Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Chiral nitrones:
studies of [1,4]-sigmatropic rearrangement and utilization in the synthesis of new iminosugars

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SUPPLEMENTARY INFORMATION

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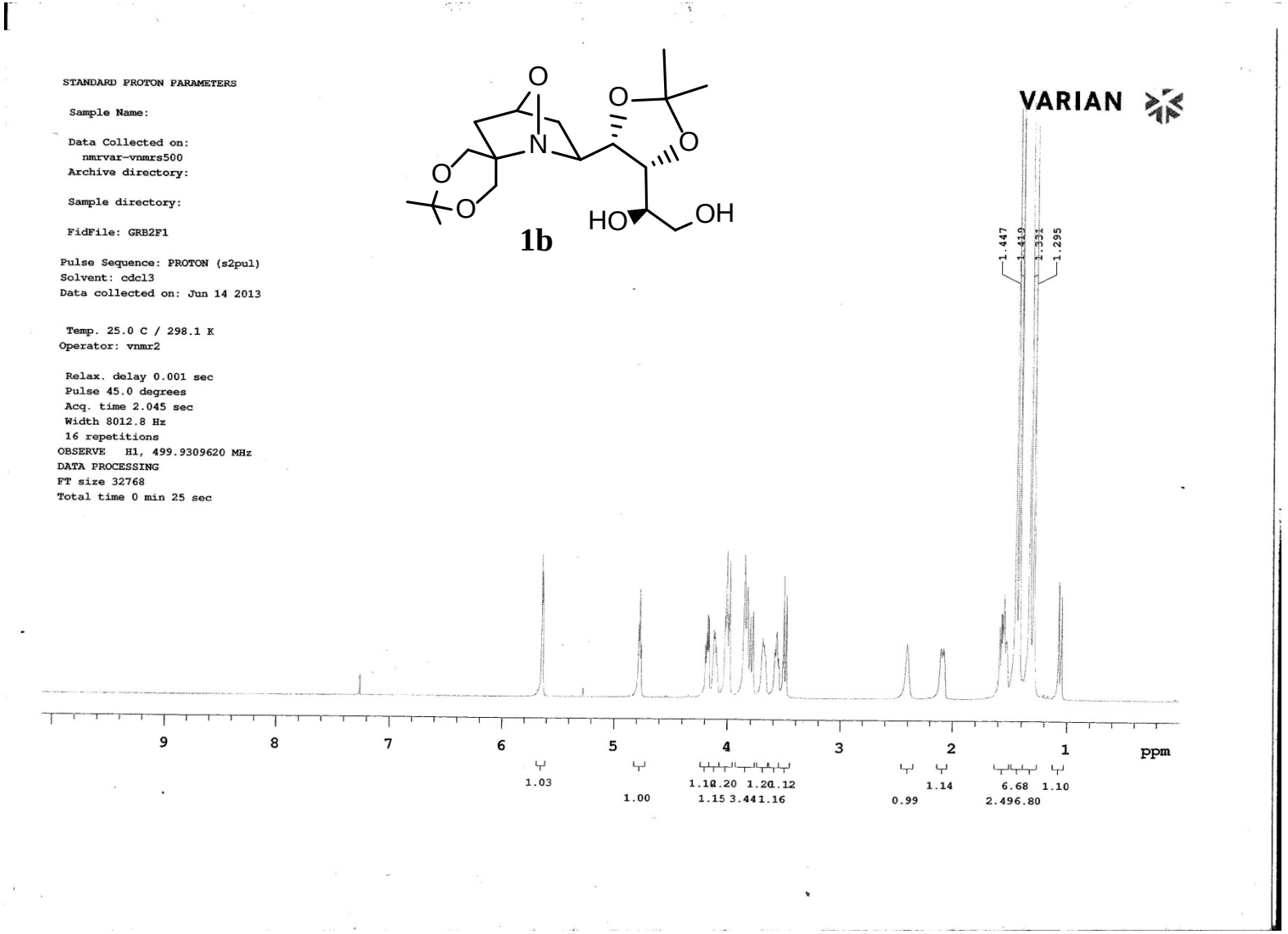
The NMR spectra copies



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

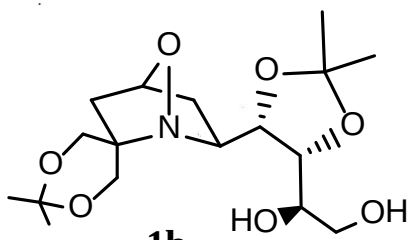
Sample directory:

FidFile: GRB2F1-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 14 2013

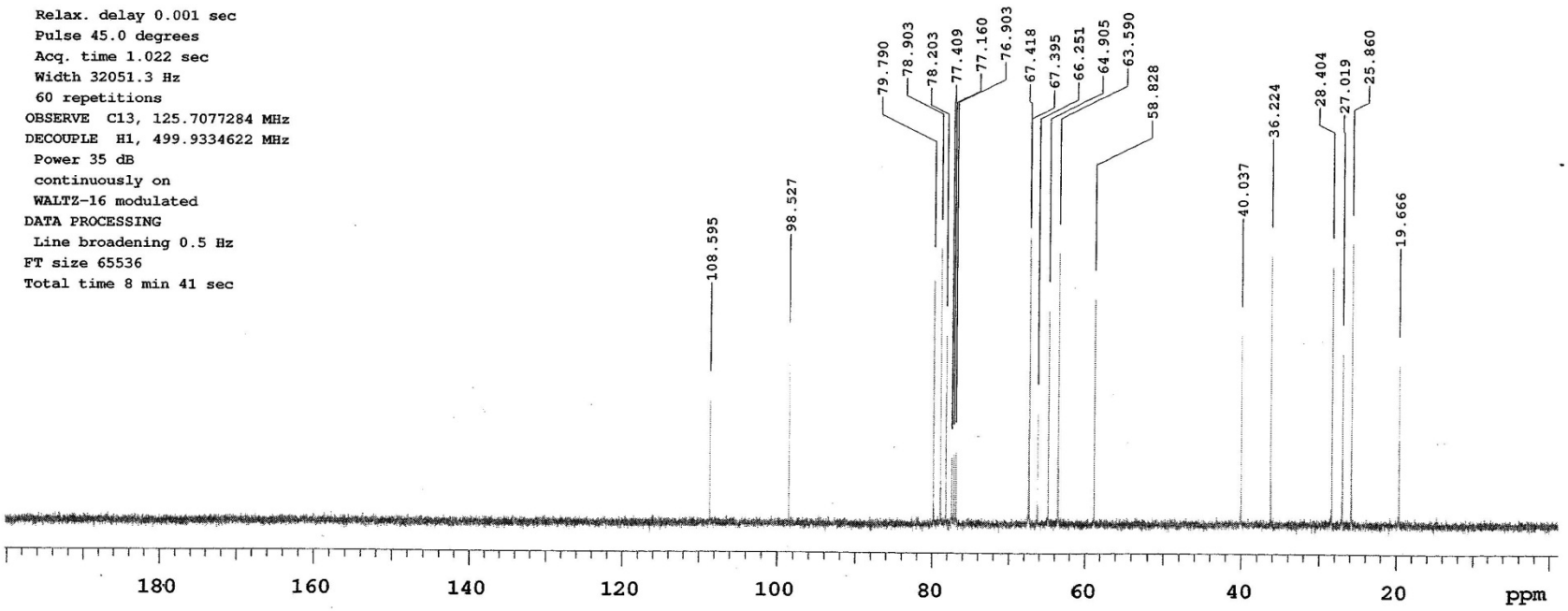
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
60 repetitions
OBSERVE C13, 125.7077284 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec



1b

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

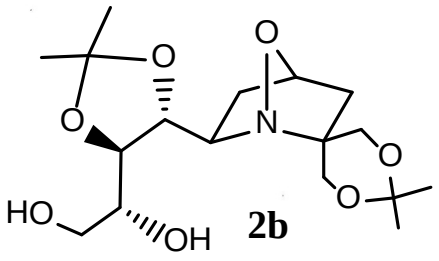
Sample directory:

FidFile: B2F2

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 21 2013

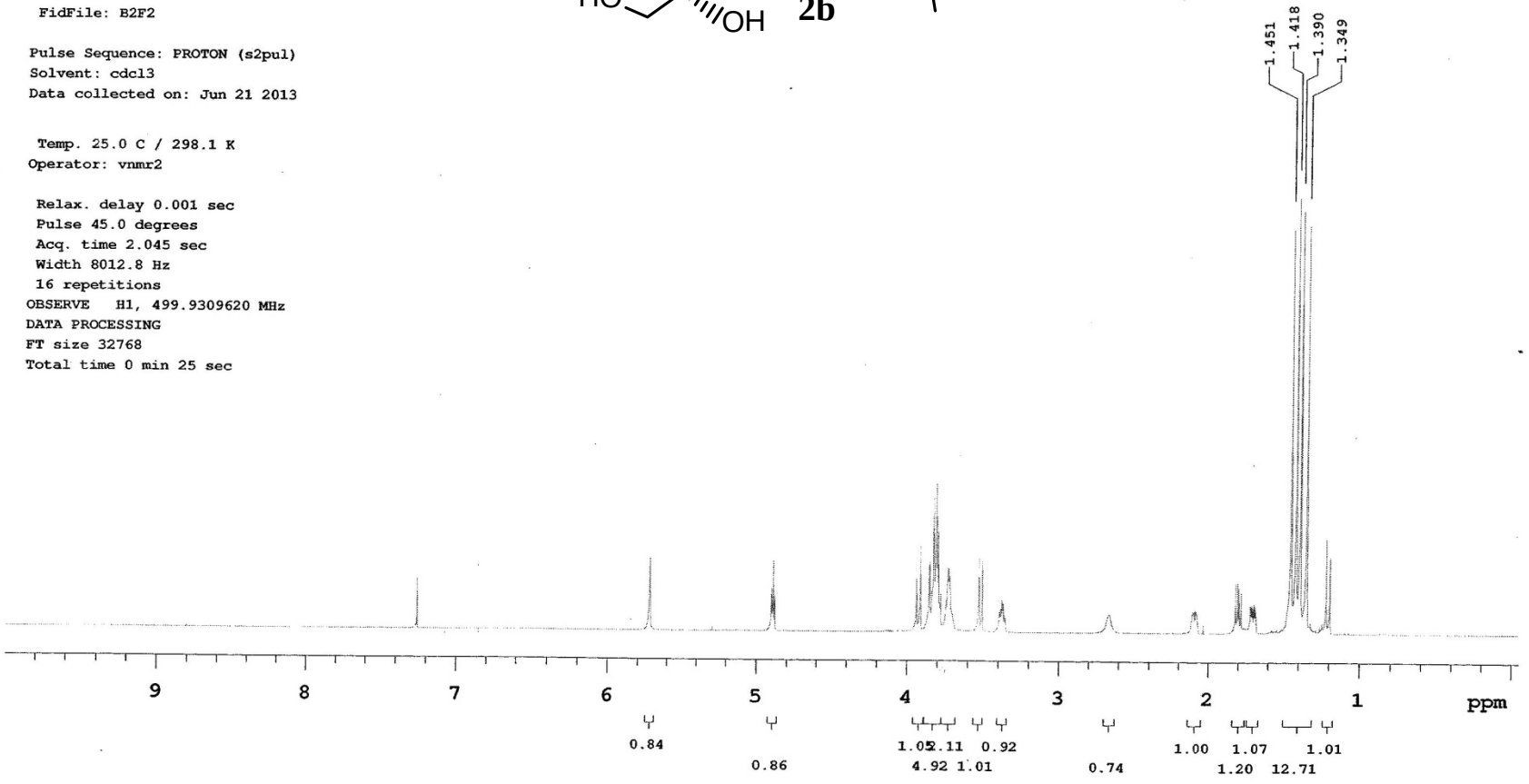
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309620 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



2b

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

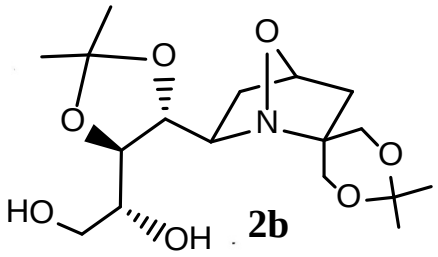
Sample directory:

FidFile: B2F2-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 21 2013

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
120 repetitions
OBSERVE C13, 125.7077215 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec



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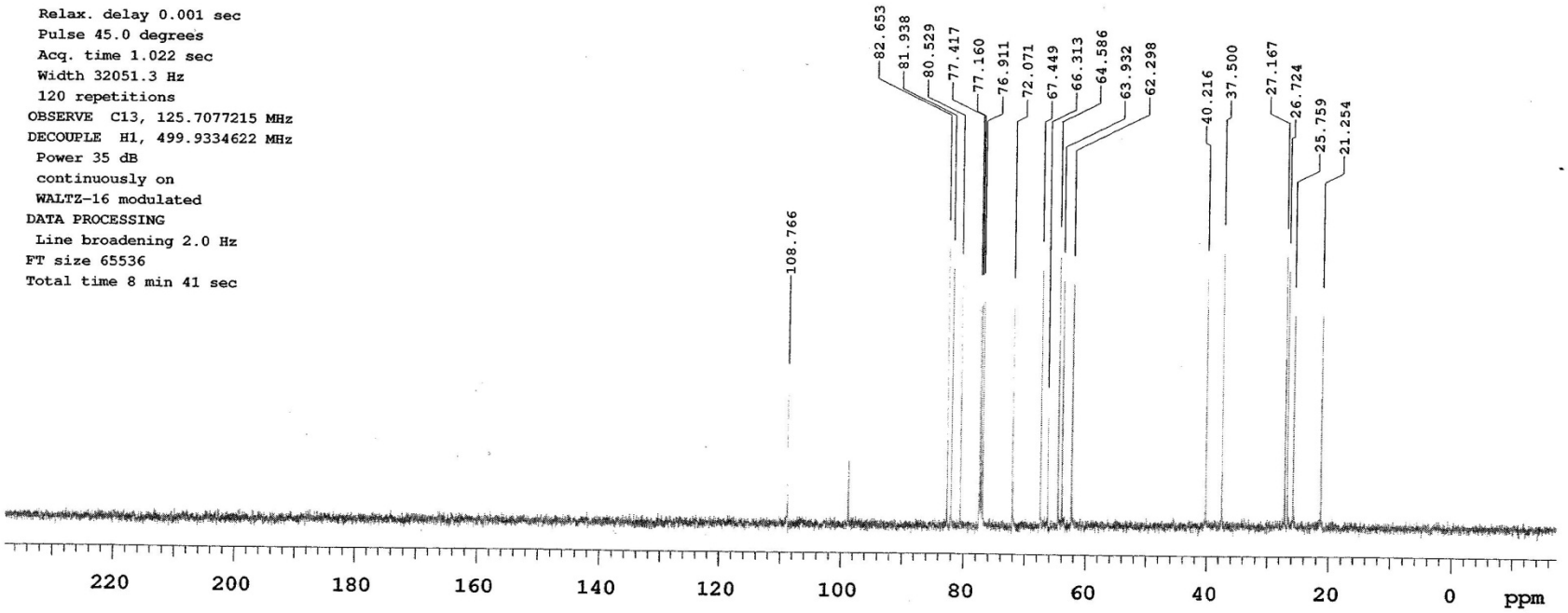
VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

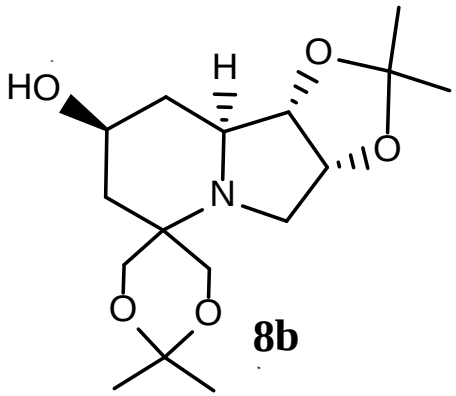
Sample directory:

FidFile: MA234-1-1

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 5 2014

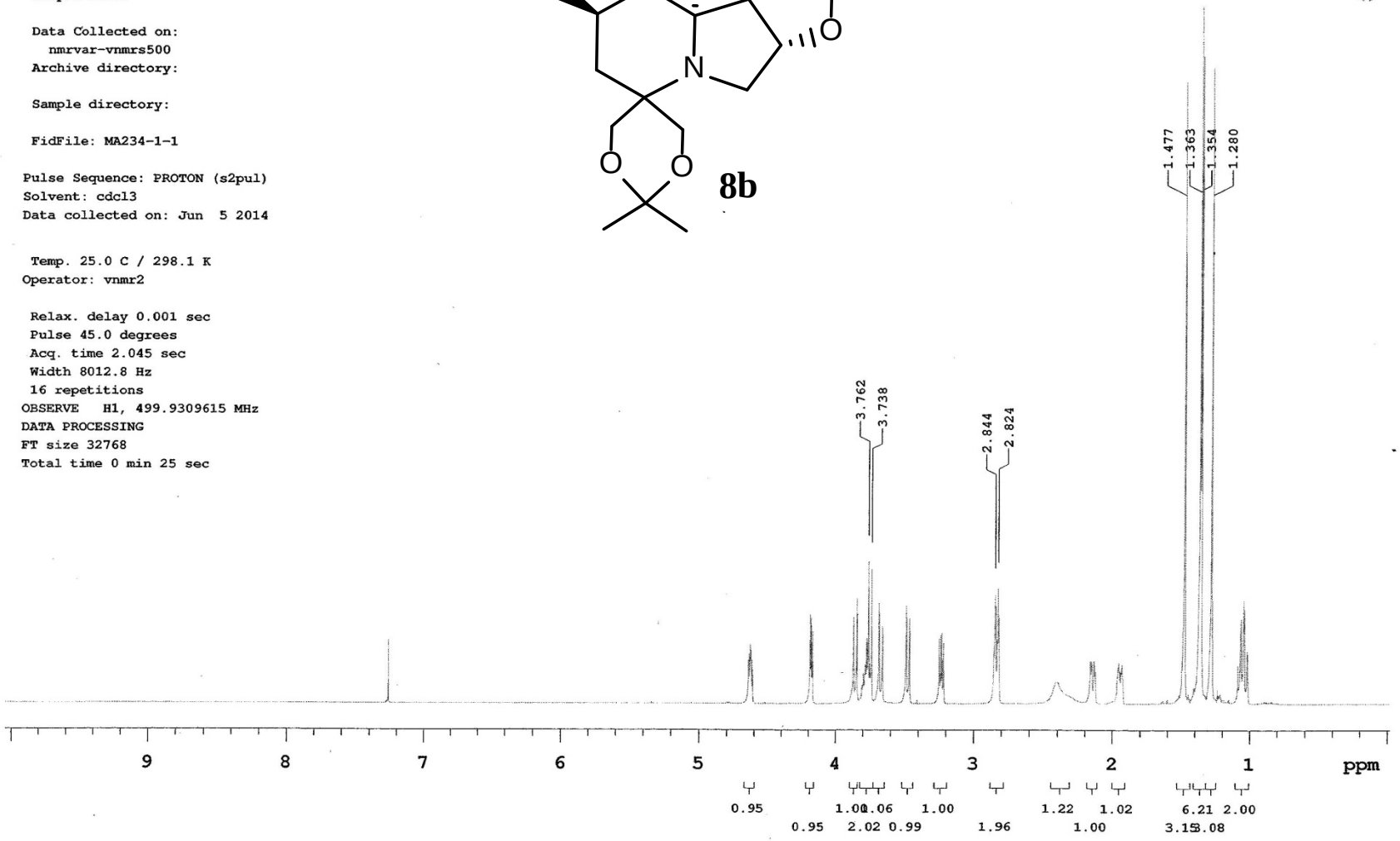
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309615 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



8b

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

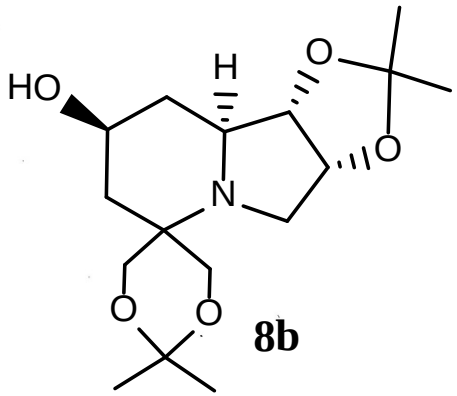
Sample directory:

FidFile: GR046-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 20 2013

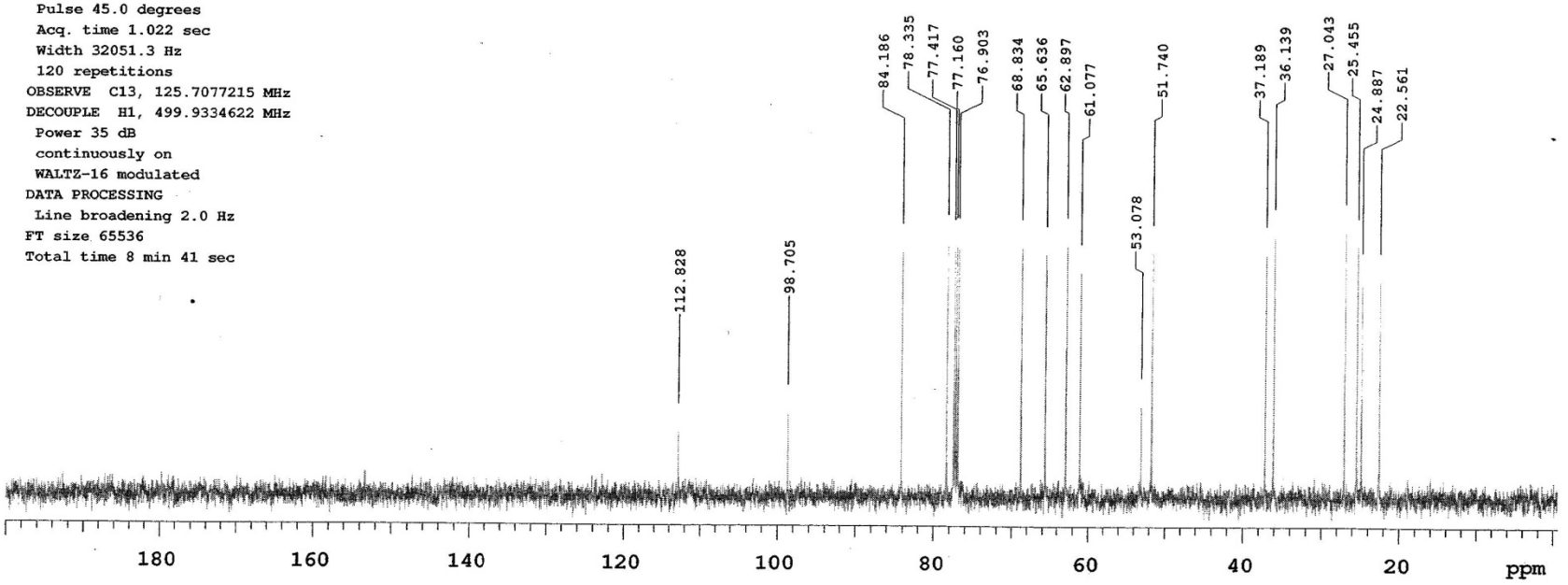
Temp. 25.0 C / 298.1 K
Operator: vnmr2

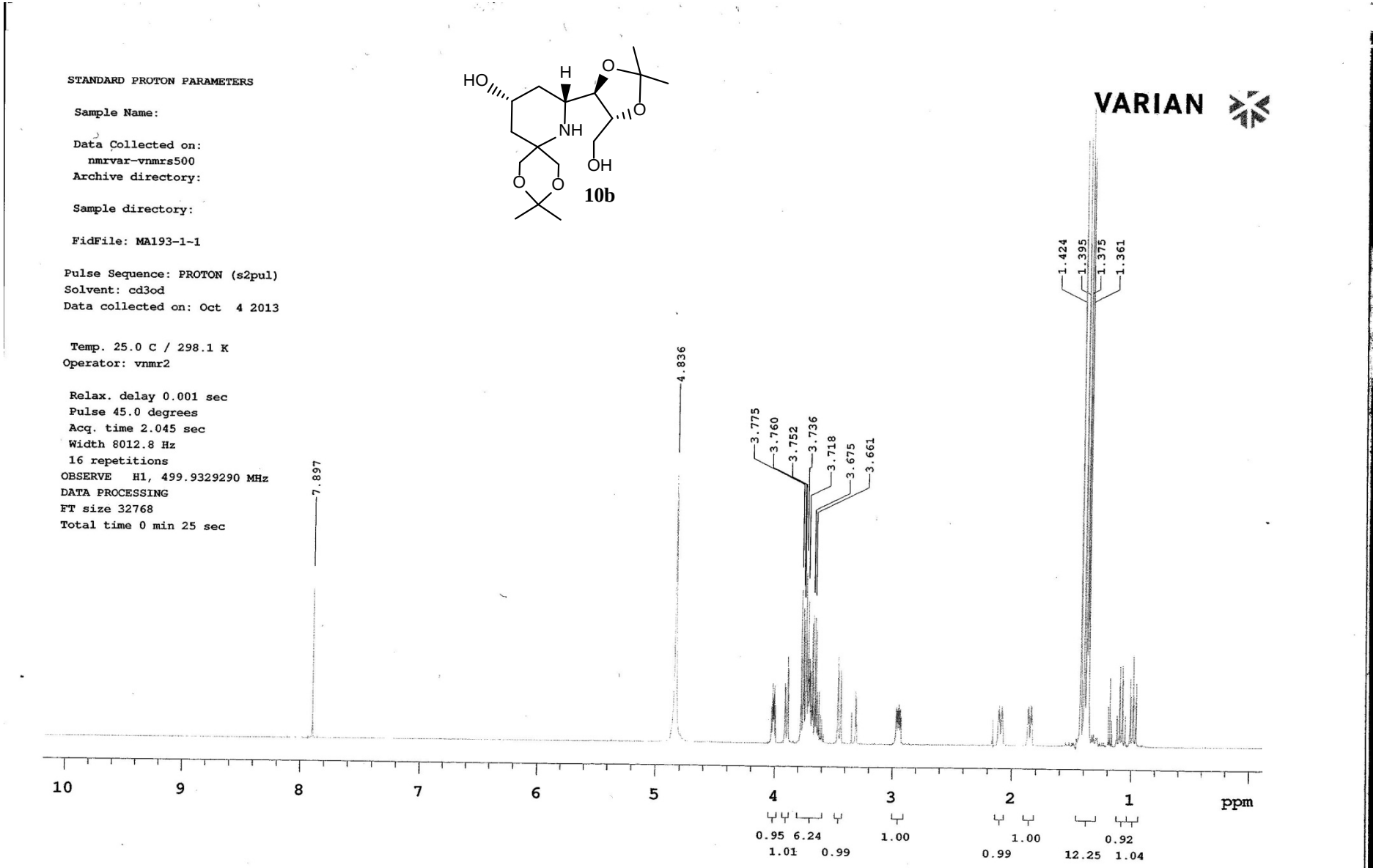
Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
120 repetitions
OBSERVE C13, 125.7077215 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec



