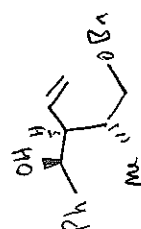


SD25F11-14
STANDARD IN OBSERVE

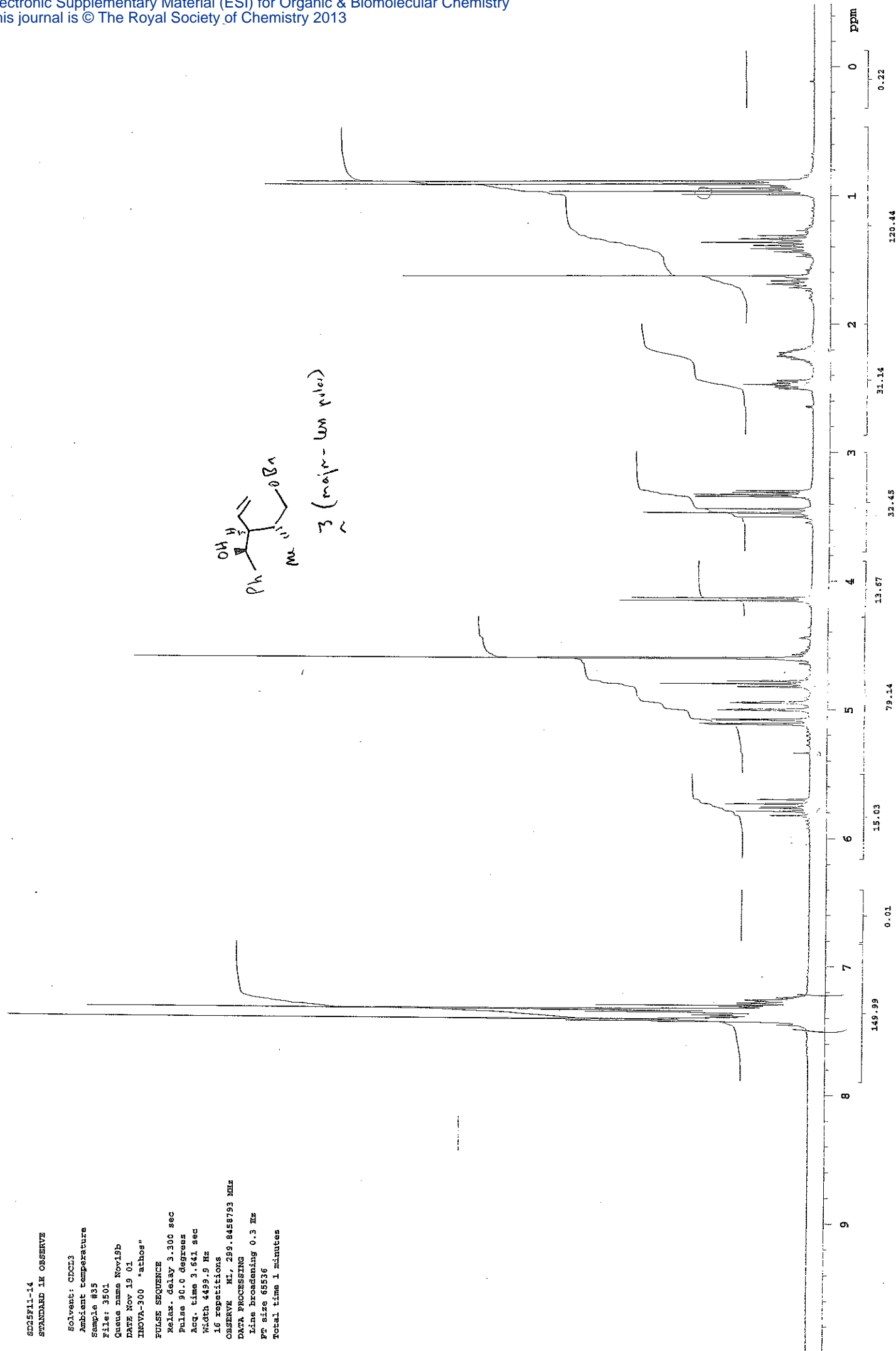
Solvent: CDCl₃
Ambient temperature
Sample #35
File: 3501
Queue name Nov19b
DATE Nov 19 01
INNOVA-300 "athos"

PULSE SEQUENCE
Relax. delay 3.300 sec
Pulse 90.0 degrees
Acq. time 3.641 sec
Width 4499.9 Hz
16 repetitions

OBSERVE ML, 299.8458793 MHz
DATA PROCESSING
Line broadening 0.3 Hz
PT size 65536
Total time 1 minutes



3 (major - LM peak)



5

SIEMENS 1344

SCHUMMERLE H. 1000000000

BAJOER
SOLLINGER
PACHO

Solvent: CDCl₃

Acquisition date: 2013-01-15

Sample ID: 435

Q1 file: 1344-2013-01-15

Q2 file: 1344-2013-01-15

Q3 file: 1344-2013-01-15

Q4 file: 1344-2013-01-15

Q5 file: 1344-2013-01-15

Q6 file: 1344-2013-01-15

Q7 file: 1344-2013-01-15

Q8 file: 1344-2013-01-15

Q9 file: 1344-2013-01-15

Q10 file: 1344-2013-01-15

Q11 file: 1344-2013-01-15

Q12 file: 1344-2013-01-15

Q13 file: 1344-2013-01-15

Q14 file: 1344-2013-01-15

Q15 file: 1344-2013-01-15

Q16 file: 1344-2013-01-15

Q17 file: 1344-2013-01-15

Q18 file: 1344-2013-01-15

Q19 file: 1344-2013-01-15

Q20 file: 1344-2013-01-15

Q21 file: 1344-2013-01-15

Q22 file: 1344-2013-01-15

Q23 file: 1344-2013-01-15

Q24 file: 1344-2013-01-15

Q25 file: 1344-2013-01-15

Q26 file: 1344-2013-01-15

Q27 file: 1344-2013-01-15

Q28 file: 1344-2013-01-15

Q29 file: 1344-2013-01-15

Q30 file: 1344-2013-01-15

Q31 file: 1344-2013-01-15

Q32 file: 1344-2013-01-15

Q33 file: 1344-2013-01-15

Q34 file: 1344-2013-01-15

Q35 file: 1344-2013-01-15

Q36 file: 1344-2013-01-15

Q37 file: 1344-2013-01-15

Q38 file: 1344-2013-01-15

Q39 file: 1344-2013-01-15

Q40 file: 1344-2013-01-15

Q41 file: 1344-2013-01-15

Q42 file: 1344-2013-01-15

Q43 file: 1344-2013-01-15

Q44 file: 1344-2013-01-15

Q45 file: 1344-2013-01-15

Q46 file: 1344-2013-01-15

Q47 file: 1344-2013-01-15

Q48 file: 1344-2013-01-15

Q49 file: 1344-2013-01-15

Q50 file: 1344-2013-01-15

Q51 file: 1344-2013-01-15

Q52 file: 1344-2013-01-15

Q53 file: 1344-2013-01-15

Q54 file: 1344-2013-01-15

Q55 file: 1344-2013-01-15

Q56 file: 1344-2013-01-15

Q57 file: 1344-2013-01-15

Q58 file: 1344-2013-01-15

Q59 file: 1344-2013-01-15

Q60 file: 1344-2013-01-15

Q61 file: 1344-2013-01-15

Q62 file: 1344-2013-01-15

Q63 file: 1344-2013-01-15

Q64 file: 1344-2013-01-15

Q65 file: 1344-2013-01-15

Q66 file: 1344-2013-01-15

Q67 file: 1344-2013-01-15

Q68 file: 1344-2013-01-15

Q69 file: 1344-2013-01-15

Q70 file: 1344-2013-01-15

Q71 file: 1344-2013-01-15

Q72 file: 1344-2013-01-15

Q73 file: 1344-2013-01-15

Q74 file: 1344-2013-01-15

Q75 file: 1344-2013-01-15

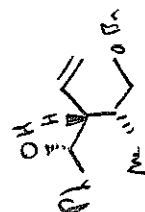
Q76 file: 1344-2013-01-15

Q77 file: 1344-2013-01-15

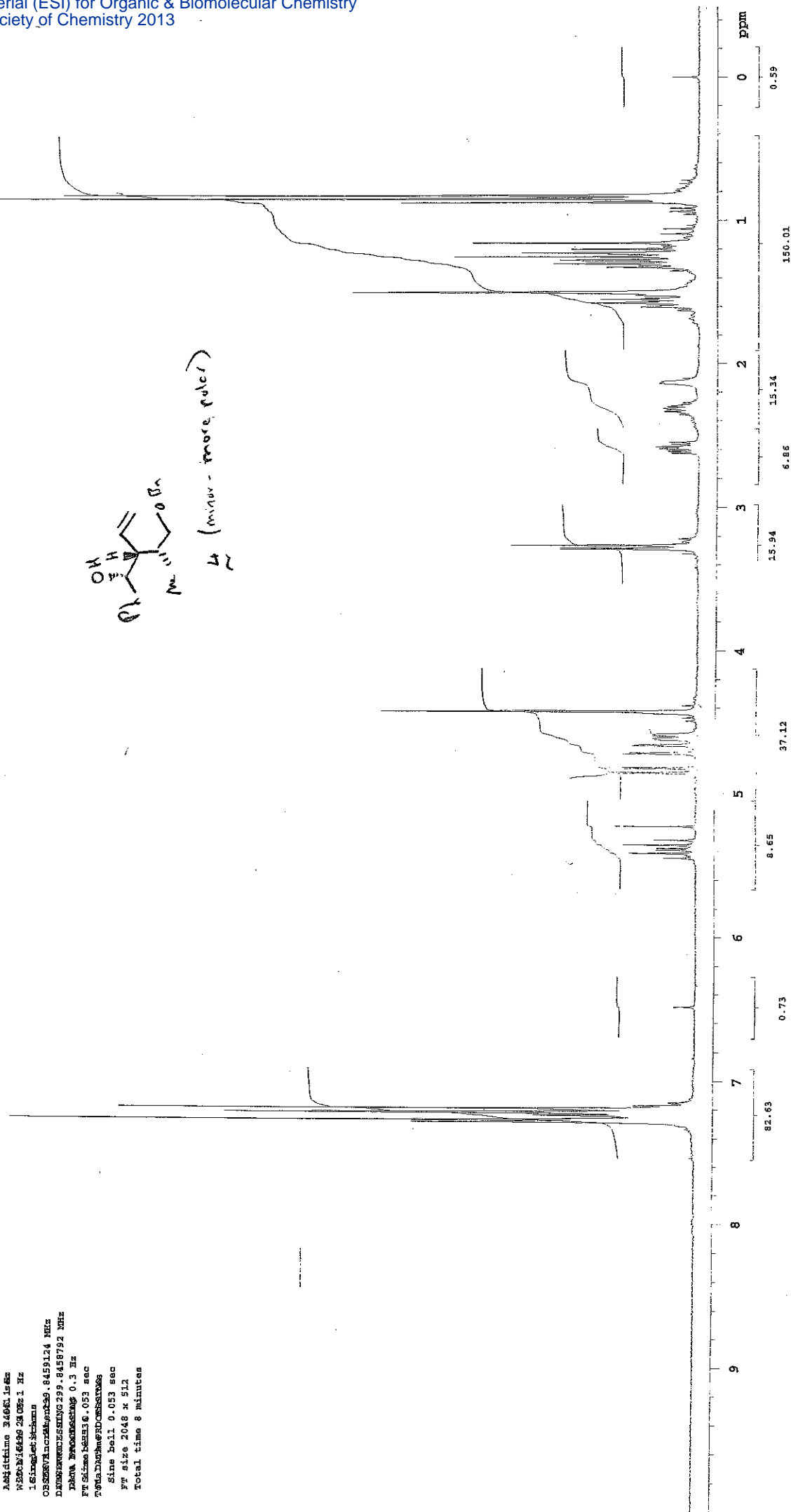
Q78 file: 1344-2013-01-15

Q79 file: 1344-2013-01-15

Q80 file: 1344-2013-01-15



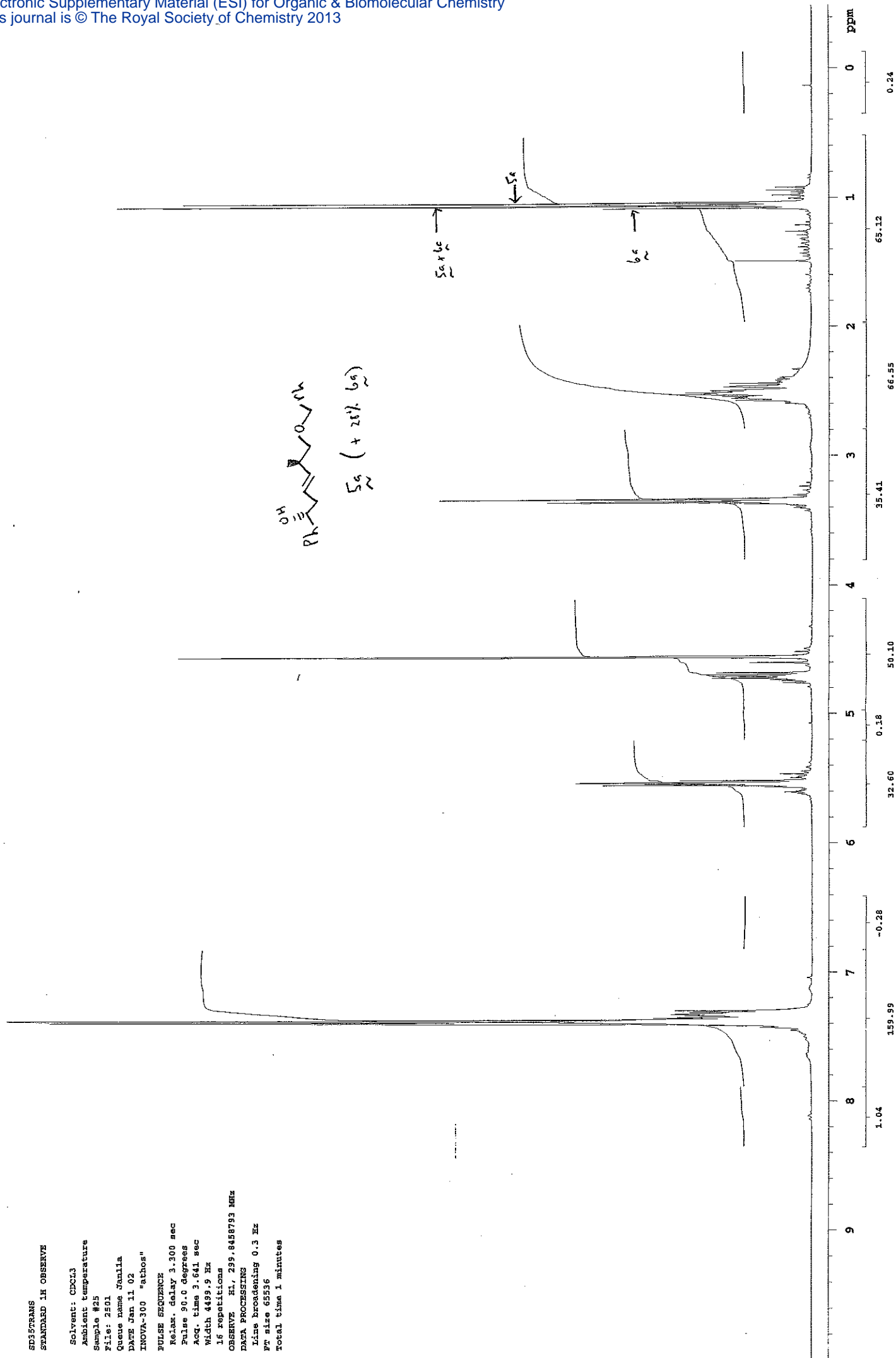
42 (minor - more polar)



PULSE SEQUENCE
Relax. delay 3.300 sec
Pulse 90.0 degrees
Acq. time 3.641 sec
Width 4499.9 Hz
16 repetitions

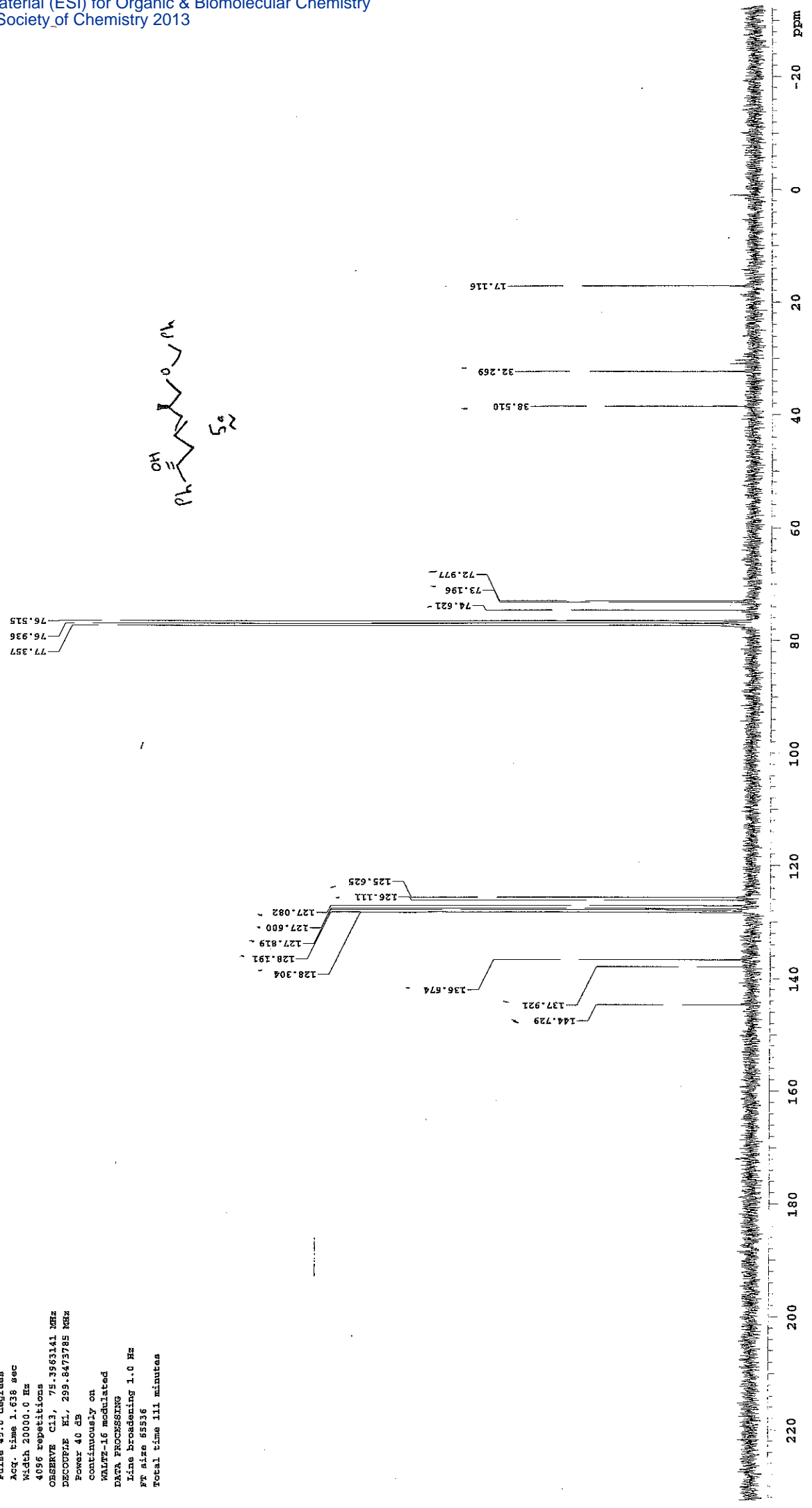
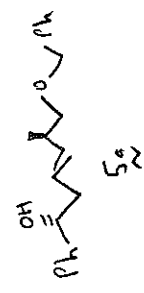
CC(C)(CO)C=C[C@H](O)C

5g (+ 20% loss)



8427.1622-28
13C OBSERVE

Solvent: CDCL3
Ambient temperature
Sample #31
File: 3101
Queue name Nov28b
Date Nov 29 01
INOVA-300 "athos"
PULSE SEQUENCE
Pulse 45.0 degrees
Acq. time 1.638 sec
Width 20000.0 Hz
4096 repetitions
OBSERVE C13, 75.3563141 MHz
DECOUPLE E1, 299.8473785 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 111 minutes



Solvent: CDCl₃

52# STAIRS

Queene name Feb28a

INOVA-300 "Athog"

Relax. delay 3.300 sec

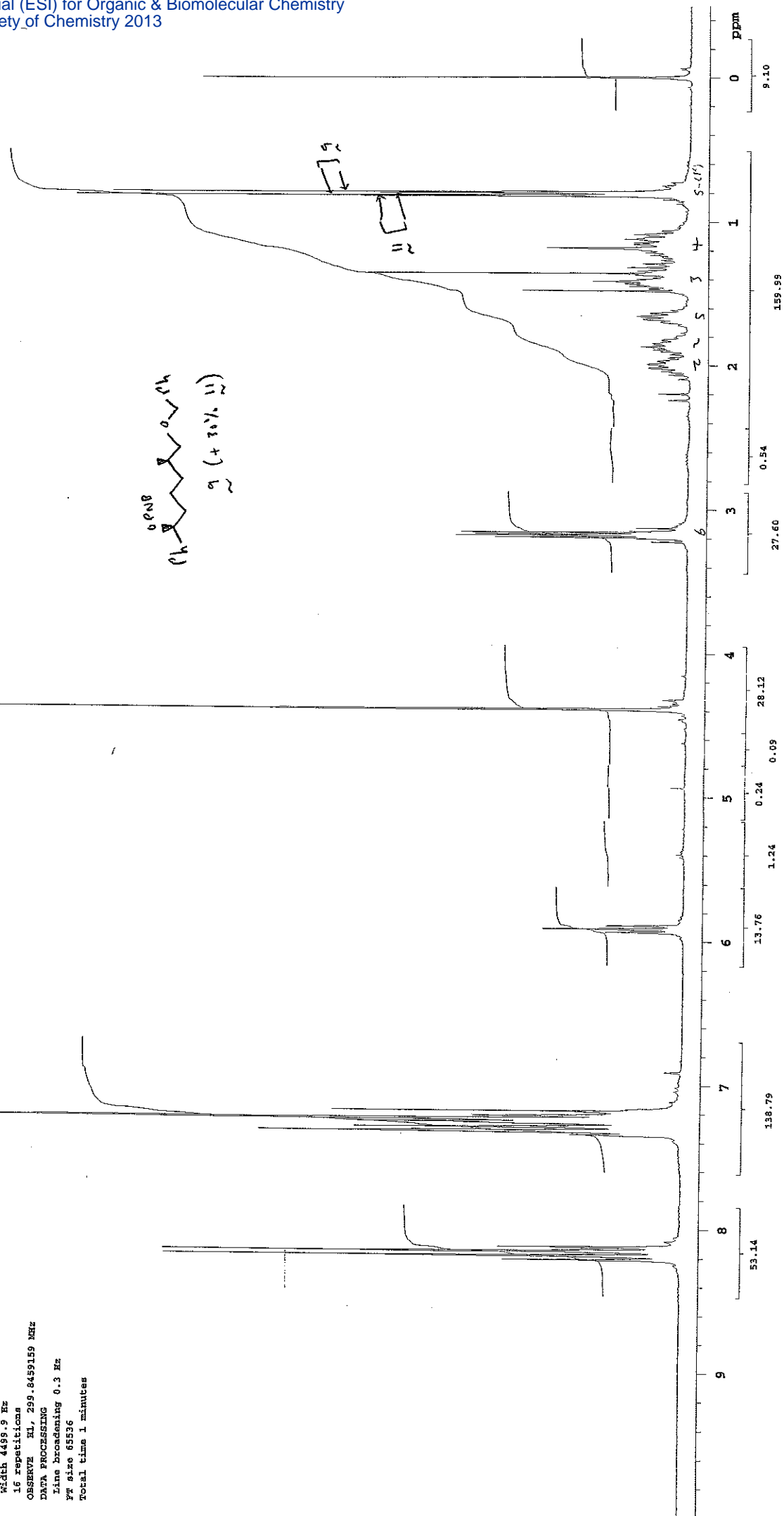
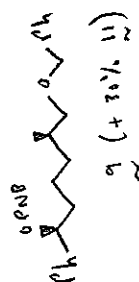
Acc. time 3.641 sec

Width 4499.9 Hz

OBSERVE AL, 291

Line broadening

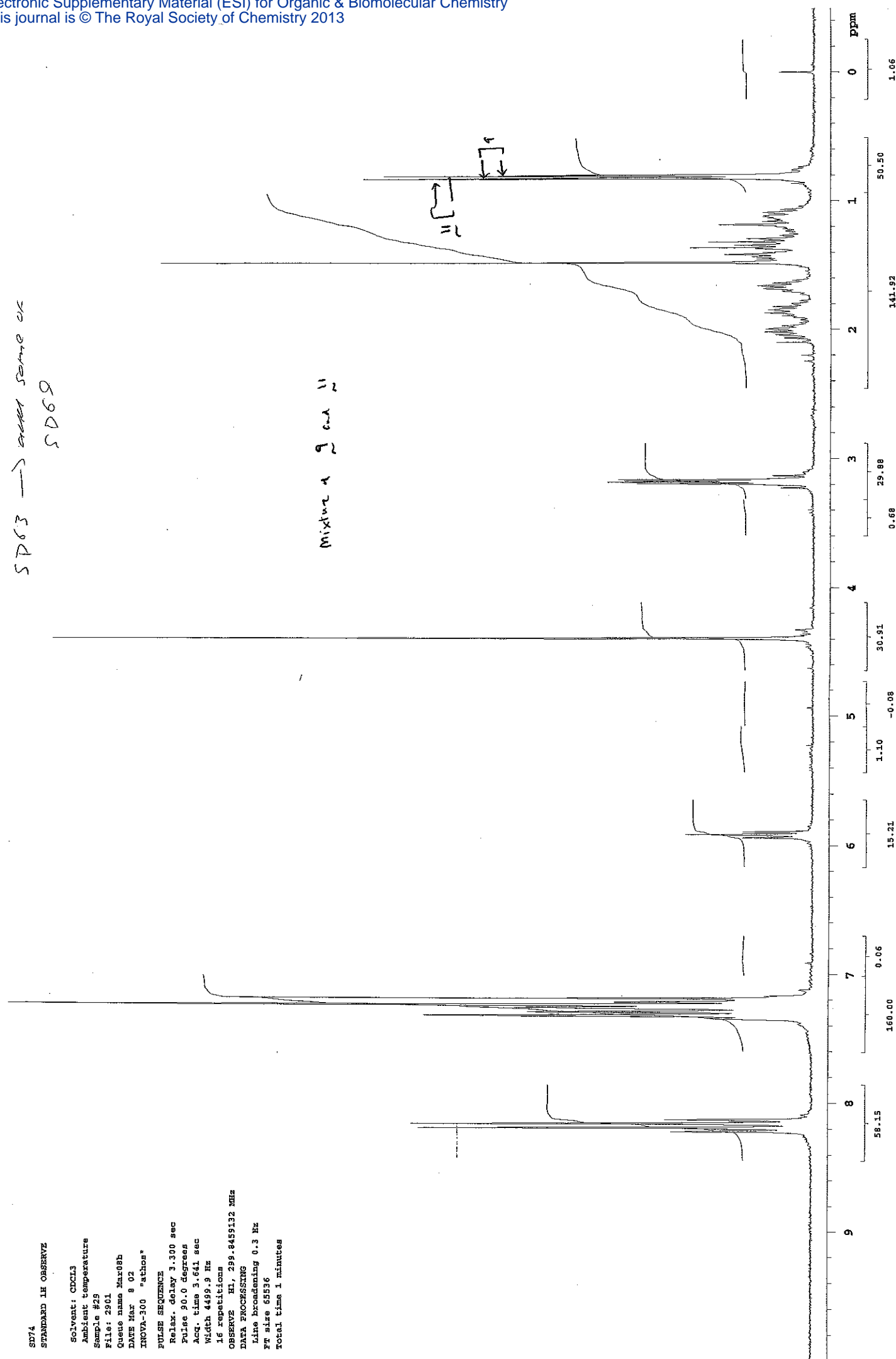
total time 1 minutes



SD63 → entry same as
SD69

Mixture 1 g ca 11

SD74
STANDARD IN OBSERVE
Solvent: CDCl3
Ambient temperature
Sample #29
File: 2301
Queue name Mar08b
DATE Mar 8 02
INOVA-300 "athos"
PULSE SEQUENCE
Relax. delay 3.300 sec
Pulse 90.0 degrees
Acq. time 3.641 sec
Width 4499.9 Hz
16 repetitions
OBSERVE H1, 299.8459132 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 minutes



