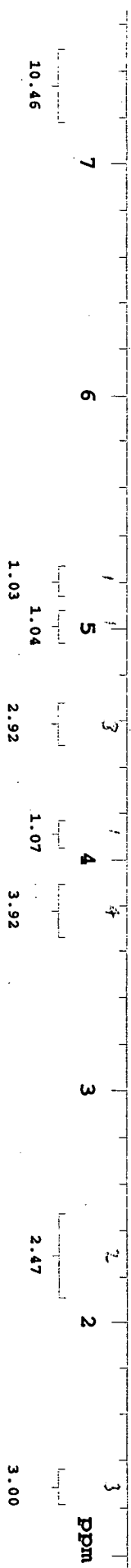
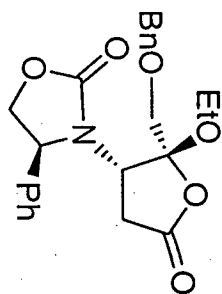
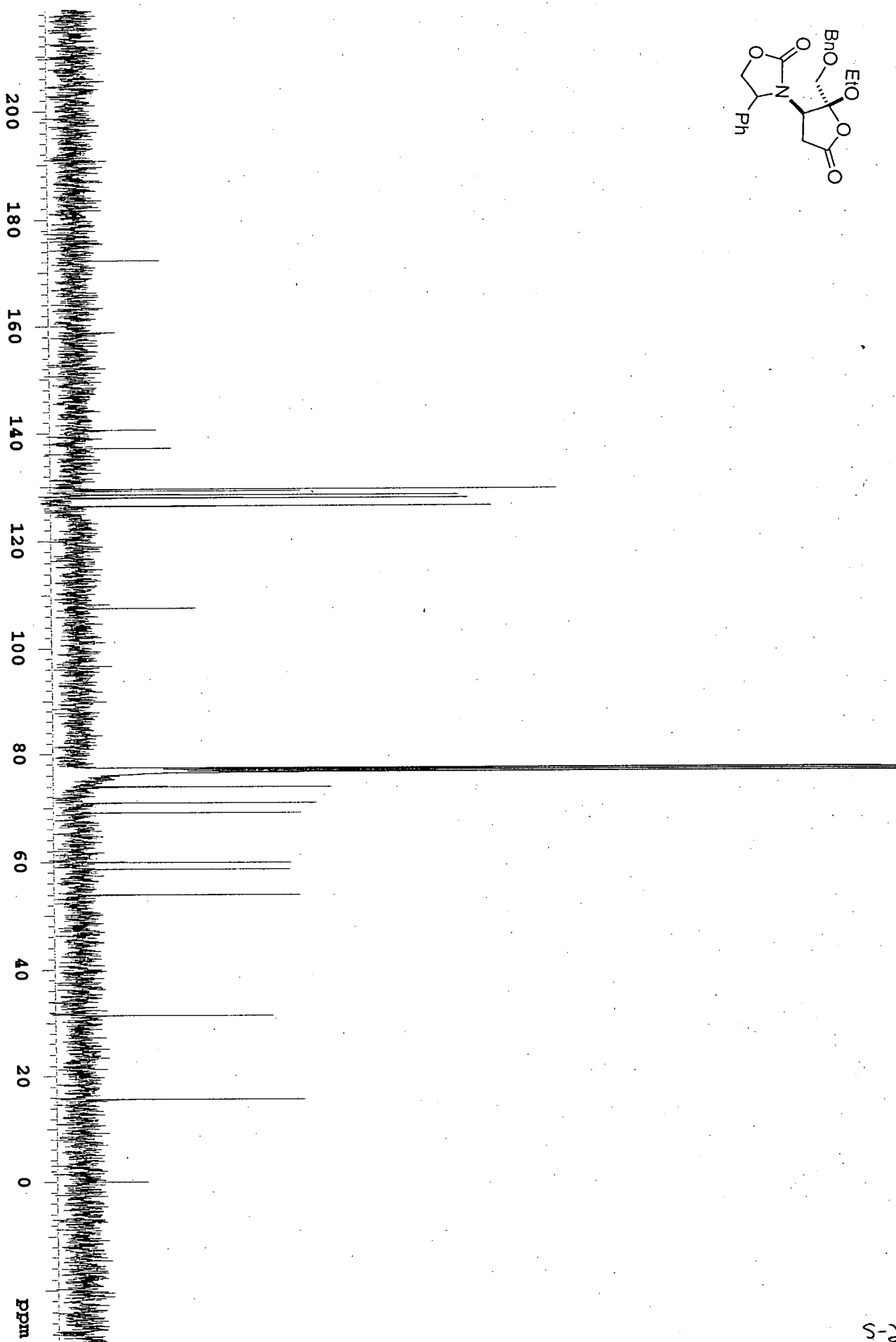
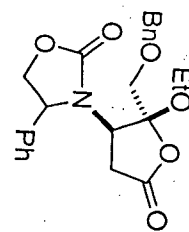
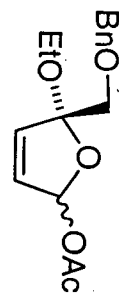


SSSI362P22+23

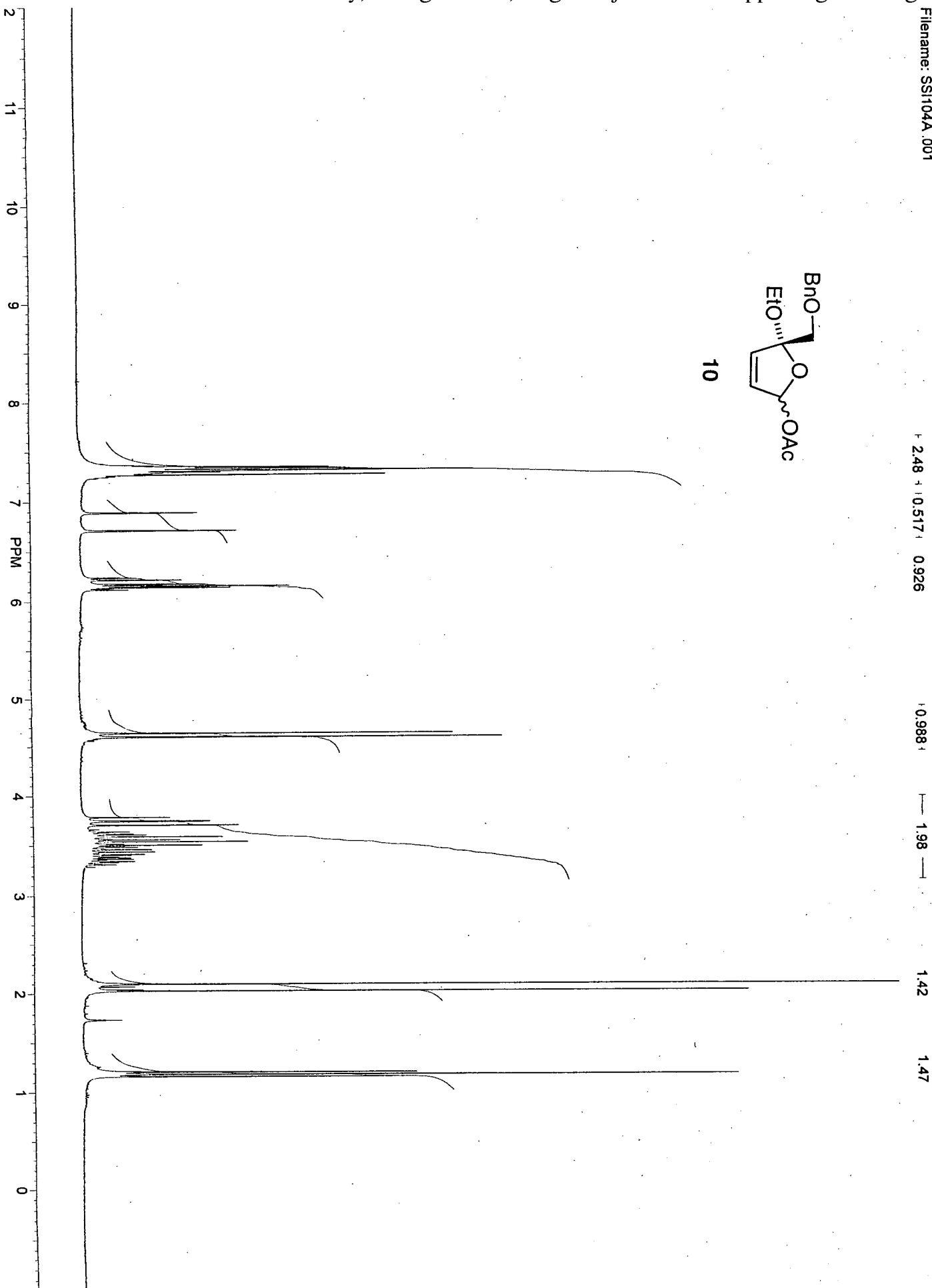


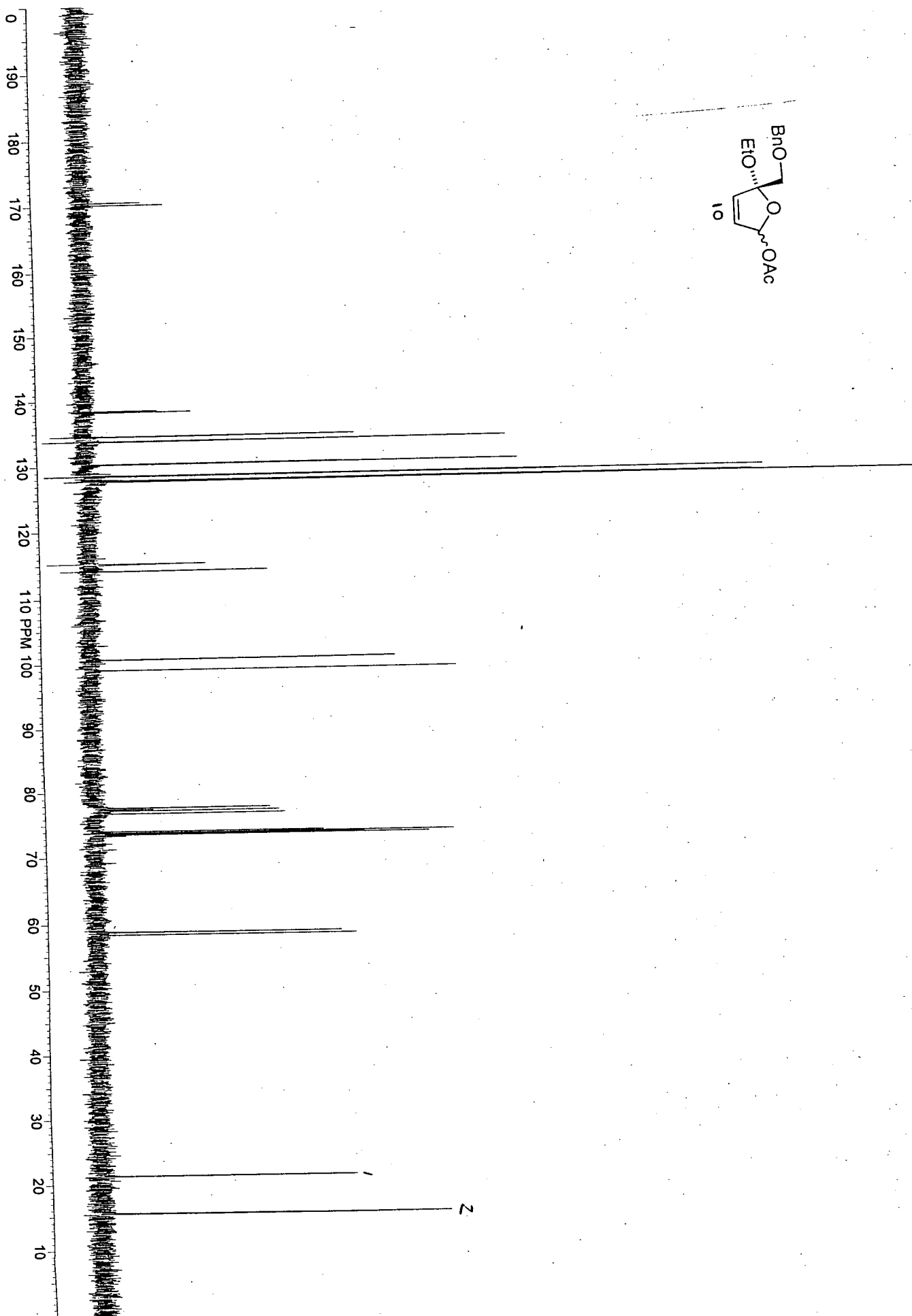


Filename: SS104A.001



10





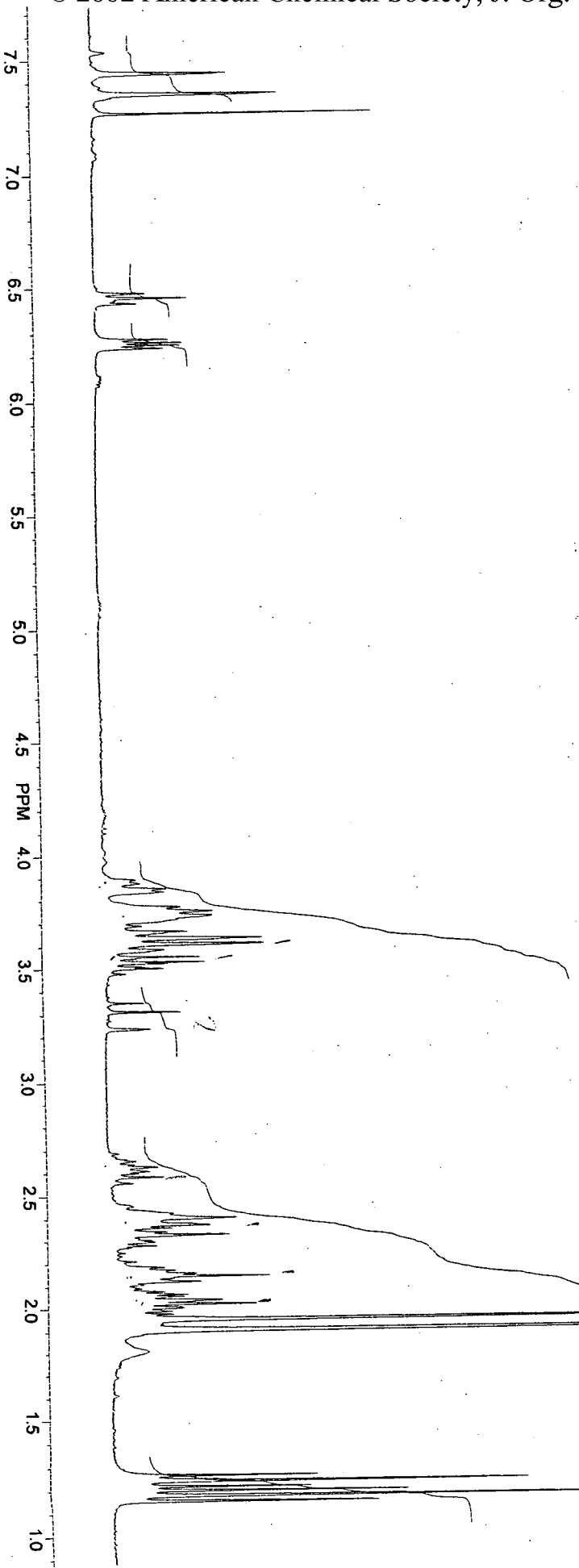
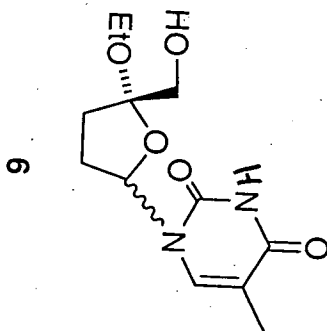
31230CR
 1.95
 EQFIL S2PUL
 300.157 MHz
 19.986 ppm
 2.66667 sec
 0 sec
 6.66666 usec
 16
 60EMP
 N

