb	22000	dfrq2	DEC2		
bs	18	dn2		0	
lpwr	38	dpwr2		1	
pw	8.0	dof2		0	
p1	28.0	dmm2		n	
d1	2.000	dmm2		c	
d2	0.007	dmtf2		10000	
d3	0.000	dseq2			
tof	0	dres2		1.0	
nt	20000	homo2		n	
ct	1296	PROCESSING			
gain	not used	lb	1.20		
11	not used	wtfile			
1n	n	proc			
dp	n	fn	not used		
hs	y	math			
	nh	warr			
	wn	wexp			
	ws	wbs			
	wnt	procp1ot			
DISPLAY					
sp	-529.2				
wp	32051.3				
vs	125				
sc	0				
hzm	200				
hzm	160.26				
ts	500.00				
rfl	14565.3				
rtp	6158.3				
tn	2				
ins	1.000				
nm	cdc	ph			



58

1H IN ACETONE-D6
 40°C N



SF 360.136
 SY 120.0
 O1 8140.000
 SI 32768
 TD 32768
 SW 6024.096
 HZ/PT .368
 PM 3.0
 RD 0.0
 AG 2.720
 RG 40.0
 NS 32.0
 TE 297.0
 FM 7600.0
 O2 0.0
 DP 40L P0
 LB 0.0
 GB 0.0
 CX 36.00
 CY 0.0
 F1 10.500P
 F2 105.024
 PPM/CM 292
 SR 5901.12

~~BRUKER~~

SP

MANU LALL, MSL-III-79A IN CD3CN, APT

170.359

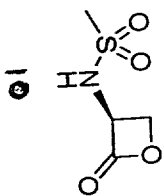
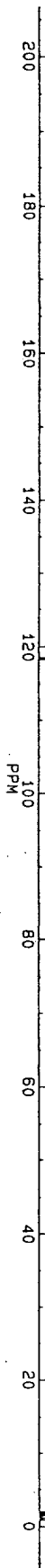
118.298

68.354

61.674

42.603

2.123
1.845
1.571
1.298
1.020
.747
.472



DE170F.103
AU PROG:
X251AU
DATE 3-1-99
TIME 8:32

SF 112.0
O1 7500.000
SI 32768
TD 32768
SW 18518.519
HZ/PT 1.130

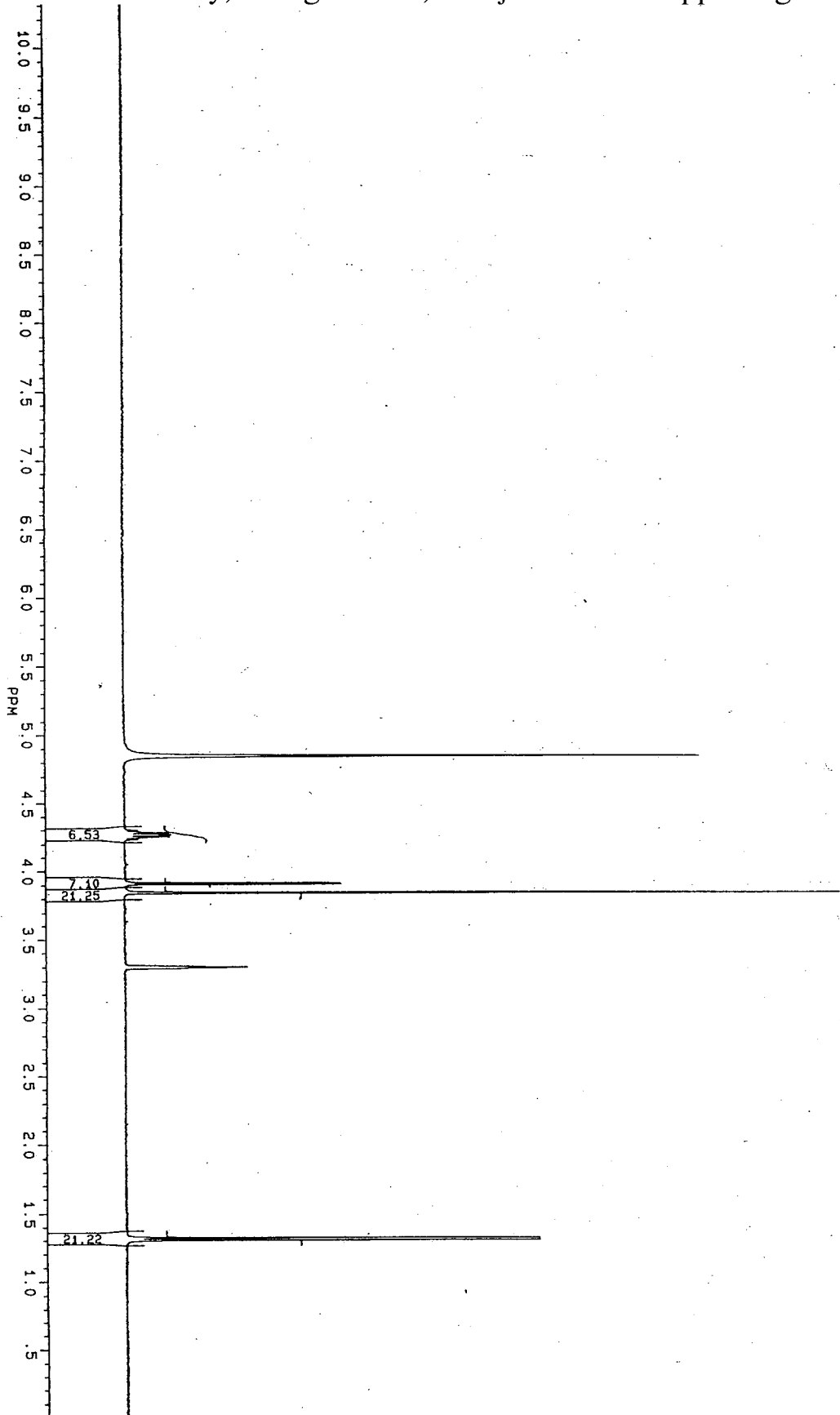
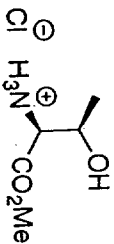
PM 0.0
AQ 0.0
RG 800.885
NS 7821
TE 297

FM 23200
O2 6400.000
DP 18H.CPD

LB 1.200
CB 0.0
CX 36.00
CY 10.00
F1 210.001P
F2 -5.994P
HZ/CM 482.803
RPM/CM 5.000
SR -1079.74

D1 2.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 2.00
D3 .0070000
P6 8.40
D4 .0001000
RGA
RD 0.0
PM 0.0
DE 33.80
NS 7821
DS 2

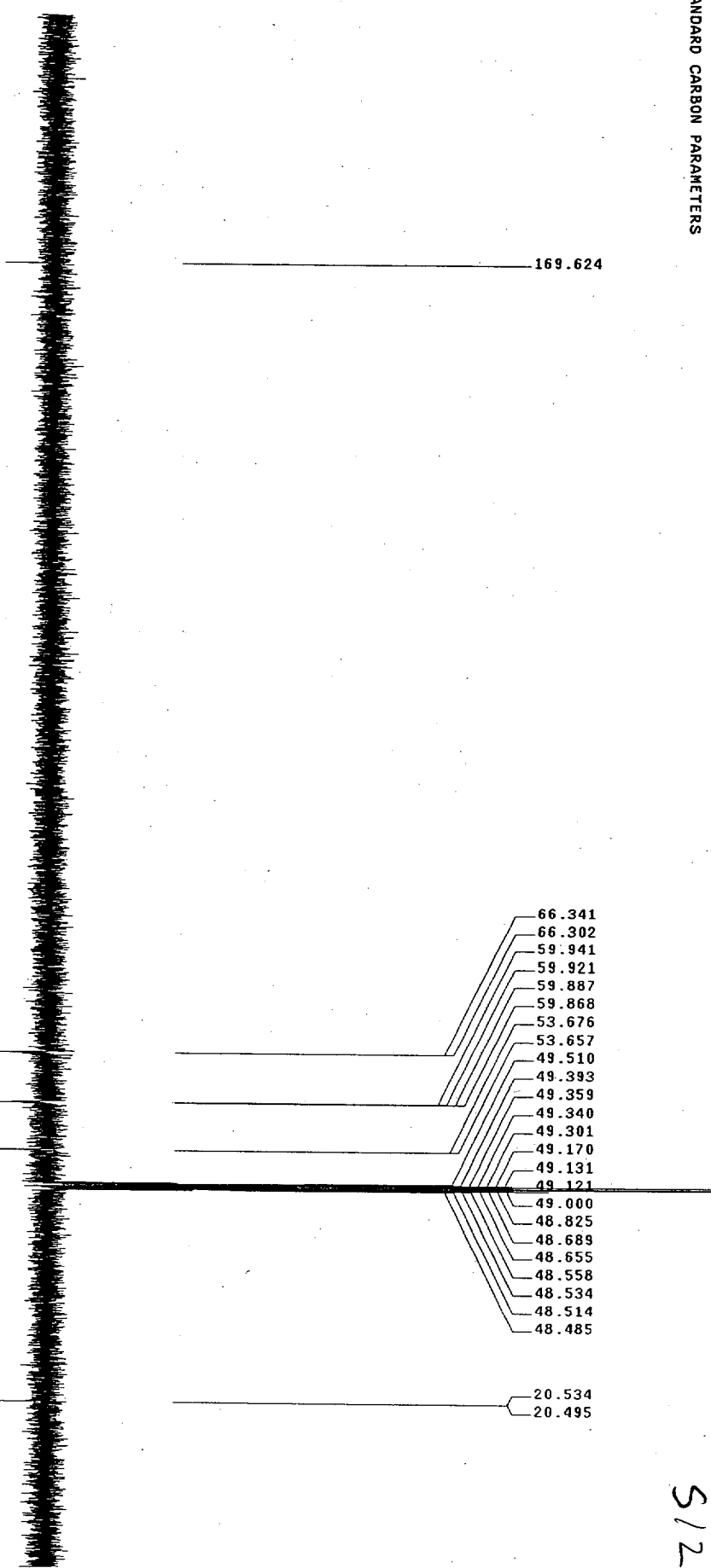
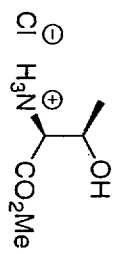
B
510

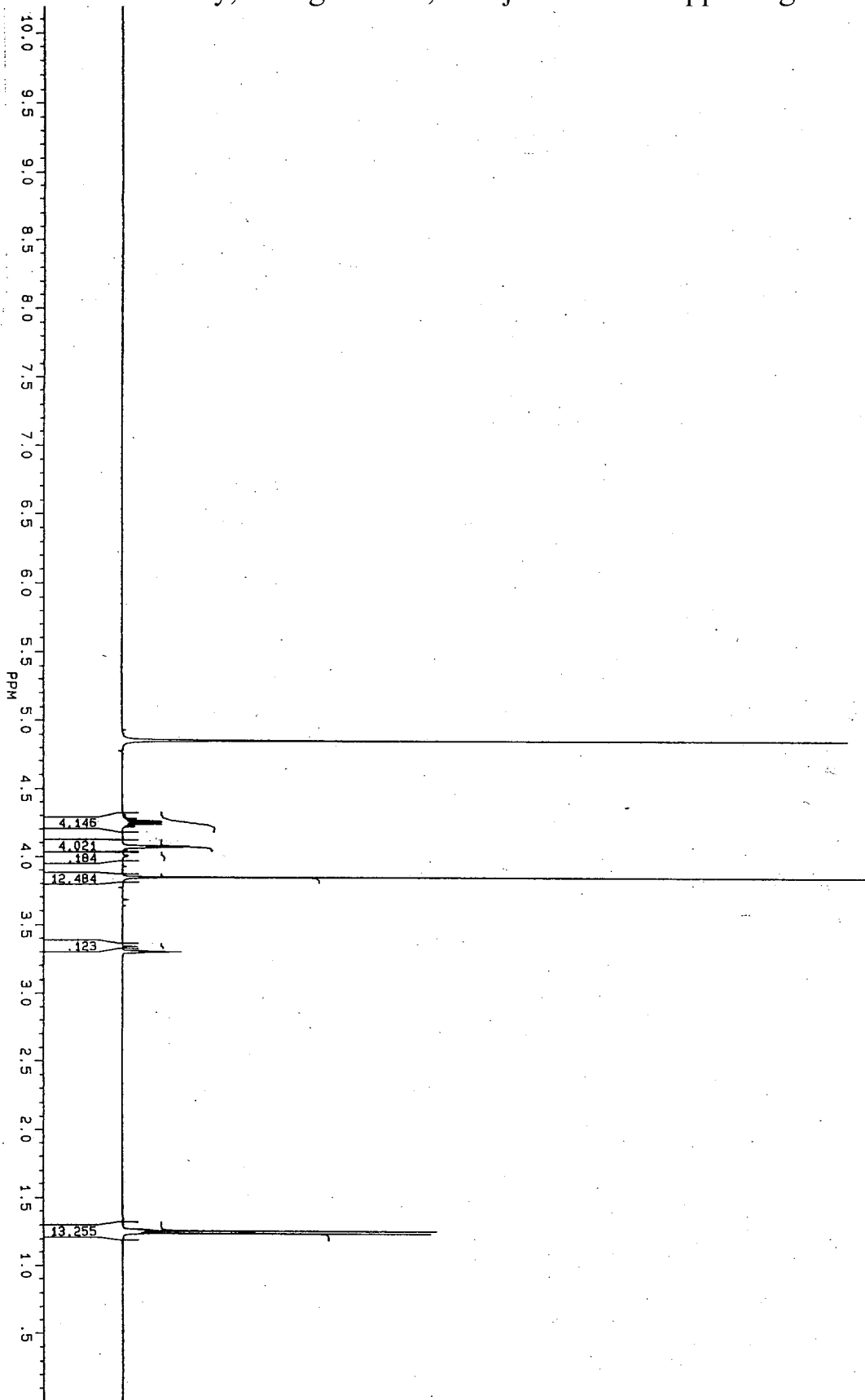
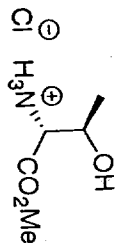


OX2190
 DATE 20-5-99
 TIME 12:59
 SF 360.135
 SY 120.0
 O1 7600.000
 SI 32788
 TD 32788
 SW 6024.096
 HZ/PT .368
 PM 3.0
 RD 0.0
 AG 2.720
 RG 320
 NS 32
 TE 297
 FM 7600
 DP 02 4790.000
 40L P0
 LB 0.0
 GB 0.0
 CX 36.00
 CT 0.0
 F1 10.500P
 F2 10.001P
 HZ/CM 105.024
 PPM/CM .292
 SR 5404.45



200
180
160
140
120
100
80
60
40
20
ppm





HOF7180.001
 DATE 20-5-99
 TIME 11:25
 SF 360.135
 SY 120.0
 O1 7800.000
 S1 32788
 T0 32788
 SM 5024.096
 HZ/PT .368
 PM 3.0
 RD 0.0
 AG 2.720
 RS 200
 NS 32
 TE 297
 FM 7600
 O2 4790.000
 DP 40L P0
 LB 0.0
 GB 0.0
 CX 36.00
 CY 0.0
 F1 10.5008
 F2 105.024
 HZ/CM 105.024
 PPM/CM .292
 SR 4852.20



MANU. LALL. MSL-III-157A IN CD3OD, APTXH

BX
S/4

UJ020F.101
AU PROG:
X25 AU
DATE 1-7-99
TIME 18:52

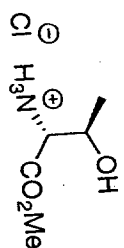
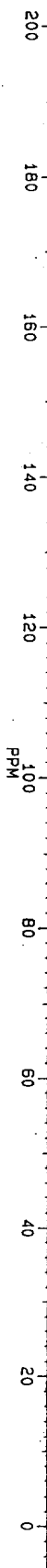
SF 112.0
O1 7478.000
SI 32758
TD 32758
SW 18518.519
HZ/PT 1.130

