

Supplementary Information

Divergent synthetic approach to 6''-modified α -GalCer analogues

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SAMPLE: NP002

File: /home/data/Nora/NP002/Proton_12Oct2009_1.fid

Date: Oct 12 2009

Solvent: dms

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_12Oct2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4798.5 Hz

64 repetitions

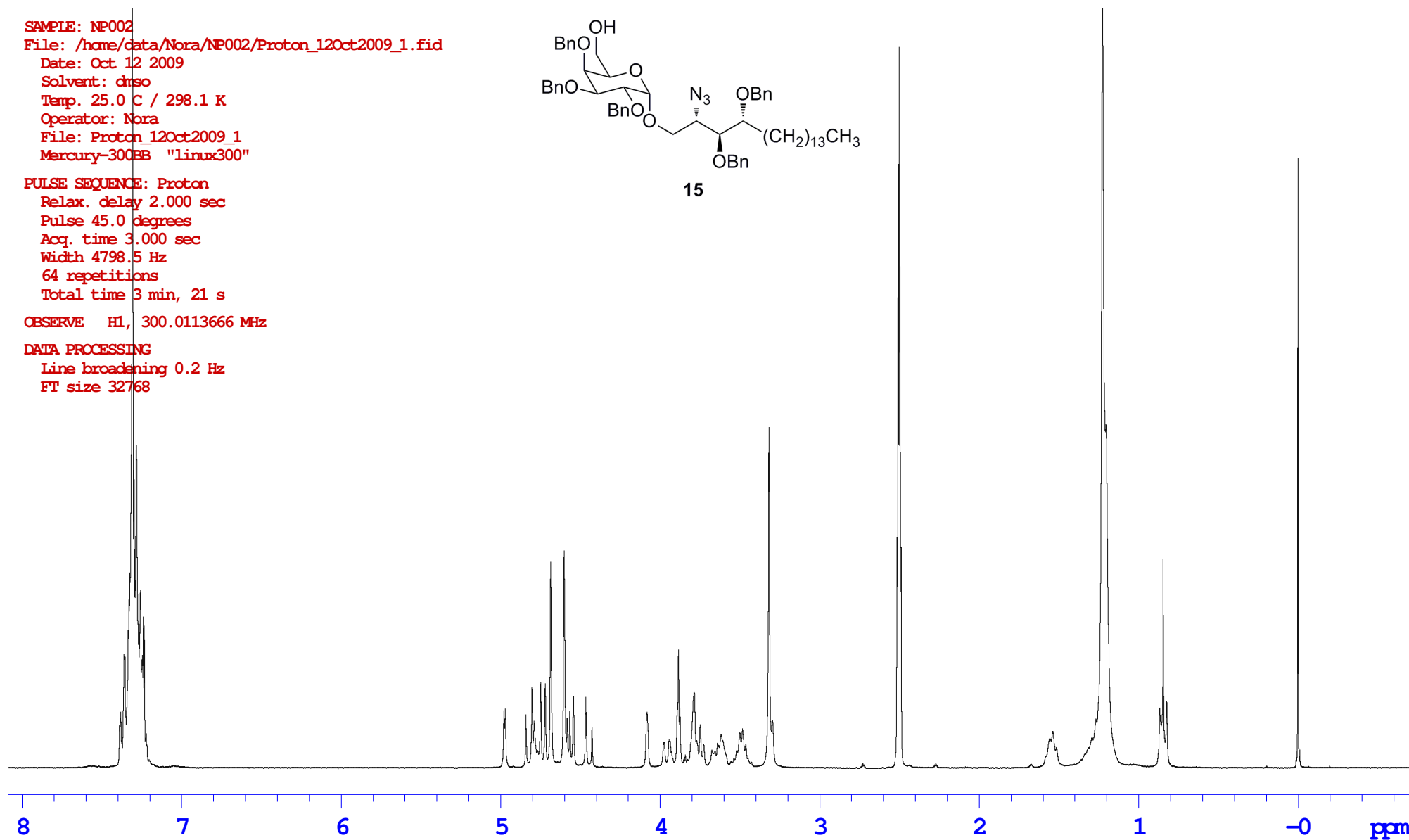
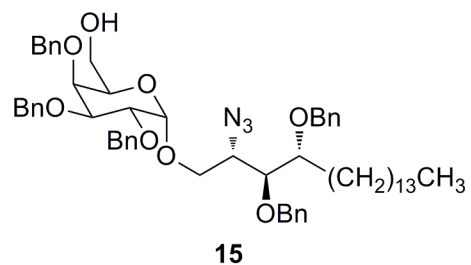
Total time 3 min, 21 s

OBSERVE H1, 300.0113666 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768



SAMPLE: NP002

File: /home/data/Nora/NP002/Carbon_12h_07Oct2009_1.fid

Date: Oct 7 2009

Solvent: dmso

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_12h_07Oct2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon_12h

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

14400 repetitions

Total time 12 hr, 37 min, 36 s

OBSERVE C13, 75.4379015 MHz

DECOUPLE H1, 300.0128784 MHz

Power 33 dB

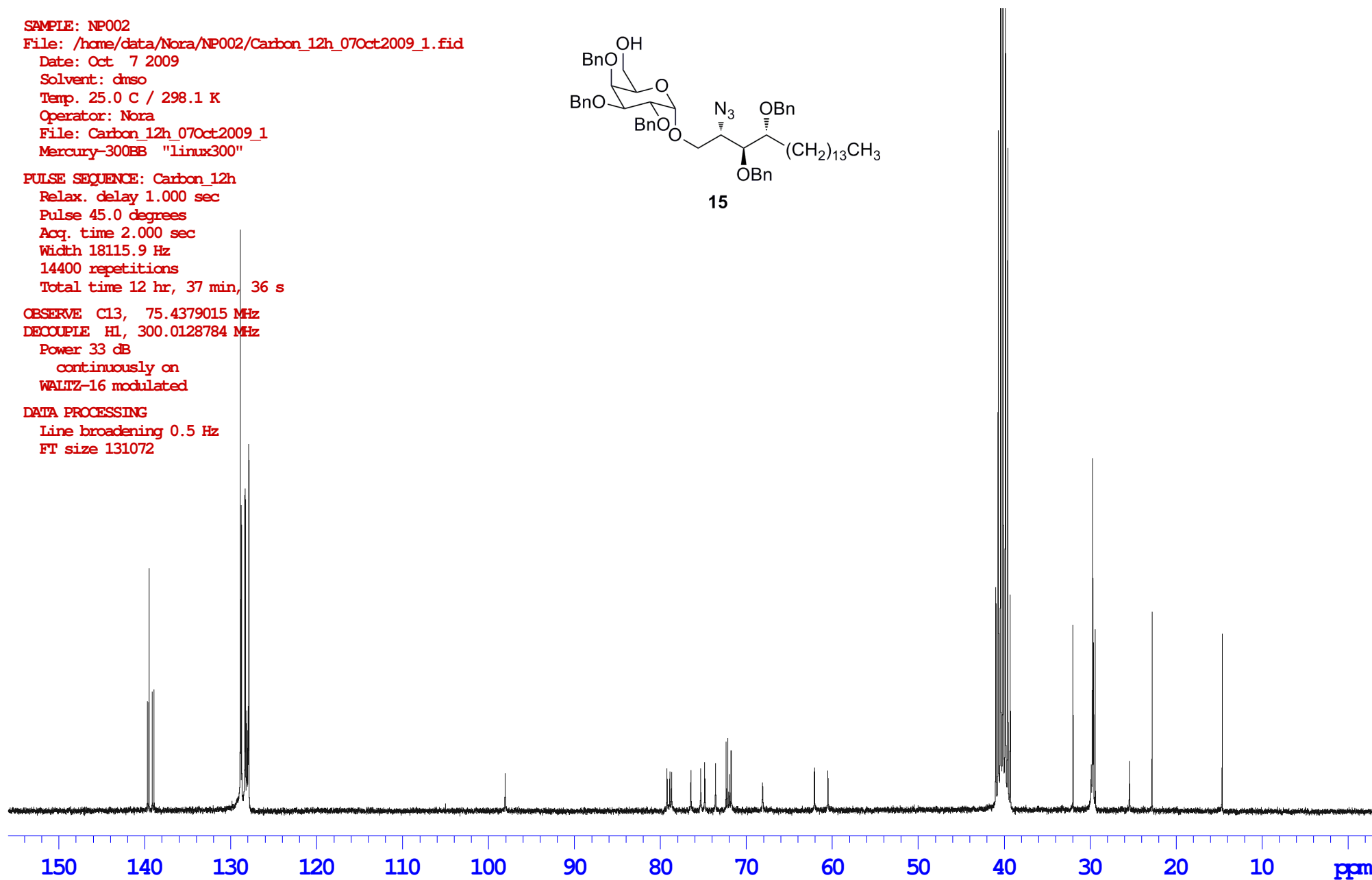
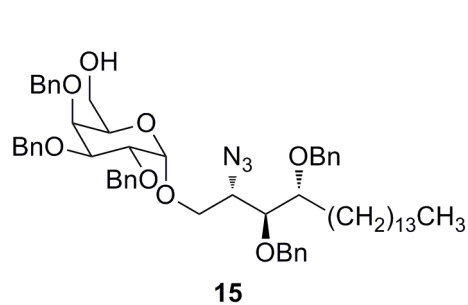
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



SAMPLE: NP222

File: /home/data/Nora/NP222/Proton_Minsw_19Jan2009_1.fid

Date: Jan 19 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_19Jan2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.004 sec

Width 2540.7 Hz

64 repetitions

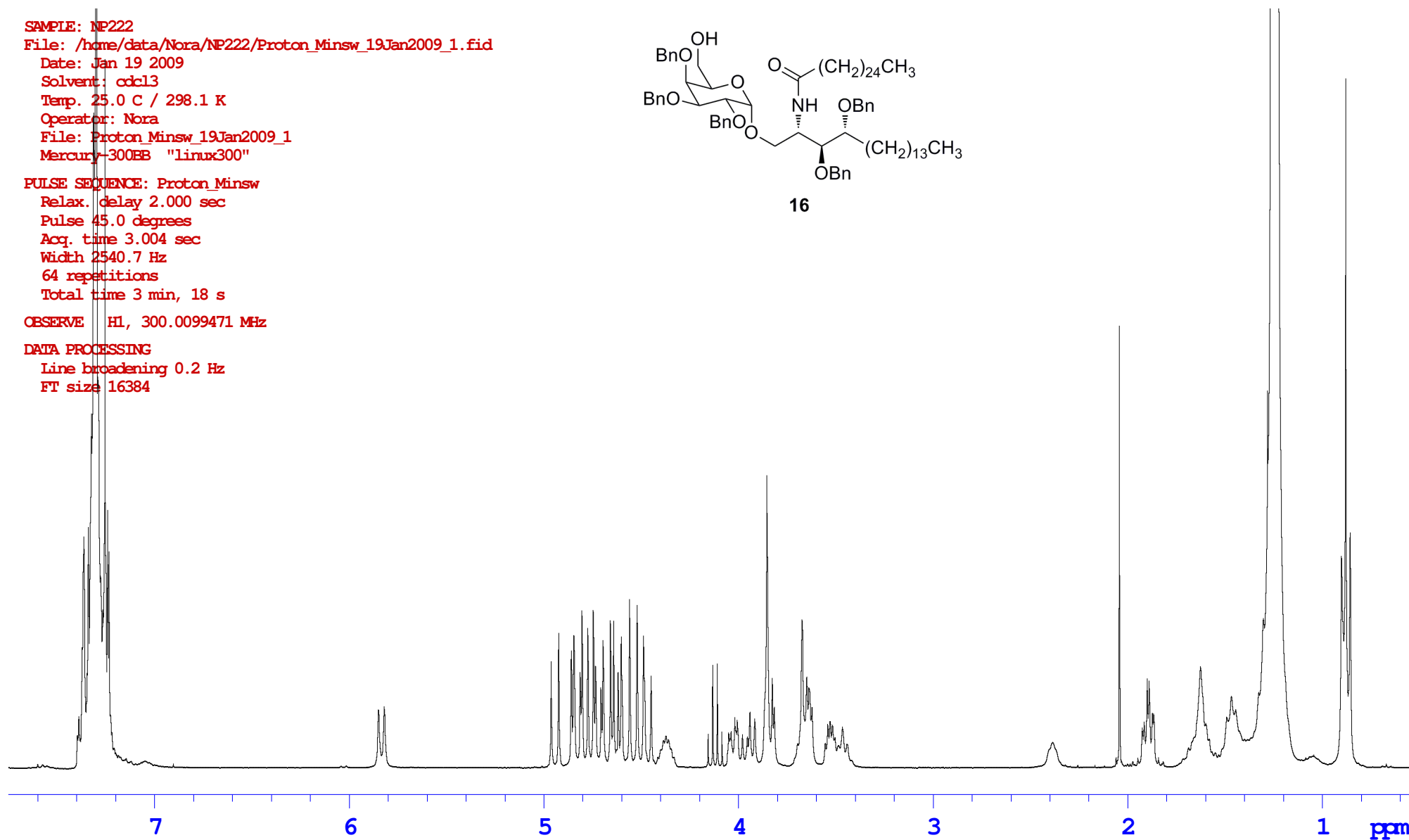
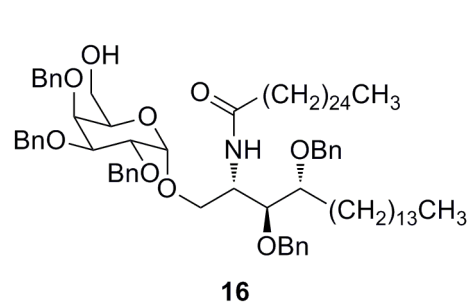
Total time 3 min, 18 s