8b

VARIAN




STANDARD PROTON PARAMETERS
Sample Name:
Data Collected on:
nmrvar-vnmrs500
Archive directory:
Sample directory:
FidFile: MA193-1-1
Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Oct 4 2013
Temp. 25.0 C / 298.1 K
Operator: vnmr2
Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9329290 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec
HO
H
O
O
NH
OH
O
O
10b
VARIAN
7.897
4.836
3.775
3.760
3.752
3.736
3.718
3.675
3.661
1.424
1.395
1.375
1.361
10
9
8
7
6
5
4
3
2
1
ppm
0.95 6.24
1.01 0.99
1.00
0.99
1.00
0.92
12.25 1.04

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

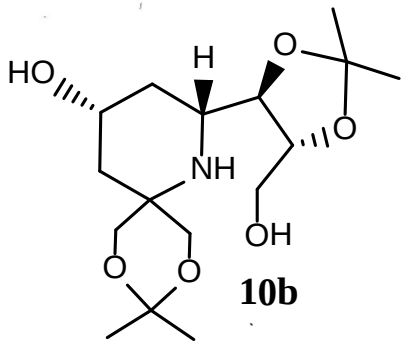
Sample directory:

FidFile: MA193-1-1-c

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Oct 4 2013

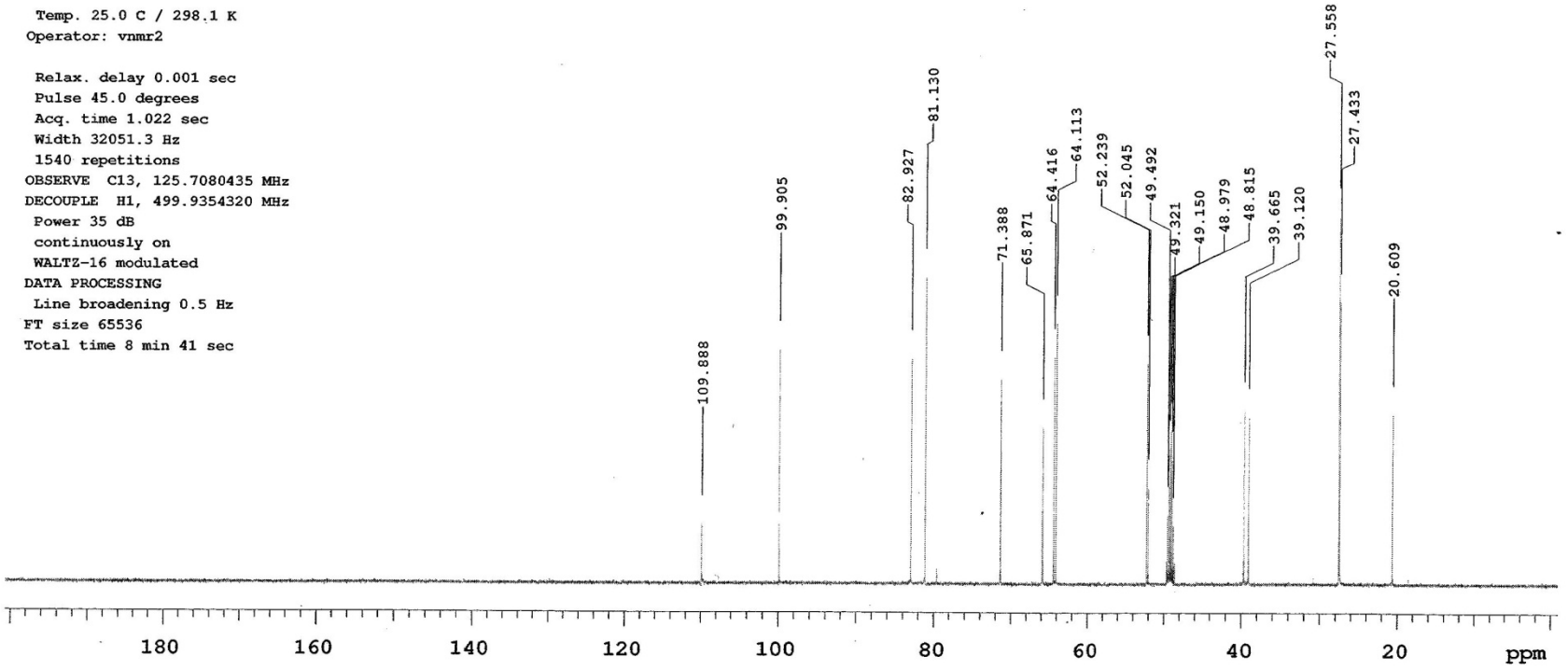
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
1540 repetitions
OBSERVE C13, 125.7080435 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec



10b

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

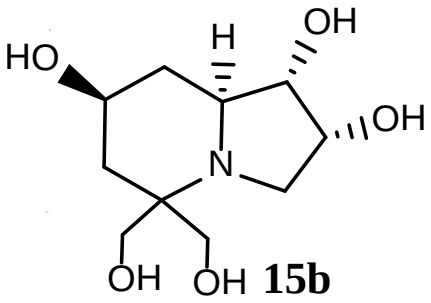
Sample directory:

FidFile: MA-235-2-1

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Jul 14 2014

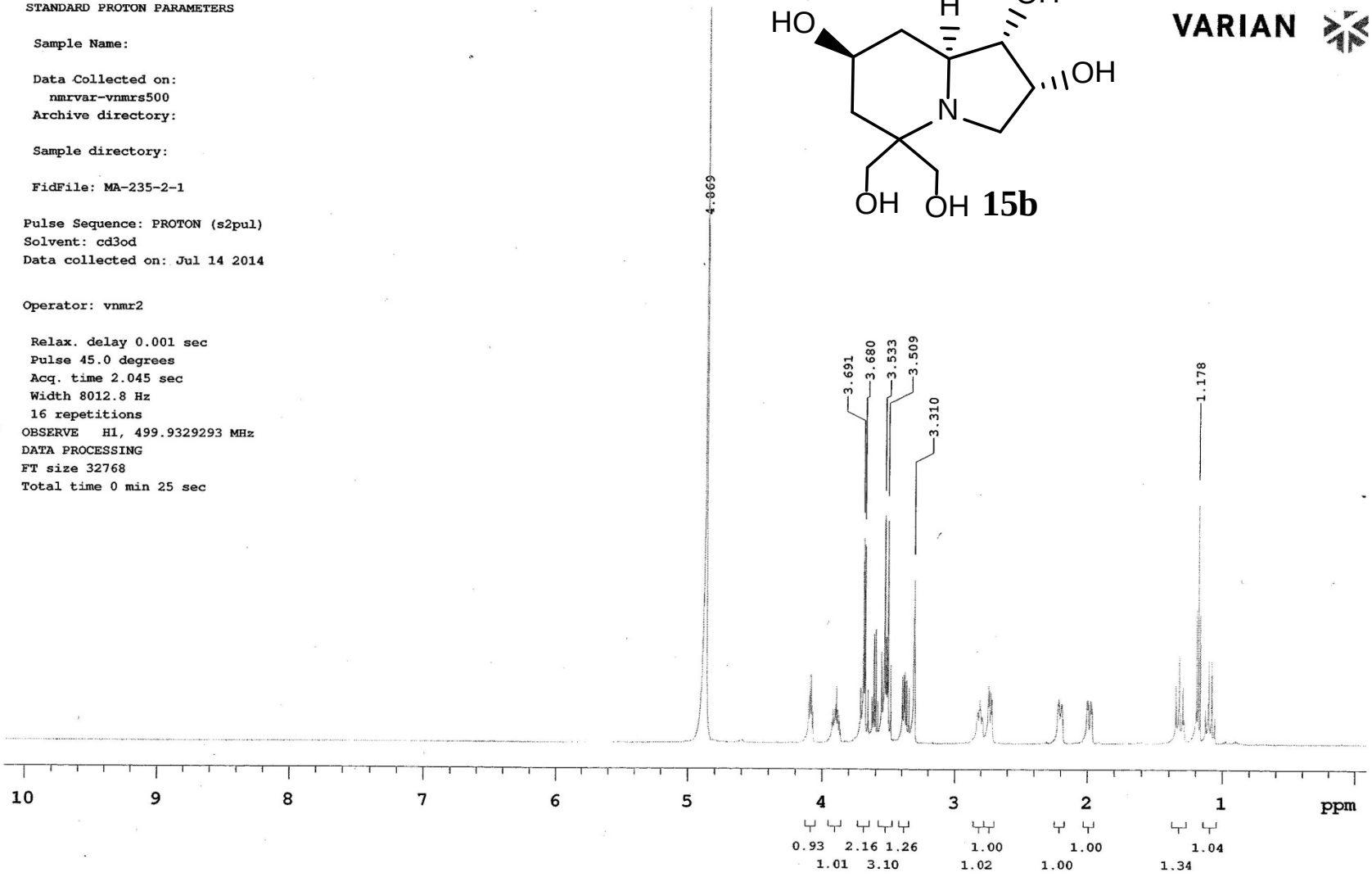
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9329293 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



15b

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

FidFile: MA235-2-1-c

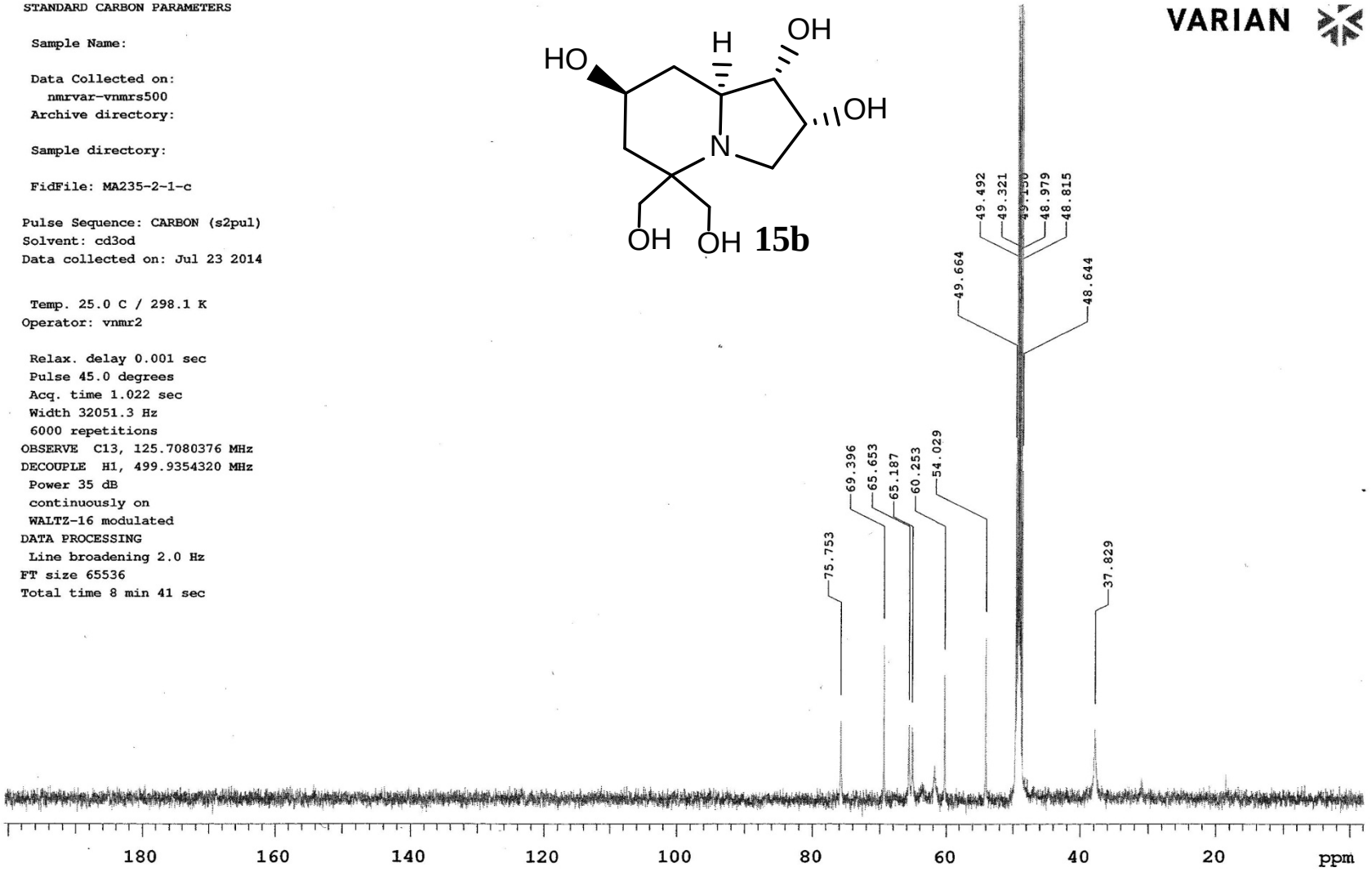
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Jul 23 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
6000 repetitions
OBSERVE C13, 125.7080376 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec

15b

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

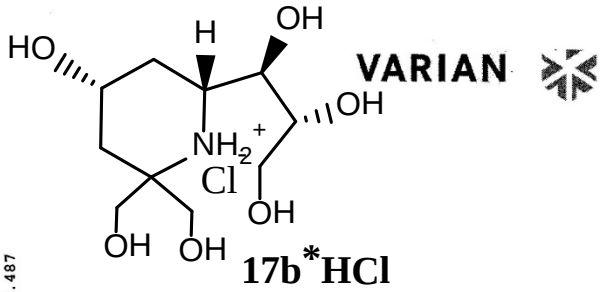
Sample directory:

FidFile: MA260-1-1

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Oct 30 2014

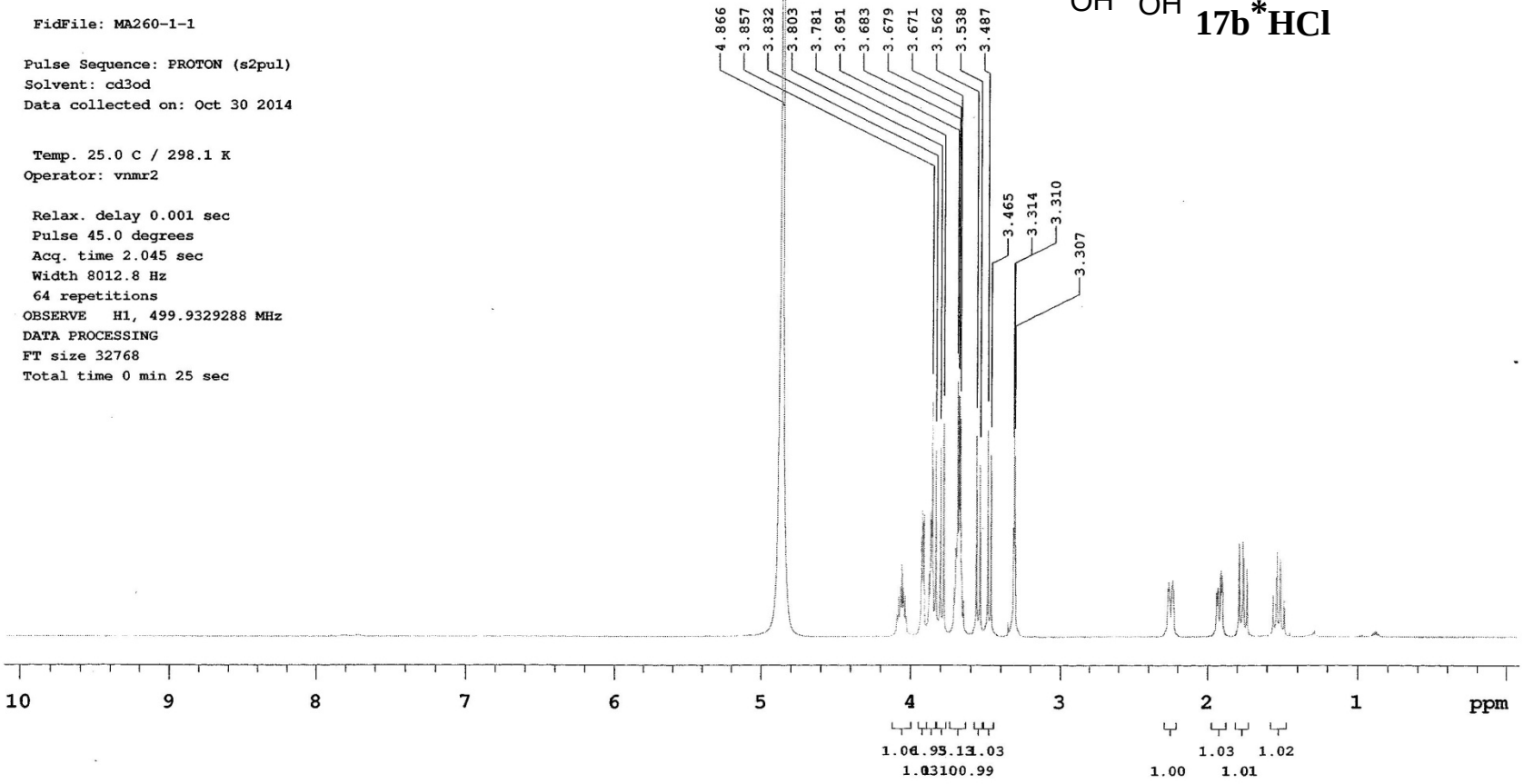
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
64 repetitions
OBSERVE H1, 499.9329288 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



VARIAN

17b*HCl



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

FidFile: MA260-1-1-c

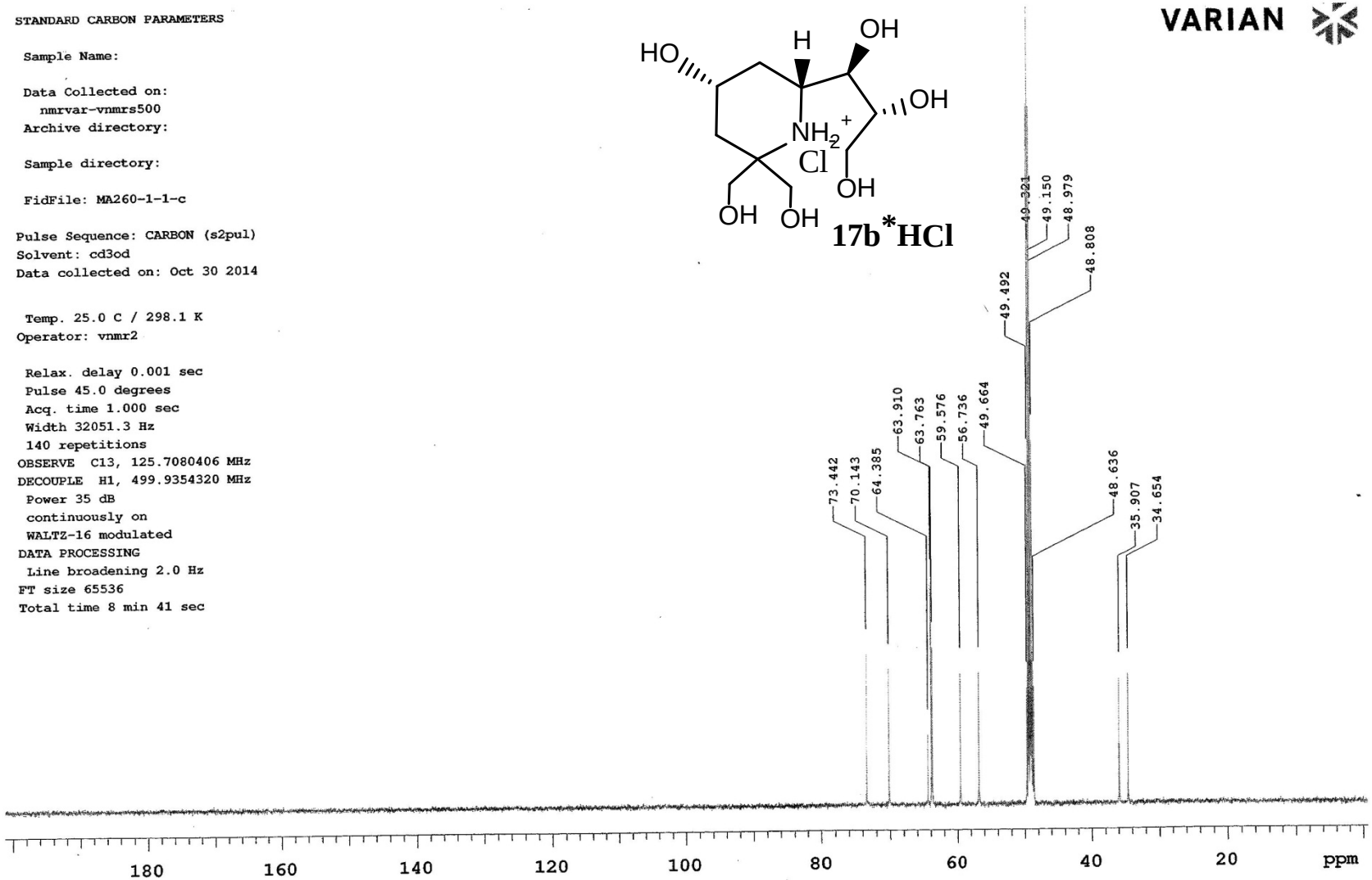
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Oct 30 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.000 sec
Width 32051.3 Hz
140 repetitions
OBSERVE C13, 125.7080406 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec

17b*HCl

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

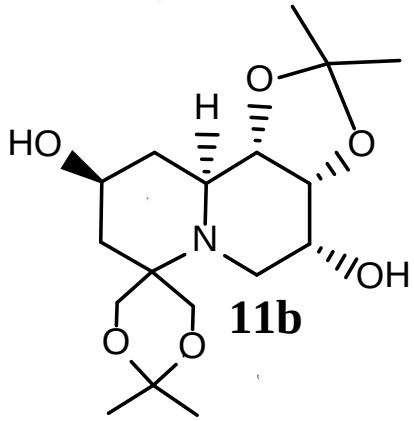
Sample directory:

