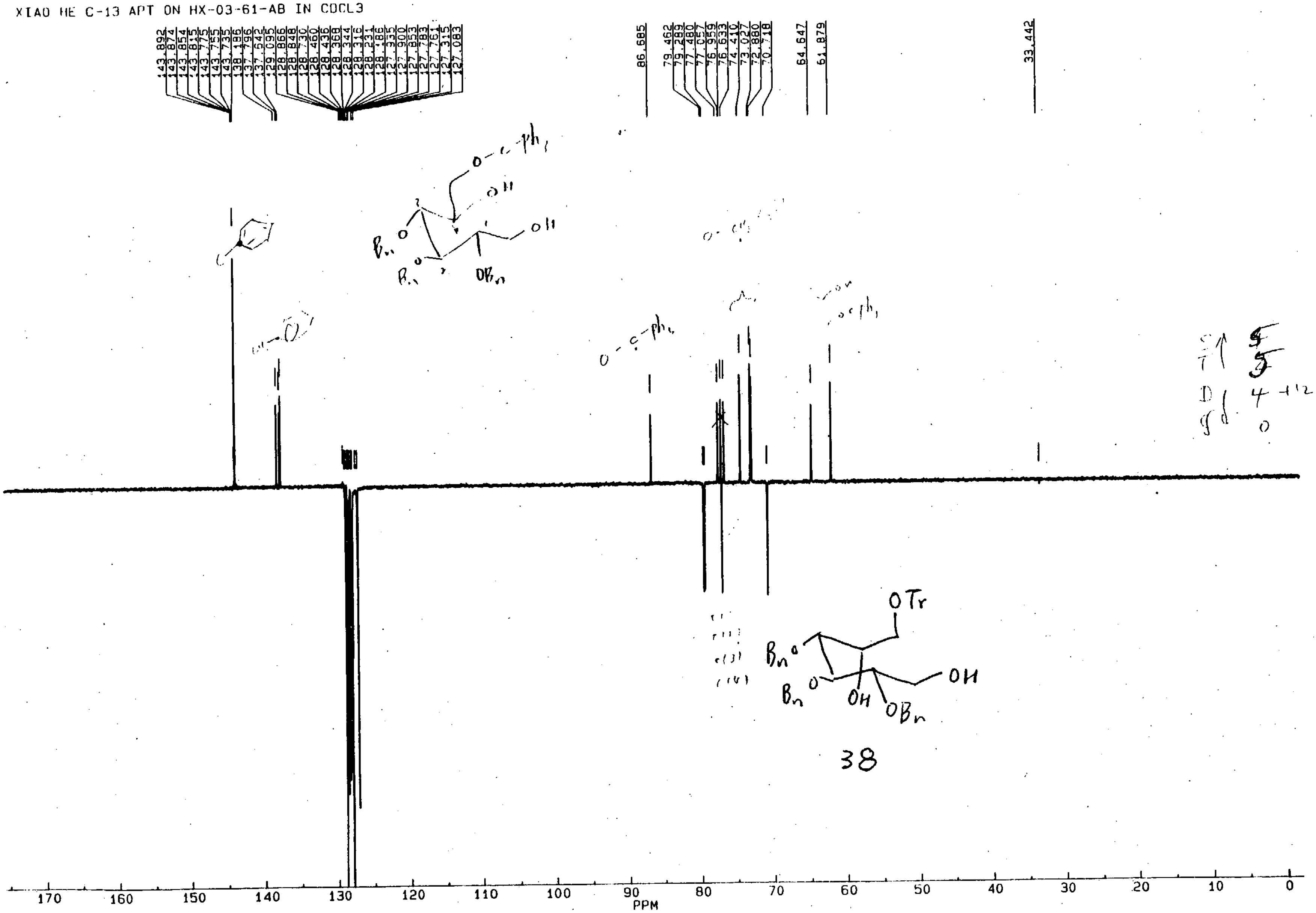
41

XIAO HE C-13 APT ON HX-03-61-AB IN CDCL3



38

BRUKER

SF270F.102
AU PROG:
X25.AU
DATE 28-9-95

SF 75.469
SY 112.0
O1 7000.000
SI 65536
TD 32768
SW 22727.273
HZ/PT .694

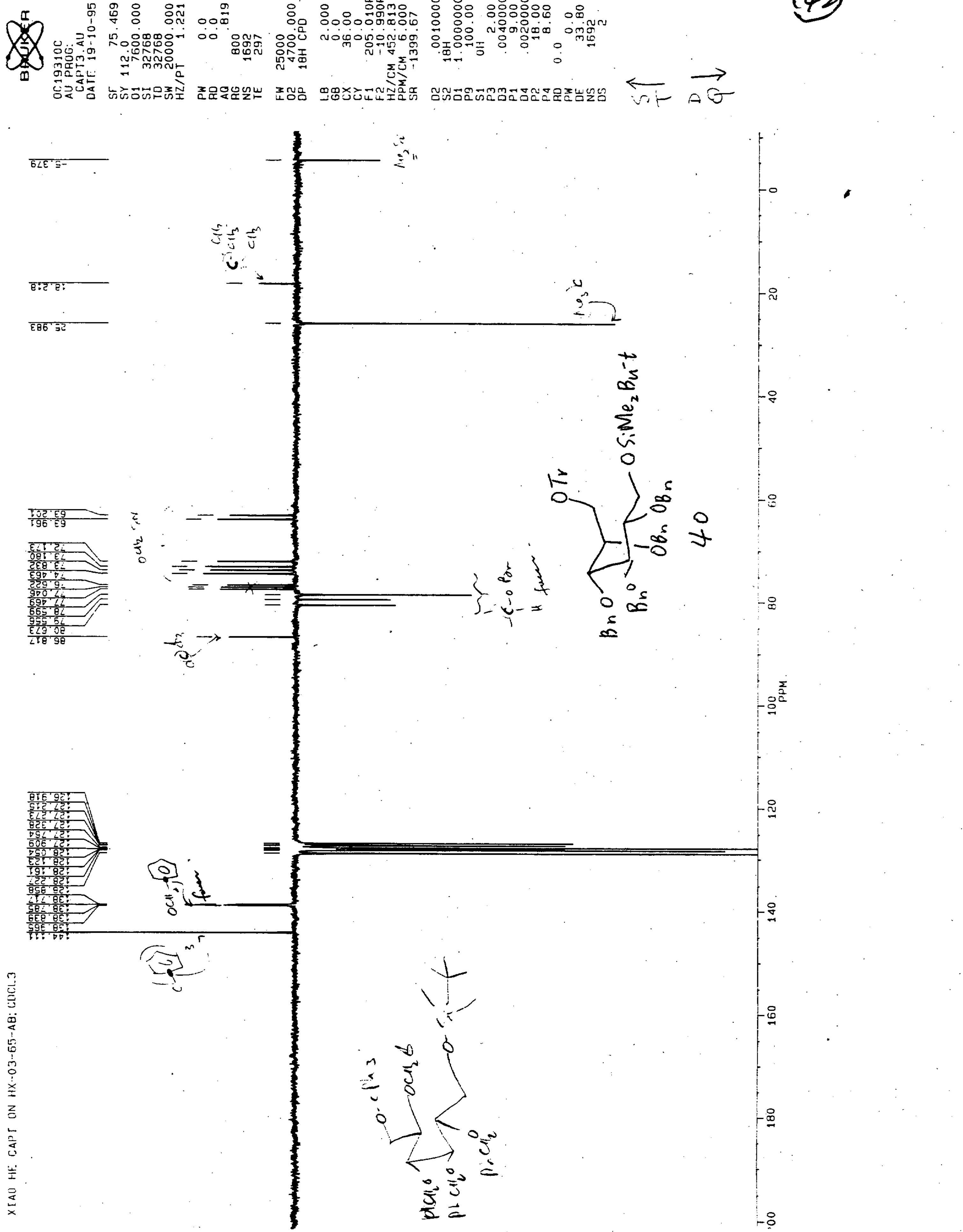
PW 0.0
RD 0.0
AQ .721
RG 800
NS 5000
TE 297

FW 28500
O2 4425.000
DP 18H CPD

LB .700
GB .010
CX 36.00
CY 0.0
F1 178.007P
F2 -1.986P
HZ/CM 377.328
PPM/CM 5.000
SR -1399.89

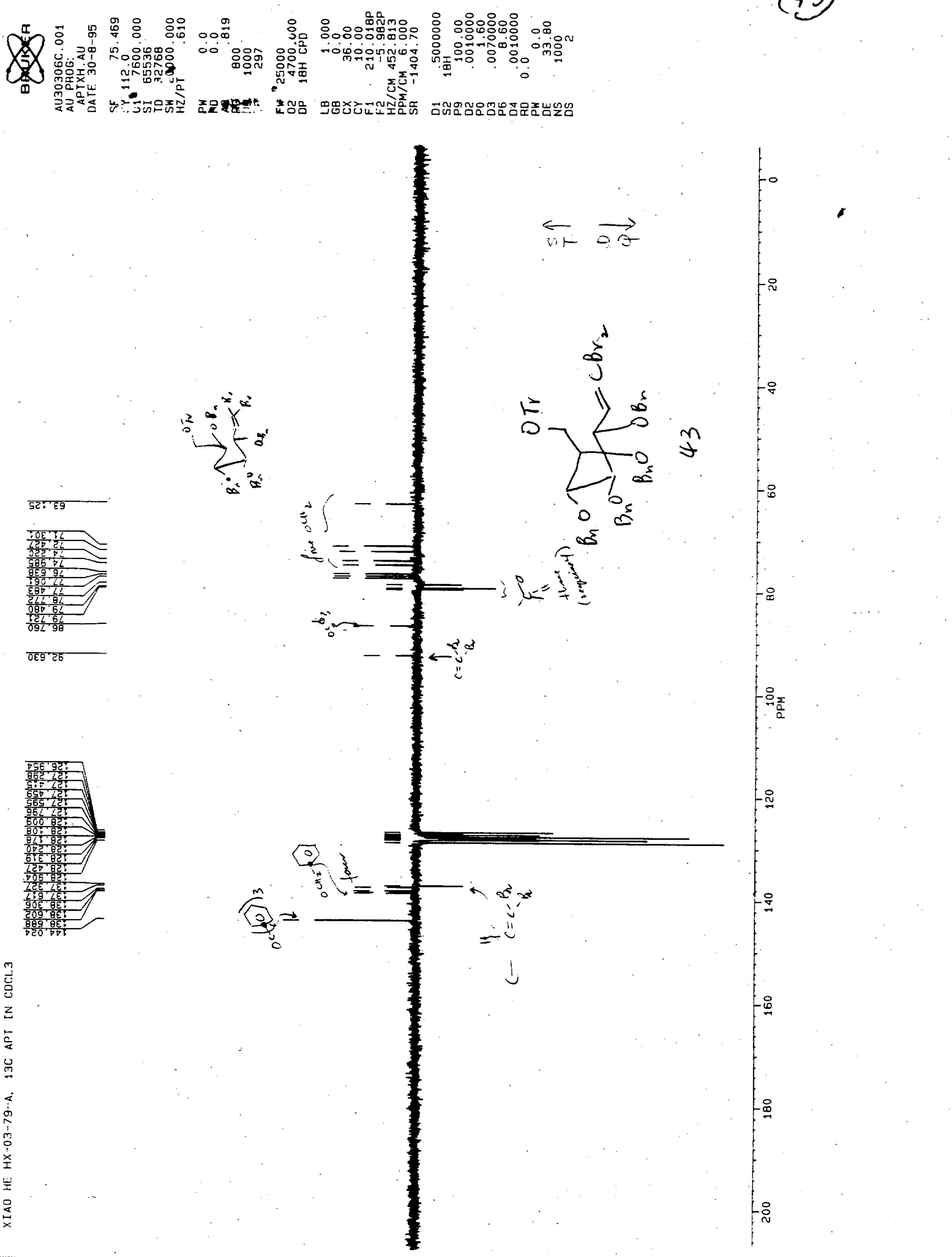
D1 2.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 2.00
D3 .0070000
P6 8.40
D4 .0010000
RGA
RD 0.0
PW 0.0
DE 30.00
NS 5000
DS 2

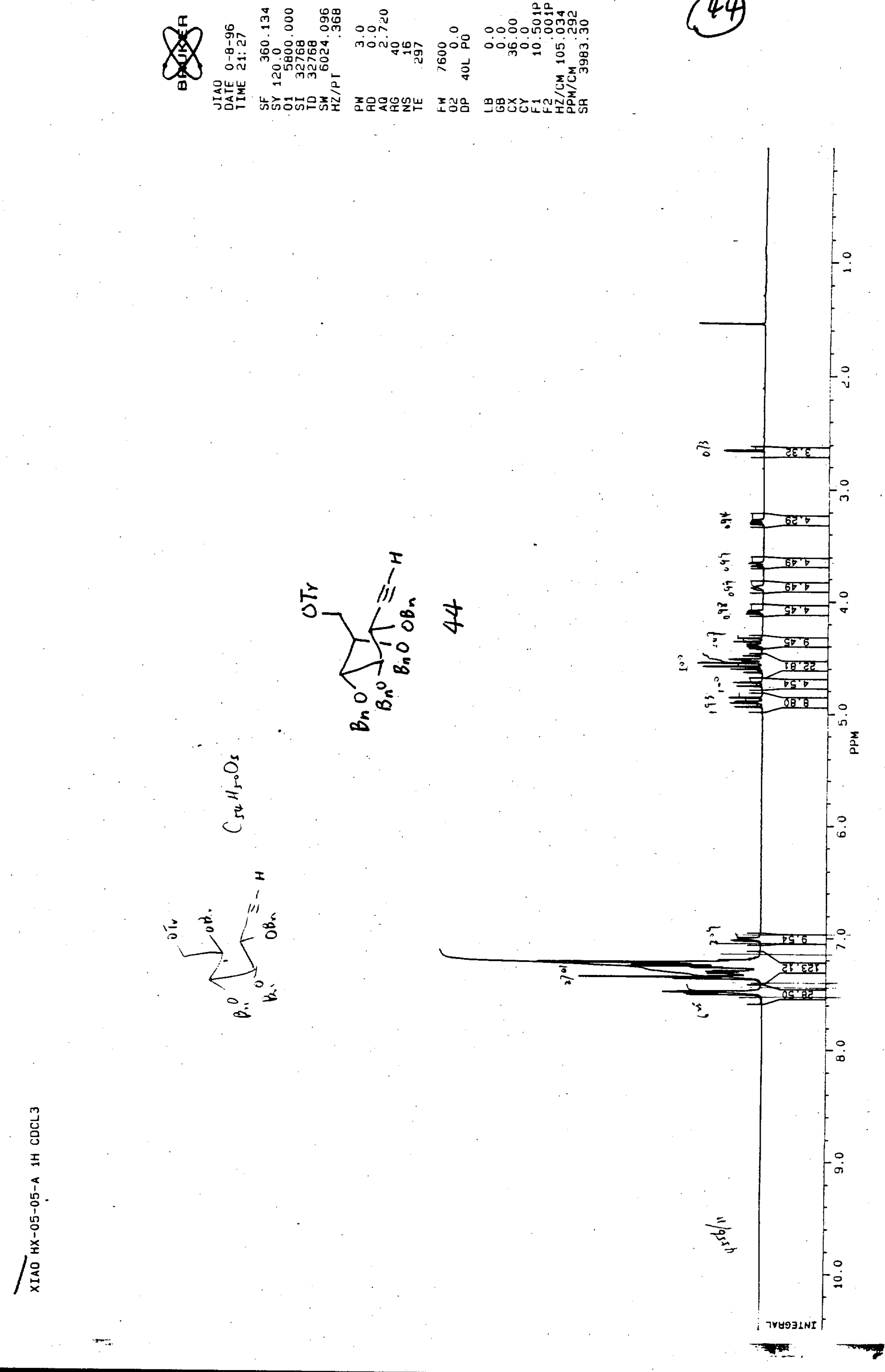
(42)

