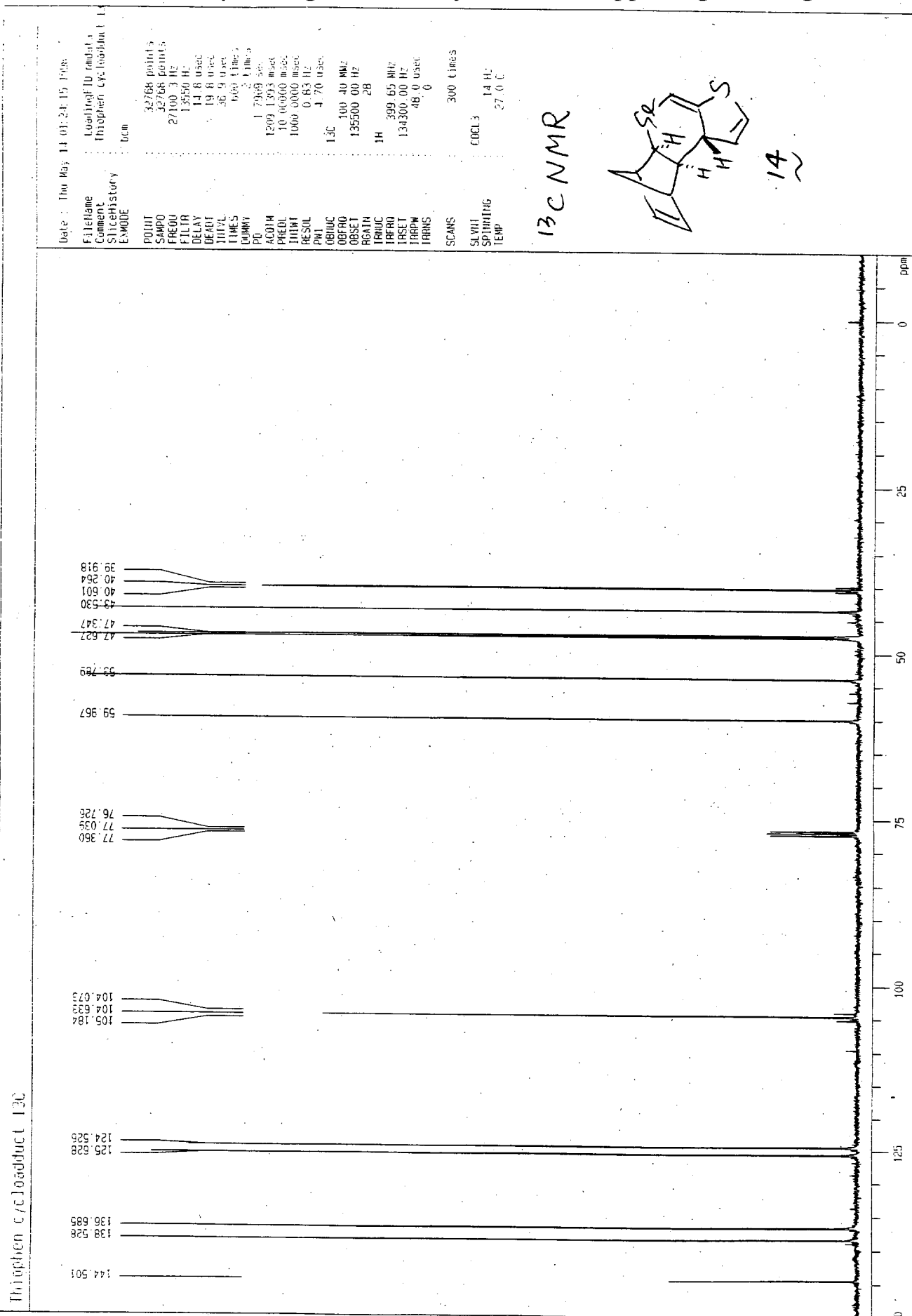
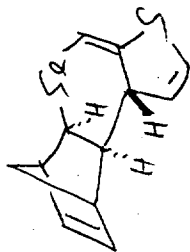




Thiophen cycloadduct 77Se

77Se NMR



14

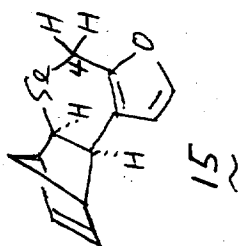
06126

Date : Thu May 11 01:42:32 1998
 Filename : LoadingFile.nmr1at
 Comment : Thiophen cycloadduct 77
 SliceHistory : bcn
 E.MODE :
 POINT : 32768 points
 SAMPD : 32768 points
 FREQD : 100000.0 Hz
 FTLTR : 50000 Hz
 DELAY : 4.0 usec
 DEATH : 10.0 usec
 INITVL : 10.0 usec
 TINES : 600 times
 DUMMY : 2 times
 PC : 2 6.53 sec
 ACQTM : 327.6800 msec
 PREDL : 10.00000 msec
 TUNIT : 0.5000 msec
 RESOL : 3.05 Hz
 PH1 : 6.40 usec
 ORNUC : 77Se
 OBPRG : 76 20 MHz
 OBSET : 79699.81 Hz
 AGATN : 23
 IANUC : 1H
 IAFRO : 399.65 MHz
 IASET : 134300.00 Hz
 IARPW : 48.0 usec
 IARNS : 0
 SCANS : 120 times
 SLVNT : CDCl3
 SPINNING : 14 Hz
 TEMP : 27.3 C

1000 750 500 250 0 ppm

AT

¹H NMR



0.0001

0.0724

7.2870
7.2420
7.2328

7.26 7.25 7.24 7.23 ppm

6.1787
6.1810
6.1815
6.1828
6.2090
6.2094
6.2199
6.2239

6.2643
6.2648
6.2654
6.2790

6.2825
6.2933

6.3013
6.3110

6.32 6.30 6.28 6.26 6.24 6.22 6.20 6.18 ppm

0 ppm

2

4

6

8

10

12

User: GML I		File: H		Date: 07-27-98		XLA 200	
Pulse Sequence: STD1H				SAMPLE			
Probe: DUAL5				USE "TEXT" TO ENTER SAMPLE DATA			
Temp: --- °C				Solvent: CDCl3			
EXPERIMENT				PLT/PROCESSING			
FN: 32	K: RE	sec: CD	sec: CD	Hz: 170.2	Offset: 170.2	Hz: 200	Power: 20
LB: 18	Hz: AF	sec: CD	sec: CD	Hz: 2901.1	Start: -219.6	Hz: 200	Power: 20
Width: 2901.1	Hz: Start	Width: 219.6	Hz: Start	Power: 20	Power: 20	Power: 20	Power: 20
Nucleus: 1,750				Mode: NNN			
Spec Width: 2901.1				Modulation: Mode C			
Acq Time: 5.648				Pulse Width: 5.6			
Pulse Width: 5.6				Transients: 40			
Nucleus: 1,750				Freq: 200			
Spec Width: 2901.1				Offset: 400			
Acq Time: 5.648				Delay: 0.350			
Pulse Width: 5.6				Transients: 40			

User: GML I
File: H
Date: 07-27-98
XLA 200

USE "TEXT" TO ENTER SAMPLE DATA

Pulse Sequence: STD1H
Probe: DUAL5
Temp: °C
Solvent: CDCL3

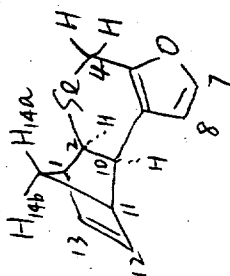
EXPERIMENT
F1: 32 K RE sec CD sec
L8: Hz AF sec CD
Width: 54.4 Hzppm Start: 682.7 Hzppm
Reference: _____

PL07/PROCESSING
Offset: 170.2 Hz
Power: 20 dB
Modulation: Mode C
Freq: 200 Hz
Power Mode: _____
Nucleus: 13C
Mode: NMR
Modulation: Mode C
Pulse Width: _____ μ sec

DECOUPLE
Nucleus: 13C
Freq: 200 MHz
Spec. Width: 2901.1 Hz
Offset: 400 Hz
Acq. Time: 5.648 sec
Delay: 0.350 sec
Pulse Width: 5.8 μ sec
Transients: 40

OBSERVE

¹H NMR (expansion)



