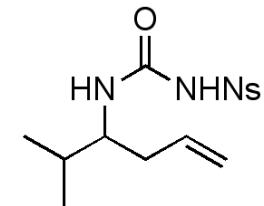


# **Catalyst-Controlled C-O versus C-N Allylic Functionalization of Terminal Olefins**

Iulia I. Strambeanu and M. Christina White\*

*Roger Adams Laboratory, Department of Chemistry, University of Illinois, Urbana, Illinois 61801*

## **Supporting Information: Spectral Data**



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: iPr\_SM

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 45.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

16 repetitions

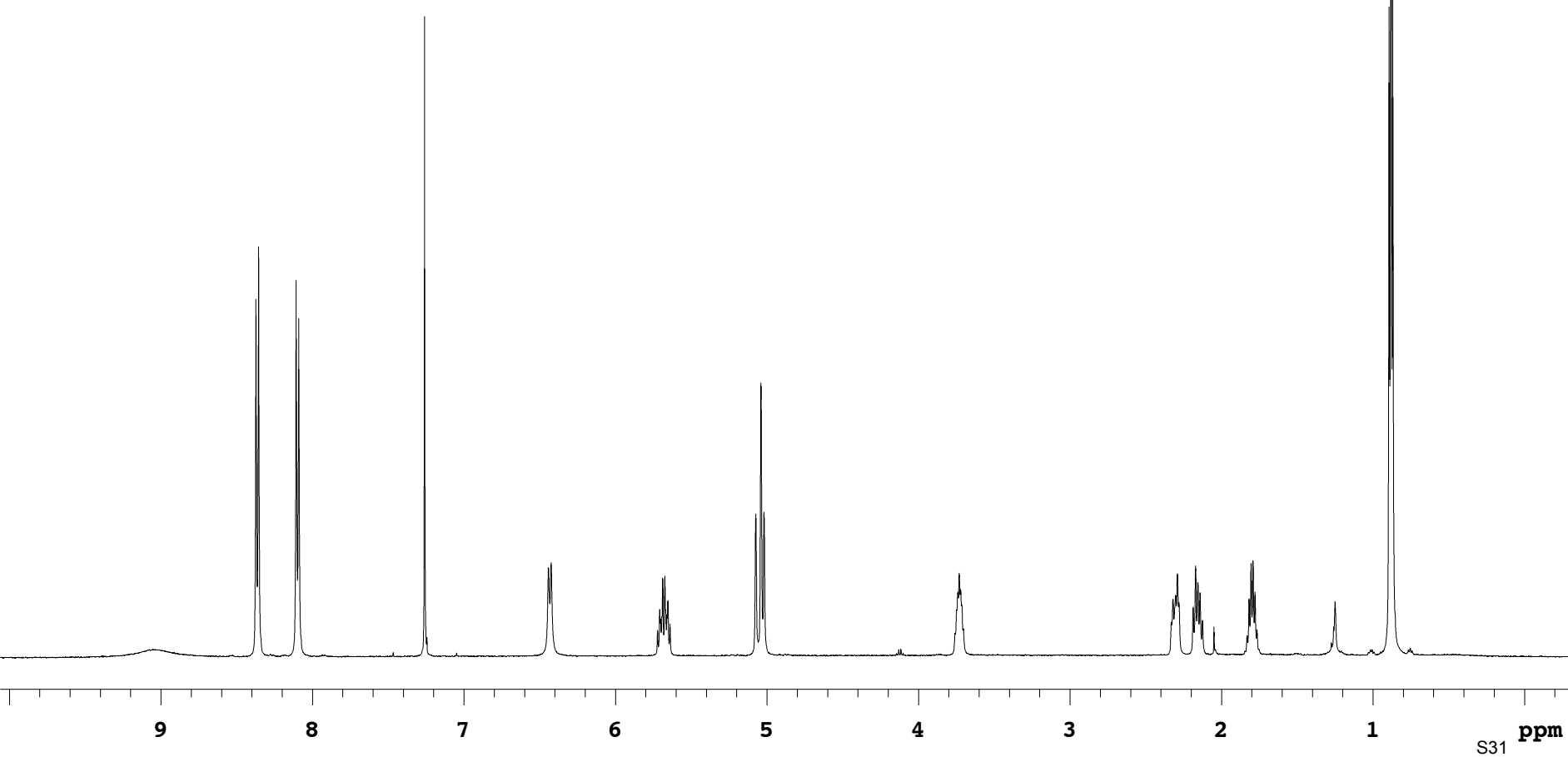
OBSERVE H1, 499.4299002 MHz

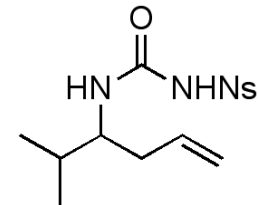
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 3 min, 45 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: iPr\_SM\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

984 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

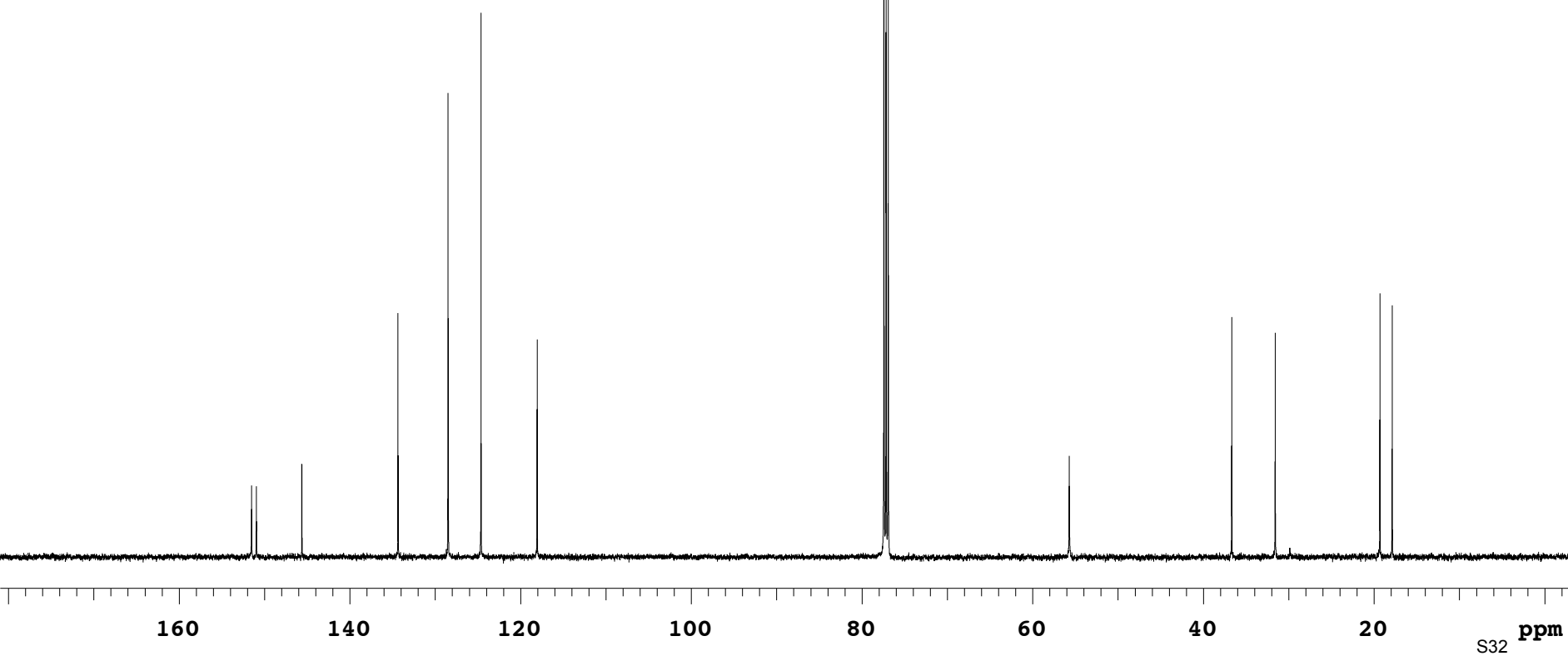
WALTZ-16 modulated

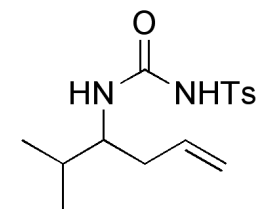
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 28 min, 8 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: IIS.105.IX

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

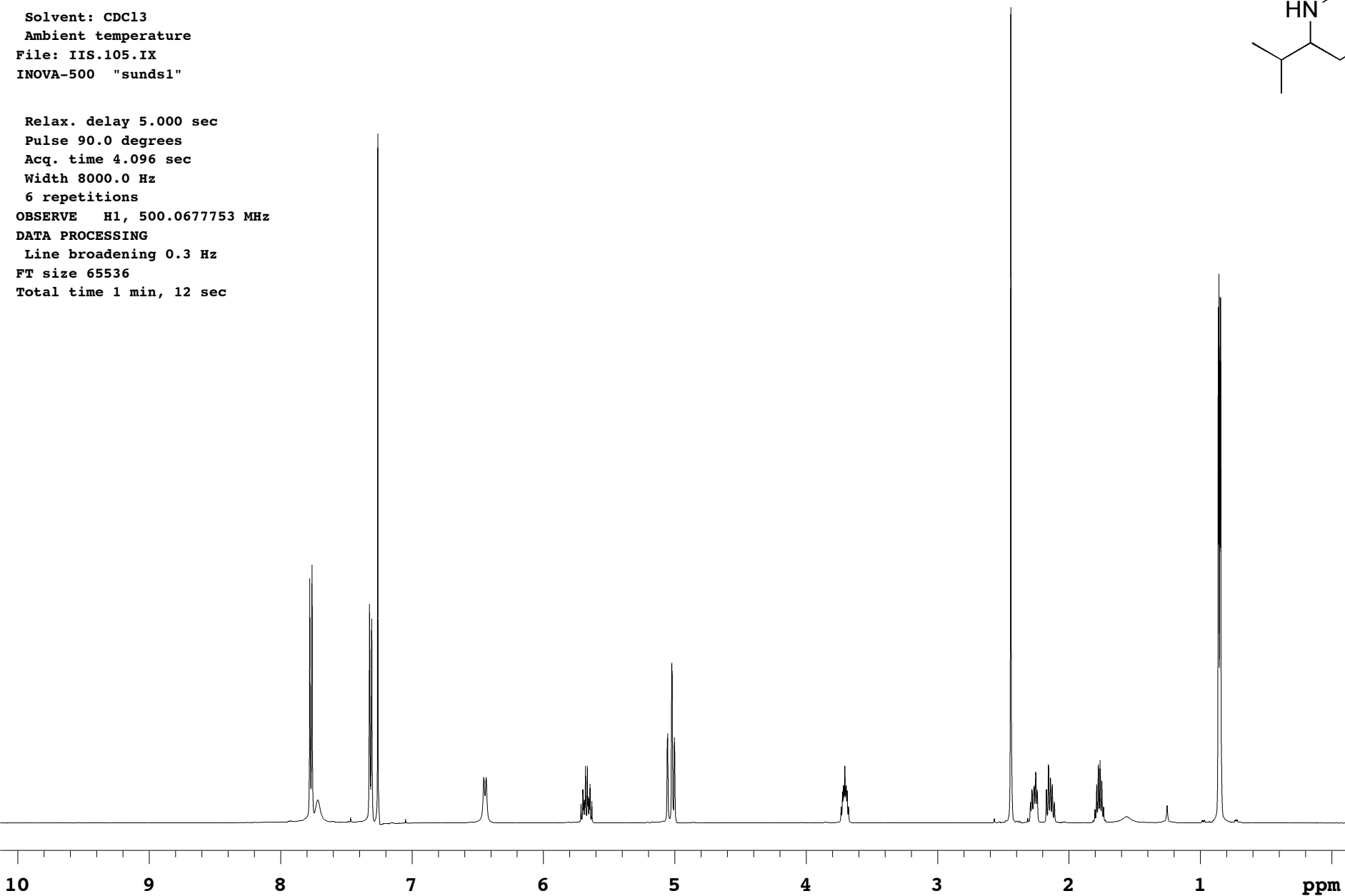
OBSERVE H1, 500.0677753 MHz

DATA PROCESSING

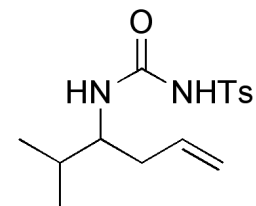
Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec







Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: Ts.SM.C13

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

658 repetitions

OBSERVE C13, 125.5817522 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

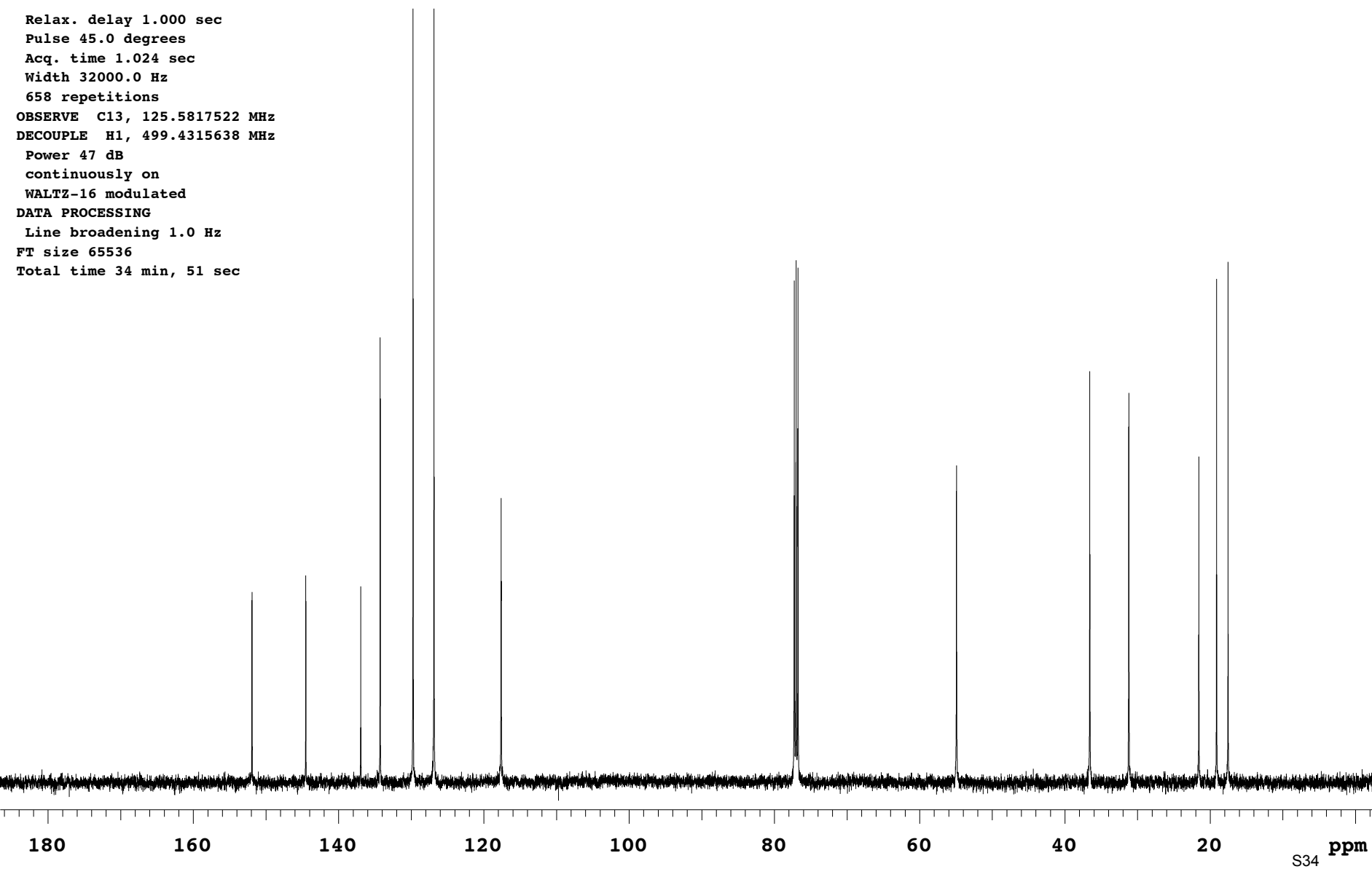
WALTZ-16 modulated

DATA PROCESSING

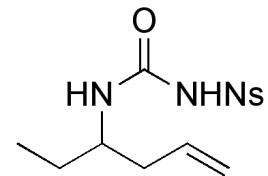
Line broadening 1.0 Hz

FT size 65536

Total time 34 min, 51 sec



# Strambeanu and White



Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "ui500nb"

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

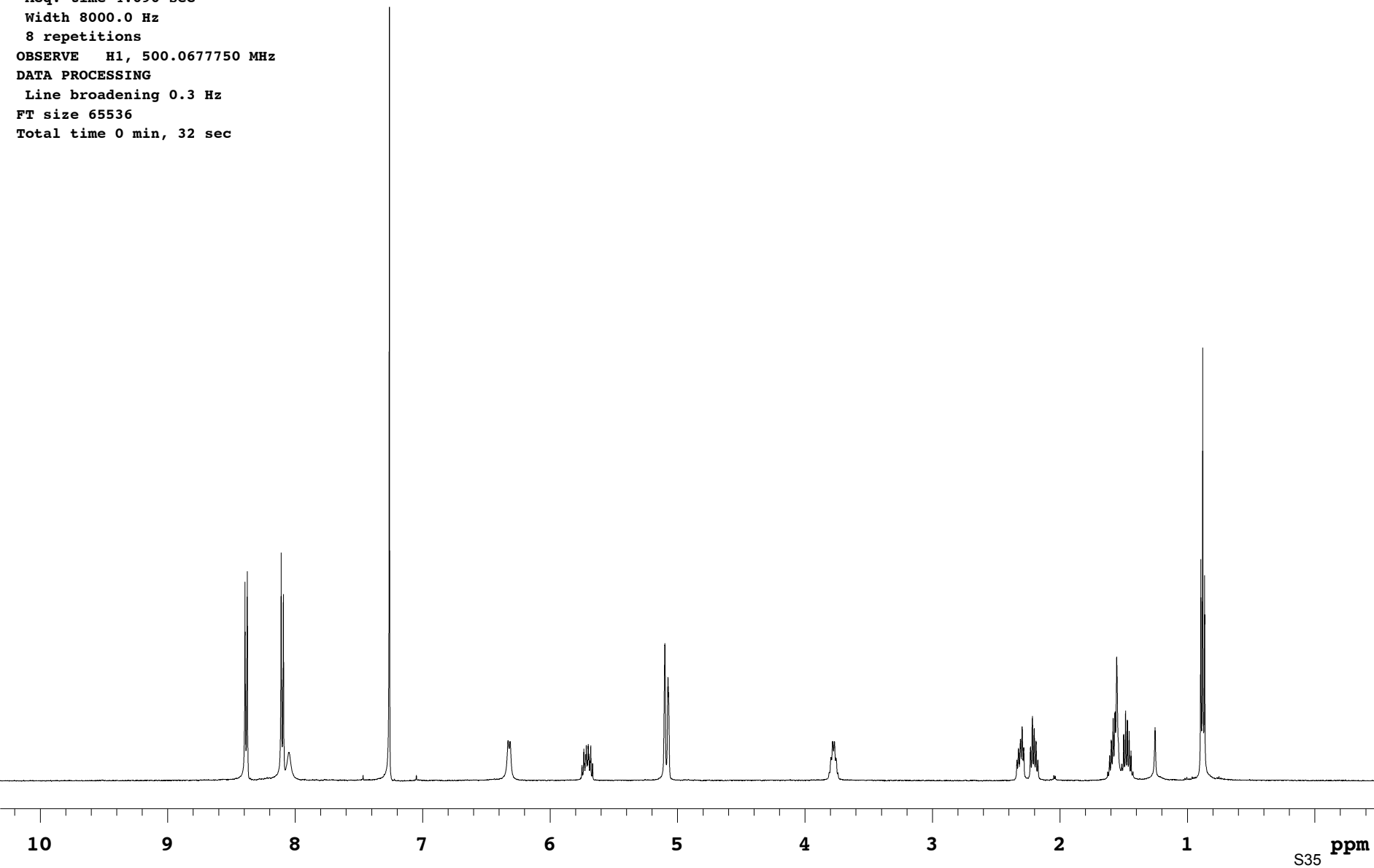
OBSERVE H1, 500.0677750 MHz

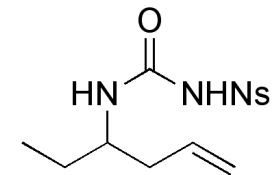
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 0 min, 32 sec



*Strambeanu and White*

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "u500"

Relax. delay 1.000 sec

Pulse 28.1 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

716 repetitions

OBSERVE C13, 125.6473175 MHz

DECOUPLE H1, 499.6923275 MHz

Power 45 dB

continuously on

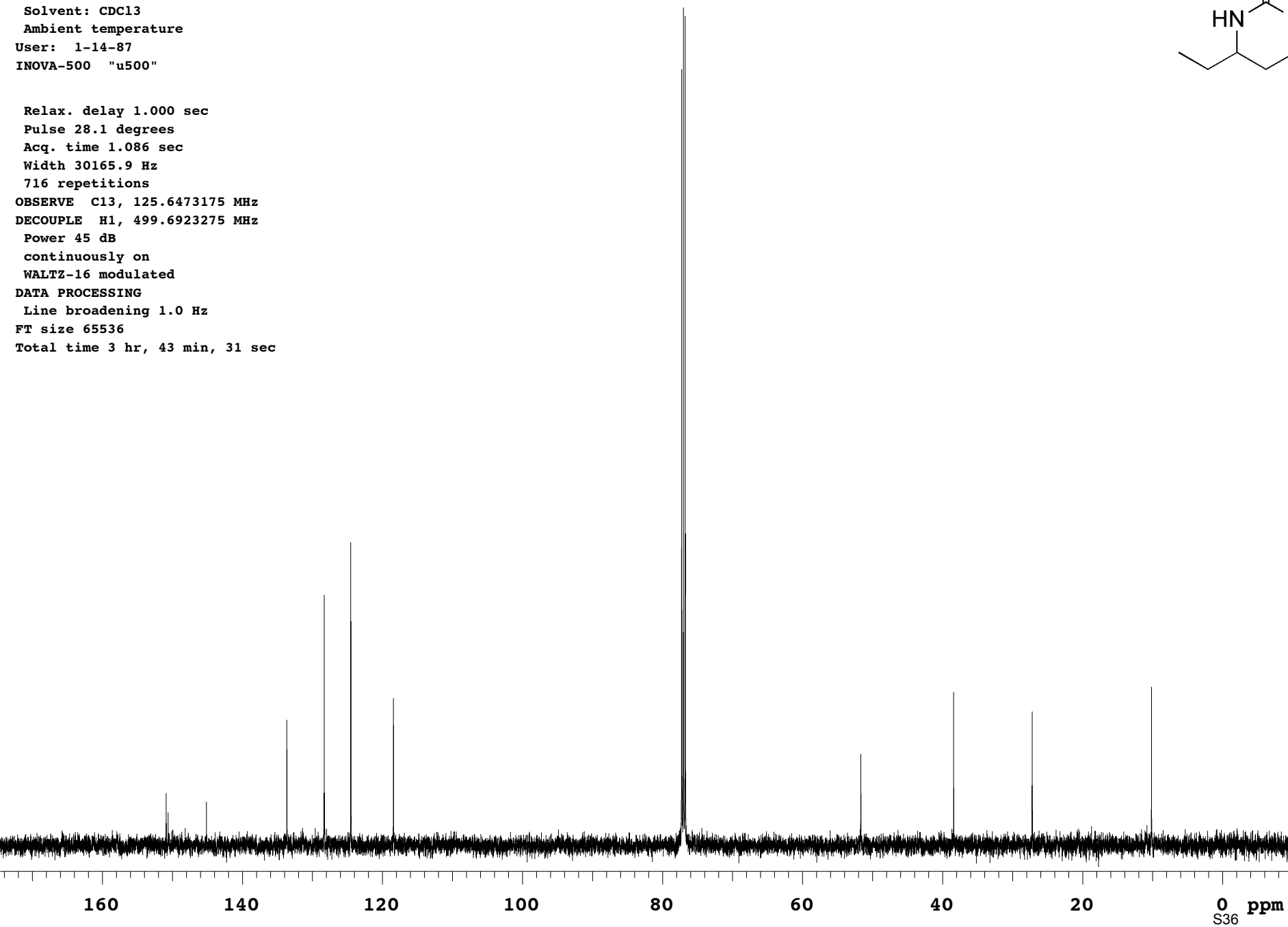
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

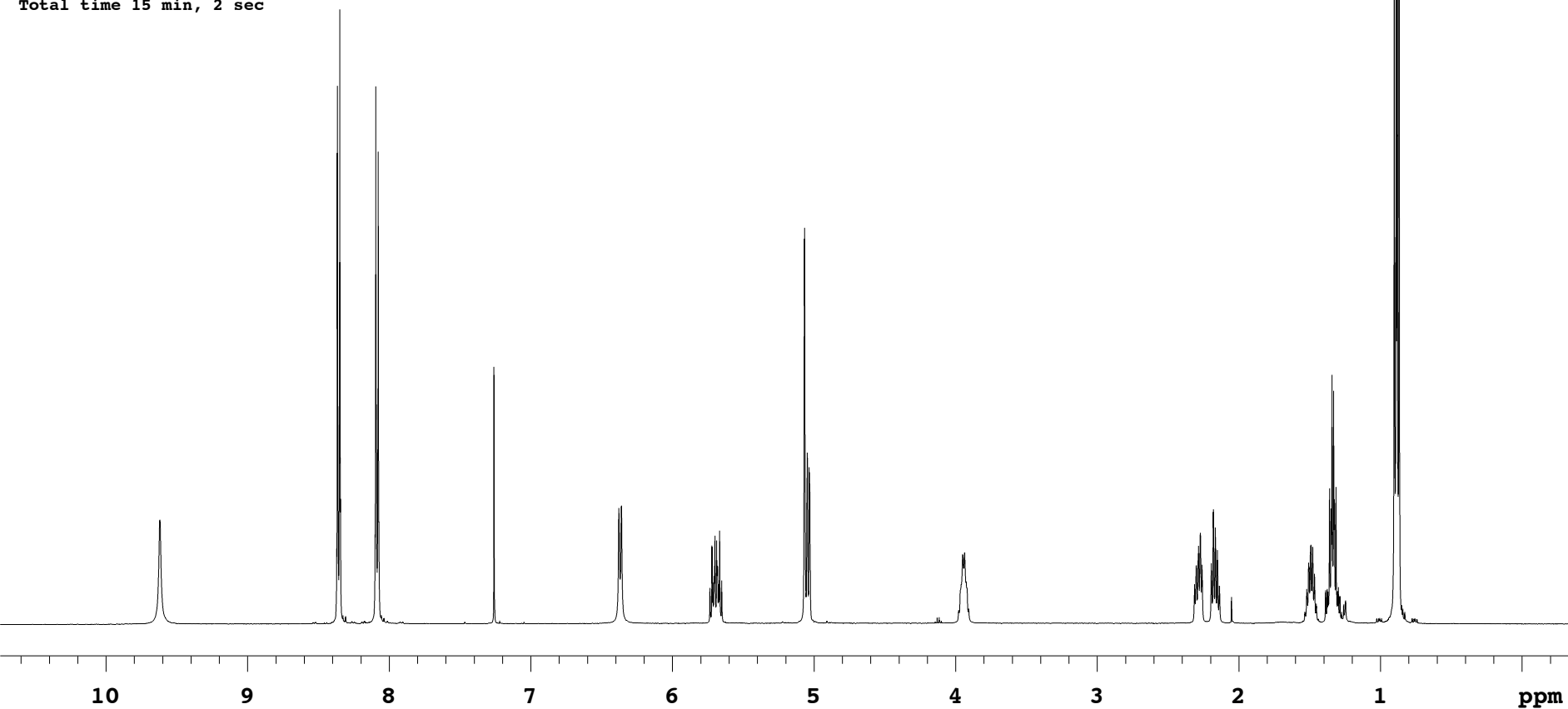
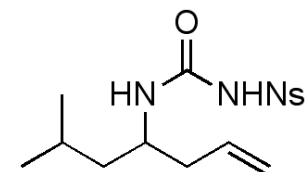
Total time 3 hr, 43 min, 31 sec

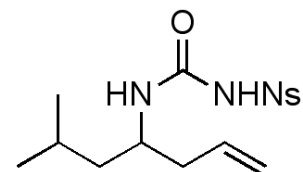


Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>  
Ambient temperature  
File: iBu\_SM  
INOVA-500 "sunds1"

Relax. delay 10.000 sec  
Pulse 45.0 degrees  
Acq. time 4.096 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.4299007 MHz  
DATA PROCESSING  
Line broadening 0.3 Hz  
FT size 65536  
Total time 15 min, 2 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: iBu\_SM\_C

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

370 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 49 dB

continuously on

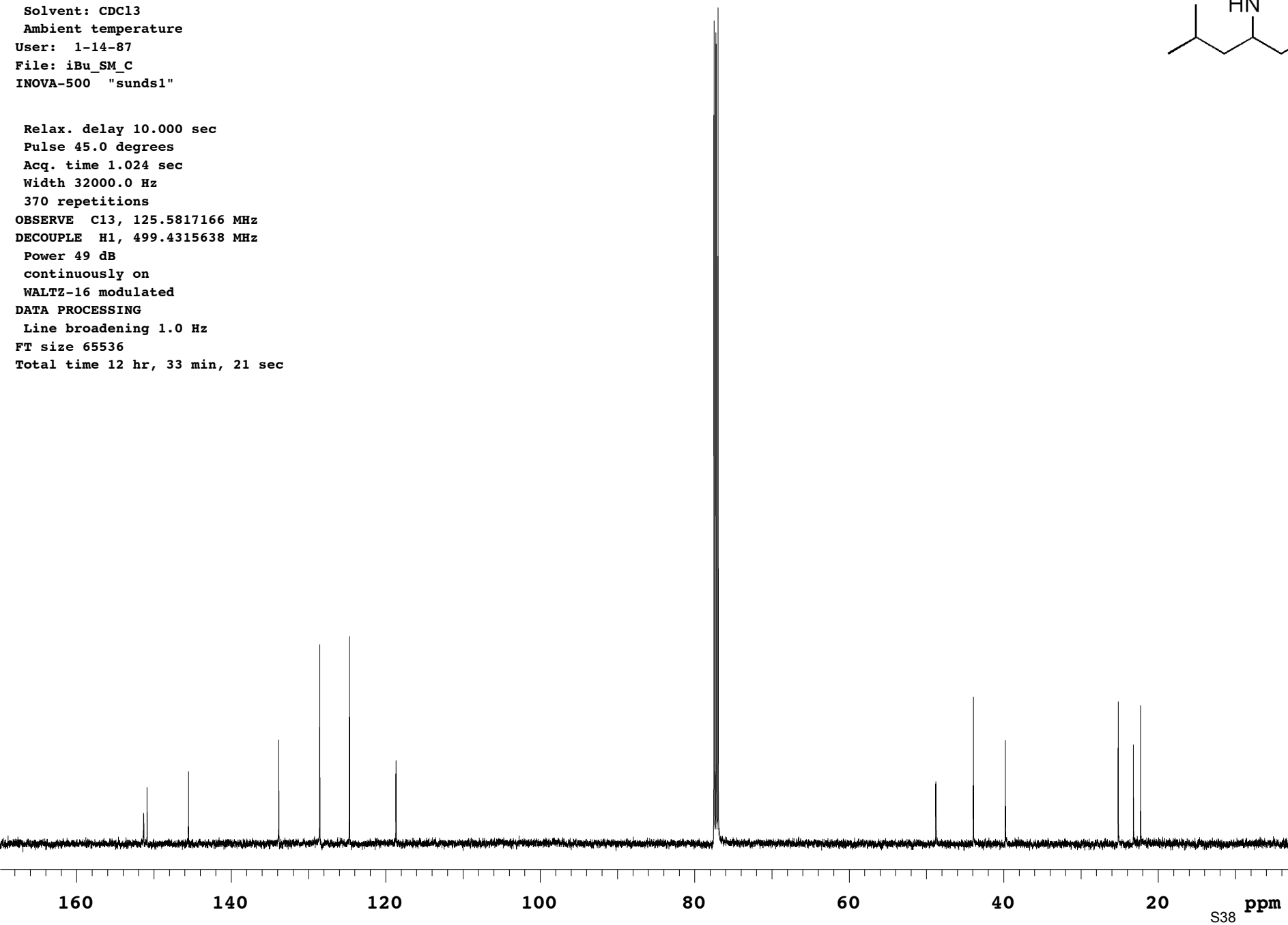
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 12 hr, 33 min, 21 sec



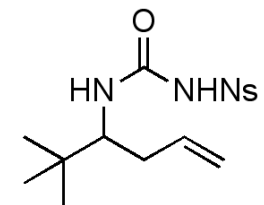
Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: tBu\_SM

INOVA-500 "sunds1"



Relax. delay 10.000 sec

Pulse 45.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

10 repetitions

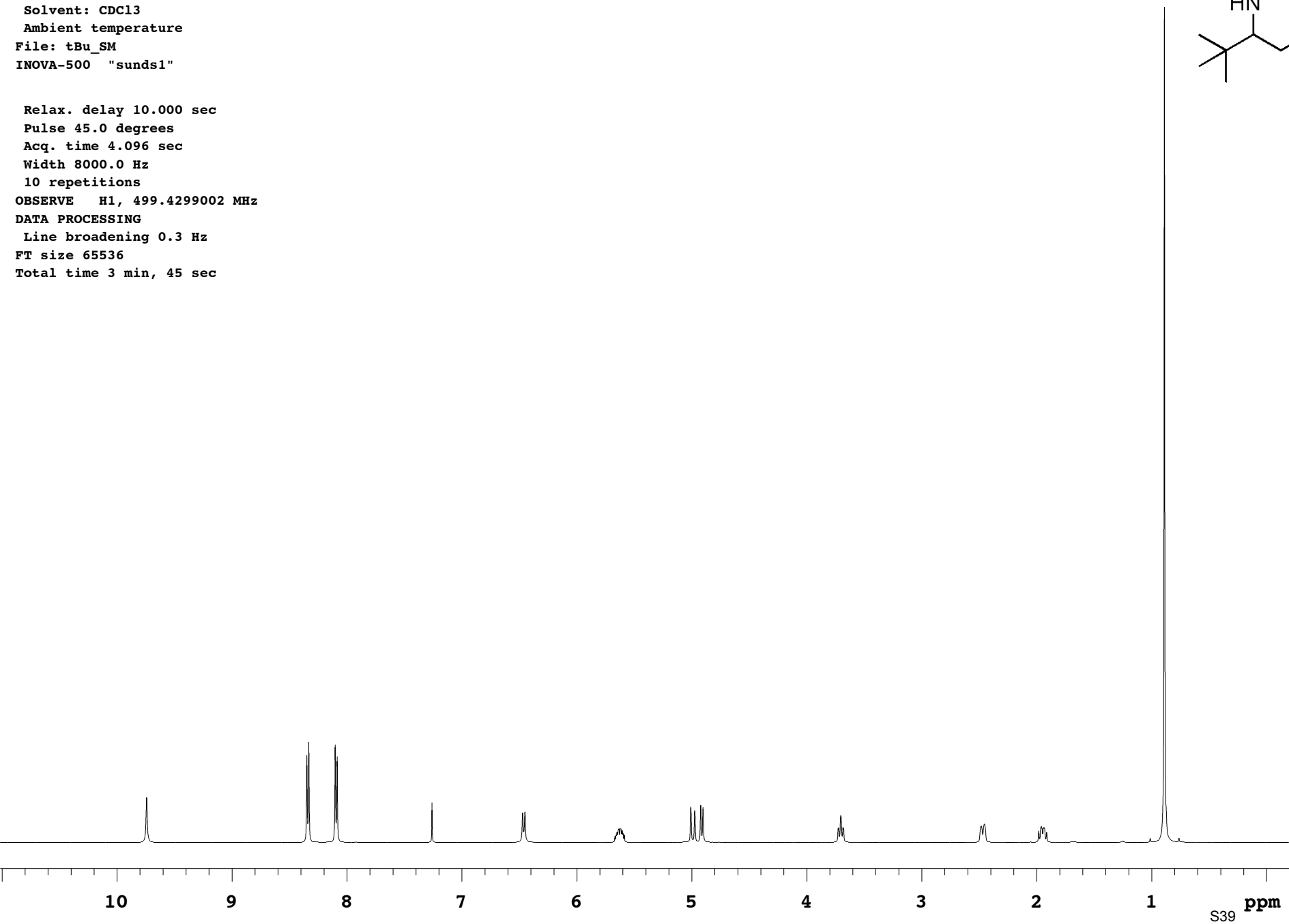
OBSERVE H1, 499.4299002 MHz

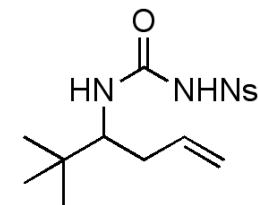
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 3 min, 45 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: tBu\_SM\_C

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

304 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 49 dB

continuously on

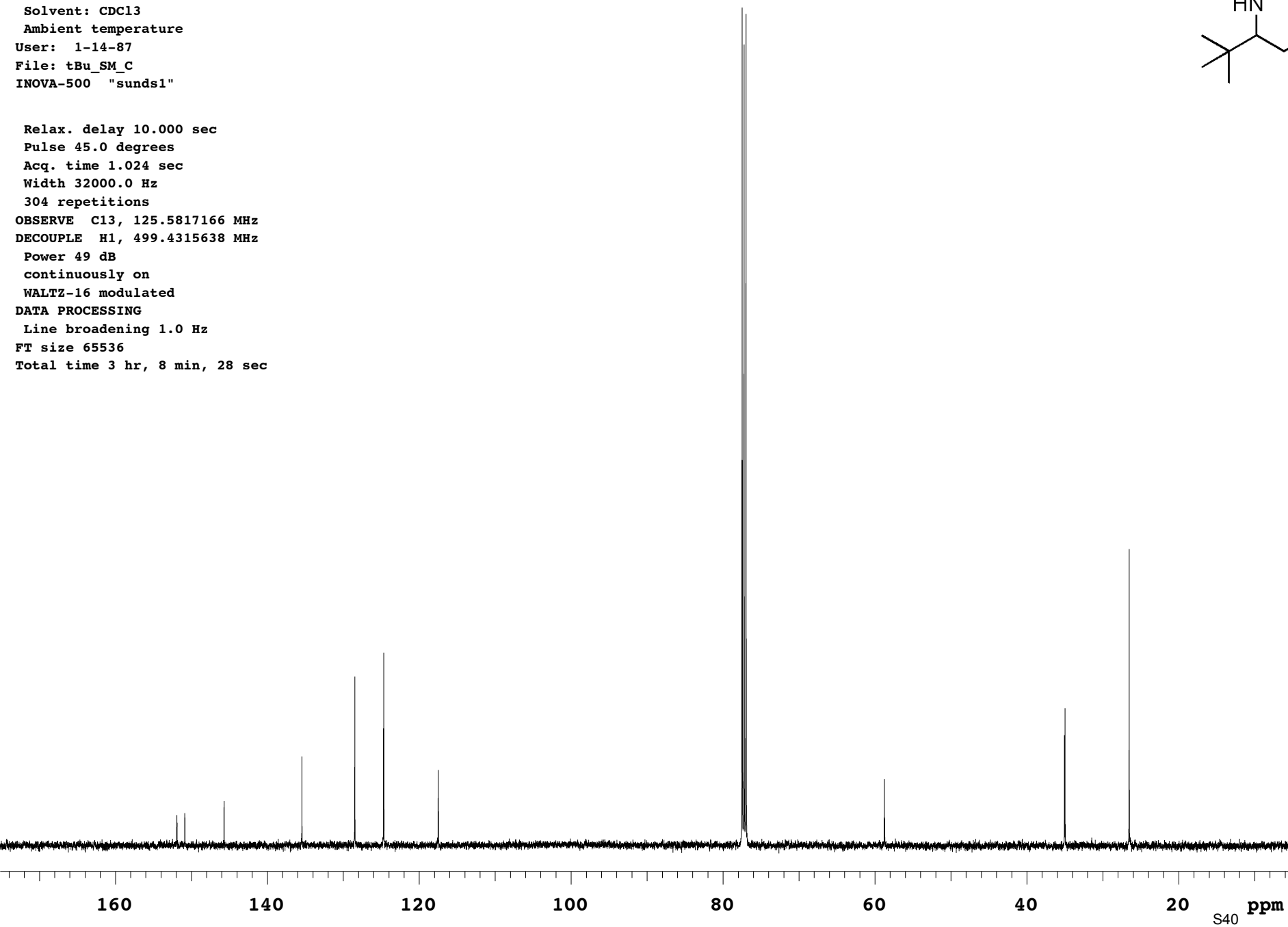
WALTZ-16 modulated

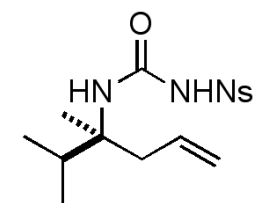
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 8 min, 28 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: quat\_SM

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

12 repetitions

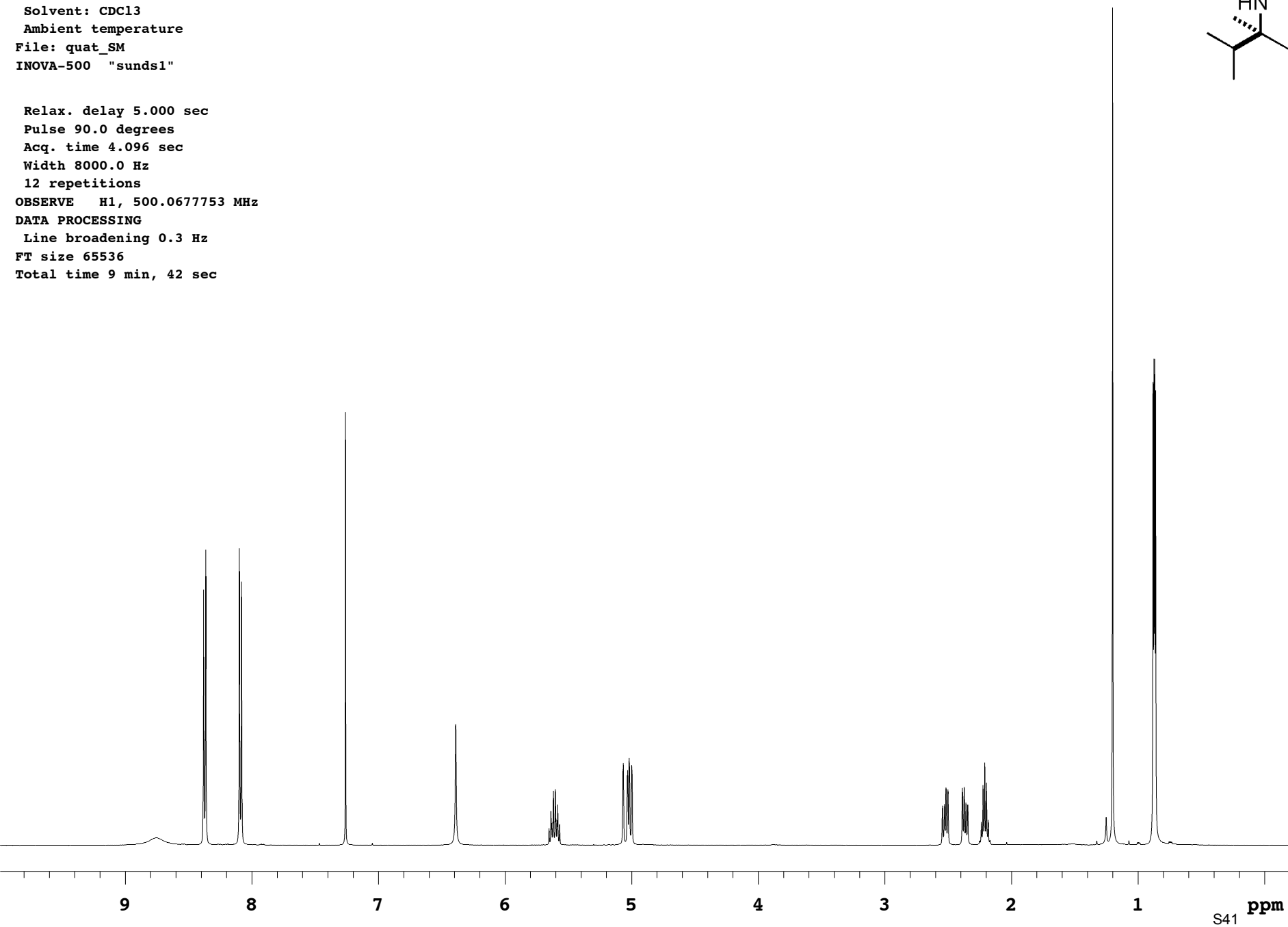
OBSERVE H1, 500.0677753 MHz

DATA PROCESSING

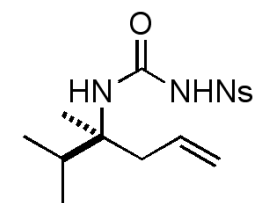
Line broadening 0.3 Hz

FT size 65536

Total time 9 min, 42 sec







Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: quat\_SM\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

726 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

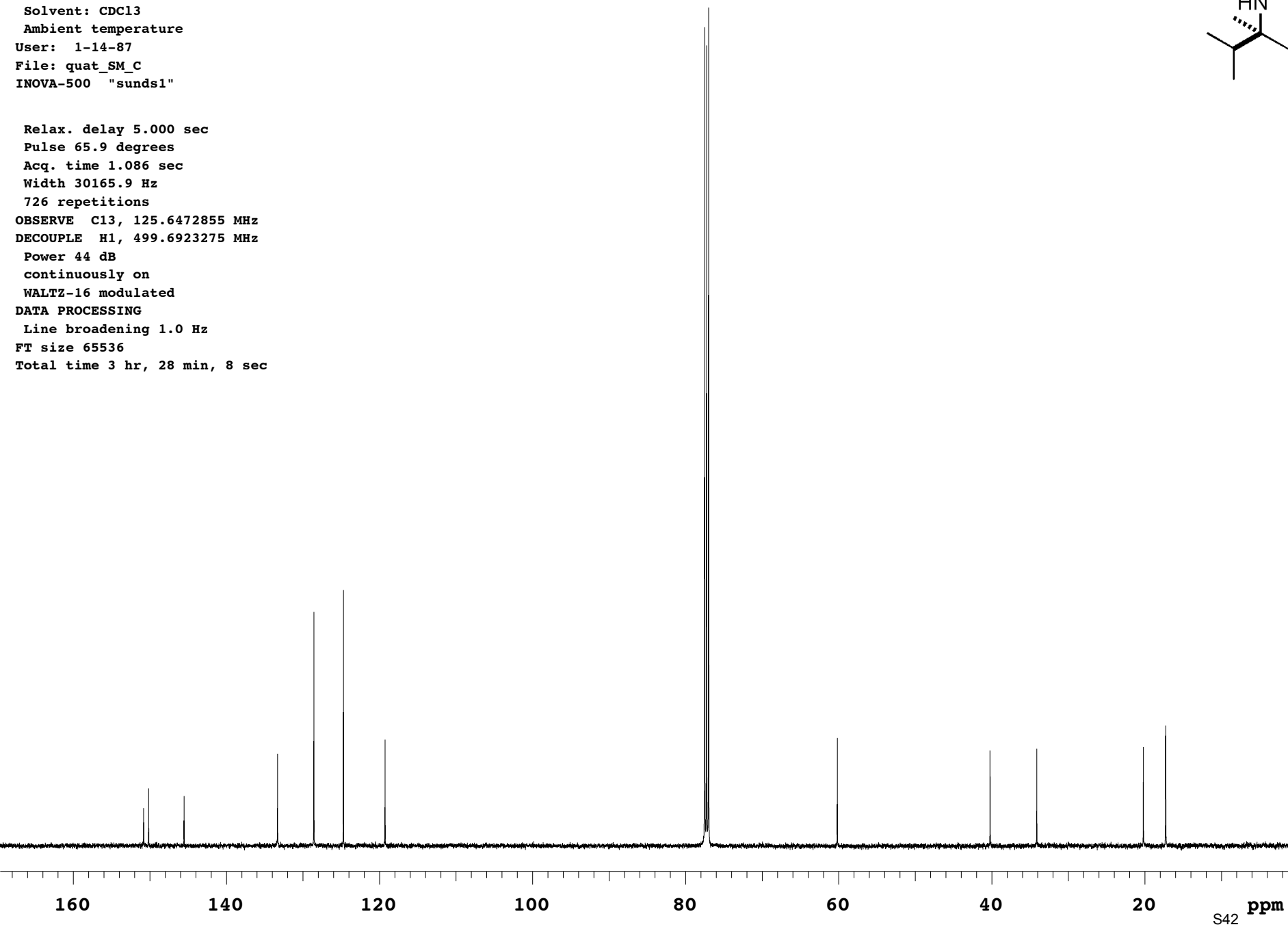
WALTZ-16 modulated

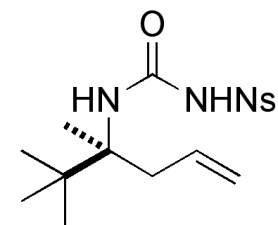
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 28 min, 8 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: IIS.88.IX

