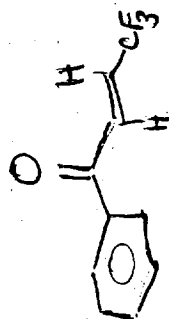


S41

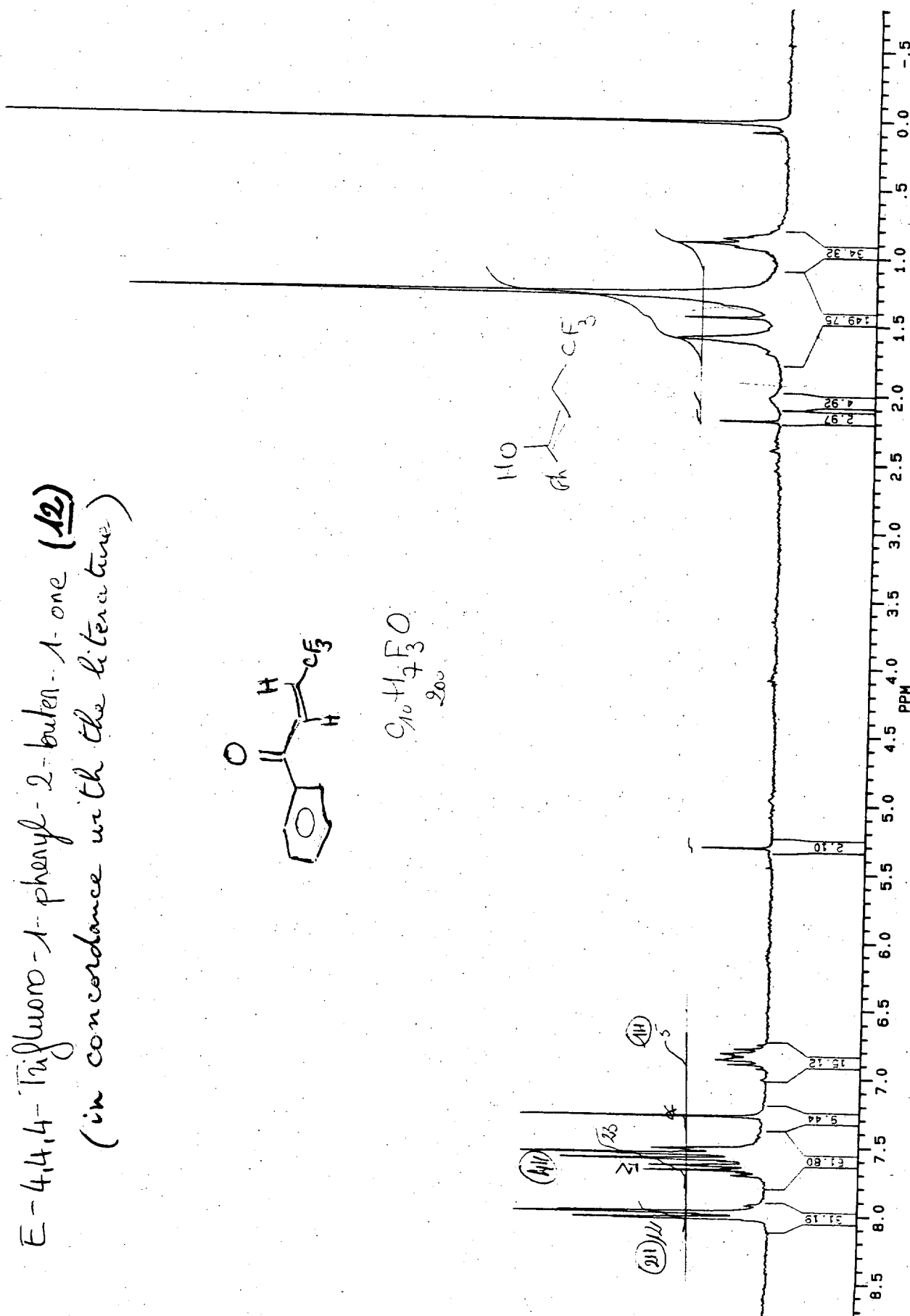
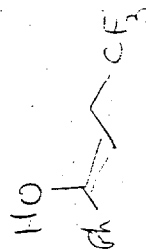
¹H NMR

SLV1150F1/1H/CDCL3

E-4,4,4-Trifluoro-1-phenyl-2-buten-1-one (12)
(in concordance with the literature)



C₁₀H₇FO
200

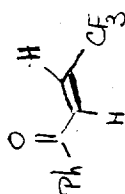


BRUKER

FE030F.115
AU PROG:
X00-AU
DATE 3-2-97
TIME 20:19
SF 200.132
SY 200.0
O1 3449.899
SI 32768
TD 32768
SM 4032.258
HZ/PT 246
PW 0.0
HD 0.0
AQ 4.063
RG 80
NS 16
TE 297
FW 5100
O2 2228.997
DP 63L P0
LB 300
GB 0.0
CX 35.00
CY 20.00
F1 9.203F
F2 807F
HZ/CM 57.238
PPM/CM 286
SR 2337.48

SLV1150F1/19F COUPLE

19F NMR



12

$J_{HF} = 7.7 \text{ Hz}$

449.2645
449.2645
449.2645

449.2645

-66

-64

-62

PPM

~~BRUKER~~

VII150F1F.MAO
DATE 4-2-97
TIME 16:08

SF 188.31
SY 188.0
O1 9759.03
SI 65536
TD 65536
SW 125000.00
HZ/PT 3.81

PW 3.0
RD 1.00
AQ 20
RG 120
NS 297
TE

FW 250000
O2 4582.8
DP 30L P0

LB 3.0
GB 0.00
CX 35.01
CY 20.01
F1 -11486.01
F2 -12443.51
HZ/CM 27.31
PPM/CM 1.1
SR 22629.81

543

$m = 158 \text{ mg}$

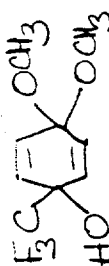
$= 0.24 n_A + 1.1 n_B$

$n_A + n_B + n_C =$

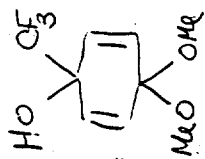
$^1\text{H NMR}$

SL VI 64 F2 H1/CDCL3

1-Trifluoromethyl-1-hydroxy-4,4-dimethoxy-2,5-cyclohexadiene (9f)



9f (A)



11-0.27

11-0.27 67% (72%)

BRUKER

SL64F2H.ME1
DATE 16-10-11
TIME 9:08

SF 200.13
SY 200.0
O1 4000.000

SI 32788
TD 32788
SW 4032.21

HZ/PT 2.2

PW 3.5
RD 1.00

AQ 4.00

RG 10
NS 16

TE 297

FW 5100
O2 2930.40

DP 151.00

LB 30

GB 0.0

CX 35.00

CY 0.0

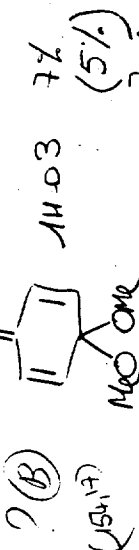
F1 9.15

F2 9.81

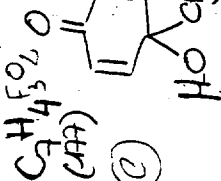
HZ/CM 57.23

PPM/CM 25.25

SH 2338.80

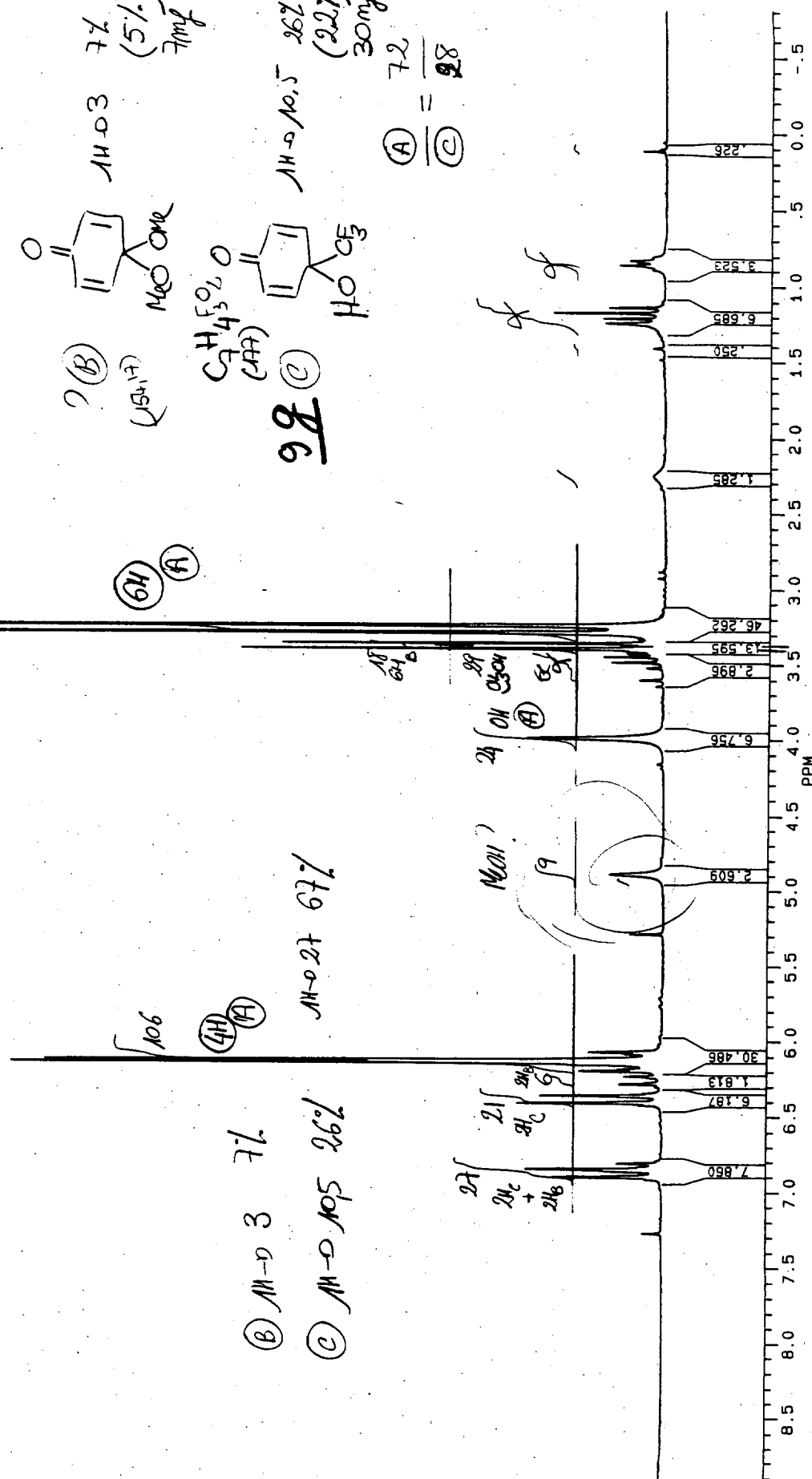


7% (5%)
7mg



7% (22%)
30mg

$$\frac{(A)}{(C)} = \frac{72}{98}$$



(B) 11-0.3 7%

(C) 11-0.105 26%

11-0.27 67%

MeOH

9

24

OH

24

OH

24

OH

24

OH

24

OH

24

OH

24

OH

S44

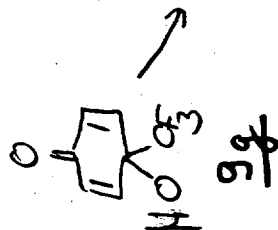
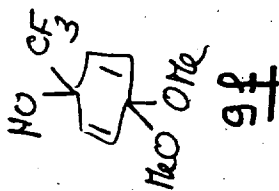


SLV164F2 MA
DATE 15-10-00
TIME 17:44
SF 188.3
SY 188.0
O1 9759.0
SI 65536
TD 65536
SW 125000.0
HZ/PT 3.8
PW 3.0
RD 0.0
AQ 0.2
RG 10
NS 120
TE 297
FW 250000
O2 3227.0
DP 15H CPD
LB 1.0
GB 0.0
CX 35.0
CY 20.0
F1 -57.0
F2 -103.6
HZ/CM 251.0
PPM/CM 1.3
SR 22652.7

SLV164F2 19F DECOUPLE

-81.6572
-80.7845
-79.6510

19 F NMR



-60 -70 -80 -90 -100 PPM

S45



SL64F2C.ME10
DATE 16-10-96
TIME 11:54

SF 50.323
SY 50.0
Q1 8396.387
SI 65536
TD 65536
SW 12500.000
HZ/PT .381

PW 6.0
RD 2.000
AQ 2.621
RG 400
NS 800
TE 297

FW 15700
Q2 3154.531
DP 15H CPD

LB 1.000
GB 0.0
CX 35.00
CY 20.00
F1 209.9931
F2 -5.0101
HZ/CM 309.132
PPM/CM 6.143
SR 3314.39

SL VI-64 F2 C13/CDCL3

15.028
14.063

29.679

50.391
49.874

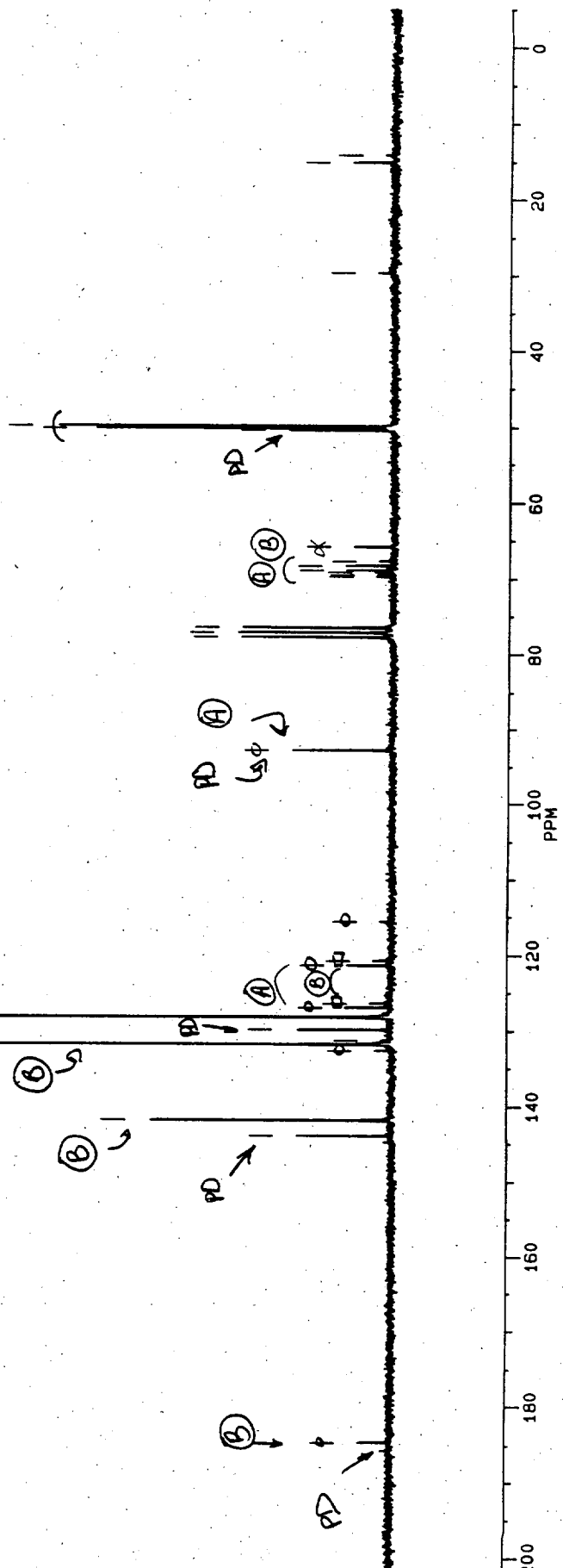
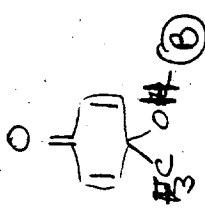
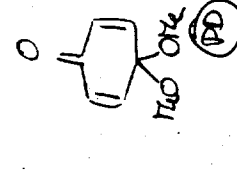
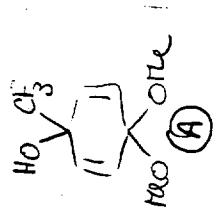
77.205
76.436
75.126
74.406
69.474
68.126
68.091
67.607
65.809