H4

H4

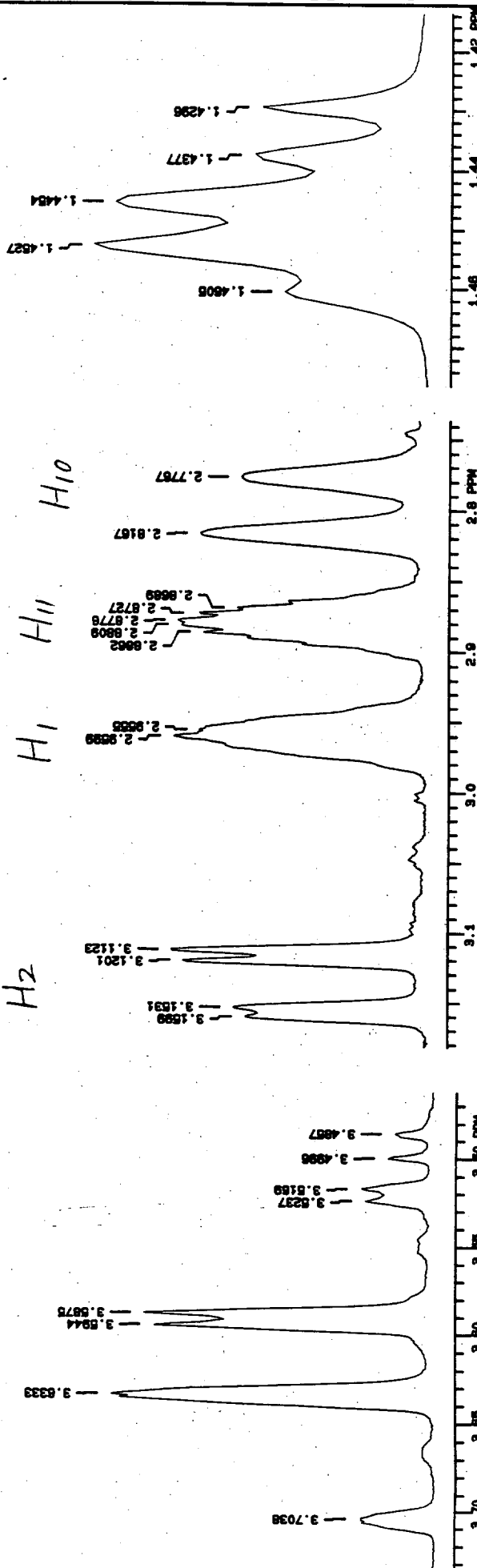
H2

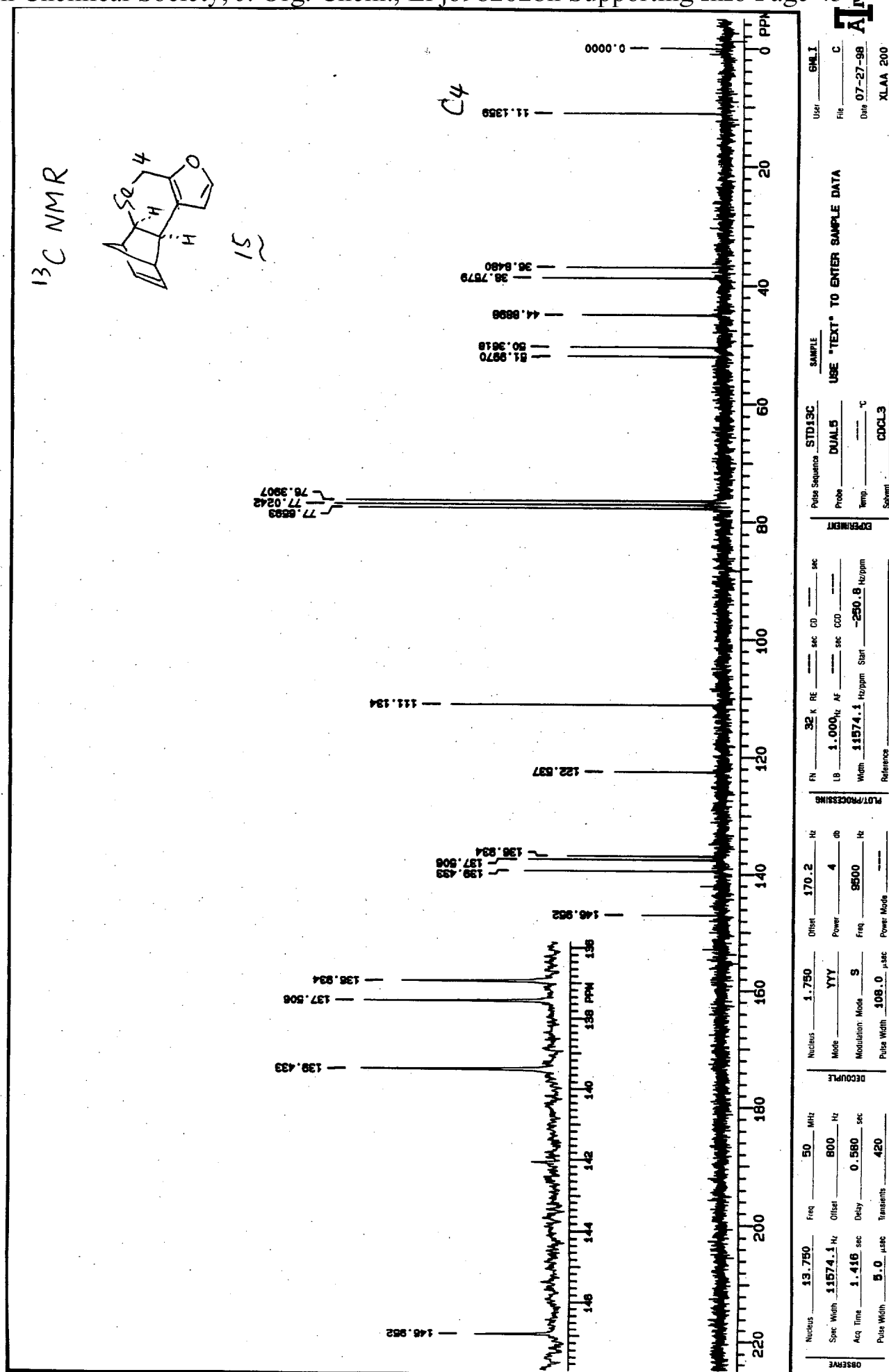
H1

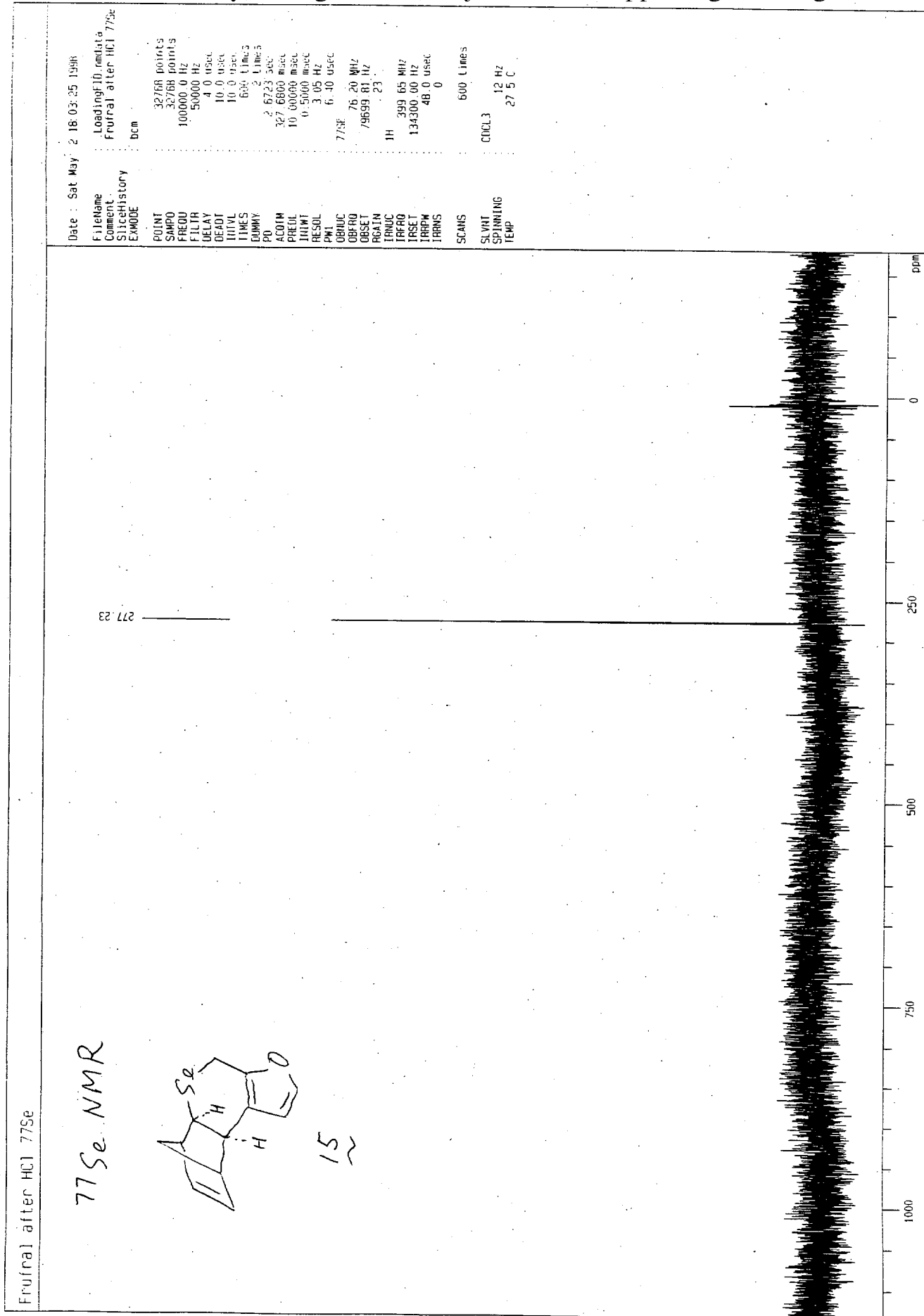
H11

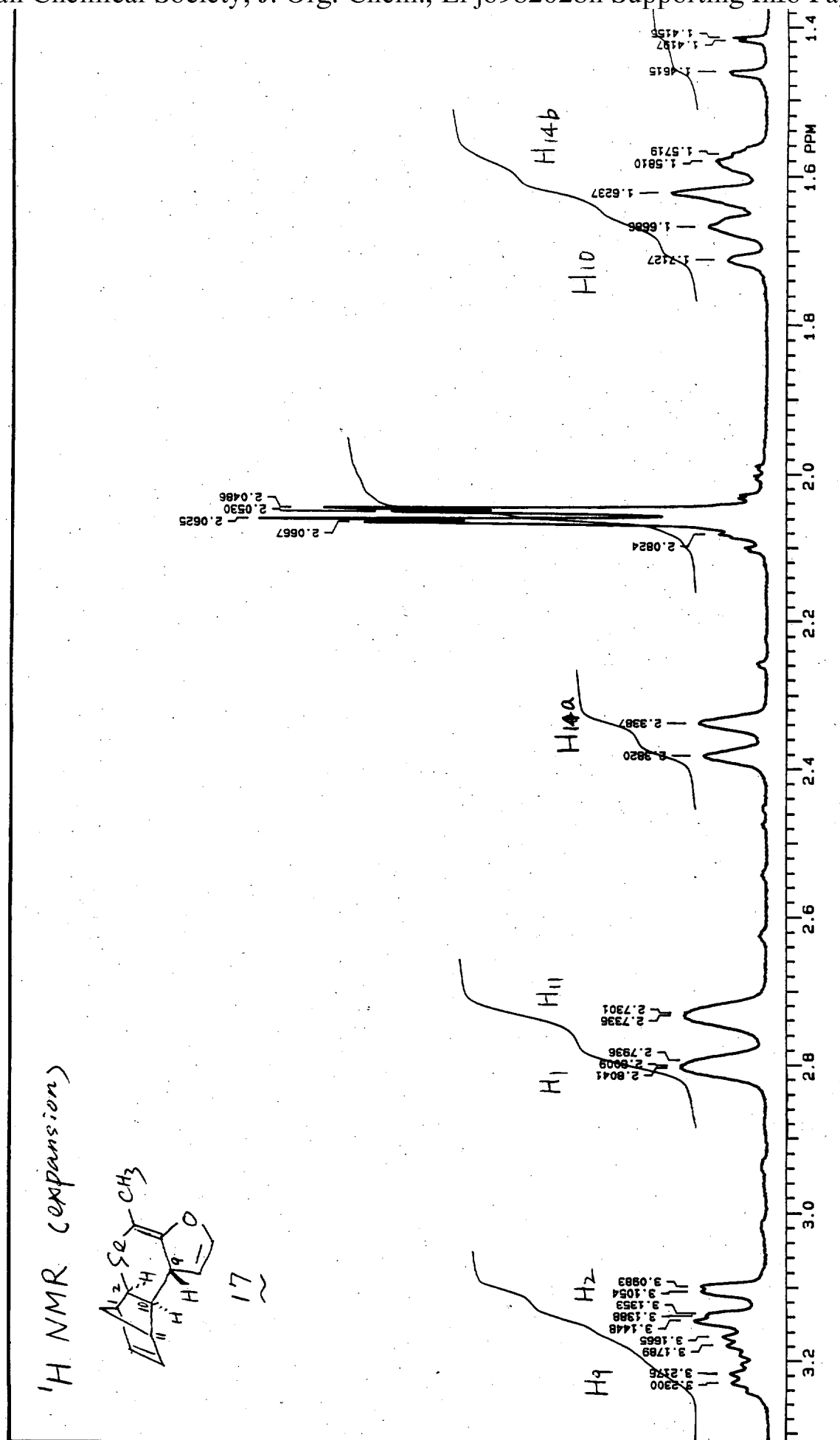
H10

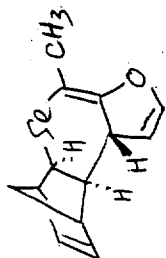
H14a, H14b



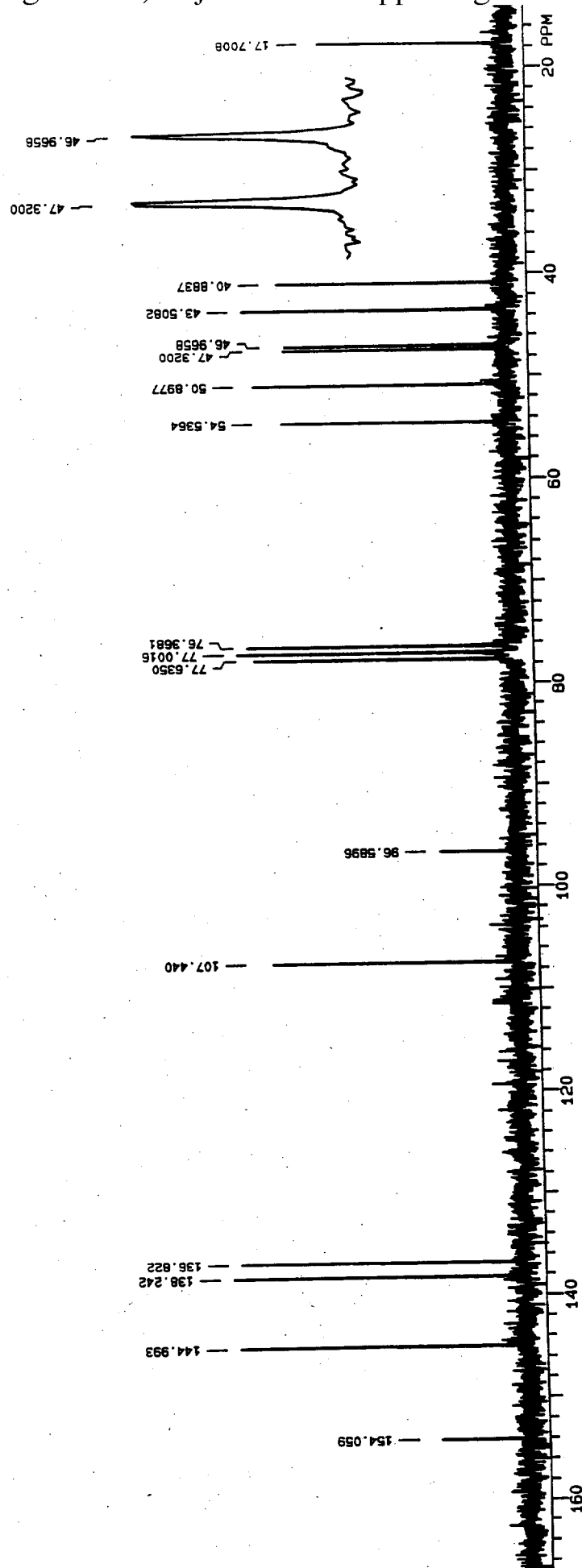






^{13}C NMR

17)



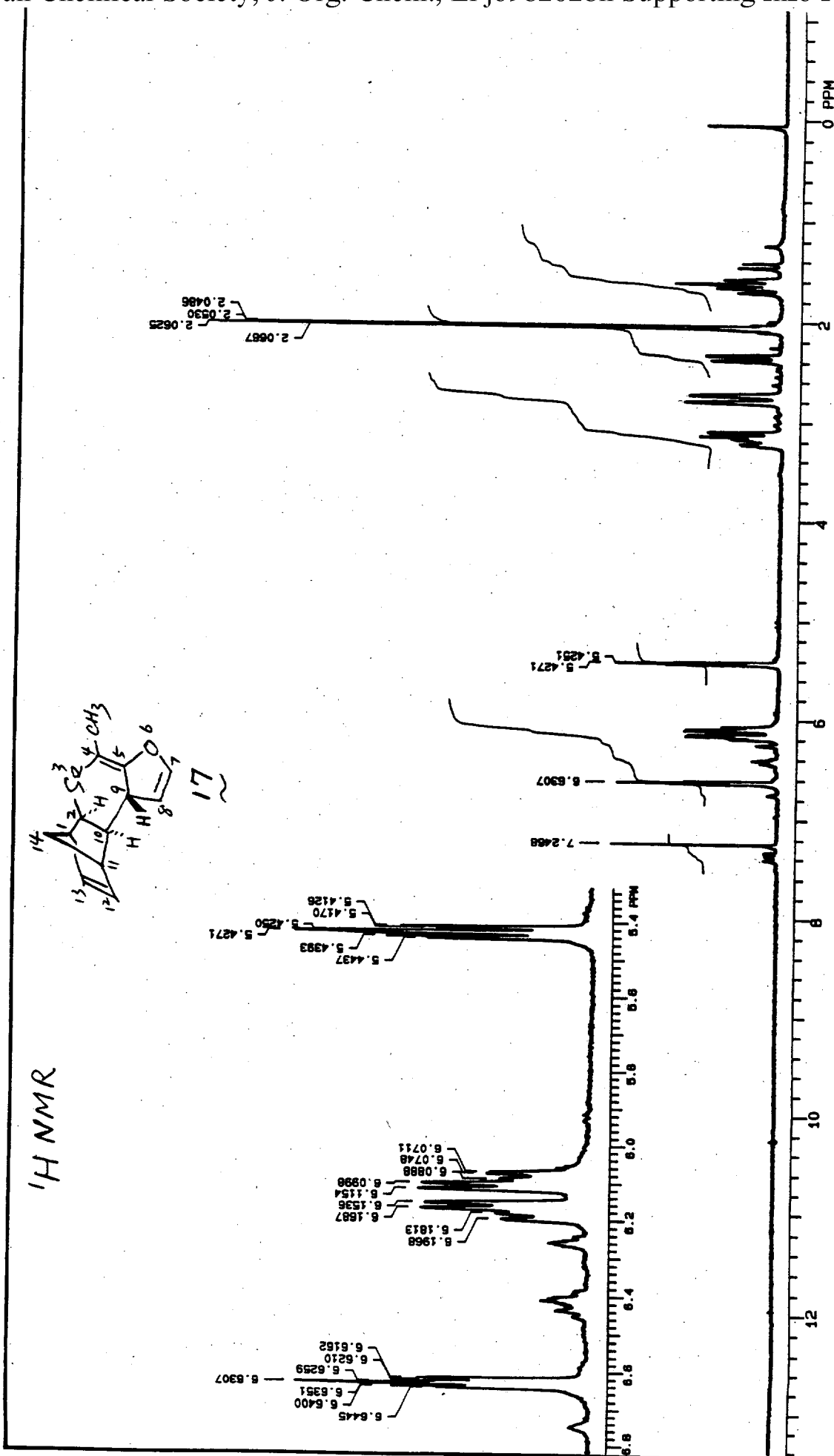
SAMPLE _____
USE "TEXT" TO ENTER SAMPLE DATA

Pulse Sequence	STD13C
Probe	DUAL5
Temp	--- °C
Sample	CDCL3

FN 32 K RE SEC CD SEC
 LB 1.000 Hz AF SEC C/D SEC
 Wdth 7711.8 Hz/ppm Start 693.0 Hppm

Nucleus **1.750** Offset **170.2** Hz
 Mode **YYY** Power **4** db
 Modulation Mode **S** Freq. **9300** Hz

Nucleus 13.750 Freq 50 MHz
Spec Width 11574.1 Hz Offset 800 Hz
Acq Time 1.418 sec Delay 0.580 sec



USE "TEXT" TO ENTER SAMPLE DATA

EXPERIMENT

Pulse Sequence: STD1H

Probe: DUALB

Temp: °C

Solvent: CDCL3

Reference: TMS

Acq Time: 5.848 sec

Spec Width: 2801.1 Hz

Decouple: 1.750

Modulation Mode: C

Power: 20

Offset: 170.2 Hz

Power Mode: μsec

Pulse Width: 20

Transients: 20

Delay: 0.350 sec

Offset: 400 Hz

Frequency: 200 MHz

NUC1: 1.750

NUC2: 200

NUC3: 200

NUC4: 200

NUC5: 200

NUC6: 200

NUC7: 200

NUC8: 200

NUC9: 200

NUC10: 200

NUC11: 200

NUC12: 200

NUC13: 200

NUC14: 200

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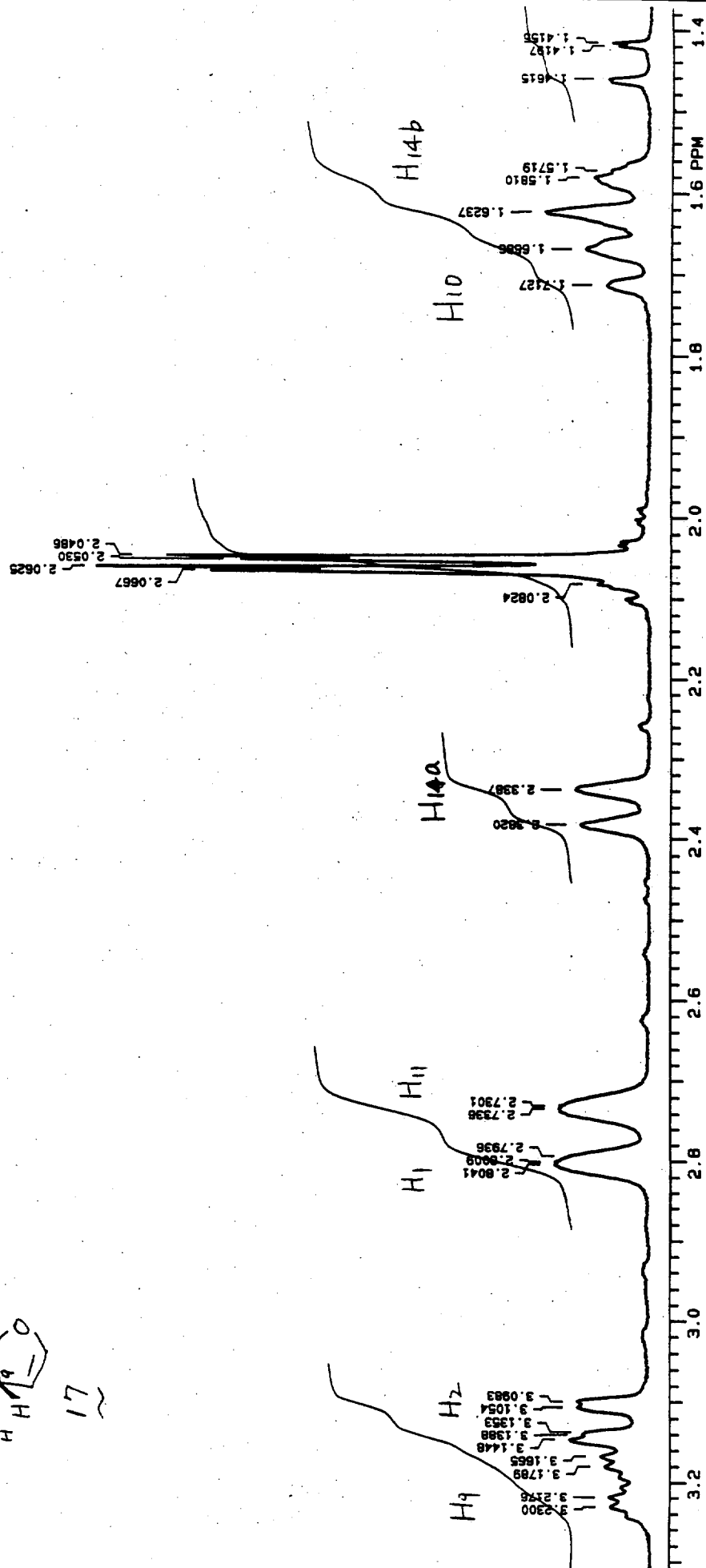
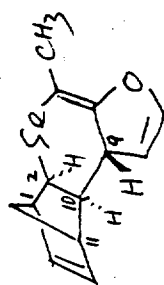
NUC722: 200

