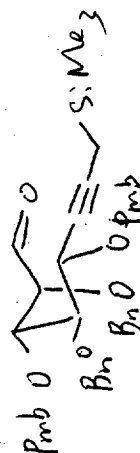
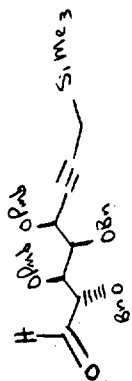


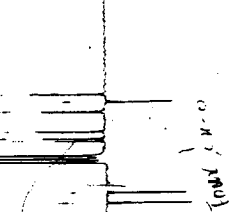
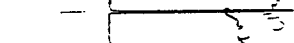
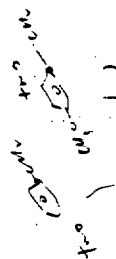
(1) of 2

5

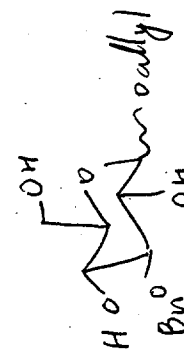
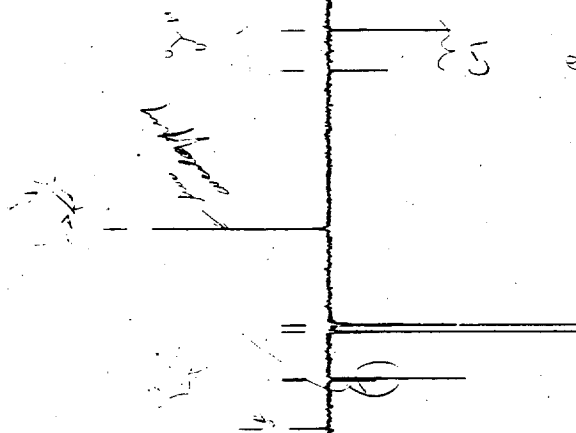
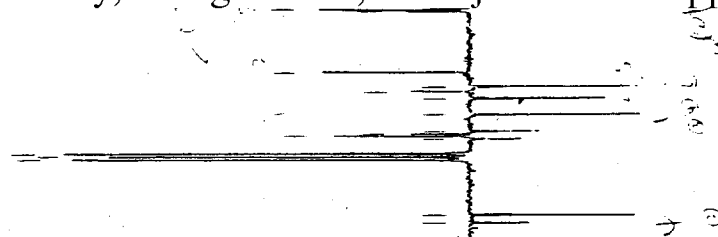
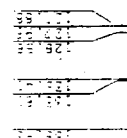
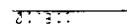
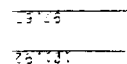
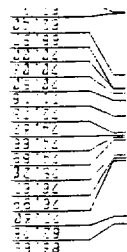


(2Z) of 2

5



150. H¹F MP 0-1.55.1



(2) of 2 8

5

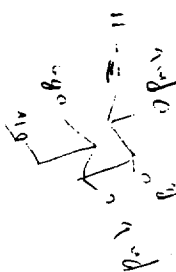


SE290F .101
AU PROG:
X25 AU
DATE 29-9-97
TIME 23:14
SF 75.469
SY 112.0
O1 7500.000
S1 32768
T0 32768
SM 20000.000
HZ/PT 1.221
PW 0.0
RD 0.0
AQ 0.819
RG 800
NS 8400
TE 297
FW 25000
D2 4700.000
DP 18H CPD
LB 2.000
GB 0.0
CX 36.00
CY 10.00
F1 210.002P
F2 -5.999P
HZ/CM 452.813
PPM/CM 6.000
SR -1407.75
D1 2.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 1.60
D3 .0070000
P6 8.60
D4 .0001000
HGA 0.0
RD 0.0
PW 33.80
DE 8400
NS 2
DS

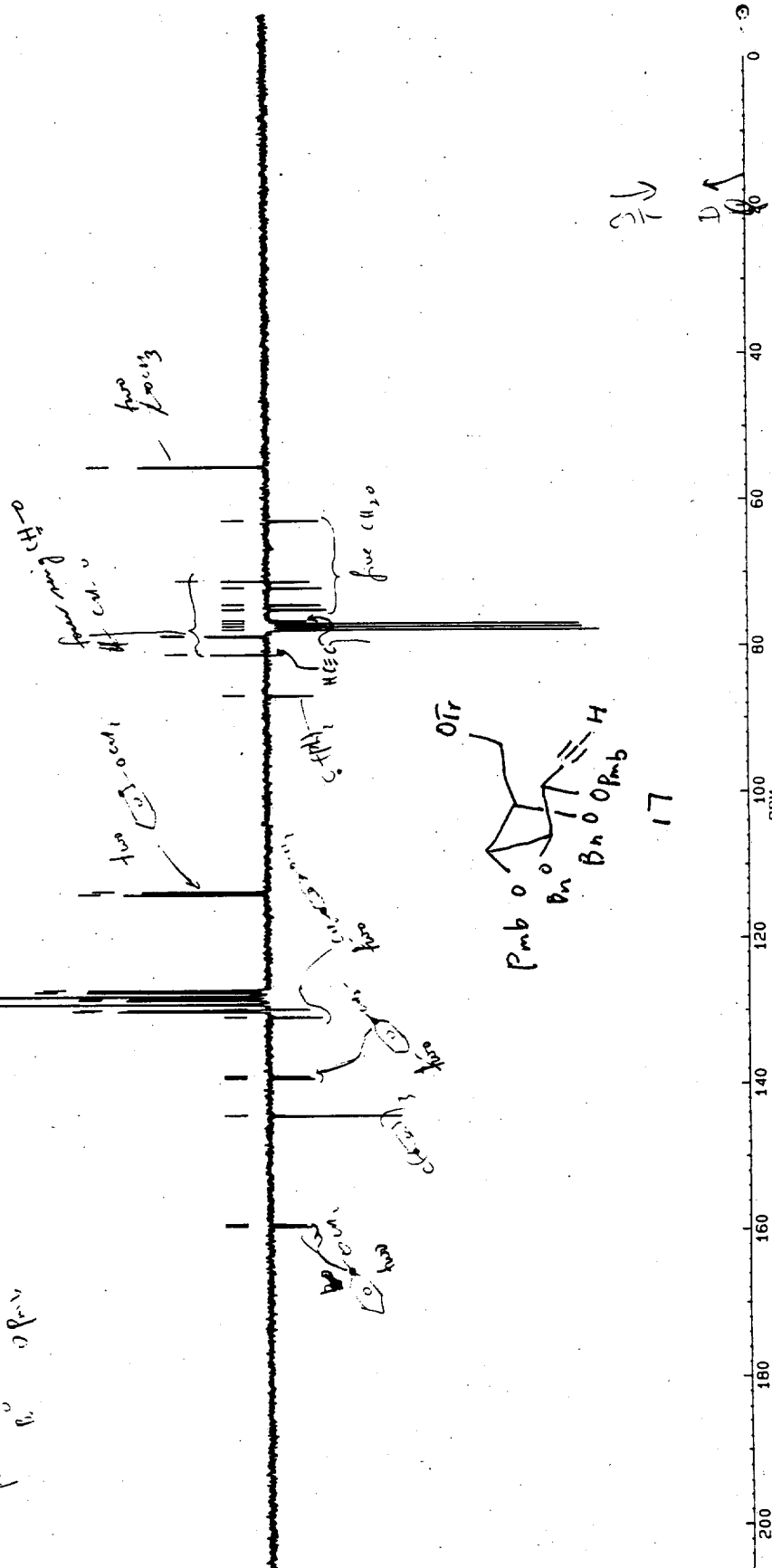
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71.930
74.231
74.840
76.290
76.658
77.053
77.477
78.477
78.509
86.686
86.696

113.808
113.460
126.944
127.245
127.312
127.787
128.104
128.290
128.697
129.508
129.538
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130.744
139.030
144.116

159.326
159.008

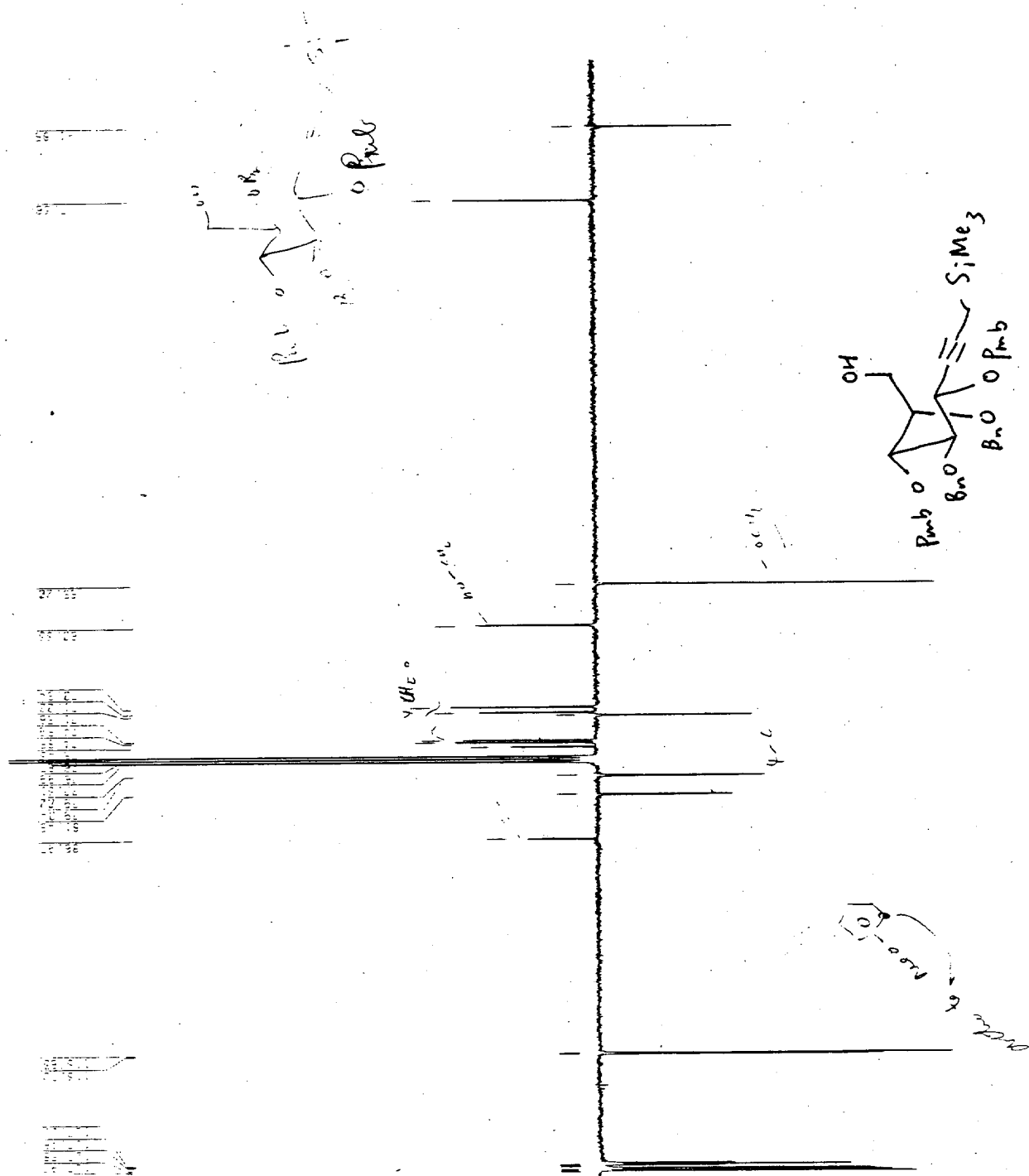


$C_{61}H_{91}O_7$



17

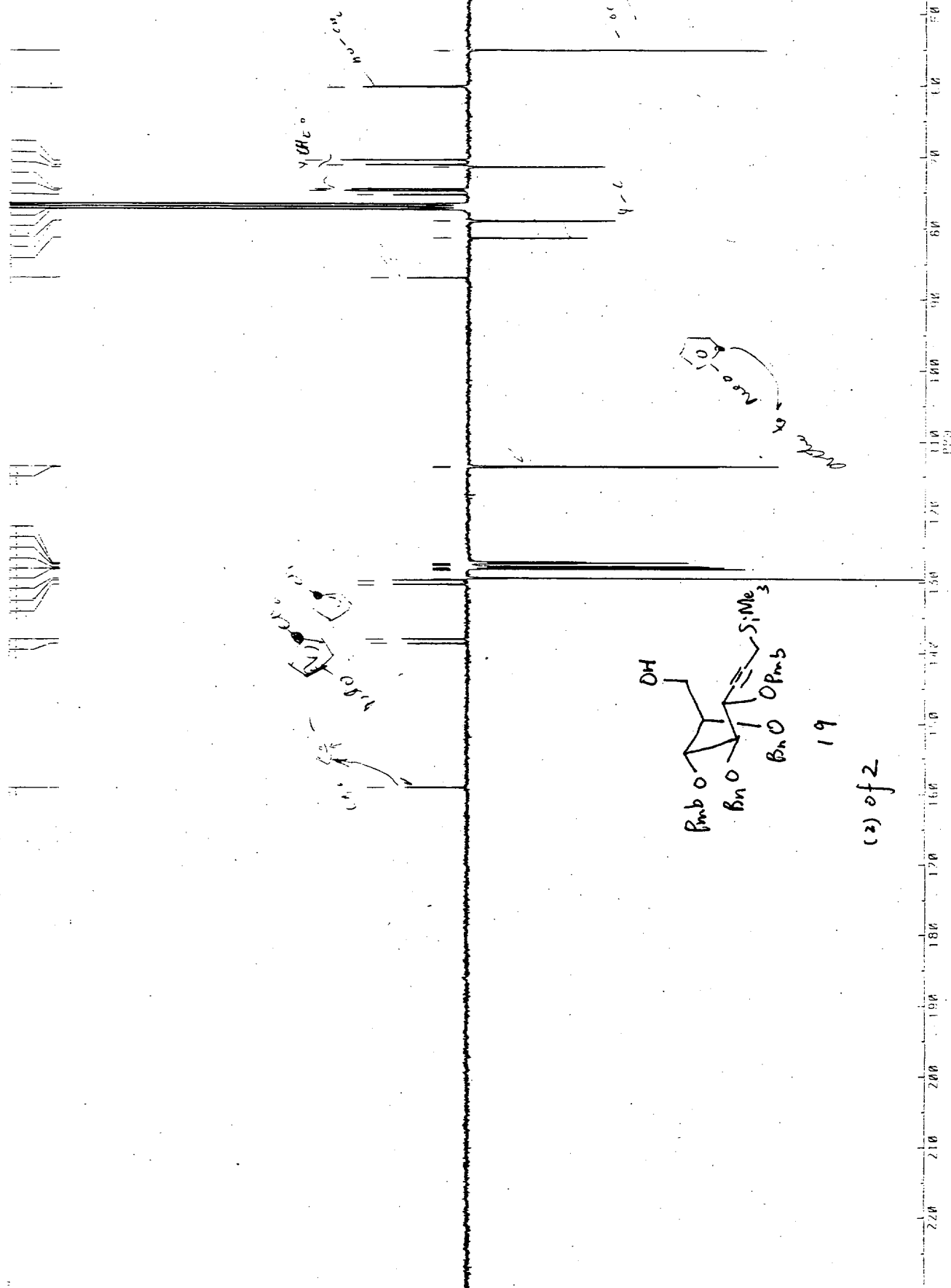
(6)