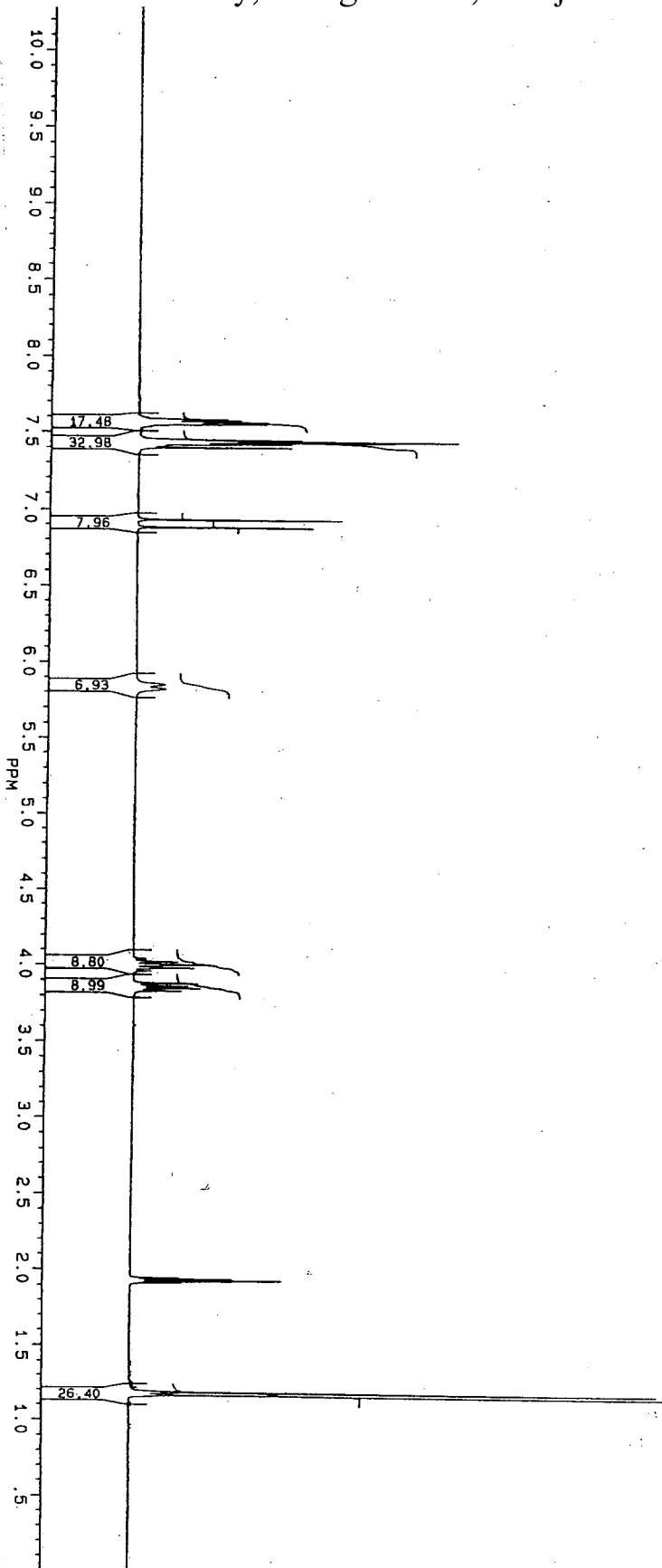
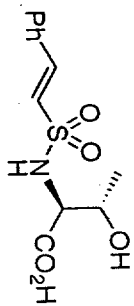
PW 0.0
RD 0.0
RG 800
R6 900
NS 297

FW 23200
O2 5595.000
DP 18H.CPD

LB 2.000
GB 0.0
CX 36.00
CY 0.0
F1 240.001P
F2/CM 452.834
PPM/CM 6.000
SR -1214.68

D1 5000000
S1 18H
P9 100.00
D2 0010000
S2 18H
P0 1.60
D3 0070000
P6 8.40
D4 0001000
RGA
RD 0.0
PM 0.0
DE 36.30
NS 9000
DS 2



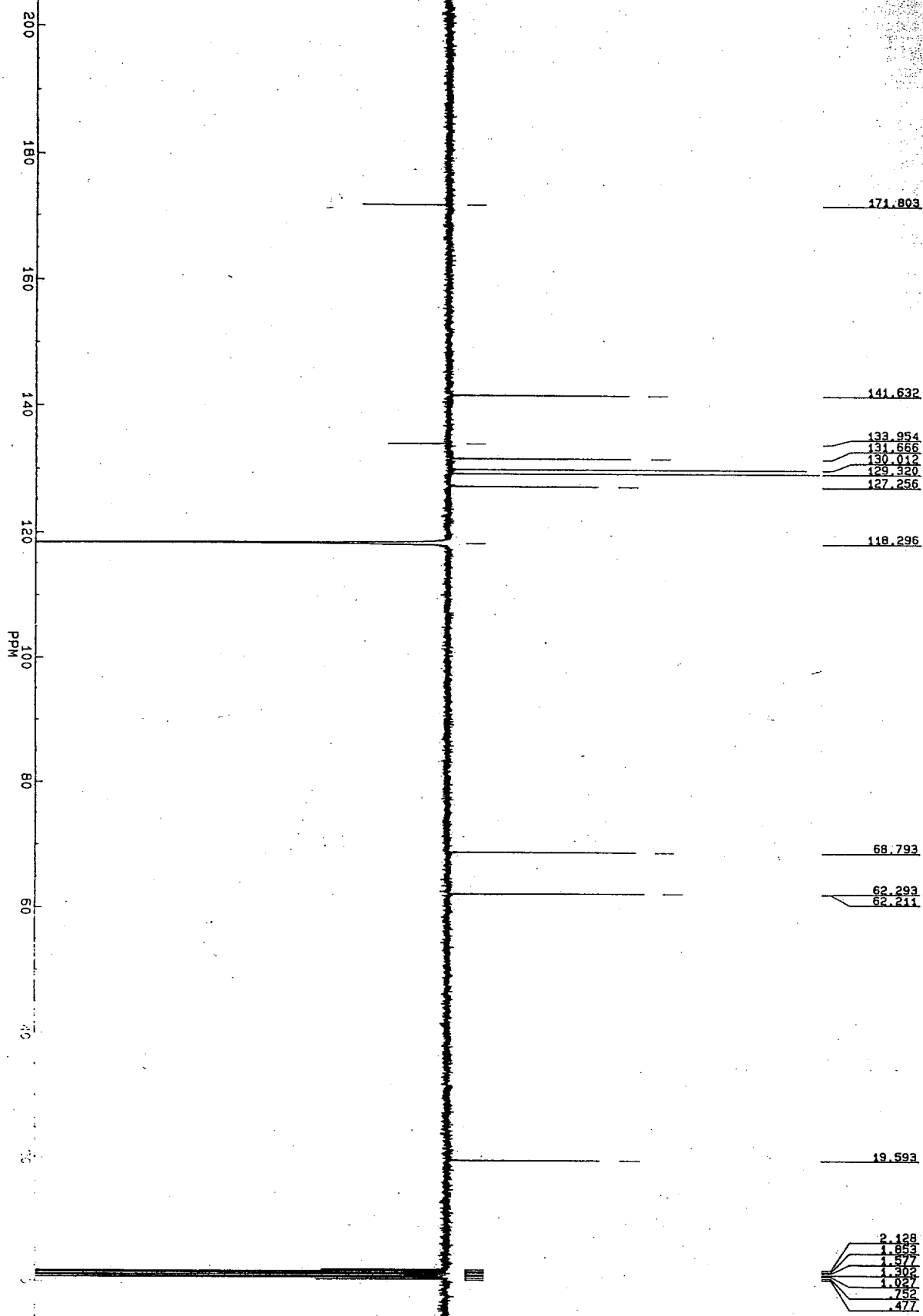
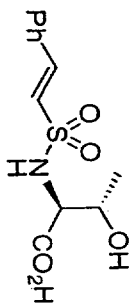


FID1
 DATE 18-6-99
 SF 300.135
 SY 100.0500000
 O1 6700.000
 SI 32768
 TD 32768
 SM 4504.505
 HZ/PT .275
 PM 4.0
 RD 0.0
 AG 3.637
 RG 100
 NS 32
 TE 297
 FW 5700
 O2 14000.000
 DP 12L P0
 LB 0.0
 GB 0.0
 CX 36.00
 CY 0.0
 F1 10.500P
 F2 0.000P
 HZ/CM 87.328
 PM/CM 292
 SR 4965.47



S/5

MANU LALL APT ON SAMPLE MSL-III-143A



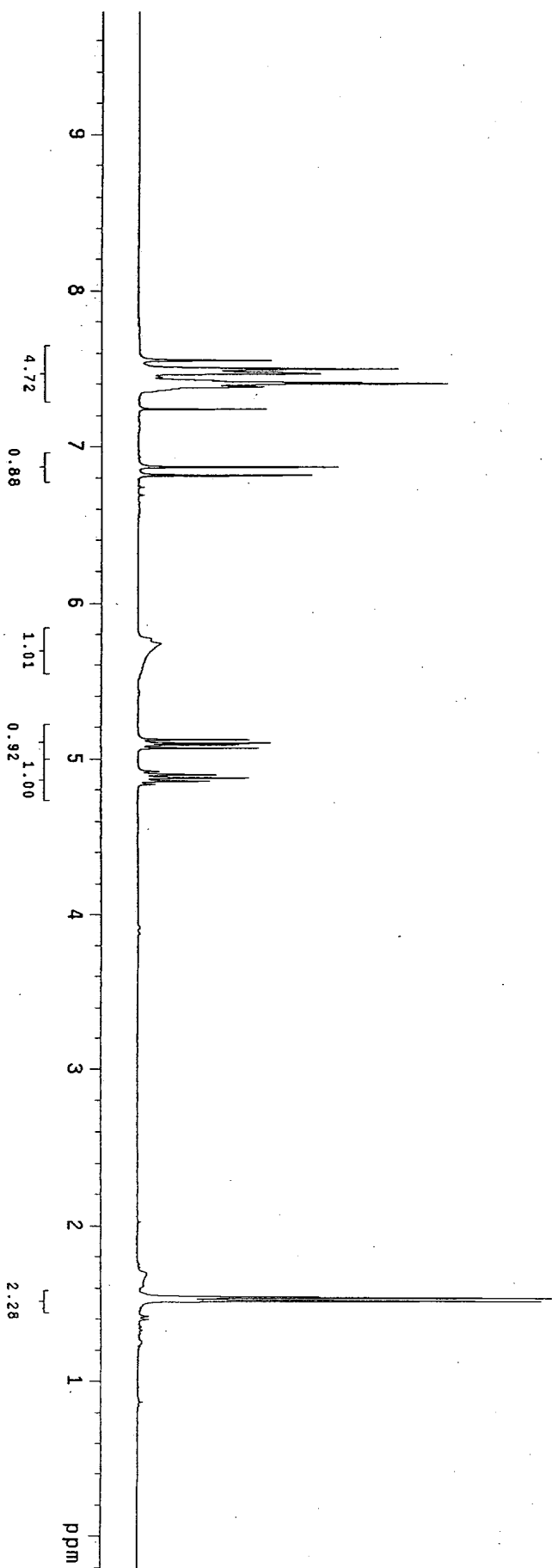
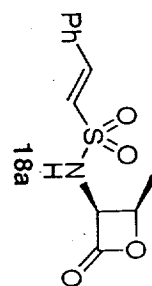
- 171.803
- 141.632
- 133.954
- 131.666
- 130.012
- 129.320
- 127.256
- 118.296
- 68.793
- 62.293
- 62.211
- 19.593
- 2.128
- 1.853
- 1.577
- 1.302
- 1.027
- 0.752
- 0.477

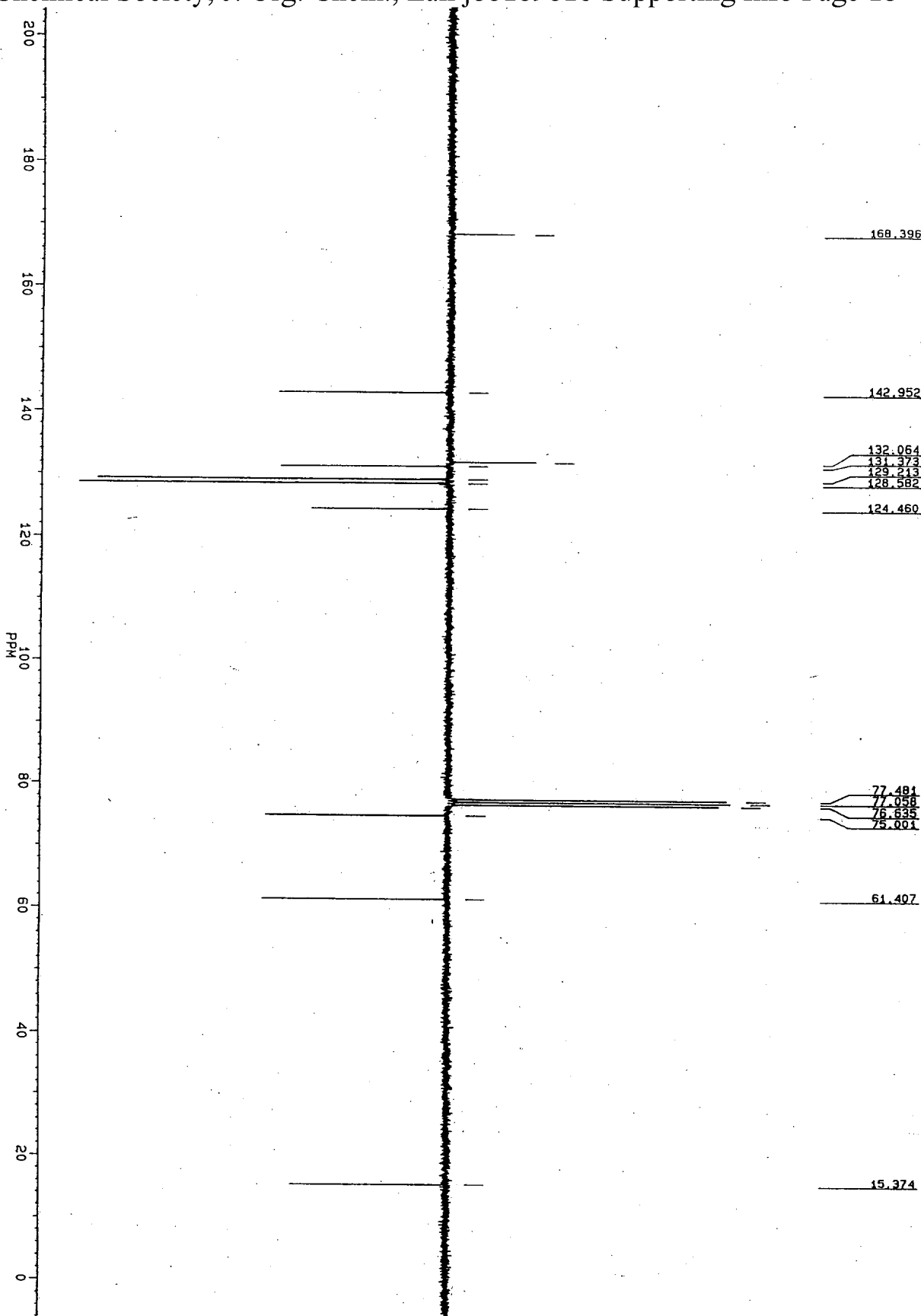
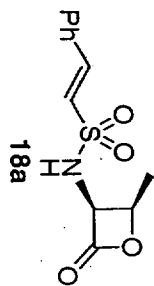
UN180F:101
 AU PROG: X25, AU
 DATE 8-7-99
 TIME 20:34
 SF 75.459
 SI 112.0
 S1 7500.000
 SI 65536
 TD 32768
 SW 18518.519
 HZ/PT .565
 PW 0.0
 RD 0.0
 AG .885
 RG 800
 NS 4800
 TE 297
 FW 23200
 O2 6400.000
 DP 18H CPD
 LB 1.000
 GB 010
 CX 36.00
 CY 10.00
 F1 210.001P
 F2 6.001P
 HZ/CM 452.819
 PPM/CM 6.000
 SR -1079.74
 D1 2.0000000
 S1 18H
 P9 100.00
 D2 0010000
 S2 18H
 P0 2.00
 D3 0070000
 P6 8.40
 D4 0001000
 RGA
 RD 0.0
 PD 0.0
 DE 33.80
 NS 4800
 DS 2



S/6

300 MHz 1D in CDCl3 (ref. to CDCl3 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C
date: Jul 20 1999 seqf11: s2pu1 hz/mm: 12.51 spectrometer: 1300 file: exp
acq.time [s]: 2.0 relax.time [s]: 3.0 sweep width [Hz]: 3001 dig.res. [Hz/pt]: 0.09

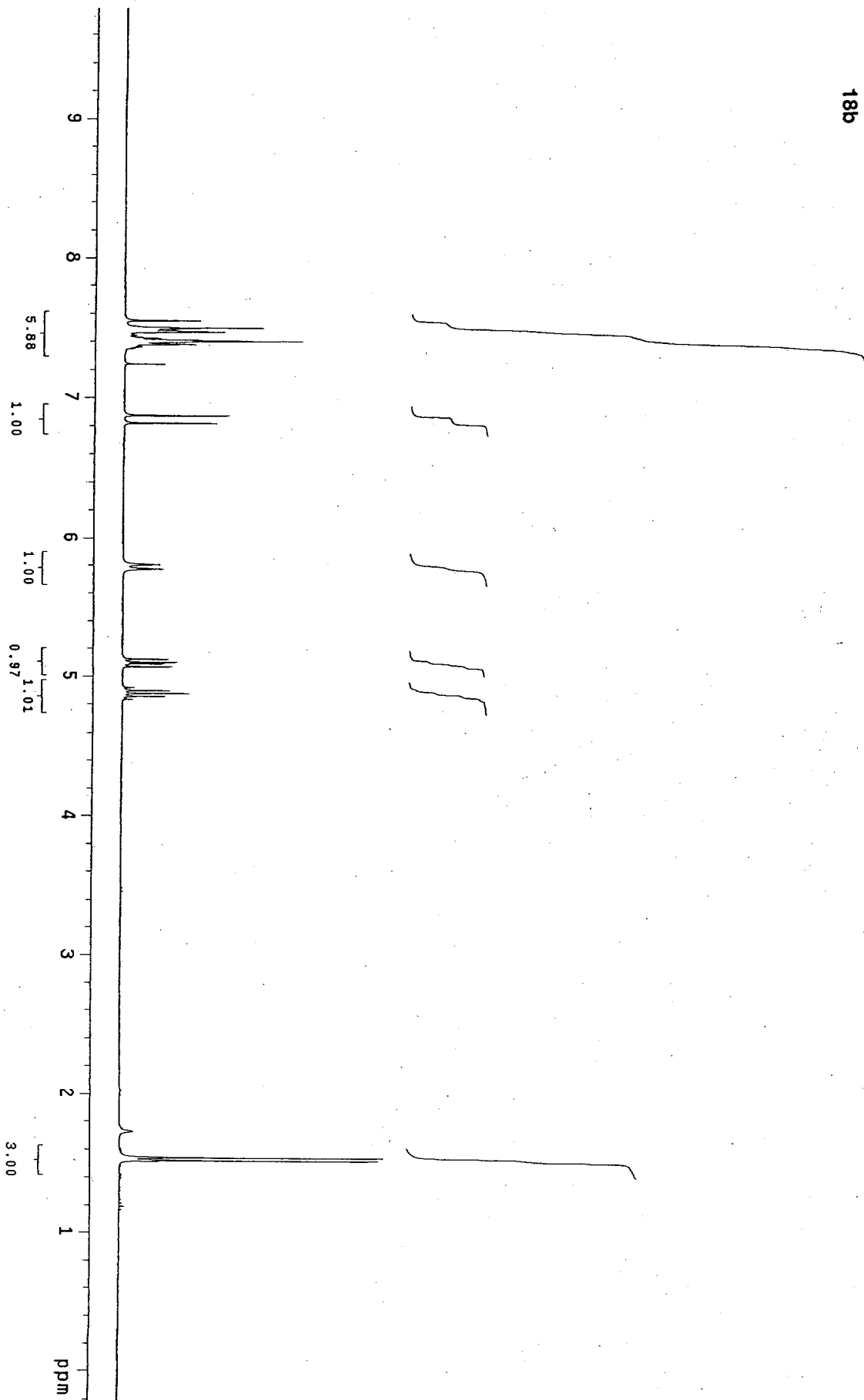
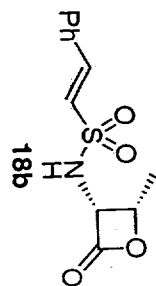