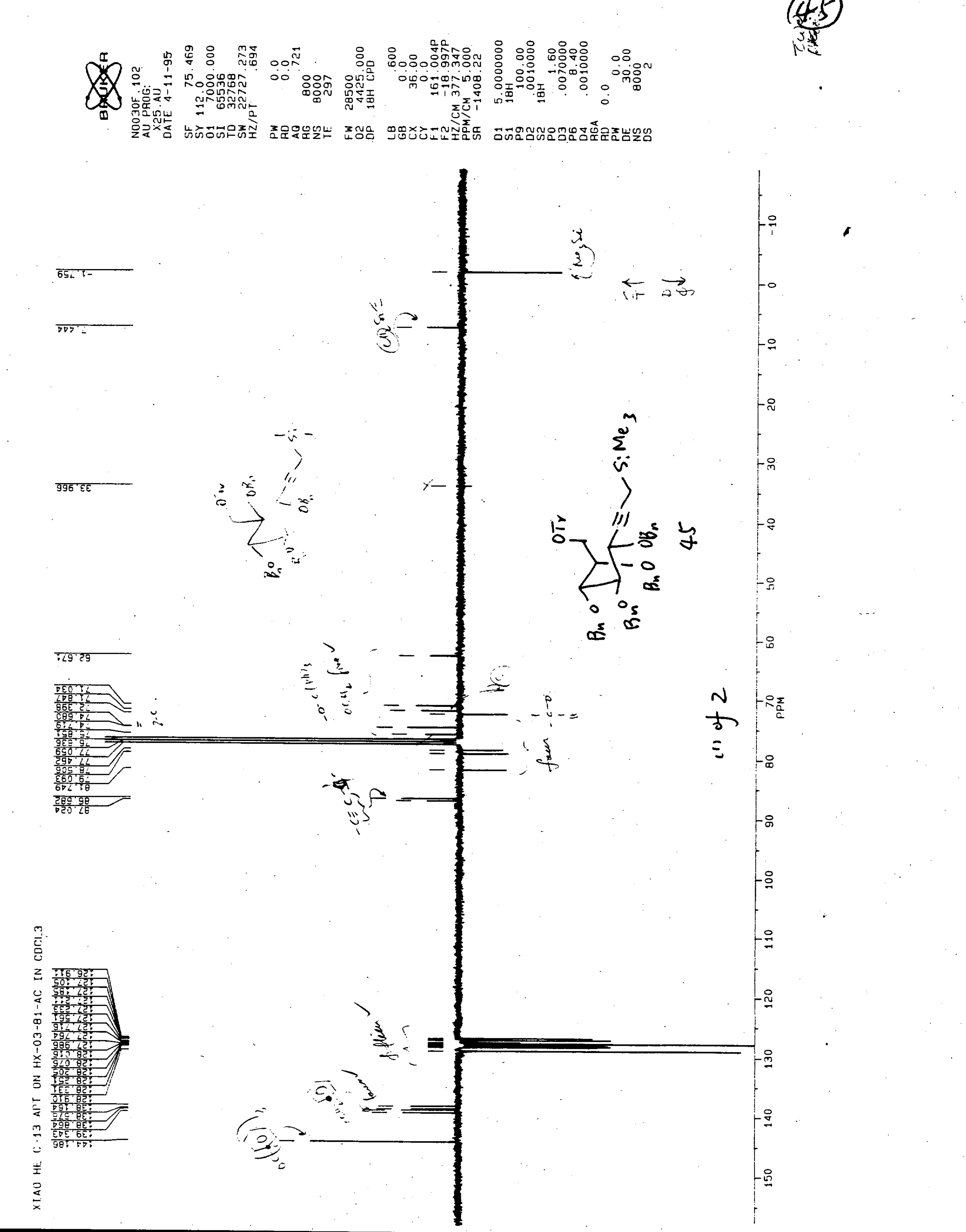


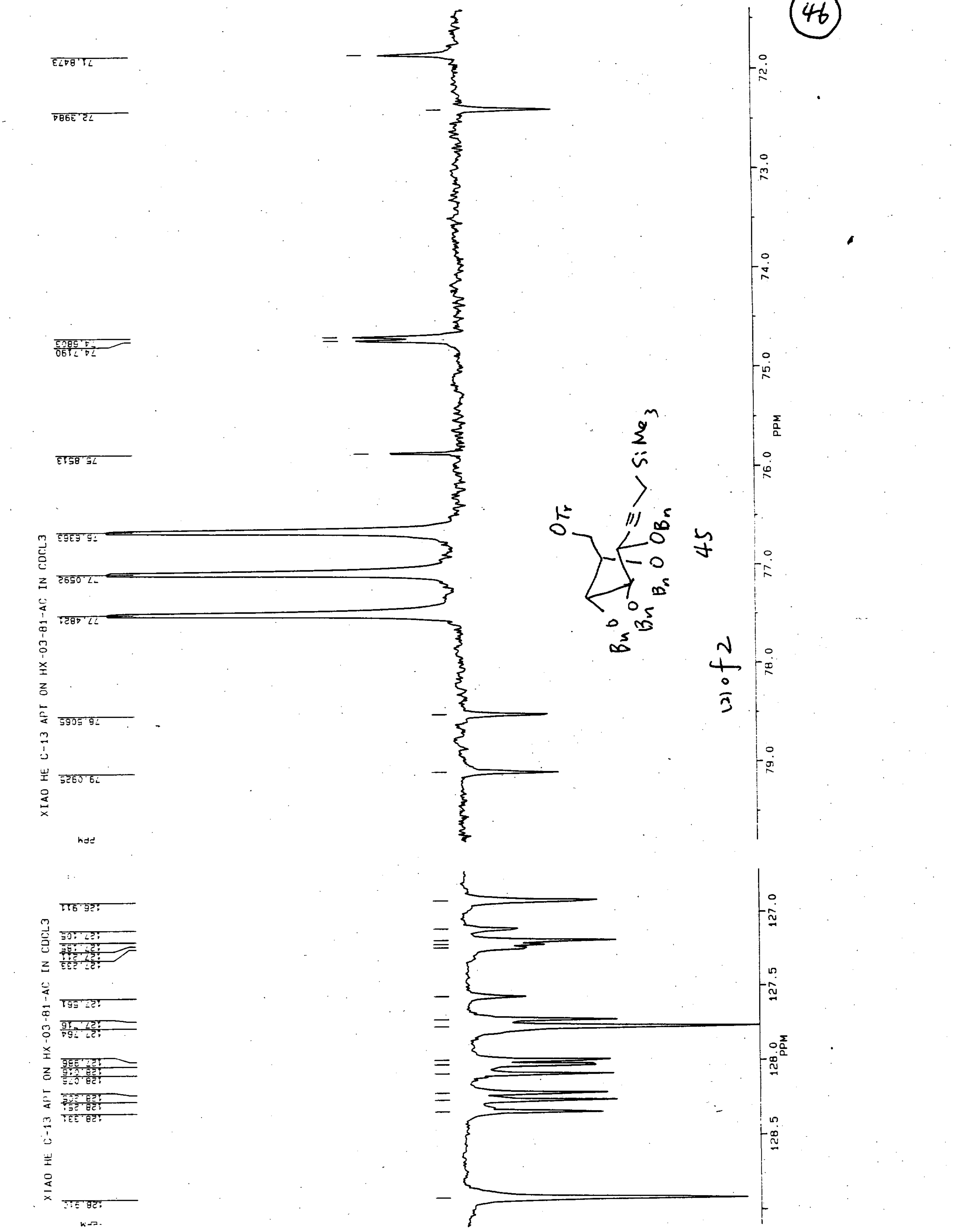
BRUKER
0C19310C
AU PROG:
CAPT3.AU
DATE 19-10-95
SF 75.469
SY 112.0
O1 7600.000
SI 32768
TD 32768
SW 20000.000
HZ/PT 1.221
PW 0.0
RD 0.0
AQ .819
RG 800
NS 1692
TE 297
FW 25000
O2 4700.000
DP 18H CPD
LB 2.000
GB 0.0
CX 36.00
CY 0.0
F1 205.010P
F2 -10.990P
HZ/CM 452.813
PPM/CM 6.000
SR -1399.67
D2 .0010000
S2 18H
D1 1.0000000
P9 100.00
S1 0H
P3 2.00
D3 .0040000
P1 9.00
D4 .0020000
P2 18.00
P4 8.60
RD 0.0
PW 0.0
DE 33.80
NS 1692
DS 2
-5.379
18.218
25.983
XIAO HK CAPT ON HX-03-65-AB; CDCL3
PPM
0
20
40
60
80
100
120
140
160
180
200
OTr
OSiMe2Bu-t
OBn
BnO
40

(43)

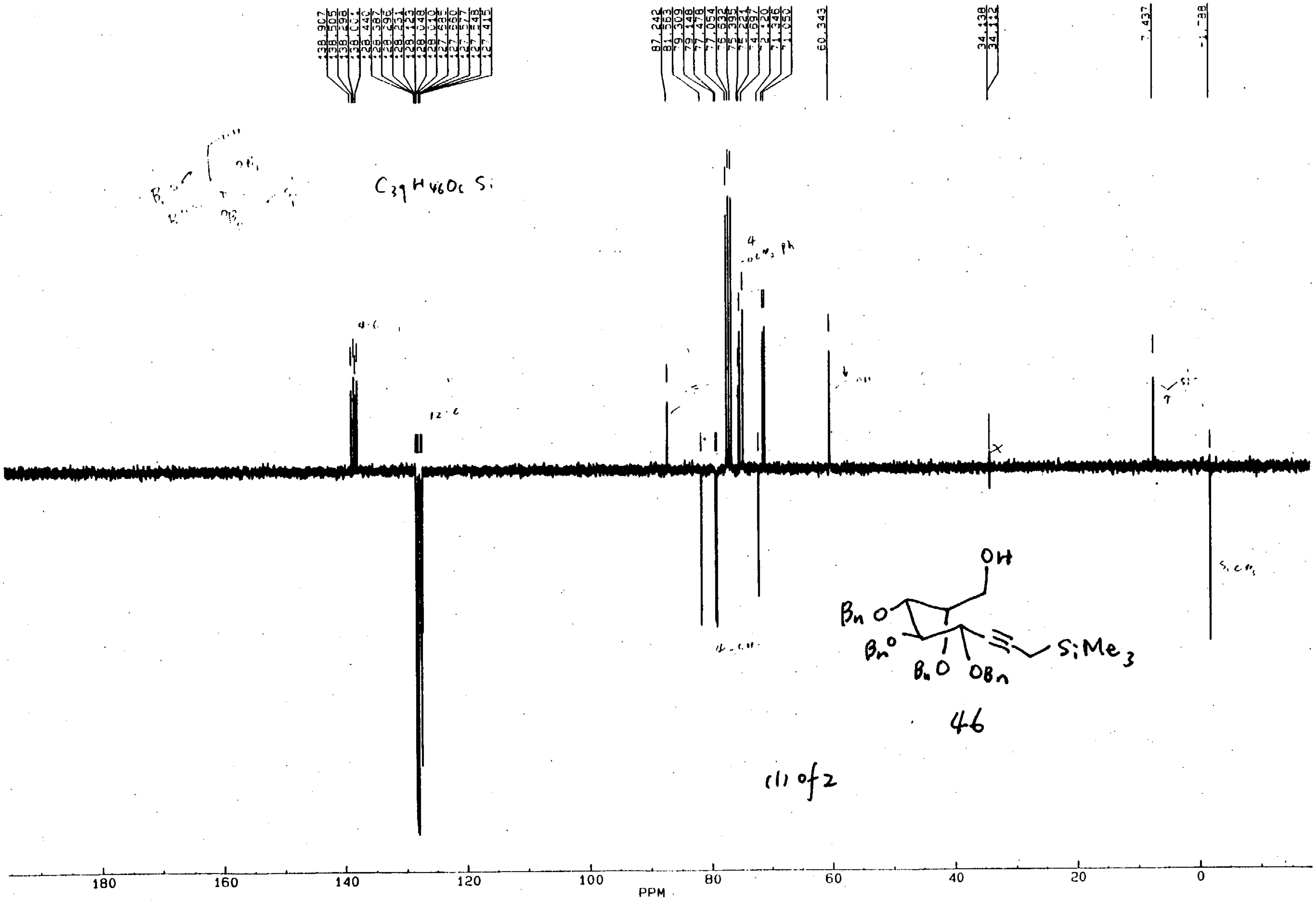



XIAO HX-05-05-A 1H CDCL3
JIAO
DATE 0-8-96
TIME 21:27
SF 360.134
SY 120.0
O1 5800.000
SI 32768
TD 32768
SW 6024.096
HZ/PT .368
PW 3.0
RD 0.0
AQ 2.720
RG 40
NS 16
TE 297
FW 7600
O2 0.0
DP 40L PO
LB 0.0
GB 0.0
CX 36.00
CY 0.0
F1 10.501P
F2 .001P
HZ/CM 105.034
PPM/CM .292
SR 3983.30
PPM
INTEGRAL
44


XIAO HE C-13 APT ON HX-03-81-AC IN CDCL3
N0030F.102
AU PROG:
X25.AU
DATE 4-11-95
SF 75.469
SY 112.0
O1 7000.000
SI 65536
TD 32768
SW 22727.273
HZ/PT .694
PW 0.0
RD 0.0
AQ .721
RG 800
NS 8000
TE 297
FW 28500
O2 4425.000
DP 18H CPD
LB .600
GB 0.0
CX 36.00
CY 0.0
F1 161.004P
F2 -18.997P
HZ/CM 377.347
PPM/CM 5.000
SR -1408.22
D1 5.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 1.60
D3 .0070000
P6 8.40
D4 .0010000
RGA 0.0
RD 0.0
PW 0.0
DE 30.00
NS 8000
DS 2
PPM
45
"1 of 2"


(46)
XIAO HE C-13 APT ON HX-03-81-AC IN CDCL3
PPM
45
(2) of 2

XIAO 13C{1H} APT ON HX-03-85-AB IN CDCL3

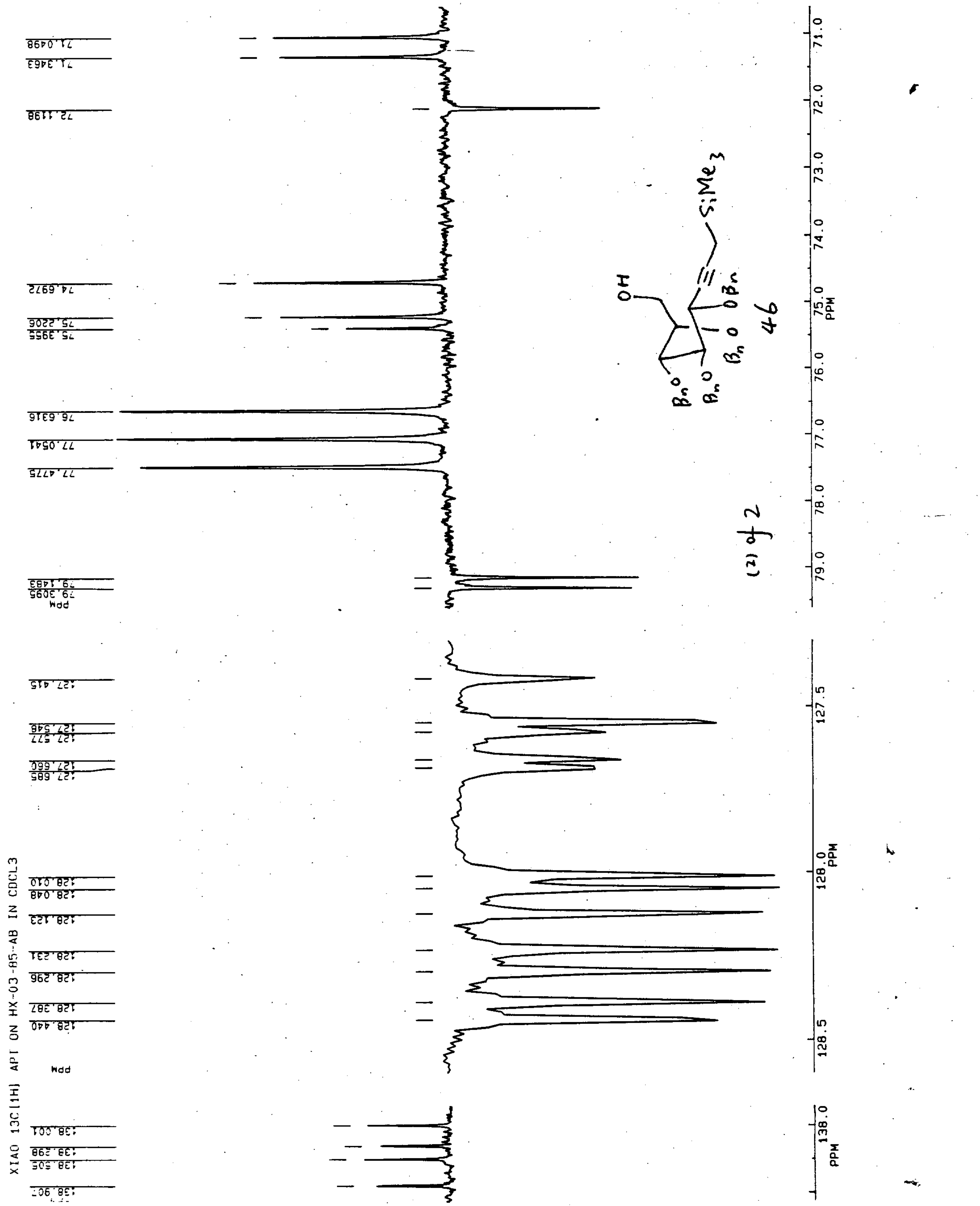


BRUKER

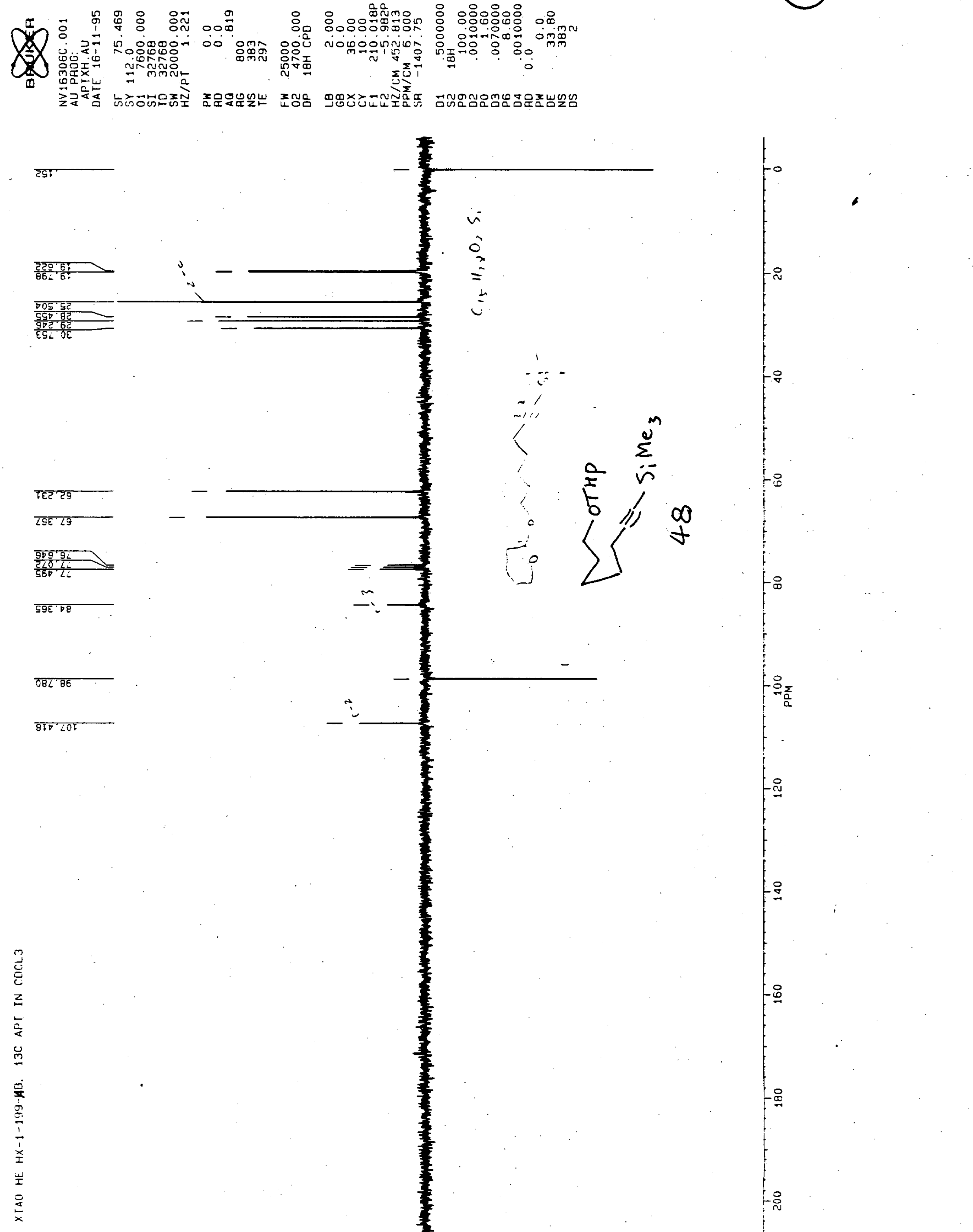
MY070F.102
AU PROG:
X25.AU
DATE 3-7-96
TIMF 4:26