NUC723: 200

NUC724: 200

NUC725: 200

NUC726: 2

¹H NMR (expansion)

DETERMINE

Nucleus: ¹H, Freq: 200 MHz, Spec Width: 200.1 Hz, Acq Time: 5.648 sec, Pulse Width: 5.8 μsec

RECOUPLE

Decouple: 200 Hz, Delay: 0.350 sec, Transients: 20

PLT/PROCESSING

FN: 32 K, RE: 387.4 Hz, AF: 274.3 Hz, Width: 387.4 Hz, Start: 274.3 Hz, Reference: 274.3 Hz

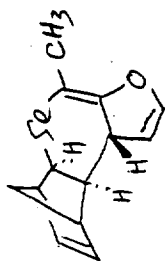
DOCUMENT

Pulse Sequence: STD1H, DUALS: USE *TEXT* TO ENTER SAMPLE DATA, Probe: CDCL₃, Temp: °C, Solvent: CDCL₃

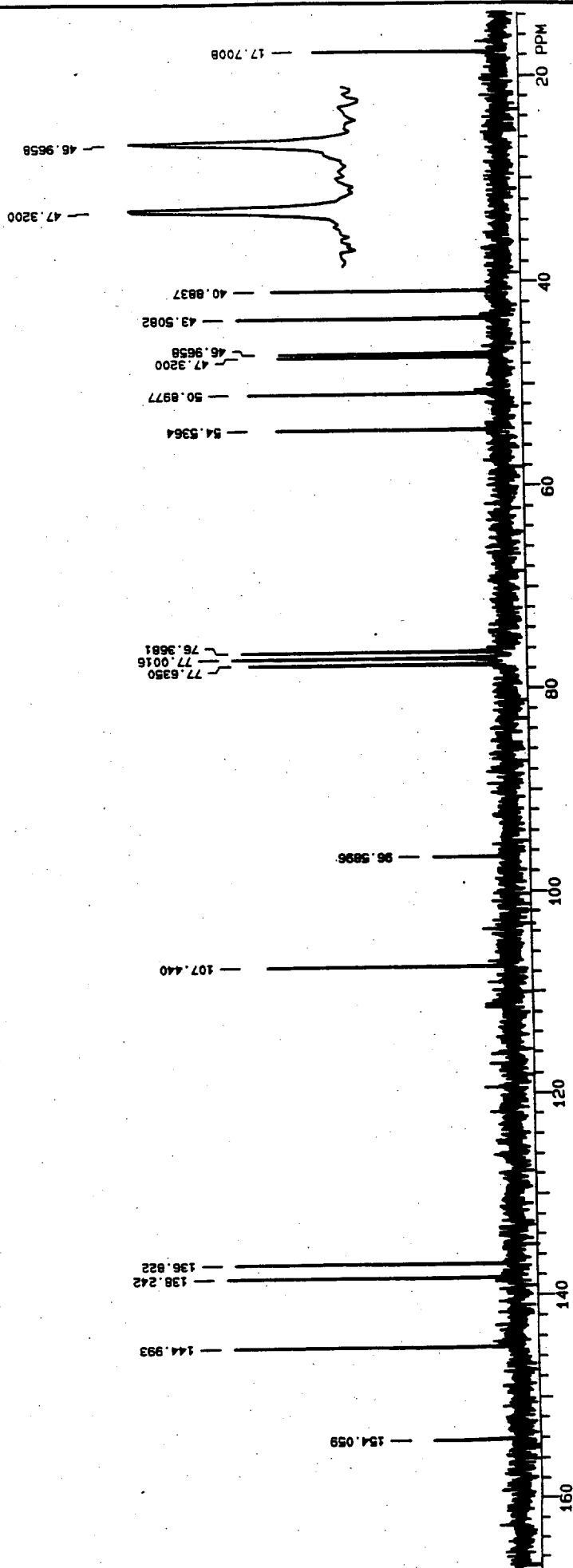
USER: GML, User: H, File: 12-18-97, Date: 12-18-97, XLAA 200

AT

¹³C NMR



17



OBSERVE				RECOUPLE				PULP/PROCESSING				EXPERIMENT				SAMPLE			
Nucleus	13.750	Freq	50 MHz	Nucleus	1.750	Offset	170.2 Hz	FN	32	K	RE	sec	CD	sec	Pulse Sequence	STD13C	USE "TEXT" TO ENTER SAMPLE DATA		
Spec Width	11574.1 Hz	Offset	800 Hz	Mode	YYY	Power	4 db	LB	1.000	Hz	AF	sec	CD	sec	Probe	DUAL5			
Acq Time	1.418 sec	Delay	0.580 sec	Modulation Mode	S	Freq	9300 Hz	Width	7713.8	Hz/ppm	Start	893.0	Hz/ppm		Temp		°C		
Pulse Width	0.0 μsec	Transmit	200	Pulse Width	108.0 μsec	Power Mode		Reference							Solvent	CDCL3			

Acetylthiophene cycloadduct 1H

Date: Fri May 19 15:43:33 1999
 Filename: 11000001
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 Solvent: CDCl3
 E-90000

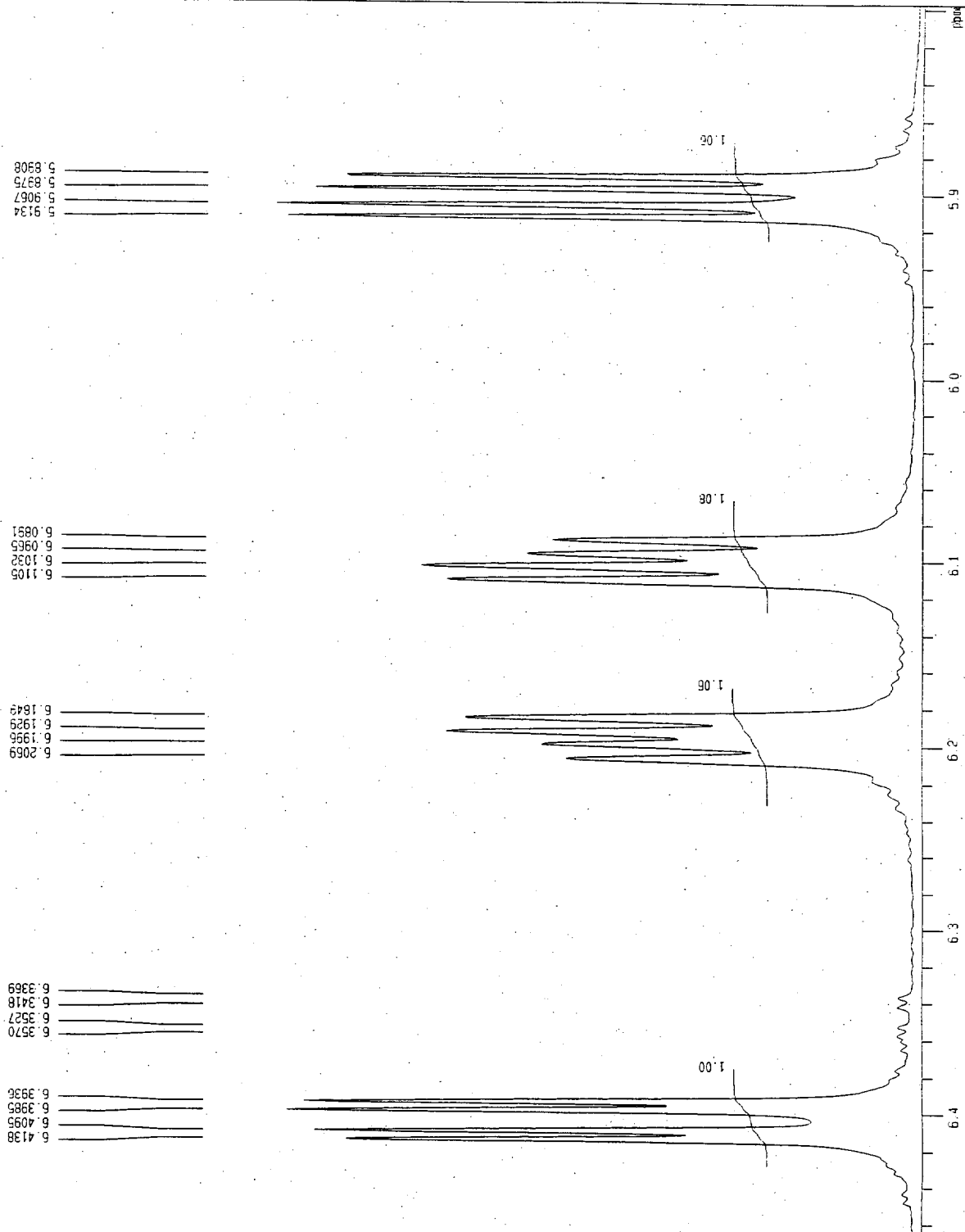
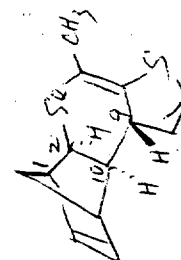
1H NMR (400 MHz) data:

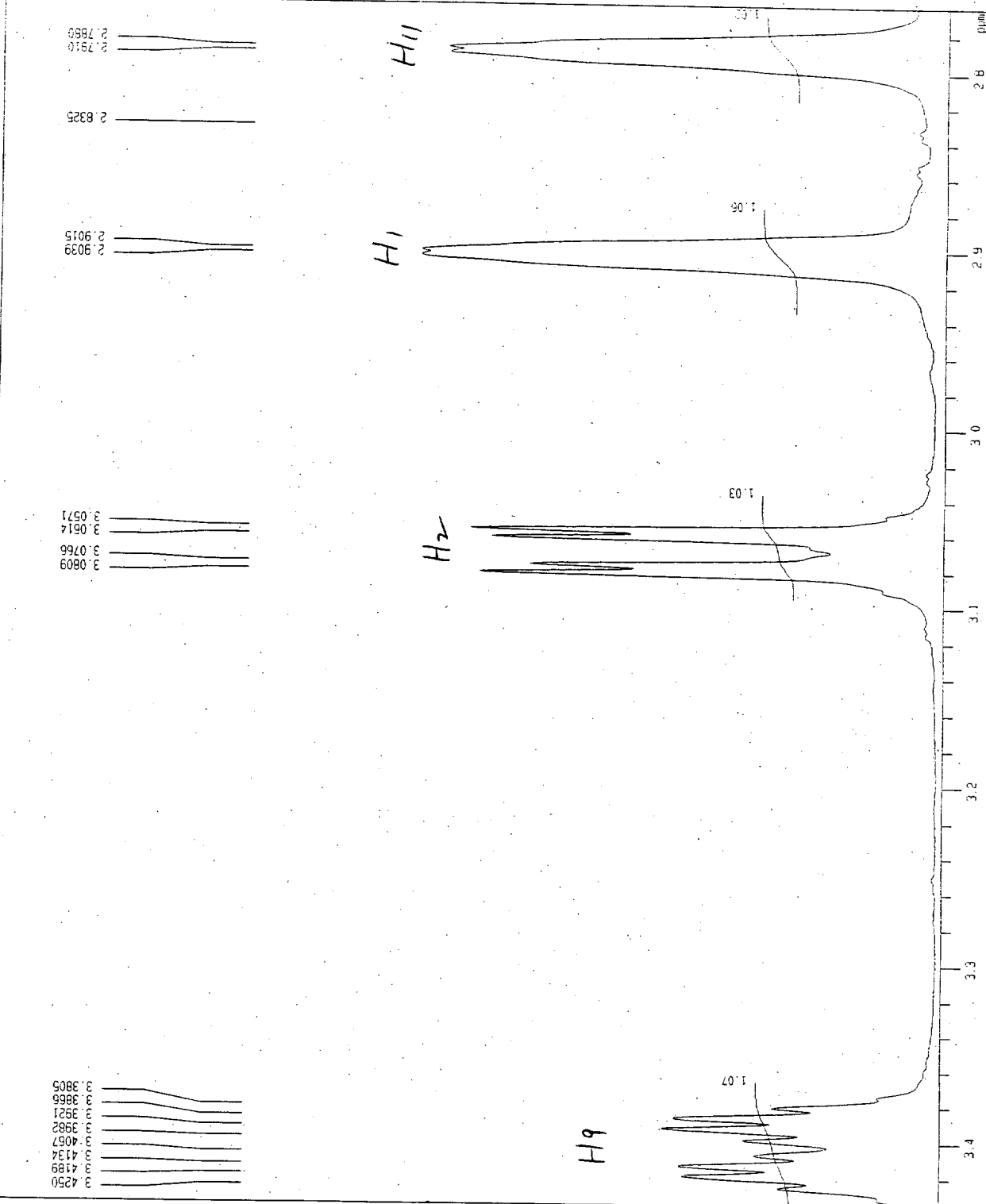
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6.8665	1.00	H5
6.8537	1.00	H6
6.7701	1.00	H7
6.7610	1.00	H8
6.4138	1.00	H9
6.4095	1.00	H10
6.3985	1.00	H11
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6.3570	1.00	H13
6.3527	1.00	H14
6.3418	1.00	H15
6.3369	1.00	H16
6.2069	1.00	H17
6.1956	1.00	H18
6.1829	1.00	H19
6.1849	1.00	H20
6.1105	1.00	H21
6.1032	1.00	H22
6.0965	1.00	H23
6.0891	1.00	H24
5.9134	1.00	H25
5.9067	1.00	H26
5.8975	1.00	H27
5.8908	1.00	H28
5.4250	1.00	H29
5.4189	1.00	H30
5.4134	1.00	H31
5.4067	1.00	H32
5.3982	1.00	H33
5.3921	1.00	H34
5.3866	1.00	H35
5.3805	1.00	H36
5.3809	1.00	H37
5.3766	1.00	H38
5.3614	1.00	H39
5.3571	1.00	H40
5.3512	1.00	H41
5.3457	1.00	H42
5.3395	1.00	H43
5.3335	1.00	H44
5.3277	1.00	H45
5.3210	1.00	H46
5.3138	1.00	H47
5.3067	1.00	H48
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5.2744	1.00	H53
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5.1944	1.00	H65
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5.1814	1.00	H67
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5.1614	1.00	H70
5.1544	1.00	H71
5.1477	1.00	H72
5.1414	1.00	H73
5.1344	1.00	H74
5.1277	1.00	H75
5.1214	1.00	H76
5.1144	1.00	H77
5.1077	1.00	H78
5.1014	1.00	H79
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5.0814	1.00	H82
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5.0077	1.00	H93
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4.6277	1.00	H150
4.6214	1.00	H151
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4.6077	1.00	H153
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3.1		