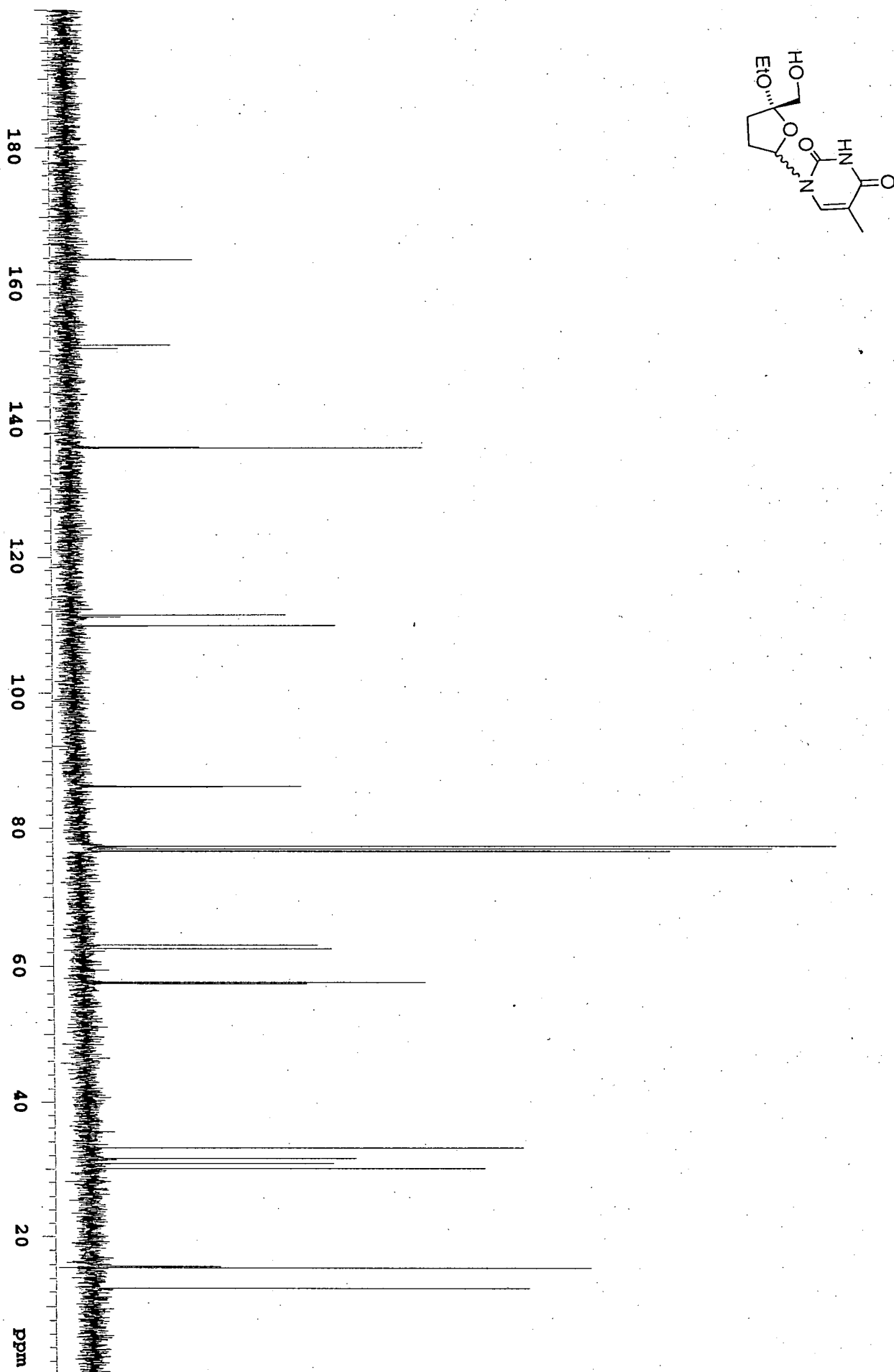
0.708 1.03

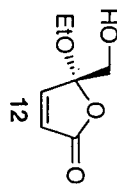
8 0.637

18.4

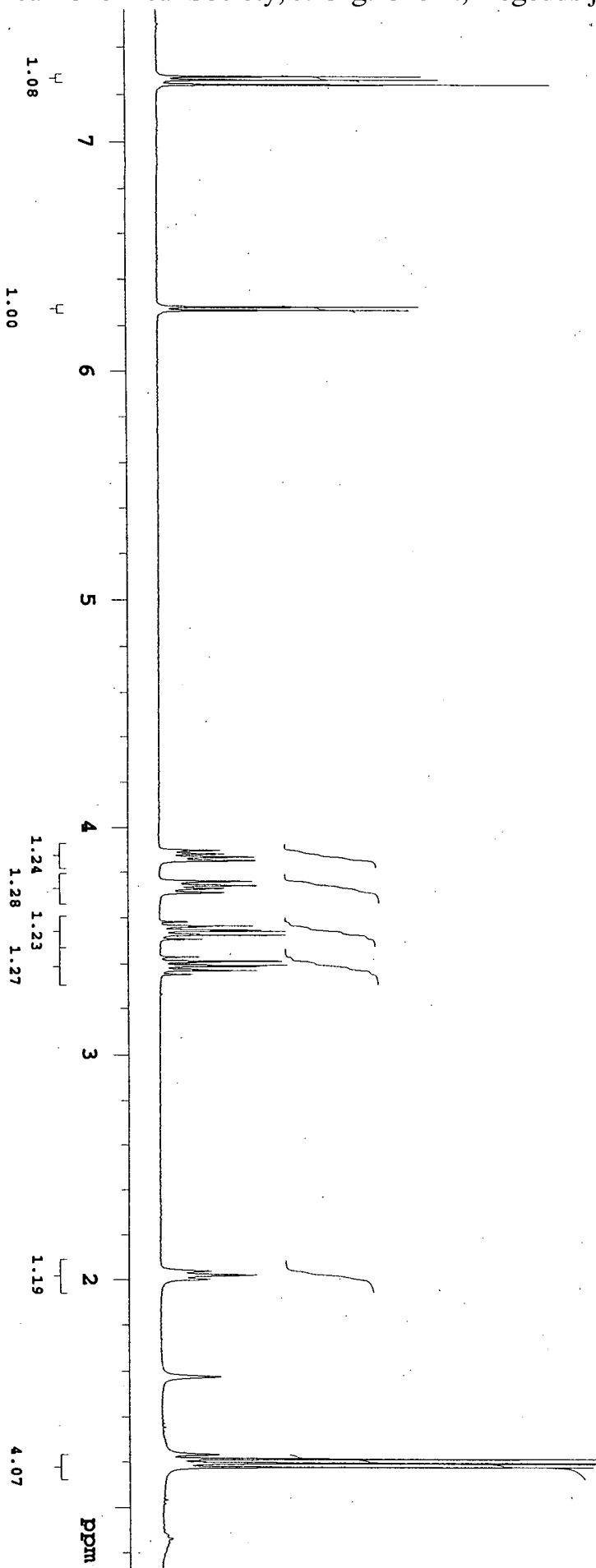
6

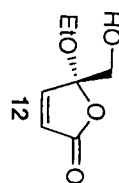
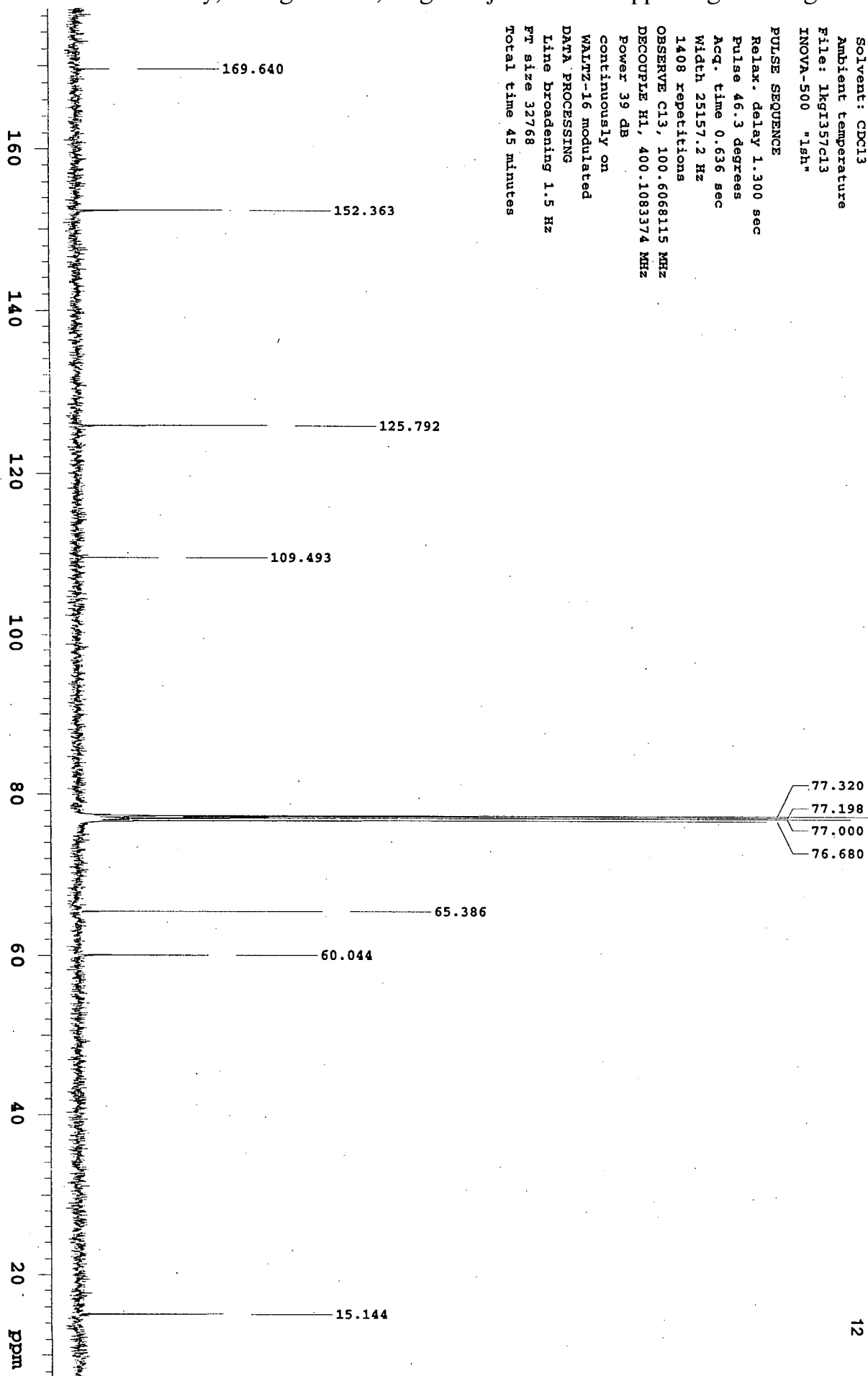






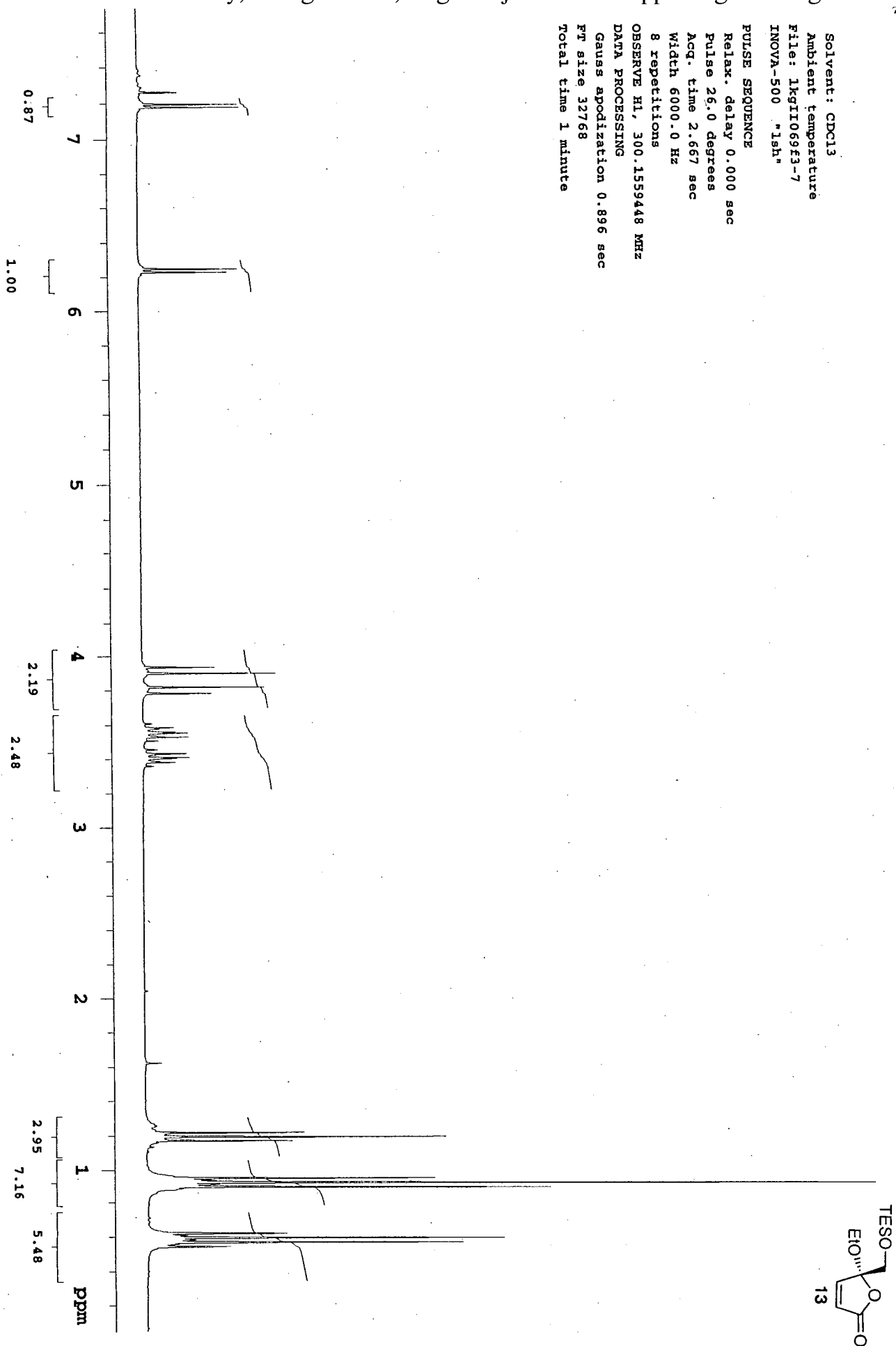
Solvent: CDCl₃
 Ambient temperature
 File: PROTON
 INOVA-500 "1sh"
 PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.559 sec
 Width 4801.3 Hz
 16 repetitions
 OBSERVE H1, 400.1063232 MHz
 DATA PROCESSING
 Sq. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 1 minute





Solvent: CDCl₃
 Ambient temperature
 File: 1kg11069f3-7
 INOVA-500 "1sh"

PULSE SEQUENCE
 Relax. delay 0.000 sec
 Pulse 26.0 degrees
 Acq. time 2.667 sec
 Width 6000.0 Hz
 8 repetitions
 OBSERVE H1, 300.1559448 MHz
 DATA PROCESSING
 Gauss apodization 0.896 sec
 FT size 32768
 Total time 1 minute



13C OBSERVE

Solvent: CDCl3
 Ambient temperature
 File: lkg1069c13-2
 INOVA-500 "1sh"

PULSE SEQUENCE

Relax. delay 1.000 sec
 Pulse 46.3 degrees
 Acq. time 0.696 sec
 Width 23000.0 Hz
 240 repetitions

OBSERVE C13, 75.4742813 MHz
 DECOUPLE H1, 300.1574402 MHz

Power 40 dB

continuously on

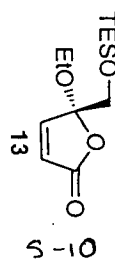
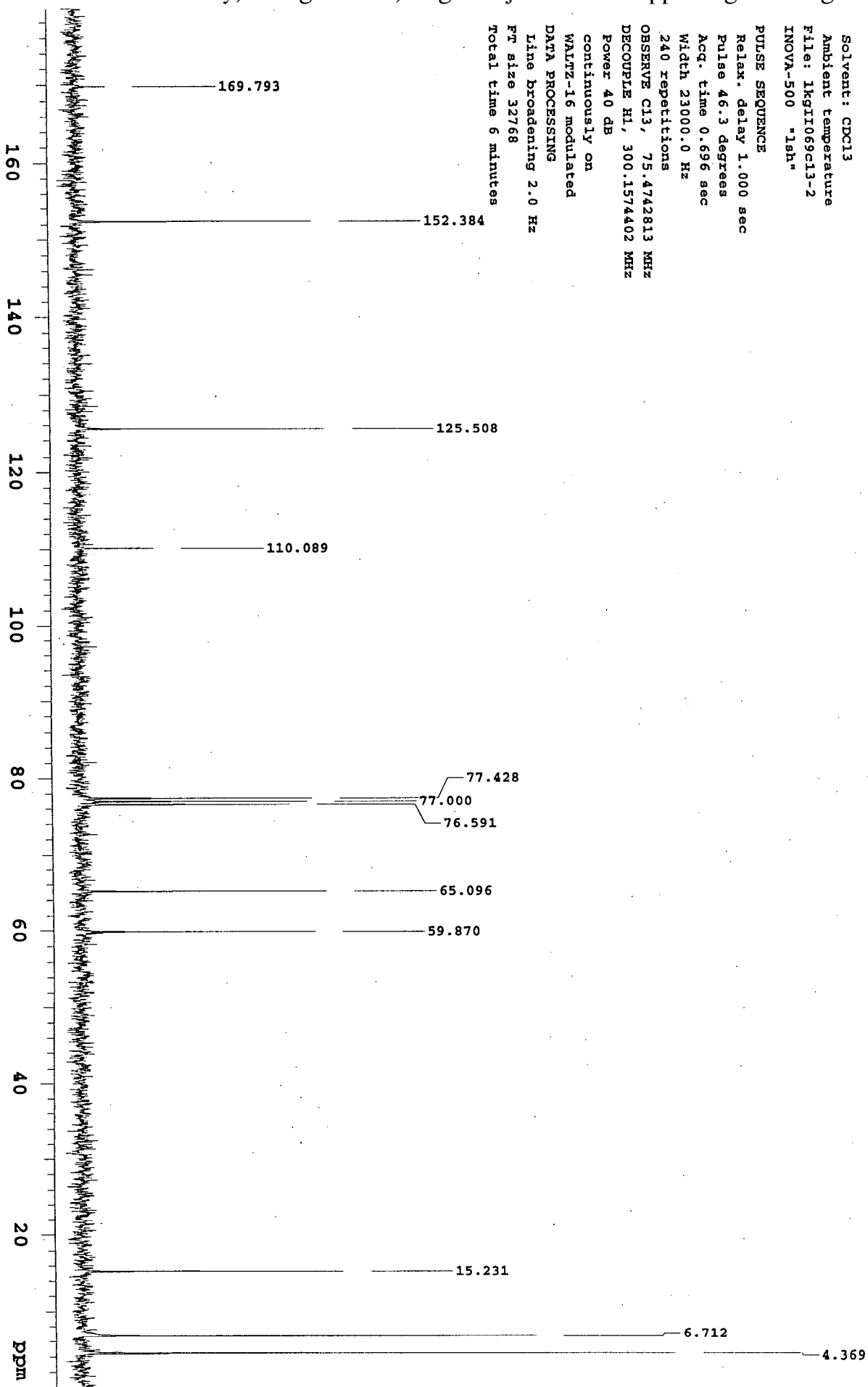
WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