19

(1) of 2

7



(2) of 2

(9)



AP090F 101
AU PROG:
X25.1 AU
DATE 9-4-97
TIME 23:26

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

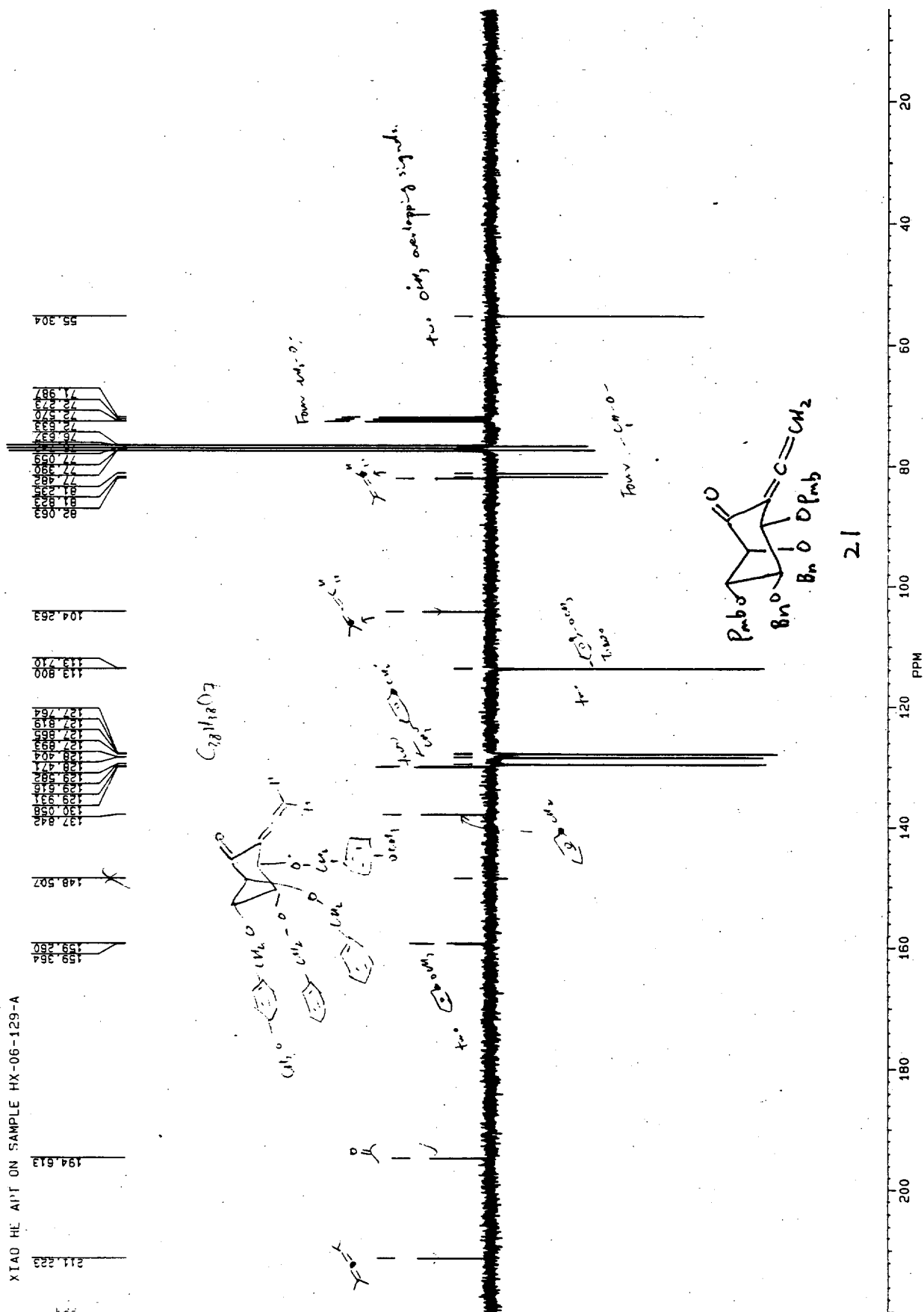
PW 0.0
RG 0.0
AQ .721
RG 800
NS 9600
TE 297

FW 28500
O2 4425.000
DP 18H CPD

LB 1.000
GB 0.0
CX 36.00
CY 0.0
F1 220.999P
F2 4.999P
HZ/CM 452.812
PPM/CM 6.000
SR -1408.91

D1 2.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 2.00
D3 .0070000
P6 8.40
D4 .0010000

RG 0.0
RD 0.0
PW 0.0
DE 30.00
NS 9600
DS 2



Two Phases



NV100F.103
AU PROG:
X25.AU
DATE 10-1-98
TIME 6:09

SF	75.469
SY	112.0
01	7600.000
SI	65536
TD	32768
SW	20000.000
HZ/PT	.610

PW	0.0
RD	0.0
AG	.819
RG	800
NS	9600
TE	297

FW 25000
02 4700.000
DP 18H CPD

LB	GB	CB
600	0.0	35.00

CY 10.00
F1 210.002P
F2 -5.990P
HZ/CM 452.796
PPM/CM 6.000
SR -1408.97

D1 2.0000000

SI 18H 100 00

D2 100.00
D3 .0010000

52	18H	1.60
90		

03.0070000

P6 8.60
D4 .0001000

RG A
00

FD	0.0
PW	0.0

DE 33.80
NS 9600

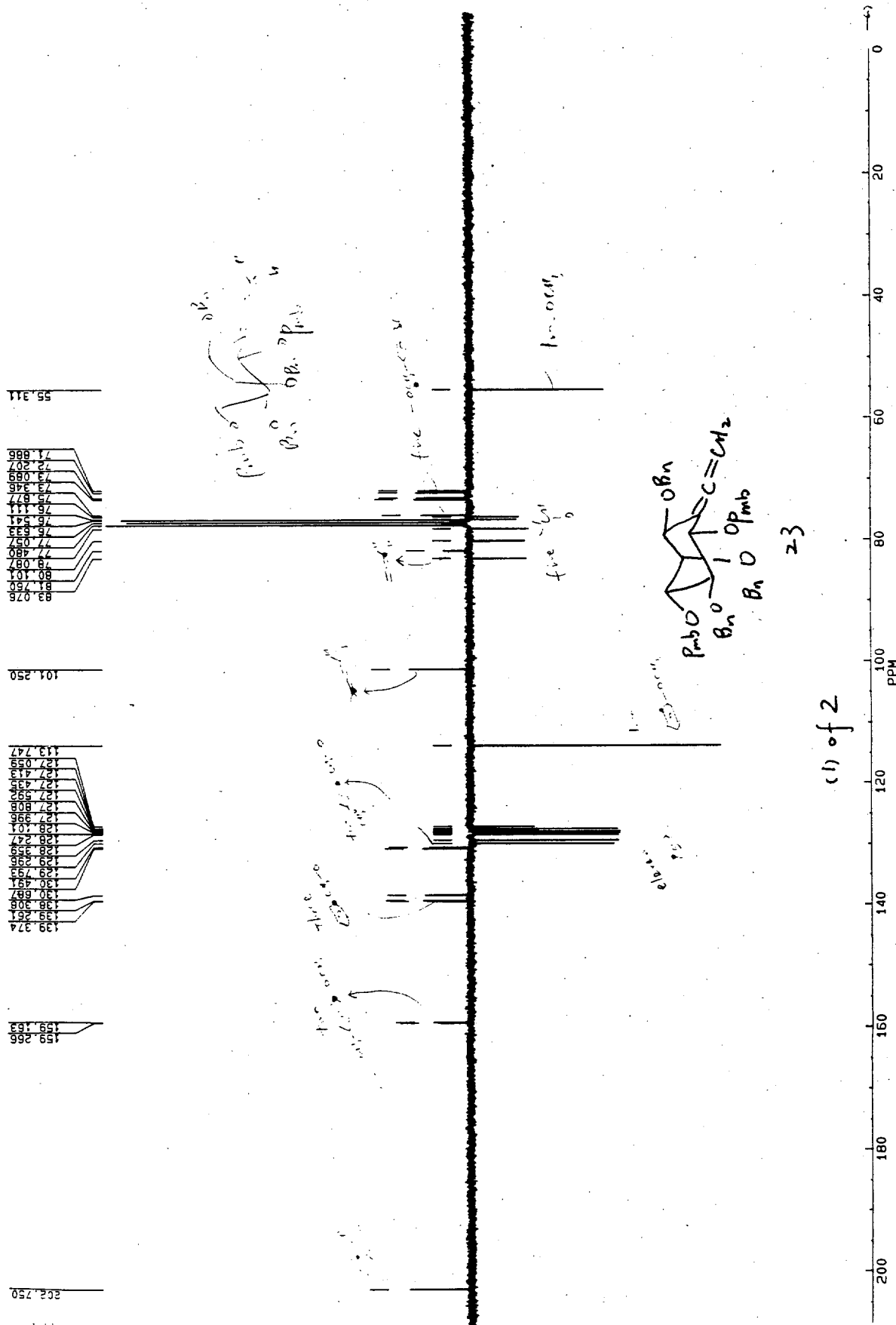
25

1

Two 1

1

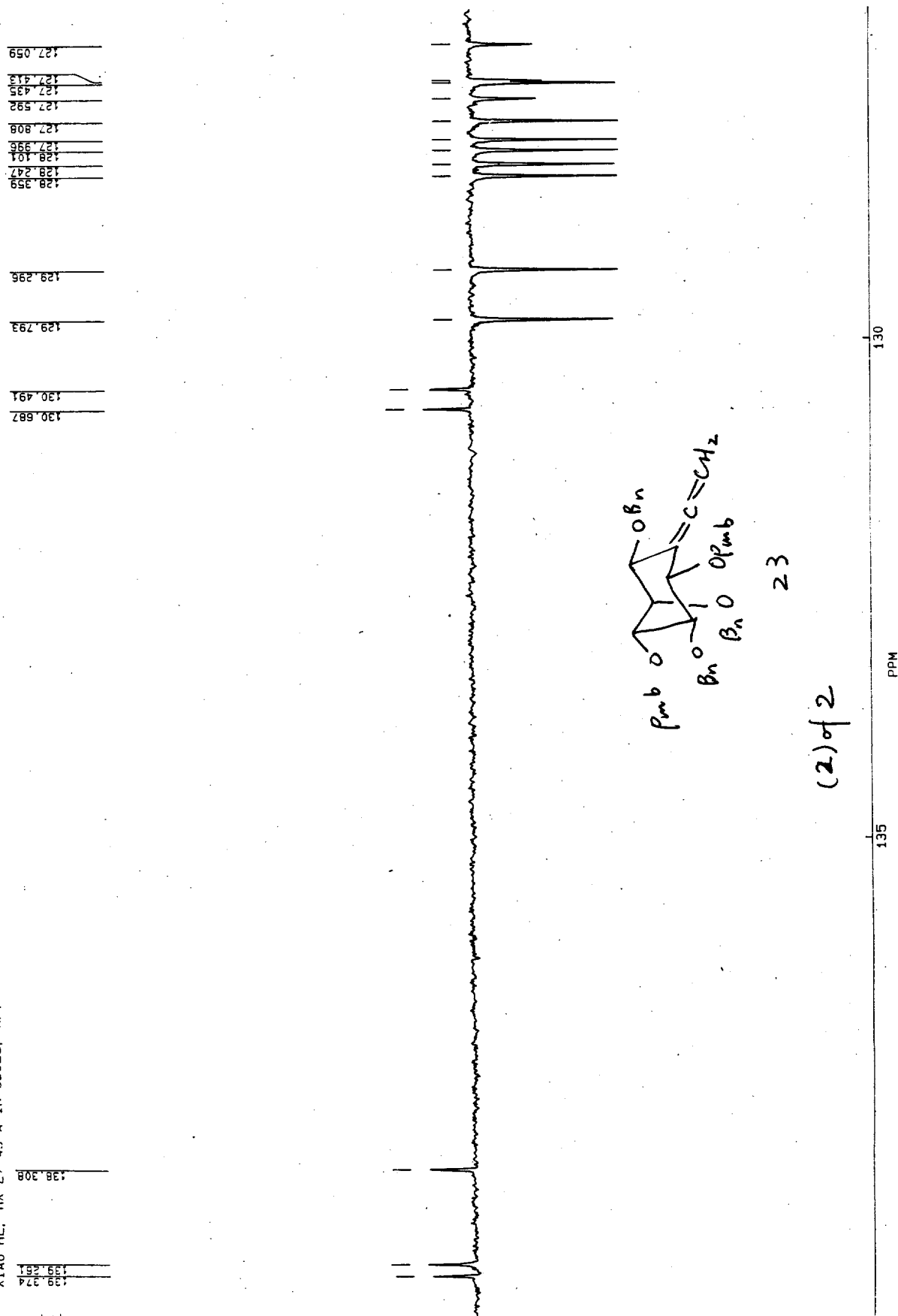
10



(12)

XIAO HE, HX-27-45-A IN CDCL₃, APT

NV100F.103
 AU PROG:
 X25.AU
 DATE 10-1-98
 TIME 6:09
 SF 75.469
 SY 112.0
 O1 7600.000
 SI 65536
 TD 32768
 SW 20000.000
 HZ/PT .610
 PW 0.0
 RD 0.0
 AD .819
 RG 800
 NS 9600
 TE 297
 FM 25000
 O2 4700.000
 DP 18H CPD
 LB .600
 GB 0.0
 CY 36.00
 CY 10.00
 F1 139.843P
 F2 126.709P
 HZ/CM 27.534
 PPM/CM .365
 SR -1408.97
 D1 2.0000000
 S1 18H
 P9 100.00
 D2 .0010000
 S2 18H
 P0 1.60
 D3 .0070000
 P6 8.60
 D4 .0001000
 RGA 0.0
 RD 0.0
 PW 0.0
 DE 33.80
 NS 9600
 DS 2