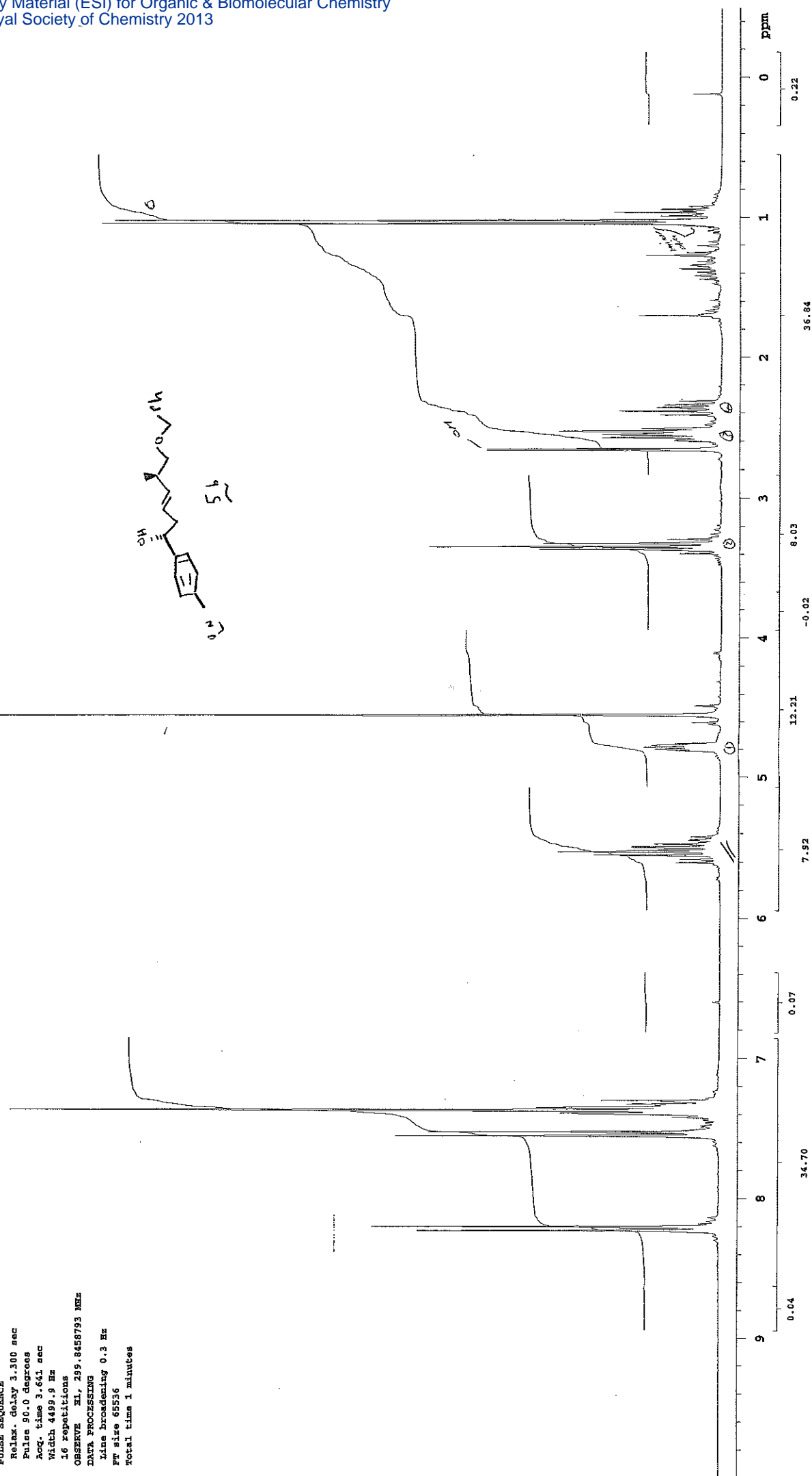
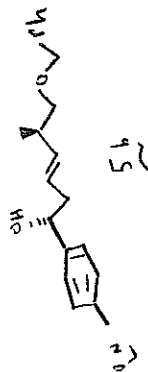
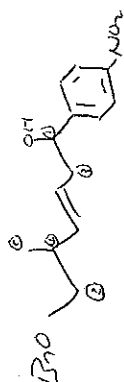
SD88CDCL3
STANDARD 1H OBSERVE

Solvent: CDCl3
Ambient temperature
File: 2401
Queue name Max28a
DATE Mar 28 02
INNOVA-300 "solids"

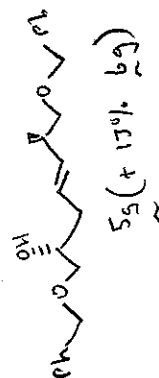
```

PULSE SEQUENCE
Relax. delay 3.300 sec
Pulse 90.0 degrees
Acq. time 3.641 sec
Width 4499.9 Hz
16 repetitions
OBSERVE XI, 299.845879
-----
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 1 minutes

```



Sam Donnelly/sd450



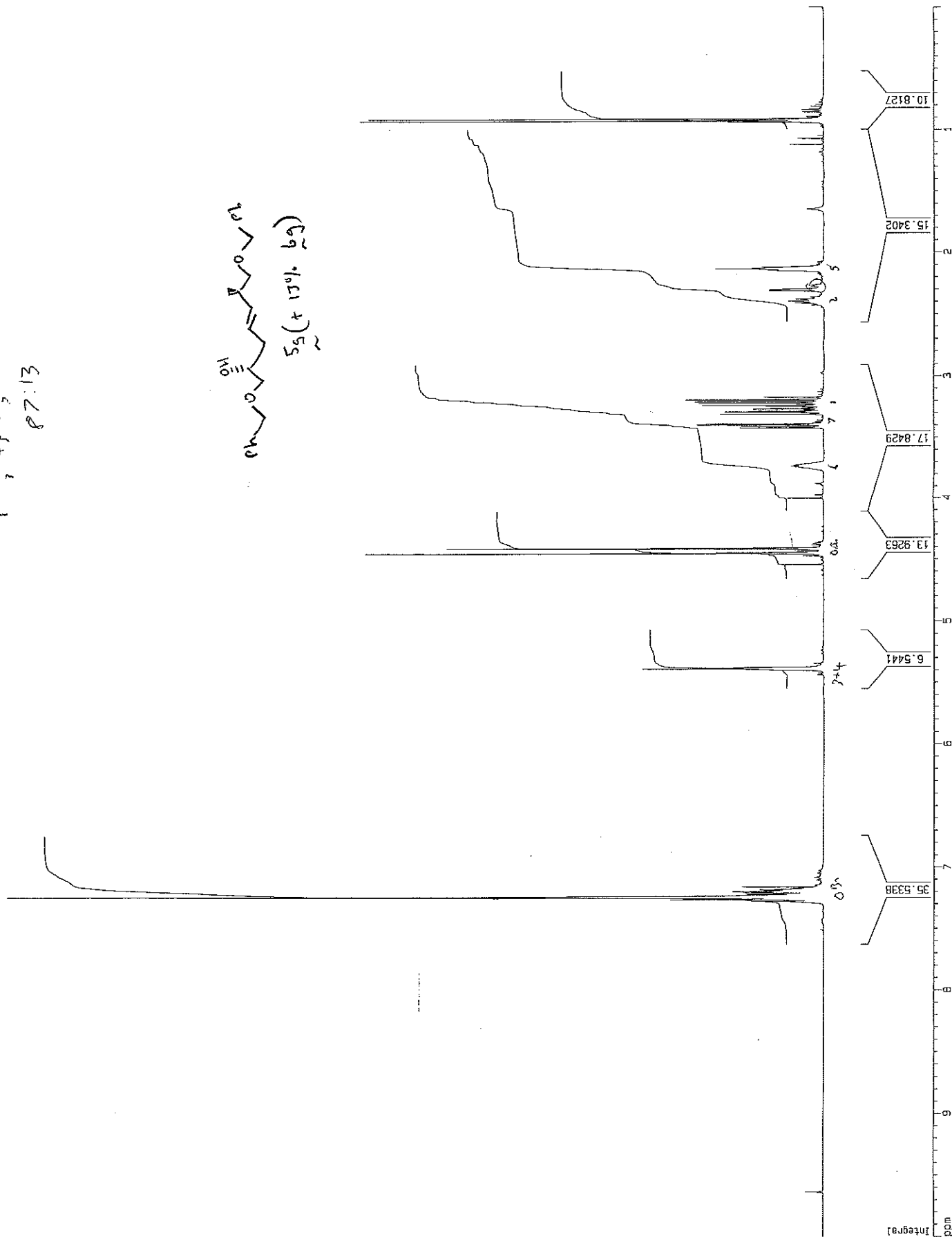
Current Data Parameters
NAME 031017014
EXPNO 10
PROCNO 1
USER pdd

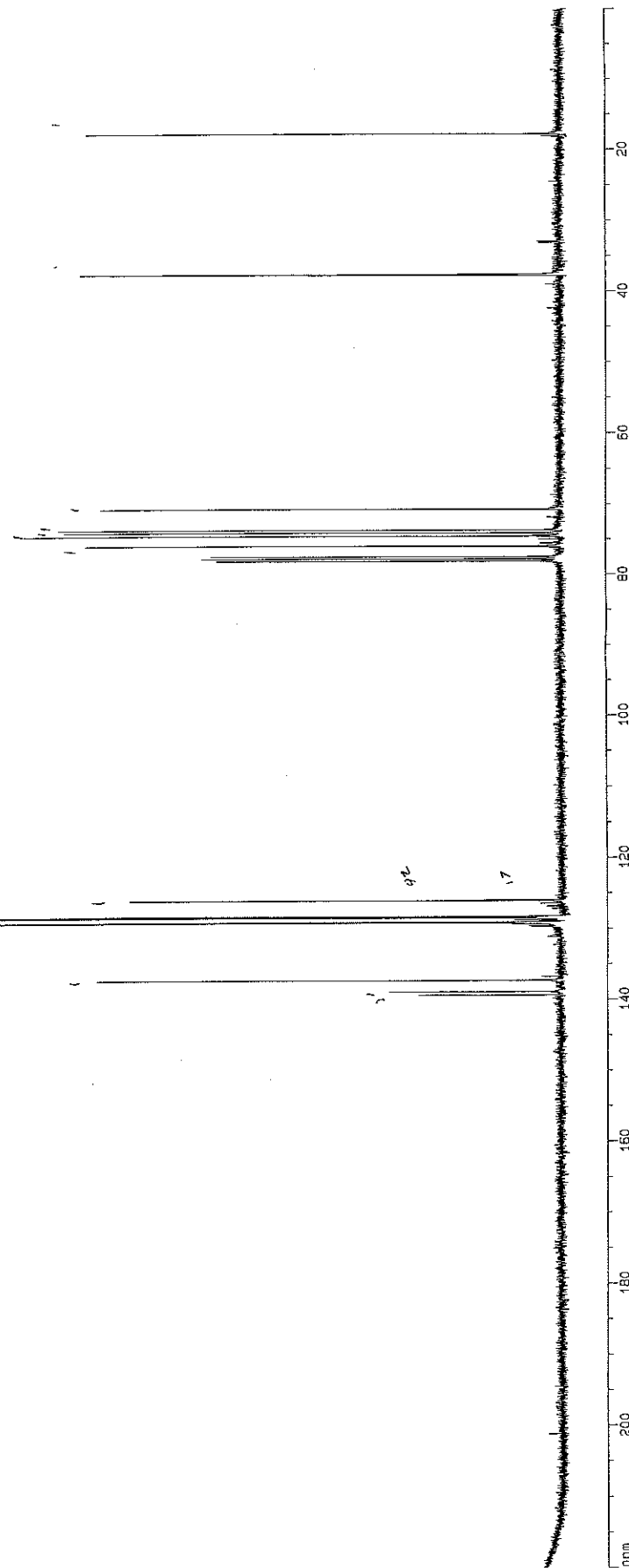
F2 - Acquisition Parameters
Date_ 20031017
Time 20.15
INSTRUM dpx400
PROBHD 5 mm QNP 1H/1
PULPROG zg45
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 7062.147 Hz
FIDRES 0.107760 Hz
AQ 4.639989 sec
RG 32
DW 70.800 usec
DE 5.00 usec
TE 300.0 K
D1 5.36000013 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -3.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300482 MHz
WDW EM
SSB 0
LB 0.19 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 33.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.30303 ppm/cm
HZCM 121.25153 Hz/cm





Sam Donnelly/sd435f2



52

Current Data Parameters
NAME 031003034
EXPNO 10
PROCNO 1
USER pdd

F2 - Acquisition Parameters
Data... 20031004
Time 0.19
INSTRUM dpx400
PROBHD 5 mm GNP 1H/1
PULPROG zg45
TD 65536
SOLVENT CDCl3
NS 32
DS 0
SWH 7052.147 Hz
FIDRES 0.107750 Hz
AQ 4.6399989 sec
RG 71.8
DW 70.800 usec
DE 5.00 usec
TE 300.0 K
D1 5.36000013 sec

===== CHANNEL f1 =====
NUC1 1H
P1 9.50 usec
PL1 -3.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300136 MHz
WDW EM
SSB 0
LB 0.19 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 33.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 0.30303 ppm/cm
HZCM 121.25152 Hz/cm



Sam Donnelly/sd435f1

Current Data Parameters
NAME 031003033
EXPNO 12
PROCNO 1
USER pdd

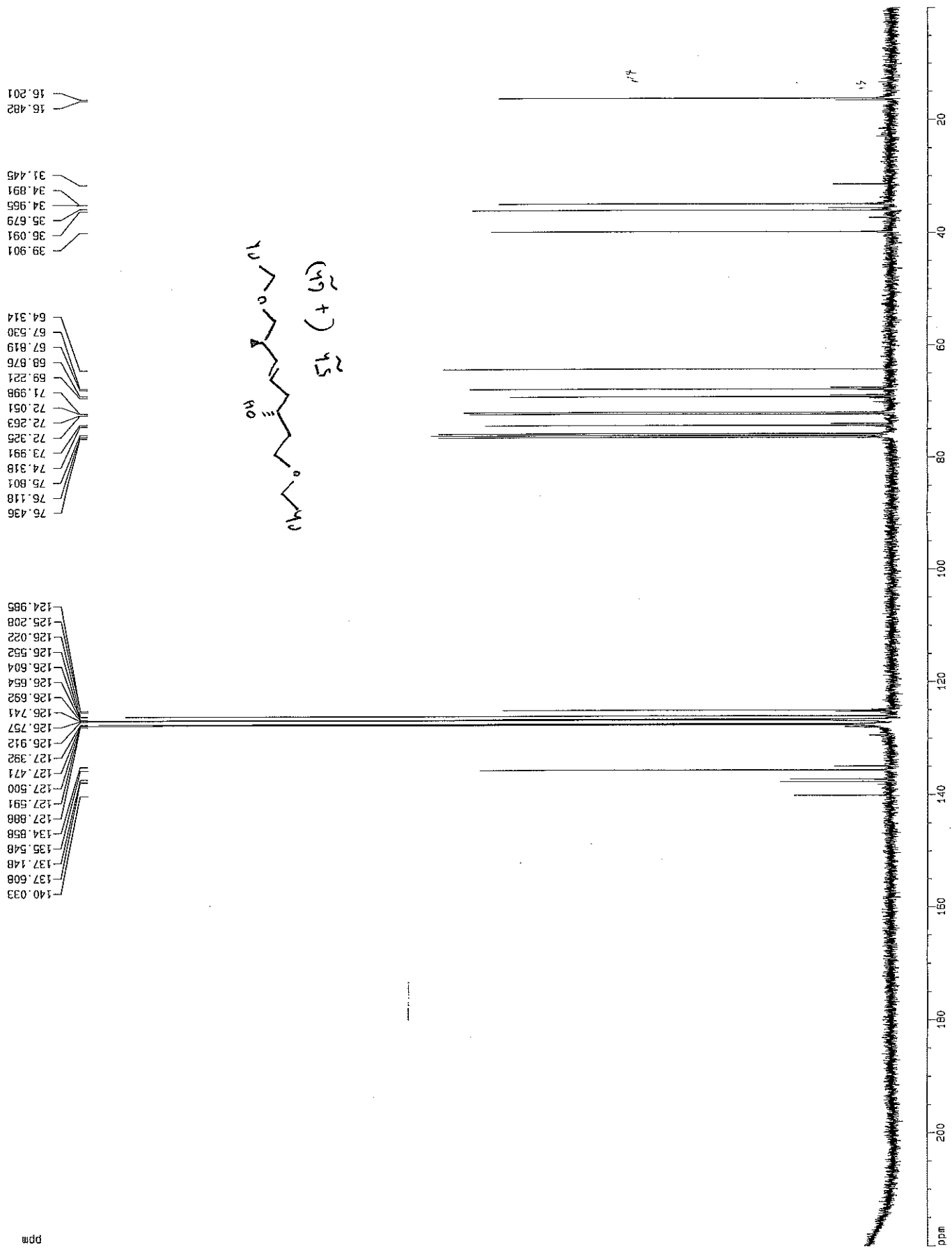
F2 - Acquisition Parameters
Date_ 20031004
Time 0.02
INSTRUM cdx400
PROBHD 5 mm QNP 1H/1
PULPROG zgpg45
TD 65536
SOLVENT CDCl3
NS 800
DS 2
SWH 24691.357 Hz
FIDRES 0.376750 Hz
AQ 1.3271540 sec
RG 322.5
DW 20.250 usec
DE 5.00 usec
TE 300.0 K
D1 0.69999999 sec
D11 0.03000000 sec
D12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.70 usec
PL1 -3.00 dB
SFO1 100.6227903 MHz

===== CHANNEL f2 =====
CPOPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 18.00 dB
PL13 19.00 dB
SFO2 400.1315005 MHz

F2 - Processing parameters
SI 65536
SF 100.6128641 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 33.00 cm
F1P 220.000 ppm
F1 22134.83 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 6.66667 ppm/cm
HZCM 670.75244 Hz/cm



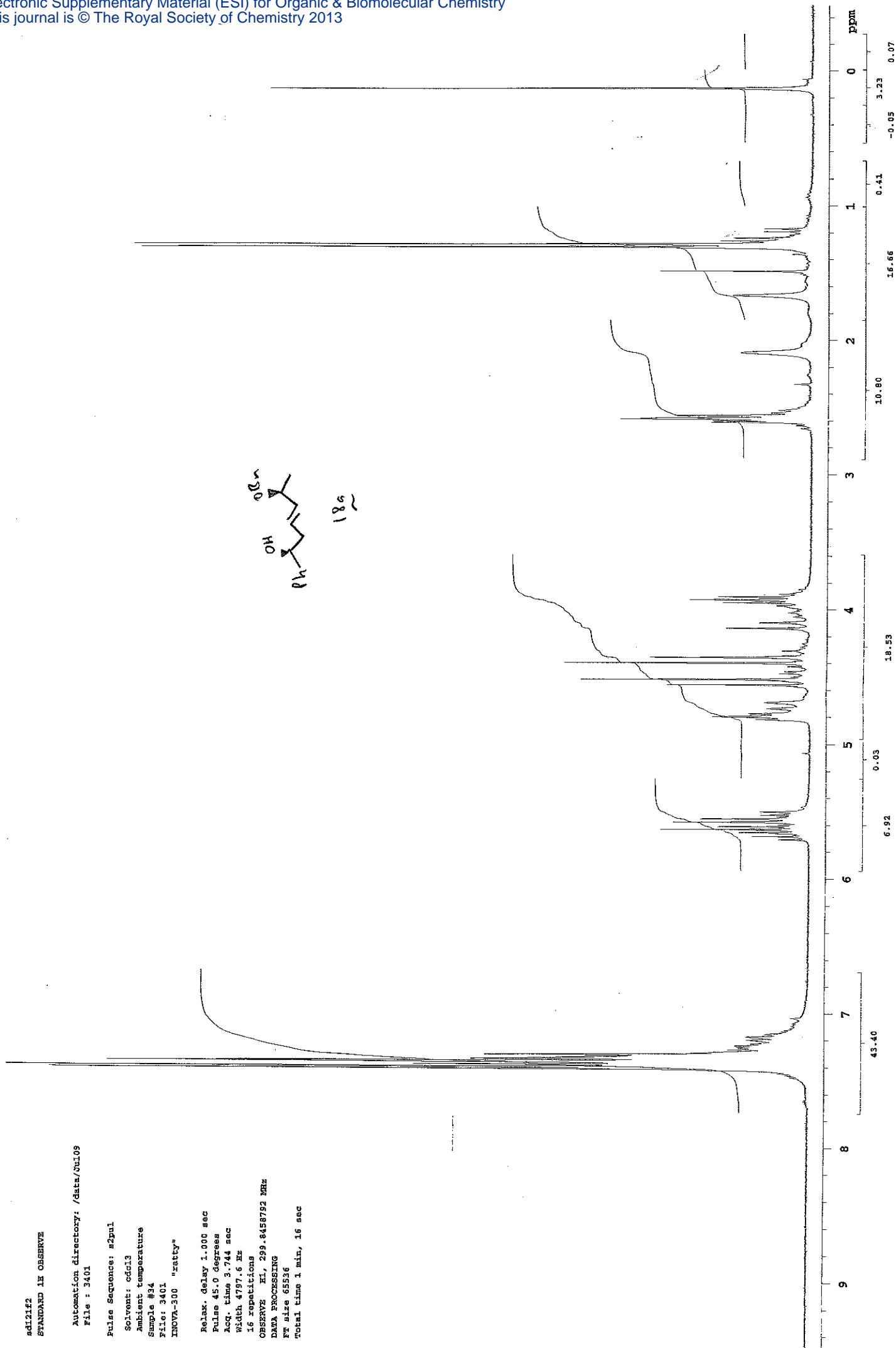
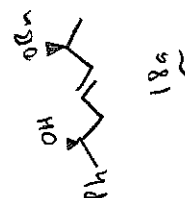
ad12122
STANDARD IN OBSERVE

Automation directory: /data/Vul09
File : 3401

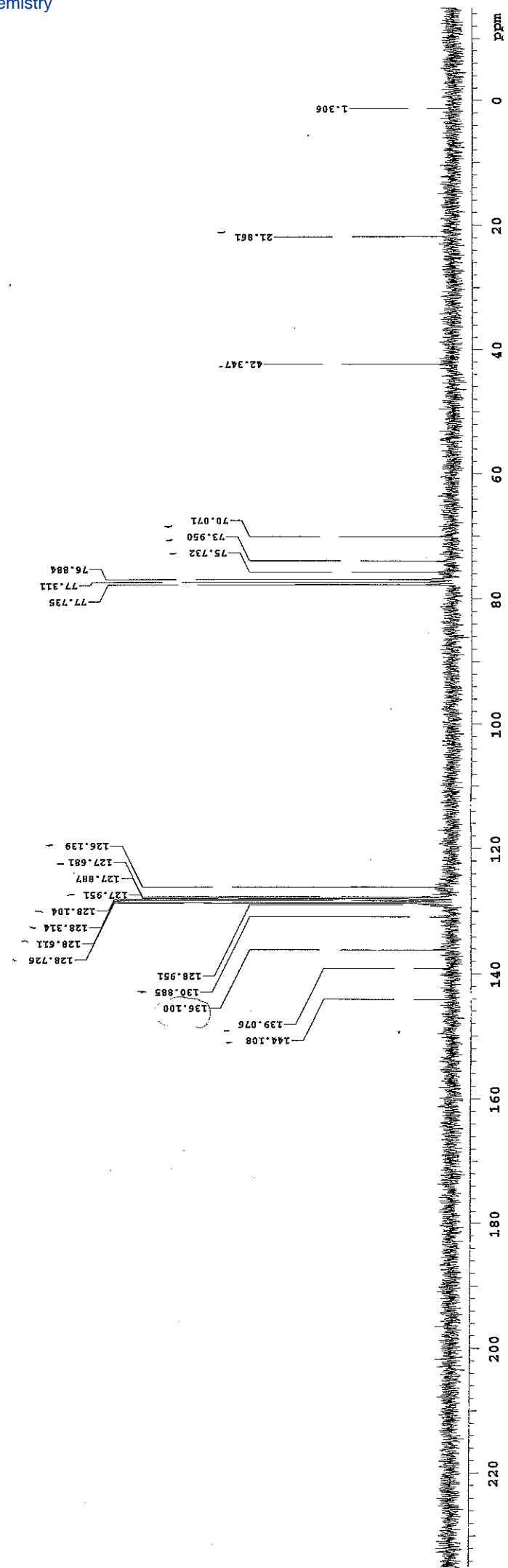
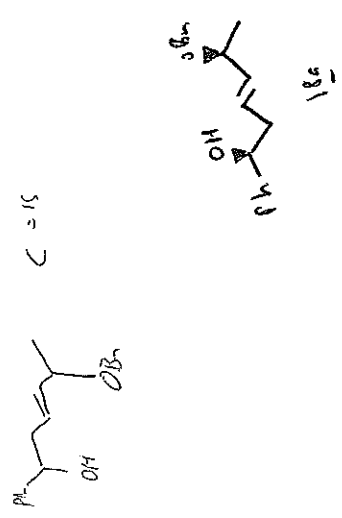
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #34
File: 3401
INOVA-300 "ratty"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.744 sec
Width 4797.6 Hz
16 repetitions

OBSERVE XL, 299.8458792 MHz
DATA PROCESSING
Ft size 65536
Total time 1 min, 16 sec



sd121f2
STANDARD 1H OBSERVE
Automation directory: /data/Jul09
File : 3402
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #34
File: 3402
INOVA-300 "ratty"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18850.1 Hz
256 repetitions
OBSERVE CH3, 75.3962883 MHz
DECOUPLE H1, 299.8473786 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 12 min, 2 sec

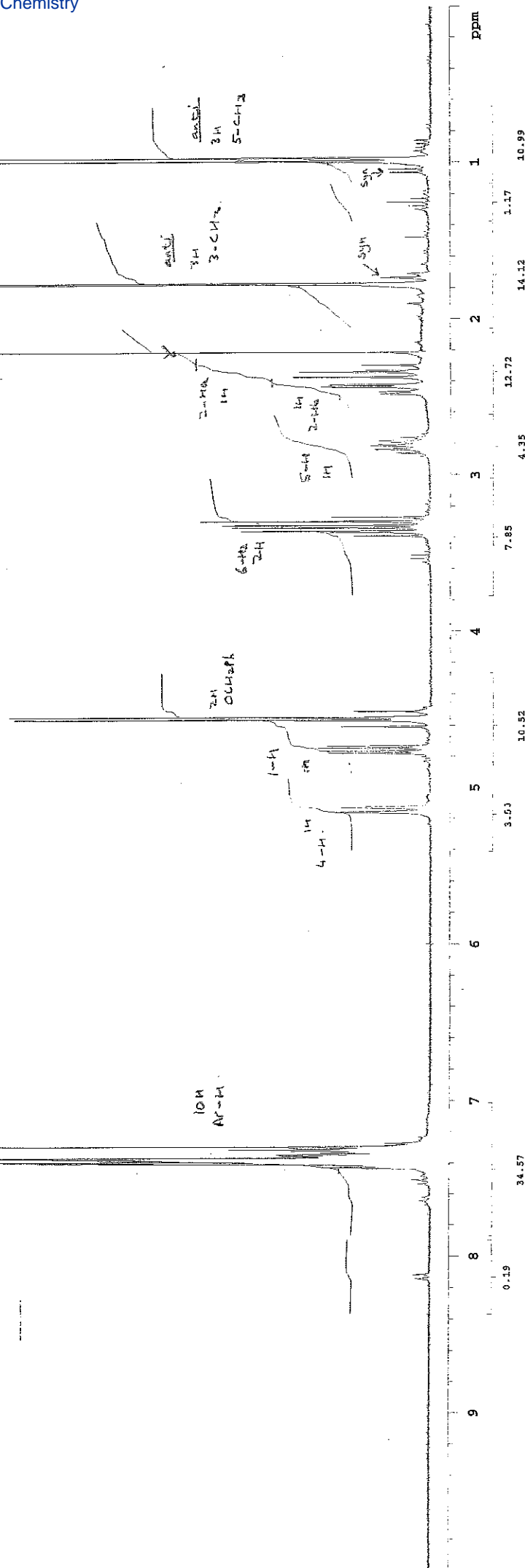
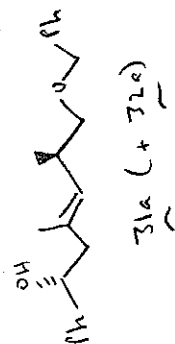
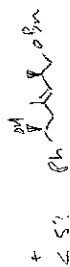
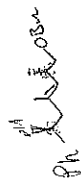


nb006
STANDARD 1H OBSERVE

Automation directory: /data/nmrdata/Sep16
File : 3601

Pulse Sequence: zgpg30
Solvent: cdcl3
DATE Sep 16 2005
Sample #36
File: 3601
INNOVA-300 "zatty"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.744 sec
Width 4797.6 Hz
16 repetitions
OBSERVE E1, 299.8458792 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 16 sec