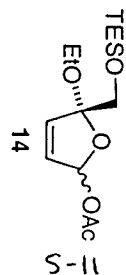
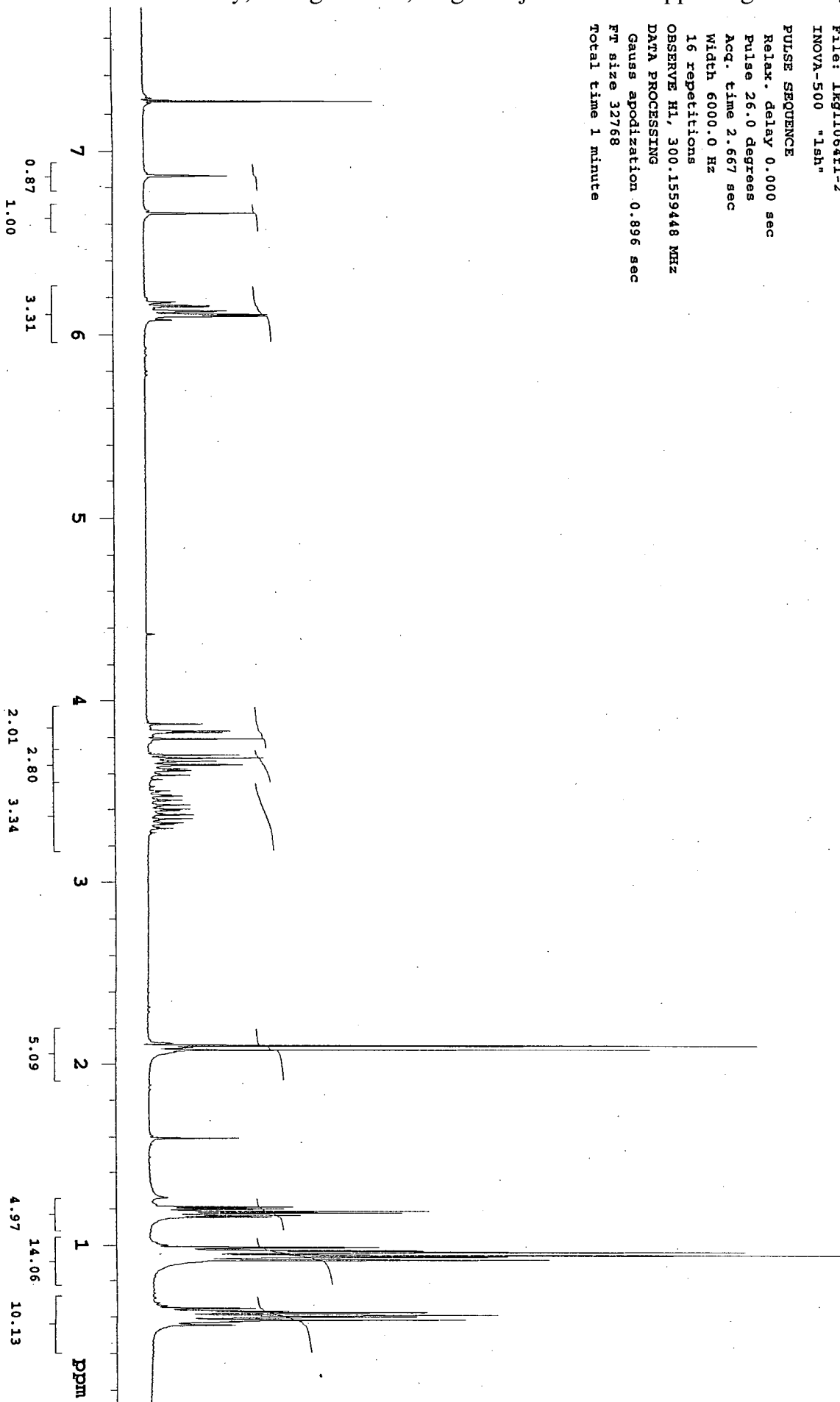
FT size 32768

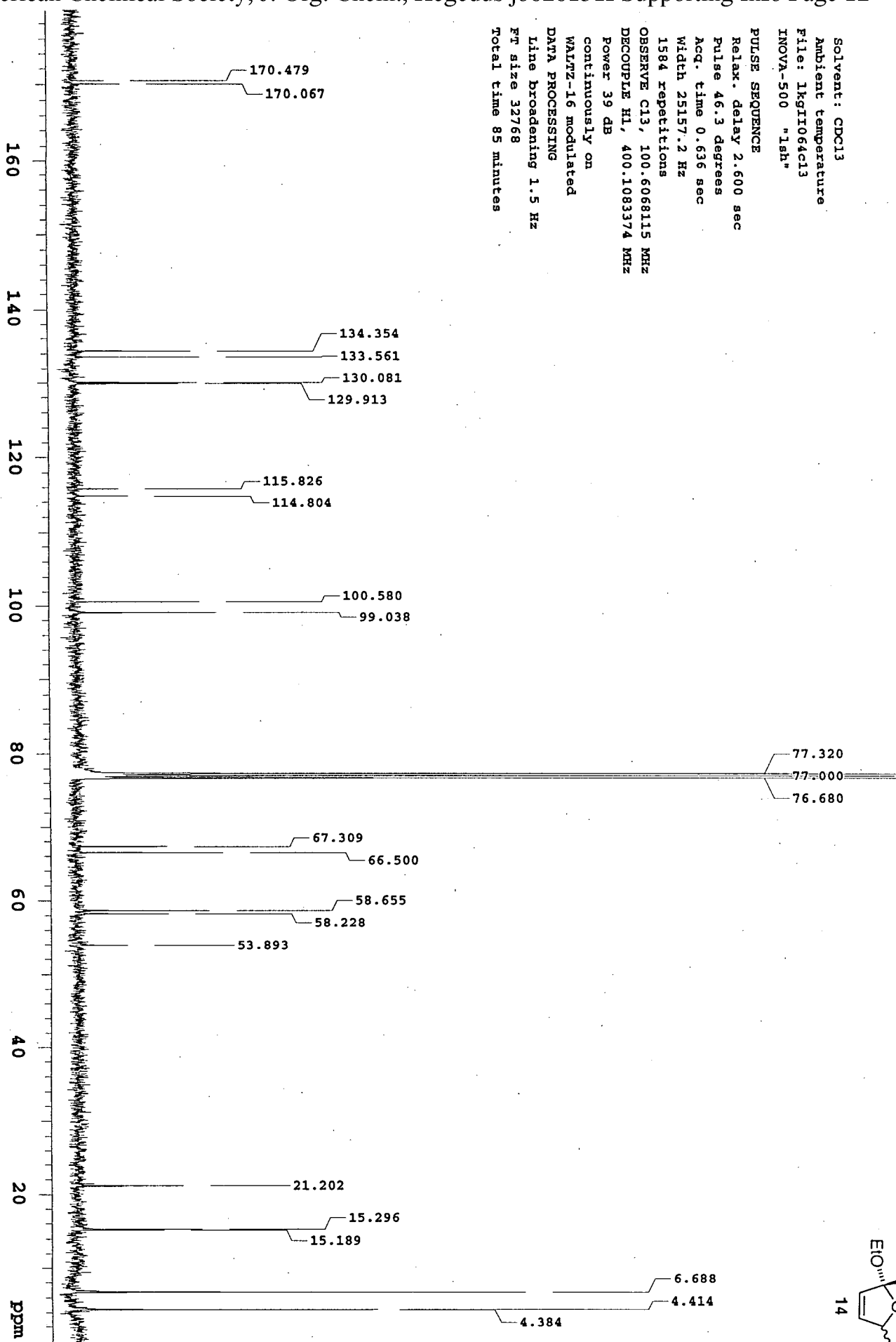
Total time 6 minutes



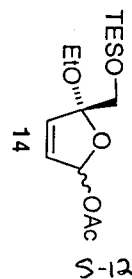
Solvent: CDCl₃
 Ambient temperature
 File: lkg1064f1-2
 INOVA-500 "1sh"

PULSE SEQUENCE
 Relax. delay 0.000 sec
 Pulse 26.0 degrees
 Acq. time 2.667 sec
 Width 6000.0 Hz
 16 repetitions
 OBSERVE H1, 300.1559448 MHz
 DATA PROCESSING
 Gauss apodization 0.896 sec
 FT size 32768
 Total time 1 minute



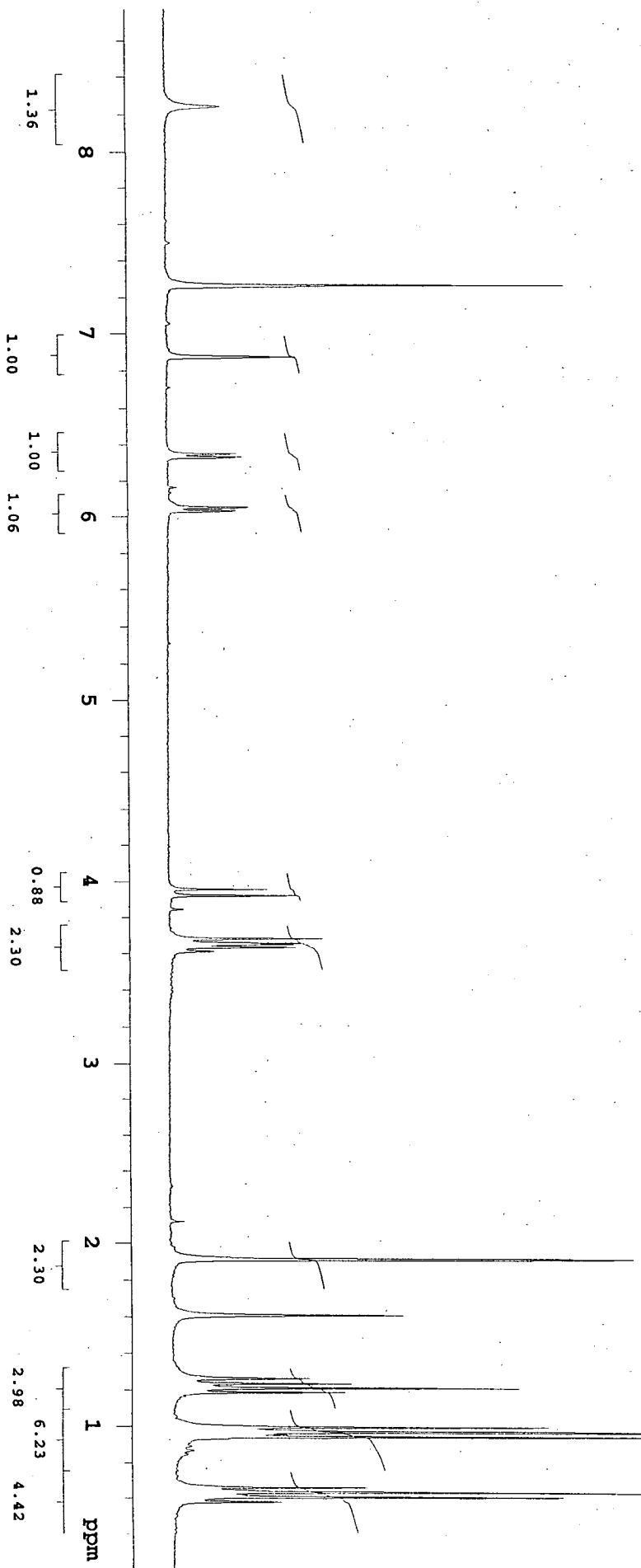
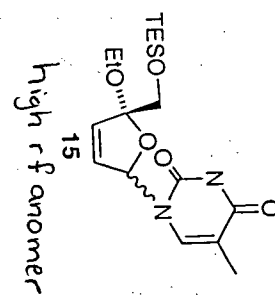


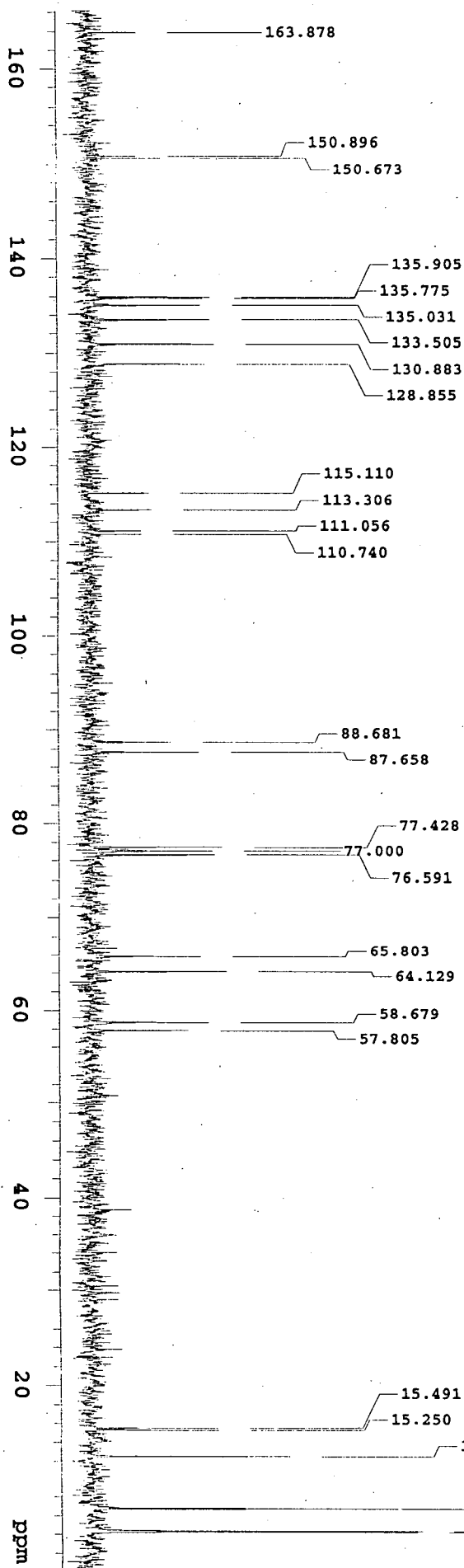
Solvent: CDCl₃
 Ambient temperature
 File: 1kgit064c13
 INOVA-500 "1sh"
 PULSE SEQUENCE
 Relax. delay 2.600 sec
 Pulse 46.3 degrees
 Acq. time 0.636 sec
 Width 25157.2 Hz
 1584 repetitions
 OBSERVE C13, 100.606815 MHz
 DECOUPLE H1, 400.1083374 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 32768
 Total time 85 minutes



Solvent: CDCl₃
 Ambient temperature
 File: 1kg1100f70-5
 INOVA-500 "1sh"

PULSE SEQUENCE
 Relax. delay 0.000 sec
 Pulse 26.0 degrees
 Acq. time 2.667 sec
 Width 6000.0 Hz
 16 repetitions
 OBSERVE H1, 300.1559448 MHz
 DATA PROCESSING
 Gauss apodization 0.896 sec
 FT size 32768
 Total time 1 minute



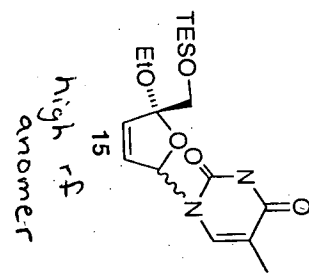


13C OBSERVE

Solvent: CDCl₃
 Ambient temperature
 File: 1kg1094c13-2
 INOVA-500 "1sh"

PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 46.3 degrees
 Acq. time 0.696 sec
 Width 23000.0 Hz
 32 repetitions

OBSERVE C13, 75.4742813 MHz
 DECOUPLE H1, 300.1574402 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 32768
 Total time 1 minute



1kg1105f34-64

Solvent: CDCl₃

Ambient temperature

File: 1kg1105f34-64

Mercury-300 "xllan"

PULSE SEQUENCE

Relax. delay 0.000 sec

Pulse 26.0 degrees

Acq. time 2.667 sec

Width 6000.0 Hz

4 repetitions

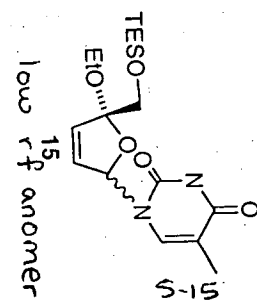
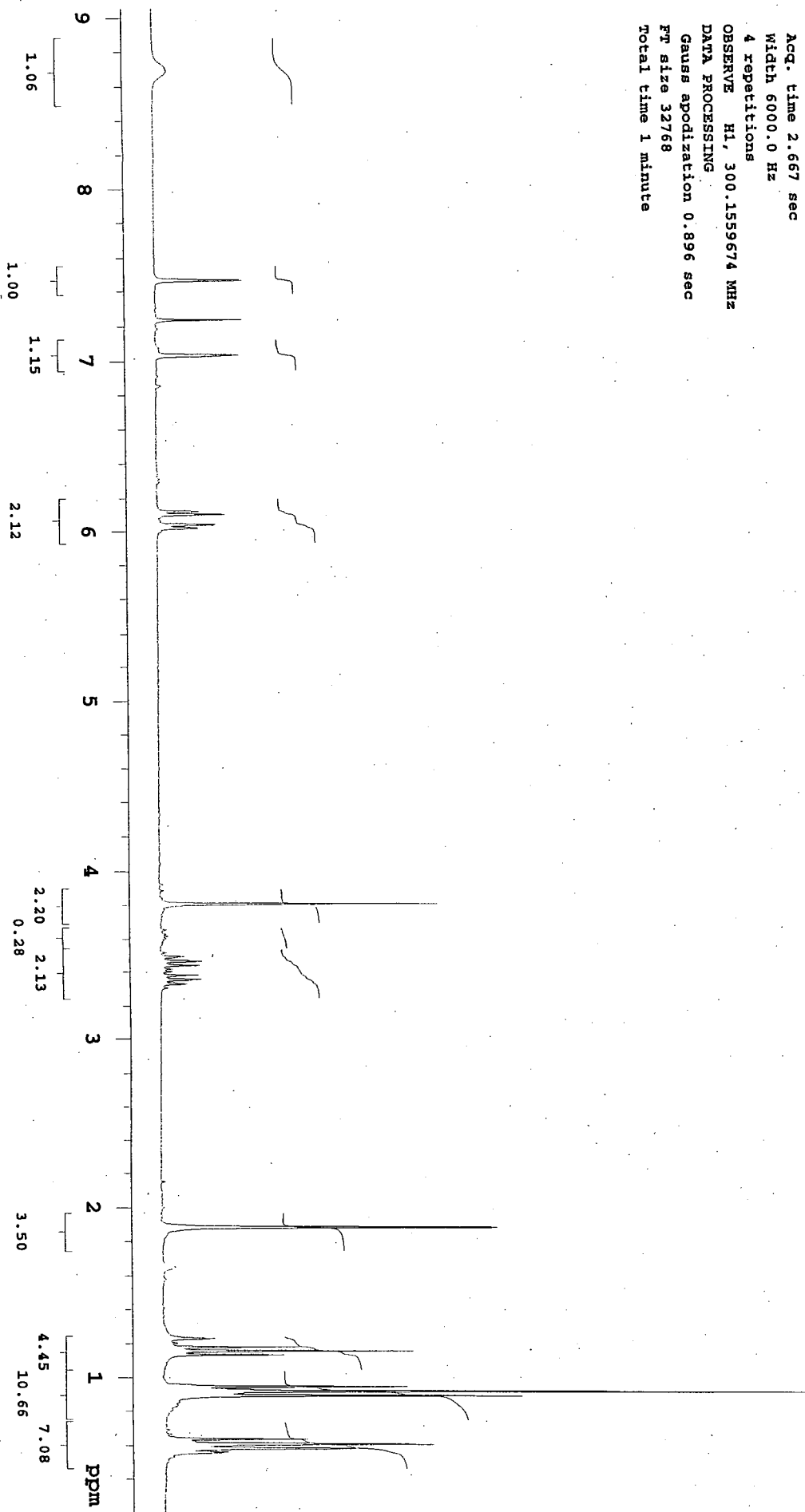
OBSERVE H1, 300.1559674 MHz