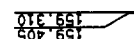
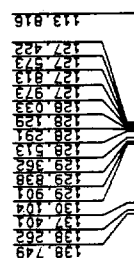
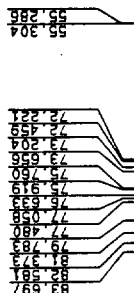
Two PA

(13)

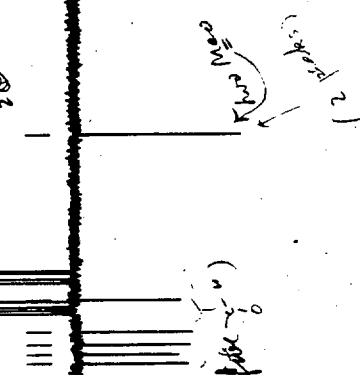
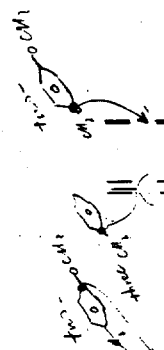
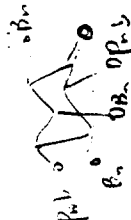


OC060F.102
AU PROG:
X25-AU
DATE 7-10-97
TIME 1:10
SF 75.469
SY 112.0
O1 7600.000
SI 65536
ID 32768
SM 20000.000
HZ/PT .610
PW 0.0
RD 0.0
AQ .819
RG 800
NS 4000
TE 297
FW 25000
O2 4700.000
DP 18H CPD
LB 1.000
GB 0.0
CX 36.00
CY 11.00
F1 212.000P
F2 -4.001P
HZ/CM 452.813
PPM/CM 6.000
SR -1407.14
D1 2.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 1.50
D3 .0070000
P6 8.60
D4 .0001000
RGA 0.0
RD 0.0
PW 33.80
DE 4000
NS 2
DS

XIAO HE 13C [1H] APT ON HX-06-143-A IN CDCL3

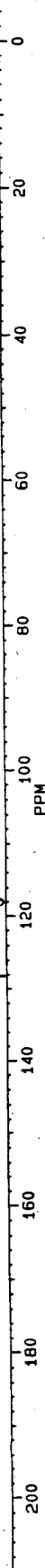


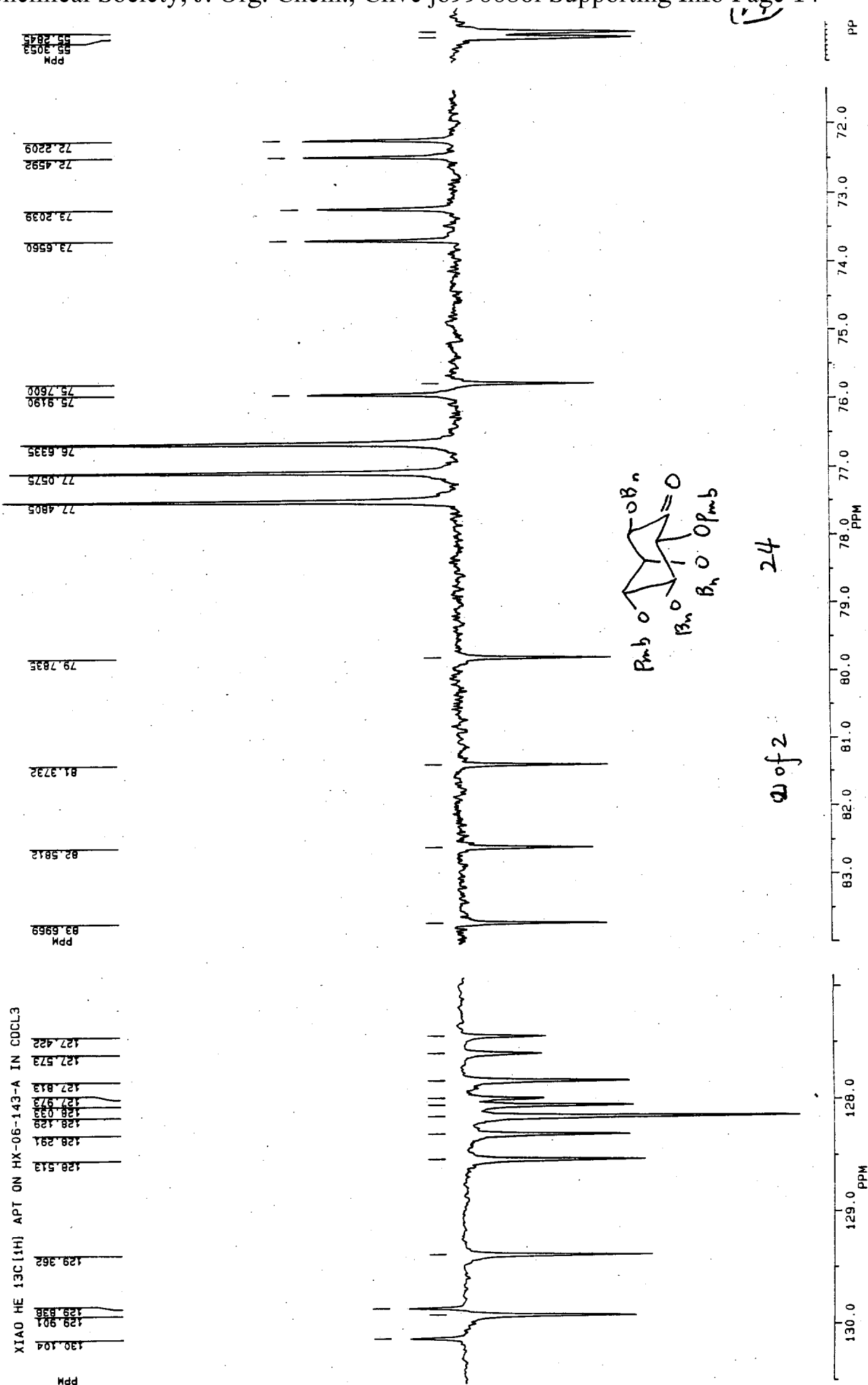
4: due O₂



24

(1) of 2



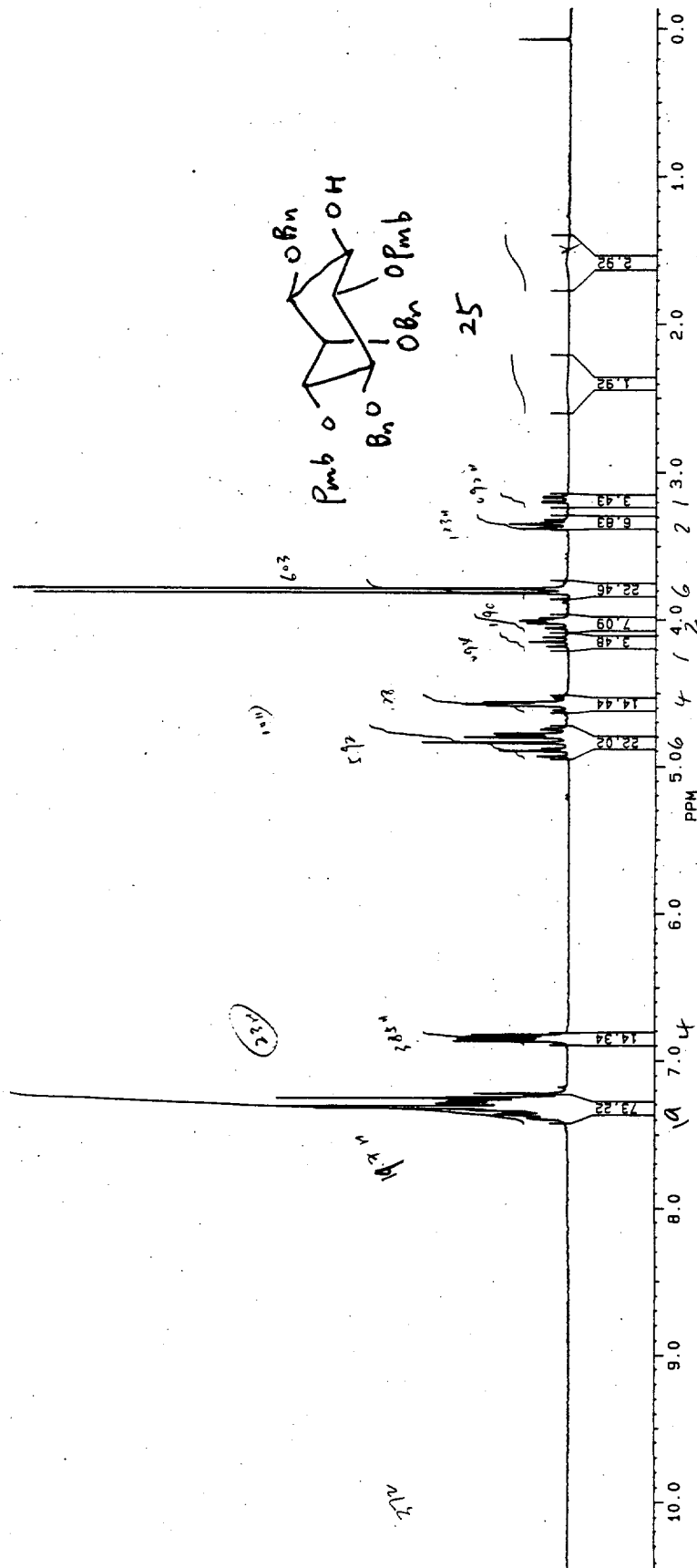
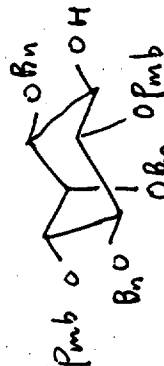
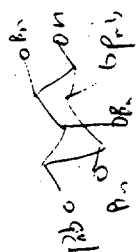


15



KAS122A
DATE 28-7-97
SF 300.133
SY 100.0500000
O1 5200.000
SI 32768
TD 32768
SM 4504.505
HZ/PT 275
PW 3.0
RD 0.0
AQ 3.637
RG 400
NS 64
TE 297
FW 5700
O2 0.0
DP 12L P0
LB 0.0
GB 0.0
CX 36.00
CY 0.0
F1 10.666P
F2 -133P
HZ/CM 90.033
PPM/CM 300
SR 3368.36

C₄₃H₄₆O₈



16
Tuck/Kent



AU20399C
AU PROG:
CAPT3 AU
DATE 20-8-96
TIME 13:14

SF 75.469
SY 112.0
D1 7300.000
SI 32768
TD 32768
SM 21739.130
HZ/PT 1.327

PW 0.0
RG 0.0
AQ 0.754
RG 800
NS 1235
TE 297

FW 27200
D2 4800.000
DP 18H CPD

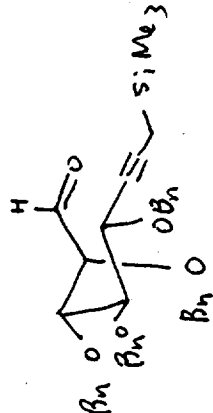
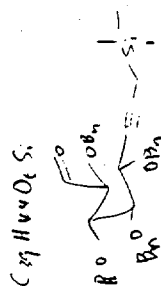
LB 1.200
GB 0.10
CX 36.00
CY 8.00
F1 215.012P
F2 -18.980P
HZ/CM 490.530
PPM/CM 6.500
SR -1407.39

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
R0 0.0
PW 0.0
DE 31.30
NS 1235
DS 2

7.392
-1.789

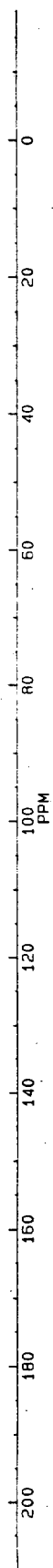
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70.922
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70.892
70.882
70.872
70.862
70.852
70.842
70.832
70.822
70.812
70.802
70.792
70.782
70.772
70.762
70.752
70.742
70.732
70.722
70.712
70.702
70.692
70.682
70.672
70.662
70.652
70.642
70.632
70.622
70.612
70.602
70.592
70.582
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70.562
70.552
70.542
70.532
70.522
70.512
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70.462
70.452
70.442
70.432
70.422
70.412
70.402
70.392
70.382
70.372
70.362
70.352
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70.332
70.322
70.312
70.302
70.292
70.282
70.272
70.262
70.252
70.242
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70.012
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71.002
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70.892
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70.852
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70.822
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70.802
70.792
70.782
70.772
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70.732
70.722
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70.642
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70.542
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70.512
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70.402
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70.072
70.062
70.052
70.042
70.032
70.022
70.012
70.002



XIAO HE 13C CAPT ON-HX-03-89-A4; CDCL3

201.257



(18)