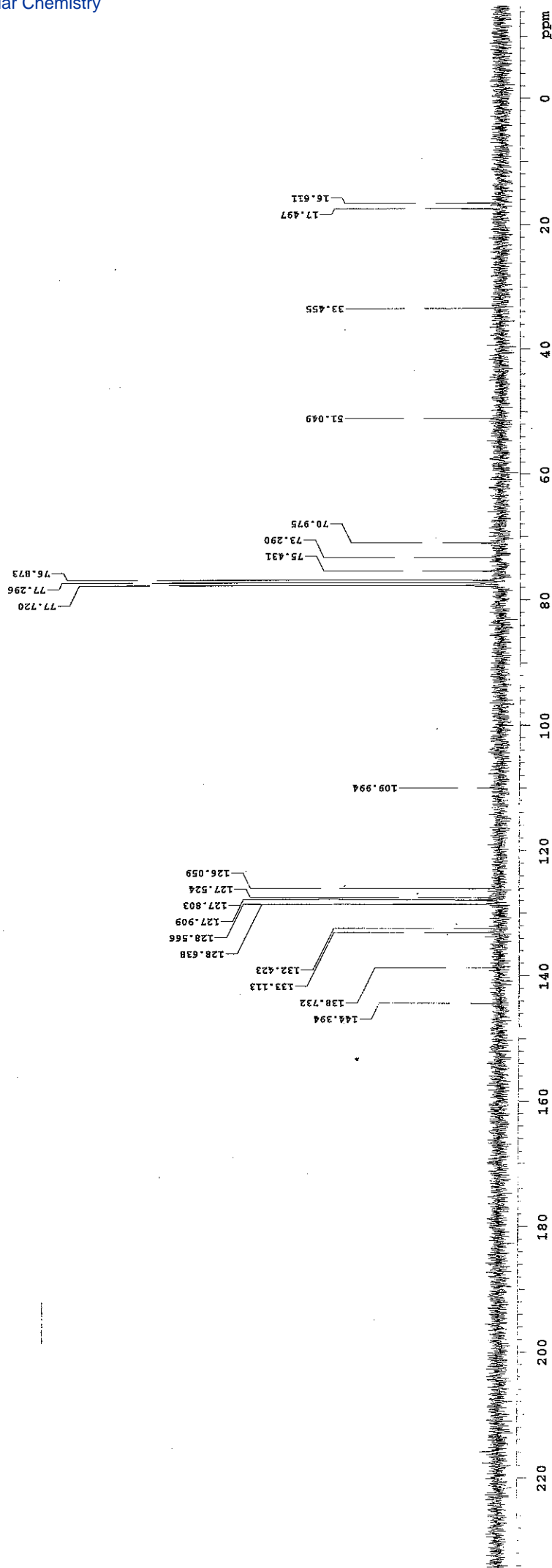
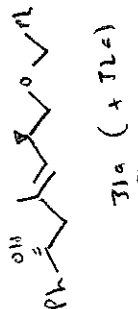


zb006
STANDARD IN OBSERVE

Automation directory: /data/mrdata/Sep19
File : 4102

Pulse Sequence: s2pul
Solvent: cdcl3
DATE Sep 20 2005
Sample #41
File: 4102
INNOVA-300 "ratty"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18850.1 Hz
256 repetitions
OBSERVE C13, 75.3962883 MHz
DECOUPLE H1, 299.8473786 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Ft size 131072
Total time 12 min, 2 sec



Automation directory: /data/nmrdata/Sep23

File : 4501

Pulse Sequence: s2pul

Solvent: cdcl3

DATE Sep 25 2005

Sample #45

File: 4502

NOVA-300 "zatty"

Relax. delay 1.000 sec

Schedule D - Estimated Tax

PAGE NO.: 00077668
Acc. time 3,744 sec

ACQ. FILE 3-744 SEC
WITH 4797-6 HZ

Width 497.6 Hz

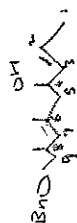
16 repetitions

OBSERVE HL, 299.8458792 MHz

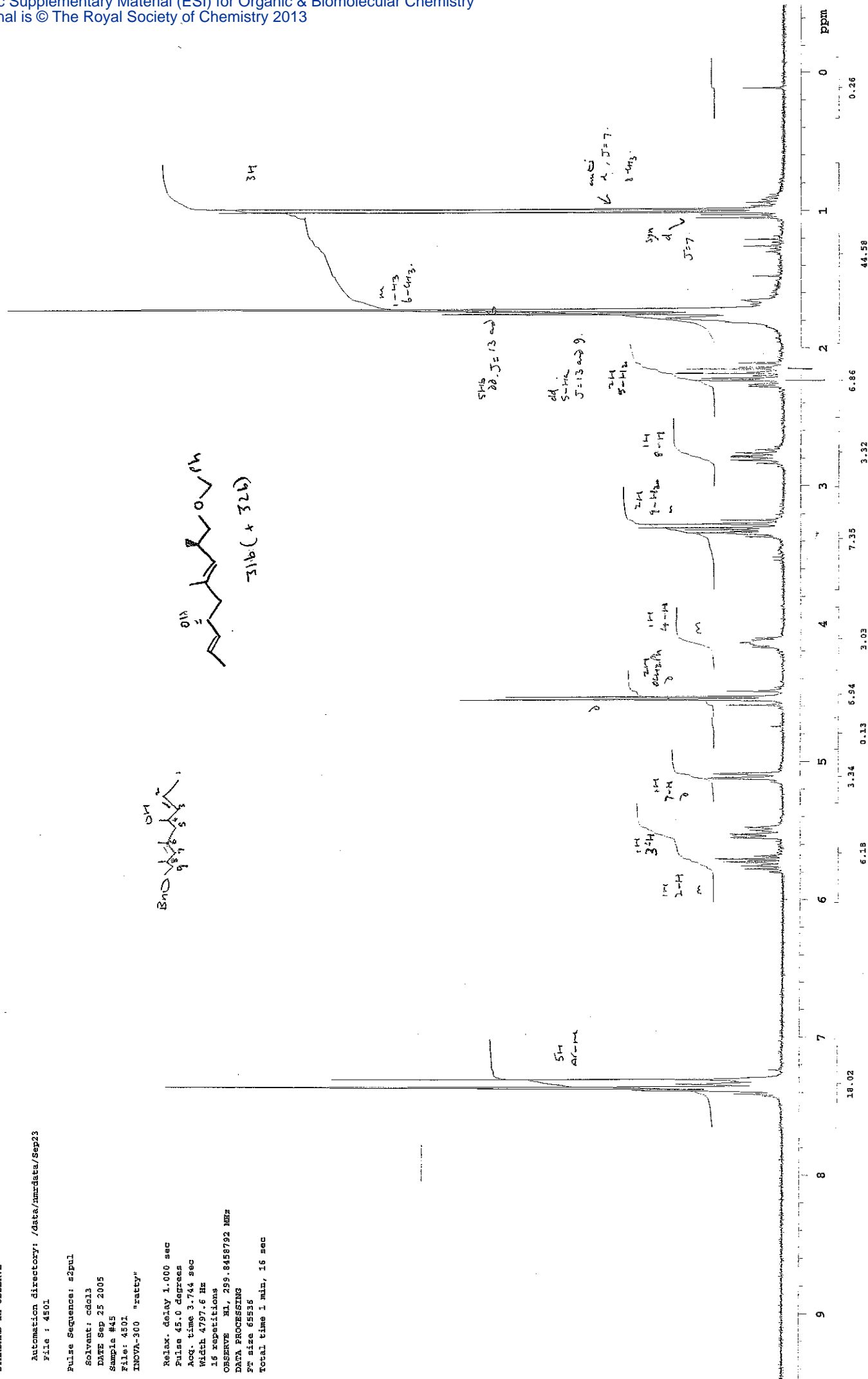
DATA PROCESSING

WY size 65536

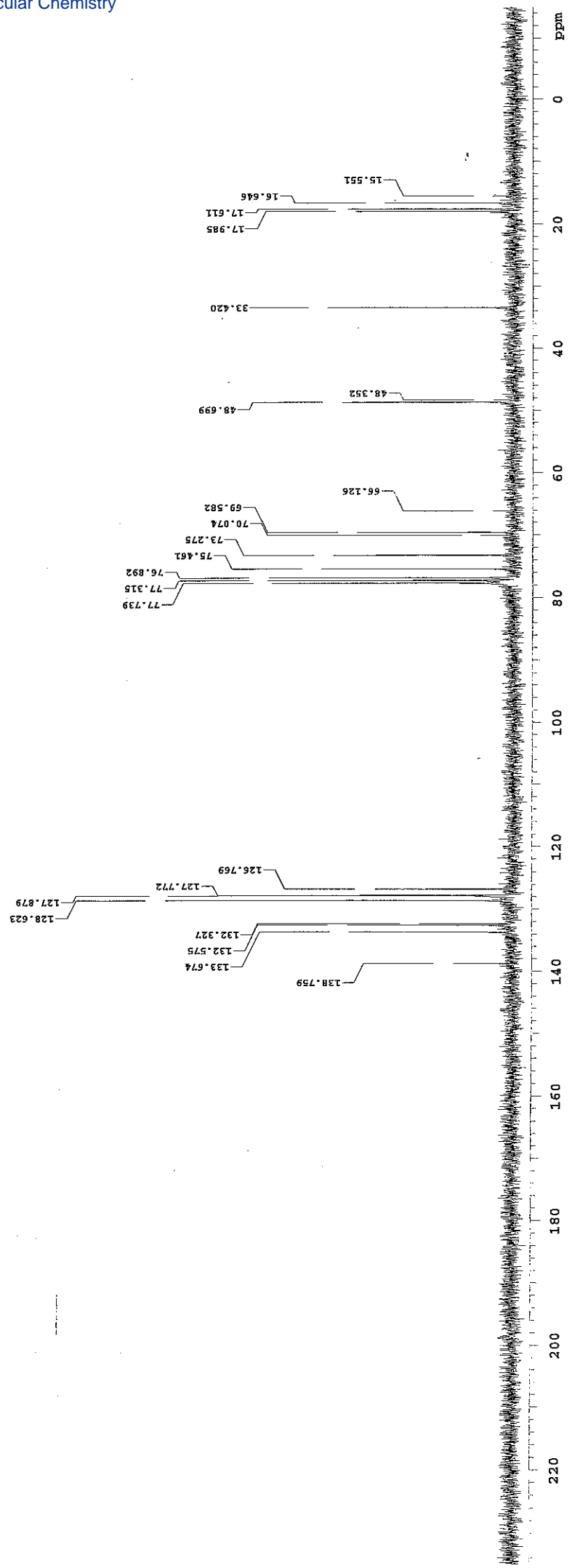
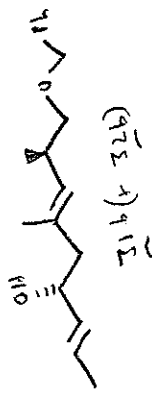
Total time 1 min, 16 sec



$-316(+326)$

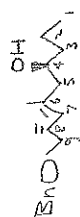


nb008
13C OBSERVE
pad=2 run with kindr0 before acquisition
Automation directory: /data/nmrdata/Sep27
File : 1801
Pulse Sequence: s2pul
Solvent: cdcl3
Date Sep 27 2005
Sample #18
File: 1801
INOVA-300 "ratty"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18850.1 Hz
256 repetitions
OBSERVE C13, 75.3562883 MHz
DECOUPLE H1, 259.8473786 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 12 min, 2 sec



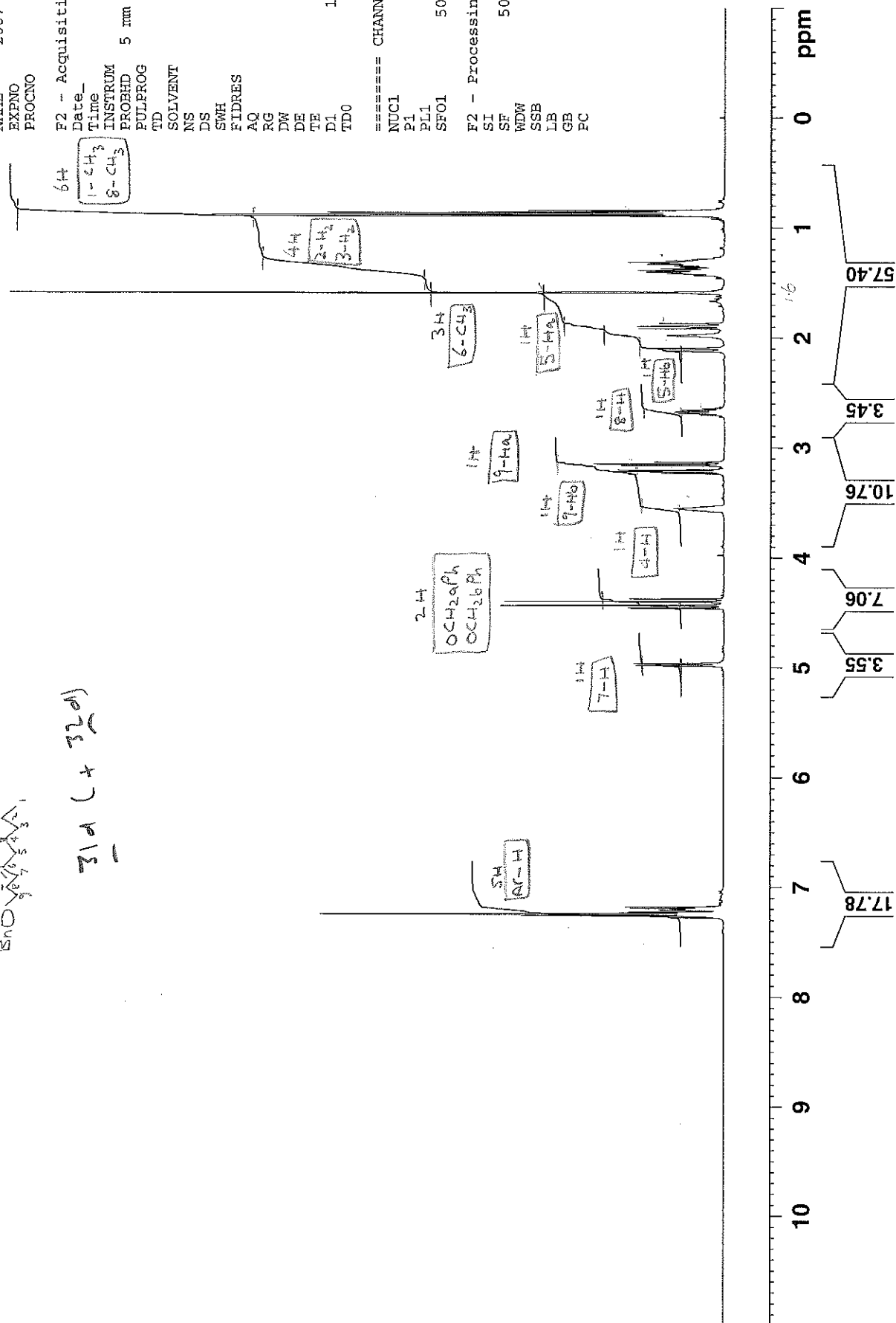


nb090
mPROTON CDCl₃ /opt/topspin ejt 41



3.1 d (+ 32 d)

Current Data Parameters
NAME 2007-06-08-ejt-41
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070608
Time 14.49
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 36
DW 48.400 usec
DE 13.76 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 7.80 usec
PL1 3.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300471 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



C₁₈H₂₈O₂
FW = 276.21

nb090

mCARBON CDCl₃ /opt/topspin ejt 38



138.49
132.64
131.94
128.35
127.60
127.50

77.31
77.05
76.80
75.24
73.00
67.67

48.23
39.11
33.14

19.02
17.34
16.39
14.19

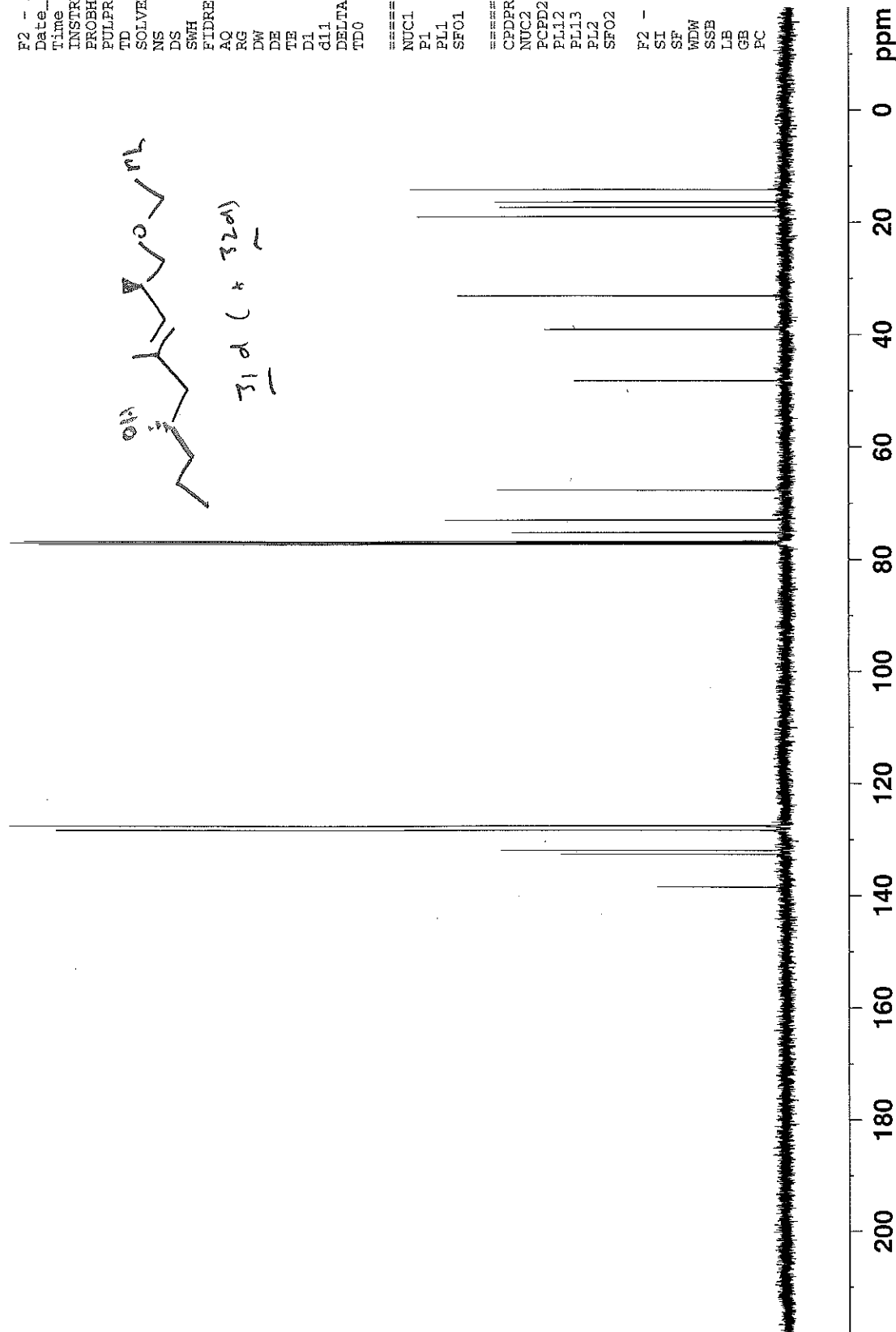
Current Data Parameters
NAME 2007-06-11-ejt-38
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070611
Time 12.35
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 256
DS 2
SMH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 512
DW 16.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

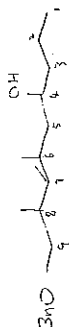
===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 -4.20 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 23.47 dB
PL13 120.00 dB
PL2 3.25 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



C₁₈ H₃₆ O₂

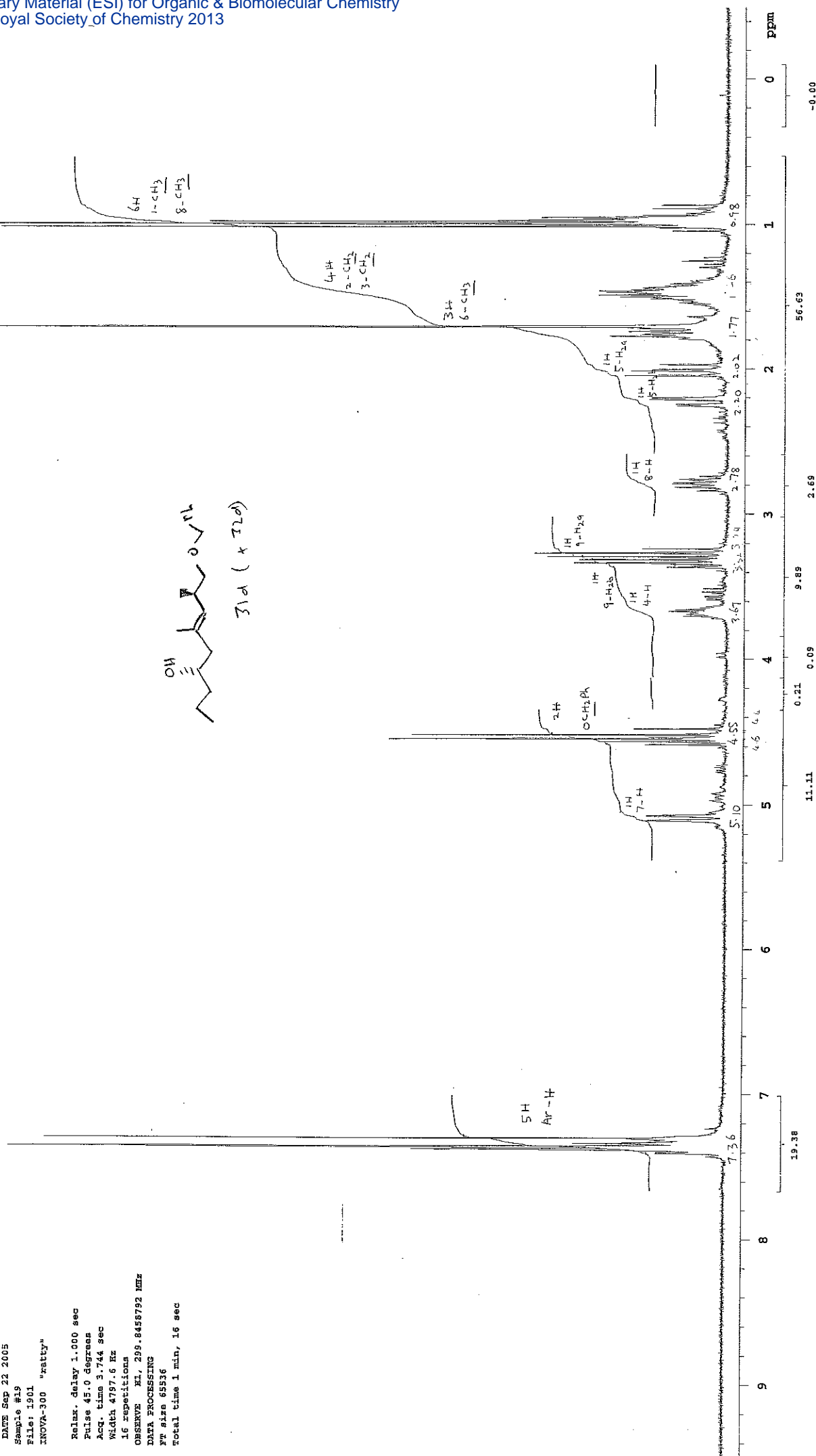


nb007
STANDARD 1H OBSERVE

Automation directory: /data/nmrdata/Sep22
File : 1901

Pulse Sequence: s2pul
Solvent: cdcl3
DATE Sep 22 2005
Sample #19
File: 1901
INOVA-300 "fatty"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.744 sec
Width 4797.6 Hz
16 repetitions
OBSERVE EI, 299.8458792 MHz
DATA PROCESSING
Ft size 65536
Total time 1 min, 16 sec

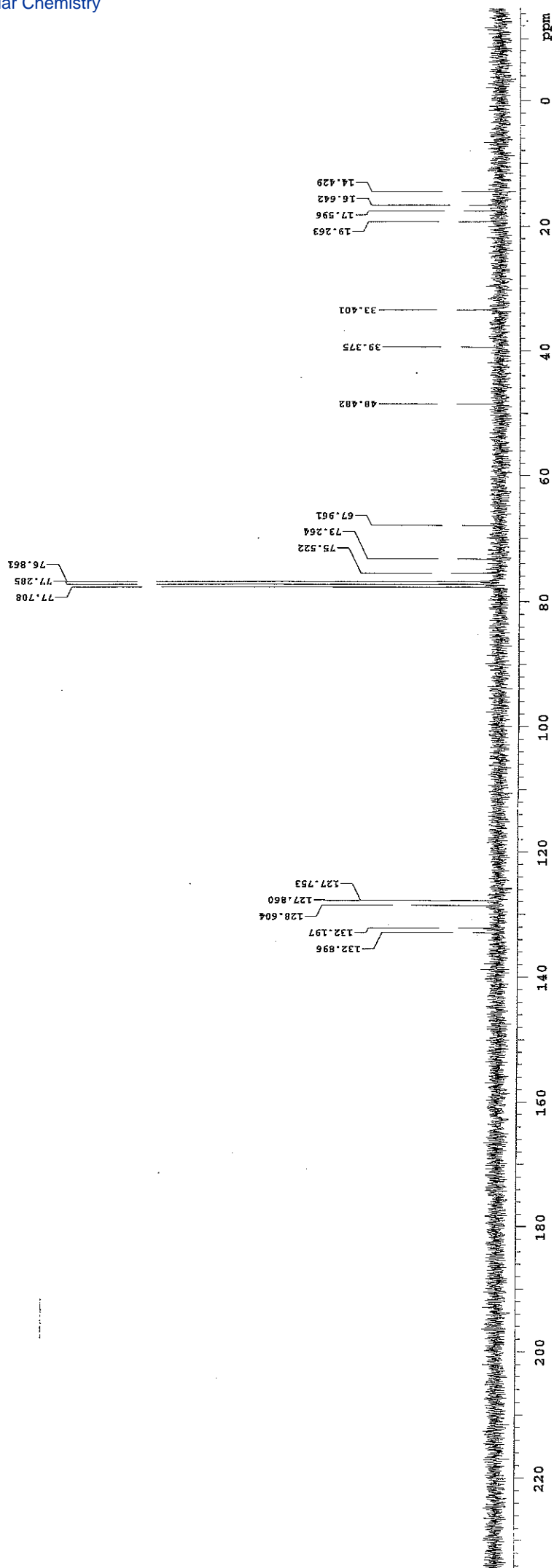
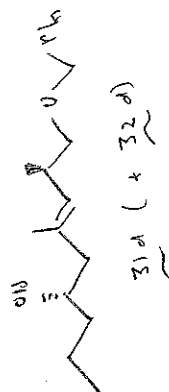


nb007
STANDARD 1H OBSERVE2

Automation directory: /data/nmrdata/Sep22
File : 1902

Pulse Sequence: s2pul
Solvent: cdcl3
DATE Sep 22 2005
Sample #19
File: 1902
INOVA-300 "ratty"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18850.1 Hz
256 repetitions
OBSERVE CH3, 75.3962883 MHz
DECOUPLE H1, 299.8473786 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 12 min, 2 sec