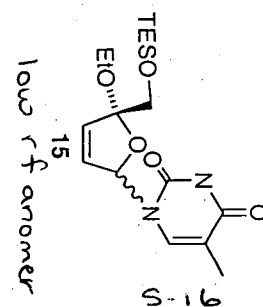
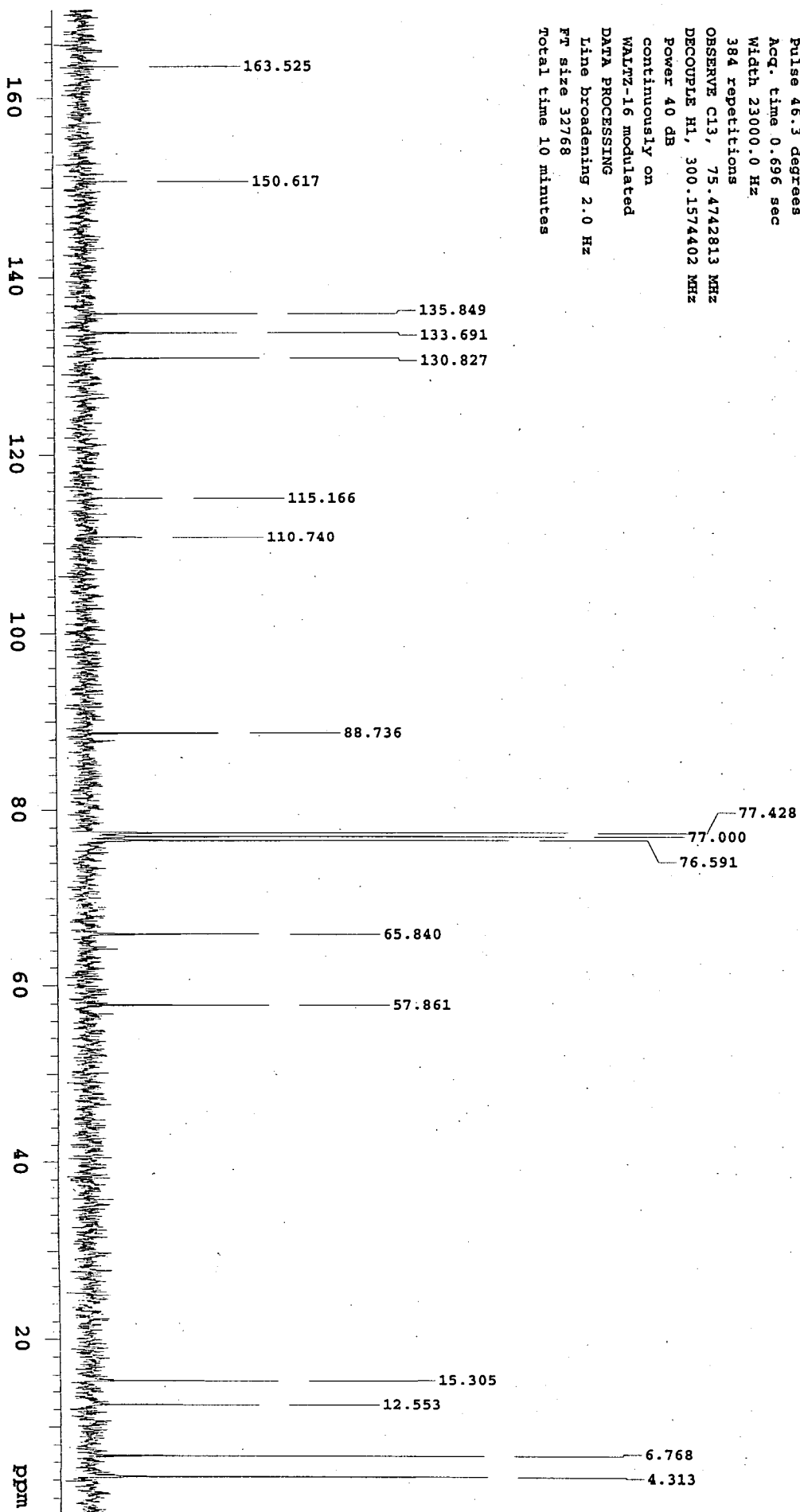
DATA PROCESSING

Gauss apodization 0.896 sec

FT size 32768

Total time 1 minute





1kg1095 prep TLC low band

Solvent: CDCl₃

Ambient temperature

File: 1kg1096h

INOVA-500 "1sh"

PULSE SEQUENCE

Relax. delay 0.000 sec

Pulse 26.0 degrees

Acq. time 2.667 sec

Width 6000.0 Hz

16 repetitions

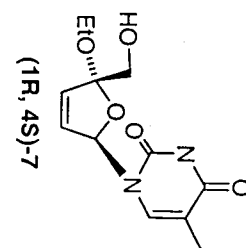
OBSERVE H1, 300.1559448 MHz

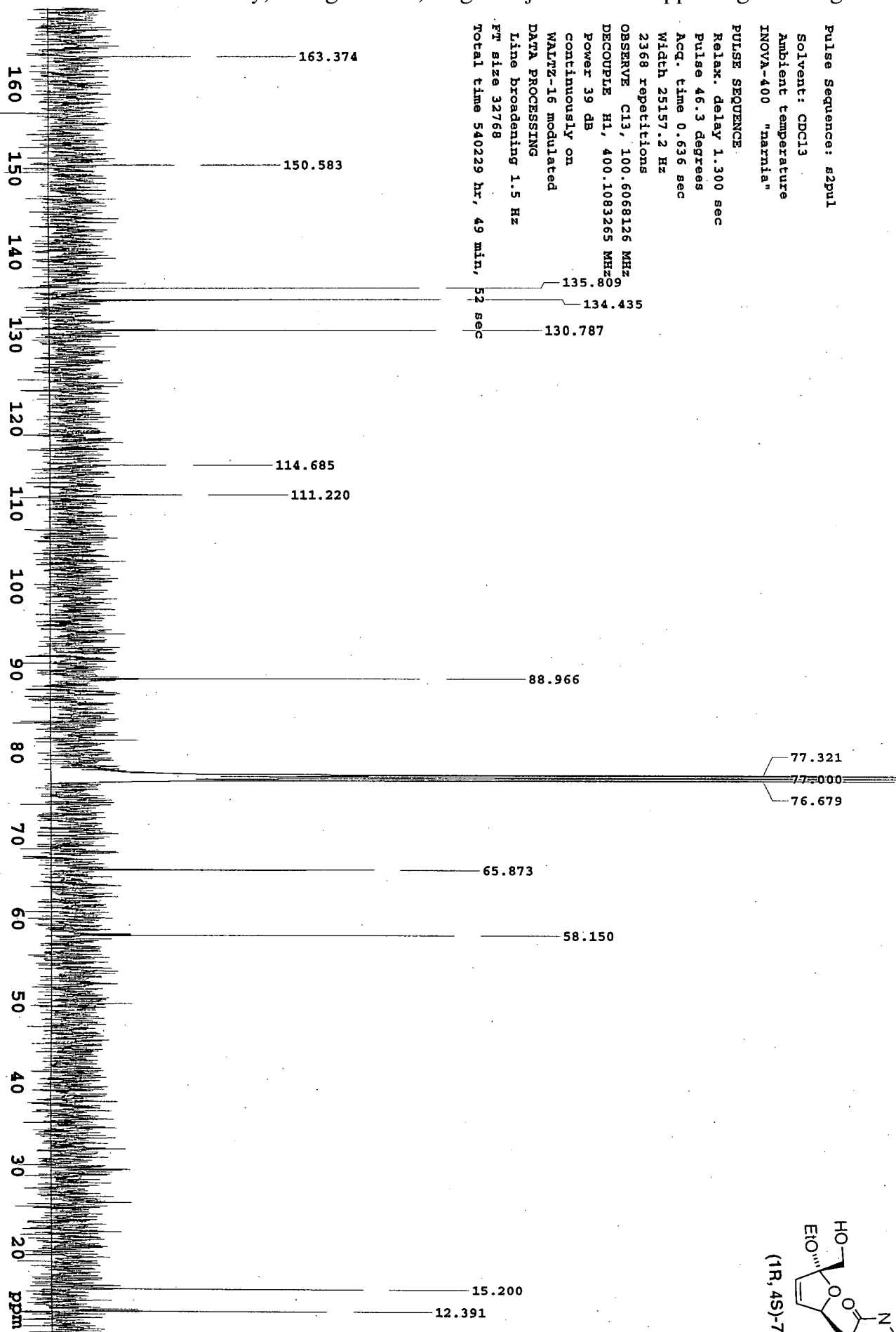
DATA PROCESSING

Gauss apodization 0.896 sec

FT size 32768

Total time 1 minute

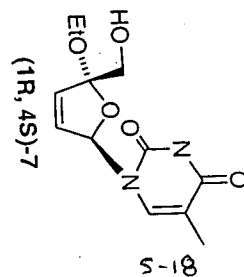




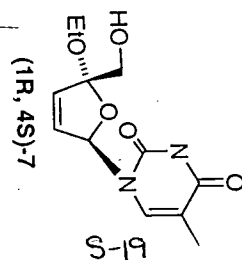
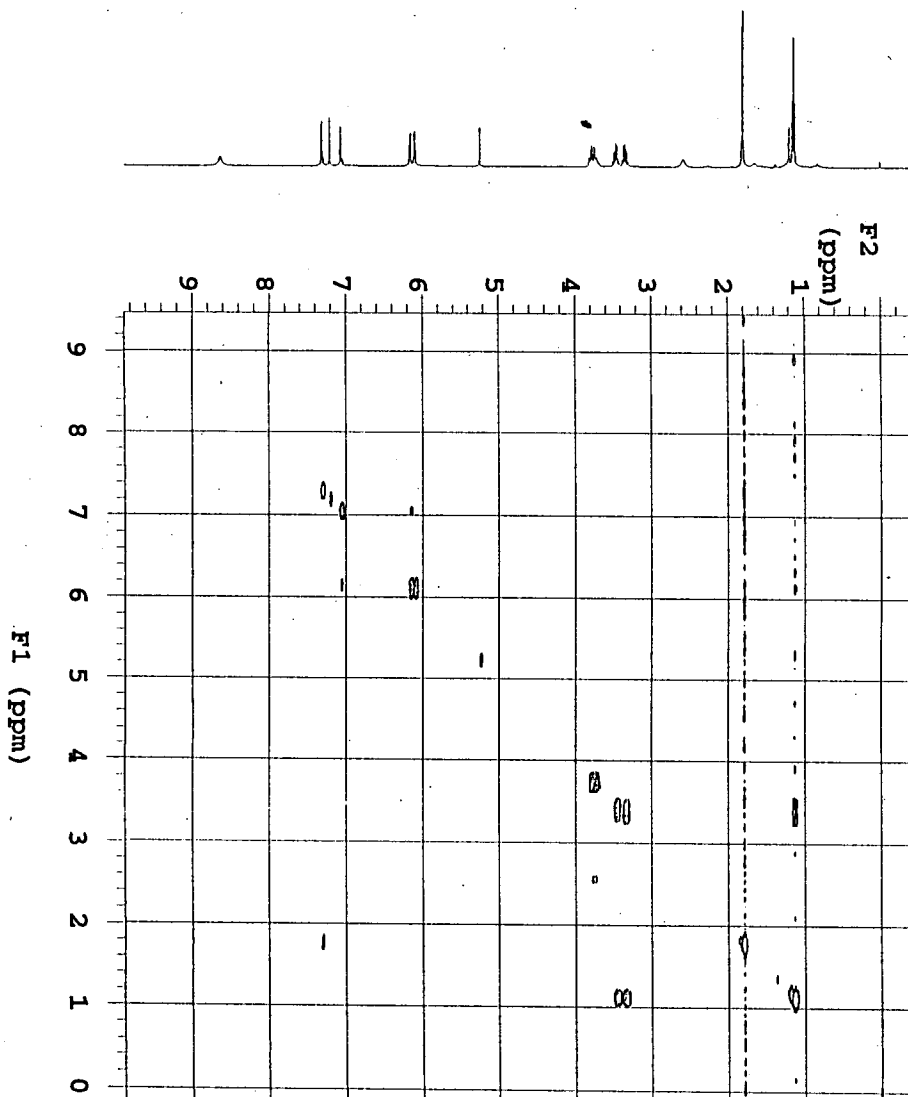
Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 INOVA-400 "narnia"

PULSE SEQUENCE
 Relax. delay 1.300 sec
 Pulse 46.3 degrees
 Acq. time 0.636 sec
 Width 25157.2 Hz
 2368 repetitions

OBSERVE C13, 100.6068126 MHz
 DECOUPLE H1, 400.1083265 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 32768
 Total time 540229 hr, 49 min, 52 sec



Pulse Sequence: gCOSY
 Solvent: CDCl₃
 Ambient temperature
 File: gCOSY
 INOVA-400 "narnia"
 PULSE SEQUENCE: gCOSY
 Relax. delay 1.000 sec
 Acq. time 0.213 sec
 Width 4801.9 Hz
 2D Width 4801.9 Hz
 2 repetitions
 200 increments
 OBSERVE H1, 400.1063415 MHz
 DATA PROCESSING
 Sq. sine bell 0.107 sec
 F1 DATA PROCESSING
 Sq. sine bell 0.021 sec
 FT size 2048 x 1024
 Total time 8 min, 38 sec



Pulse Sequence: NOESY1D

Solvent: CDCl₃

Ambient temperature

File: 1kgtrinoesyl

INOVA-400 "nairia"

PULSE SEQUENCE: NOESY1D

Relax. delay 1.000 sec

Pulse 90.0 degrees

Mixing 0.500 sec

Acq. time 2.505 sec

Width 6387.7 Hz

2048 repetitions

OBSERVE H1, 400.1063260 MHz

DATA PROCESSING

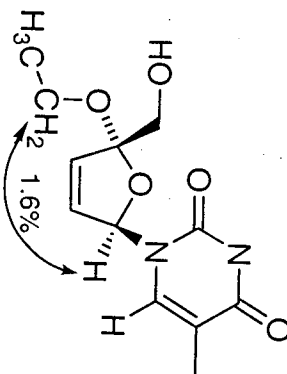
Line broadening 0.4 Hz

Sq. sine bell 2.505 sec

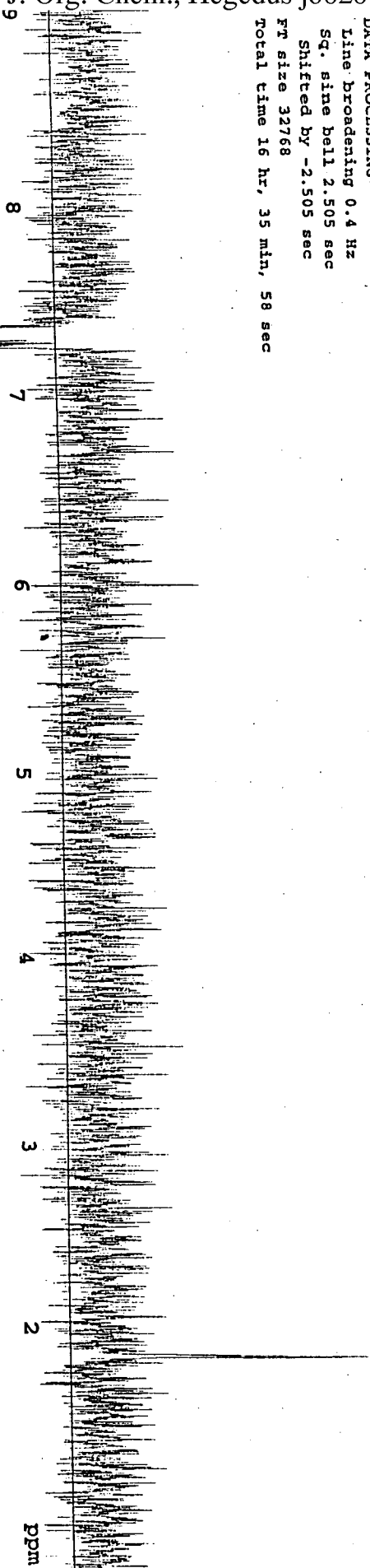
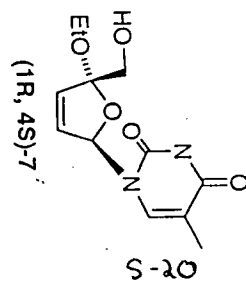
Shifted by -2.505 sec