SF	75.469
SY	112.0
O1	7000.000
SI	65536
TD	32768
SW	22727.273
HZ/PT	.694
PW	0.0
RD	0.0
AQ	.721
RG	800
NS	6000
TE	297
FW	28500
O2	4425.000
DP	18H CPD
LB	.700
GB	.010
CX	36.00
CY	10.00
F1	198.005P
F2	-17.986P
HZ/CM	452.793
PPM/CM	6.000
SR	-1407.52
D1	2.0000000
S1	18H
P9	100.00
D2	.0010000
S2	18H
P0	2.00
D3	.0070000
P6	8.40
D4	.0010000
RGA	
RD	0.0
PW	0.0
DE	30.00
NS	6000
DS	2

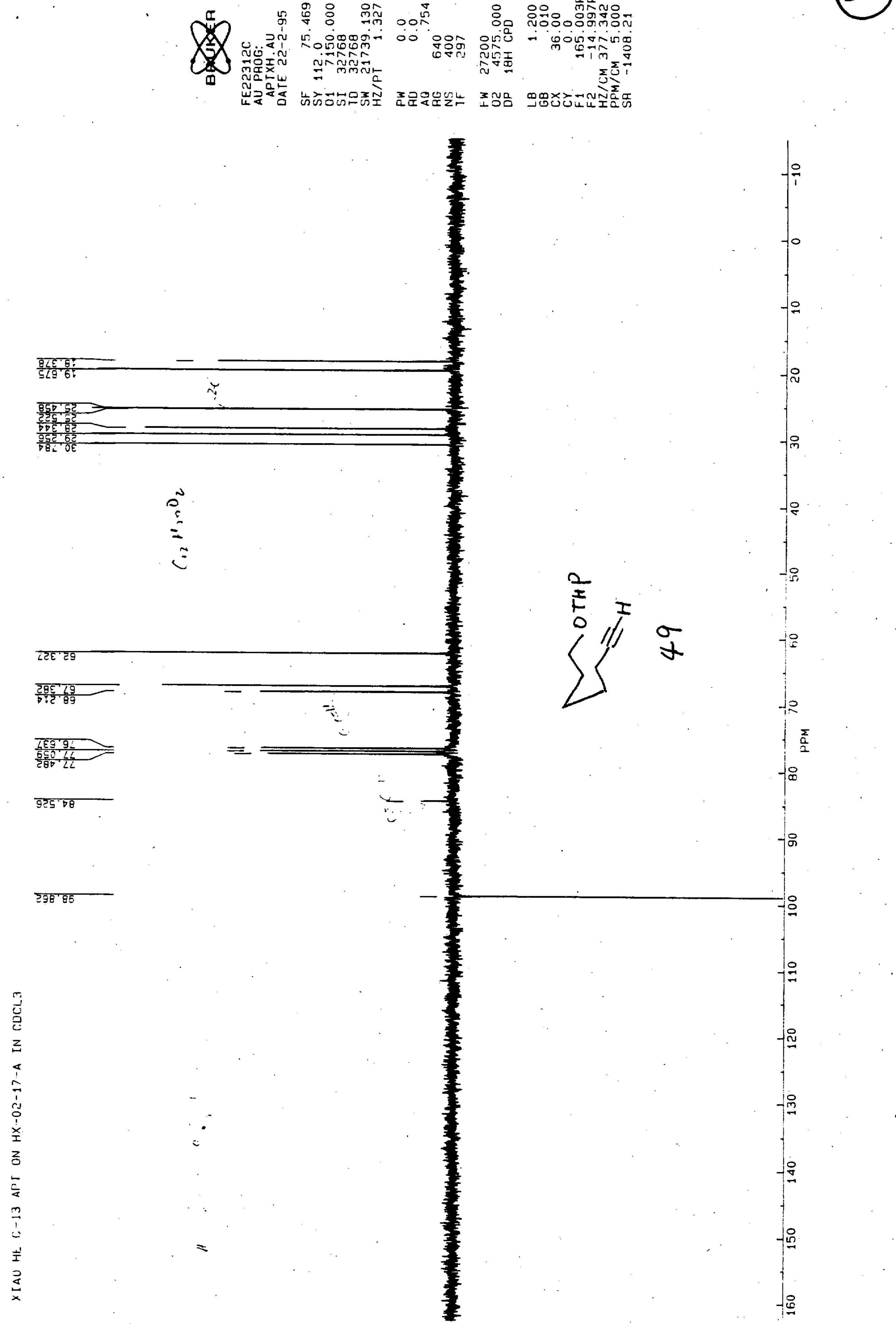
(47)


XIAO 13C{1H} APT ON HX-03-85-AB IN CDCL3
71.0498
71.3463
72.1198
74.6972
75.2206
75.3955
76.6316
77.0541
77.4775
79.1483
79.3095
PPM
127.415
127.548
127.577
127.660
127.685
128.010
128.048
128.123
128.231
128.296
128.387
128.440
PPM
138.001
138.298
138.505
138.907
SiMe3
OH
BnO
BnO
BnO
OBn
46
(2) of 2
PPM

49

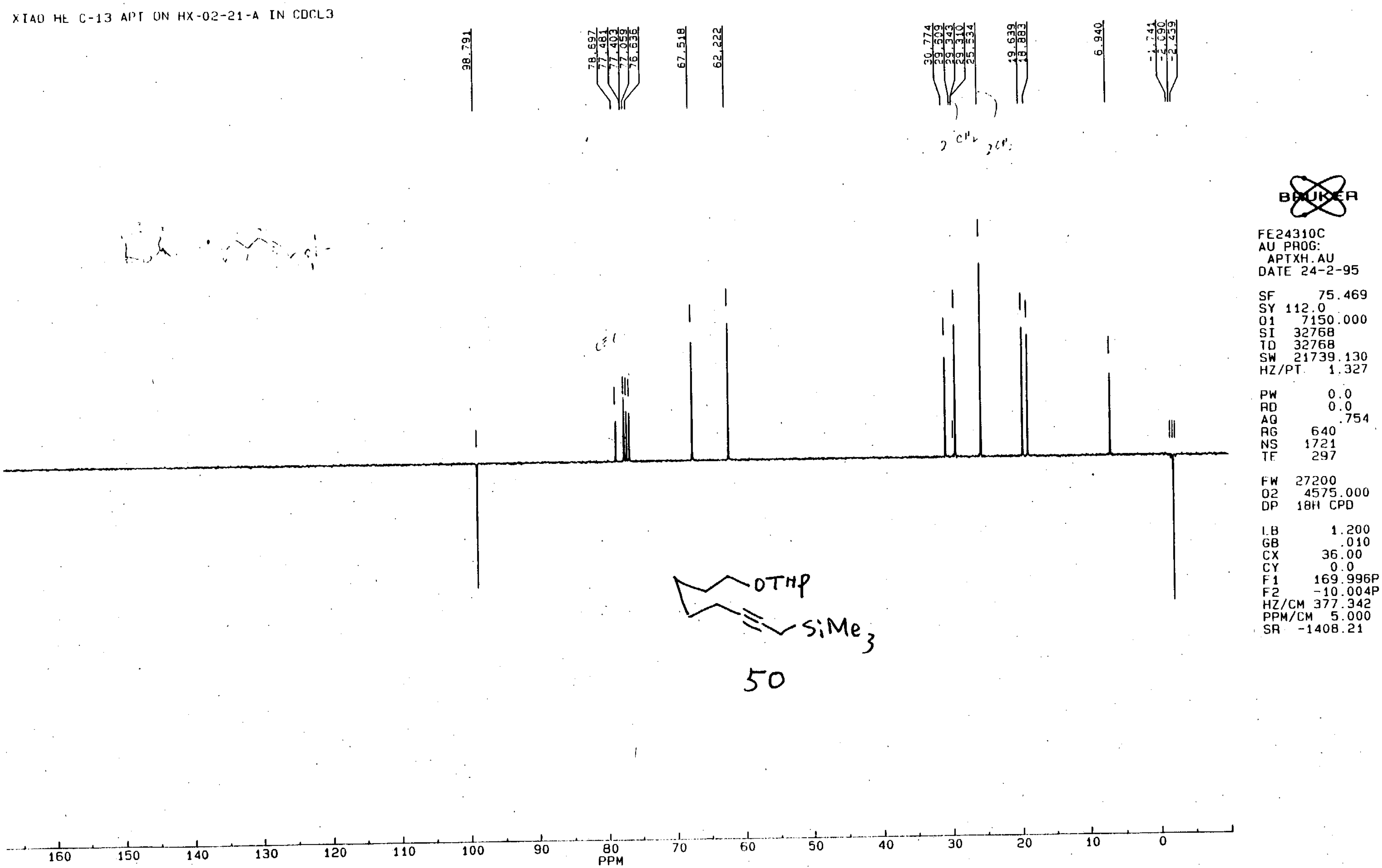

BRUKER
NV16306C.001
AU PROG:
APTXH.AU
DATE 16-11-95
SF 75.469
SY 112.0
O1 7600.000
SI 32768
TD 32768
SW 20000.000
HZ/PT 1.221
PW 0.0
RD 0.0
AQ .819
RG 800
NS 383
TE 297
FW 25000
O2 4700.000
DP 18H CPD
LB 2.000
GB 0.0
CX 36.00
CY 10.00
F1 210.018P
F2 -5.982P
HZ/CM 452.813
PPM/CM 6.000
SR -1407.75
D1 .5000000
S2 18H
P9 100.00
D2 .0010000
P0 1.60
D3 .0070000
P6 8.60
D4 .0010000
RD 0.0
PW 0.0
DE 33.80
NS 383
DS 2
.152
19.622
19.798
25.504
28.455
29.246
30.753
62.231
67.357
76.646
77.072
77.495
84.365
98.780
107.418
$C_{15}H_{28}O_2Si$
OTHP
SiMe3
48
0
20
40
60
80
100
PPM
120
140
160
180
200
XTAO HE HX-1-199-48. 13C APT IN CDCL3

50

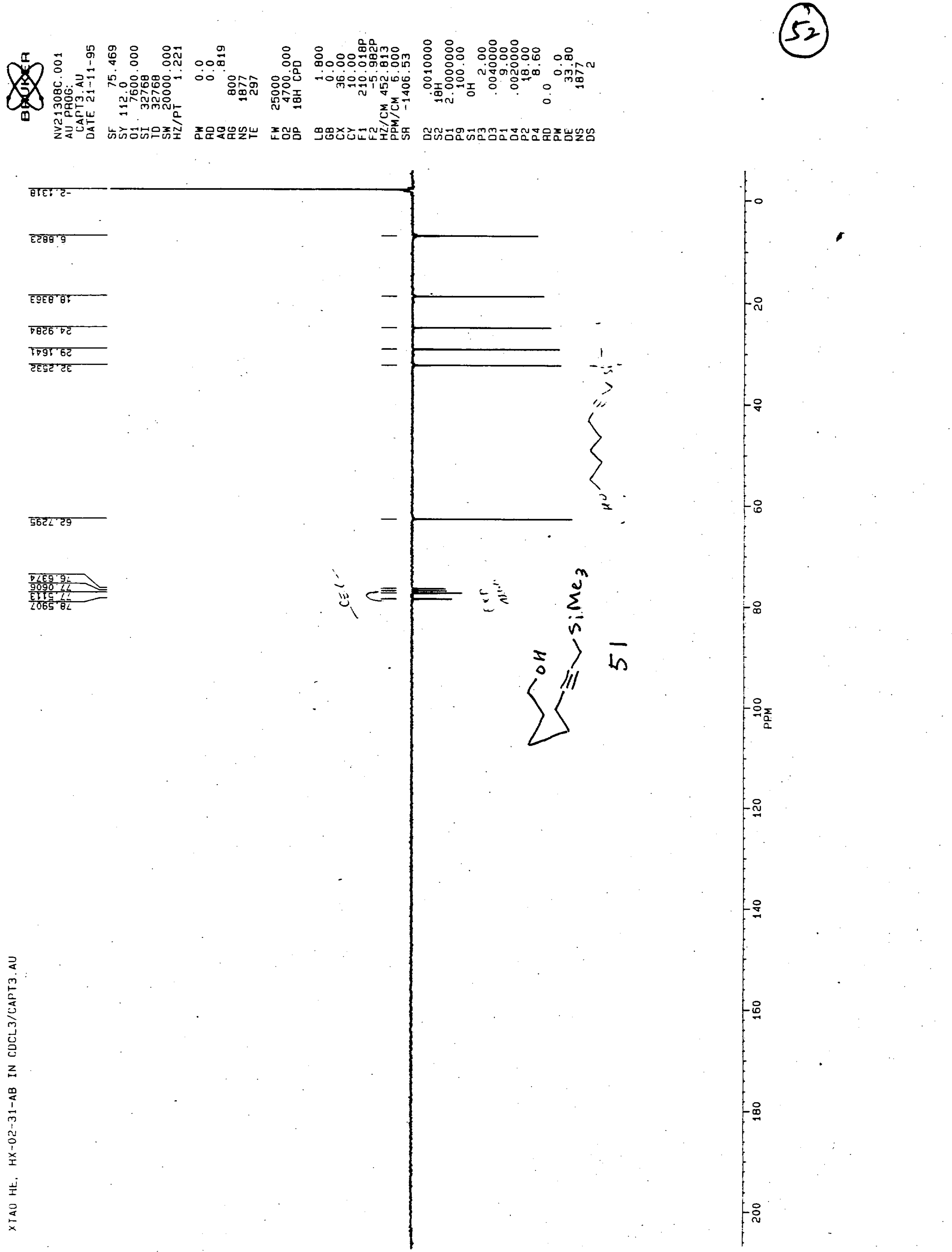


FE22312C
AU PROG:
APTXH.AU
DATE 22-2-95
SF 75.469
SY 112.0
O1 7150.000
SI 32768
TD 32768
SW 21739.130
HZ/PT 1.327
PW 0.0
RD 0.0
AQ .754
RG 640
NS 400
TE 297
FW 27200
O2 4575.000
DP 18H CPD
LB 1.200
GB .010
CX 36.00
CY 0.0
F1 165.003P
F2 -14.997P
HZ/CM 377.342
PPM/CM 5.000
SR -1408.21
18.378
19.675
25.458
26.522
28.344
29.250
30.784
62.327
67.382
68.214
76.637
77.059
77.482
84.526
98.862
$C_{12}H_{20}O_2$
OTHP
H
49
PPM
XIAU HE C-13 APT ON HX-02-17-A IN CDCL3