Acetylthiophene cycloadduct III

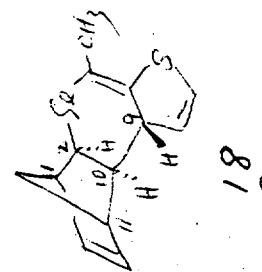
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 PREP: 10.0000 sec
 INVT: 10.0000 sec
 PASC: 6.34 Hz
 PHA: 6.34 Hz
 ORDC: 6.34 Hz
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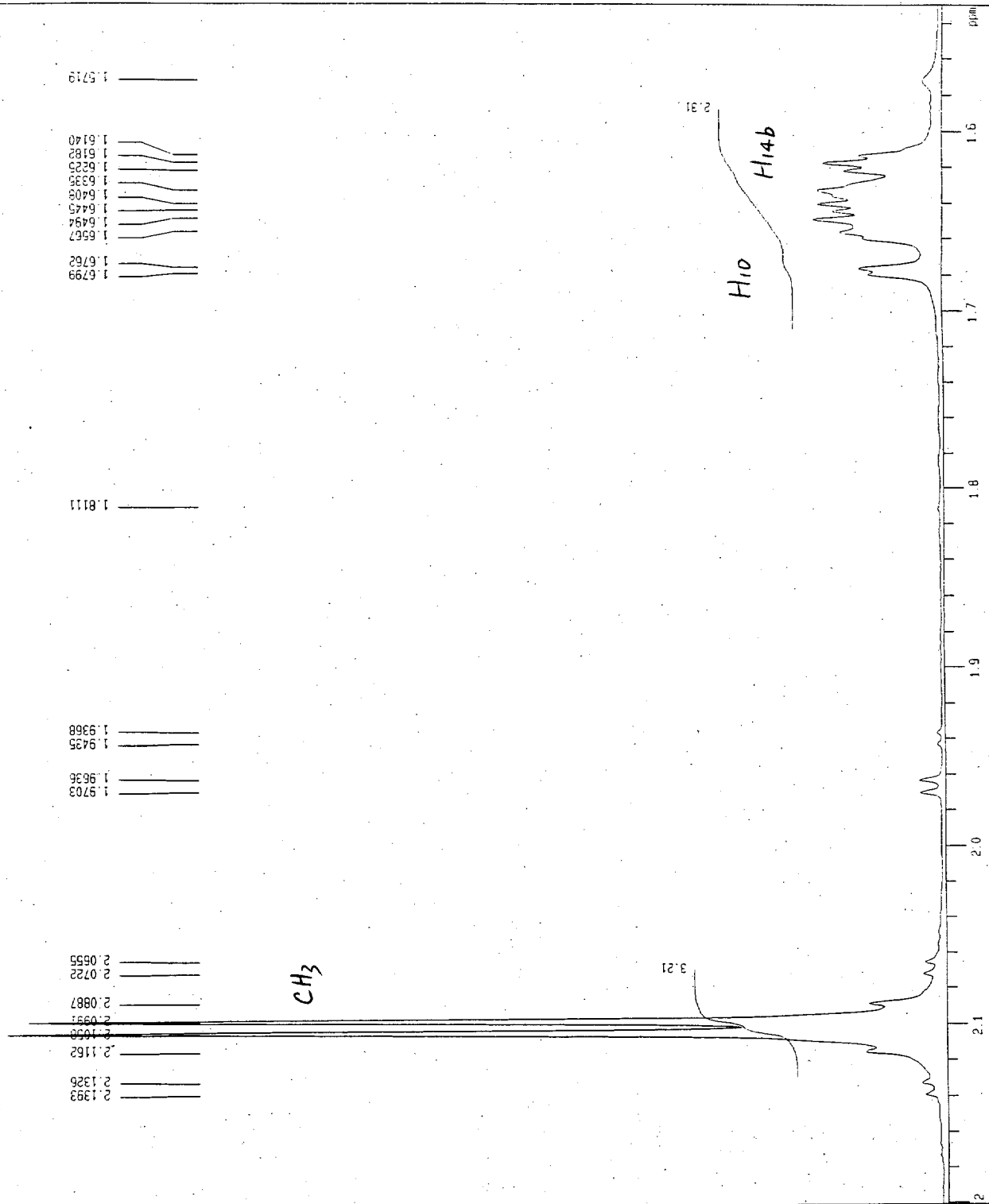
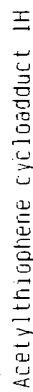
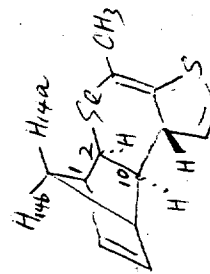
¹H NMR
 (expansion)

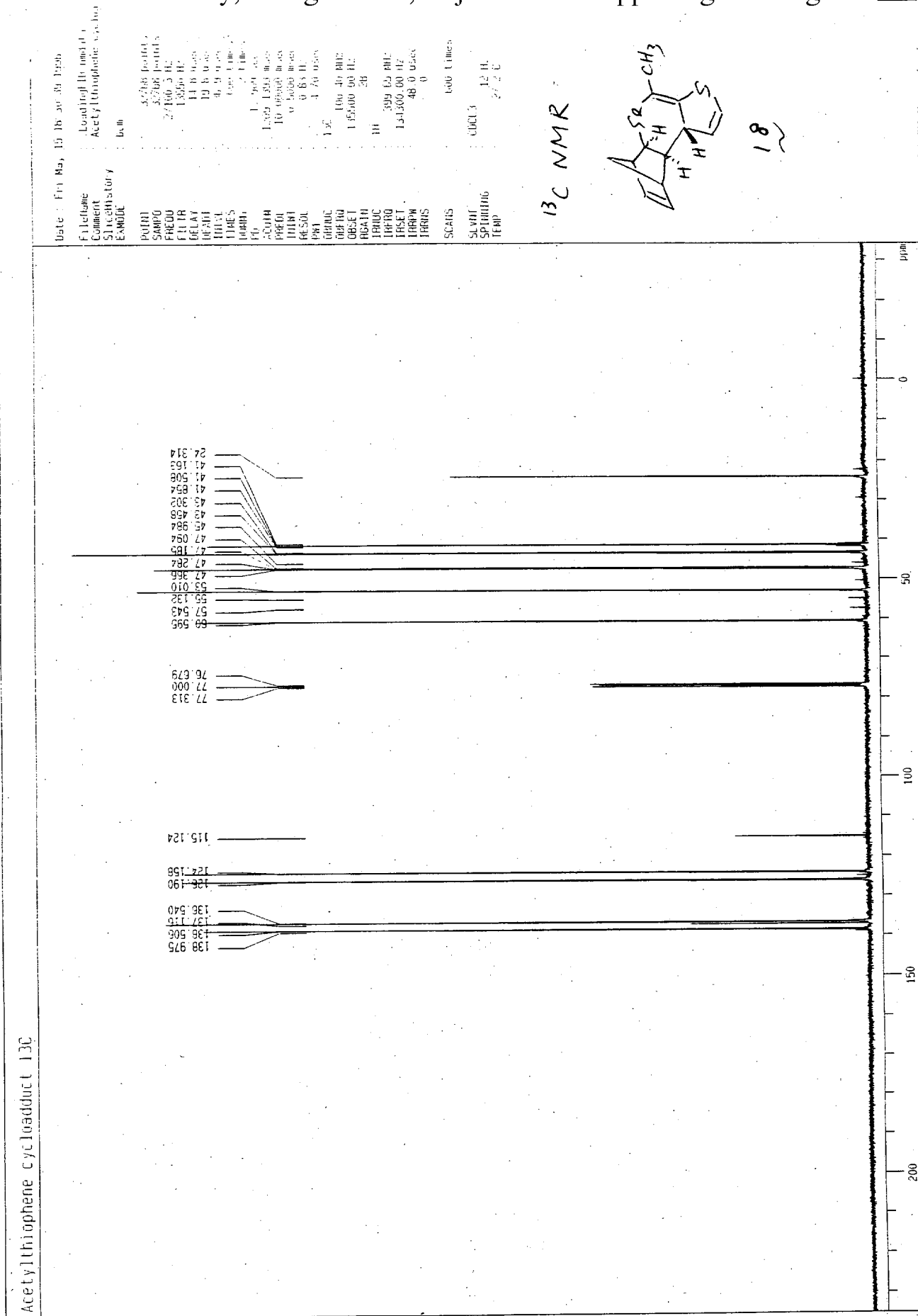




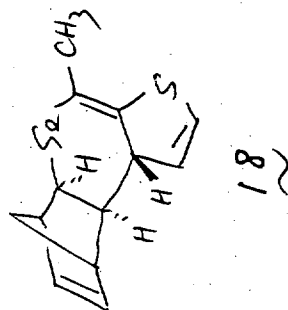
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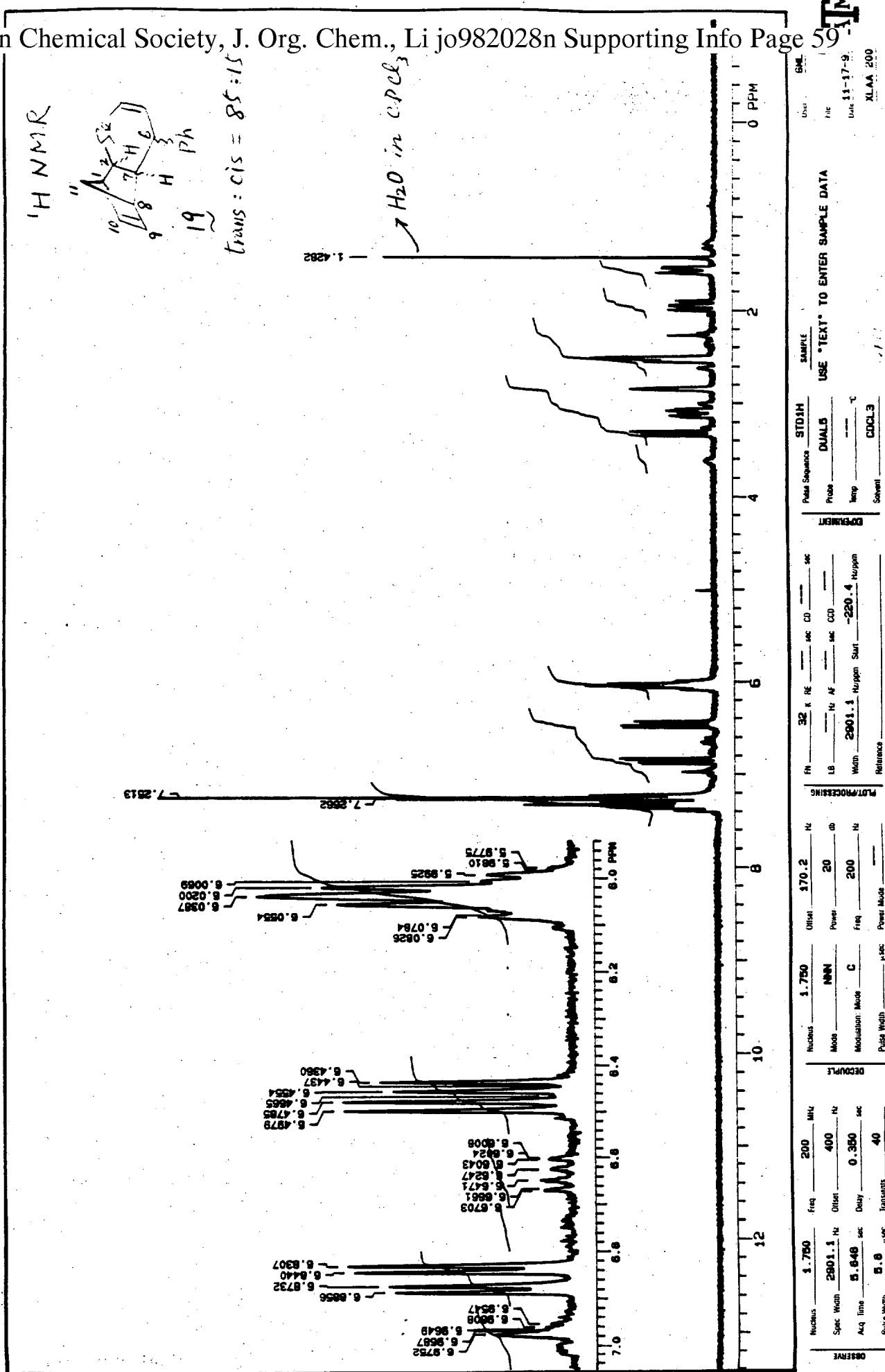


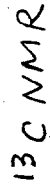
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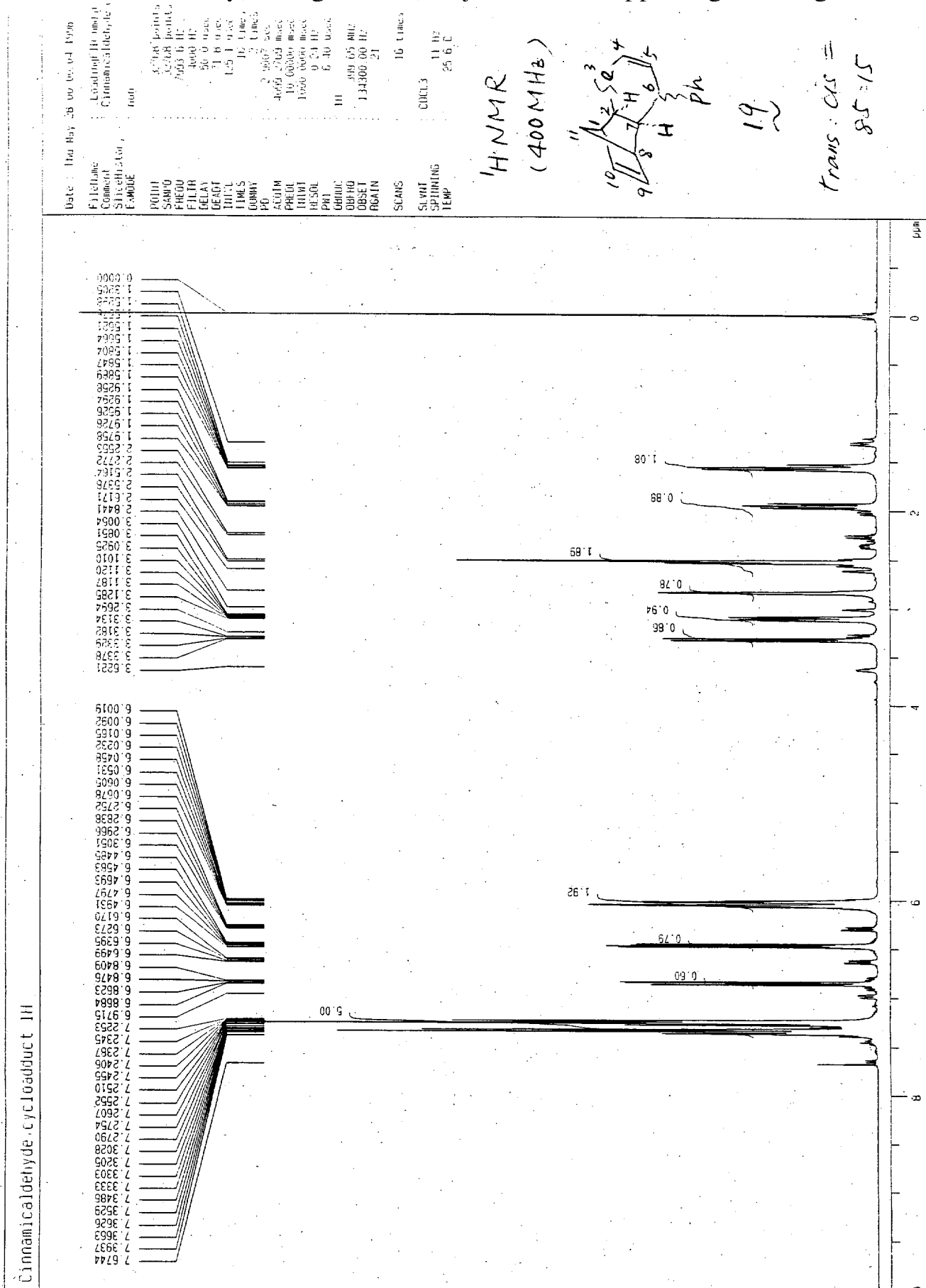