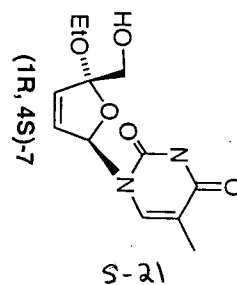
FT size 32768

Total time 16 hr, 35 min, 58 sec

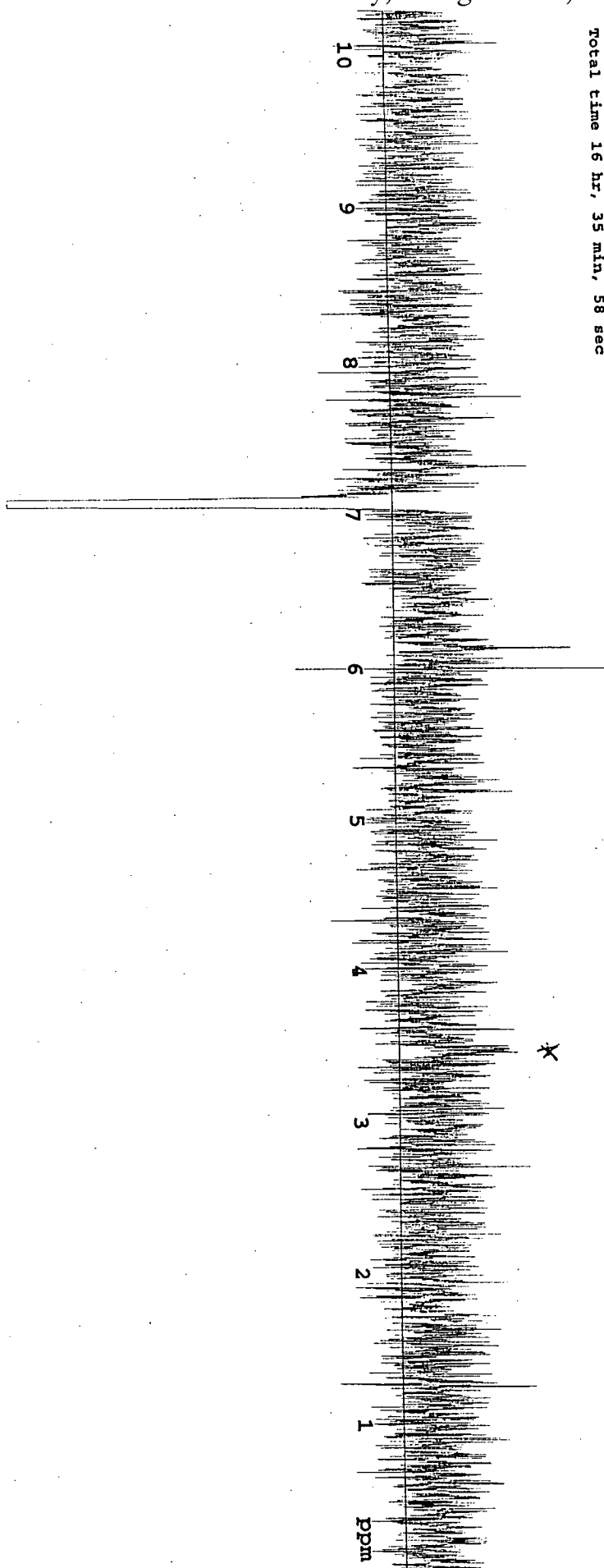


nOe studies for
(1R, 4S) anomer



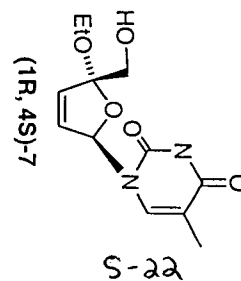
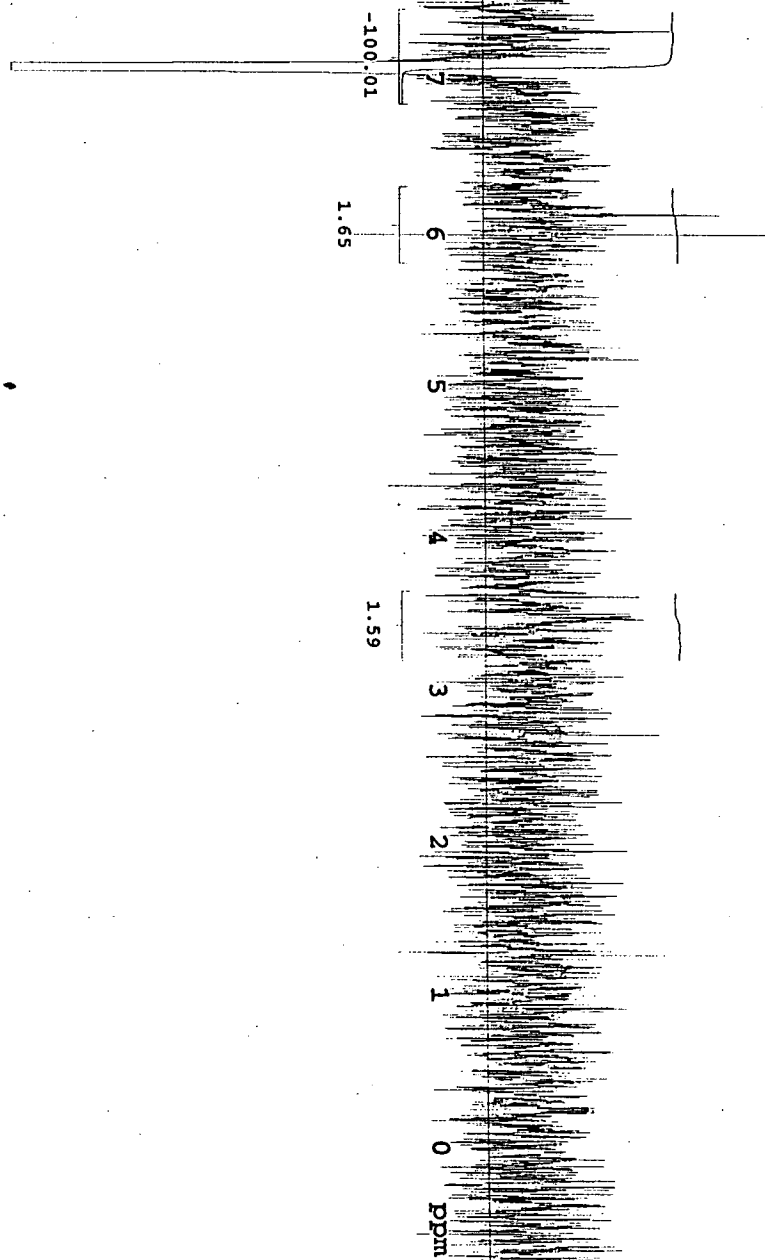


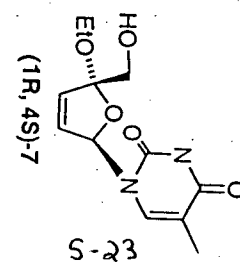
Pulse Sequence: NOESY1D
 Solvent: CDCl₃
 Ambient temperature
 File: 1kg1noesy1
 INOVA-400 "narnia"
 PULSE SEQUENCE: NOESY1D
 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Mixing 0.500 sec
 Acq. time 2.505 sec
 Width 6387.7 Hz
 2048 repetitions
 OBSERVE H1, 400.1063260 MHz
 DATA PROCESSING
 Line broadening 0.4 Hz
 Sq. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 16 hr, 35 min, 58 sec



Solvent: CDCl₃
 Ambient temperature
 File: 1kgilnoesyl-95bh
 INOVA-500 "1sh"

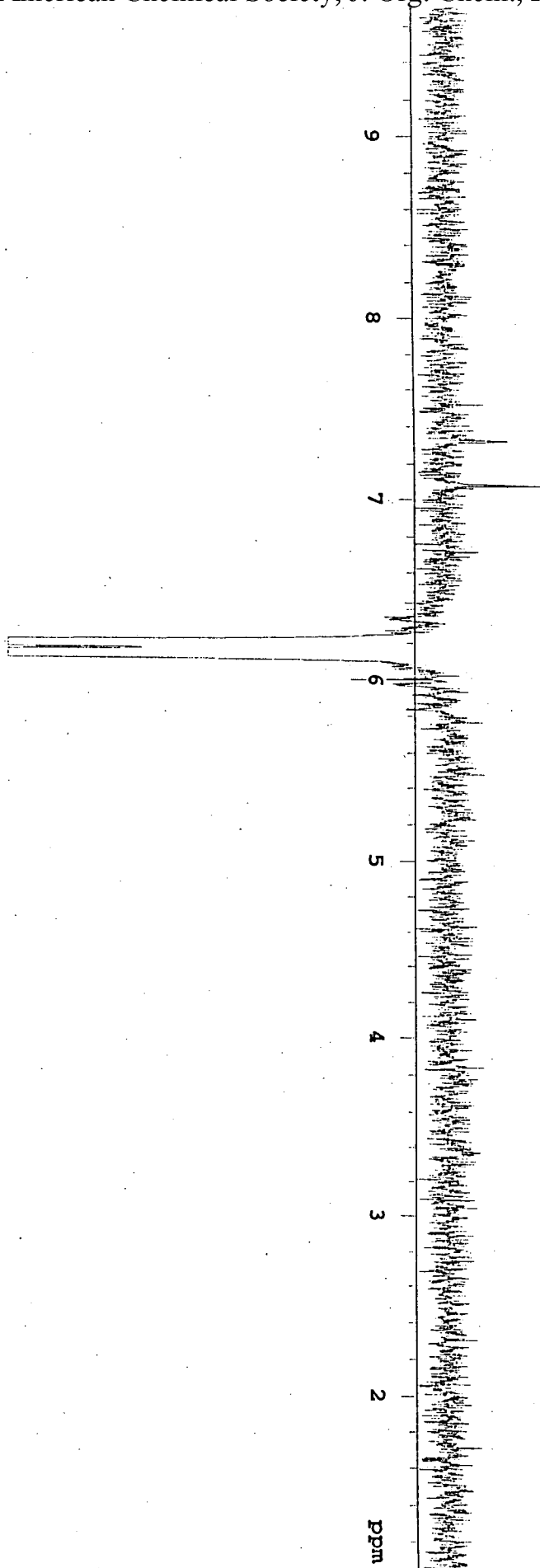
PULSE SEQUENCE: NOESY1D
 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Mixing 0.500 sec
 Acq. time 2.505 sec
 Width 6387.7 Hz
 2048 repetitions
 OBSERVE H1, 400.1063232 MHz
 DATA PROCESSING
 Line broadening 0.4 Hz
 Sq. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 15.9 hours

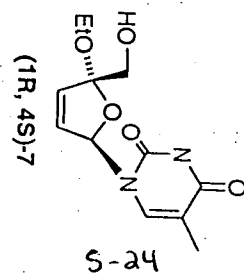




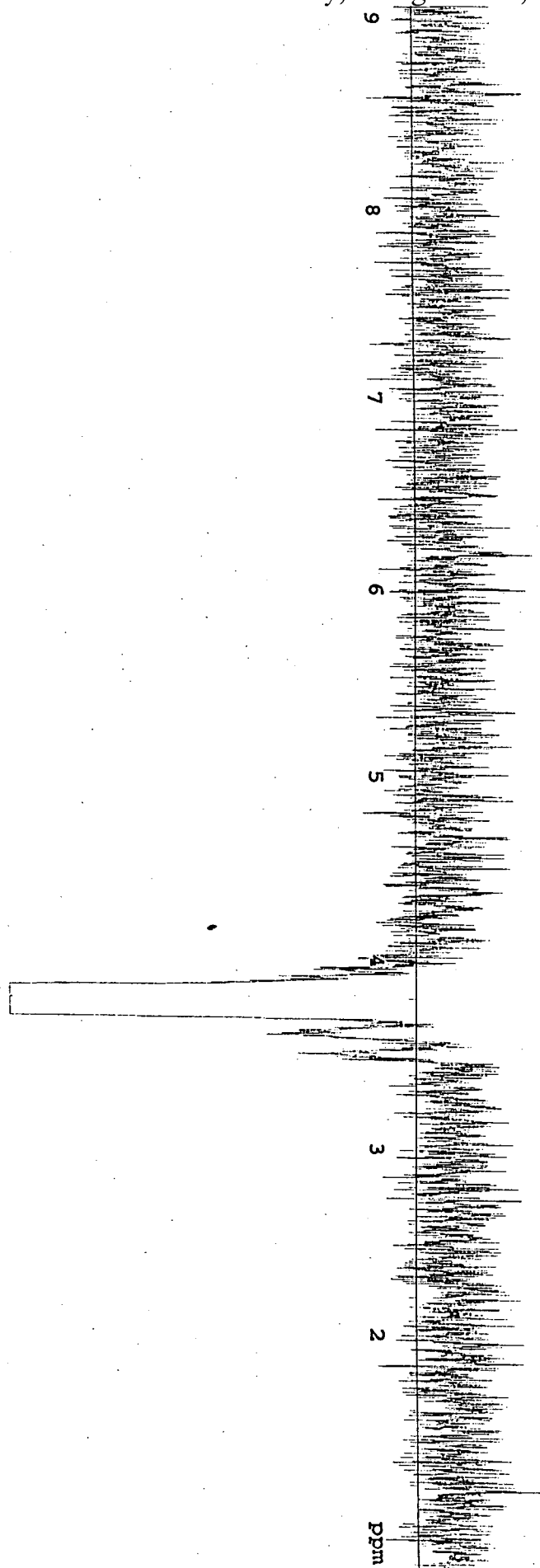
Pulse Sequence: NOESYD
 Solvent: CDCl₃
 Ambient temperature
 INOVA-400 "narnia"
 PULSE SEQUENCE: NOESYD
 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Mixing 0.500 sec
 Acq. time 2.505 sec
 Width 6387.7 Hz
 2048 repetitions
 OBSERVE H1, 400.1063260 MHz
 DATA PROCESSING
 Line broadening 0.4 Hz
 Sq. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 11 hr, 43 min, 38 sec

9
8
7
6
5
4
3
2
ppm





Pulse Sequence: NOESY1D
 Solvent: CDCl₃
 Ambient temperature
 INOVA-400 "narnia"
 PULSE SEQUENCE: NOESY1D
 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Mixing 0.500 sec
 Acq. time 2.505 sec
 Width 6387.7 Hz
 2048 repetitions
 OBSERVE H1, 400.1063260 MHz
 DATA PROCESSING
 Line broadening 0.4 Hz
 Sq. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 11 hr, 43 min, 38 sec



Pulse Sequence: NOESY1D

Solvent: CDCl₃
Ambient temperature
INOVA-400 "narnia"

PULSE SEQUENCE: NOESY1D

Relax. delay 1.000 sec

Pulse 90.0 degrees

Mixing 0.500 sec

Acq. time 2.505 sec

Width 6387.7 Hz

2048 repetitions

OBSERVE H1, 400.1063260 MHz

DATA PROCESSING

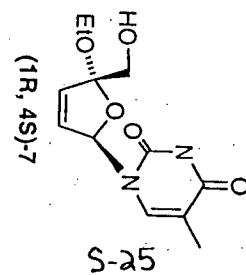
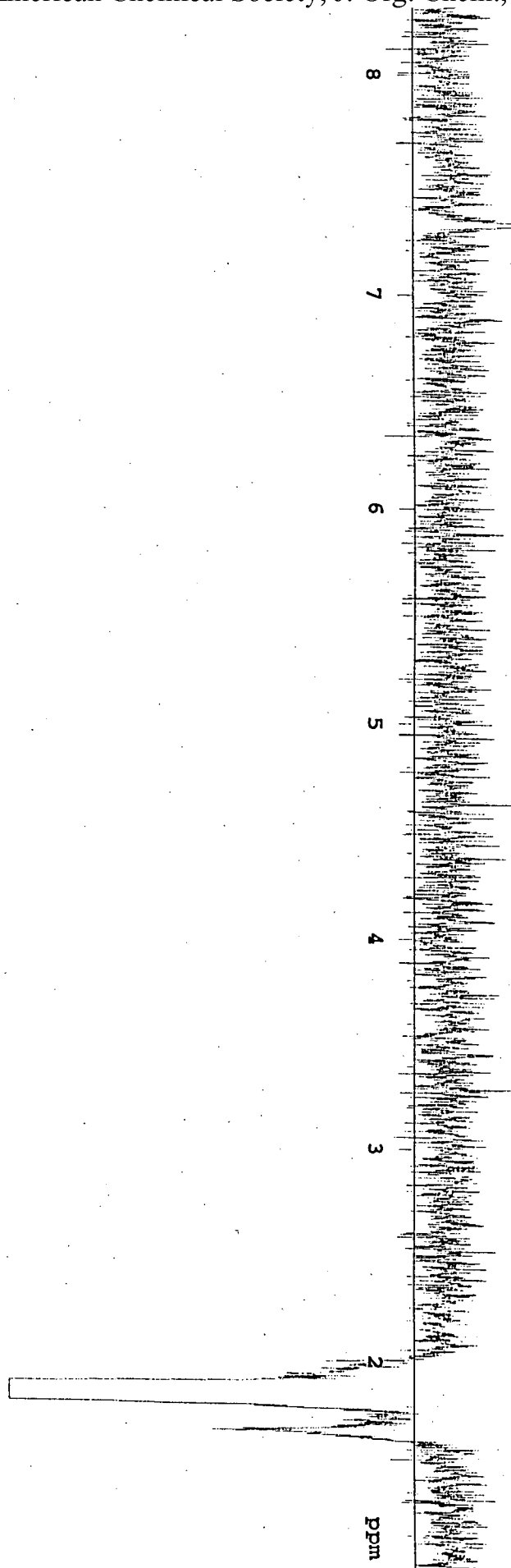
Line broadening 0.4 Hz

Sq. sine bell 2.505 sec

Shifted by -2.505 sec

FT size 32768

Total time 11 hr, 43 min, 38 sec



Pulse Sequence: NOESY1D

Solvent: CDCl₃

Ambient temperature

INOVA-400 "narnia"

PULSE SEQUENCE: NOESY1D

Relax. delay 1.000 sec

Pulse 90.0 degrees

Mixing 0.500 sec

Acq. time 2.505 sec

Width 6387.7 Hz

2048 repetitions

OBSERVE H1, 400.1063260 MHz

DATA PROCESSING

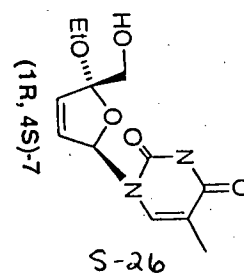
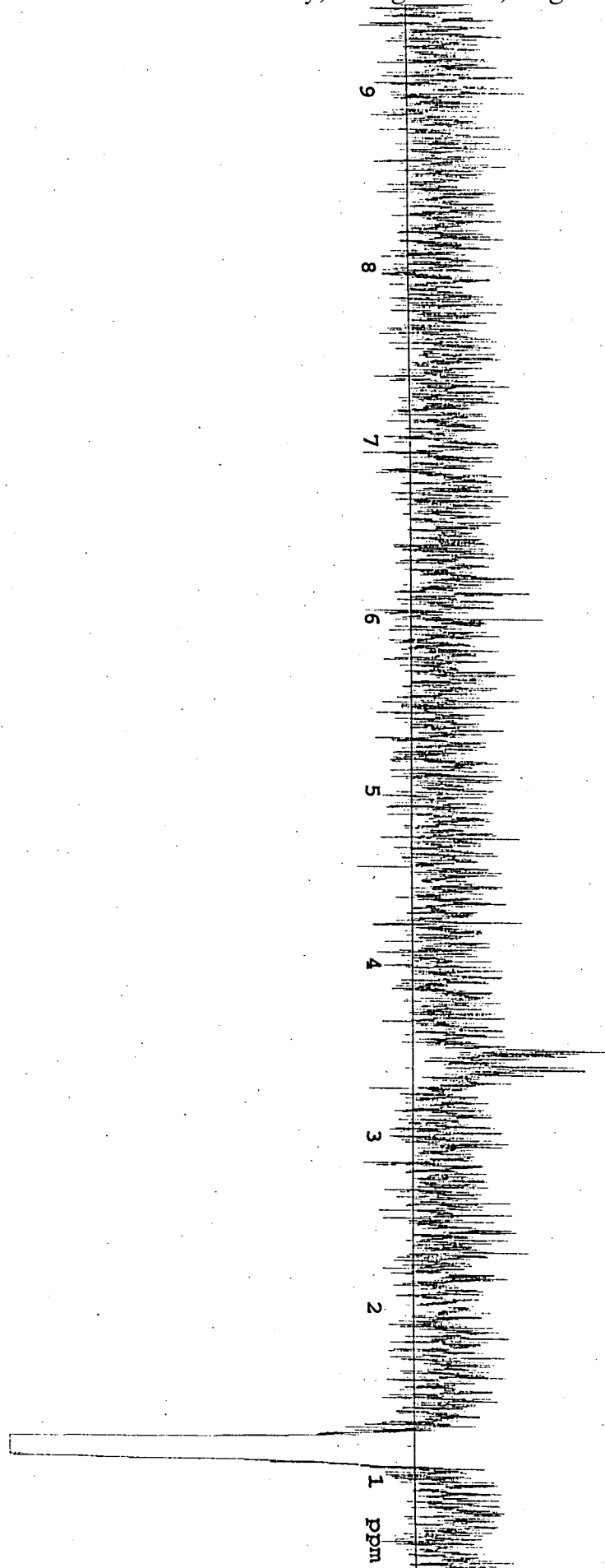
Line broadening 0.4 Hz