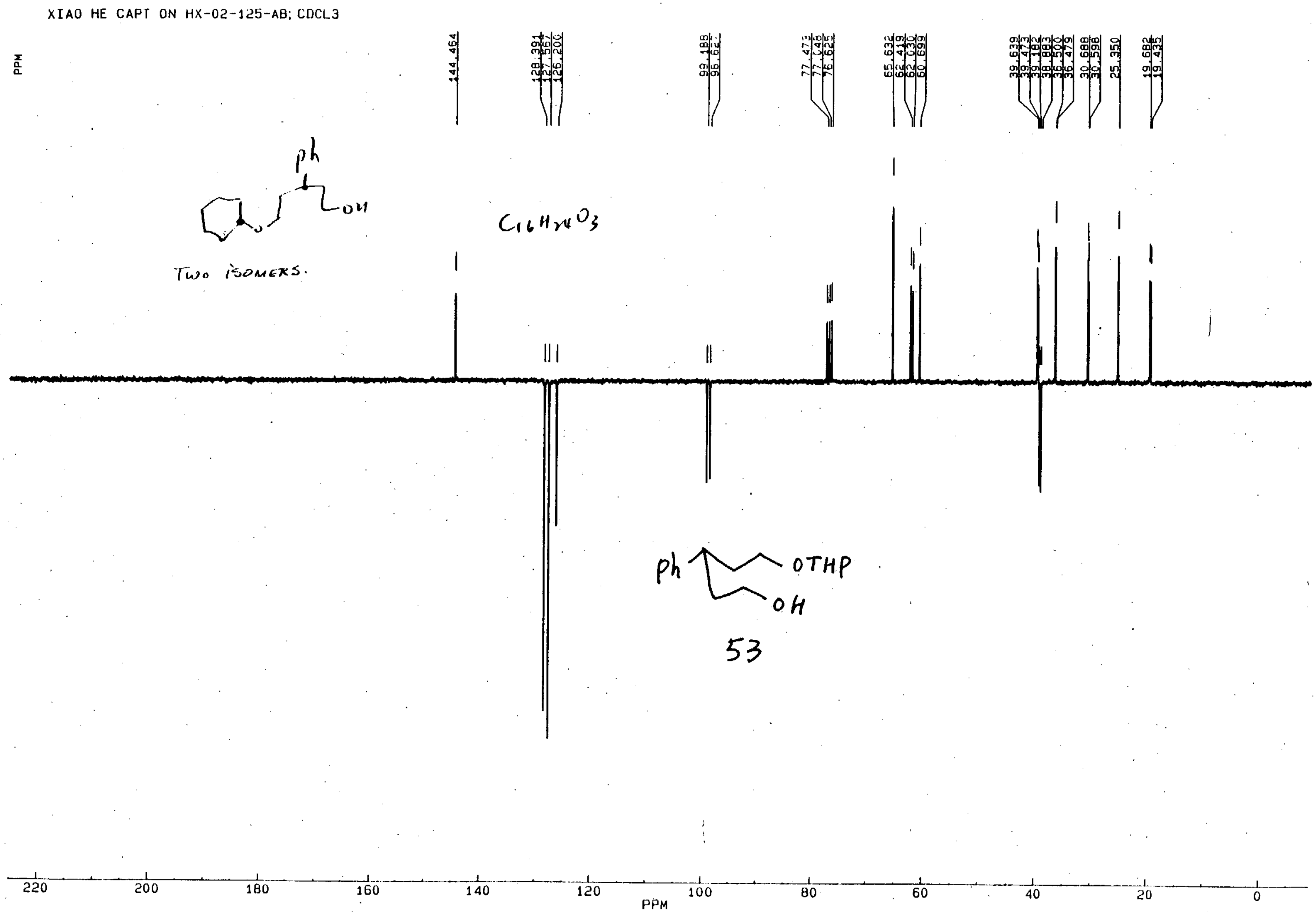
(51)


XIAO HE C-13 APT ON HX-02-21-A IN CDCL3
98.791
78.697
77.481
77.403
77.059
76.636
67.518
62.222
30.774
29.509
29.343
29.310
25.534
19.639
18.883
6.940
-1.741
-2.090
-2.439
2 CH2
2 CH2
PPM
BRUKER
FE24310C
AU PROG:
APTXH.AU
DATE 24-2-95
SF 75.469
SY 112.0
O1 7150.000
SI 32768
TD 32768
SW 21739.130
HZ/PT 1.327
PW 0.0
RD 0.0
AQ .754
RG 640
NS 1721
TE 297
FW 27200
O2 4575.000
DP 18H CPD
LB 1.200
GB .010
CX 36.00
CY 0.0
F1 169.996P
F2 -10.004P
HZ/CM 377.342
PPM/CM 5.000
SR -1408.21
OTHP
SiMe3

50



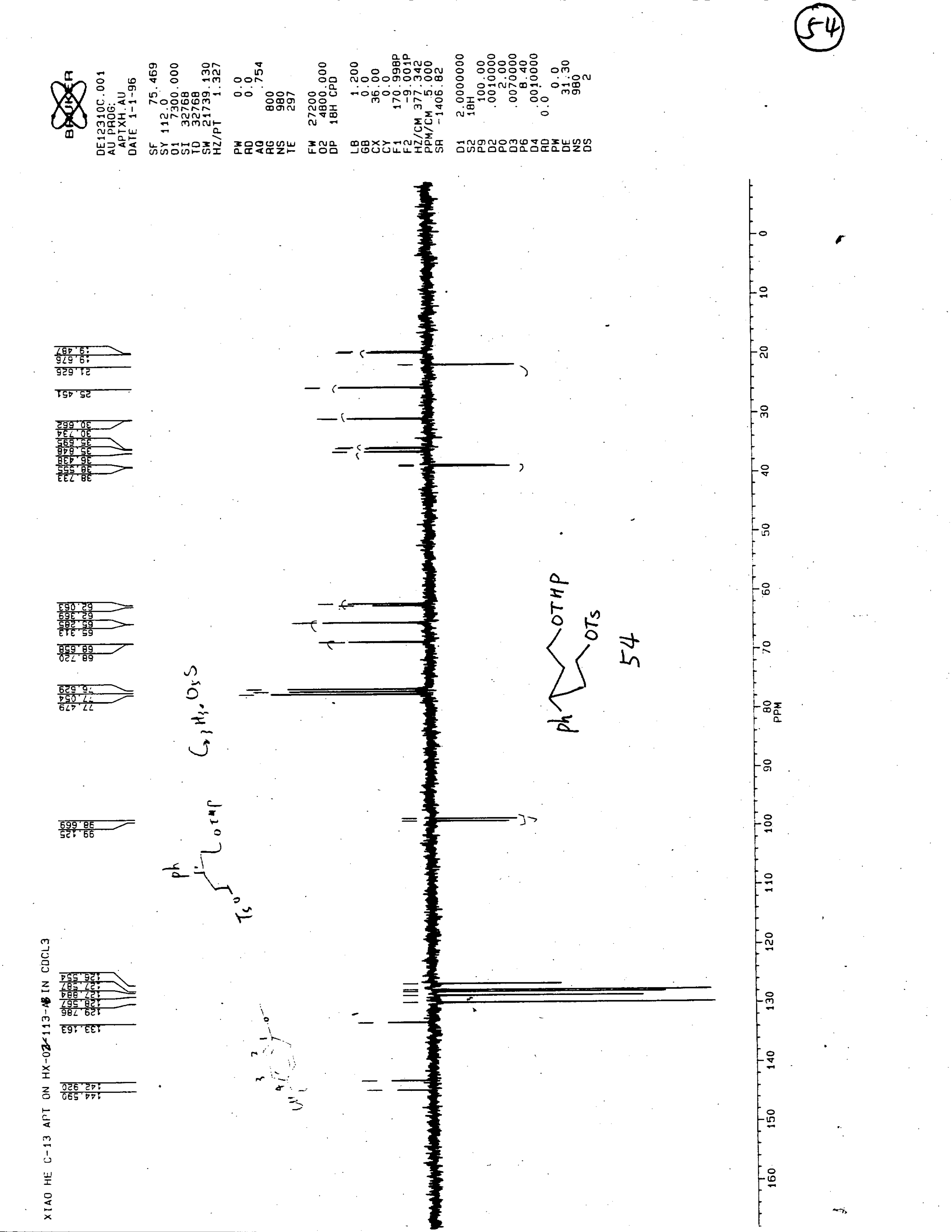
53



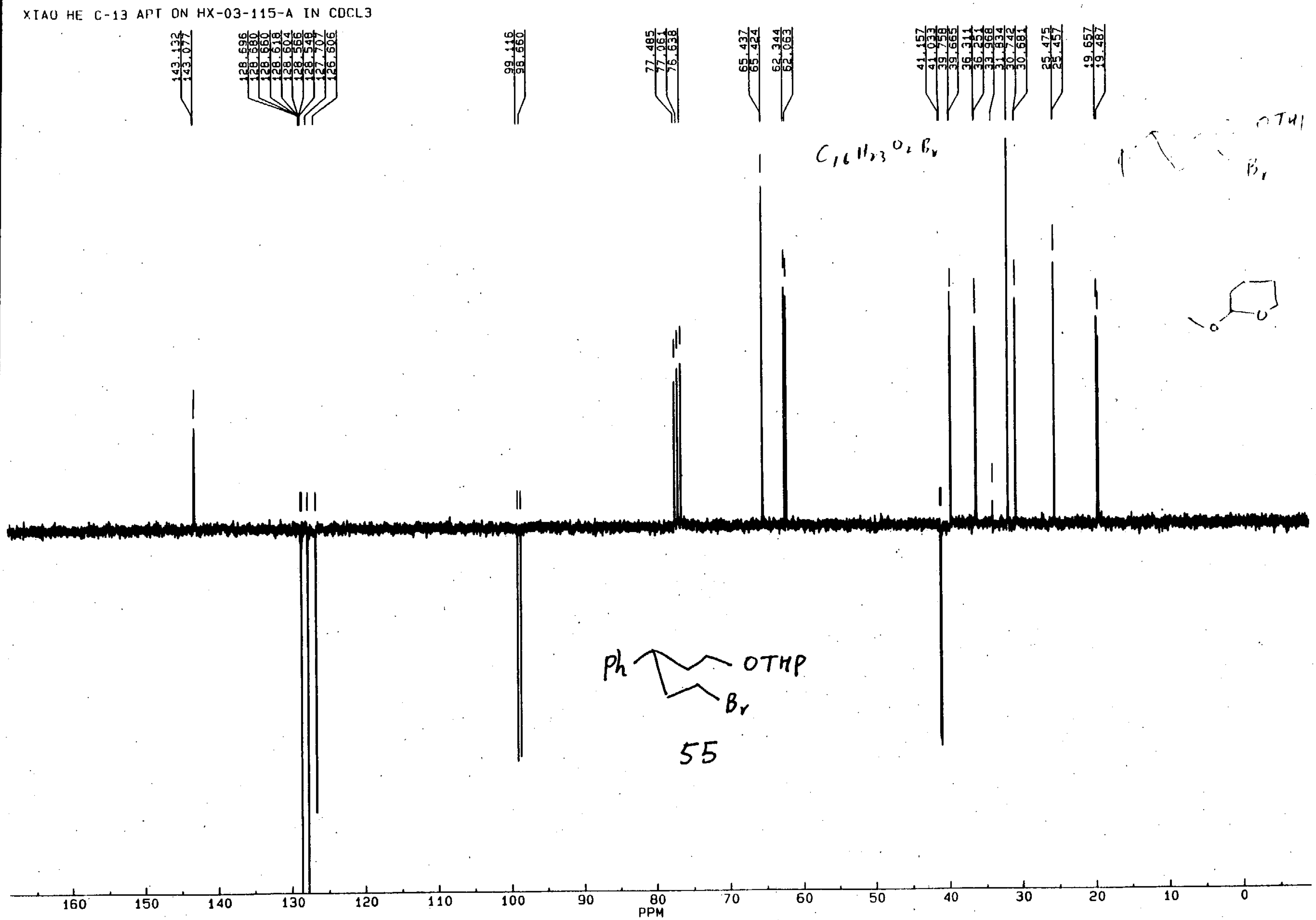
BRUKER

DE06310C
AU PROG:
CAPT3.AU
DATE 6-12-95

SF	75.469
SY	112.0
O1	7300.000
SI	32768
TD	32768
SW	21739.130
HZ/PT	1.327
PW	0.0
RD	0.0
AQ	.754
RG	800
NS	1527
TE	297
FW	27200
O2	4800.000
DP	18H CPD
LB	1.200
GB	.010
CX	36.00
CY	10.00
F1	224.998
F2	-8.994
HZ/CM	490.530
PPM/CM	6.500
SR	-1400.76
D2	.001000
S2	18H
D1	2.000000
P9	100.00
S1	0H
P3	2.00
D3	.004000
P1	9.00
D4	.002000
P2	18.00
P4	8.60
RD	0.0
PW	0.0
DE	31.30
NS	1527
DS	2