NV29303C
AU PH06:
CAPT3.AU
DATE 29-11-95

SF 75.469
SY 112.0
SI 7300.000
ID 32768
SM 21739.130
HZ/PT 1.327

PW 0.0
RG 800
NS 835
TE 297

FM 27200
D2 4700.000
DP 18H CPD

LB 2.000
GB 0.0
CX 36.00
CY 10.00
F1 214.999P
F2 -18.993P
HZ/CM 490.530
PPM/CM 6.500
SR -1407.75

D2 .0010000
S2 18H
D1 2.0000000
P9 100.00
S1 0H

P3 2.00
D3 .0040000
P1 9.00
D4 .0020000
P2 19.00
P4 8.60
P5 0.0
P6 0.0
DE 35.16
NS 835
DS 2

-2.444
-2.096

6.910

18.664

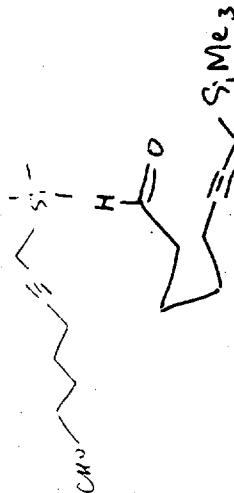
21.234

28.740

43.369

78.004
77.918
77.481
77.056
76.534

C=C

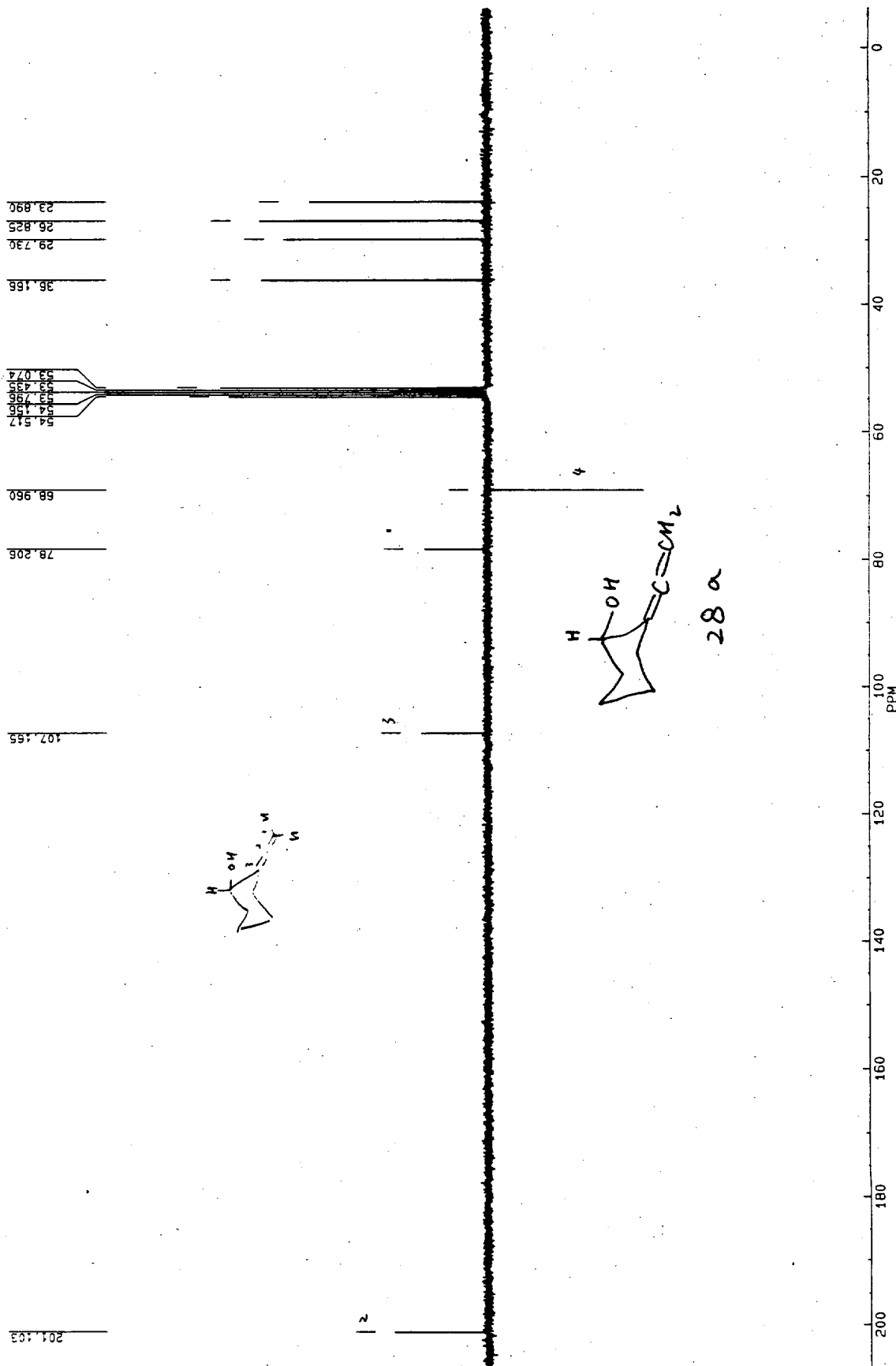


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19

XIAO HE C-13 APT ON HX-03-119-AB IN CD2CL2



BLUKE

DE20301C.001
AU PROG:
X25.AU
DATE 9-1-96

SF 75.469
SY 112.0
O1 11100.000
SI 65536
TD 32768
SM 25000.000
HZ/PT .763

PW 0.0
RD 0.0
AG .655
RG 800
NS 6778
TE 297

FW 31300
O2 5200.000
DP 18H CPD

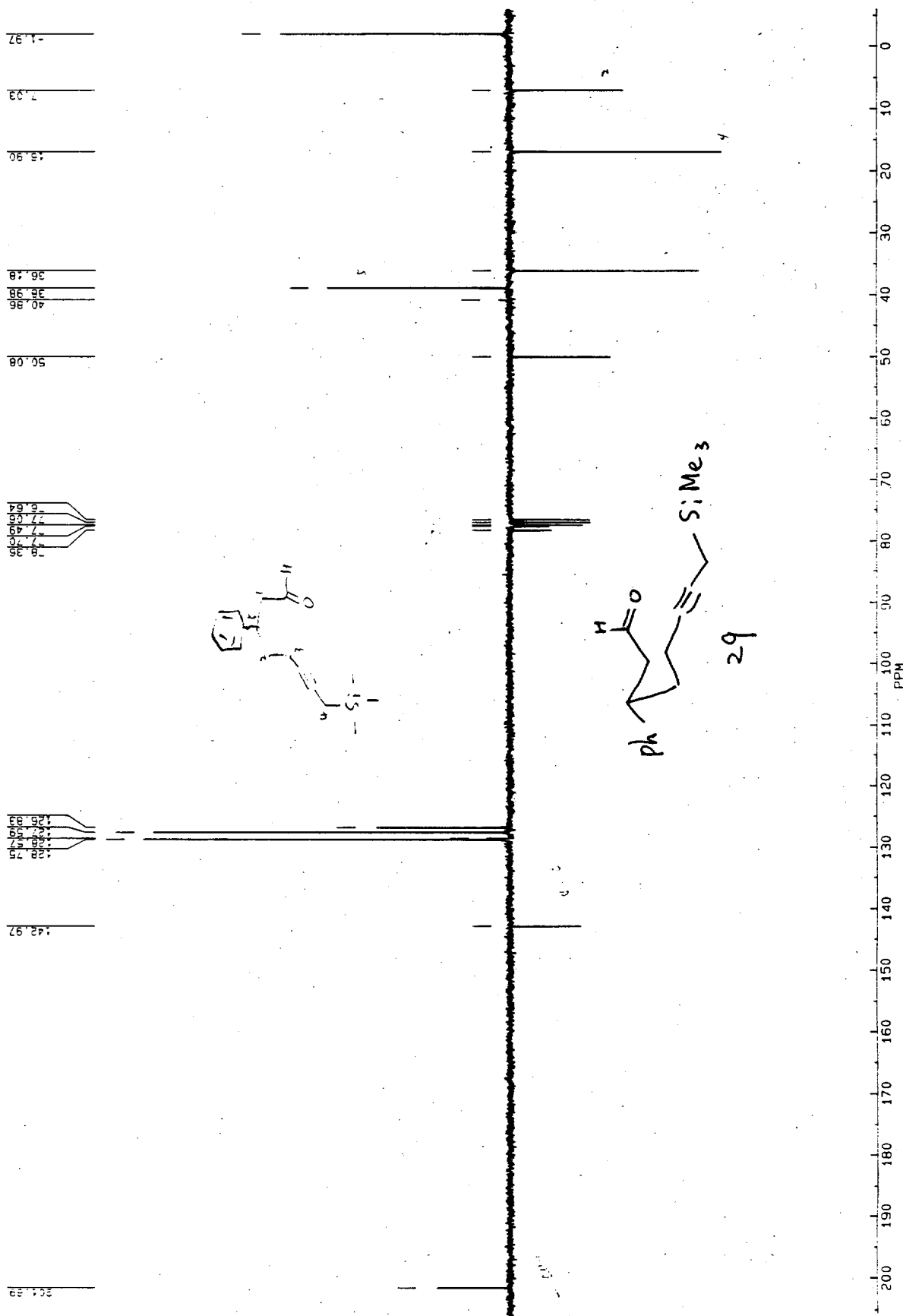
LB .760
GB 0.0
CX 36.00
CY 0.0
F1 210.000P
F2 -5.997P
HZ/CM 452.805
PPM/CM 6.000
SR 708.15

D1 8.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H
P0 1.60
D3 .0080000
P6 8.40
D4 .0010000
RGA 0.0
RD 0.0
PW 30.90
DE 6778
NS 0
DS 0

20



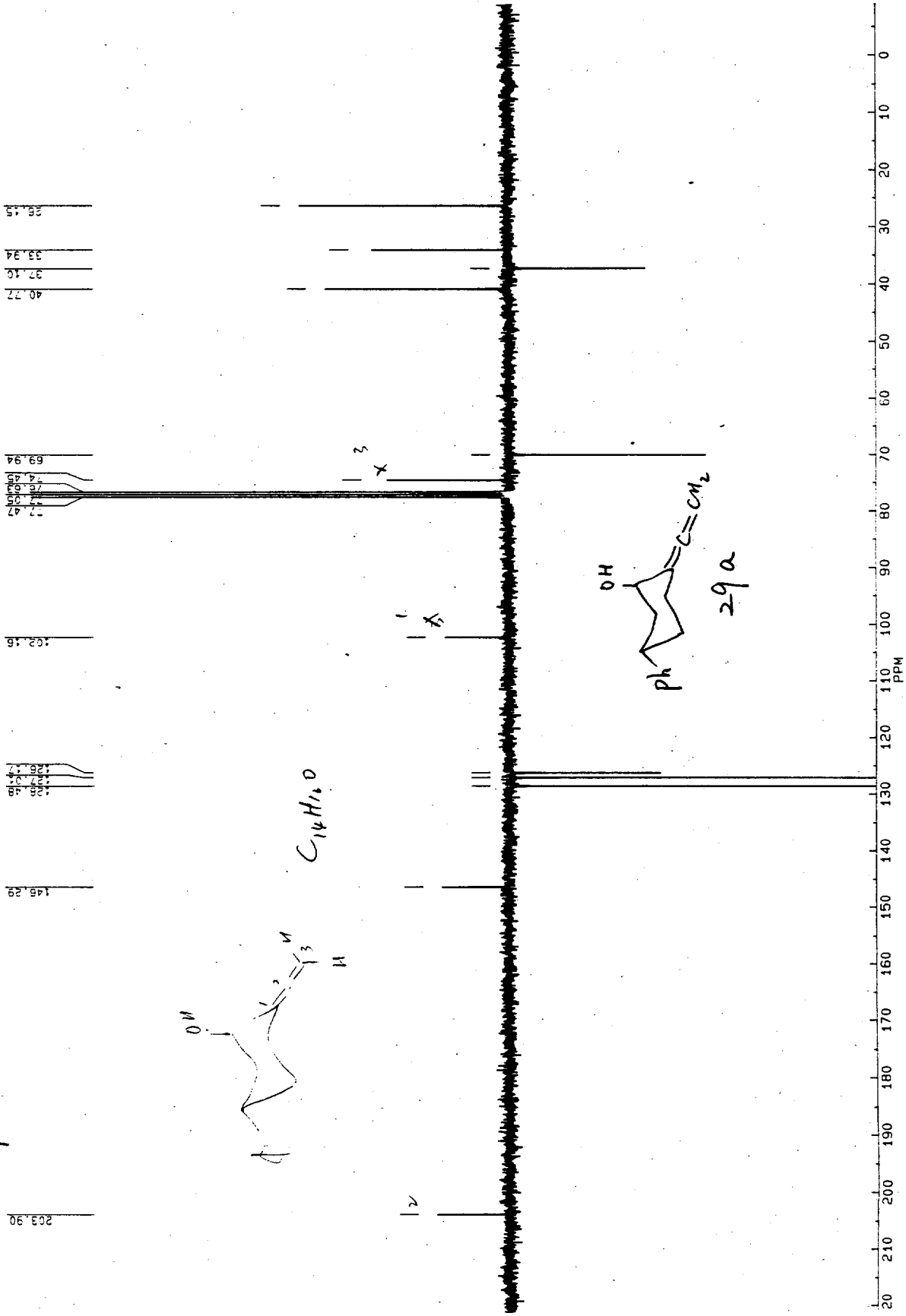
MY24308C
AU PROG:
APTXH.AU
DATE 24-5-95
SF 75.469
SI 112.0
O1 7300.000
SI 32768
TD 32768
SW 21739.130
HZ/PT 1.327
PW 0.0
RD 0.0
AQ 800.754
RG 1107
TE 297
FW 27200
O2 4800.000
DP 18H CPD
LB 1.200
GB 0.010
CX 36.00
CY 10.00
F1 210.011P
F2 5.995P
HZ/CM 452.823
BPM/CM 6.000
SR -1409.47