SF. sine bell 2.505 sec

Shifted by -2.505 sec

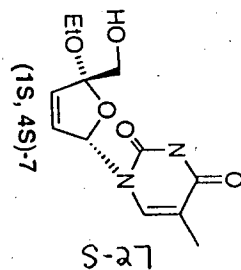
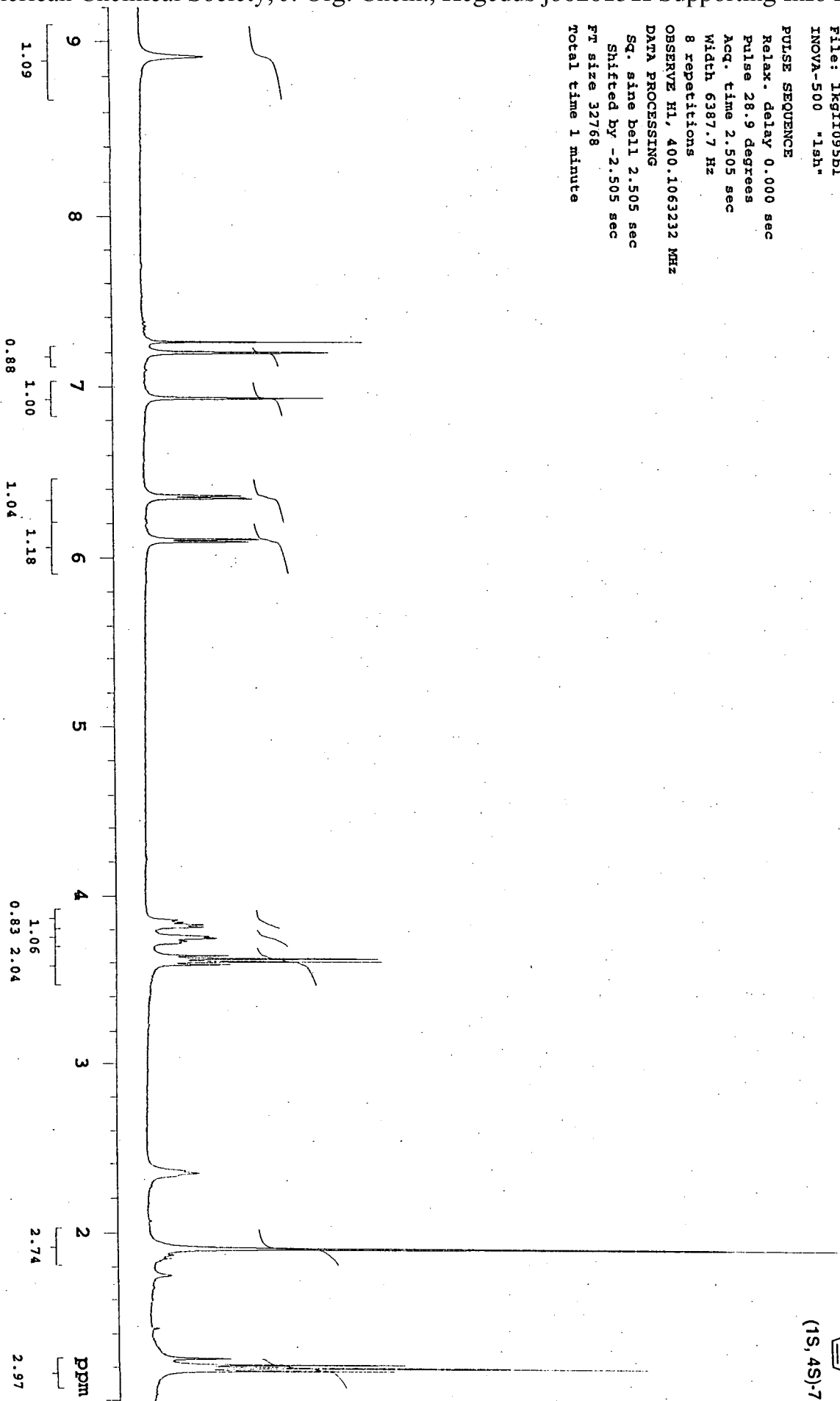
FT size 32768

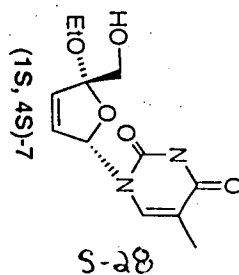
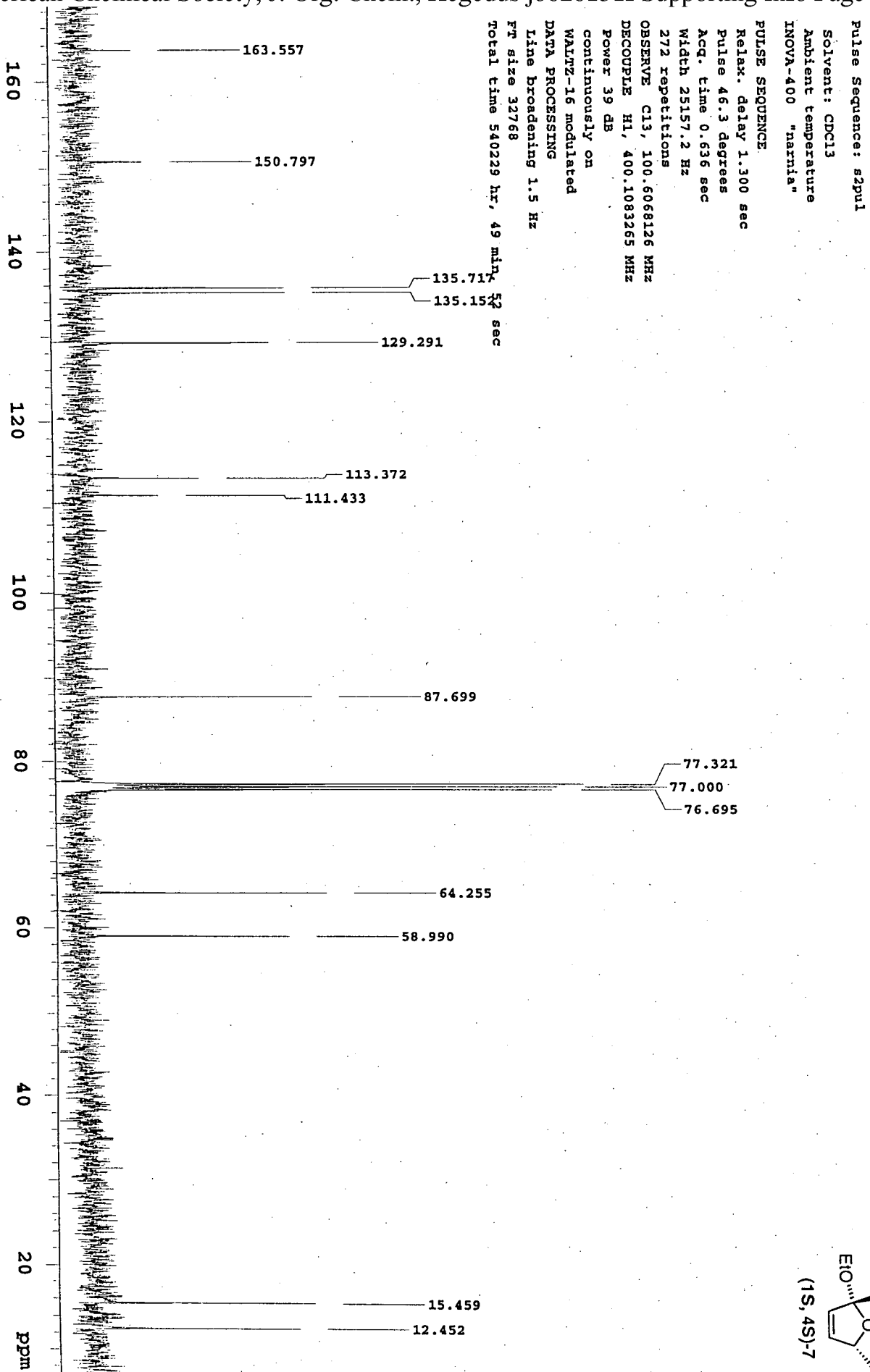
Total time 11 hr, 43 min, 38 sec



Solvent: CDCl₃
 Ambient temperature
 File: lkgit095b1
 INOVA-500 "1sh"

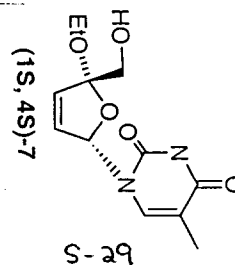
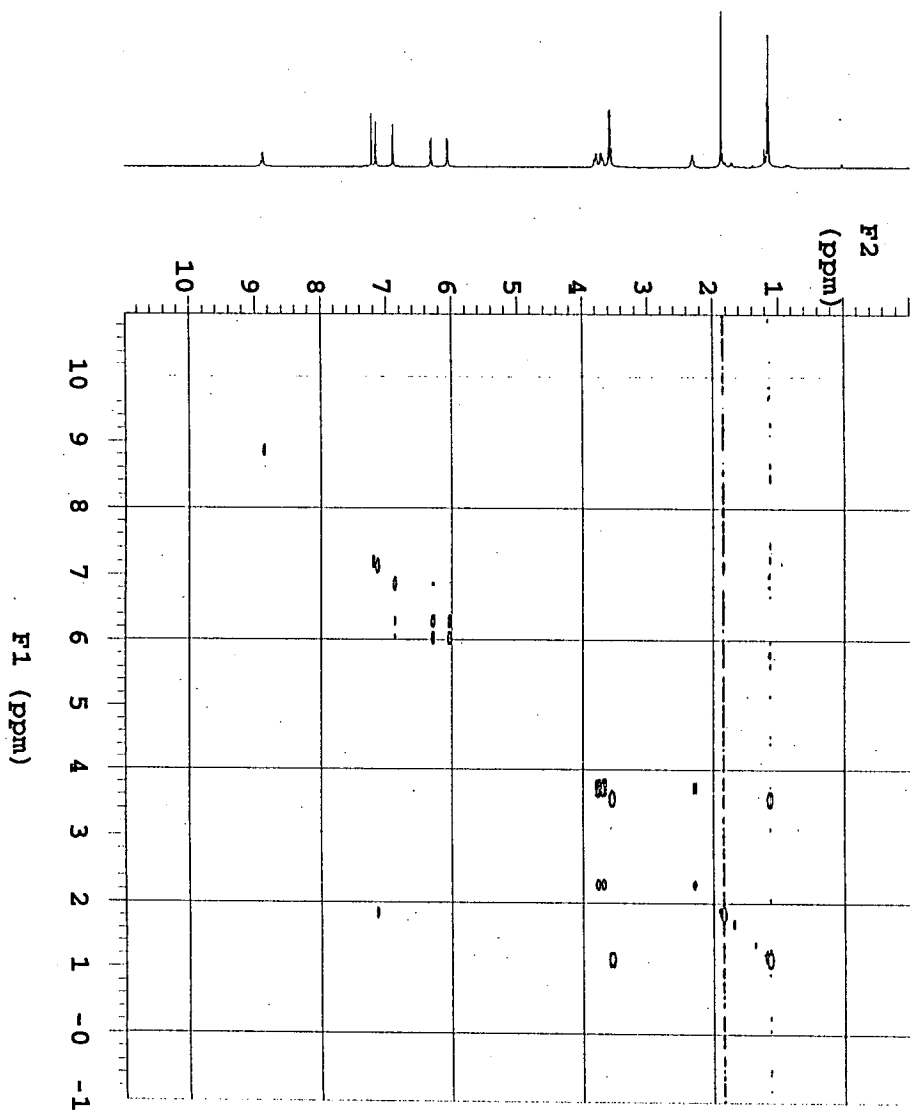
PULSE SEQUENCE
 Relax. delay 0.000 sec
 Pulse 28.9 degrees
 Acq. time 2.505 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 400.1063232 MHz
 DATA PROCESSING
 Sd. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 1 minute





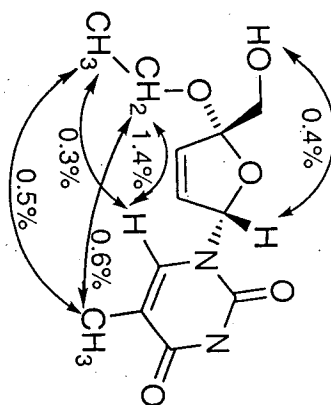
Pulse Sequence: gcosy
 Solvent: CDCl₃
 Ambient temperature
 File: gcosy
 INOVA-400 "narnia"

PULSE SEQUENCE: gcosy
 Relax. delay 1.000 sec
 Acq. time 0.213 sec
 Width 4801.9 Hz
 2D Width 4801.9 Hz
 2 repetitions
 200 increments
 OBSERVE H1, 400.1063412 MHz
 DATA PROCESSING
 Sq. sine bell 0.107 sec
 F1 DATA PROCESSING
 Sq. sine bell 0.021 sec
 FT size 2048 x 1024
 Total time 8 min, 38 sec

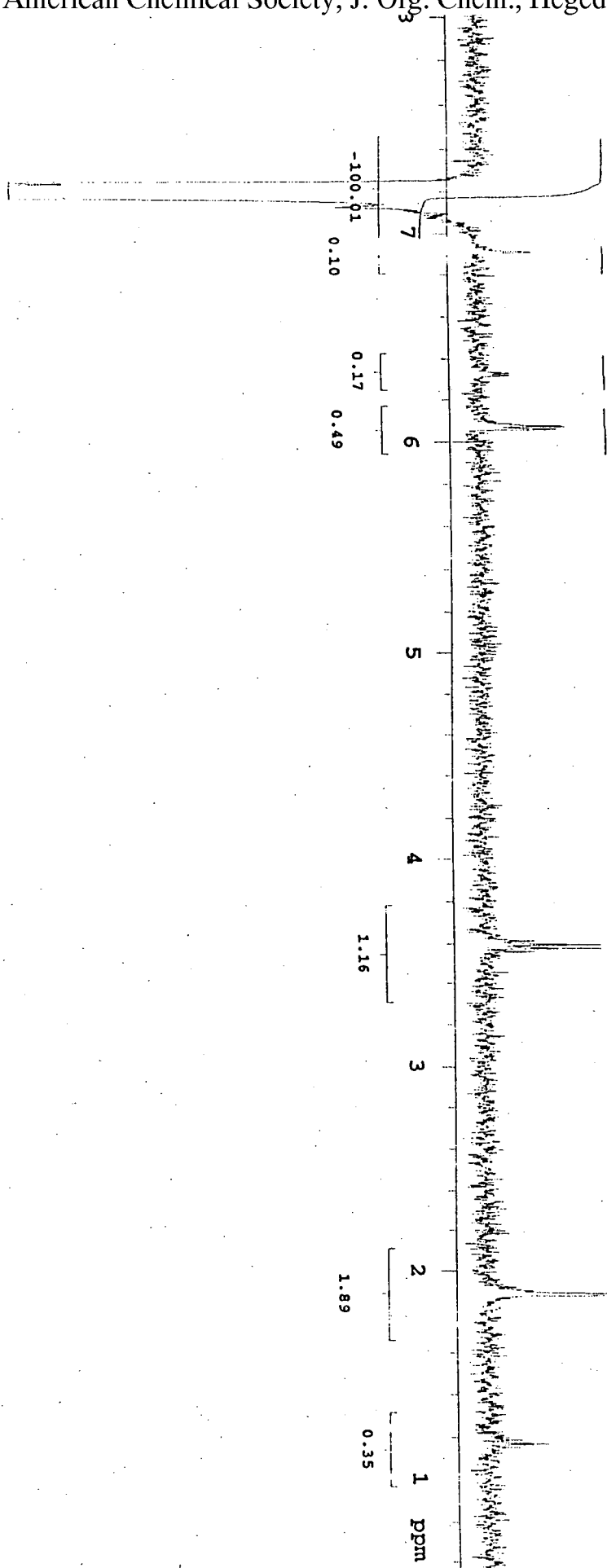
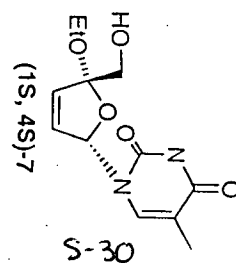


Solvent: CDCl₃
Ambient temperature
File: 1kgit095b1noesy1-2
INOVA-500 "1sh"

PULSE SEQUENCE: NOESTYD
Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 2.505 sec
Width 6387.7 Hz
2048 repetitions
OBSERVE H1, 400.1063232 MHz
DATA PROCESSING
Line broadening 0.4 Hz
Sq. sine bell 2.505 sec
Shifted by -2.505 sec
FT size 32768
Total time 4.6 hours