54
XIAO HE C-13 APT ON HX-02-113-AB IN CDCL3
DATE 1-1-96
PPM

55

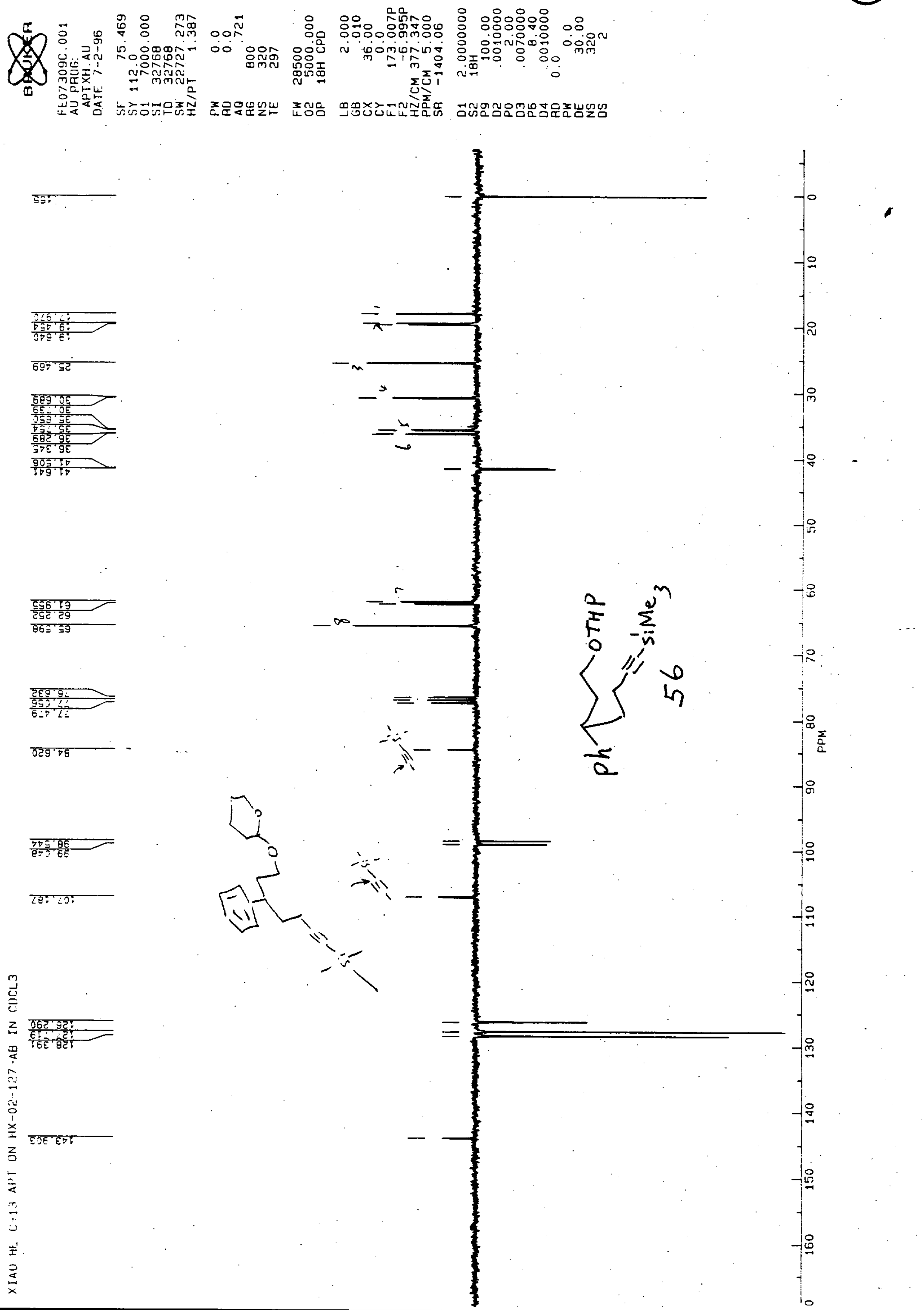


BRUKER

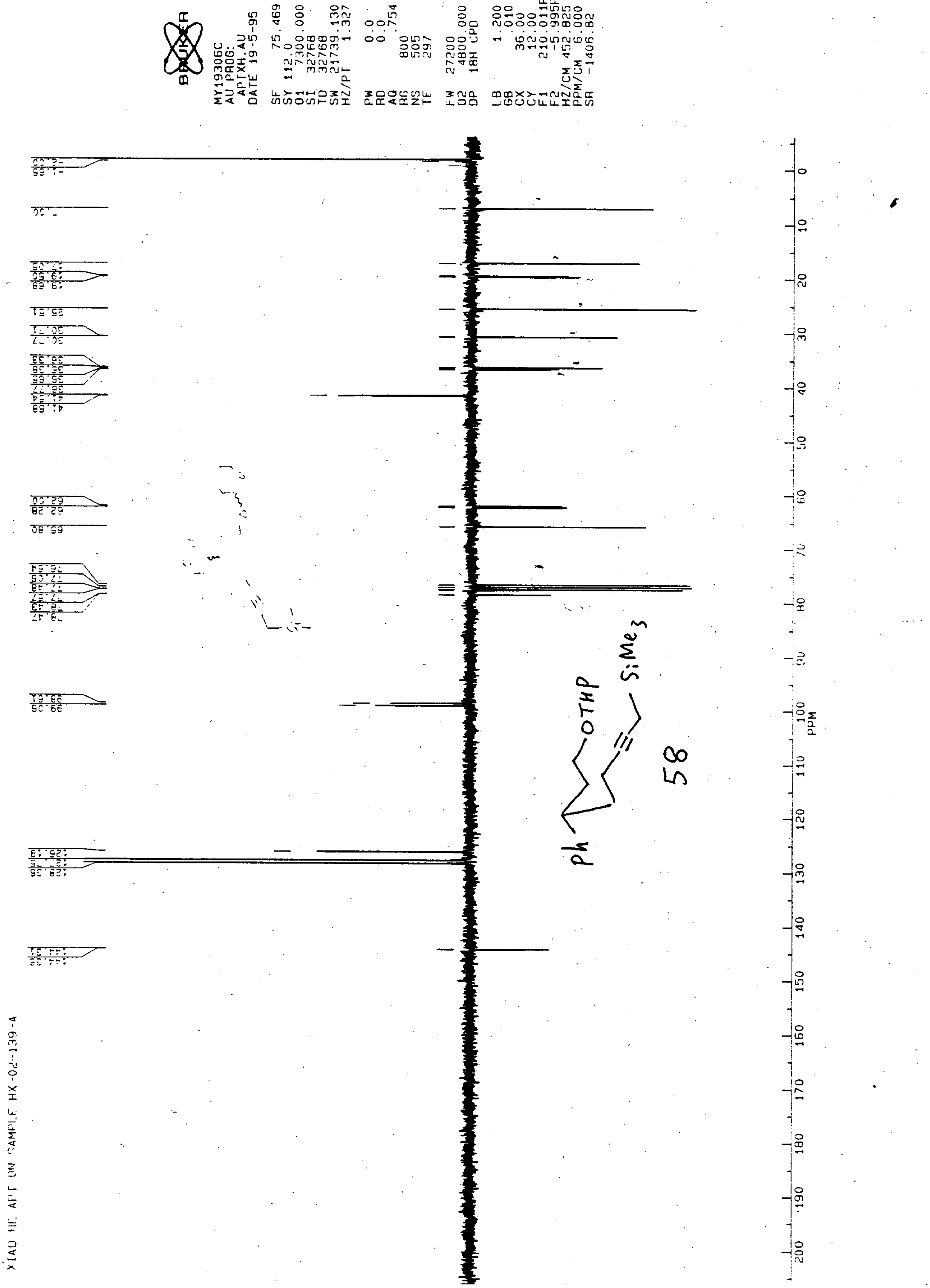
DE12308C.001
AU PROG:
APTXH.AU
DATE 1-1-96

SF	75.469
SY	112.0
O1	7300.000
SI	65536
TD	32768
SW	21739.130
HZ/PT	.663
PW	0.0
RD	0.0
AQ	.754
RG	800
NS	1200
TE	297
FW	27200
O2	4800.000
DP	18H CPD
LB	.700
GB	.010
CX	36.00
CY	0.0
F1	170.998P
F2	-9.001P
HZ/CM	377.342
PPM/CM	5.000
SR	-1405.49
D1	2.0000000
S2	18H
P9	100.00
D2	.0010000
P0	2.00
D3	.0070000
P6	8.40
D4	.0010000
RD	0.0
PW	0.0
DE	31.30
NS	1200
DS	2

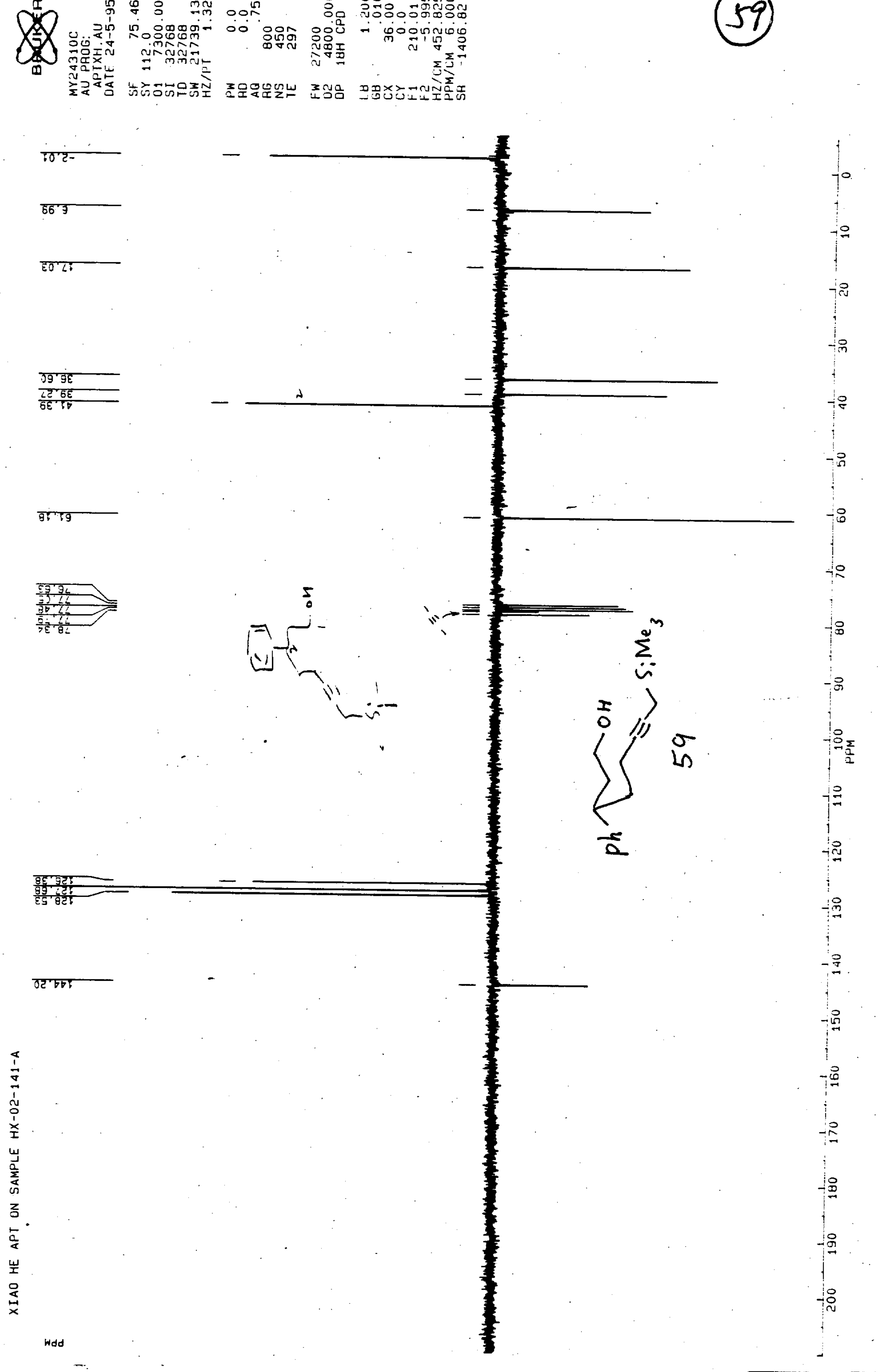
56



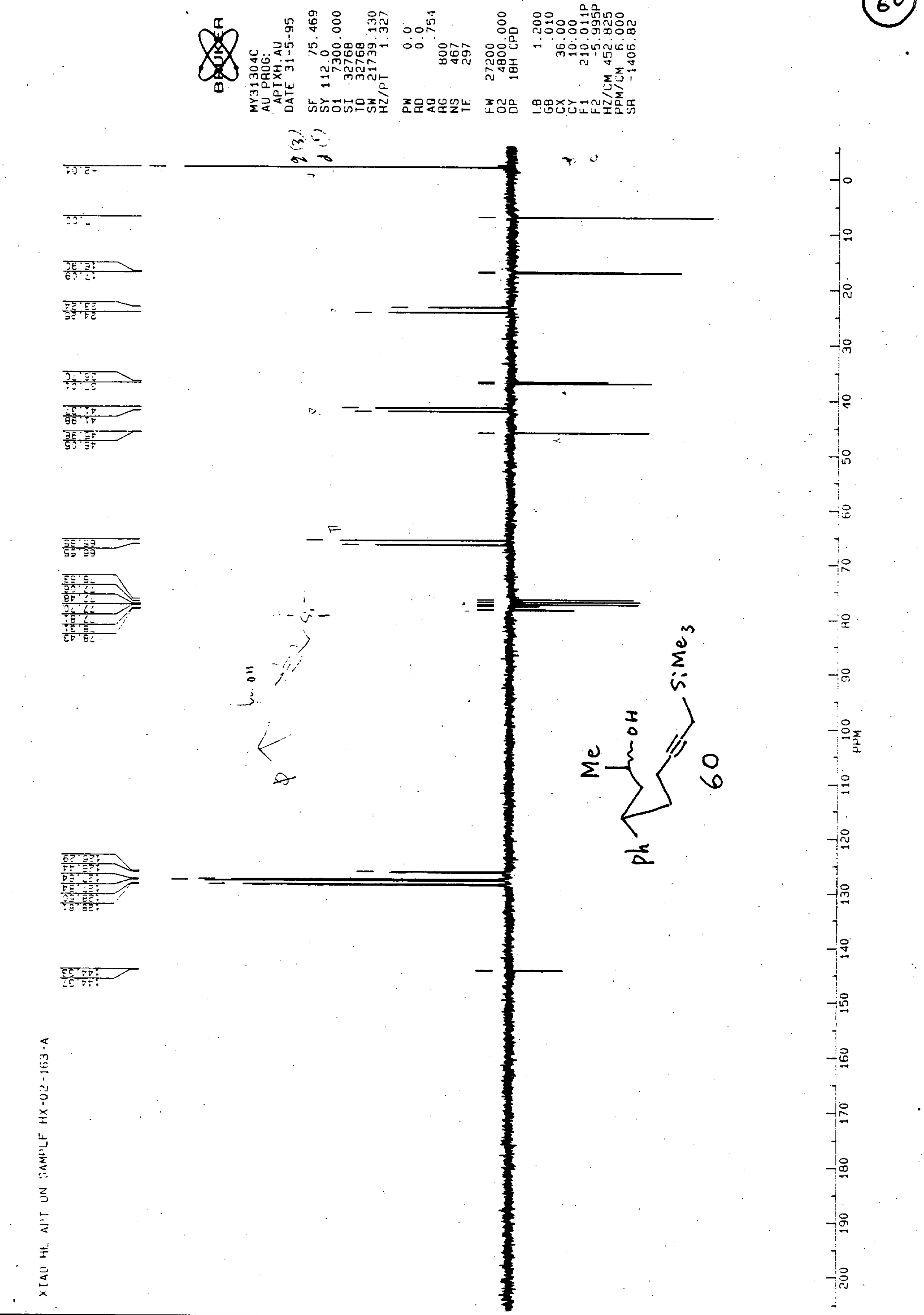
57
BRUKER
MY11311C
AU PROG:
APTXH.AU
DATE 11-5-95
SF 75.469
SY 112.0
O1 7300.000
SI 32768
TD 32768
SW 21739.130
HZ/PT 1.327
PW 0.0
RD 0.0
AQ .754
RG 800
NS 349
TE 297
FW 27200
O2 4800.000
DP 18H CPD
LB 1.200
GB .010
CX 36.00
CY 12.00
F1 210.011P
F2 -5.995P
HZ/CM 452.825
PPM/CM 6.000
SR -1401.51
Ph
OTHP
H
57
PPM
XIAO HE APT ON SAMPLE HX-02-129-A


MY19306C
AU PROG:
APTXH.AU
DATE 19-5-95
SF 75.469
SY 112.0
O1 7300.000
SI 32768
TD 32768
SW 21739.130
HZ/PT 1.327
PW 0.0
RD 0.0
AQ .754
RG 800
NS 505
TE 297
FW 27200
O2 4800.000
DP 18H CPD
LB 1.200
GB .010
CX 36.00
CY 12.00
F1 210.011P
F2 -5.995P
HZ/CM 452.825
PPM/CM 6.000
SR -1406.82
Ph
OTHP
SiMe3
58
PPM
XIAO HE APT ON SAMPLE HX-02-139-A

59

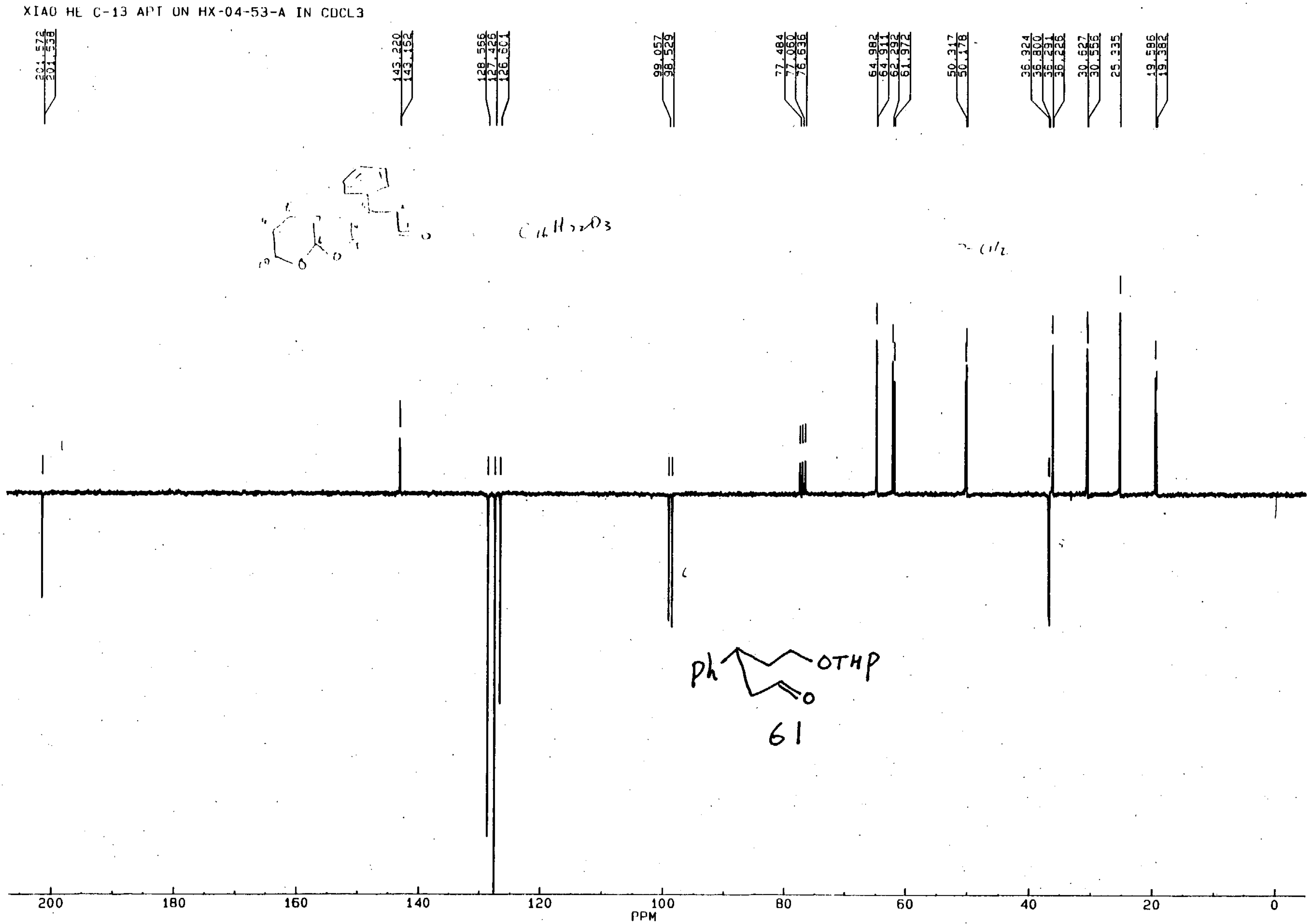

XIAO HE APT ON SAMPLE HX-02-141-A
MY24310C
AU PROG:
APTXH.AU
DATE 24-5-95
-2.01
6.99
17.03
36.60
39.27
41.39
61.18
78.34
144.20
PPM
Ph
OH
SiMe3
59

60


MY31304C
AU PROG:
APTXH.AU
DATE 31-5-95
SF 75.469
SY 112.0
O1 7300.000
SI 32768
TD 32768
SW 21739.130
HZ/PT 1.327
PW 0.0
RD 0.0
AQ .754
RG 800
NS 467
TE 297
FW 27200
O2 4800.000
DP 18H CPD
LB 1.200
GB .010
CX 36.00
CY 10.00
F1 210.011P
F2 -5.995P
HZ/CM 452.825
PPM/CM 6.000
SR -1406.82
PPM
Me
OH
SiMe3
Ph
60
XIAO HL APT ON SAMPLE HX-02-163-A

(61)