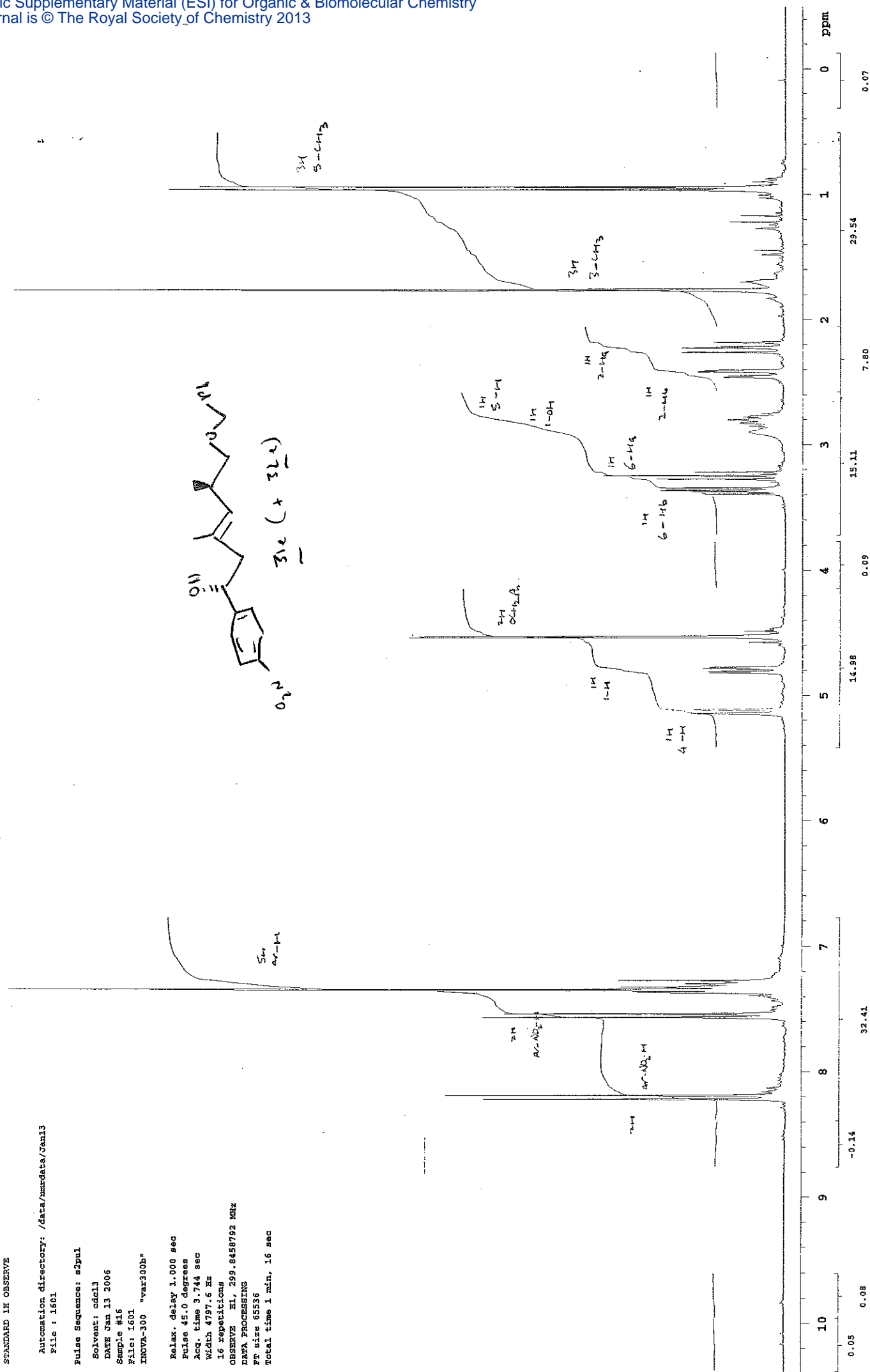
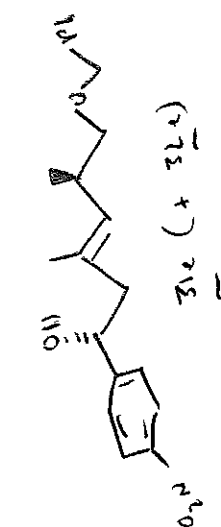


h2009L
STANDARD 1H OBSERVE

Automation directory: /data/wwrdata/Jan13
File : 1601

Pulse Sequence: s2pul
Solvent: cdcl3
DATE Jan 13 2006
Sample #16
File: 1601
INOVA-300 "var300b"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.744 sec
Width 4797.6 Hz
16 repetitions
OBSERVE E1, 299.8458792 MHz
DATA PROCESSING
FT size 65536
Total time 1 min, 16 sec



kb008r

13C OBSERVE

pad=2 run with fmdx0 before acquisition

Automation directory: /data/nmrdata/Jan13

File : 2101

Pulse Sequence: s2yn1

Solvent: cdcl3

DATE Jan 13 2006

Sample #21

File: 2101

INNOVA-300 "var300b"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.815 sec

Width 18850.1 Hz

256 repetitions

OBSERVE C13, 75.3962883 MHz

DECOUPLE H1, 299.6473786 MHz

Power 37 dB

continuously on

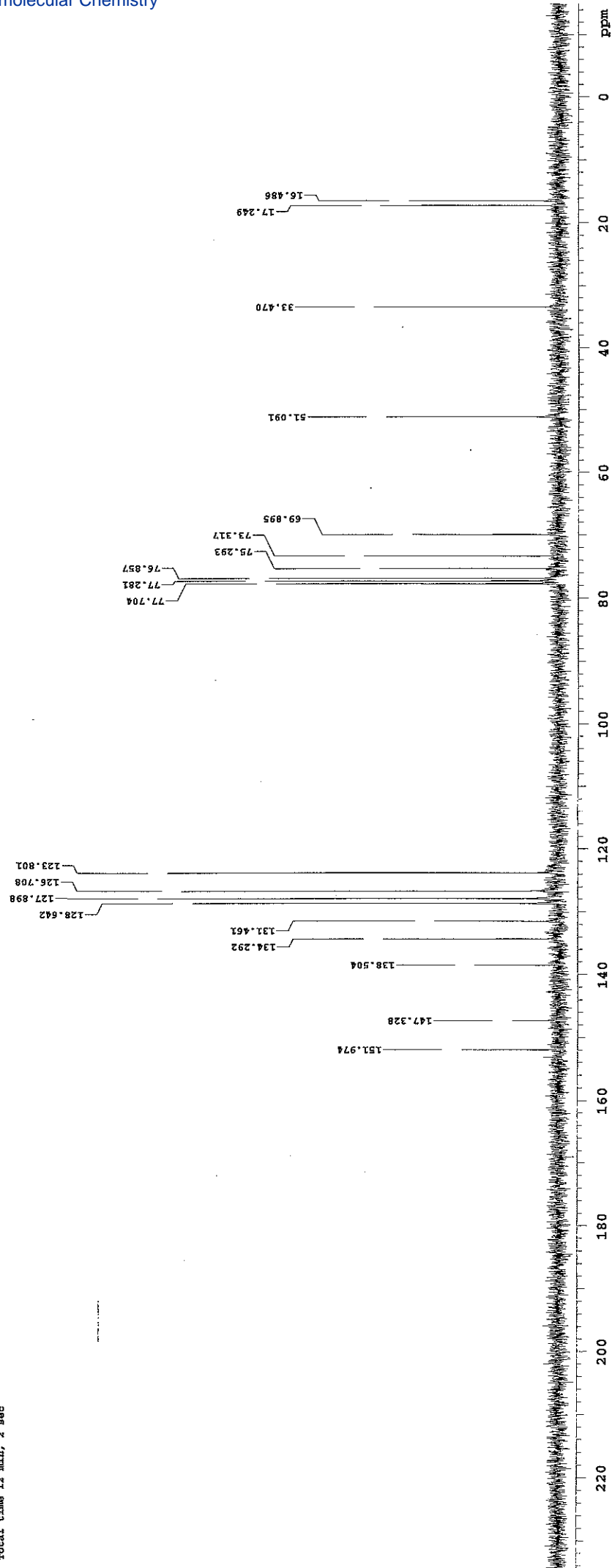
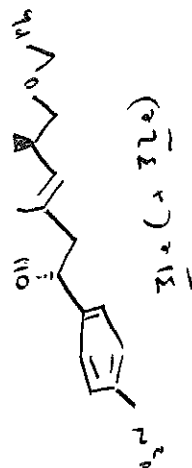
WALTZ-16 Modulated

DATA PROCESSING

Line broadening 1.0 Hz

PT size 131072

Total time 12 min, 2 sec

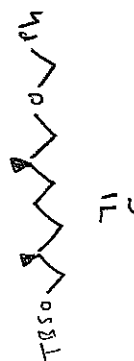


sd57
STANDARD IN OBSERVE

Automation directory: /data/nmrdata/feb27
File : 4102

Pulse Sequence: #2pul
Solvent: cdcl3
Ambient temperature
Sample #41
File: 4102
XNOVA-300 "ratby"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.744 sec
Width 4797.6 Hz
16 repetitions
OBSERVE H1, 299.8458792 MHz
DATA PROCESSING
Ft size 65536
Total time 1 min, 16 sec



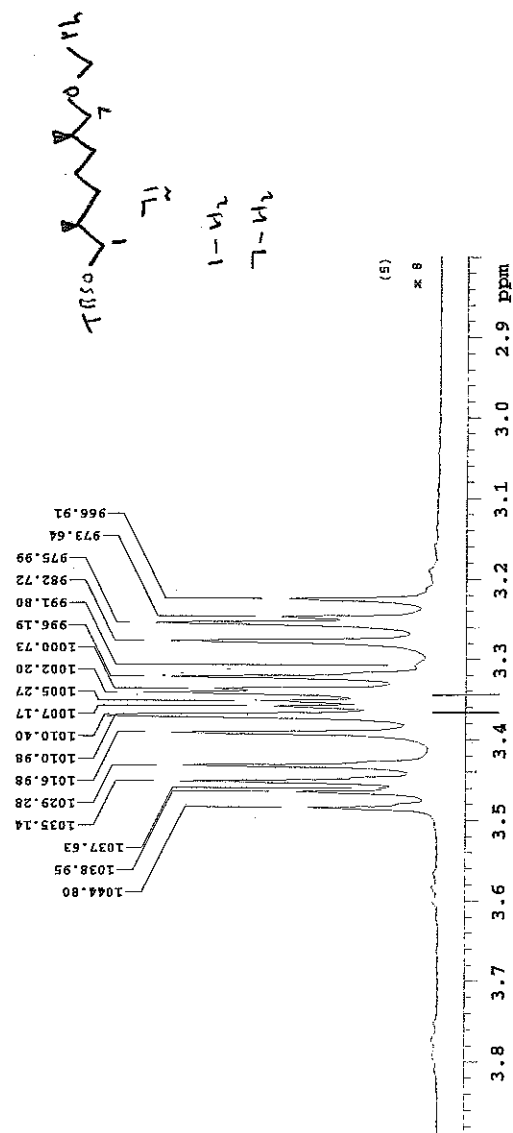
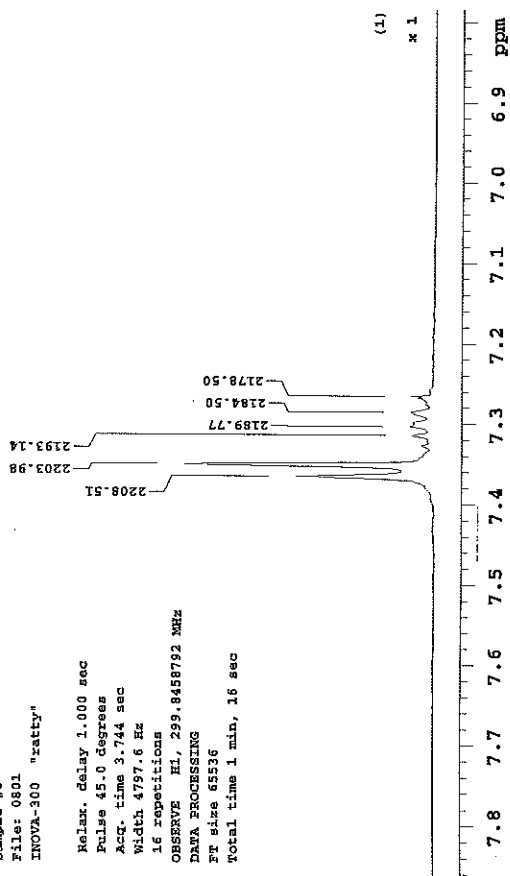
Expansions at 2.00 Hz/run

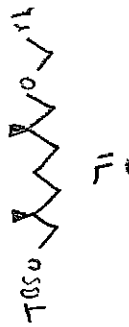
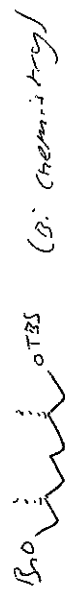
STANDARD 1H OBSERVE
ED553

Automation directory: /data/nmrdata/feb25
File : 0801

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #8
File: 0801
INOVA-300 "ratty"

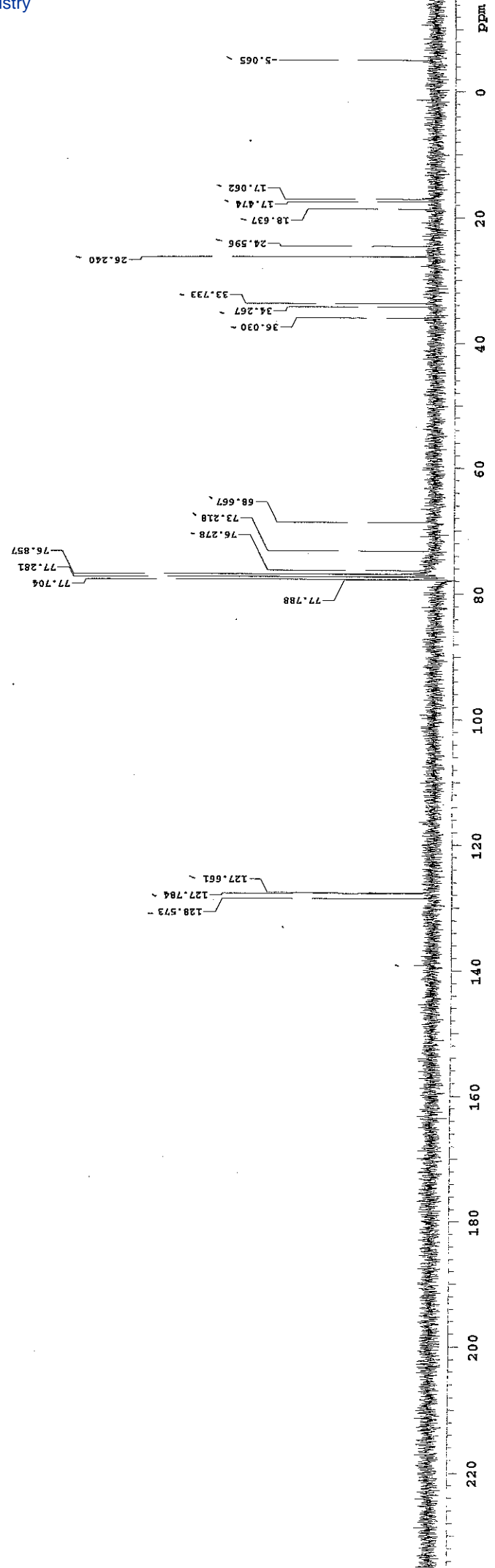
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.744 sec
Width 4797.6 Hz
16 repetitions
OBSERVE H1, 299.8458792
DATA PROCESSING
FT size 65536
Total time 1 min, 16 sec





11

sd557
13C OBSERVE
pad-2 run with findz0 before acquisition
Automation directory: /data/nmrdata/Mar26
File : 0102
Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #1
File: 0102
INOVA-300 "ratby"
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 1850.1 Hz
256 repetitions
OBSERVE C13, 75.3562883 MHz
DECOUPLE H1, 299.8473786 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Ft size 131072
Total time 12 min, 2 sec



Automation directory: /data/mmrdata/Mar25

File : 4501

Pulse Sequence: s2pul

solvent: cdcl3

Ambient temperature

Sample #45

File: 4501

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.744 sec

Width 4797.6 Hz

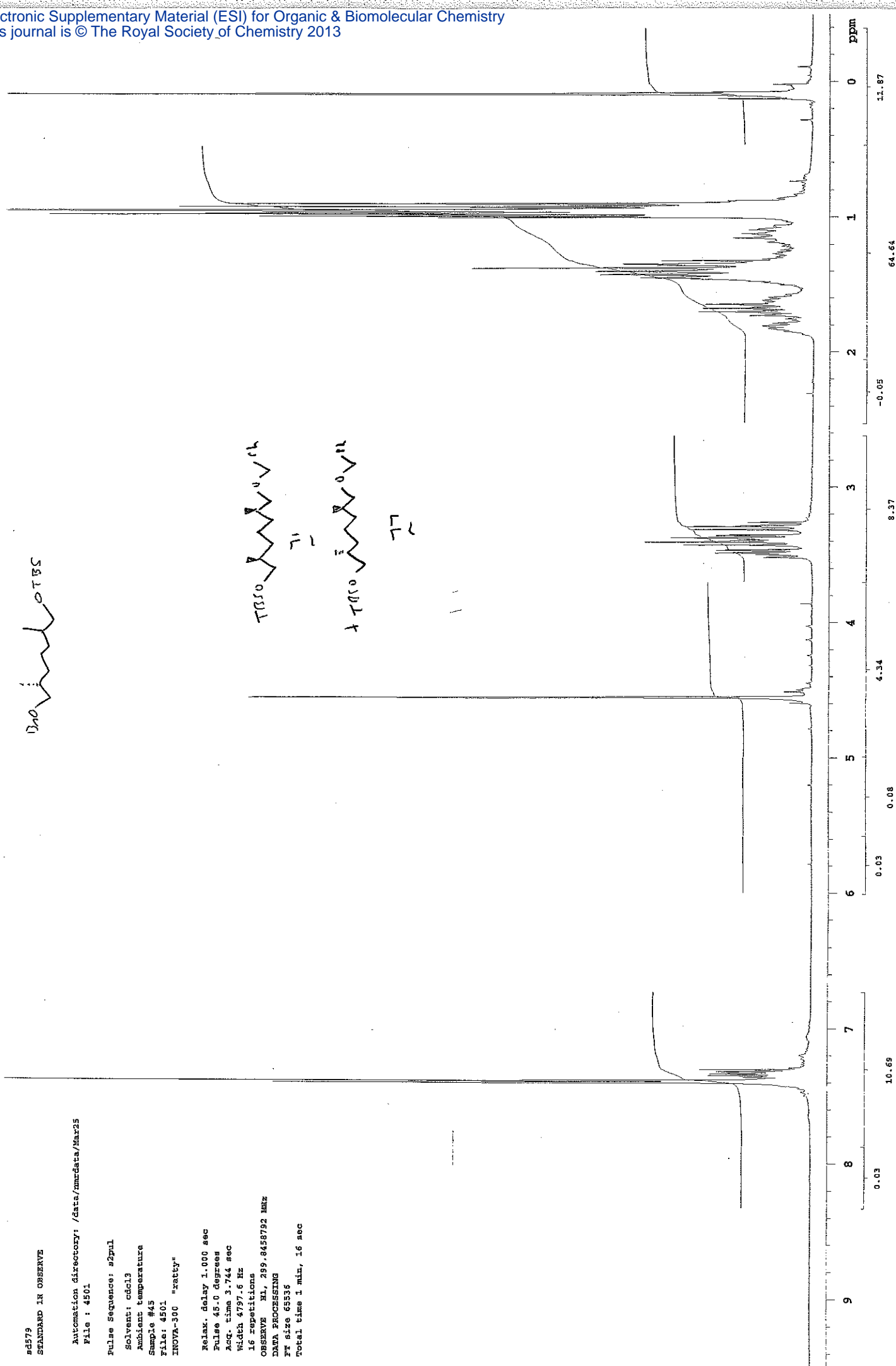
16 repetitions

OBSERVE H1, 299.8458792 MHz

DATA PROCESSING

PT size 65535

Total time 1 min, 16 sec



0.03

10.69

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5

— K

— **4**

25

2013

Expansions at 2.00 Hz/mm

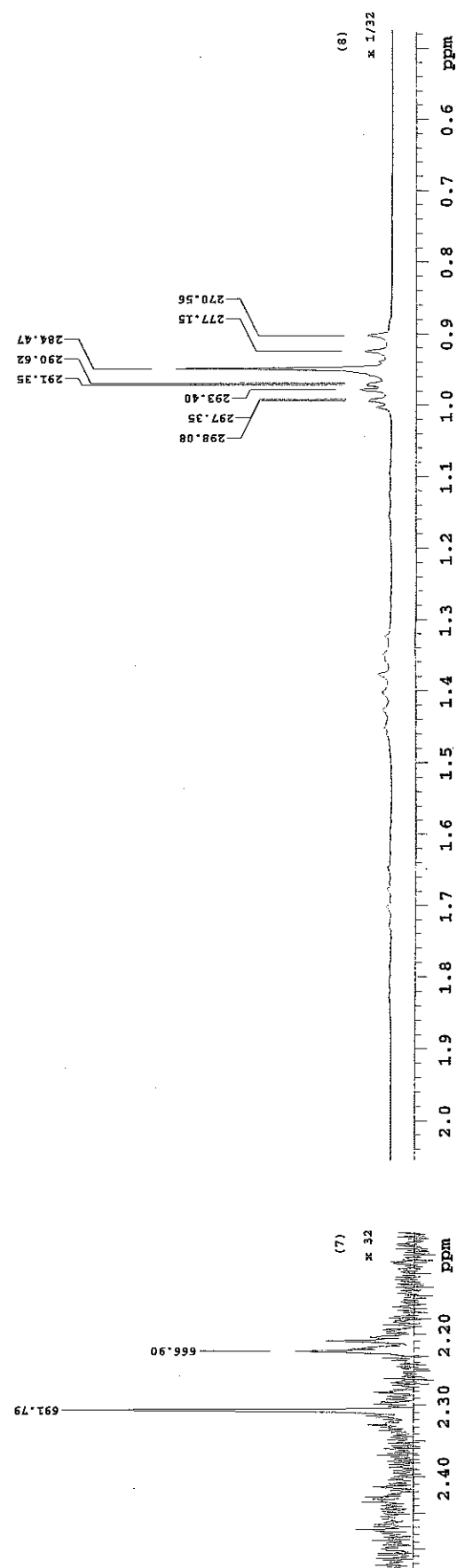
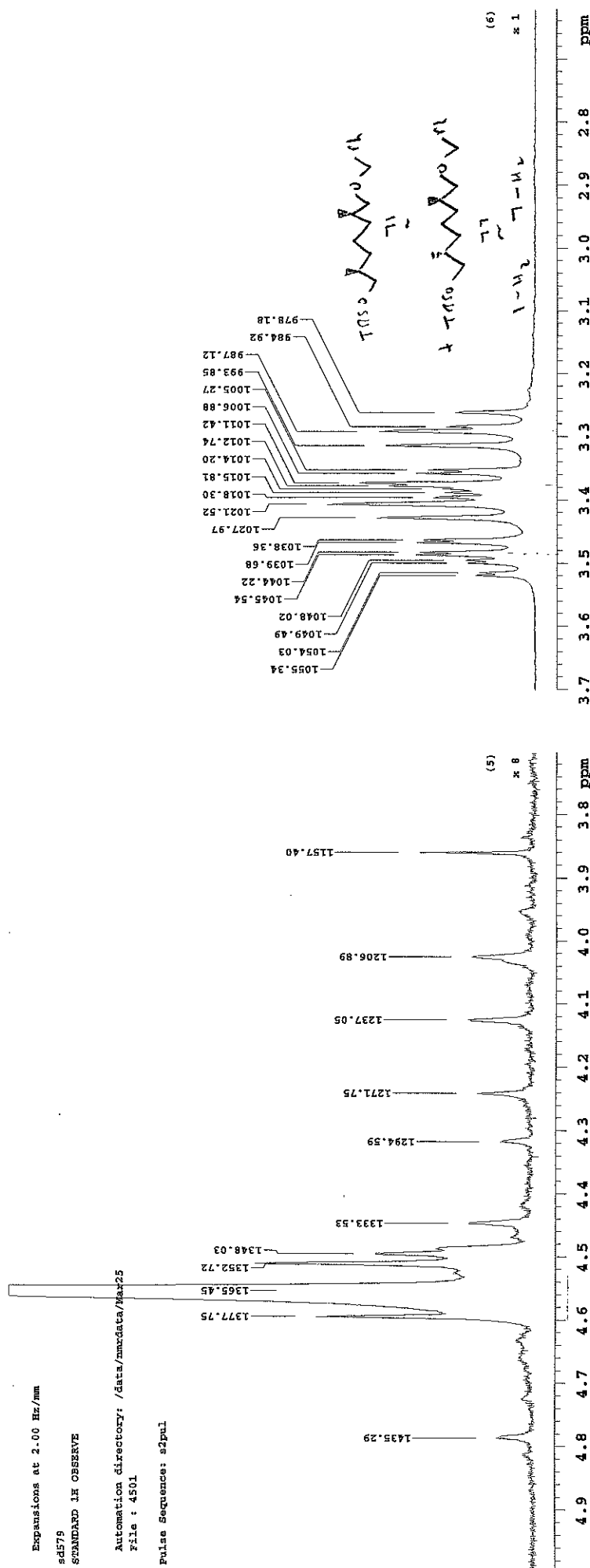
64579

STANDARD JH OBSERVE

Automation directory: /data/nmrdata/Mar25
File : 4501

File : 4501

Pulse Sequence: s2pul



ad590

STANDARD 1K OBSERVE

Automation directory: /data/mrdata/Apr06
File: 1302

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Sample #13

File: 1302

INOVA-300 "ratty"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.744 sec

Width 4797.6 Hz

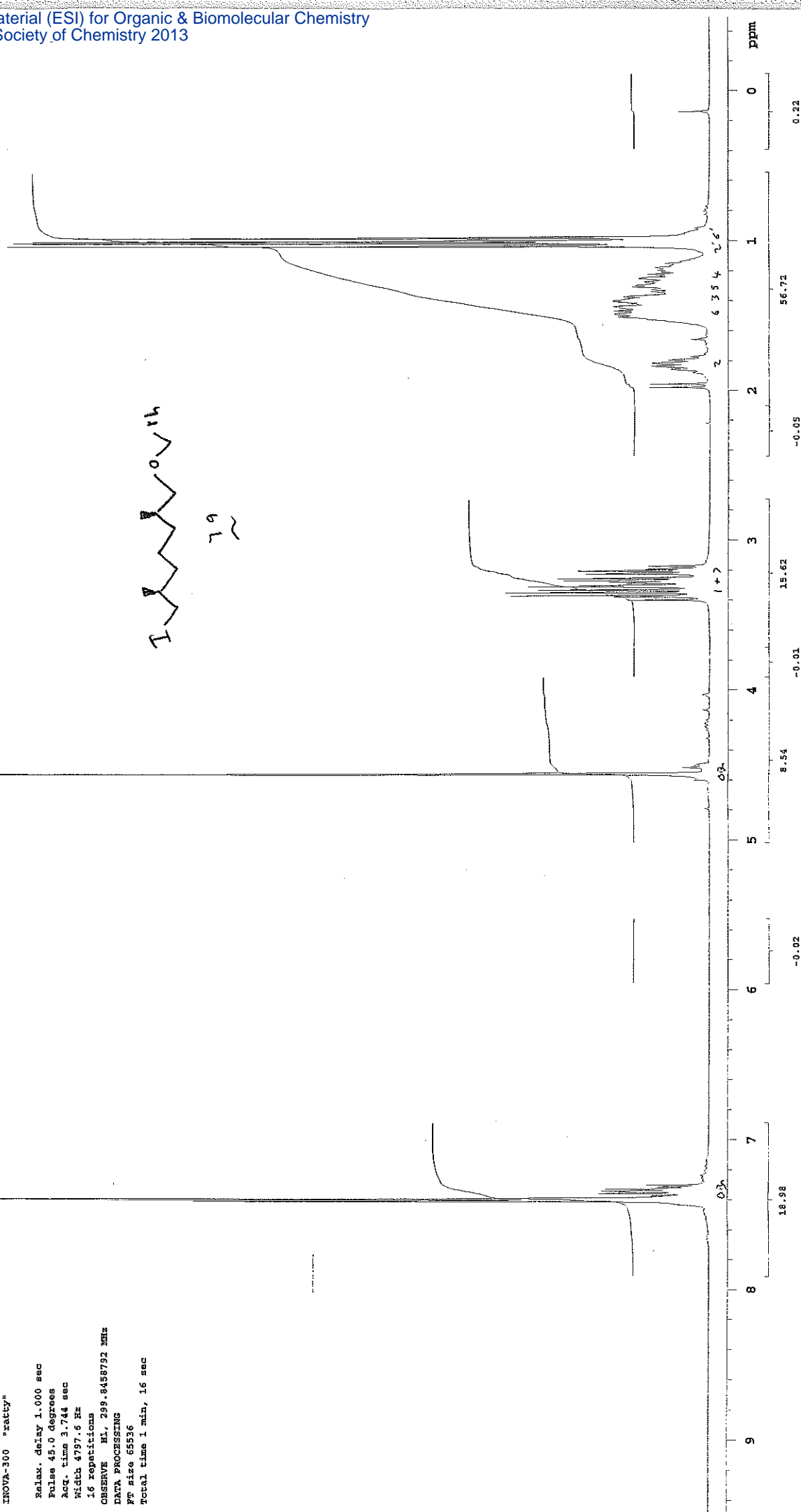
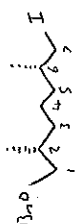
16 repetitions