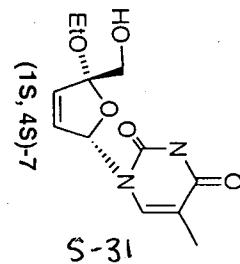
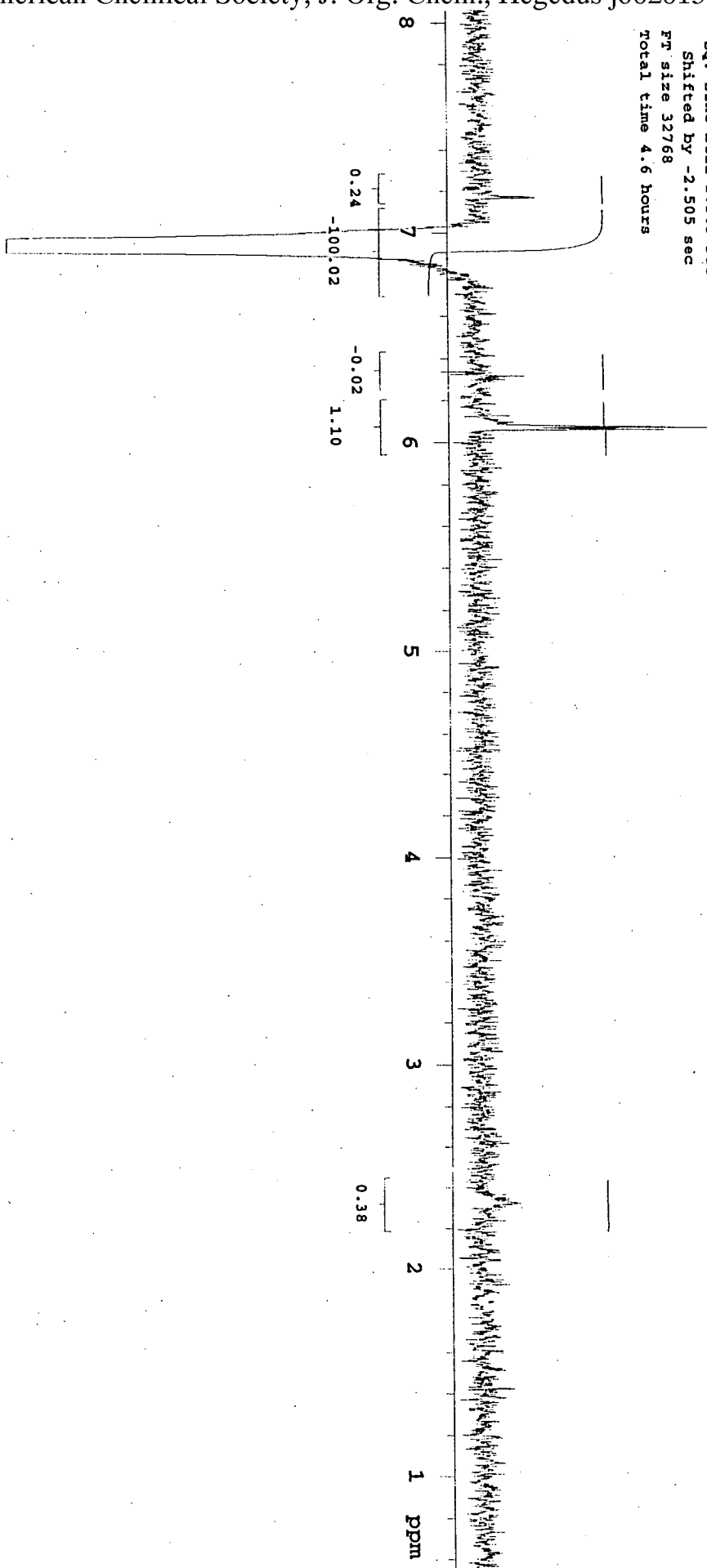


nOe studies for
(1S, 4S) anomer



Solvent: CDCl₃
 Ambient temperature
 File: lkg1095b1noesy1-2
 INOVA-500 "1sh"

PULSE SEQUENCE: NOESYD
 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Mixing 0.500 sec
 Acq. time 2.505 sec
 Width 6387.7 Hz
 2048 repetitions
 OBSERVE H1, 400.1063232 MHz
 DATA PROCESSING
 Line broadening 0.4 Hz
 Sq. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 4.6 hours



ds (3)

Pulse Sequence: NOESY1D

Solvent: CDCl₃
Ambient temperature
INOVA-400 "narnia"

PULSE SEQUENCE: NOESY1D

Relax. delay 1.000 sec

Pulse 90.0 degrees

Mixing 0.500 sec

Acq. time 2.505 sec

Width 6387.7 Hz

2048 repetitions

OBSERVE H1, 400.1063260 MHz

DATA PROCESSING

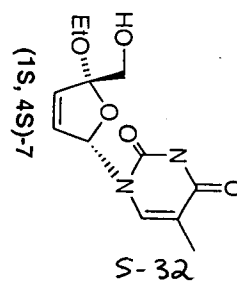
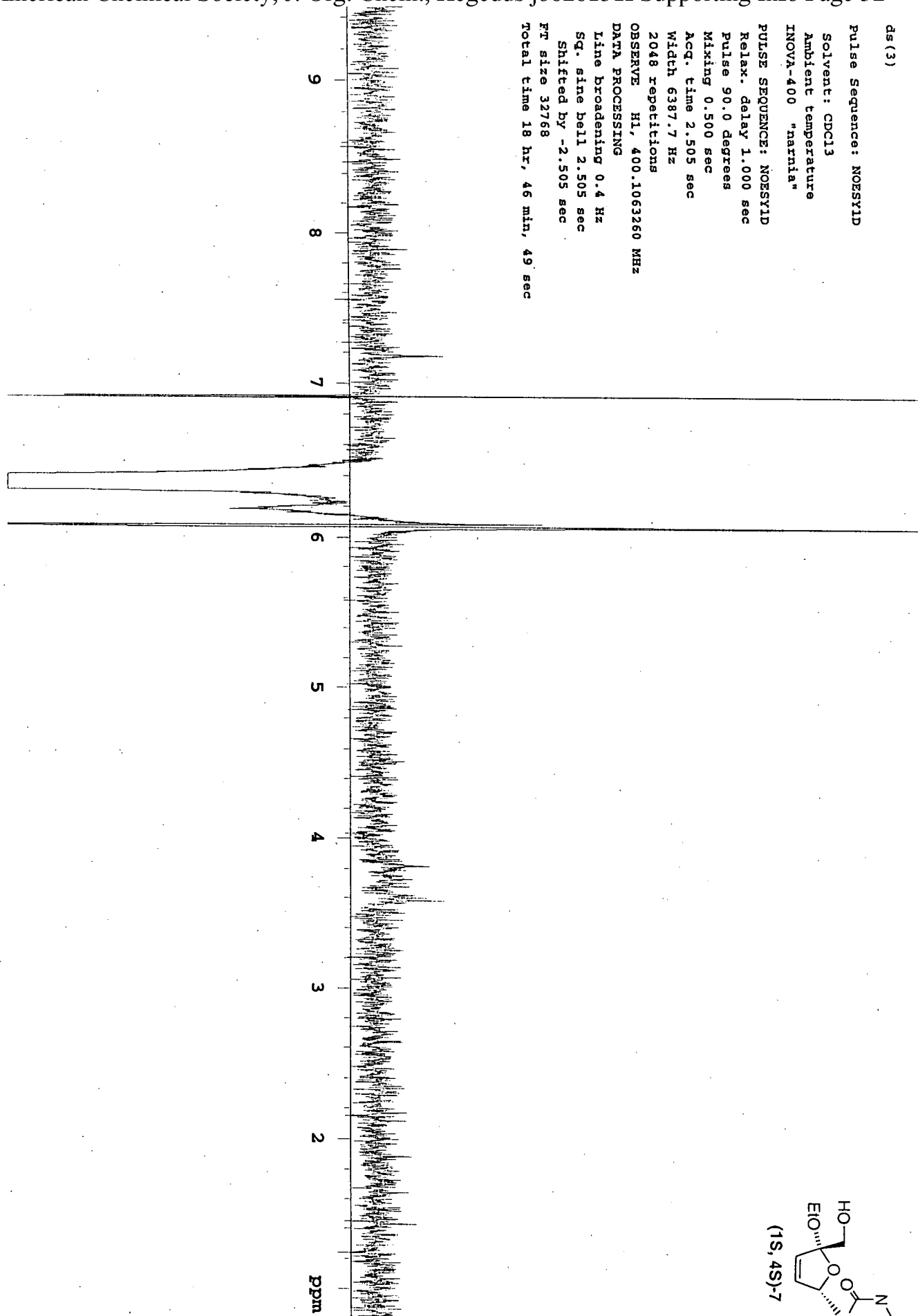
Line broadening 0.4 Hz

Sq. sine bell 2.505 sec

Shifted by -2.505 sec

FT size 32768

Total time 18 hr, 46 min, 49 sec



Pulse Sequence: NOESYD

Solvent: CDCl₃
Ambient temperature
INOVA-400 "narda"

PULSE SEQUENCE: NOESY1D

Relax. delay 1.000 sec

Pulse 90.0 degrees

Mixing 0.500 sec

Acq. time 2.505 sec

Width 6387.7 Hz

2048 repetitions
CH 400 1063260 MHz
OBSERVE

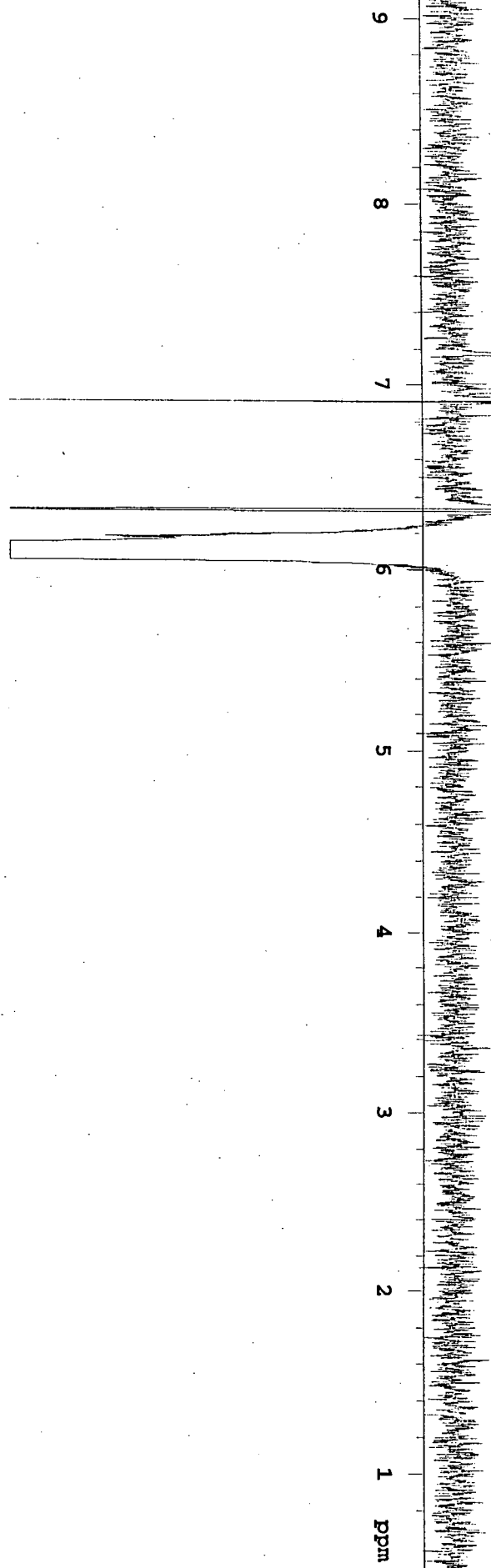
DATA PROCESSING

Line broadening 0.4 Hz

Sq. sine bell 2.505 sec

Shifted by

FT size 32768



ds(5)

Pulse Sequence: NOESY1D

Solvent: CDCl₃

Ambient temperature

INOVA-400 "narnia"

PULSE SEQUENCE: NOESY1D

Relax. delay 1.000 sec

Pulse 90.0 degrees

Mixing 0.500 sec

Acq. time 2.505 sec

Width 6387.7 Hz

2048 repetitions

OBSERVE H1, 400.1063260 MHz

DATA PROCESSING

Line broadening 0.4 Hz

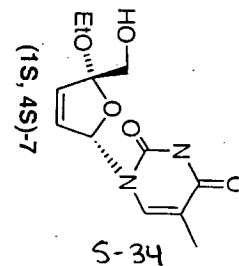
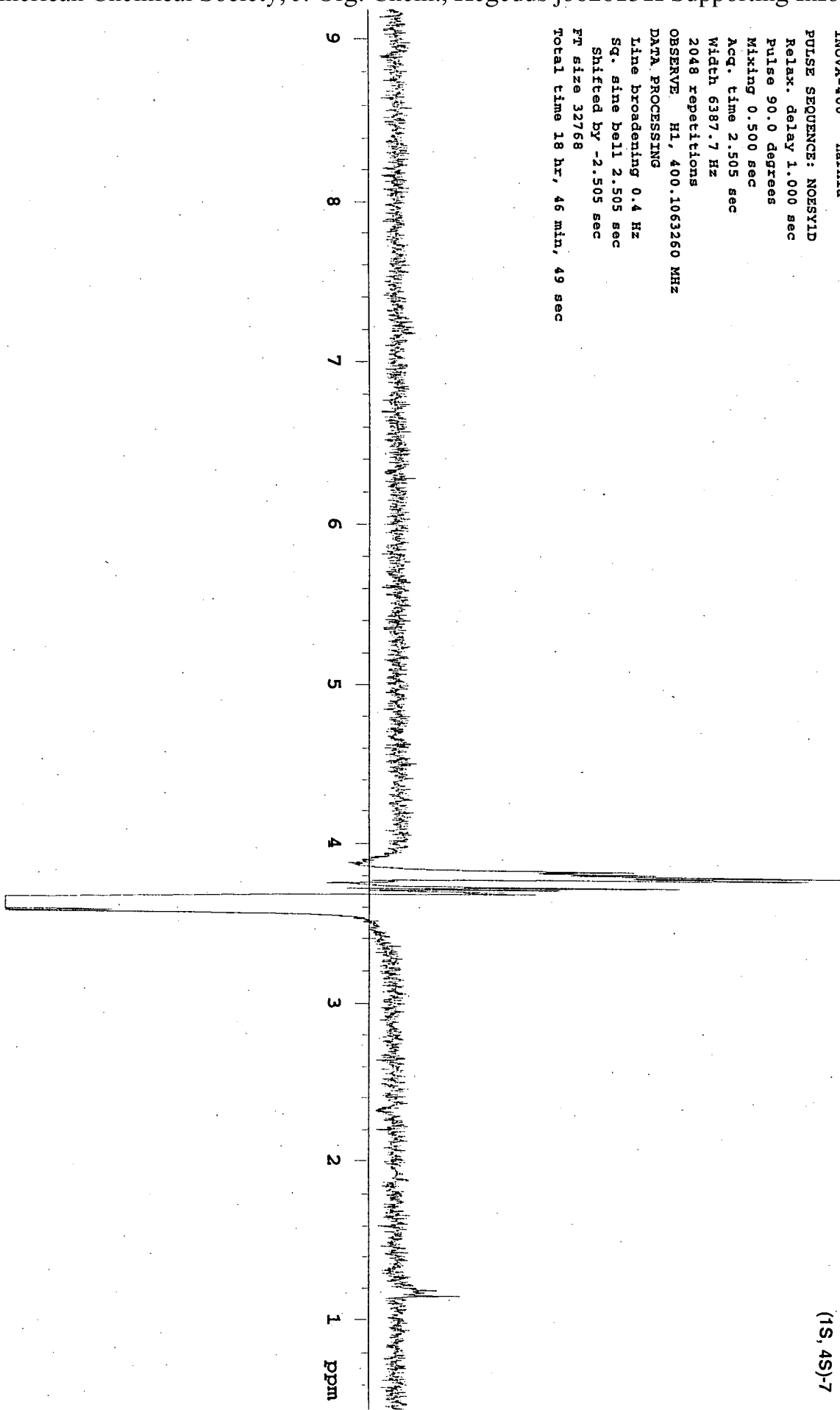
Sq. sine bell 2.505 sec

Shifted by -2.505 sec

FT size 32768

Total time 18 hr, 46 min, 49 sec

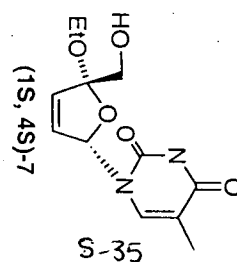
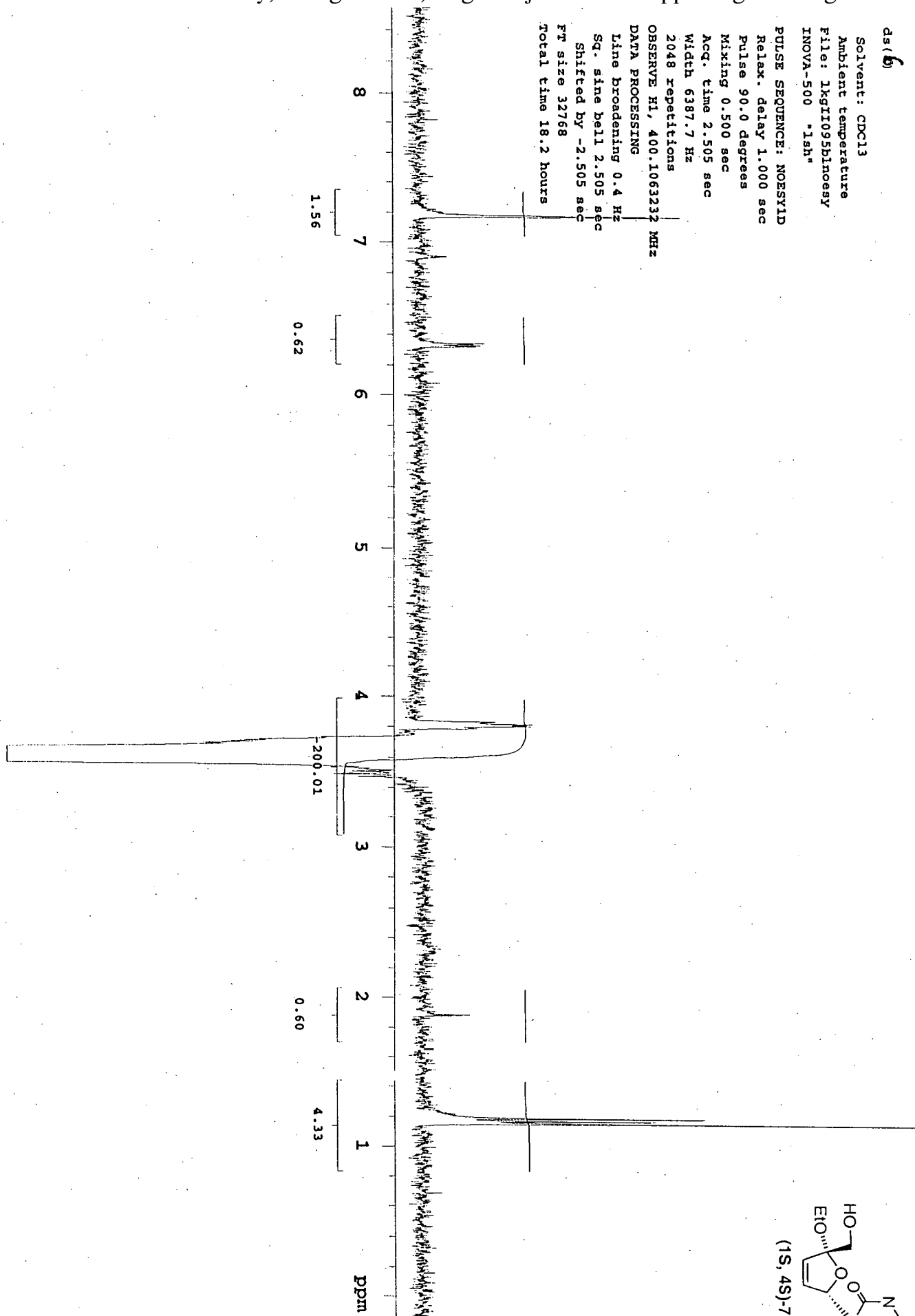
9
8
7
6
5
4
3
2
1 ppm



ds(6)