XTAU HE APT ON SAMPLE HX-02-147-A

21

XIAO HE, HX-02-149-A IN CDCL3/APT



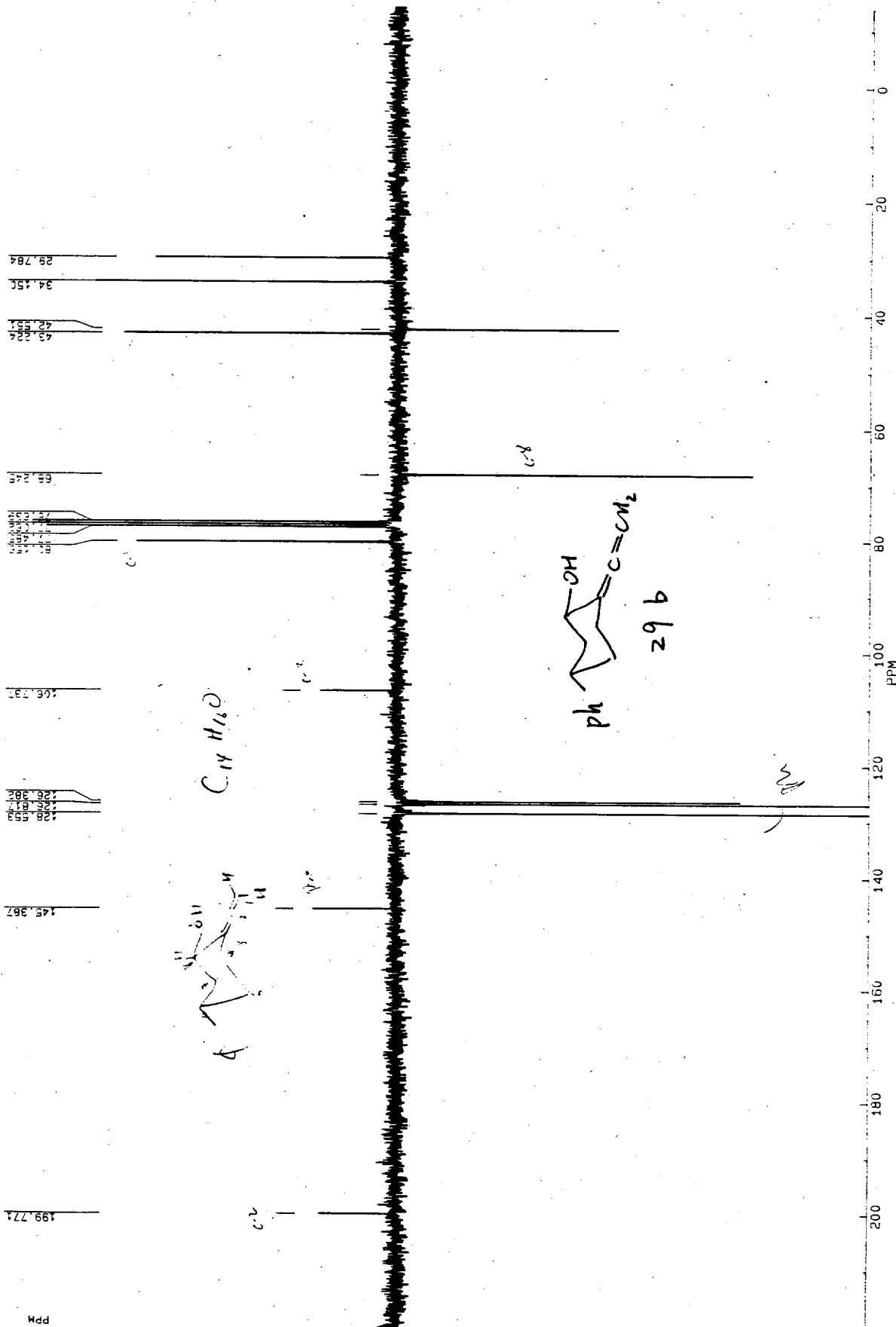
MY300F 101
AU PROG:
X25-AU
DATE 31-5-95
SF 75.469
SY 112.0
O1 7000.000
SI 32768
TO 32768
SM 22727.273
HZ/PT 1.387
PW 0.0
RD 0.0
AG 0.721
RG 800
NS 3000
TE 297
FW 28500
O2 4425.000
DP 18H CPD
LB 1.700
GB 0.010
CX 36.00
CY 0.0
F1 224.996P
F2 -8.990P
HZ/CM 490.516
PPM/CM 6.500
SR -1408.85

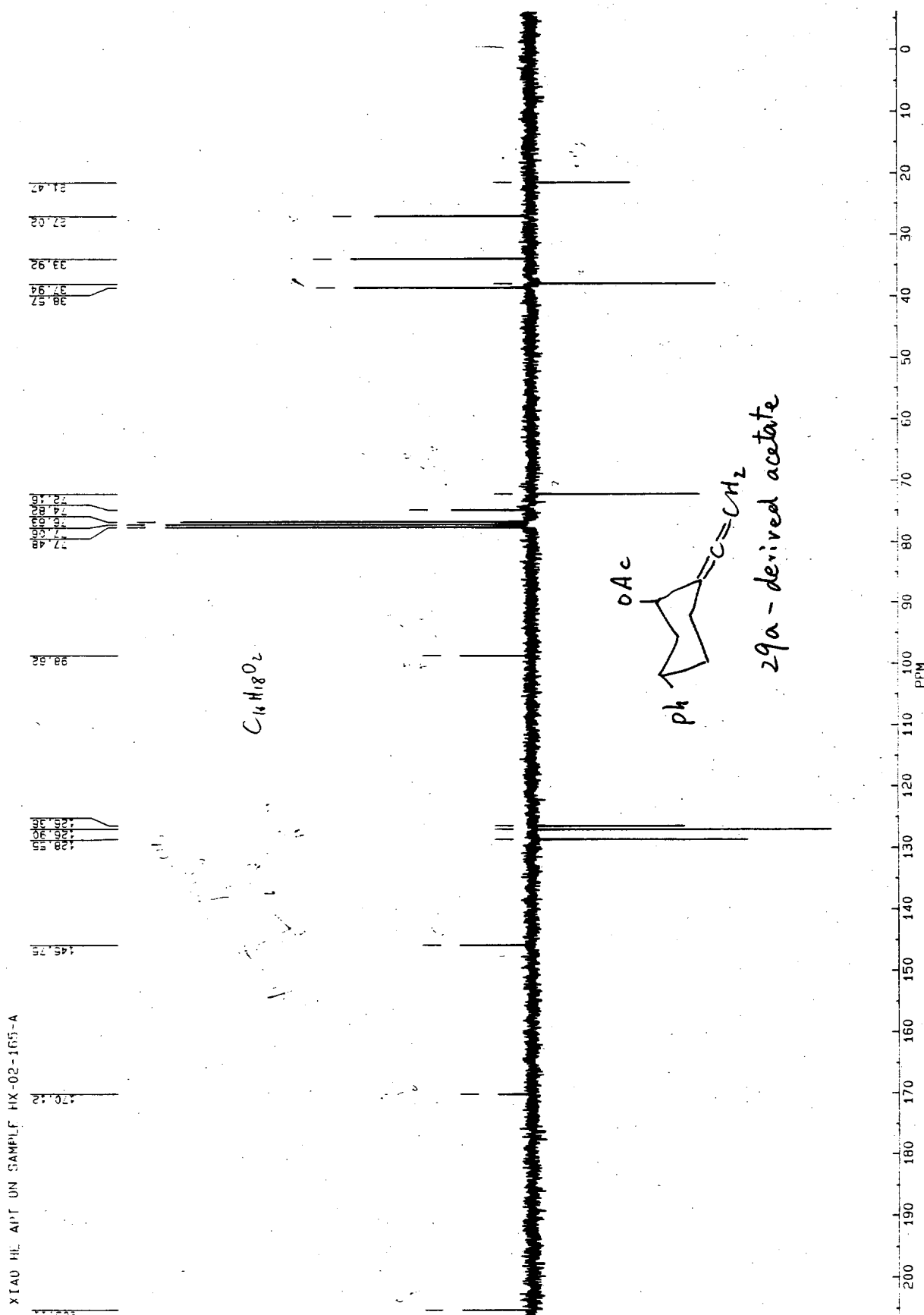


FE260F.101
AU PHOG:
X25 AU
DATE 6-4-96
SF 75.469
SY 112.0
O1 7000.000
S1 32768
TD 32768
SW 22727.273
HZ/PT 1.387
PW 0.0
RD 0.0
AG 800
RG 7000
TE 297
FW 28500
U2 4425.000
DP 18H CPD.
LB 2.000
GB 0.010
CX 36.00
CY 0.0
F1 219.996
F2 -13.989
HZ/CM 490.516
PPM/CM 6.500
SR -1408.85
D1 1.000000
S1 18H
P9 100.00
D2 .001000
S2 18H
P0 1.70
D3 .007000
P6 8.40
D4 .001000
HGA 0.0
RD 0.0
PW 0.0
DE 30.00
NS 7000
DS 2

22

XIAO HE APT, ON HX-03-147-A; CDCL3



[illegible]

25



FE210F.102
AU PROG:
X25. AU
DATE 2-4-96

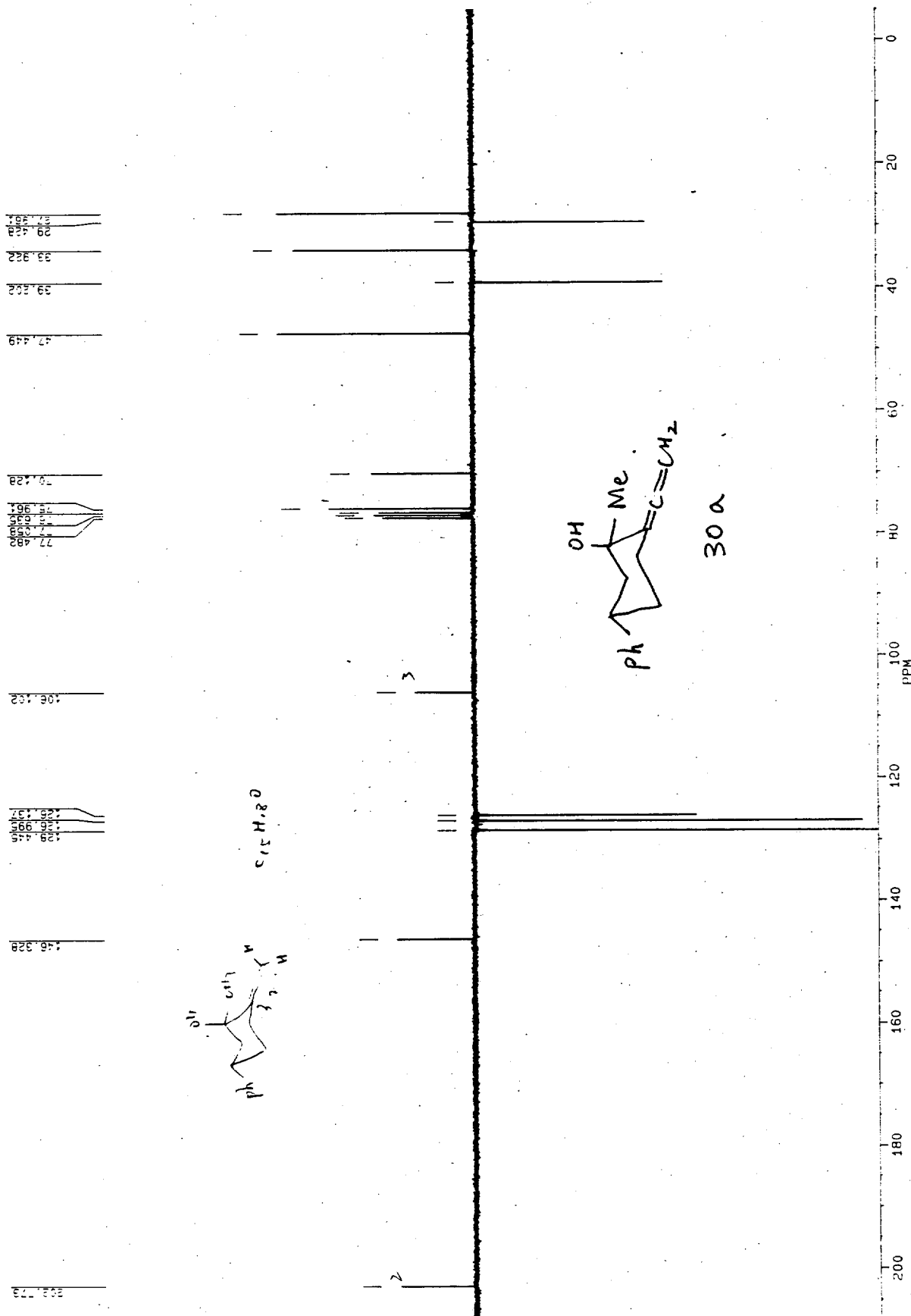
SF	75.469
SY	112.0
O1	7000.000
SI	65536
TD	32768
SW	22727.273
HZ/PT	.694

PW	0.0
RD	0.0
AG	.721
RG	800
NS	3000
TE	297

FW 28500
02 4425.000
DP 18H CPD

LB	700
GB	0.0
CX	36.00
CY	0.0
F1	211.0000
F2	-5.0000
HZ/CM	452.812
PPM/CM	6.000
SA	-1406.83

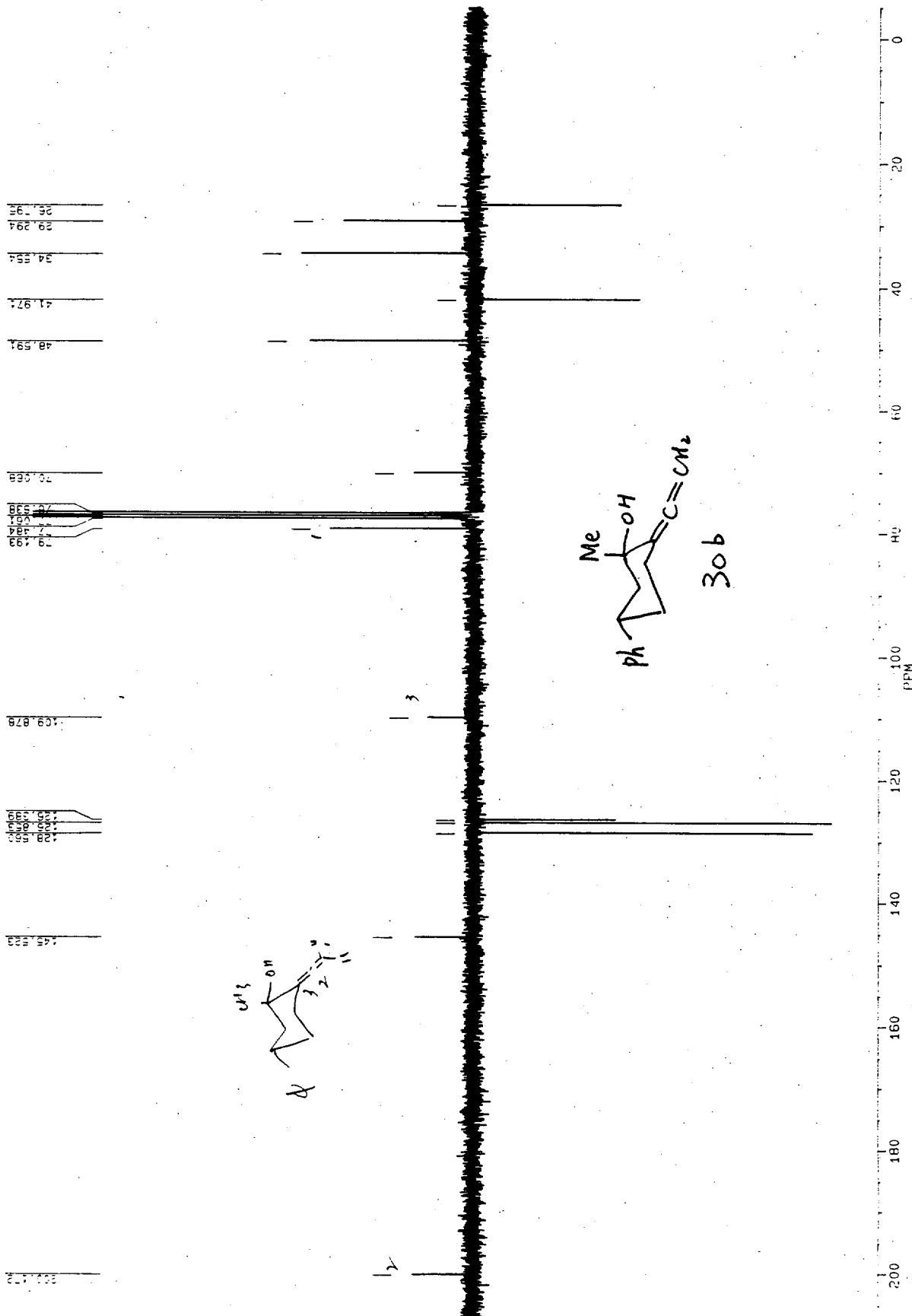
D1	2.0000000
S1	18H
P9	100.00
S2	.0010000
S2	18H
P0	2.00
D3	.0070000
P6	8.40
D4	.0010000
RG	0.0
RD	0.0
PW	30.00
DE	3000
NS	2
DS	