92.874

132.503
131.738
131.487
129.827
128.206
126.943
126.589
121.280
120.698
115.620

143.871
141.804

184.503



546



SL64F20.ME1
AU PROG:
DEPT135.AU
DATE 16-10-
TIME 12:15

SF 50.3
SY 50.0
OI 8396.3
SI 65536
TD 65536
SM 12500.0
HZ/PT 3.3

PW 0.0
RD 0.0
AQ 2.6
RG 400
NS 260
TE 297

FW 15700
O2 3154.5
DP 15H D0

LB 1.01
GB 0.0
CX 35.01
CY 10.01
F1 210.01
F2 -5.01
HZ/CM 309.1
PPM/CM 6.1
SR 3314.3

SL VI 64 F2 DEPT/CDCL3

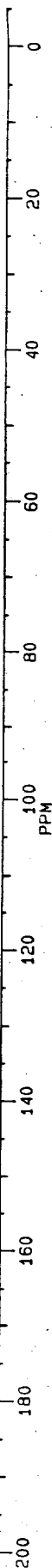
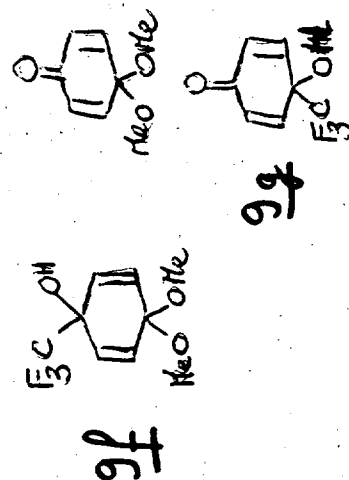
15.032

50.384
50.164
49.879

65.817

131.728
129.928
128.219

141.827
143.882



547


 VI64F2II.ME1
 DATE 16-10-99
 TIME 15:38

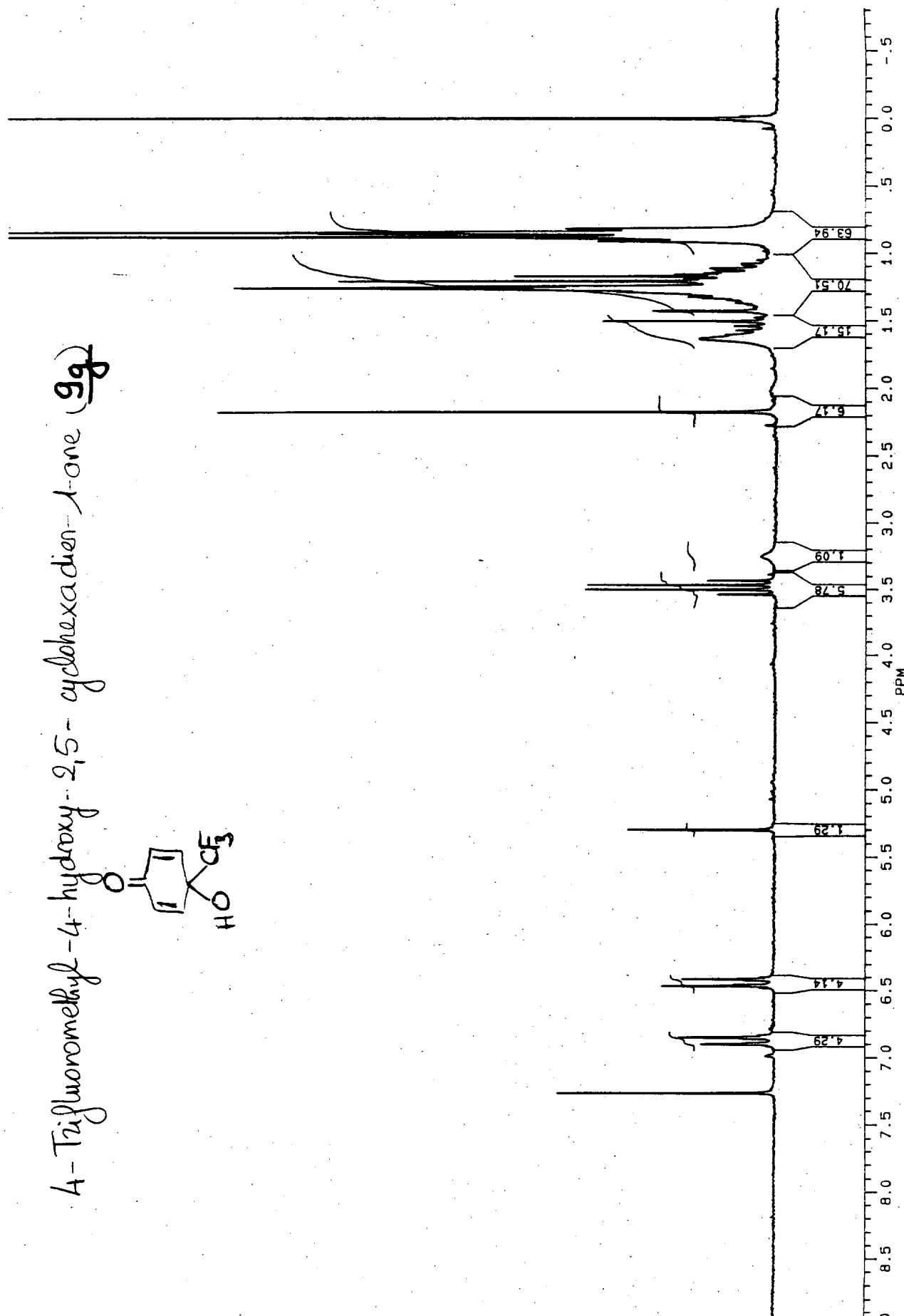
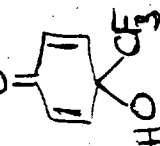
 SF 200.13
 SY 200.0
 O1 4000.06
 SI 32768
 TD 32768
 SW 4032.25
 HZ/PT 24

 PW 3.5
 RD 1.00
 AQ 4.00
 RG 40
 NS 16
 TE 297

 FW 5100
 O2 2930.40
 DP 15L P0

 LB 30
 GB 0.0
 CX 35.00
 CY 20.00
 F1 9.20
 F2 7.80
 HZ/CM 57.20
 PPM/CM 2339.20
 SR 2339.20
¹H NMR

SLVI64F2II/1H/CDCL3

4-Trifluoromethyl-4-hydroxy-2,5-cyclohexadien-1-one (9g)

548



SL64F2II.ME:
DATE 16-10-01
TIME 15:32

SF 188.31
SY 188.0
Q1 9759.0

SI 65536
TD 65536
SW 125000.01

HZ/PT 3.8
PW 3.00
AQ 1.01

RG 10
NS 120
TE 297

FW 250000
Q2 4582.8
DP 30L P0

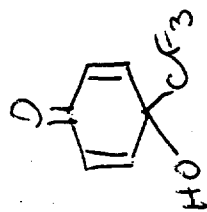
LB 1.00
GB 0.00
CX 35.00

CY 20.00
F1 11.00
F2 -95.22

HZ/CM 571.8
PPM/CM 3.00
SR 22652.7

SLV164F2II

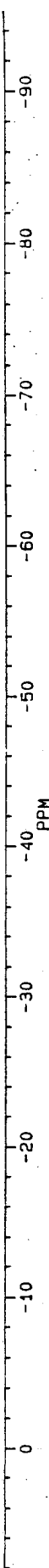
¹³F NMR



92

-0.087

-79.6723



S49

~~BRUKER~~

SL64F2CS.JE
AU PROG:
X02.AU
DATE 17-10-
TIME 0:04

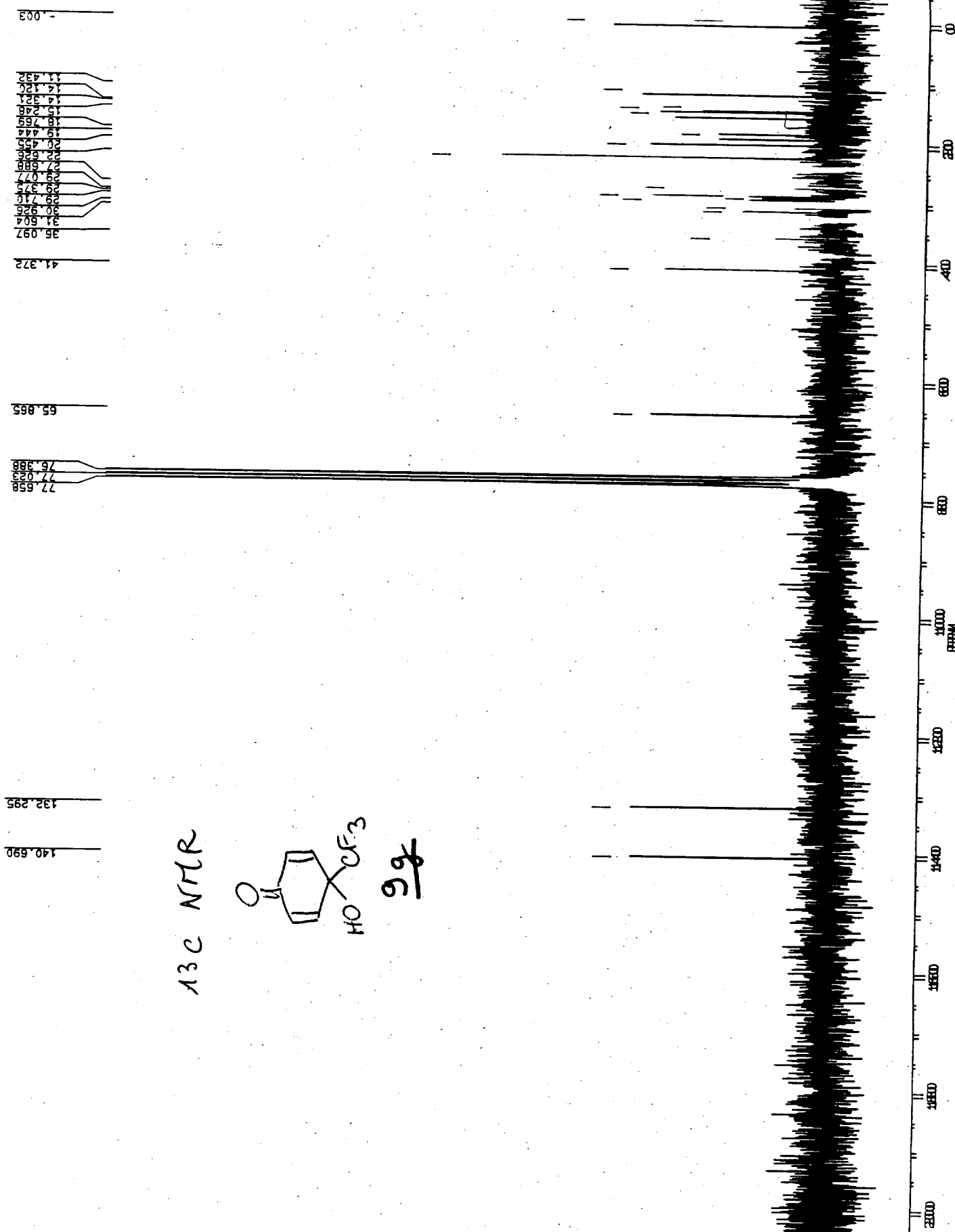
SF 50.30
SY 50.0
O1 8396.31
SI 65536
TD 65536
SM 12500.01
HZ/PT .31

PW 0.0
RD 0.0
AQ 2.61
RG 640
NS 2000
TE 297

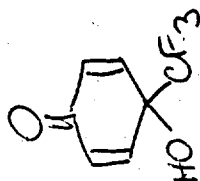
FW 15700
O2 3154.51
DP 15H D0

LB 1.00
GB 0.0
CX 35.00
CY 0.0
F1 209.95
F2 -5.00
HZ/CM 309.13
PPM/CM 6.14
SR 3315.21

SLV164F2II/13C/CDCL3



¹³C NMR



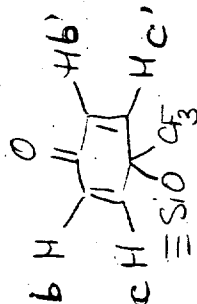
92

¹H NMR

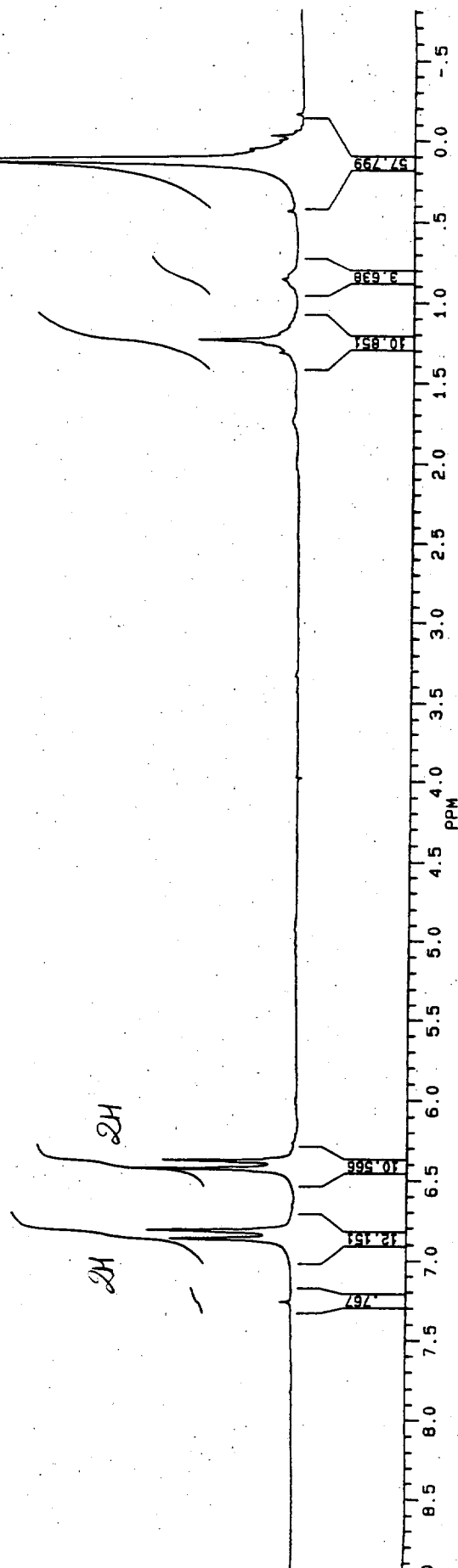
S50

SLV68F2/1H/CDCL3

4-Trifluoromethyl-4-trimethylsilyloxy-2,5-cyclohexadien-1-one (10g)



2H



BRUKER

SLV68F2H.04
DATE 28-6-9
TIME 19:58

SF 200.1
SY 200.0
O1 4000.0
SI 32768
TD 32768
SW 4032.2
HZ/PT 2

PW 3.5
RD 1.0
AQ 4.0
RG 10
NS 16
TE 297

FW 5100
O2 2930.4
DP 15L P0

LB 3
GB 0.0
CX 35.0
CY 0.0
F1 9.2
F2 9.8
HZ/CM 57.2
PPM/CM 2340.7
SR 2340.7

S51



SLV68F2F.0E
DATE 28-6-9
TIME 19:54

SF 188.3
SY 188.0
O1 9759.0
SI 65536
TD 65536
SW 125000.0
HZ/PT 3.8

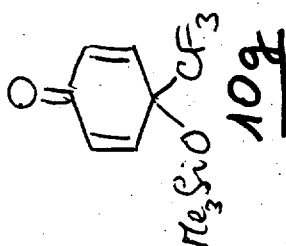
PW 3.0
RG 1.0
AQ 1.2
RG 10
NS 120
TE 297