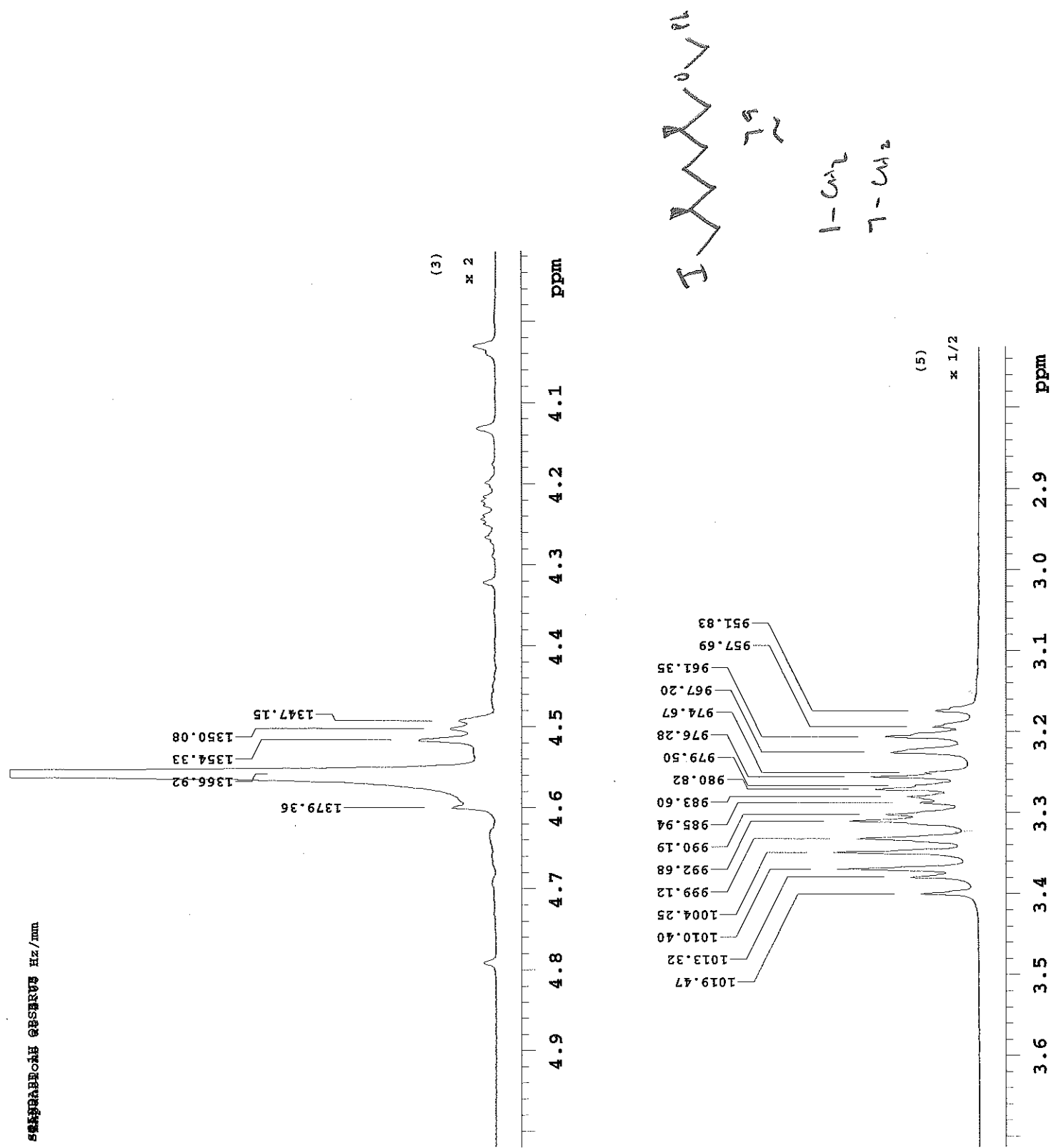
OBSERVE M1, 299.8458792 MHz

DATA PROCESSING

FT size 65536

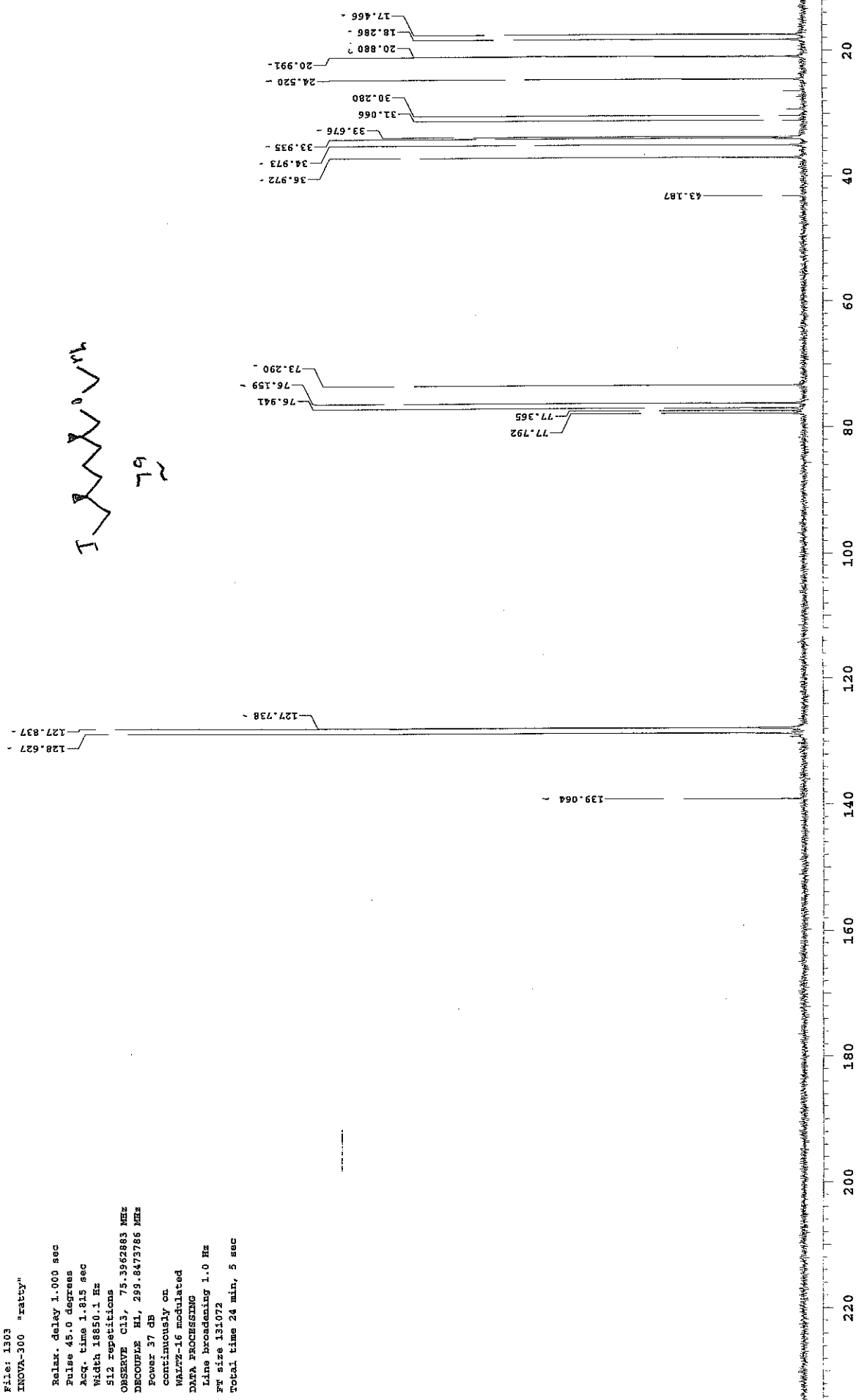
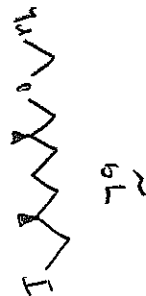
Total time 1 min, 16 sec





Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #13
File: 1303
INOVA-300 "ratty"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 1850.1 Hz
512 repetitions
OPERATION C13, 75.3962883 MHz
DECOUPLE H1, 299.8473786 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
F1 size 131072
Total time 24 min, 5 sec



sd584

STANDARD 1H OBSERVE

Automation directory: /data/nmrdata/Mar30

File : 3902

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Sample #39

File: 3902

INOVA-300 "raty"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.744 sec

Width 4797.6 Hz

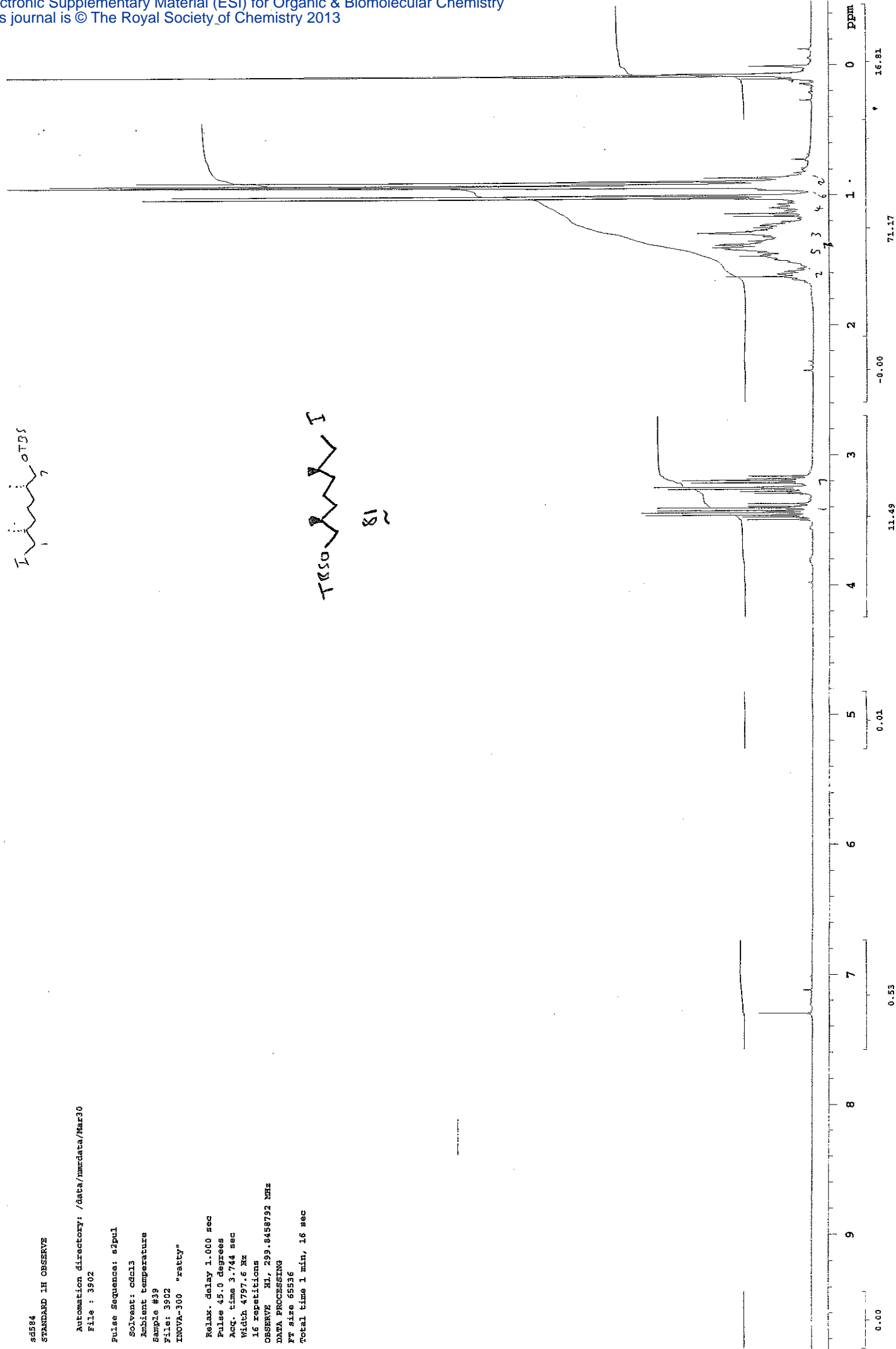
16 repetitions

OBSERVE RU, 299.8458792 MHz

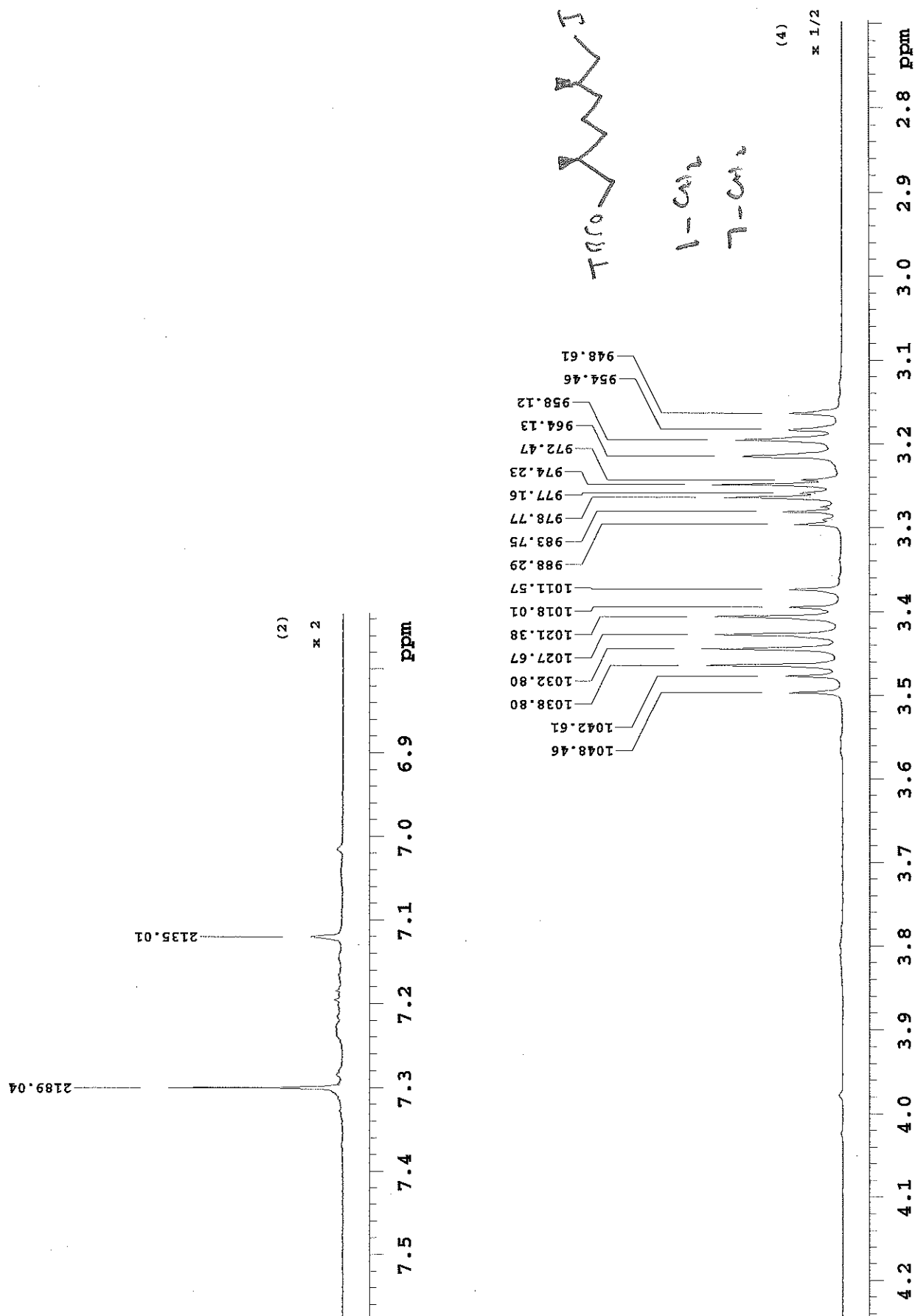
DATA PROCESSING

FT size 65536

Total time 1 min, 16 sec



Expansions at 2.00 Hz/mm



13C OBSERVE

pad=2 run with findz before acquisition

Pulse Sequence: s2pul

Solvent: cdcl3

Ambient temperature

Sample #35

File: 3501

INOVA-300 "ratty"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.815 sec

Width 18850.1 Hz

64 repetitions

OBSERVE C13, 75.3962883 MHz

DECOUPLE H1, 299.8473786 MHz

Power 37 dB

continuously on

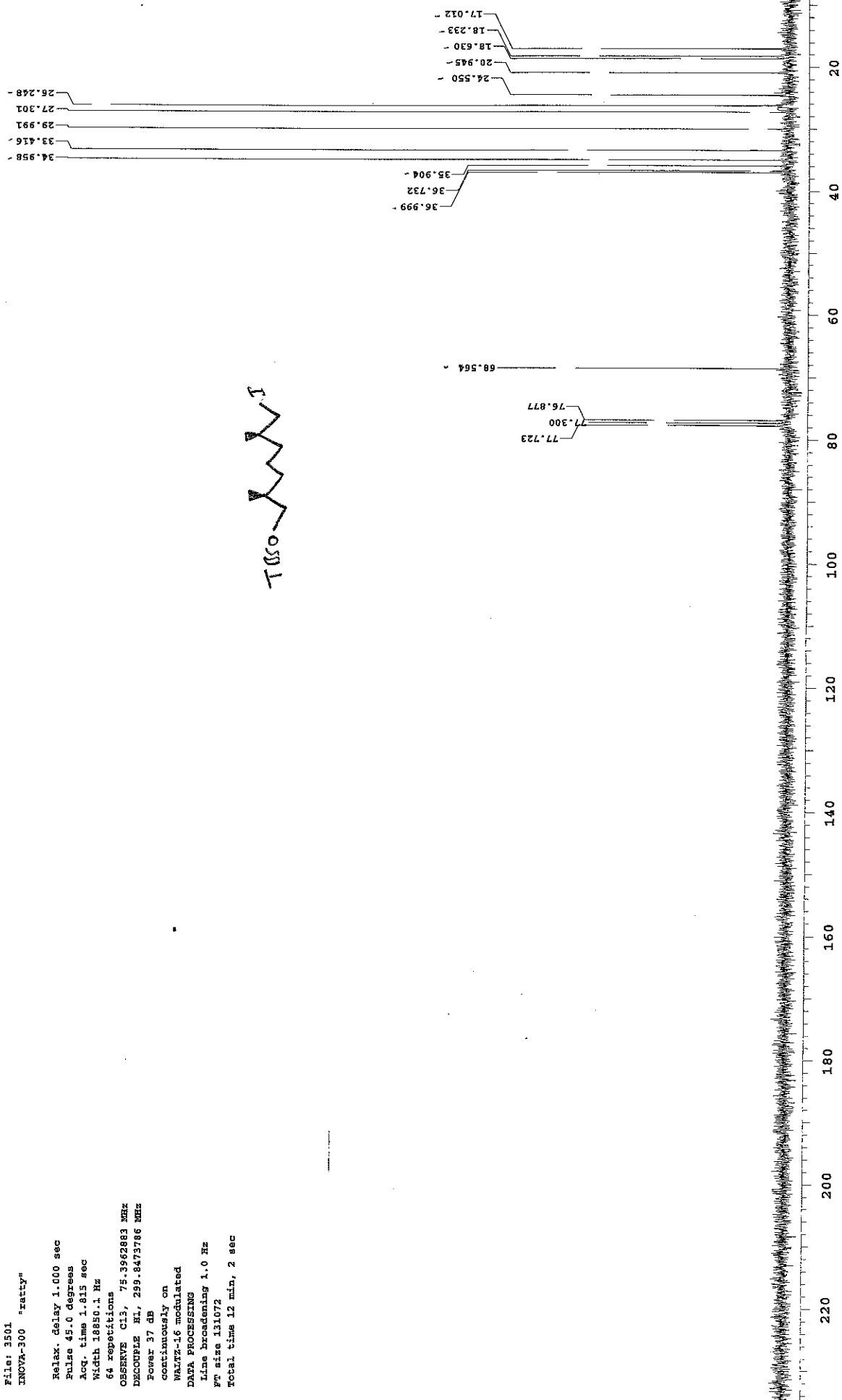
WALTZ-16 modulated

DATA PROCESSING

Line broadening

mm size 131072

Total time 12 m

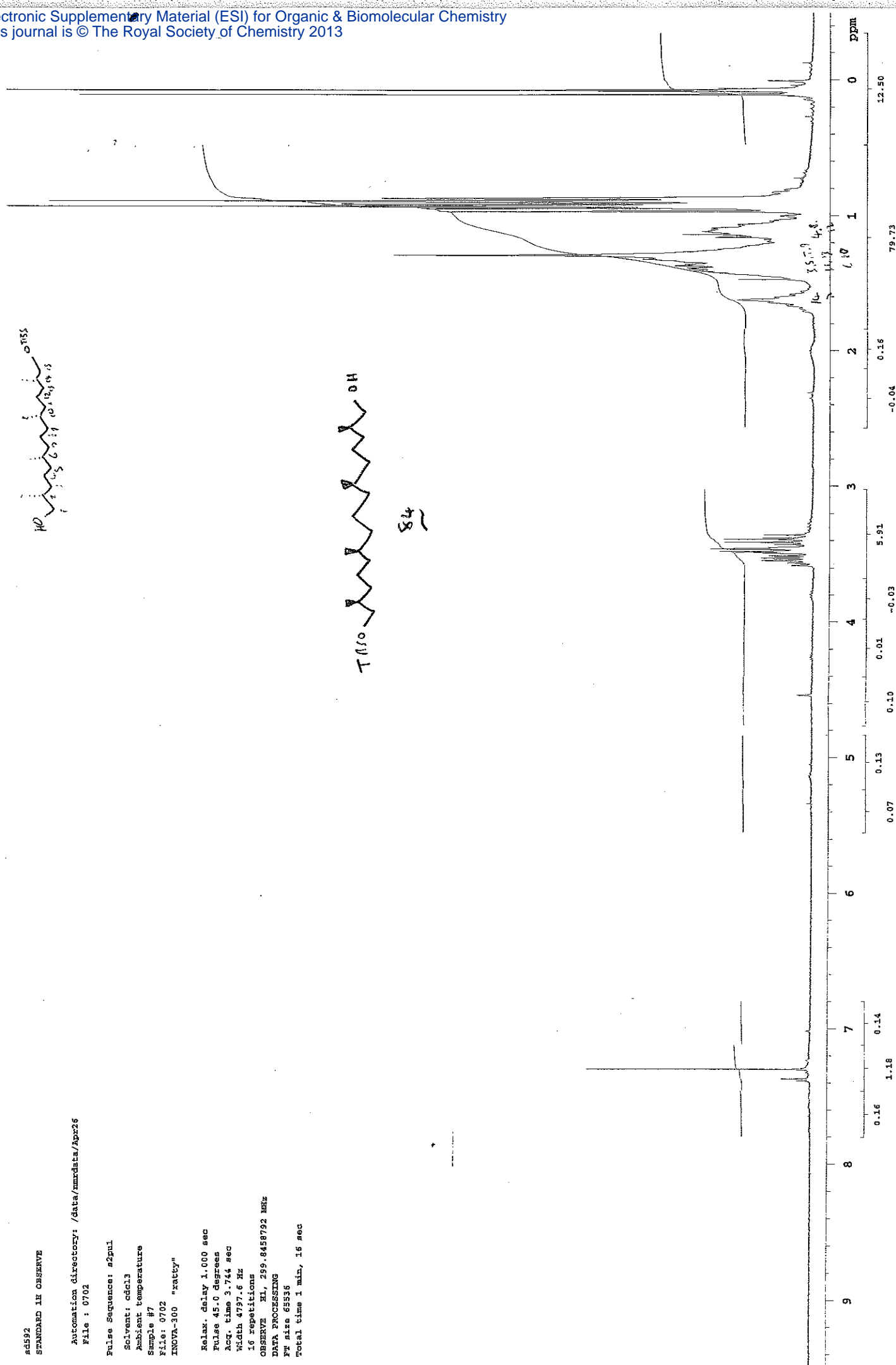
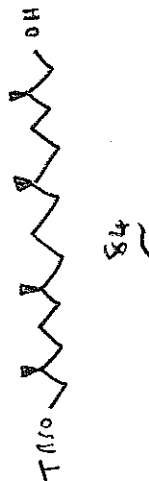
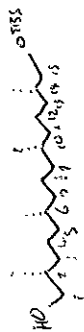


sd592
STANDARD 1H OBSERVE

Automation directory: /data/nmrdata/Apr26
File : 0702

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #7
File: 0702
INOVA-300 "ratty"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 3.744 sec
Width 4797.6 Hz
16 repetitions
OBSERVE XL, 299.8458792 MHz
DATA PROCESSING
F2 size 65536
Total time 1 min, 16 sec

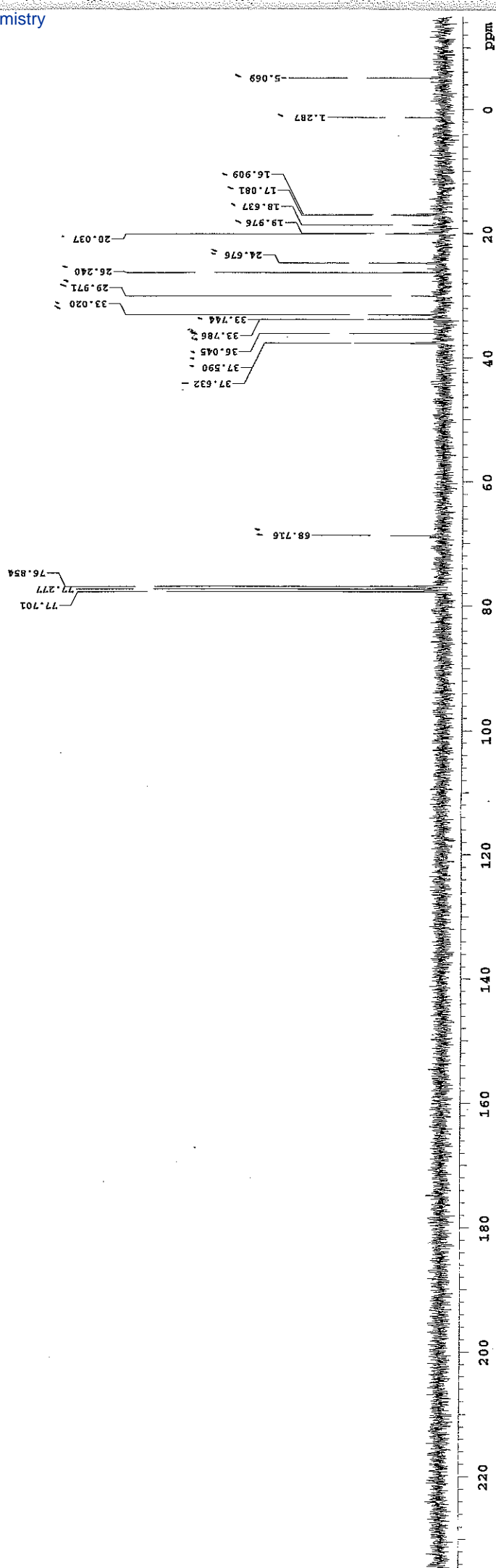
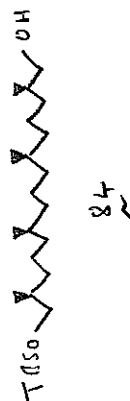