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

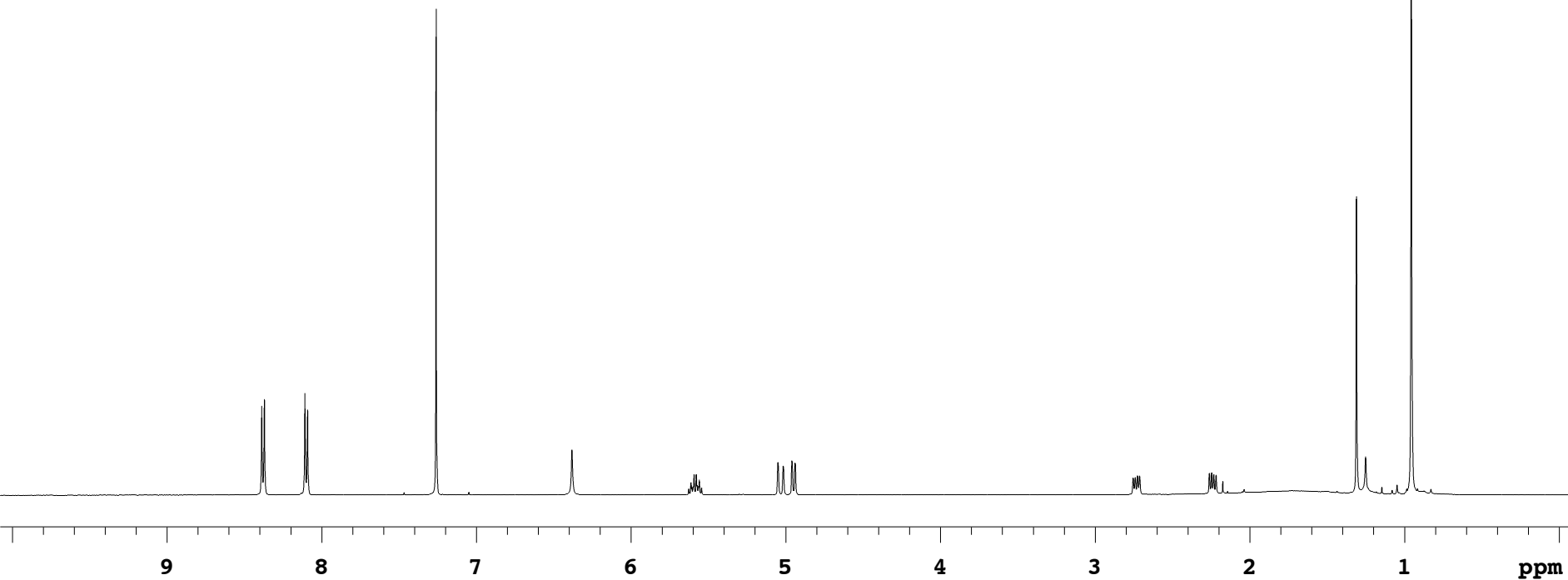
OBSERVE H1, 500.0677750 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

942 repetitions

OBSERVE C13, 125.5817473 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

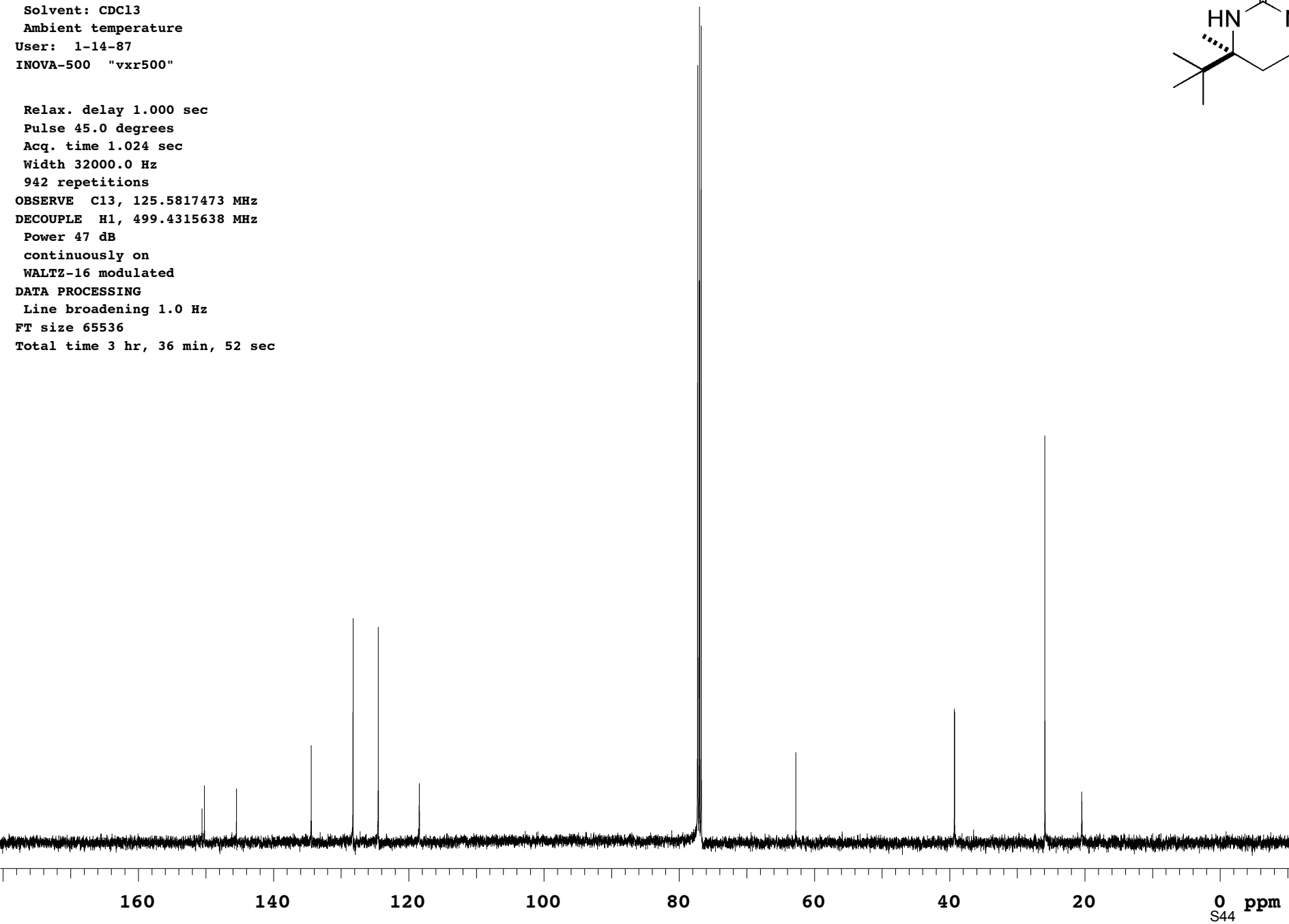
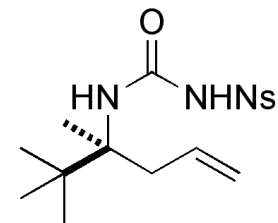
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 36 min, 52 sec



## Strambeanu and White

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "ui500nb"

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

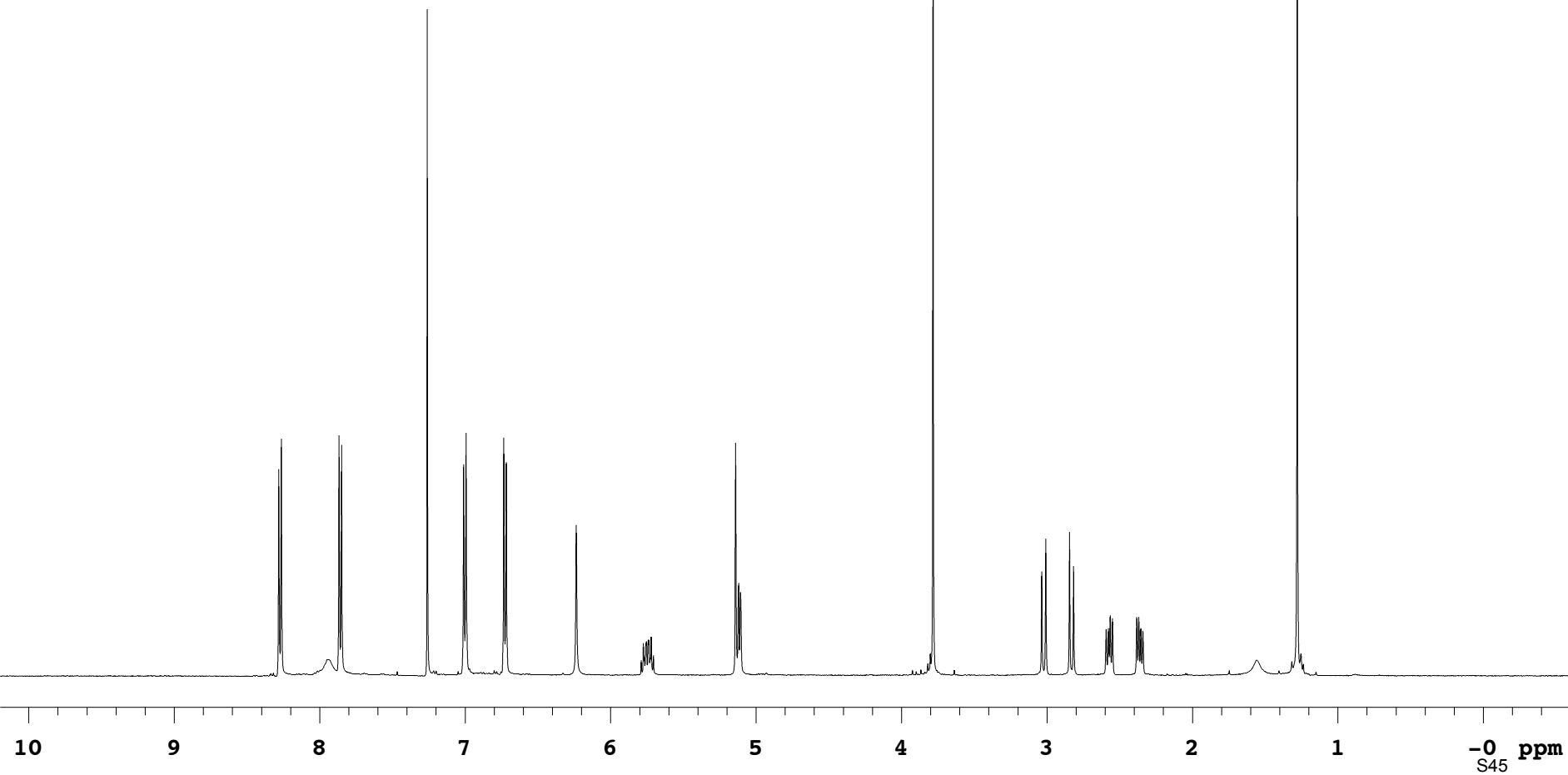
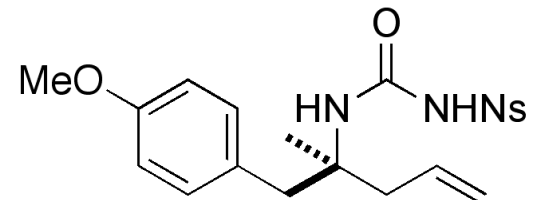
OBSERVE H1, 500.0677750 MHz

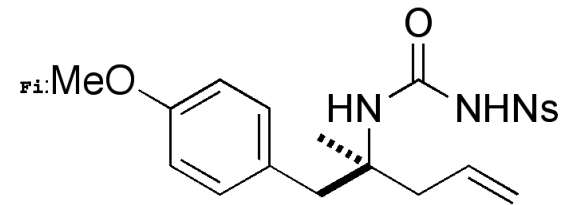
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 0 min, 32 sec





STANDARD CARBON PARAMETERS

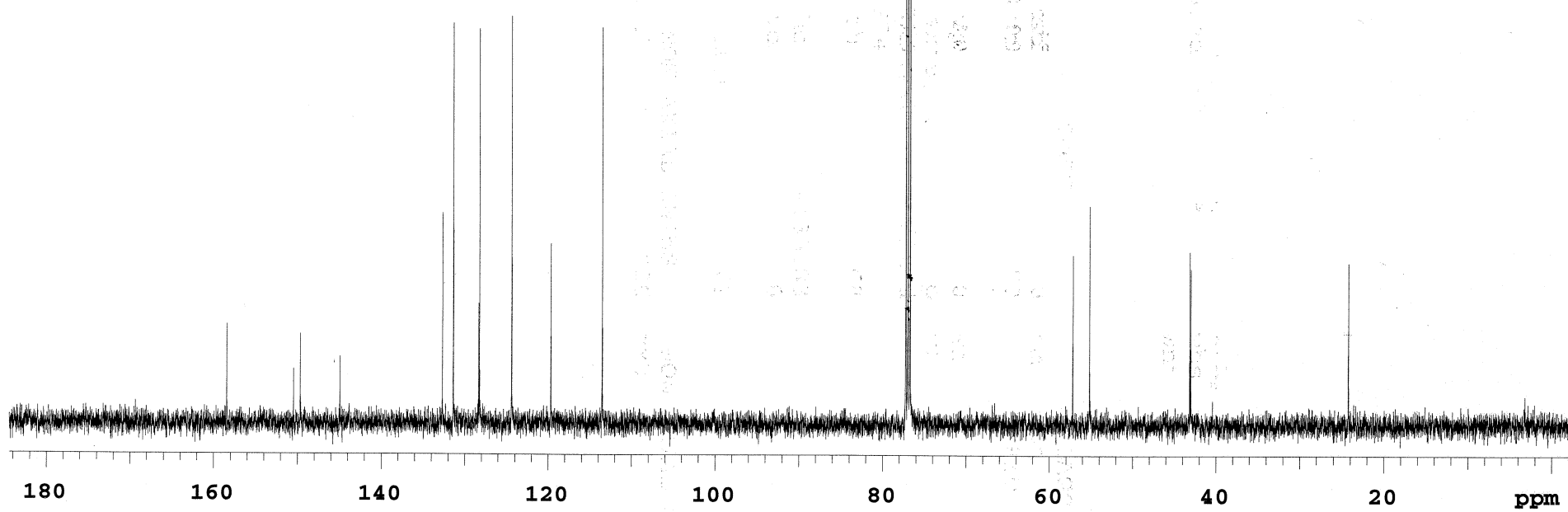
Pulse Sequence: s2pul

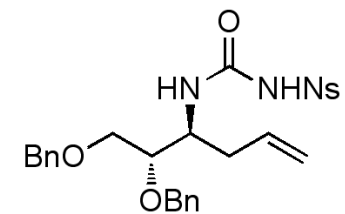
Solvent: CDCl3  
 Ambient temperature  
 User: 1-14-87  
 INOVA-500 "u500"

Relax. delay 1.000 sec  
 Pulse 28.1 degrees  
 Acq. time 1.086 sec  
 Width 30165.9 Hz  
 906 repetitions  
 OBSERVE C13, 125.6473166 MHz  
 DECOUPLE H1, 499.6923275 MHz  
 Power 45 dB  
 continuously on  
 WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz  
 FT size 65536  
 Total time 3 hr, 43 min, 31 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: OBn\_anti\_SM

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 45.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

64 repetitions

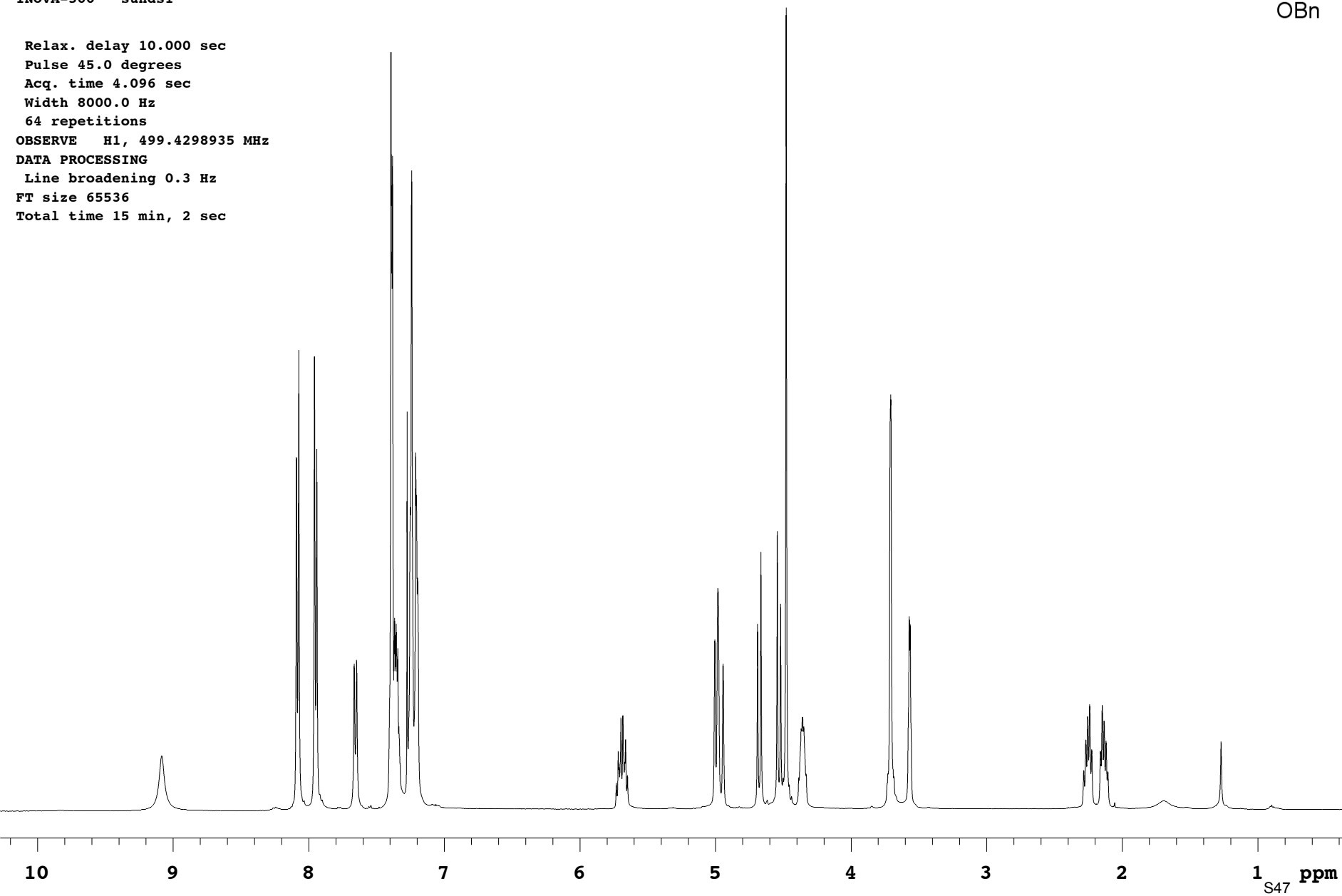
OBSERVE H1, 499.4298935 MHz

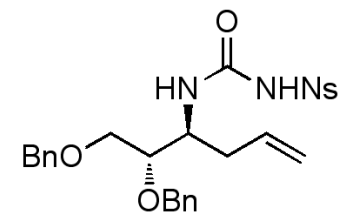
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 15 min, 2 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Temp. 20.0 C / 293.1 K

User: 1-14-87

File: OBn\_anti\_SM\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

1200 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

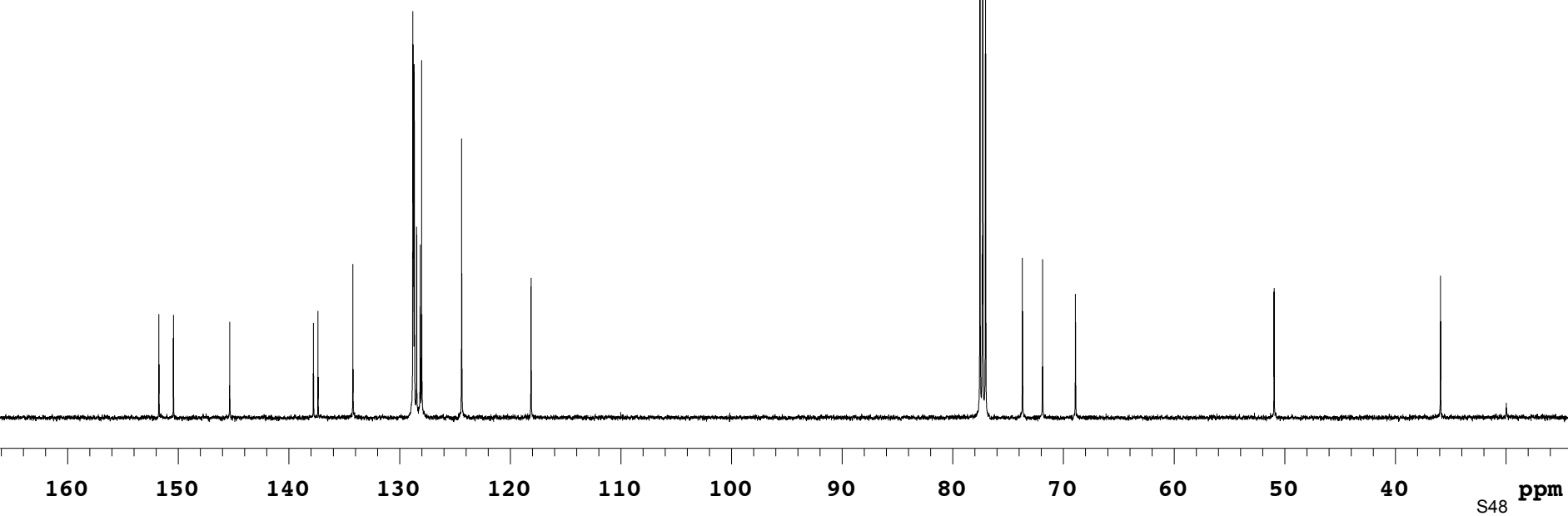
WALTZ-16 modulated

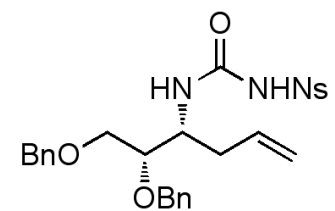
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2 hr, 32 min, 28 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: OBn\_syn\_SM1

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

16 repetitions

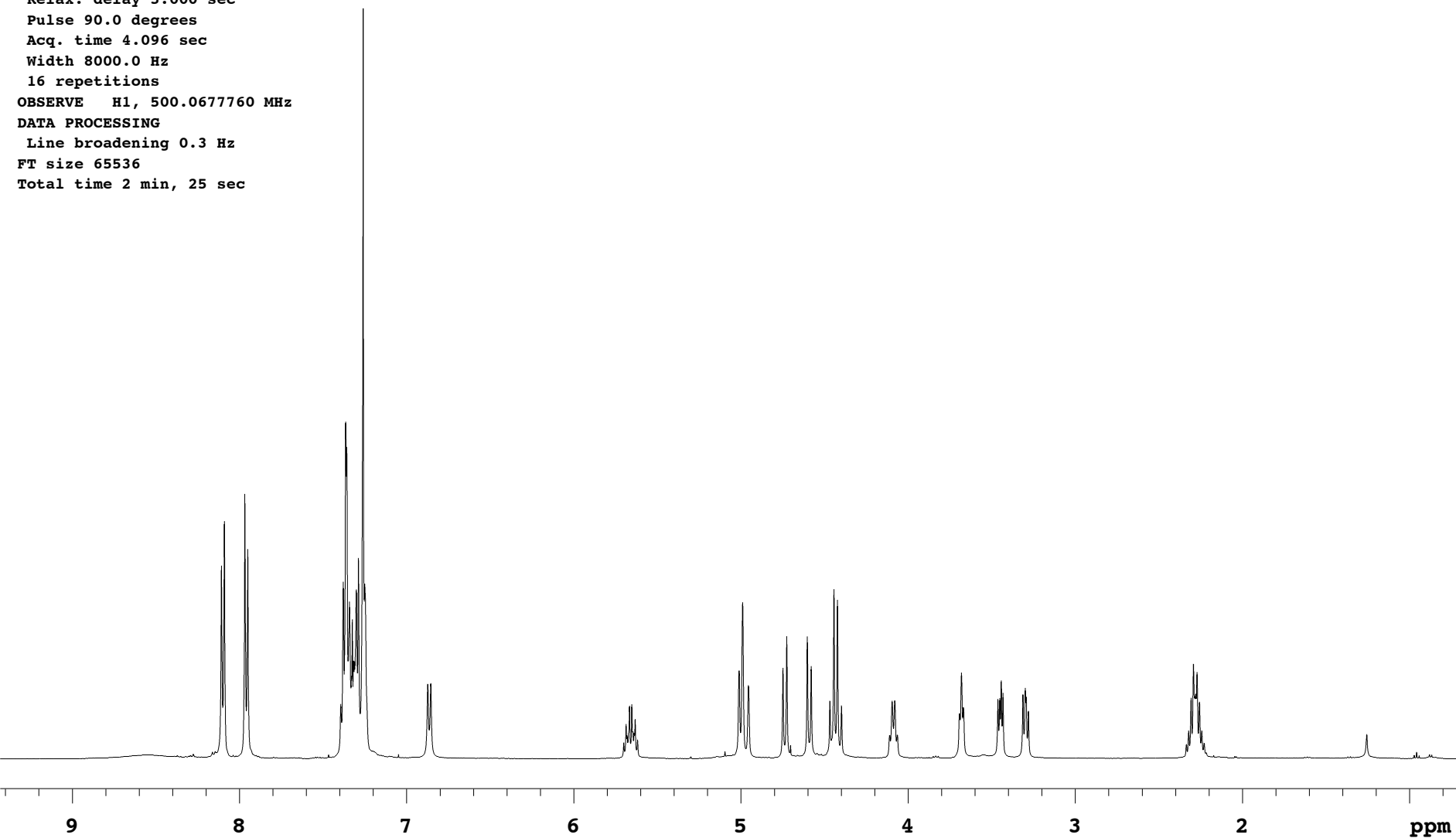
OBSERVE H1, 500.0677760 MHz

DATA PROCESSING

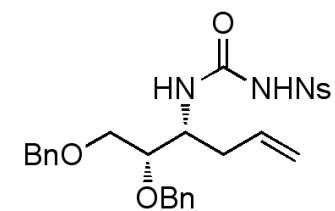
Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec







Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: OBn\_syn\_SM\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

428 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

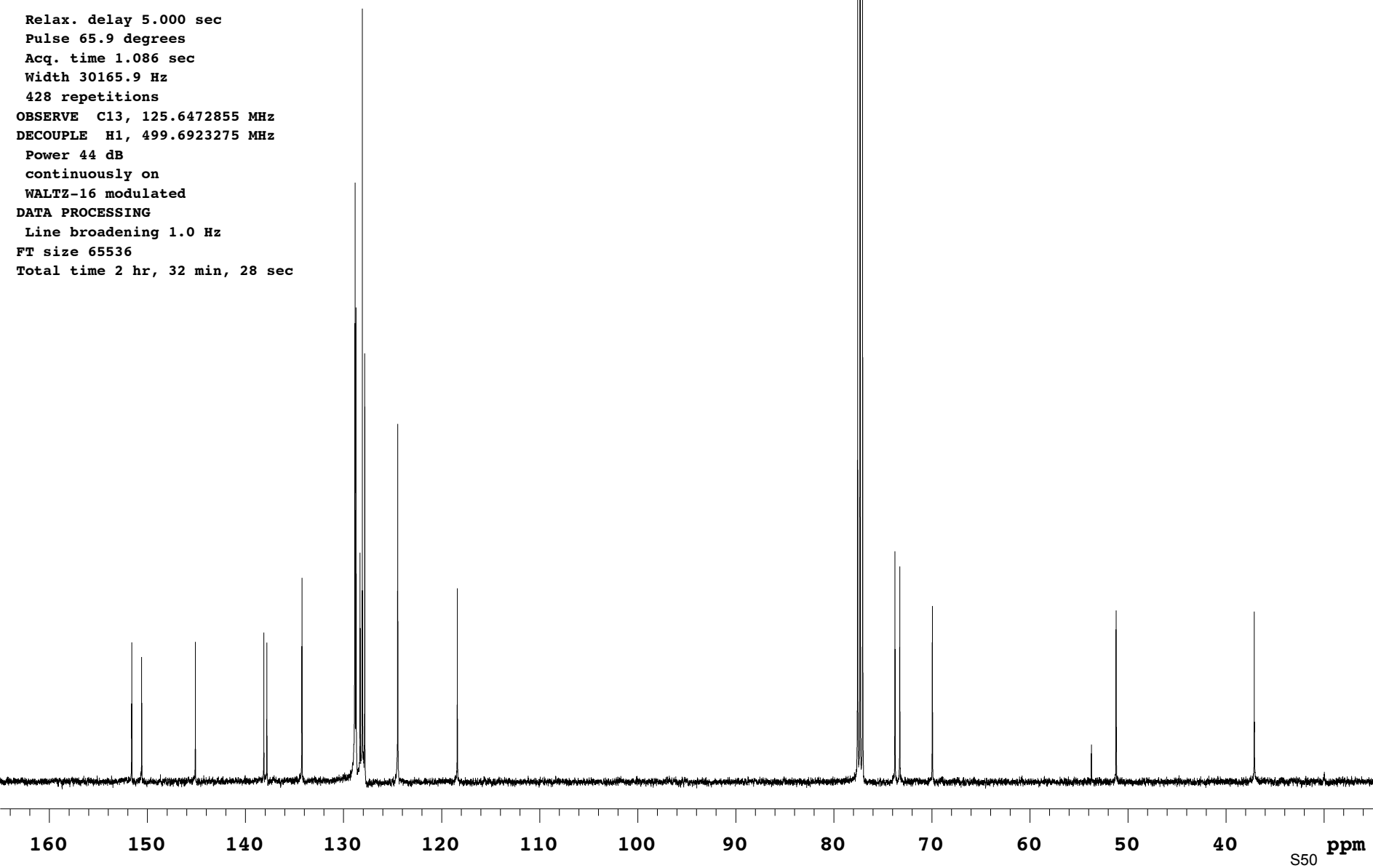
WALTZ-16 modulated

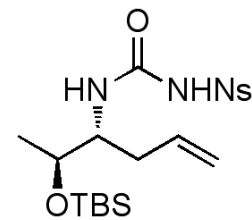
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2 hr, 32 min, 28 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: OTBSAntiUrea

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 61.6 degrees

Acq. time 4.665 sec

Width 7024.9 Hz

12 repetitions

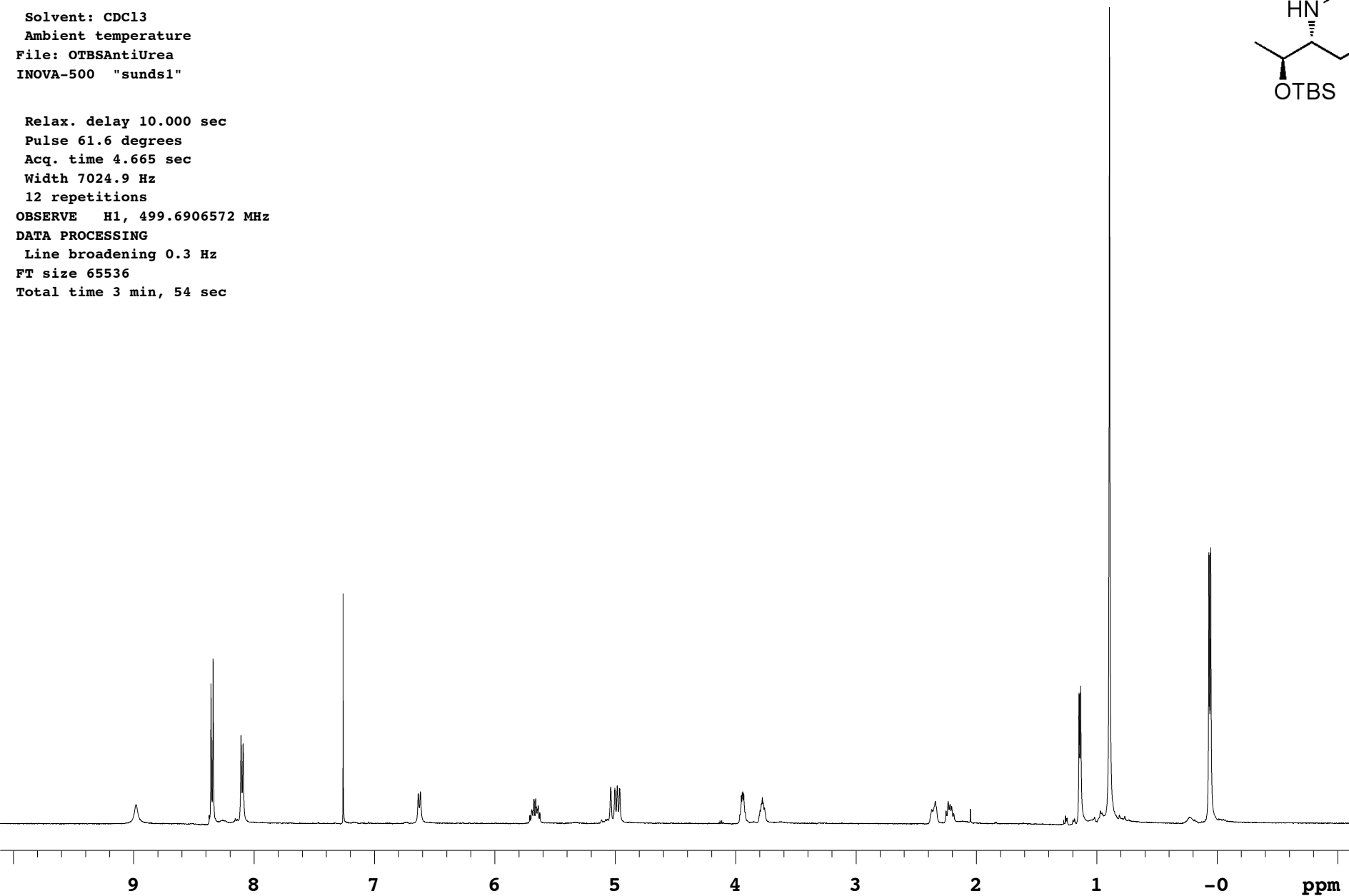
OBSERVE H1, 499.6906572 MHz

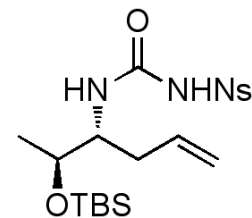
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 3 min, 54 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: OTBSAntiUreaCarb

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

1504 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

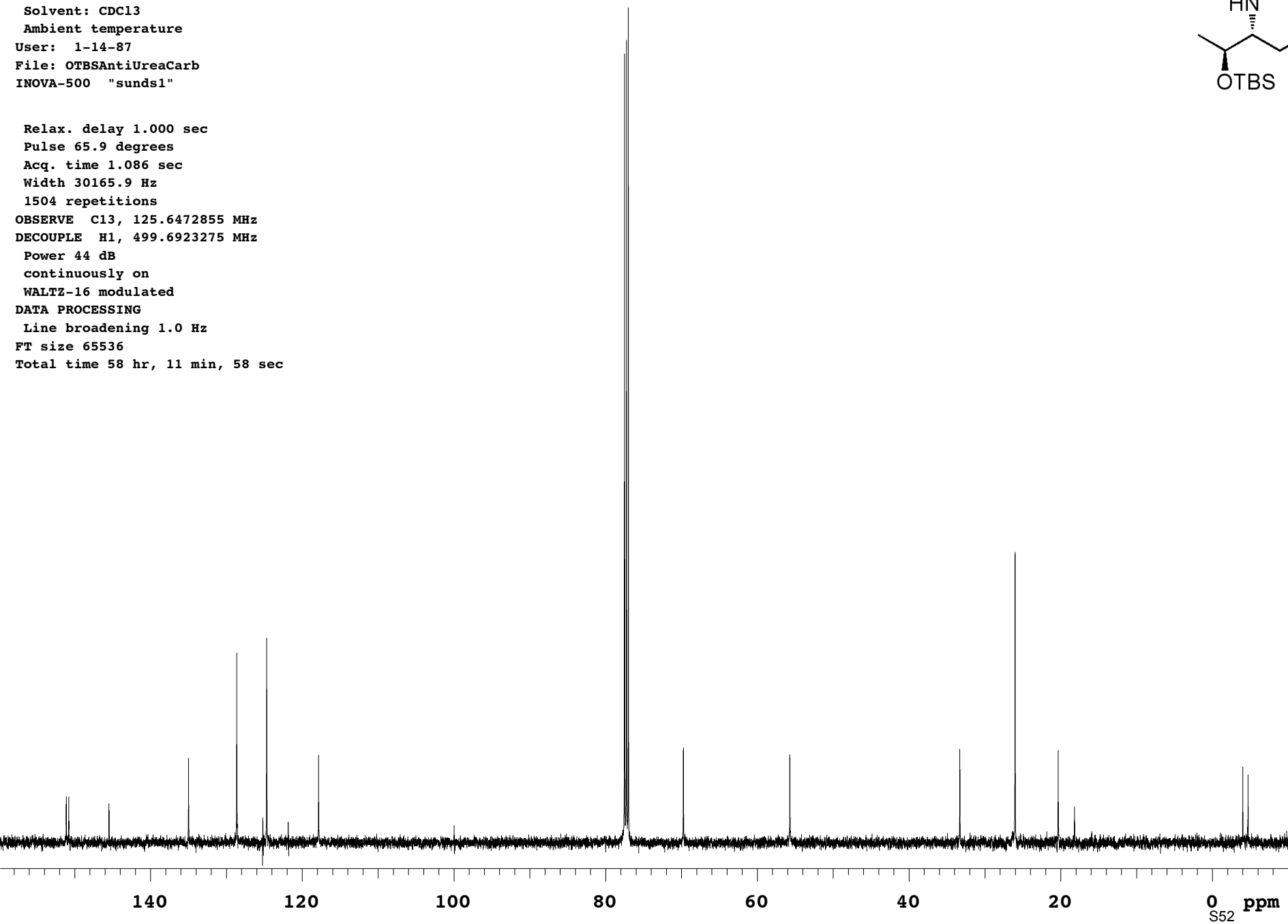
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

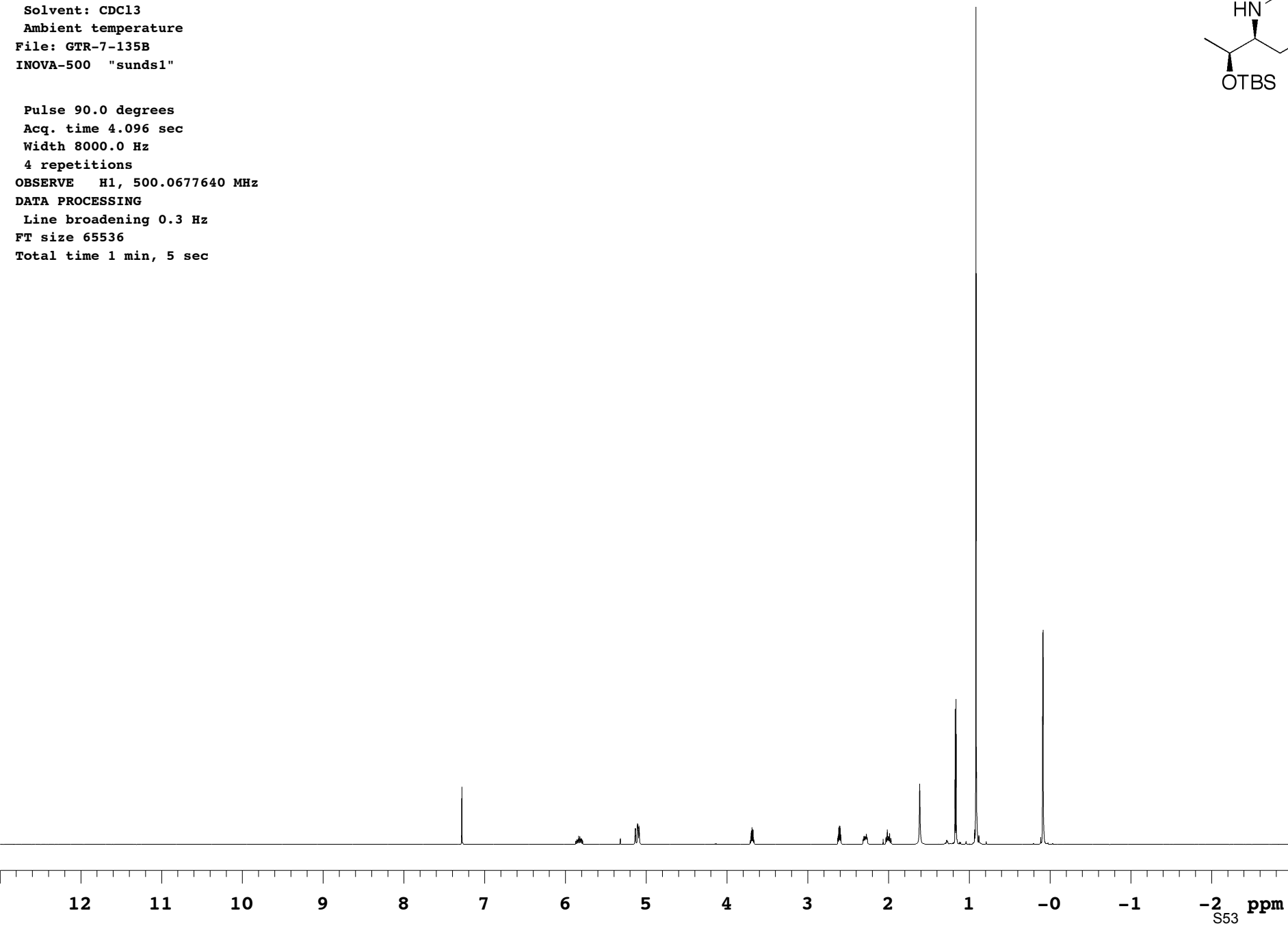
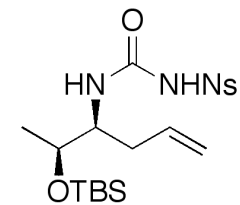
Total time 58 hr, 11 min, 58 sec

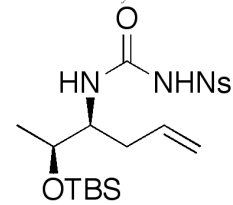


Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>  
Ambient temperature  
File: GTR-7-135B  
INOVA-500 "sunds1"

Pulse 90.0 degrees  
Acq. time 4.096 sec  
Width 8000.0 Hz  
4 repetitions  
OBSERVE H1, 500.0677640 MHz  
DATA PROCESSING  
Line broadening 0.3 Hz  
FT size 65536  
Total time 1 min, 5 sec

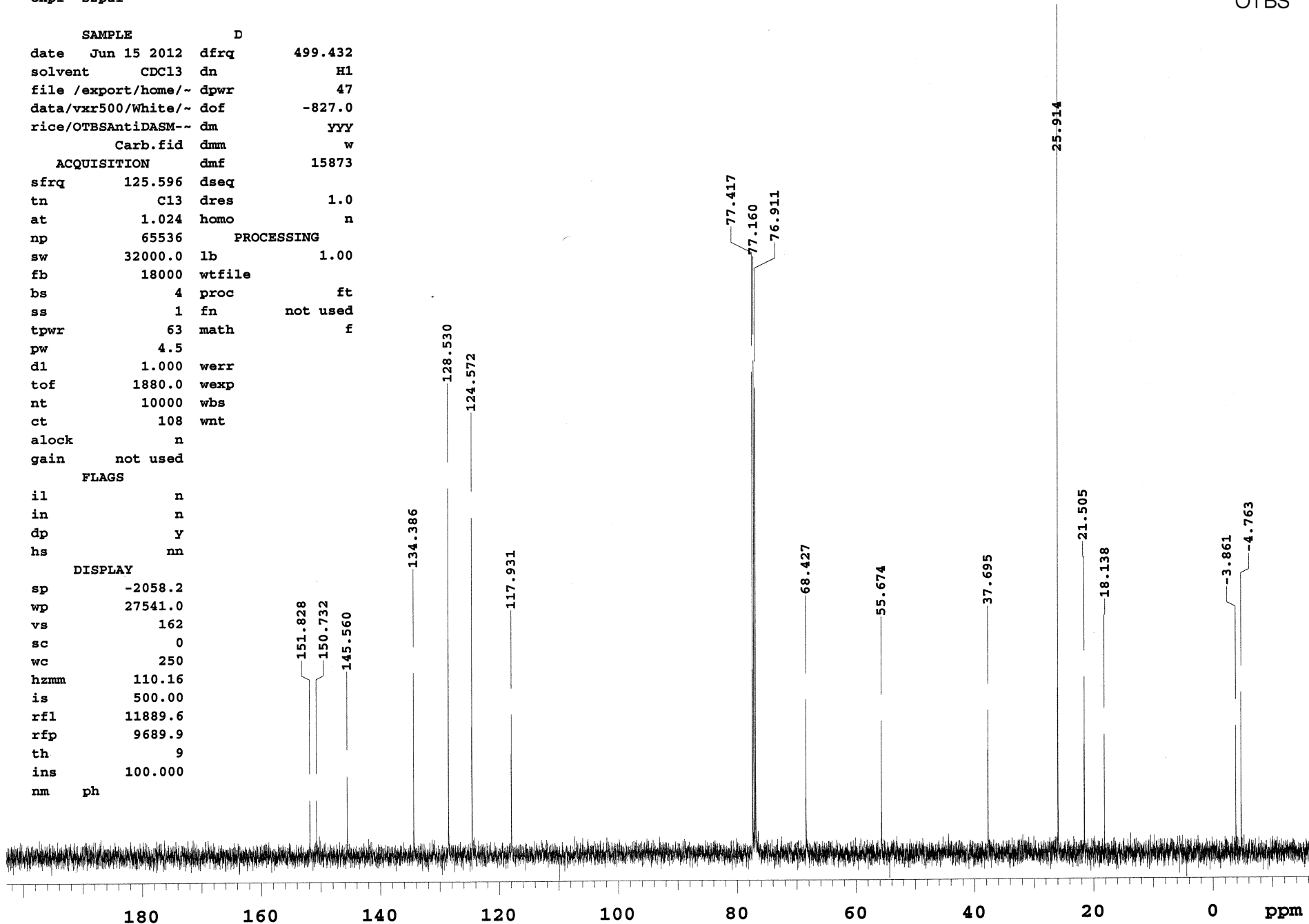




STANDARD CARBON PARAMETER

expl s2pul

SAMPLE		D
date	Jun 15 2012	dfrq 499.432
solvent	CDC13	dn H1
file	/export/home/~	dpwr 47
data/vxr500/White/~	dof -827.0	
rice/OTBSAntiDASM--	dm YYY	
Carb.fid	dmm w	
ACQUISITION		dmf 15873
sfrq	125.596	dseq
tn	C13	dres 1.0
at	1.024	homo n
np	65536	PROCESSING
sw	32000.0	lb 1.00
fb	18000	wtfile
bs	4	proc ft
ss	1	fn not used
tpwr	63	math f
pw	4.5	
d1	1.000	werr
tof	1880.0	wexp
nt	10000	wbs
ct	108	wnt
alock	n	
gain	not used	
FLAGS		
il	n	
in	n	
dp	y	
hs	nn	
DISPLAY		
sp	-2058.2	
wp	27541.0	
vs	162	
sc	0	
wc	250	
hzmm	110.16	
is	500.00	
rfl	11889.6	
rfp	9689.9	
th	9	
ins	100.000	
nm	ph	



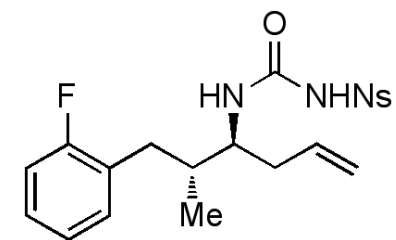
Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: FPhdiamineSM

INNOVA-500 "sunds1"



Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

16 repetitions

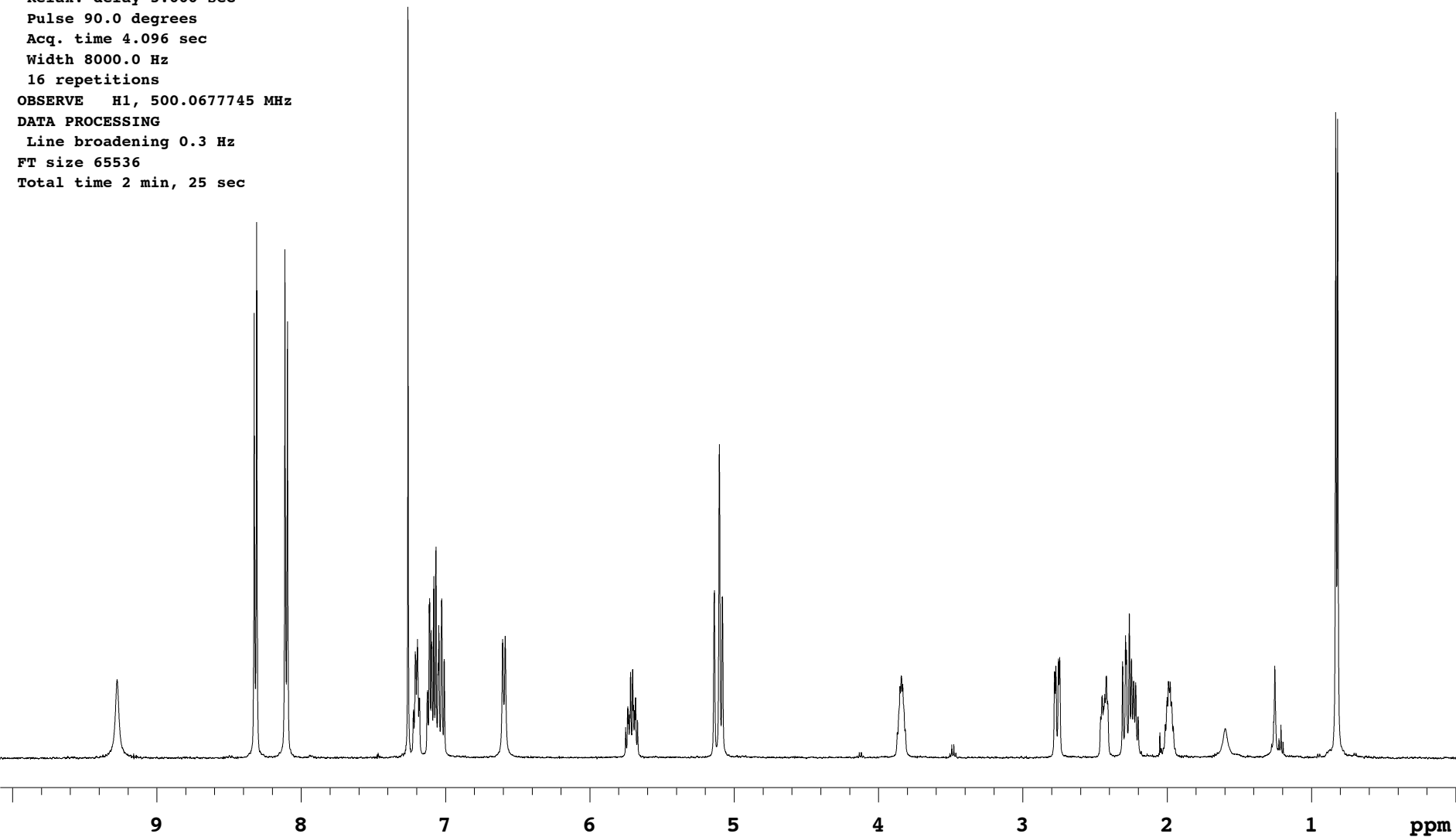
OBSERVE H1, 500.0677745 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: FPhSynDiamSMBest