OBSERVE H1, 300.0099471 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 16384



SAMPLE: NP222

File: /home/data/Nora/NP222/Carbon_12h_19Jan2009_1.fid

Date: Jan 19 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_12h_19Jan2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon_12h

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

14400 repetitions

Total time 12 hr, 37 min, 36 s

OBSERVE C13, 75.4375432 MHz

DECOUPLE H1, 300.0114533 MHz

Power 33 dB

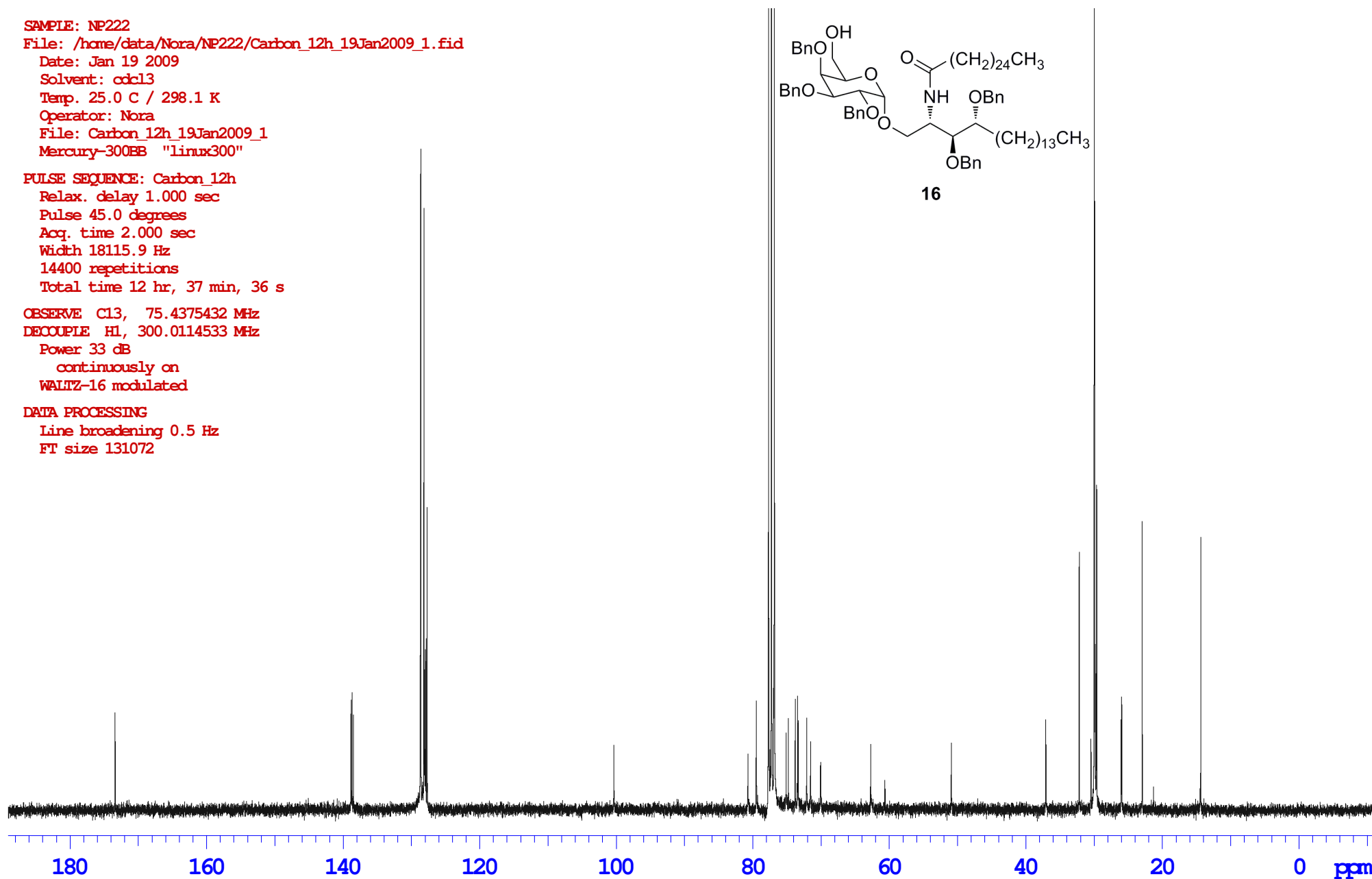
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



SAMPLE: NP004

File: /home/data/Nora/NP004/Proton_Minsw_14Oct2009_1.fid

Date: Oct 14 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_14Oct2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.003 sec

Width 2525.3 Hz

32 repetitions

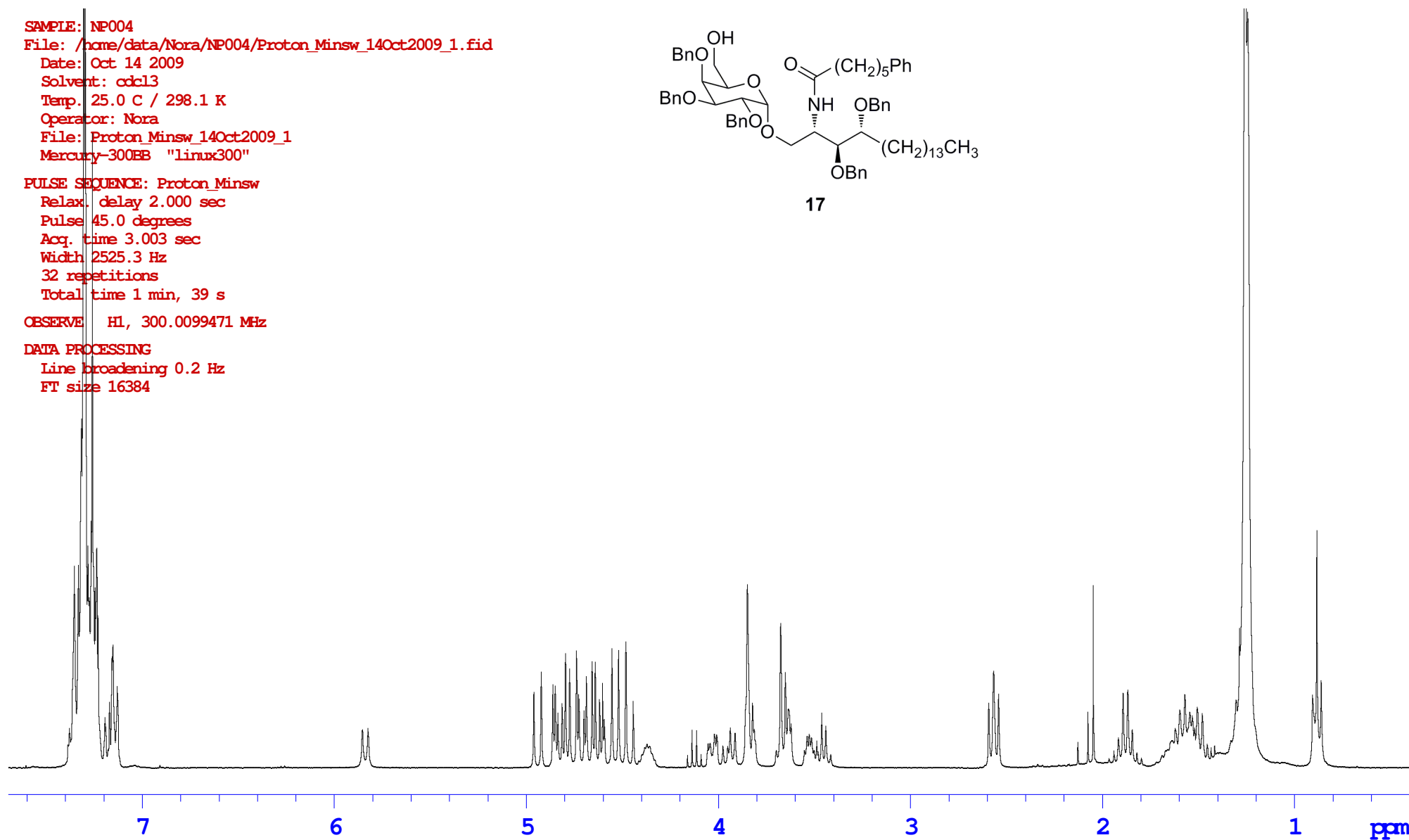
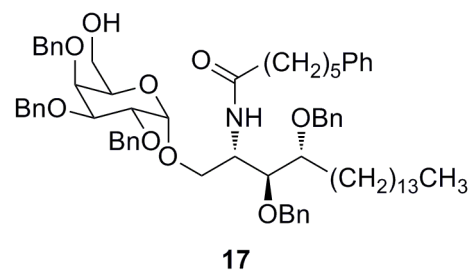
Total time 1 min, 39 s

OBSERVE H1, 300.0099471 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 16384



SAMPLE: NP004

File: /home/data/Nora/NP004/Carbon_14Oct2009_1.fid

Date: Oct 14 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_14Oct2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon

Relax. delay 1.000 sec

Pulse 40.2 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

11000 repetitions

Total time 9 hr, 38 min, 46 s

OBSERVE C13, 75.4375432 MHz

DECOUPLE H1, 300.0114533 MHz

Power 33 dB

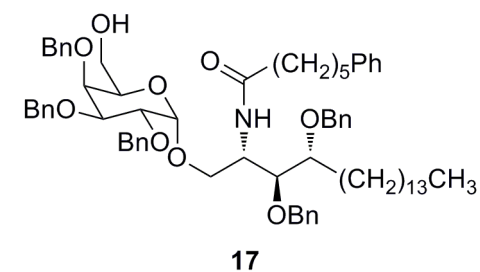
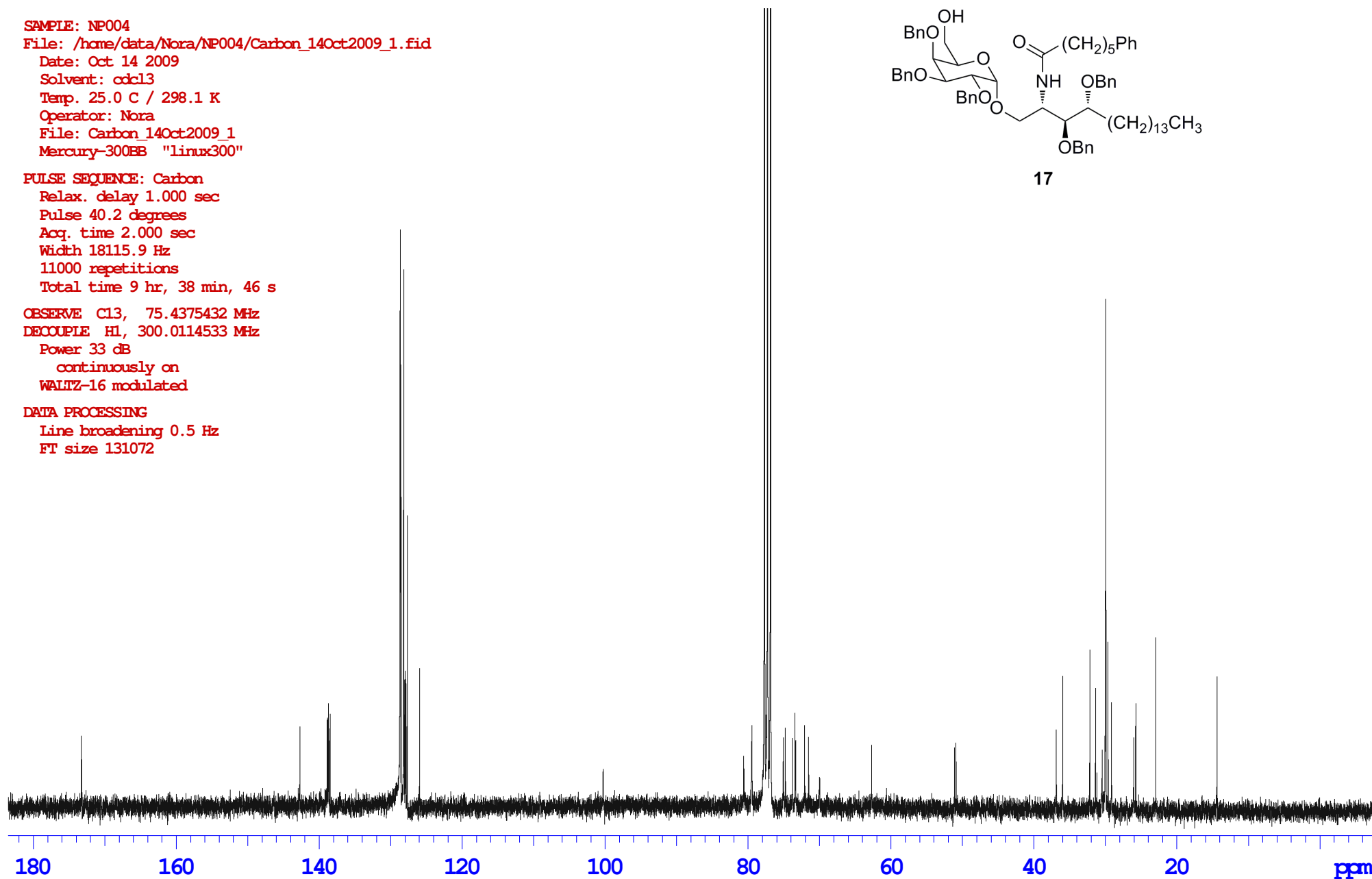
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



SAMPLE: NP009

File: /home/data/Nora/NP009/Proton_Minsw_15Nov2009_1.fid

Date: Nov 15 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_15Nov2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.002 sec

Width 2812.1 Hz

32 repetitions

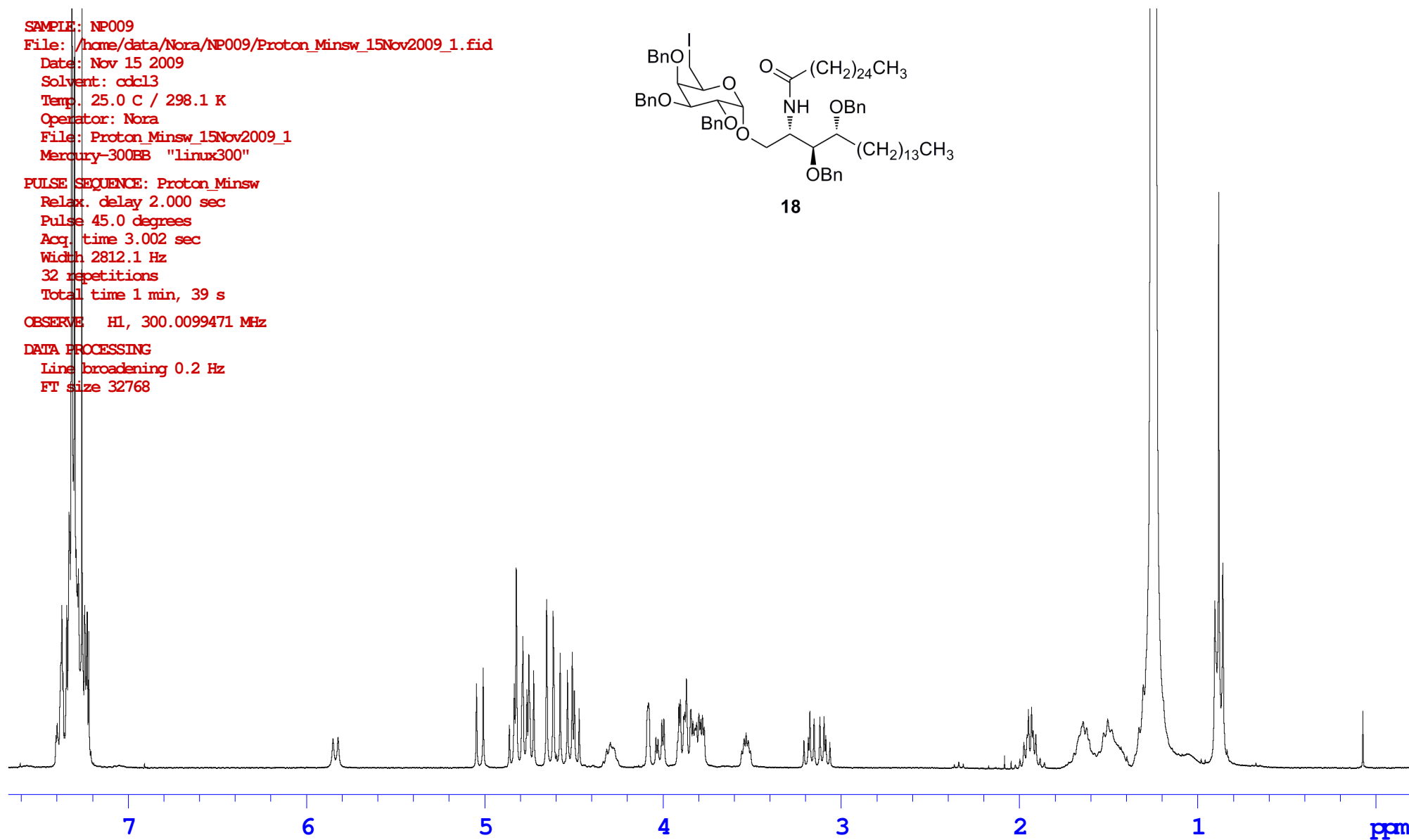
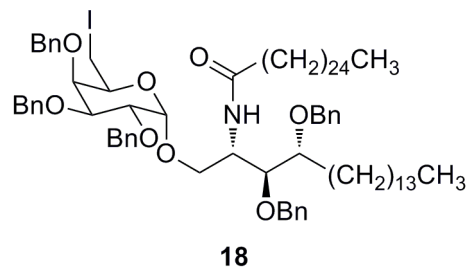
Total time 1 min, 39 s

OBSERVE H1, 300.0099471 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768



SAMPLE: NP009

File: /home/data/Nora/NP009/Carbon_12h_15Nov2009_1.fid

Date: Nov 15 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_12h_15Nov2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon_12h

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

17000 repetitions

Total time 14 hr, 54 min, 21 s

OBSERVE C13, 75.4378240 MHz

DECOUPLE H1, 300.0114533 MHz

Power 33 dB

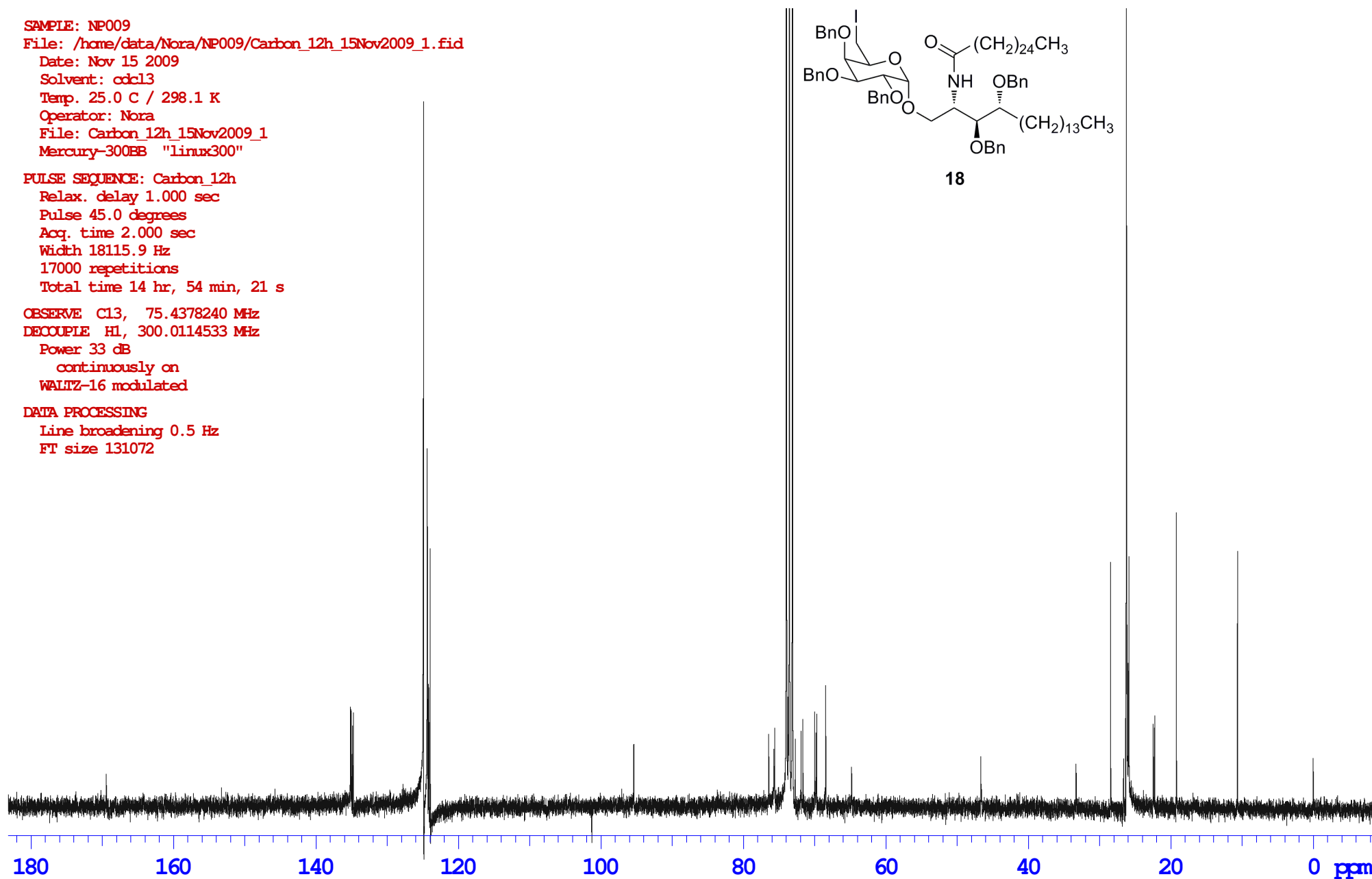
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