STANDARD 1H OBSERVE
ssd592

Automation directory: /data/xmrdata/2pr25
File : 0703

Pulse Sequence: s2pul
Solvent: cdcl3
Ambient temperature
Sample #7
File: 0703
INOVA-300 "xatxy"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.815 sec
Width 18850.1 Hz
256 repetitions
OBSERVE C13, 75.3952893 MHz
DECOUPLE H1, 299.8473786 MHz
Power 37 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Fw size 131072
Fw time 12 min, 2 sec

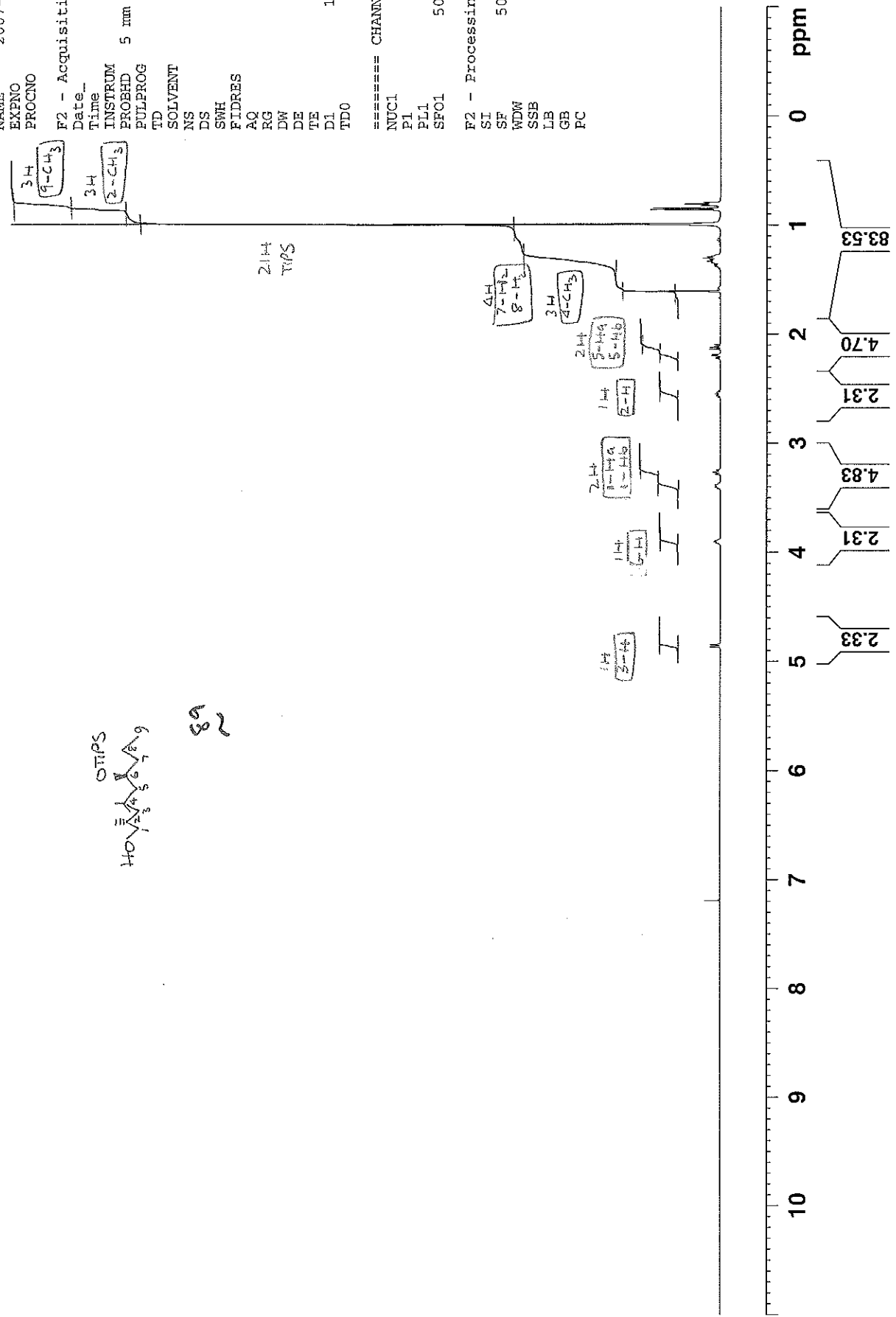


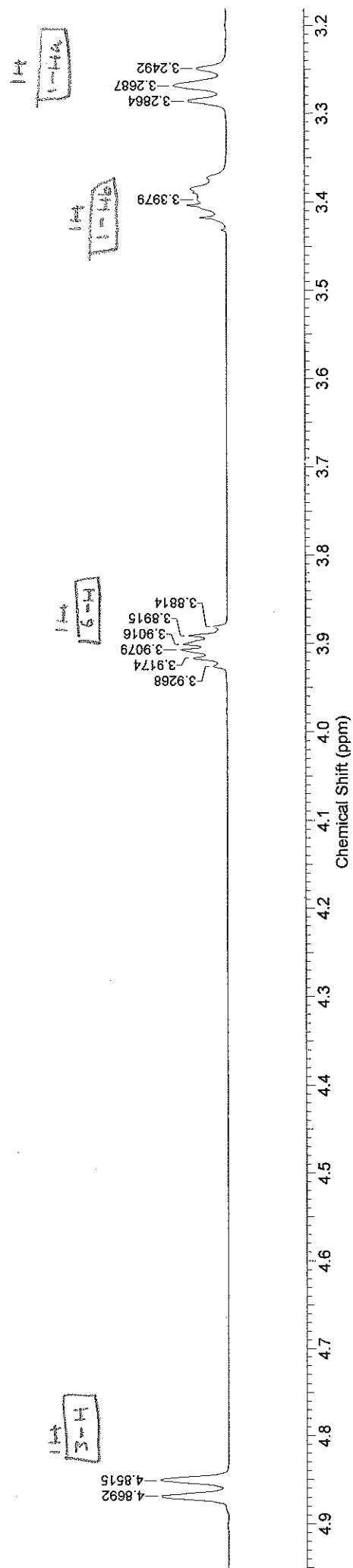
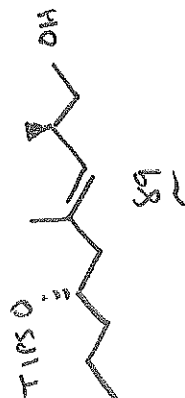


C₂₀H₄₂O₂Si⁺
FW = 342.30

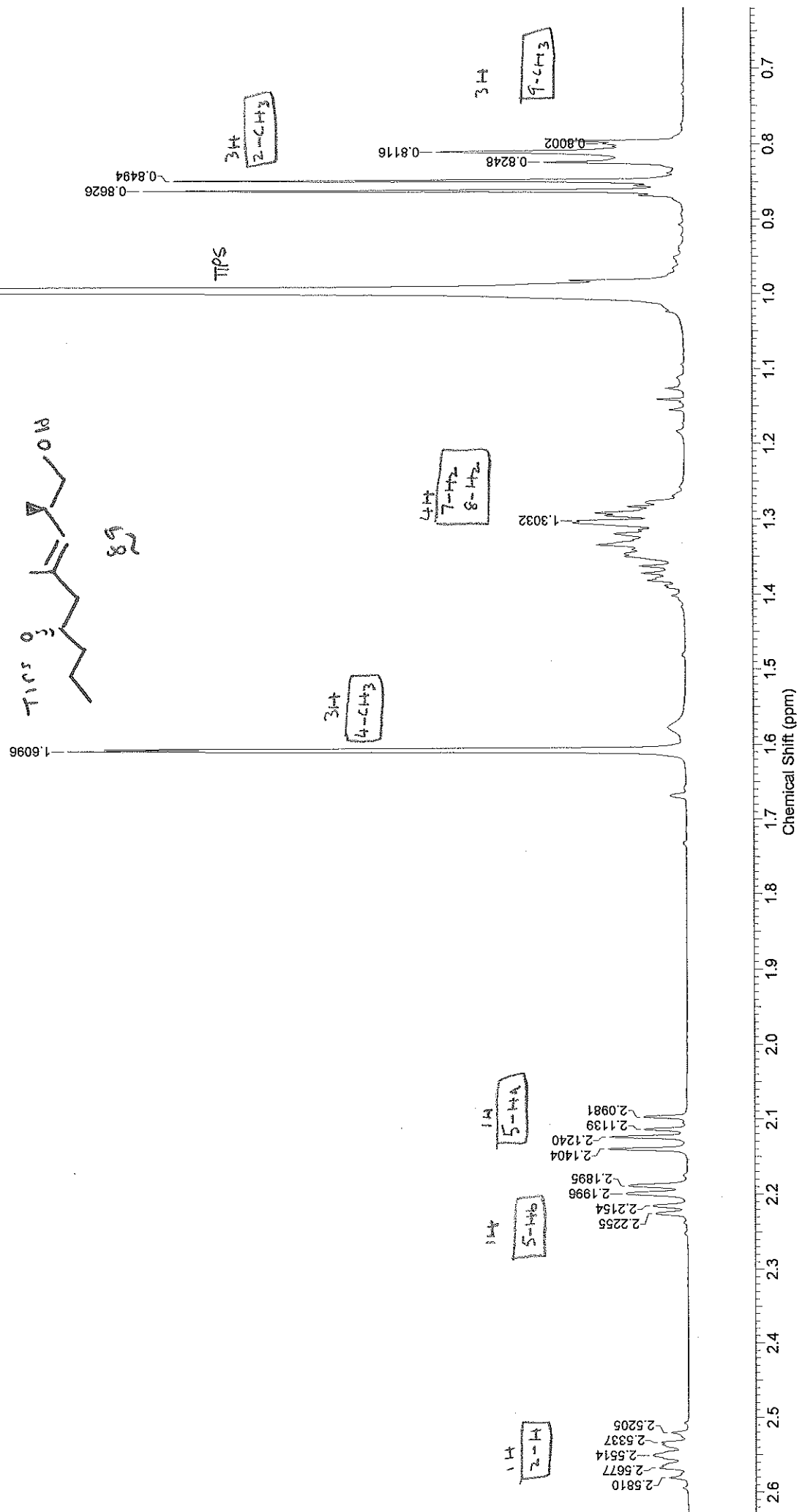
nb101
mPROTON CDCl₃ /opt/topspin ejt 32

Current Data Parameters
NAME 2007-07-05-ejt-32
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070705
Time 14.47
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDCl₃
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 36
DW 48.400 usec
DE 13.76 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 7.80 usec
PL1 3.25 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300415 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





nb101 mPROTON CDCl3 /opt/topspin ejt 32



nb101
mCARBON CDCl₃ /opt/topspin ejt 1



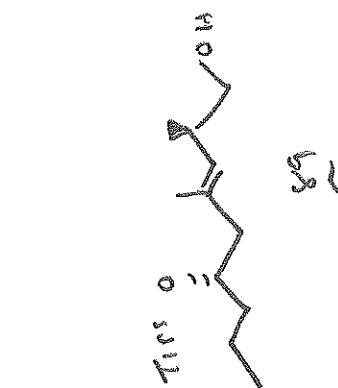
129.68
135.21

77.31
77.06
76.80
70.68
67.89

47.63

38.51
35.44

18.25
17.77
17.13
16.95
14.41
12.71



Current Data Parameters
NAME 2007-07-05-ejt-1
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070706
Time 10.23
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 256
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 512
DW 16.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 -4.20 dB
SF01 125.7703643 MHz

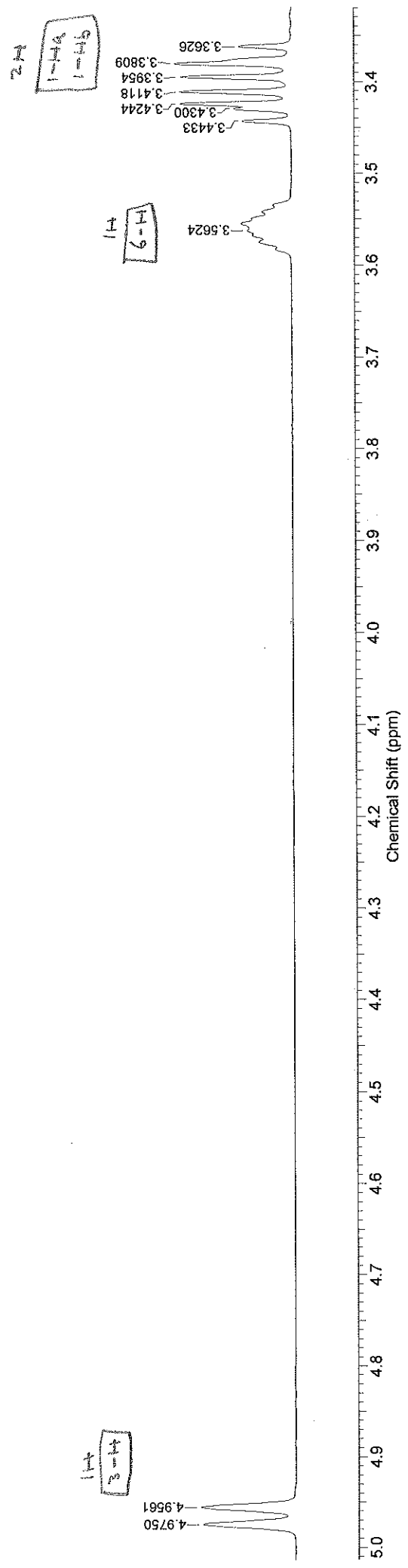
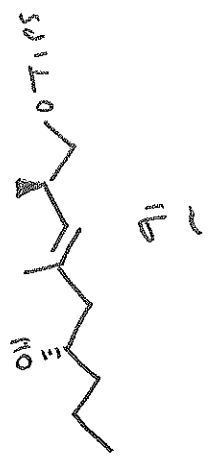
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 23.47 dB
PL13 120.00 dB
PL2 3.25 dB
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 1.40

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

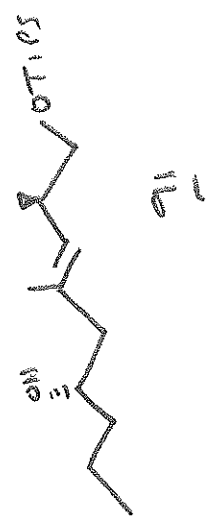
nb112 mPROTON CDCl3 /opt/topspin ejt 7

2007-08-08-EJT-7_010000FID

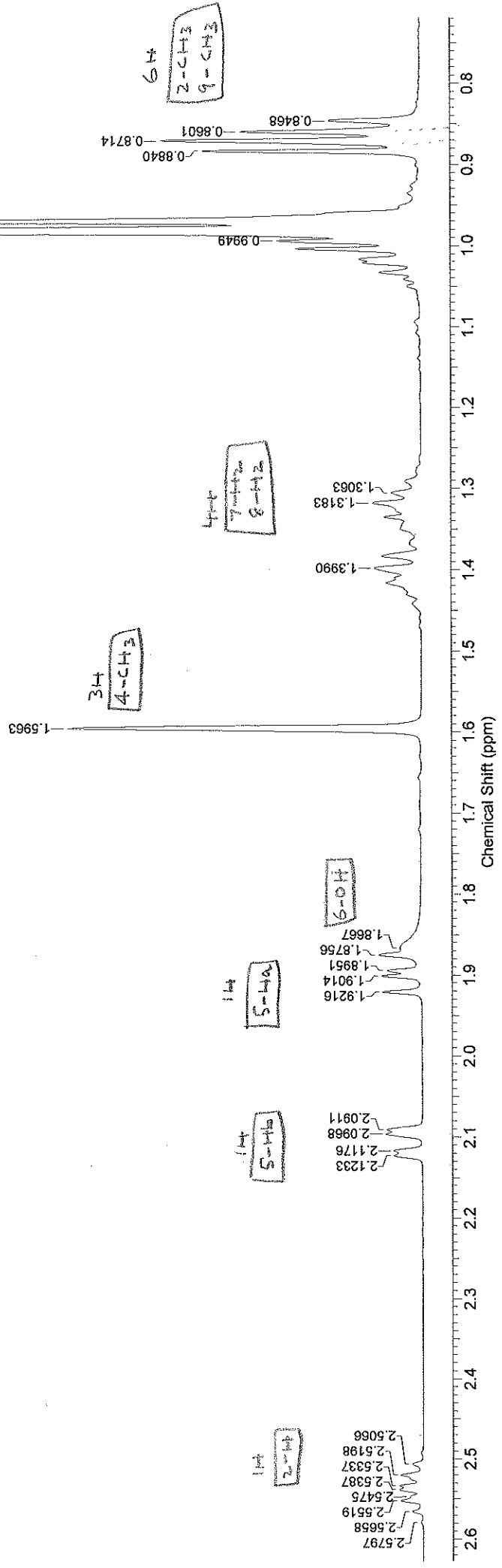


nb112 mPROTON CDCl3 /opt/topspin ejt 7

2007-08-08-EJT-7_010000FID

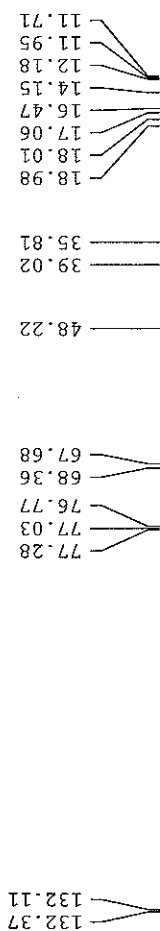


5d11





nb110
mCARBON CDCl3 /opt/topspin vnmr1 3



Current Data Parameters
NAME 2007-07-23-vnmr1-3
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070723
Time 13.43
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 512
DW 16.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 -4.20 dB
SF01 125.7703643 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 23.47 dB
PL13 120.00 dB
PL2 3.25 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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



$2 = 4$
 $4 = 4$
 $6 = 4 \checkmark$
 34

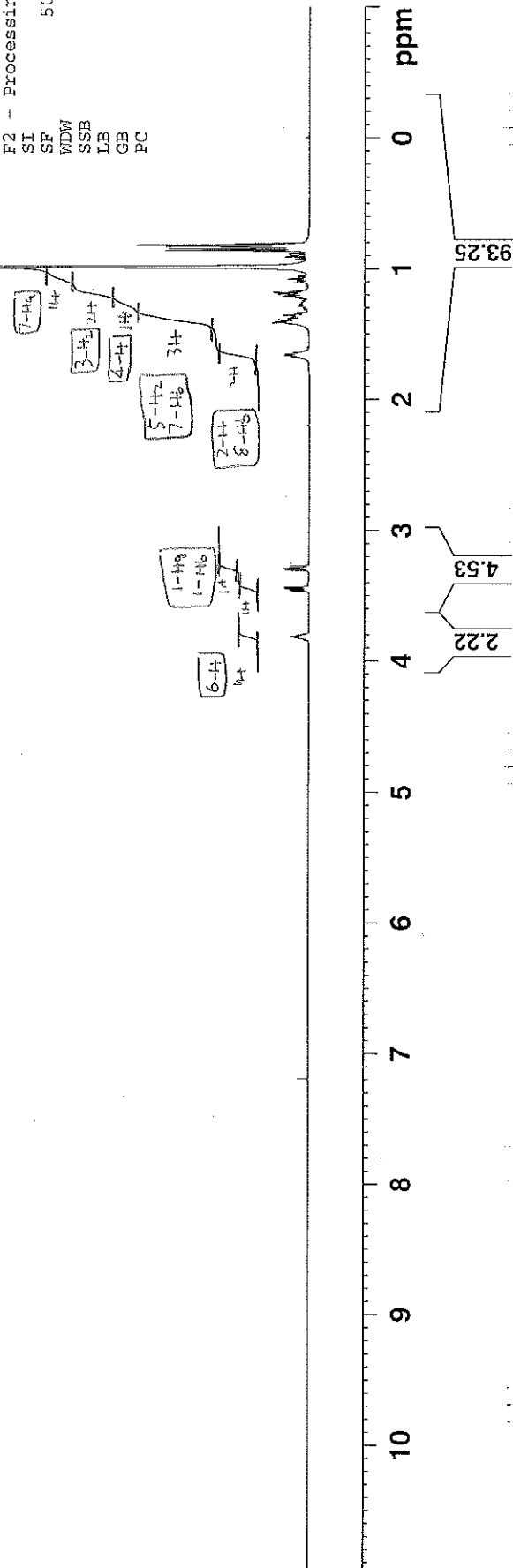
10

$$\begin{array}{r} 2-CH_3 \\ 2-CH_3 \\ 2-CH_3 \\ \hline 9H \end{array}$$

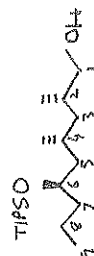

```
Current Data Parameters
NAME      2007-08-03-ejt-21
EXPNO     10
PROCNO    1

===== CHANNEL f1 =====
1H
7.80 usec
3.25 dB
500.1330885 MHz

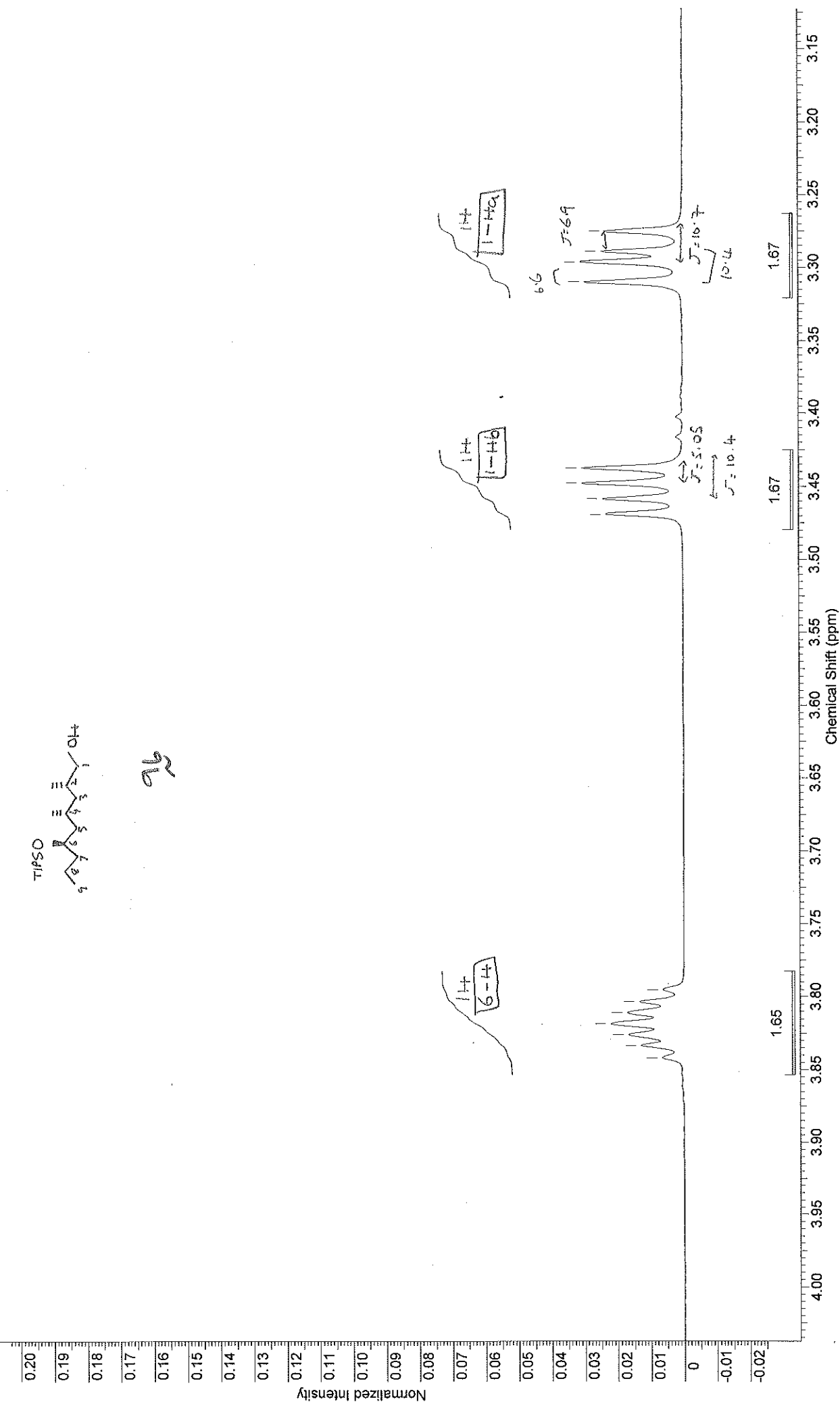
===== Processing parameters =====
SI          .32768
FF          500.1300405 MHz
WDW         EM
SSB         0
GB          0.30 Hz
EC          1.00
```

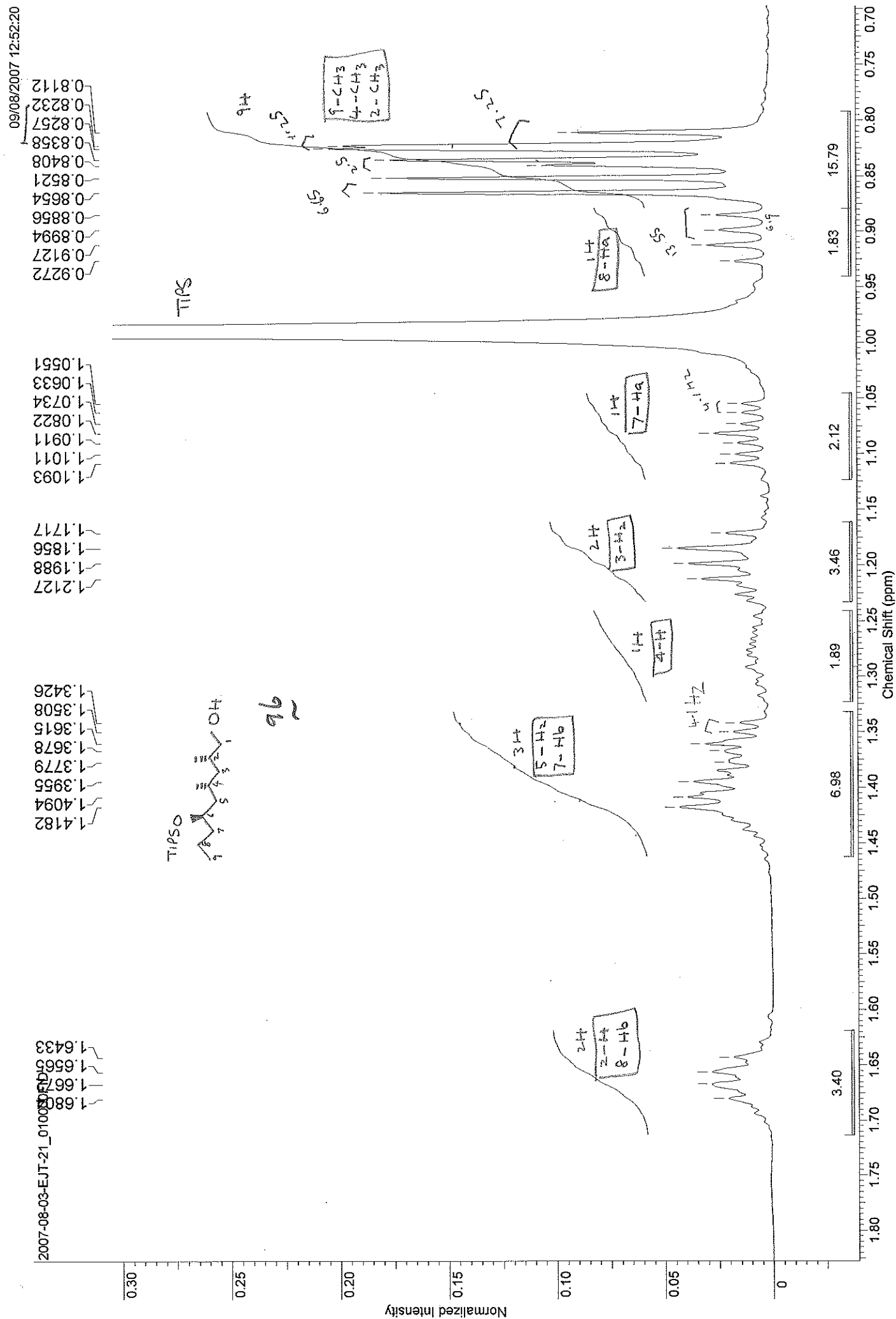


3.8419
3.8338
3.8262
3.8186
3.8111
3.8035
3.7953



—3.3099
—3.2967
—3.2891
—3.2753





nb115
mCARBON CDCl3 /opt/topspin ejt 21



44.24
41.76
40.34
33.04
30.30
29.70
27.00
26.44
20.73
20.56
18.27
18.24
18.08
17.72
17.39
14.52
14.37
13.12
12.89
12.76
12.71
12.65
12.36