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 36.5 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

488 repetitions

OBSERVE C13, 125.6472956 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

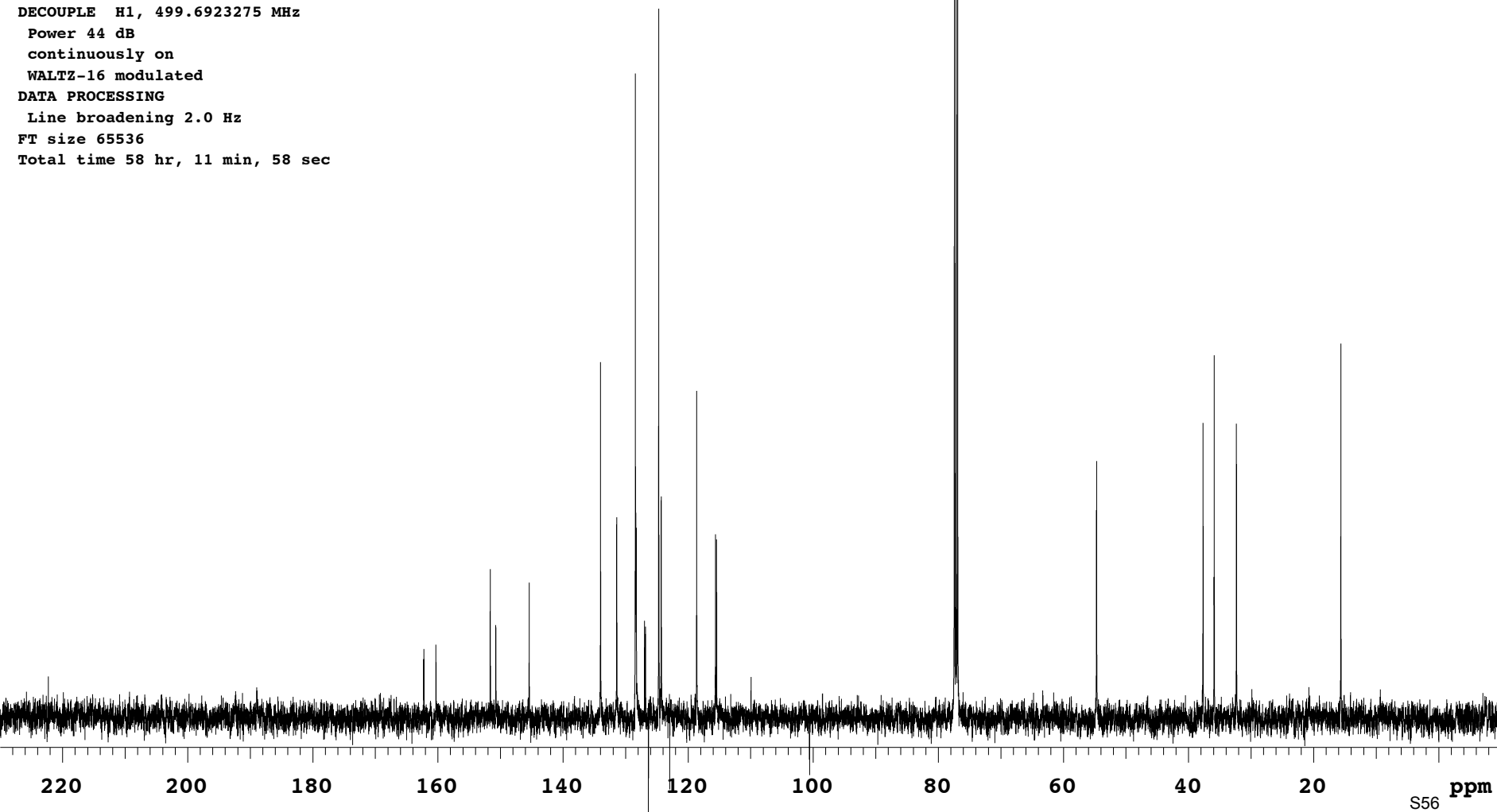
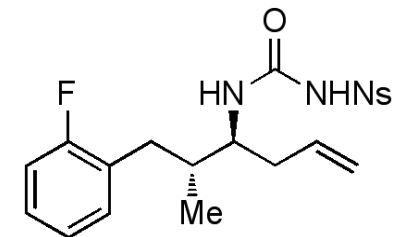
WALTZ-16 modulated

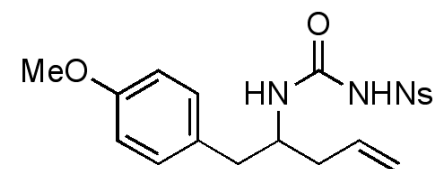
DATA PROCESSING

Line broadening 2.0 Hz

FT size 65536

Total time 58 hr, 11 min, 58 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: OMe\_SM

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

10 repetitions

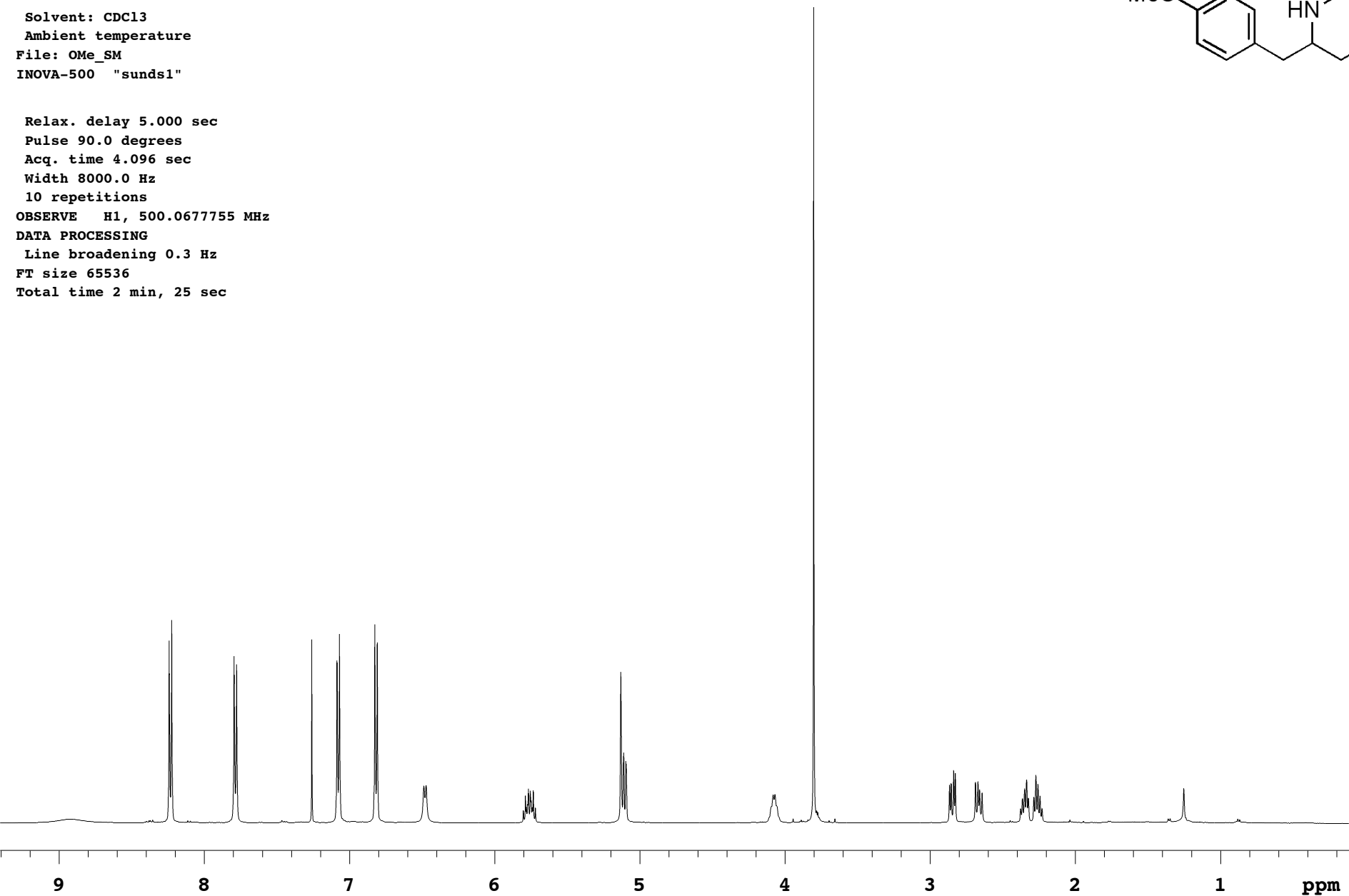
OBSERVE H1, 500.0677755 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: OMe\_SM\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

906 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 48 dB

continuously on

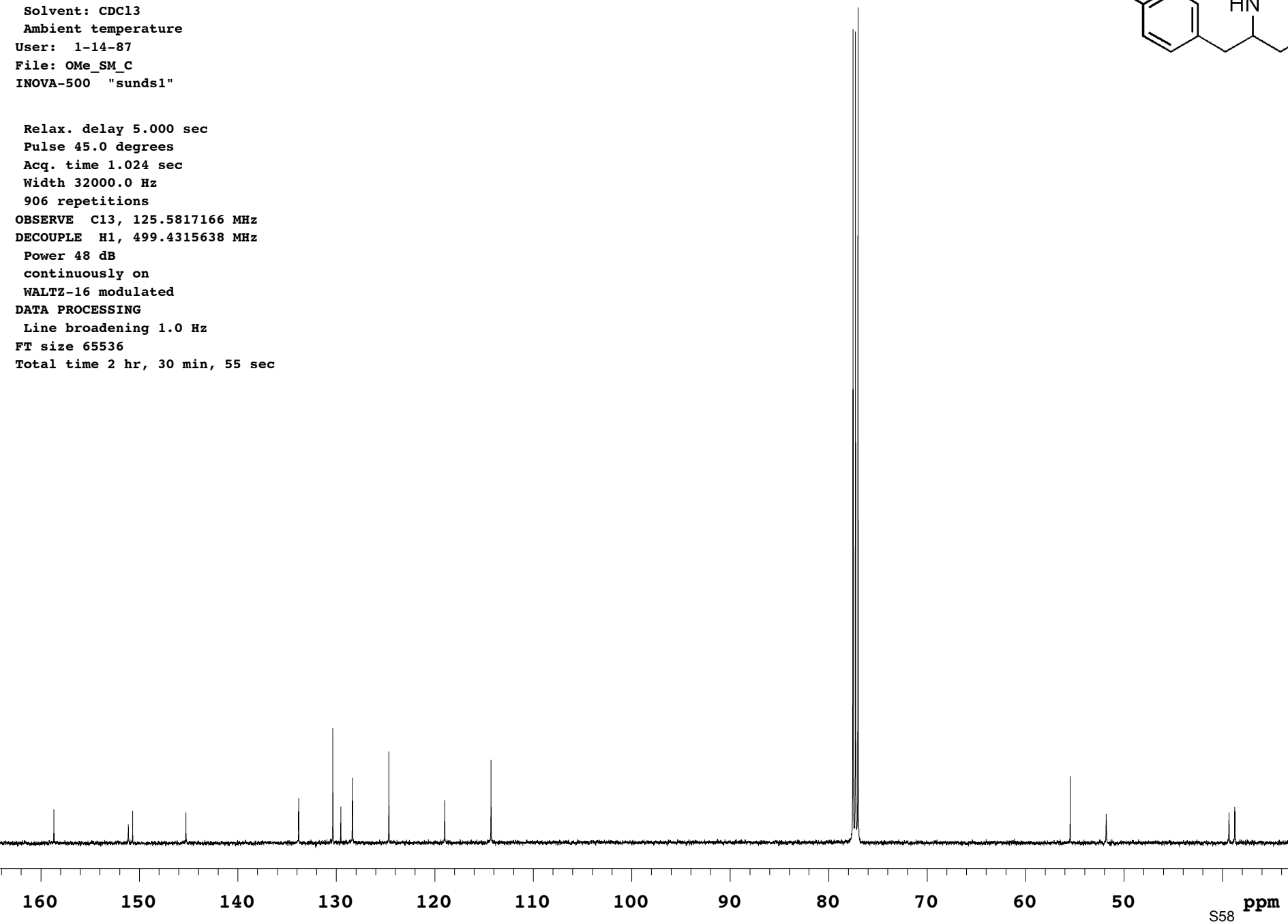
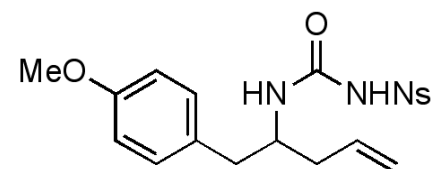
WALTZ-16 modulated

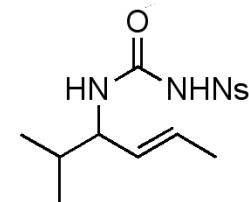
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2 hr, 30 min, 55 sec

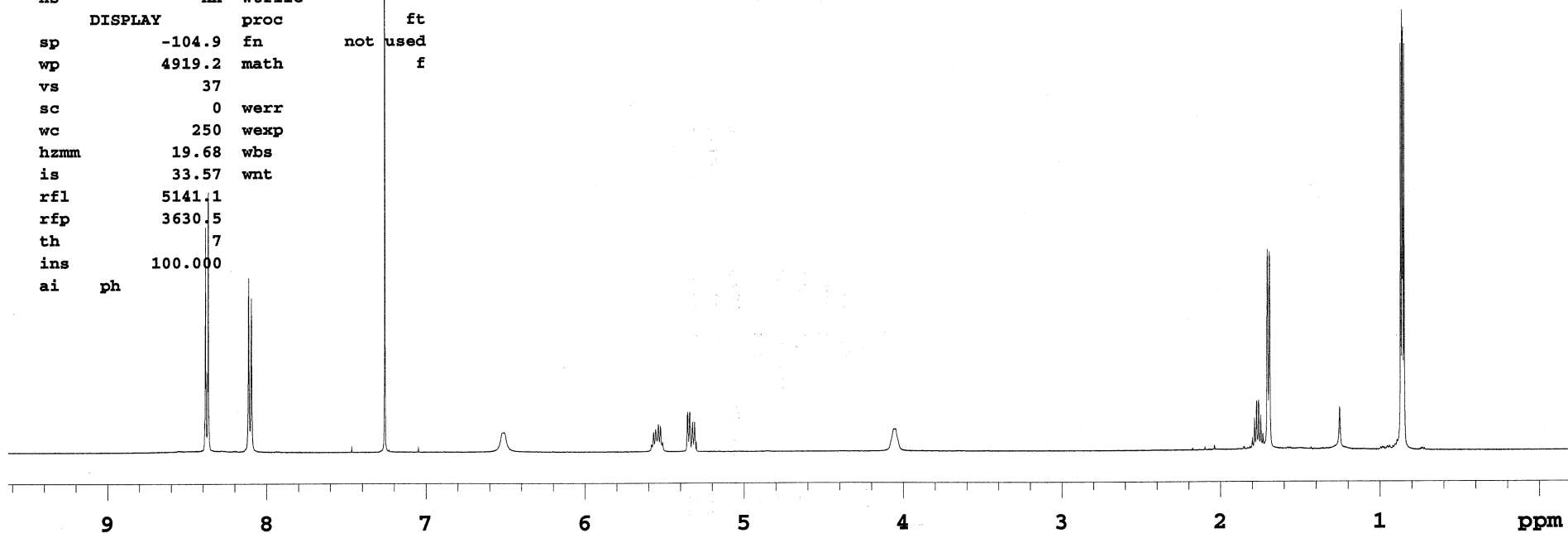


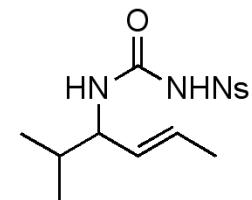


## STANDARD PROTON PARAMETERS

exp1 s2pu1

SAMPLE		DEC. & VT	
date	Mar 9 2010	dfrq	500.070
solvent	CDC13	dn	H1
file	exp	dpwr	18
ACQUISITION		dof	
sfrq	500.070	dm	nnn
tn	H1	dmm	c
at	4.096	dmf	200
np	65536	dseq	
sw	8000.0	dres	1.0
fb	4000	homo	n
bs	2	DEC2	
tpwr	55	dfrq2	0
pw	9.0	dn2	
d1	5.000	dpwr2	1
tof	0	dof2	0
nt	12	dm2	n
ct	12	dmm2	c
alock	n	dmf2	200
gain	not used	dseq2	
FLAGS		dres2	
il	n	homo2	n
in	n	PROCESSING	
dp	y	lb	0.30
hs	nn	wtfile	
DISPLAY		proc	
sp	-104.9	fn	not used
wp	4919.2	math	f
vs	37		
sc	0	werr	
wc	250	wexp	
hzmm	19.68	wbs	
is	33.57	wnt	
rfl	5141.1		
rfp	3630.5		
th	7		
ins	100.000		
ai	ph		





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: Int\_Olefin

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

400 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

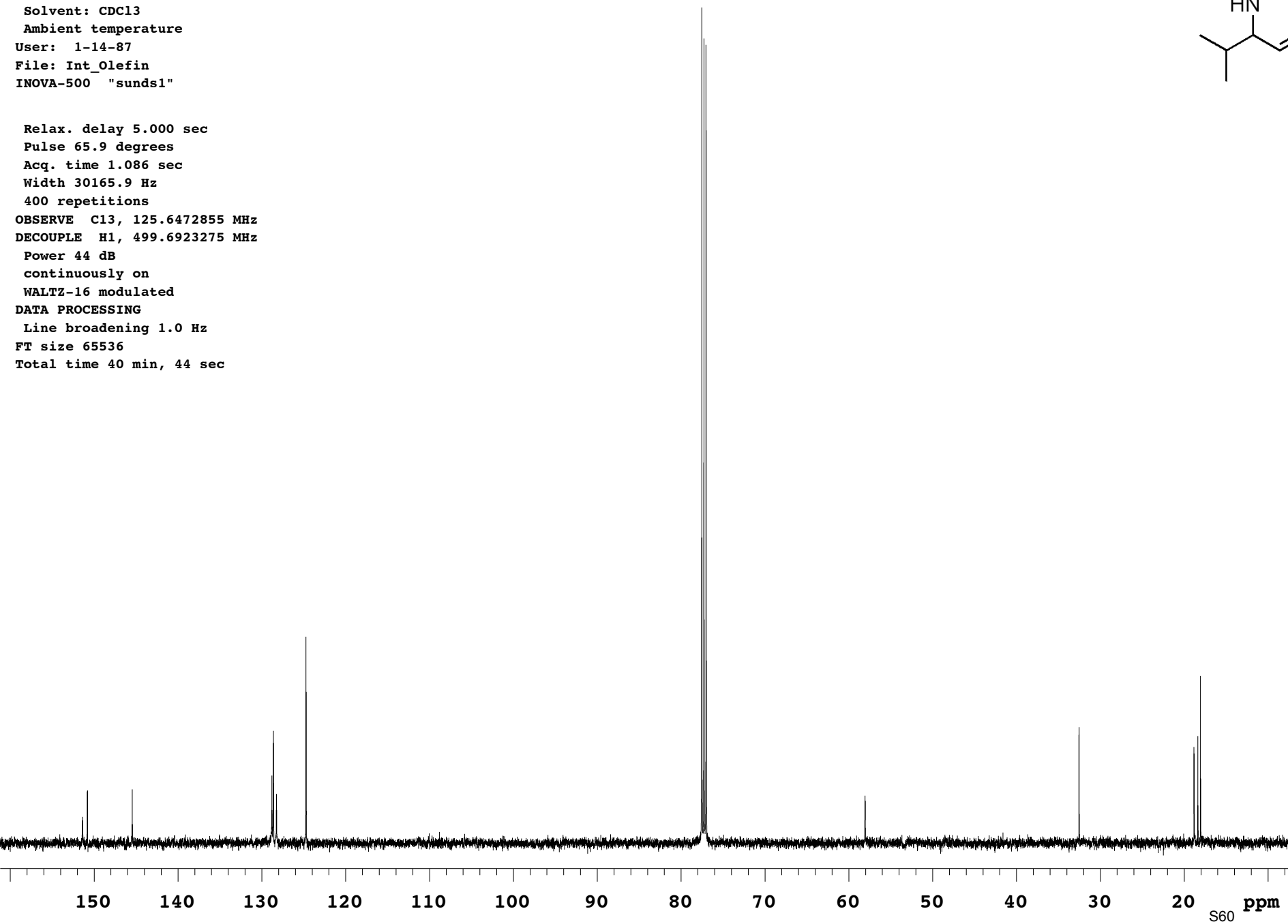
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 40 min, 44 sec



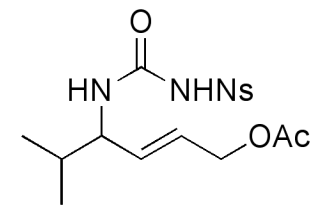
Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: allylicOAc\_SM

INOVA-500 "sunds1"



Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

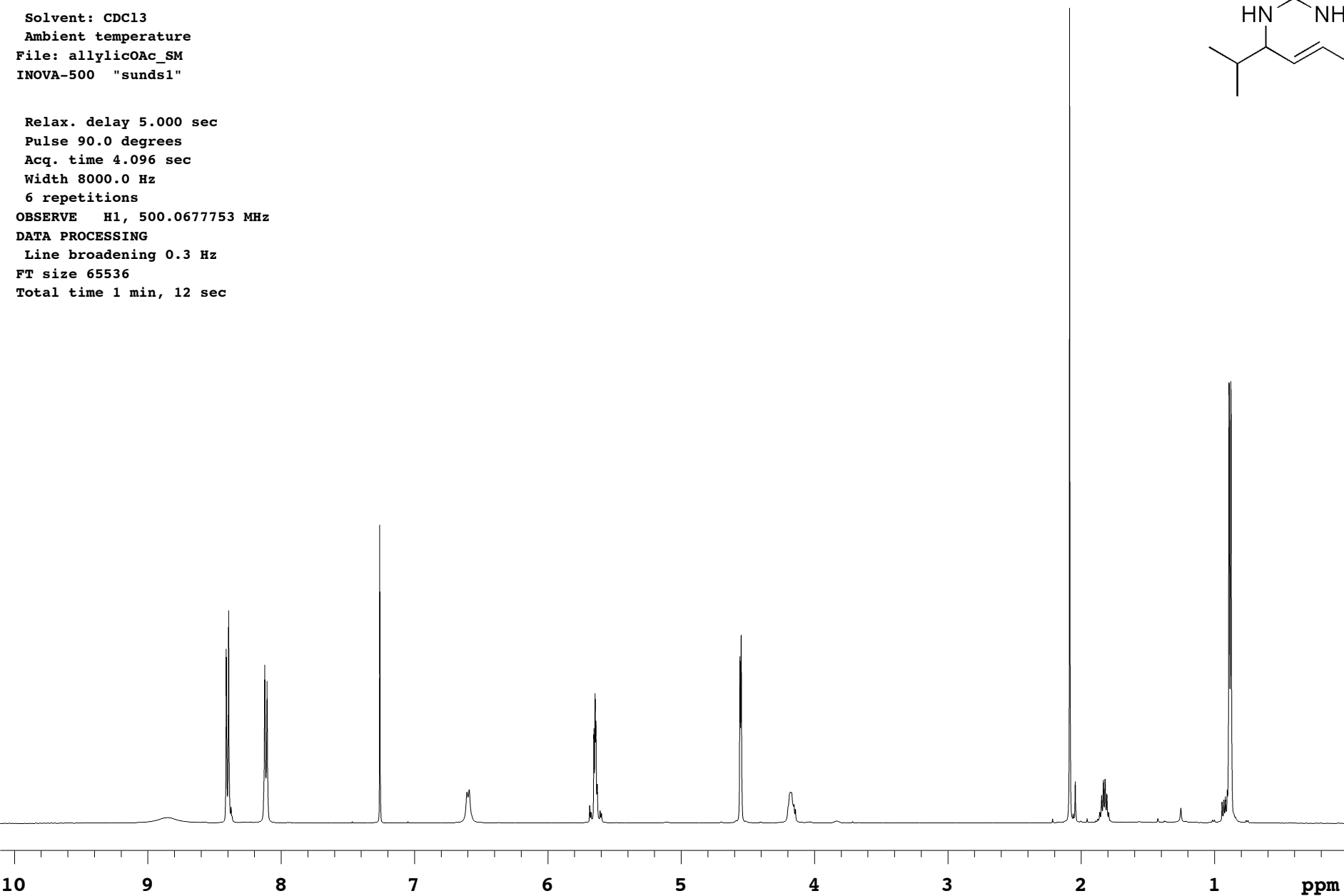
OBSERVE H1, 500.0677753 MHz

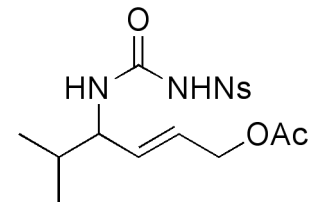
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: allylicOAc\_SM\_C

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

1470 repetitions

OBSERVE C13, 125.5817492 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

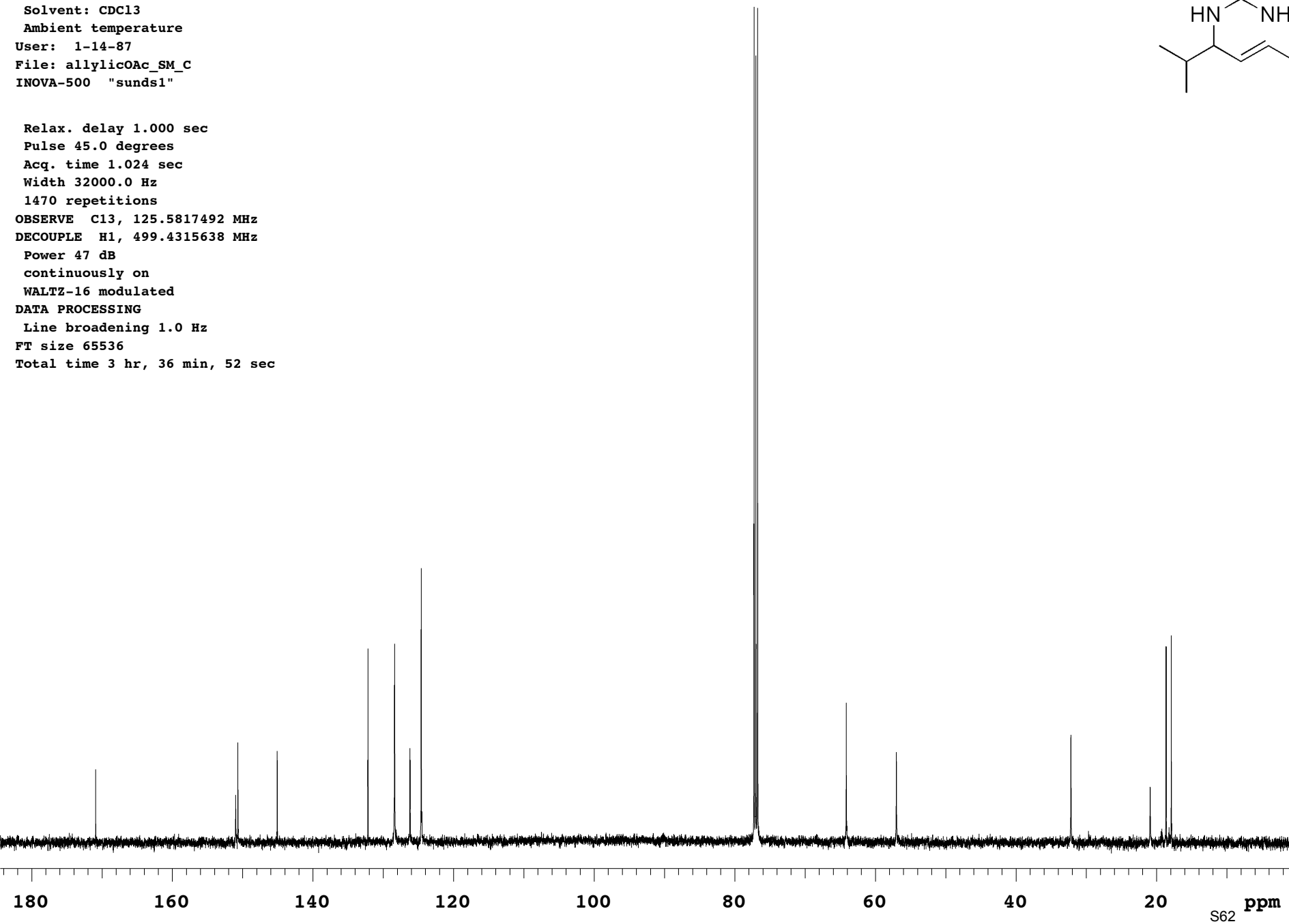
WALTZ-16 modulated

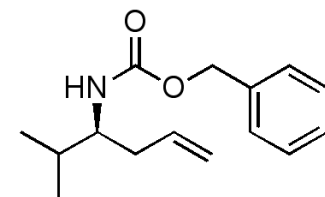
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 36 min, 52 sec





Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

File: IIS.31.VIII.col

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

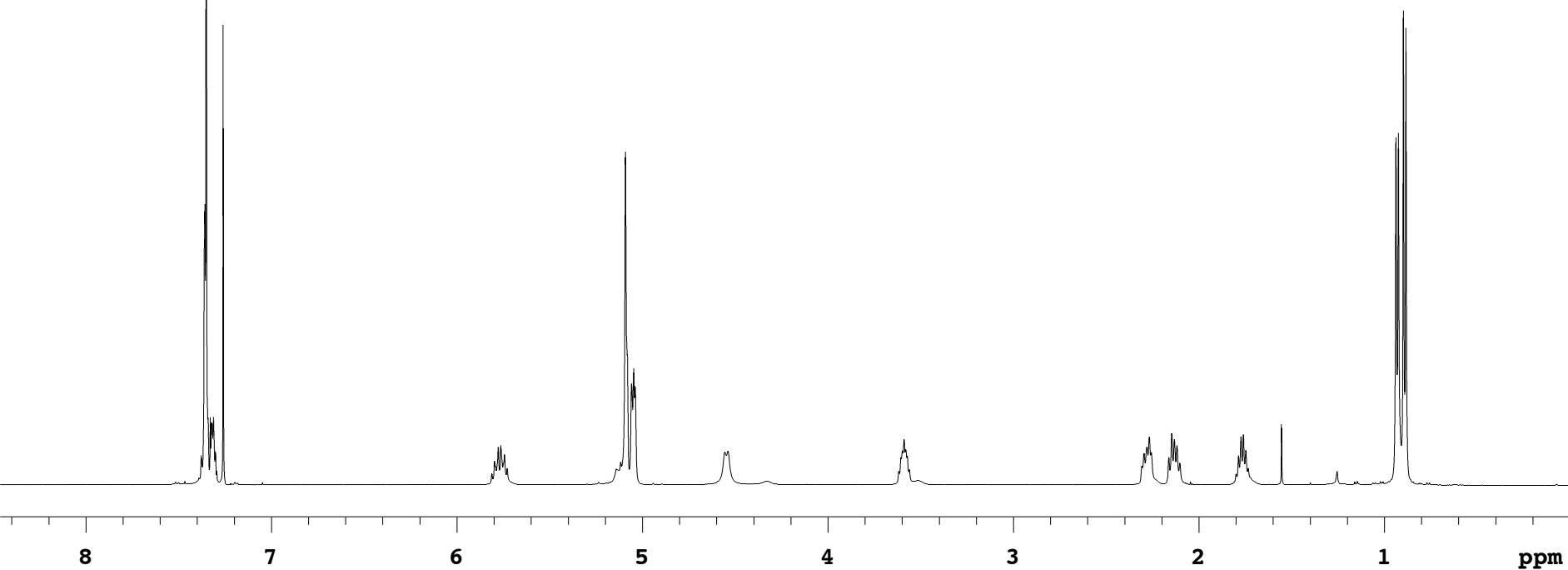
OBSERVE H1, 500.0677748 MHz

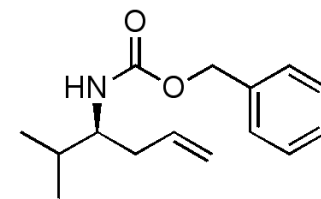
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

User: 1-14-87

File: IIS.31.VIII.col

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

182 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 48 dB

continuously on

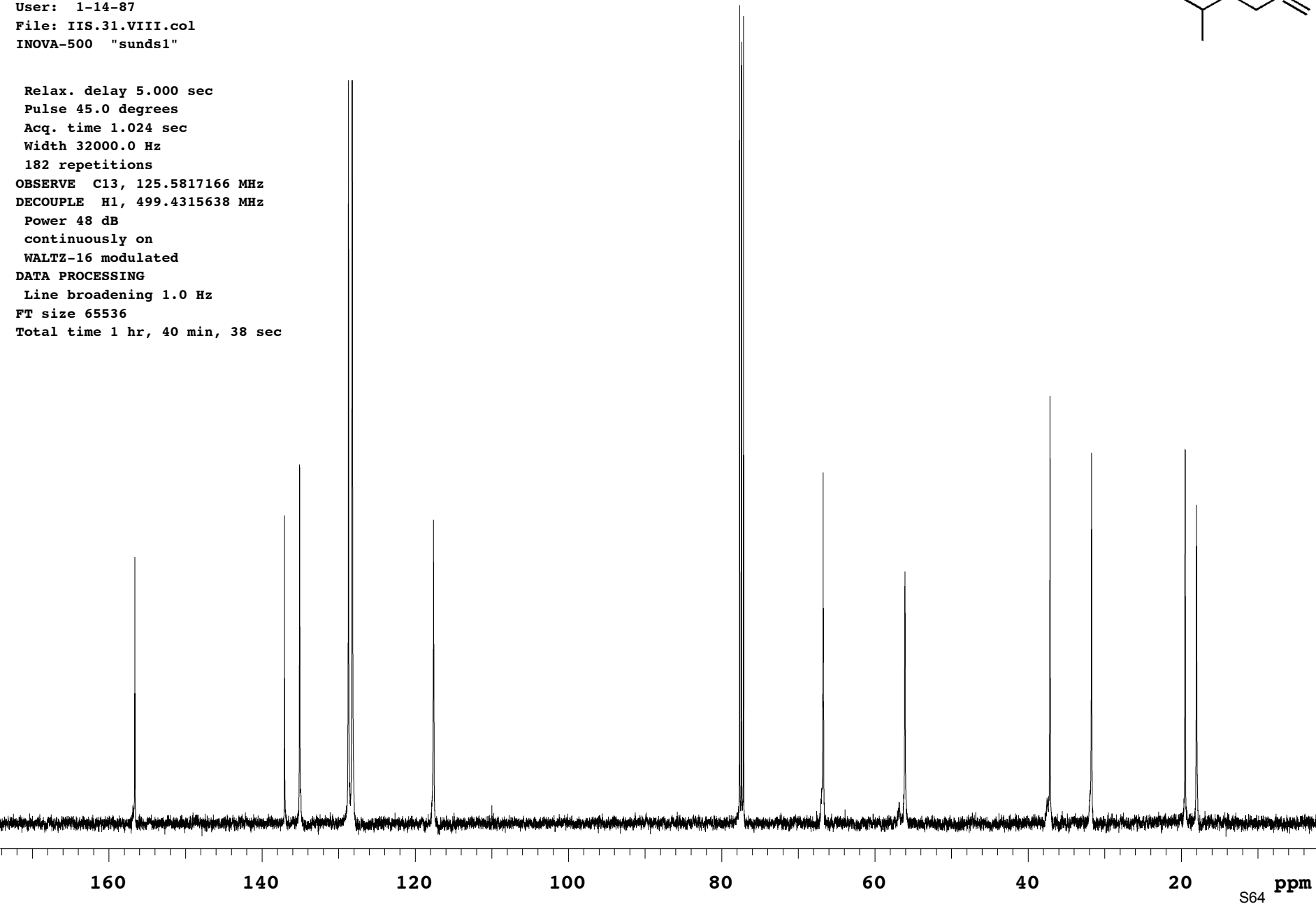
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1 hr, 40 min, 38 sec



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: iPrSynDiamine

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

16 repetitions

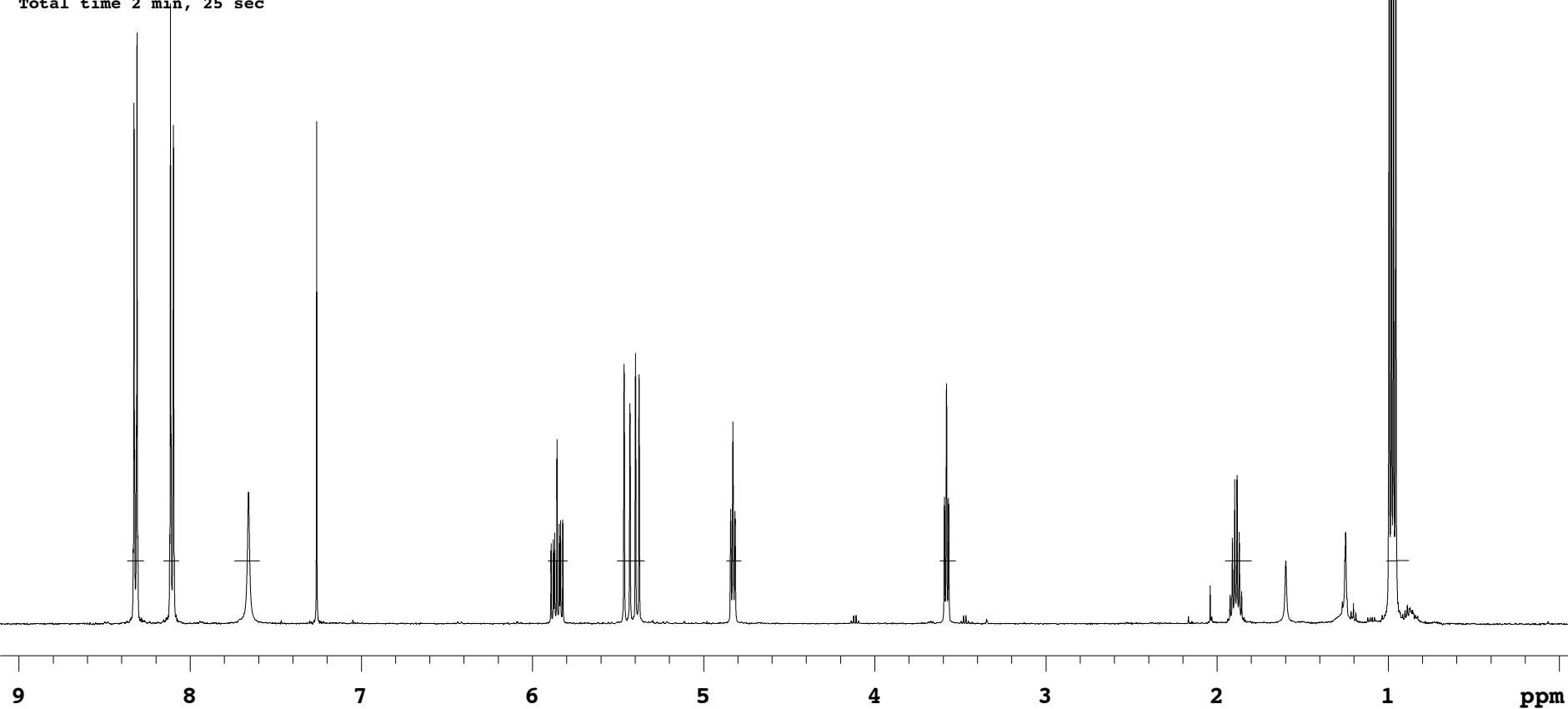
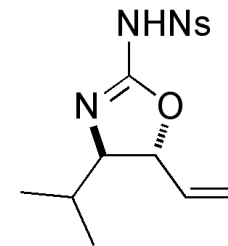
OBSERVE H1, 500.0677743 MHz

DATA PROCESSING

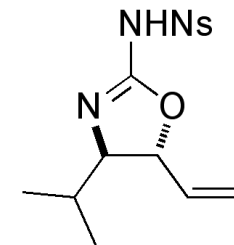
Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec







Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: iPrSynDiamineCarb

INOVA-500 "sunds1"

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

544 repetitions

OBSERVE C13, 125.5817483 MHz

DECOUPLE H1, 499.4315638 MHz

Power 48 dB

continuously on

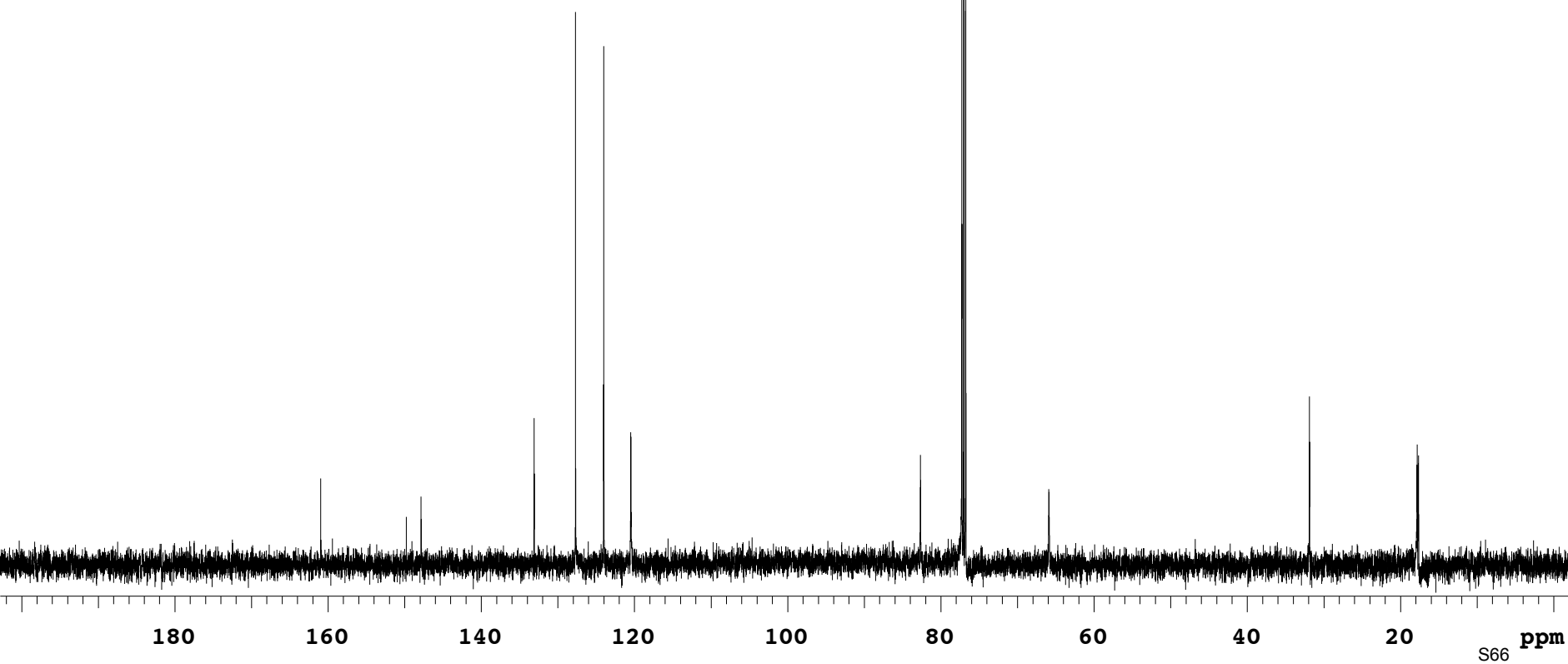
WALTZ-16 modulated

DATA PROCESSING

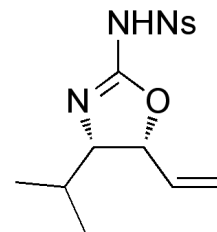
Line broadening 1.0 Hz

FT size 65536

Total time 2 hr, 52 min, 10 sec



Strambeanu and White



Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: syn\_oxazoline

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

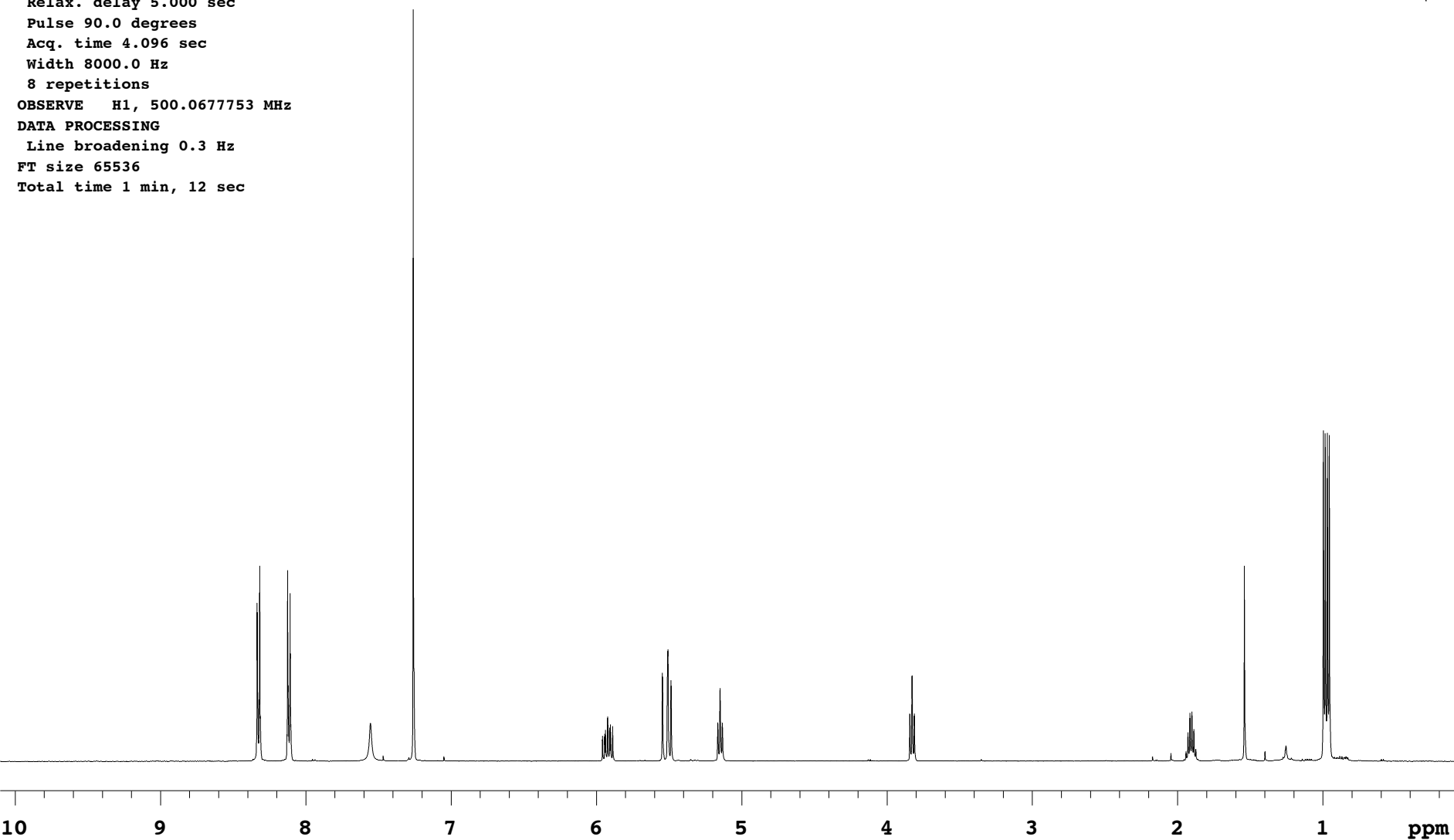
OBSERVE H1, 500.0677753 MHz

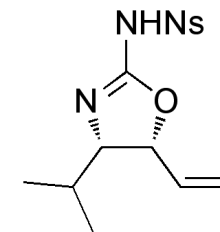
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