SAMPLE: NP007

File: /home/data/Nora/NP007/Proton_Minsw_27Oct2009_2.fid

Date: Oct 27 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_27Oct2009_2

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.002 sec

Width 2812.1 Hz

32 repetitions

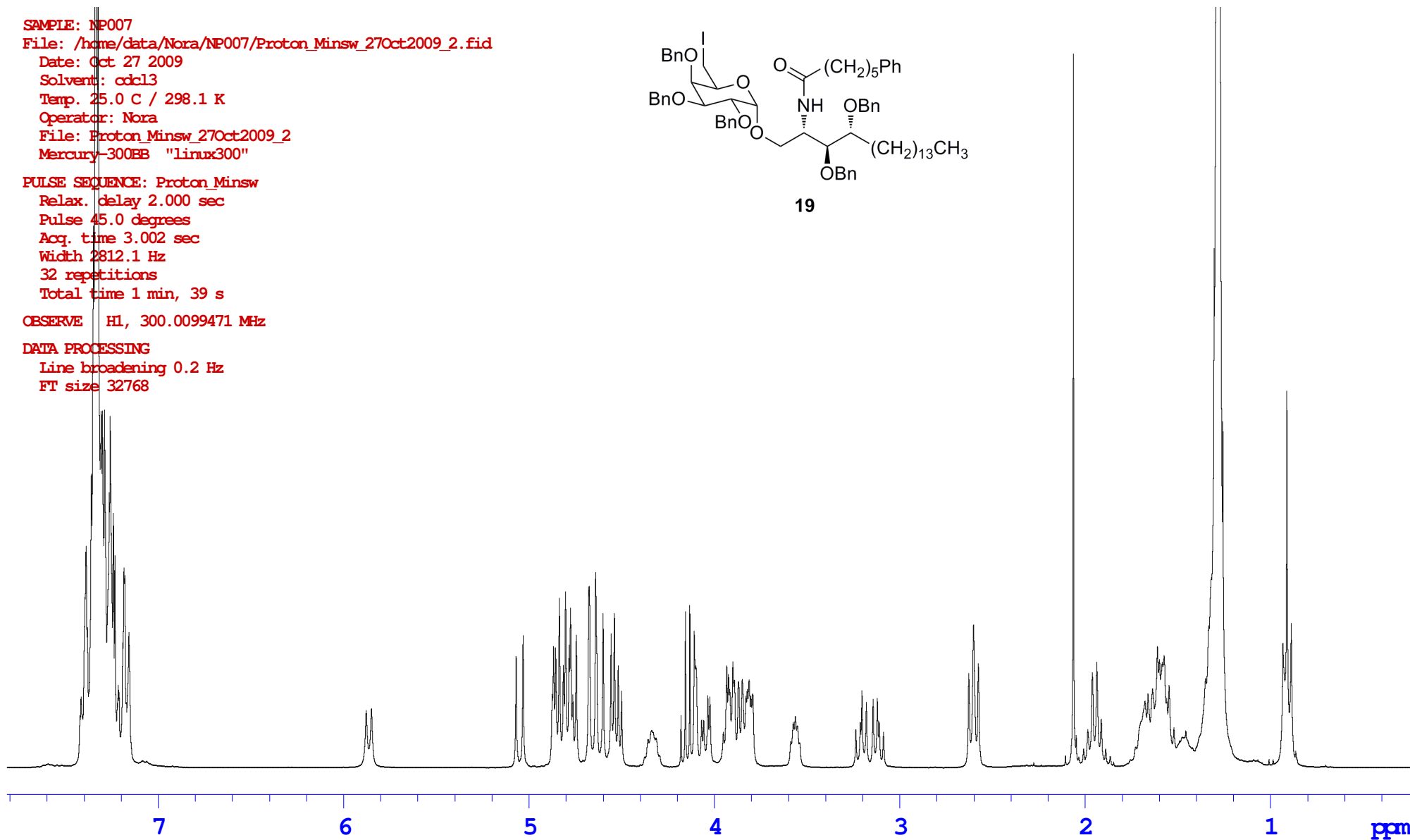
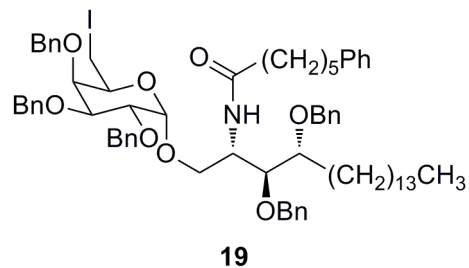
Total time 1 min, 39 s

OBSERVE H1, 300.0099471 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768



SAMPLE: NP007

File: /home/data/Nora/NP007/Carbon_27Oct2009_1.fid

Date: Oct 27 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_27Oct2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon

Relax. delay 1.000 sec

Pulse 40.2 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

1100 repetitions

Total time 58 min, 4 s

OBSERVE C13, 75.4378278 MHz

DECOUPLE H1, 300.0114533 MHz

Power 33 dB

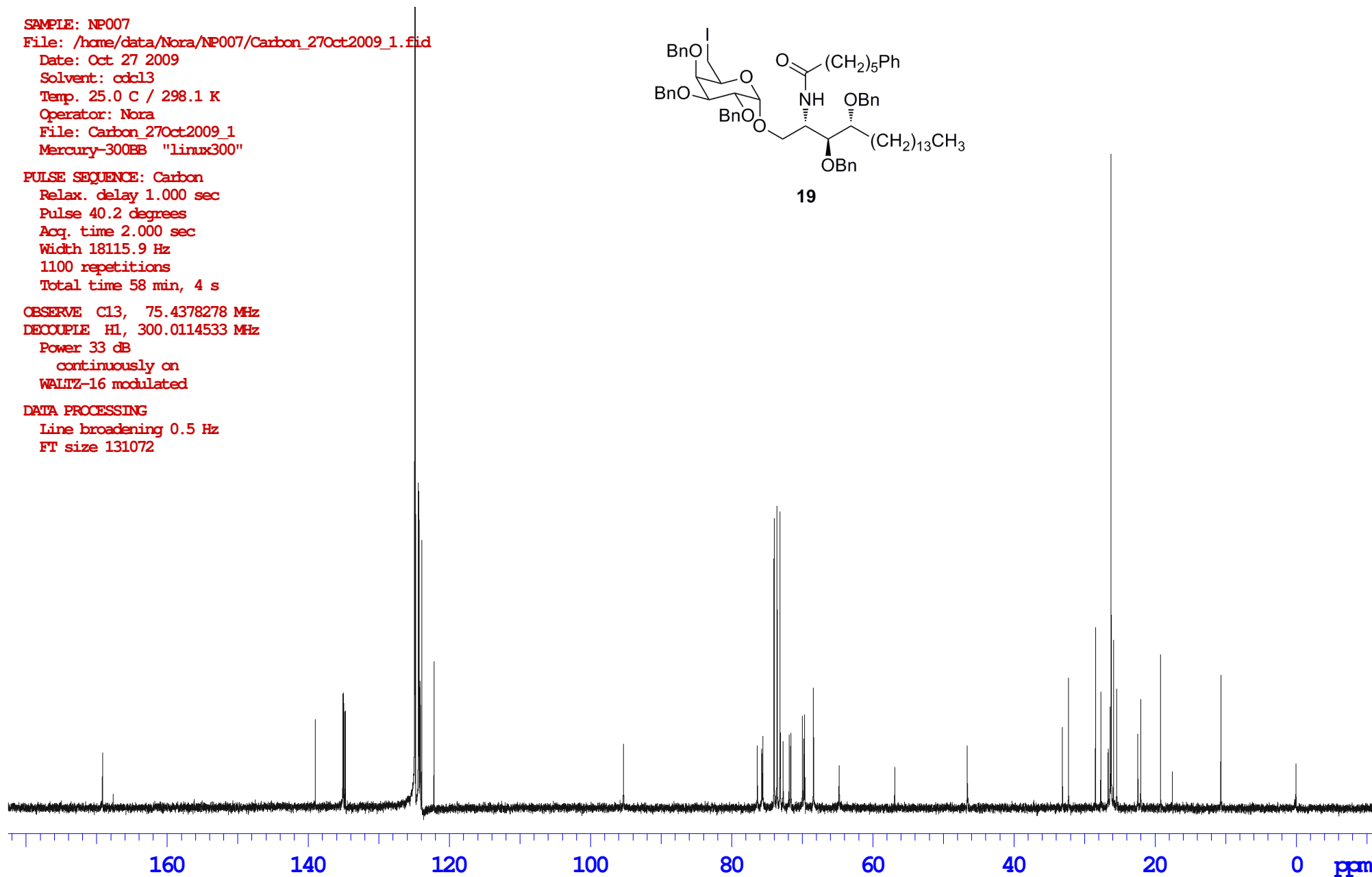
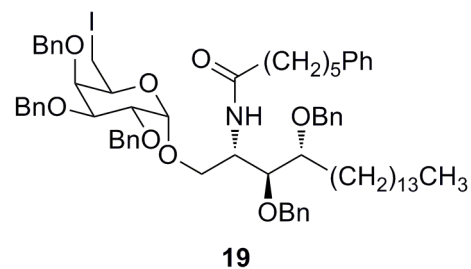
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



SAMPLE: NP223

File: /home/Data/Nora/NP223/Proton_Minsw_17Jun2009_1.fid

Date: Jun 17 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_17Jun2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.001 sec