FW 250000
O2 4582.8
DP 30L P0

LB 3.1
GB 0.0
CX 35.0
CY 20.0
F1 -74.2
F2 -82.8
HZ/CM 46.1
PPM/CM 2.2
SA 22626.0

SLV68F2/19F COUPLE

19F NMR



-81.2115
-80.1584
-80.0656

-76.4127

-82

-80

PPM

-78

-76

552

~~SECRET~~

SL68F2C.LU07
AU PROG:
X02.AU
DATE 29-6-96
TIME 15:16

SF 50.32
SY 50.0
O1 8396.3E
SI 65536
TD 65536
SW 12500.0E
HZ/PT .3E

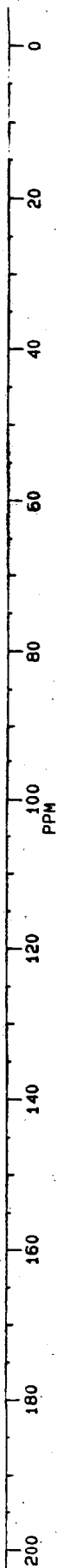
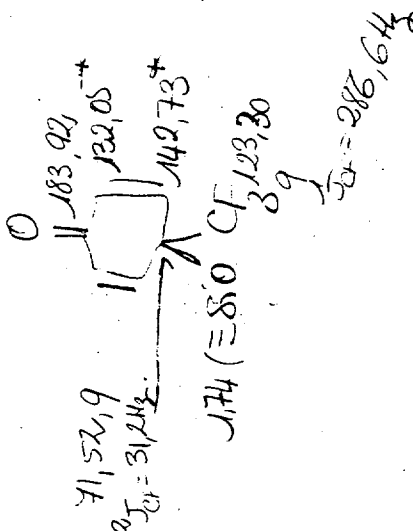
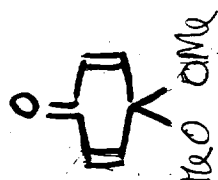
PW 0.0
RD 0.0
AQ 2.6E
RG 640
NS 1800
TE 297

FW 15700
O2 3154.5E
DP 15H.D0

LB 1.0E
GB 0.0
CX 35.0E
CY 20.0E
F1 210.0E
F2 -4.9E
HZ/CM 309.1E
PPM/CM 6.1E
SR 3313.6E

¹³C NMR

SLV68F2/13C/CDCL3

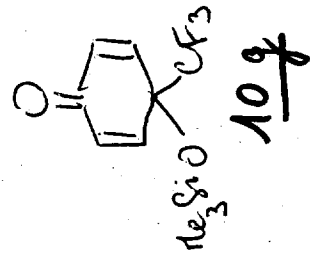
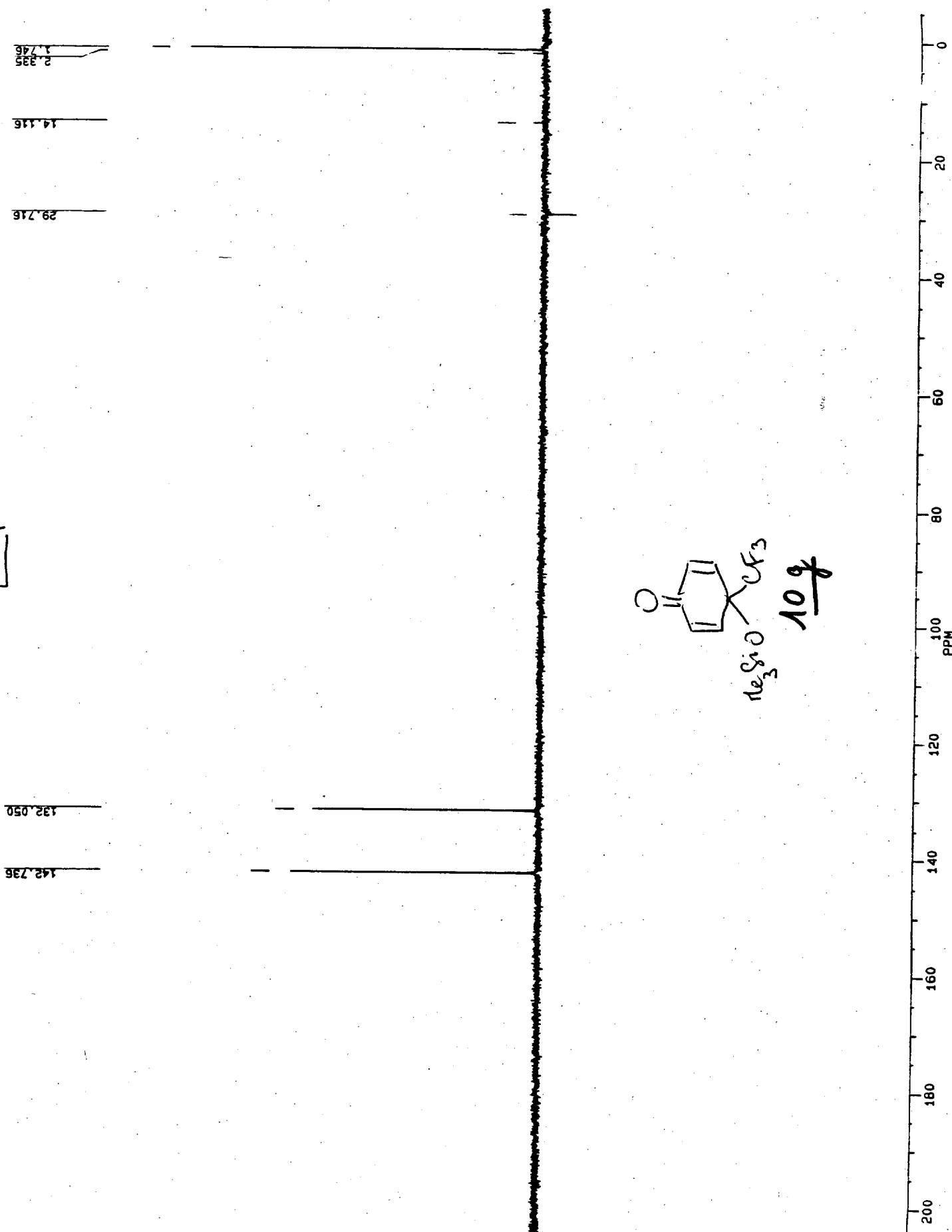


553



SLV68F2D.LU0
 AU PROG:
 X09 AU
 DATE 29-6-9
 TIME 16:20
 SF 50.3
 SY 50.0
 O1 8396.3
 SI 65536
 TD 65536
 SM 12500.0
 HZ/PT 3.3
 PW 0.0
 RD 0.0
 AG 2.6
 RG 400
 NS 800
 TE 297
 FW 15700
 O2 3154.5
 OP 15H 00
 LB 1.0
 GB 0.0
 CX 35.0
 CY 10.0
 F1 209.870
 F2 -5.1
 HZ/CM 309.1
 PPM/CM 6.1
 SR 3313.6

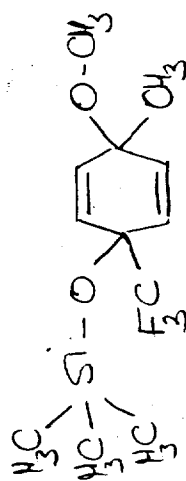
SLV68F2/DEPT



¹H NMR

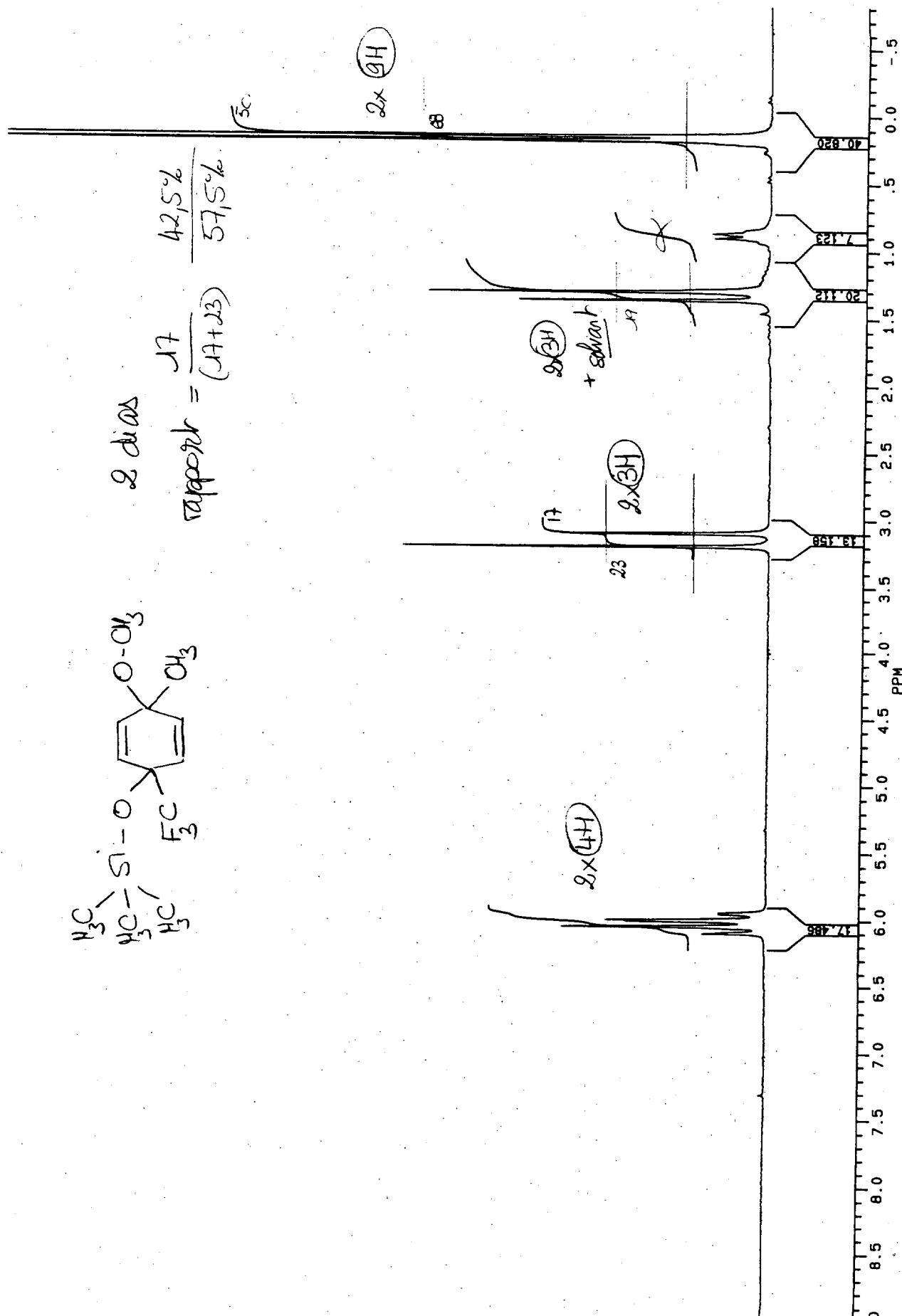
Mixture of 10h-cis and 10h-trans

SLVIF2/1H/CDCL3



2 dias

$$\text{rapport} = \frac{17}{(17+23)} = \frac{42,5\%}{57,5\%}$$



~~BAUJE~~

SLVIF2/1H/CDCL3
DATE 30-9-99
TIME 18:35

SF 200.1
SY 200.0
O1 4000.0
SI 32768
TD 32768
SW 4032.2
HZ/PT 12

PW 3.5
RG 1.0
AQ 4.0
RG 4
NS 16
TE 297

FW 5100
O2 2930.4
DP 15L PO

LB 3
GB 0.0
CX 35.0
CY 20.0
F1 9.2
F2 8
HZ/CH 57.2
PPM/CM 2
SR 2331.6

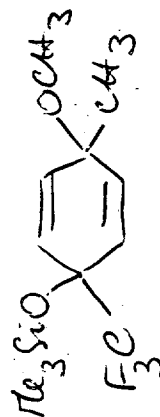
SL VI-F2 FLUOR COUPLE

19F NMR

SSS

-81.1097

-81.7788



10h (cis + trans)



SLF2FC.MA10
DATE 1-10-9
TIME 8:33

SF 188.3
SY 188.0
O1 9759.0
SI 65536
TD 65536
SM 125000.0
HZ/PT 3.8

PW 3.0
RG 1.0
AQ 1.2
RG 16
NS 120
TE 297

FW 250000
O2 4582.8
DP 30L P0

LB 1.0
GB 0.0
CX 35.0
CY 20.0
F1 -15064.2
F2 -15762.3
HZ/CM 19.9
PPM/CM 1.1
SR 22622.1

44%

56%

-82

PPM

S 56

~~SECRET~~

SLF2C.MA10
AU PROG:
X02.AU
DATE 30-9-98
TIME 21:48
SF 50.32
SY 50.0
O1 8396.3f
SI 65536
TD 65536
SW 12500.0f
HZ/PT .3f
PW 0.0
RD 0.0
AQ 2.6f
RG 640
NS 2000
TE 297
FW 15700
O2 3154.5f
DP 15H D0
LB 1.0f
GB 0.0
CX 35.0f
CY 0.0
F1 3668.6f
F2 3318.84
HZ/CM 9.95
PPM/CM .15
SR 3311.37