1240 repetitions

OBSERVE C13, 125.5817483 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

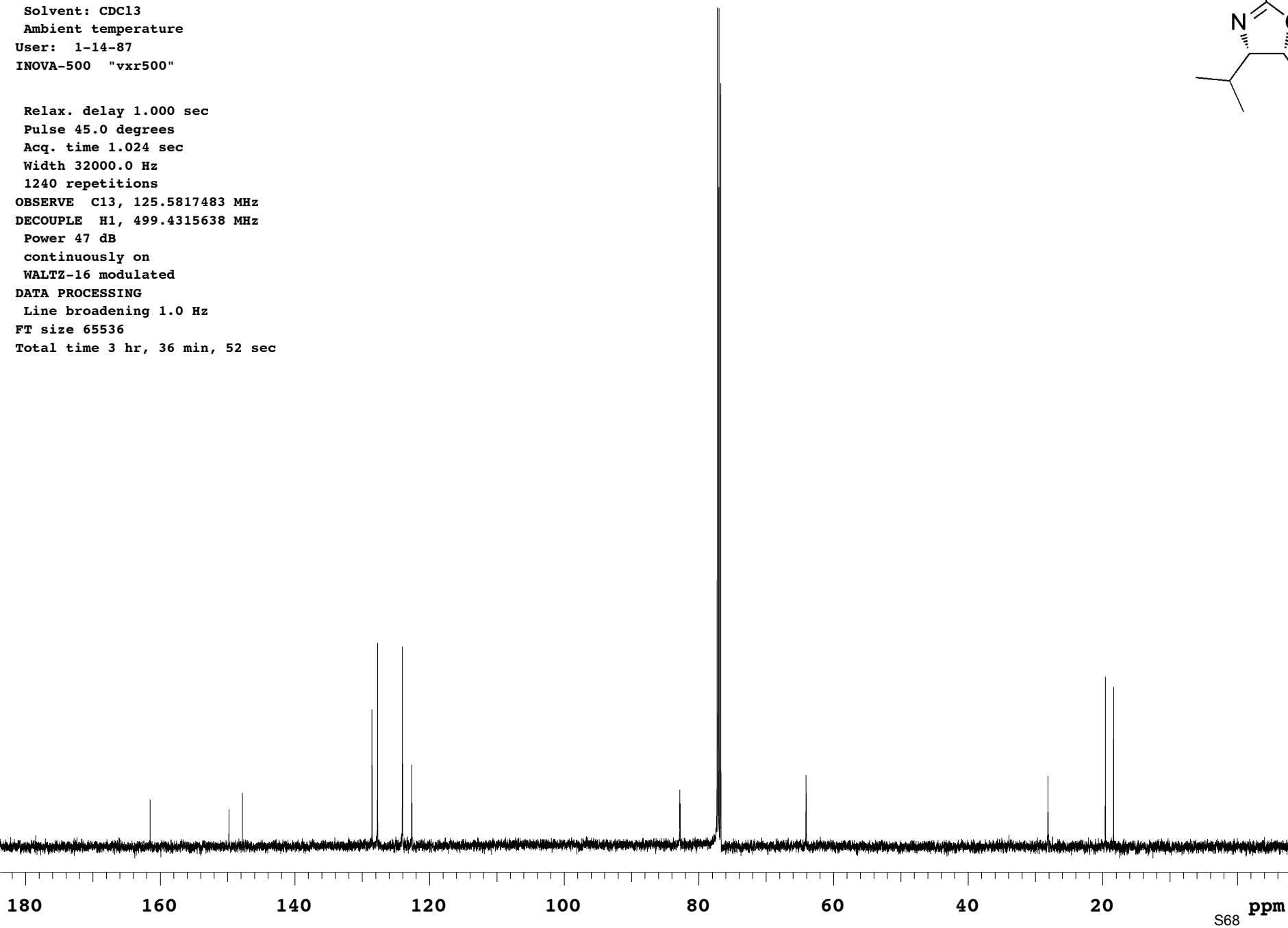
WALTZ-16 modulated

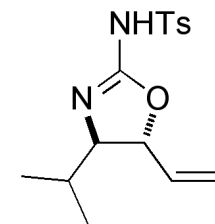
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 36 min, 52 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: iPrTs\_oxazoline\_H

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

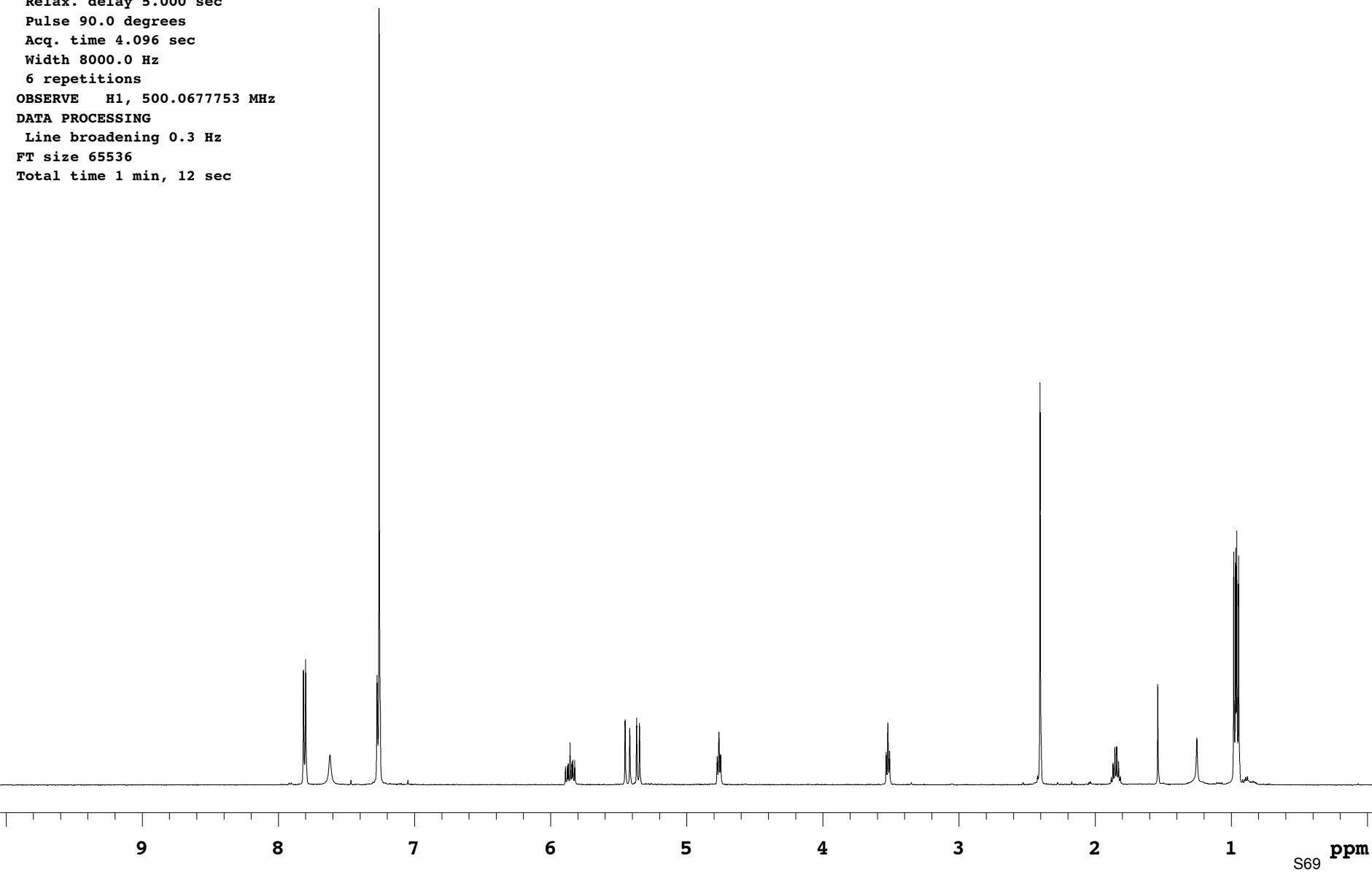
OBSERVE H1, 500.0677753 MHz

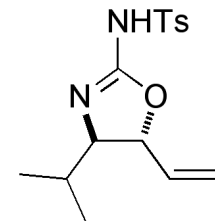
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: iPrTs\_ox\_C1

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 28.1 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

1000 repetitions

OBSERVE C13, 125.6473193 MHz

DECOUPLE H1, 499.6923275 MHz

Power 45 dB

continuously on

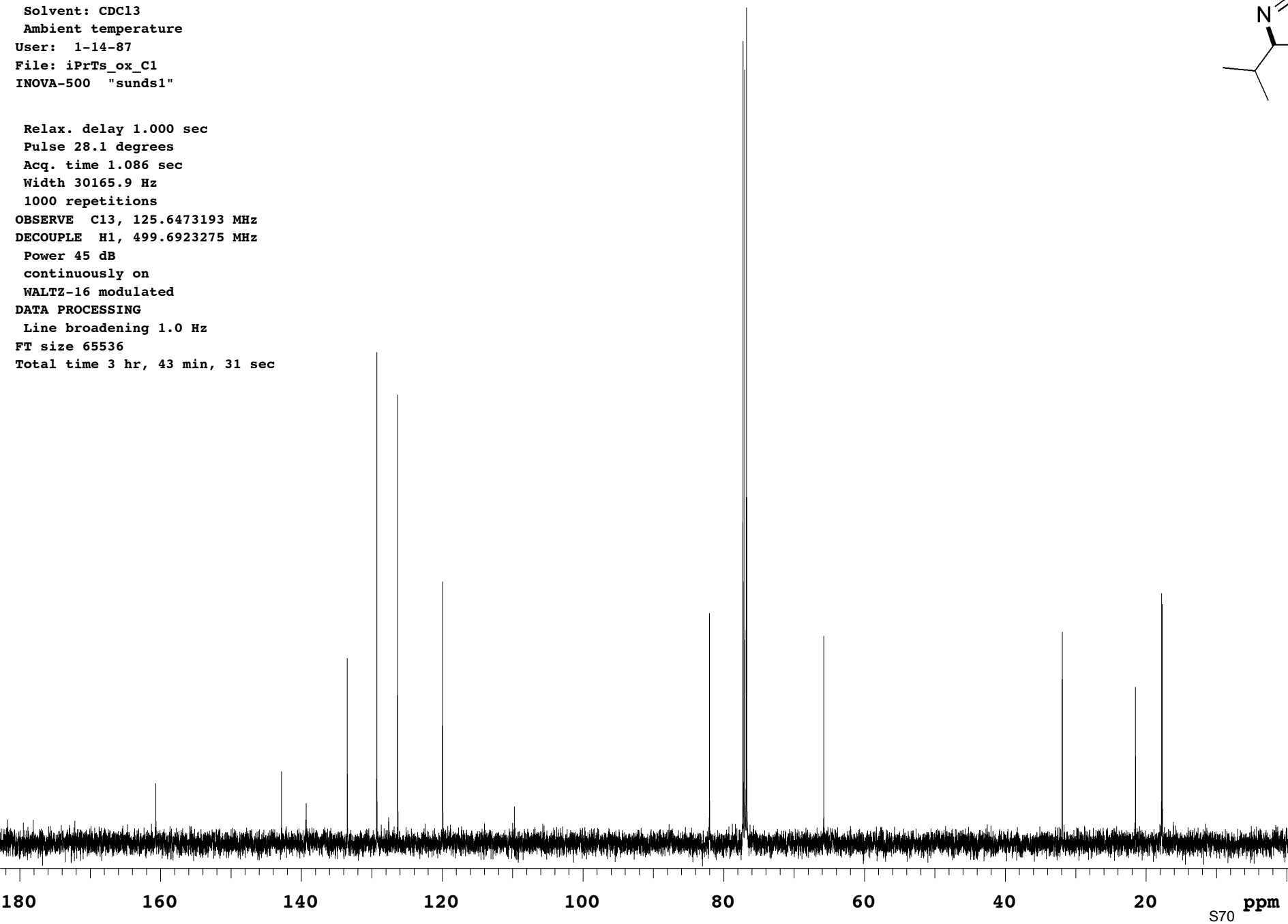
WALTZ-16 modulated

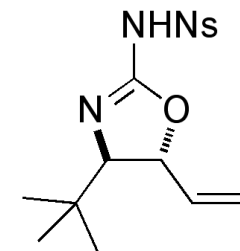
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 43 min, 31 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: tBuSynDiamine

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 61.6 degrees

Acq. time 4.665 sec

Width 7024.9 Hz

12 repetitions

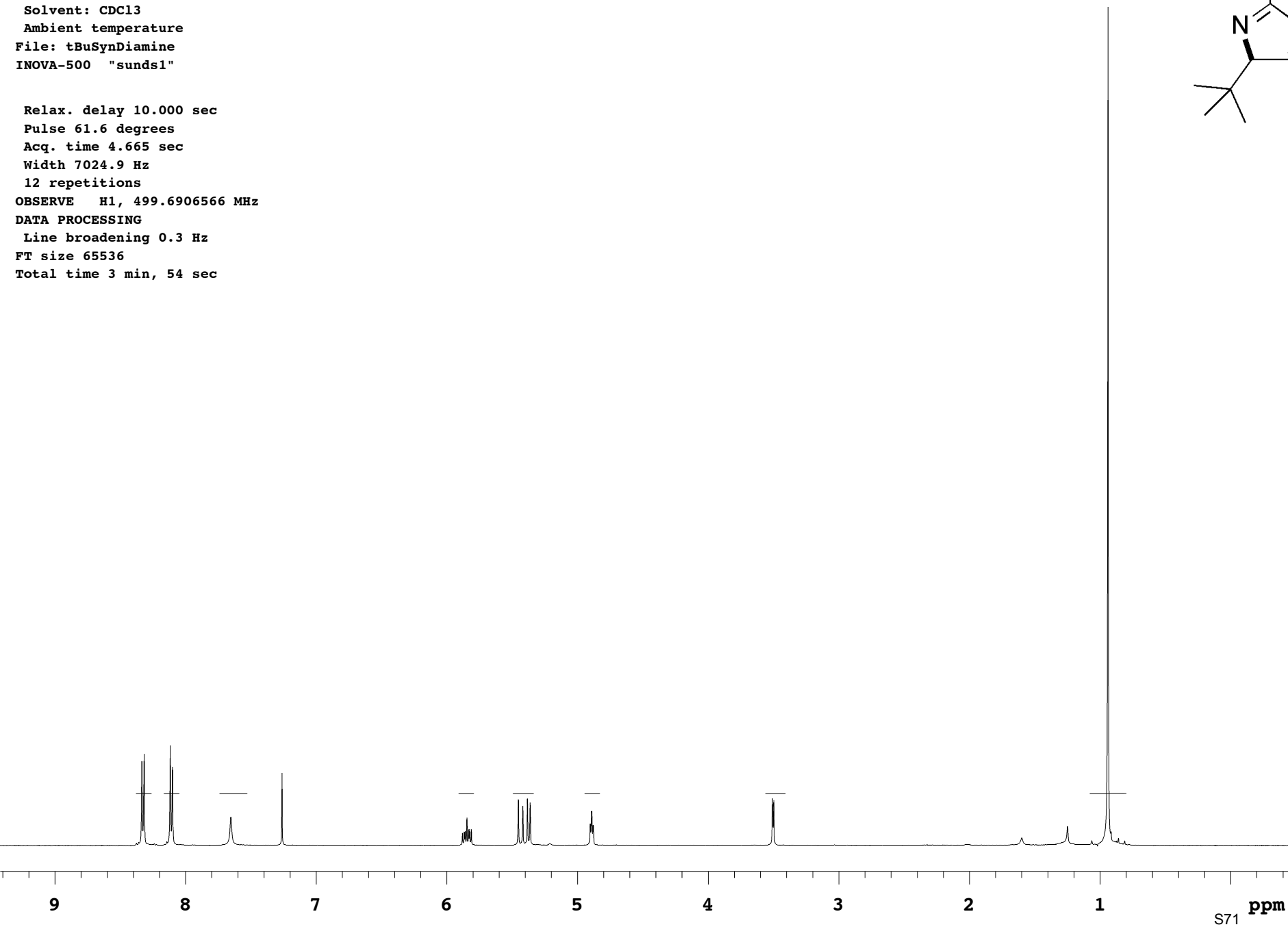
OBSERVE H1, 499.6906566 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 3 min, 54 sec



Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: tBuSynDiamineCarb

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

414 repetitions

OBSERVE C13, 125.6473020 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

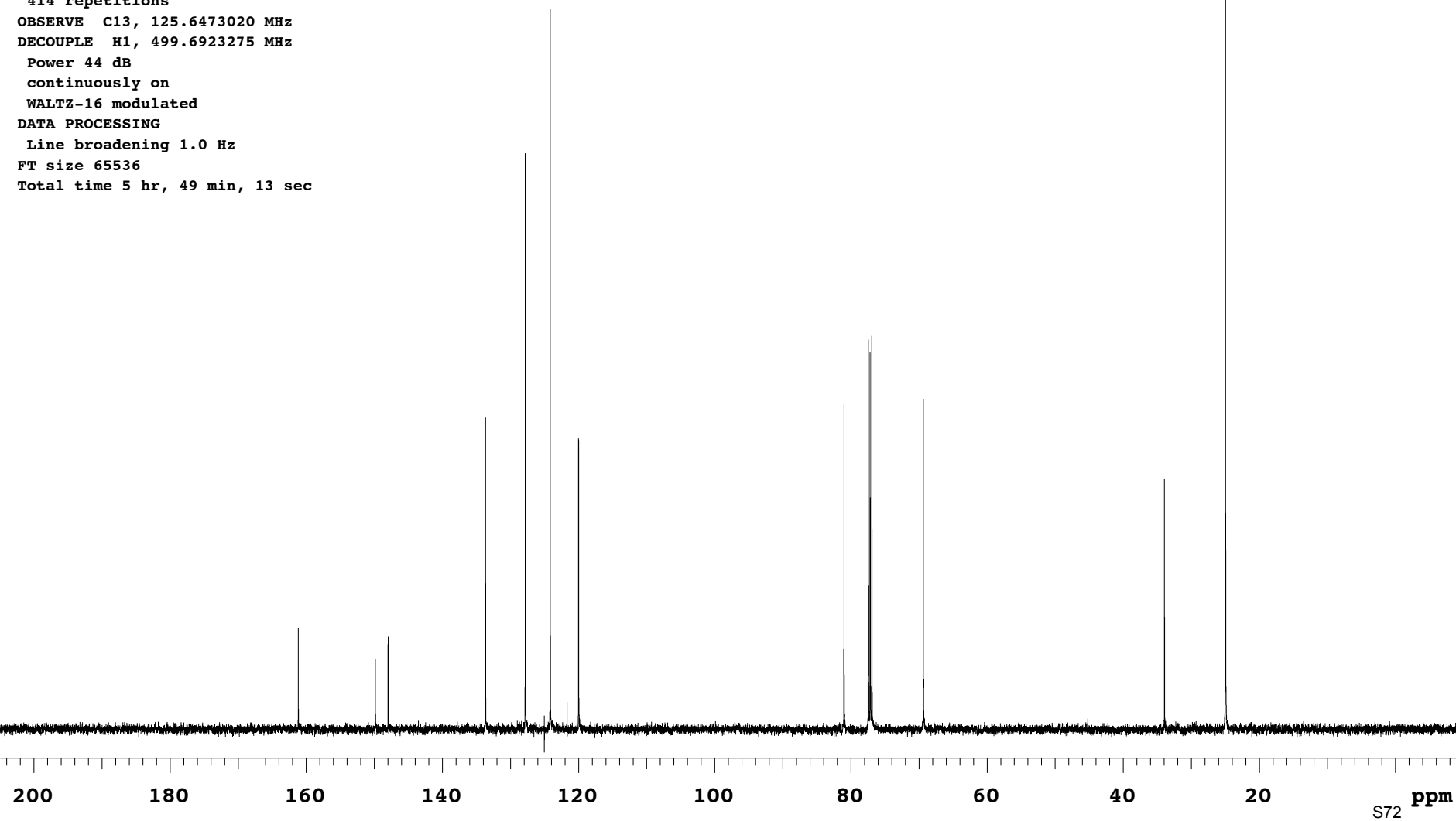
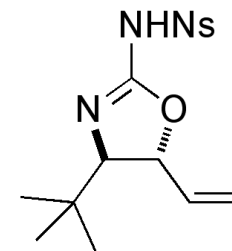
WALTZ-16 modulated

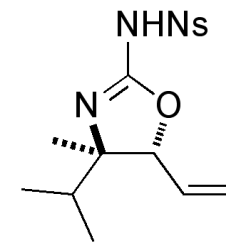
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 5 hr, 49 min, 13 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: TertiarySynDiamine

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 45.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

16 repetitions

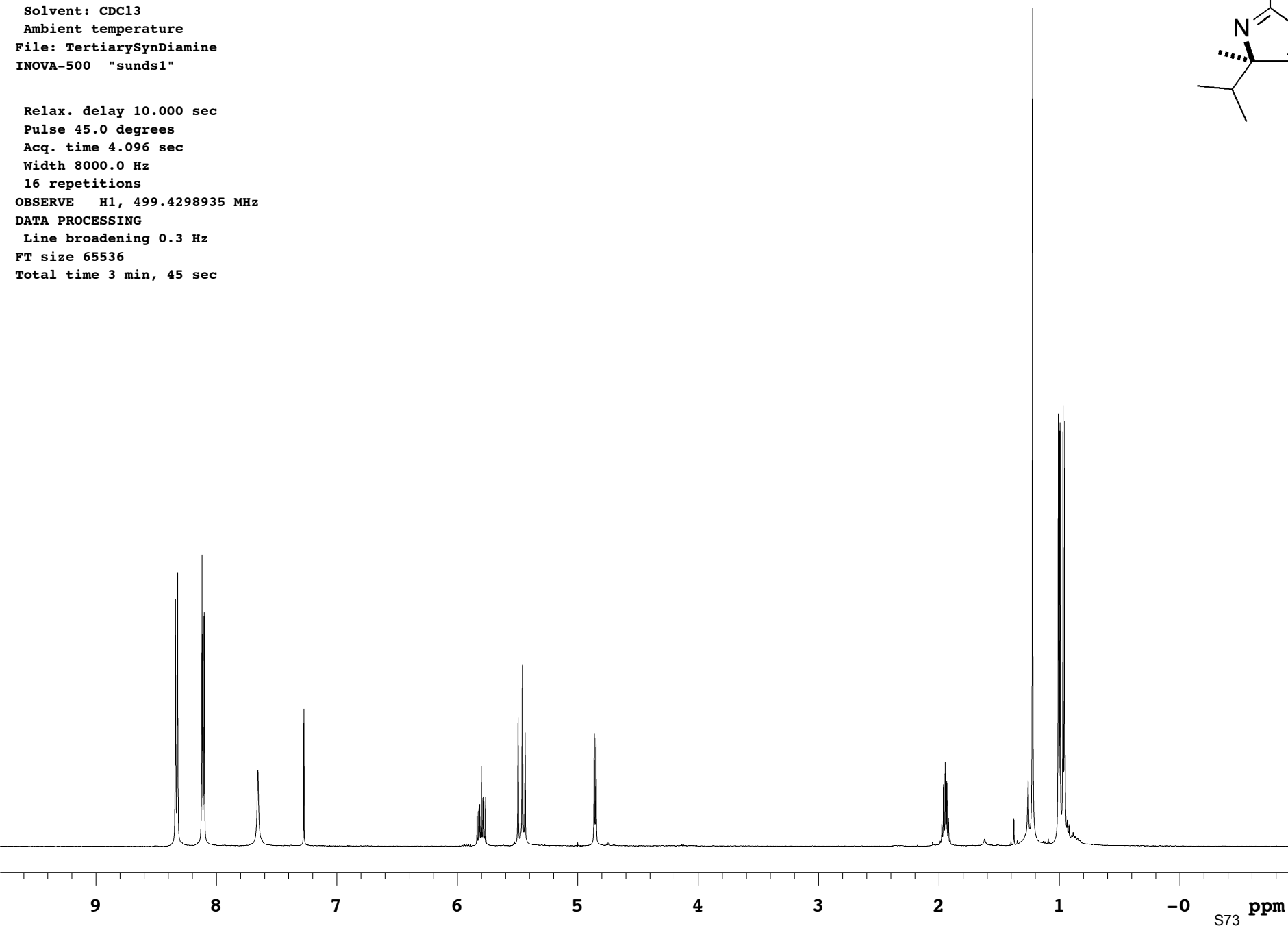
OBSERVE H1, 499.4298935 MHz

DATA PROCESSING

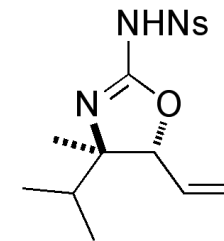
Line broadening 0.3 Hz

FT size 65536

Total time 3 min, 45 sec







Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: TertiarySynDiamineCarb

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

498 repetitions

OBSERVE C13, 125.5817185 MHz

DECOUPLE H1, 499.4315638 MHz

Power 44 dB

continuously on

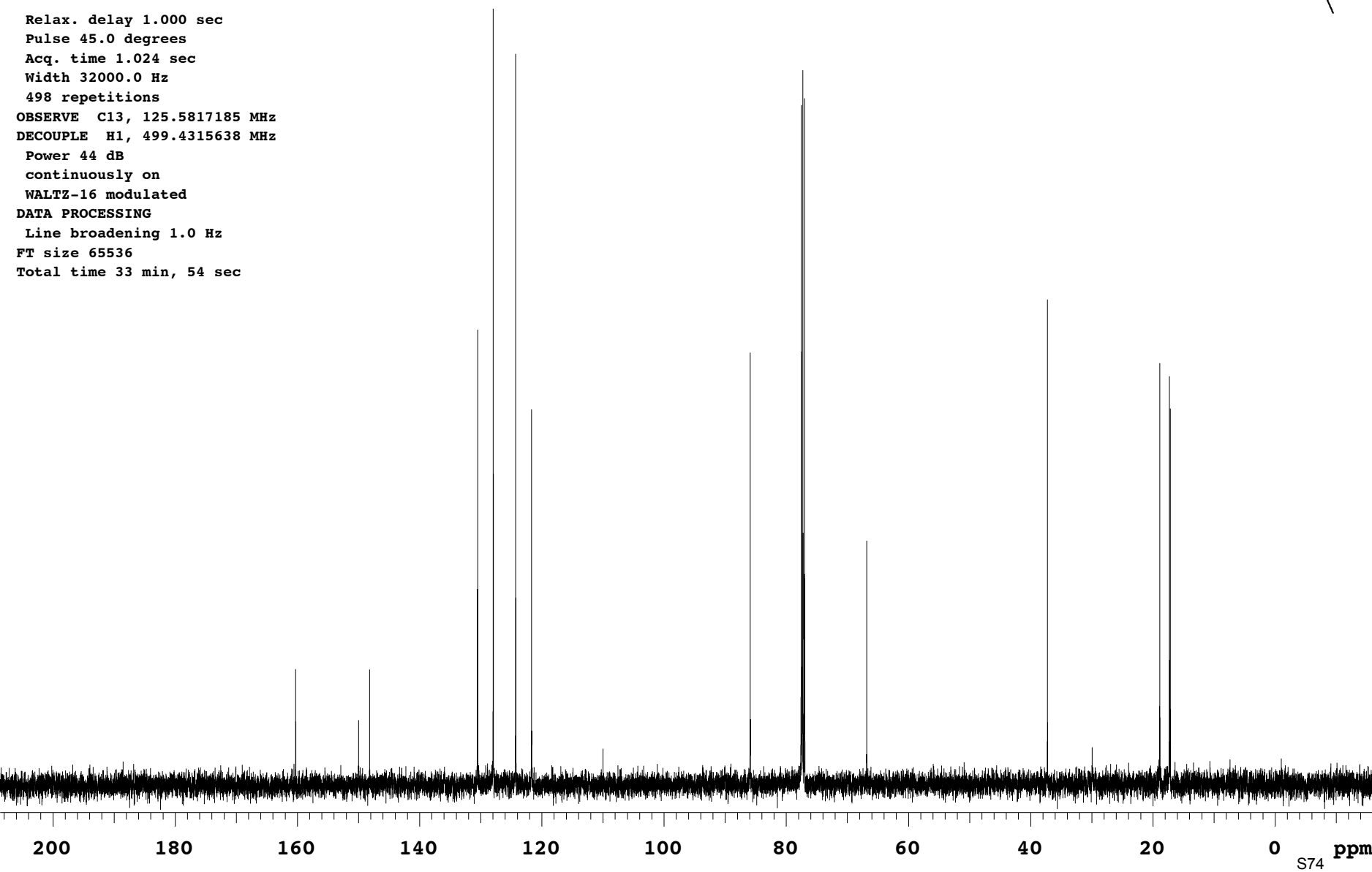
WALTZ-16 modulated

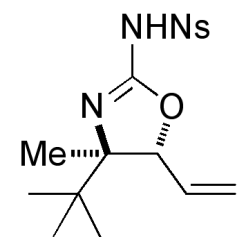
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 33 min, 54 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: tBuMe\_P\_H1

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

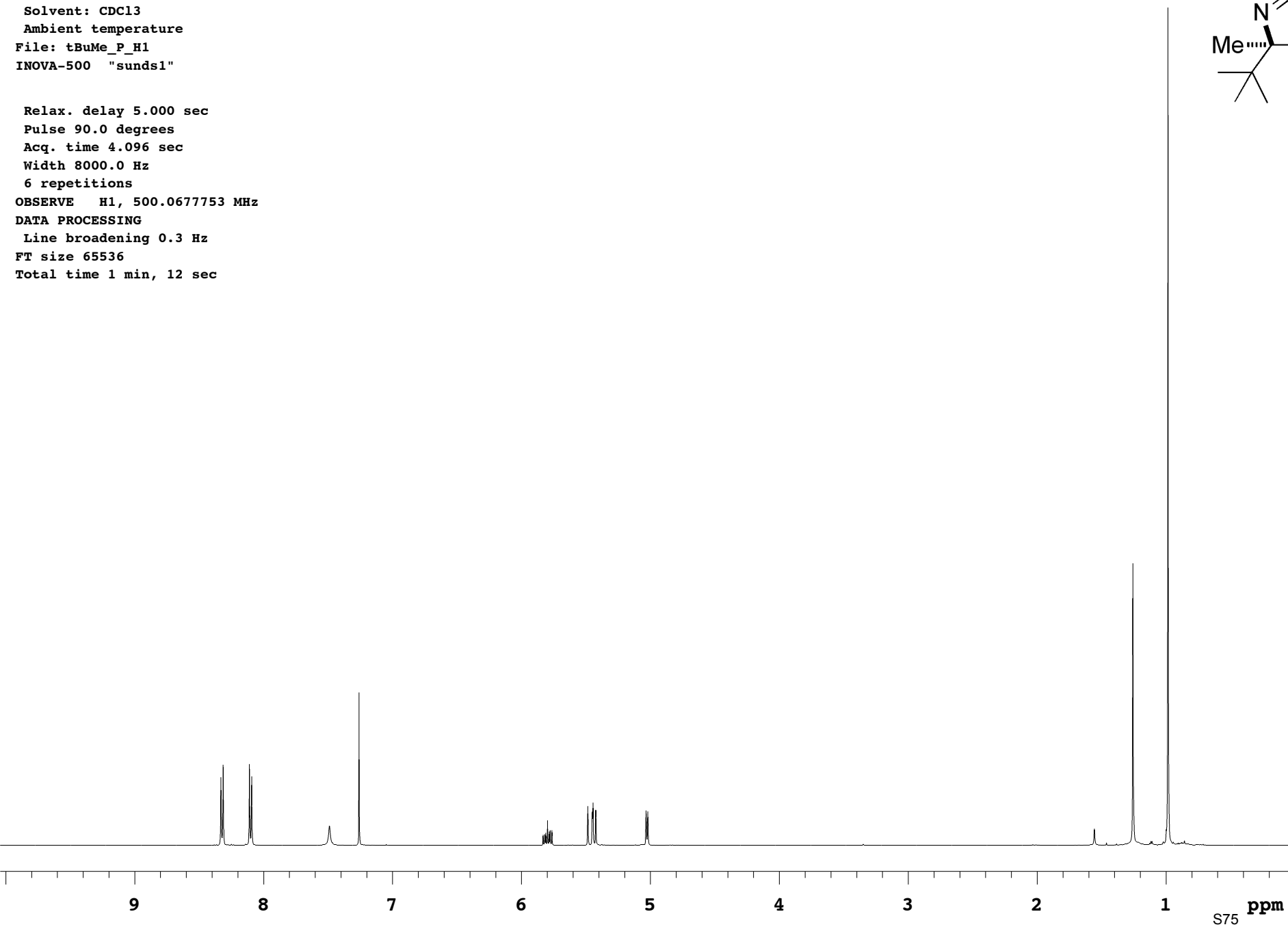
OBSERVE H1, 500.0677753 MHz

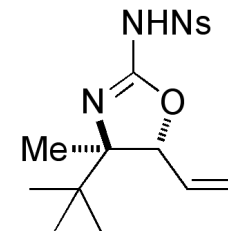
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

250 repetitions

OBSERVE C13, 125.5817473 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

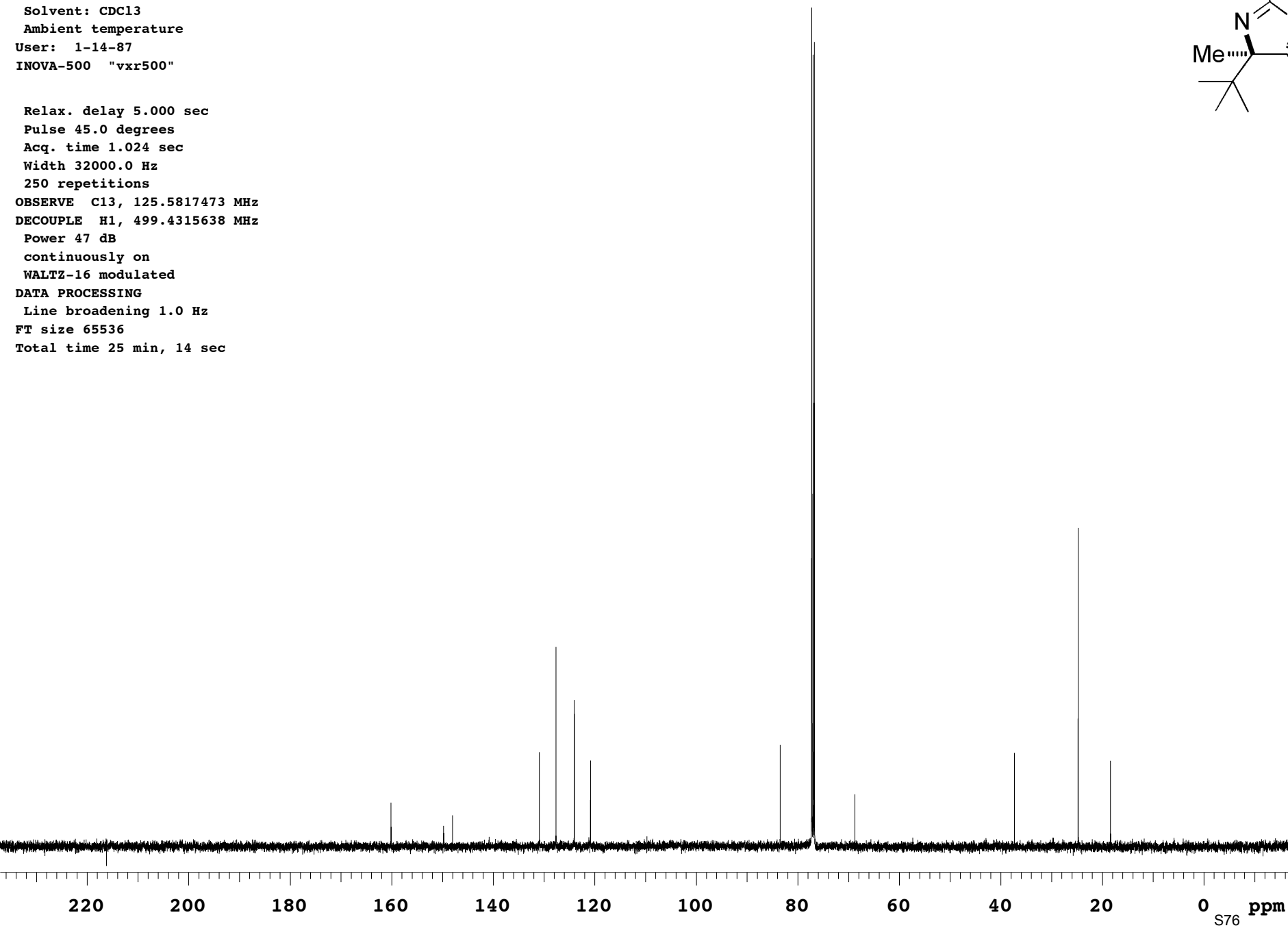
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 25 min, 14 sec



Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: OMePh\_P\_H1

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

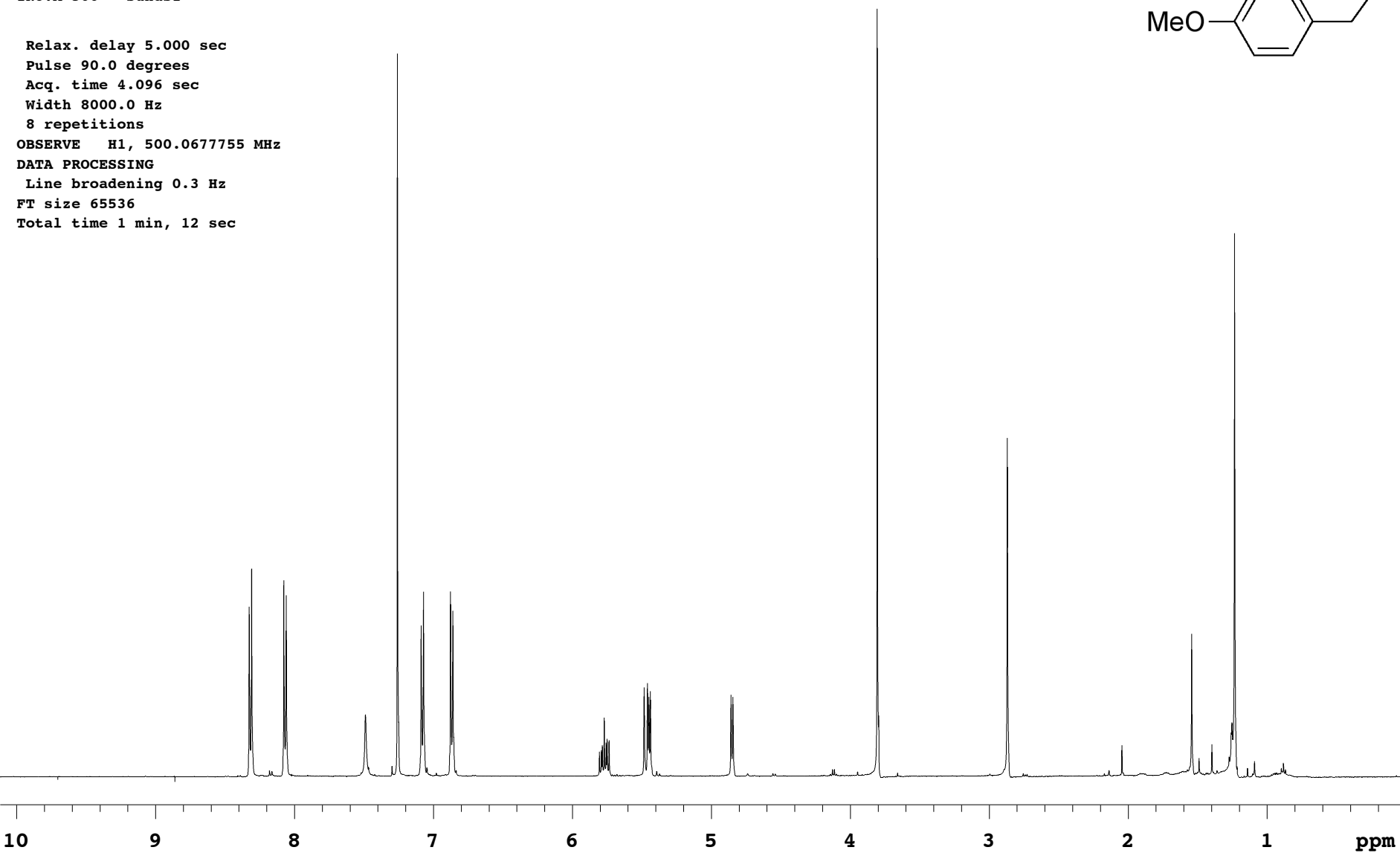
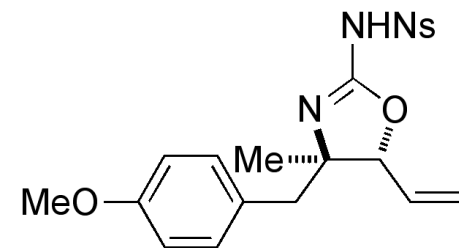
OBSERVE H1, 500.0677755 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

574 repetitions

OBSERVE C13, 125.5817492 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

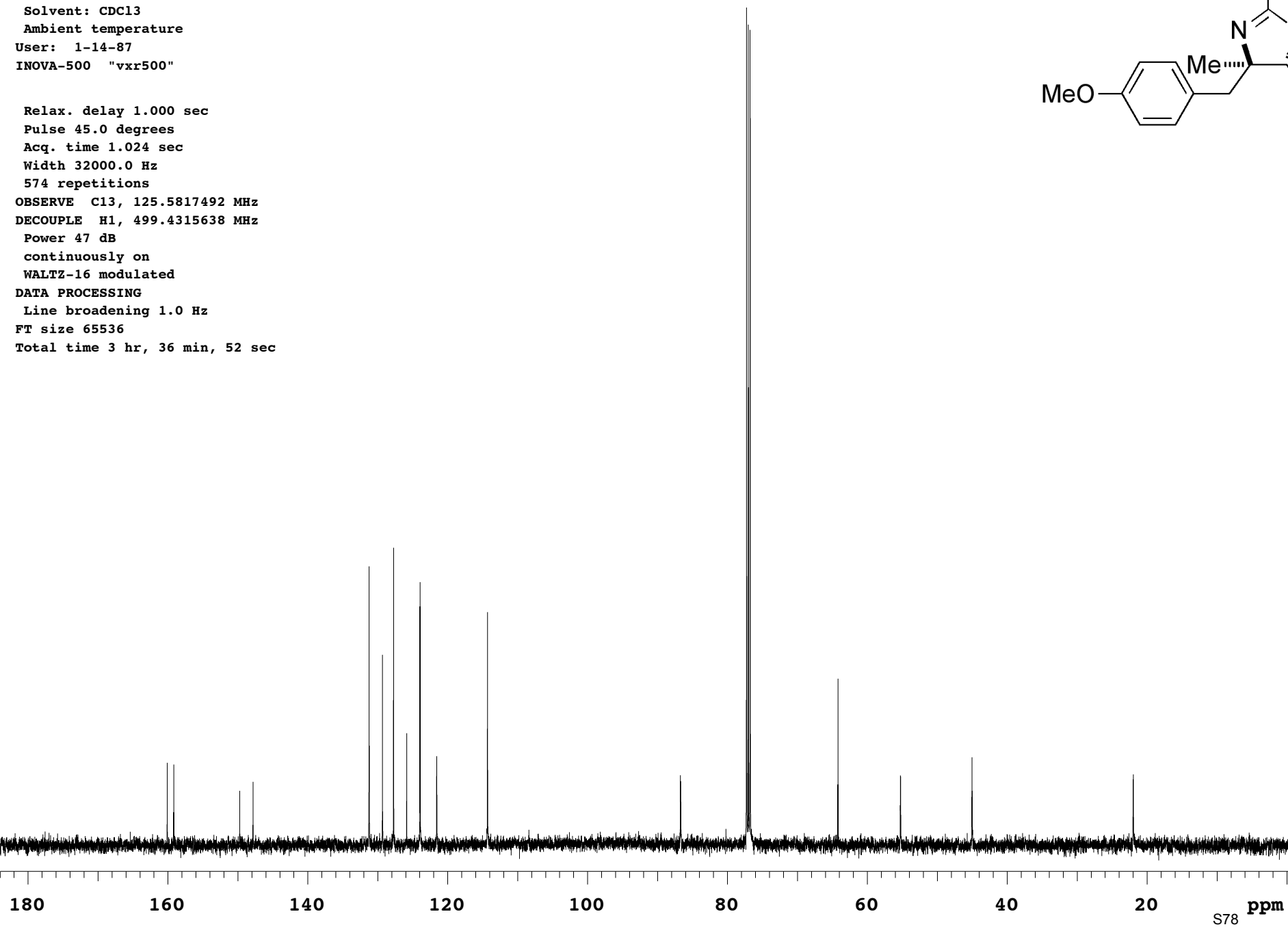
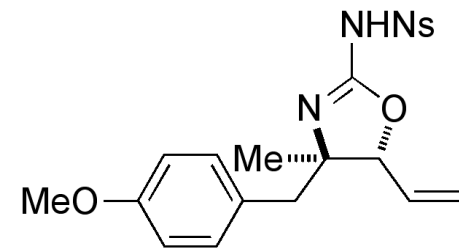
WALTZ-16 modulated

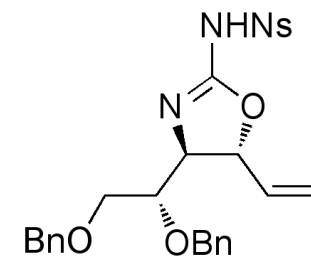
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 36 min, 52 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: DiBenzSynDiamine

INOVA-500 "u500"

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

32 repetitions

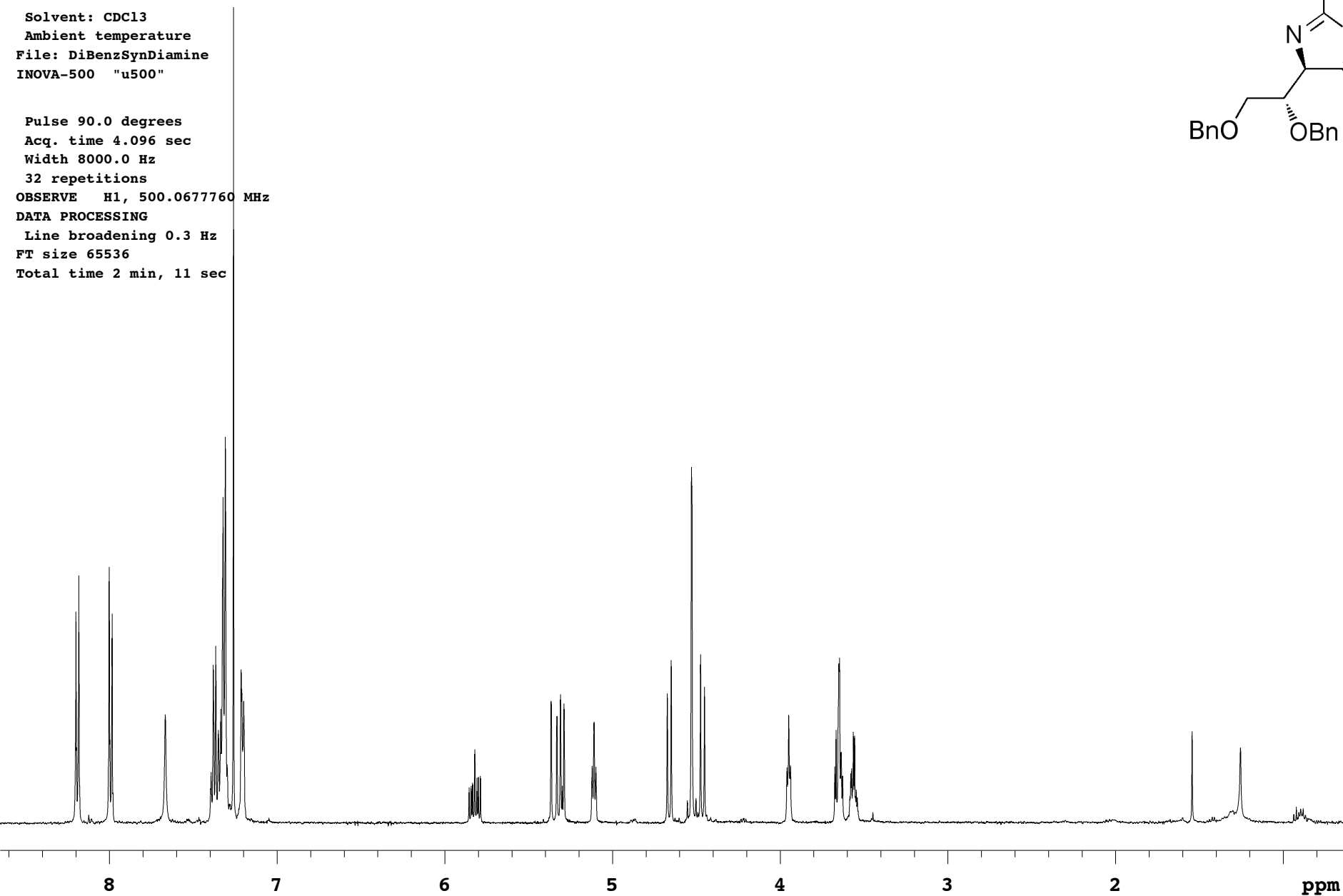
OBSERVE H1, 500.0677760 MHz

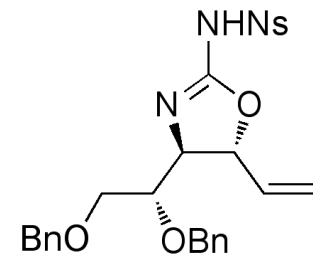
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 11 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: DiBenzSynDiamineCarb