26

XTAU HE C-13 APT ON HX-02-185-BC IN CDCL3

SF 75.469
 SY 112.0
 O1 7000.000
 SI 65536
 TD 32768
 SM 22727.273
 HZ/PT 594
 PW 0.0
 RD 0.0
 AG 721
 RG 800
 NS 10000
 TE 297
 FW 28500
 O2 4425.000
 DP 18H CPD
 LB 700
 GB 0.0
 CX 36.00
 CY 0.0
 F1 211.000P
 F2 -5.000P
 HZ/CM 452.812
 PM/CM 5.000
 SR -1410.30
 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 10000
 DS 2



728.207

2.2.5.4. *Knowledge*

40,529	39,245	36,609	33,892
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23374

33

BRUKER
MR11307C.001
AU PROG;
APTXX.AU

MR11307C.001
AU PROG:
APTXXH.AU
DATE 10-5-96

6SF	75.469
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6GI	65536
6ID	32768
6SW	21739.130
6HZ/PI	.663

W	0.0
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AG	.754
RG	800
NS	1682
IE	297

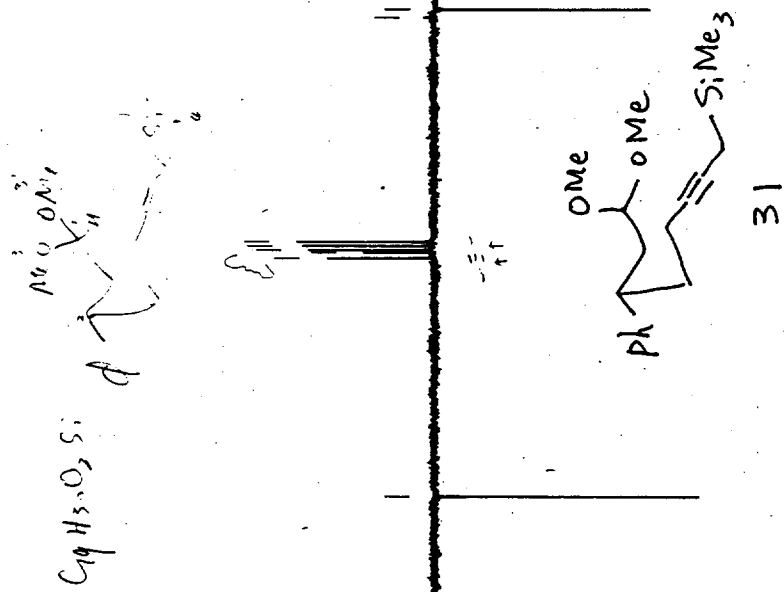
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B		.700
SB		.010

13C	36.00
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19F	-9.995P
1H	377.342
2H	5.000
3H	-1408.15

01	2.0000000
02	18H
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04	.0010000
05	2.00
06	.0070000

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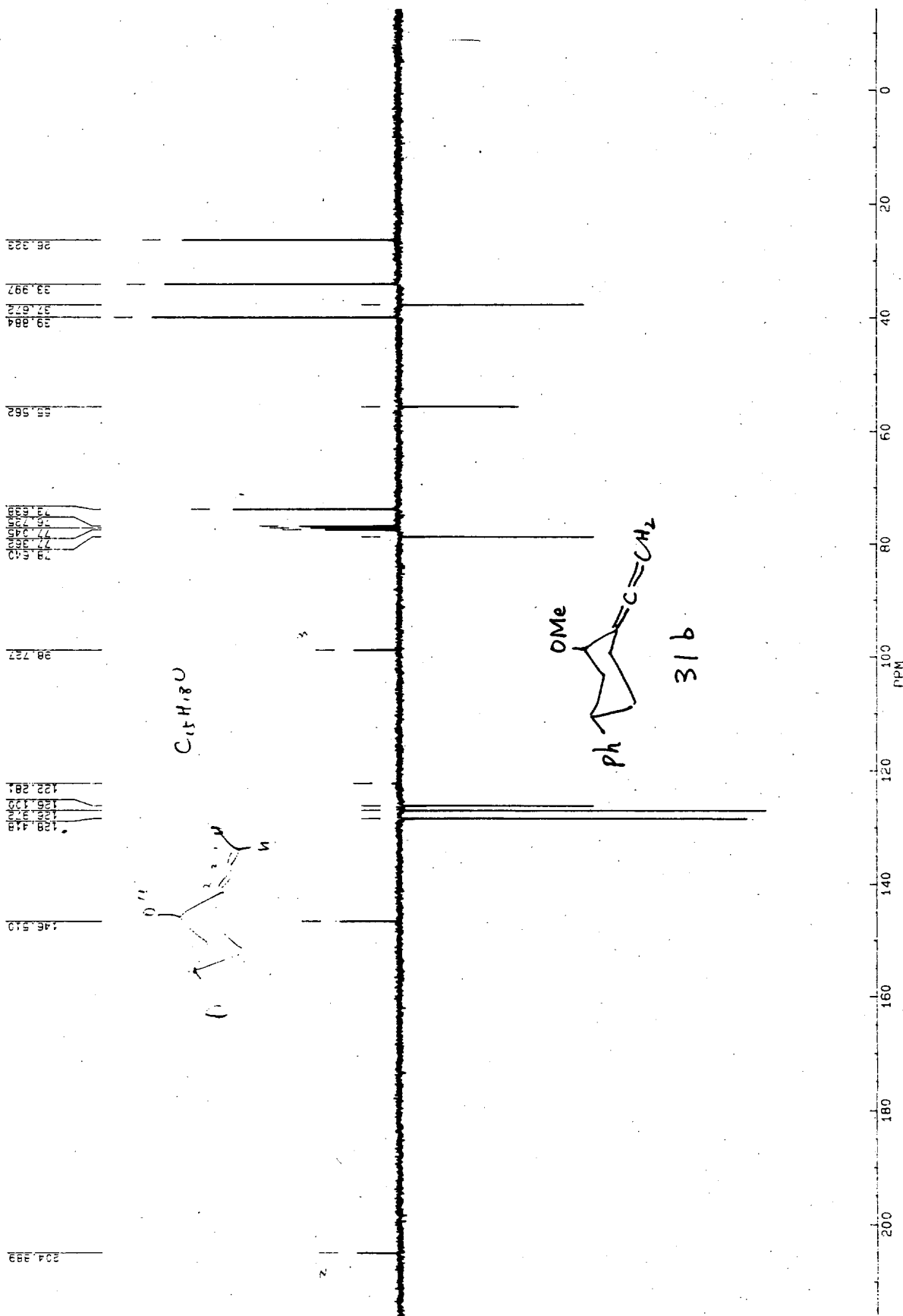
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28



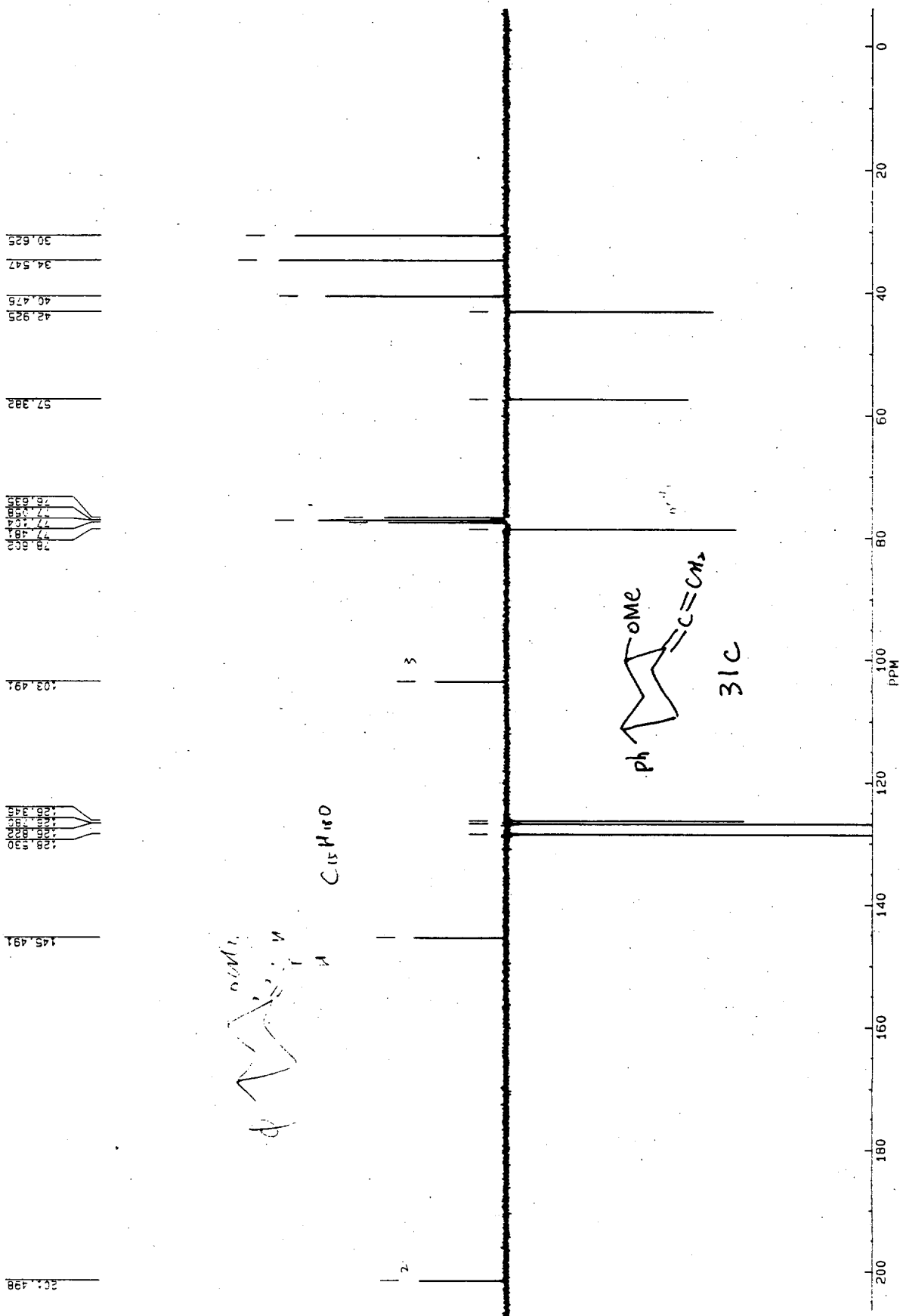
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 RD 0.0
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 RG 400
 NS 1812
 TE 297
 FW 36800
 O2 6400.000
 DP 15H CPD
 LB 1.700
 GR 0.0
 CX 36.00
 CY 10.00
 F1 220.000H
 F2 -13.998P
 HZ/CM 653.984
 PPM/CM 6.500
 SH -128.88
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 D1 1.0000000
 P9 95.00
 OH
 S1 3.00
 P3 .0040000
 D3 13.00
 P1 .0020000
 D4 .0020000
 P2 26.00
 P4 13.00
 RU 0.0
 PW 0.0
 DE 23.80
 NS 1812
 DS 2



29



MR120F.103
AU PROG:
X25 AU
DATE 1-6-96
SF 75.469
SY 112.0
D1 7000.000
SI 65536
TD 32768
SW 22727.273
HZ/PT .694
PW 0.0
RD 0.0
RG 800
NS 4000
TE 297
FW 28500
D2 4425.000
DP 18H CPD
LB 700
GB .010
CX 36.00
CY 0.0
F1 209.998P
F2 -6.002P
HZ/CM 452.812
PPM/CM 6.000
SH -1406.83
D1 2.0000000
S1 18H
P9 100.00
D2 .0010000
S2 18H 2.00
P0 .0070000
D3 8.40
D4 .0010000
RGA 0.0
RD 0.0
PW 30.00
DE 4000
NS 2
DS



~~BAUER~~

AU080F.102
AU PRUG:
X25-AU
DATE 9-8-96
TIME 3:02

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SY 112.0
SI 7000.000
TD 32768
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HZ/PT 1.387