FidFile: MA219-2-1

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 5 2014

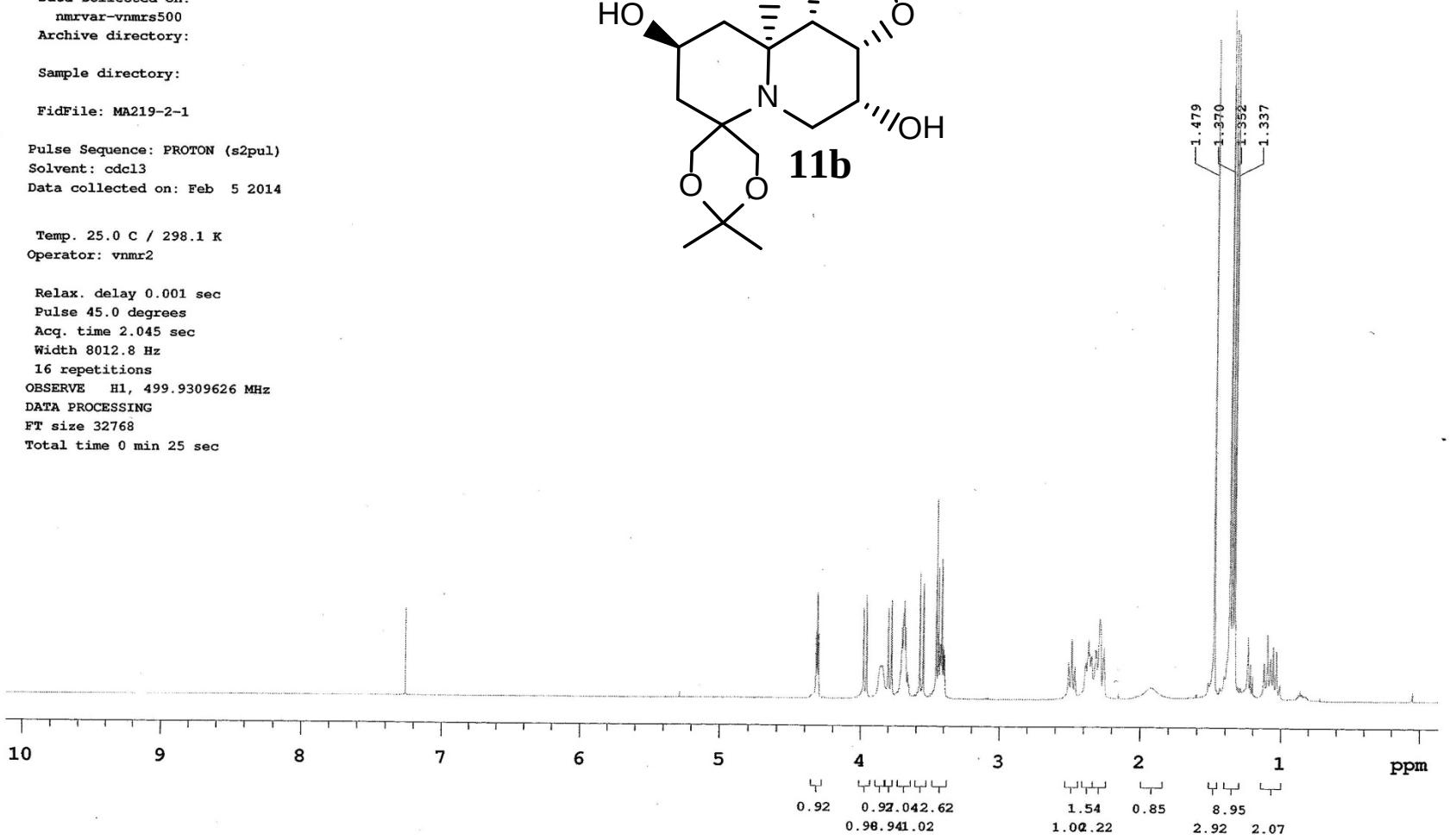
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309626 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



11b

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

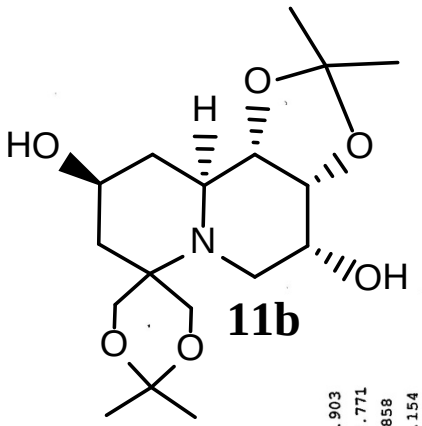
Sample directory:

FidFile: MA219-2-1-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 5 2014

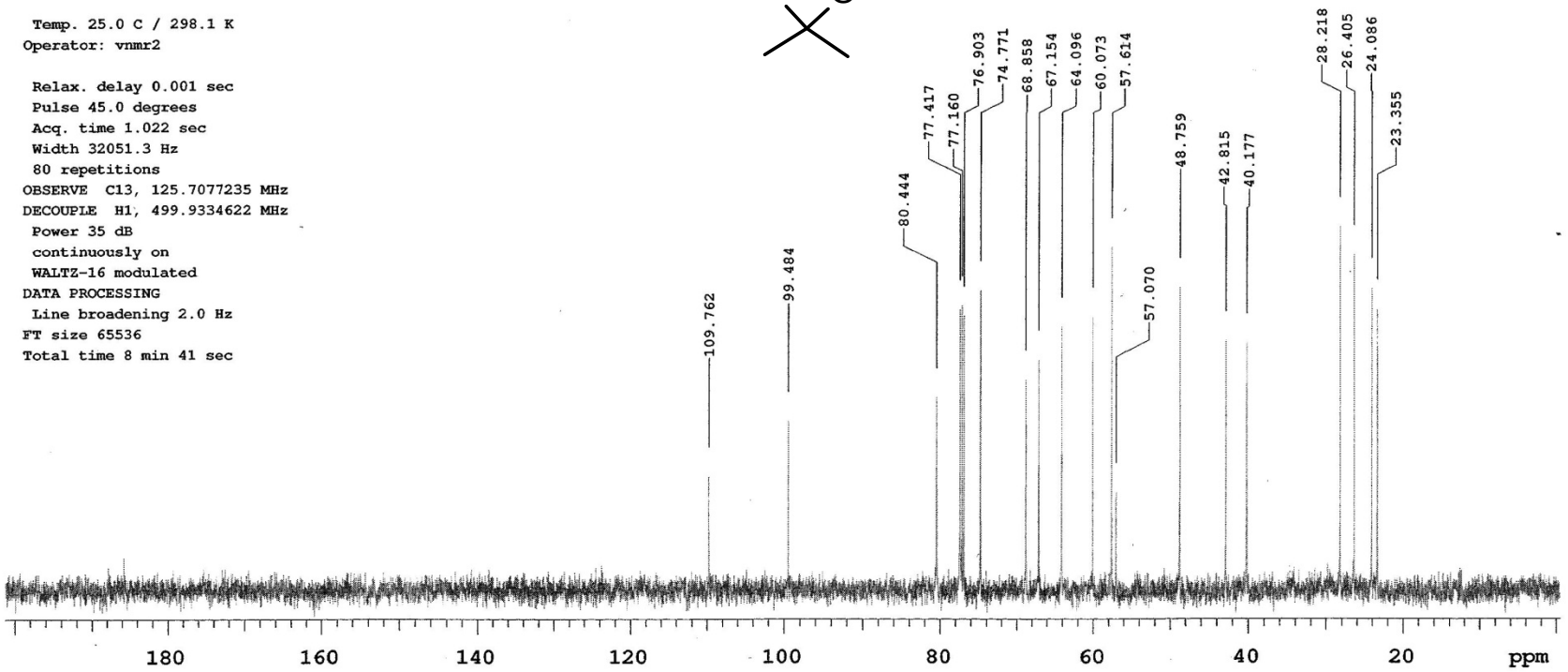
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
80 repetitions
OBSERVE C13, 125.7077235 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec



11b

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

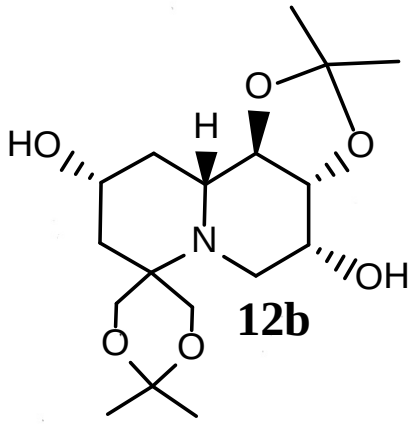
Sample directory:

FidFile: MA221-2-1

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 10 2014

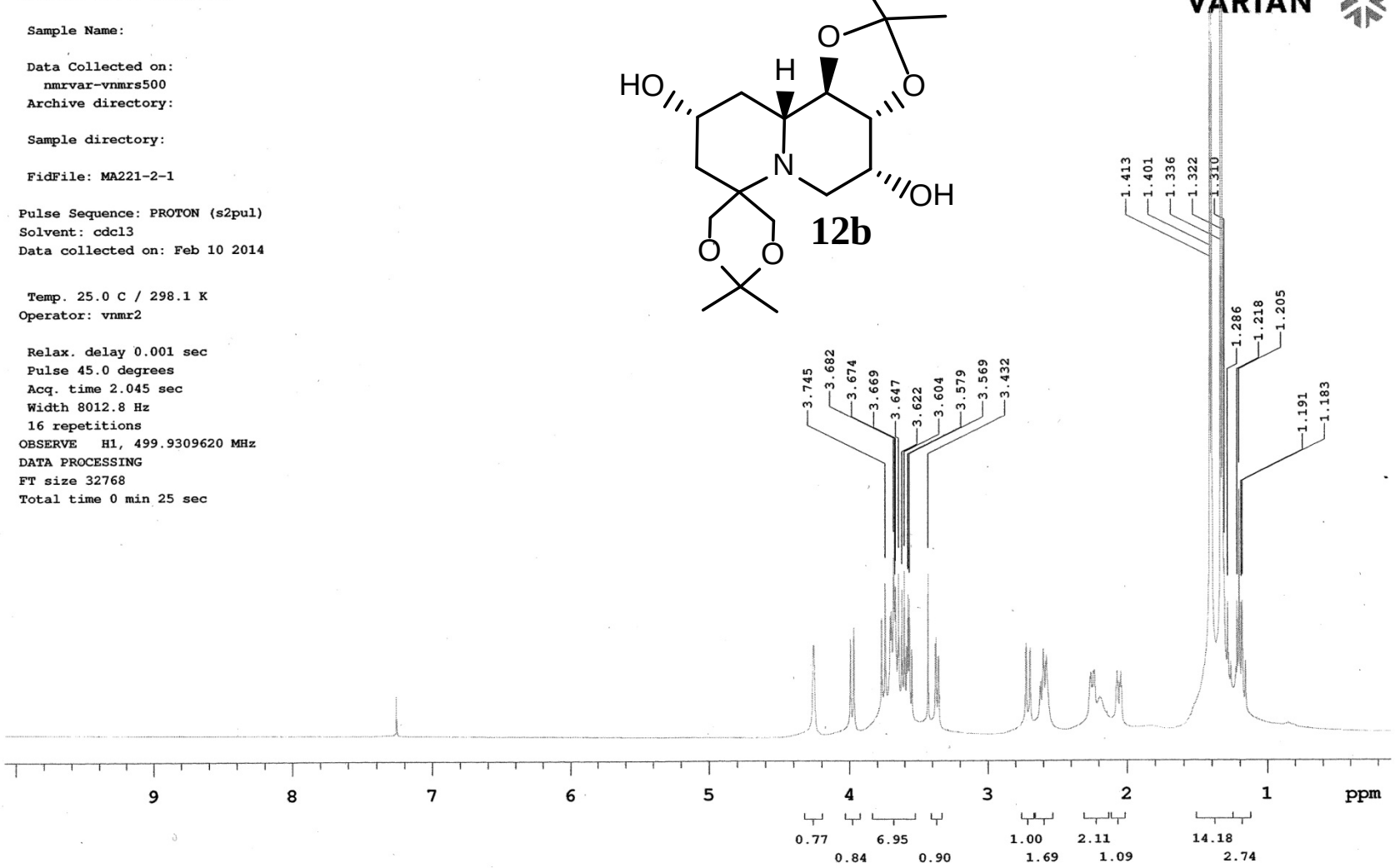
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309620 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



12b

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

FidFile: MA215-1-1a-c

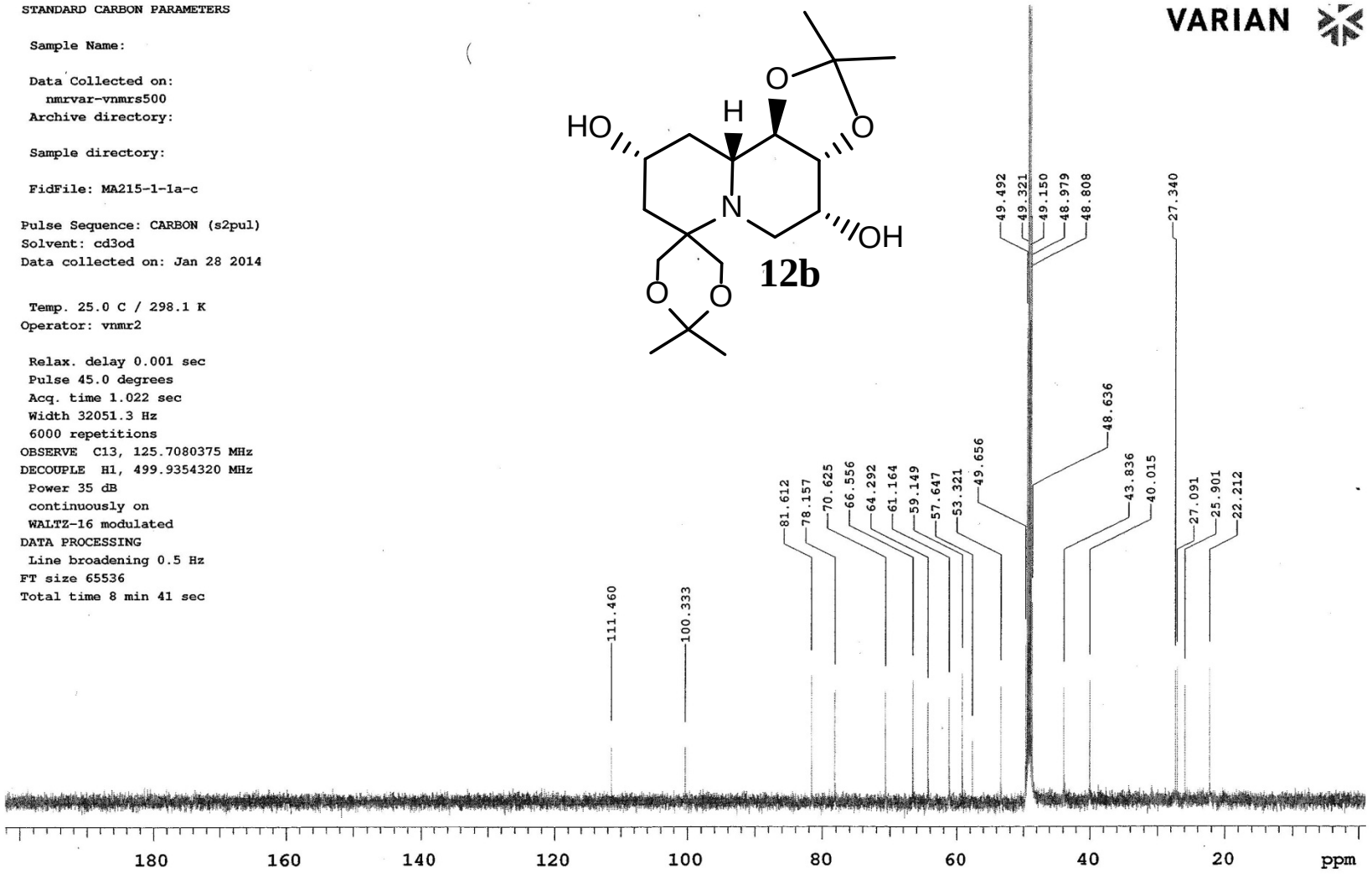
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Jan 28 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
6000 repetitions
OBSERVE C13, 125.7080375 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec

12b

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

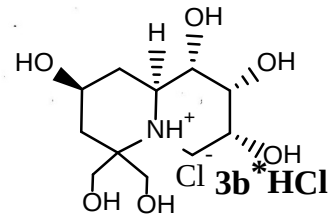
Sample directory:

FidFile: MA228-3-1

Pulse Sequence: PRESAT
Solvent: d2o
Data collected on: Apr 24 2014

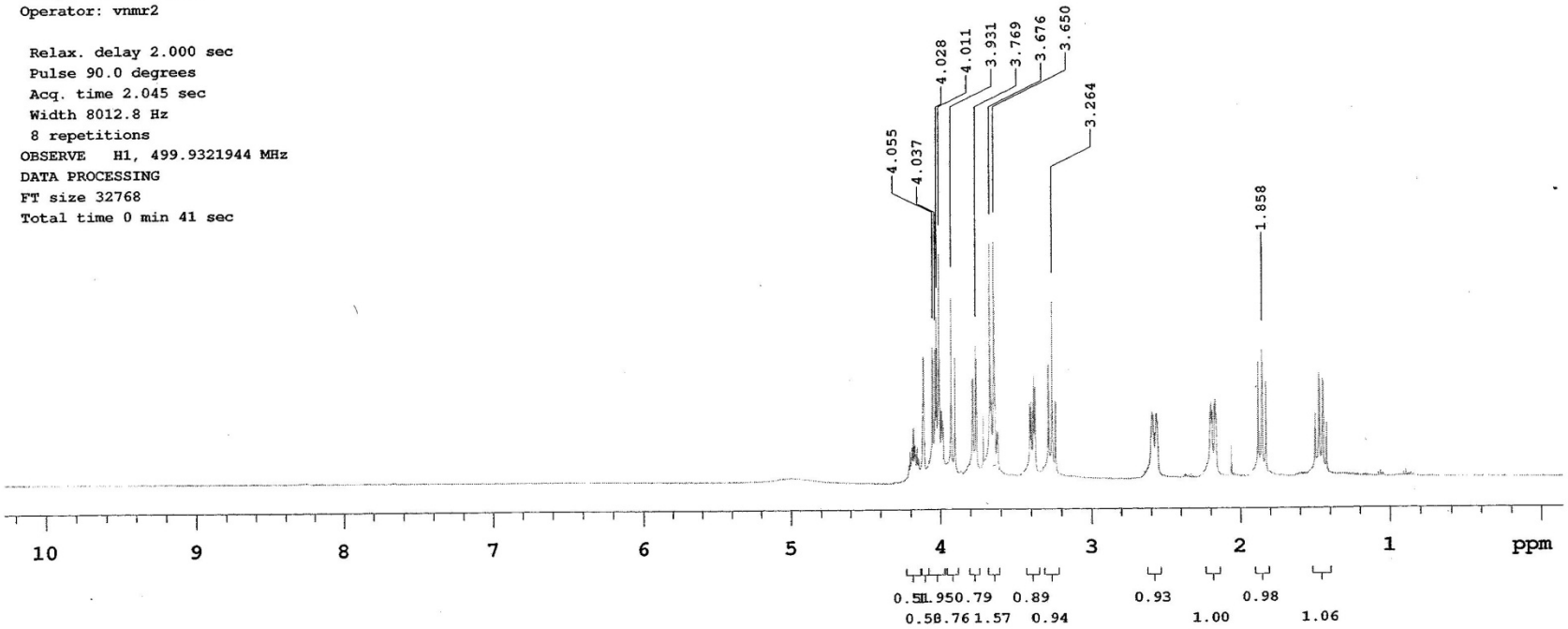
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.9321944 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 41 sec



3b*HCl

VARIAN



STANDARD PROTON PARAMETERS

Sample Name: nd228-4-1

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

FidFile: PROTON

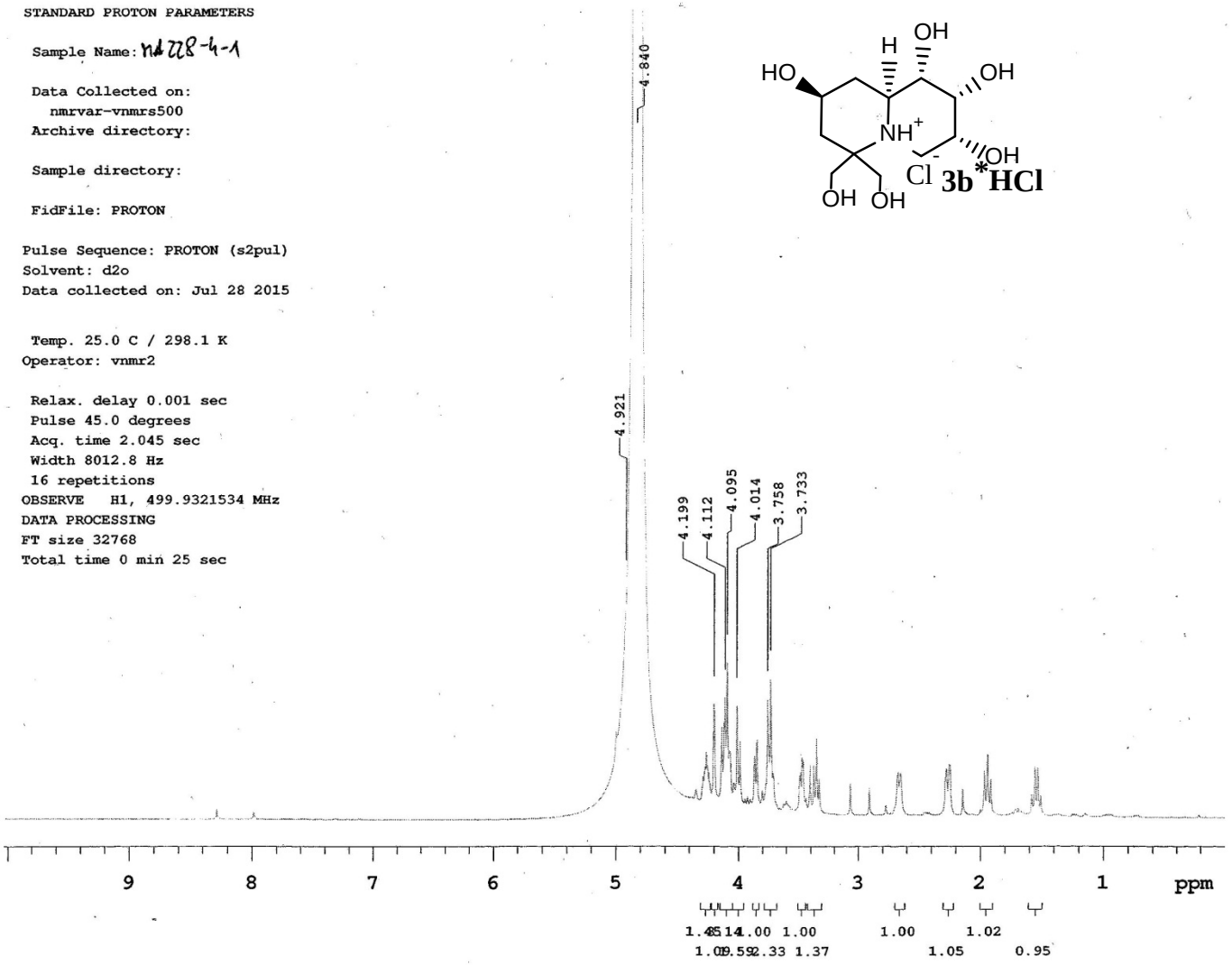
Pulse Sequence: PROTON (s2pul)
Solvent: d2o
Data collected on: Jul 28 2015

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9321534 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

3b*HCl

VARIAN



VARIAN

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

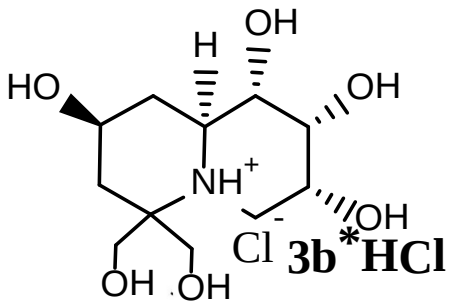
Sample directory:

FidFile: MA228-3-1-c

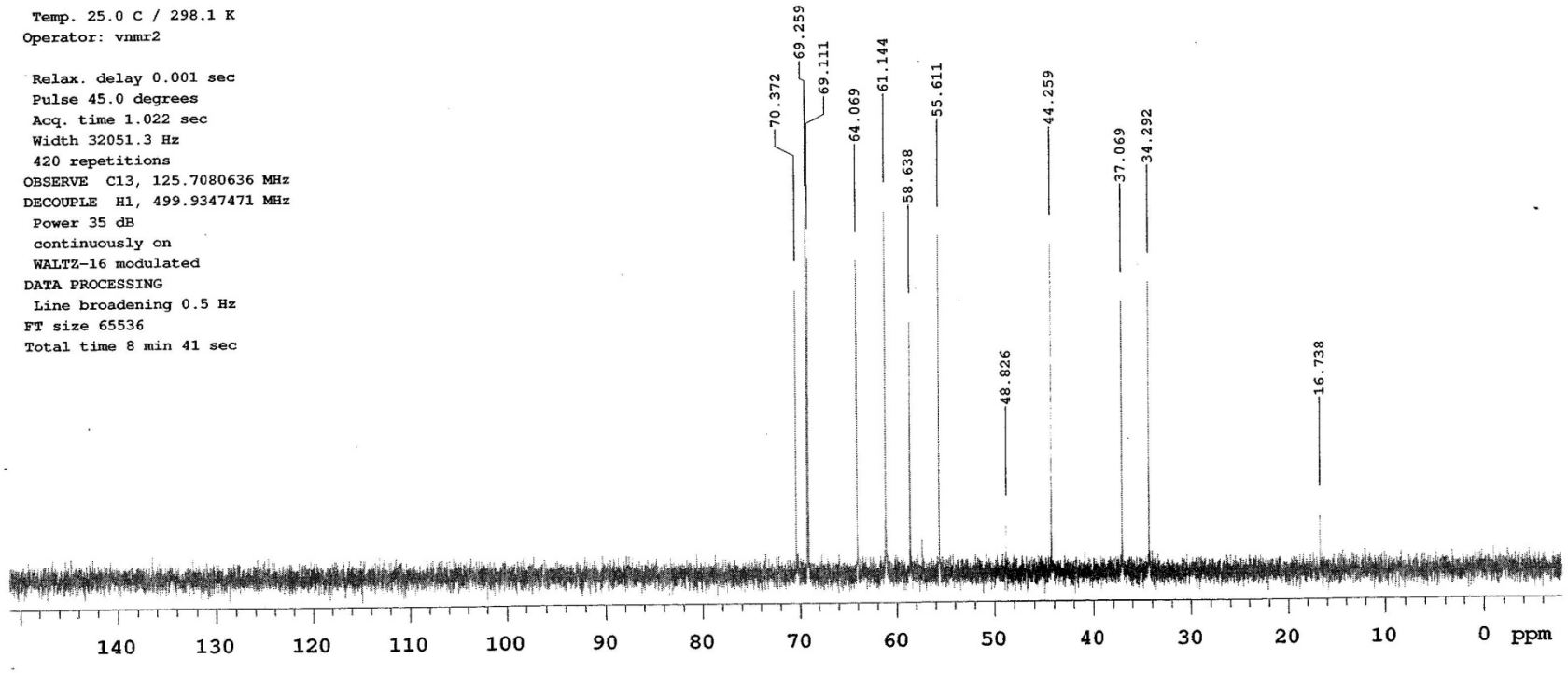
Pulse Sequence: CARBON (s2pul)
Solvent: d2o
Data collected on: Mar 28 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
420 repetitions
OBSERVE C13, 125.7080636 MHz
DECOUPLE H1, 499.9347471 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec



3b*HCl



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

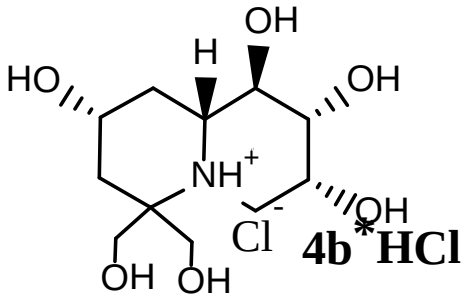
Sample directory:

FidFile: NA229-1-1-a

Pulse Sequence: PRESAT
Solvent: d2o
Data collected on: Apr 30 2014

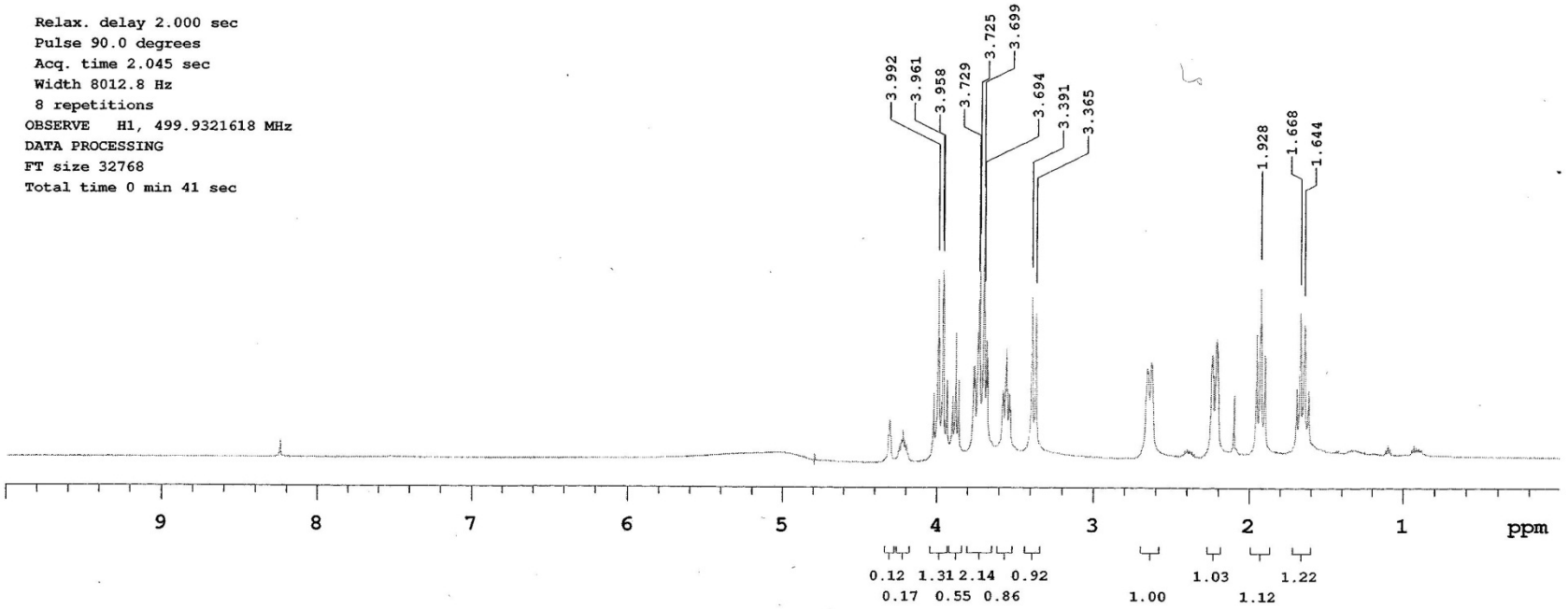
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.9321618 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 41 sec



4b*HCl

VARIAN



STANDARD PROTON PARAMETERS

Sample Name: HA228-5-1

Data Collected on:
nmrvar-vnmrs500
Archive directory:

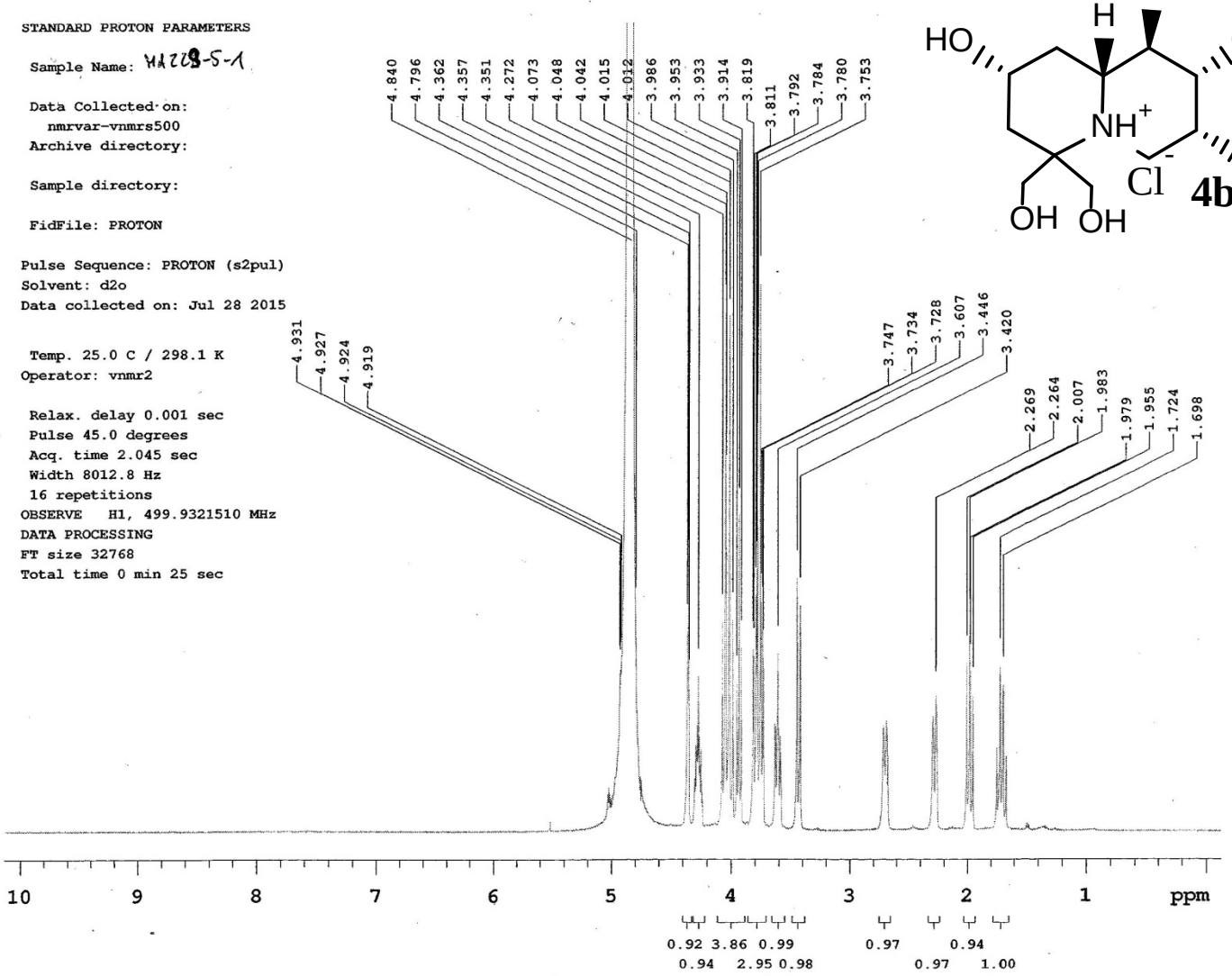
Sample directory:

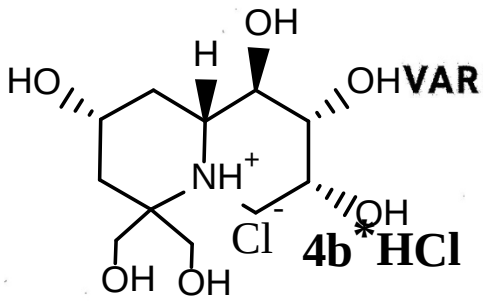
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: d2o
Data collected on: Jul 28 2015

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9321510 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec





4b*HCl

VARIAN

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

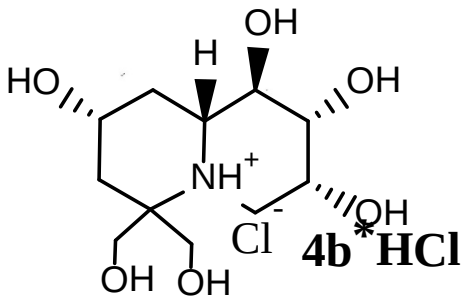
Sample directory:

FidFile: MA229-1-1-a-c

Pulse Sequence: CARBON (s2pul)
Solvent: d2o
Data collected on: Apr 30 2014

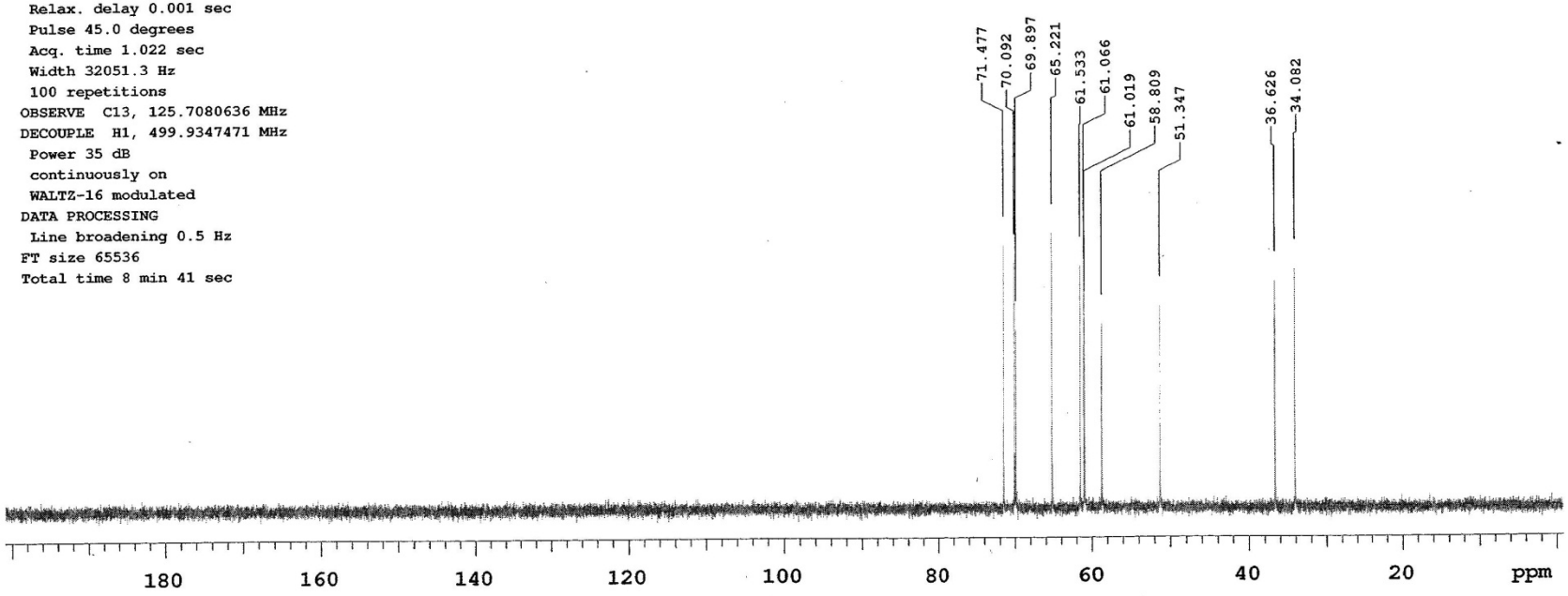
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
100 repetitions
OBSERVE C13, 125.7080636 MHz
DECOUPLE H1, 499.9347471 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec



4b*HCl

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

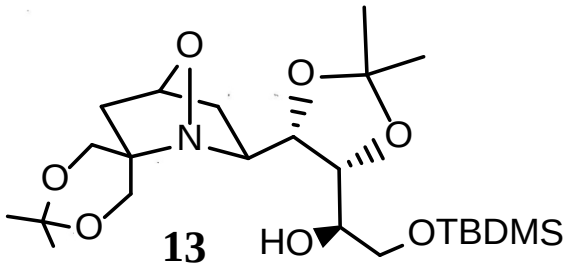
Sample directory:

FidFile: MA180-1-1

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 26 2013

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309610 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



13

VARIAN

7.260
4.798
3.937
3.822
3.817
3.521
3.497
1.486
1.429
1.349
1.315
1.139
1.116
0.918
0.913
0.907
0.086
0.080

10 9 8 7 6 5 4 3 2 1 ppm

0.89 0.90 0.95 1.98 2.73 2.41 2.03 1.00 2.93 3.14 3.16 1.16 5.47 9.52 5.44

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

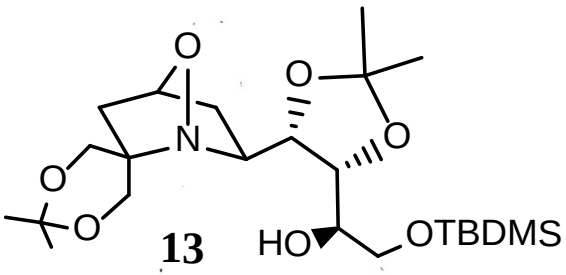
FidFile: MA180-1-1-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 26 2013

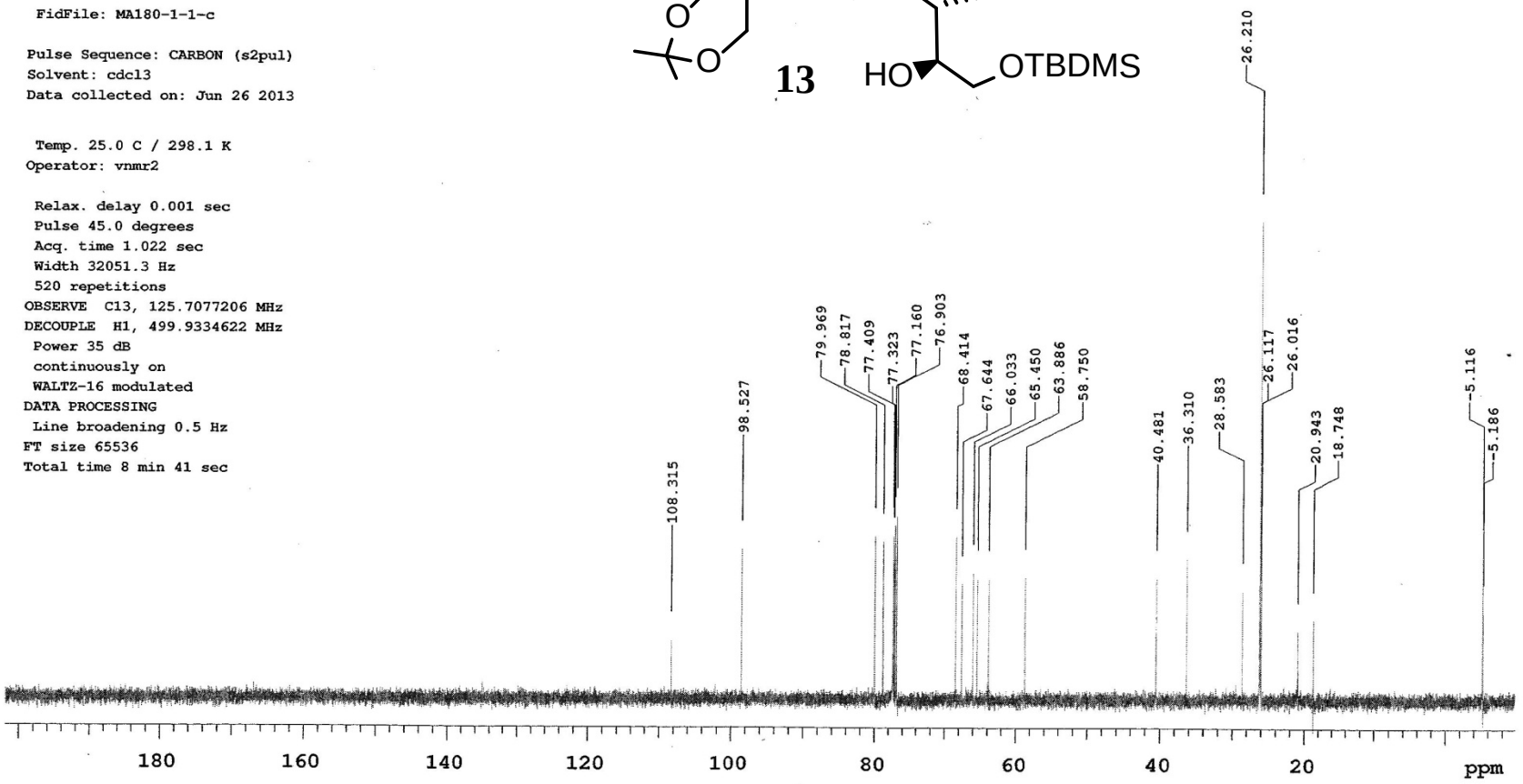
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
520 repetitions
OBSERVE C13, 125.7077206 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec

VARIAN



13



~~GR042_MPLC~~

STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

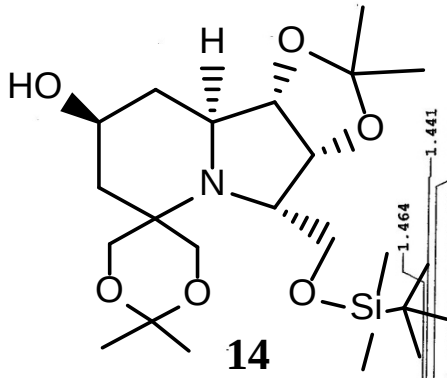
Sample directory:

FidFile: PROTON

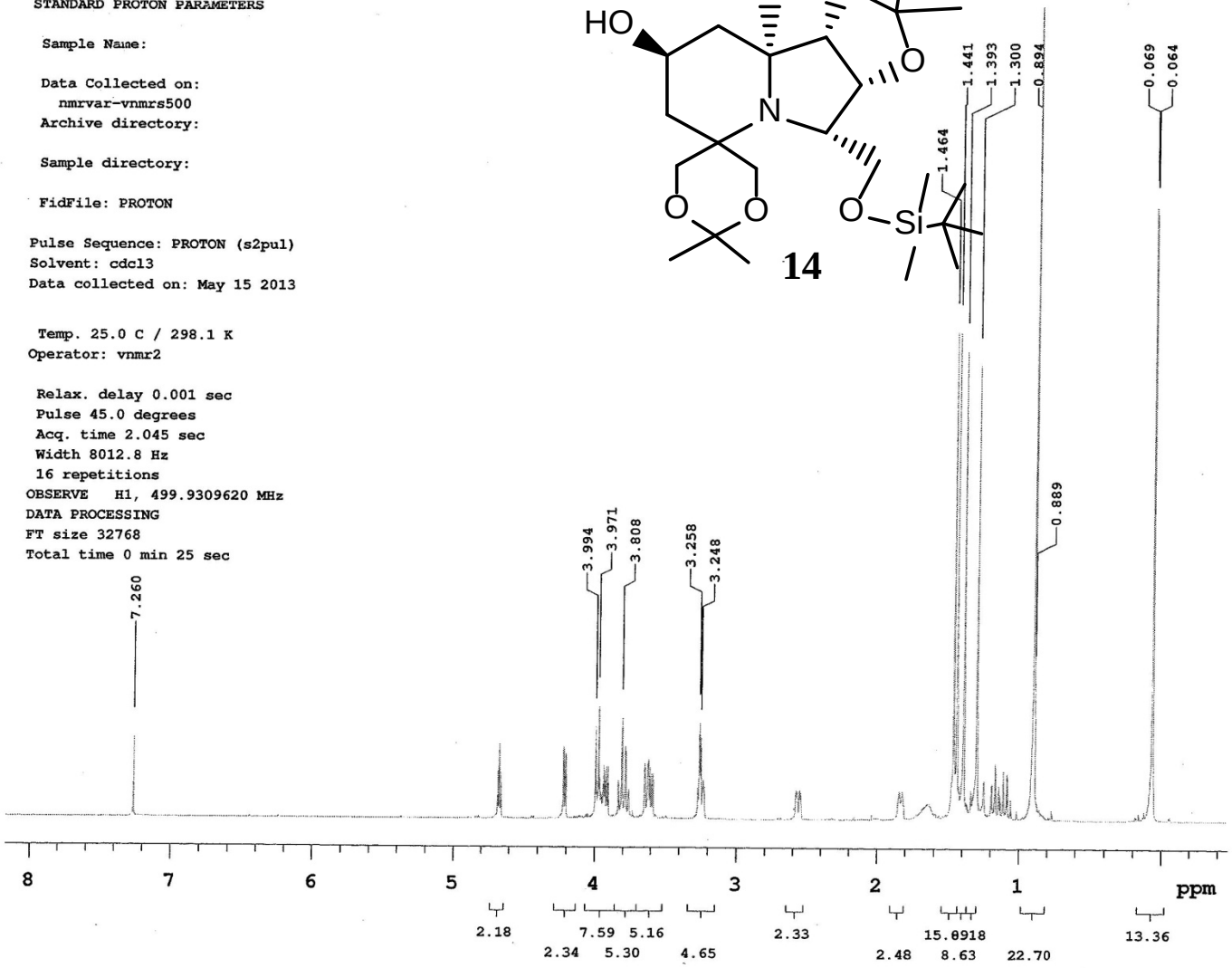
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 15 2013