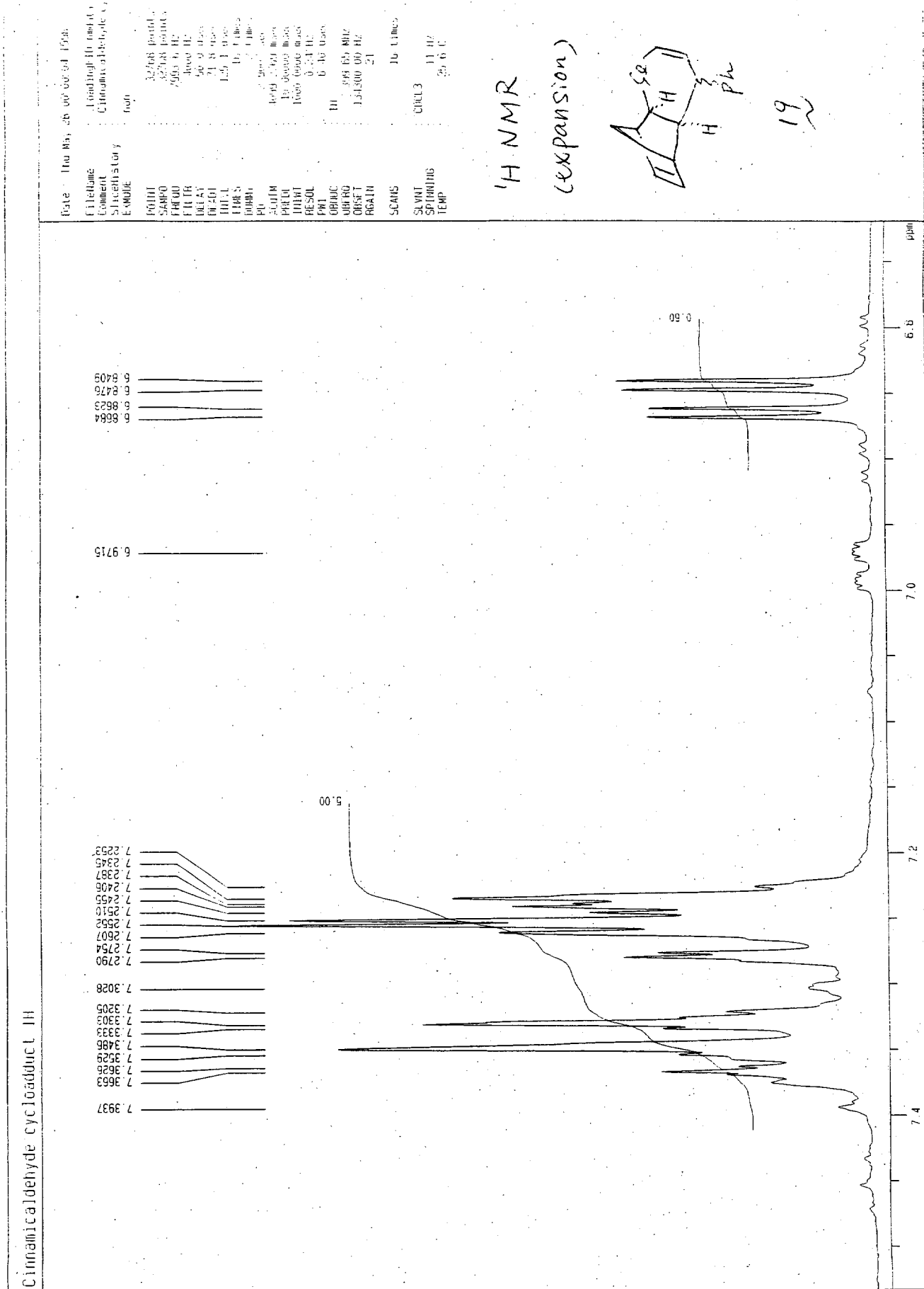
^{77}Se NMR

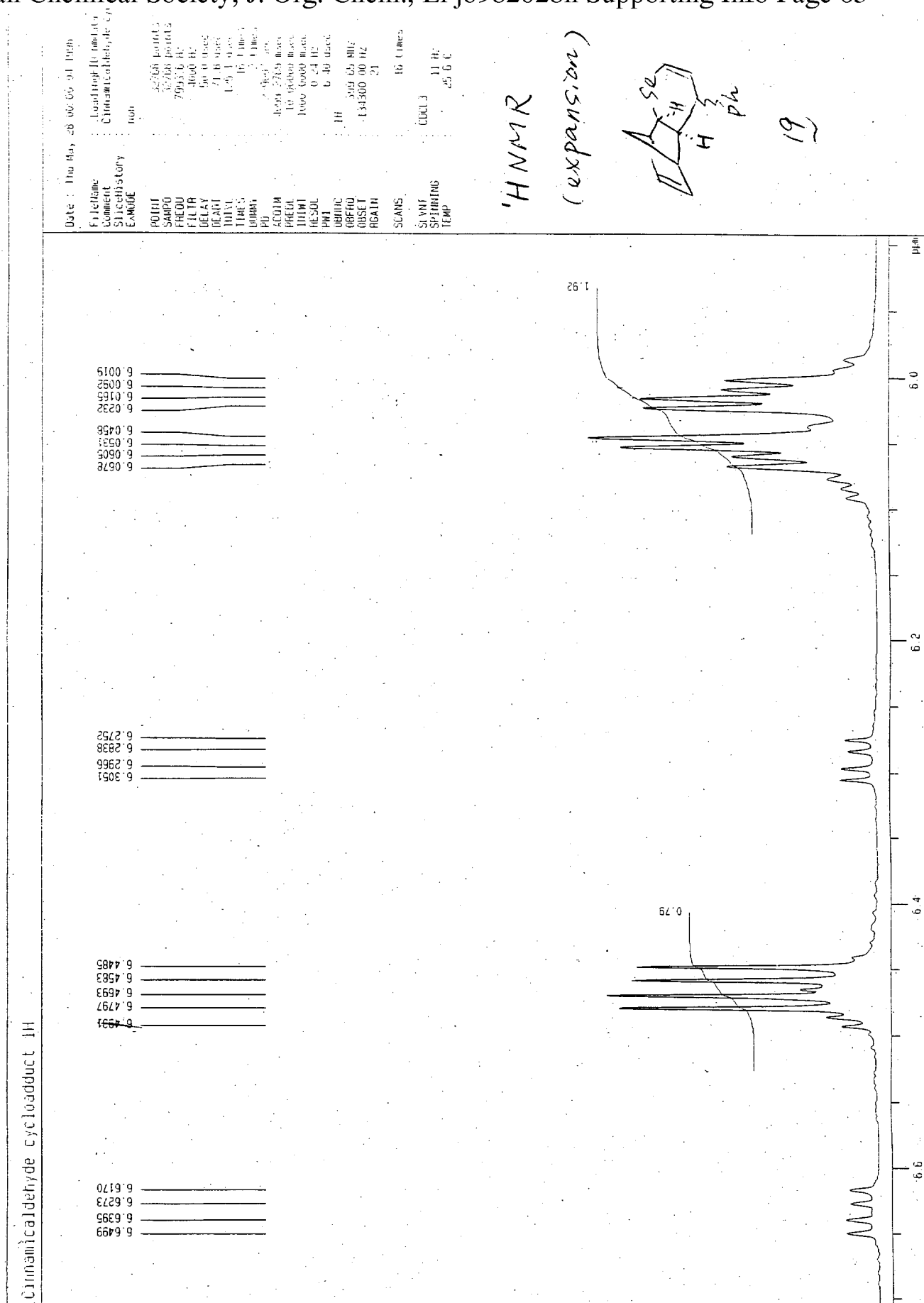
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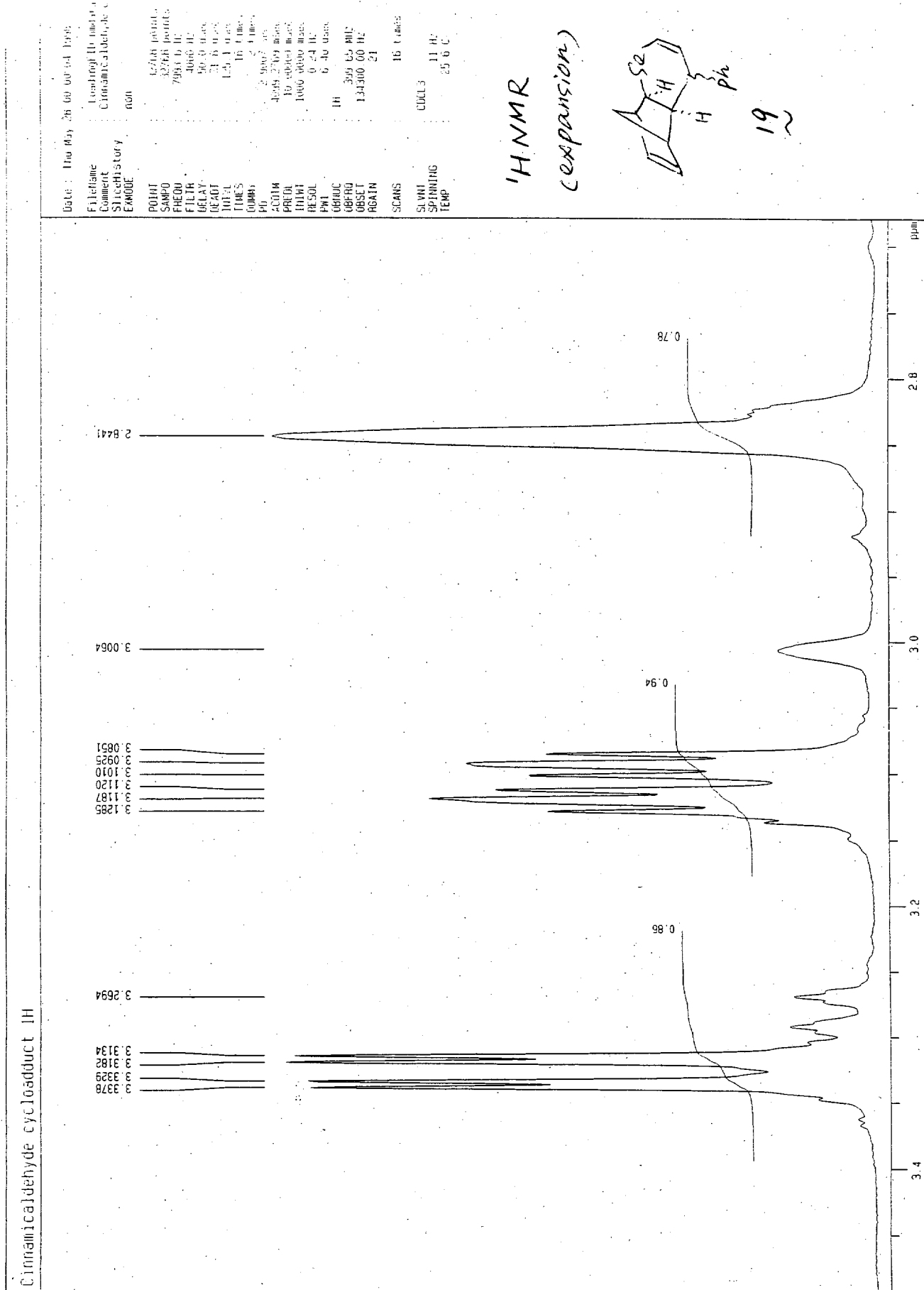