SLVIF2/13C/CDCL3

69.4282

70.0311

70.3577

70.6380

70.7623

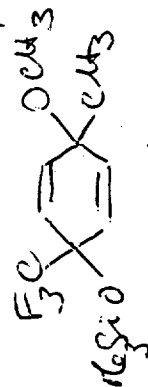
70.9720

71.2105

71.5861

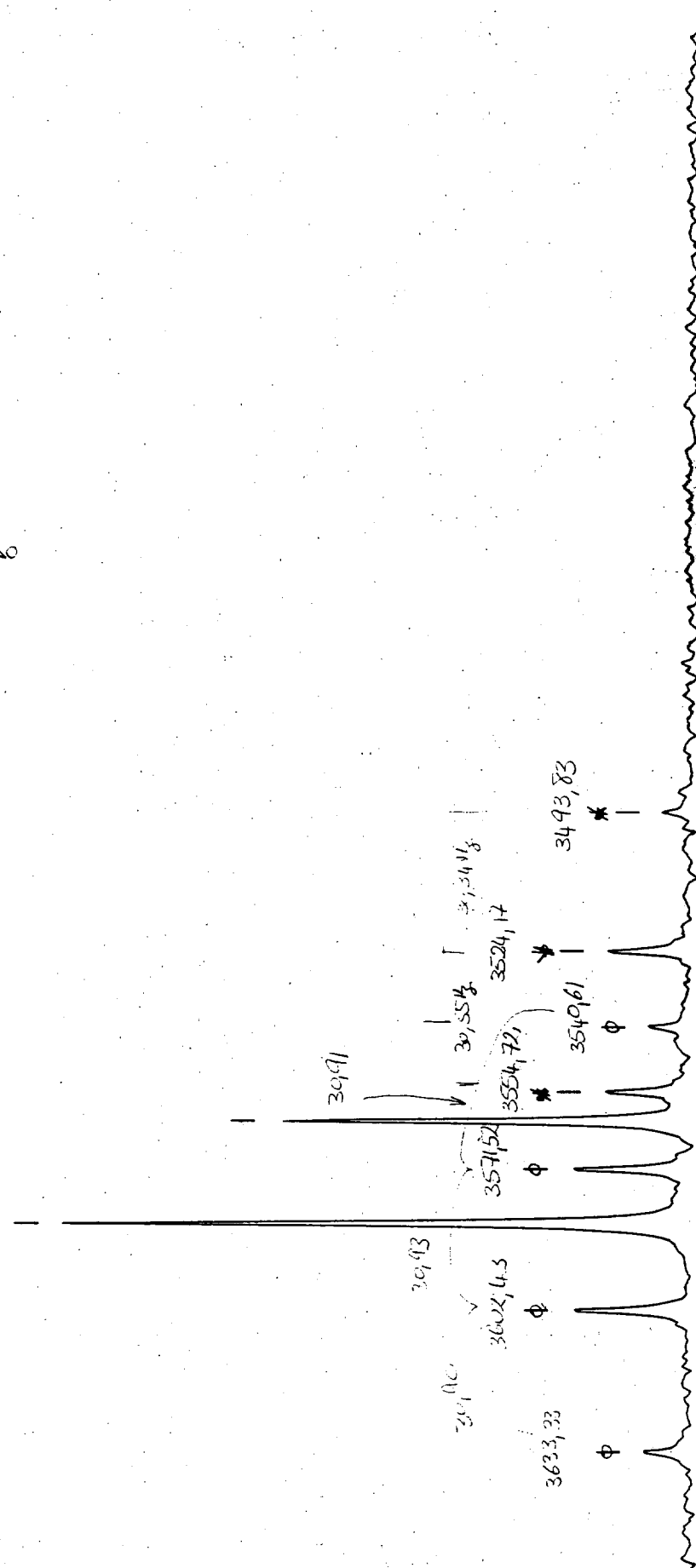
72.2092

¹³C NMR



10h cis + trans

$\delta = 2$
b



557

BRUKER

SLF2C, MA10
AU PROG:
X02.AU
DATE 30-9-96
TIME 21: 48

SF 50.32
SY 50.0
O1 8396.38
SI 65536
TD 65536
SM 12500.00
HZ/PT .38

PW 0.0
RD 0.0
AQ 2.62
RG 640
NS 2000
TE 297

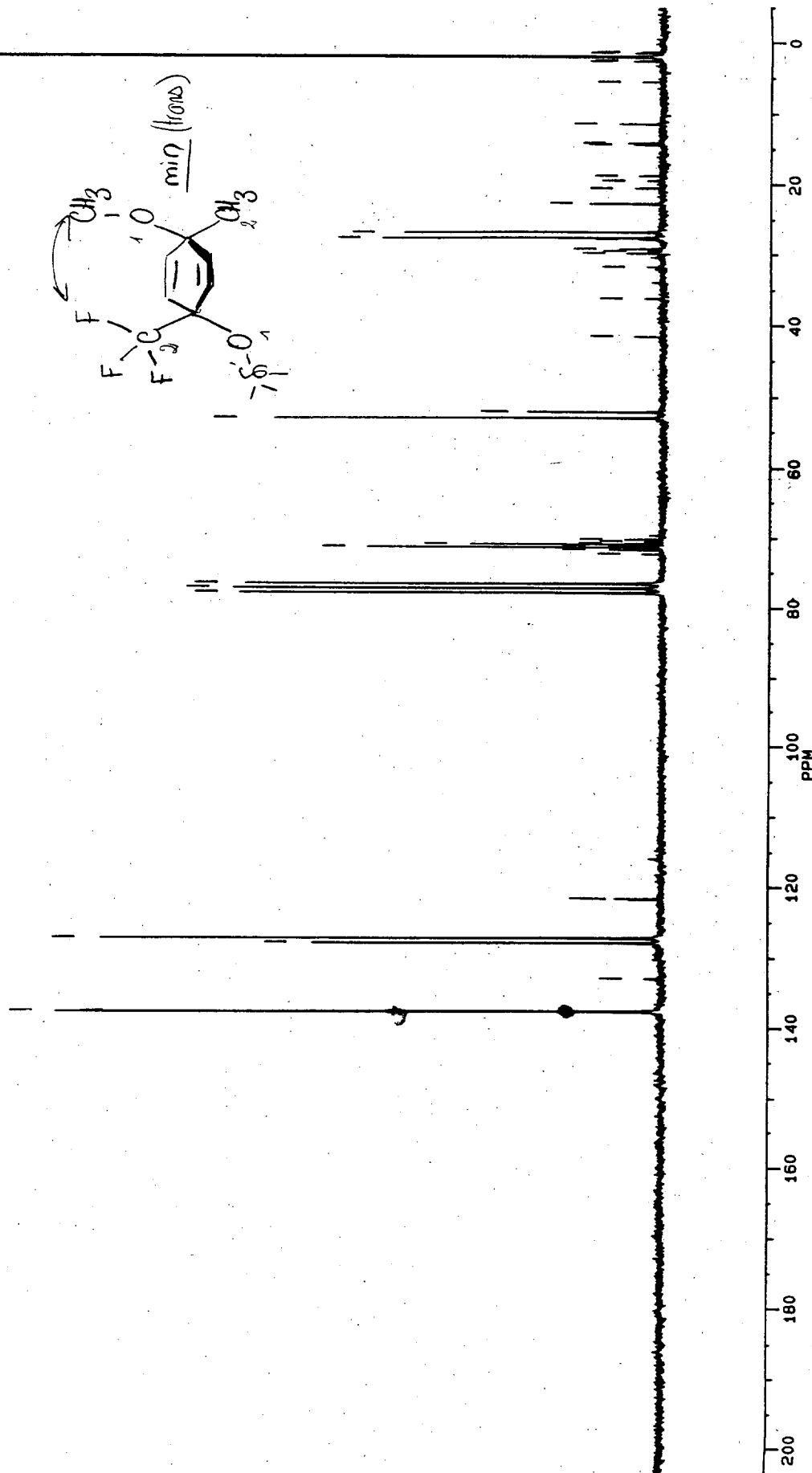
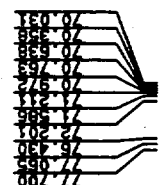
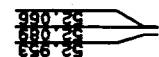
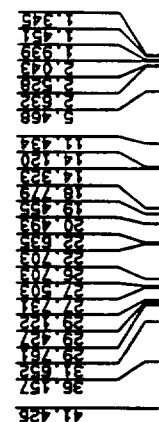
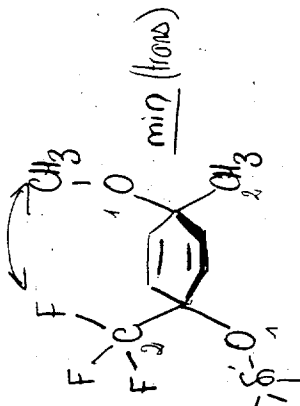
FW 15700
O2 3154.53
DP 15H D0

LB 1.00
GB 0.0
CX 35.00
CY 0.0
F1 210.00
F2 -5.00
HZ/CM 309.13
PPM/CM 6.14
SR 3311.34

SLV1F2/13C/CDCL3

¹³C NMR

10h-trans



55



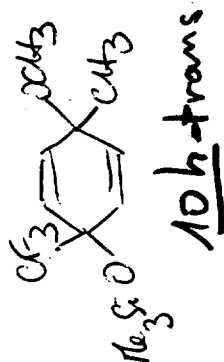
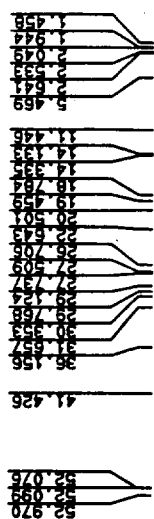
SLF2D.MA10
AU PROG:
X09.AU
DATE 30-9-98
TIME 23:09

SF 50.32
SY 50.0
O1 8396.38
SI 65536
TD 65536
SW 12500.00
HZ/PT 38

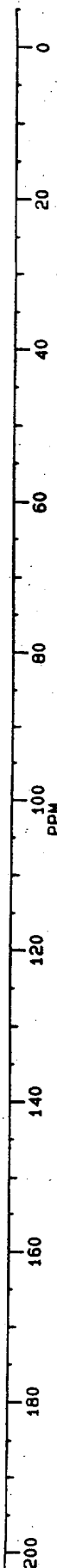
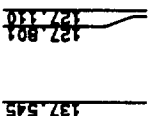
PW 0.0
RD 0.0
AQ 2.62
RG 640
NS 1000
TE 297

FW 15700
O2 3154.53
DP 15H 00

LB 1.00
GB 0.0
CX 35.00
CY 10.00
F1 210.00
F2 -5.00
HZ/CM 309.13
PPM/CM 6.14
SR 3311.34



SLVIF2/DEPT

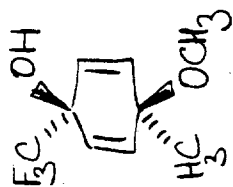


559

¹H NMR

SL VI-50 Fg H1/CDCL3

1-Trifluoromethyl-1-hydroxy-4-methoxy-2,5-cyclohexadiene (9h-cis)



~~BRUKER~~

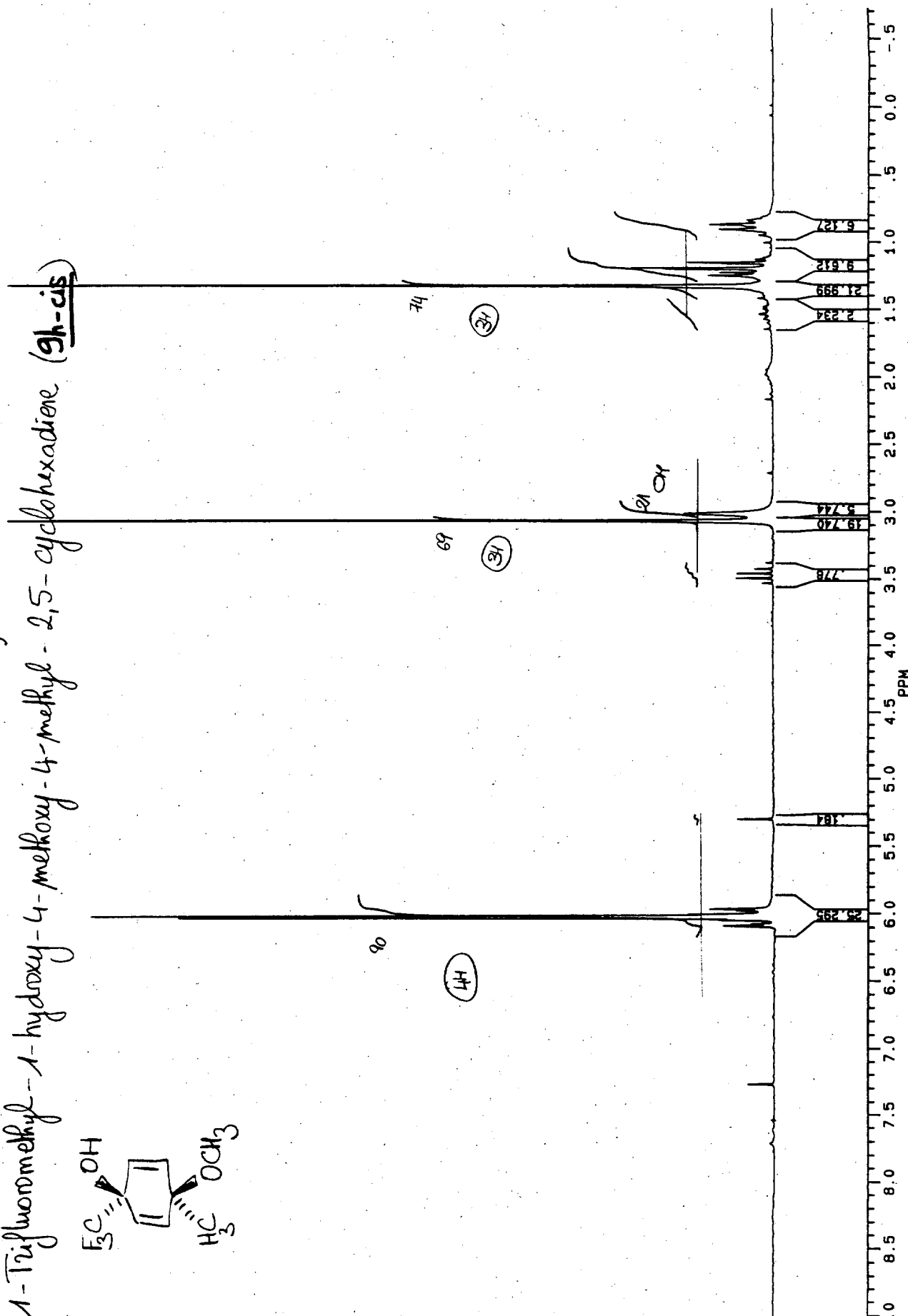
SL50F3H JE1C
DATE 3-10-96
TIME 9:05

SF 200.13
SY 200.0
O1 4000.00
SI 32768
TD 32768
SW 4032.24
HZ/PT 24

PW 3.5
RD 1.00
AQ 4.00
RG 10
NS 16
TE 297

FW 5100
O2 2930.40
DP 15L P0

LB 30
GB 0.0
CX 35.00
CY 0.0
F1 9.20
F2 7.20
HZ/CM 57.20
PPM/CM 2.20
SR 2338.80

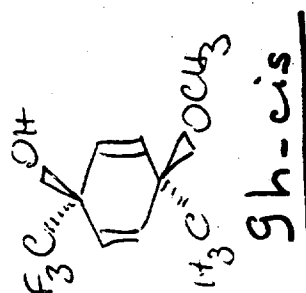


S60

SLV150F3/19F DECOUPLE

19F NMR

-80.6294



~~BIOMER~~

SLV150F3 ME
DATE 2-10-99
TIME 17:06

SF 188.3
SY 188.0
O1 9759.0
SI 65536
TD 65536
SM 125000.0
HZ/PT 3.8
PW 3.0
RD 0.0
AQ 0.2
RG 10
NS 120
TE 297

FW 250000
O2 3227.0
DP 15H CPD
LB 1.0
GB 0.0
CX 35.0
CY 20.0
F1 -61.9
F2 -98.0
HZ/CM 194.5
PPM/CM 1.0
SR 22622.1

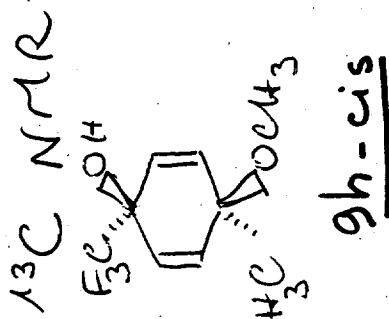
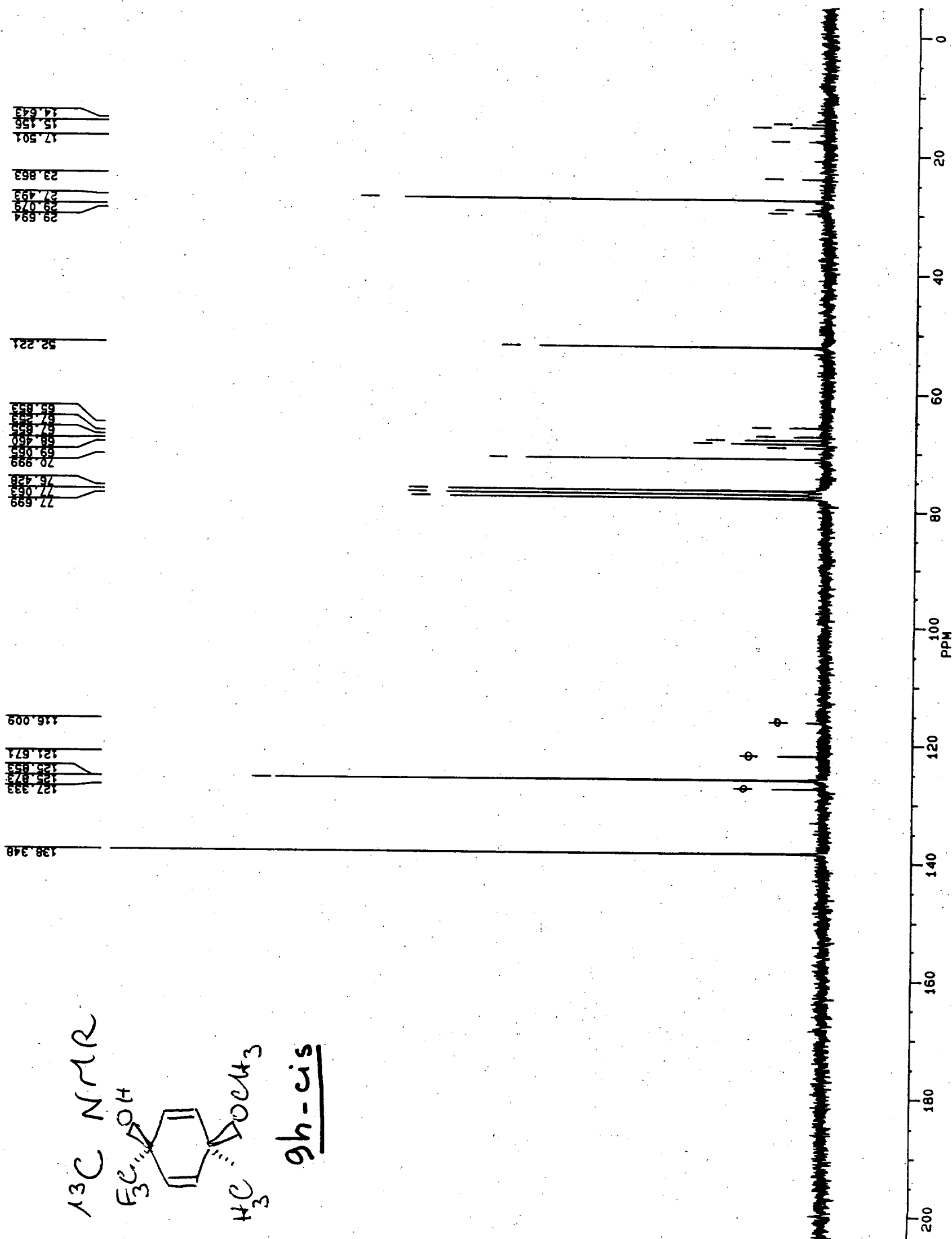