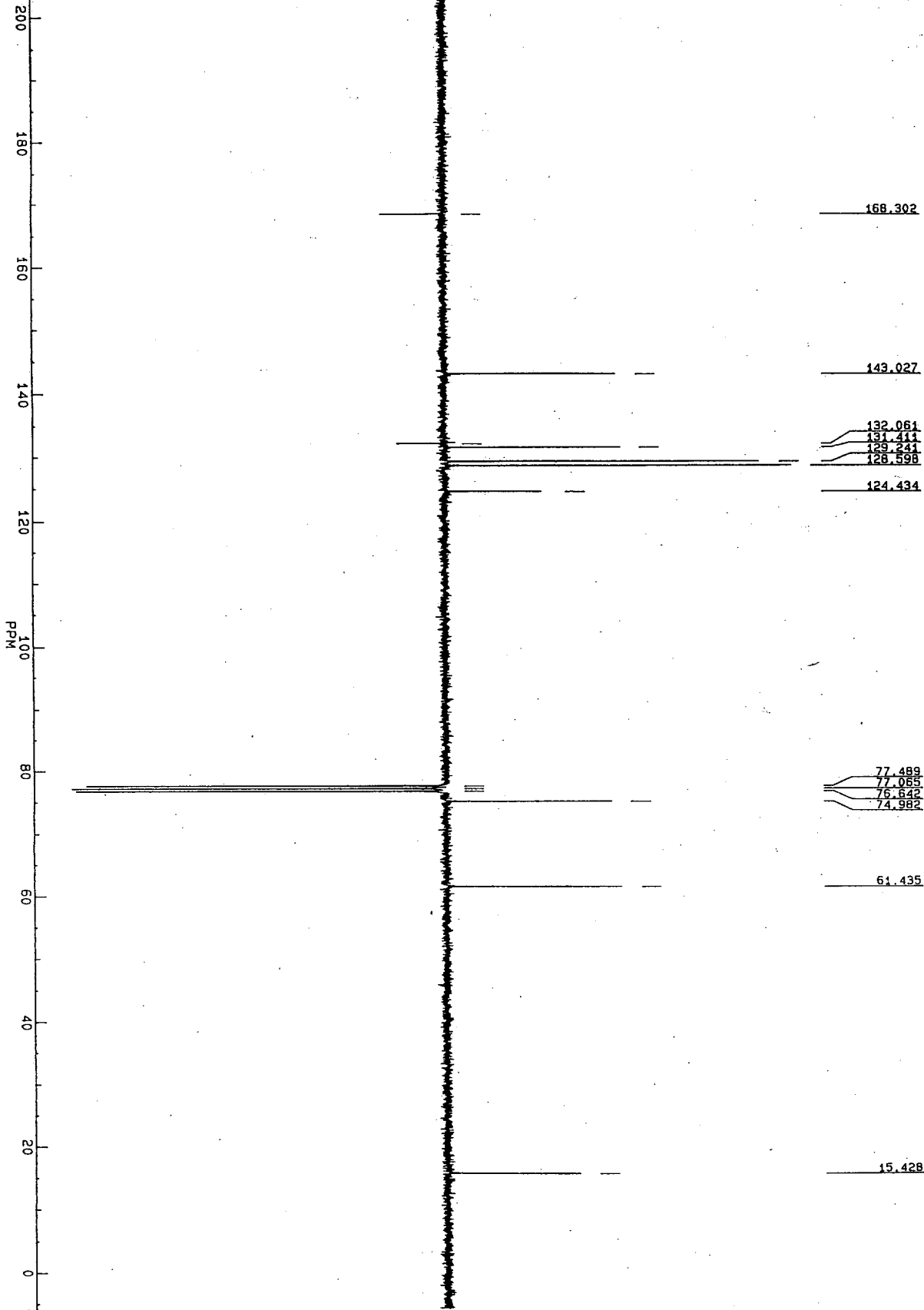
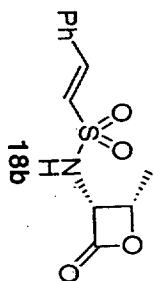
JI230F.104
 AU PROG: X25.AU
 DATE 1-9-99
 TIME 0:30
 SF 75.469
 SY 112.0
 O1 7000.000
 S1 63536
 TD 32769
 SW 22727.273
 HZ/PT .694
 PW 0.0
 RD 0.0
 AG 800.721
 RG 3500
 NS 297
 TE
 FW 28500
 O2 4425.000
 DP 18H CPD
 LB 1.000
 GB 0.0
 CX 36.00
 CY 10.00
 F1 210.007P
 F2 8.002P
 HZ/CM 452.832
 PPM/CM 6.000
 SR -1408.22
 D1 2.0000000
 S1 18H
 P9 100.00
 D2 0010000
 S2 18H
 P0 2.00
 D3 .0070000
 P6 8.40
 D4 .0001000
 RGA
 RD 0.0
 PM 0.0
 DE 30.00
 NS 3500
 DS 2

BALIX 5/8

300 MHz ID in CDCl3 (ref. to CDC13 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C
date: Jul 19 1999 seqfil: s2pu1 hz/mm: 12.51 spectrometer: 1300
acq.time [s]: 2.0 Relax. time [s]: 3.0 sweep width [Hz]: 3001 dig.res. [Hz/pt]: 0.09 file: exp



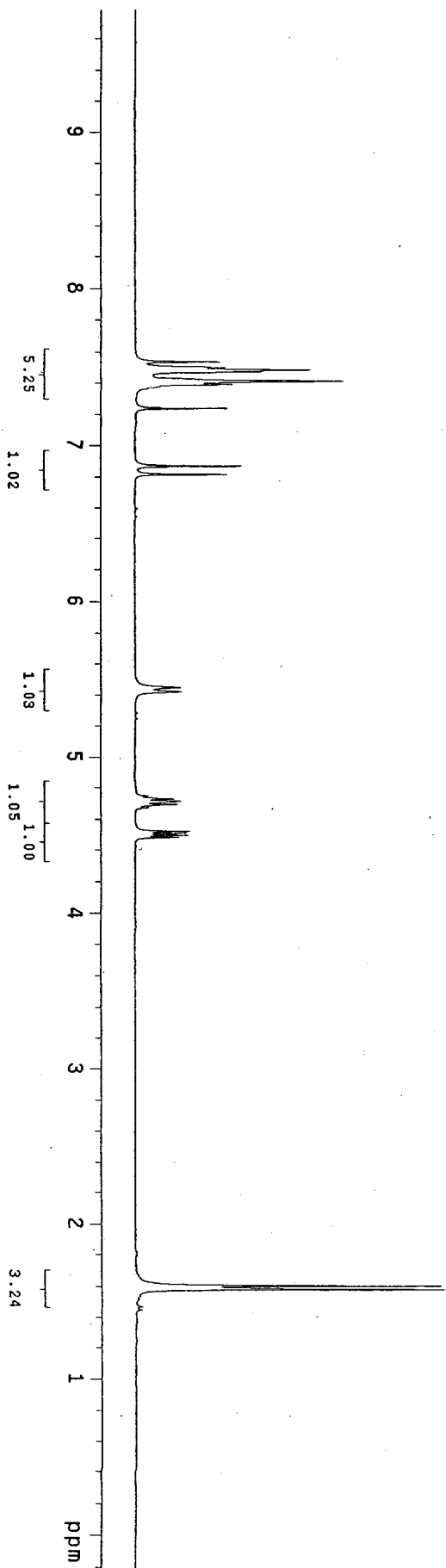
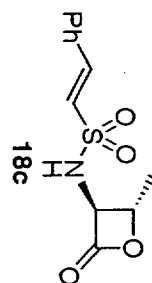
S 19



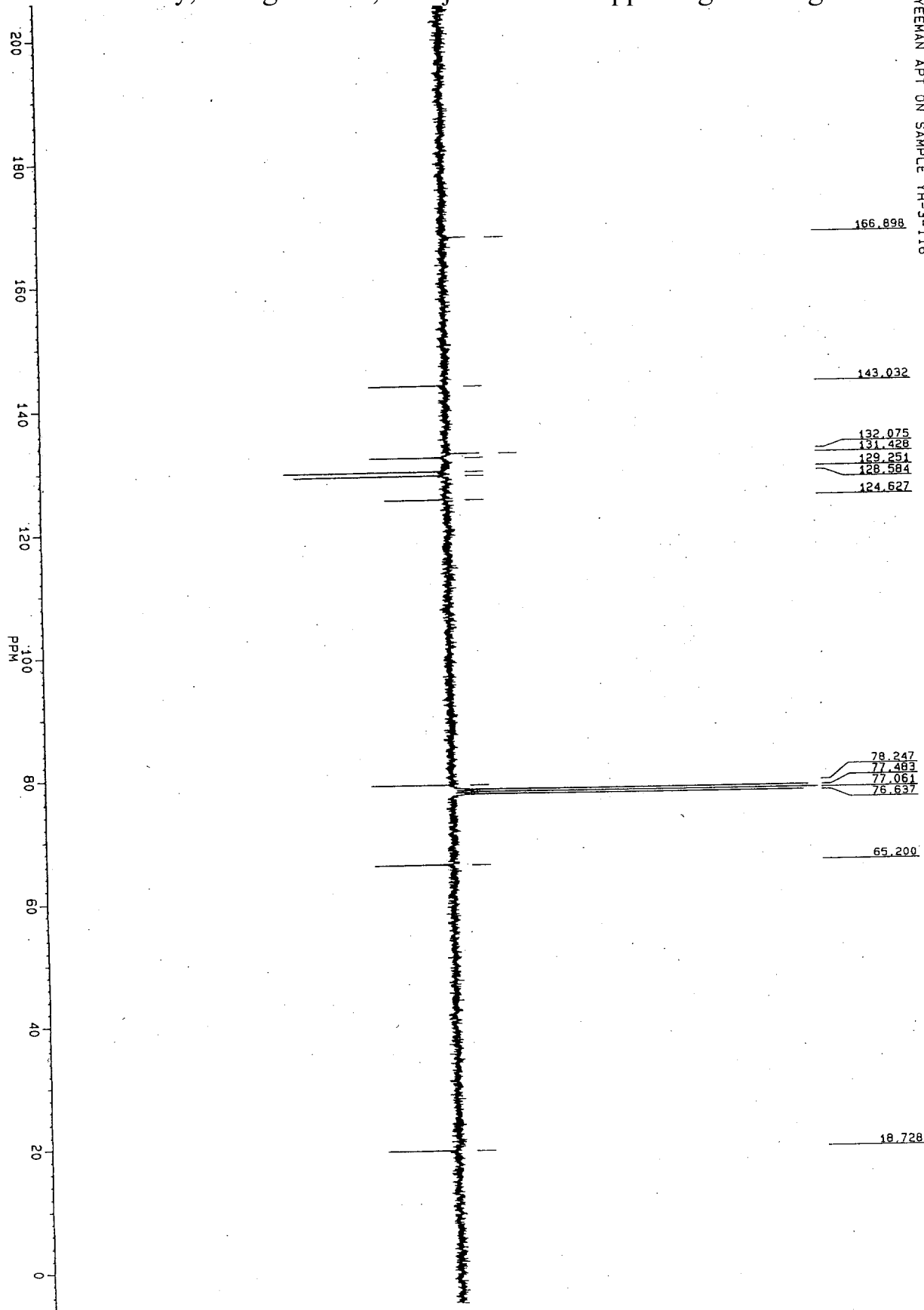
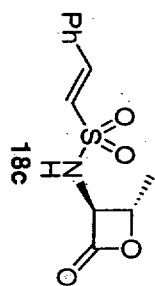
JL220F.103
 AU PROG: 103
 X25 AU
 DATE 10-8-99
 TIME 6.18
 SF 75.459
 SY 112.0
 O1 7000.000
 SI 32768
 TD 32768
 SW 22727.273
 HZ/PT 1.387
 PW 0.0
 RD 0.0
 AG 721
 RG 800
 NS 4800
 TE 297
 FW 28500
 DP 4425.000
 DP 18H.CPD.
 LB 1.200
 GB 0.20
 CX 36.00
 CY 10.00
 F1 210.007P
 F2/CH -5.984P
 PPM/CH 452.793
 SR 5.000
 SR -1409.60
 D1 2.0000000
 S1 18H
 S9 100.00
 D2 .0010000
 S2 18H
 P0 2.00
 D3 .0070000
 P6 8.40
 D4 .0001000
 RGA
 RD 0.0
 RN 0.0
 DE 30.00
 NS 4800
 DS 2

B
 J
 U
 R
 520

300 MHz 1D 1h CDCl3 (ref. to CDCl3 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C
date: Jul 21 1999 seqfil: s2pu1 hz/mm: 12.51 spectrometer: 1300
acq.time [s]: 2.0 Relax. time [s]: 3.0 sweep width [Hz]: 3001 dig.res. [Hz/pt]: 0.09 file: exp