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

206 repetitions

OBSERVE C13, 125.6472876 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

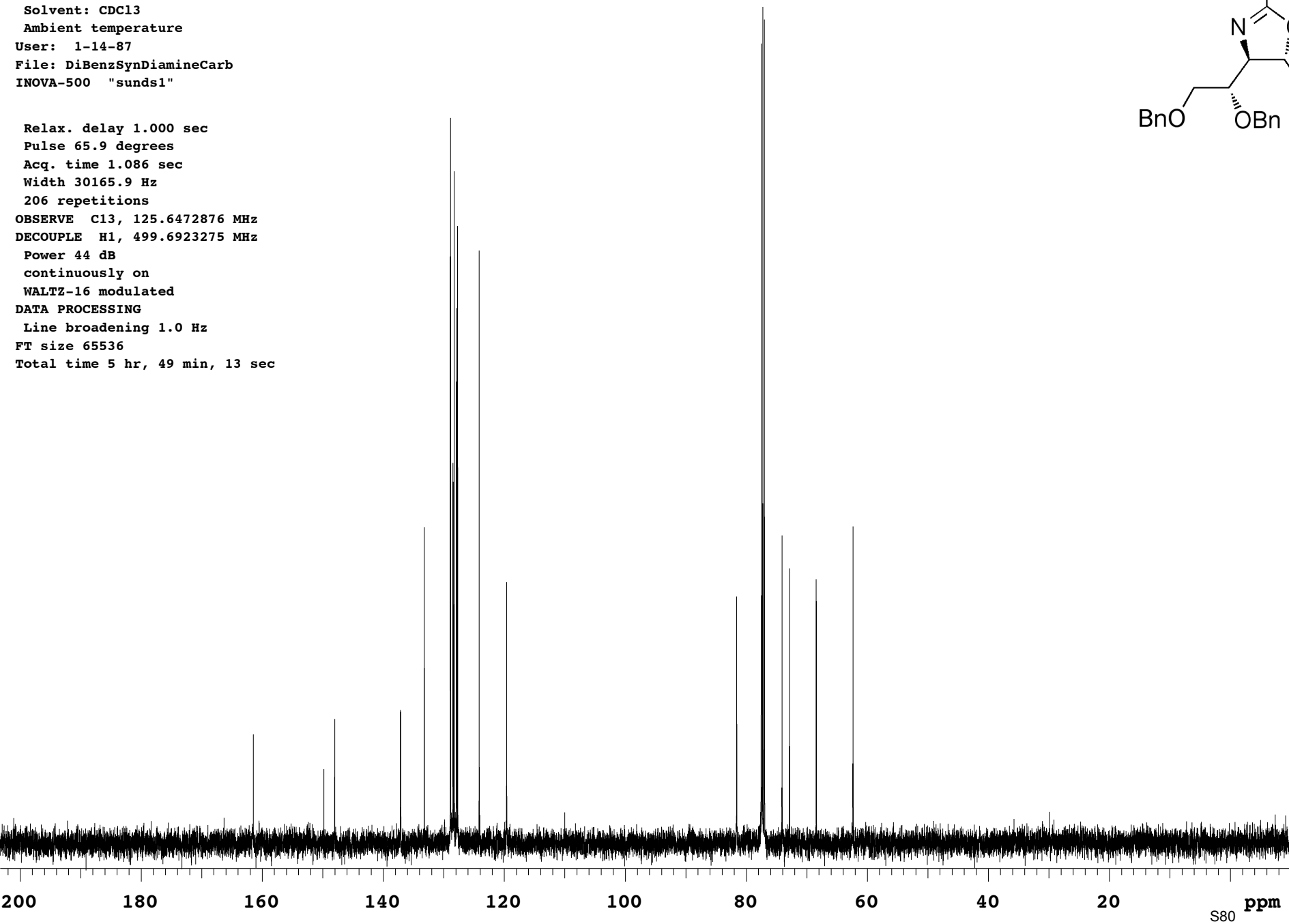
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 5 hr, 49 min, 13 sec



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: FPhSynDiamine

INOVA-500 "sunds1"

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

108 repetitions

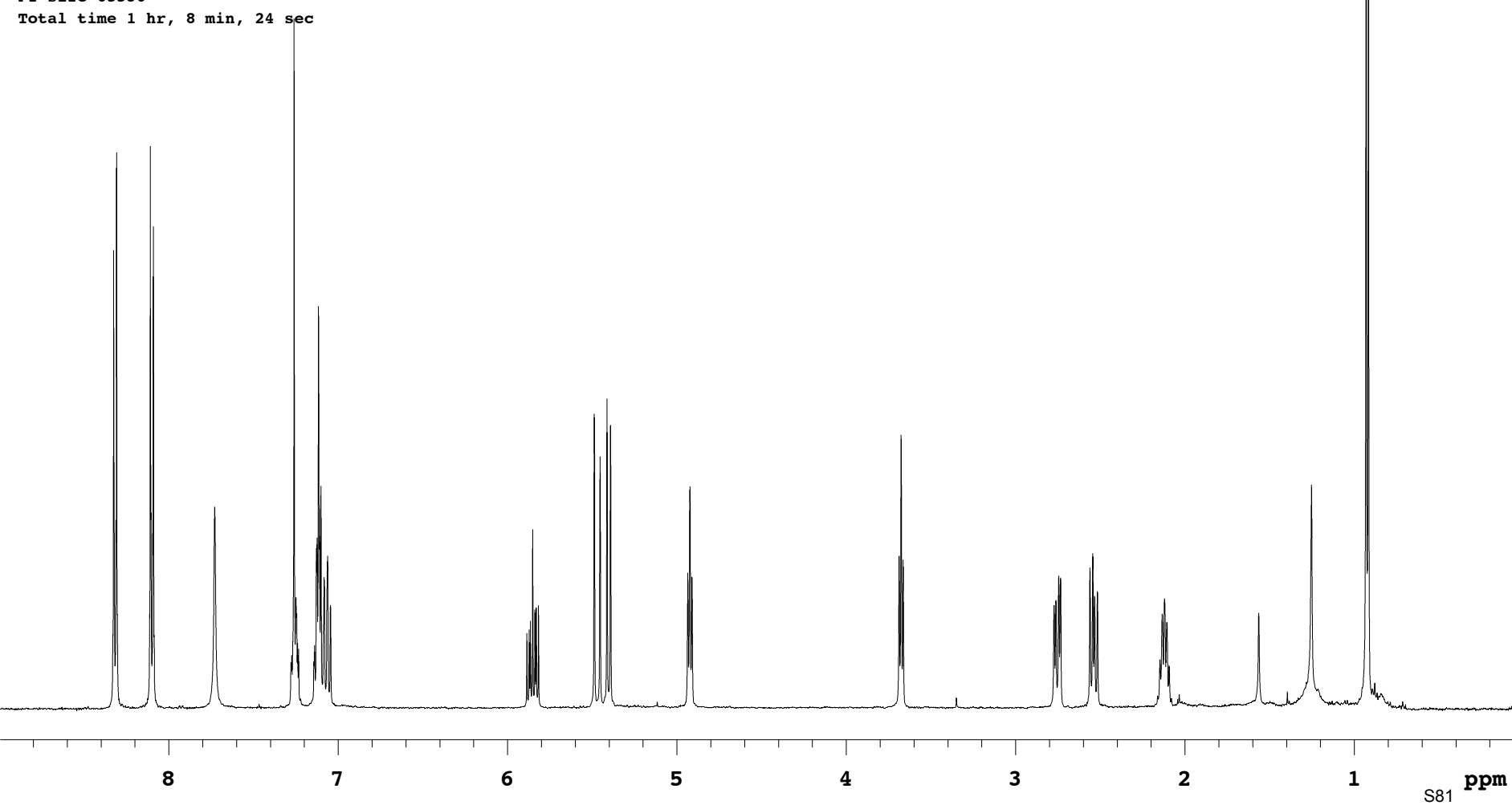
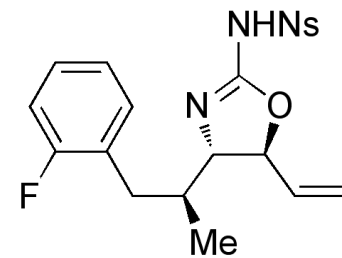
OBSERVE H1, 500.0677750 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 hr, 8 min, 24 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: FPhSynDiamineCarbBest

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 36.5 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

784 repetitions

OBSERVE C13, 125.6472974 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

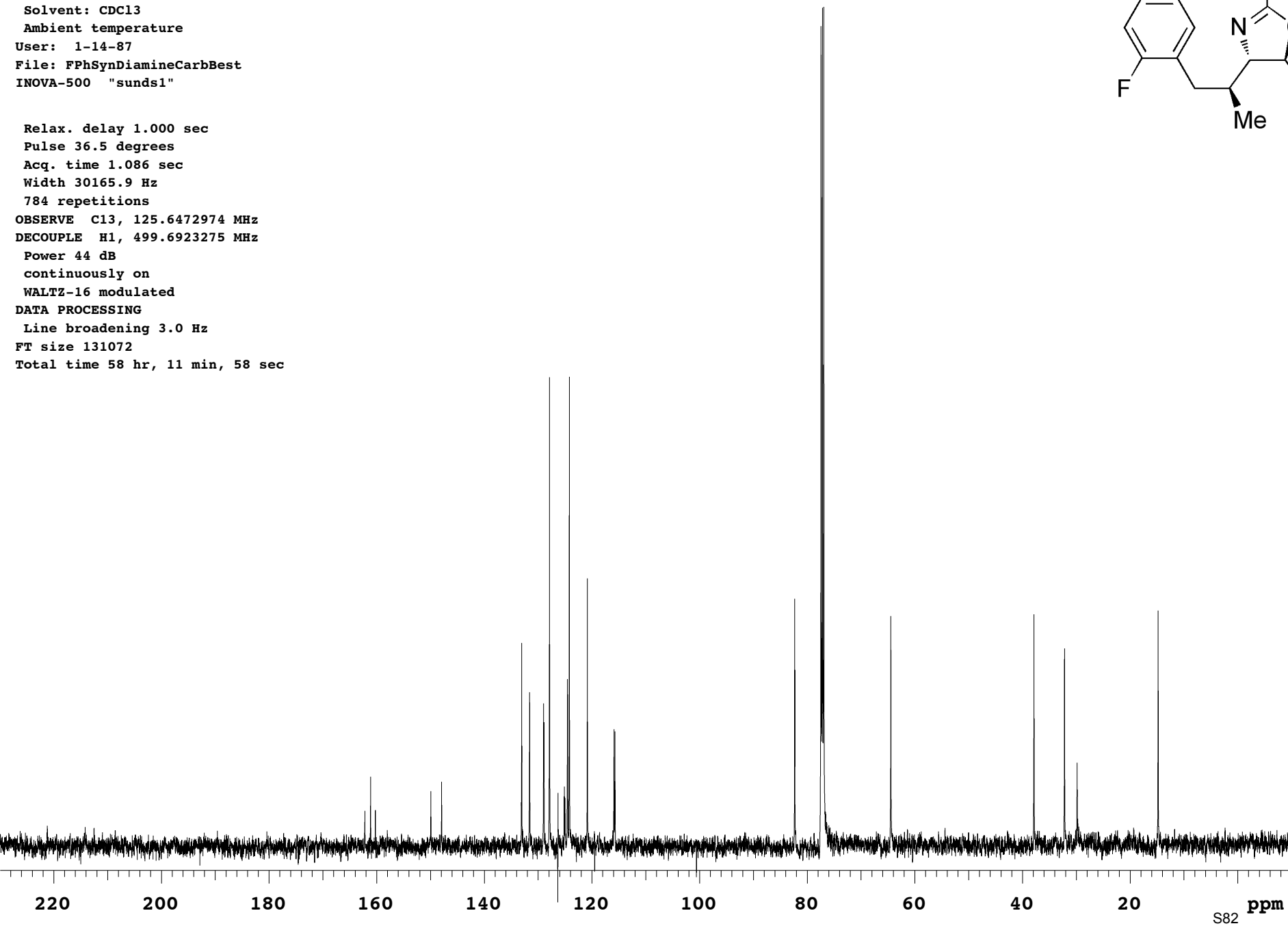
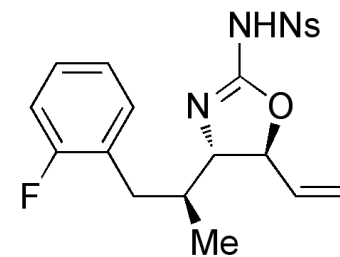
WALTZ-16 modulated

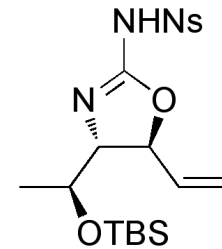
DATA PROCESSING

Line broadening 3.0 Hz

FT size 131072

Total time 58 hr, 11 min, 58 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: OTBSAntiSynDiamine

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 61.6 degrees

Acq. time 4.665 sec

Width 7024.9 Hz

8 repetitions

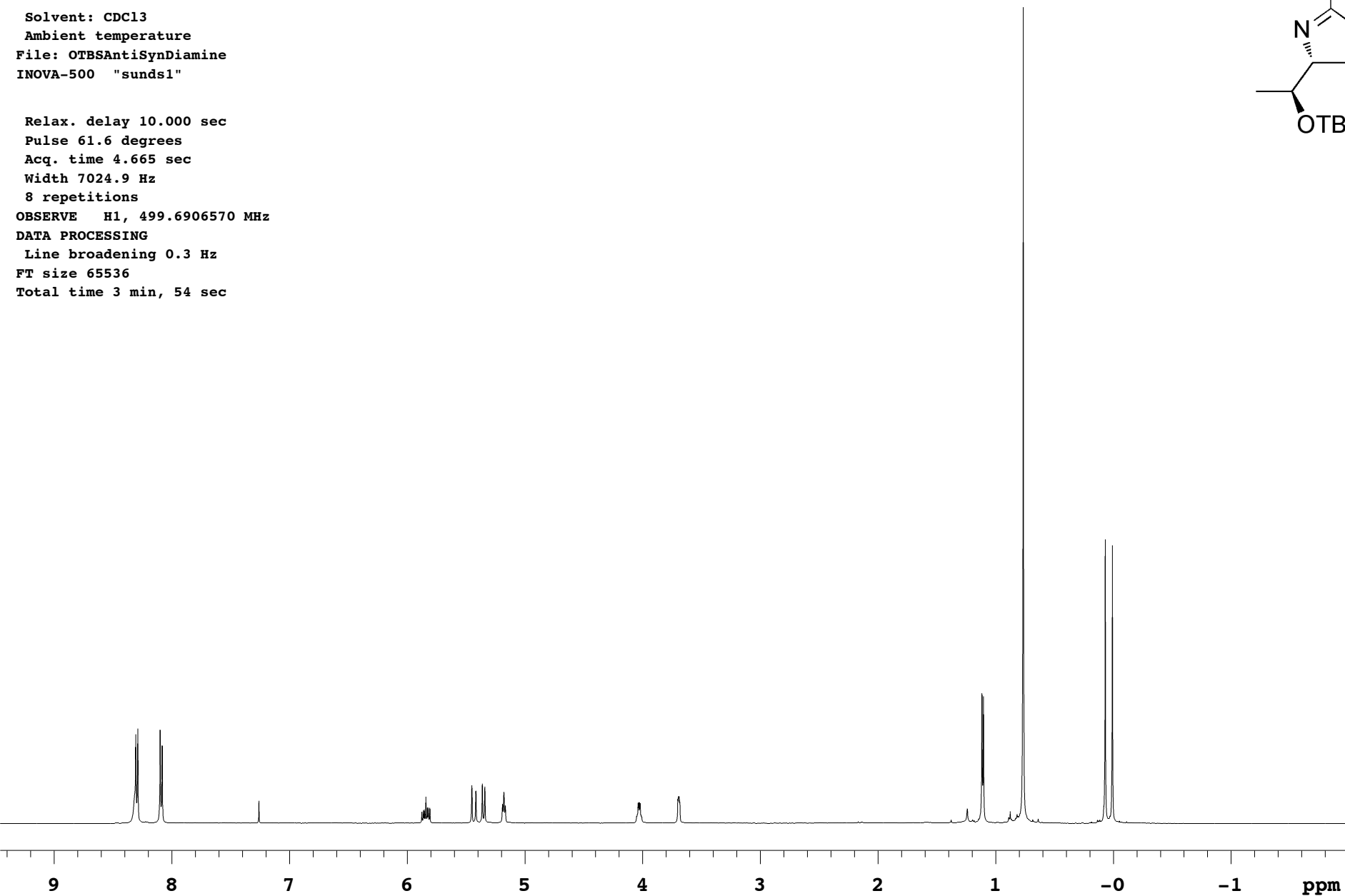
OBSERVE H1, 499.6906570 MHz

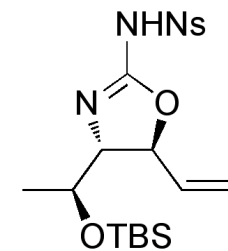
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 3 min, 54 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: OTBSAntiSynDiaminCarb

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

84 repetitions

OBSERVE C13, 125.6473011 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

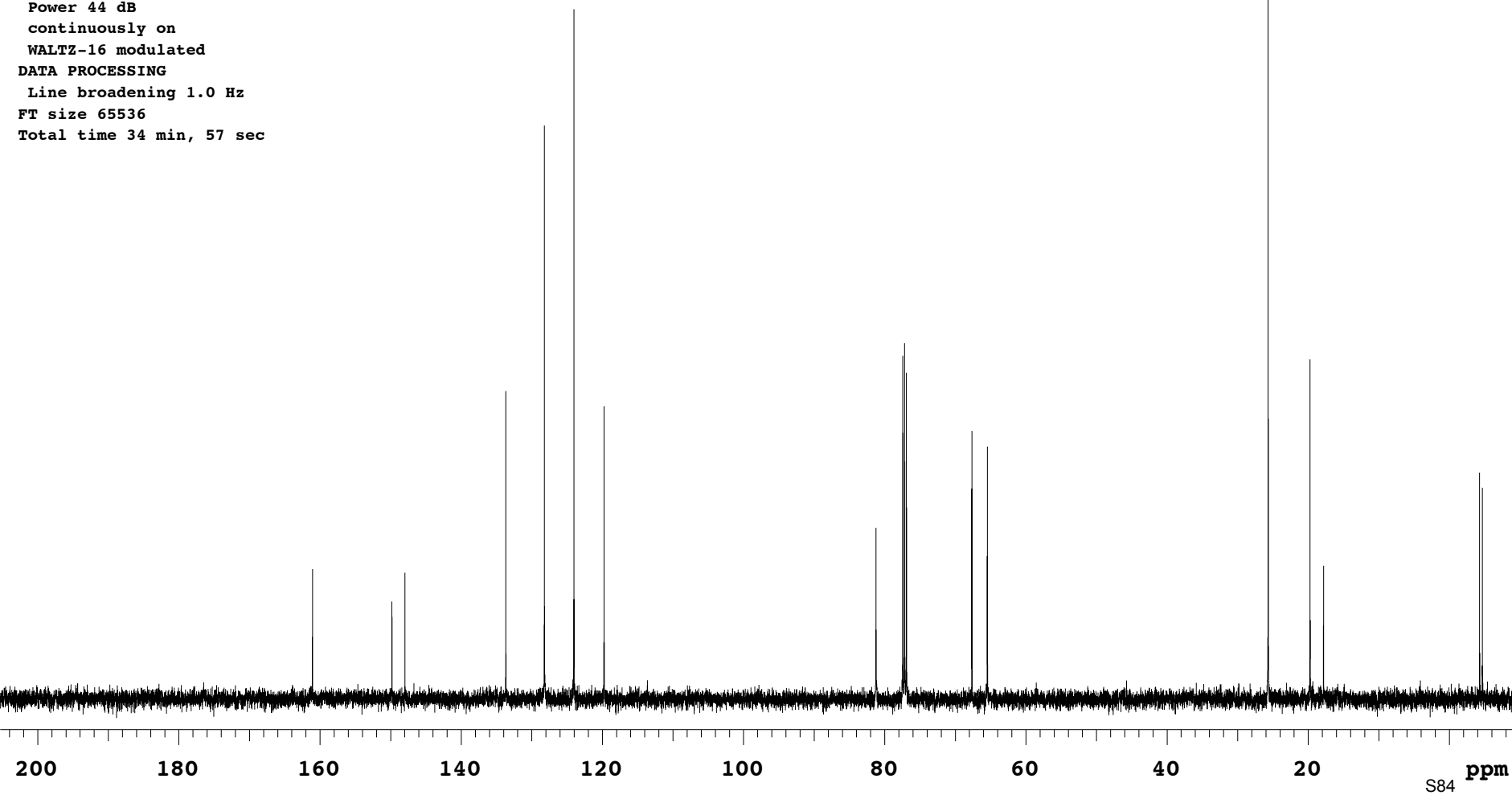
WALTZ-16 modulated

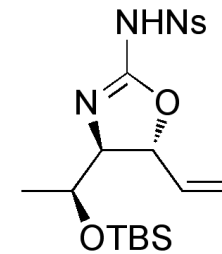
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 34 min, 57 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: OTBSynSynDiamine

INOVA-500 "sunds1"

Relax. delay 10.000 sec

Pulse 45.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

62 repetitions

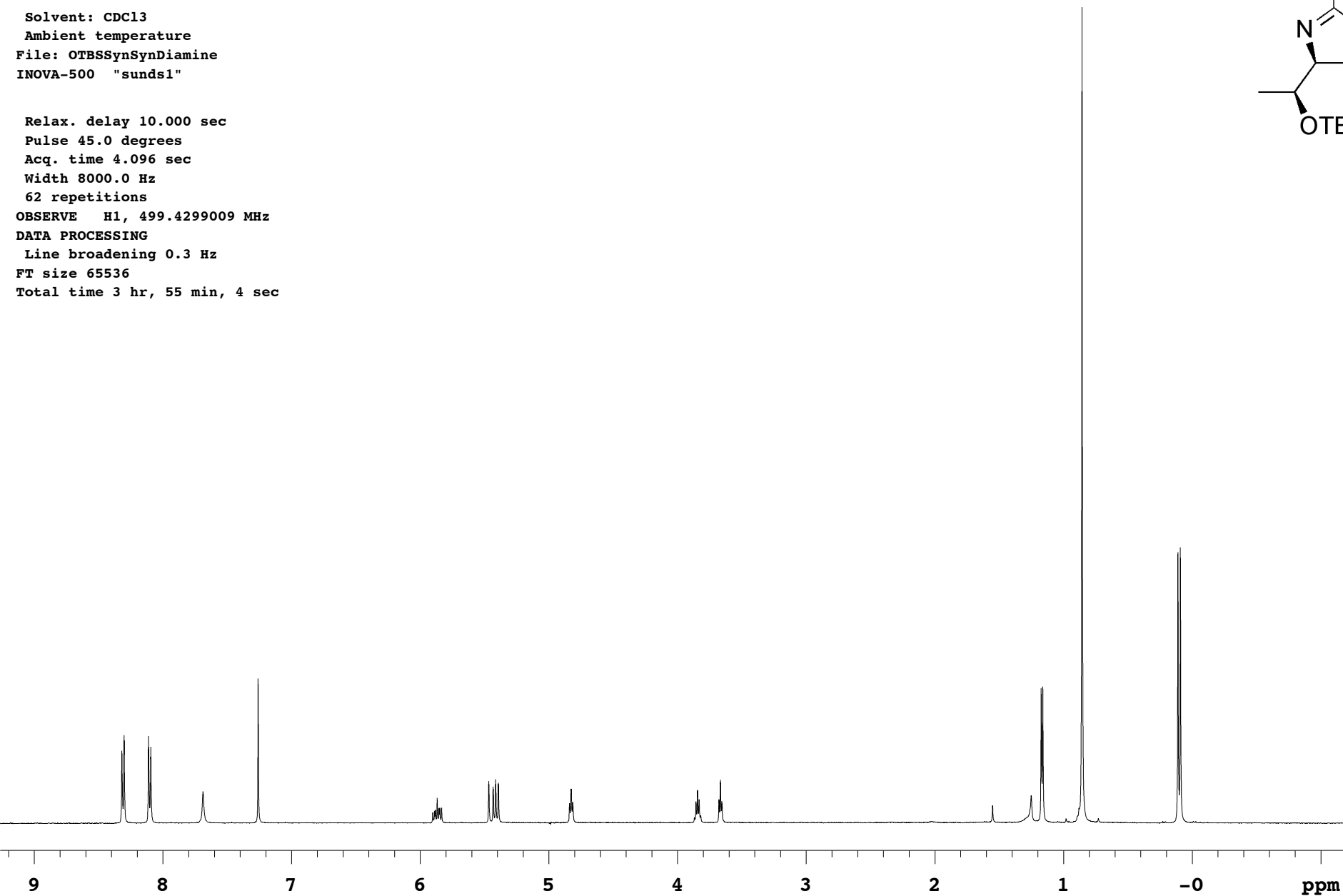
OBSERVE H1, 499.4299009 MHz

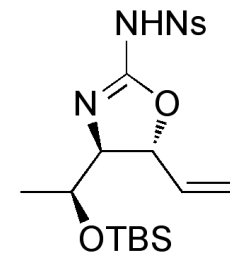
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 3 hr, 55 min, 4 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: OTBSynSynDiamineCarb

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

100 repetitions

OBSERVE C13, 125.6472965 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

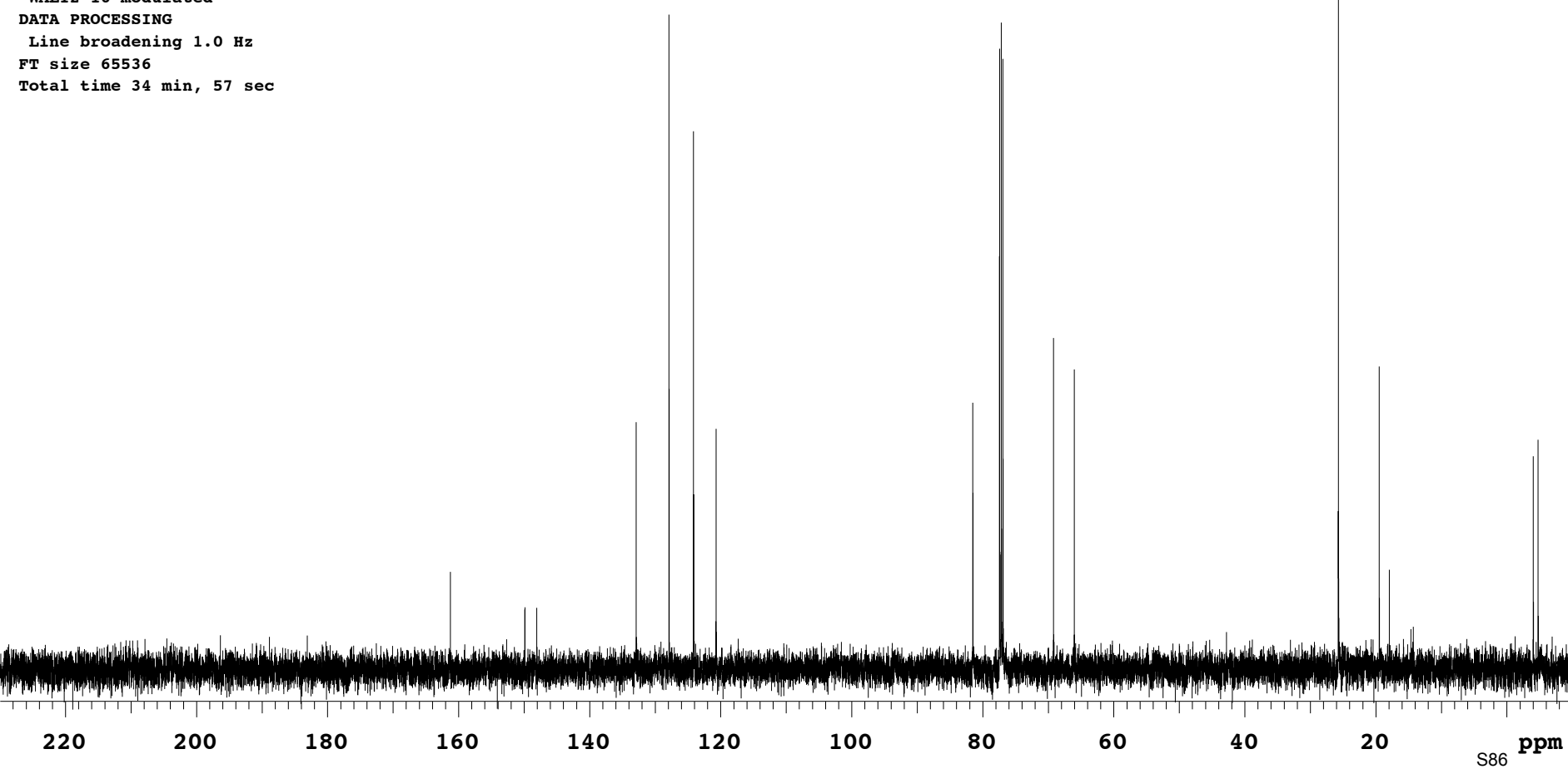
WALTZ-16 modulated

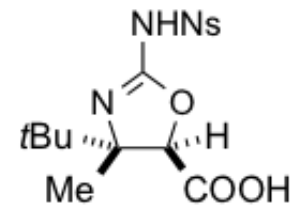
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 34 min, 57 sec





Pulse Sequence: s2pul

Solvent: CD3CN

Ambient temperature

File: oxazoline.acid.H

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

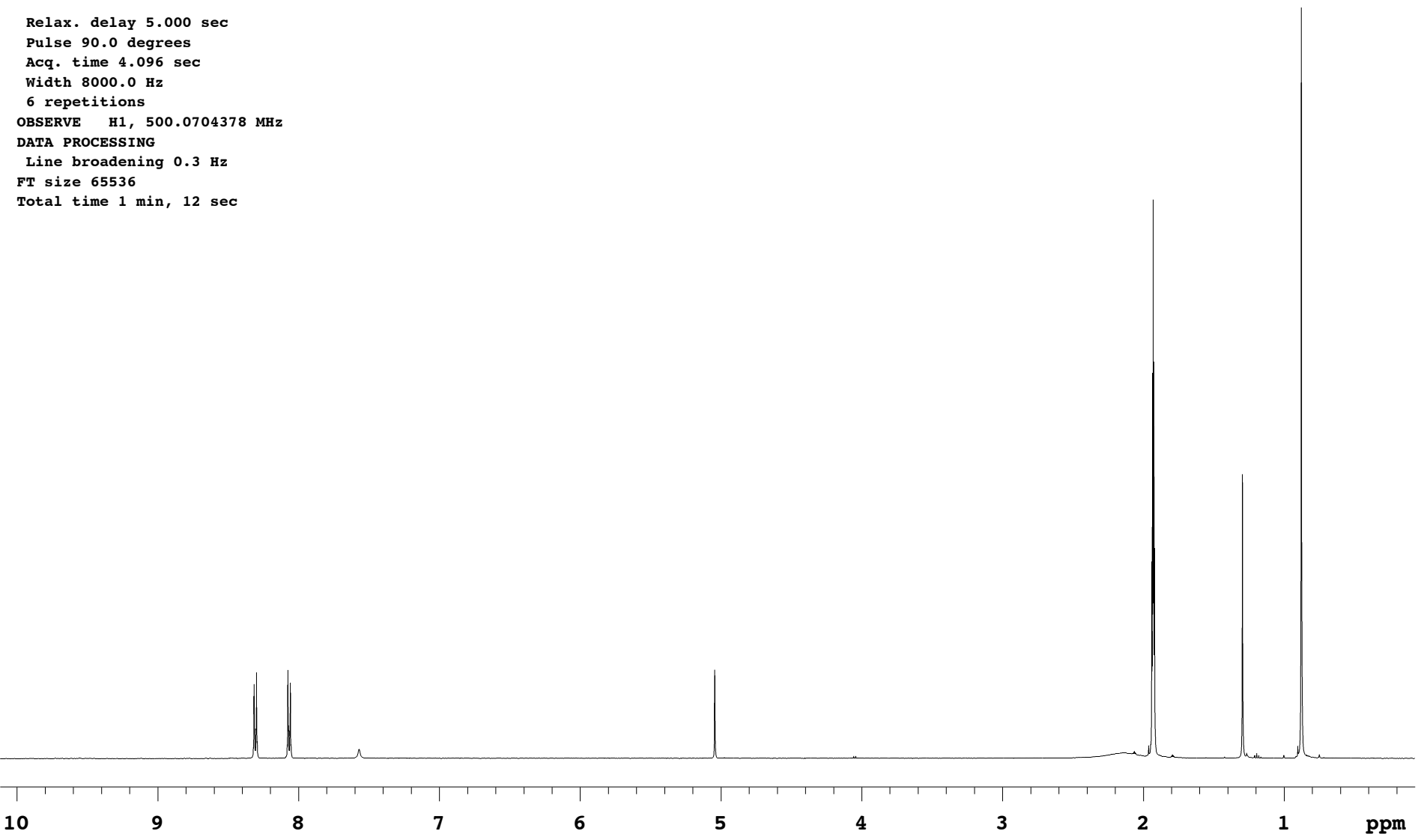
OBSERVE H1, 500.0704378 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec



Pulse Sequence: s2pul

Solvent: CD3OD

Ambient temperature

User: 1-14-87

INOVA-500 "u500"

Relax. delay 10.000 sec

Pulse 28.1 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

150 repetitions

OBSERVE C13, 125.6476336 MHz

DECOUPLE H1, 499.6942963 MHz

Power 45 dB

continuously on

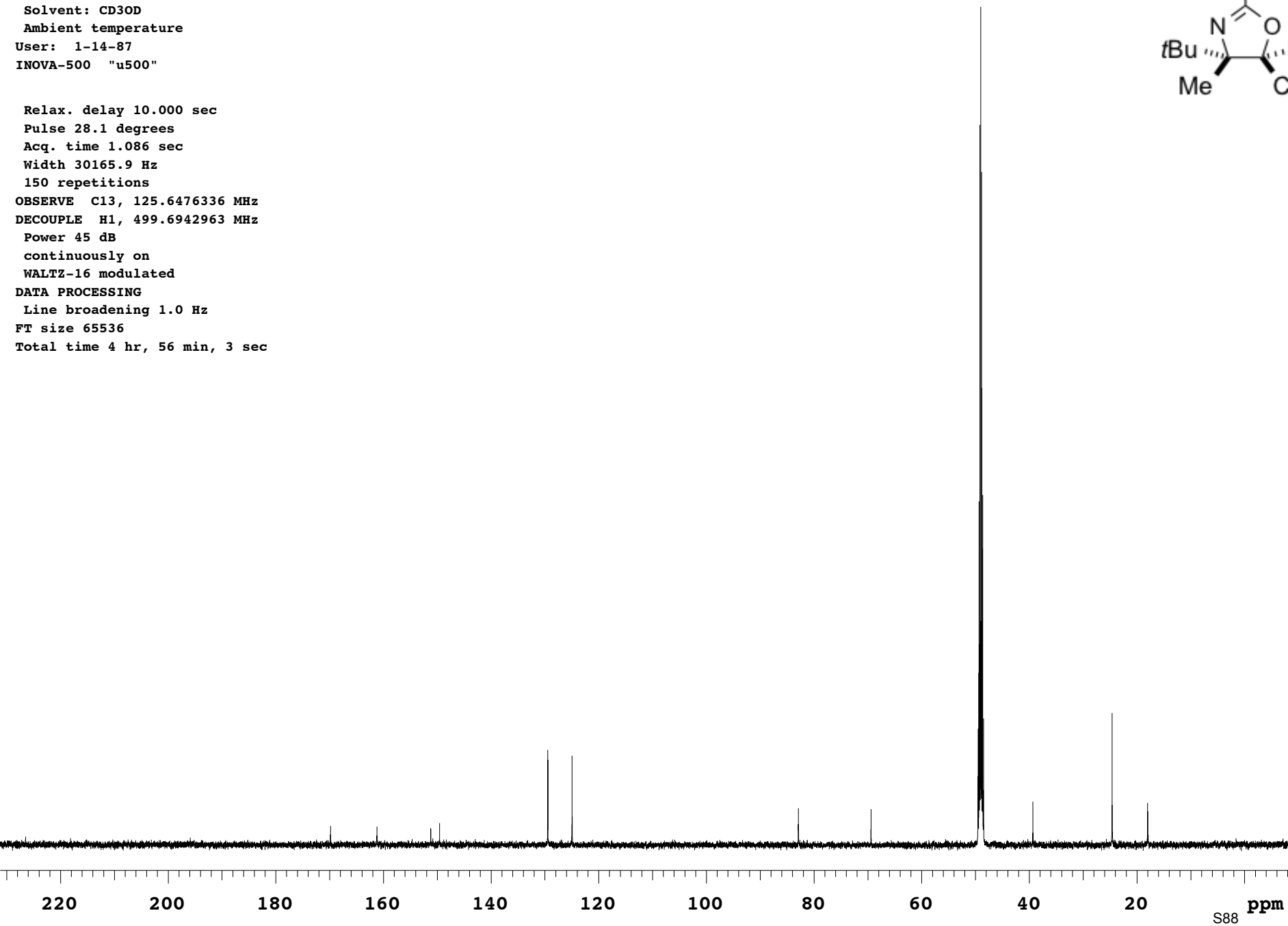
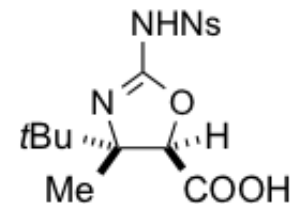
WALTZ-16 modulated

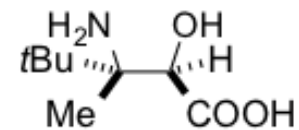
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 4 hr, 56 min, 3 sec





Pulse Sequence: s2pul

Solvent: D2O

Ambient temperature

File: IIS.aminoalcoholacid.H

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

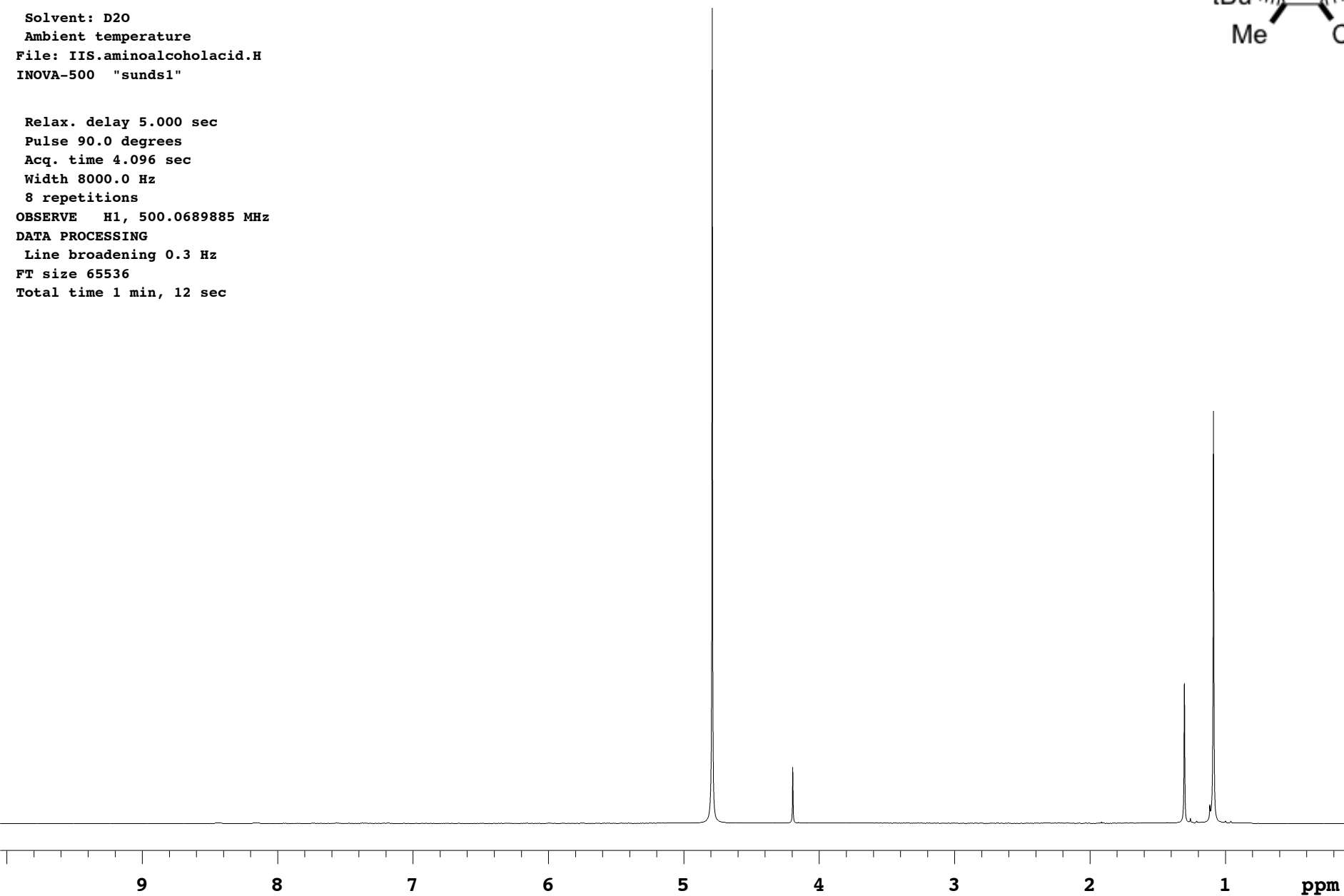
OBSERVE H1, 500.0689885 MHz

DATA PROCESSING

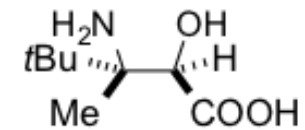
Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec







Pulse Sequence: s2pul

Solvent: D<sub>2</sub>O

Ambient temperature

User: 1-14-87

File: iis.128.x.col.c13

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

12800 repetitions

OBSERVE C13, 125.5820394 MHz

DECOUPLE H1, 499.4328473 MHz

Power 47 dB

continuously on

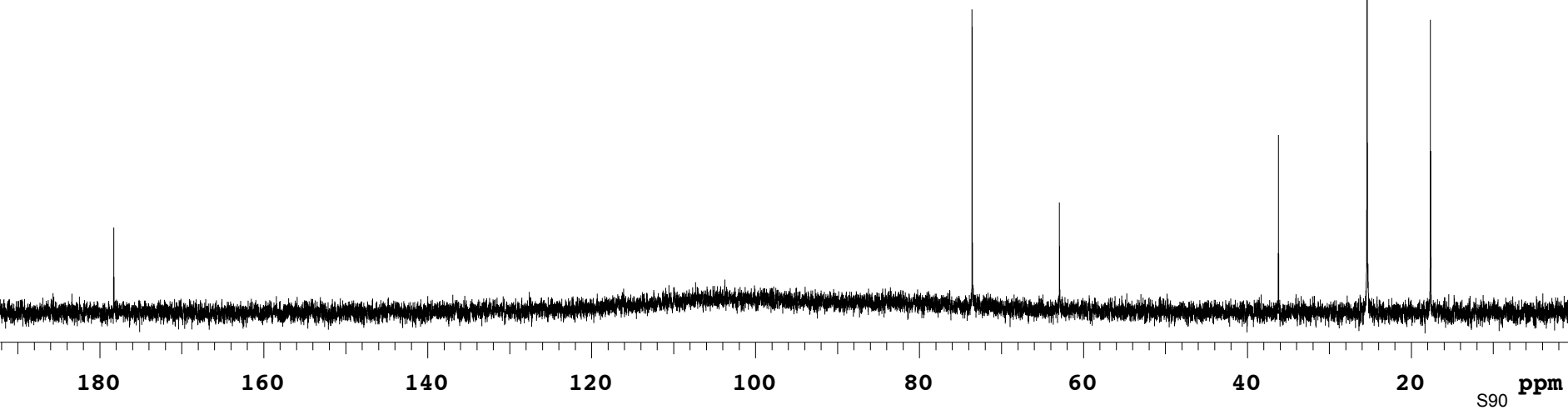
WALTZ-16 modulated

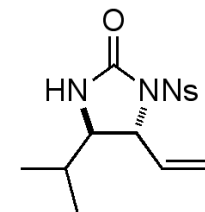
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 7 hr, 13 min, 43 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: iPr\_P

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

12 repetitions

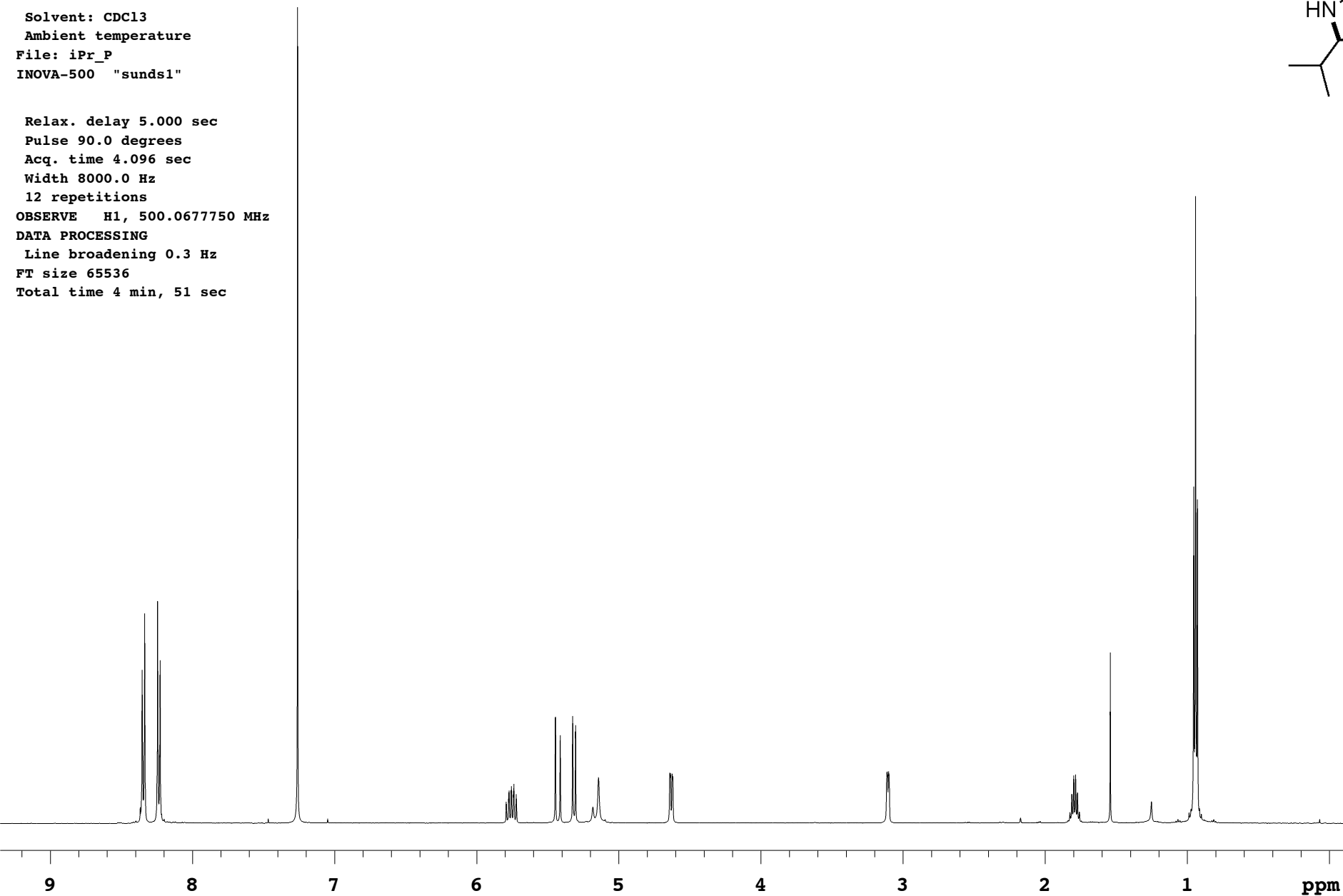
OBSERVE H1, 500.0677750 MHz

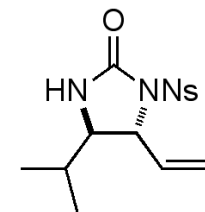
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 4 min, 51 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: iPr\_P\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