S61



SL50F3C.VE1
AU PROG:
X02.AU
DATE 4-10-91
TIME 0:59
SF 50.31
SY 50.0
O1 8396.31
SI 65536
TD 65536
SM 12500.01
HZ/PT .31
PW 0.0
RD 0.0
AQ 2.61
RG 400
NS 1000
TE 297
FM 15700
O2 3154.51
DP 15H D0
LB 1.00
GB 0.0
CX 35.00
CY 0.0
F1 210.00
F2 -5.00
HZ/CM 308.13
PPM/CM 6.14
SR 3313.25

SLV150F3/13C/CDCL3



S62

~~BRUKER~~

SL50F3D VE10
AU PROG:
X09-AU
DATE 3-10-96
TIME 23:39

SF 50.32
SY 50.0
O1 8396.38
SI 65536
TD 65536
SW 12500.00
HZ/PT 38

PW 0.0
RD 0.0
AQ 2.62
RG 640
NS 400
TE 297

FW 15700
O2 3154.53
DP 15H D0

LB 1.00
GB 0.0
CX 35.00
CY 10.00
F1 210.00
F2 -5.00
HZ/CM 309.13
PPM/CM 6.14
SR 3313.25

15.163
17.505

23.867
27.491
29.729

40.921

52.229

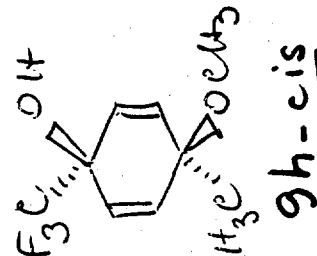
65.858

125.882

138.337

175.572

SLV150F3/DEPT



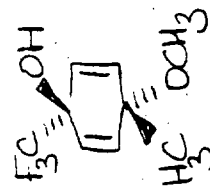
0 20 40 60 80 100 120 140 160 180 200 PPM

S63

¹H NMR

SL VI-50 F4 H1/CDCL3

1-(1-hydroxy-4-methoxy-2,5-dicyclohexadiene-2-yl)-2,2,2-trifluoroethyl



BRUKER

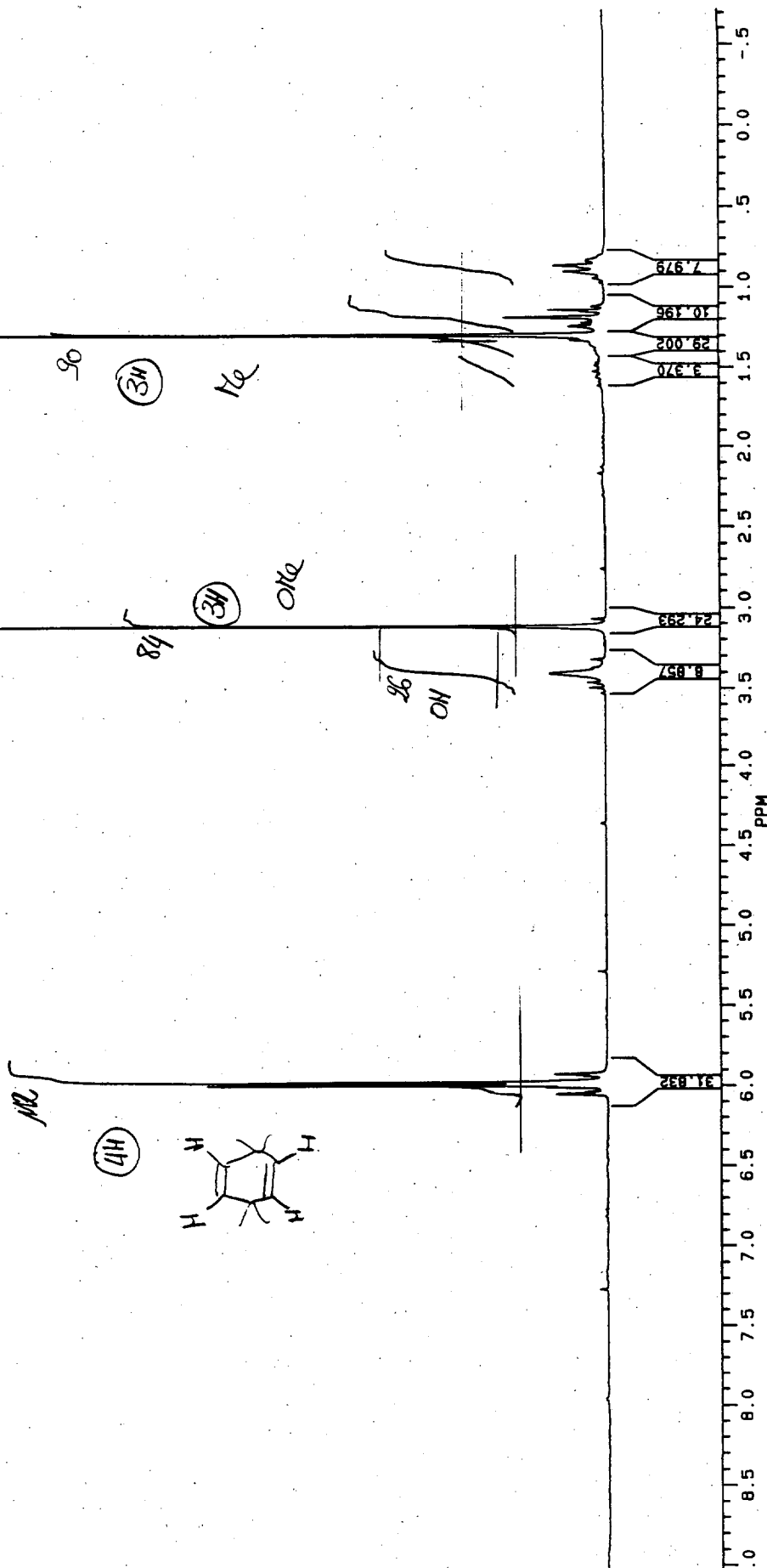
SL50F4H JE1C
DATE 3-10-96
TIME 9:15

SF 200.13
SY 200.0
O1 4000.00
SI 32768
TD 32768
SW 4032.25
HZ/PT 21

PW 3.5
RD 1.00
AQ 4.00
RG 8
NS 16
TE 297

FM 5100
D2 2930.40
DP 15L P0

LB 30
GB 0.00
CX 35.00
CY 0.00
F1 9.20
F2 7.70
HZ/CM 57.20
PPM/CM 2338.81
SA 2338.81



SG

~~BAUER~~

SL50F4FD JE10
DATE 3-10-96
TIME 9:17

SF 188.313
SY 188.0
O1 9759.030
SI 65536
TD 65536
SM 125000.000
HZ/PT 3.815

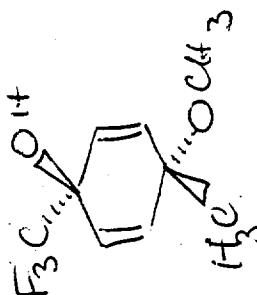
PW 3.0
RD 0.0
AQ 0.262
RG 10
NS 120
TE 297

FW 250000
O2 3227.000
DP 15H CPD

LB 1.000
GB 0.0
CX 35.00
CY 20.00
F1 -15129.08H
F2 -15827.17H
HZ/CM 19.945
PPM/CM 106
SR 22622.18

SL VI-50 F4 FLUOR DECOUPLE

19 F NMR



9h-trans

-80.6469

-81.2926

-82

PPM

-84

S65

~~BRUKER~~

SL50F4C JE11
AU PROG:
X02.AU
DATE 2-10-98
TIME 23:52

SF 50.32
SY 50.0
SI 8396.31
SI 65536
TD 65536
SW 12500.00
HZ/PT 31

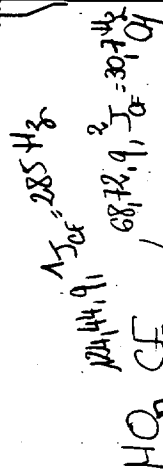
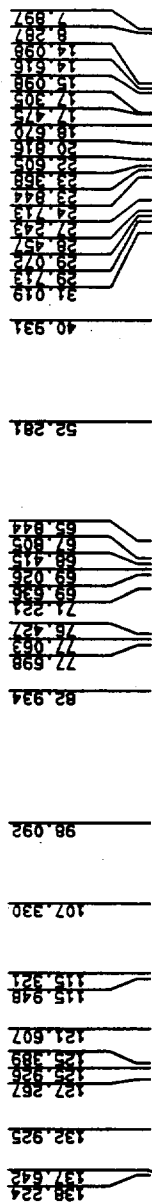
PW 0.0
RD 0.0
AQ 2.61
RG 640
NS 1000
TE 297

FW 15700
O2 3154.51
DP 15H D0

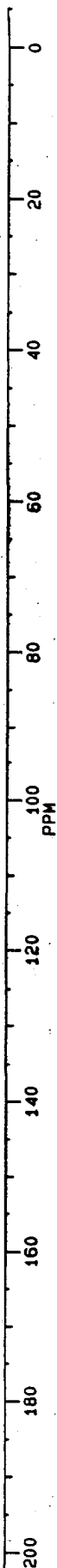
LB 1.00
GB 0.00
CX 35.00
CY 20.00
F1 210.00
F2 -5.00
HZ/CM 309.13
PPM/CM 6.14
SR 3313.28

¹³C NMR

SLV150F4/13C/CDCL3



gh-trans



56



SL50F4D JE1
AU PROG:
X09 AU
DATE 2-10-9
TIME 22:32
SF 50.3
SY 50.0
O1 8396.3
SI 65536
TD 65536
SW 12500.0
HZ/PT 3.3
PW 0.0
RD 0.0
AQ 2.6
RG 640
NS 400
TE 297
FW 15700
O2 3154.5
DP 15H D0
LB 1.0
GB 0.0
CX 35.0
CY 10.0
F1 209.9
F2 -5.0
HZ/CM 309.1
PPM/CM 6.1
SR 3313.2

14.626
15.106
17.482
20.820
23.848
27.247
29.722

40.927

52.291

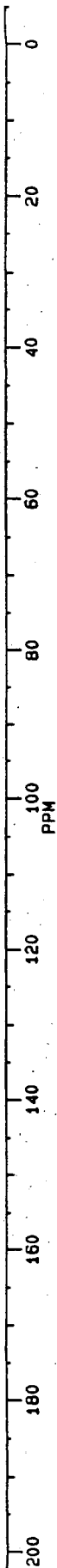
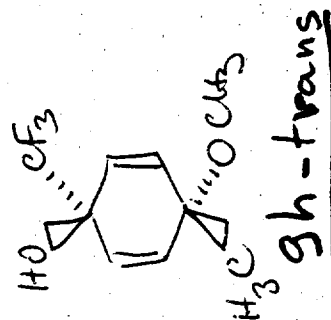
65.855

71.230

125.383

137.633

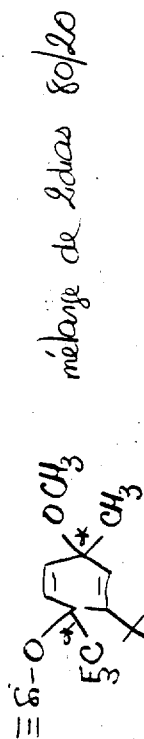
SLV50F4/DEPT



¹H NMR

SL VIII 40 F2 H1/CDCL3

Mixture of 10i-cis and 10i-trans



irradiation sur $\delta = 0.07$ ppm dans H_2O
 $\delta = 2.97$ ppm

S67

BRUKER

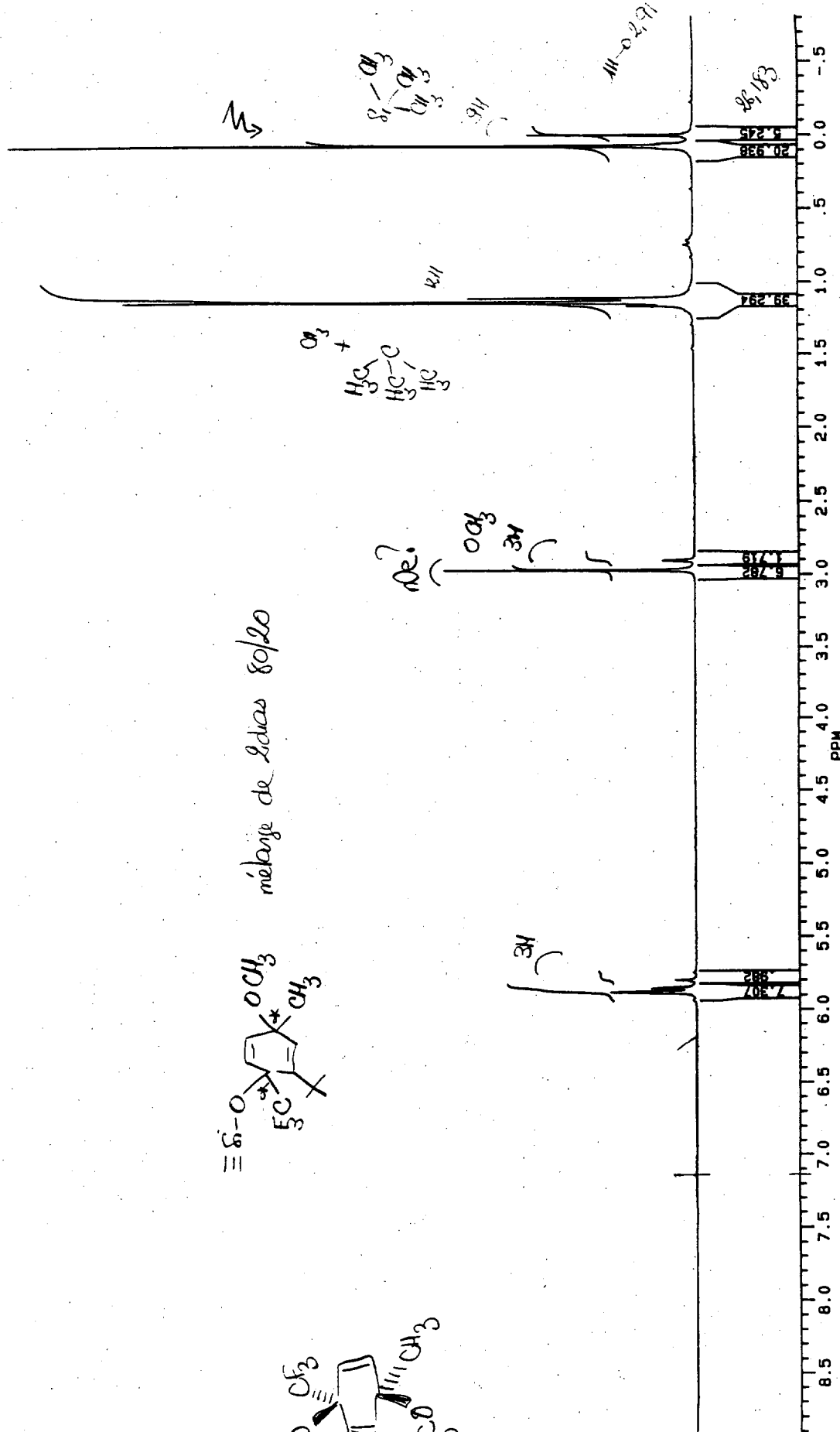
SL40F2H.ME04
DATE 30-4-97
TIME 10:56

SF 200.13
 SY 200.0
 O1 4000.00
 SI 32768
 TD 32768
 SW 4032.25
 HZ/PT 24

PW 3.5
 RD 1.00
 AQ 4.06
 RG 4
 NS 8
 TE 297

FW 5100
 D2 2930.40
 DP 15L P0

LB 30
 GB 0.0
 CX 35.00
 CY 0.0
 F1 9.20
 F2 9.80
 HZ/CM 57.23
 PPM/CM 28
 SR 2365.83



568

BRUKER

DATE 30-4-99
TIME 10:49

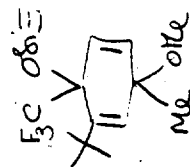
CF 100.13
CY 100.13
C1 100.13
C2 100.13
C3 100.13
C4 100.13
C5 100.13
C6 100.13
C7 100.13
C8 100.13
C9 100.13
C10 100.13
C11 100.13
C12 100.13
C13 100.13
C14 100.13
C15 100.13
C16 100.13
C17 100.13
C18 100.13
C19 100.13
C20 100.13
C21 100.13
C22 100.13
C23 100.13
C24 100.13
C25 100.13
C26 100.13
C27 100.13
C28 100.13
C29 100.13
C30 100.13
C31 100.13
C32 100.13
C33 100.13
C34 100.13
C35 100.13
C36 100.13
C37 100.13
C38 100.13
C39 100.13
C40 100.13
C41 100.13
C42 100.13
C43 100.13
C44 100.13
C45 100.13
C46 100.13
C47 100.13
C48 100.13
C49 100.13
C50 100.13
C51 100.13
C52 100.13
C53 100.13
C54 100.13
C55 100.13
C56 100.13
C57 100.13
C58 100.13
C59 100.13
C60 100.13
C61 100.13
C62 100.13
C63 100.13
C64 100.13
C65 100.13
C66 100.13
C67 100.13
C68 100.13
C69 100.13
C70 100.13
C71 100.13
C72 100.13
C73 100.13
C74 100.13
C75 100.13
C76 100.13
C77 100.13
C78 100.13
C79 100.13
C80 100.13
C81 100.13
C82 100.13
C83 100.13
C84 100.13
C85 100.13
C86 100.13
C87 100.13
C88 100.13
C89 100.13
C90 100.13
C91 100.13
C92 100.13
C93 100.13
C94 100.13
C95 100.13
C96 100.13
C97 100.13
C98 100.13
C99 100.13
C100 100.13