XIAO HL C-13 APT ON HX-04-53-A IN CDCL3



BRUKER

JN17308C.001
AU PROG:
CAPT3.AU
DATE 1-9-96
TIME 13:06

SF 75.469
SY 112.0
O1 7300.000
SI 32768
TD 32768
SW 21739.130
HZ/PT 1.327

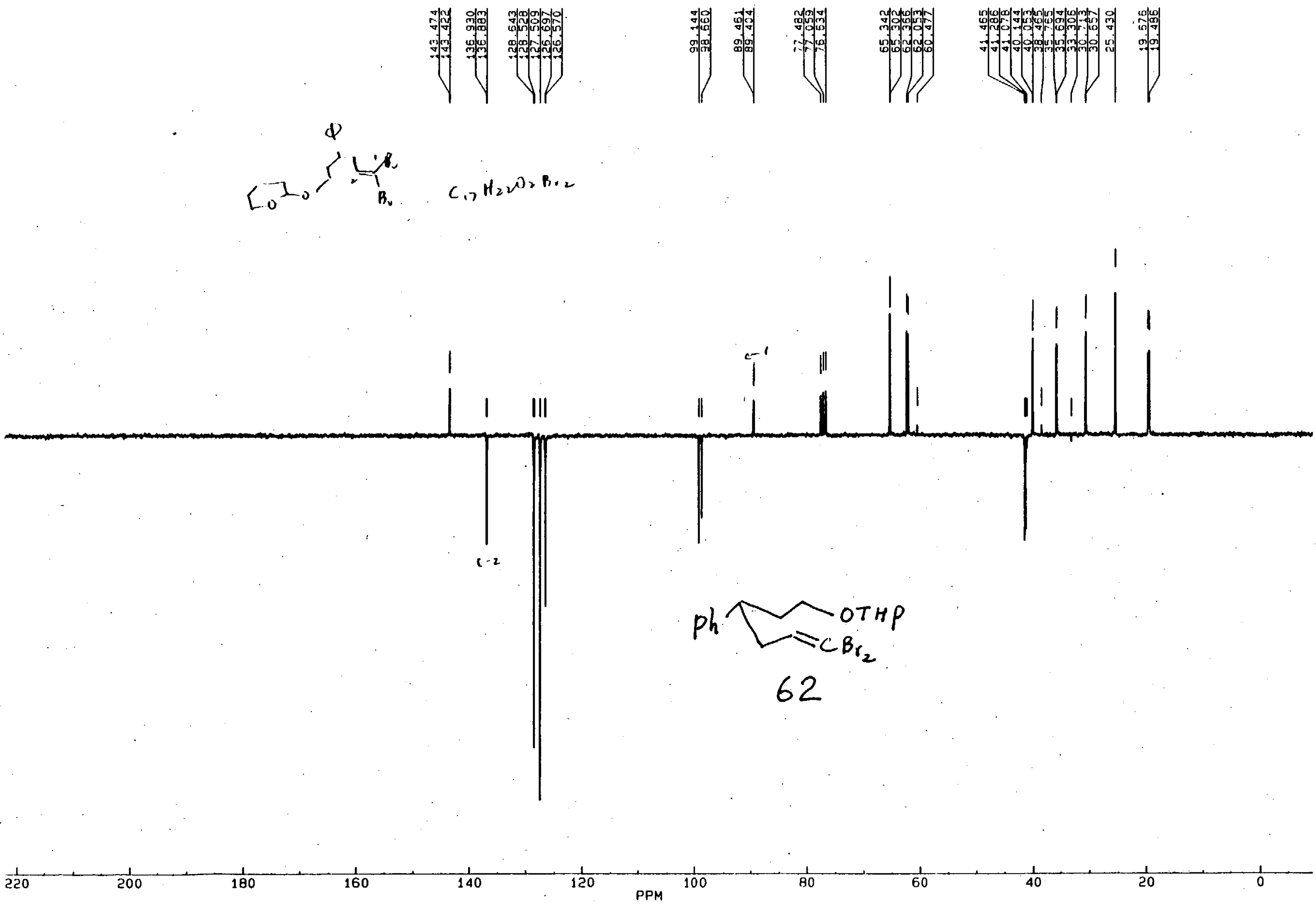
PW 0.0
RD 0.0
AQ .754
RG 800
NS 1260
TE 297

FW 27200
O2 4800.000
DP 18H CPD

LB 1.200
GB .010
CX 36.00
CY 0.0
F1 210.996P
F2 -4.993P
HZ/CM 452.788
PPM/CM 6.000
SR -1398.86

D2 .0010000
S2 18H
D1 2.0000000
P9 100.00
S1 0H
P3 2.00
D3 .0040000
P1 9.00
D4 .0020000
P2 18.00
P4 8.60
RD 0.0
PW 0.0
DE 31.30
NS 1260
DS 2

XIAO HE APT ON HX-04-65-A; CDCL3



62

BRUKER

JN060F.105
AU PROG:
X25.AU
DATE 2-8-96
TIME 2:46

SF 75.469
SY 112.0
O1 7000.000
SI 32768
TD 32768
SW 22727.273
HZ/PT 1.387

PW 0.0
RD 0.0
AQ .721
RG 800
NS 2000
TE 297

FW 28500
O2 4425.000
DP 18H CPD

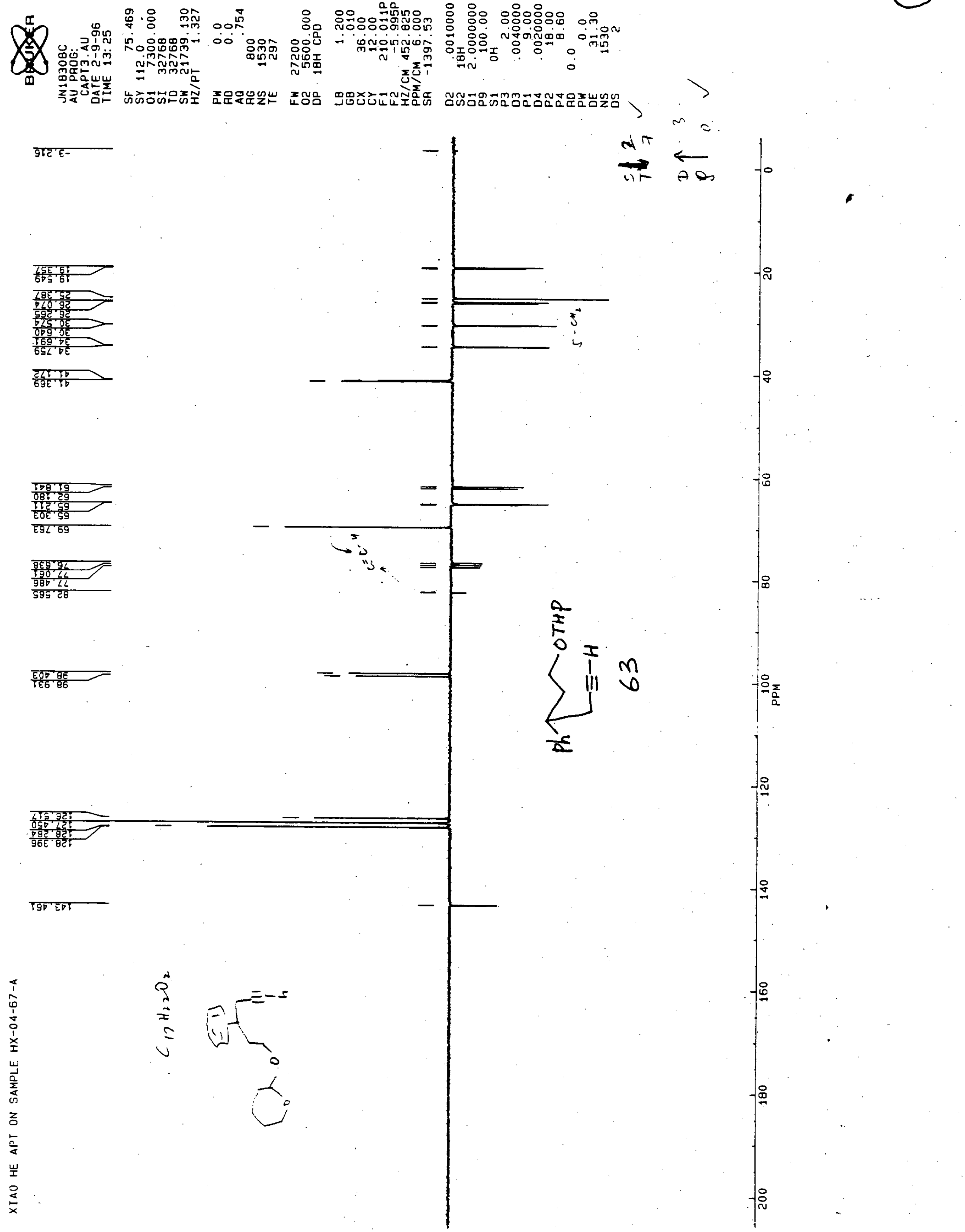
LB 2.000
GB .010
CX 36.00
CY 10.00
F1 224.996P
F2 -8.990P
HZ/CM 490.516
PPM/CM 6.500
SR -1401.91

D1 1.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 1.80
D3 .0070000
P6 8.40
D4 .0010000
RGA
RD 0.0
PW 0.0
DE 30.00
NS 2000
DS 2

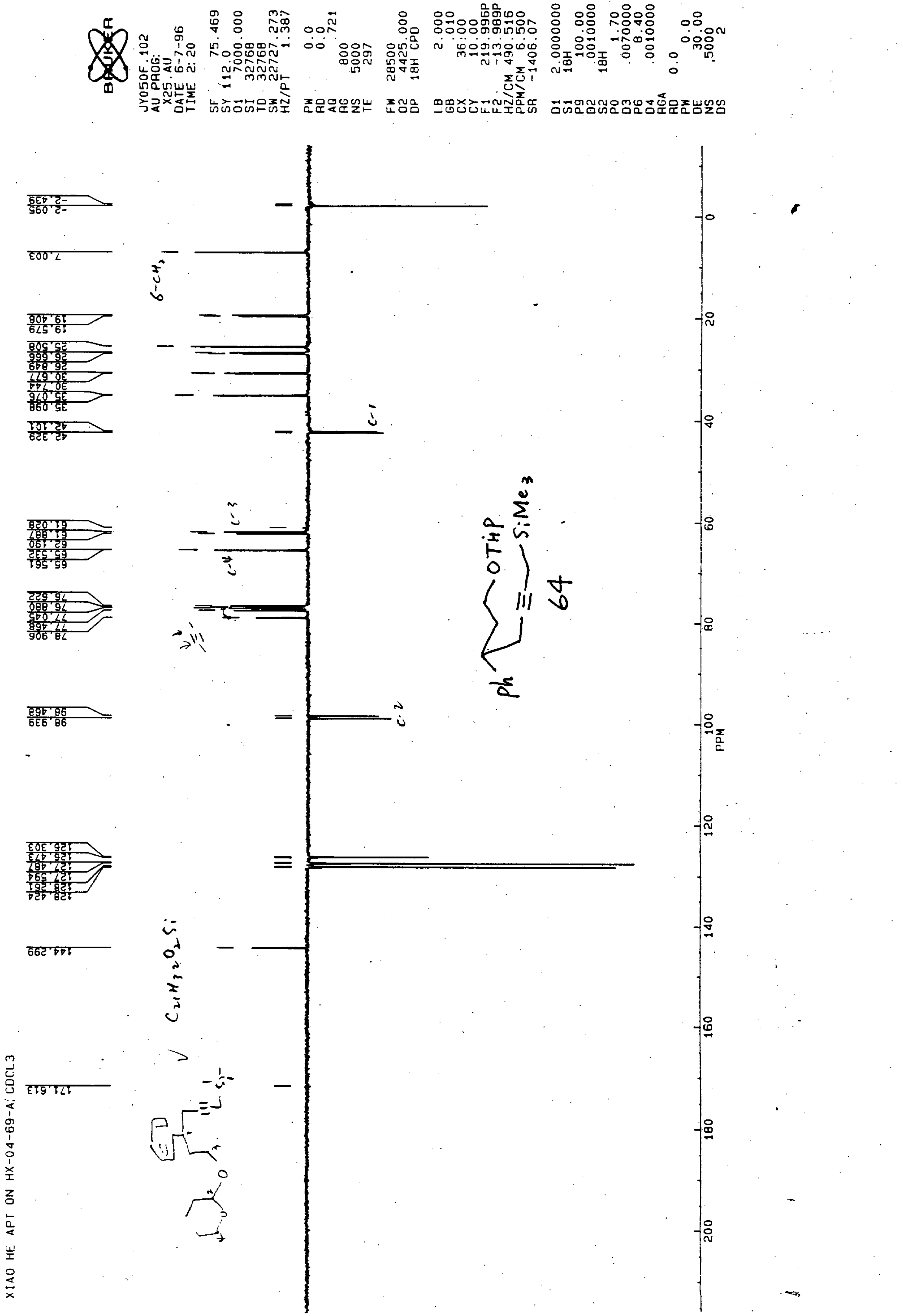
S T 7
D Q 3+3

62

63



(64)


XIAO HE APT ON HX-04-69-A; CDCL3
JY050F.102
AU PROG:
X25.AU
DATE 6-7-96
TIME 2:20
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7.003
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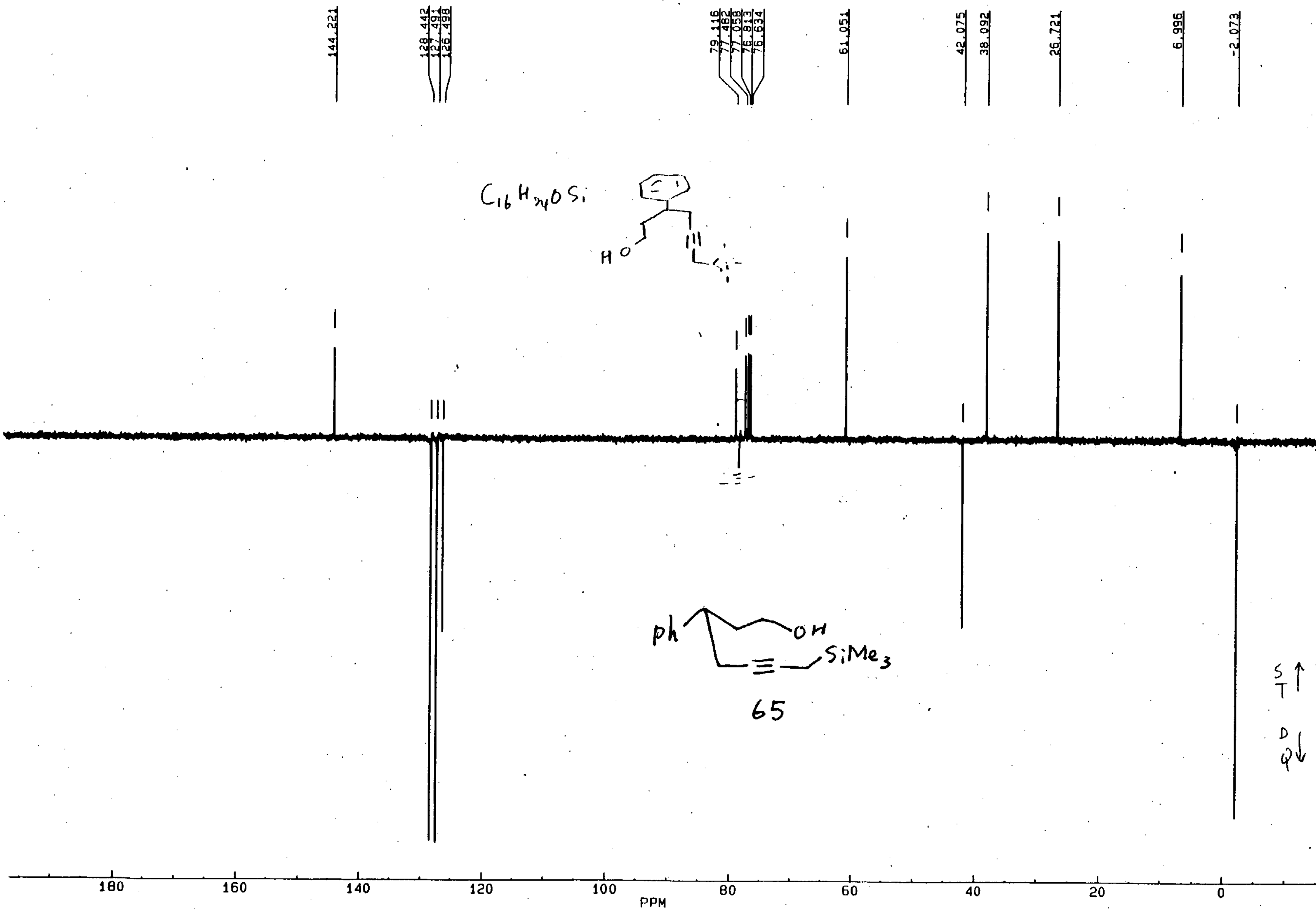
25.508
26.666
26.849
30.677
30.744
35.076
35.098
42.101
42.329
61.028
61.887
62.190
65.332
65.561
76.622
76.880
77.045
77.468
78.906
98.468
98.939
126.303
126.473
127.487
127.594
128.261
128.424
144.299
171.613
6-CH3
C-1
C-3
C-4
C-2
OTHP
SiMe3
64
Ph
C21H32O2Si
PPM