444 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 48 dB

continuously on

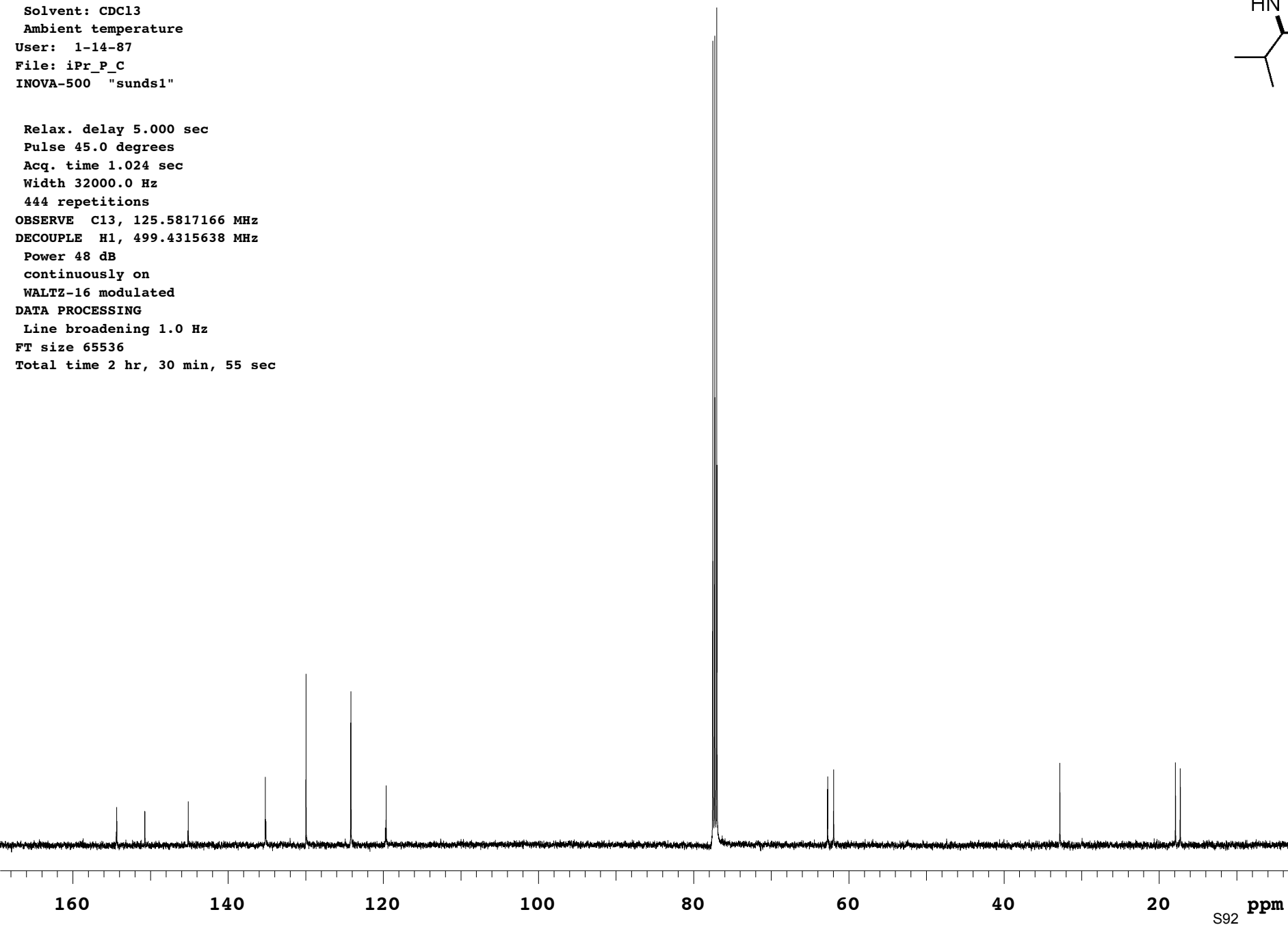
WALTZ-16 modulated

DATA PROCESSING

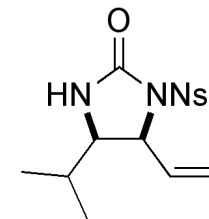
Line broadening 1.0 Hz

FT size 65536

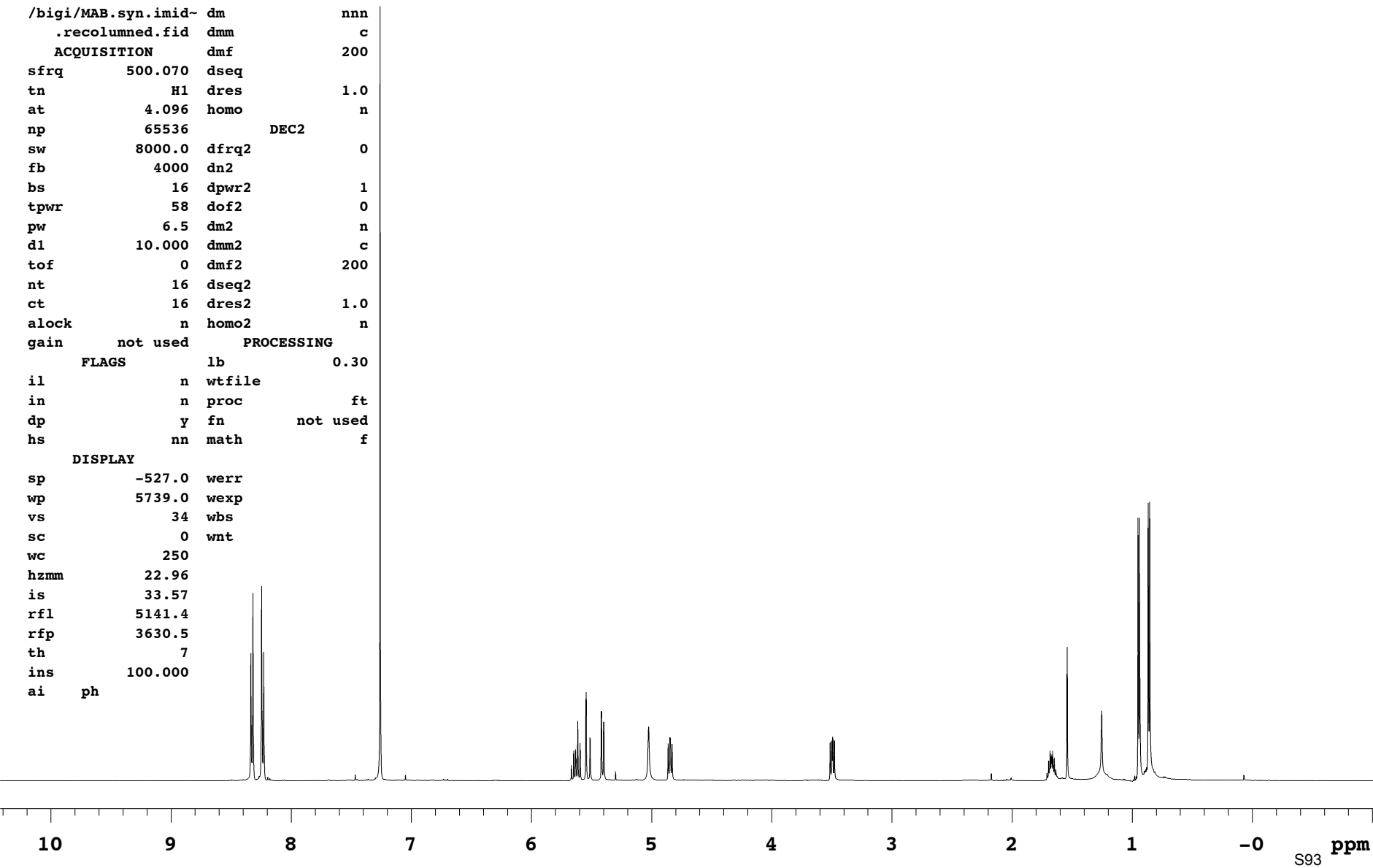
Total time 2 hr, 30 min, 55 sec



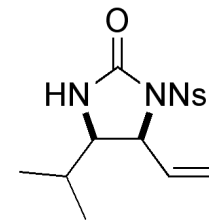
expl s2pul



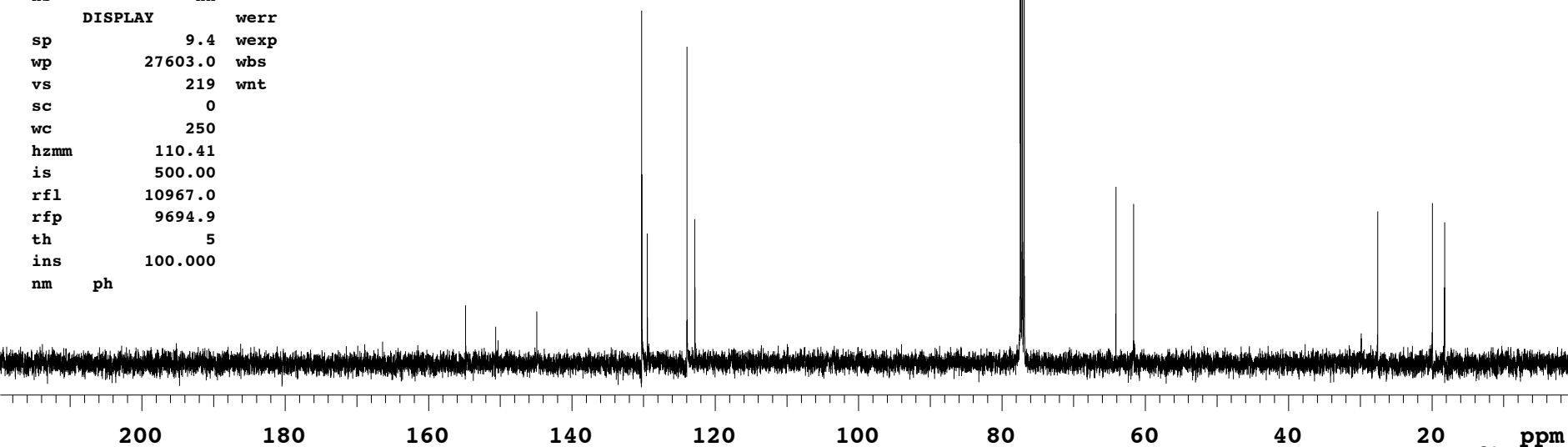
SAMPLE		DEC	
date	Jan 3 2013	dfrq	
solvent	CDC13	dn	
file	/export/home/~	dpwr	
data/ui500nb/White~		dof	
/bigi/MAB.syn.imid~		dm	nnn
.recolumned.fid		dmm	c
ACQUISITION		dmf	200
sfrq	500.070	dseq	
tn	H1	dres	1.0
at	4.096	homo	n
np	65536	DEC2	
sw	8000.0	dfrq2	0
fb	4000	dn2	
bs	16	dpwr2	1
tpwr	58	dof2	0
pw	6.5	dm2	n
d1	10.000	dmm2	c
tof	0	dmf2	200
nt	16	dseq2	
ct	16	dres2	1.0
alock	n	homo2	n
gain	not used	PROCESSING	
FLAGS		lb	0.30
il	n	wtfile	
in	n	proc	ft
dp	y	fn	not used
hs	nn	math	f
DISPLAY			
sp	-527.0	werr	
wp	5739.0	wexp	
vs	34	wbs	
sc	0	wnt	
wc	250		
hzmm	22.96		
is	33.57		
rfl	5141.4		
rfp	3630.5		
th	7		
ins	100.000		
ai	ph		

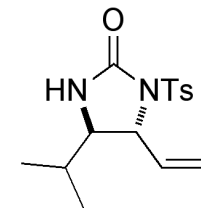


expl s2pul



SAMPLE		DEC. & VT	
date	Jan 3 2013	dfrq	499.692
solvent	CDC13	dn	H1
file	/export/home/~	dpwr	45
data/u500/White/bi-		dof	-827.6
gi/MAB.syn.imid.ca-		dm	YYY
rbon.fid		dmm	w
ACQUISITION		dmf	
sfrq	125.661	dseq	20202
tn	C13	dres	90.0
at	1.086	homo	n
np	65536	DEC2	
sw	30165.9	dfrq2	0
fb	17000	dn2	
bs	16	dpwr2	1
ss	1	dof2	0
tpwr	60	dm2	n
pw	6.0	dmm2	c
d1	1.000	dmf2	10000
tof	1884.7	dseq2	
nt	1500	dres2	1.0
ct	1184	homo2	n
alock	n	PROCESSING	
gain	not used	lb	1.00
FLAGS		wtfile	
il	n	proc	ft
in	n	fn	not used
dp	y	math	f
hs	nn		
DISPLAY		werr	
sp	9.4	wexp	
wp	27603.0	wbs	
vs	219	wnt	
sc	0		
wc	250		
hzmm	110.41		
is	500.00		
rfl	10967.0		
rfp	9694.9		
th	5		
ins	100.000		
nm	ph		





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: iPrTs\_anti\_diamine

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

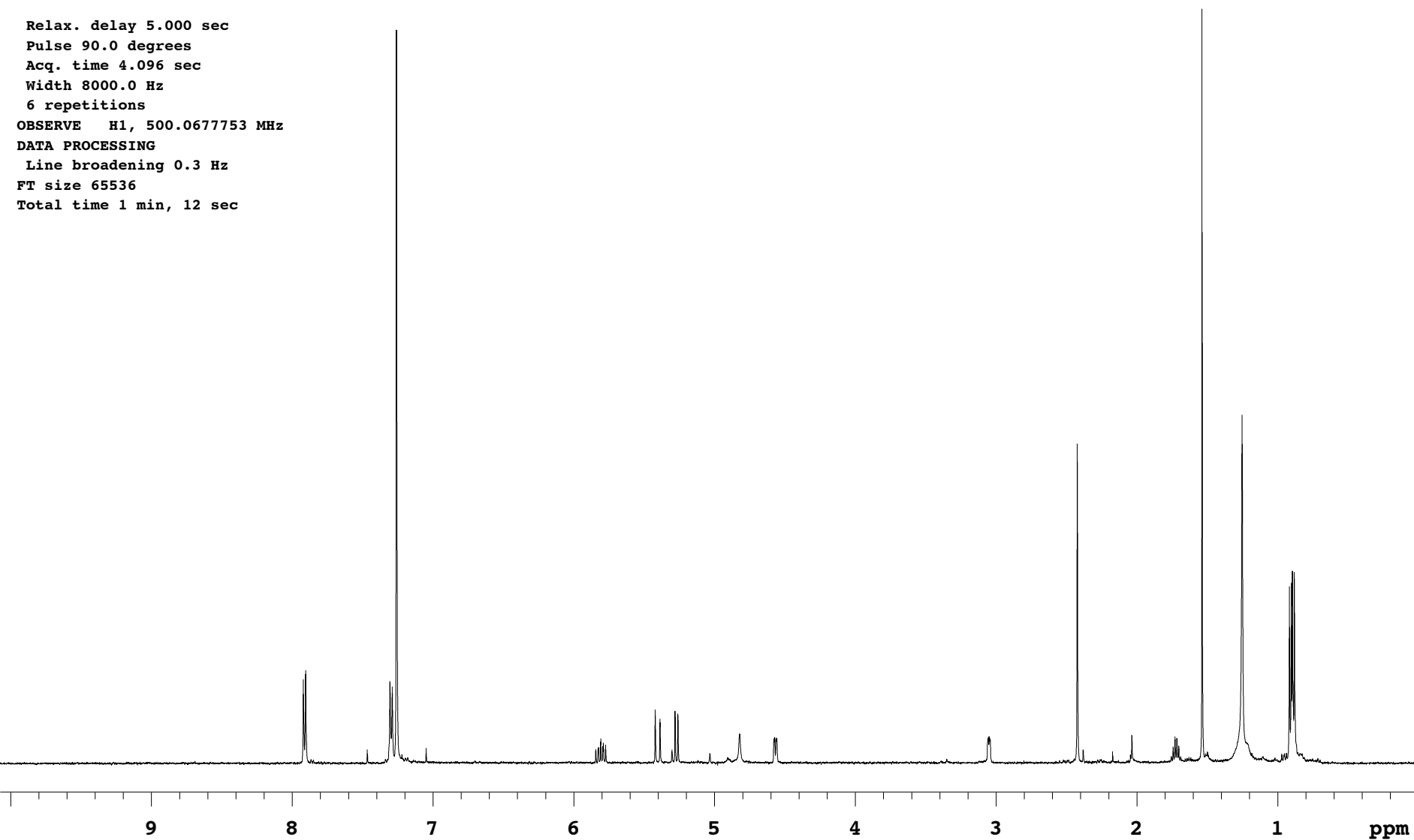
OBSERVE H1, 500.0677753 MHz

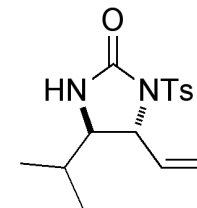
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

3526 repetitions

OBSERVE C13, 125.5817483 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

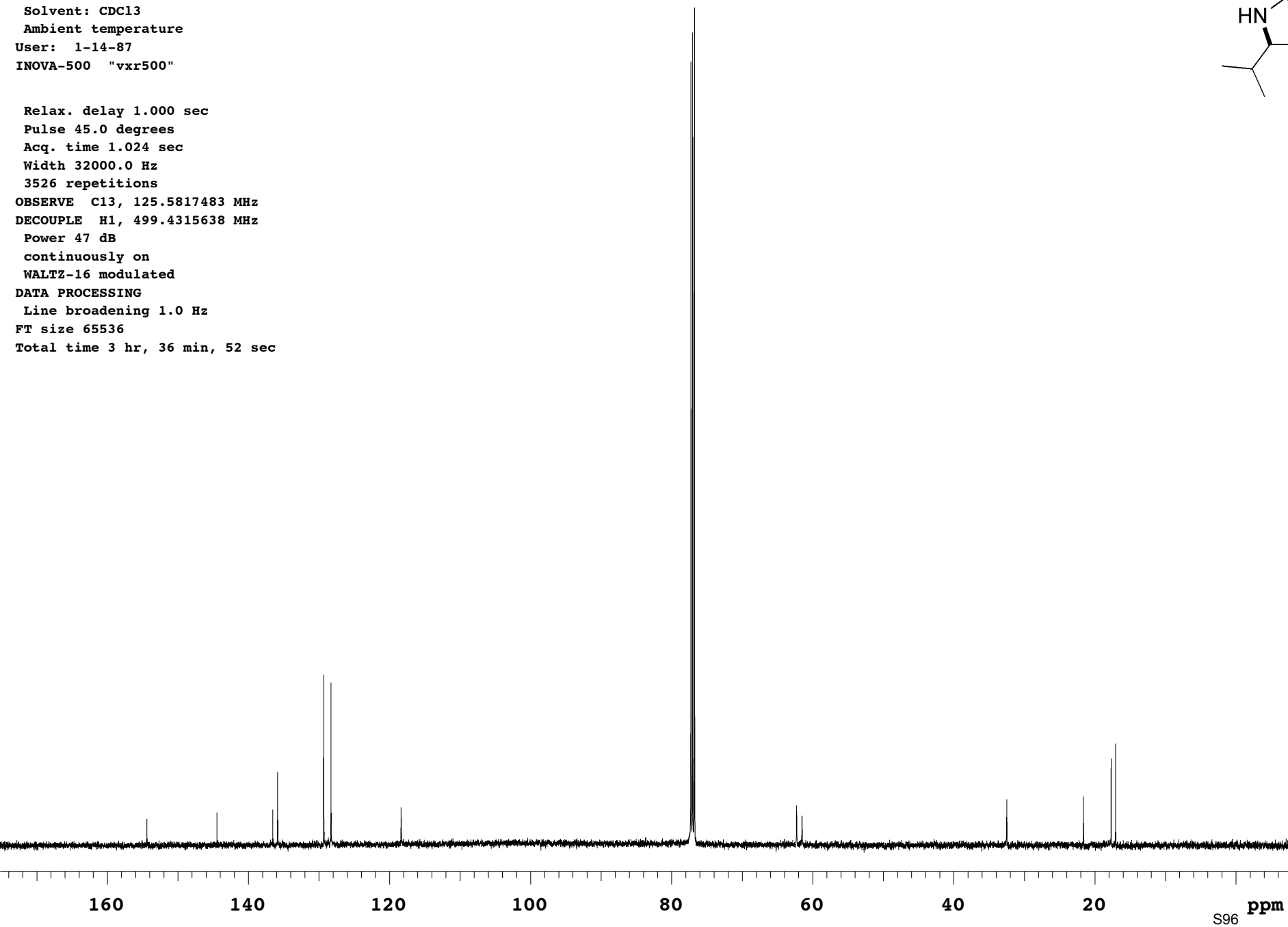
WALTZ-16 modulated

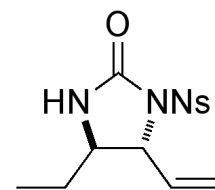
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 36 min, 52 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: Et\_P2

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

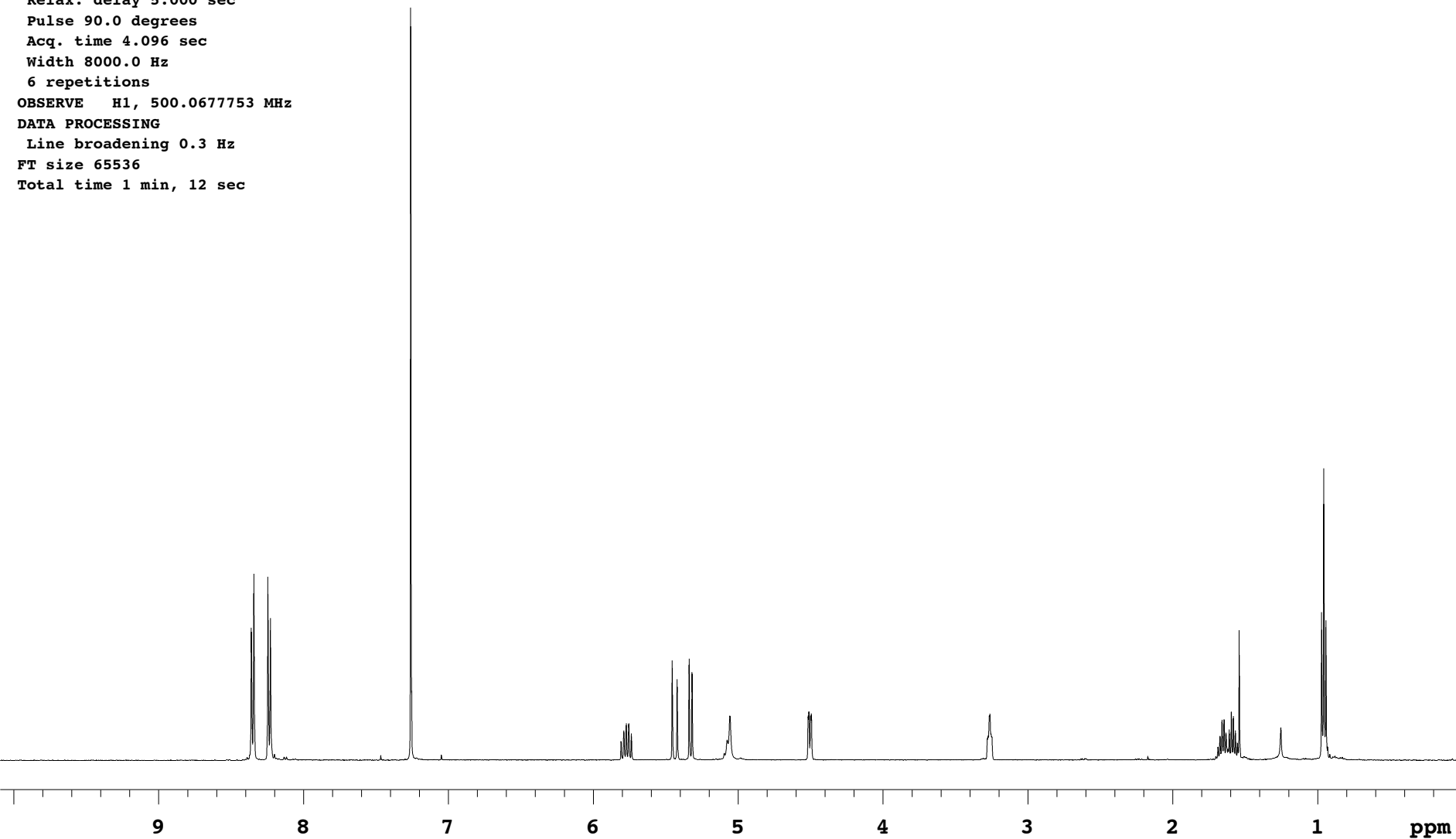
OBSERVE H1, 500.0677753 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

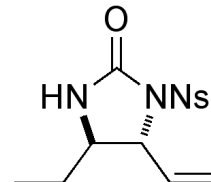
Total time 1 min, 12 sec





Et\_P

# Strambeanu and White



Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

INOVA-500 "u500"

Relax. delay 1.000 sec

Pulse 28.1 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

480 repetitions

OBSERVE C13, 125.6473203 MHz

DECOUPLE H1, 499.6923275 MHz

Power 45 dB

continuously on

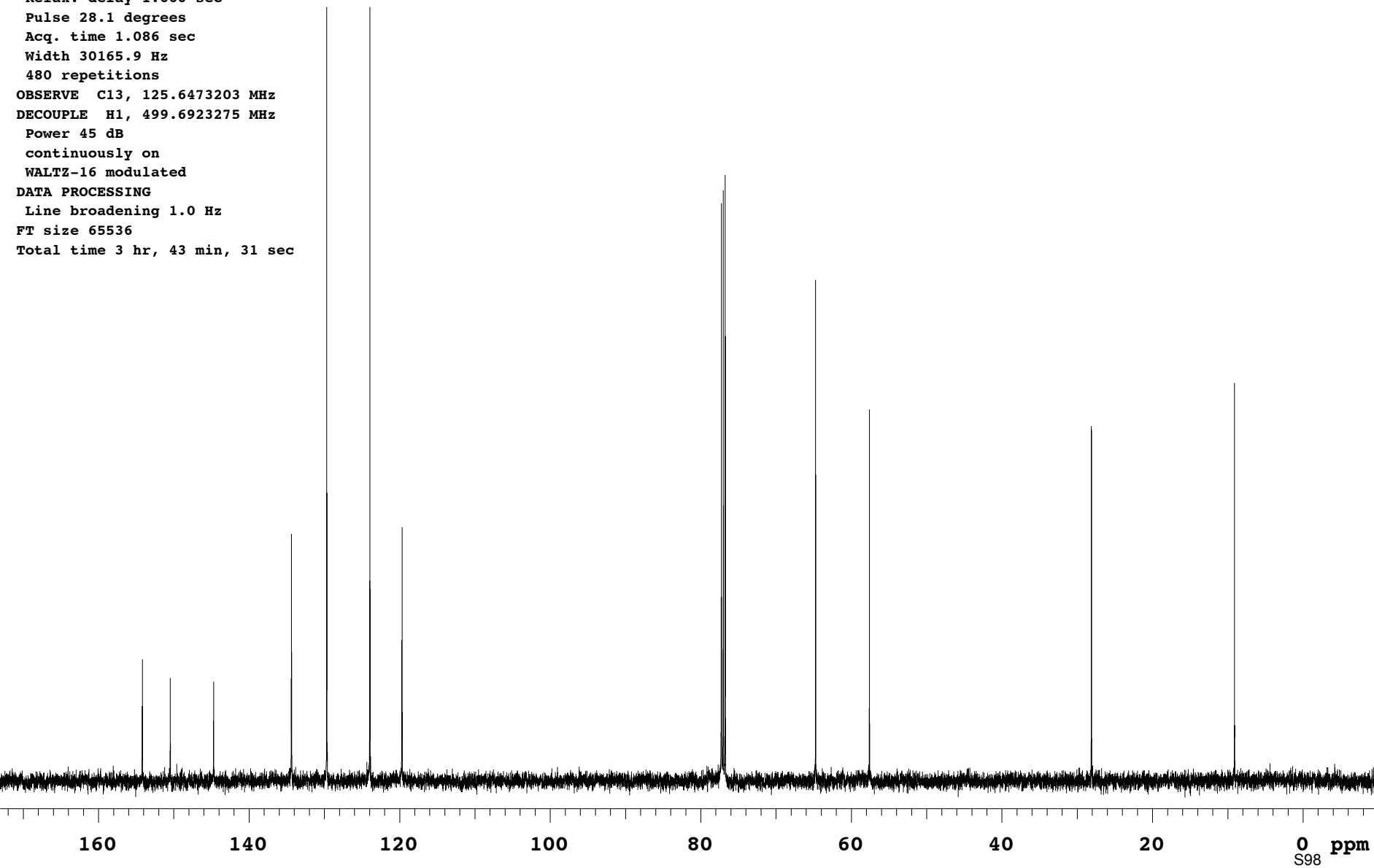
WALTZ-16 modulated

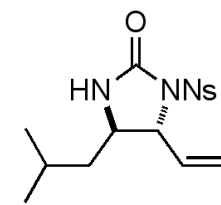
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 43 min, 31 sec





STANDARD PROTON PARAMETERS

Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

INOVA-500 "ui500nb"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

12 repetitions

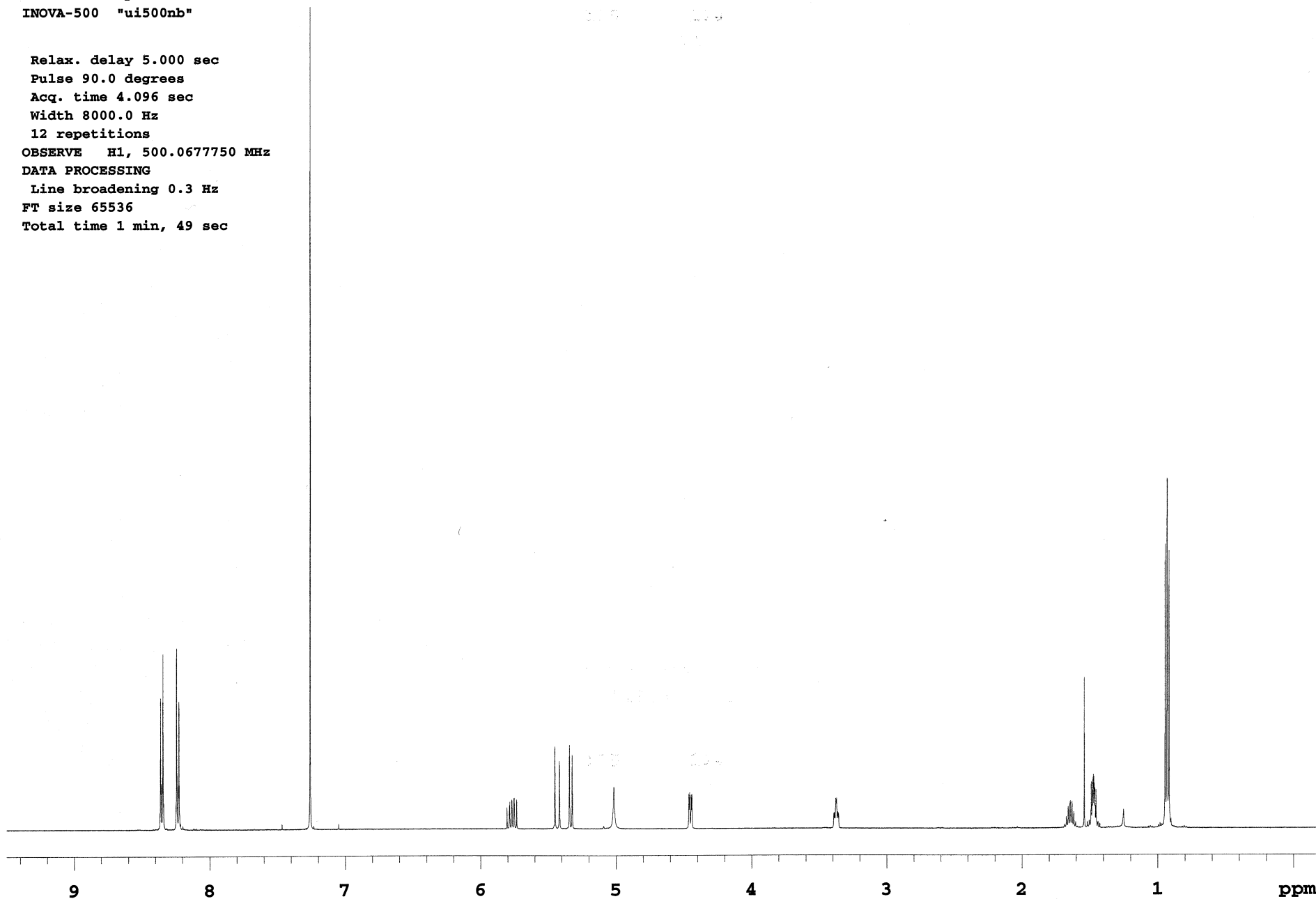
OBSERVE H1, 500.0677750 MHz

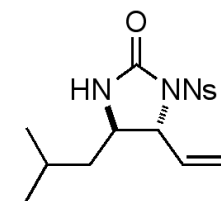
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 49 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: iBu\_P

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

228 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

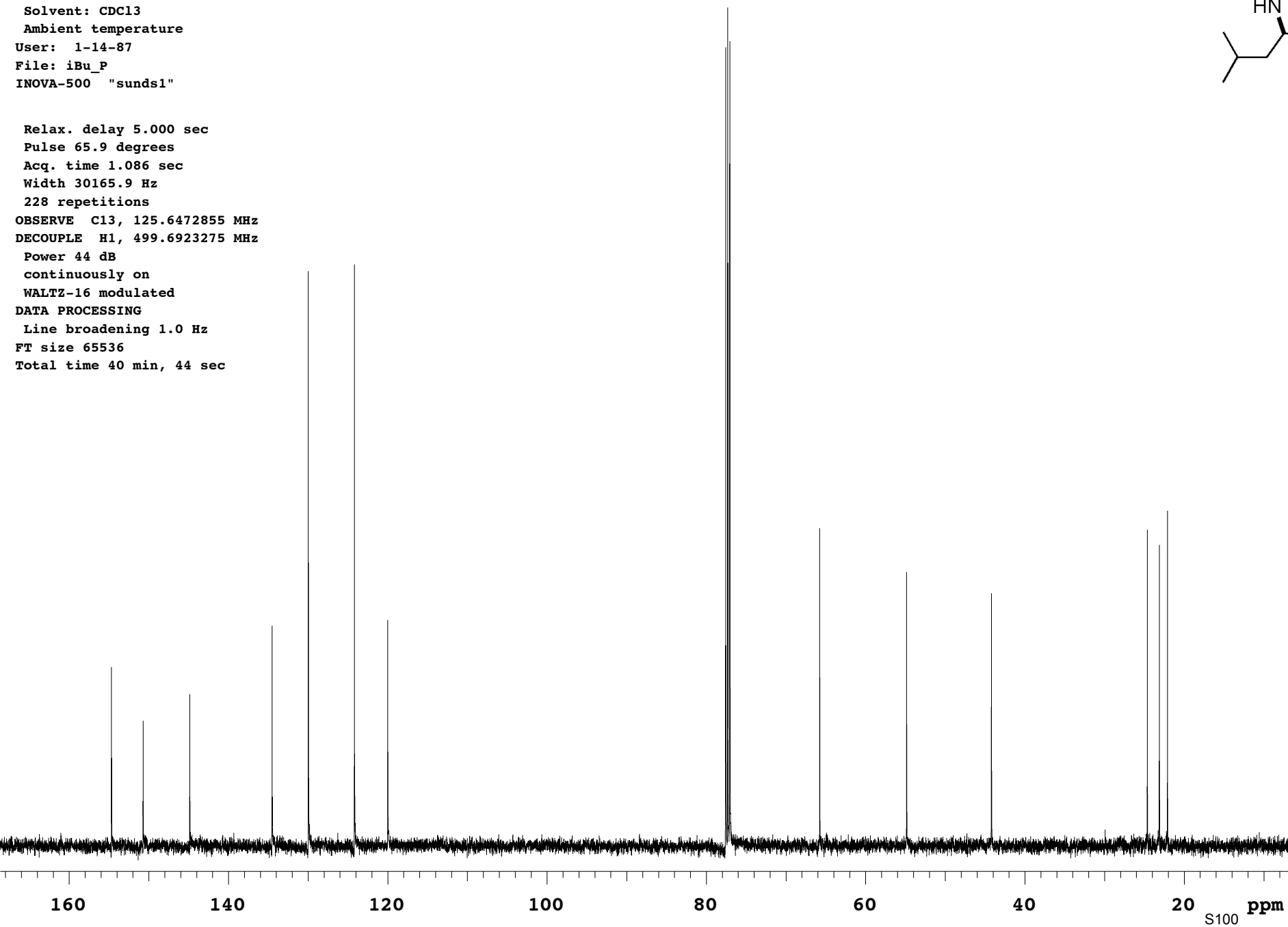
WALTZ-16 modulated

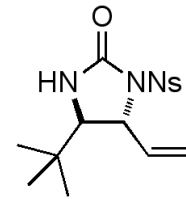
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 40 min, 44 sec





STANDARD PROTON PARAMETERS

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "ui500nb"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

12 repetitions

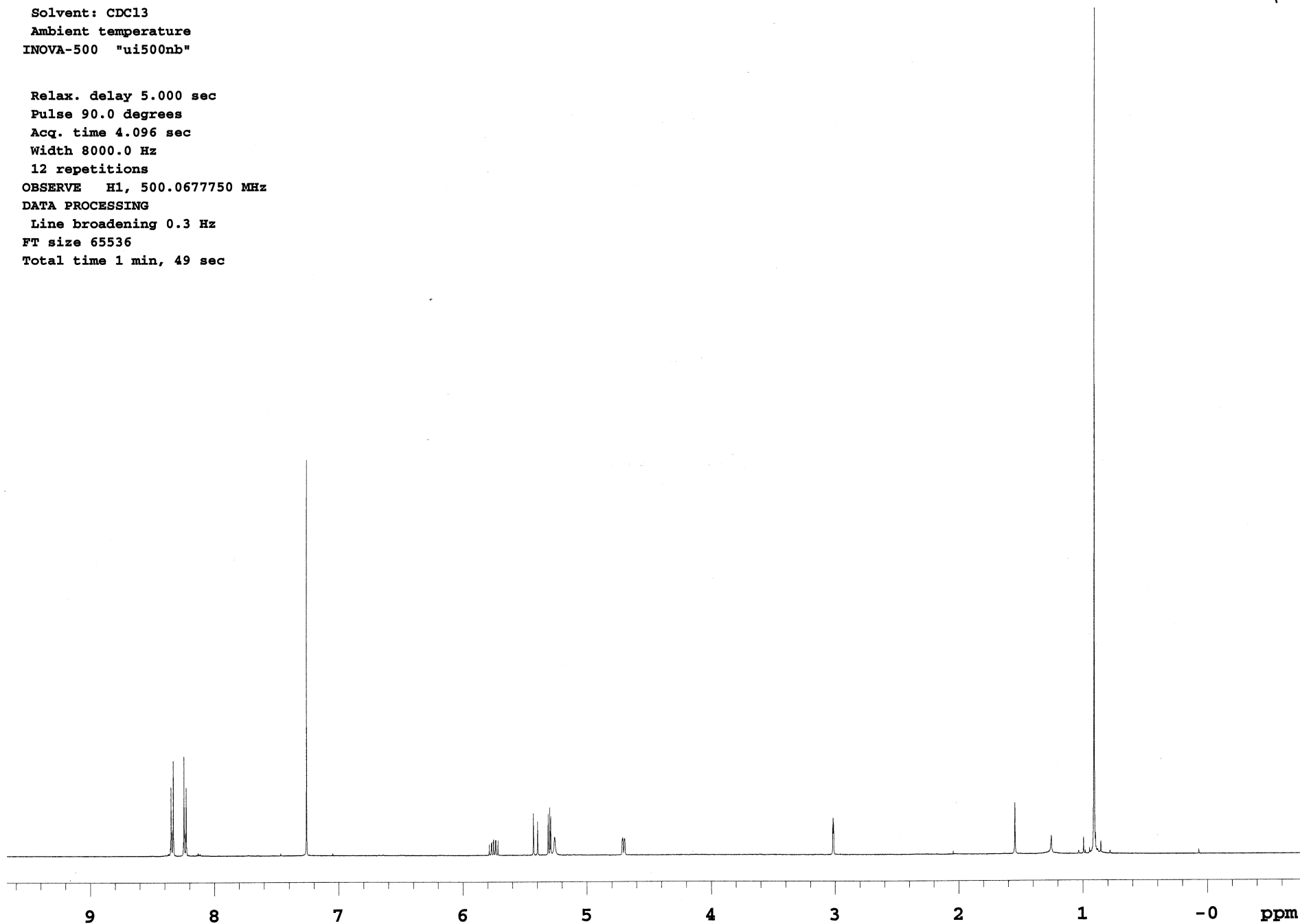
OBSERVE H1, 500.0677750 MHz

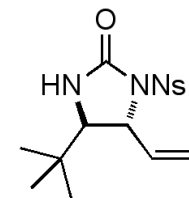
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 49 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: tBu\_P

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

216 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

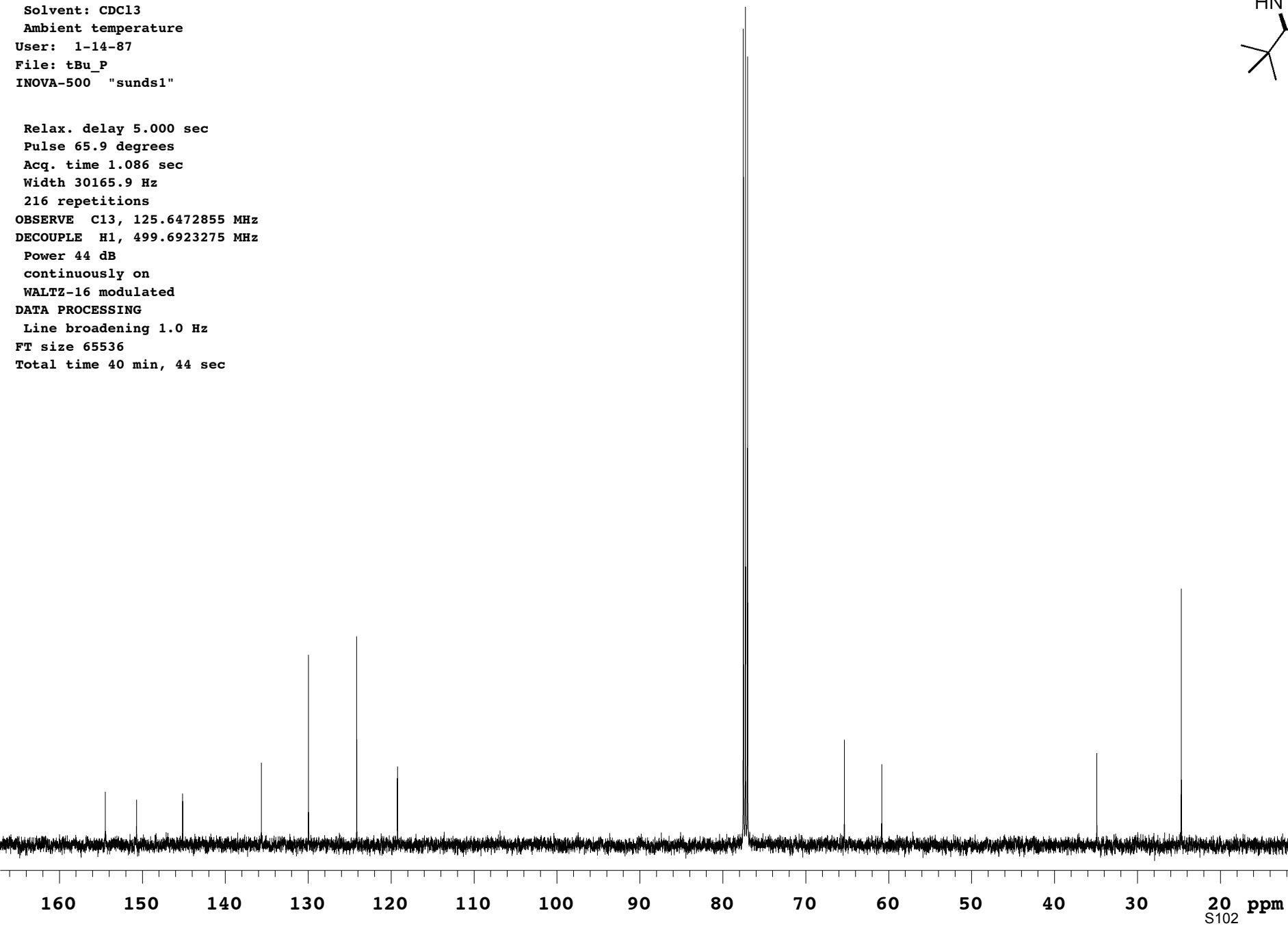
WALTZ-16 modulated

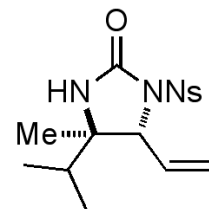
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 40 min, 44 sec





Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

File: quat\_P

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

10 repetitions

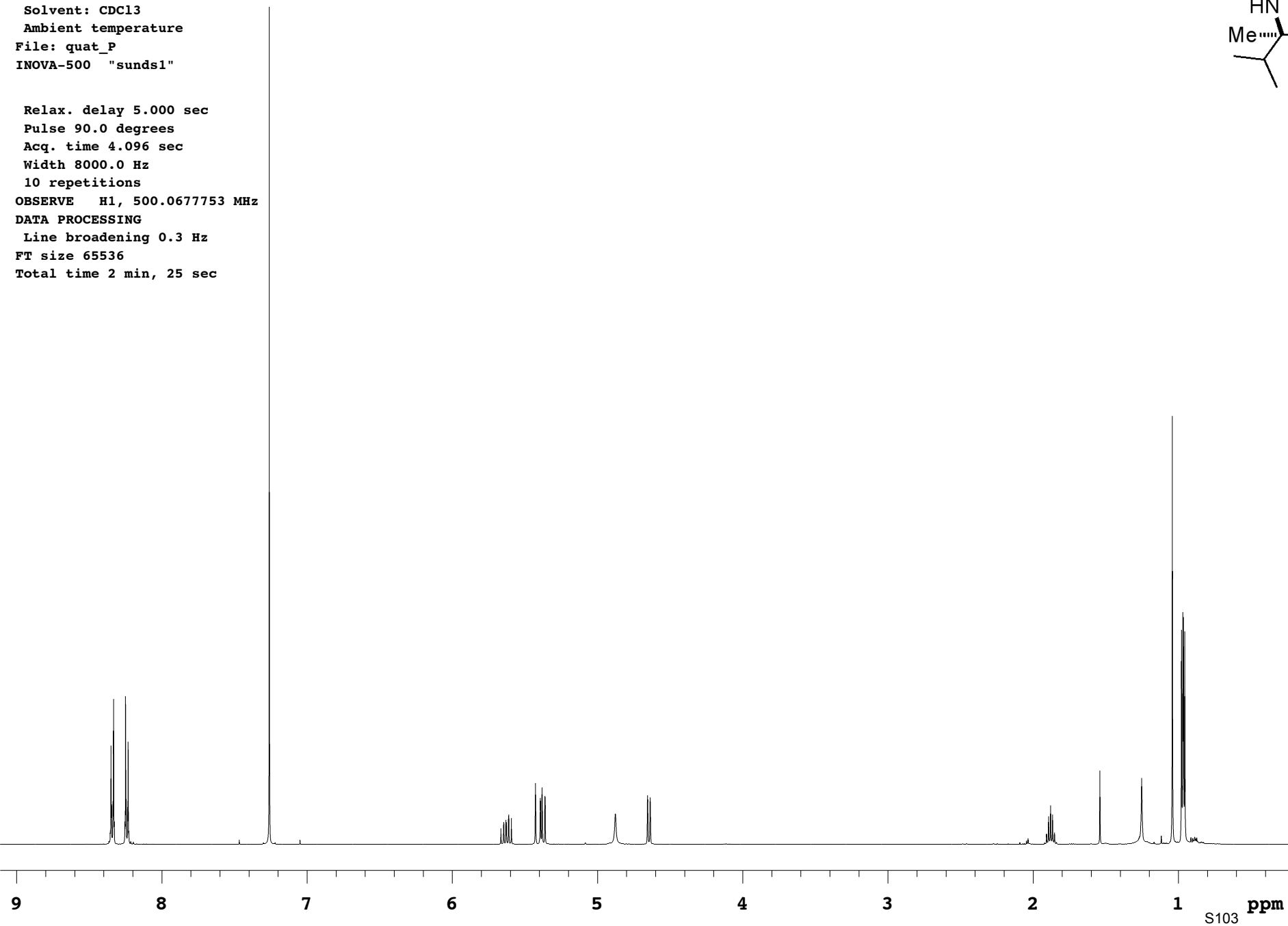
OBSERVE H1, 500.0677753 MHz

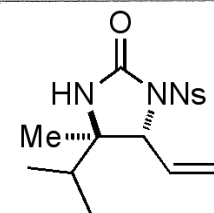
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec





## STANDARD CARBON PARAMETERS

Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

360 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 44 dB

continuously on

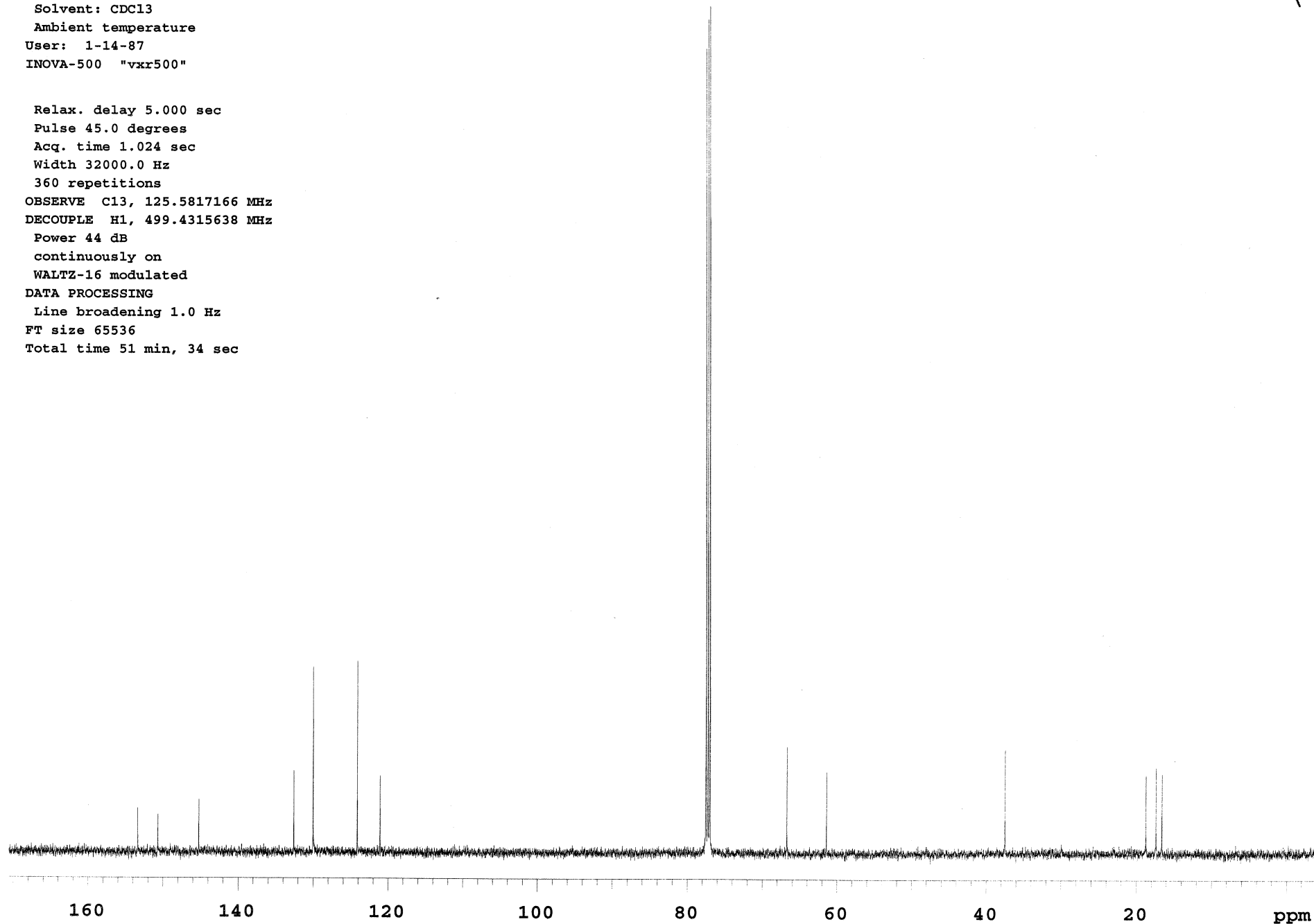
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 51 min, 34 sec



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: tBuMe\_P\_anti

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 47.8 degrees

Acq. time 4.665 sec

Width 7024.9 Hz

8 repetitions

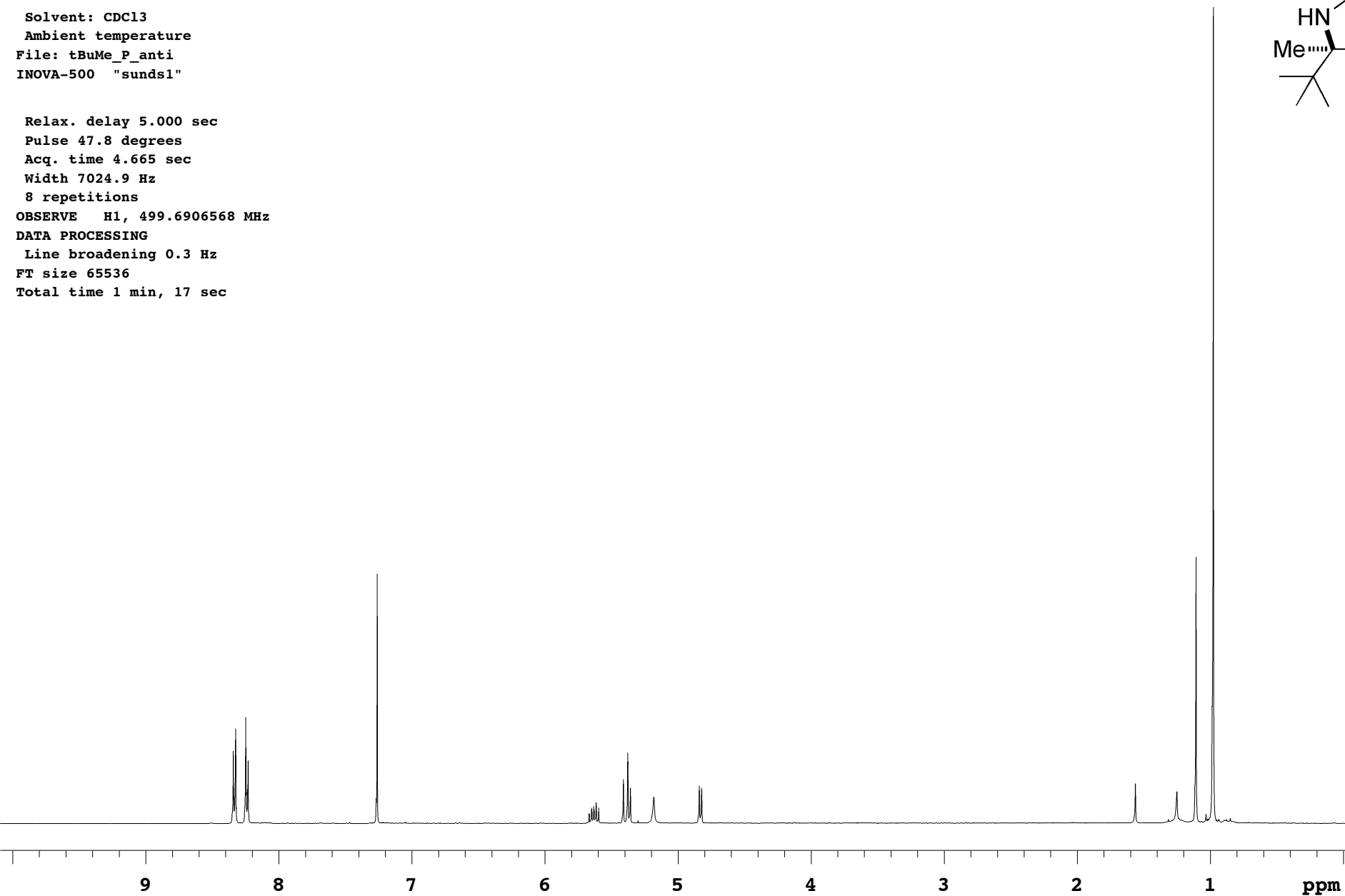
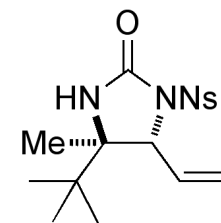
OBSERVE H1, 499.6906568 MHz

DATA PROCESSING

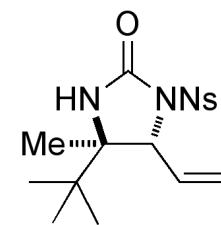
Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 17 sec







Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: tBuMe\_P\_anti\_C13

INOVA-500 "sunds1"

Relax. delay 1.000 sec

Pulse 28.1 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

914 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 45 dB

continuously on

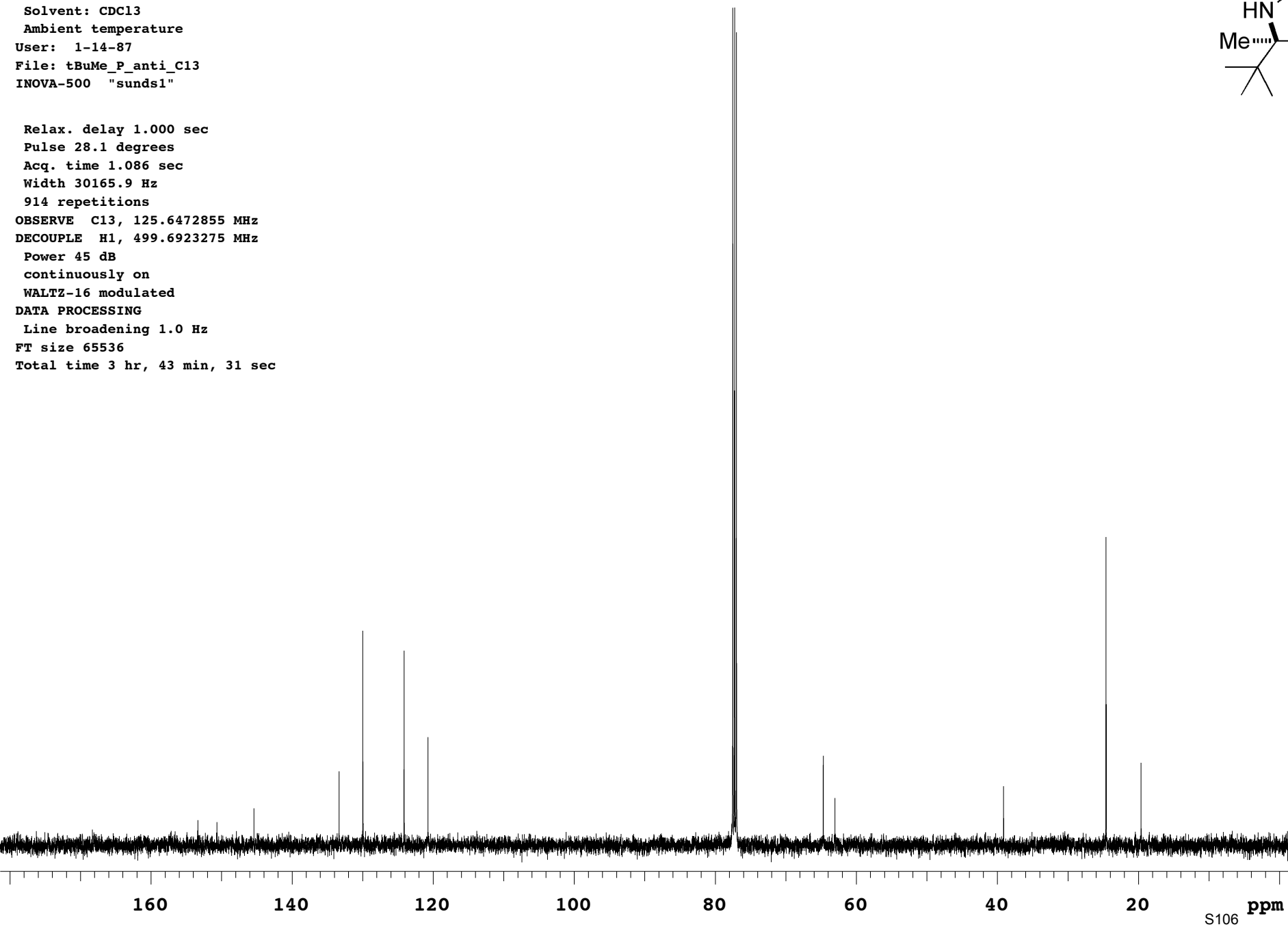
WALTZ-16 modulated

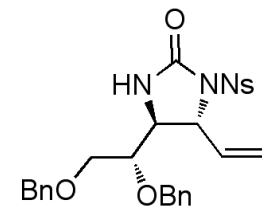
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 3 hr, 43 min, 31 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

File: OBn\_anti\_P

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

12 repetitions

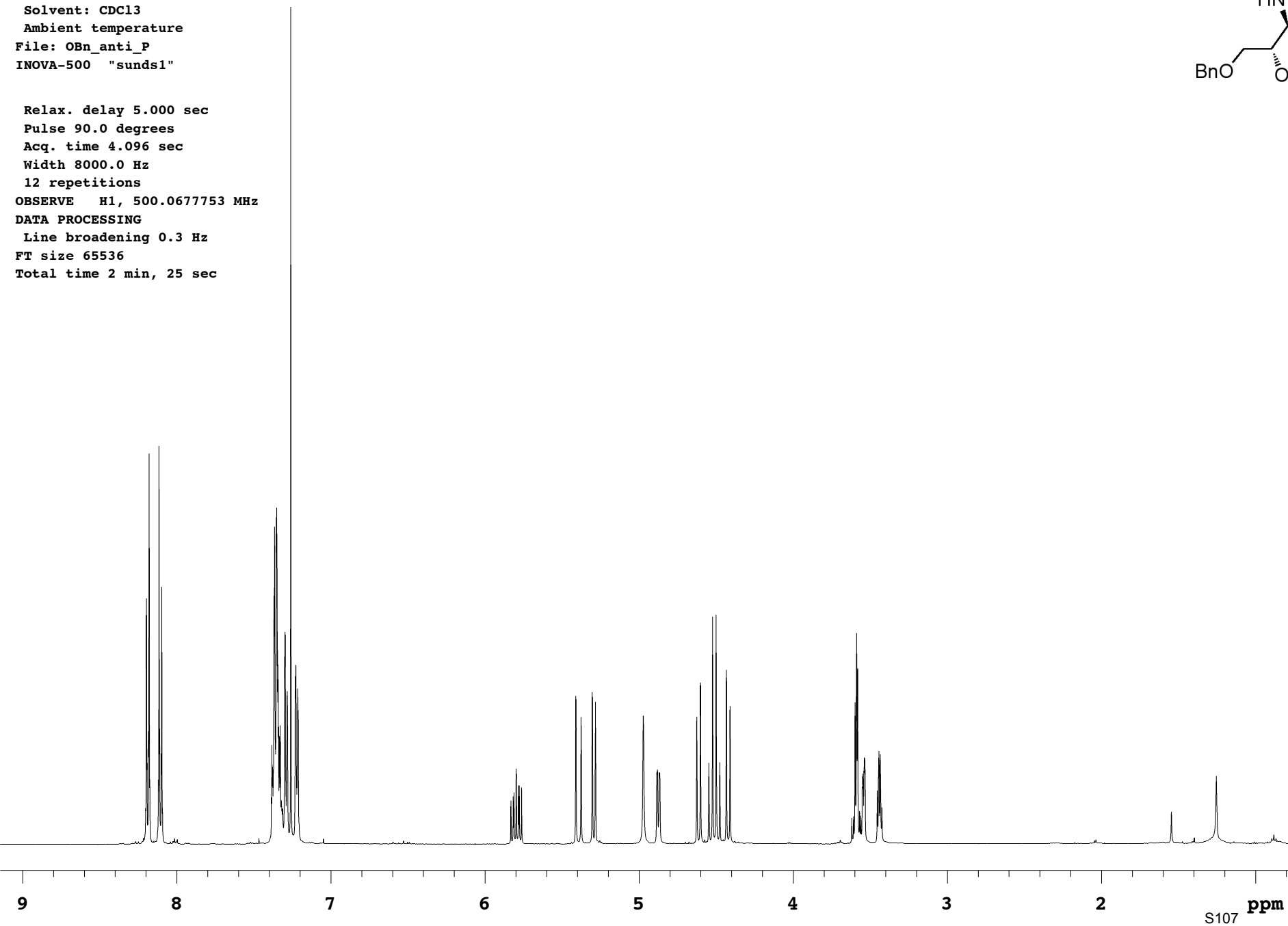
OBSERVE H1, 500.0677753 MHz

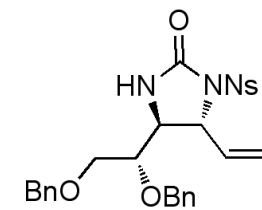
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec





Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: 1-14-87

File: OBn\_anti\_P\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 65.9 degrees

Acq. time 1.086 sec

Width 30165.9 Hz

1200 repetitions

OBSERVE C13, 125.6472855 MHz

DECOUPLE H1, 499.6923275 MHz

Power 44 dB

continuously on

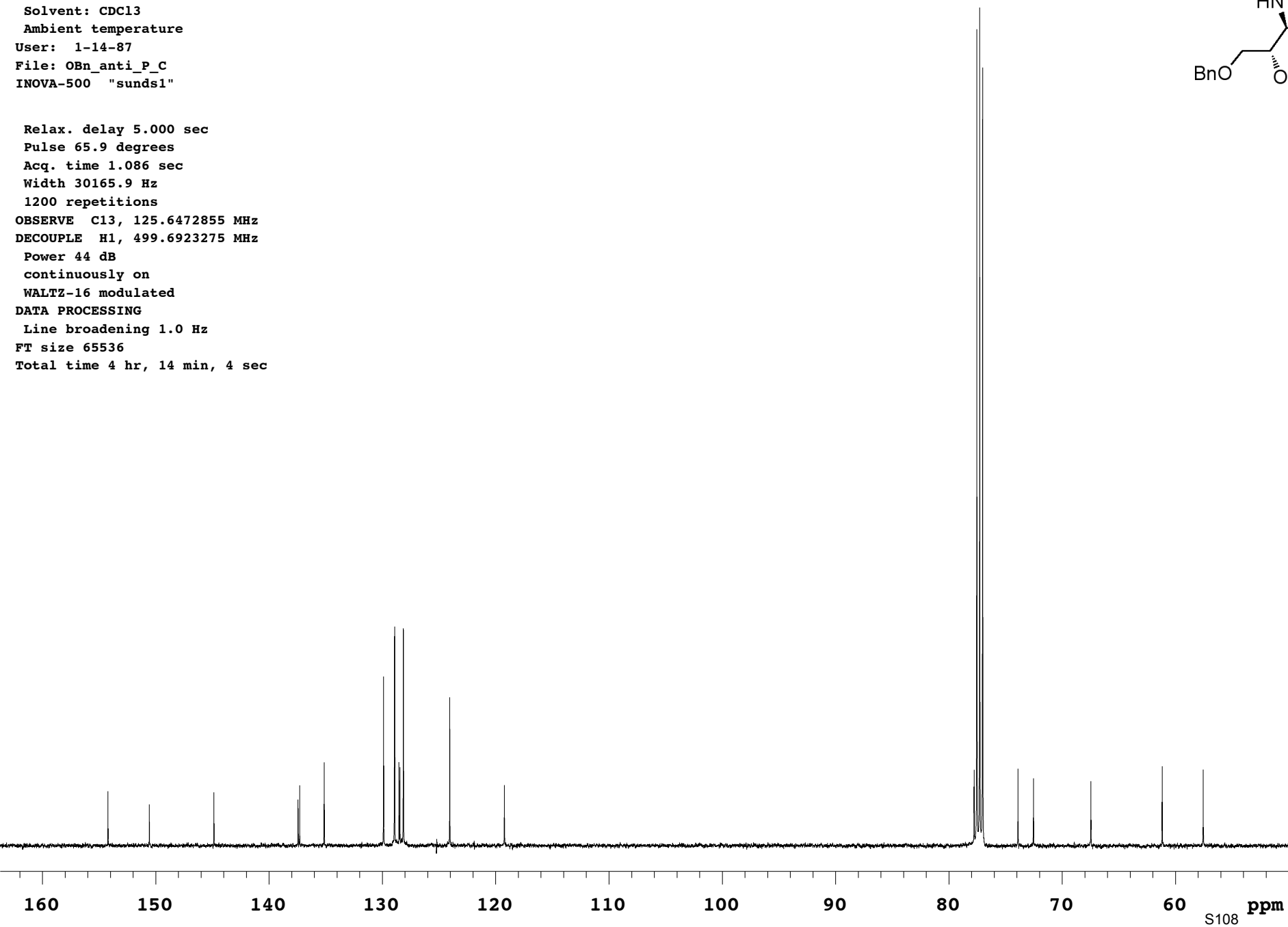
WALTZ-16 modulated

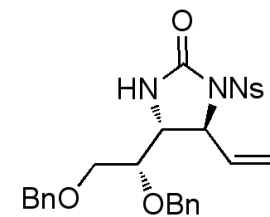
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 4 hr, 14 min, 4 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

File: OBn\_syn\_P

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

12 repetitions

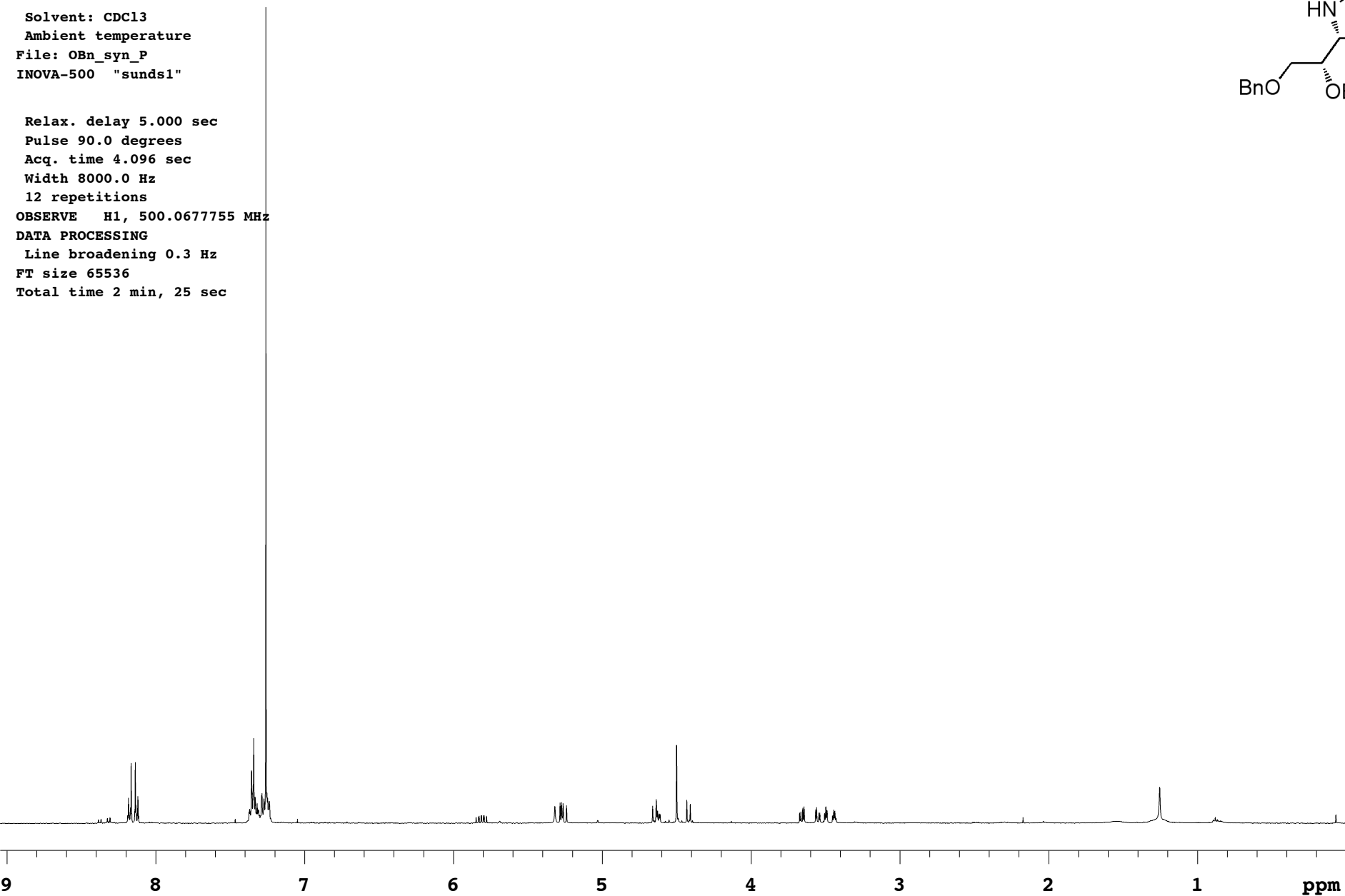
OBSERVE H1, 500.0677755 MHz

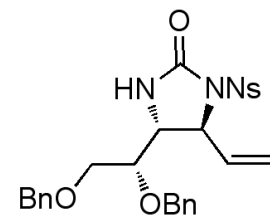
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec





Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: OBn\_syn\_P\_C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

1014 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 48 dB

continuously on

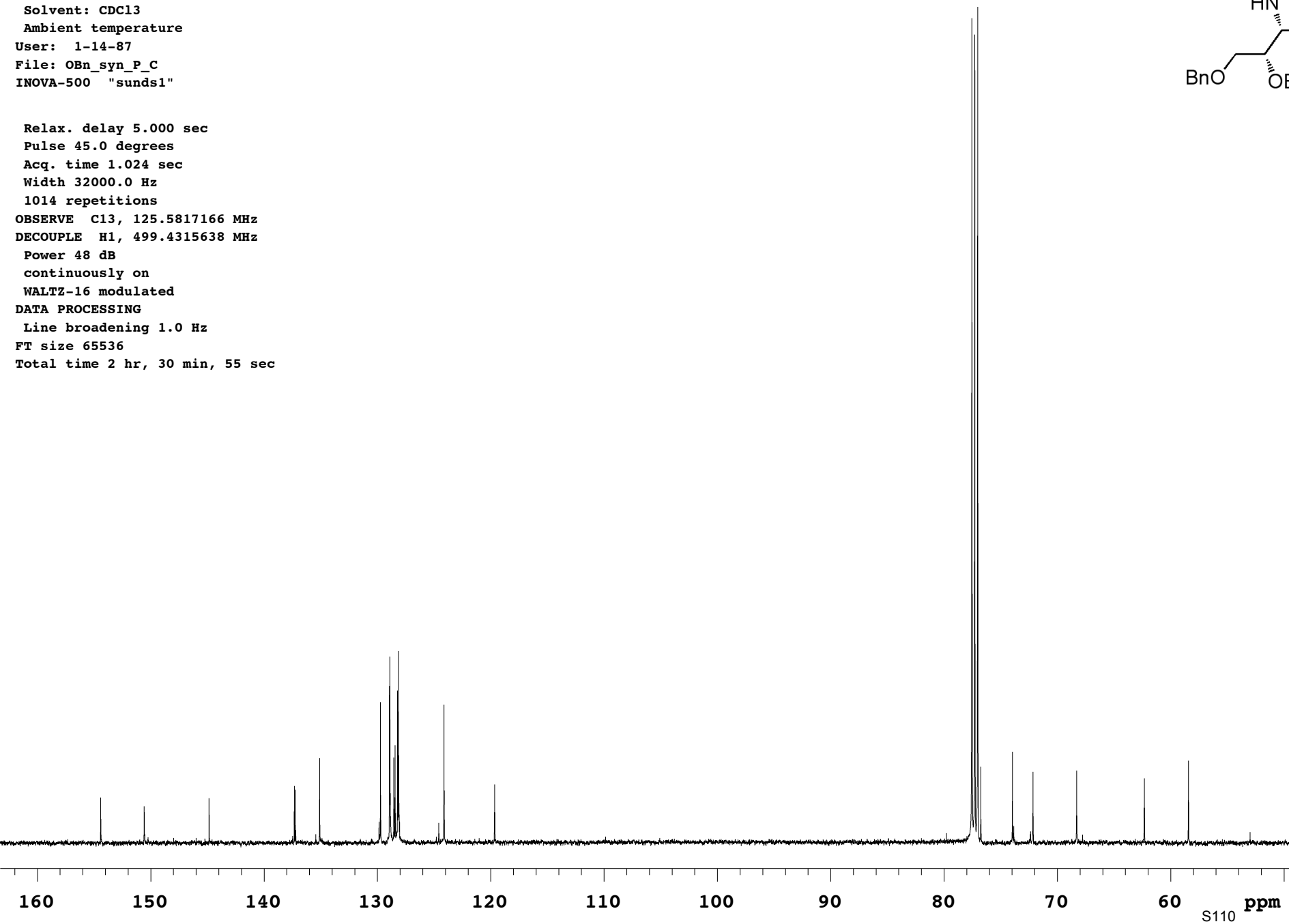
WALTZ-16 modulated

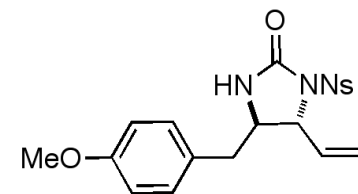
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2 hr, 30 min, 55 sec





Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

File: OMe\_P

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

10 repetitions

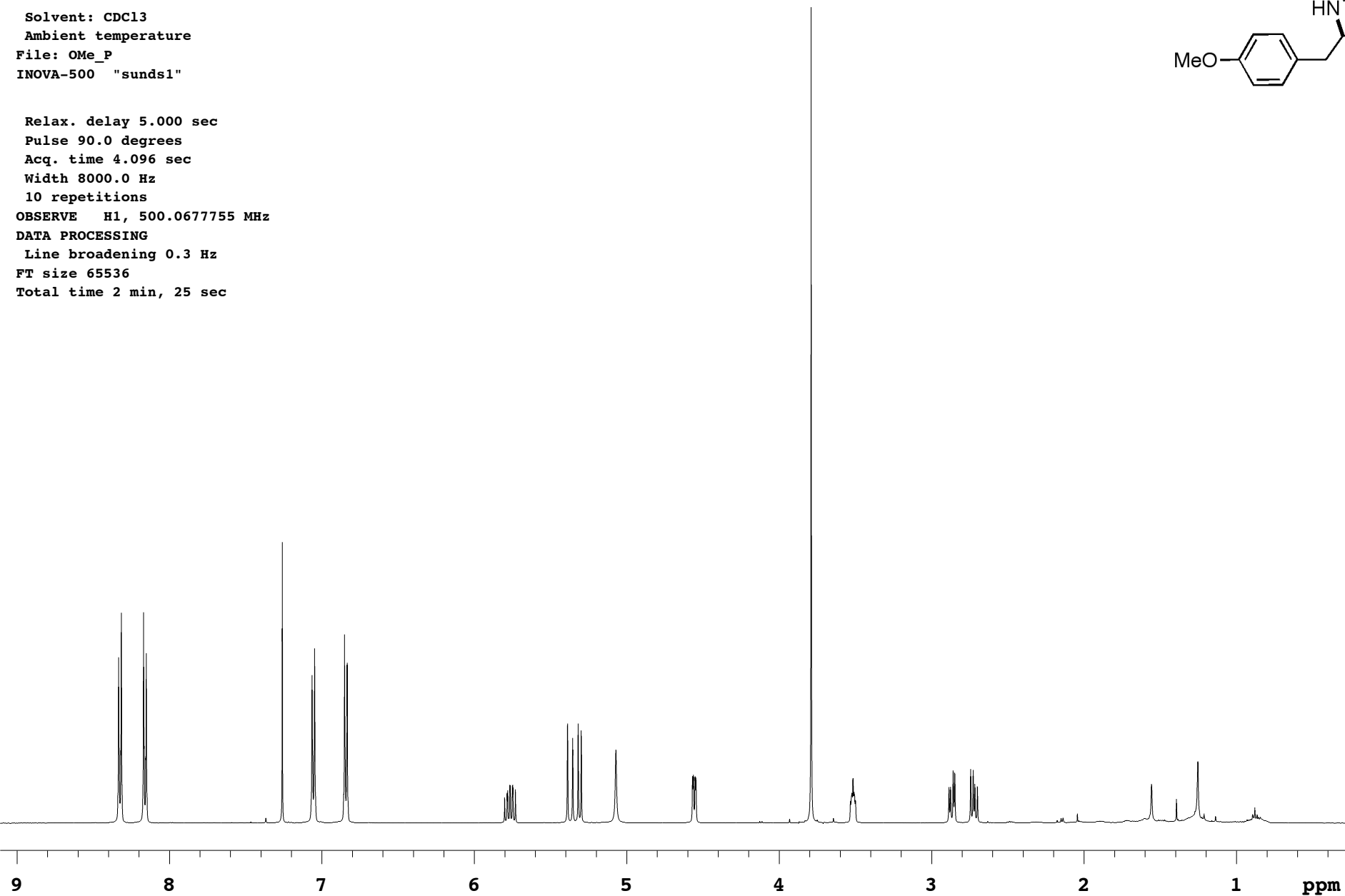
OBSERVE H1, 500.0677755 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 2 min, 25 sec



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

File: OMe\_P\_C13

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

974 repetitions

OBSERVE C13, 125.5817166 MHz

DECOUPLE H1, 499.4315638 MHz

Power 49 dB

continuously on

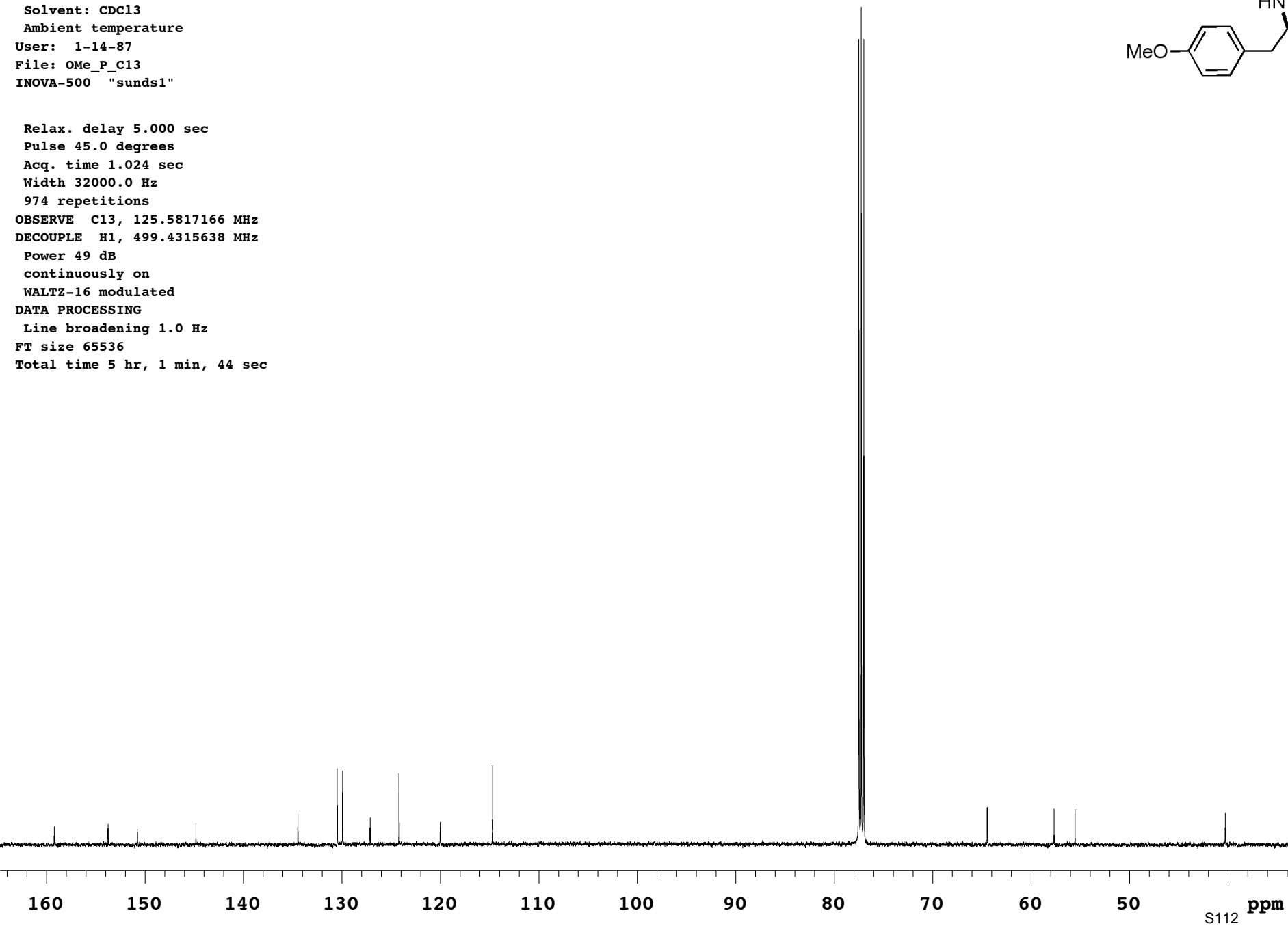
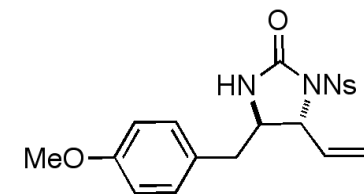
WALTZ-16 modulated

DATA PROCESSING

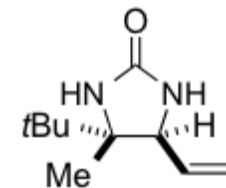
Line broadening 1.0 Hz

FT size 65536

Total time 5 hr, 1 min, 44 sec



## Strambeanu and White



Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

INOVA-500 "ui500nb"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

6 repetitions

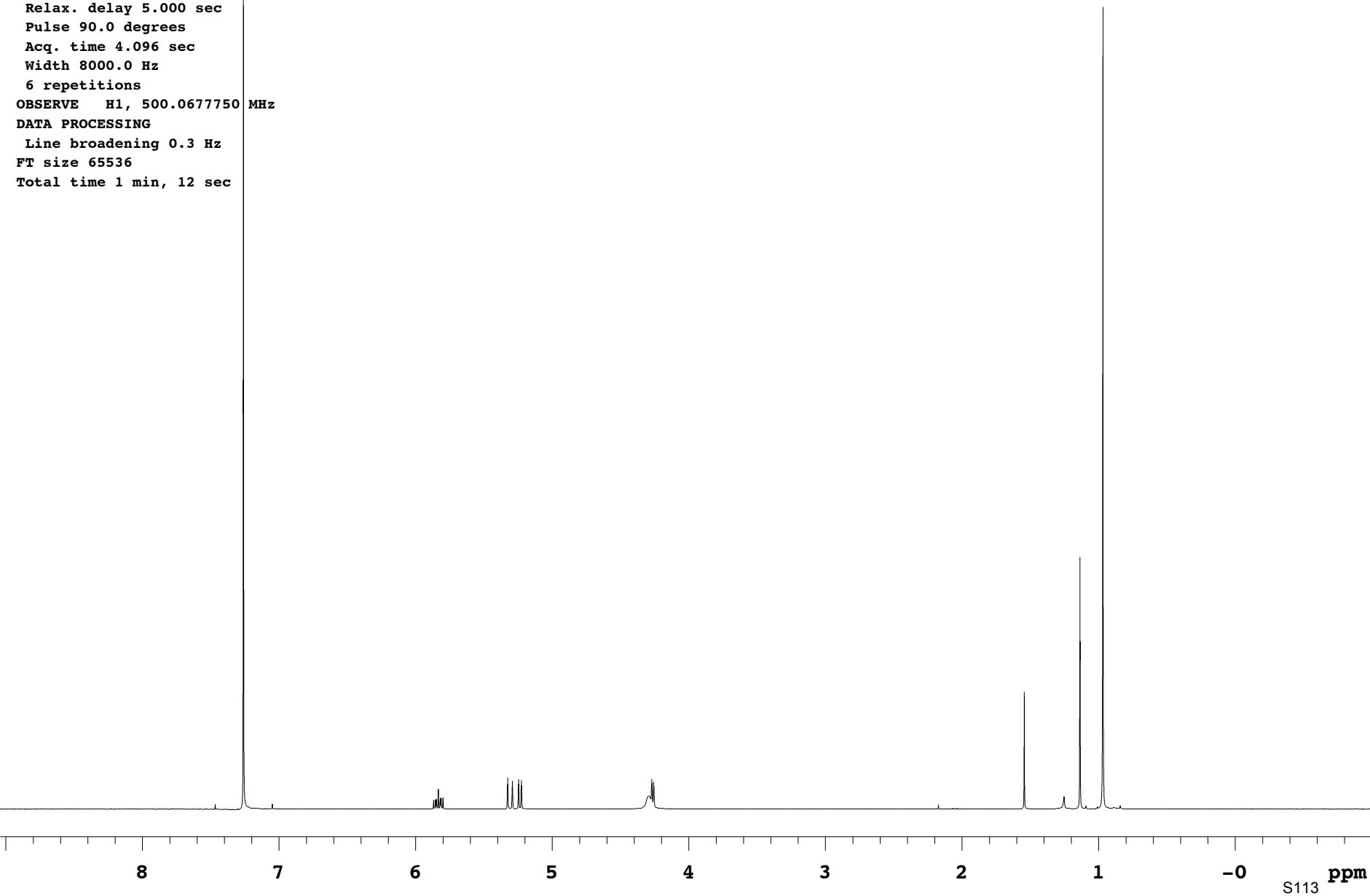
OBSERVE H1, 500.0677750 MHz

DATA PROCESSING

Line broadening 0.3 Hz

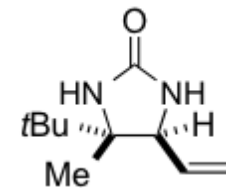
FT size 65536

Total time 1 min, 12 sec





## Strambeanu and White



Pulse Sequence: s2pul

Solvent: CDCl<sub>3</sub>

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

348 repetitions

OBSERVE C13, 125.5817483 MHz

DECOUPLE H1, 499.4315638 MHz

Power 47 dB

continuously on

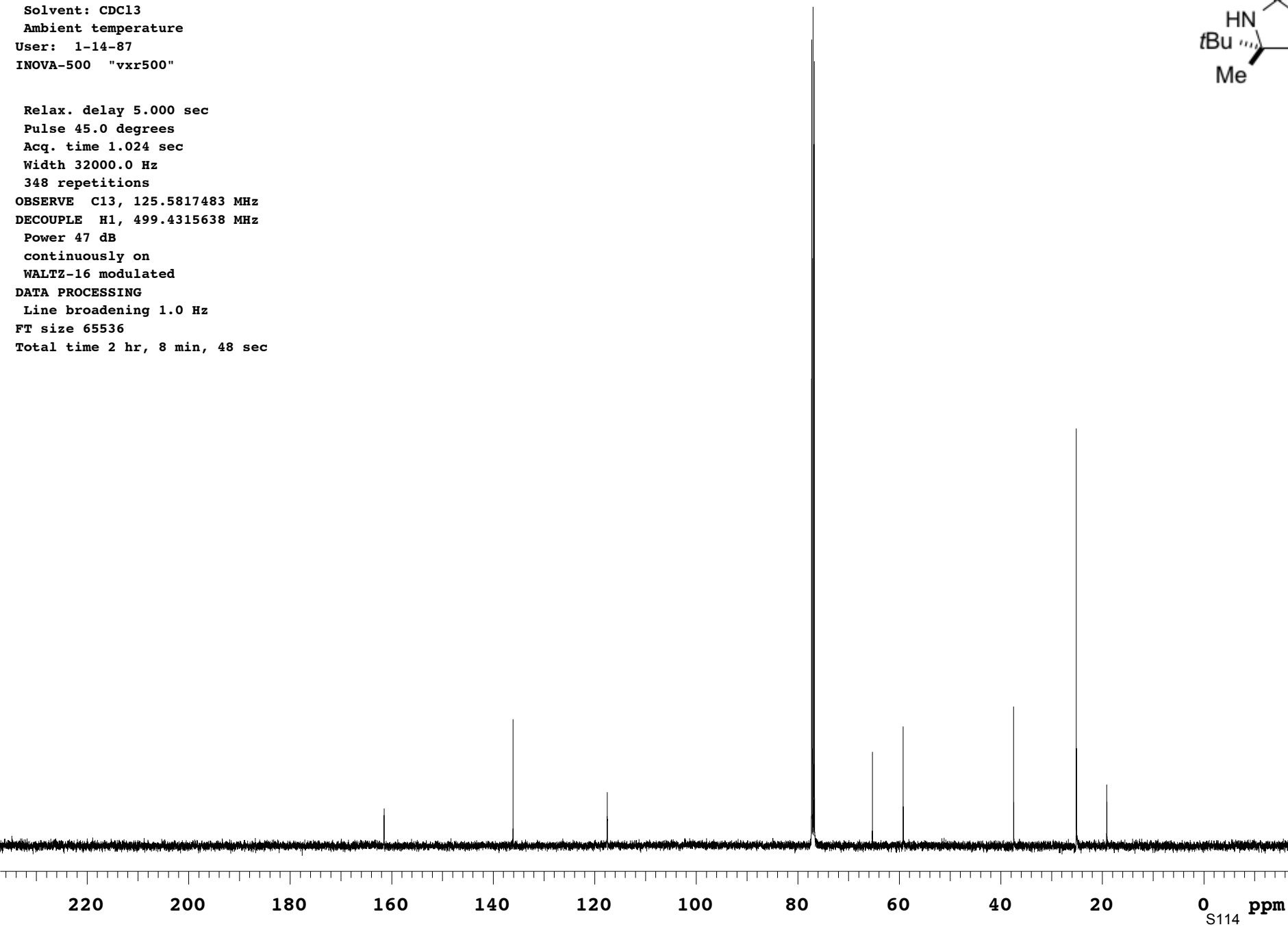
WALTZ-16 modulated

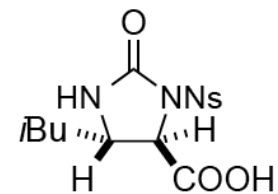
DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2 hr, 8 min, 48 sec





Pulse Sequence: s2pul

Solvent: CD3CN

Ambient temperature

INOVA-500 "vxr500"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

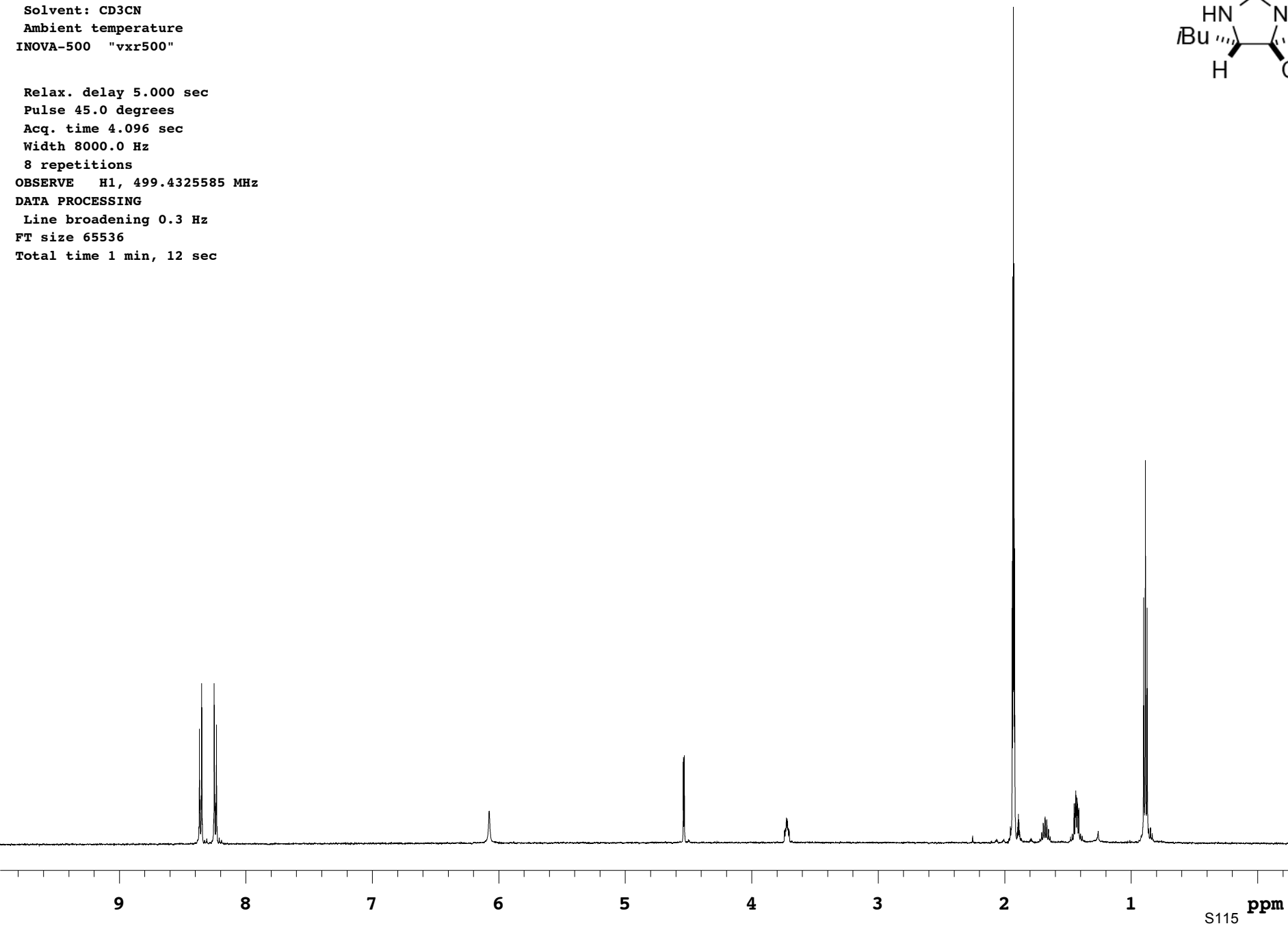
OBSERVE H1, 499.4325585 MHz

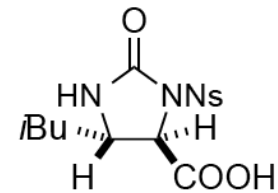
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: CD3CN