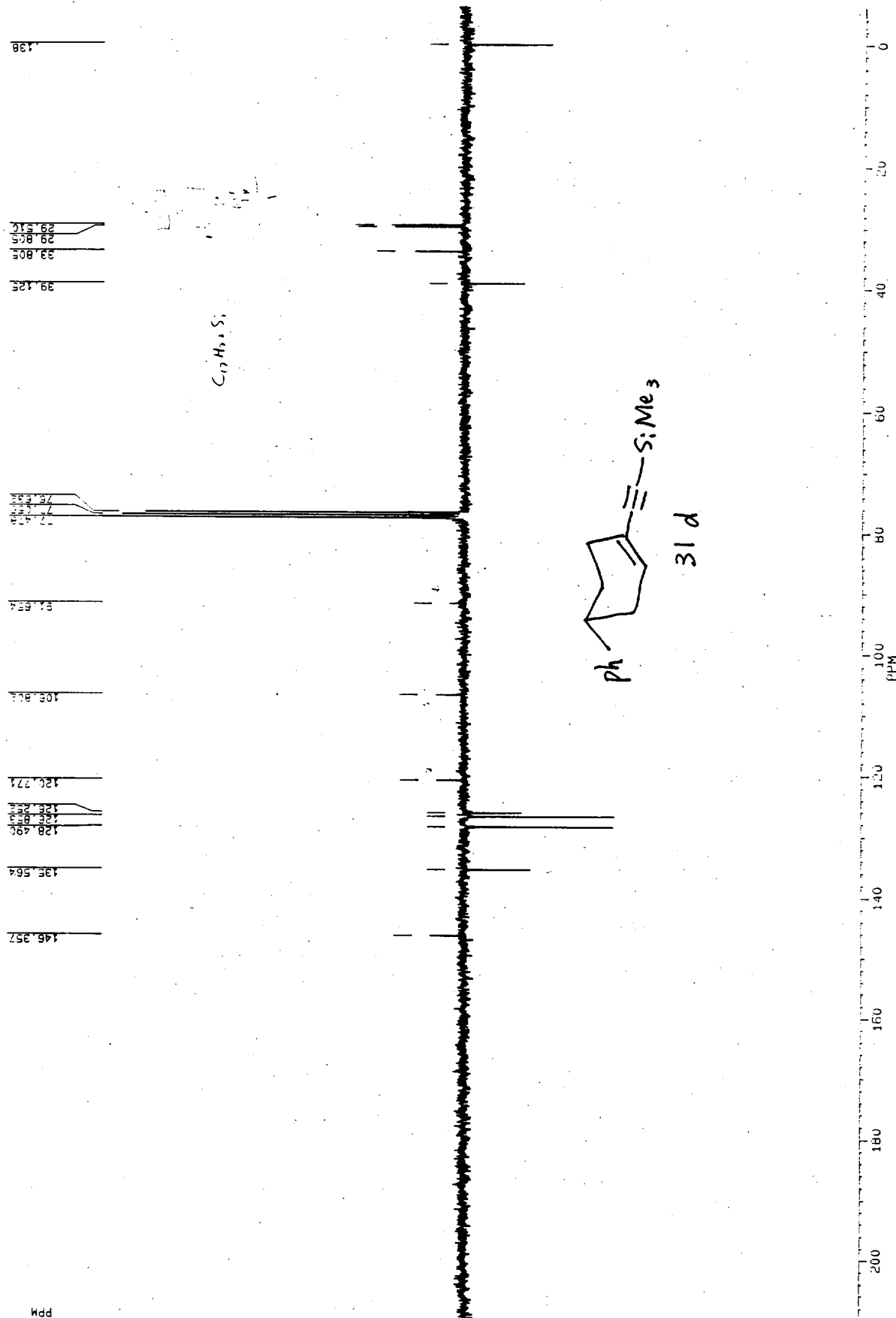
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HD 0.0
AG 721
RG 800
NS 7877
TE 297

FM 28500
Q2 4425.000
DP 18H CPD
IB 2.000
GB 0.0
CX 36.00
CY 10.00
F1 210.030
F2 -5.965
HZ/CM 452.793
PPM/CM 6.000
SR -1409.60

D1 2.000000
S1 18H
P9 100.00
D2 .001000
S2 18H
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P6 8.60
D4 .000100
HGA
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PW 0.0
DE 30.00
NS 7877
US 2

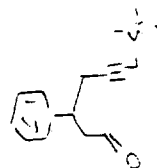
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XIAO HE HX-04-167-A, 13C APT IN CDCL3

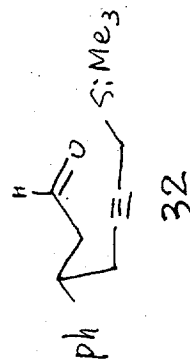


31

XIAO HE C-13 APT ON HX-04-73-A IN CDCL3



($H_{22}OS$)



32



JN140F.104
AU PROG:
X25. AU
DATE 11-8-96
TIME 6:11

SF 75.459
SY 112.0
D1 7000.000
SI 65536
TD 32768
SW 22727.273
HZ/PT .694

PW 0.0
RD 0.0
AG 800
RG 5000
NS 297
TE

FW 28500
Q2 4425.000
DP 18H CPD

LB 1.000
GB 0.0
CX 36.00
CY 0.0
F1 208.004P
F2 -7.997P
H2/CM 452.812
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 0.0
RD 0.0
PW 0.0
DE 30.00
NS 5000
DS 2

5↑ 3
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P 15
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SF	75.469
SY	112.0
O1	7000.000
SI	65536
TD	32768
SW	22727.273
HZ/PT	.594

FW 28500
02 4425.000
08 18H CPD

CX	36.00
CY	0.0
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F2	5.0000

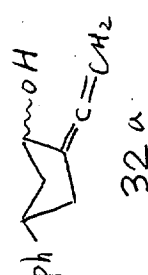
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32 16H 2.00
PO 0070000
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NS	DS	7000	2

$\frac{1}{2}$





JN140F.103
 AU PROG:
 X25-AU
 DATE 11-8-96
 TIME 2:15
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 TD 32768
 SW 22727.273
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 AQ .721
 RG 800
 NS 8000
 TE 297
 FW 28500
 O2 4425.000
 DP 18H CPD
 LB 1.000
 GB 0.0
 CX 36.00
 CY 0.0
 F1 209.998P
 F2 -5.965P
 HZ/CM 452.735
 PPM/CM 5.939
 SR -1409.60
 D1 2.0000000
 S1 18H
 P9 100.00
 D2 .0010000
 S2 18H
 P0 2.00
 D3 .0070000
 P5 8.40
 D4 .0010000
 RGA 0.0
 RD 0.0
 PW 0.0
 DE 30.00
 NS 8000
 DS 2

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$C_{13}H_{13}Cl$

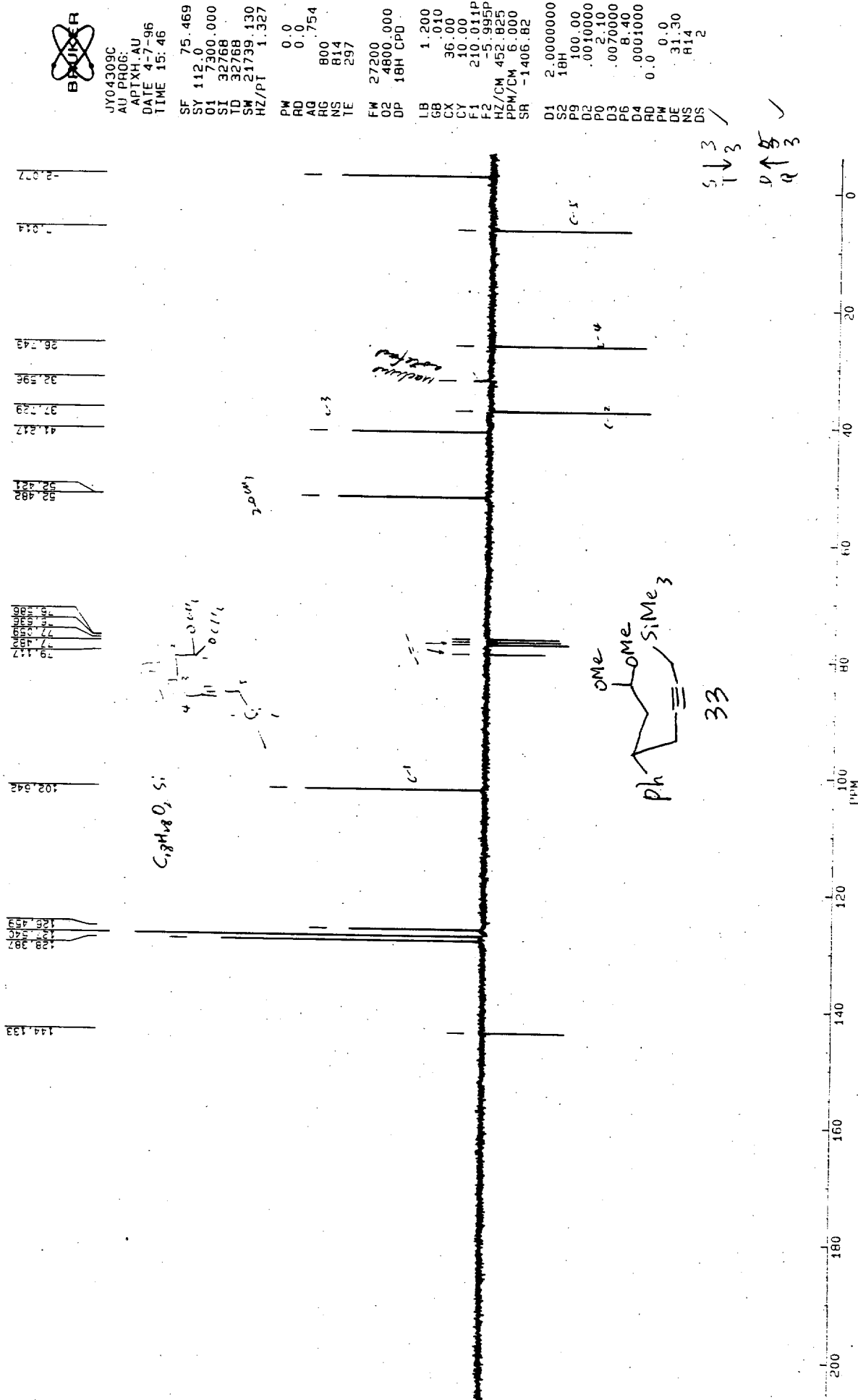
Cl 4



32b

(34)