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9309620 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



14



VARIAN

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

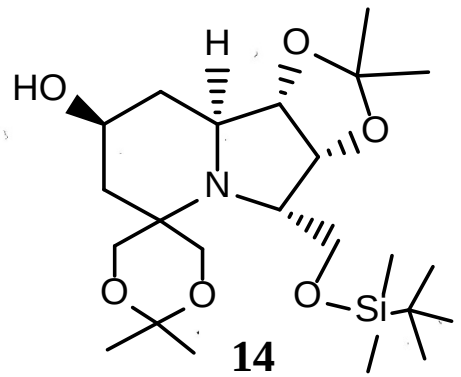
Sample directory:

FidFile: GR042-MPLC-c

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 15 2013

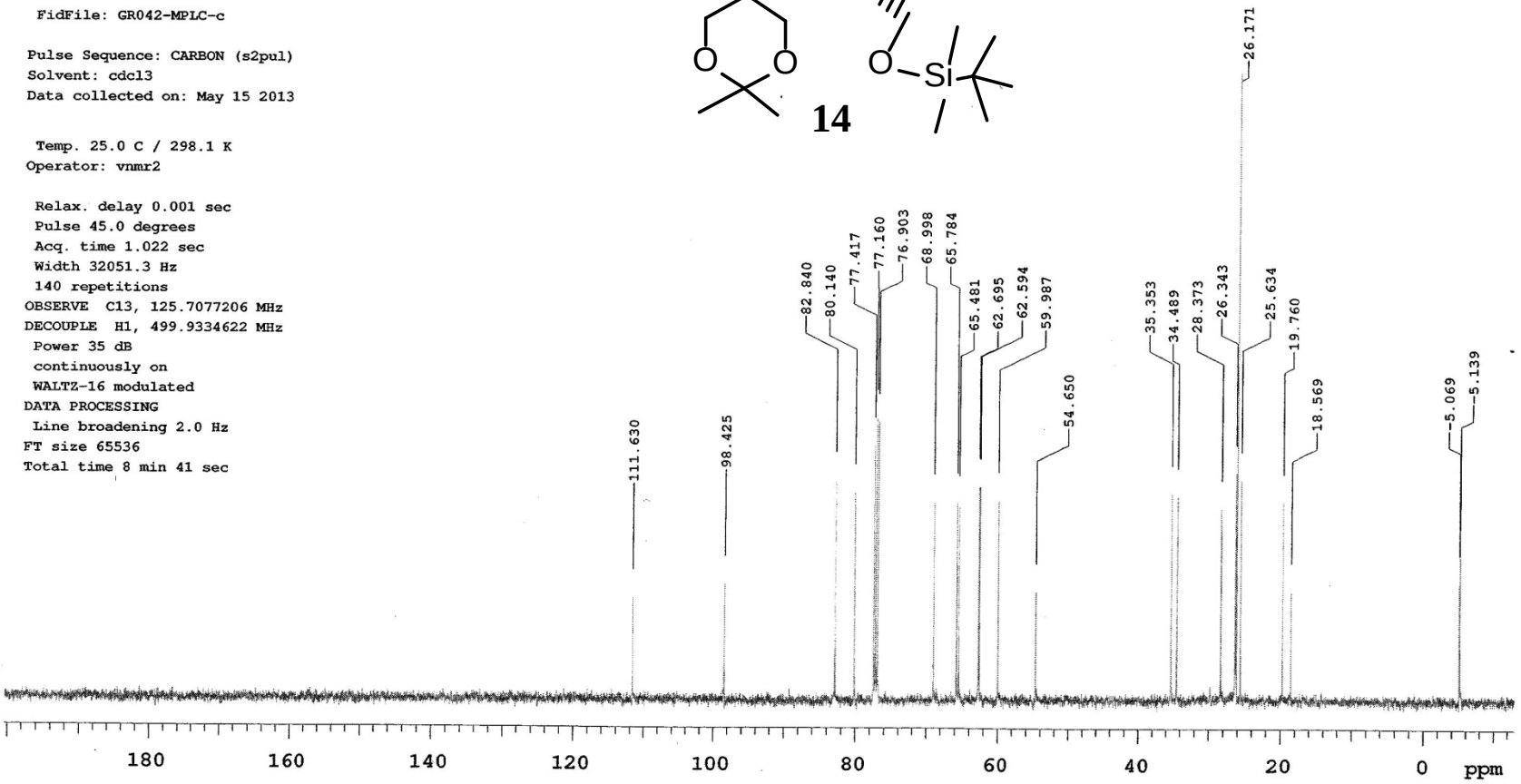
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
140 repetitions
OBSERVE C13, 125.7077206 MHz
DECOUPLE H1, 499.9334622 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec



14

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

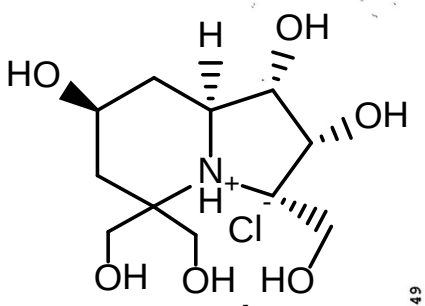
Sample directory:

FidFile: RE043-2

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Apr 28 2014

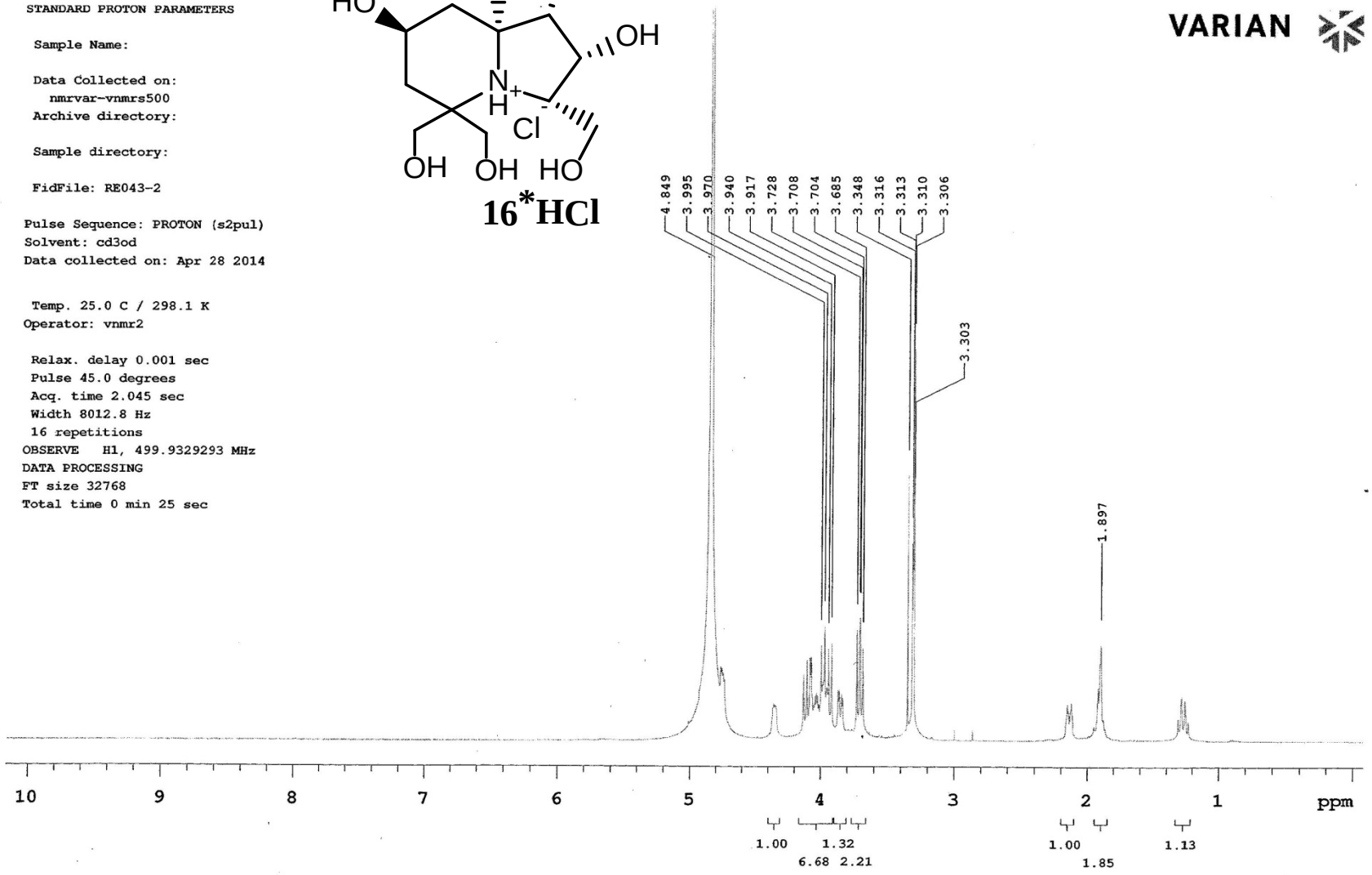
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9329293 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



16*HCl

VARIAN



Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

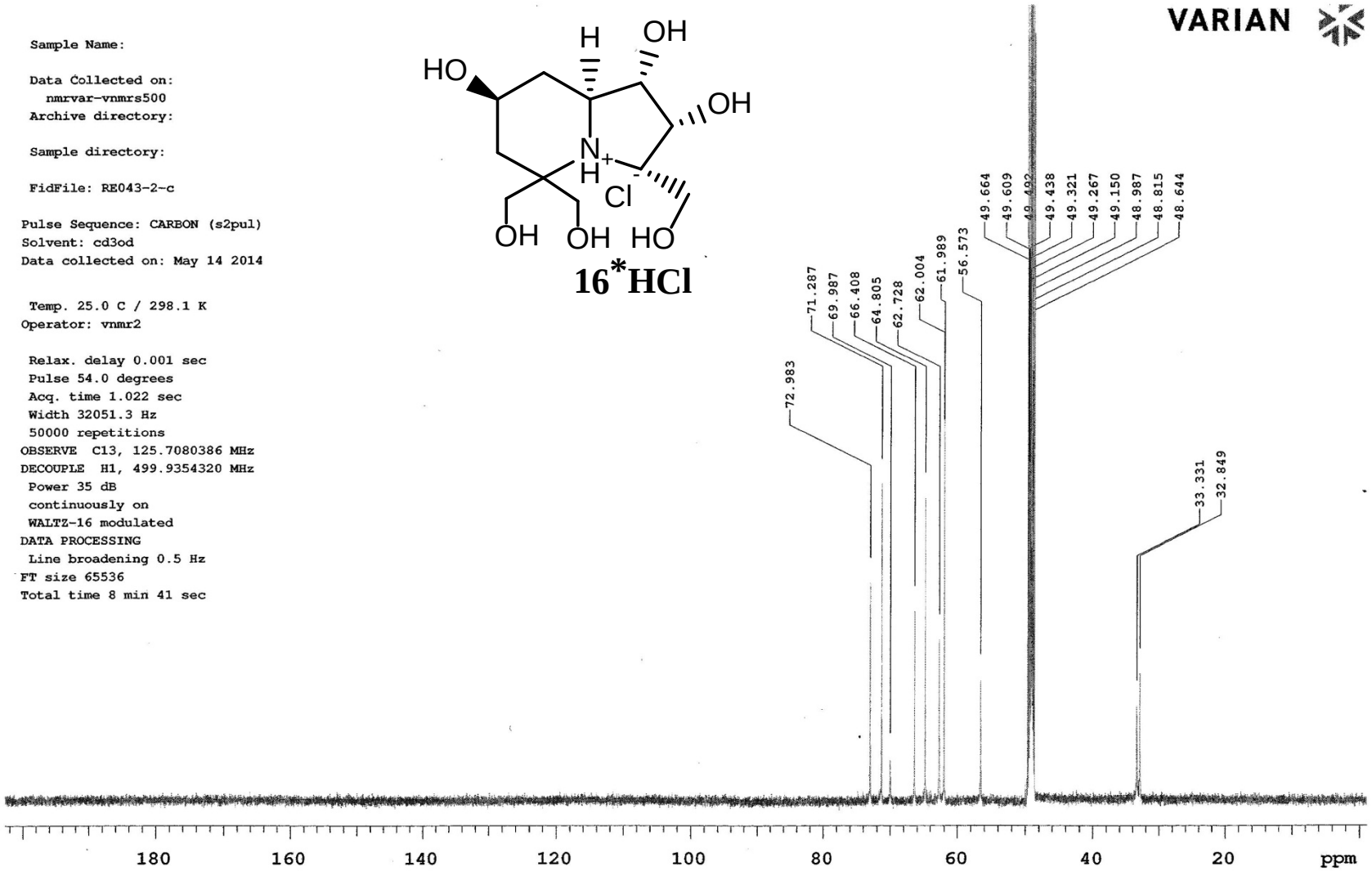
FidFile: RE043-2-c

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: May 14 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 54.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
50000 repetitions
OBSERVE C13, 125.7080386 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec

16*HCl



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

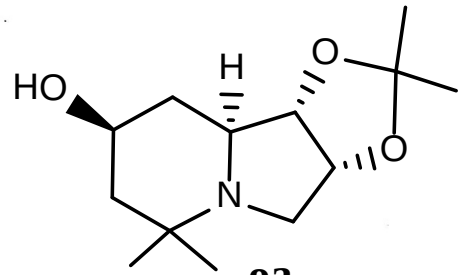
Sample directory:

FidFile: SELRE-04

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Jun 18 2013

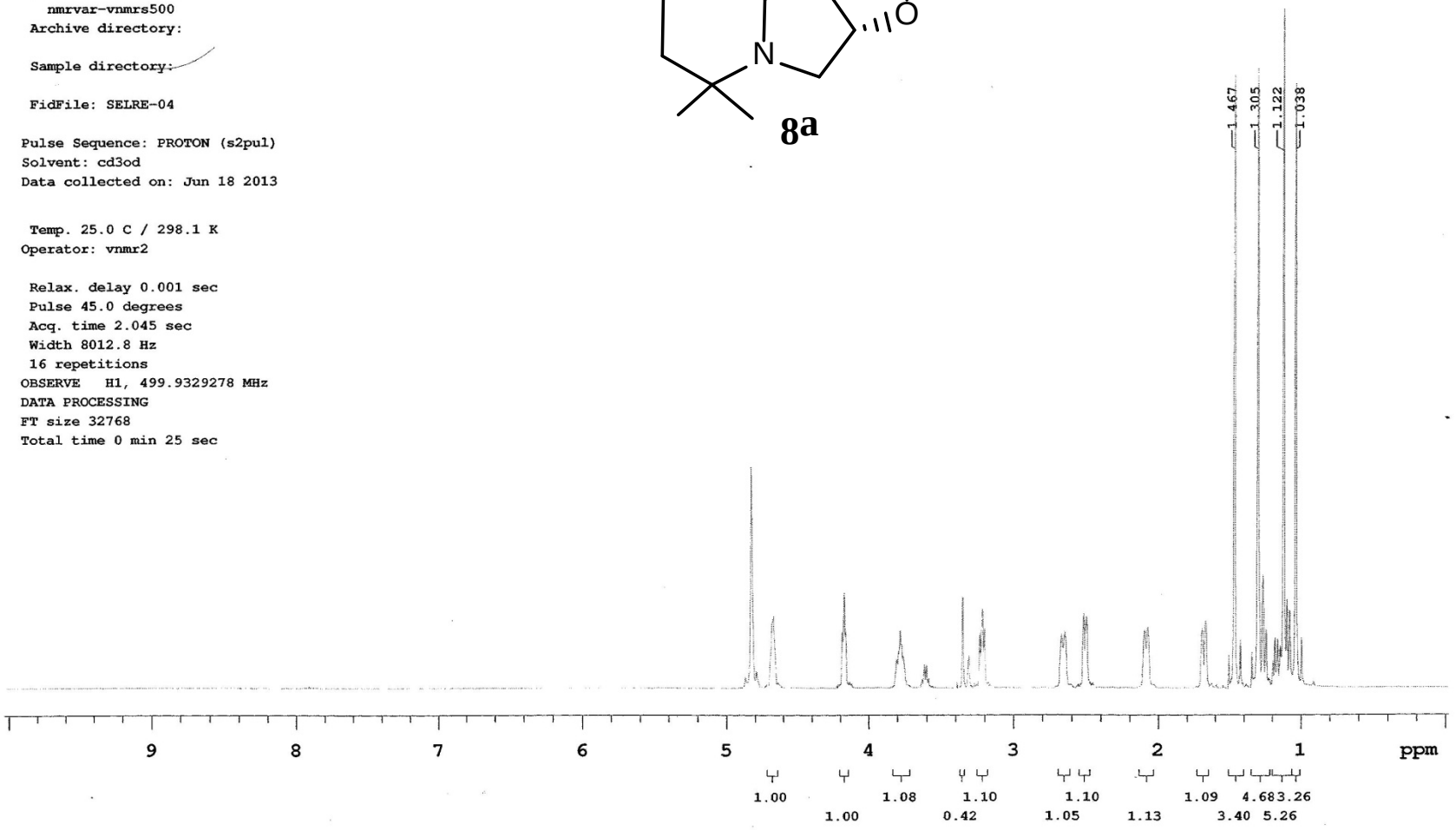
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9329278 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



8a

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

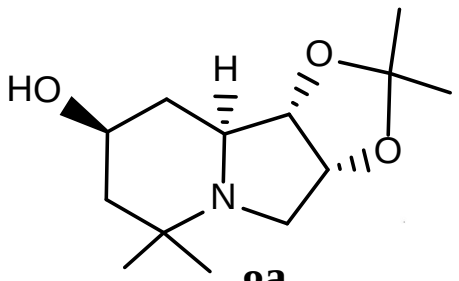
Sample directory:

FidFile: SELRE04-c

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Jun 21 2013

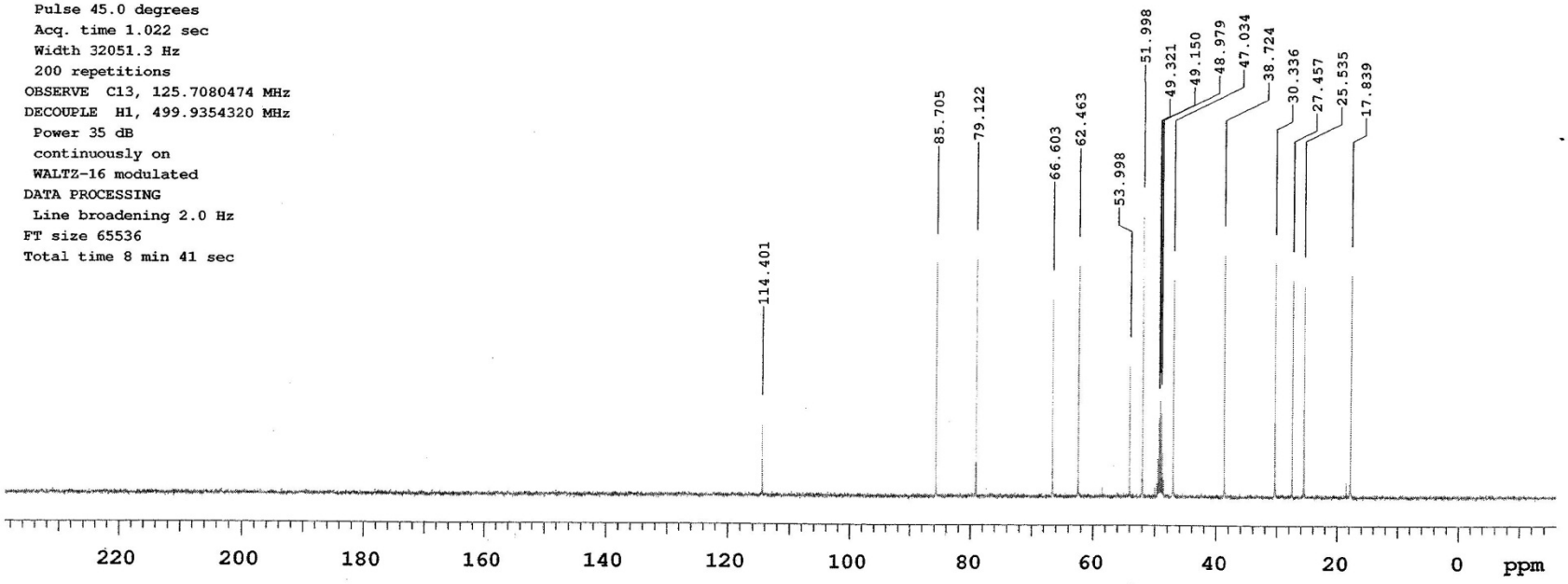
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
200 repetitions
OBSERVE C13, 125.7080474 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec



8a

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

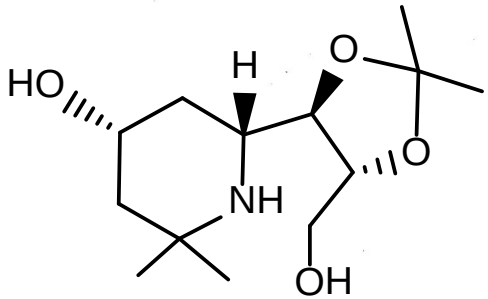
Sample directory:

FidFile: SELRE02B

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Jun 24 2013

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9329293 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



10a

VARIAN

4.851
3.710
3.688
3.680
3.597
3.587
3.573
3.317
3.313
3.310
3.307
3.303
1.382
1.375
1.360
1.170
1.132
1.111

9 8 7 6 5 4 3 2 1 ppm

1.09 0.91 2.36 5 2.01
1.00
1.02
1.11
6.58
8.84

STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

FidFile: SELRE02B-c

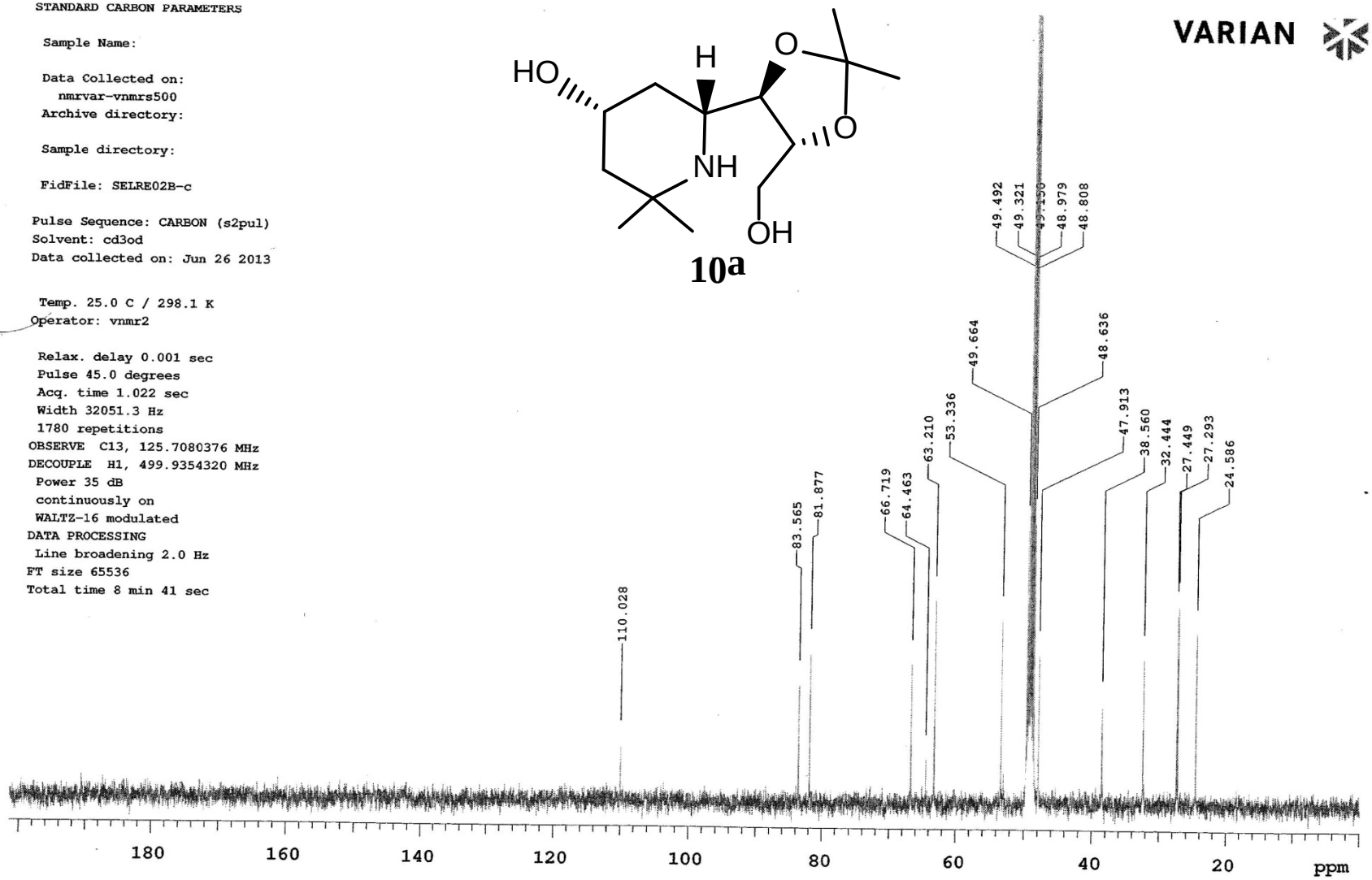
Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Jun 26 2013