Current Data Parameters
NAME 2007-08-03-ejt-21
EXPNO 22
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070804
Time 7.55
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SMH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 512
DW 16.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 -4.20 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 20.00 dB
PL13 23.00 dB
PL2 3.25 dB
SFO2 500.1320005 MHz

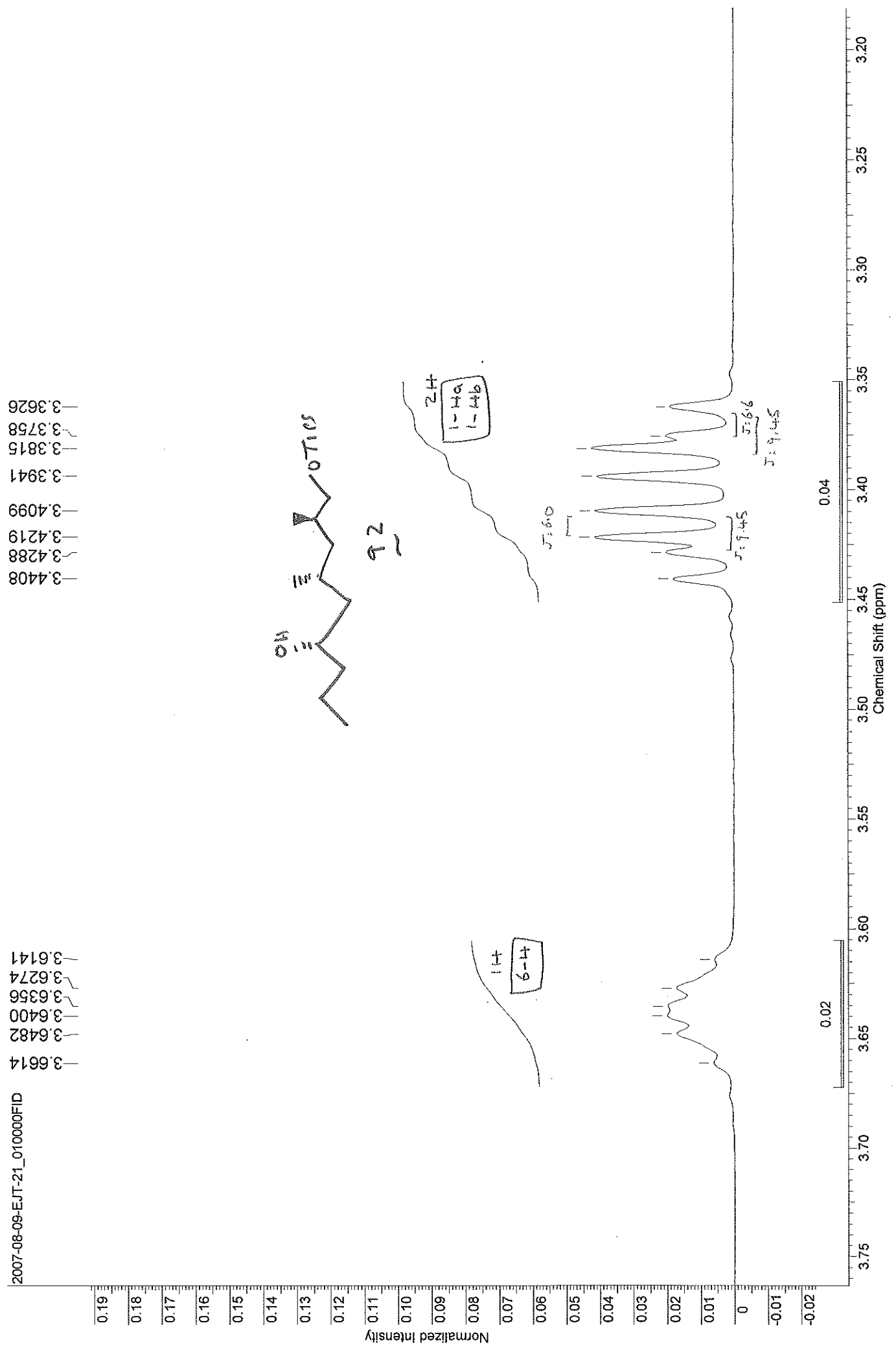
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



96

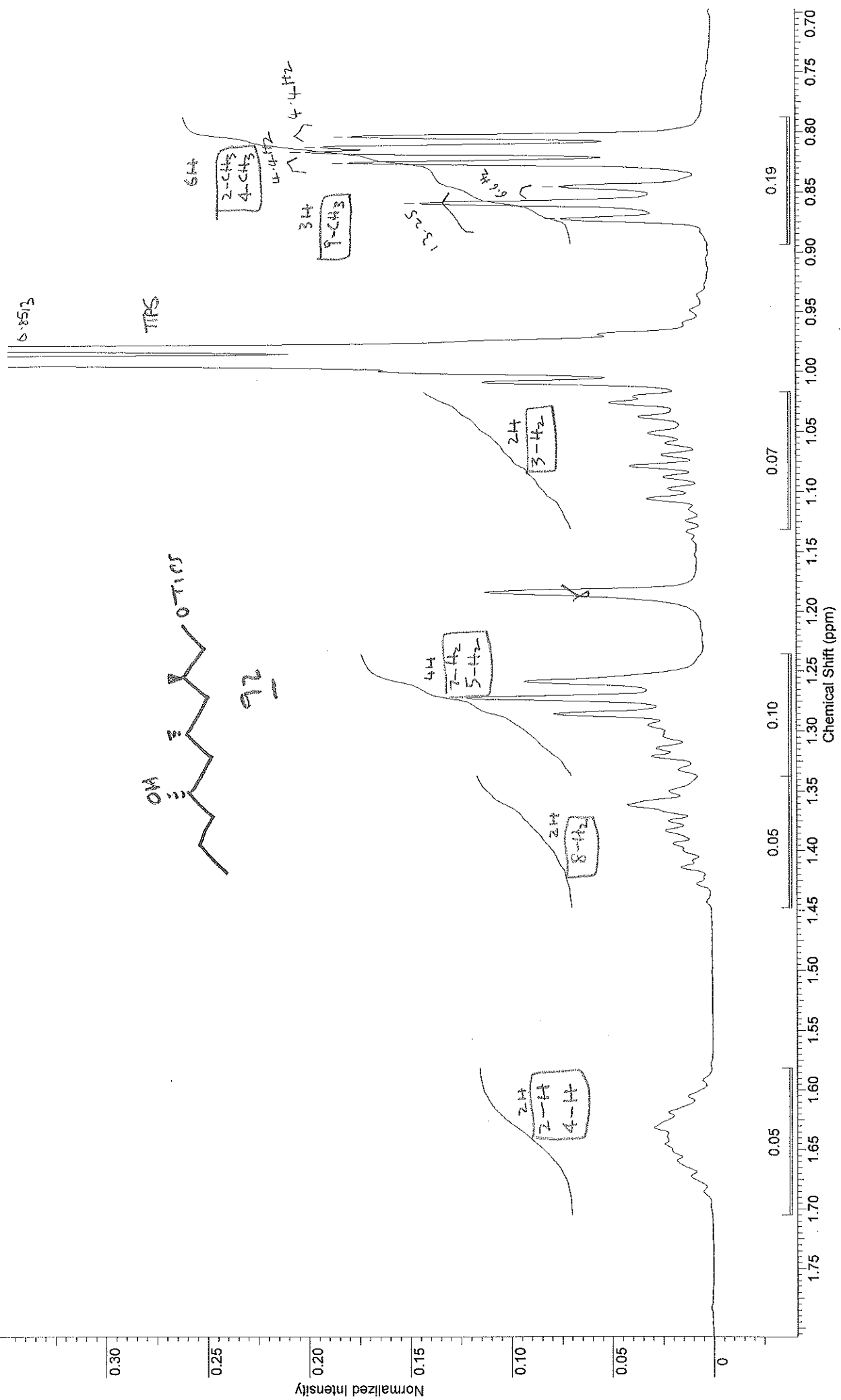
200 180 160 140 120 100 80 60 40 20 0 ppm

09/08/2007 12:54:27

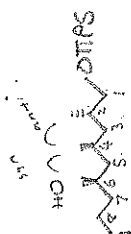
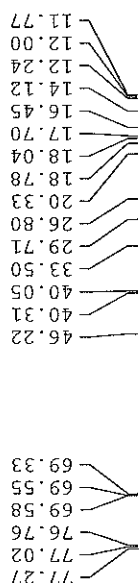


09/08/2007 12:57:20

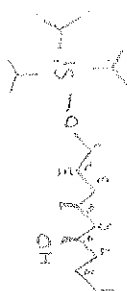
2007-08-09-EJT-21_010000FID



nb122 -B
mCARBON CDCl₃ /opt/topspin ejt 42



92



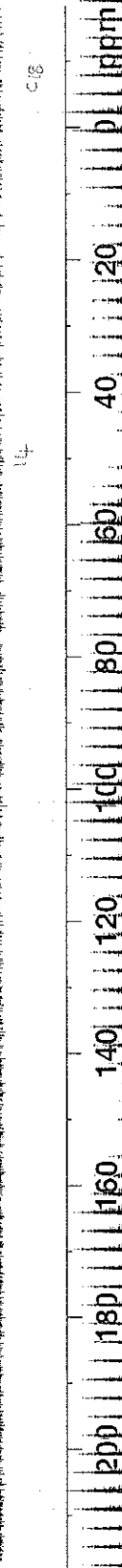
Current Data Parameters
NAME 2007-08-09-ejt-42
EXPNO 10
PROCNO 1

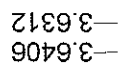
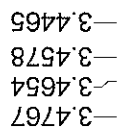
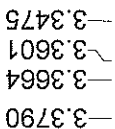
F2 - Acquisition Parameters
Date_ 20070809
Time 13.08
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 256
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 512
DW 16.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

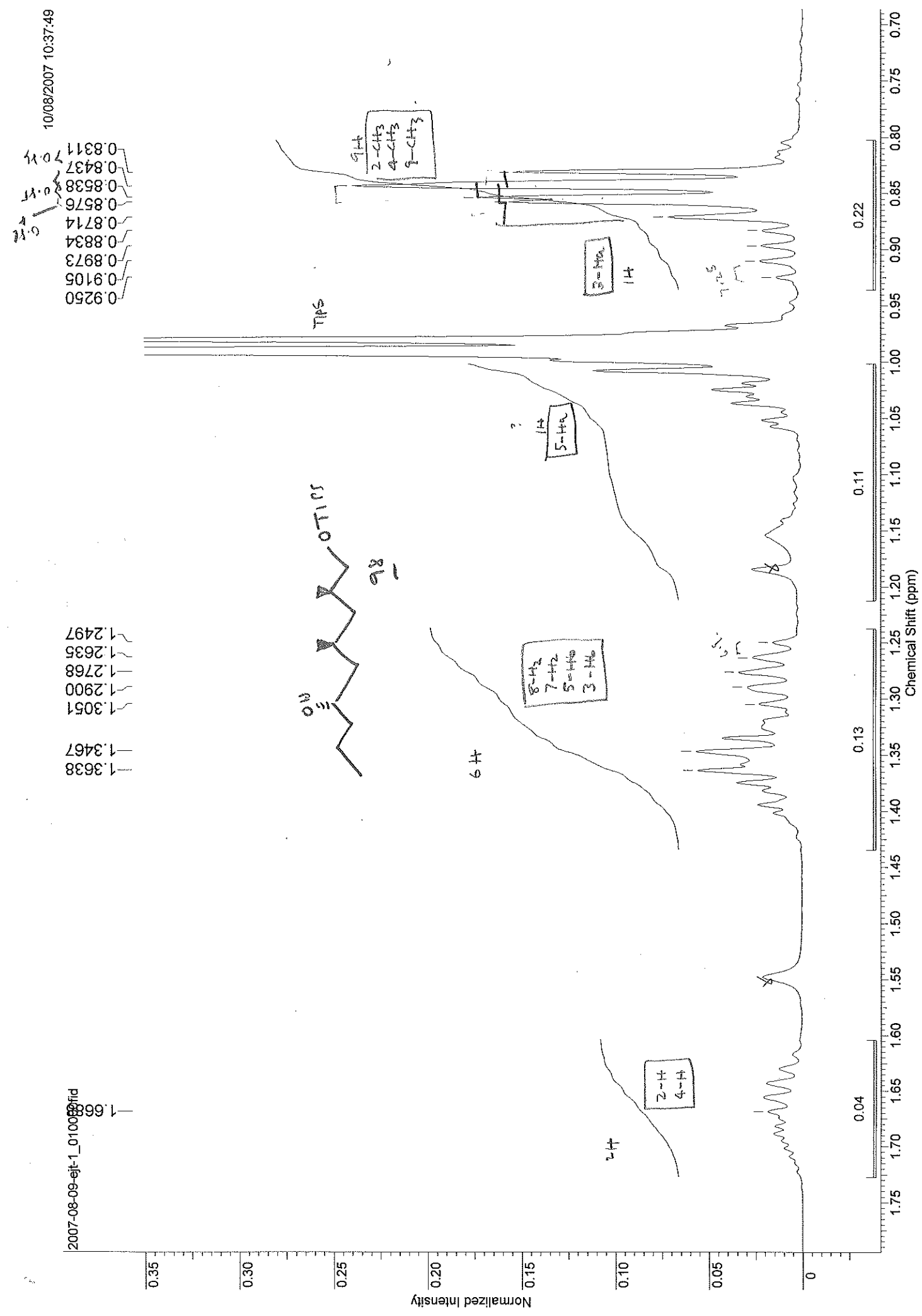
===== CHANNEL f1 =====
NUC1 13C
P1 11.50 usec
PL1 -4.20 dB
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 20.00 dB
PL3 23.00 dB
PL2 3.25 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40









| | 1970 | 1980 | 1990 | 2000 |
|---------------------|--------|--------|--------|--------|
| 1. Total population | 117.27 | 177.02 | 276.76 | 369.34 |
| 2. Male | 58.66 | 89.34 | 138.66 | 198.66 |
| 3. Female | 58.61 | 87.68 | 138.10 | 170.68 |
| 4. Urban population | 44.78 | 71.90 | 104.64 | 133.33 |
| 5. Male | 20.20 | 33.33 | 48.63 | 63.26 |
| 6. Female | 24.58 | 38.57 | 56.00 | 70.43 |
| 7. Rural population | 72.49 | 105.12 | 172.10 | 236.00 |
| 8. Male | 38.00 | 58.00 | 89.90 | 135.00 |
| 9. Female | 34.49 | 47.12 | 82.20 | 101.00 |

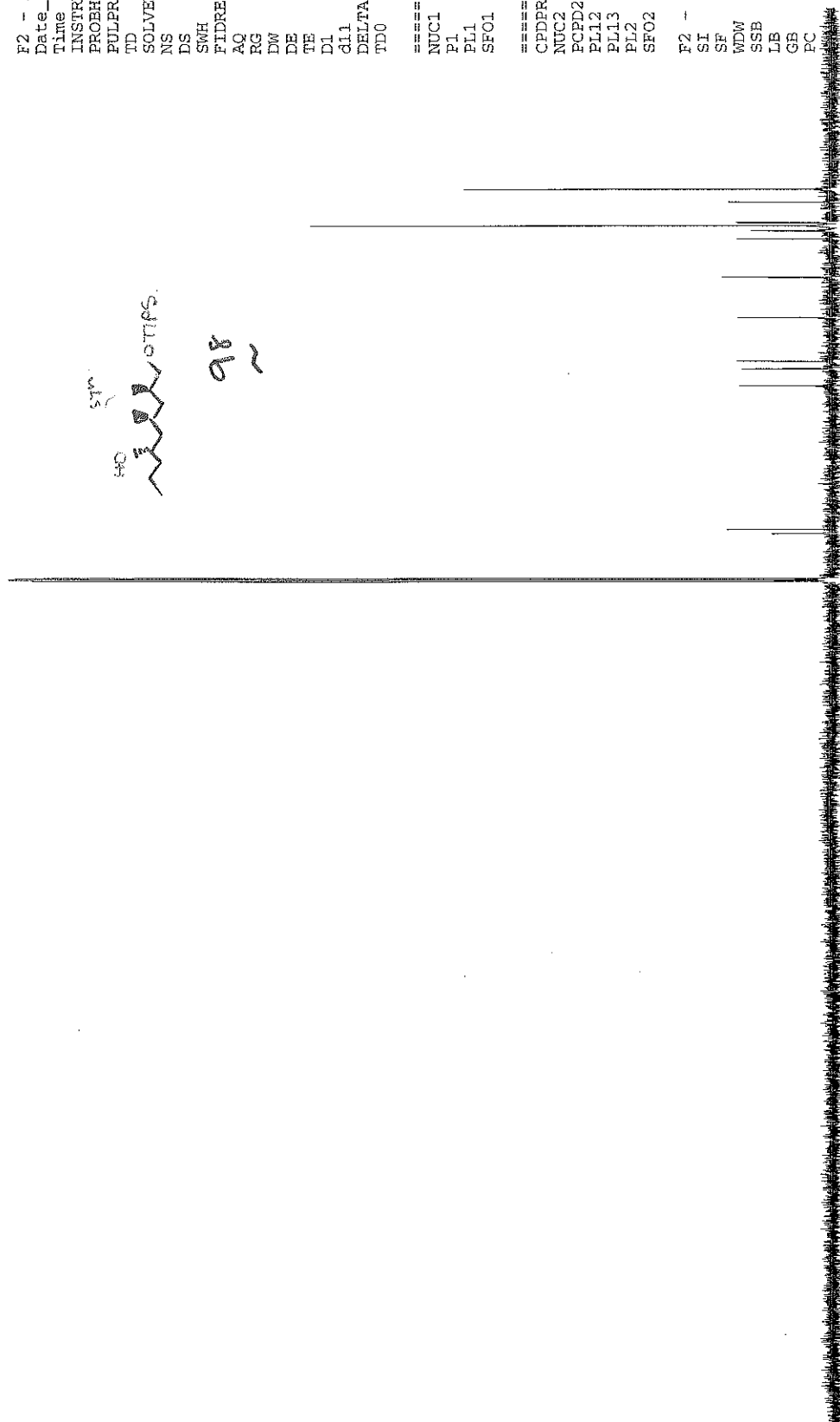
| | |
|-------------------------|-------------------|
| Current Data Parameters | 2007-08-10-ejt-46 |
| NAME | |
| EXPNO | 20 |
| PROCNO | 1 |

| F2 - Acquisition Parameters | |
|-----------------------------|----------------|
| Date_ | 20070812 |
| Time | 6.36 |
| INSTRUM | spect |
| PROBHD | 5 mm TXI 1H/D- |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 256 |
| DS | 2 |
| SWH | 29761.904 Hz |
| F2FREQS | 0.454131 Hz |
| AQ | 1.1010548 sec |
| RG | 512 |
| OR | 16.800 usec |
| DE | 6.00 usec |
| TE | 300.0 K |
| DT | 2.0000000 sec |
| al1 | 0.0300000 sec |
| DELTA | 1.89999998 sec |
| TD0 | 1 |

```
===== CHANNEL f1 =====
NUC1      13C
P1        11.50 usec
PL1       -4.20 dB
SF01      125.7703643 MHz
```

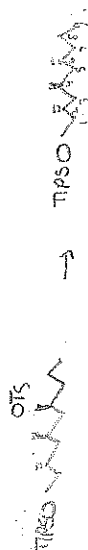
```
===== CHANNEL f2 =====
CPDRG2      waltz16
NUC2        1H
            80.00 usec
            20.00 dB
            23.00 dB
            3.25 dB
            500.132000 MHz
```

| | |
|----------------------------|-----------------|
| F2 - Processing parameters | |
| SI | 32768 |
| SSF | 125.7577890 MHz |
| WDW | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |



| α | $f(x)$ |
|----------|--------|
| 0 | 0 |
| 20 | 18 |
| 40 | 10 |
| 60 | 12 |
| 80 | 11 |
| 100 | 10 |
| 120 | 10 |
| 140 | 10 |
| 160 | 10 |
| 180 | 10 |
| 200 | 10 |

nb220
mPROTON CDCI3 {C:\bruk400data\2008\Feb} ejt 27



TIPS

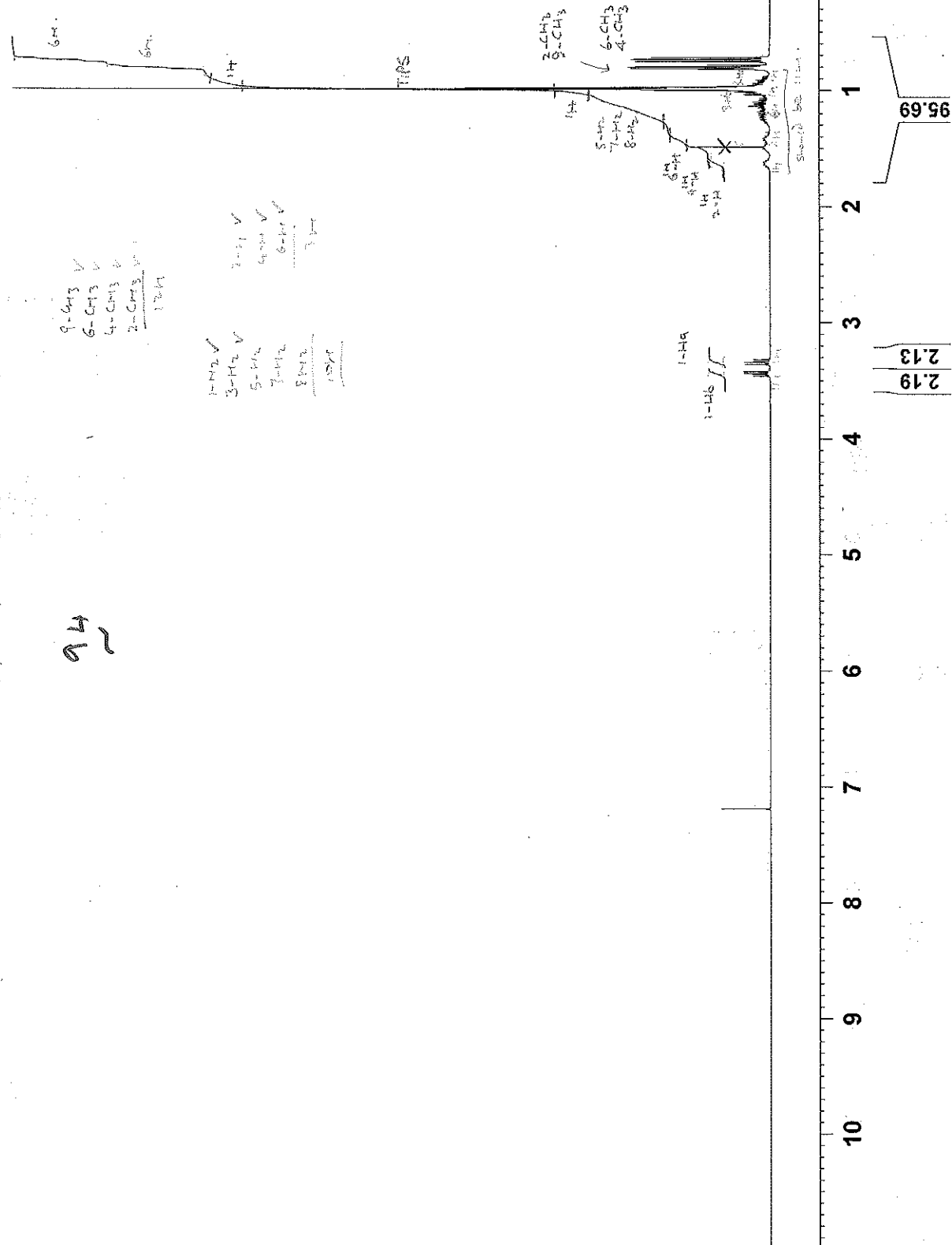
94

C21H46OS
FW = 342.33



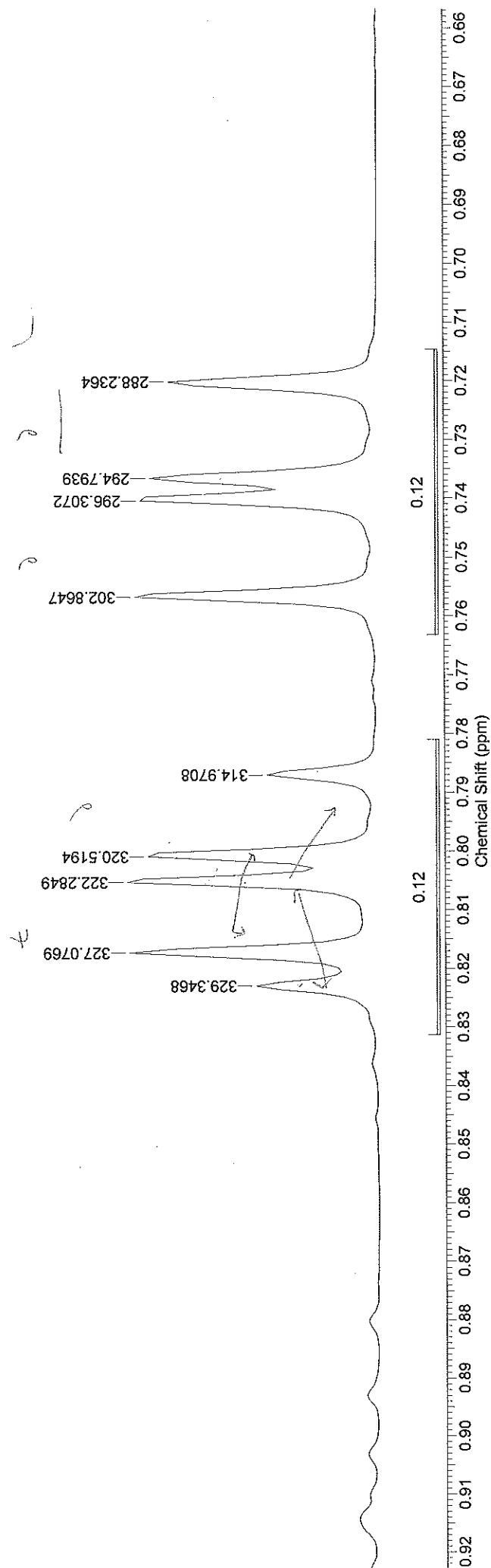
NAME 2008-02-29-ejt-27
EXPNO 10
PROCNO 1
Date_ 20080229
Time 14.17
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCI3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 101
DW 60.500 usec
DE 9.40 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300338 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



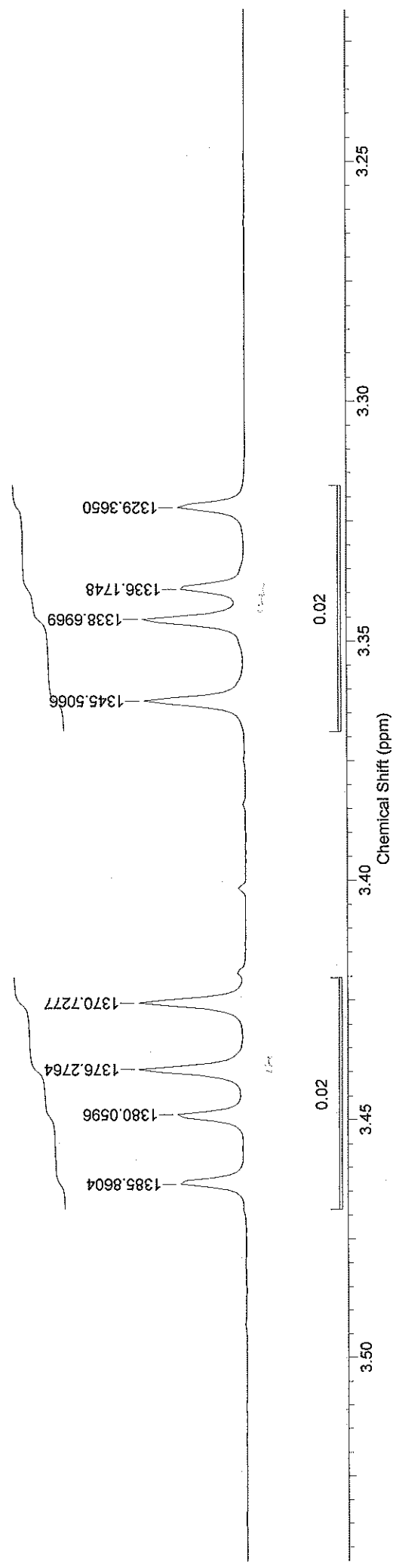
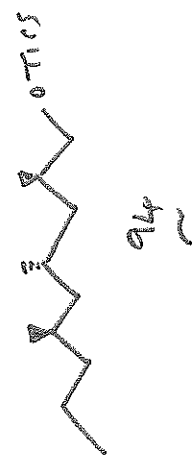
nb220 mPROTON CDCl3 {C:\bruk400data\2008\Feb\} ejt 27