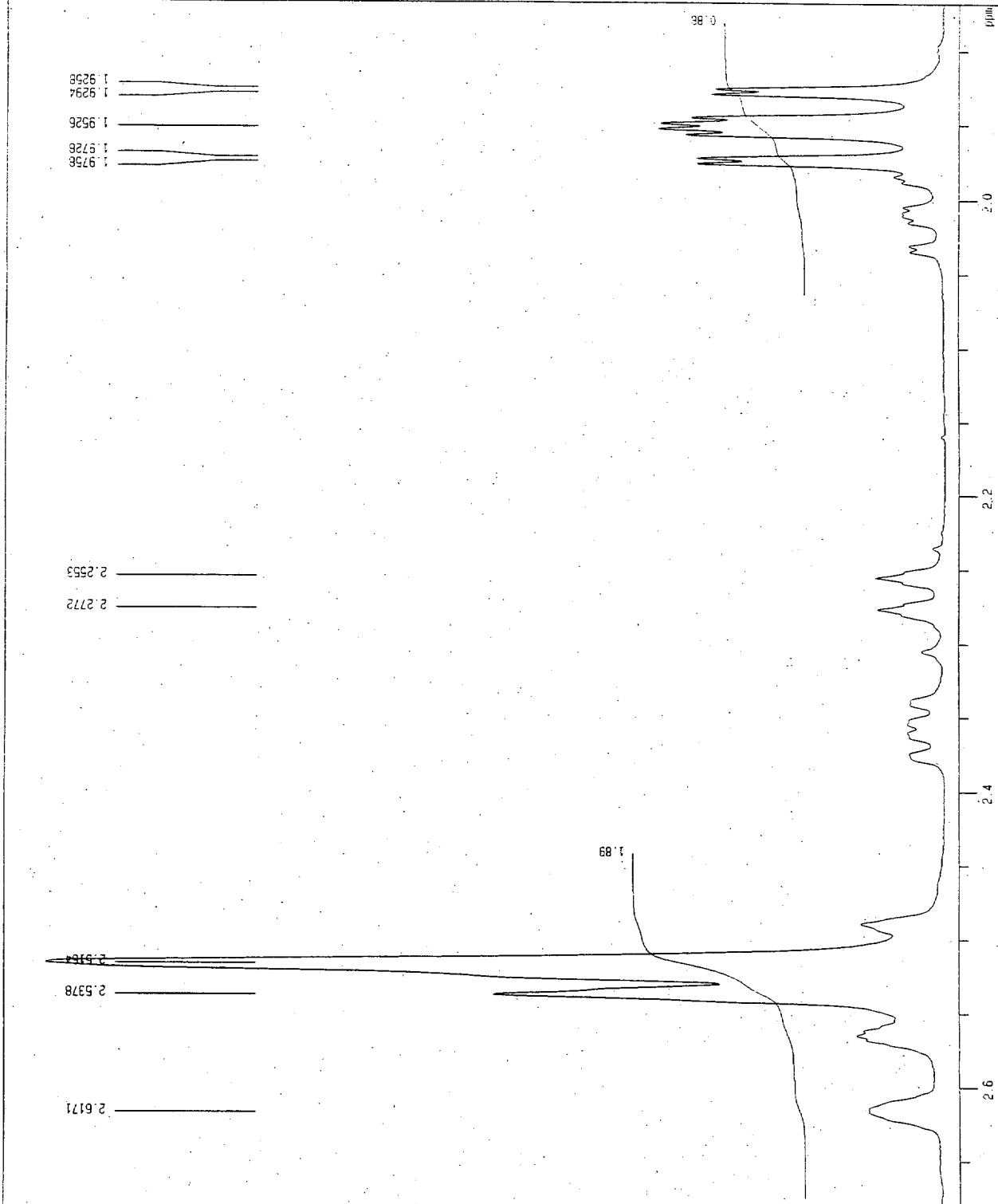


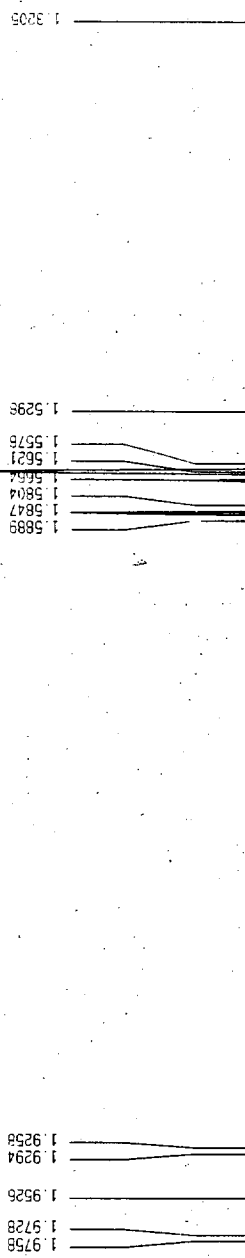






Cinnamicaldehyde cycloadduct 1H



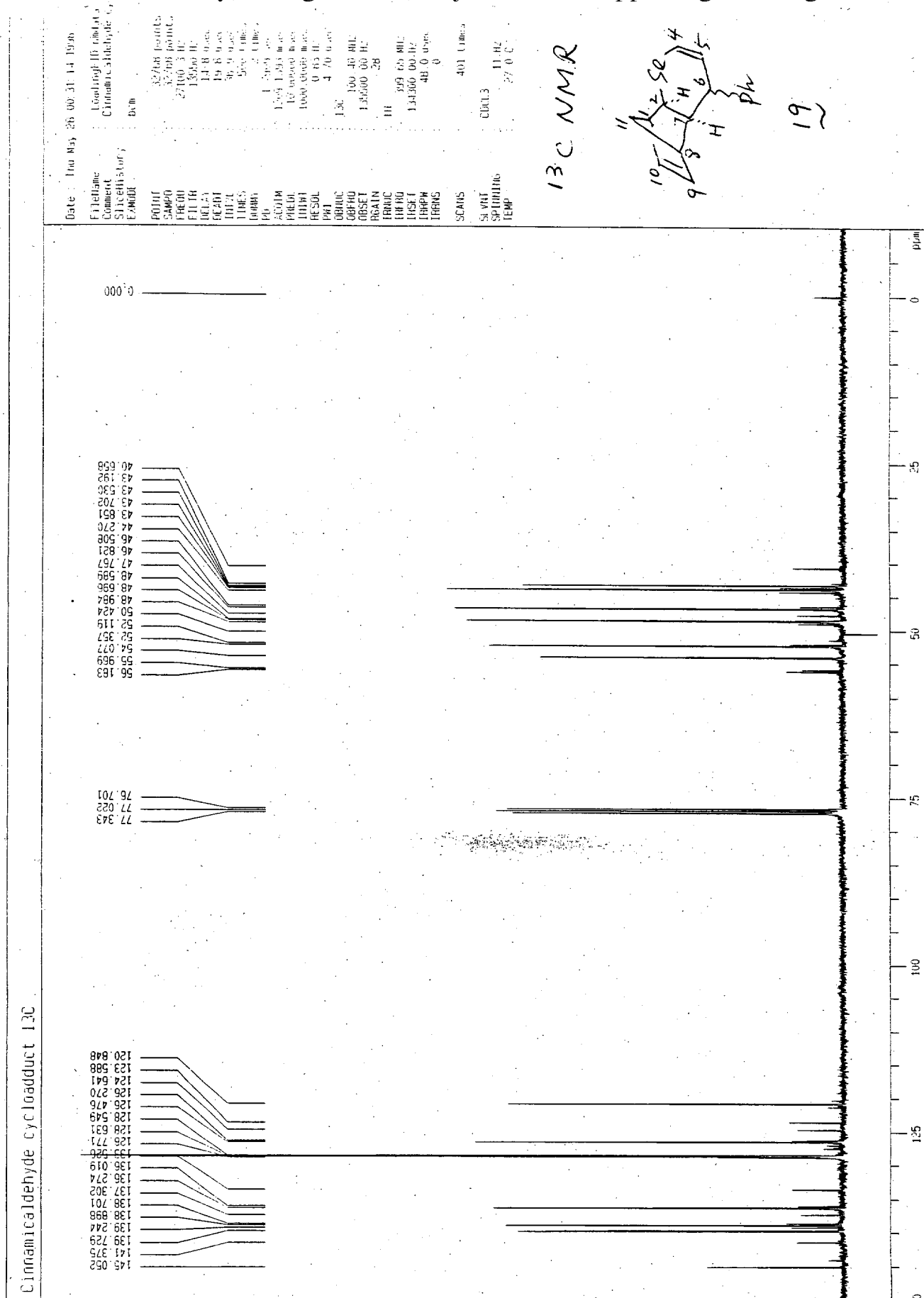


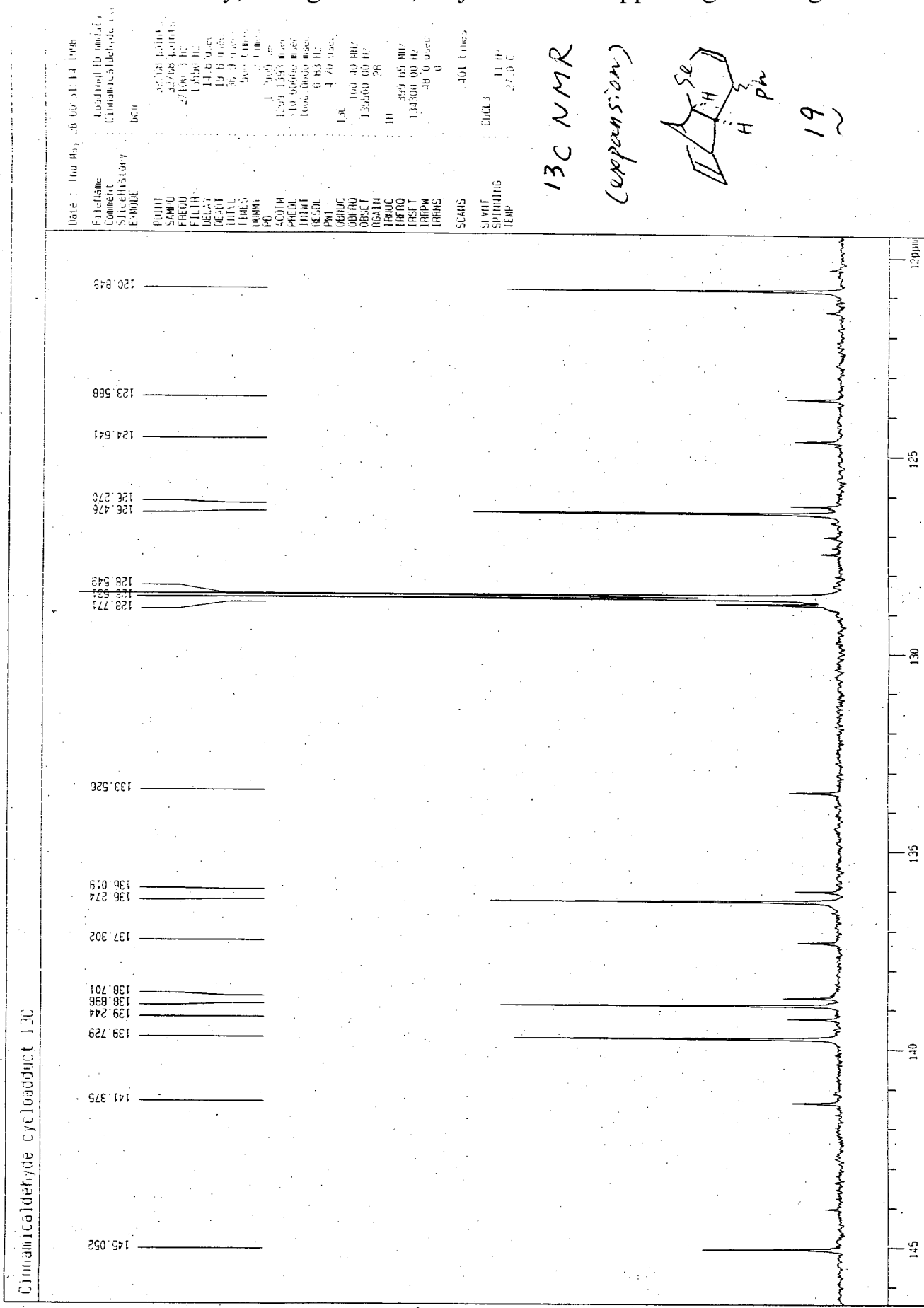
$^1\text{H NMR}$ (expansion)

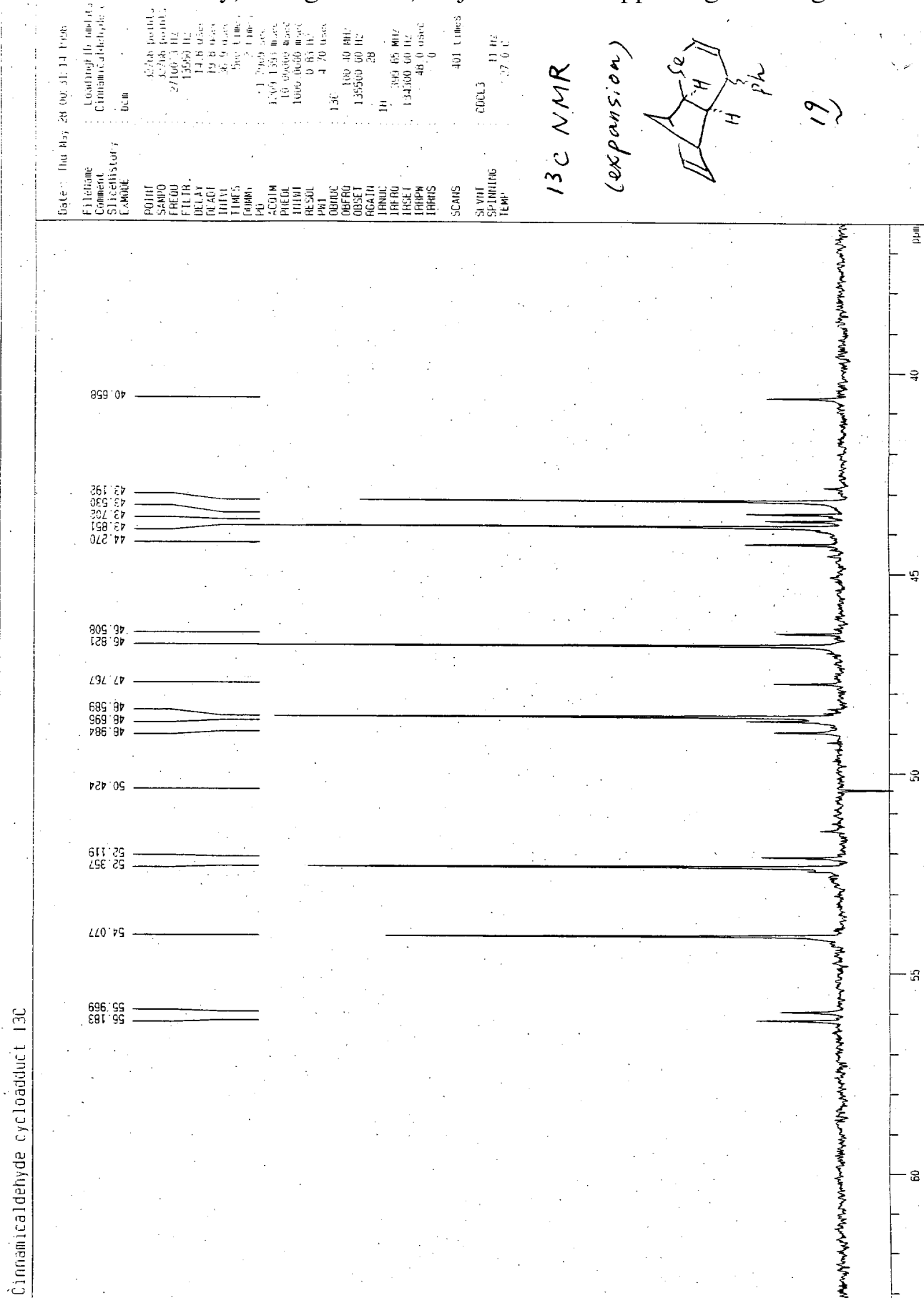


61

[illegible]

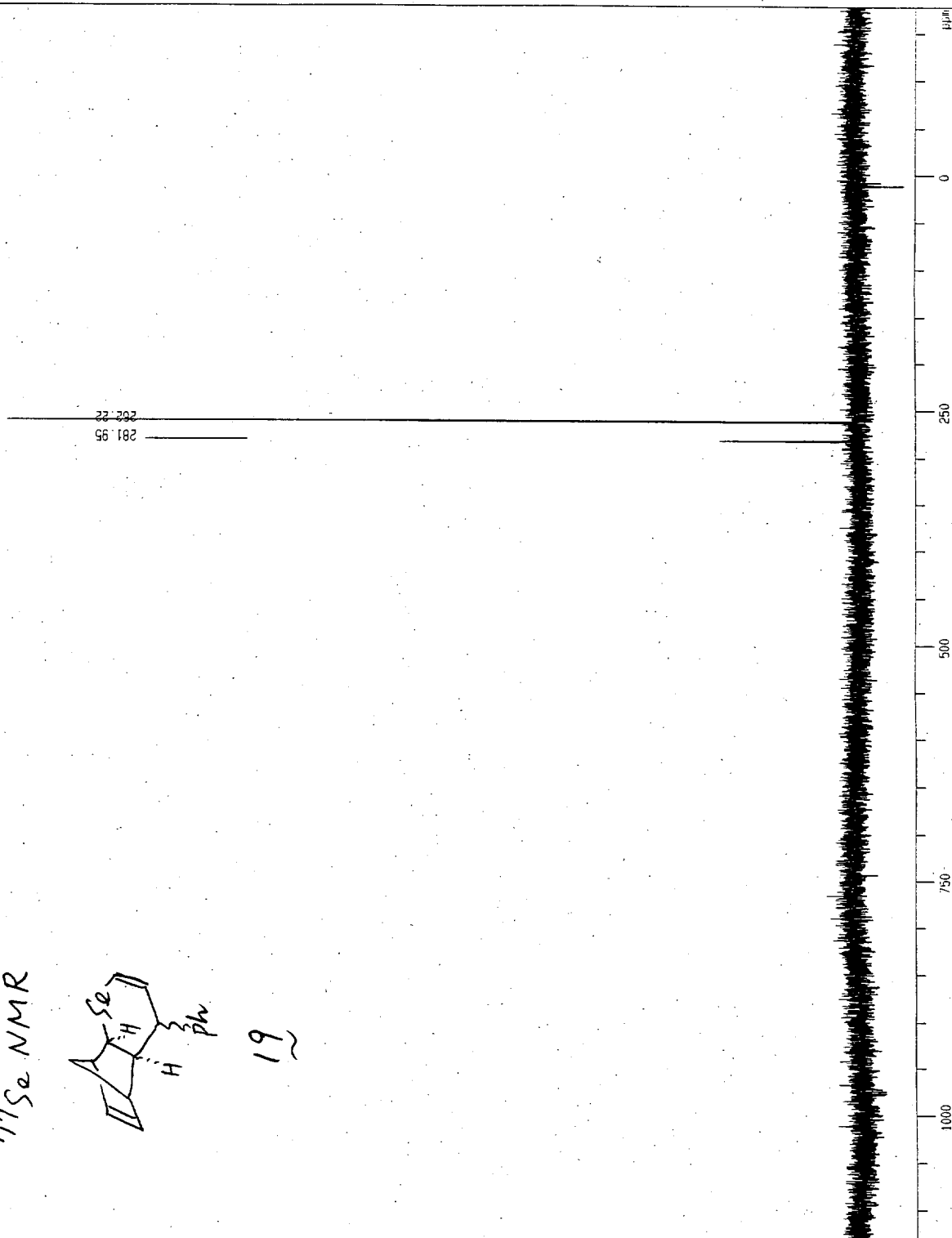






^{77}Se NMR

19



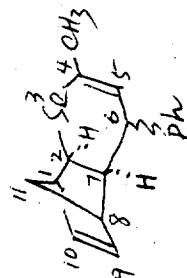
Benzalacetone cycloadduct 1H

Date: Wed May 27 23:09:22 1998

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 E-MODE: non

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 TITVL: 125.1 usec
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 RUNNY: 2 times
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 PRELO: 10.00000 msec
 TUMI: 1000.0000 msec
 RESOL: 0.24 Hz
 PNH: 6.40 usec
 OBNUC: 1H
 OBFRQ: 399.65 MHz
 OBSET: 134300.00 Hz
 RGAIN: 17
 SCANS: 16 times
 SLVNT: CDCL3
 SPINNT: 13 Hz
 TEM: 22.8 C
¹H NMR