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
1780 repetitions
OBSERVE C13, 125.7080376 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 8 min 41 sec

10a

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

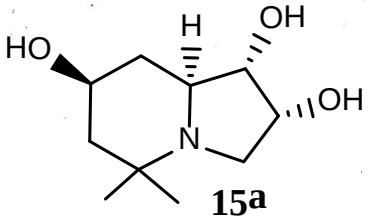
Sample directory:

FidFile: RE044-1

Pulse Sequence: PRESAT
Solvent: d2o
Data collected on: May 23 2014

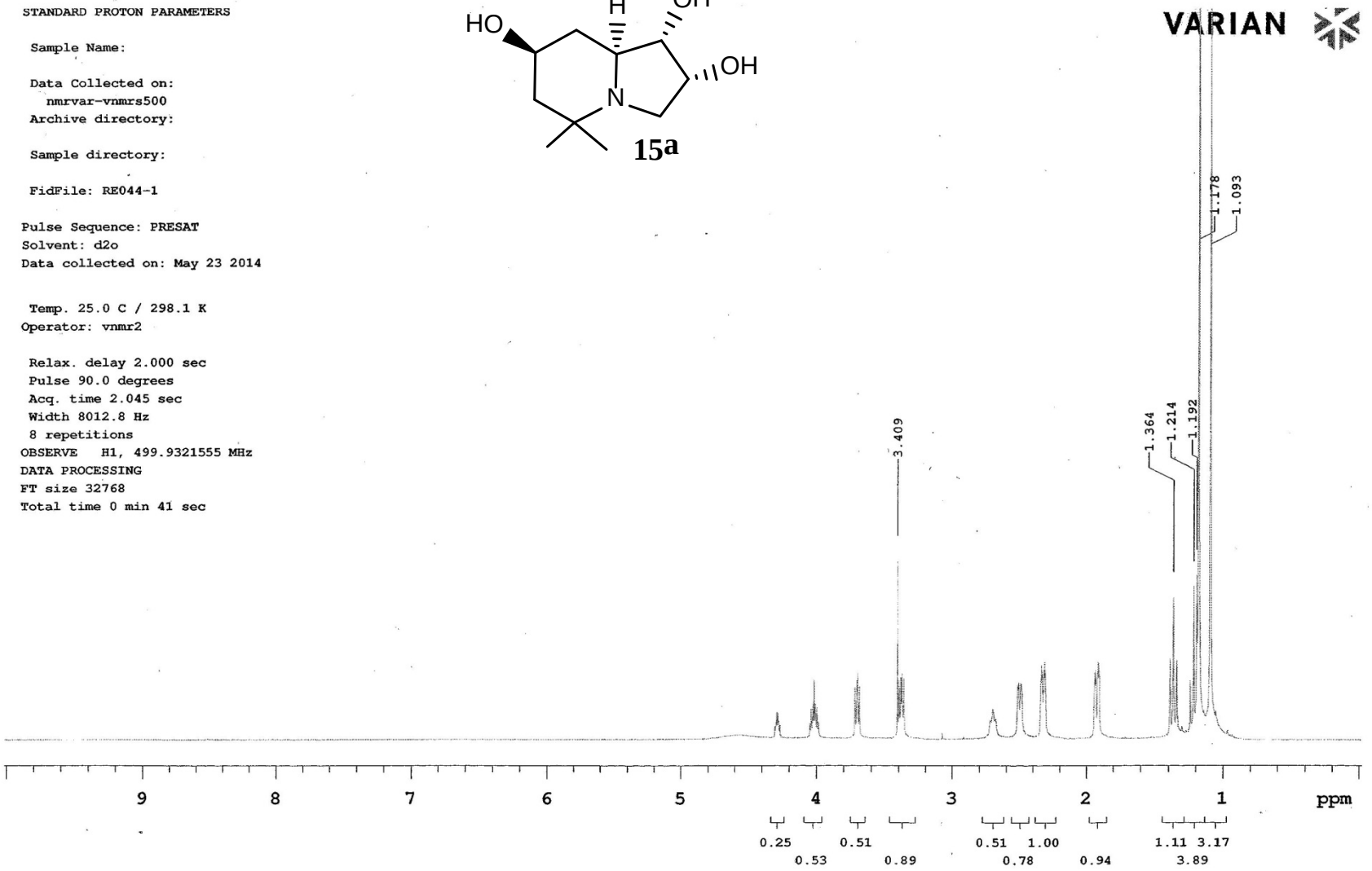
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
8 repetitions
OBSERVE H1, 499.9321555 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 41 sec



15a

VARIAN



STANDARD PROTON PARAMETERS

Sample Name: RE064-3

Data Collected on:
nmrvar-vnmrs500
Archive directory:

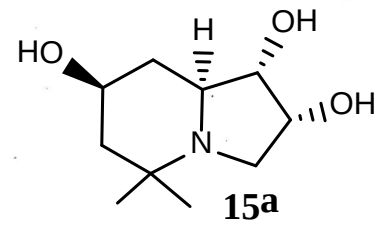
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: d2o
Data collected on: Jul 28 2015

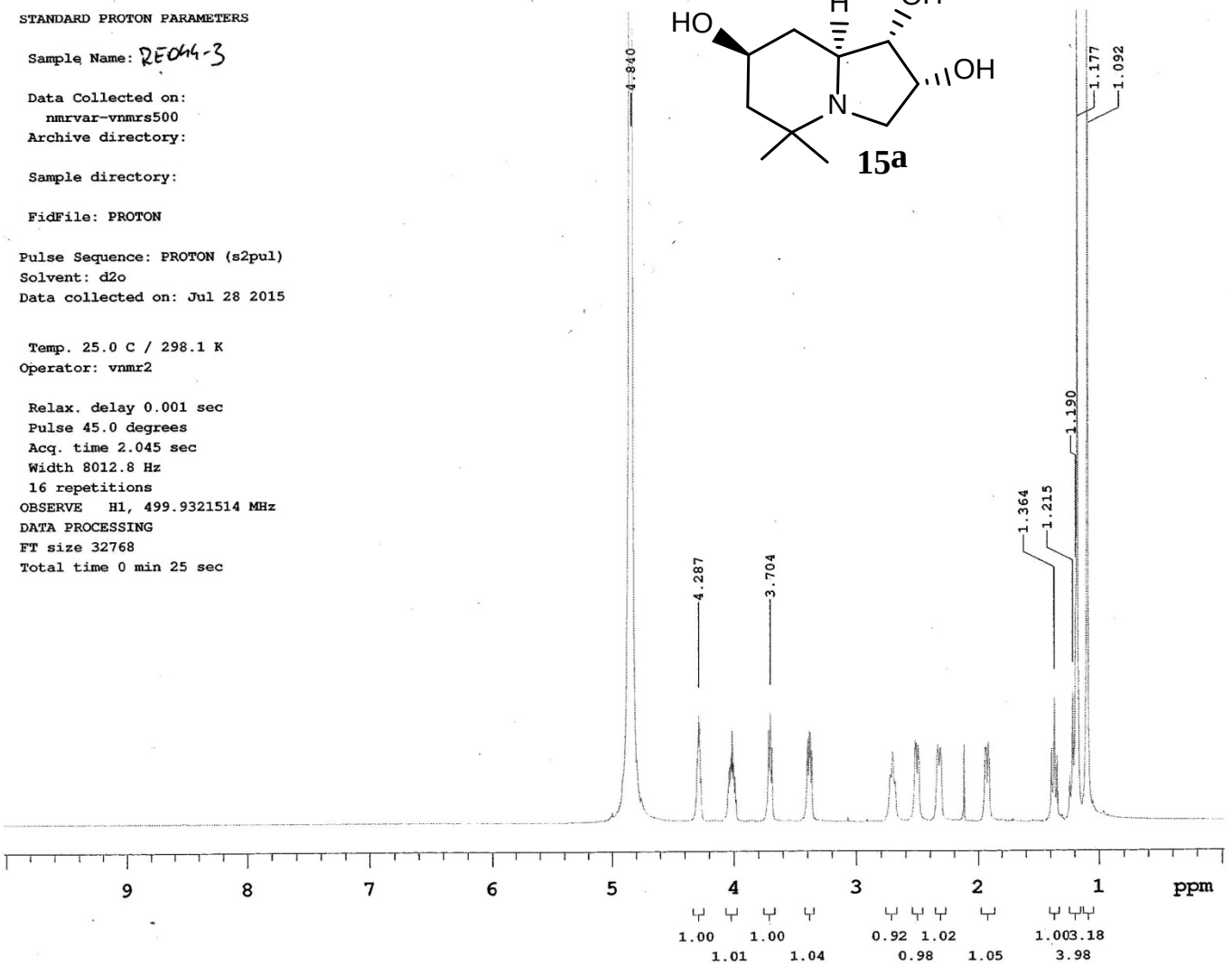
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
16 repetitions
OBSERVE H1, 499.9321514 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec



15a

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

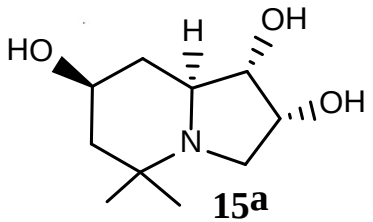
FidFile: RE044-1-c-apt-d2o

Pulse Sequence: APT
Solvent: d2o
Data collected on: May 28 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr2

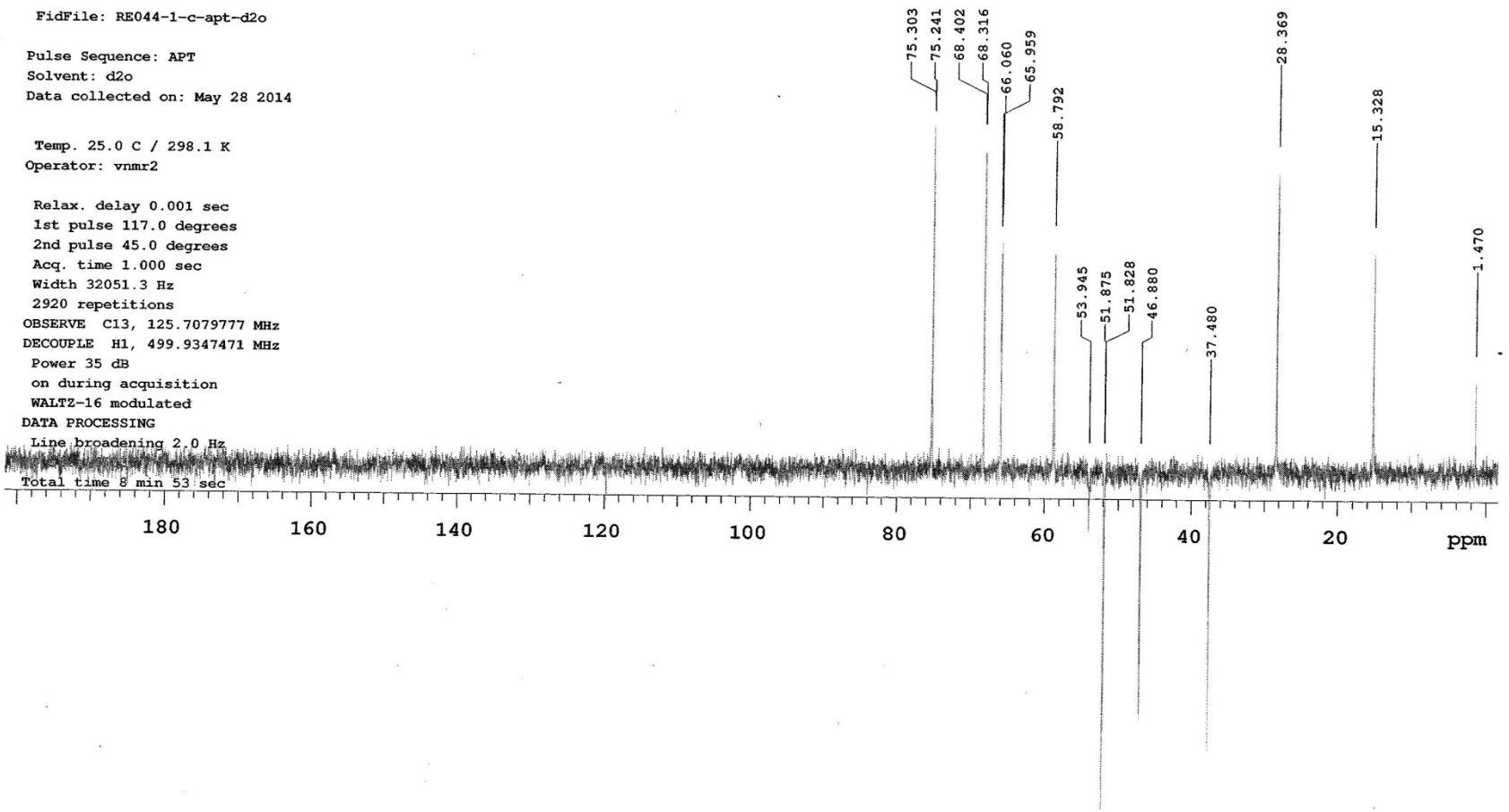
Relax. delay 0.001 sec
1st pulse 117.0 degrees
2nd pulse 45.0 degrees
Acq. time 1.000 sec
Width 32051.3 Hz
2920 repetitions
OBSERVE C13, 125.7079777 MHz
DECOUPLE H1, 499.9347471 MHz
Power 35 dB
on during acquisition
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz

Total time 8 min 53 sec



15a

VARIAN



STANDARD PROTON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

Sample directory:

FidFile: MA262-1-1

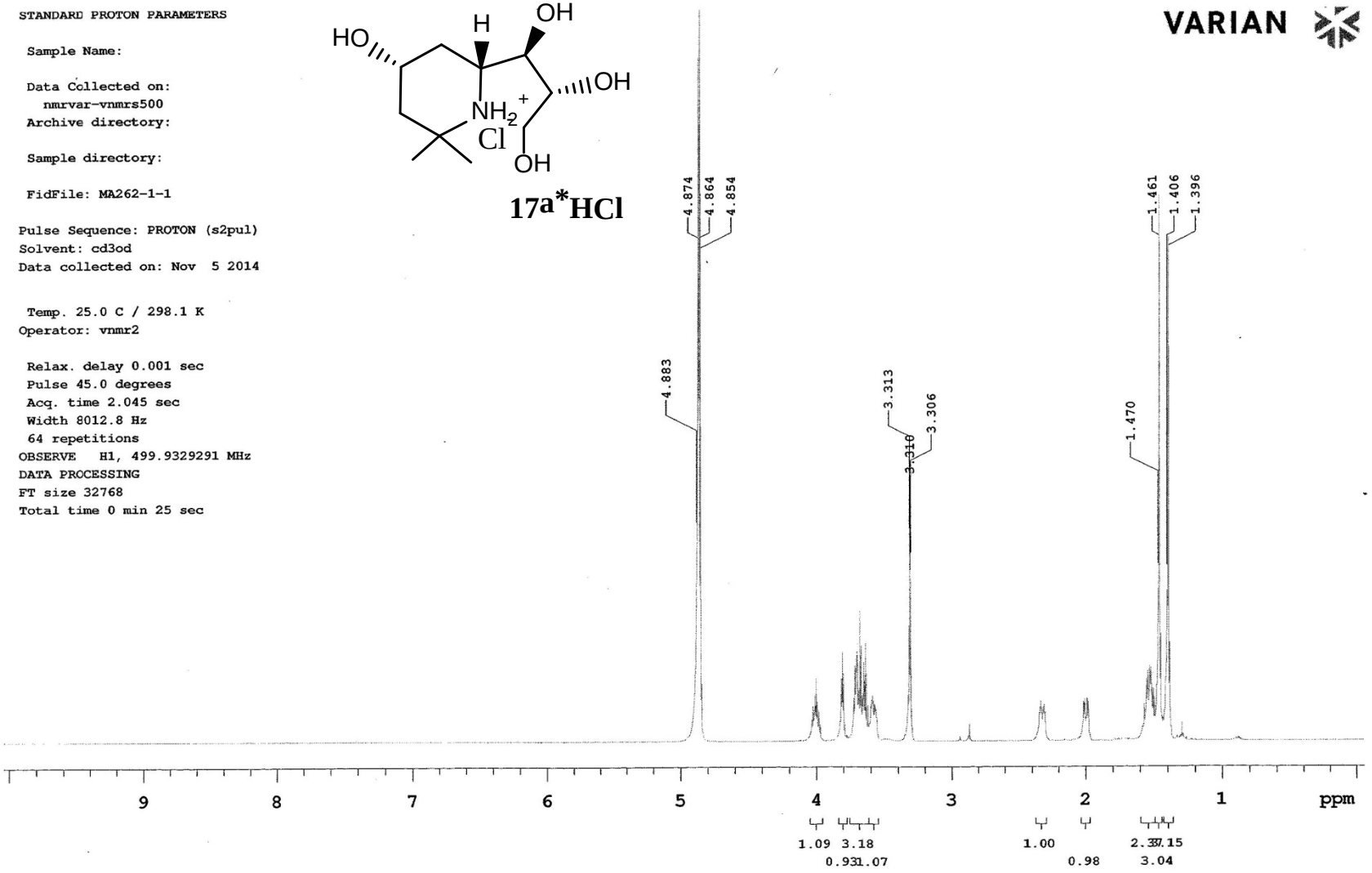
Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Nov 5 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 2.045 sec
Width 8012.8 Hz
64 repetitions
OBSERVE H1, 499.9329291 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

17a*HCl

VARIAN



STANDARD CARBON PARAMETERS

Sample Name:

Data Collected on:
nmrvar-vnmrs500
Archive directory:

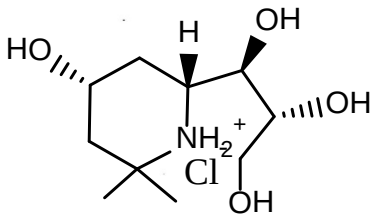
Sample directory:

FidFile: MA262-1-1-c

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Nov 5 2014

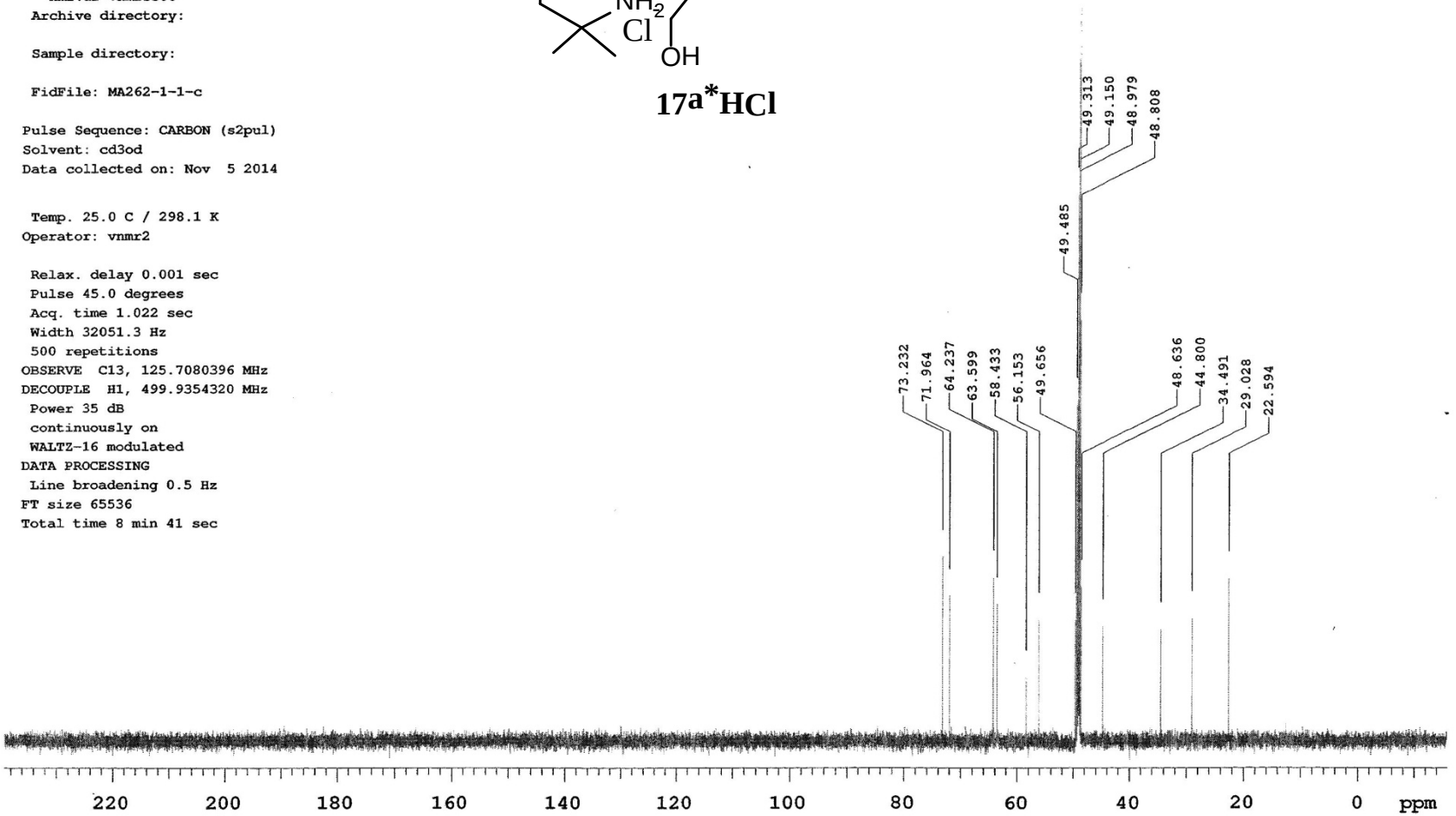
Temp. 25.0 C / 298.1 K
Operator: vnmr2

Relax. delay 0.001 sec
Pulse 45.0 degrees
Acq. time 1.022 sec
Width 32051.3 Hz
500 repetitions
OBSERVE C13, 125.7080396 MHz
DECOUPLE H1, 499.9354320 MHz
Power 35 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 8 min 41 sec



17a*HCl

VARIAN



Configuration elucidation

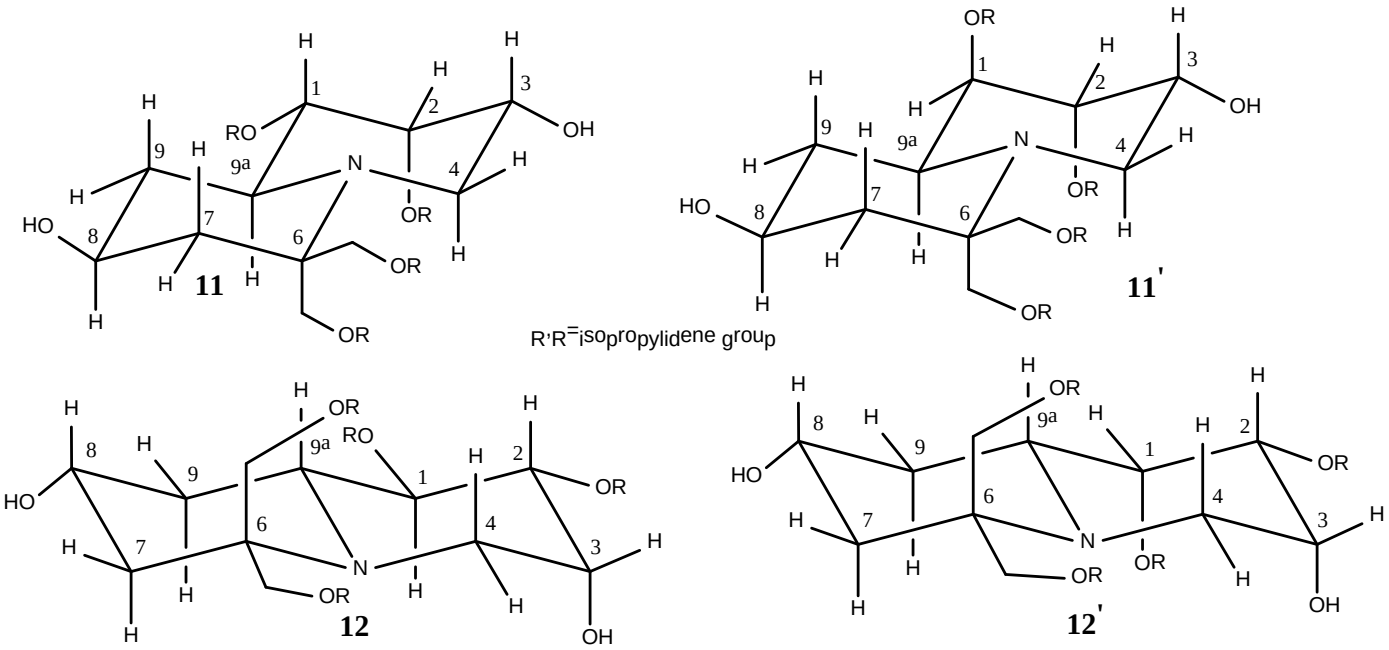


Figure S1. Conformation of quinolizidines **11**, **12** and hypothetical **11'**, **12'**.