SL VIII 40 F2 FLUOR DECOUPLE

¹⁹F NMR

-75.7595
-75.6635

-75.0349



10 i (cis + trans)

-73.5124

60b

PPM

-74

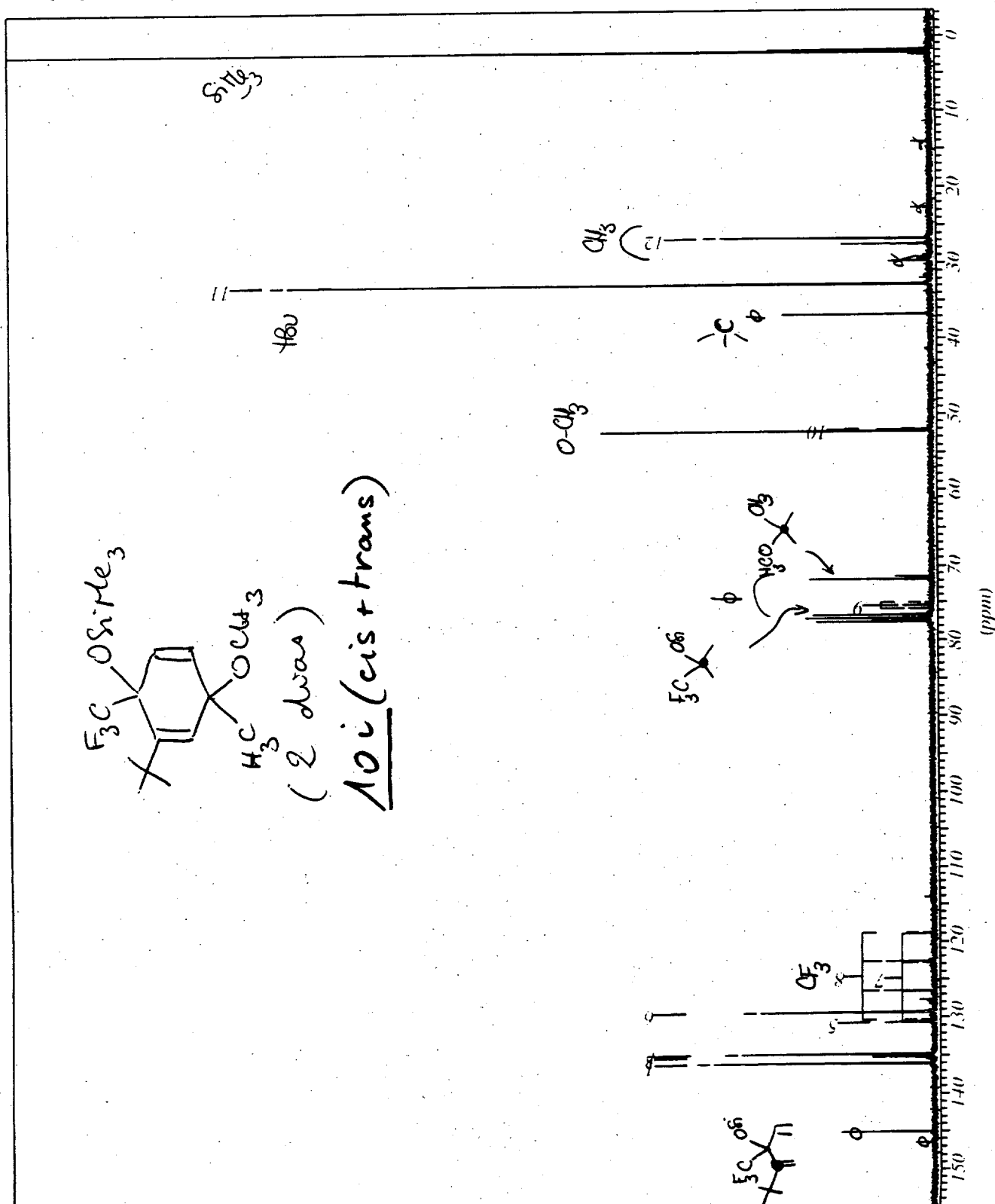
-76

S69

¹³C NMR

SL VIII-40 F2

SL VIII-40 F2



*** Current Data Parameters ***

NAME : AMSI8402

EXPNO : 2

PROCNO : 1

*** Acquisition Parameters ***

AQ_mod : qseq

AUNM : X02.AU

BF1 : 75.4665950 MHz

DS : 2

NS : 2400

O1 : 6466.00 Hz

O2 : 5225.00 Hz

RO : 20 Hz

SF01 : 75.4730610 MHz

SW : 245.3805 ppm

SW_h : 18518.519 Hz

TD : 65536

TE : 297 K

*** Processing Parameters ***

LB : 0.00 Hz

TI : SLVIII40F213C

*** Aspect 3000 Parameters ***

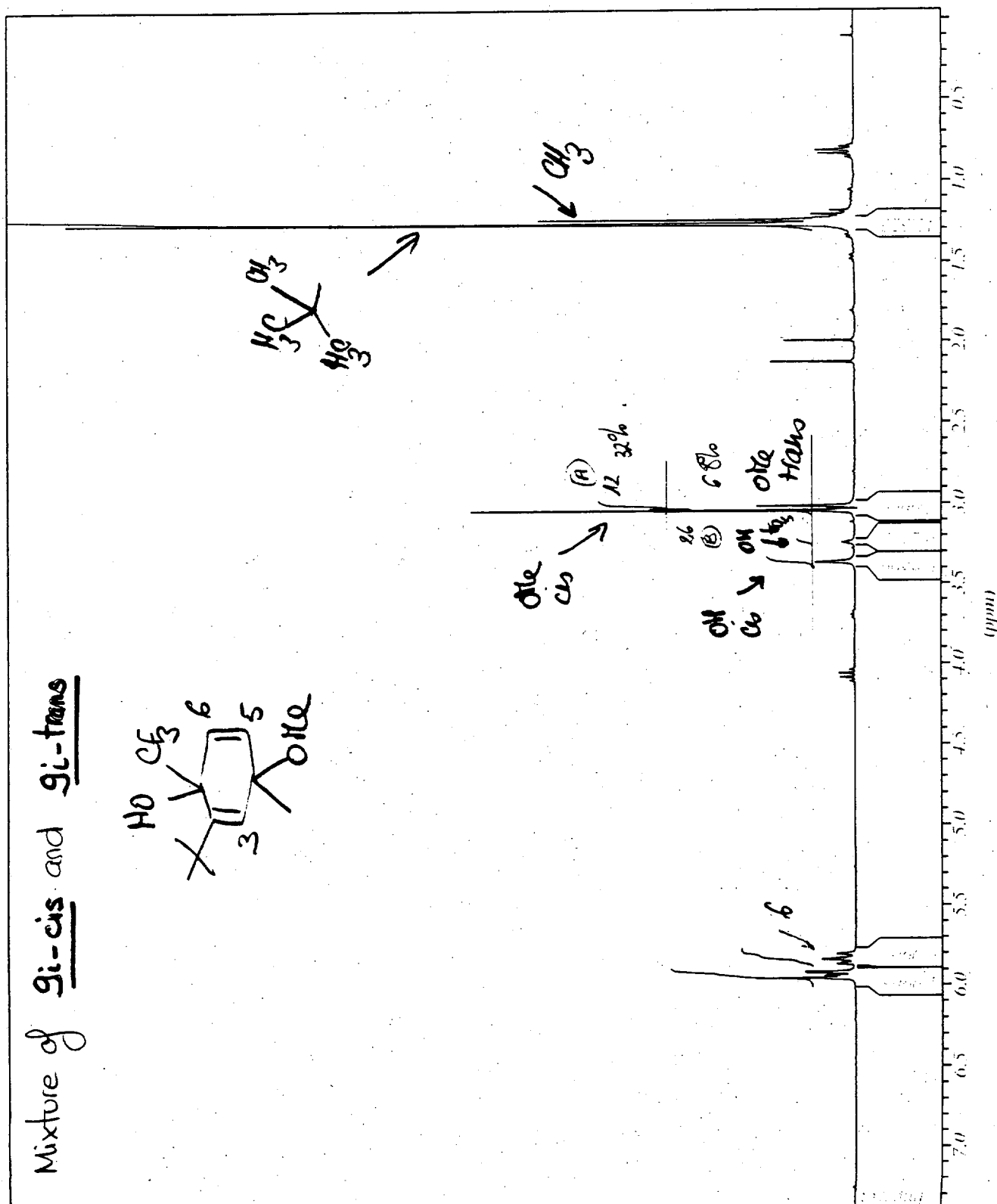
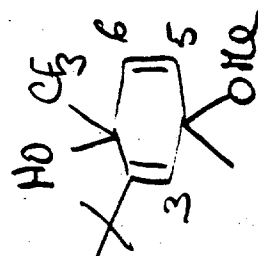
P100 : 0

S70

¹⁴NMR

JA VIII 4612

Mixture of gi-cis and gi-trans



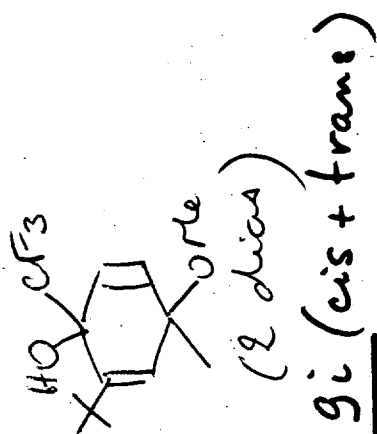
Current Data Parameters	
NAME	AMST462
EXPNO	1
PROCNO	1
Acquisition Parameters	
AQ_mod	qseq
AUNM	ZGILRGA
BF1	300.1300000 MHz
DS	2
NS	32
Q1	6048.00 Hz
Q2	3200.00 Hz
RO	20 Hz
SF01	300.1300480 MHz
SW	20.0711 ppm
SW_H	6024.096 Hz
TD	32768
TE	297 K
Processing Parameters	
GB	0.00 Hz
HI	1H, CDCL3
Aspect 3000 Parameters	
PH00	0

S 77

¹⁹F NMR

SLV11146F2/19F COUPLE

-72.5256
-75.2171



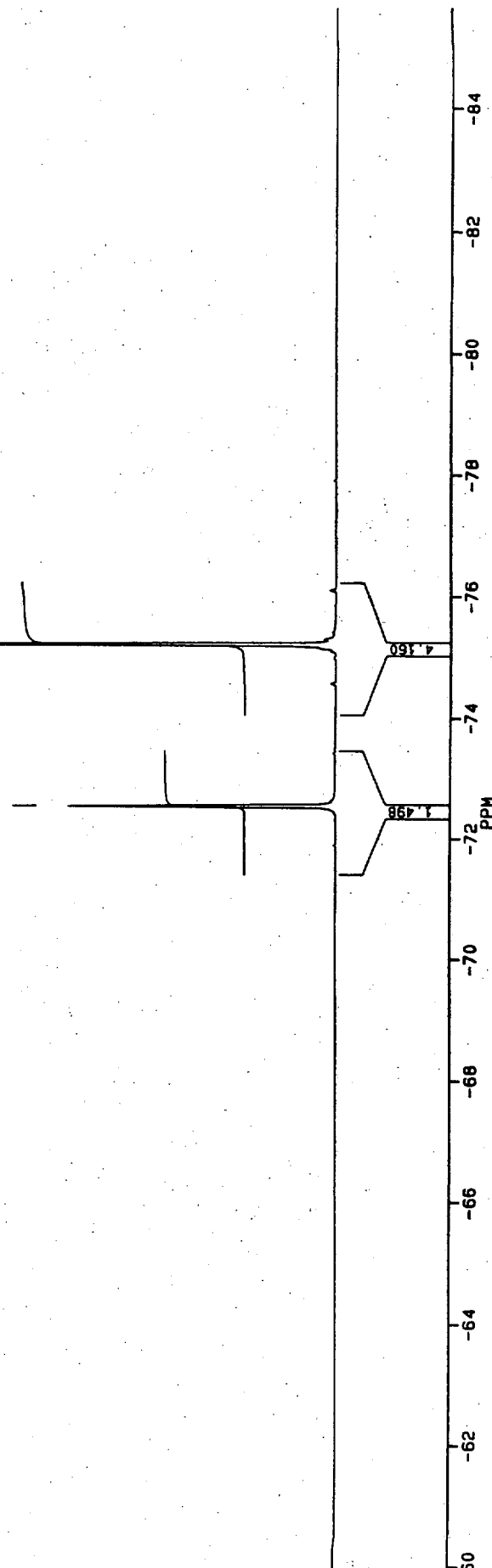
SL46F2-VE05
DATE 2-5-97
TIME 17: 41

SF 188.3
SY 188.0
Q1 9759.0
SI 65536
TD 65536
SM 125000.0
HZ/PT 3.8

PW 3.0
RD 1.0
AQ 1.2
RG 10
NS 120
TE 297

FW 250000
Q2 4582.8
DP 30L PD

LB 3.0
GB 0.0
CX 35.0
CY 20.0
F1 -11157.9
F2 -16120.9
HZ/CW 141.7
PPM/CW .7
SR 22595.4



S72

¹³C NMR

SL VIII-16 F2

*** Current Data Parameters

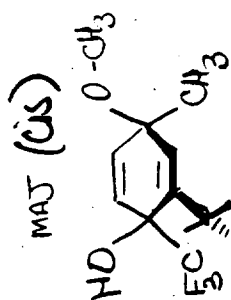
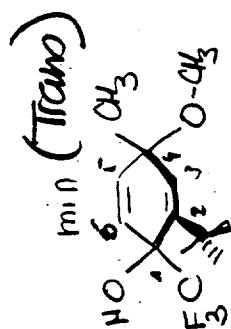
NAME : AMIS18462
 EXPNO : 2
 PROCNO : 1

*** Acquisition Parameters ***

AQ_mod : qseq
 AUNM : X02.AU
 BF1 : 75.1696001 MHz
 DS : 2
 NS : 2400
 OL : 6466.00 Hz
 O2 : 5225.00 Hz
 RO : 20 Hz
 SFO1 : 75.4760661 MHz
 SW : 245.3805 ppm
 SW_Hz : 18518.519 Hz
 TD : 65536
 TE : 297 K

*** Processing Parameters ***

LB : 0.00 Hz
 TI : SLVH146F213C
 *** Aspect 3000 Parameters ***
 PHOC : 0

cis-transcis-cis

K19

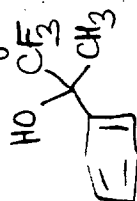
CH₃CO₂SCH₃CO₂S
transC₄aCH₃CO₂S
transC₄CO₂S
transC₄CO₂S
transC₃CO₂S
transC₃CO₂SC₄CO₂SC₄CO₂SC₄CO₂SC₄CO₂SC₄CO₂SC₄CO₂SC₄CO₂S