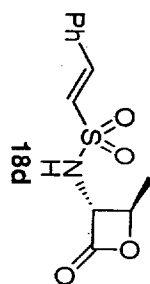


S 21

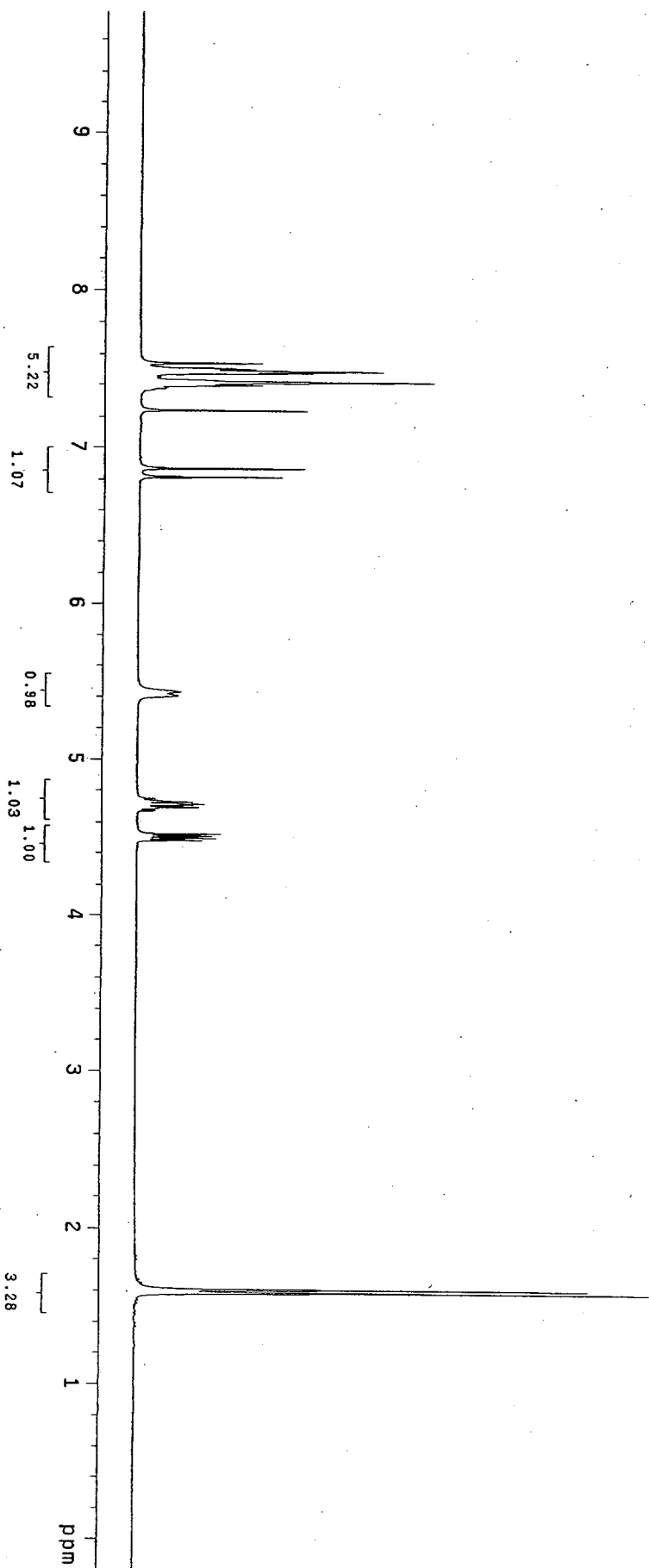


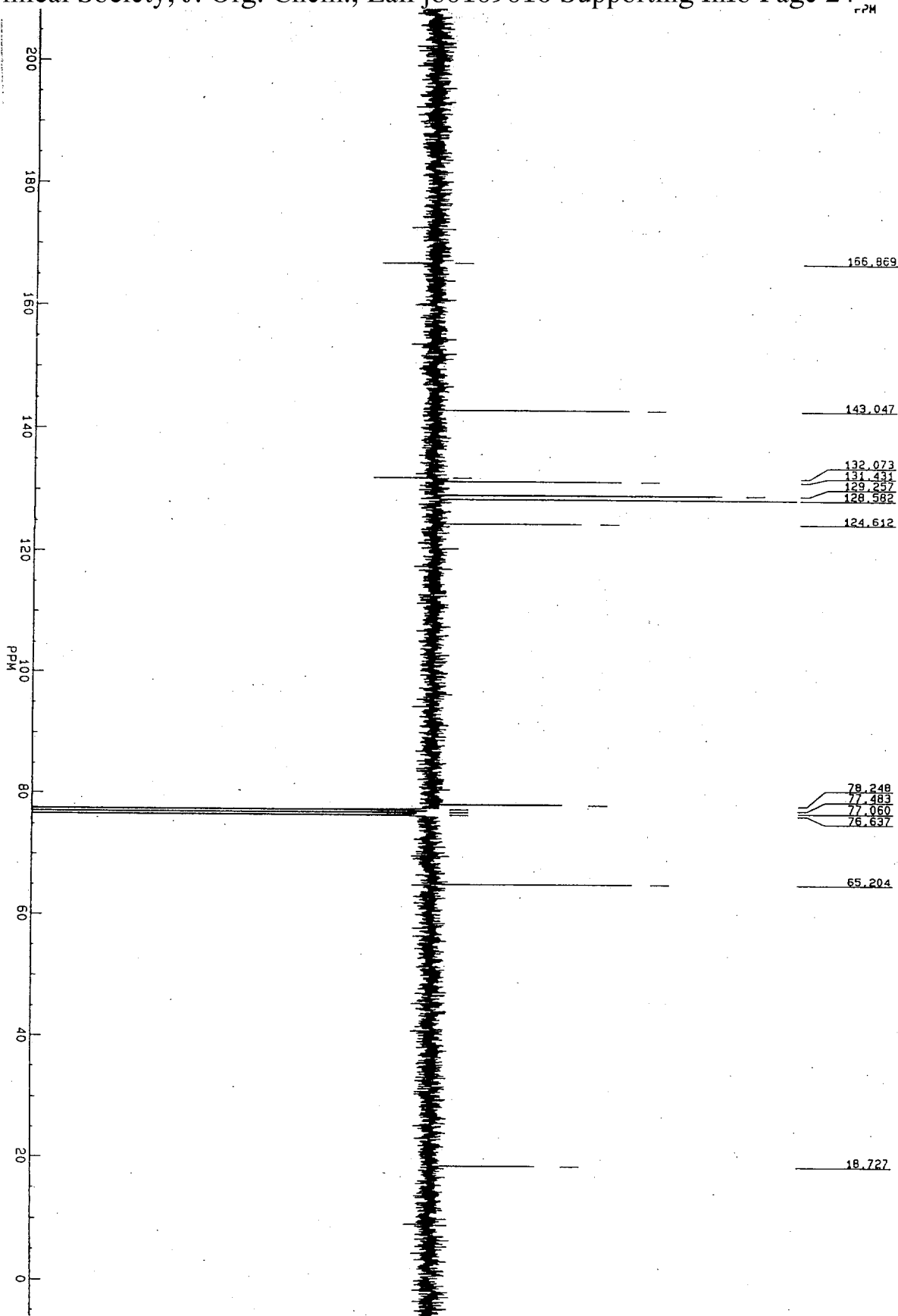
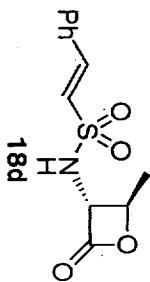
JL239F.105
 AU:PH06:
 X25:AU
 DATE:1-9-99
 TIME:3:21
 SF 112.0
 SY 75.469
 O1 7000.000
 S1 65536
 T10 32768
 S11 27272.273
 HL/PT 694
 PW 0.0
 R0 0.0
 R3 0.0
 R6 721
 R8 800
 R9 800
 S5 3600
 S6 297
 TE
 FW 28500
 D2 44225.000
 DP 181 CPU
 LB 2.000
 GB 0.0
 CX 36.00
 CY 10.00
 F1 210.007P
 F2 -6.002P
 HZ/CM 452.832
 PPM/CM 5.000
 SR -1409.50
 D1 2.0000000
 S1 18H
 P9 100.00
 D2 .0010000
 S2 18H
 P0 2.00
 D3 .0070000
 P3 8.40
 D4 .0001000
 RGA
 RD 0.0
 PW 0.0
 DE 30.00
 NS 3600
 DS 2

BAKER
 522



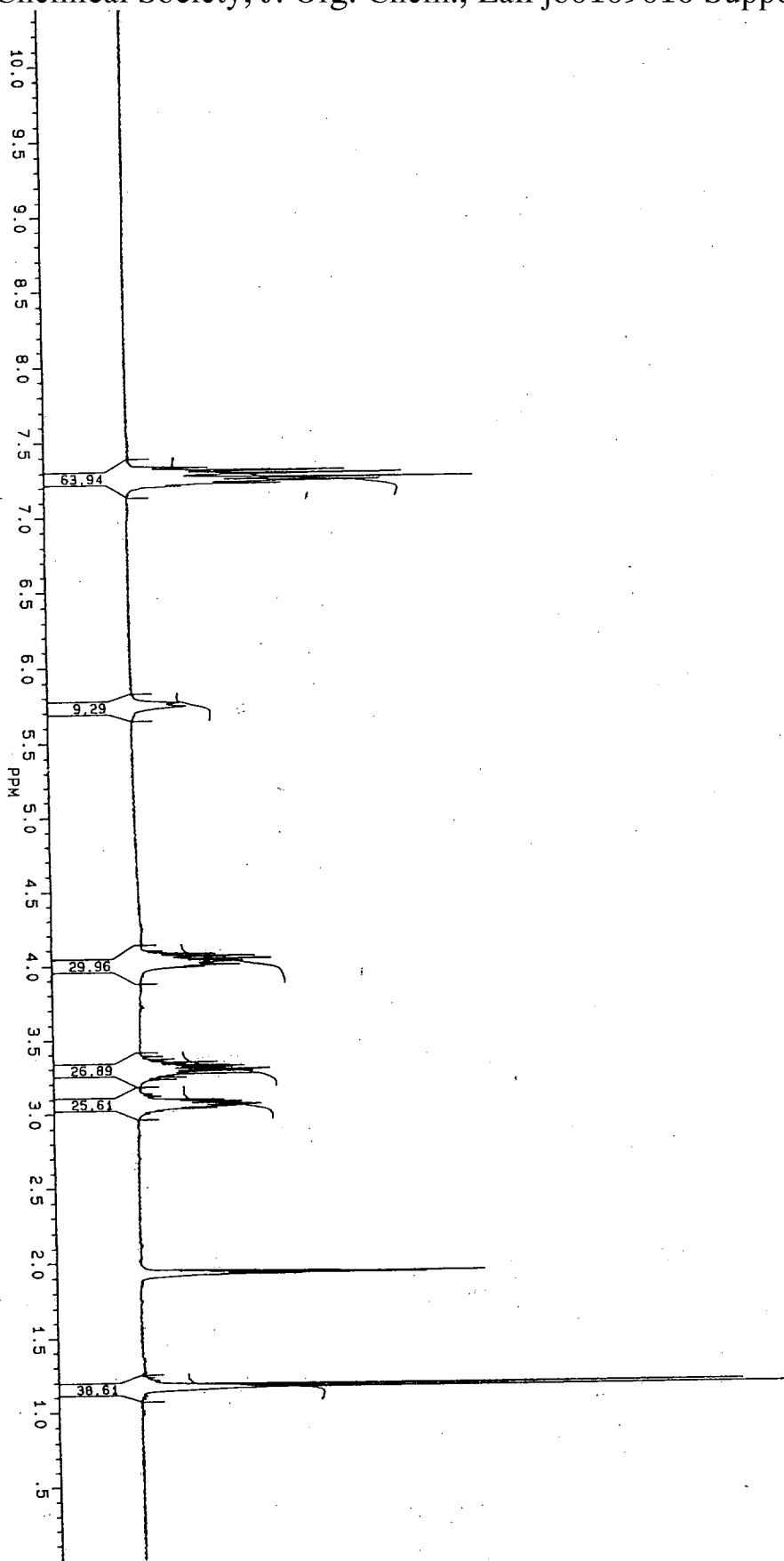
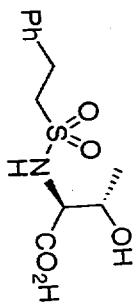
300 MHz 1D in CDCl3 (ref. to CDCl3 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C
date: Jul 21 1999 seqfil: s2pu1
acq.time [s]: 2.0 Relax.time [s]: 3.0 hz/mm: 12.50
Spectrometer: 1300
dig.res. [Hz/pt]: 0.09
file: exp





JL220F.104
 AU PRG: X25.AU
 DATE: 10-8-99
 TIME: 9:14
 SF 112.0 75.469
 SY 142.0
 O1 7000.000
 S1 32768
 TD 32768
 SW 22727.273
 HZ/PT 1.387
 PW 0.0
 RD 0.0
 AG 0.721
 RG 800
 NS 3645
 TE 297
 FW 28500
 O2 4425.000
 DP 18H CPD
 LB 1.200
 GB 0.010
 CX 36.00
 CY 10.00
 C1 10.00
 F1 210.007P
 F2 452.793
 HZ/CM 5.000
 PPM/CM 6.000
 SR -1409.60
 O1 2.0000000
 S1 18H
 P9 100.00
 O2 0010000
 S2 18H
 P6 2.00
 O3 .0070000
 P3 8.40
 O4 .0001000
 RGA
 RD 0.0
 PW 0.0
 DE 30.00
 NS 3645
 DS 2

B
 X
 R
 524

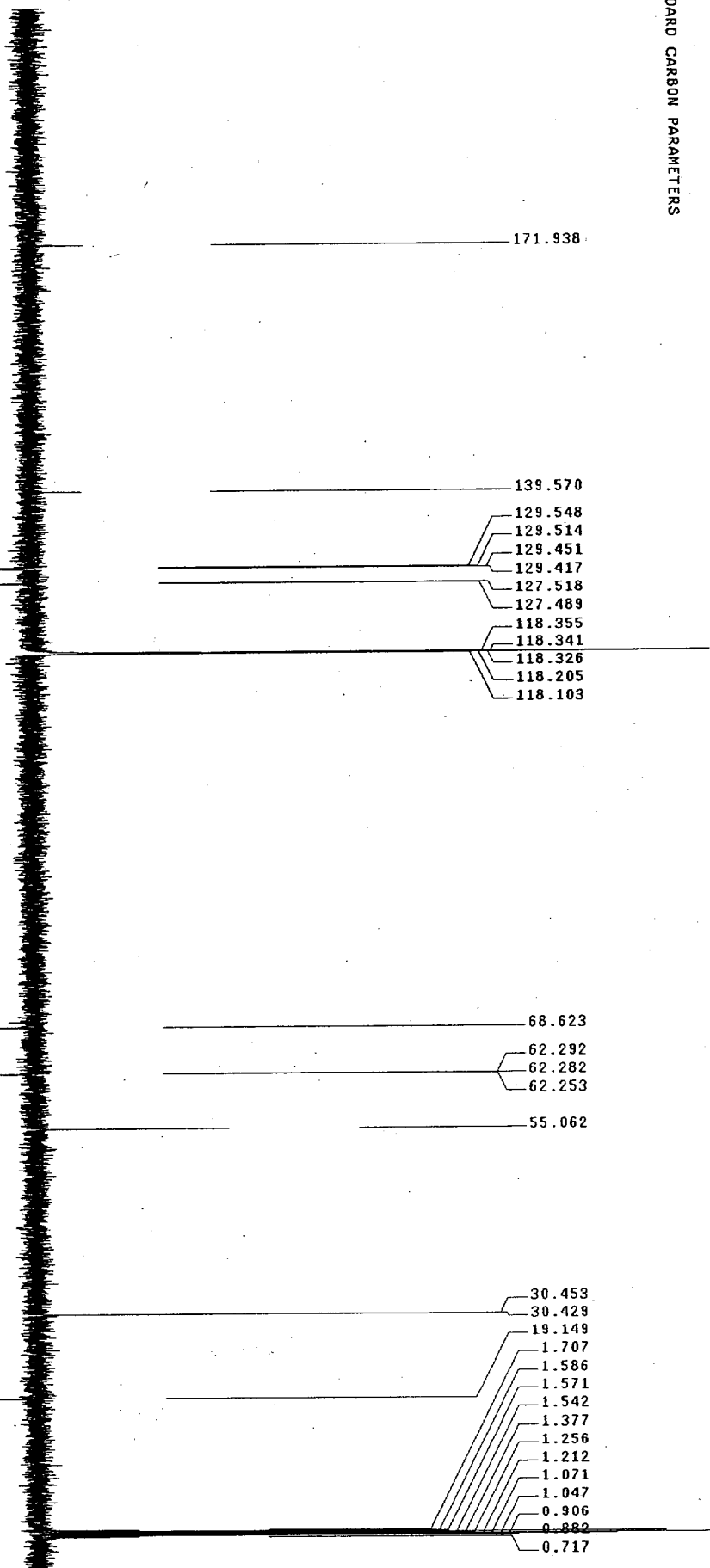
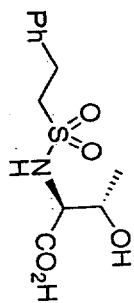


OX2190
 DATE 20-5-99
 TIME 10:10
 SF 360.136
 SY 120.0
 O1 8100.000
 SI 32768
 TD 32768
 SM 6024.096
 HZ/PT .368
 PM 3 0
 RD 0 0
 AG 2.720
 RG 200
 NS 32
 TE 297
 FM 7500
 O2 0 0
 DP 40L P0
 LB 0 0
 GB 0 0
 CX 36.00
 CY 0 0
 F1 10.900P
 F2 105.024
 PPM/CM 292
 SR 5901.12

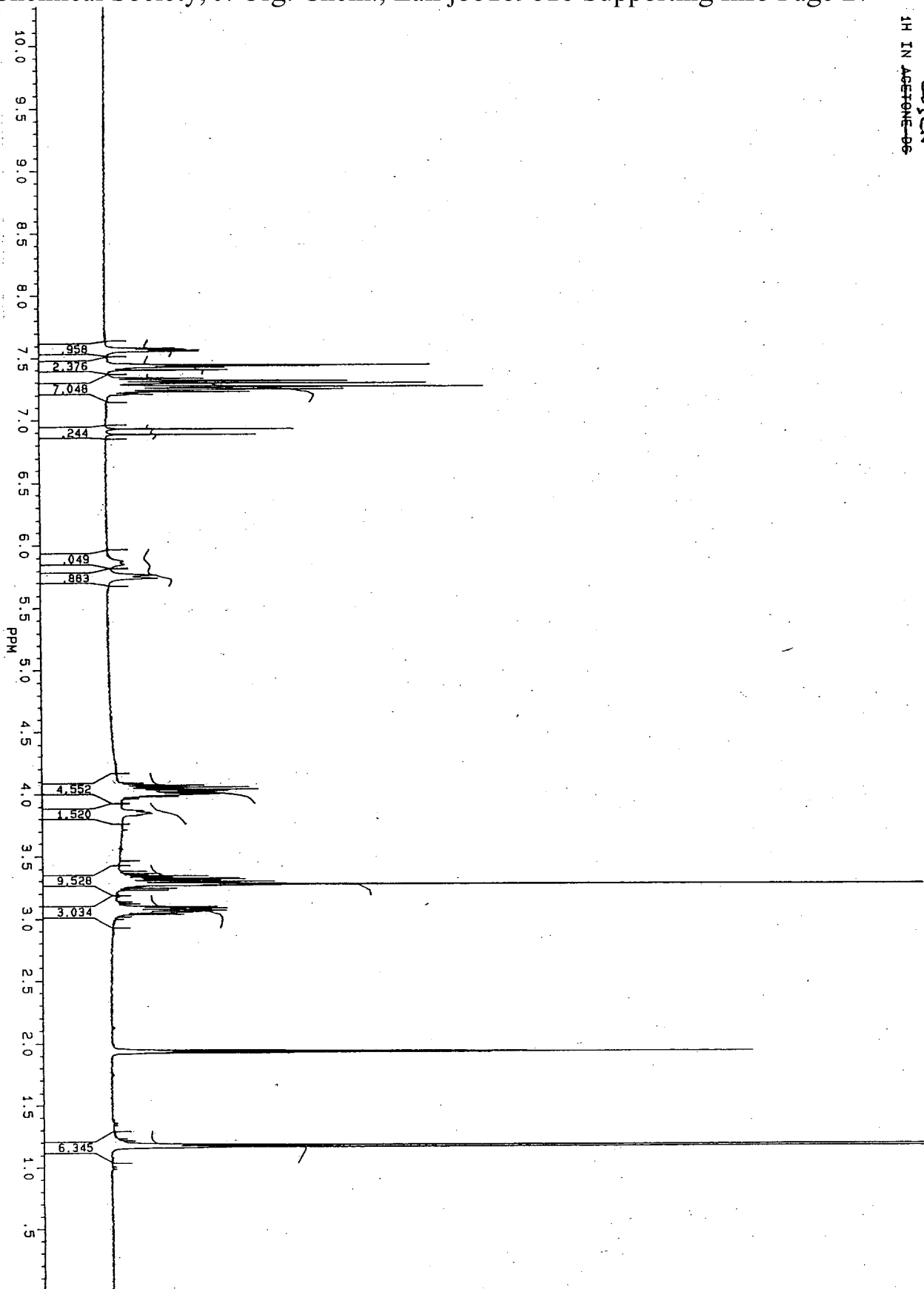
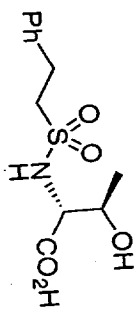