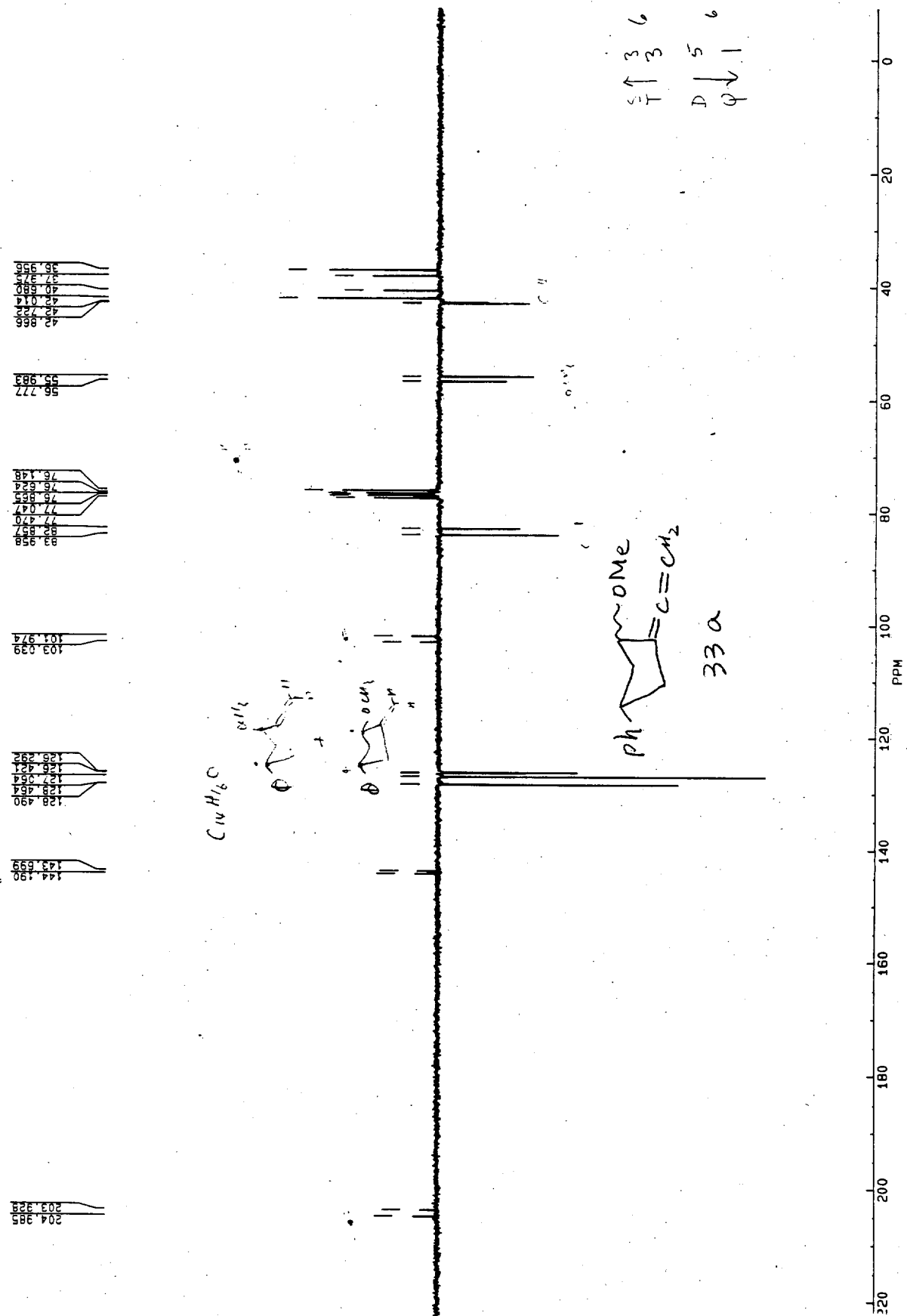
XIAO HE APT ON SAMPLE HX-04-95-A



35

XIAO HE APT ON HX-04-105-A; CDCL3

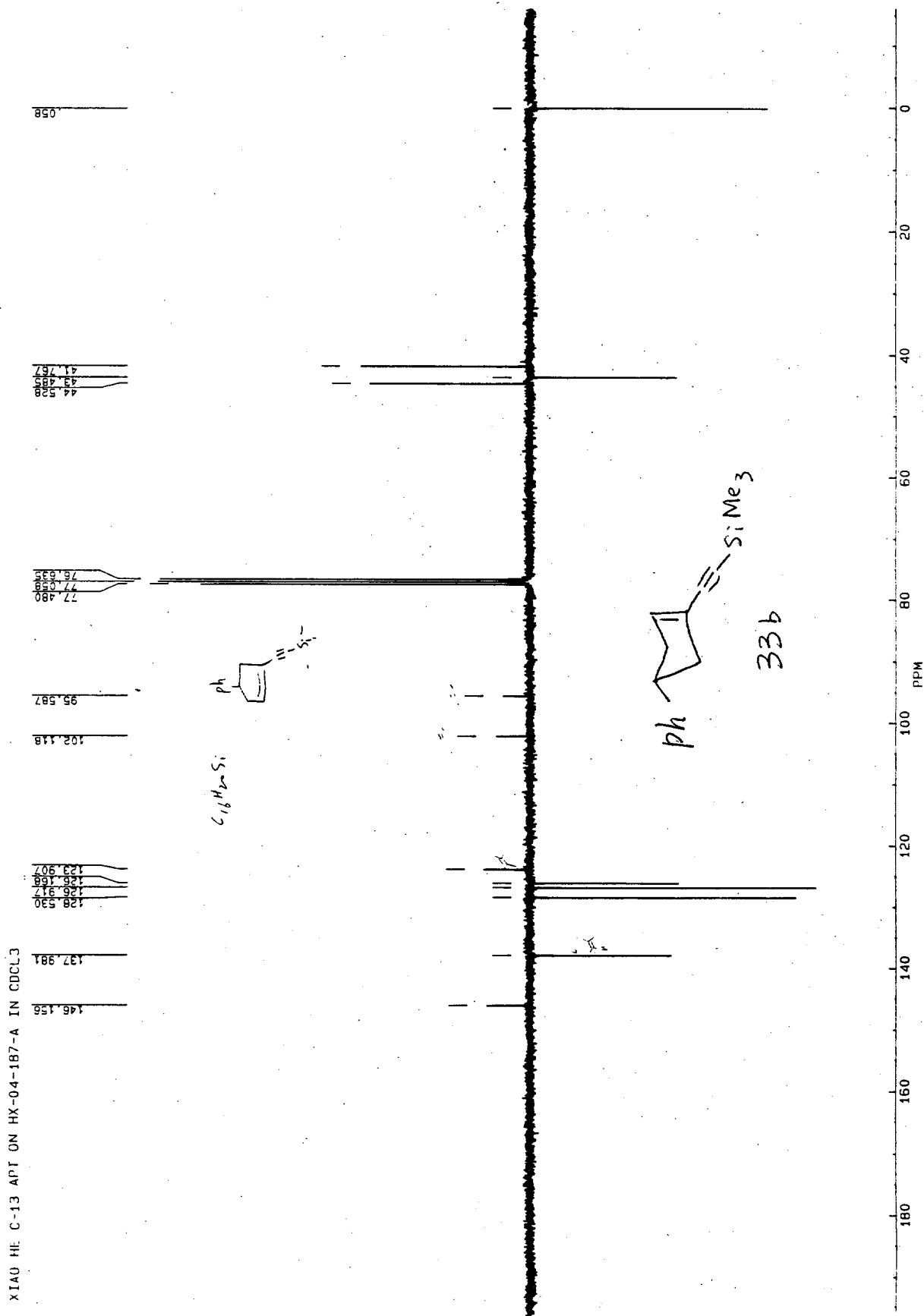
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 RD 0.0
 AG 0.721
 RG 800
 NS 8000
 TE 297
 FW 28500
 O2 4425.000
 DP 18H CPD
 LB 1.700
 GB 36.00
 CX 36.00
 CY 9.00
 F1 225.014P
 F2 -8.971P
 HZ/CM 490.516
 PPM/CM 5.500
 SR -1407.46
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 S1 18H
 P9 100.00
 D2 .0010000
 S2 18H
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 D4 .0010000
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 RD 0.0
 PW 30.00
 NS 8000
 DS 2



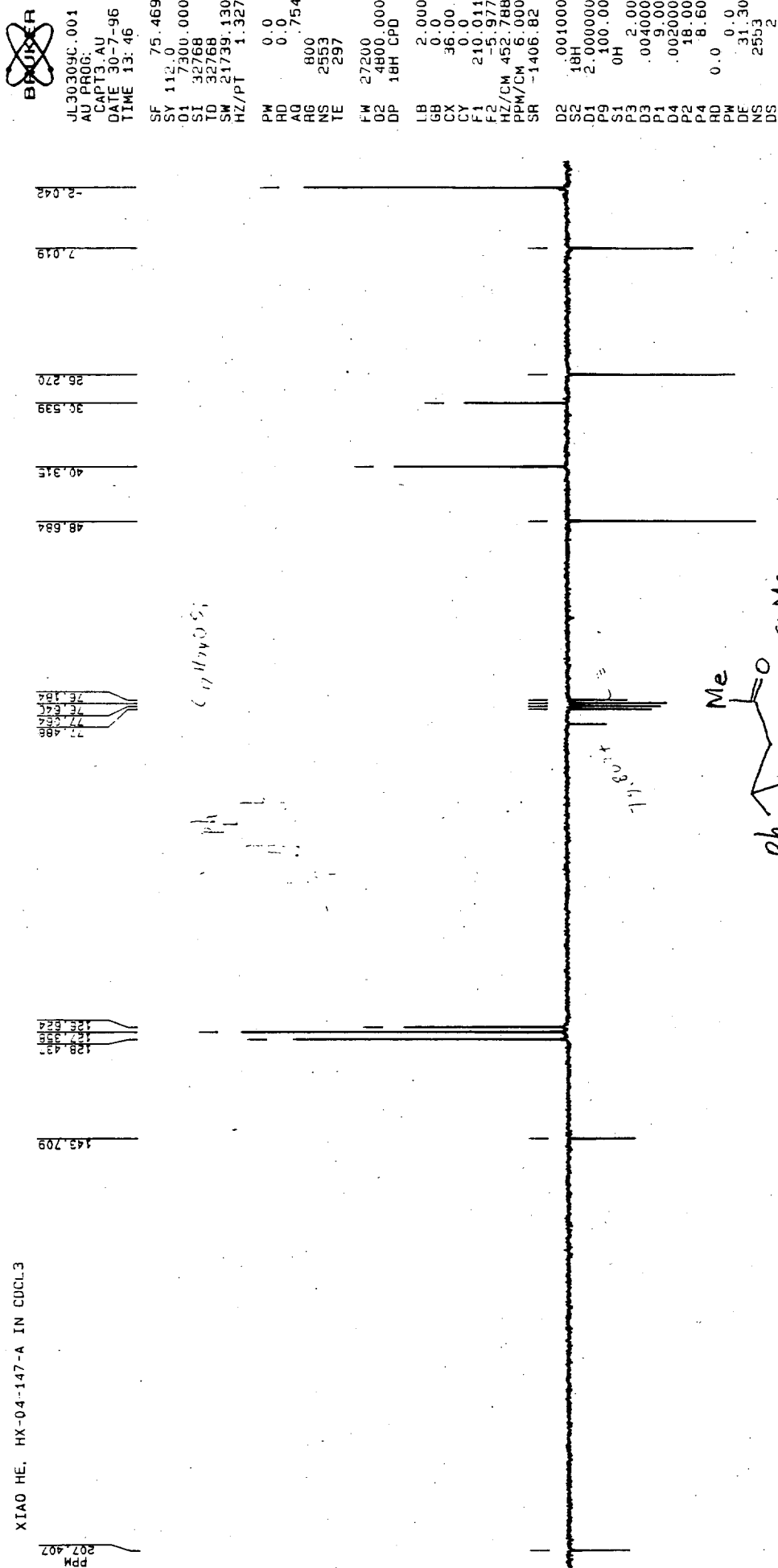
36

BRUKER

AU16301C.001
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 DATE 5-9-96
 TIME 9: 08
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 SM 25000.000
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 RG 800
 NS 12060
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 FW 31300
 O2 4425.000
 DP 18H CPD
 LB .900
 GB .010
 CX 36.00
 CY 0.0
 F1 200.000P
 F2 -15.997P
 HZ/CM 452.805
 PPM/CM 6.000
 SR -1409.60
 D1 2.0000000
 S1 18H
 P9 100.00
 D2 .0010000
 S2 18H
 P0 2.00
 D3 .0070000
 P6 8.40
 D4 .0010000
 RGA 0.0
 RD 0.0
 PW 0.0
 DE 30.90
 NS 12060
 DS 2



(37)

XIAO HE, HX-04-147-A IN CDCl₃

38



JL291F.102
AU PR06:
X25. AU
DATE 30-7-96
TIME 9:27

SF 75.469
SI 112.0
SI 7000.000
SI 32768
SI 32768
SI 32768
SI 22727.273
HZ/PT 1.387

PW 0.0
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RG 800
NS 11670
TE 297

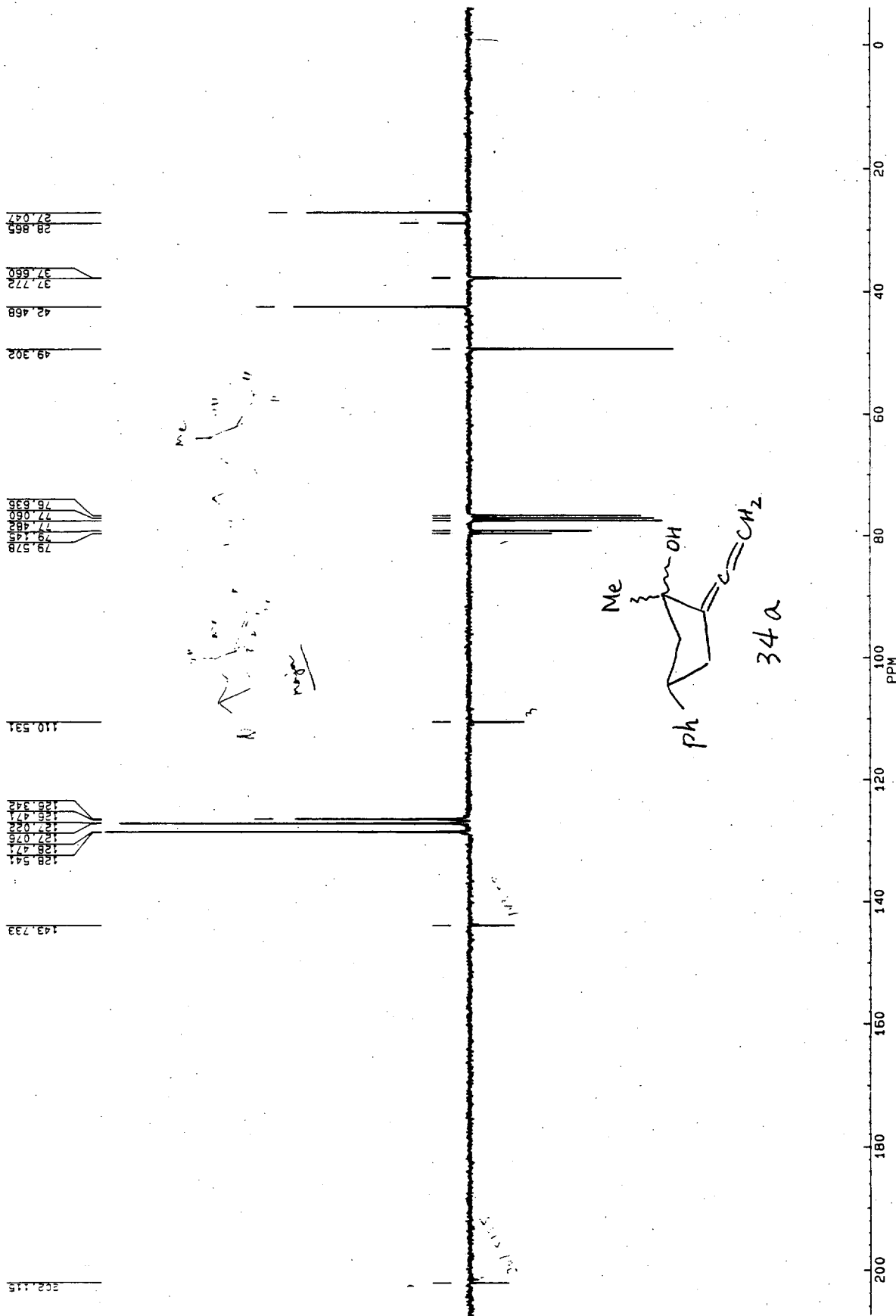
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O2 4425.000
DP 18H CPD

LB 2.000
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CX 36.00
CY 10.00
F1 210.007P
F2 -5.984P
HZ/CM 452.793
PPI/CM 6.000
SR -1408.22

D1 2.0000000
S1 18H
P9 100.00
D2 0.0010000
S2 18H

P0 2.00
D3 0.0070000
P6 8.40
D4 0.0001000
RGA

RD 0.0
PW 0.0
DE 30.00
NS 11670
DS



XIAO HE, HX-04-149-A IN CDCL3

39

BRUKER

DE07320C
AU PROG:
CAPT3.AU
DATE 7-12-95

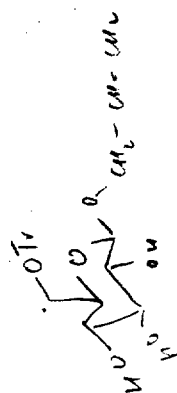
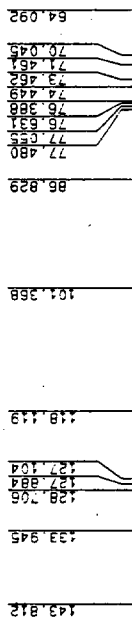
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NS 1751
TE 297

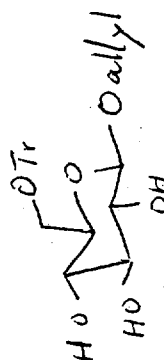
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LB 1.200
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CY 11.00
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F2 8.934P
HZ/CM 490.530
PPM/CM 6.500
SR -1404.74

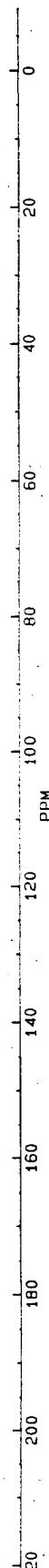
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S2 18H
D1 2.0000000
P9 100.00
S1 OH
D3 .0040000
P1 9.00
D4 .0020000
P2 18.00
P4 8.60
RD 0.0
PW 0.0
DE 31.30
NS 1751
DS 2



C₂₈H₃₀O₆



35



40



SE110F.103
AU PROG:
X25.AU
DATE 11-9-95
SF 75.469
SI 112.0
SI 17000.000
SI 32768
SI 32768
SI 32768
SI 22727.273
HZ/PT 1.387
PW 0.0
RD 0.0
AQ 0.721
RG 800
NS 6000
TE 297
FW 28500
D2 4425.000
DP 16H CPD
LB 2.000
GB 36.00
CX 36.00
CY 11.00
F1 225.492P
F2 -8.494P
HZ/CM 490.516
PPM/CM 6.500
SR -1404.69
D1 1.0000000
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 6000
DS 2