(ppm)

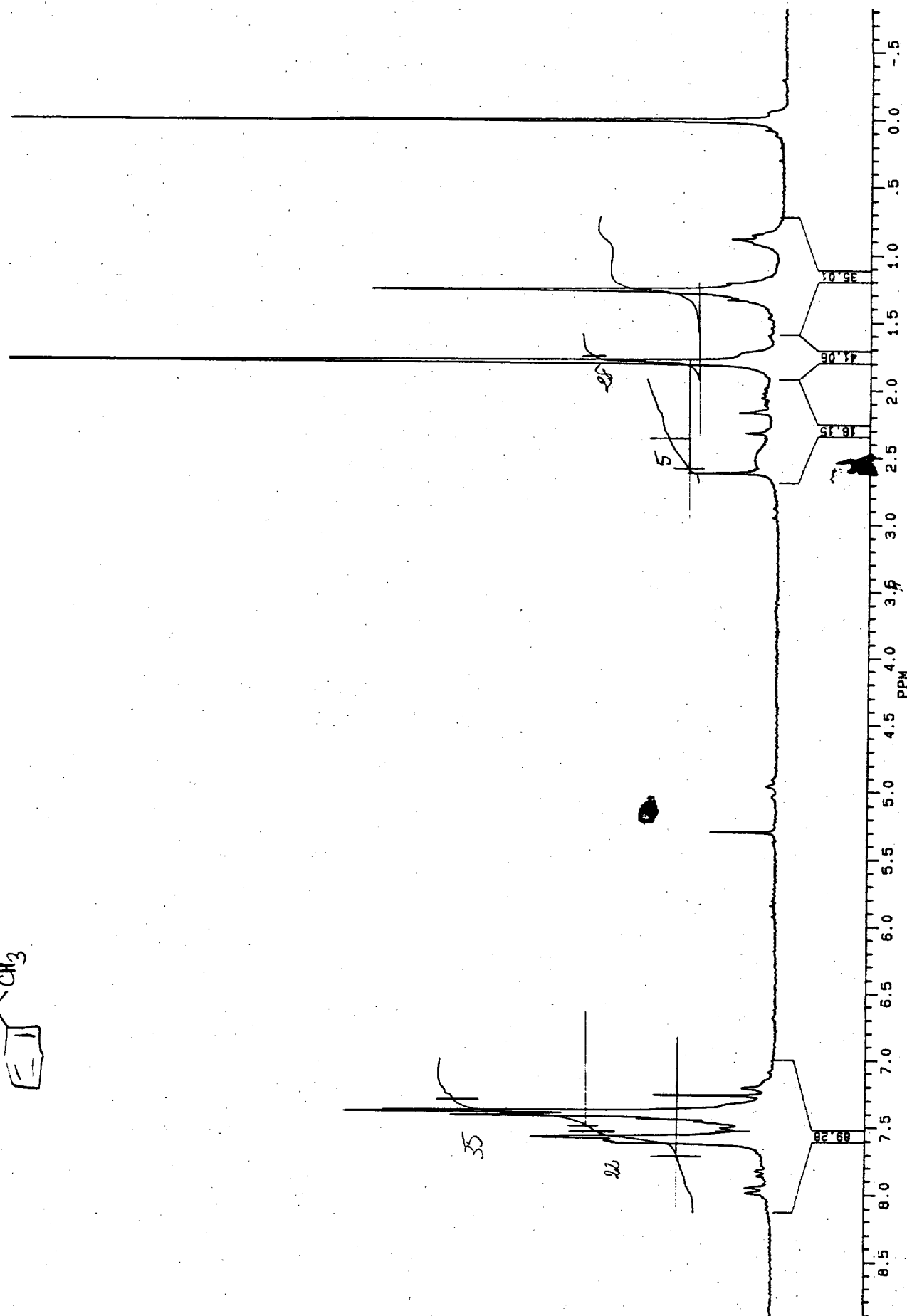
573

¹H NMR

1-Methyl-1-phenyl-2,2,2-trifluoroethanol



SLV40F3/1H/CDCL3



~~BAUKEF~~

SLV40F3.LU0
DATE 17-6-9
TIME 17:23

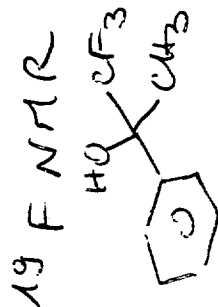
SF 200.1
SY 200.0
O1 4000.0
SI 32768
TD 32768
SM 4032.2
HZ/PT .2

PW 3.5
RD 1.0
AQ 4.0
RG 40
NS 16
TE 297

FW 5100
O2 2930.4
DP 15L P0

LB 3
GB 0.0
CX 35.0
CY 20.0
F1 9.1
F2 1.8
HZ/CM 57.2
PPM/CM .2
SR 2340.2

S74



SLV-40 F3 FLUOR COUPLE

-81.4542

~~BAUR~~

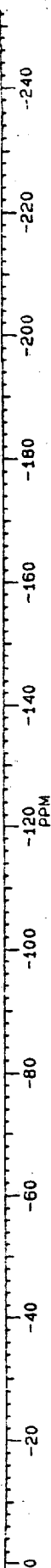
SL40F3FC.MAC
DATE 18-6-98
TIME 9:24

SF 188.31
SY 188.0
31 9759.05
37 65536
TD 65536
SW 125000.00
HZ/PT 3.81

PW 5.0
RD 1.00
AQ 20
RG 10
NS 120
TE 297

FW 250000
02 4582.83
01 391.00

LR 1.01
GB 0.0
CX 35.01
CY 29.01
F1 7.31
F2 252.51
FZ/CM 1.5981
PPM/CM 7.41
SR 22637.41



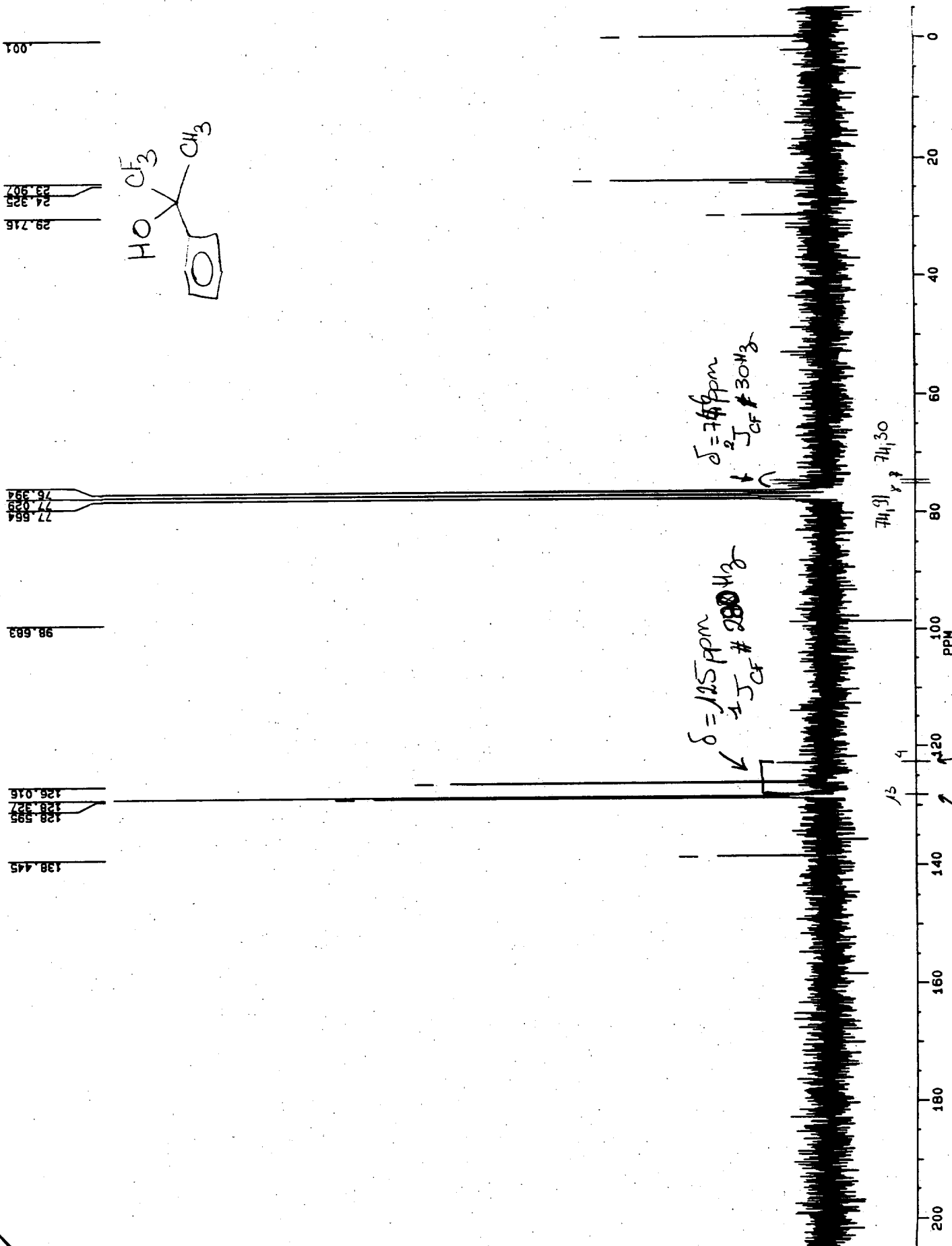
S75



SL40F3C.ME0F
AU PROG:
X02.AU
DATE 18-6-98
TIME 23:52
SF 50.31
SY 50.0
OI 8396.3KHz
SI 65536
TD 65536
SM 12500.01
HZ/PT .31
PW 0.0
RD 0.0
AQ 2.61
RG 640
NS 1200
TE 297
FM 15700
O2 3154.5
DP 15H D0
LB 1.01
GB 0.0
CX 35.01
CY 0.0
F1 209.91
F2 5.01
HZ/CM 309.1
PPM/CM 6.1
SR 3315.5

¹³C NMR

SLV40F3/13C/CDCL3



S76

~~BRUKER~~

SL40F3D.ME0E
AU PROG:
X09.AU
DATE 18-6-96
TIME 22:16

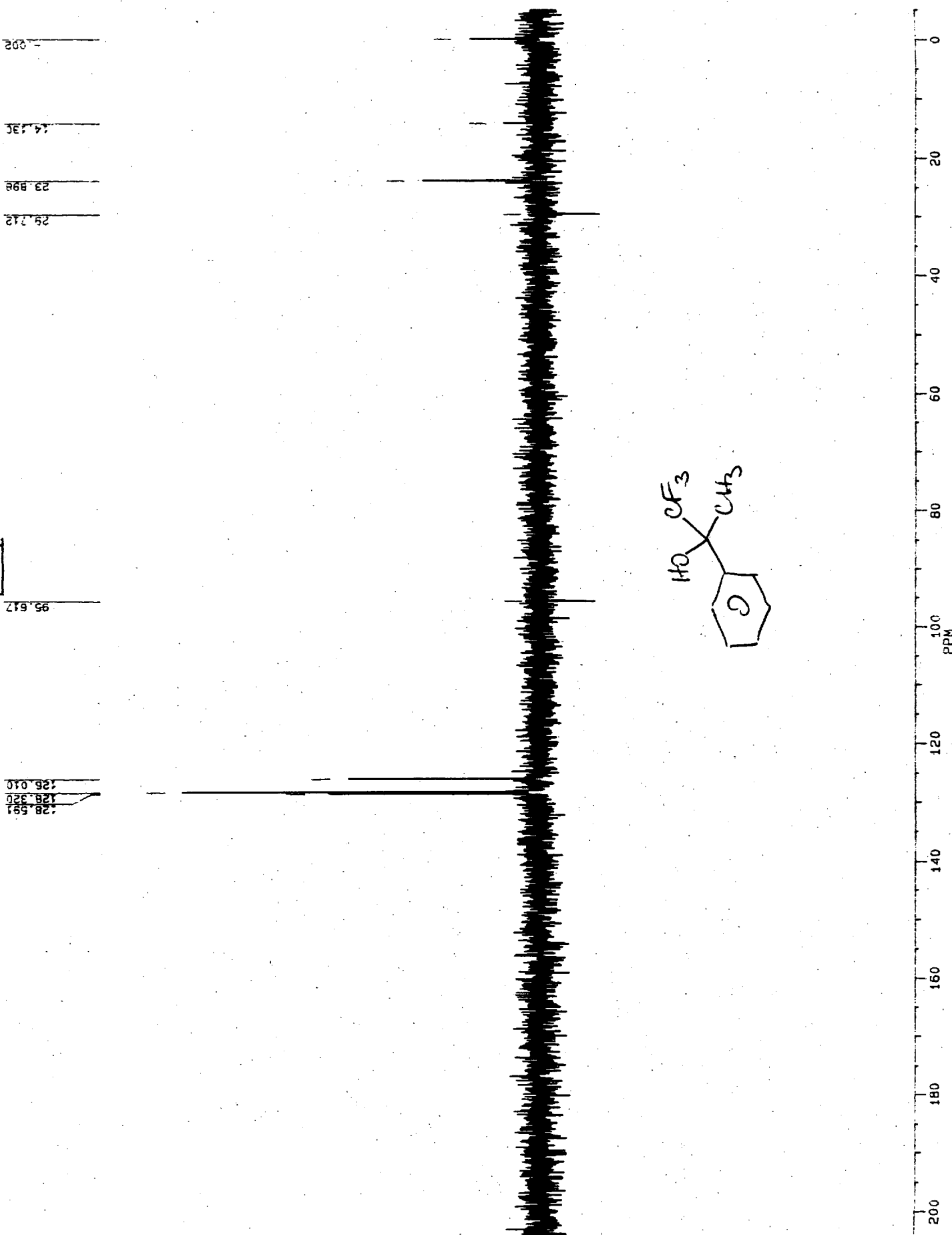
SF 50.31
SY 50.00
O1 8396.31
SI 65536
TD 65536
SM 12500.00
HZ/PT 31.31

PW 0.0
RD 0.0
AQ 2.61
RG 640
NS 500
TE 297

FW 15700
O2 3154.51
DP 15H D0

L8 1.00
G8 0.0
CX 35.00
CY 10.00
F1 209.90
F2 -5.00
HZ/CM 309.11
PPM/CM 6.11
SR 3315.91

SLV40F3 DEPT

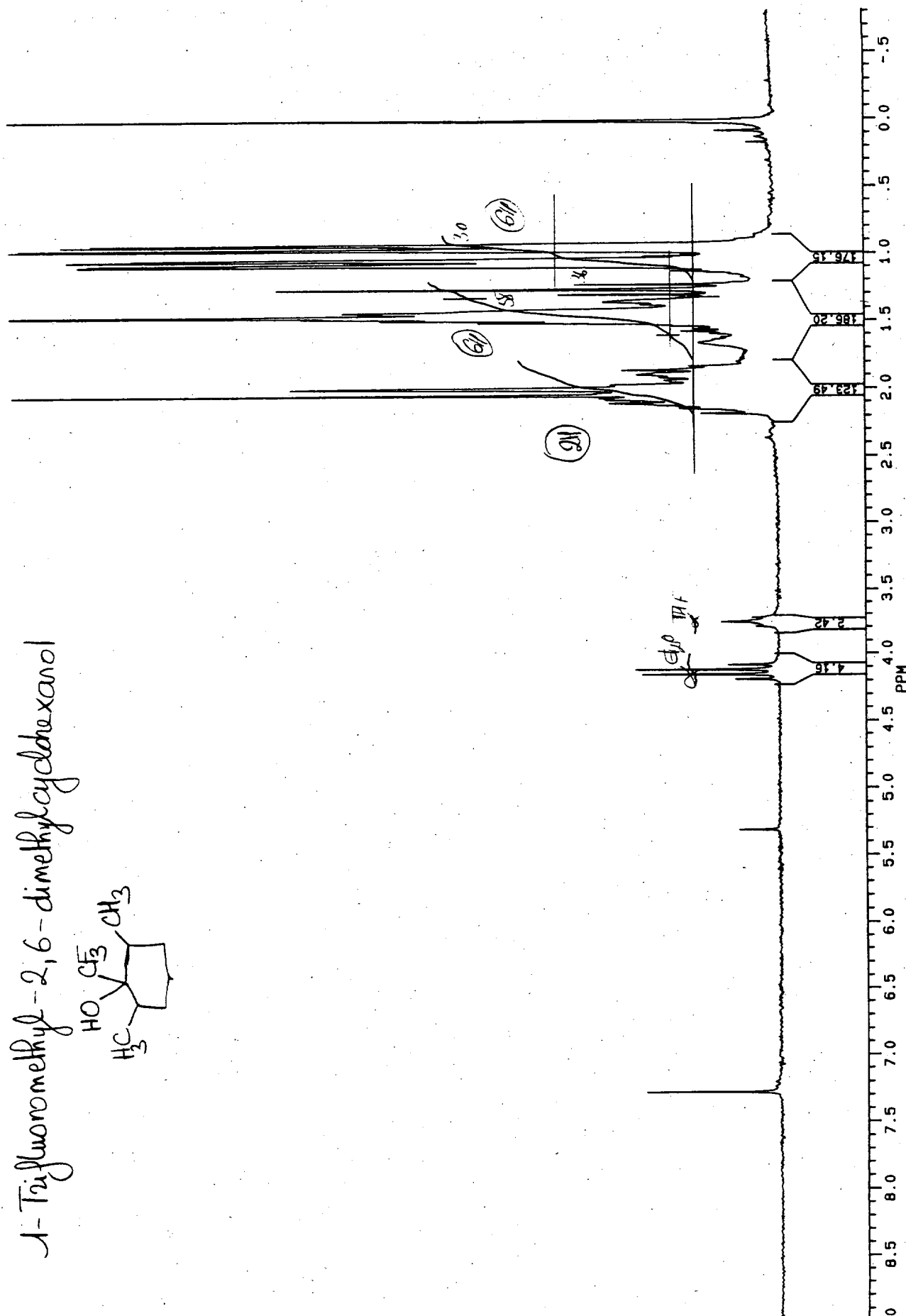
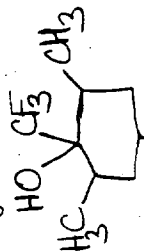