STANDARD CARBON PARAMETERS

200
180
160
140
120
100
80
60
40
20
ppm



1H IN ACETONE-D6

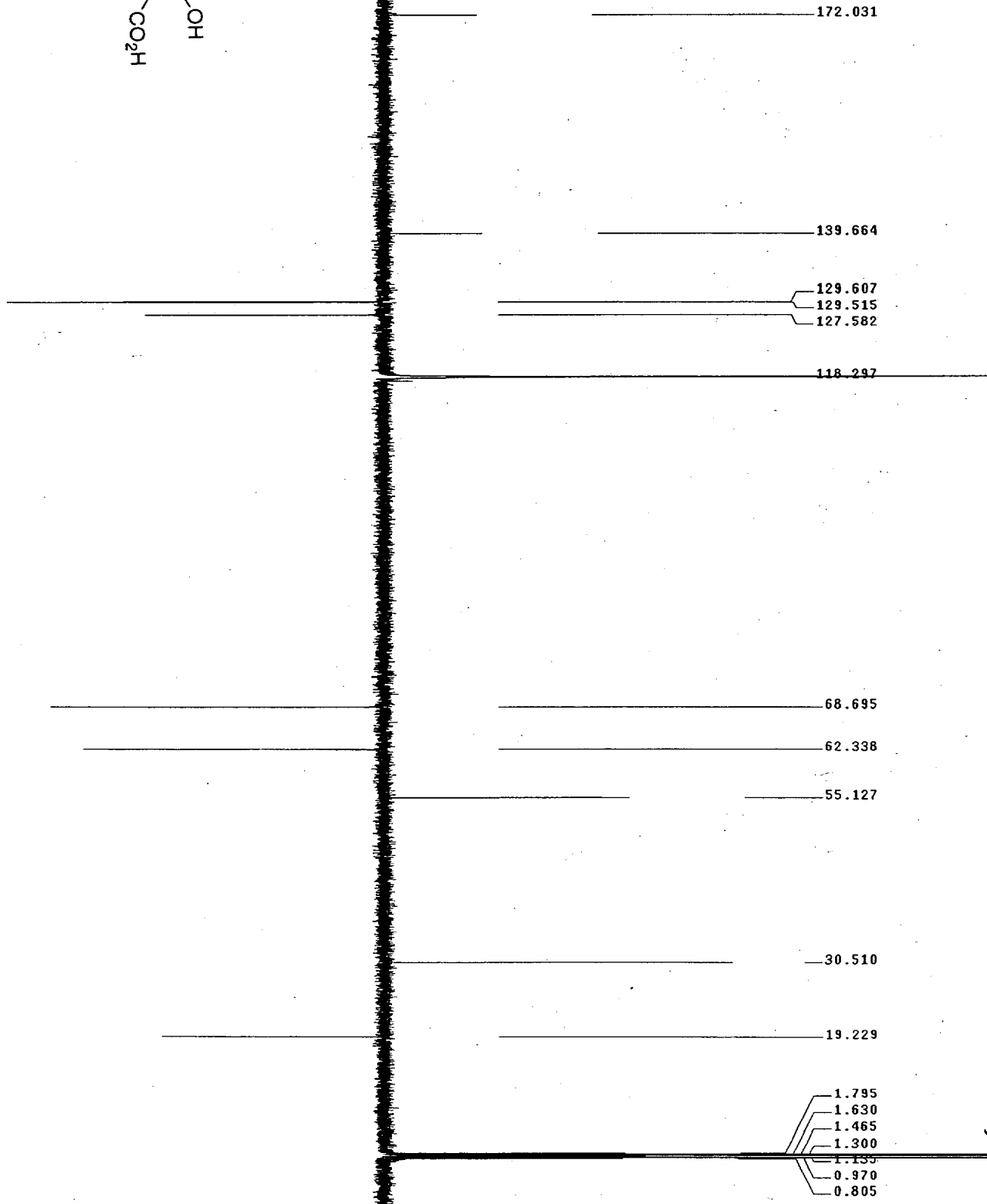
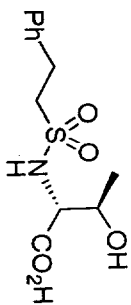


SF 120.0 360.136
 SY 120.0
 O1 8100.000
 ST 32768
 TD 32768
 SW 5024.096
 HZ/PT 388
 PM 3.0
 RD 0.0
 RG 100
 NS 32
 TE 297
 FW 7600
 OZ 0.0
 DP 40L P0
 LB 0.0
 GB 0.0
 CX 36.00
 CY 0.0
 F1 10.500P
 F2 105.024
 PPM/DW 292
 SR 3900.73



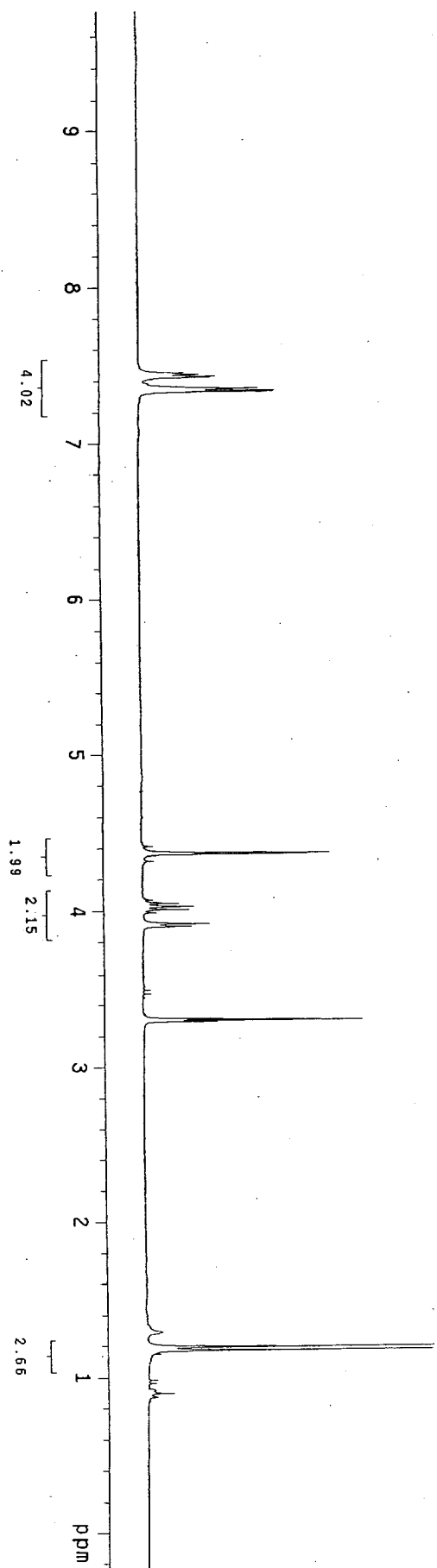
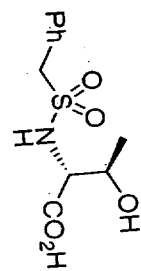
S 27

200
180
160
140
120
100
80
60
40
20
ppm

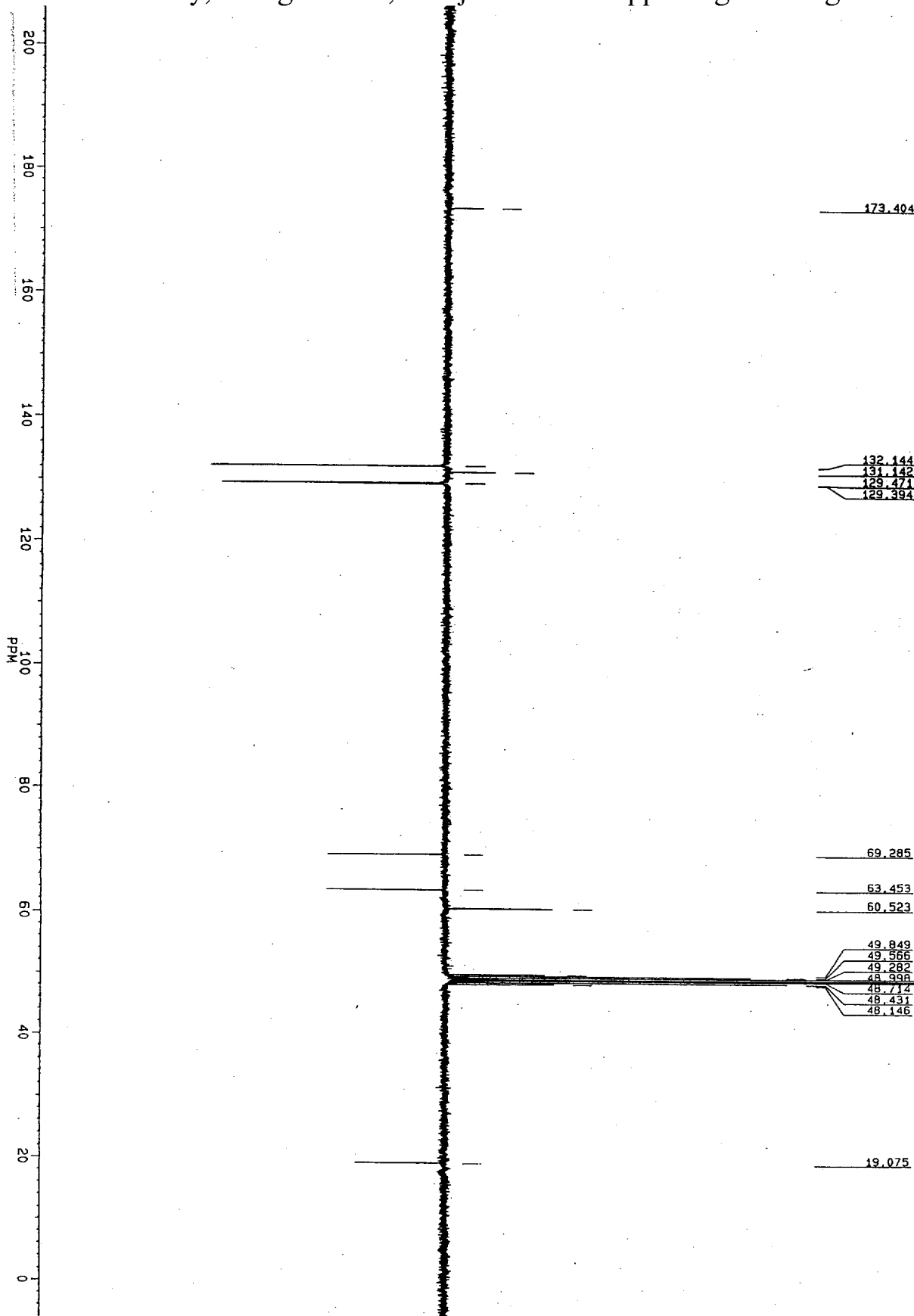
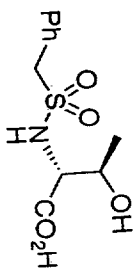


S 228

300 MHz 1D in CD3OD (ref. to CD3OD @ 3.30 ppm), temp 27.5 C -> actual temp =27.0 C
date: Aug 4 1998 seqfil: s2pu1 hz/mm: 12.51 spectrometer: 1300
acq.time [s]: 2.0 relax. time [s]: 3.0 sweep width [Hz]: 3001 dig.res. [Hz/pt]: 0.09 file: exp



YEEMAN YR-3-136, 13C APT IN C030D

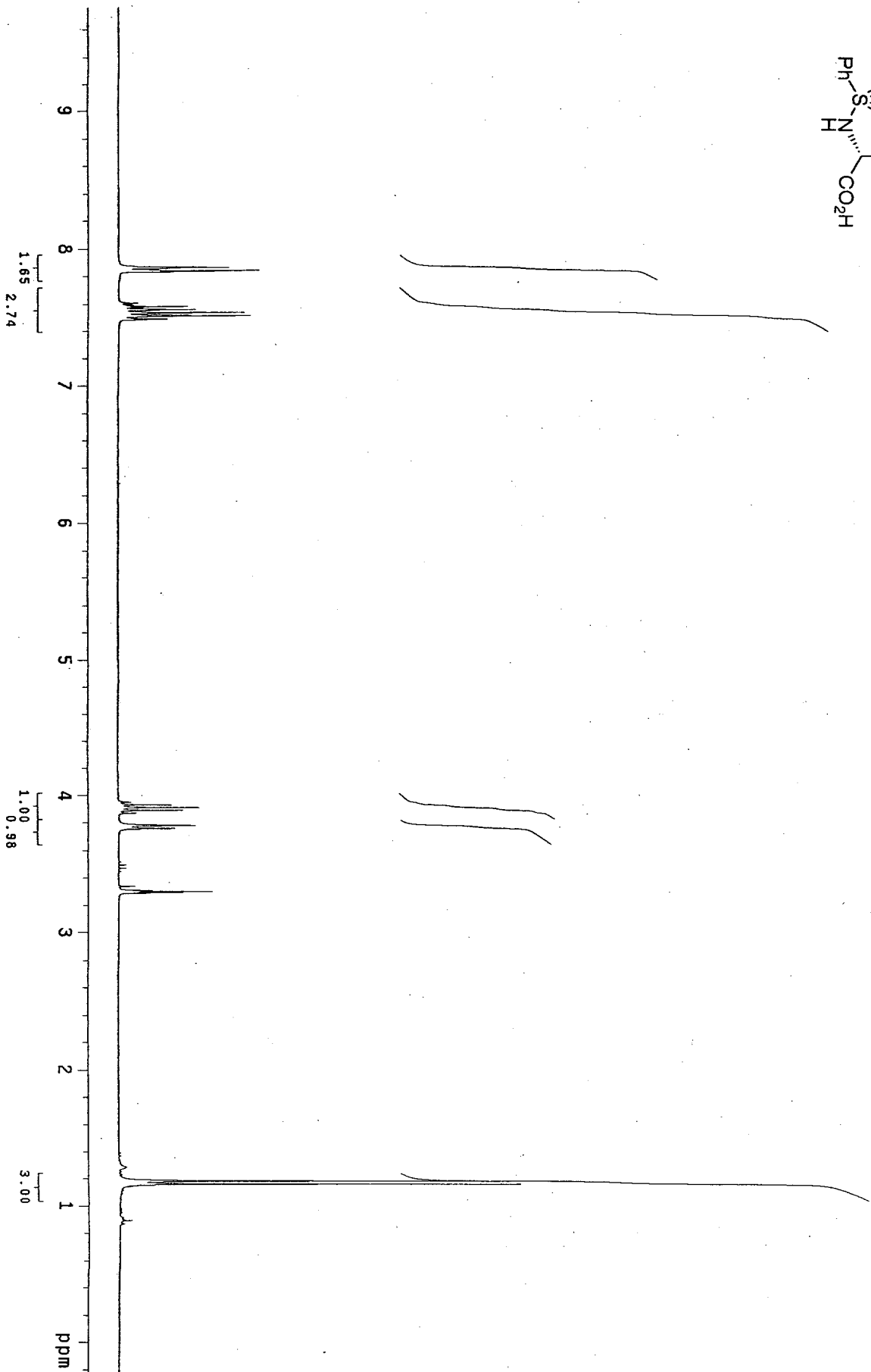
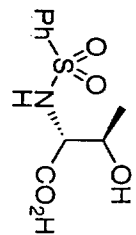


SF 75.469
 SY 112.0
 O1 17478.000
 ST 65536
 TD 32928
 SK 32468
 SH 18518.519
 HZ/PT 565
 PM 0.0
 RD 0.0
 AG 800
 RG 885
 NS 10000
 TE 297
 FM 23200
 O2 3595.000
 DP 18H.CPD
 LB 1.000
 GB 0.0
 CX 36.00
 CY 20.00
 F1 210.008P
 F2 -15.987P
 HZ/CN 452.803
 DM/CN 8.000
 SH -1328.27
 D1 500.0000
 S1 18H
 P9 100.00
 D2 .0010000
 SS2 18H
 P0 1.70
 D3 .0070000
 P8 8.880
 D4 .0001000
 RGA
 RD 0.0
 PW 0.0
 DE 36.30
 NS 10000
 DS 2