Solvent: CDCl₃
Ambient temperature
File: 1kg1095b1nccsy
INOVA-500 "1sh"

PULSE SEQUENCE: NOESYD
Relax. delay 1.000 sec
Pulse 90.0 degrees
Mixing 0.500 sec
Acq. time 2.505 sec
Width 6387.7 Hz
2048 repetitions
OBSERVE H1, 400.1063232 MHz
DATA PROCESSING
Line broadening 0.4 Hz
Sq. sine bell 2.505 sec
Shifted by -2.505 sec
FT size 32768
Total time 18.2 hours

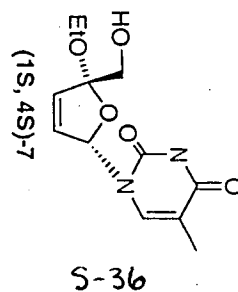
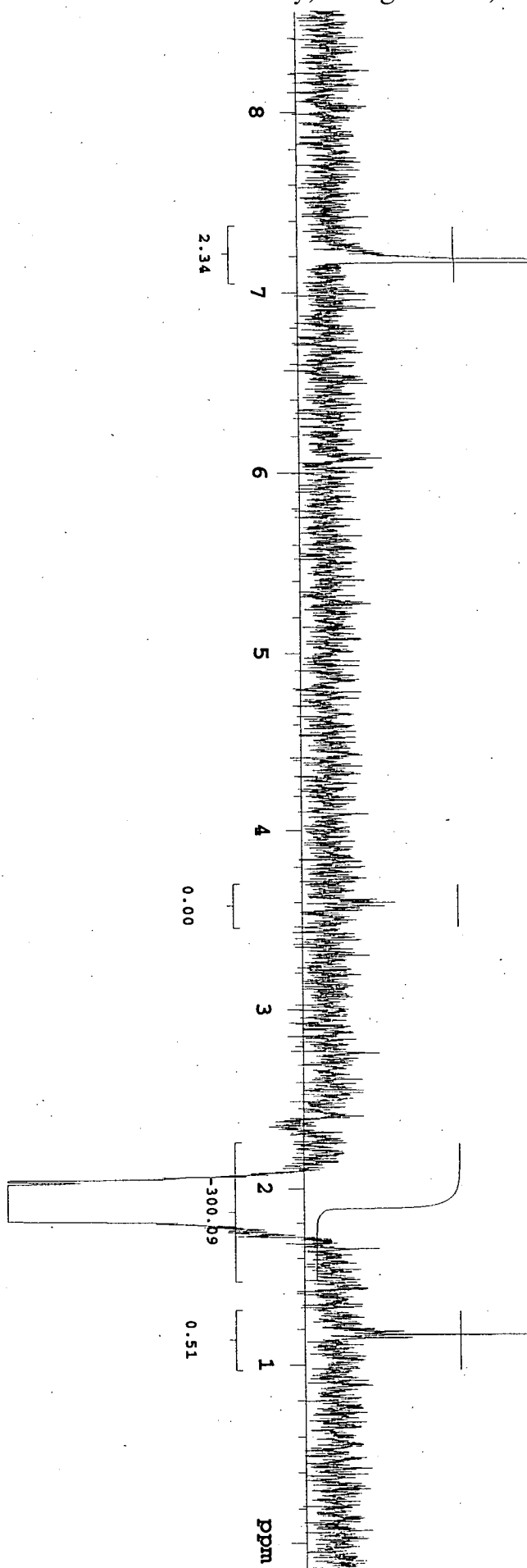


Solvent: CDCl₃
 Ambient temperature
 File: 1kgit095b1ncesy
 INOVA-500 "1sh"

PULSE SEQUENCE: NOESY1D
 Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Mixing 0.500 sec
 Acq. time 2.505 sec
 Width 6387.7 Hz
 2048 repetitions

OBSERVE H1, 400.1063232 MHz
 DATA PROCESSING

Line broadening 0.4 Hz
 Sq. sine bell 2.505 sec
 Shifted by -2.505 sec
 FT size 32768
 Total time 18.2 hours



Solvent: CDCl₃

Ambient temperature

File: 1kgTI095b1noesy

INOVA-500 "15h"

PULSE SEQUENCE: NOESY1D

Relax. delay 1.000 sec

Pulse 90.0 degrees

Mixing 0.500 sec

Acq. time 2.505 sec

Width 6387.7 Hz

2048 repetitions

OBSERVE H1, 400.1063232 MHz

DATA PROCESSING

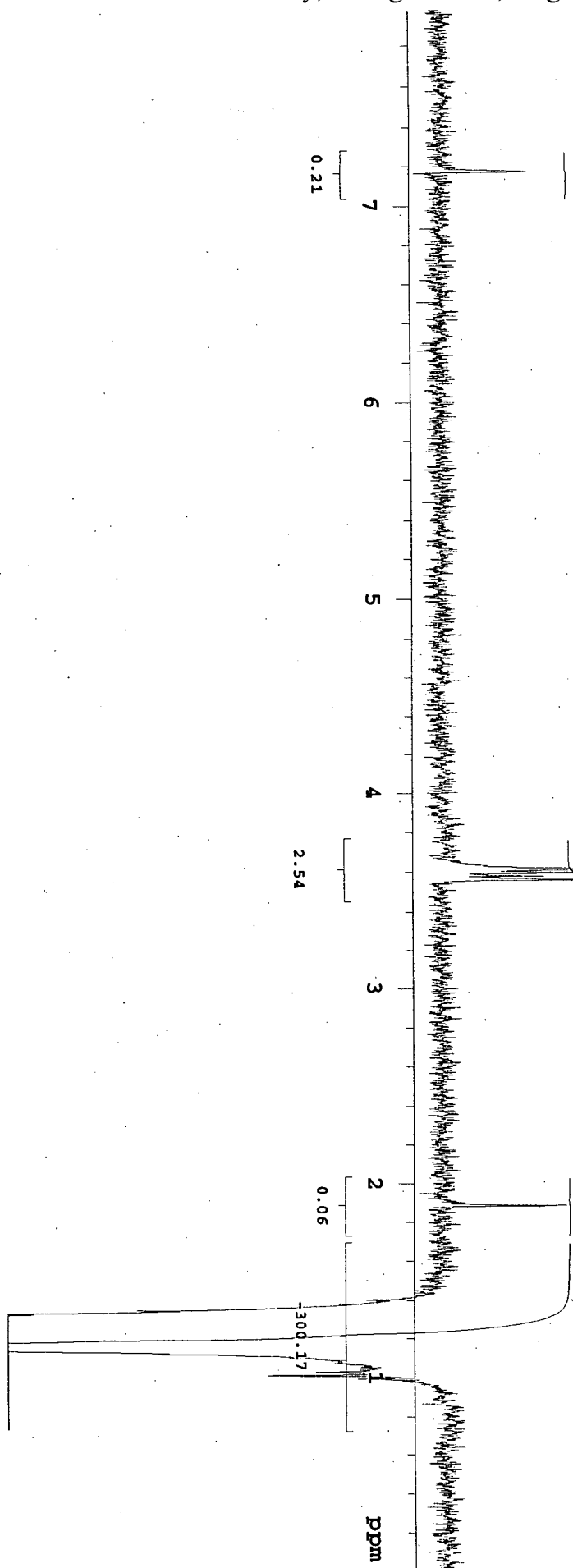
Line broadening 0.4 Hz

Sq. sine bell 2.505 sec

Shifted by -2.505 se

FT size 32768

Total time 18.2 hours



STANDARD 1H OBSERVE

Solvent: CDCl₃
Ambient temperature
File: lkg1477f12-25
INOVA-500 "1sh"

PULSE SEQUENCE

Relax. delay 0.000 sec

Pulse 30.0 degrees

Acq. time 2.666 sec

Width 6000.6 Hz

20 repetitions

OBSERVE H1, 300.1149292 MHz

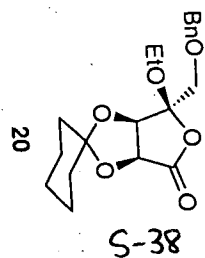
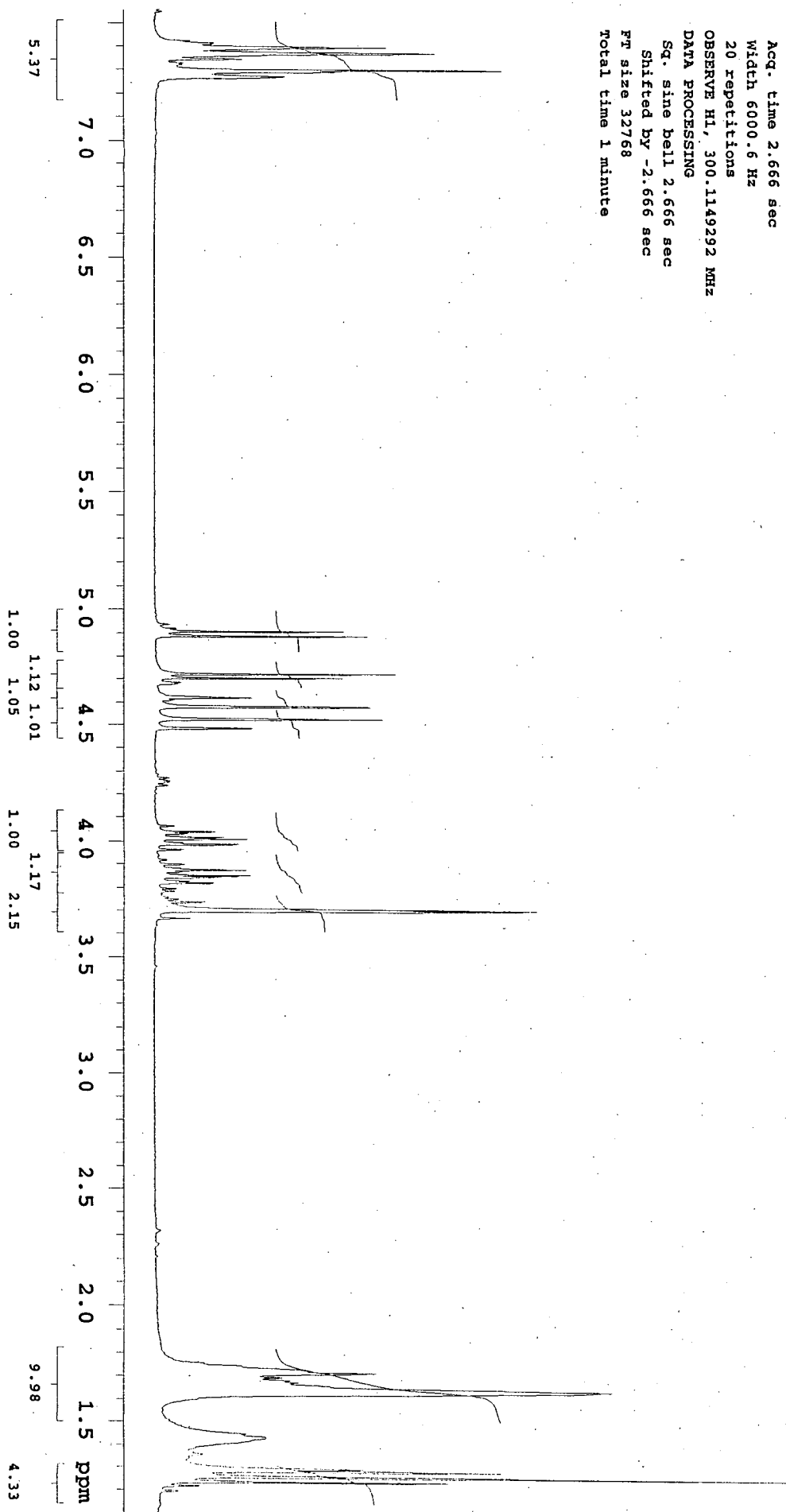
DATA PROCESSING

Sq. sine bell 2.666 sec

Shifted by -2.666 sec

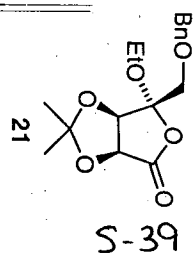
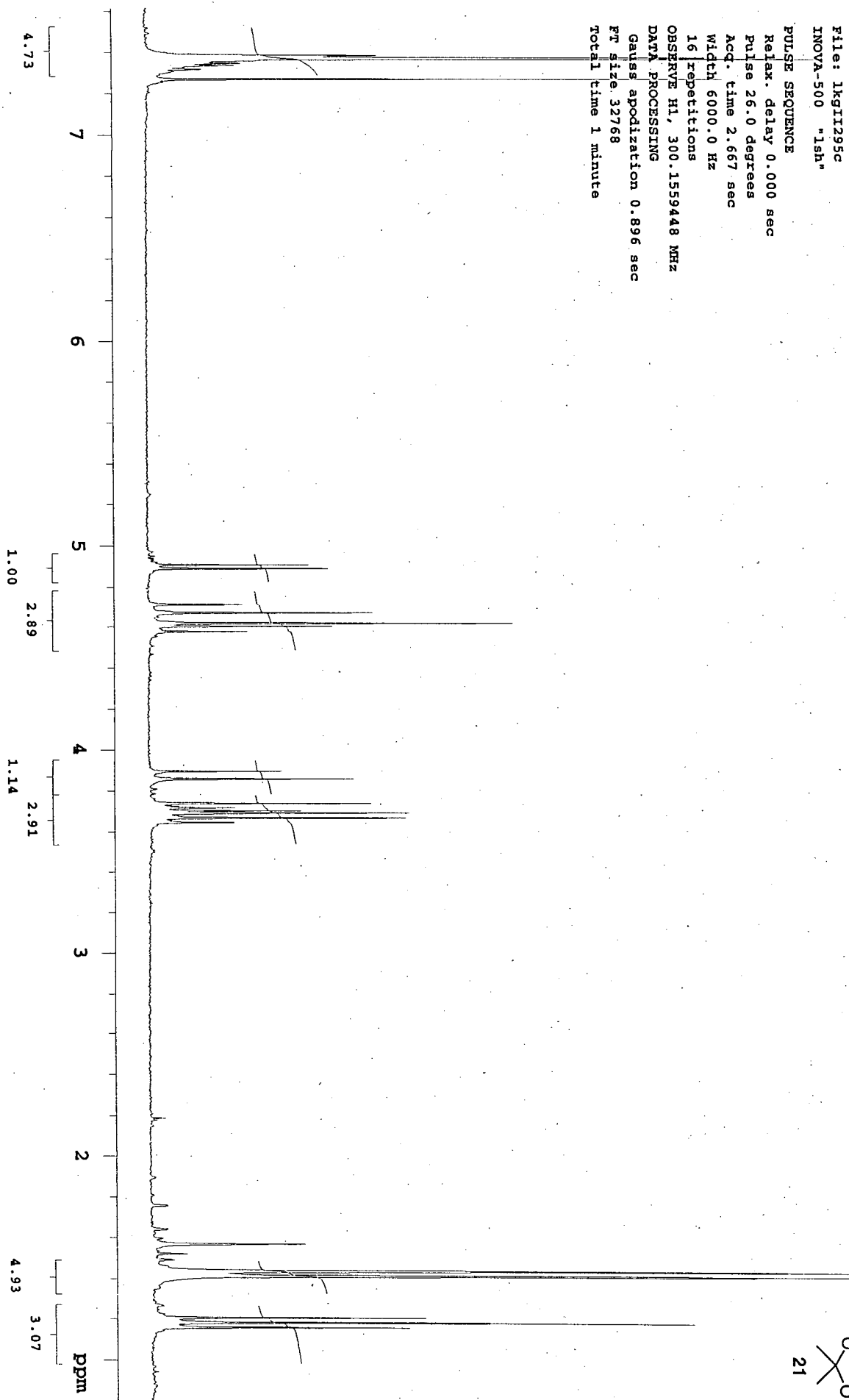
FT size 32768

Total time 1 minute



Solvent: CDCl₃
 Ambient temperature
 File: 1kg1295c
 INOVA-500 "1sh"

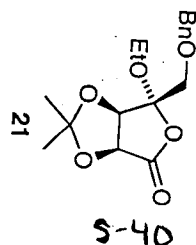
PULSE SEQUENCE
 Relax. delay 0.000 sec
 Pulse 26.0 degrees
 Acq. time 2.667 sec
 Width 6000.0 Hz
 16 repetitions
 OBSERVE H1, 300.1559448 MHz
 DATA PROCESSING
 Gauss apodization 0.896 sec
 FT size 32768
 Total time 1 minute



3C OBSERVE

keys

EQF 30S2PUL
FRC 75.4812 MHz
W 264.967 ppm
T 0.8 sec
T 1 sec
W 6.65 usec
T 602
EMF 20N



5-40