Ambient temperature

User: 1-14-87

File: imid.acid.C

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

1516 repetitions

OBSERVE C13, 125.5822916 MHz

DECOUPLE H1, 499.4342058 MHz

Power 47 dB

continuously on

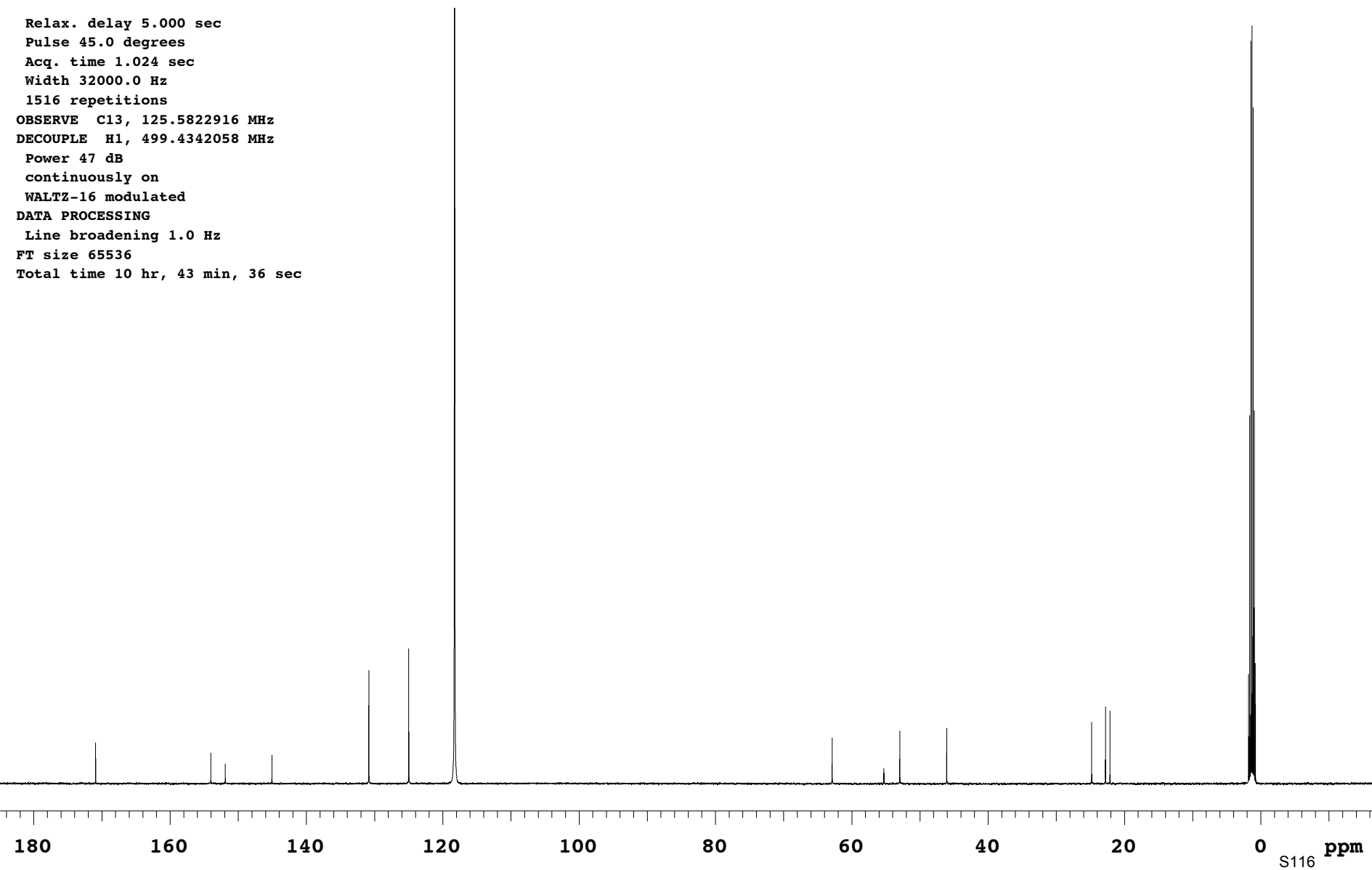
WALTZ-16 modulated

DATA PROCESSING

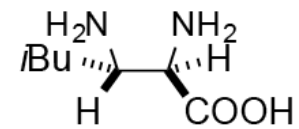
Line broadening 1.0 Hz

FT size 65536

Total time 10 hr, 43 min, 36 sec



## Strambeanu and White



Pulse Sequence: s2pul

Solvent: D2O

Ambient temperature

File: diamineH

INOVA-500 "sunds1"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 4.096 sec

Width 8000.0 Hz

8 repetitions

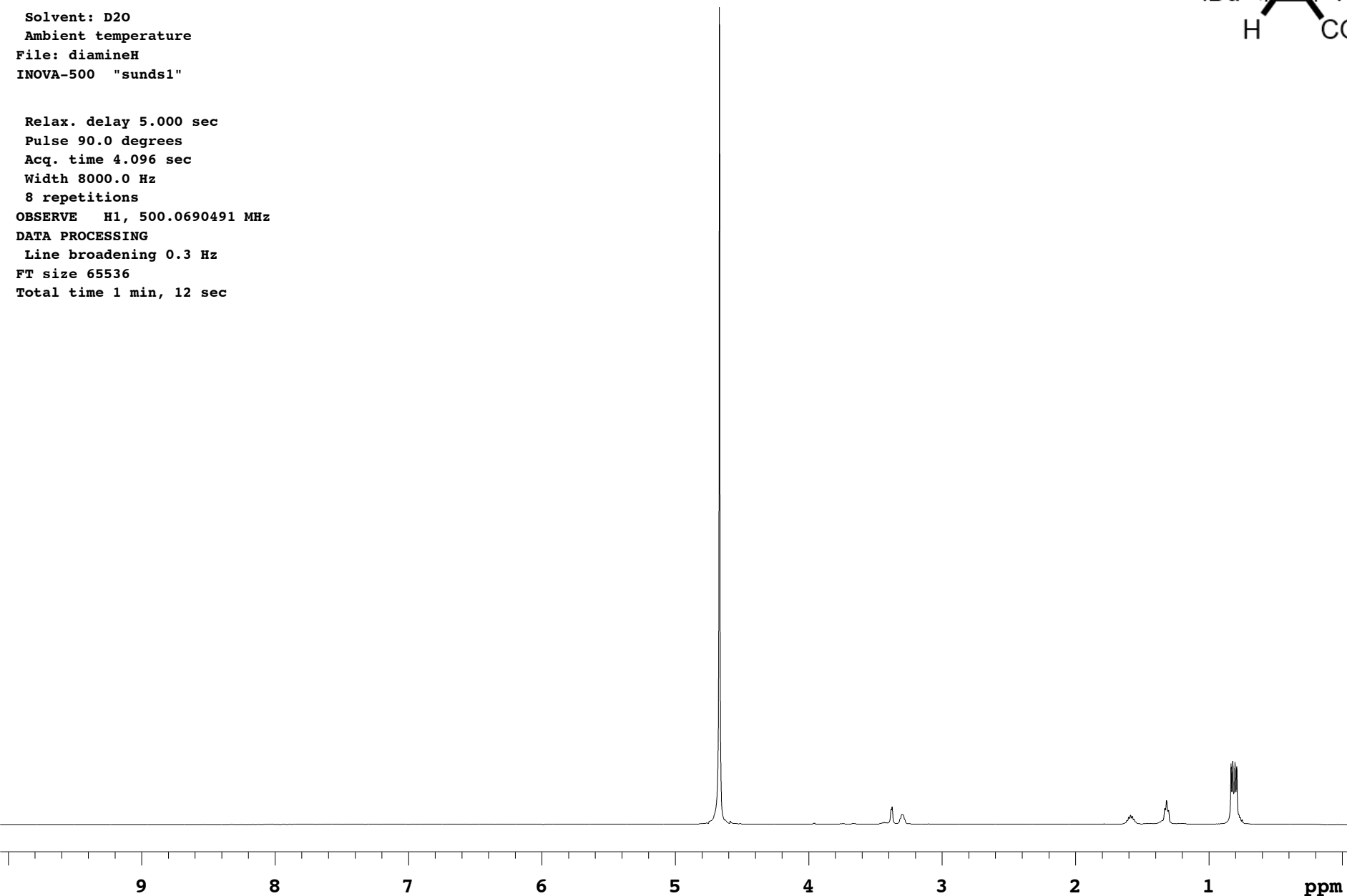
OBSERVE H1, 500.0690491 MHz

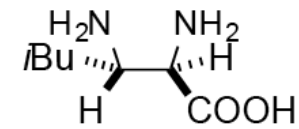
DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 1 min, 12 sec





Pulse Sequence: s2pul

Solvent: D<sub>2</sub>O

Ambient temperature

User: 1-14-87

INOVA-500 "vxr500"

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 1.024 sec

Width 32000.0 Hz

6654 repetitions

OBSERVE C13, 125.5820394 MHz

DECOUPLE H1, 499.4328473 MHz

Power 47 dB

continuously on

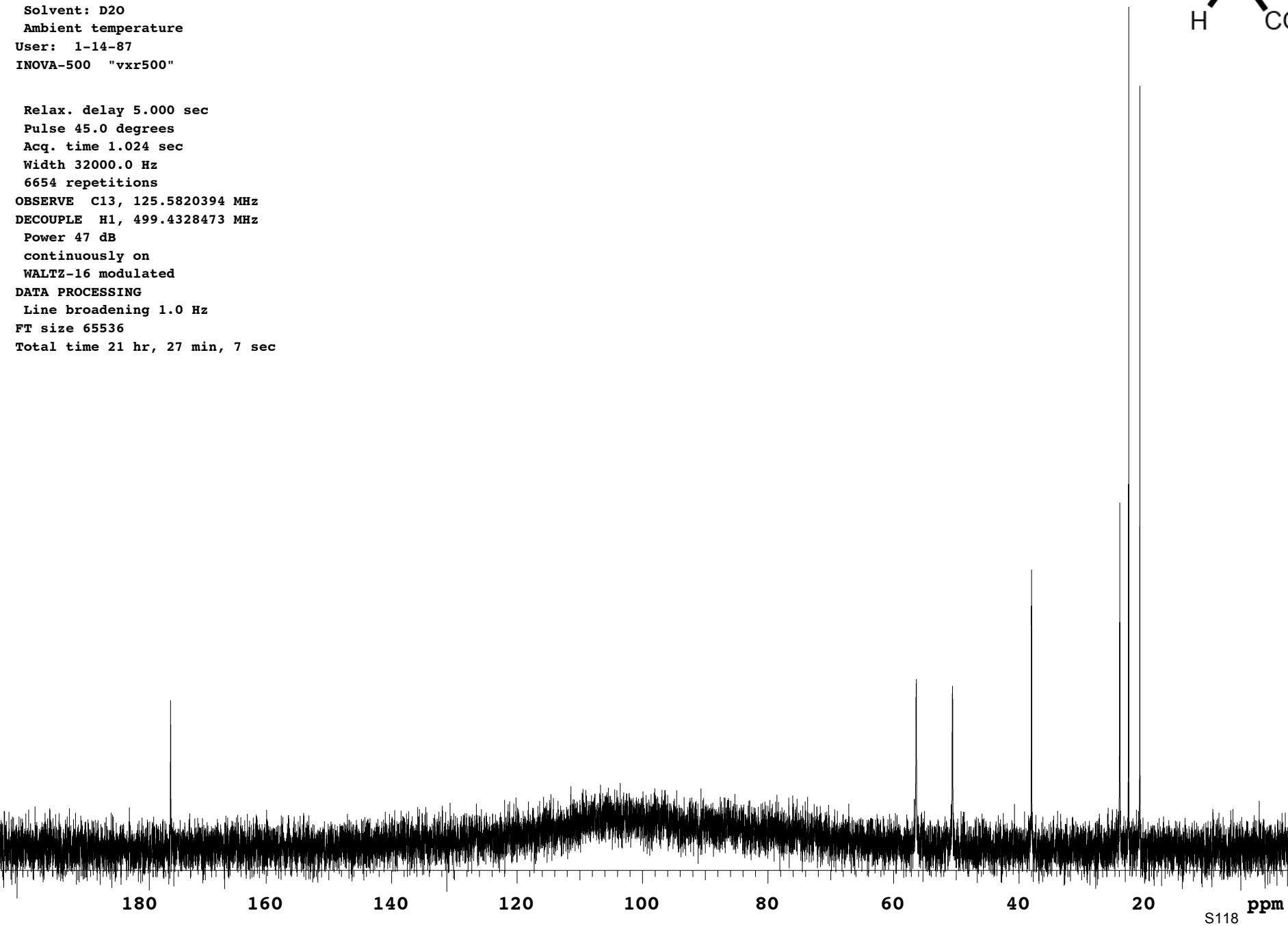
WALTZ-16 modulated

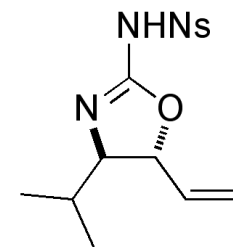
DATA PROCESSING

Line broadening 1.0 Hz

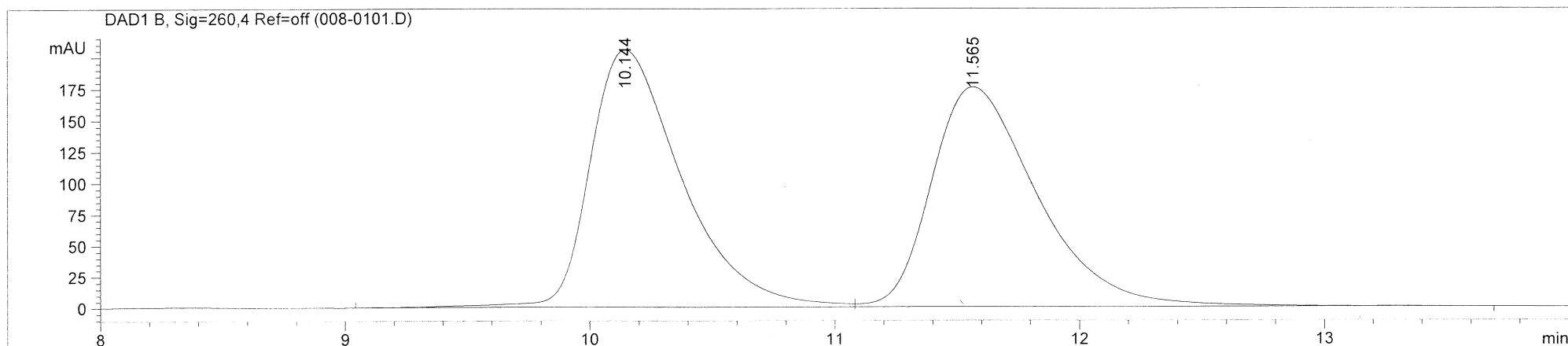
FT size 65536

Total time 21 hr, 27 min, 7 sec





Racemic

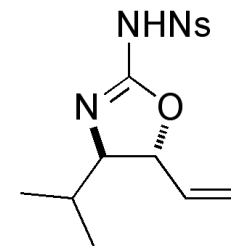


=====  
 Area Percent Report  
 =====

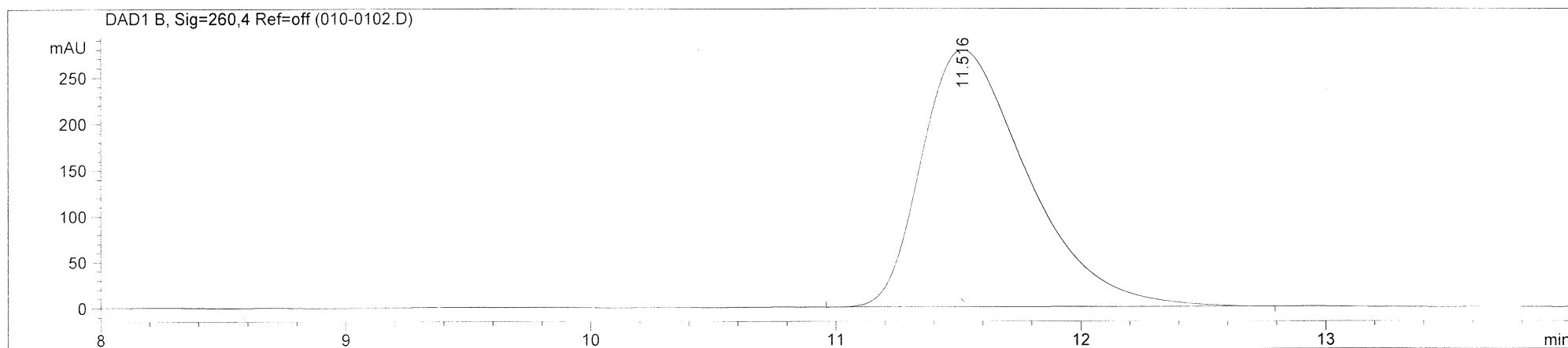
Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=260,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.144	BV	0.3960	5356.85693	205.33366	50.1807
2	11.565	VB	0.4624	5318.27441	175.77657	49.8193



Enantiopure



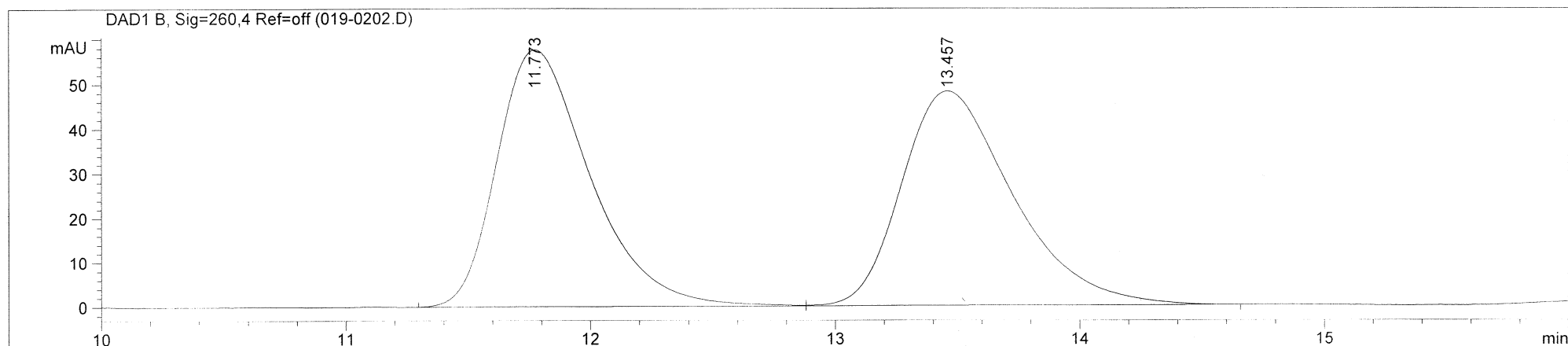
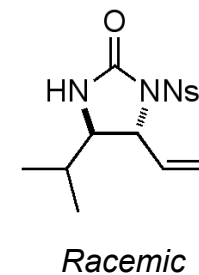
=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=260,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.516	PV	0.4622	8389.36816	278.40936	100.0000

Totals : 8389.36816 278.40936



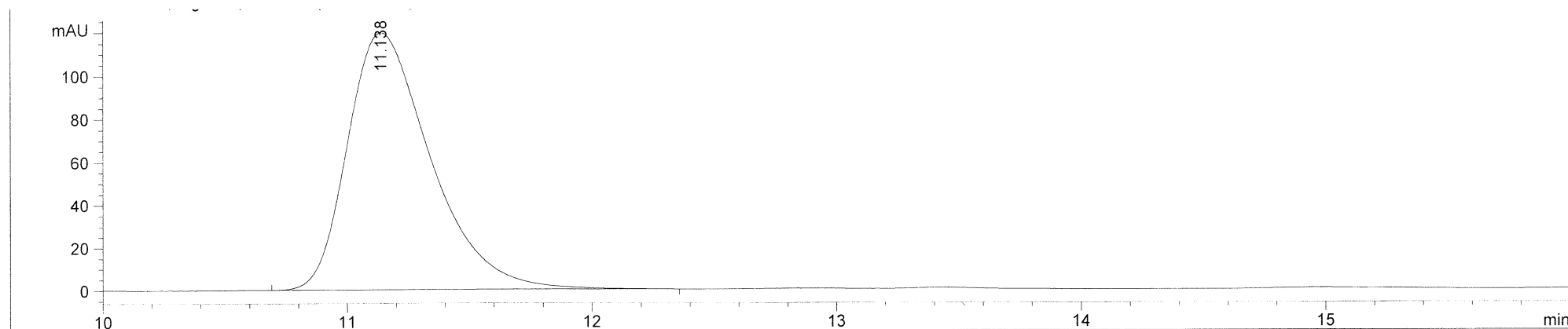
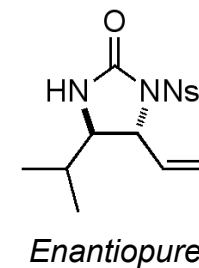
=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 B, Sig=260,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.773	BV	0.3956	1529.78955	57.56527	50.0723
2	13.457	VB	0.4796	1525.37341	48.11532	49.9277





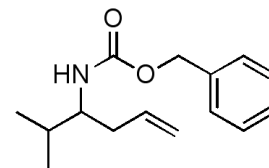
=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

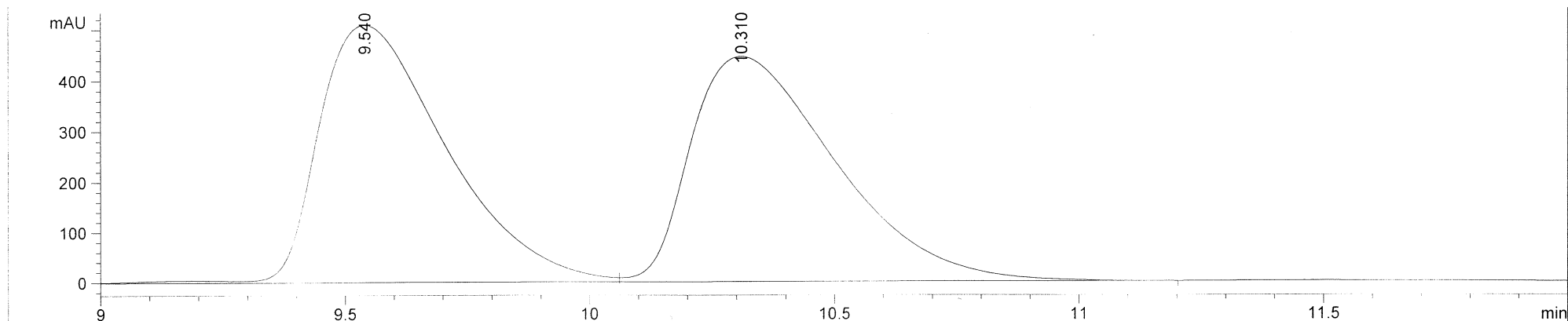
Signal 1: DAD1 B, Sig=260,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.138	BB	0.3629	2831.71143	119.47504	100.0000

Totals : 2831.71143 119.47504



Racemic



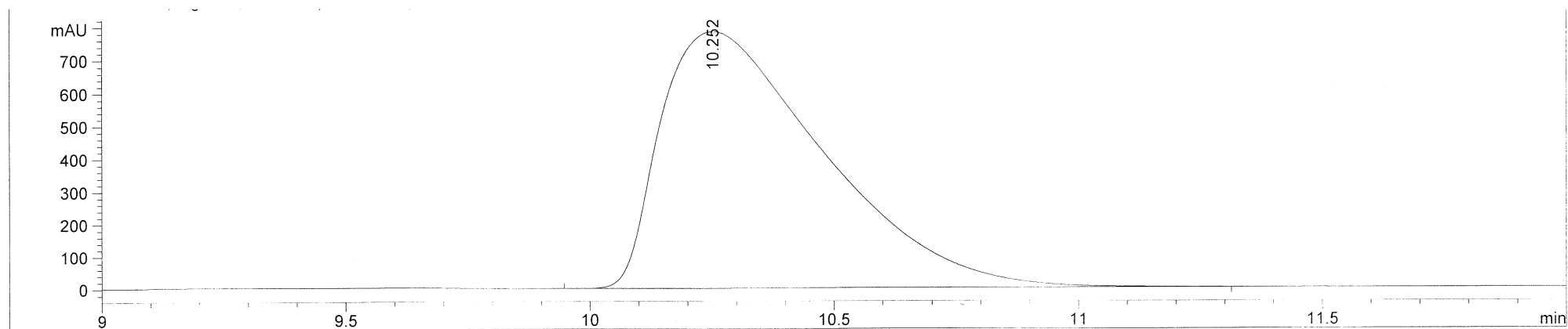
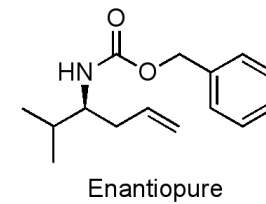
=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.540	BV	0.2809	9244.64160	508.78873	50.1515
2	10.310	VB	0.3214	9188.77930	446.07635	49.8485

Totals : 1.84334e4 954.86508



=====  
 Area Percent Report  
 =====

Sorted By : Signal  
 Multiplier : 1.0000  
 Dilution : 1.0000  
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 C, Sig=214,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.645	BV	0.0982	1863.58533	292.37411	8.3579
2	5.723	BB	0.1200	2214.77856	282.25439	9.9329
3	10.252	BB	0.3537	1.82190e4	783.78644	81.7092

expl NOESY1D

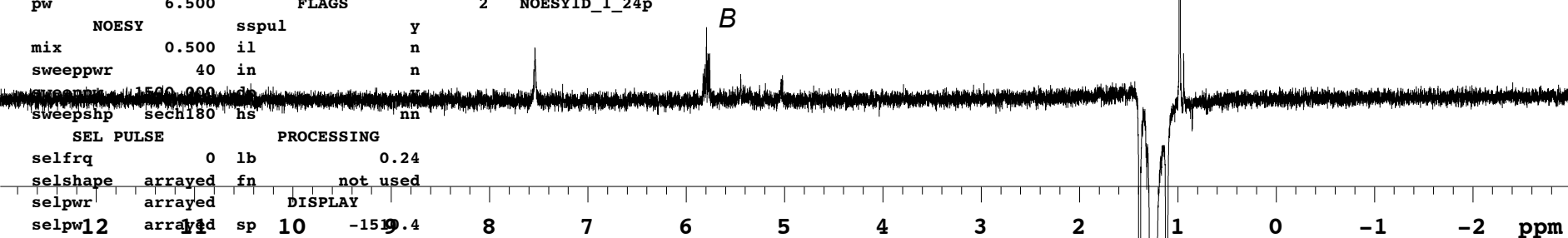
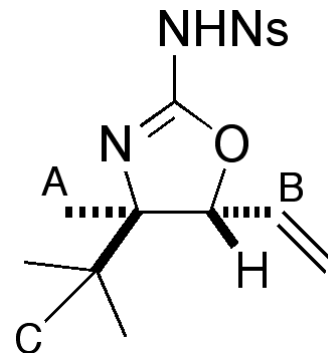
ACQUISITION		DECOU			
sw	8000.0	dn			
at	4.096	dm			
np	65536		SAM		
fb	4000	date	Jz		
bs	16	solvent	CDC13	i	selpw
ss	-2	file	/export/home/~	1	32788.8
d1	1.000	data	White/big1/MA~	2	32788.8
nt	128	B.tBu.Me.oxazoline~			
ct	128	.noesy1.fid		i	selpwr
TRANSMITTER		SPECIAL		1	7
tn	H1	temp	not used	2	7
sfrq	500.070	gain	60		
tof	0	spin	not used	i	selshape
tpwr	58	pw90	6.500	1	NOESY1D_1_24p
pw	6.500	FLAGS		2	NOESY1D_1_24p

NOESY		sspul		y
mix	0.500	il		n
sweepwr	40	in		n
freq	1500.000	h1		n
sweepshp	sech180	hs		nn

SEL PULSE		PROCESSING	
selfrq	0	lb	0.24
selshape	arrayed	fn	not used
selpwr	arrayed		

DISPLAY		
selpw12	arrayed	sp 10 -1519.4
GRADIENT		wp 7999.8

gzlv11	857	vs	4349
gt1	0.000500	sc	0
gzlv12	3430	wc	250
gt2	0.005000	hzmm	32.00
gstab	0.000500	is	33.57
hsglv1	4288	rfl	1510.6
hsgt	0.010000	rpf	0
PRESATURATION		th	7
satfrq	0	ins	100.000
satpwr	0	ai	ph
satdly	0		
satmode	n		

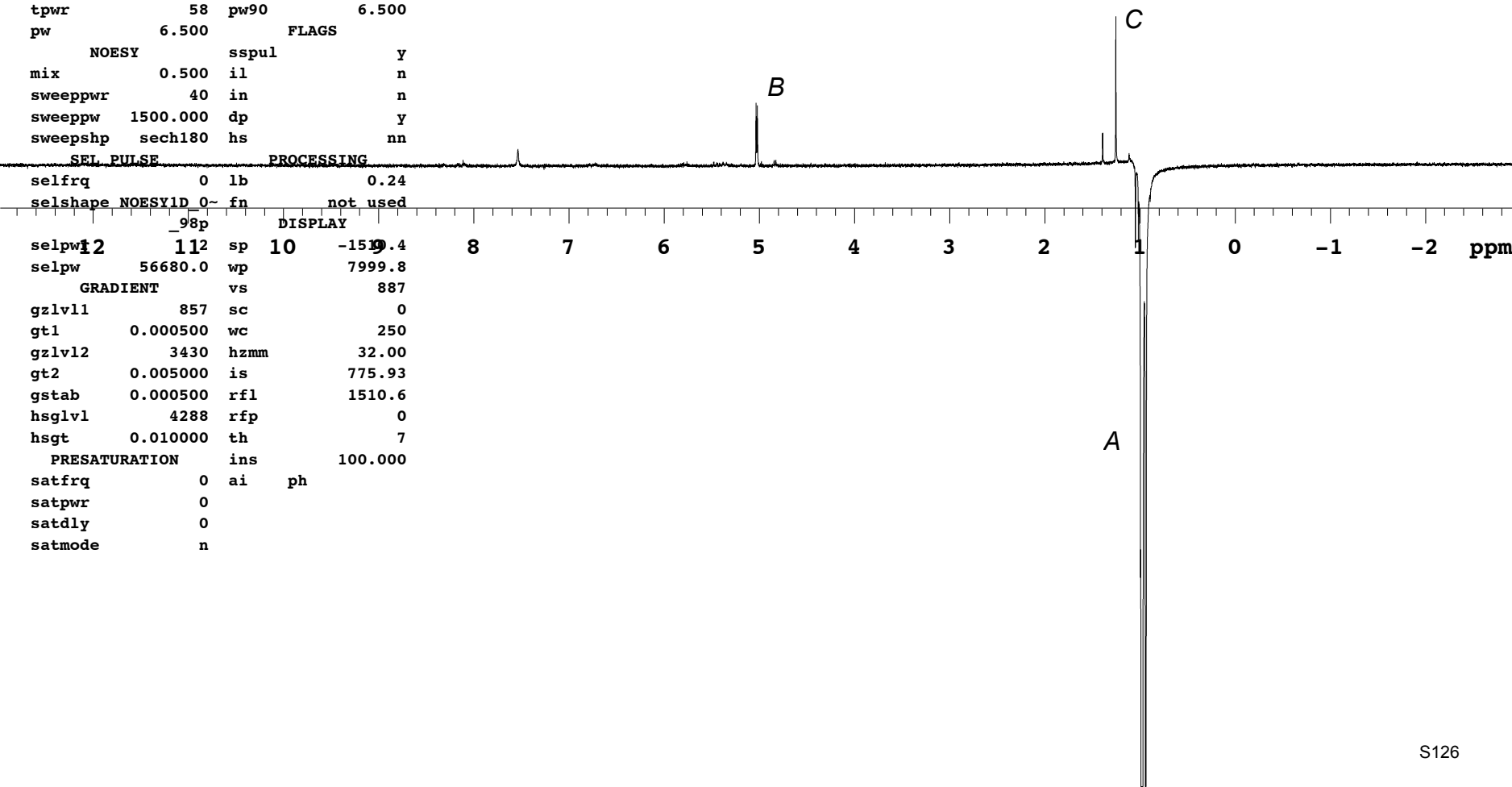
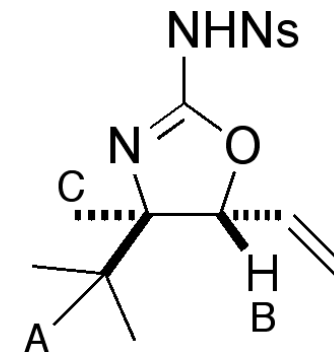


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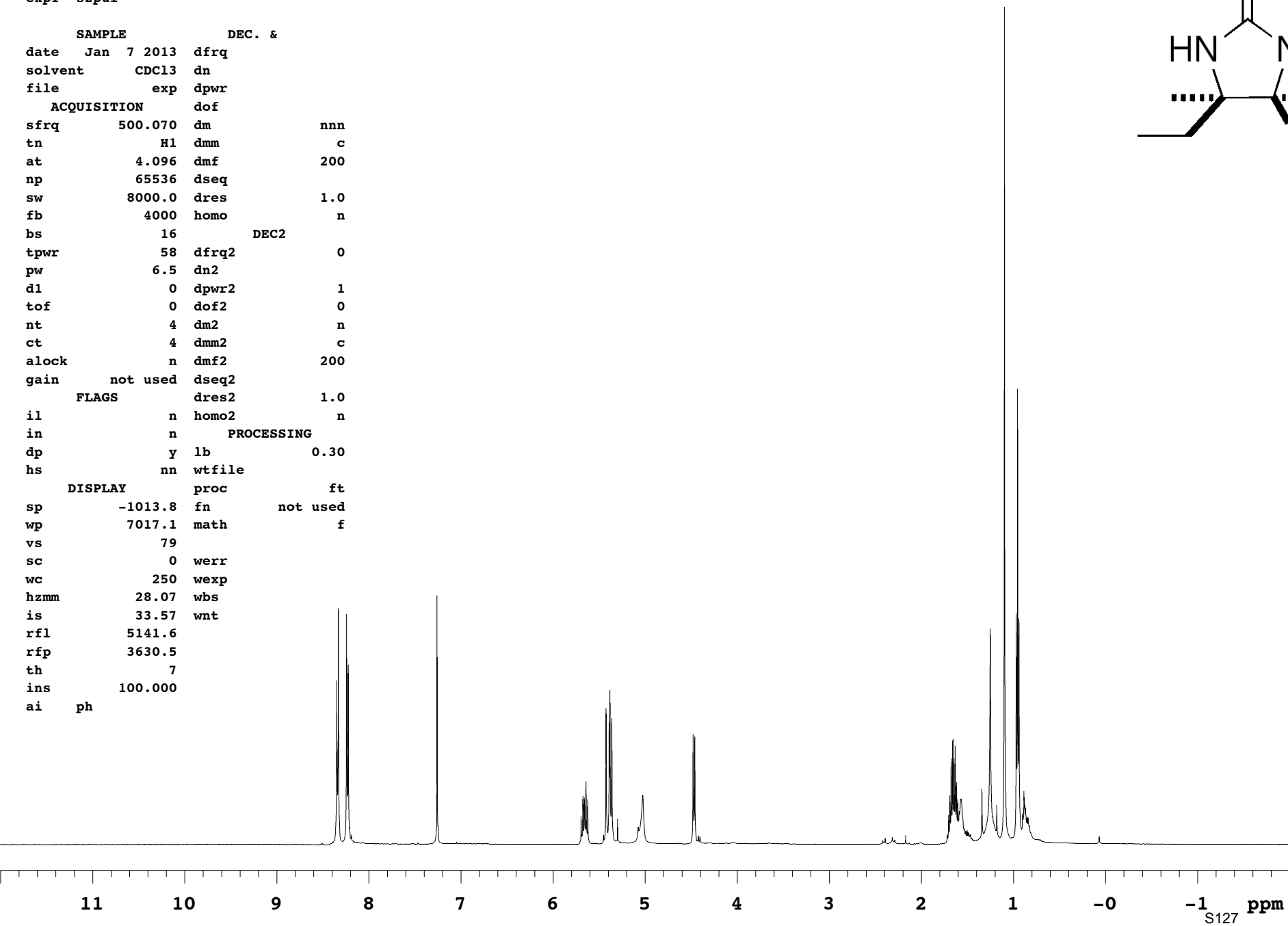
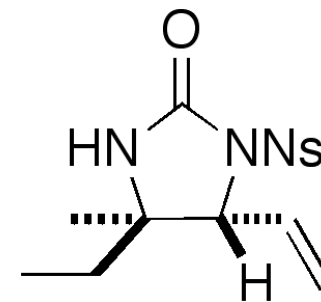
expl NOESY1D

ACQUISITION		DECOUPL	
sw	8000.0	dn	
at	4.096	dm	
np	65536	SAMPL	
fb	4000	date	Jan
bs	16	solvent	CDC13
ss	-2	file	/export/home/~
d1	1.000	data	White/big1/MA~
nt	128	B.tBu.Me.oxazoline~	
ct	128	.noesy2.fid	
TRANSMITTER		SPECIAL	
tn	H1	temp	not used
sfrq	500.070	gain	60
tof	0	spin	not used
tpwr	58	pw90	6.500
pw	6.500	FLAGS	
	NOESY	sspul	y
mix	0.500	il	n
sweepwr	40	in	n
sweeppw	1500.000	dp	y
sweepshp	sech180	hs	nn
SEL PULSE		PROCESSING	
selfrq	0	lb	0.24
selshape	NOESY1D 0~	fn	not used
	98p	DISPLAY	
selpw1	112	sp	10 -1519.4
selpw	56680.0	wp	7999.8
GRADIENT		vs	
gzlv11	857	sc	0
gt1	0.000500	wc	250
gzlv12	3430	hzmm	32.00
gt2	0.005000	is	775.93
gstab	0.000500	rfl	1510.6
hsglv1	4288	rpf	0
hsgt	0.010000	th	7
PRESATURATION		ins	
satfrq	0	ai	ph
satpwr	0		
satdly	0		
satmode	n		



expl s2pul

SAMPLE		DEC. &	
date	Jan 7 2013	dfrq	
solvent	CDC13	dn	
file	exp	dpwr	
ACQUISITION		dof	
sfrq	500.070	dm	nnn
tn	H1	dmm	c
at	4.096	dmf	200
np	65536	dseq	
sw	8000.0	dres	1.0
fb	4000	homo	n
bs	16	DEC2	
tpwr	58	dfrq2	0
pw	6.5	dn2	
d1	0	dpwr2	1
tof	0	dof2	0
nt	4	dm2	n
ct	4	dmm2	c
alock	n	dmf2	200
gain	not used	dseq2	
FLAGS		dres2	1.0
il	n	homo2	n
in	n	PROCESSING	
dp	y	lb	0.30
hs	nn	wtfile	
DISPLAY		proc	ft
sp	-1013.8	fn	not used
wp	7017.1	math	f
vs	79		
sc	0	werr	
wc	250	wexp	
hzmm	28.07	wbs	
is	33.57	wnt	
rfl	5141.6		
rfp	3630.5		
th	7		
ins	100.000		
ai	ph		



expl NOESY1D

ACQUISITION		DI	
sw	8000.0	dn	
at	4.096	dm	
np	65536		
fb	4000	date	
bs	16	solvent	CDC13
ss	-2	file	/export/home/~
d1	1.000	data/White/big1/MA~	
nt	128	B.Me.Et.imid.noesy~	
ct	128	.fid	

TRANSMITTER		SPECIAL	
tn	H1	temp	not used
sfrq	500.070	gain	60
tof	0	spin	not used
tpwr	58	pw90	6.500
pw	6.500	FLAGS	

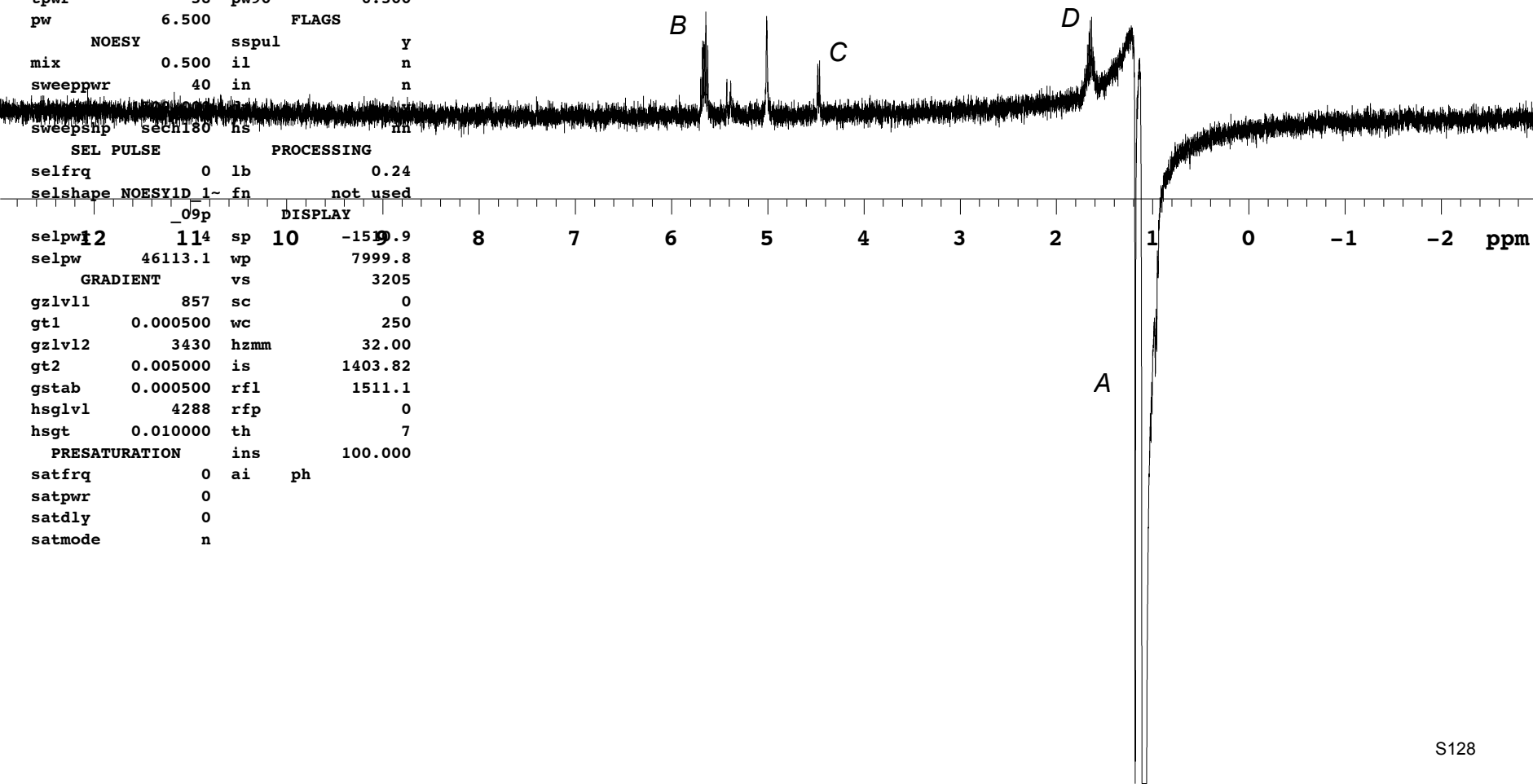
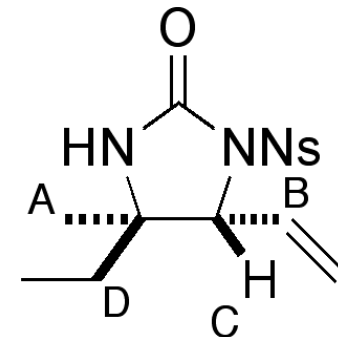
NOESY		sspul	
mix	0.500	il	n
sweeppwr	40	in	n
sweepshp	sech180	hs	in

SEL PULSE		PROCESSING	
selfrq	0	lb	0.24
selshape	NOESY1D_1~	fn	not used

		DISPLAY	
selpw1	114	sp	10
selpw	46113.1	wp	7999.8

GRADIENT		vs	
gzlv11	857	sc	0
gt1	0.000500	wc	250
gzlv12	3430	hzmm	32.00
gt2	0.005000	is	1403.82
gstab	0.000500	rfl	1511.1
hsglv1	4288	rpf	0
hsgt	0.010000	th	7

PRESATURATION		ins	
satfrq	0	ai	ph
satpwr	0		
satdly	0		
satmode	n		



expl NOESY1D

ACQUISITION		DE	
sw	8000.0	dn	
at	4.096	dm	
np	65536		
fb	4000	date	
bs	16	solvent	CDC13
ss	-2	file	/export/home/~
d1	1.000	data	White/big/MA~
nt	128	B.Me.Et.imid.noesy~	
ct	128		2.fid

TRANSMITTER		SPECIAL	
tn	H1	temp	not used
sfrq	500.070	gain	60
tof	0	spin	not used
tpwr	58	pw90	6.500
pw	6.500	FLAGS	

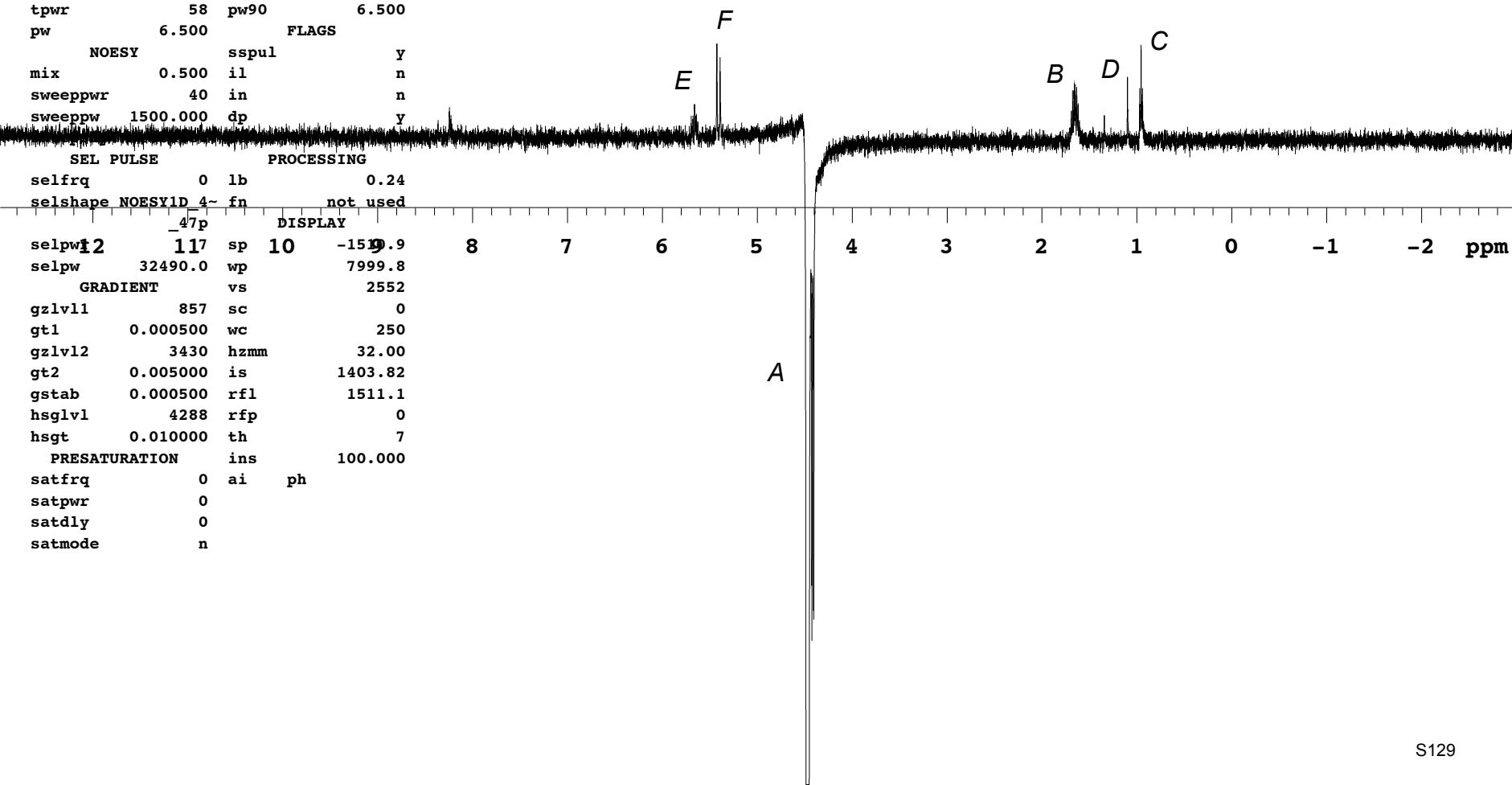
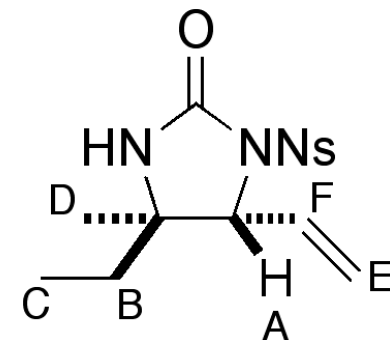
NOESY		sspul	
mix	0.500	il	n
sweeppwr	40	in	n
sweeppw	1500.000	dp	y

SEL PULSE		PROCESSING	
selfrq	0	lb	0.24
selshape	NOESY1D 4~	fn	not used

		DISPLAY	
selpw1	117	sp	10
selpw	32490.0	wp	7999.8

GRADIENT		vs	
gzlv11	857	sc	0
gt1	0.000500	wc	250
gzlv12	3430	hzmm	32.00
gt2	0.005000	is	1403.82
gstab	0.000500	rfl	1511.1
hsglv1	4288	rpf	0
hsgt	0.010000	th	7

PRESATURATION		ins	
satfrq	0	ai	ph
satpwr	0		
satdly	0		
satmode	n		





expl NOESY1D

ACQUISITION		DE	
sw	8000.0	dn	
at	4.096	dm	
np	65536		
fb	4000	date	
bs	16	solvent	CDC13
ss	-2	file	/export/home/~
d1	1.000	data	White/big/MA~
nt	128	B.Me.Et.imid.noesy~	
ct	101		3.fid

TRANSMITTER		SPECIAL	
tn	H1	temp	not used
sfrq	500.070	gain	60
tof	0	spin	not used
tpwr	58	pw90	6.500
pw	6.500	FLAGS	

NOESY		sspul	
mix	0.500	il	n
sweppwr	40	in	n
sweppw	1500.000	dp	y

SEL PULSE		PROCESSING	
selfrq	0	lb	0.24
selshape	NOESY1D_1~	fn	not used

_64p		DISPLAY	
selpw1	110	sp	10
selpw	23095.5	wp	1519.9
		vs	7999.8

GRADIENT		vs	
gzlv11	857	sc	0
gt1	0.000500	wc	250
gzlv12	3430	hzmm	32.00
gt2	0.005000	is	1403.82
gstab	0.000500	rfl	1511.1
hsglv1	4288	rpf	0
hsgt	0.010000	th	7

PRESATURATION		ins	
satfrq	0	ai	ph
satpwr	0		
satdly	0		
satmode	n		