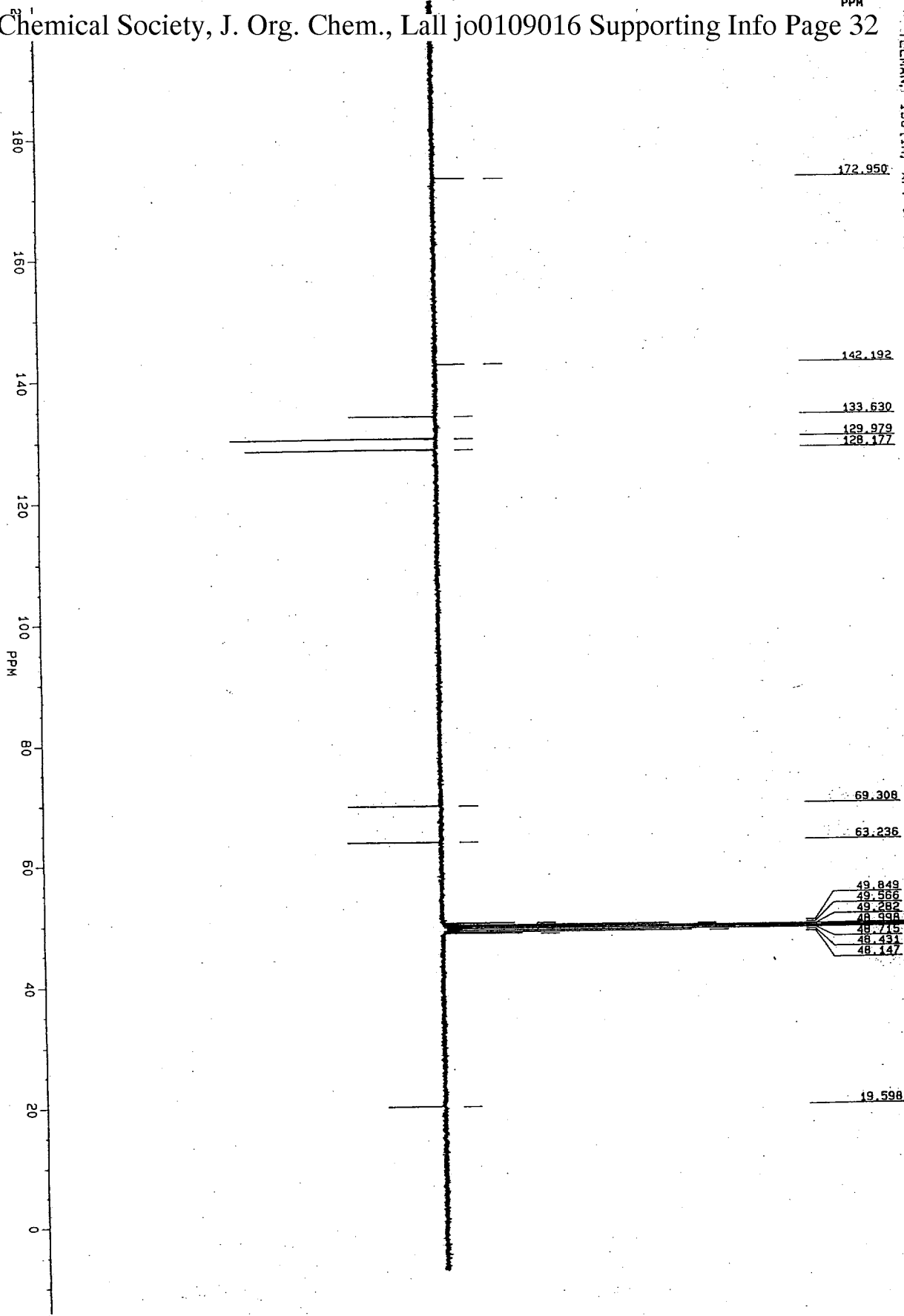
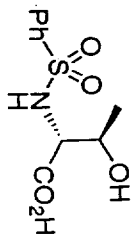
BDIKER
 330

300 MHz 1D 1h CD30D (ref. to CD30D @ 3.30 ppm), temp 27.5 C -> actual temp =27.0 C

date: Aug 30 1999 seqfil: s2pu1 hz/mm: 12.50 spectrometer: 1300 file: exp
acq.time [s]: 2.0 Relax.time [s]: 3.0 sweep width [Hz]: 3001 dig.res. [Hz/pt]: 0.09



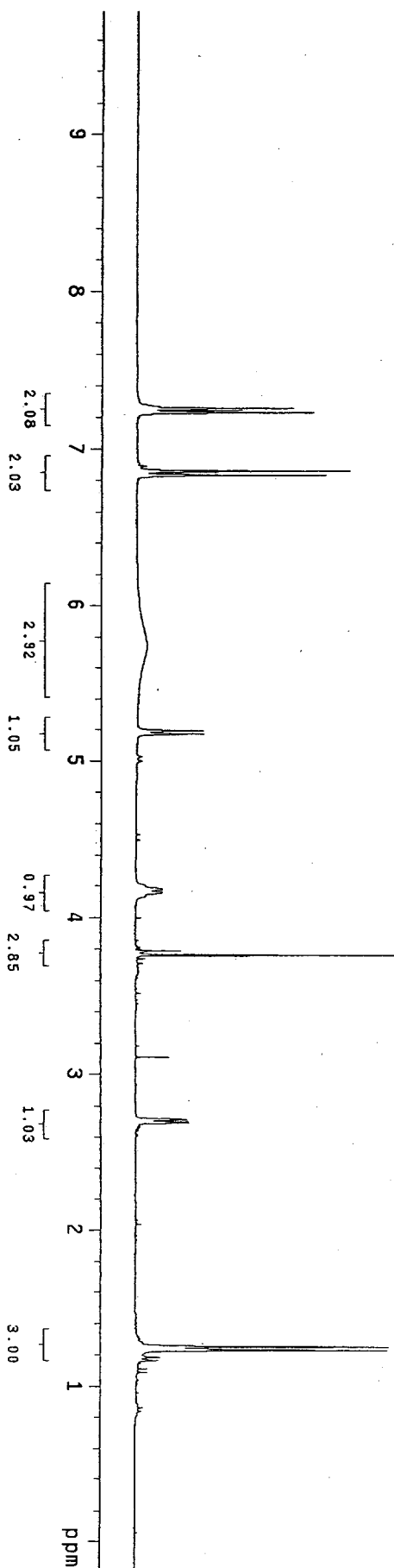
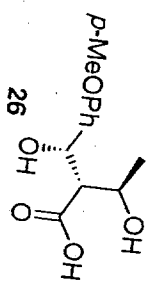
YEE MAN, 13C [1H] APT ON VR-3-188 IN CD3OD



AU310F.101
 AU PROG:
 X25, AU
 DATE 10-10-99
 TIME 21:42
 SF 75.469
 SY 112.0
 O1 7478.000
 S1 65536
 T1 32768
 SW 18518.519
 HZ/PT 565
 PM 0.0
 RD 0.0
 AG 885
 RG 800
 NS 8000
 TE 297
 FW 23200
 O2 3895.000
 DP 18H.CPD
 LB 1.000
 GB 0.0
 CX 36.00
 CY 0.0
 F1 202.003P
 F2 -13.992P
 HZ/CM 452.803
 PPM/CM 6.000
 SR -1214.12
 D1 1.2000000
 S1 18H
 P9 100.00
 D2 .0010000
 S2 18H
 P6 1.70
 D3 .0065600
 P6 8.40
 D4 .0010000
 RGA
 RD 0.0
 PM 0.0
 DE 36.30
 NS 8000
 DS 2

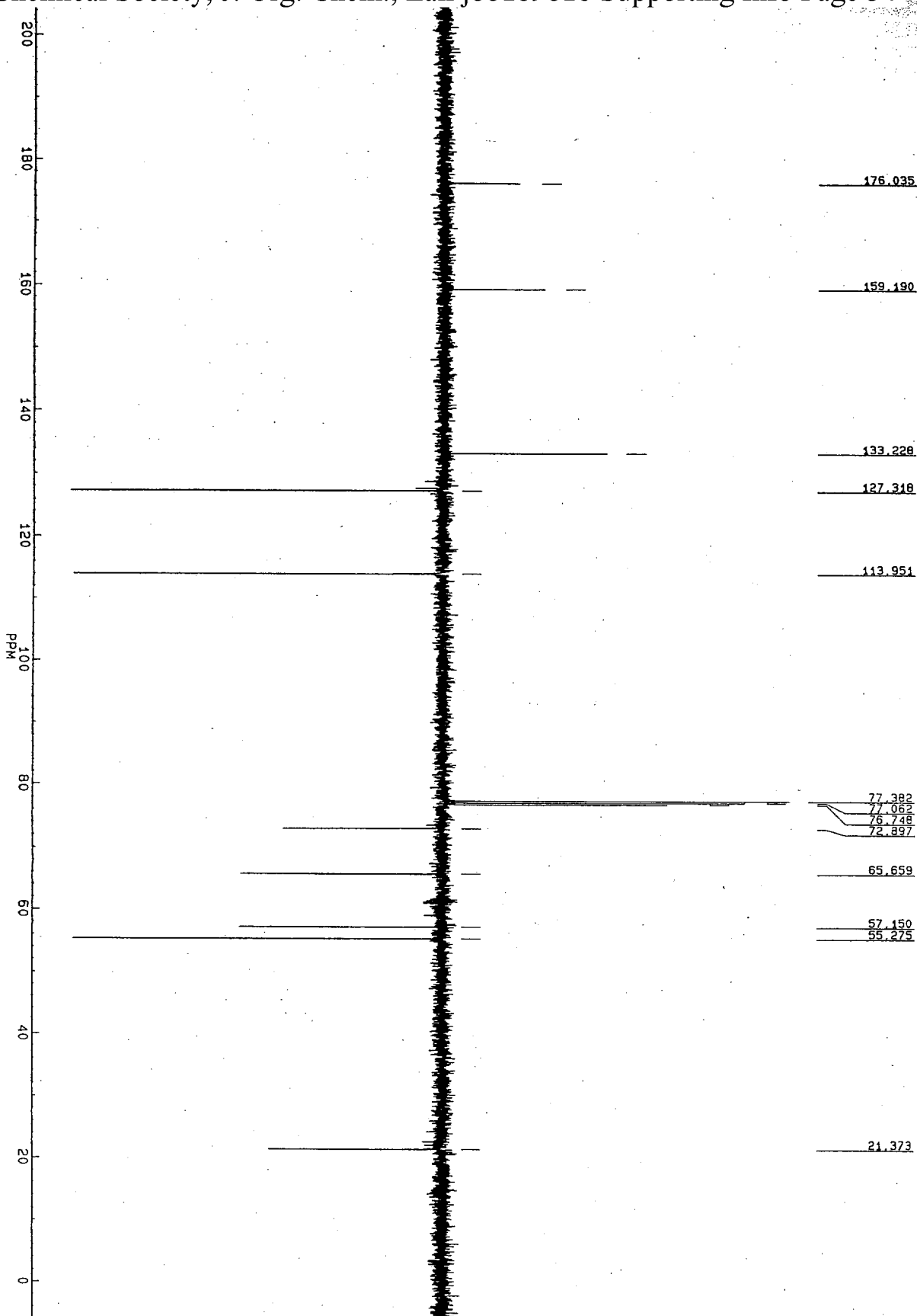
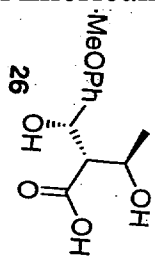
B
 532

300 MHz 1D 1H CDCl3 (ref. to CDCl3 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C
date: Nov 18 1999 seqfil: s2pu1 hz/mm: 12.50 spectrometer: j300 file: exp
acq.time [s]: 2.0 relax.time [s]: 3.0 sweep width [Hz]: 3001 dg.res. [Hz/pt]: 0.09
Pulse Sequence: s2pu1



S33

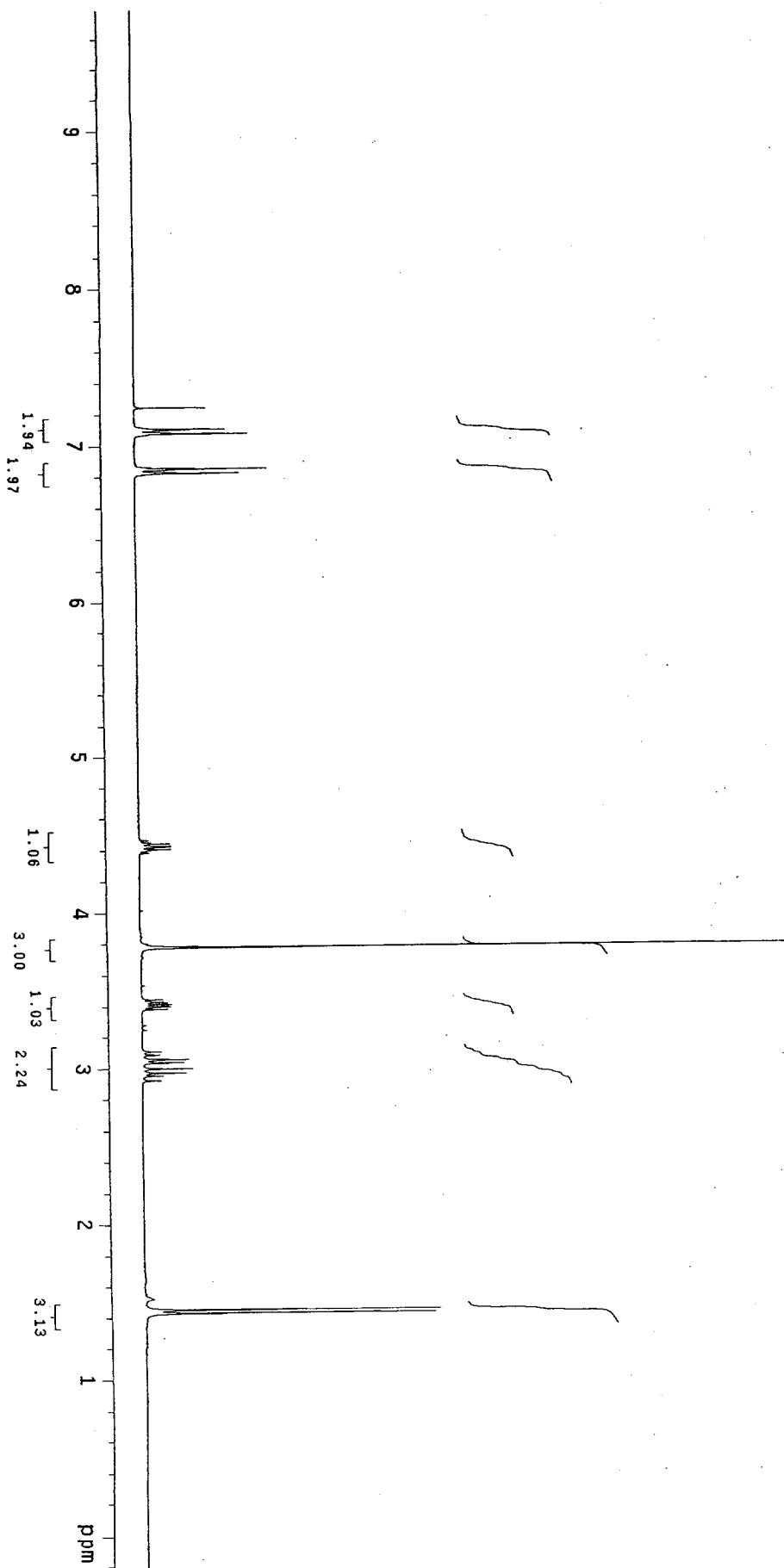
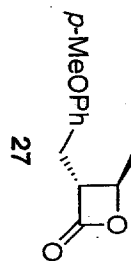
YEMAN, YR-4-28C IN CDCL3, APTXH



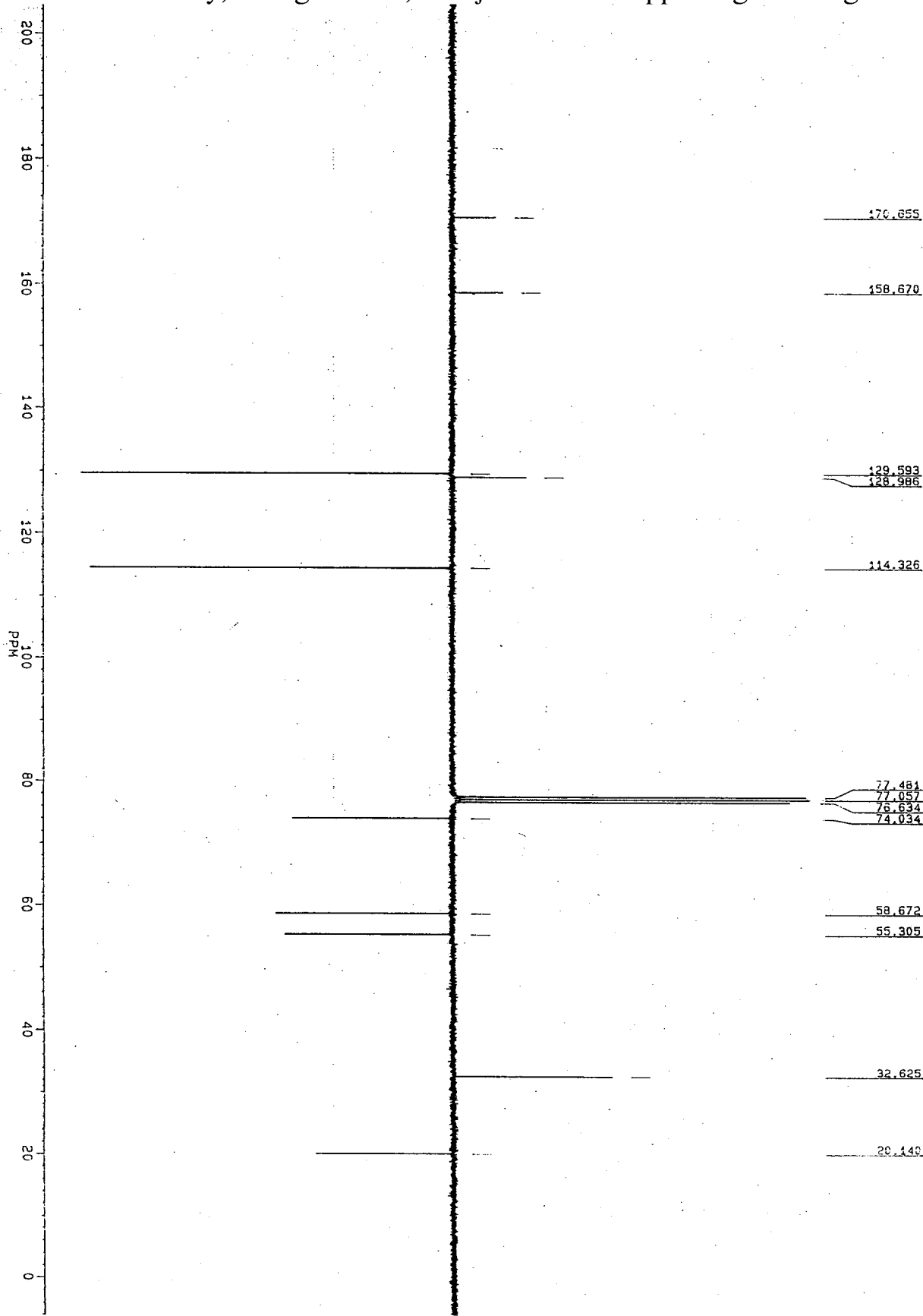
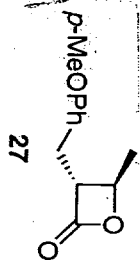
NV18407C.001
 AU PROG: APTXH.AU
 DATE 18-11-99
 TIME 16:03
 SF 100.614
 Q1 12000.000
 Q2 32768
 Q3 32768
 Q4 29411.765
 HZ/PT 1.795
 PW 0.0
 RD 0.0
 AG 0.557
 RG 400
 NS 2509
 TE 297
 FW 36800
 O2 6300.000
 DP 15H CPD
 LB -300
 TX 36.00
 CY 40.00
 F1 210.001P
 F2 -5.994P
 HZ/CM 603.670
 PPM/CM 6.000
 SR -129.88
 D1 .7000000
 S2 15H
 P9 95.00
 D2 .0010000
 P0 2.30
 D3 .0070000
 P6 13.00
 D4 .0001000
 RD 0.0
 PW 0.0
 DE 23.80
 NS 2509
 DS 2