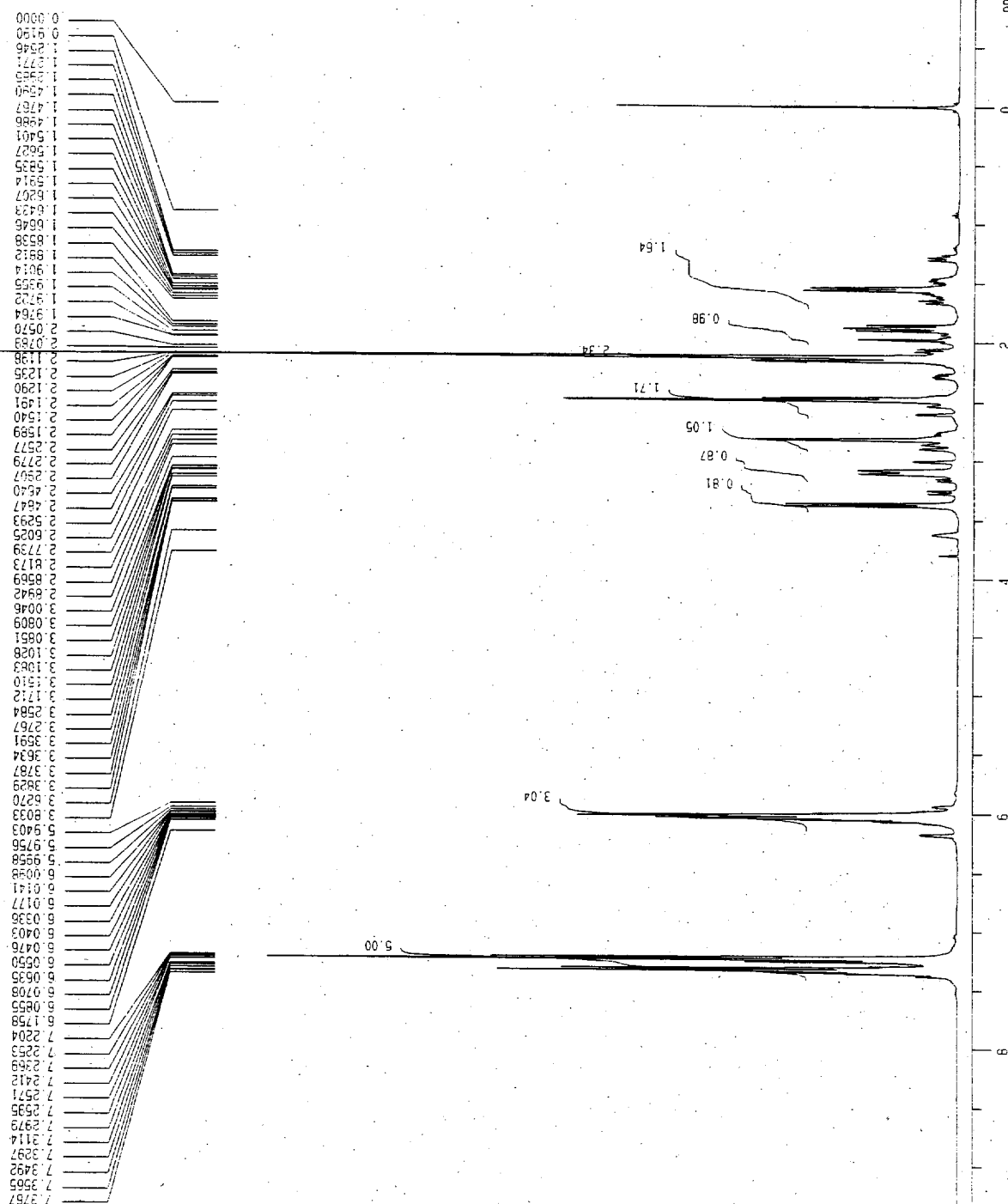
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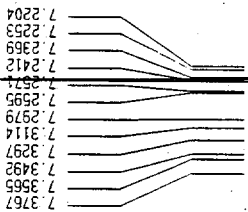
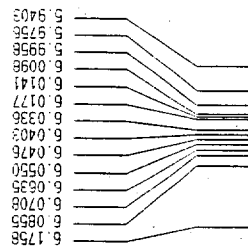
20

Trans: cis =

82:18



Benzalacetone cycloadduct 1H

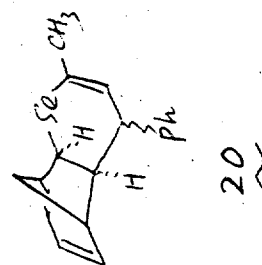


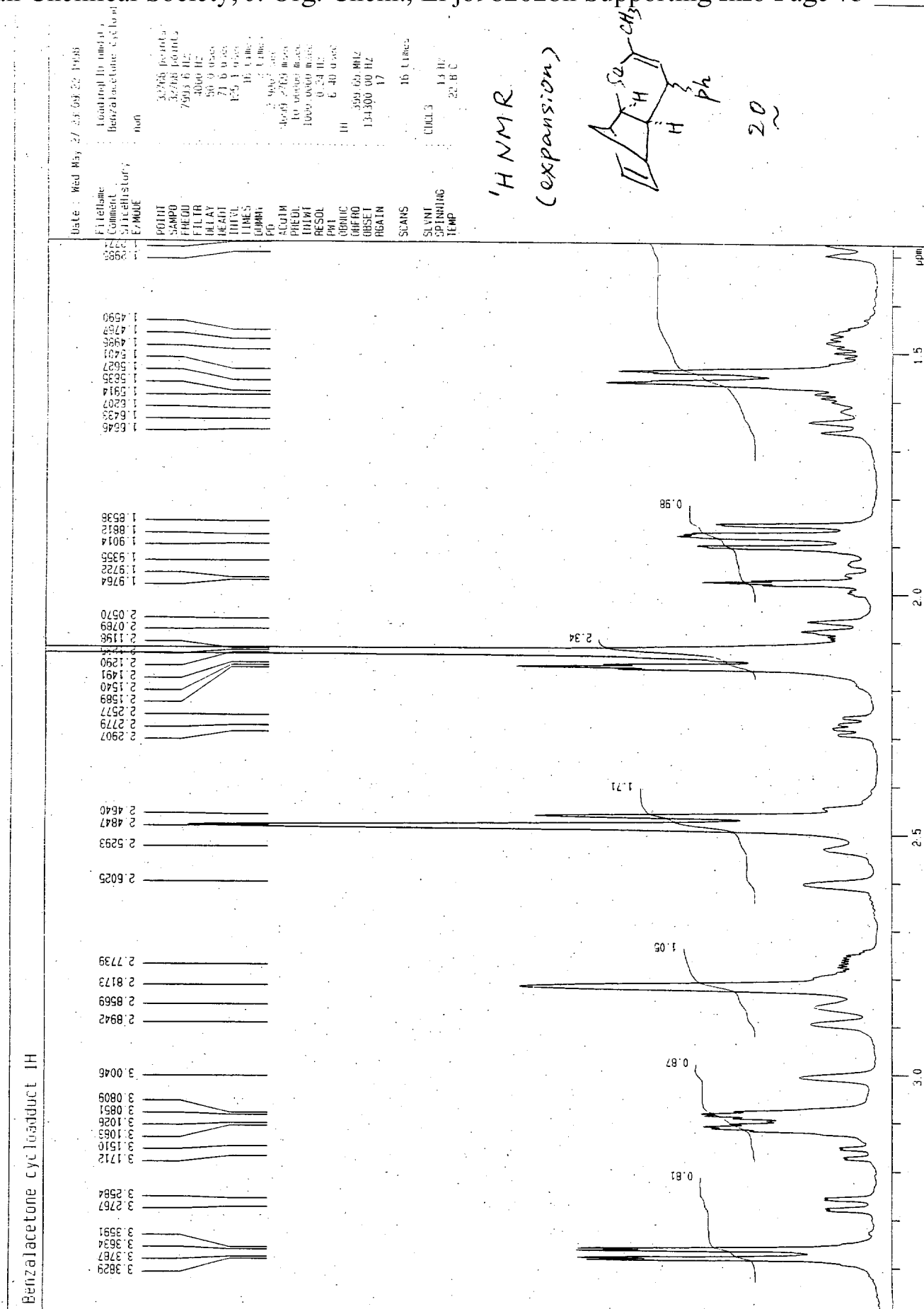
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 Comment: Benzalacetone cycloadduct
 Spectral history
 LAMODE

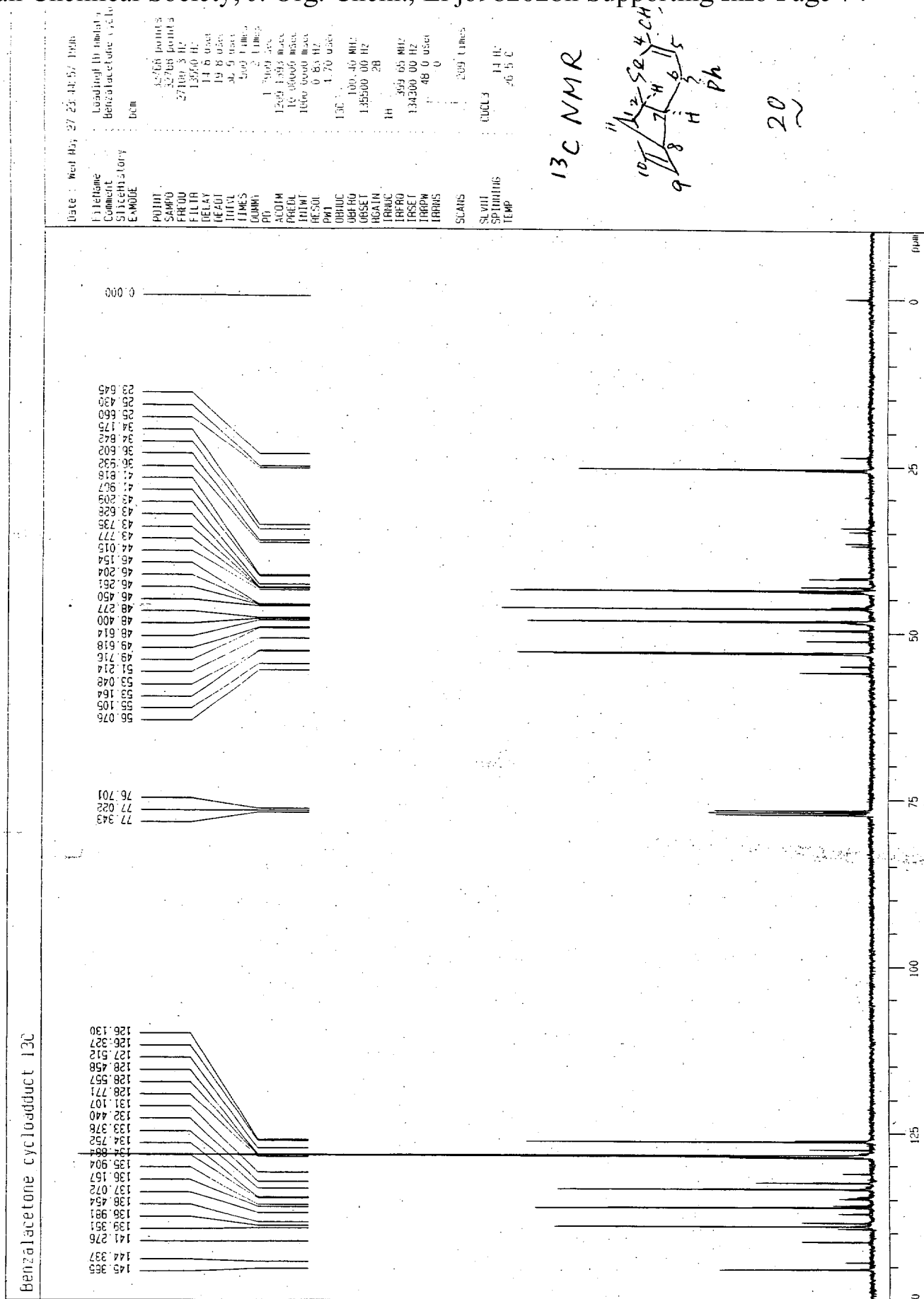
POINT 32768 points
 SAMPLE 32768 points
 FREQ 7993.6 Hz
 FILTER 4000 Hz
 DELAY 50.00 sec
 DEATH 71.60 sec
 TITVL 125.1 Hz
 TIMES 10 Times
 GAIN 2.500
 ACCUM 4059.7759 MHz
 PNUC 10 00000 MHz
 TITVL 1000.0000 MHz
 H2SOL 0.21 Hz
 PH1 6.40 sec
 CPMOL 399.05 MHz
 CPMOL 134300.00 Hz
 OFFSET 17
 RGAIN 10 Times

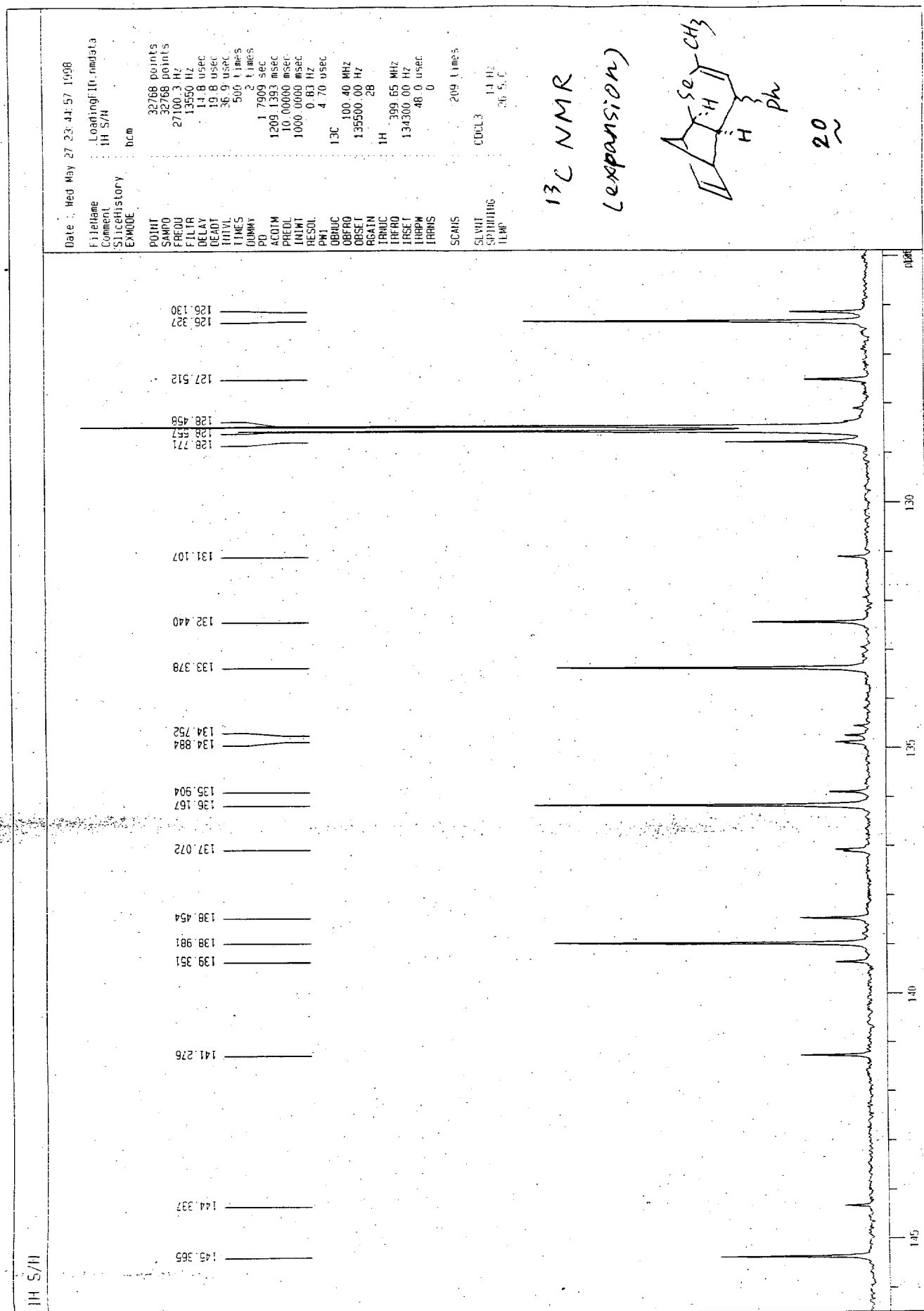
SCANS 10 Times
 SOLVH CUCU3
 SPINNING 13 Hz
 TEMP 22.8 C