Single crystal X-Ray analysis of **13** revealed the configuration of cycloaddition-generated stereogenic centers as S, S. The structural assignment of **13** and **11** respectively was confirmed in **11** by the magnitude of coupling constant. In compound **12** H-1 must occupy an axial position and is explained by the coupling constant value between H1-H2 and it equals 9.5 Hz (typical axial/axial interaction, Figure S1). In hypothetical **12'** compound, in which epimerization did not occur, H-1 proton would occupy equatorial position which means that the coupling constants between proton H1 and H-2,H-9a would be expected in a lower value (1-5Hz). Analogical conclusion was made to determine **11** configuration. The crucial proton H-1 exhibit large coupling constant (7.9 Hz, H1-H9a interaction) and small coupling constant (4.5 Hz, H1-H2). If epimerization took place, the theoretical **11'** isomer would possess only small coupling constants for H-1 signal (ax/eq and eq/eq interactions).

Multiplicity also revealed *cis* relation between H-8 and H-9a protons in both isomers. H-8 protons were a triplet of triplets (ax/ax and ax/eq interactions) and must occupy axial position. H-9a as a doublet of doublet of doublets (two ax/ax coupling constants and one ax/eq) is established in axial position. Since X-Ray analysis of **13** consequently defined stereogenic centers C-8 and C-9a in **11** as S,S, therefore **12** must be R,R isomer on C-8 and C-9a atoms (Table S1).

Table S1. Value of coupling constants between crucial protons to determine configuration of **11** and **12**.

coupling protons	**11** J/ Hz	**12** J/ Hz
H1-H2	4.5	9.5
H2-H3	4.5	2.7
H3-$H4_{ax}$	10.7	1.5
H3-$H4_{eq}$	4.6	2.7
H8-$H9_{ax}$	11.8	11.5
H9a-$H9_{ax}$	11.5	11.7
H9a-$H9_{eq}$	3.7	2.9
H9a-H1	7.9	8.9

Glycosidase Inhibition Assays

Chemicals and enzymes for the inhibition kinetics were purchased from a commercial suppliers. Nonlinear regression analysis was performed using GraphPad Prism v.5 **(**GraphPad Software, Inc. La Jolla, CA). Inhibition assay for the inhibitory potencies of the iminosugars were determined by measuring the residual hydrolytic activities of the glycosidases of the corresponding *p*-nitrophenyl glycosides in the presence of iminosugars spectrophotometrically. Assays were carried out in 96-well plate format, each well containing 6 µL of compound, 3 µL of enzyme and 36 µL of buffer. Reaction mixture were preincubated at 30^{o}C for 3 min and the reaction was started by addition of 15 µL of substrate and incubated for 10 min at 30^{o}C. The reaction was quenched by addition of 120 µL of 1 M sodium carbonate solution. The absorbance of the resulting solution was read at 405 nm using Synergy H4 microplate reader (BioTek).

Buffer conditions and enzyme concentrations were recommended by enzymes supplier. The K_m values for each substrate/enzyme combination were determined experimentally and for the inhibition assays the substrate concentration was equal to K_m. α-Glucosidase (*Saccharomyces cerevisiae*) was assayed at 1U/mL in phosphate buffer (67 mM, pH 6,8) and α-glucosidase (rice) was assayed at 1U/mL in citrate phosphate buffer (100 mM, pH 4,0) with 0,21 mM 4-nitrophenyl α-D-glucopyranoside. β-Glucosidase (almond) was assayed at 1U/mL in citrate phosphate buffer (50 mM, pH 5.0) with 2,52 mM 4-nitrophenyl β-D-glucopyranoside. α-Galactosidase (green coffee beans) was assayed at 1U/mL in sodium phosphate buffer (100 mM, pH 6.5) with 0.83 mM 4-nitrophenyl α-D-galactopyranoside. β-Galactosidase (*Aspergillus oryzae*) was assayed at 1U/mL in citrate phosphate buffer (50 mM, pH 4,5) with 0.68 mM 4-nitrophenyl β-Dgalactopyranoside. α-mannosidase (jack bean (*Canavalia ensiformis)*) was assayed at 1U/mL in citrate phosphate buffer (50 mM, pH 4.5) with 1,17 mM 4-nitrophenyl α-D-mannpyranoside. β-Mannosidase (*Helix pomatia*) was assayed at 1U/mL in citrate phosphate buffer (50 mM, pH 4.0) with 0.65 mM 4-nitrophenyl β-D-mannopyranoside.

Table S2. Inhibitory properties of iminosugars from this work and quinolizidines from the preliminary communication.[a,b]

Enzyme	**3a**	**3b**	**4a**	**4b**	**15a**	**15b**	**16**	**17a**	**17b**
α-glucosidase from *Saccharomyces cerevisiae* (EC 3.2.1.20)	NI	NI	NI	**97**	NI	NI	NI	NI	NI
α-glucosidase from rice (EC 3.2.1.20)	**95**	NI	NI	NI	NI	**95**	NI	NI	NI
β-glucosidase from sweet almonds (EC 3.2.1.21)	NI	NI	NI	NI	NI	NI	NI	NI	NI
α-galactosidase from green coffee beans (EC 3.2.1.22)	NI	NI	NI	NI	NI	**97**	NI	NI	NI
β-galactosidase from *Aspergillus oryzae* (EC 3.2.1.23)	NI	NI	NI	NI	NI	NI	NI	NI	NI
α-mannosidase from *Canavalia ensiformis* (EC 3.2.1.24)	NI	NI	**83**	NI	NI	NI	NI	NI	NI
β-mannosidase from *Helix pomatia* (EC 3.2.1.25)	NI	NI	NI	NI	NI	NI	NI	NI	NI

[a]Percent of glycosidase remaining activity at 1 mM; [b] NI, no inhibition up to 1 mM

Cell viability test (MTT assay)

The in vitro studies were carried out on the human melanoma cell lines from two cancer stages – primary WM115 and metastatic WM266-4 which were derived from the same patient. The melanoma cells were cultured in RPMI-1640 medium (Sigma Aldrich, USA) containing L-glutamine and sodium bicarbonate and supplemented with 10% fetal bovine serum (FBS, Life Technologies, USA) as well as 1% of antibiotics mixture (10,000 U/ml penicillin – 10,000 µg/ml streptomycin, Life Technologies, USA). Cells were grown in monolayers at air/5% CO_2 atmosphere at 37 ºC in a 25 cm^2 culture flasks. When the cells were approximately 80% confluent, they were washed with phosphate-buffered saline (PBS, Life Technologies, USA) and harvested with 0.05% trypsin/EDTA solution (Life Technologies, USA). For the experiments cells were seeded at density 5×10^3 cells/ml in 96-well plates and cultured at air/5% CO^2 at 37 ºC for 24 h for MTT assay (cell viability test).

During the experiments various inhibitors were examined in the concentration 100 µM. The inhibitor stock solutions were prepared in ultrapure water (MiliQ) and the appropriate concentration was added per well. Cells were incubated at air/5% CO_2 at 37 ºC for 24 h.

The MTT [3-(4, 5-dimethylthiazol-2-yl)-2, 5-diphenyltetrazolinum bromide, Sigma-Aldrich, USA] assay was performed according to the producers protocol and used as the viability assay. MTT salt was dissolved in DMEM (Life Technologies, USA) at the concentration of 5 mg/ml. After treatment with several inhibitors, medium was removed from the wells and cells were washed with PBS buffer. Next 70 µl of the MTT solution per well was added and the plates were incubated for 4 hours at air/5% CO_2 at 37 ºC. To dissolve the purple formazan product, a 200 µl of dimethylsulfoxide (DMSO, Carl Roth, Gremany) was added to each well and shook for 10 minutes at room temperature. 25 µl of Sorensen Buffer was added per well and the absorbance of the resulting solutions was determined at 570 nm wavelengths in a microplate reader. The results were expressed as a relative viability of treated cells and untreated control cells.

Sorensen buffer - glycine 0.1M (Sigma Aldrich, USA), NaCl 0.1M (Sigma Aldrich, USA), pH:10.5 with 0.1 NaOH (Sigma Aldrich, USA)

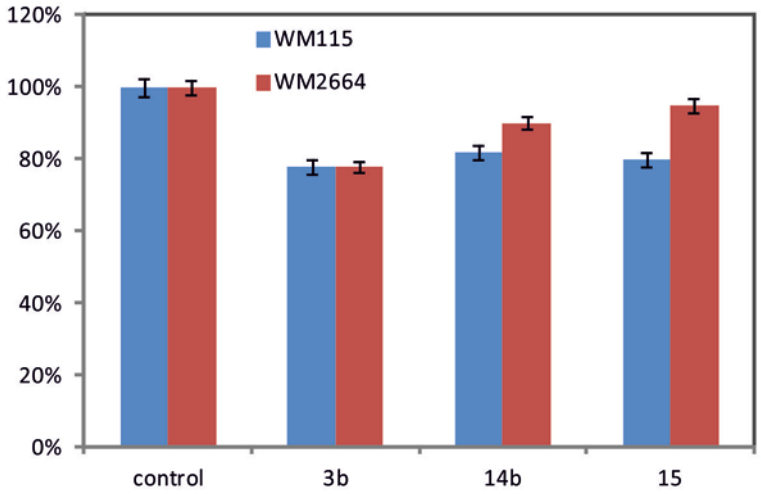


Fig. S2. Metabolic activity of melanoma primary WM115 and metastatic WM266-4 cell lines after treatment for 24 h with **3b**, **15b** and **16** at 100 µM.

X-ray Structure Determination of 13 and 15a*HCl

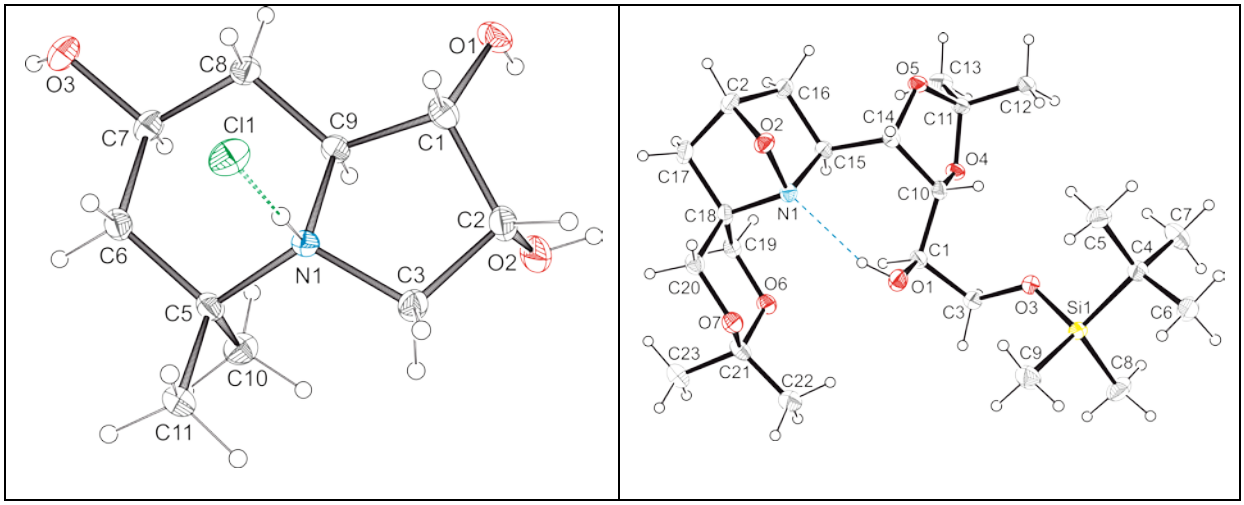


Fig. S3. Ortep[i] drawings of **15a*HCl** (left picture) and **13** (right picture) molecules with the atoms' numbering scheme. Thermal ellipsoids are shown at 50% probability. The absolute configuration was determined by anomalous dispersion consideration[ii,iii,iv].

Crystal Data for **15a*HCl**, $C_{10}H_{20}NO_3Cl$ (M = 237.72): orthorhombic, space group $P2_12_12_1$, a = 6.82581(5) Å, b = 12.02340(7) Å, c = 14.64680(9) Å, α, β, γ = 90.00°, V = 1202.05(1) Å^3, Z = 4, T = 120.0(2) K, μ(CuKα) = 2.741 mm^{-1}, ρ_{calc} = 1.314 g/cm^3, 33361 measured reflections, 2148 unique (R_{int} = 0.0329). 883 Bijvoet pairs, Flack's x = –0.003(3) [ii], Hooft's y = 0.007(3) [iv].The final R_1 = 2.17% ($I > 2\sigma(I)$) and wR_2 = 5.80% (all data). CCDC-1410262

Crystal Data for **13**, $C_{23}H_{43}NO_7Si$ (M = 473.67): orthorhombic, space group $P2_12_12_1$, a = 7.96665(7) Å, b = 10.06647(10) Å, c = 31.8330(3) Å, α, β, γ = 90.00°, V = 2552.88(4) Å^3, Z = 4, T = 100(2) K, μ(CuKα) = 1.154 mm^{-1}, ρ_{calc} = 1.232 g/cm^3, 22949 measured reflections, 4512 unique (R_{int} = 0.0394). 1909 Bijvoet pairs, Flack's x = 0.002(10) [ii], Hooft's y = -0.013(10) [iv]. The final R_1 = 2.78% ($I > 2\sigma(I)$) and wR_2 = 7.20% (all data). CCDC-1410265

Diffraction data were measured at 120.0(2) K and 100(2) K in case of **15a*HCl** and **13**, respectively with mirror monochromated Cu$K\alpha$ radiation (λ = 1.54184 Å) on an Oxford Diffraction (Agilent Technologies) κ-CCD Gemini A Ultra diffractometer. Cell refinement and data collection as well as data reduction were performed with CrysAlis^{Pro} software[v]. The empirical absorption corrections using spherical harmonics, implemented in mutli-scan algorithm, were also performed. The structures were solved by direct methods and subsequent Fourier difference synthesis while full-matrix least-squares refinement method against F^2 values was carried out using the SHELXL program [vi] implemented in OLEX2[vii] suite. All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were added to the structure model at geometrically idealized coordinates and refined as riding atoms with U_{iso}(H) = 1.2×U_{eq}(CH and CH_2) or U_{iso}(H) = 1.5×U_{eq}(CH_3). Positions of hydrogen atoms

of OH and NH groups have been found on the basis of differential Fourier map and refined freely. Molecular diagrams, depicted in Fig. S3, were generated using ORTEP-3 for Windows[i]. The crystal data and structure refinement parameters are given in Table S3.

Determination of an absolute structure and absolute configuration of the **15a*HCl** and **13** molecules was successfully conducted using anomalous dispersion effects. Referring to the Cahn–Ingold–Prelog priority rules stereocentres of **15a*HCl** have the following configuration: C2 – *R* and C1, C7, C9 – *S*, whereas C1, C10 – *R* and C2, C14, C15 – *S* in case of **13** (see Fig. S2). Flack's parameter *x*[ii] for **15a*HCl**, calculated from 868 selected quotients (Parsons' method)[iii], equals –0.003(3). Corresponding values for **13**amounted to 1844 selected quotients and *x* = 0.002(10). Further analysis of the absolute structure was performed using likelihood methods with PLATON[viii] program. A total of 883 (**15a*HCl**) and 1909 (**13**) Bijvoet pairs (coverage of 1.00) were included in the calculations. The resulting value of the Hooft's parameter *y*[iv] was 0.000(1) and -0.013(10) for **15a*HCl** and **13** respectively confirming the correctly assigned configuration.

Table S3 Crystal data for **15a*HCl** and **13**

Crystal data	**15a*HCl**	**13**
Empirical formula	$C_{10}H_{20}NO_3Cl$	$C_{23}H_{43}NO_7Si$
Crystal size (mm^3)	0.30×0.20×0.05	0.60×0.30×0.20
M_r	237.72	473.67
Crystal system	Orthorhombic	Orthorhombic
Space group	$P2_12_12_1$	$P2_12_12_1$
Temperature (K)	120.0(2)	100(2)
λ (Cu Kα radiation) (Å)	1.54184	1.54184
a (Å)	6.82581(5)	7.96665(7)
b (Å)	12.02340(7)	10.06647(10)
c (Å)	14.64680(9)	31.8330(3)
α, β, γ (°)	90.00	90.00
Volume ($Å^3$)	1202.05(1)	2552.88(4)
Z	4	4
F(000)	512	1032
ρ calc. ($g\ cm^{-3}$)	1.314	1.232
μ (mm^{-1})	2.741	1.154
Reflections collected	33361	22949
Independent reflections [*R*(int)]	2148 [3.29%]	4512 [3.94%]
Reflections with $I > 2\sigma(I)$	2128	4423
θ° range	4.76 ÷ 67.17	4.61÷ 66.68
	$-7 \le h \le 8$	$-9 \le h \le 9$
Index range	$-14 \le k \le 14$	$-11 \le k \le 11$
	$-17 \le l \le 17$	$-37 \le l \le 37$
Data/restraints/parameters	2148/0/157	4512/0/303
Weighting scheme: *a*, *b*	0.0360, 0.3460	0.0416, 0.5848
Goodness-of-fit on F^2[a]	1.034	1.041
Final *R* indices	$R_1 = 0.0217$	$R_1 = 0.0278$
($I > 2\sigma(I)$)[b]	$wR_2 = 0.0578$	$wR_2 = 0.0713$
R indices (all data)[b]	$R_1 = 0.0220$	$R_1 = 0.0286$
	$wR_2 = 0.0580$	$wR_2 = 0.0720$
Max and min electron density in the difference Fourier map($e/Å^3$)	0.214/–0.175	0.246/–0.201
Flack's parameter, *x*[ii]	–0.003(3)	0.002(10)
Hooft's parameter, *y*[iv]	0.007(3)	0.013(10)

[a] Goodness of fit = $\{[w(F_o^2-F_c^2)^2]/(n-p)\}^{1/2}$, where *n* is the number of reflections and *p* is the total number of parameters refined. [b] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Energies and Cartesian coordinates of optimized geometries.

Table S4. Absolute (hartrees) and relative (kcal/mol) electronic energies (E_0) and free energies (G_{378}) for protonated derivatives of nitrone **Ia**.

	E_0	ΔE_0	G_{378}	ΔG_{378}
IVa	-979.742251629	0.0	-979.414861	0.0
VIa	-979.676774832	41.1	-979.357701	35.8
VIIIa	-979.715997085	16.5	-979.387061	17.4

Table S5. Absolute (hartrees) and relative (kcal/mol) electronic energies (E_0) and free energies (G_{378}) for [1,4]-sigmatropic rearrangement.

	E_0	ΔE_0	G_{378}	ΔG_{378}
Ia	-979.352401756	0.0	-979.036397	0.0
(*E*)-IIa	-979.333826794	11.6	-979.019901	10.3
(*Z*)-IIa	-979.328564468	14.9	-979.019662	10.5
IIIa	-979.355197653	-1.8	-979.040519	-2.6
TS_E_1	-979.291697354	38.1	-978.982007	34.1
TS_E_2	-979.289953335	39.2	-978.979664	35.6
TS_Z_1	-979.274327852	49.0	-978.966159	44.0
TS_Z_2	-979.274698187	48.7	-978.967064	43.5

Table S6. Absolute (hartrees) and relative (kcal/mol) electronic energies (E_0) and free energies (G_{298}) for protected quinolizidines **11a** and **12a**.

	E_0	ΔE_0	G_{298}	ΔG_{298}
11a	-904.207426839	0.0	-903.863357	0.0
12a	-904.189474603	11.3	-903.846547	10.5

Table S7. Absolute (hartrees) and relative (kcal/mol) electronic energies (E_0) and free energies (G_{298}) for diols **1a** and **2a**.

	E_0	ΔE_0	G_{298}	ΔG_{298}
1a	-979,370193007	0.0	-979,026326	0.0
2a	-979,383885160	-8.6	-979,039211	-8.1

Table S8. Absolute (hartrees) and relative (kcal/mol) electronic energies (E_0) and free energies (G_{298}) for the intermediate aldehydes **IXa** and **Xa**.

	E_0	ΔE_0	G_{298}	ΔG_{298}
IXa	-864.892482441	0.0	-864.581525	0.0
Xa	-864.893376993	-0.6	-864.583420	-1.2

Table S9. Absolute (hartrees) and relative (kcal/mol) electronic energies (E_0) and free energies (G_{298}) for protected indolizidines **8a** and **9a** (hypothetical).