BX
 YR
 S34

300 MHz 1D in CDCl3 (ref. to CDC13 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C
date: Jan 12 2000 seqf11: szpu1 hz/mm: 12.51 Spectrometer: 1300 file: exp
acq.time [s]: 2.0 relax.time [s]: 3.0 Sweep width [Hz]: 3001 dig.res. [Hz/pt]: 0.09
Pulse Sequence: szpu1

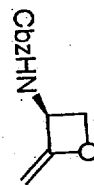


YEEMAN APT ON SAMPLE YR-4778

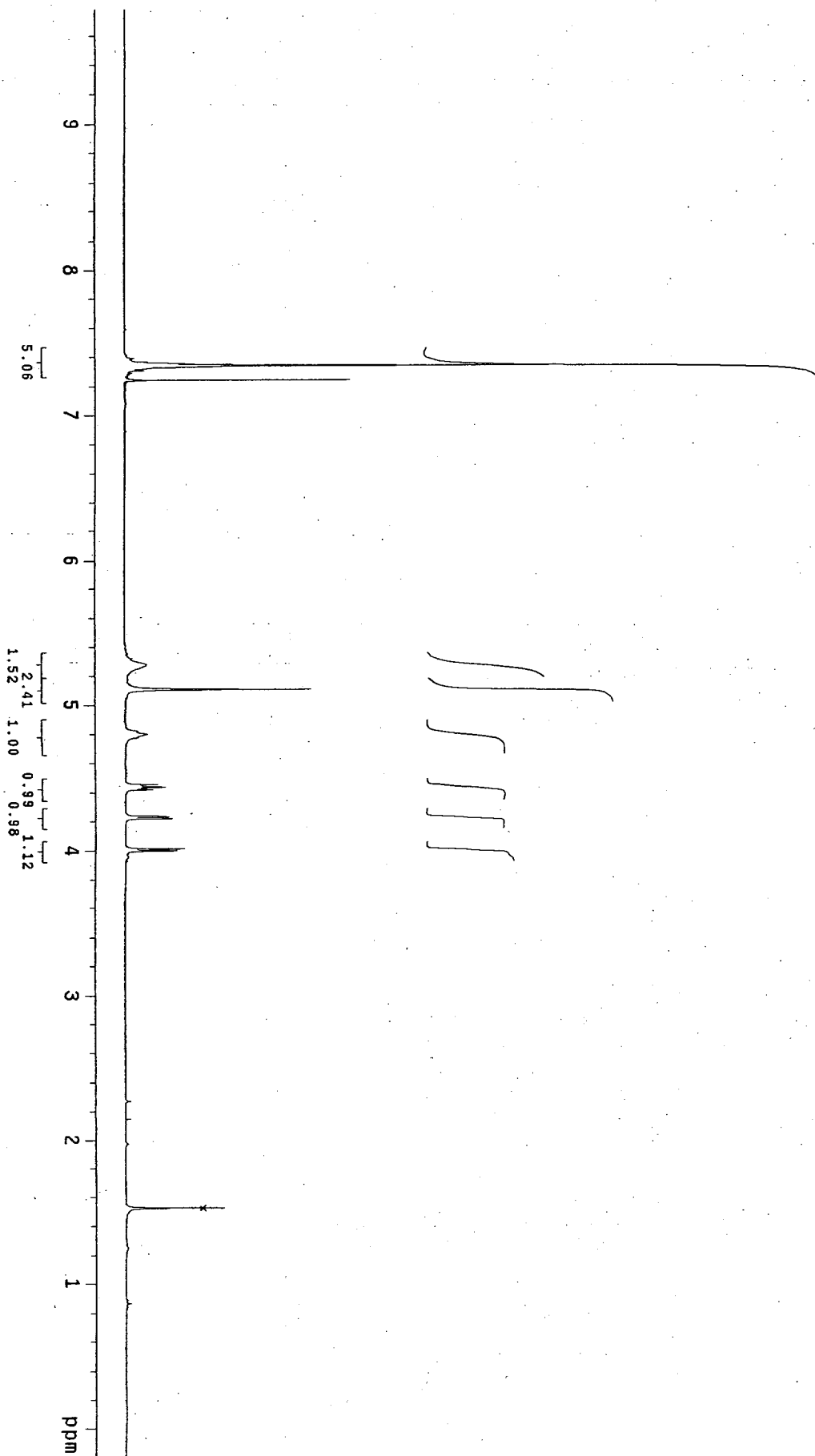


41407.108
 AU PPRR
 X25.40
 DATE 15-1-0
 ST 1437 75.489
 SI 1437 75.489
 O1 7000.090
 S1 68880
 T0 52782
 LW 3870.479
 HZ/PI 1894
 FW 5.0
 R0 5.0
 A2 5.781
 A3 5.0
 R3 5.0
 R4 5.0
 R5 5.0
 R6 5.0
 R7 5.0
 R8 5.0
 R9 5.0
 R10 5.0
 R11 5.0
 R12 5.0
 R13 5.0
 R14 5.0
 R15 5.0
 R16 5.0
 R17 5.0
 R18 5.0
 R19 5.0
 R20 5.0
 R21 5.0
 R22 5.0
 R23 5.0
 R24 5.0
 R25 5.0
 R26 5.0
 R27 5.0
 R28 5.0
 R29 5.0
 R30 5.0
 R31 5.0
 R32 5.0
 R33 5.0
 R34 5.0
 R35 5.0
 R36 5.0
 R37 5.0
 R38 5.0
 R39 5.0
 R40 5.0
 R41 5.0
 R42 5.0
 R43 5.0
 R44 5.0
 R45 5.0
 R46 5.0
 R47 5.0
 R48 5.0
 R49 5.0
 R50 5.0
 R51 5.0
 R52 5.0
 R53 5.0
 R54 5.0
 R55 5.0
 R56 5.0
 R57 5.0
 R58 5.0
 R59 5.0
 R60 5.0
 R61 5.0
 R62 5.0
 R63 5.0
 R64 5.0
 R65 5.0
 R66 5.0
 R67 5.0
 R68 5.0
 R69 5.0
 R70 5.0
 R71 5.0
 R72 5.0
 R73 5.0
 R74 5.0
 R75 5.0
 R76 5.0
 R77 5.0
 R78 5.0
 R79 5.0
 R80 5.0
 R81 5.0
 R82 5.0
 R83 5.0
 R84 5.0
 R85 5.0
 R86 5.0
 R87 5.0
 R88 5.0
 R89 5.0
 R90 5.0
 R91 5.0
 R92 5.0
 R93 5.0
 R94 5.0
 R95 5.0
 R96 5.0
 R97 5.0
 R98 5.0
 R99 5.0
 R100 5.0
 R101 5.0
 R102 5.0
 R103 5.0
 R104 5.0
 R105 5.0
 R106 5.0
 R107 5.0
 R108 5.0
 R109 5.0
 R110 5.0
 R111 5.0
 R112 5.0
 R113 5.0
 R114 5.0
 R115 5.0
 R116 5.0
 R117 5.0
 R118 5.0
 R119 5.0
 R120 5.0
 R121 5.0
 R122 5.0
 R123 5.0
 R124 5.0
 R125 5.0
 R126 5.0
 R127 5.0
 R128 5.0
 R129 5.0
 R130 5.0
 R131 5.0
 R132 5.0
 R133 5.0
 R134 5.0
 R135 5.0
 R136 5.0
 R137 5.0
 R138 5.0
 R139 5.0
 R140 5.0
 R141 5.0
 R142 5.0
 R143 5.0
 R144 5.0
 R145 5.0
 R146 5.0
 R147 5.0
 R148 5.0
 R149 5.0
 R150 5.0
 R151 5.0
 R152 5.0
 R153 5.0
 R154 5.0
 R155 5.0
 R156 5.0
 R157 5.0
 R158 5.0
 R159 5.0
 R160 5.0
 R161 5.0
 R162 5.0
 R163 5.0
 R164 5.0
 R165 5.0
 R166 5.0
 R167 5.0
 R168 5.0
 R169 5.0
 R170 5.0
 R171 5.0
 R172 5.0
 R173 5.0
 R174 5.0
 R175 5.0
 R176 5.0
 R177 5.0
 R178 5.0
 R179 5.0
 R180 5.0
 R181 5.0
 R182 5.0
 R183 5.0
 R184 5.0
 R185 5.0
 R186 5.0
 R187 5.0
 R188 5.0
 R189 5.0
 R190 5.0
 R191 5.0
 R192 5.0
 R193 5.0
 R194 5.0
 R195 5.0
 R196 5.0
 R197 5.0
 R198 5.0
 R199 5.0
 R200 5.0
 R201 5.0
 R202 5.0
 R203 5.0
 R204 5.0
 R205 5.0
 R206 5.0
 R207 5.0
 R208 5.0
 R209 5.0
 R210 5.0
 R211 5.0
 R212 5.0
 R213 5.0
 R214 5.0
 R215 5.0
 R216 5.0
 R217 5.0
 R218 5.0
 R219 5.0
 R220 5.0
 R221 5.0
 R222 5.0
 R223 5.0
 R224 5.0
 R225 5.0
 R226 5.0
 R227 5.0
 R228 5.0
 R229 5.0
 R230 5.0
 R231 5.0
 R232 5.0
 R233 5.0
 R234 5.0
 R235 5.0
 R236 5.0
 R237 5.0
 R238 5.0
 R239 5.0
 R240 5.0
 R241 5.0
 R242 5.0
 R243 5.0
 R244 5.0
 R245 5.0
 R246 5.0
 R247 5.0
 R248 5.0
 R249 5.0
 R250 5.0
 R251 5.0
 R252 5.0
 R253 5.0
 R254 5.0
 R255 5.0
 R256 5.0
 R257 5.0
 R258 5.0
 R259 5.0
 R260 5.0
 R261 5.0
 R262 5.0
 R263 5.0
 R264 5.0
 R265 5.0
 R266 5.0
 R267 5.0
 R268 5.0
 R269 5.0
 R270 5.0
 R271 5.0
 R272 5.0
 R273 5.0
 R274 5.0
 R275 5.0
 R276 5.0
 R277 5.0
 R278 5.0
 R279 5.0
 R280 5.0
 R281 5.0
 R282 5.0
 R283 5.0
 R284 5.0
 R285 5.0
 R286 5.0
 R287 5.0
 R288 5.0
 R289 5.0
 R290 5.0
 R291 5.0
 R292 5.0
 R293 5.0
 R294 5.0
 R295 5.0
 R296 5.0
 R297 5.0
 R298 5.0
 R299 5.0
 R300 5.0
 R301 5.0
 R302 5.0
 R303 5.0
 R304 5.0
 R305 5.0
 R306 5.0
 R307 5.0
 R308 5.0
 R309 5.0
 R310 5.0
 R311 5.0
 R312 5.0
 R313 5.0
 R314 5.0
 R315 5.0
 R316 5.0
 R317 5.0
 R318 5.0
 R319 5.0
 R320 5.0
 R321 5.0
 R322 5.0
 R323 5.0
 R324 5.0
 R325 5.0
 R326 5.0
 R327 5.0
 R328 5.0
 R329 5.0
 R330 5.0
 R331 5.0
 R332 5.0
 R333 5.0
 R334 5.0
 R335 5.0
 R336 5.0
 R337 5.0
 R338 5.0
 R339 5.0
 R340 5.0
 R341 5.0
 R342 5.0
 R343 5.0
 R344 5.0
 R345 5.0
 R346 5.0
 R347 5.0
 R348 5.0
 R349 5.0
 R350 5.0
 R351 5.0
 R352 5.0
 R353 5.0
 R354 5.0
 R355 5.0
 R356 5.0
 R357 5.0
 R358 5.0
 R359 5.0
 R360 5.0
 R361 5.0
 R362 5.0
 R363 5.0
 R364 5.0
 R365 5.0
 R366 5.0
 R367 5.0
 R368 5.0
 R369 5.0
 R370 5.0
 R371 5.0
 R372 5.0
 R373 5.0
 R374 5.0
 R375 5.0
 R376 5.0
 R377 5.0
 R378 5.0
 R379 5.0
 R380 5.0
 R381 5.0
 R382 5.0
 R383 5.0
 R384 5.0
 R385 5.0
 R386 5.0
 R387 5.0
 R388 5.0
 R389 5.0
 R390 5.0
 R391 5.0
 R392 5.0
 R393 5.0
 R394 5.0
 R395 5.0
 R396 5.0
 R397 5.0
 R398 5.0
 R399 5.0
 R400 5.0
 R401 5.0
 R402 5.0
 R403 5.0
 R404 5.0
 R405 5.0
 R406 5.0
 R407 5.0
 R408 5.0
 R409 5.0
 R410 5.0
 R411 5.0
 R412 5.0
 R413 5.0
 R414 5.0
 R415 5.0
 R416 5.0
 R417 5.0
 R418 5.0
 R419 5.0
 R420 5.0
 R421 5.0
 R422 5.0
 R423 5.0
 R424 5.0
 R425 5.0
 R426 5.0
 R427 5.0
 R428 5.0
 R429 5.0
 R430 5.0
 R431 5.0
 R432 5.0
 R433 5.0
 R434 5.0
 R435 5.0
 R436 5.0
 R437 5.0
 R438 5.0
 R439 5.0
 R440 5.0
 R441 5.0
 R442 5.0
 R443 5.0
 R444 5.0
 R445 5.0
 R446 5.0
 R447 5.0
 R448 5.0
 R449 5.0
 R450 5.0
 R451 5.0
 R452 5.0
 R453 5.0
 R454 5.0
 R455 5.0
 R456 5.0
 R457 5.0
 R458 5.0
 R459 5.0
 R460 5.0
 R461 5.0
 R462 5.0
 R463 5.0
 R464 5.0
 R465 5.0
 R466 5.0
 R467 5.0
 R468 5.0
 R469 5.0
 R470 5.0
 R471 5.0
 R472 5.0
 R473 5.0
 R474 5.0
 R475 5.0
 R476 5.0
 R477 5.0
 R478 5.0
 R479 5.0
 R480 5.0
 R481 5.0
 R482 5.0
 R483 5.0
 R484 5.0
 R485 5.0
 R486 5.0
 R487 5.0
 R488 5.0
 R489 5.0
 R490 5.0
 R491 5.0
 R492 5.0
 R493 5.0
 R494 5.0
 R495 5.0
 R496 5.0
 R497 5.0
 R498 5.0
 R499 5.0
 R500 5.0
 R501 5.0
 R502 5.0
 R503 5.0
 R504 5.0
 R505 5.0
 R506 5.0
 R507 5.0
 R508 5.0
 R509 5.0
 R510 5.0
 R511 5.0
 R512 5.0
 R513 5.0
 R514 5.0
 R515 5.0
 R516 5.0
 R517 5.0
 R518 5.0
 R519 5.0
 R520 5.0
 R521 5.0
 R522 5.0
 R523 5.0
 R524 5.0
 R525 5.0
 R526 5.0
 R527 5.0
 R528 5.0
 R529 5.0
 R530 5.0
 R531 5.0
 R532 5.0
 R533 5.0
 R534 5.0
 R535 5.0
 R536 5.0
 R537 5.0
 R538 5.0
 R539 5.0
 R540 5.0
 R541 5.0
 R542 5.0
 R543 5.0
 R544 5.0
 R545 5.0
 R546 5.0
 R547 5.0
 R548 5.0
 R549 5.0
 R550 5.0
 R551 5.0
 R552 5.0
 R553 5.0
 R554 5.0
 R555 5.0
 R556 5.0
 R557 5.0
 R558 5.0
 R559 5.0
 R560 5.0
 R561 5.0
 R562 5.0
 R563 5.0
 R564 5.0
 R565 5.0
 R566 5.0
 R567 5.0
 R568 5.0
 R569 5.0
 R570 5.0
 R571 5.0
 R572 5.0
 R573 5.0
 R574 5.0
 R575 5.0
 R576 5.0
 R577 5.0
 R578 5.0
 R579 5.0
 R580 5.0
 R581 5.0
 R582 5.0
 R583 5.0
 R584 5.0
 R585 5.0
 R586 5.0
 R587 5.0
 R588 5.0
 R589 5.0
 R590 5.0
 R591 5.0
 R592 5.0
 R593 5.0
 R594 5.0
 R595 5.0
 R596 5.0
 R597 5.0
 R598 5.0
 R599 5.0
 R600 5.0
 R601 5.0
 R602 5.0
 R603 5.0
 R604 5.0
 R605 5.0
 R606 5.0
 R607 5.0
 R608 5.0
 R609 5.0
 R610 5.0
 R611 5.0
 R612 5.0
 R613 5.0
 R614 5.0
 R615 5.0
 R616 5.0
 R617 5.0
 R618 5.0
 R619 5.0
 R620 5.0
 R621 5.0
 R622 5.0
 R623 5.0
 R624 5.0
 R625 5.0
 R626 5.0
 R627 5.0
 R628 5.0
 R629 5.0
 R630 5.0
 R631 5.0
 R632 5.0
 R633 5.0
 R634 5.0
 R635 5.0
 R636 5.0
 R637 5.0
 R638 5.0
 R639 5.0
 R640 5.0
 R641 5.0
 R642 5.0
 R643 5.0
 R644 5.0
 R645 5.0
 R646 5.0
 R647 5.0
 R648 5.0
 R649 5.0
 R650 5.0
 R651 5.0
 R652 5.0
 R653 5.0
 R654 5.0
 R655 5.0
 R656 5.0
 R657 5.0
 R658 5.0
 R659 5.0
 R660 5.0
 R661 5.0
 R662 5.0
 R663 5.0
 R664 5.0
 R665 5.0
 R666 5.0
 R667 5.0
 R668 5.0
 R669 5.0
 R670 5.0
 R671 5.0
 R672 5.0
 R673 5.0
 R674 5.0
 R675 5.0
 R676 5.0
 R677 5.0
 R678 5.0
 R679 5.0
 R680 5.0
 R681 5.0
 R682 5.0
 R683 5.0
 R684 5.0
 R685 5.0
 R686 5.0
 R687 5.0
 R688 5.0
 R689 5.0
 R690 5.0
 R691 5.0
 R692 5.0
 R693 5.0
 R694 5.0
 R695 5.0
 R696 5.0
 R697 5.0
 R698 5.0
 R699 5.0
 R700 5.0
 R701 5.0
 R702 5.0
 R703 5.0
 R704 5.0
 R705 5.0
 R706 5.0
 R707 5.0
 R708 5.0
 R709 5.0
 R710 5.0
 R711 5.0
 R712 5.0
 R713 5.0
 R714 5.0
 R715 5.0
 R716 5.0
 R717 5.0
 R718 5.0
 R719 5.0
 R720 5.0
 R721 5.0
 R722 5.0
 R723 5.0
 R724 5.0
 R725 5.0
 R726 5.0
 R727 5.0
 R728 5.0
 R729 5.0
 R730 5.0
 R731 5.0
 R732 5.0
 R733 5.0
 R734 5.0
 R735 5.0
 R736 5.0
 R737 5.0
 R738 5.0
 R739 5.0
 R740 5.0
 R741 5.0
 R742 5.0
 R743 5.0
 R744 5.0
 R745 5.0
 R746 5.0
 R747 5.0
 R748 5.0
 R749 5.0
 R750 5.0
 R751 5.0
 R752 5.0
 R753 5.0
 R754 5.0
 R755 5.0
 R756 5.0
 R757 5.0
 R758 5.0
 R759 5.0
 R760 5.0
 R761 5.0
 R762 5.0
 R763 5.0
 R764 5.0
 R765 5.0
 R766 5.0
 R767 5.0
 R768 5.0
 R769 5.0
 R770 5.0
 R771 5.0
 R772 5.0
 R773 5.0
 R774 5.0
 R775 5.0
 R776 5.0
 R777 5.0
 R778 5.0
 R779 5.0
 R780 5.0
 R781 5.0
 R782 5.0
 R783 5.0
 R784 5.0
 R785 5.0
 R786 5.0
 R787 5.0
 R788 5.0
 R789 5.0
 R790 5.0
 R791 5.0
 R792 5.0
 R793 5.0
 R794 5.0
 R795 5.0
 R796 5.0
 R797 5.0
 R798 5.0
 R799 5.0
 R800 5.0
 R801 5.0
 R802 5.0
 R803 5.0
 R804 5.0
 R805 5.0
 R806 5.0
 R807 5.0
 R808 5.0
 R809 5.0
 R810 5.0
 R811 5.0
 R812 5.0
 R813 5.0
 R814 5.0
 R815 5.0
 R816 5.0
 R817 5.0
 R818 5.0
 R819 5.0
 R820 5.0
 R821 5.0
 R822 5.0
 R823 5.0
 R824 5.0
 R825 5.0
 R826 5.0
 R827 5.0
 R828 5.0
 R829 5.0
 R830 5.0
 R831 5.0
 R832 5.0
 R833 5.0
 R834 5.0
 R835 5.0
 R836 5.0
 R837 5.0
 R838 5.0
 R839 5.0
 R840 5.0
 R841 5.0
 R842 5.0
 R843 5.0
 R844 5.0
 R845 5.0
 R846 5.0
 R847 5.0
 R848 5.0
 R849 5.0
 R850 5.0
 R851 5.0
 R852 5.0
 R853 5.0
 R854 5.0
 R855 5.0
 R856 5.0
 R857 5.0
 R858 5.0
 R859 5.0
 R860 5.0
 R861 5.0
 R862 5.0
 R863 5.0
 R864 5.0
 R865 5.0
 R866 5.0
 R867 5.0
 R868 5.0
 R869 5.0
 R870 5.0
 R871 5.0
 R872 5.0
 R873 5.0
 R874 5.0
 R875 5.0
 R876 5.0
 R877 5.0
 R878 5.0
 R879 5.0
 R880 5.0
 R881 5.0
 R882 5.0
 R883 5.0
 R884 5.0
 R885 5.0
 R886 5.0
 R887 5.0
 R888 5.0
 R889 5.0
 R890 5.0
 R891 5.0
 R892 5.0
 R893 5.0
 R894 5.0
 R895 5.0
 R896 5.0
 R897 5.0
 R898 5.0
 R899 5.0
 R900 5.0
 R901 5.0
 R902 5.0
 R903 5.0
 R904 5.0
 R905 5.0
 R906 5.0
 R907 5.0
 R908 5.0
 R909 5.0
 R910 5.0
 R911 5.0
 R912 5.0
 R913 5.0
 R914 5.0
 R915 5.0
 R916 5.0
 R917 5.0
 R918 5.0
 R919 5.0
 R920 5.0
 R921 5.0
 R922 5.0
 R923 5.0
 R924 5.0
 R925 5.0
 R926 5.0
 R927 5.0
 R928 5.0
 R929 5.0
 R930 5.0
 R931 5.0
 R932 5.0
 R933 5.0
 R934 5.0
 R935 5.0
 R936 5.0
 R937 5.0
 R938 5.0
 R939 5.0
 R940 5.0
 R941 5.0
 R942 5.0
 R943 5.0
 R944 5.0
 R945 5.0
 R946 5.0
 R947 5.0
 R948 5.0
 R949 5.0
 R950 5.0
 R951 5.0
 R952 5.0
 R953 5.0
 R954 5.0
 R955 5.0
 R956 5.0
 R957 5.0
 R958 5.0
 R959 5.0
 R960 5.0
 R961 5.0
 R962 5.0
 R963 5.0
 R964 5.0
 R965 5.0
 R966 5.0
 R967 5.0
 R968 5.0
 R969 5.0
 R970 5.0
 R971 5.0
 R972 5.0
 R973 5.0
 R974 5.0
 R975