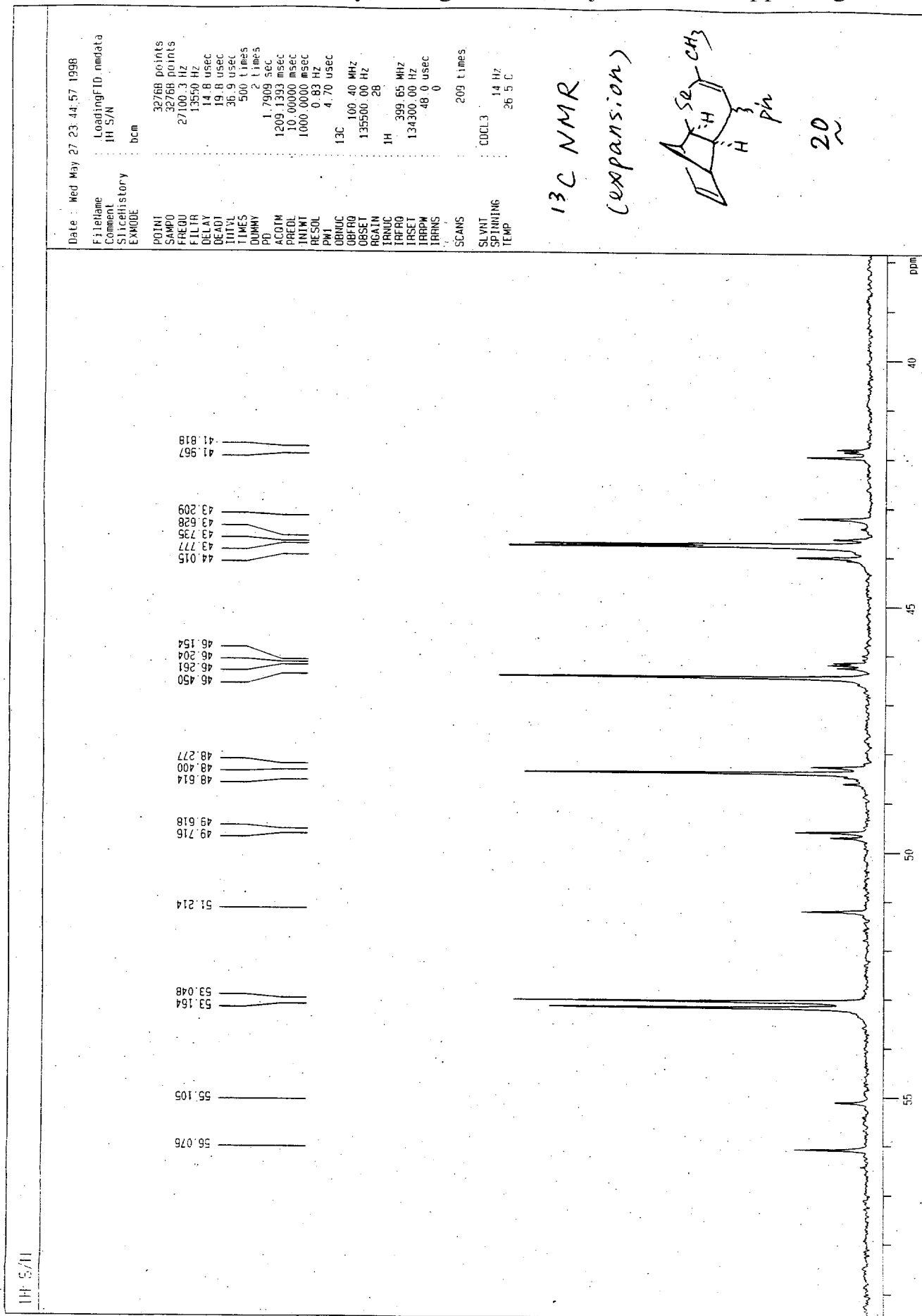
¹H NMR
 (expansion)



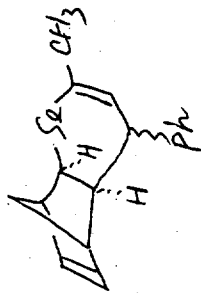




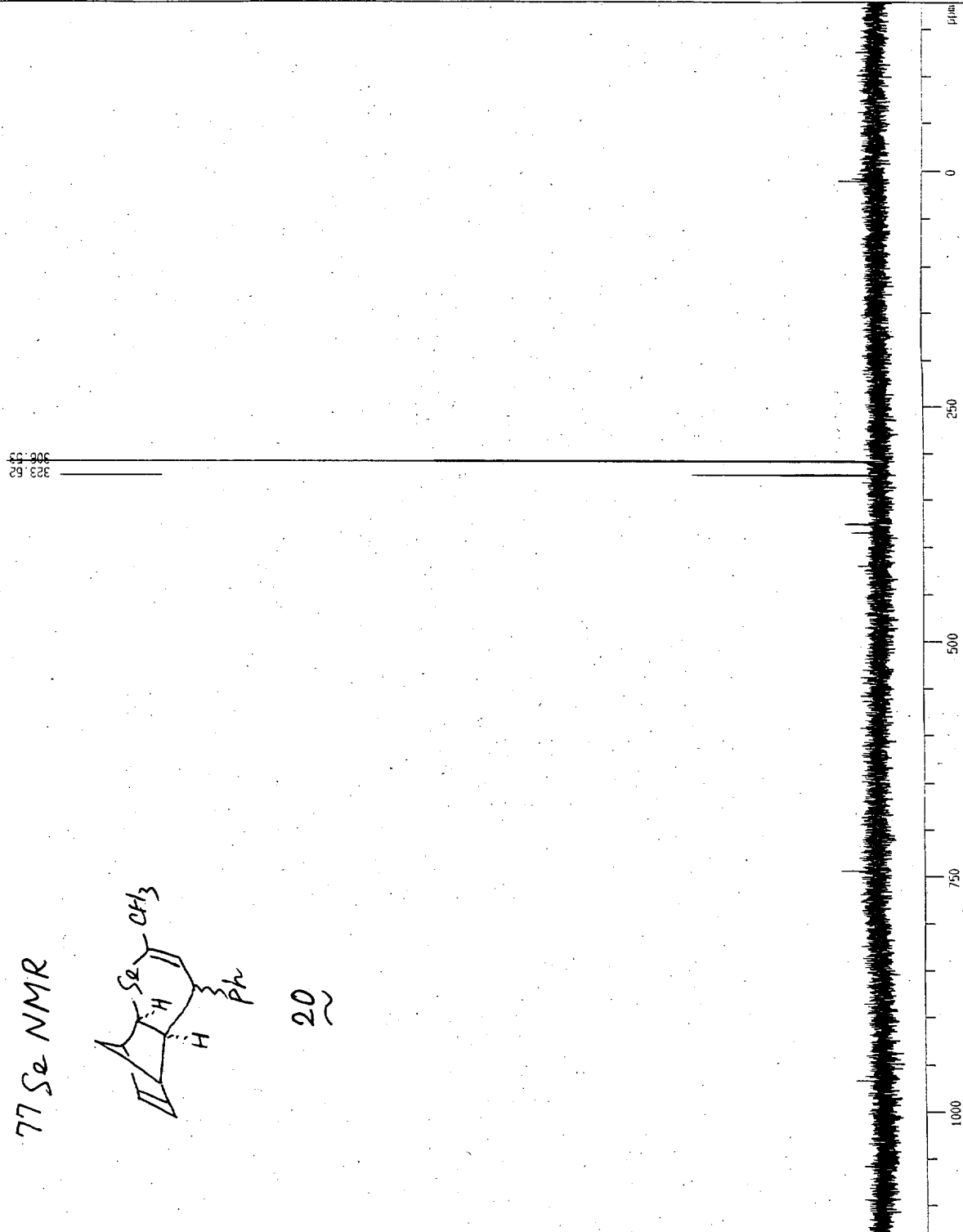




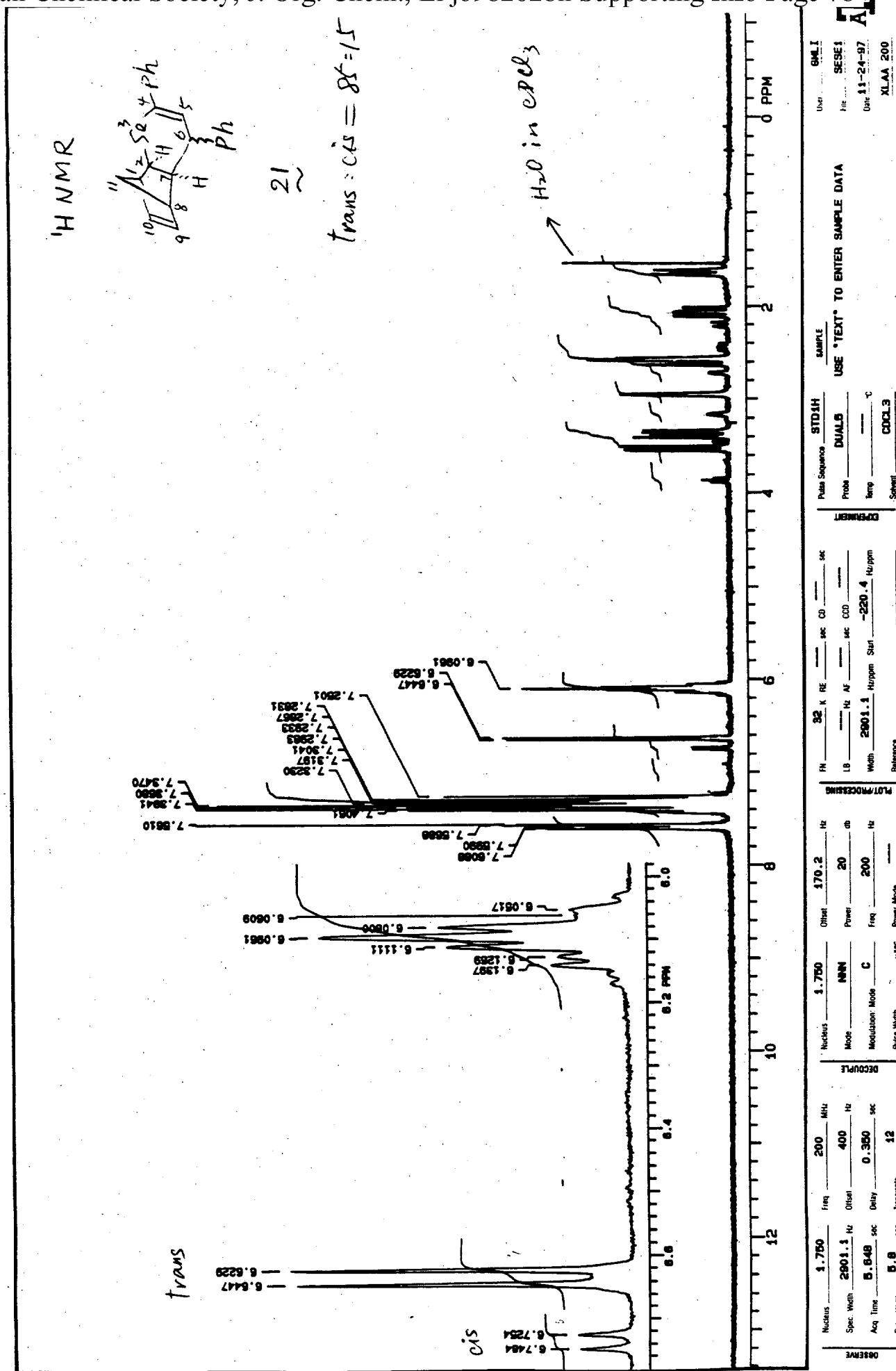
Benzalacetone cycladduct 77Se

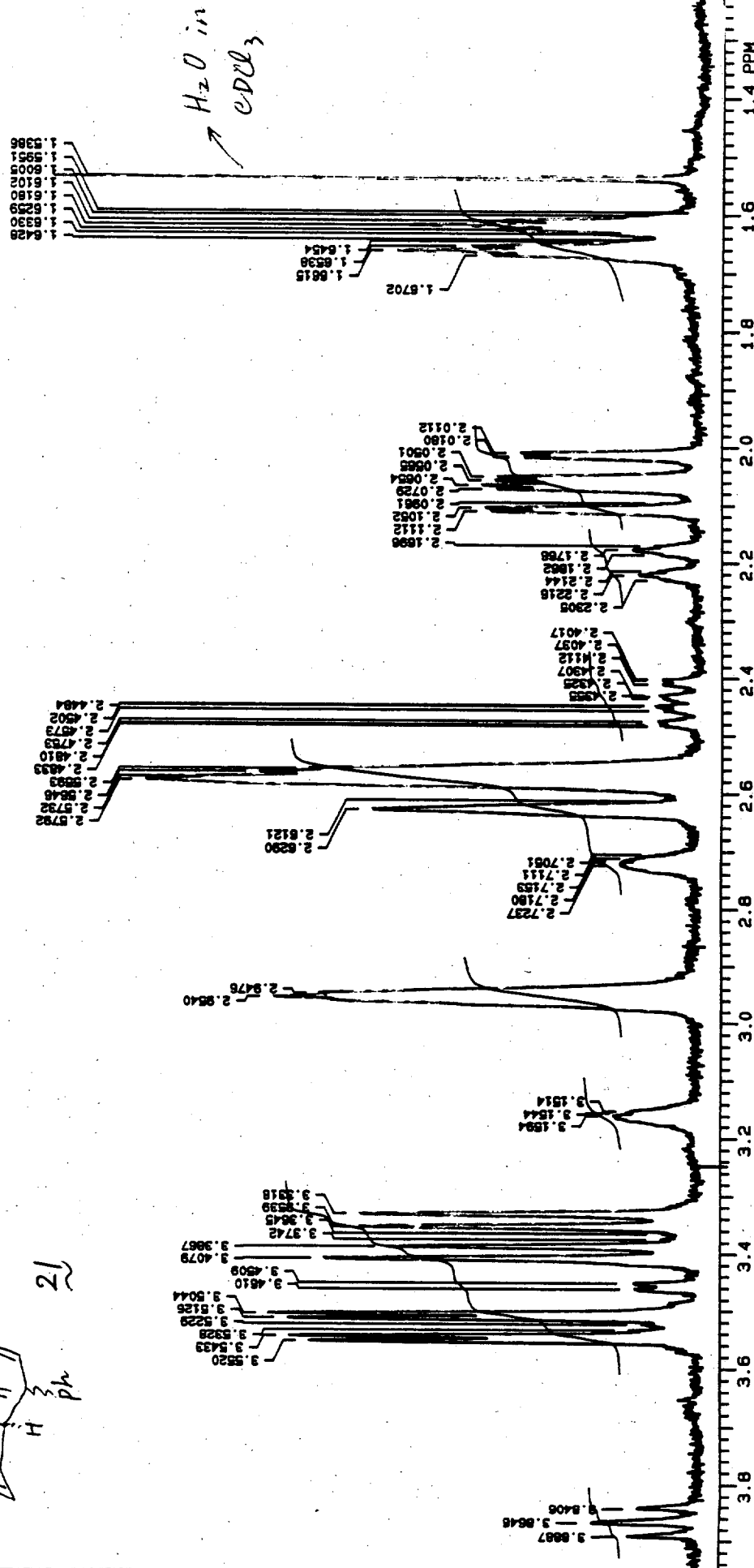
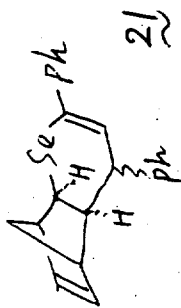
 ^{77}Se NMR

20~



Date	Time	Day	25	00	52	15	1998	
Flighttime								Load/rop 16 min 17 s
Comment								Benzalacetone cycle
Silicelystory								
EXAMIDE								ben
P01H								32766 points
SAMPO								32768 points
FH01H								Running 0 Hz
FH11H								50000 Hz
GE15V								1.0 data
RE401								10.0 data
RE111								10.0 data
TH15S								5000 times
DOH8S								2 times
PG								2.17-2.3 sec
AC01H								32768000 data
PH11H								10.0000000 data
TH11H								0.50000000
RE50L								3.05 Hz
PW1								6.40 data
GH00C								7750
OH01H								76.30 MHz
OB01C								79609.81 Hz
RE41H								25
TH00C								11
TH000								899.15 MHz
TH01C								134300.00 Hz
TH00V								40.0 data
TH00W								0
SE41S								240 times
SV11H								CLCL3
SP101H05								14 Hz
LE01								27.1 Hz



¹H NMR (expansion)

USE "TEXT" TO ENTER SAMPLE DATA

DATE 11-24-97

FILE 9891

USER GML

SAMPLE

STD1H

Pulse Sequence

PROB DUAL5

Temp °C

Solvent CDCl₃

DECREMENT

FN 32

RE Hz

CD sec

LB Hz

AF sec

CCD sec

Width 547.9

Height 241.5

Reference

PLT/PROCESSING

Nucleus 170.2

Offset Hz

Power 20

Mod 100

Modulation Mode C

Power Mode

DECUPLE

Nucleus 1.750

Spec Width 2001.1

Hz

Acq Time 5.648

sec

Delay 0.350

sec

Pulse Width 5.8

µsec

Transients 12

REVERSE