Width 2801.1 Hz

32 repetitions

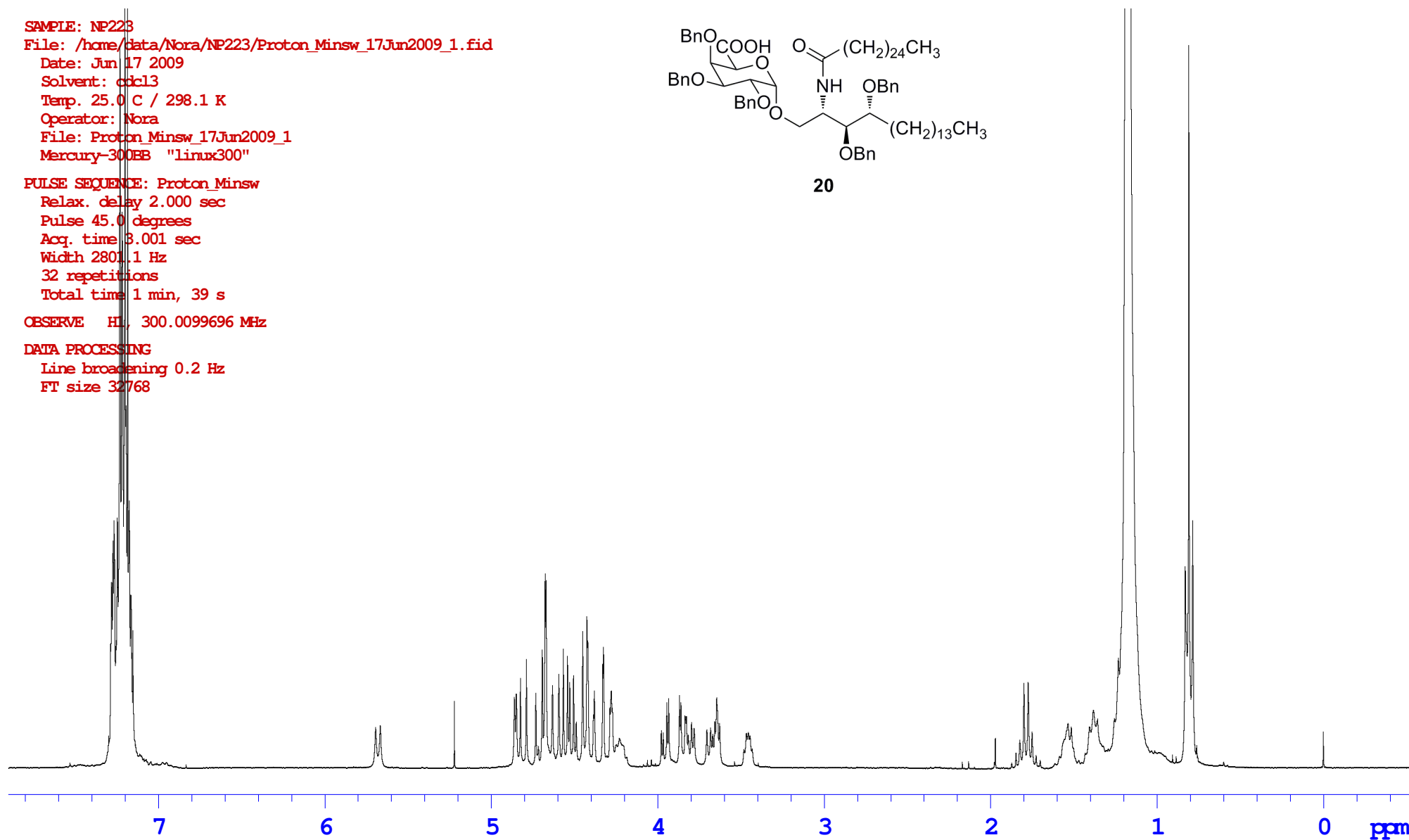
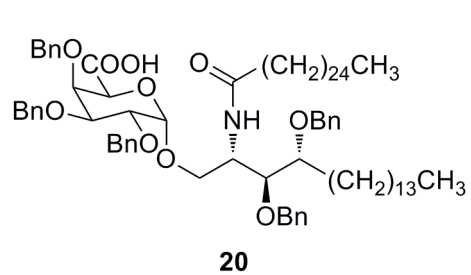
Total time 1 min, 39 s

OBSERVE H1, 300.0099696 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768



SAMPLE: NP223

File: /home/data/Nora/NP223/Carbon_18Jun2009_3.fid

Date: Jun 17 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_18Jun2009_3

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon

Relax. delay 1.000 sec

Pulse 40.2 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

13844 repetitions

Total time 15 hr, 20 min, 39 s

OBSERVE C13, 75.4375432 MHz

DECOUPLE H1, 300.0114533 MHz

Power 33 dB

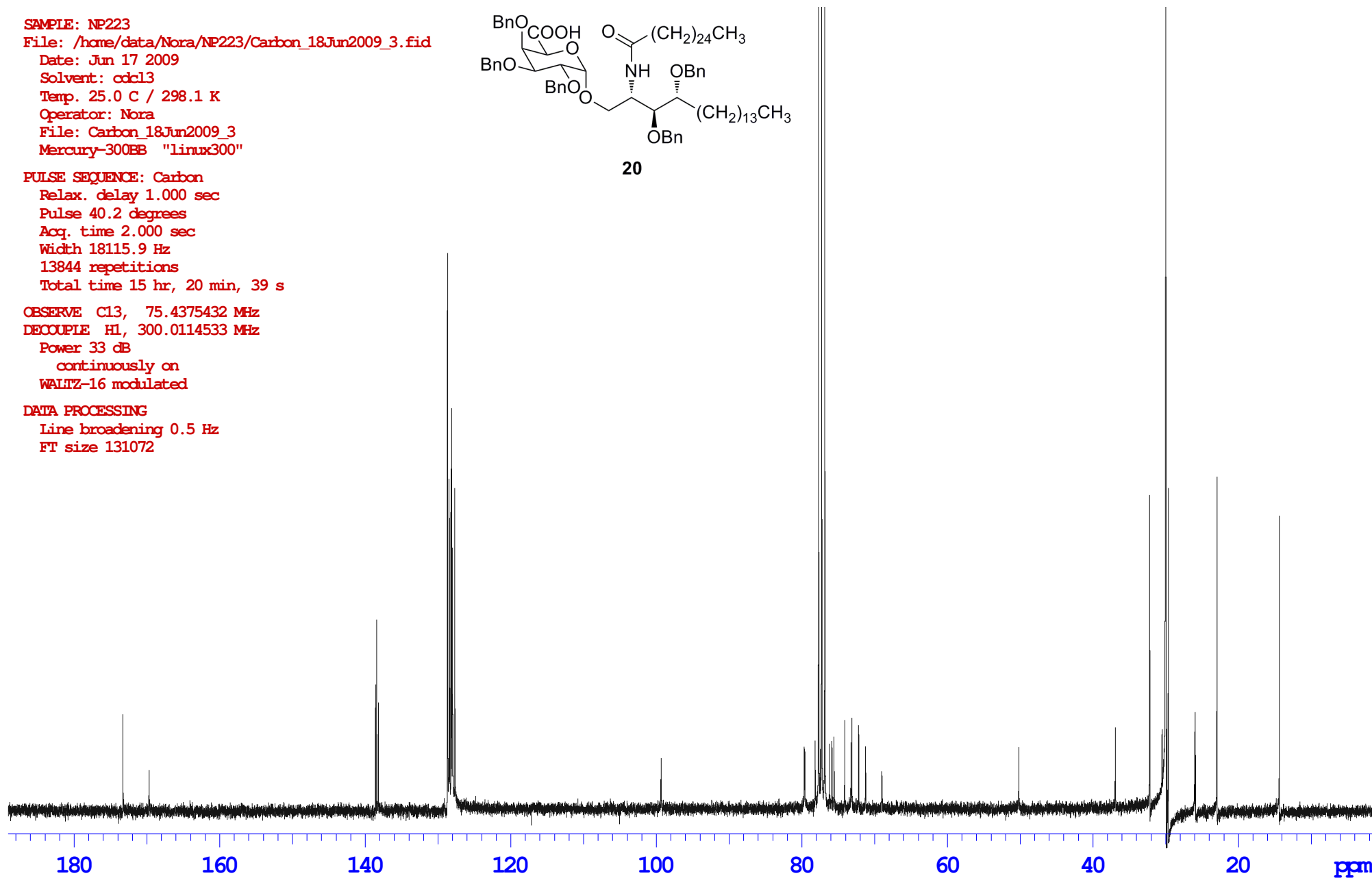
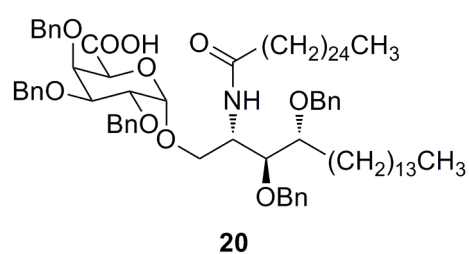
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



SAMPLE: NP005

File: /home/data/Nora/NP005/Proton_Minsw_21Oct2009_1.fid

Date: Oct 21 2009

Solvent: cdc13

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_21Oct2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.001 sec

Width 2795.6 Hz

32 repetitions

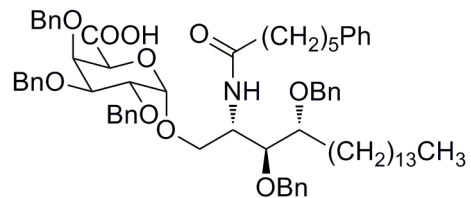
Total time 1 min, 39 s

OBSERVE H1, 300.0099471 MHz

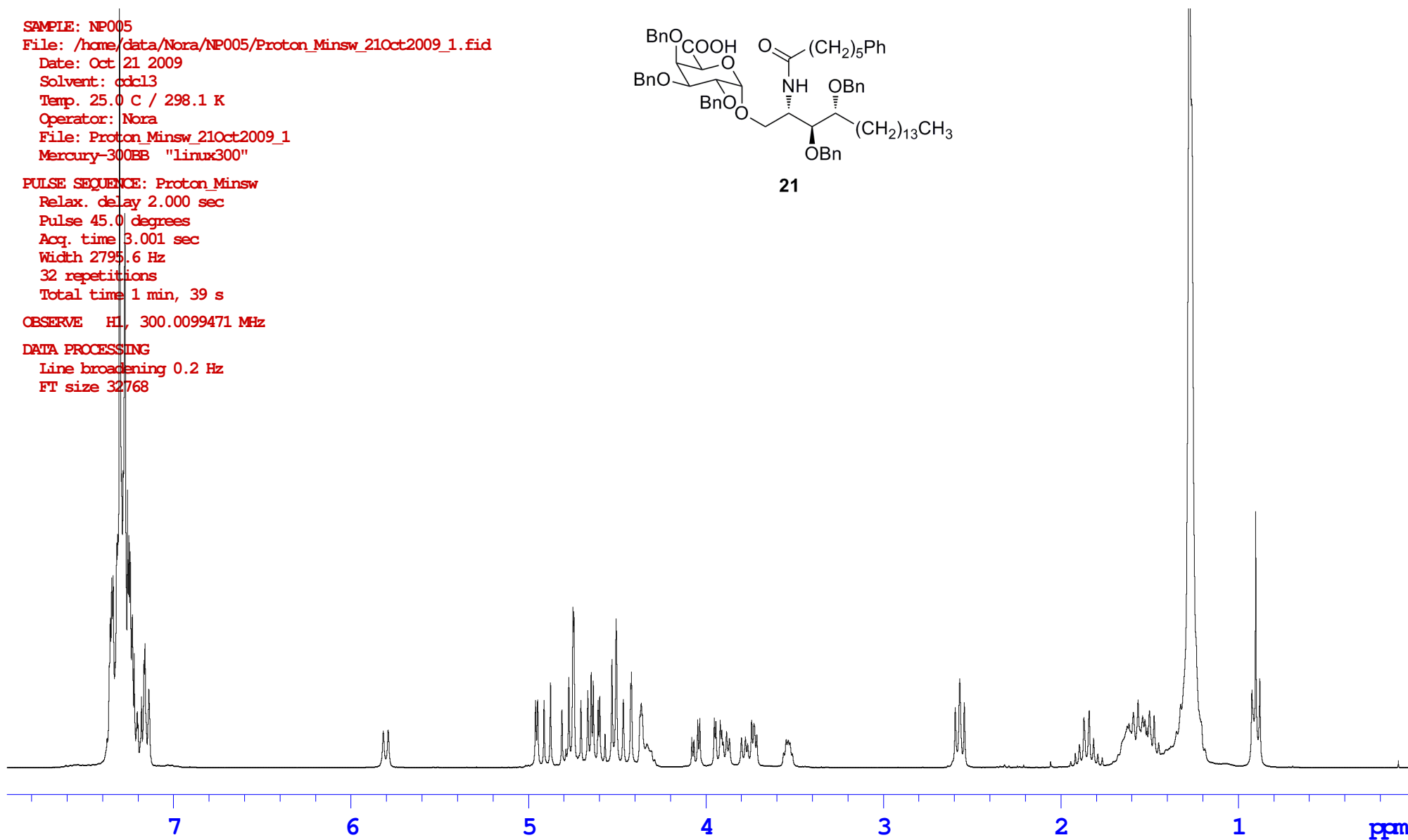
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768