300 MHz 1D 1H CDCl3 (ref. to CDCl3 @ 7.24 ppm), temp 27.5 C -> actual temp = 27.0 C
date: Feb 11 2000 seqfil: s2pu1 Spectrometer: 1300 file: exp
acq.time [s]: 2.0 relax.time [s]: 3.0 sweep width [Hz]: 3001 Dig.res. [Hz/pt]: 0.09
Pulse Sequence: s2pu1



34



S37

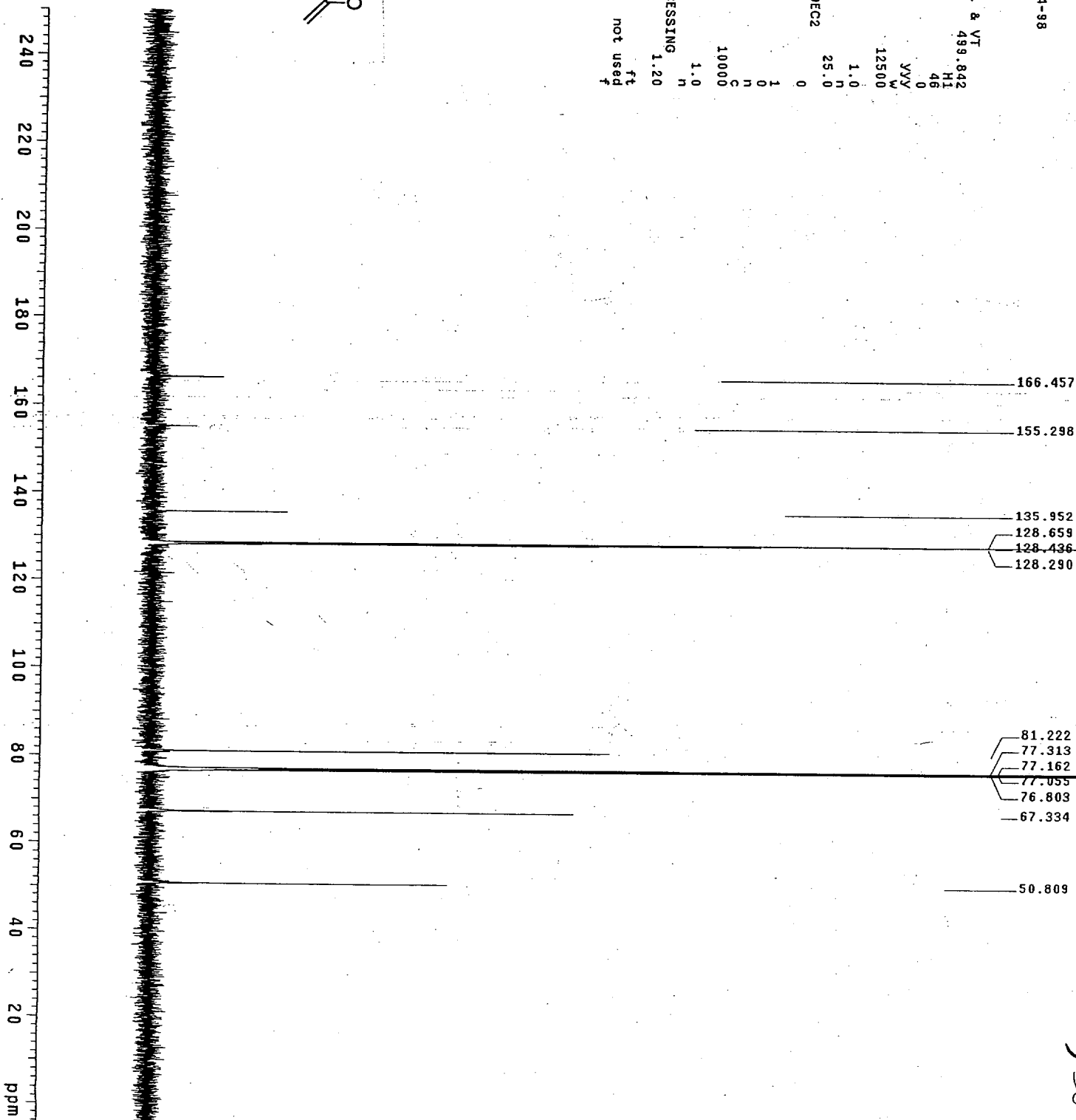
STANDARD CARBON PARAMETERS
Yeaman carbon on sample YR-4-98

```

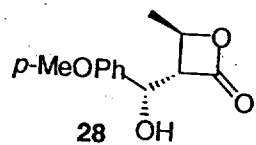
exp2  szpu1
SAMPLE  Feb 15 00  DEC. & VT  499.842
solvent  /export/home/~  dn  HI  46
file     /fids/feb1550~  dof  0
vnmr1/fids/feb1550~  dof  0
ACQUISITION  4c  dm  YVY
sfrq      125.697  dmf  12500
fn        G13  dseq
at        1.300  dres  1.0
np        104000  homo  n
sw        40000.0  temp  25.0
fb        22000
bs        16  dfrq2  0
tpwr     58  dn2
pw        8.0  dpwr2  1
d1        0  dot2
tof       0  dm2
nt       10000  dmm2  n
ct       8512  dmf2  C
alock    n  dseq2
gain     not used  dres2  1.0
        FLAGS  homo2  n
        PROCESSING  1.20
        11  n  lb  wtfile
        in  n  proc  ft
        dp  n  math  not used
        hs  n  math  f
        DISPLAY  -628.5  werr  wbsx  wnt
        wp  32051.9  werr  wbs  wnt
        vs  297  math
        wc  0  werr  wbs  wnt
        hzmm  160.25  werr  wbs  wnt
        is  500.00  werr  wbs  wnt
        rfp  12787.8  werr  wbs  wnt
        th  9886.0  werr  wbs  wnt
        ins  5  werr  wbs  wnt
        nm  1.000  werr  wbs  wnt
        cdc  ph
    
```



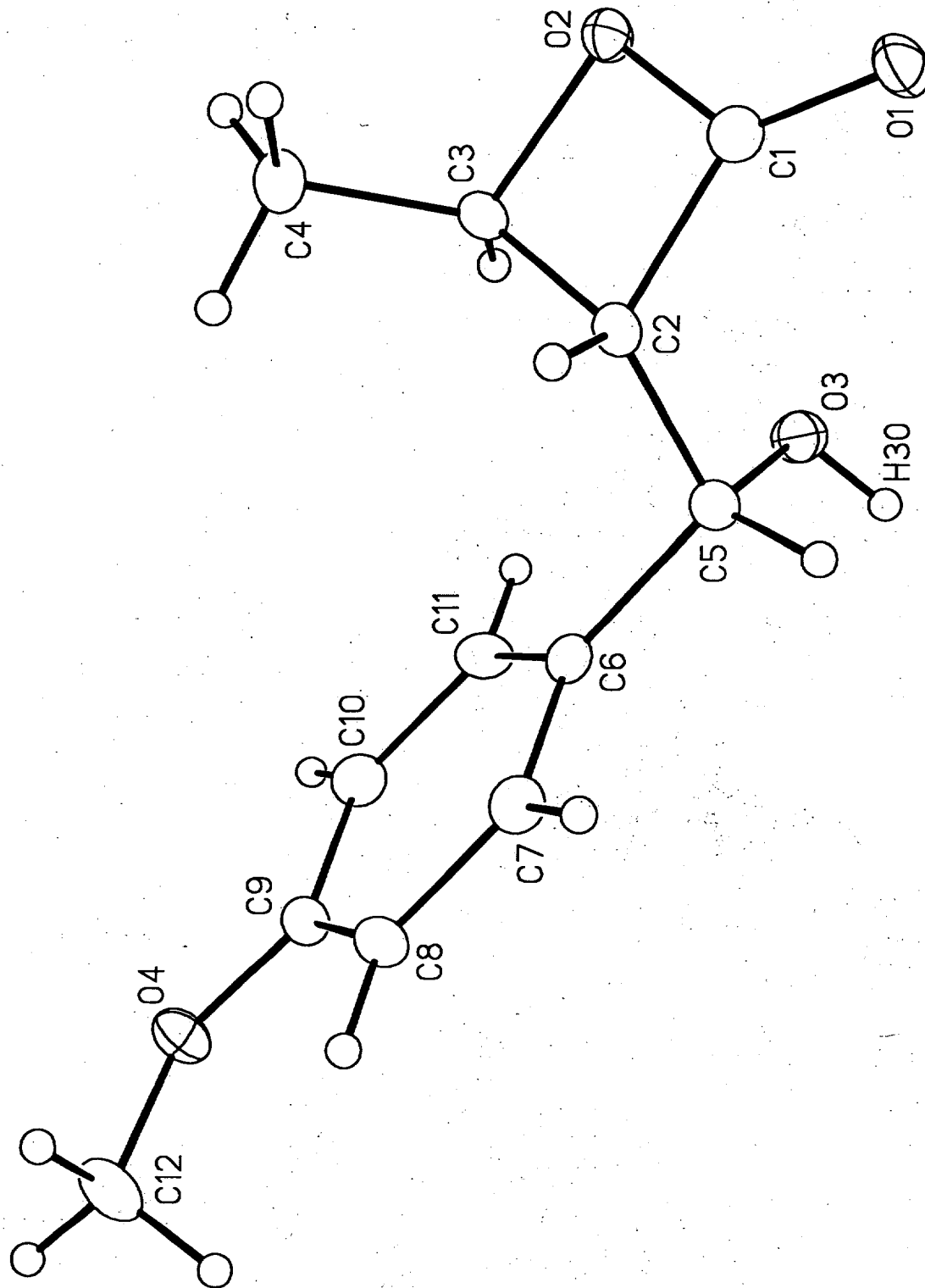
34



S 38



molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters.



List of Tables

- Table 1.** Crystallographic Experimental Details
- Table 2.** Atomic Coordinates and Equivalent Isotropic Displacement Parameters
- Table 3.** Selected Interatomic Distances
- Table 4.** Selected Interatomic Angles
- Table 5.** Torsional Angles
- Table 6.** Anisotropic Displacement Parameters
- Table 7.** Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms
- Table 8.** Observed and Calculated Structure Factor Amplitudes (supervisor's copy only)