2008-02-29-ejt-27_010000fid



2008-02-29-ejt-27_010000f1d

2008-02-29-ejt-27_010000f1d





nb220
mDEPT135night CDCl3 {C:\bruk400data\2008\Feb} ejt 27

45.67
41.58
40.17
33.48
29.70
27.25
20.08
19.54
19.35
18.06
16.81
14.41
14.39
12.01
11.71

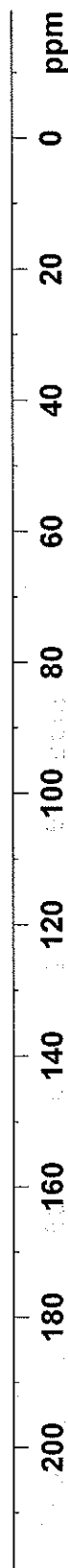
69.16



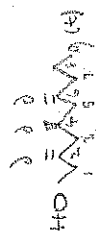
NAME 2008-02-29-ejt-27
EXPNO 12
PROCNO 1
Date_ 20080229
Time_ 17.16
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 16400
DW 20.800 usec
DE 6.50 usec
TE 294.8 K
CNS12 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
P2 16.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SF01 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.20 usec
P4 20.40 usec
PCPD2 80.00 usec
PL2 -3.60 dB
PL12 13.80 dB
PL2W 17.83863831 W
PL12W 0.32460985 W
SF02 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



nb221
mPROTONight CDCI3 {C:\bruk400data\2008\Feb} ejt 5

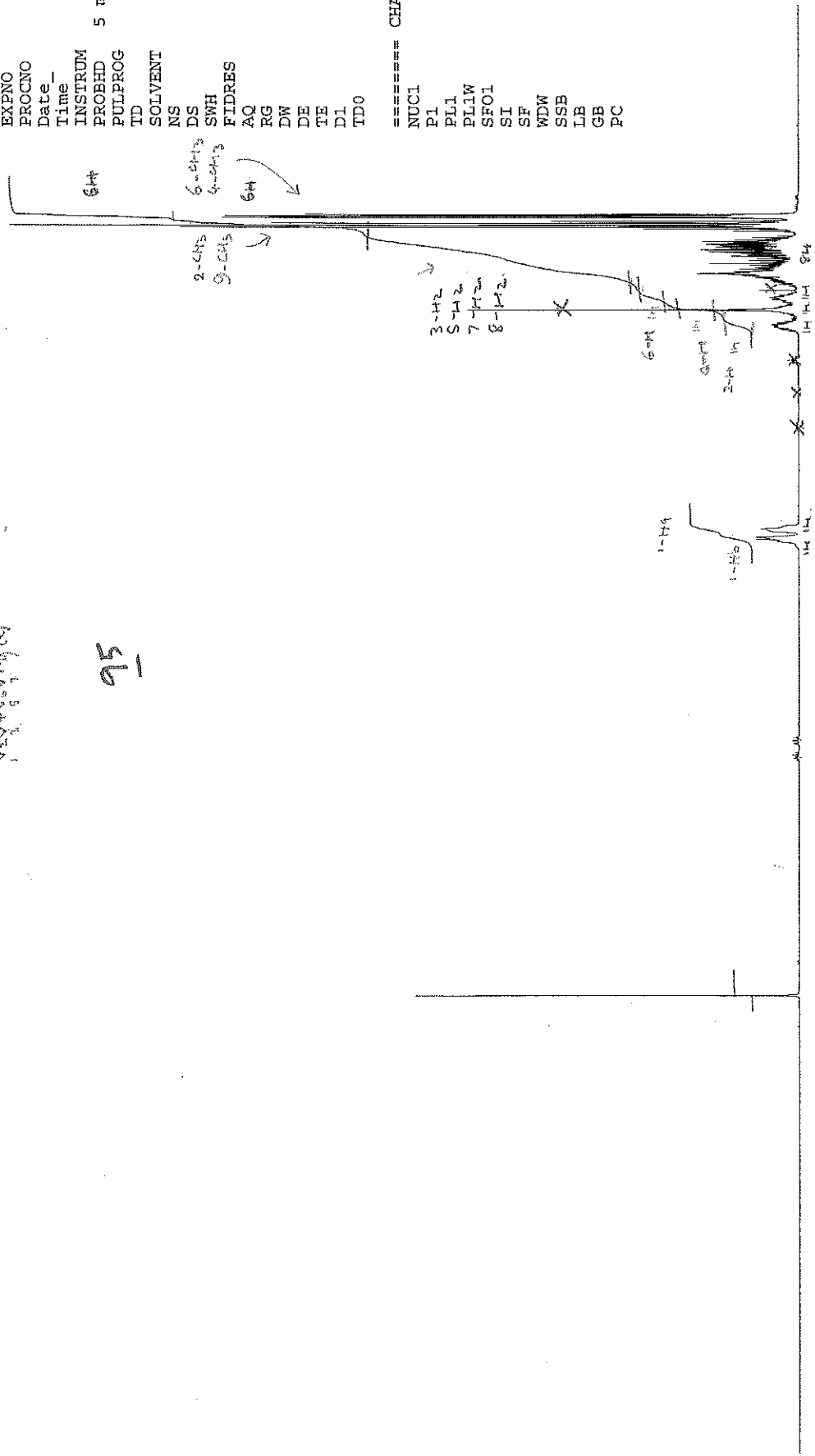


95

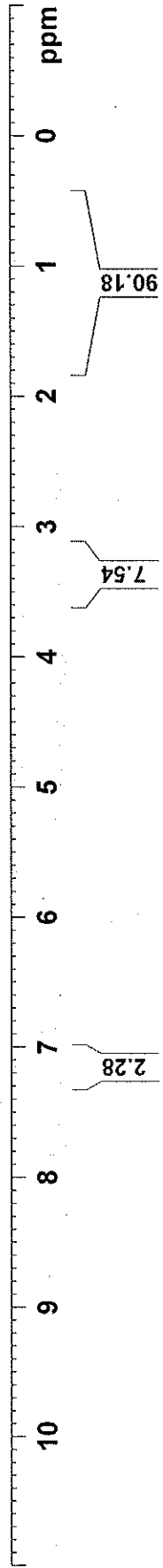


NAME 2008-03-02-ejt-5
EXPNO 10
PROCNO 1
Date_ 20080302
Time 19.52
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zg30b
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8264.463 Hz
FIDRES 0.126106 Hz
AQ 3.9649780 sec
RG 287
DW 60.500 usec
DE 9.40 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 -3.60 dB
PL1W 17.83863831 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300321 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

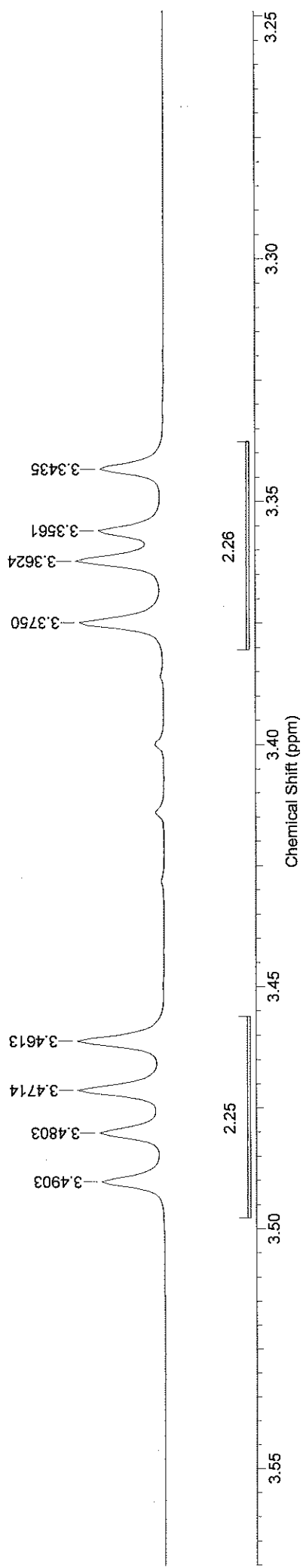


CDCl3



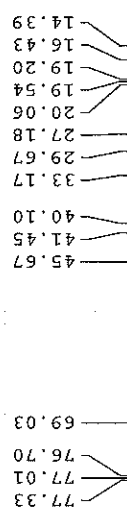
nb215 mPROTONnight CDCl3 /opt/bruk500data/2008/Feb ejt 11

2008-02-23-ejt-11_010000fid





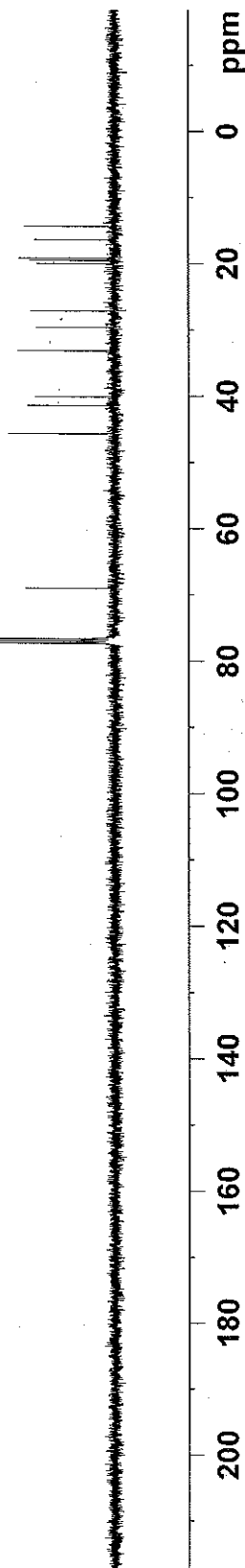
nb221
mCARBONnight CDCl3 {C:\bruk400data\2008\Feb} ejt 5



NAME 2008-03-02-ejt-5
EXPNO 12
PROCNO 1
Date_ 20080302
Time_ 20.15
INSTRUM AV400
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 23809.523 Hz
FIDRES 0.363304 Hz
AQ 1.3763061 sec
RG 512
DW 21.000 usec
DE 7.66 usec
TE 295.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.00 usec
PL1 0.00 dB
PL1W 34.91522217 W
SF01 100.6228294 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.60 dB
PL12 13.80 dB
PL13 14.00 dB
PL2W 17.83863831 W
PL12W 0.32460985 W
PL13W 0.31000000 W
SF02 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



C21H46OSi

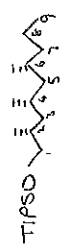
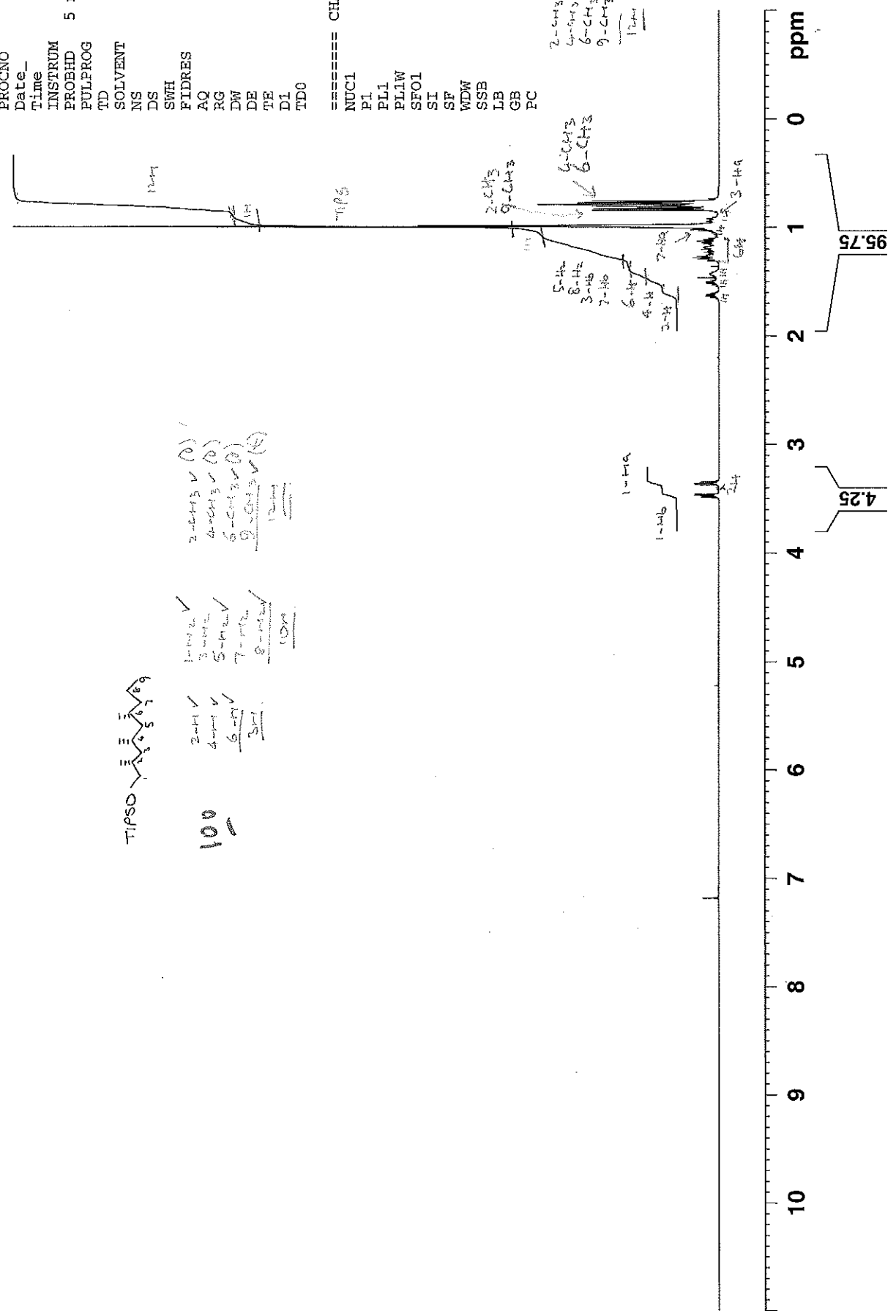
C21H46OSi
FW = 342.33

nb215
mPROTONight CDC13 /opt/bruk500data/2008/Feb ejt 36

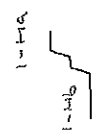


NAME 2008-02-22-ejt-36
EXPNO 10
PROCNO 1
Date_ 20080223
Time 6.09
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30b
TD 65536
SOLVENT CDC13
NS 16
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 18
DW 48.400 usec
DE 13.46 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.80 usec
PL1 3.25 dB
PL1W 12.12272263 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300460 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



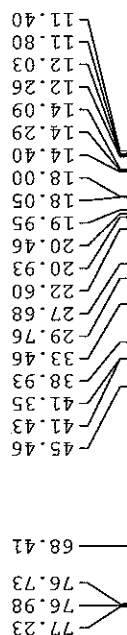
100
2-H ✓
3-H ✓
4-H ✓
5-H ✓
6-H ✓
7-H ✓
8-H ✓
9-H ✓
10-H ✓
11-H ✓
12-H ✓
13-H ✓
14-H ✓
15-H ✓
16-H ✓
17-H ✓
18-H ✓
19-H ✓
20-H ✓
21-H ✓



1-H
2-H
3-H
4-H
5-H
6-H
7-H
8-H
9-H
10-H
11-H
12-H
13-H
14-H
15-H
16-H
17-H
18-H
19-H
20-H
21-H

2-CH3
3-CH3
4-CH3
5-CH3
6-CH3
7-CH3
8-CH3
9-CH3
10-CH3
11-CH3
12-CH3
13-CH3
14-CH3
15-CH3
16-CH3
17-CH3
18-CH3
19-CH3
20-CH3
21-CH3

nb215
mCARBONnight CDC13 /opt/bruk500data/2008/Feb ejt 36



100

NAME 2008-02-23-ejt-36
EXPNO 11
PROCNO 1
Date_ 20080223
Time 6.23
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 512
DE 16.800 usec
TE 32.63 usec
D1 300.0 K
D11 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 -4.20 dB
PL1W 218.02882385 W
SF01 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.20 dB
PLI2 23.47 dB
PLI3 23.00 dB
PL2W 9.74092484 W
PLI2W 0.11523920 W
PLI3W 0.12841040 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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

nb218

mPROTON CDCl₃ {C:\bruk400data\2008\Feb} ejt 28



NAME 2008-02-29-ejt-28

EXPNO 10

PROCNO 1

Date_ 20080229

Time_ 14.21

INSTRUM AV400

PROBHD 5 mm PABBO BB-

PULPROG zg30b

TD 65536

SOLVENT CDCl₃

NS 16

DS 0

SWH 8264.463 Hz

FIDRES 0.126106 Hz

AQ 3.9649780 sec

RG 203

DW 60.500 usec

DE 9.40 usec

TE 294.0 K

D1 1.00000000 sec

TD0 1

===== CHANNEL f1 =====

NUC1 1H

P1 10.00 usec

PL1 -3.60 dB

PL1W 17.83863831 W

SFO1 400.1324710 MHz

SI 32768

SF 400.1300320 MHz

WDW EM

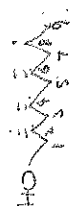
SSB 0

LB 0.30 Hz

GB 0

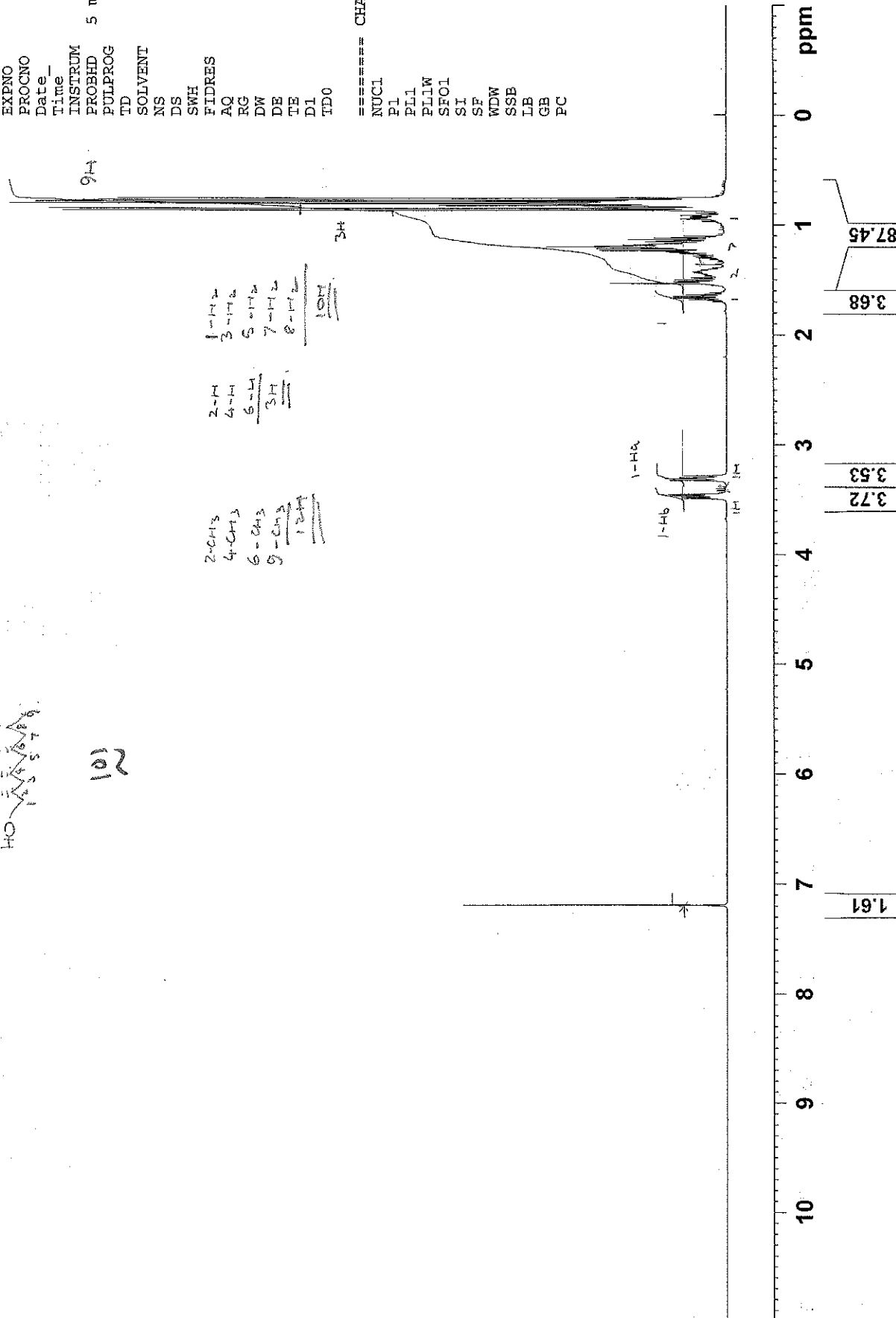
PC 1.00

C12 H26 O



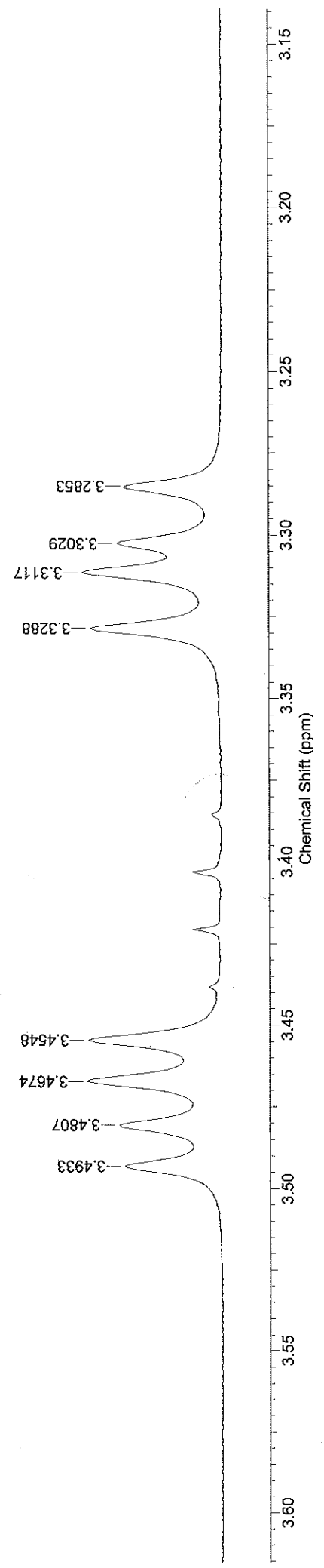
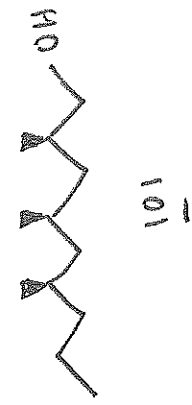
101

2-CH₃
4-CH₃
6-CH₃
9-CH₃
12-CH₃



nb218 mPROTON CDCl3 (C:\bruk400data\2008\Feb) ejt 28

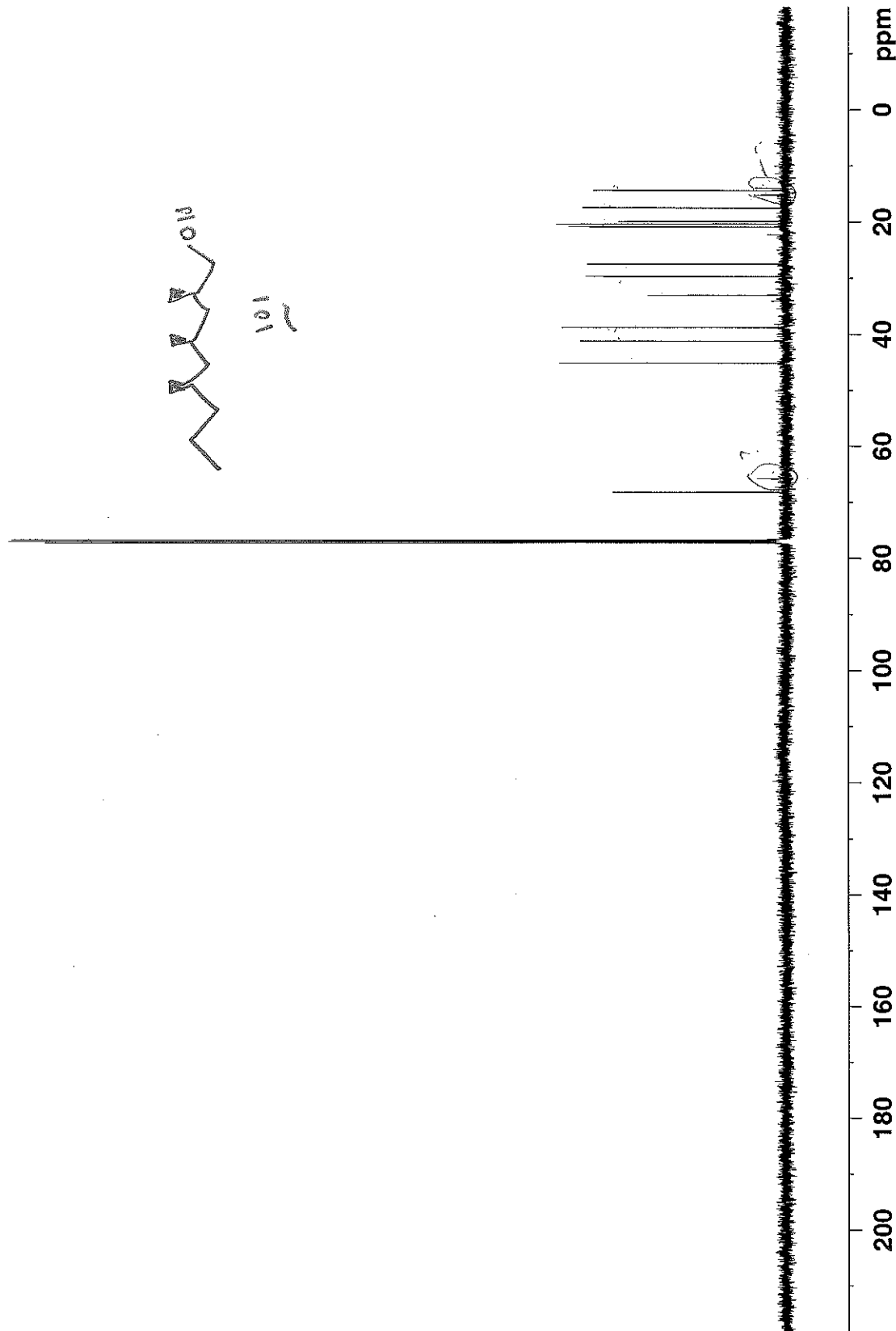
2008-02-29-ejt-28_010000fid



nb218
mCARBONnight CDCl3 /opt/bruk500data/2008/Feb ejt 32



77.25
77.00
76.74
68.28
65.84
45.17
41.27
38.83
33.10
29.74
27.54
22.32
20.91
20.42
19.94
17.53
15.25
14.41
14.03



```

NAME      2008-02-26-ejt-32
EXPNO     11
PROCNO    1
Date_     20080227
Time      9.30
INSTRUM   spect
PROBHD    5 mm TXI 1H/D-
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         256
DS         2
SWH        29761.904 Hz
FIDRES     0.454131 Hz
AQ         1.1010548 sec
RG         512
DE         16.800 usec
TE         32.63 usec
D1         300.0 K
D11        2.00000000 sec
D12        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -4.20 dB
PL1W       218.02882385 W
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waitz16
NUC2       1H
PCPD2      80.00 usec
PL2        4.20 dB
PL12       23.47 dB
PL13       23.00 dB
PL2W       9.74092484 W
PL12W      0.11523920 W
PL13W      0.12841040 W
SFO2       500.1320005 MHz
SI         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```