21



SAMPLE: NP005

File: /home/data/Nora/NP005/Carbon 12h 21Oct2009 1.fid

Date: Oct 21 2009

Solvent: cdcl_3

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon 12h 21Oct2009_1

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Mercury-300BB "linux300"
```

PULSE SEQUENCE: Carbon 12h

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

11000 repetitions

Total time 9 hr, 38 min, 46 s

OBSERVE C13, 75.4375432 MHz

DECOUPLE H1, 300.0114533 MHz

Power 33 dB

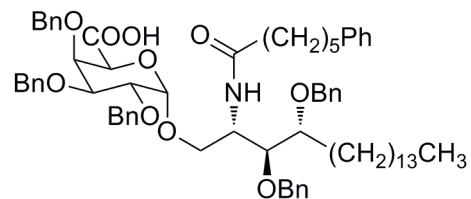
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WALTZ-16 modulated

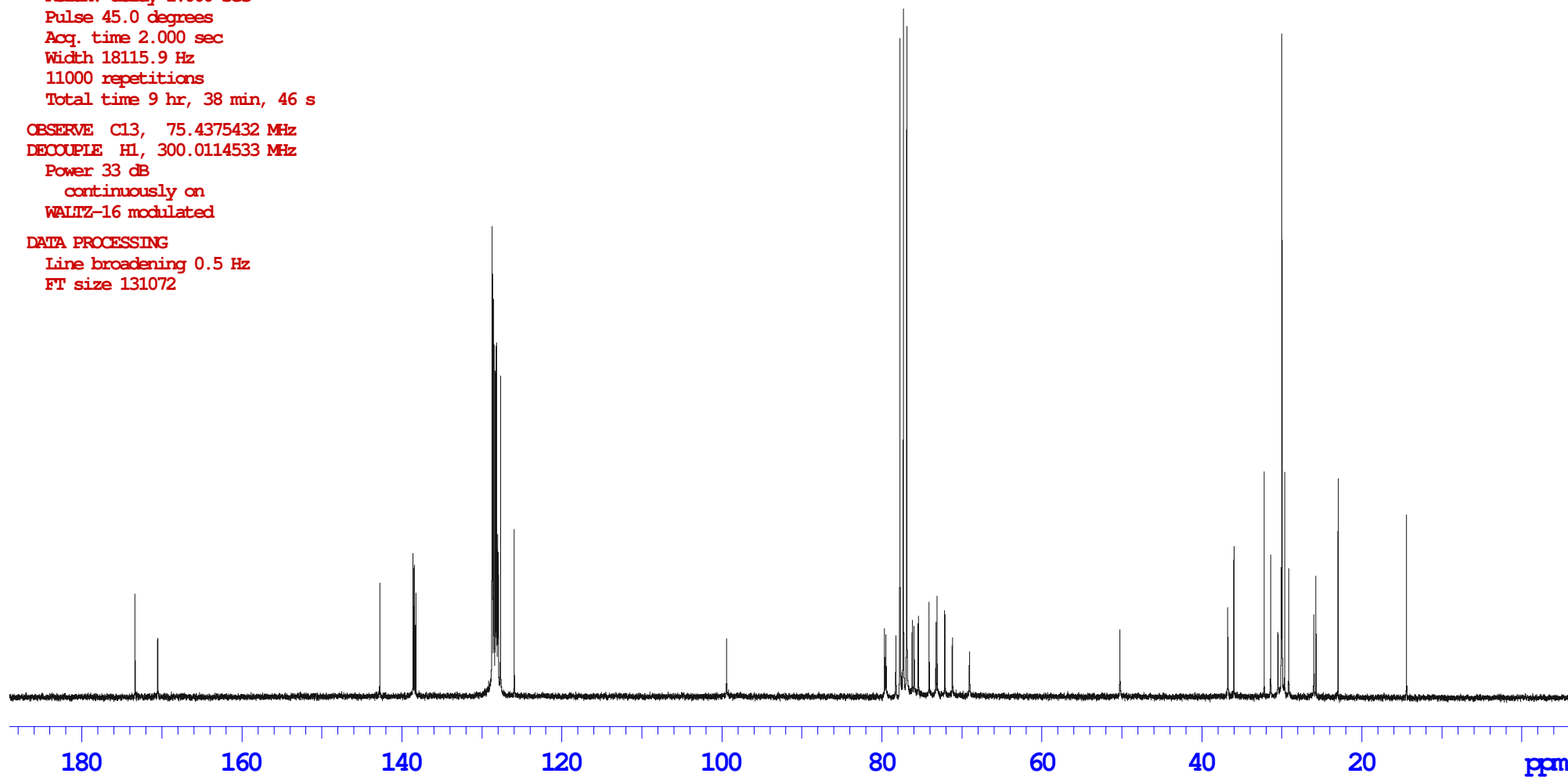
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



21



SAMPLE: NP010

File: /home/data/Nora/NP010/Proton_Minsw_10Dec2009_1.fid

Date: Dec 10 2009

Solvent: pyridine

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_10Dec2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.999 sec

Width 3039.5 Hz

32 repetitions

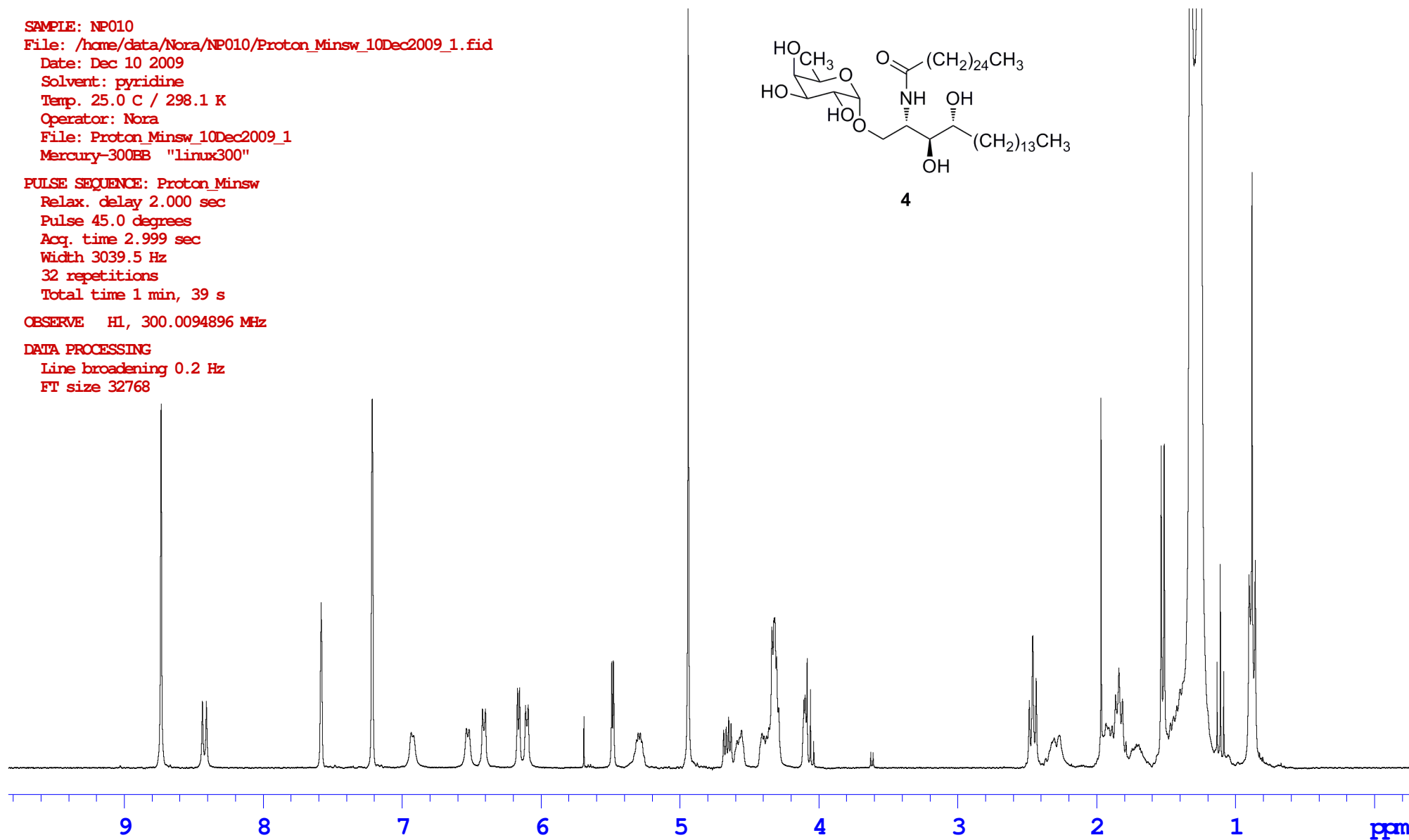
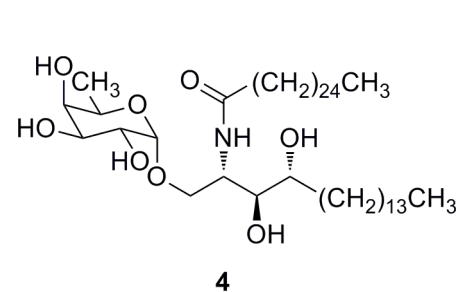
Total time 1 min, 39 s

OBSERVE H1, 300.0094896 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768



SAMPLE: NP010

File: /home/data/Nora/NP010/Carbon 12h 10Dec2009 1.fid

Date: Dec 10 2009

Solvent: pyridine

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon 12h 10Dec2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon 12h