65

XIAO HE C-13 APT ON HX-04-71-A IN CDCL3



S ↑ 3
T 4

D ↓ 4
Q 1

BRUKER

JN20308C.001
AU PROG:
CAPT3.AU
DATE 4-9-96
TIME 13:13

SF	75.469
SY	112.0
O1	7300.000
SI	65536
TD	32768
SW	21739.130
HZ/PT	.663
PW	0.0
RD	0.0
AQ	.754
RG	800
NS	1680
TE	297
FW	27200
O2	4800.000
DP	18H CPD
LB	1.000
GB	.010
CX	36.00
CY	11.00
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F2	-15.999P
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P9	100.00
S1	0H
P3	2.00
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P1	9.00
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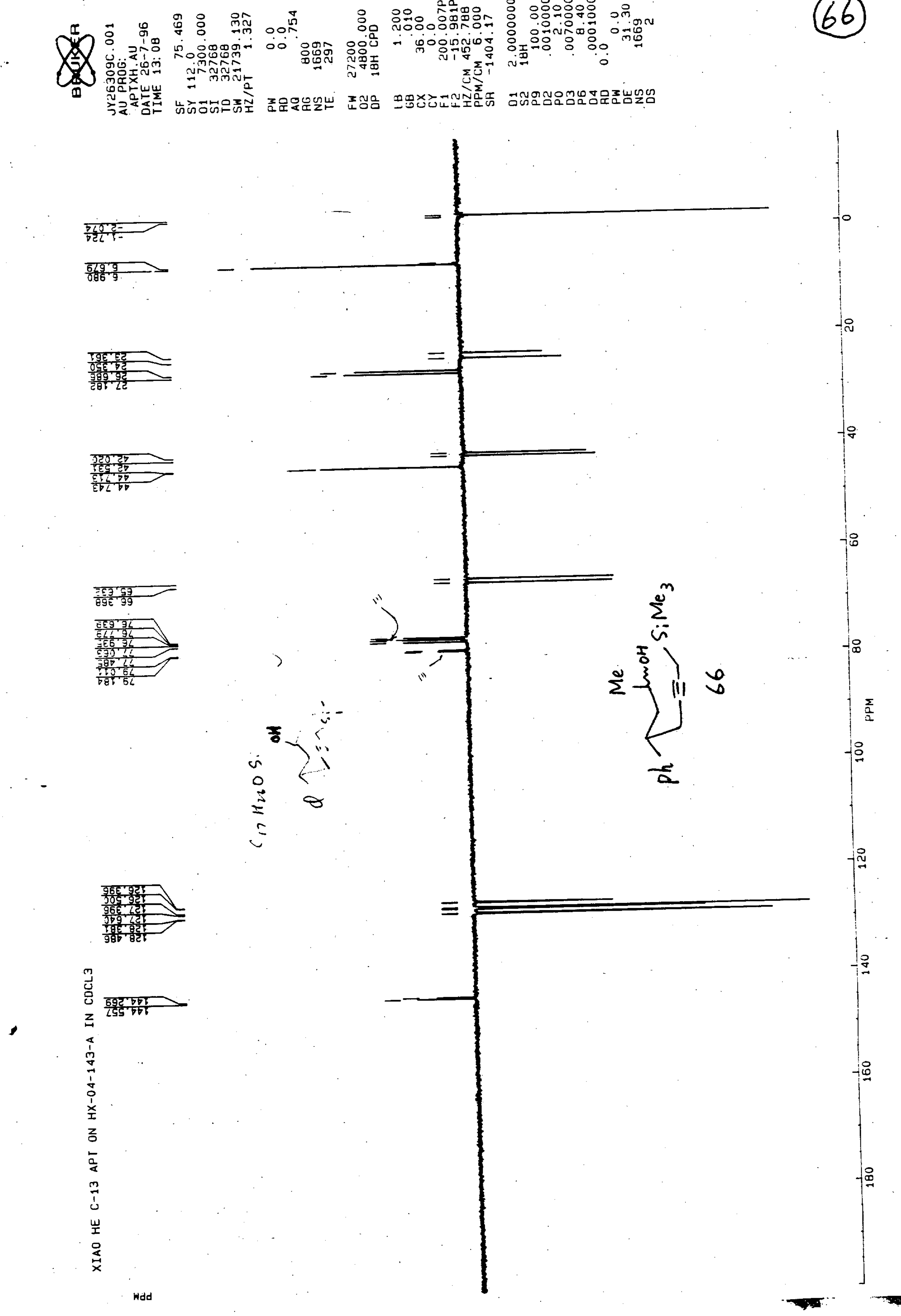
DS	2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SDL:DLC9511 3-Oct-95

Structure Determination Laboratory

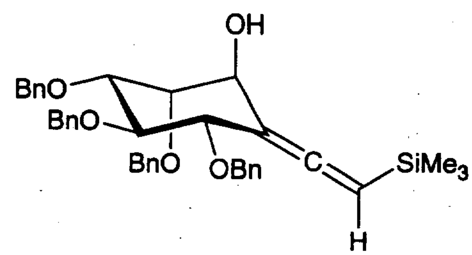
Report on the

Complete Structure Determination and Refinement of

$C_{39}H_{44}O_5Si$

for

Professor D. L. J. Clive



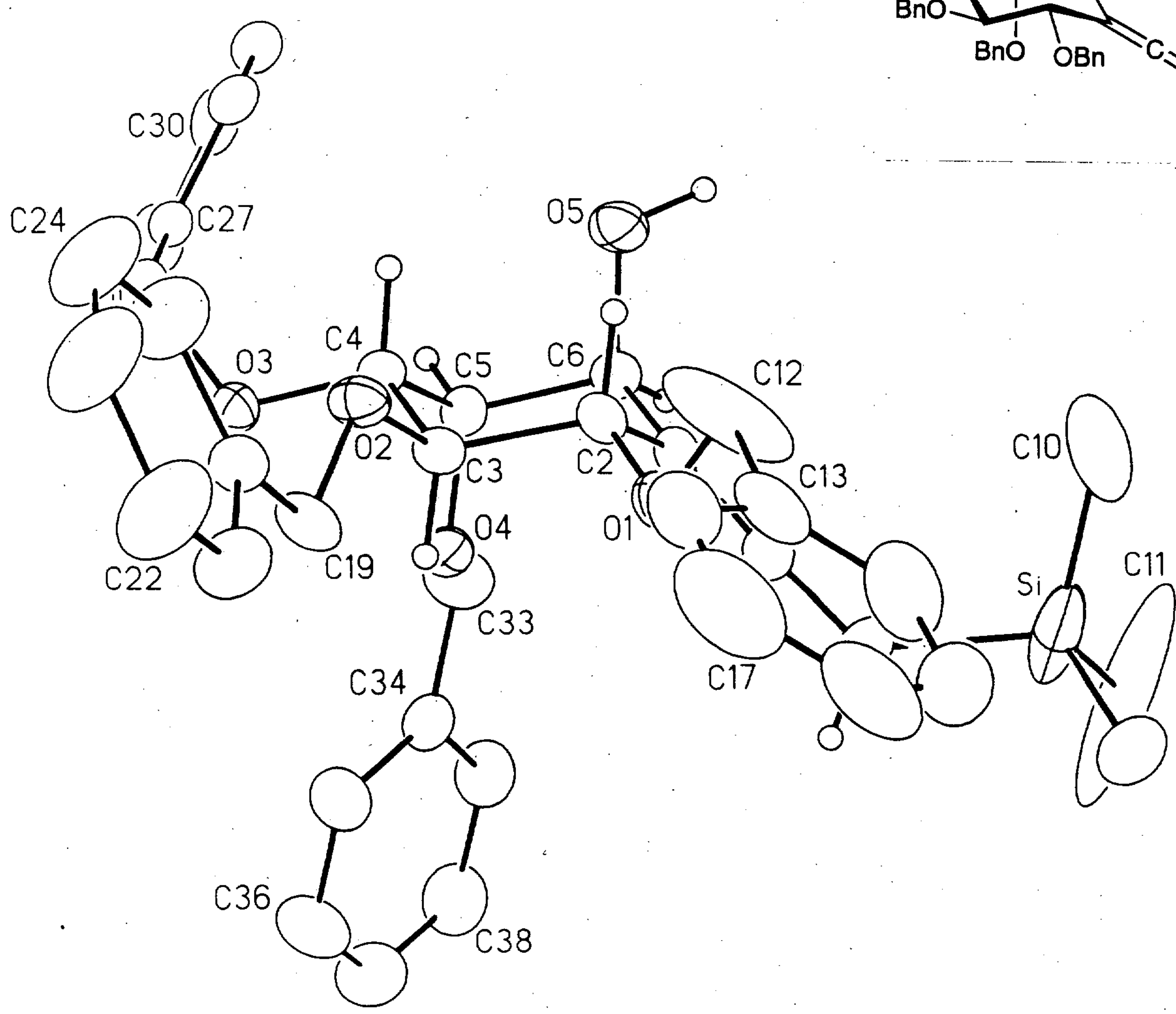
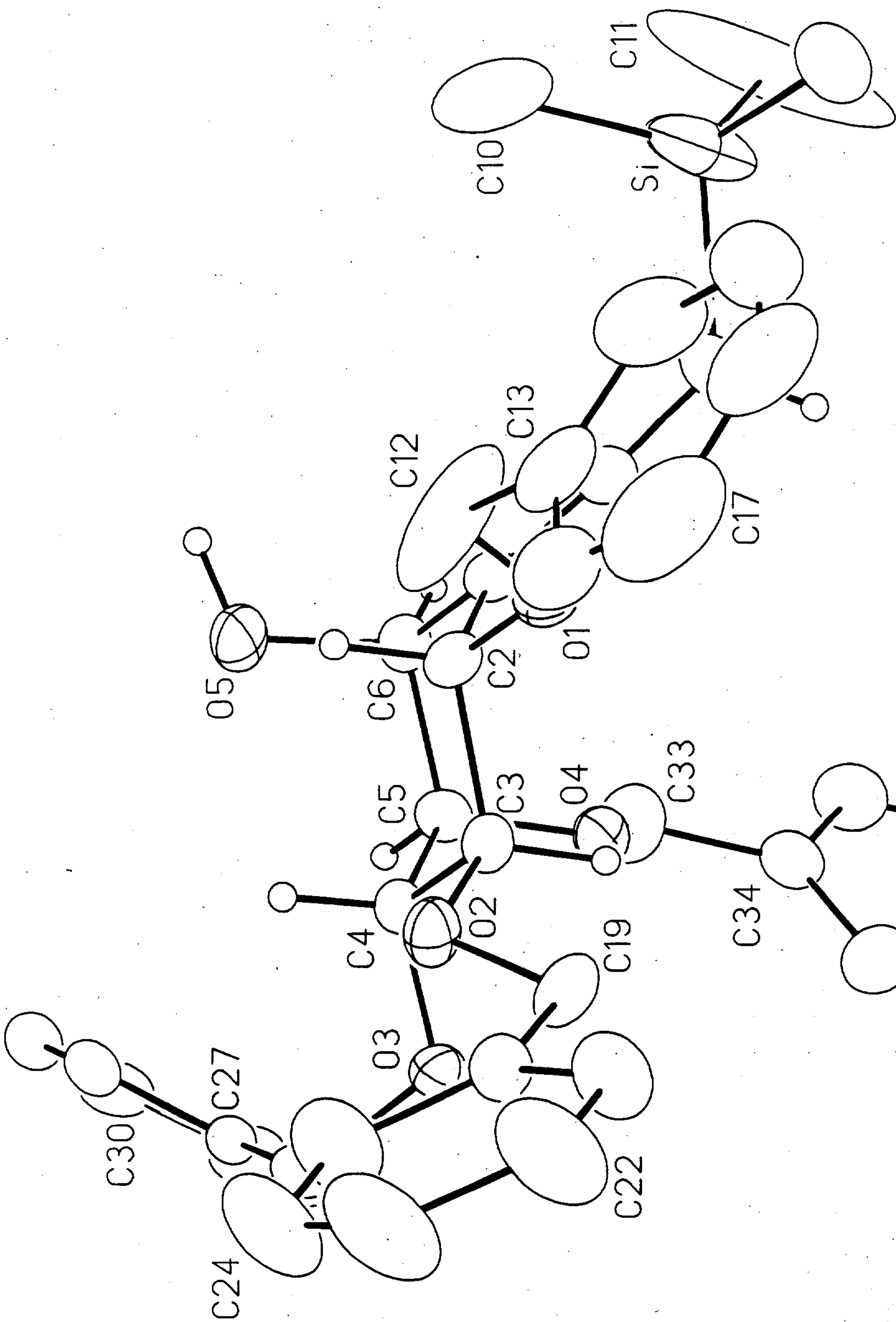


Figure Legends

Figure 1. Perspective view of the $C_{39}H_{44}O_5Si$ 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, and are not shown for the benzyl or trimethylsilyl groups.

Figure 2. View of the molecule omitting the phenyl carbons of the benzyl groups.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C13
C12
C17
O5
C6
C2
O1
C5
C3
O4
C33
C38
C34
C4
O2
C19
C36
C27
O3
C30
C22
C24

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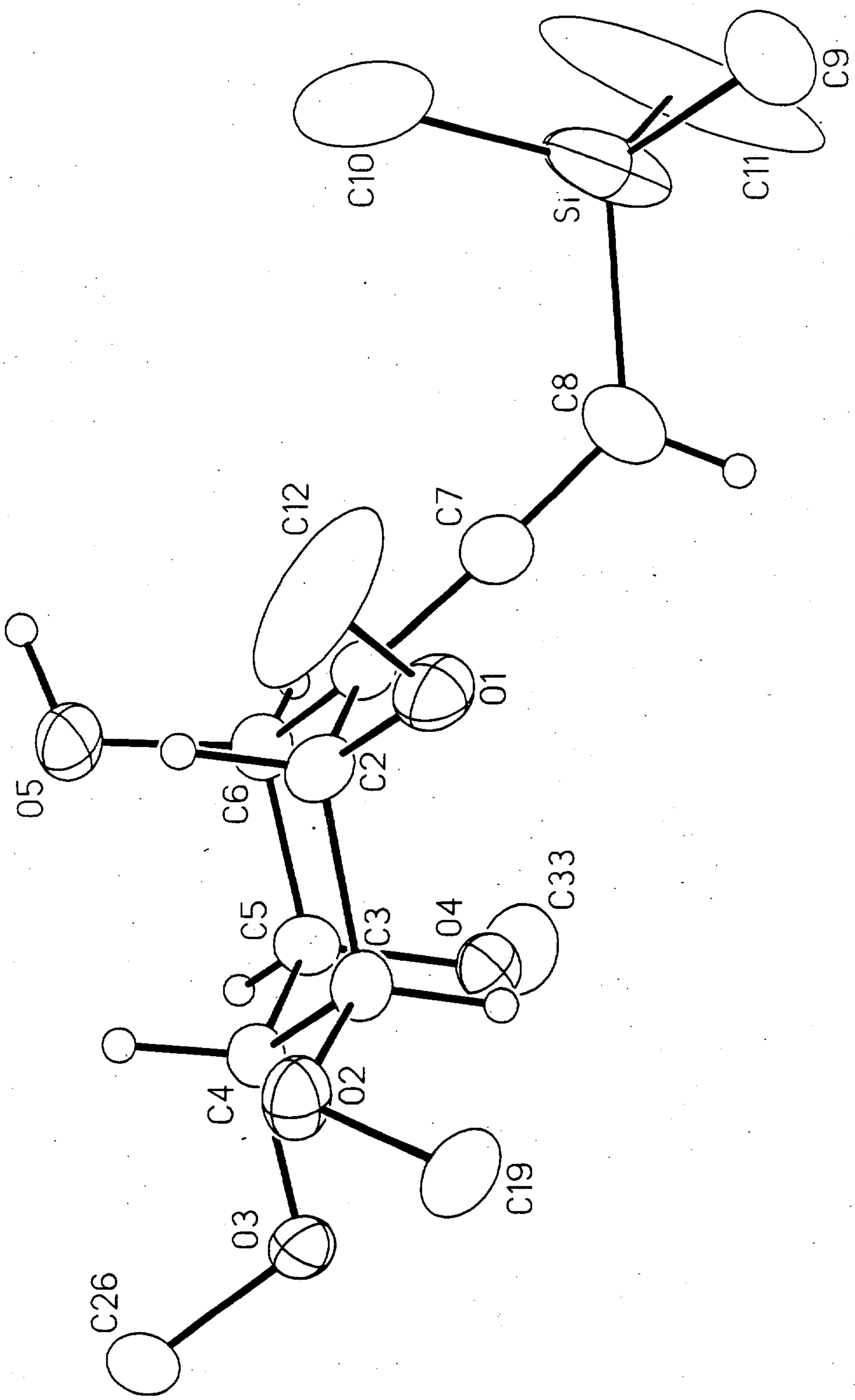

List of Tables

Table 1. Crystallographic Experimental Details

formula	$C_{39}H_{44}O_5Si$
formula weight	620.83
crystal dimensions (mm)	0.44 × 0.24 × 0.12
crystal system	monoclinic
space group	$P2_1$ (No. 4)[a]
unit cell parameters[b]	
a (Å)	11.401 (2)
b (Å)	12.219 (2)
c (Å)	13.716 (2)
β (deg)	108.353 (10)
V (Å^3)	1813.6 (5)
Z	2
ρ_{calcd} (g cm^{-3})	1.137
μ (mm^{-1})	0.105

B. Data Collection and Refinement Conditions

diffractometer	Siemens P4/RA[c]
radiation (λ [Å])	Mo Kα (0.71073)
monochromator	incident-beam, graphite crystal
temperature (°C)	–60
scan type	θ–2θ
data collection 2θ limit (deg)	50.0
total data collected	6323 ($-13 \le h \le 13$, $-14 \le k \le 14$, $0 \le l \le 16$)
independent reflections	6323

(continued)

Table 1. Crystallographic Experimental Details (continued)

number of observations (*NO*)	3100 ($F_o^2 \geq 2\sigma(F_o^2)$)
structure solution method	direct methods (*SHELXS–86*[d])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[e])
data/restraints/parameters	6315 [$F_o^2 \geq -3\sigma(F_o^2)$]/0/407
goodness-of-fit (S)[f]	1.089 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[g]	
$F_o^2 > 2\sigma(F_o^2)$	$R_1 = 0.0810$, $wR_2 = 0.1763$
all data	$R_1 = 0.1738$, $wR_2 = 0.2366$
largest difference peak and hole	0.349 and –0.318 e Å^{-3}

[a]The absolute stereochemistry of the molecule could not be assigned crystallographically but had been established via chemical means.