S77

¹H NMR

SLVIII62F3/1H/CDCL3

1-Trifluoromethyl-2,6-dimethylcyclohexanol



BRUKER

SLVIII-MEOL
DATE 21-5-9
TIME 15:30SF 200.1
SY 200.0
O1 4000.0
SI 32768
TD 32768
SW 4032.2
HZ/PT 2PW 3.5
RD 1.0
AQ 4.0
RG 10
NS 16
TE 297FW 5100
O2 2930.4
DP 15L P0LB 3
GB 0.0
CX 35.0
CY 20.0
F1 9.2
F2 9.8
HZ/CM 57.2
PPM/CM 2338.2
SR 2338.2

578

~~BRUKER~~

SLV11162.ME
DATE 21-5-9
TIME 15:25

SF 188.3
SY 188.0

O1 9759.0
SI 65536

TD 65536
SM 125000.0

HZ/PT 3.8

PW 3.0
RD 1.0

AG 21
RG 10

NS 72
TE 297

FW 250000
O2 4582.8

DP 30L P0

LB 30
GB 0.0

CX 35.00
CY 20.00

F1 -59.71
F2 -80.44

HZ/CM 111.45
PPM/CM 59

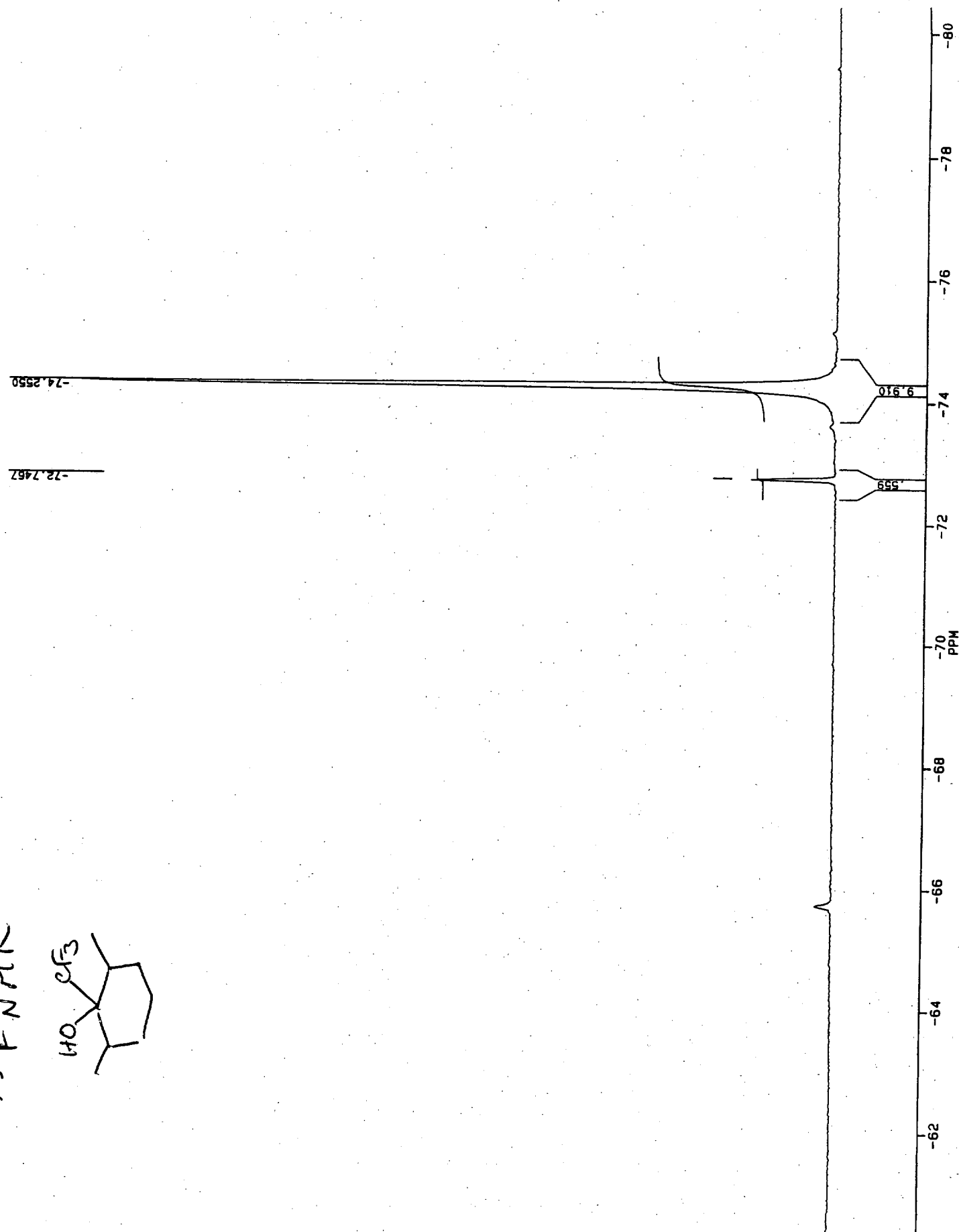
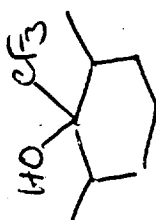
SR 22606.93

SLV11162F3/19F COUPLE

-74.2550

-72.7467

19 F NMR



S79

¹³C NMR

SL VIII-62 F3

*** Current Data Parameters

NAME : AMIS023

EXPNO : 2

PROCNO : 1

*** Acquisition Parameters ***

AQ_mod : qseq

AUNM : X02.AU

BF1 : 75.0652111 MHz

DS : 2

NS : 3200

OL : 6466.00 Hz

O2 : 5225.00 Hz

RO : 20 Hz

SF01 : 75.4716771 MHz

SW : 215.3805 ppm

SW_h : 18518.519 Hz

TD : 65536

TE : 297 K

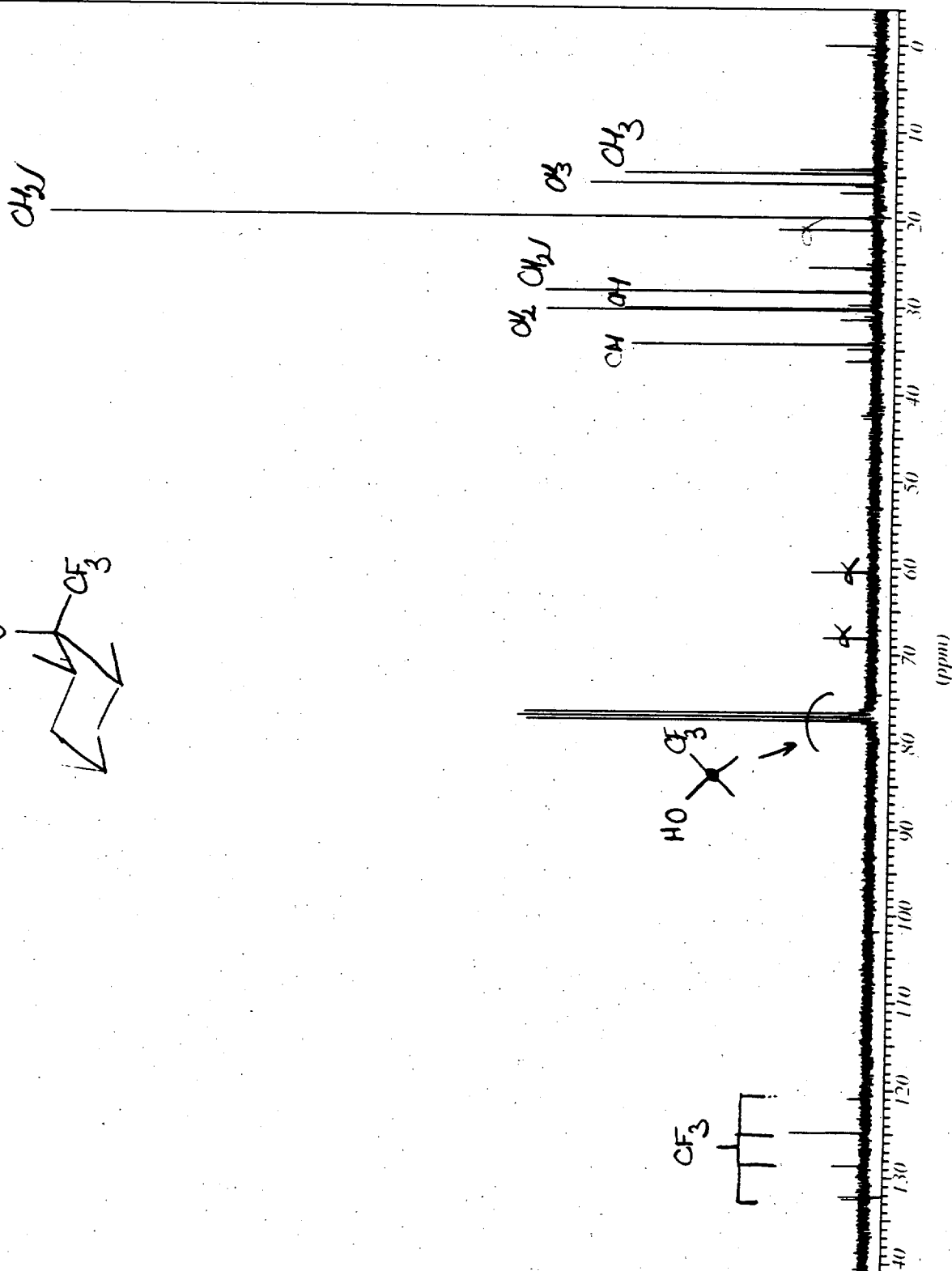
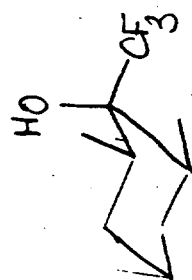
*** Processing Parameters ***

LB : 0.60 Hz

TI : SLVH02F3/130/C

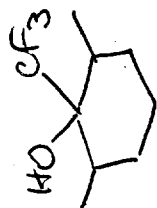
*** Aspect 3000 Parameters ***

PH0C : 0



¹³C NMR DEPT

S80



*** Current Data Parameters

NAME : AMISI623

EXPNO : 3

PROCNO : 1

*** Acquisition Parameters ***

AQ_mod : qseq

AUNM : X09.AU

BF1 : 75.1652111 MHz

DS : 2

NS : 2400

O1 : 6466.00 Hz

O2 : 5225.00 Hz

RO : 20 Hz

SF01 : 75.4716771 MHz

SW : 245.3805 ppm

SW_h : 18518.519 Hz

TD : 65536

TE : 297 K

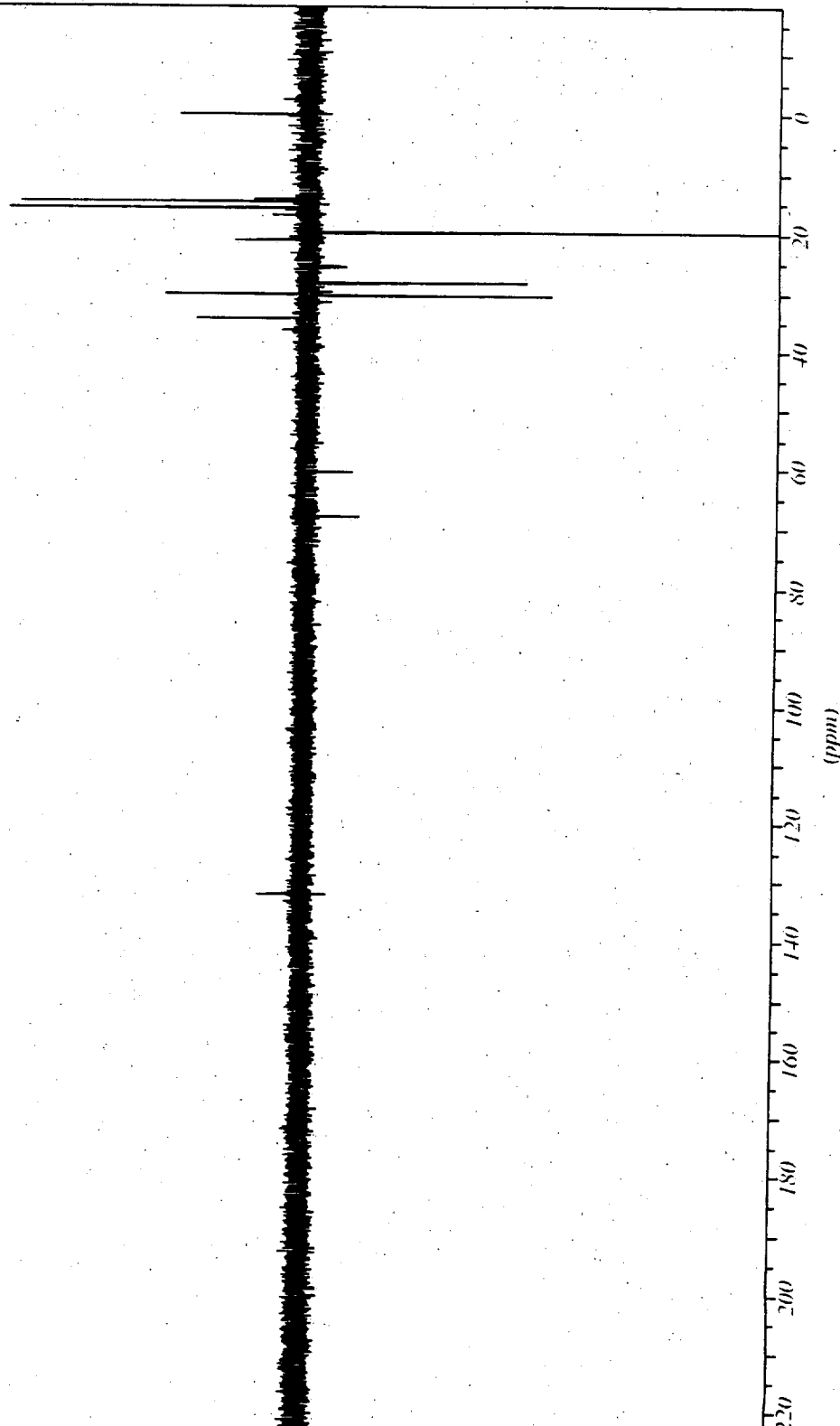
*** Processing Parameters ***

LB : 0.00 Hz

TI : ESI-VIII62F3-DEPT

*** Aspect 3000 Parameters ***

PHOC : 0



SL VIII-62 F3

VIII62F3-DEPT