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

14400 repetitions

Total time 12 hr, 37 min, 36 s

OBSERVE C13, 75.4375198 MHz

DECOUPLE H1, 300.0113603 MHz

Power 33 dB

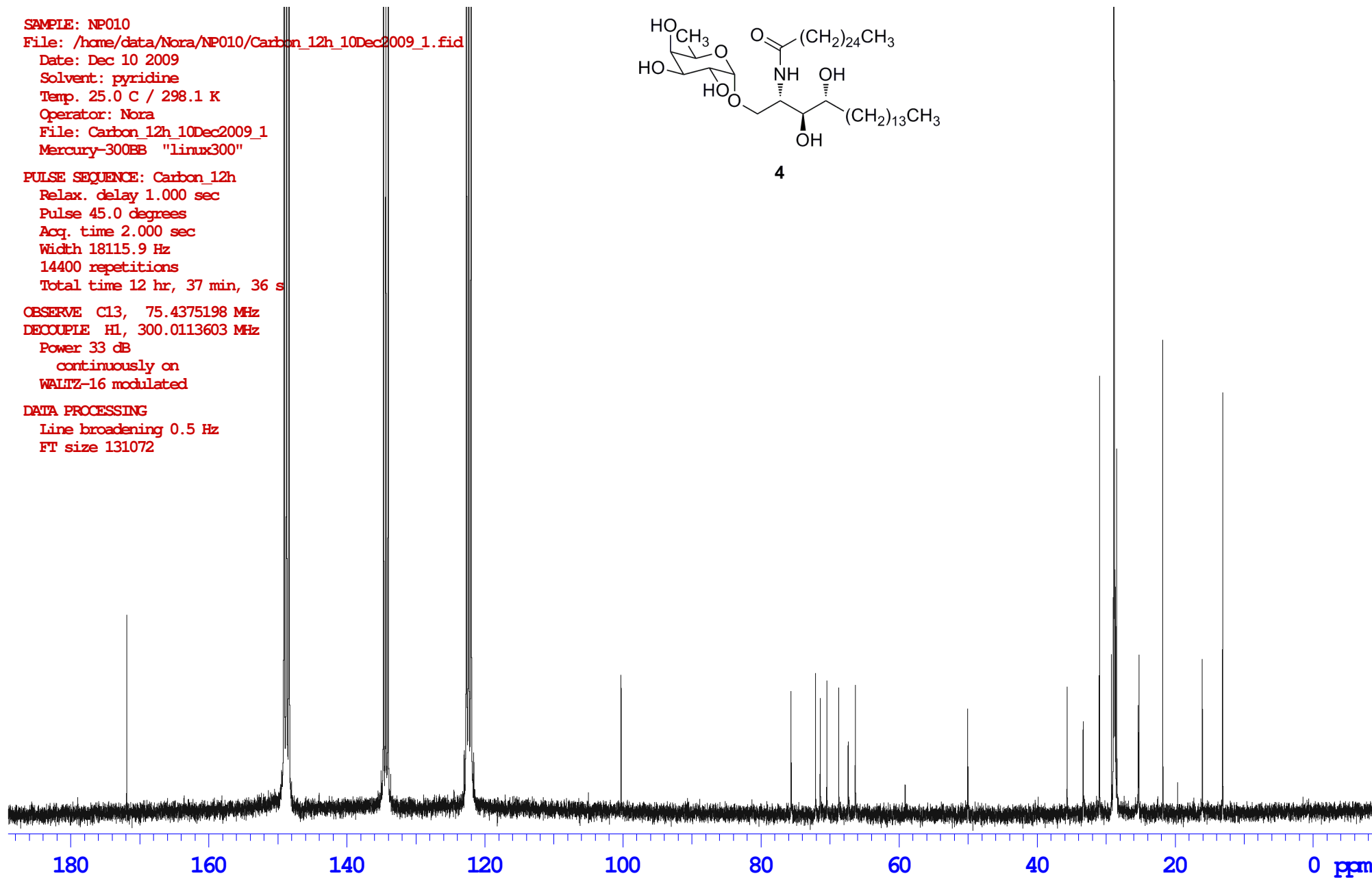
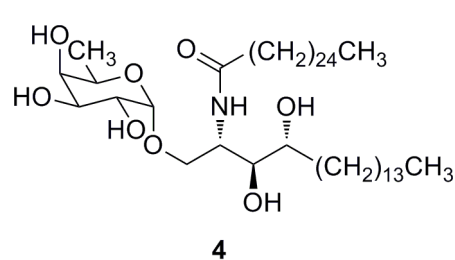
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072



SAMPLE: NP008

File: /home/data/Nora/NP008/Proton_Minsw_10Nov2009_1.fid

Date: Nov 10 2009

Solvent: cd3od

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Proton_Minsw_10Nov2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Proton_Minsw

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.998 sec

Width 3026.6 Hz

32 repetitions

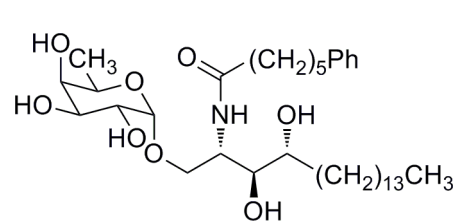
Total time 1 min, 39 s

OBSERVE H1, 300.0111287 MHz

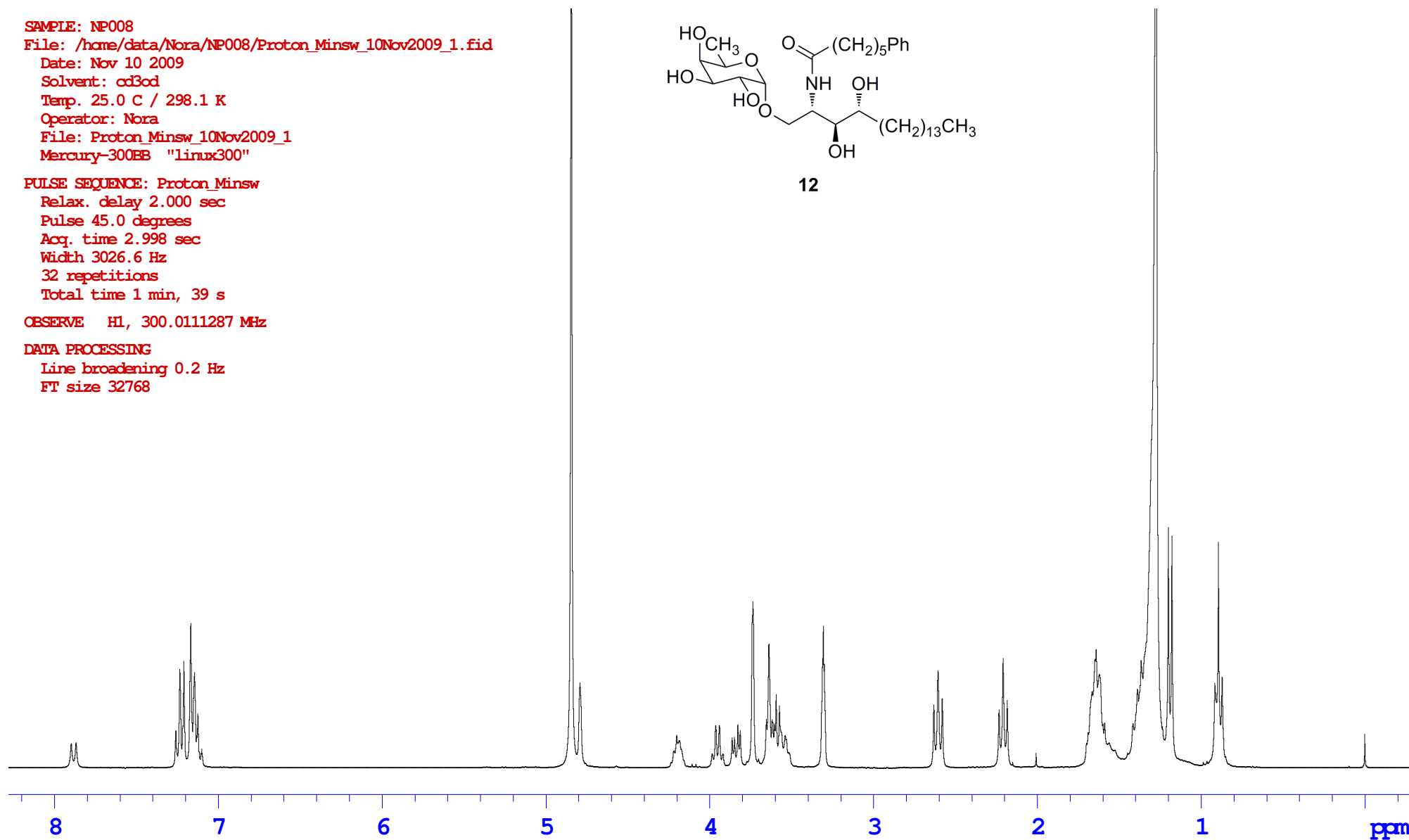
DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768



12



SAMPLE: NP008

File: /home/data/Nora/NP008/Carbon_10Nov2009_1.fid

Date: Nov 10 2009

Solvent: cd3od

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_10Nov2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon

Relax. delay 1.000 sec

Pulse 40.2 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

15000 repetitions

Total time 13 hr, 9 min, 10 s

OBSERVE C13, 75.4378404 MHz

DECOUPLE H1, 300.0126353 MHz

Power 33 dB

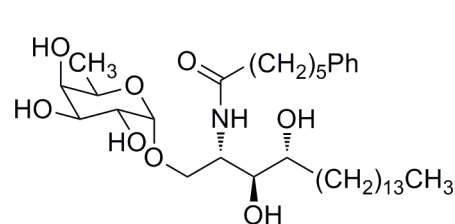