[b]Obtained from least-squares refinement of 28 reflections with $23.1° < 2\theta < 25.6°$.

[c]Programs for diffractometer operation and data collection and reduction were those of the *XSCANS* system supplied by Siemens.

[d]Sheldrick, G. M. *Acta Crystallogr.* 1990, *A46*, 467.

[e]Sheldrick, G. M. *J. Appl. Cryst.*, in preparation. Refinement on F_o^2 for all reflections except for 8 having $F_o^2 < -3\sigma(F_o^2)$. Weighted R-factors wR_2 and all goodnesses of fit S are based on F_o^2; conventional R-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. R-factors based on F_o^2 are statistically about twice as large as those based on F_o, and R-factors based on ALL data will be even larger.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0550P)^2 + 1.9911P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters

Atom	x	y	z	U_{eq}, Å^2
O1	0.0736(5)	-0.1483(4)	0.2919(3)	0.0691(14)*
O2	-0.1369(4)	-0.2070(4)	0.1269(4)	0.0639(13)*
O3	-0.1153(4)	-0.1985(4)	-0.0694(4)	0.0632(13)*
O4	0.1403(4)	-0.1638(4)	-0.0143(3)	0.0595(13)*
O5	0.0347(5)	0.0937(4)	0.0613(5)	0.082(2)*
C1	0.1538(7)	-0.0476(5)	0.1743(5)	0.059(2)*
C2	0.0427(7)	-0.0930(6)	0.1955(5)	0.062(2)*
C3	-0.0250(6)	-0.1741(6)	0.1112(5)	0.054(2)*
C4	-0.0553(6)	-0.1193(5)	0.0065(5)	0.053(2)*
C5	0.0607(6)	-0.0750(6)	-0.0134(5)	0.060(2)*
C6	0.1244(7)	0.0082(6)	0.0698(5)	0.062(2)*
C7	0.2668(8)	-0.0671(6)	0.2305(6)	0.068(2)*
C8	0.3796(8)	-0.0834(7)	0.2901(6)	0.092(3)*
C9	0.5072(9)	-0.0795(8)	0.5179(7)	0.105(3)*
C10	0.3782(23)	0.1195(10)	0.4087(13)	0.444(25)*
C11	0.6184(16)	0.0335(24)	0.3804(10)	0.509(30)*
C12	0.0263(19)	-0.1000(9)	0.3604(9)	0.223(10)*
C13	0.0437(17)	-0.1696(9)	0.4544(8)	0.099(4)*
C14	0.1503(15)	-0.1669(11)	0.5273(14)	0.134(4)*
C15	0.1703(16)	-0.2285(16)	0.6138(12)	0.148(6)*
C16	0.0819(26)	-0.2903(12)	0.6275(11)	0.163(9)*
C17	-0.0250(20)	-0.2946(12)	0.5534(17)	0.158(6)*
C18	-0.0439(13)	-0.2320(13)	0.4664(12)	0.127(4)*
C19	-0.1328(7)	-0.3147(6)	0.1643(6)	0.069(2)*
C20	-0.2439(7)	-0.3393(6)	0.1946(5)	0.058(2)*
C21	-0.2377(8)	-0.4192(8)	0.2649(7)	0.088(3)*
C22	-0.3401(10)	-0.4428(11)	0.2966(9)	0.131(4)*
C23	-0.4463(10)	-0.3934(11)	0.2554(9)	0.129(5)*
C24	-0.4577(9)	-0.3170(11)	0.1815(9)	0.125(4)*
C25	-0.3559(10)	-0.2905(9)	0.1507(7)	0.107(3)*
C26	-0.2279(6)	-0.1594(6)	-0.1429(5)	0.064(2)*
C27	-0.2055(6)	-0.0751(6)	-0.2142(6)	0.055(2)*
C28	-0.2335(7)	0.0325(7)	-0.2069(6)	0.069(2)*

Table 2. Atomic Coordinates and Displacement Parameters (continued)

Atom	x	y	z	U_{eq}, Å^2
C29	-0.2121(8)	0.1117(7)	-0.2724(8)	0.085(3)*
C30	-0.1618(9)	0.0775(9)	-0.3455(8)	0.091(3)*
C31	-0.1311(8)	-0.0290(9)	-0.3539(6)	0.089(3)*
C32	-0.1531(7)	-0.1048(7)	-0.2882(6)	0.074(2)*
C33	0.2160(9)	-0.1430(8)	-0.0751(7)	0.096(3)*
C34	0.2911(7)	-0.2442(7)	-0.0818(5)	0.069(2)*
C35	0.2503(8)	-0.3481(8)	-0.0768(6)	0.081(2)*
C36	0.3180(9)	-0.4373(8)	-0.0851(7)	0.098(3)*
C37	0.4303(10)	-0.4228(11)	-0.1051(8)	0.109(3)*
C38	0.4710(10)	-0.3205(12)	-0.1102(8)	0.112(4)*
C39	0.4025(9)	-0.2293(9)	-0.0982(6)	0.091(3)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table 3. Selected Interatomic Distances (Å)

Atom1	Atom2	Distance
Si	C8	1.841(9)
Si	C9	1.827(9)
Si	C10	1.83(2)
Si	C11	1.821(15)
O1	C2	1.426(8)
O1	C12	1.358(11)
O2	C3	1.417(7)
O2	C19	1.409(7)
O3	C4	1.428(7)
O3	C26	1.442(7)
O4	C5	1.417(8)
O4	C33	1.399(9)
O5	C6	1.441(8)
C1	C2	1.493(10)
C1	C6	1.526(10)
C1	C7	1.297(10)
C2	C3	1.534(9)
C3	C4	1.522(9)
C4	C5	1.531(8)
C5	C6	1.530(9)
C7	C8	1.304(10)
C12	C13	1.505(14)
C13	C14	1.31(2)
C13	C18	1.31(2)
C14	C15	1.36(2)
C15	C16	1.32(2)
C16	C17	1.32(2)
C17	C18	1.38(2)
C19	C20	1.482(9)
C20	C21	1.359(11)
C20	C25	1.366(11)
C21	C22	1.398(12)
C22	C23	1.311(13)
C23	C24	1.353(13)
C24	C25	1.392(12)
C26	C27	1.496(9)
C27	C28	1.364(10)
C27	C32	1.378(10)
C28	C29	1.394(11)
C29	C30	1.367(12)
C30	C31	1.362(13)
C31	C32	1.369(11)
C33	C34	1.523(12)
C34	C35	1.361(11)
C34	C39	1.370(10)
C35	C36	1.360(11)
C36	C37	1.403(12)
C37	C38	1.343(14)
C38	C39	1.400(13)

Table 4. Selected Interatomic Angles (deg)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C8	Si	C9	109.9(4)	C14	C13	C18	118.8(12)
C8	Si	C10	107.7(6)	C13	C14	C15	120.8(13)
C8	Si	C11	108.8(7)	C14	C15	C16	121.0(16)
C9	Si	C10	109.4(8)	C15	C16	C17	118.4(17)
C9	Si	C11	106.8(6)	C16	C17	C18	120.0(17)
C10	Si	C11	114.2(12)	C13	C18	C17	121.0(14)
C2	O1	C12	113.6(7)	O2	C19	C20	111.0(6)
C3	O2	C19	113.1(5)	C19	C20	C21	119.1(7)
C4	O3	C26	113.7(5)	C19	C20	C25	123.4(7)
C5	O4	C33	112.6(6)	C21	C20	C25	117.3(8)
C2	C1	C6	113.5(6)	C20	C21	C22	120.5(9)
C2	C1	C7	124.1(7)	C21	C22	C23	121.2(10)
C6	C1	C7	121.5(7)	C22	C23	C24	119.9(10)
O1	C2	C1	112.3(6)	C23	C24	C25	119.7(10)
O1	C2	C3	108.2(5)	C20	C25	C24	121.2(9)
C1	C2	C3	110.5(6)	O3	C26	C27	112.8(5)
O2	C3	C2	109.4(5)	C28	C27	C32	118.2(7)
O2	C3	C4	108.7(5)	C26	C27	C28	121.6(7)
C2	C3	C4	109.8(5)	C26	C27	C32	120.2(7)
O3	C4	C3	107.7(5)	C27	C28	C29	122.0(8)
O3	C4	C5	110.6(5)	C28	C29	C30	117.4(8)
C3	C4	C5	111.8(5)	C29	C30	C31	122.2(9)
O4	C5	C4	108.8(5)	C30	C31	C32	119.0(9)
O4	C5	C6	111.1(5)	C27	C32	C31	121.3(8)
C4	C5	C6	109.6(6)	O4	C33	C34	110.7(7)
O5	C6	C1	109.9(6)	C33	C34	C35	123.2(8)
O5	C6	C5	105.3(5)	C33	C34	C39	118.0(8)
C1	C6	C5	108.4(5)	C35	C34	C39	118.8(9)
C1	C7	C8	177.3(9)	C34	C35	C36	122.1(8)
Si	C8	C7	128.4(8)	C35	C36	C37	119.5(10)
O1	C12	C13	112.0(9)	C36	C37	C38	118.6(10)
C12	C13	C14	118.7(17)	C37	C38	C39	121.4(9)
C12	C13	C18	122.5(18)	C34	C39	C38	119.6(9)

Table 5. Torsional Angles (deg)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C9	Si	C8	C7	116.4(8)	O3	C4	C5	O4	-57.4(6)
C10	Si	C8	C7	-2.7(13)	O3	C4	C5	C6	-179.1(5)
C11	Si	C8	C7	-127.0(12)	C3	C4	C5	O4	62.7(7)
C12	O1	C2	C1	115.7(11)	C3	C4	C5	C6	-59.0(7)
C12	O1	C2	C3	-122.1(10)	O4	C5	C6	O5	179.2(5)
C2	O1	C12	C13	171.1(12)	O4	C5	C6	C1	-63.2(7)
C19	O2	C3	C2	-106.6(6)	C4	C5	C6	O5	-60.4(7)
C19	O2	C3	C4	133.6(6)	C4	C5	C6	C1	57.2(7)
C3	O2	C19	C20	171.3(6)	C1	C7	C8	Si	-15.7(173)
C26	O3	C4	C3	130.8(6)	O1	C12	C13	C14	81.8(16)
C26	O3	C4	C5	-106.7(6)	O1	C12	C13	C18	-98.7(16)
C4	O3	C26	C27	70.1(8)	C12	C13	C14	C15	180.0(11)
C33	O4	C5	C4	152.6(6)	C18	C13	C14	C15	0.4(18)
C33	O4	C5	C6	-86.6(7)	C12	C13	C18	C17	-179.9(11)
C5	O4	C33	C34	-174.7(6)	C14	C13	C18	C17	-0.4(18)
C6	C1	C2	O1	177.7(5)	C13	C14	C15	C16	-1.7(22)
C6	C1	C2	C3	56.8(8)	C14	C15	C16	C17	2.8(25)
C7	C1	C2	O1	7.9(10)	C15	C16	C17	C18	-2.7(25)
C7	C1	C2	C3	-113.0(8)	C16	C17	C18	C13	1.6(21)
C2	C1	C6	O5	56.6(7)	O2	C19	C20	C21	-155.9(7)
C7	C1	C6	O5	-133.3(7)	O2	C19	C20	C25	28.4(11)
C2	C1	C6	C5	-58.0(8)	C19	C20	C21	C22	178.7(9)
C7	C1	C6	C5	112.1(8)	C25	C20	C21	C22	-5.3(13)
C2	C1	C7	C8	-76.5(168)	C19	C20	C25	C24	179.6(9)
C6	C1	C7	C8	114.5(167)	C21	C20	C25	C24	3.7(14)
O1	C2	C3	O2	62.9(7)	C20	C21	C22	C23	4.0(17)
O1	C2	C3	C4	-177.9(6)	C21	C22	C23	C24	-0.8(20)
C1	C2	C3	O2	-173.8(5)	C22	C23	C24	C25	-0.8(20)
C1	C2	C3	C4	-54.5(7)	C23	C24	C25	C20	-0.8(18)
O2	C3	C4	O3	-61.8(7)	O3	C26	C27	C28	-108.0(7)
O2	C3	C4	C5	176.5(5)	O3	C26	C27	C32	70.7(8)
C2	C3	C4	O3	178.6(5)	C26	C27	C28	C29	179.5(7)
C2	C3	C4	C5	56.8(7)	C32	C27	C28	C29	0.8(10)

Table 5. Torsional Angles (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C26	C27	C32	C31	-179.7(7)	C33	C34	C35	C36	178.6(9)
C28	C27	C32	C31	-1.0(10)	C39	C34	C35	C36	1.7(13)
C27	C28	C29	C30	0.2(11)	C33	C34	C39	C38	-176.7(9)
C28	C29	C30	C31	-1.2(13)	C35	C34	C39	C38	0.4(13)
C29	C30	C31	C32	1.1(14)	C34	C35	C36	C37	-3.6(14)
C30	C31	C32	C27	0.0(12)	C35	C36	C37	C38	3.4(16)
O4	C33	C34	C35	30.3(11)	C36	C37	C38	C39	-1.4(17)
O4	C33	C34	C39	-152.7(7)	C37	C38	C39	C34	-0.5(16)

Table 6. Anisotropic Displacement Parameters (U_{ij}, Å^2)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si	0.158(3)	0.146(3)	0.096(2)	0.046(2)	-0.050(2)	-0.087(3)
O1	0.094(4)	0.063(3)	0.049(3)	-0.003(3)	0.019(3)	0.003(3)
O2	0.062(3)	0.050(3)	0.083(3)	0.014(3)	0.027(3)	0.003(2)
O3	0.068(3)	0.045(3)	0.065(3)	0.002(2)	0.004(3)	-0.005(2)
O4	0.062(3)	0.056(3)	0.061(3)	0.014(2)	0.020(2)	-0.003(3)
O5	0.072(3)	0.045(3)	0.118(5)	0.012(3)	0.018(3)	-0.001(3)
C1	0.067(5)	0.044(4)	0.058(4)	-0.004(3)	0.006(4)	-0.003(4)
C2	0.071(5)	0.049(4)	0.061(5)	-0.009(4)	0.016(4)	0.001(4)
C3	0.052(4)	0.045(4)	0.065(4)	0.003(3)	0.020(3)	0.003(3)
C4	0.051(4)	0.041(4)	0.061(4)	0.005(3)	0.009(4)	0.002(3)
C5	0.068(5)	0.045(4)	0.056(5)	0.014(3)	0.003(4)	-0.009(4)
C6	0.062(5)	0.043(4)	0.075(5)	0.011(4)	0.012(4)	-0.003(4)
C7	0.087(6)	0.049(4)	0.060(5)	0.009(4)	0.012(5)	-0.010(4)
C8	0.082(6)	0.092(7)	0.084(6)	0.021(5)	-0.002(5)	-0.009(5)
C9	0.096(6)	0.122(8)	0.086(7)	0.012(6)	0.014(5)	0.014(6)
C10	0.716(49)	0.054(8)	0.258(20)	-0.028(10)	-0.279(27)	0.055(15)
C11	0.293(23)	1.035(74)	0.109(11)	0.164(23)	-0.066(13)	-0.473(38)
C12	0.517(30)	0.098(9)	0.106(9)	0.022(7)	0.173(14)	0.099(13)
C13	0.177(13)	0.063(7)	0.065(7)	-0.012(5)	0.048(8)	0.017(8)
C14	0.160(13)	0.126(11)	0.127(11)	-0.027(10)	0.062(10)	-0.043(10)
C15	0.167(14)	0.140(15)	0.100(12)	-0.028(10)	-0.008(10)	0.036(11)
C16	0.337(31)	0.085(10)	0.071(9)	0.002(8)	0.068(14)	0.023(14)
C17	0.240(21)	0.113(11)	0.174(15)	-0.010(13)	0.141(16)	-0.028(12)
C18	0.130(11)	0.108(11)	0.126(12)	-0.043(9)	0.018(8)	0.017(9)
C19	0.083(6)	0.046(5)	0.093(6)	-0.004(4)	0.049(5)	-0.003(4)
C20	0.063(5)	0.053(4)	0.060(4)	0.008(4)	0.021(4)	0.000(4)
C21	0.066(6)	0.099(7)	0.104(7)	0.020(6)	0.031(5)	-0.002(5)
C22	0.085(8)	0.174(12)	0.128(9)	0.058(9)	0.027(7)	-0.022(8)
C23	0.072(7)	0.196(13)	0.120(9)	0.053(9)	0.029(7)	-0.023(8)
C24	0.060(6)	0.183(13)	0.129(9)	0.030(9)	0.025(6)	0.003(7)
C25	0.101(8)	0.133(9)	0.083(7)	0.036(6)	0.026(6)	0.003(7)
C26	0.053(4)	0.066(5)	0.066(5)	0.001(4)	0.009(4)	-0.008(4)