continuously on

WALTZ-16 modulated

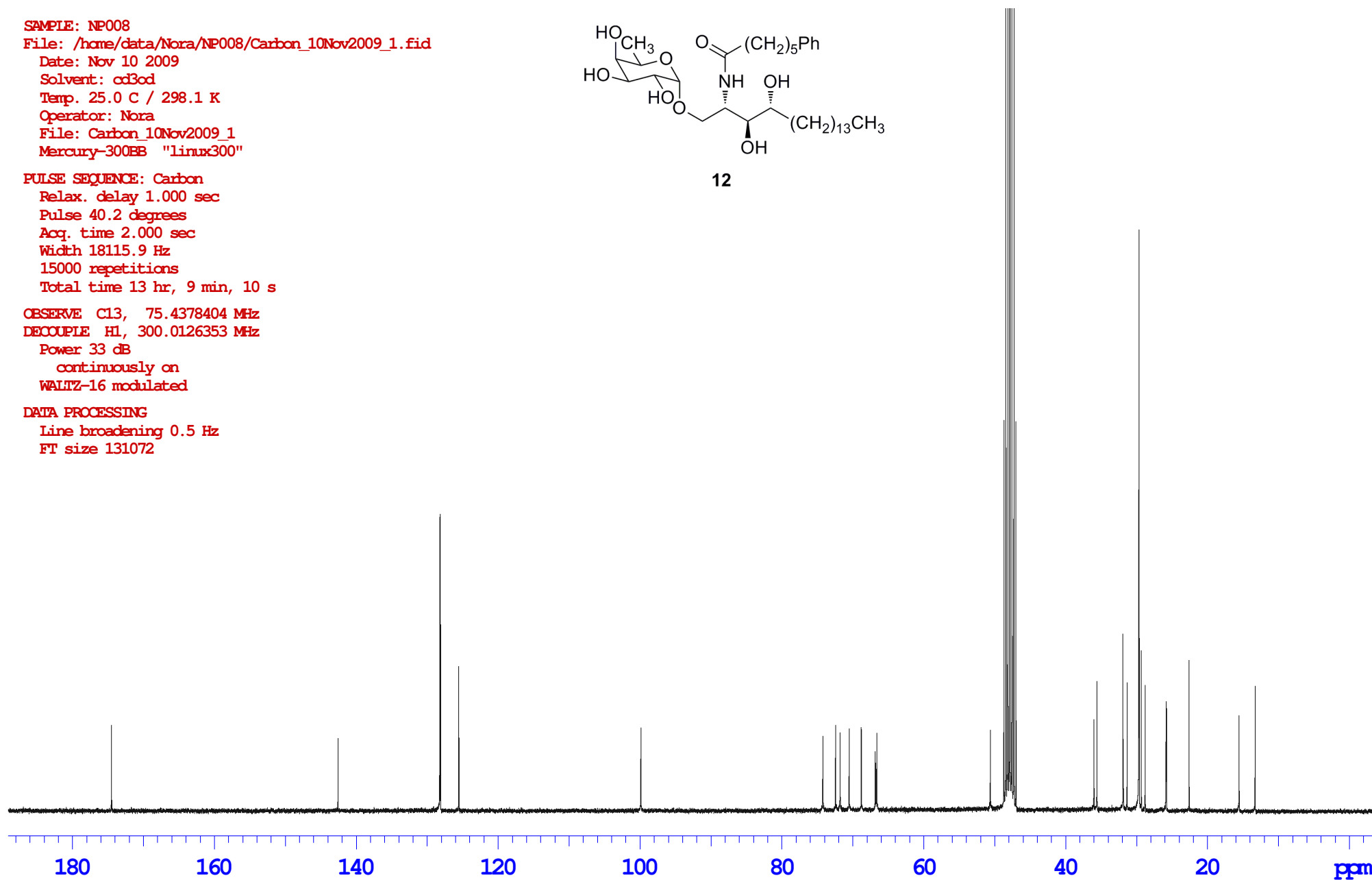
DATA PROCESSING

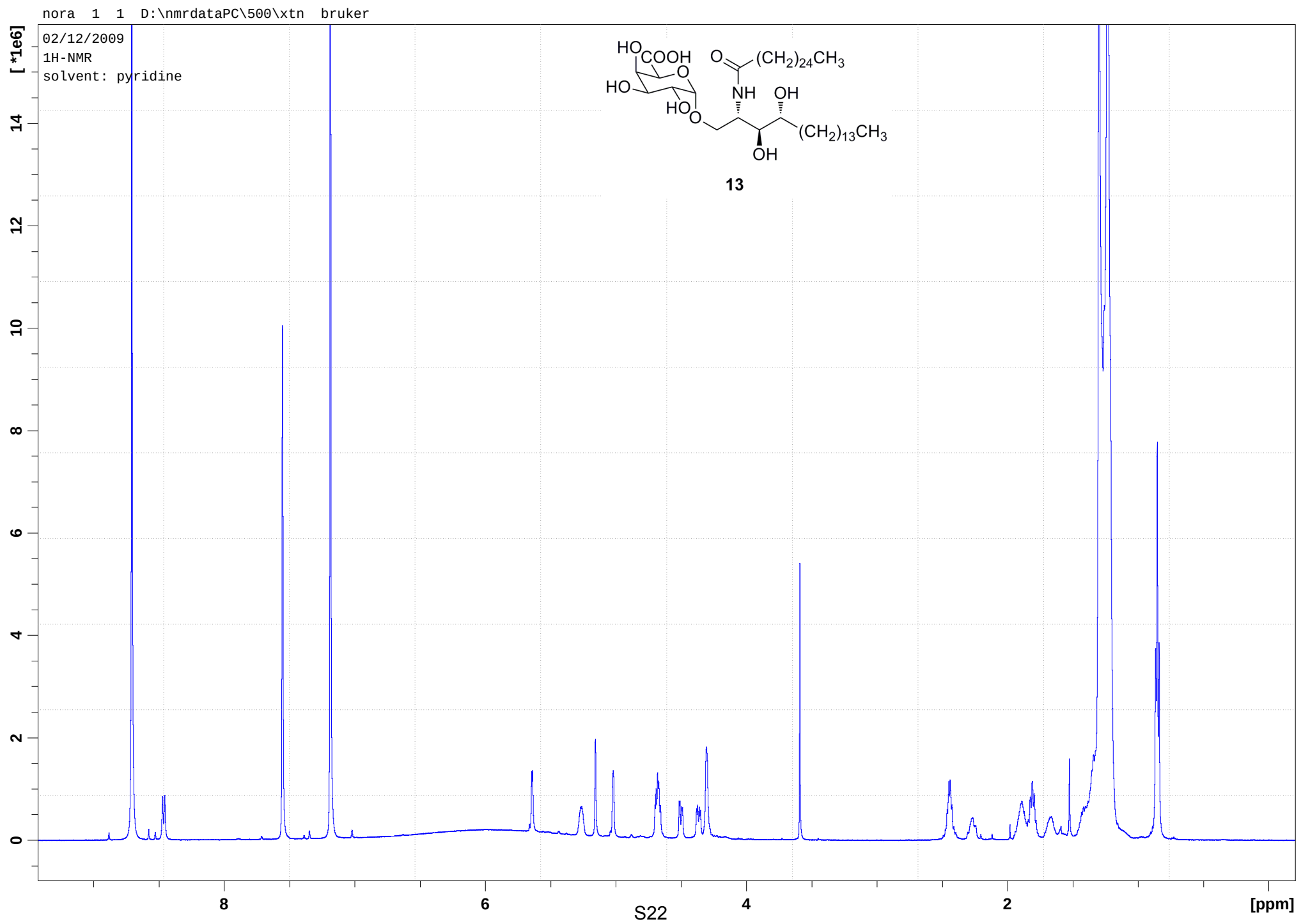
Line broadening 0.5 Hz

FT size 131072



12





SAMPLE: NP244

File: /home/data/Nora/NP244/Carbon_12h_06Aug2009_1.fid

Date: Aug 6 2009

Solvent: pyridine

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_12h_06Aug2009_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon_12h

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

17500 repetitions

Total time 15 hr, 20 min, 39 s

OBSERVE C13, 75.4375198 MHz

DECOUPLE H1, 300.0113603 MHz

Power 33 dB

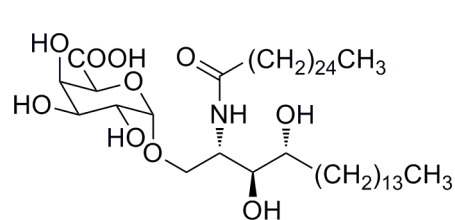
continuously on

WALTZ-16 modulated

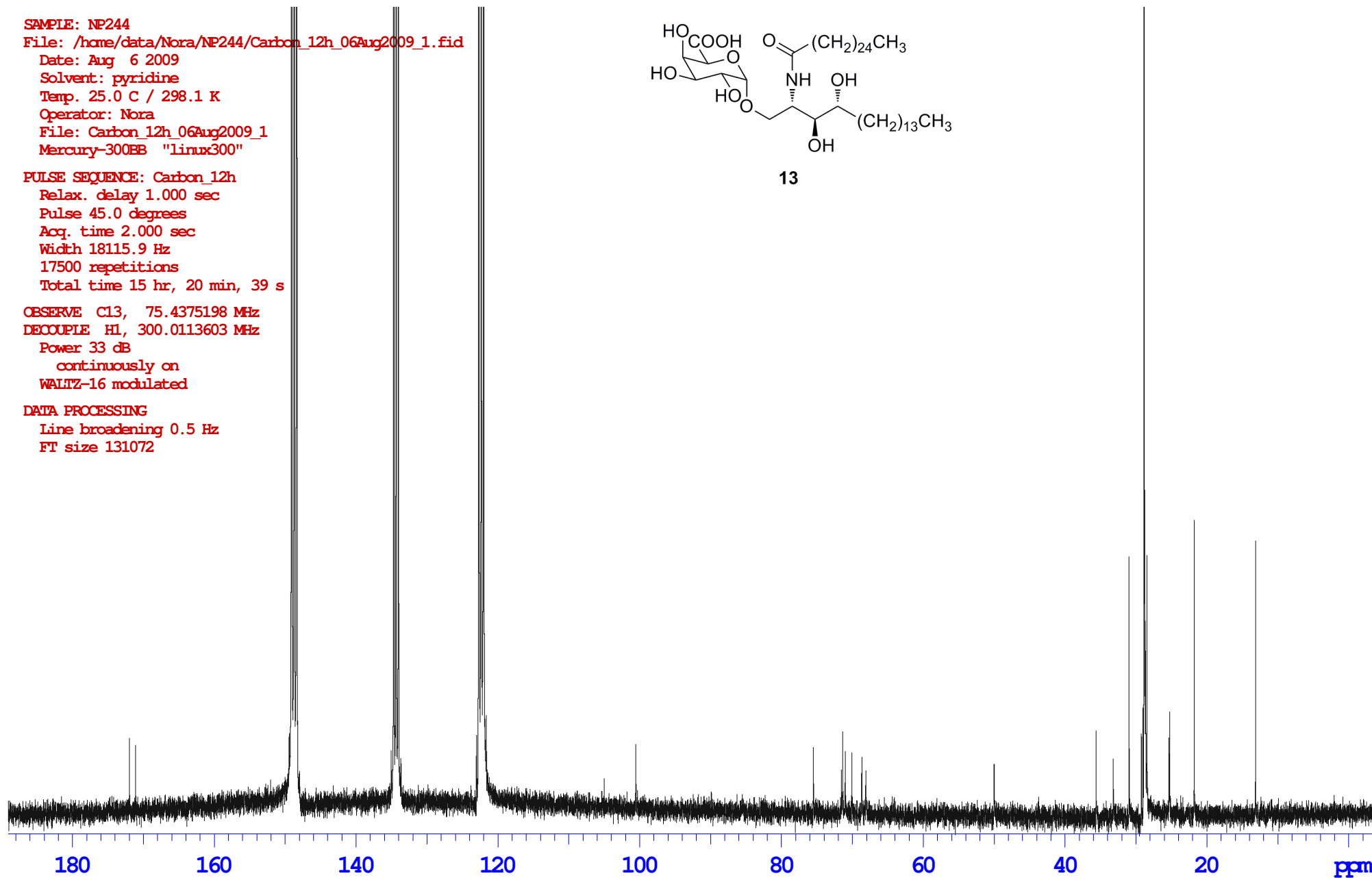
DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

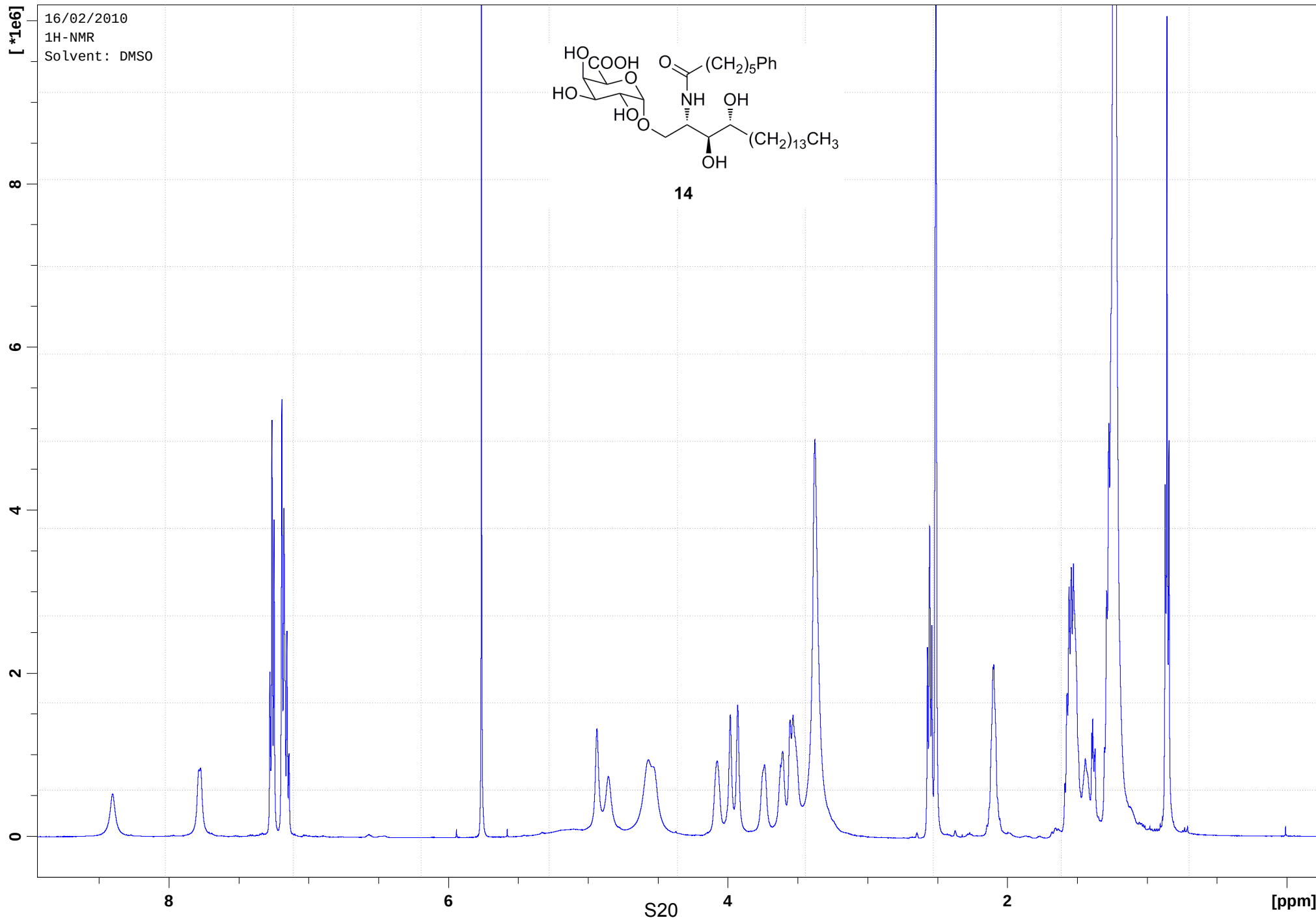


13



¹H-NMR

Solvent: DMSO



SAMPLE: NP006

File: /home/data/Nora/NP006/Carbon_12h_25Jan2010_1.fid

Date: Jan 25 2010

Solvent: dmsO

Temp. 25.0 C / 298.1 K

Operator: Nora

File: Carbon_12h_25Jan2010_1

Mercury-300BB "linux300"

PULSE SEQUENCE: Carbon_12h

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.000 sec

Width 18115.9 Hz

16960 repetitions

Total time 15 hr, 46 min, 57 s

OBSERVE C13, 75.4379015 MHz

DECOUPLE H1, 300.0128784 MHz

Power 33 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 131072