	E_0	ΔE_0	G_{298}	ΔG_{298}
8a	-789,668497102	0.0	-789,357553	0.0
9a	-789,636871881	19.8	-789,324012	21.0

IVa

C	-2.4657294018	-1.7683347546	-1.4921881667
O	-2.5960237883	-1.2165605545	-0.1774738244
C	-3.1726071476	-0.8496992211	-2.4710585212
O	-1.0285775477	-1.7440751687	-1.7544113933
C	-0.3251023037	-1.44779963	-0.5708638034
O	-0.0266309527	-0.8514666779	2.3427691302
O	-1.9340222211	-0.0169986999	3.8894080476
C	-2.948914568	-3.2121683635	-1.5521369487
C	2.3909773681	2.2433965092	0.8701935781
C	4.6771641561	2.0091363783	-1.1885958068
C	0.3379053777	-0.1081713132	-0.7655937031
C	3.6512950529	0.9304413461	-0.9553602849
N	1.4277700601	0.2490331019	-0.1788864837
C	-1.426437186	-1.5353807821	0.5397820011
C	-1.2994191684	-0.588870853	1.7242438677
C	5.1513904387	2.3436782593	-2.3889840815
O	1.9749850737	-0.5755771985	0.7664719139
C	2.2770670026	1.4810182213	-0.4584845042
C	-2.3844119834	-0.7884049522	2.778938038
C	1.6051256529	2.3380193758	-1.5310828096
H	-4.2472479738	-0.8476303125	-2.2742192985
H	-2.7970342467	0.1715184924	-2.3723195483
H	-3.0063597928	-1.1946728551	-3.4938737038
H	0.4654005342	-2.1864994529	-0.3890627769
H	-0.1038198902	-0.508454383	3.2541546326
H	-2.4655838204	-0.2233886777	4.6687755135
H	-2.7532399358	-3.6276997224	-2.5433374676
H	-4.0236113588	-3.255840114	-1.3593278641
H	-2.4338987036	-3.8354060582	-0.8167573231
H	2.9718582379	3.152824442	0.706574846
H	2.8924493243	1.6463611223	1.6335962448
H	1.4040573892	2.5407813283	1.2374670441
H	5.0678793818	2.5091051738	-0.3040934208
H	-0.0736897831	0.5702086323	-1.5023598734
H	4.024390235	0.2217754453	-0.209359888
H	3.4820137198	0.373900444	-1.884116898
H	-1.4353308862	-2.571720226	0.9065190413
H	-1.3356384695	0.4526908694	1.3764398876
H	5.9153712111	3.105698427	-2.5044224222
H	4.8099512535	1.8554079329	-3.2985279064
H	1.2536911035	-0.7018702719	1.4734584229
H	-3.3491263838	-0.4427686944	2.3906514039
H	-2.4635775355	-1.8544017313	3.0344536927
H	0.6395022359	2.7345878798	-1.2025370208
H	1.4806912355	1.8015858603	-2.4767433446
H	2.2619100044	3.185757427	-1.7329452181

VIa

C	-1.2954673382	-2.6601189899	0.367306112
O	-1.3926371789	-1.4564473939	1.1345516485
C	-2.7184904565	-2.9692790714	-0.0753710563
O	-0.4911240755	-2.3357256395	-0.785394225
C	0.2747989381	-0.0916605198	0.1312060721
O	-0.4819160759	-0.5379515693	3.7184152278
O	-1.7643972063	1.8536489524	3.5696561876
C	-0.6601945106	-3.7933385087	1.1722624759
C	0.8142911384	0.190226967	-3.2364245876
C	2.8023501647	3.5176039836	-2.6538824425
C	1.576172156	0.2442277389	-0.0834945897
C	2.2857929511	2.2504197938	-3.285381941
N	2.094475451	0.8517368185	-1.2239983125
C	-0.188331312	-0.7701009416	1.3856201475
C	-0.4187637676	0.2362235012	2.5481637964
C	4.09119766	3.7653922335	-2.4158834246
O	3.3110095354	0.9309182052	-1.2917419787
C	1.2895887459	1.4186068743	-2.4346860464
C	-1.6862525841	1.0778060432	2.3822876722
C	0.1266904743	2.2988421173	-1.938666963
H	-3.3616971714	-3.1260651324	0.793631524
H	-3.1099499819	-2.1346248258	-0.6607319316
H	-2.7327934564	-3.8707337875	-0.6923423064
H	0.1055890579	-3.0735790544	-0.9710149305
H	-0.504653129	0.1515088896	-0.5747450561
H	-0.8543695279	0.0451499813	4.3995150116
H	-2.6775266989	2.133882156	3.7090670843
H	0.3767848986	-3.5740922963	1.4430779942
H	-0.6736541969	-4.7235730431	0.5958090708
H	-1.2263589447	-3.9537397106	2.0916999452
H	0.2523805256	0.5532272862	-4.1011666693
H	1.6665515947	-0.386422529	-3.6058694735
H	0.1637119883	-0.471141611	-2.6601974982
H	2.0645419579	4.2840613677	-2.4221198156
H	2.3681538076	-0.0190828313	0.6096241858
H	3.1159014162	1.6169015474	-3.6046986593
H	1.7160015073	2.4990312791	-4.1902135824
H	0.6025967749	-1.4368664148	1.7557301748
H	0.4484969184	0.9184528983	2.5728409577
H	4.416270724	4.7121923001	-1.9968060423
H	4.8672615623	3.0405088223	-2.645702584
H	-1.6113709044	1.7166682532	1.4862056485
H	-2.5479062162	0.4119079038	2.2668159406
H	-0.1697747017	2.9479518047	-2.7663089904
H	0.4210497849	2.9421019313	-1.1065494972
H	-0.7582032984	1.7295762204	-1.6557982732

VIIIa

C	0.4937544603	1.6312354039	-1.0820699284
O	1.7938125783	1.6067221874	-0.5406758378
O	-0.5138501142	1.6390583337	0.0319436025
O	1.3571676821	1.5505433001	2.2724134486
C	1.4705990114	0.3566972718	1.5376996497
C	0.1876734542	0.5376840742	-2.0955741825
O	1.4653366745	-1.6765846087	-0.231141141
O	3.8099775238	2.7849331486	-0.5150241592
C	0.3233142471	3.032239523	-1.6528584011
C	-2.7719124656	-0.1091000524	2.0689757072
C	-3.8077945277	-1.9000051969	-0.2129539522
C	0.0800883502	-0.1998671853	1.2809913719
C	-2.4190562694	-1.3150801551	-0.1774680585
N	-0.831239191	0.4265761048	0.6270400898
C	2.3108370213	0.5316988018	0.2572585143
C	2.5742138074	-0.8020171681	-0.4572855785
C	-4.5319396405	-2.0356733853	-1.3239988303
C	-2.324730081	0.0288200772	0.6042828139
C	3.8503632298	-1.4831319262	0.0512251006
C	-3.1175006835	1.1375522188	-0.0894266457
H	1.1667077902	2.2675904809	1.6470345934
H	1.9765915939	-0.3647145027	2.1839696184
H	-0.8096909845	0.6923329023	-2.5127384395
H	0.9080406169	0.6241329366	-2.9127422716
H	0.2573826973	-0.4672744058	-1.6794200057
H	1.8065115994	-2.5746976948	-0.3971574724
H	4.5170448197	-3.3285711785	-0.1448720753
H	-0.6741644192	3.1572876916	-2.0768255516
H	0.4827182785	3.7805477261	-0.8742592077
H	1.0672480444	3.184208065	-2.4373362073
H	-2.3000700676	-0.9558691111	2.5759853115
H	-3.850785874	-0.2728807113	2.0962737871
H	-2.5562686658	0.8035610765	2.6306472365
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H	-0.2285612443	-1.1225920501	1.7565637237
H	-2.0662325331	-1.152635337	-1.2001481154
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H	3.2705474594	0.9435777294	0.5863887761
H	2.6956337577	-0.6127499595	-1.5316730799
H	-5.5179709129	-2.4884214222	-1.3061206891
H	-4.1630040279	-1.7128657829	-2.2944941213
H	4.7306624269	-0.9142499546	-0.2767266334
H	3.8546251535	-1.5240613562	1.1513037919
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H	-3.0384387461	2.0875295257	0.4417855272
H	-2.8030573039	1.2857406481	-1.1237164323

Ia

C	-2.9209930673	1.4928528738	1.3554646896
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O	-1.7505893433	1.3957425229	2.2000229454
C	-0.5942662761	1.7779424478	1.4565450901
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O	-0.3715473403	3.2245803535	-3.380586498
C	-3.825172278	2.5957821966	1.9059233877
C	3.1063827078	-0.4224754042	-0.5345212964
C	4.5458088293	-1.4648980561	1.9813237847
C	0.2195726189	0.5479912547	1.1760543702
C	3.4240432507	-0.4645403794	2.014951889
N	1.5034604278	0.6301236919	0.9798513709
C	-1.2033667373	2.5149566364	0.2303014381
C	-0.4091242888	2.5140448719	-1.0739899906
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C	2.4202591739	-0.5799942934	0.8305615678
C	-1.1832088068	3.1604356991	-2.2240228874
C	1.6465724631	-1.8974424184	0.898274487
H	-4.4951611722	0.2010017784	0.6341276472
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H	-3.9351991646	-0.1755271817	2.278207207
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H	1.3767303881	2.8122415625	-0.3132362596
H	0.4815290129	3.5570081201	-3.059455653
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H	-4.7283769841	2.6858288732	1.296182515
H	-3.303651241	3.5560034799	1.9055863284
H	2.3648987802	-0.4434239004	-1.3392902682
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H	3.6459785965	0.5239586296	-0.5846801737
H	5.2682445471	-1.3576404789	1.1730388416
H	-0.2456155957	-0.4244659508	1.2143320078
H	3.8243487381	0.5539194948	1.9899464021
H	2.8621631744	-0.5723114316	2.9504686727
H	-1.3824442043	3.5612351788	0.5196990617
H	-0.1770335768	1.4764452599	-1.3613112798
H	5.5693422035	-3.1163365315	2.8211924176
H	4.0421342703	-2.575234565	3.7127671896
H	-2.0702789455	2.5693166531	-2.4649031054
H	-1.5153626499	4.1635023685	-1.9058456358
H	2.3639600196	-2.7171135274	0.8167748923
H	1.1223235165	-2.0199263981	1.8507847505
H	0.9296598255	-1.9948617635	0.0775922047

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C	-3.4371808044	2.0423343393	-1.6342058733
O	-1.6341653537	0.8530512684	-0.6025928249
C	-0.3580965275	1.1849674052	-0.1511238536
O	1.958074367	2.4653671616	-1.6766838114
O	1.4472086137	4.4386146897	-3.377429466
C	-3.0479616282	2.151721375	0.8849641089
C	0.396873594	0.2432883306	0.4331591742
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C	0.5727934023	4.3418057192	-2.2470563115
C	2.2182663426	-0.4319268312	1.9954183929
O	2.1786194374	1.6704265708	0.8988837353
C	1.7801005242	-1.9191813986	1.8375127568
C	2.433269973	-2.8750643435	2.8003566688
C	3.7521380036	-0.3313730983	2.0139023584
C	1.6198537284	0.1773209928	3.2755947436
C	1.7934407583	-3.5354140686	3.7663369522
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H	-2.9203962858	1.9508363712	-2.5918827403
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H	-2.2676443168	2.0883037793	1.6480687965
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H	0.3328171179	3.1964634089	0.2971061564
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H	3.501638189	-3.0420309125	2.671490107
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H	4.0576389481	0.7150821226	2.0053963326
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O	-1.209219556	0.1911921557	-0.6481911215
C	-0.1947164183	0.6400036947	0.1719978672
O	1.5782417184	2.7757794421	1.4225608275
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C	2.2309304627	-2.3997507881	2.01599247
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C	3.4469983029	-1.3807468997	0.0353463293
C	3.3860246714	-4.4376642271	-0.0569923669
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H	-3.3819110962	2.1800690103	-2.2615007506
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H	-0.7174681598	-2.1296952571	-0.3738908687
H	3.0833925048	-3.0174504489	2.3119542623
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H	4.3622421642	-1.9224516398	0.2876585174
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H	4.3304089101	-4.0783161009	-0.4661306665
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IIIa

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O	-2.9865470328	0.3658938366	1.6759167324
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O	-0.2100315314	0.1631099448	-1.7469845383
O	-1.2762304508	1.1400165994	-4.0447875214
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C	2.570896226	-1.1424309144	0.8588629384
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C	-1.5898449066	0.498327618	-1.7372748905
C	4.9109817555	-0.5713444296	1.5816485049
O	-0.0143363774	-1.880852677	0.0098045159
C	1.4303504895	-1.4944411539	1.8570325792
C	-1.7605913697	1.5894591588	-2.794498943
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H	-5.7032385703	0.3886754208	1.8449684855
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H	-0.0953539009	-0.6883986328	-1.2658306533
H	-0.4300993494	0.7129986758	-3.8374288565
H	-4.2915189966	2.4224392873	2.719273949
H	-4.663299562	3.2305723913	1.1797751161
H	-2.9741412813	3.0222371432	1.6924311171
H	2.2968313172	-3.2956267218	2.6966750102
H	1.2689019597	-3.5797635089	1.268456937
H	0.5357784863	-3.2138385899	2.8420229309
H	4.1796077199	-2.5261596934	1.4950972491
H	-0.5683235474	0.2304208041	2.4083398526
H	2.3611202535	-1.6895248726	-0.065816067
H	2.5031838751	-0.0735592777	0.6242148707
H	-1.3553918934	1.7968808659	-0.0349173322
H	-2.2104796774	-0.3646029735	-2.0239210269
H	5.9030260929	-0.8665340501	1.9097157934
H	4.7422651353	0.4930839767	1.4365380914
H	-2.8177918908	1.841138299	-2.9103639442
H	-1.2280775405	2.4953780922	-2.4561582329
H	0.7452651021	-0.8910090545	3.8463888417
H	1.5642464022	0.4071811918	2.9377079218
H	2.498269709	-0.9186774951	3.6182058119

TS_E_1

H	-0.0511350233	0.3157888496	-1.0541726135
O	-0.7883595519	1.0584170038	-0.422187051
N	-1.0701613013	0.1195024636	0.5304962854
C	-0.1341527867	-0.8327067997	0.5148303939
H	-0.3449909194	-1.7893590563	0.9771072355
C	0.9051964457	-0.6581993813	-0.4507207436
O	1.4261714266	-1.8911318996	-0.8733615449
C	2.8538541934	-1.9179825895	-0.6334687691
O	3.1558580592	-0.6907079416	0.01294654
C	2.1396349597	0.2623750606	-0.3268706918
H	2.3689277076	0.7217815482	-1.2996597926
C	3.1879933082	-3.0555497777	0.3211575169
H	2.6349069476	-2.9267093341	1.2545693829
H	4.2579027315	-3.0584690372	0.5474070617
H	2.9205756675	-4.0172372019	-0.1245841114
C	3.5627405495	-2.0299436651	-1.9820697147
H	3.3211993169	-1.1690736704	-2.6105882504
H	3.2421275167	-2.9362531717	-2.5029536033
H	4.6460502045	-2.068740853	-1.8391608445
C	2.1339086144	1.3739515244	0.7307449713
H	1.7081233074	0.9831812032	1.6678592212
O	1.4102375272	2.5083154064	0.2750094178
H	0.4882512999	2.2274625743	0.1212775094
C	3.5437974322	1.8950710274	1.0232357559
H	4.0197100371	2.1820793281	0.070458949
H	4.1499314113	1.1125008681	1.4834304403
O	3.481548918	2.9854590516	1.9232169283
H	2.7711070088	3.5488682898	1.5793632249
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C	-3.0506045062	1.3293028395	1.275996382
H	-2.5303018597	1.682628584	2.1714943026
H	-4.1172795239	1.269983638	1.5020794525
H	-2.8958210549	2.0555585302	0.4762937887
C	-3.2383124422	-0.5431071879	-0.419967618
H	-3.0314622328	0.1377742021	-1.2483554736
H	-4.3201471247	-0.5765479235	-0.2664977839
H	-2.8953042196	-1.5446980597	-0.6984470494
C	-2.6451957318	-1.0659451623	2.0182736221
H	-1.9809413505	-0.7492488113	2.8306352249
H	-2.2948254013	-2.0473534752	1.6720934264
C	-4.0441377453	-1.2348815279	2.5502270522
H	-4.7850218658	-1.6213961429	1.8512730588
C	-4.4121989178	-0.9778643849	3.805168369
H	-5.4305511591	-1.141396924	4.1441551724
H	-3.7076548686	-0.6000062402	4.5420588842

TS_E_2

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C	0.1937923844	0.3851457762	0.7561598673
H	-0.3878624014	-0.4339215489	1.1620340729
C	-0.1938951159	1.0933554474	-0.4180825979
O	-1.2374960784	0.4399626311	-1.0930748148
C	-2.228375801	1.4041310068	-1.483283616
O	-1.5348031383	2.6419337453	-1.5087367222
C	-0.5340431629	2.6212787076	-0.495484448
H	-0.951196532	2.952977168	0.4677035195
C	-2.6943093402	1.0797693872	-2.8926902087
H	-1.8366771853	1.0873384912	-3.5681102436
H	-3.4221066375	1.8221066038	-3.2301870186
H	-3.1616655301	0.0920914336	-2.917792145
C	-3.3649583894	1.4248440378	-0.4583032219
H	-4.1030663789	2.1849912009	-0.7286806488
H	-2.9830428944	1.6539673291	0.5404218379
H	-3.8594241819	0.4503162504	-0.4211369822
C	0.5609061755	3.6270672519	-0.875251118
H	1.1440671827	3.2334178539	-1.7219166319
O	1.3984876573	3.8995270993	0.2422474061
H	1.9108013022	3.0866946929	0.4103124465
C	-0.0205441939	4.9852933038	-1.277200498
H	-0.700451357	5.3303382258	-0.4794847526
H	-0.5990767372	4.8927759416	-2.1983489619
O	1.0237247235	5.9119566669	-1.5063506184
H	1.633370314	5.7818700417	-0.7631759302
C	2.321122146	-0.5258253803	1.7932095494
C	2.80682204	-1.5158713596	0.7212320784
H	3.5151361898	-2.230131141	1.14933502
H	3.3113304196	-0.9740278226	-0.0816684406
H	1.96852789	-2.0734002076	0.2911230323
C	3.501504065	0.2133368814	2.4368101877
H	4.1654957348	-0.5007067791	2.9287639198
H	3.1493053382	0.9266940806	3.1881571152
H	4.065317764	0.7595130117	1.6787713913
C	1.4496522536	-1.2168372413	2.8752243662
H	0.6363508066	-1.764501584	2.3809564766
H	0.9898359995	-0.4454571133	3.5035780166
C	2.2018409993	-2.1910179243	3.7431059812
H	2.6495272603	-3.0455500902	3.2368814581
C	.3202537476	-2.0903281922	5.0668245922
H	2.8530973679	-2.8360446549	5.6487947798
H	1.883782634	-1.261517586	5.6188982373

TS_Z_1

H	-0.0458026074	-0.7414123251	-1.2039255297
O	-1.103931938	-1.3080832206	-1.0201068608
N	-1.480318044	-0.4191543284	-0.0774033805
C	-0.4444765638	0.2513310904	0.4148140764
H	-0.6036967805	1.1822634548	0.9426870867
C	0.814512411	-0.1665865343	-0.1199701349
O	1.3089739958	-1.459537571	0.2784448396
C	2.600079407	-1.5581567297	-0.2917564866
O	3.1290734699	-0.2130246742	-0.2868811464
C	2.0600473731	0.7103450853	-0.0530504801
H	2.058534993	1.4738922801	-0.842347676
C	3.4518960986	-2.4307751209	0.6194864543
H	4.4809840514	-2.4663135611	0.2523970691
H	3.05453837	-3.4489427021	0.6495150891
H	3.4473480032	-2.0190003845	1.6309848819
C	2.5541184619	-2.0673981502	-1.7338679177
H	3.5583319774	-2.0634715389	-2.166899417
H	1.9164760868	-1.4204707565	-2.3409771738
H	2.1568000638	-3.0858185273	-1.7671636672
C	2.2952128425	1.4185848901	1.2897691274
H	2.1832496506	0.6818953355	2.101332925
O	1.3142065822	2.4483905042	1.4062813032
H	1.6418206527	3.0243812662	2.1148596076
C	3.6839295327	2.0423454839	1.3859475899
H	3.8500187115	2.6953965637	0.5161364734
H	4.4516368459	1.260780772	1.3911757519
O	3.6858540381	2.8014359519	2.6018332016
H	4.4592738724	3.3777686822	2.6023878525
C	-2.9204562029	-0.034514632	-0.0692340833
C	-3.1678845775	0.9994447881	1.0345330798
H	-4.2362007503	1.2210567756	1.0822745386
H	-2.6518900216	1.9419238543	0.8330118473
H	-2.8518802399	0.627683534	2.0142423354
C	-3.259383859	0.542297041	-1.4529942591
H	-2.7133978418	1.4755660796	-1.622085398
H	-4.3310405841	0.7434500474	-1.5215936964
H	-2.983586921	-0.1688980386	-2.2335970182
C	-3.7080047906	-1.3515367658	0.2040916481
H	-3.3576891998	-1.7457821945	1.1678300052
H	-3.4146311241	-2.0759588962	-0.5602282979
C	-5.205461473	-1.209646068	0.2330643133
H	-5.629142855	-0.623584543	1.0486564267
C	-6.0357893058	-1.7723795795	-0.6459909476
H	-7.112871195	-1.6561588499	-0.5701065367
H	-5.6671173697	-2.378359343	-1.4700827932

TS_Z_2

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O	-0.195303907	-1.7730853777	-0.1431379099
N	0.6648471178	-1.4972466005	0.8553483245
C	0.6119981823	-0.2193075421	1.2142640273
H	1.4377766646	0.2039324678	1.7738749125
C	-0.3705353033	0.5435893627	0.4992898426
O	-1.7481661719	0.3007485728	0.8070285453
C	-2.479206406	1.3827934622	0.2492577628
O	-1.5995886776	2.5210774392	0.3172195311
C	-0.2531460429	2.0625124397	0.4294170138
H	0.184974726	2.4777905342	1.3524360927
C	-2.8633251046	1.105315728	-1.2062984665
H	-1.9745775523	0.8689367594	-1.7969881359
H	-3.3454209392	1.9834868602	-1.6443070202
H	-3.5515624763	0.2572019504	-1.2625341221
C	-3.6823738007	1.6462416033	1.1424385813
H	-4.3483343357	0.7793867407	1.1471901315
H	-4.2371047509	2.5148737667	0.778401767
H	-3.3423767934	1.8417386276	2.1613729466
C	0.5895279483	2.553634027	-0.756425455
H	0.0934122698	2.2656993216	-1.6932690231
O	1.9024215597	1.9748462023	-0.6900725525
H	1.8187212431	1.0573487638	-0.9824653068
C	0.8017255168	4.062312965	-0.7589303996
H	1.2568921776	4.3576418186	0.2019569256
H	-0.1648138318	4.5659332395	-0.8435183312
O	1.5989677434	4.4664745216	-1.8571144163
H	2.3670073571	3.8764622892	-1.8420077934
C	1.784171416	-2.4650985251	1.0538250169
C	2.6279251848	-2.0390984462	2.2594319936
H	2.01309811	-1.9406830281	3.1589994035
H	3.1565652126	-1.0973161852	2.0861971962
H	3.3856556374	-2.8035397883	2.4429431263
C	1.1431939307	-3.8382062573	1.3096014968
H	0.5111309476	-3.799954005	2.2015014324
H	1.9171307336	-4.5926254785	1.4708749263
H	0.5216285817	-4.1367233811	0.4632944722
C	2.621651477	-2.4449863691	-0.2606965348
H	3.0421554295	-1.438211921	-0.377966534
H	1.9187598179	-2.6070030455	-1.0856868714
C	3.7297572708	-3.4588846972	-0.3198416648
H	3.4281691985	-4.5042707967	-0.3721067498
C	5.0303300099	-3.1630412233	-0.3362794828
H	5.7902514865	-3.9359591974	-0.3985108025
H	5.3832374699	-2.1349680725	-0.3006096021

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C	-2.146759382	2.0911802446	-0.5502283219
C	-2.7234775308	1.6410011084	0.7832257834
C	-2.3561101838	0.1880773579	1.1664904951
N	-0.8728183566	0.0291630239	1.0944466621
C	-0.2464274782	0.4609618201	-0.1688885328
C	-0.6348436539	1.9039150384	-0.5125625758
C	-0.3865542922	-1.2602853459	1.6302266512
C	0.6718358081	-1.9665428263	0.7848054691
C	1.8049467806	-0.9900816905	0.4549112111
C	1.282527188	0.3865331685	-0.0174985883
O	2.5540462395	-1.4942473966	-0.6526904544
C	2.9326753221	-0.3738337049	-1.464653931
O	1.8917741932	0.583256601	-1.2959884238
C	2.9592892751	-0.8165871922	-2.9185422354
C	4.2712931056	0.1948352152	-0.9854708745
O	-2.5169755359	3.459404514	-0.7261545345
O	0.0709915445	-2.4670698261	-0.3978352263
C	-2.8107001478	-0.009835561	2.6266380674
C	-3.1106044449	-0.8118356154	0.2548516464
H	-2.5712022129	1.4842913141	-1.3662924197
H	-3.8134853584	1.7461833527	0.7709304466
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H	-0.512404413	-0.1935154341	-1.0127621412
H	-0.230996359	2.5832139905	0.2489949811
H	-0.1768611346	2.1666477462	-1.4737808315
H	0.0354524298	-1.1128550059	2.63637506
H	-1.2046386884	-1.9782337952	1.7409499518
H	1.0796434935	-2.7980299836	1.3830006507
H	2.450854825	-0.8789562412	1.3362999913
H	1.6028848341	1.1712528757	0.681690574
H	3.2041276778	0.0305080904	-3.5641292873
H	3.7092950345	-1.5980203139	-3.0655924654
H	1.9769051474	-1.2013659205	-3.2014354884
H	5.0624090173	-0.5535333595	-1.0844212809
H	4.5393142623	1.0742460279	-1.5771599053
H	4.2099470537	0.4958173543	0.0641304322
H	-2.138082648	3.7577888443	-1.5637204834
H	0.8004391775	-2.5677643887	-1.0306615111
H	-2.2275097352	0.6309742145	3.2949070258
H	-2.7074848807	-1.0445530246	2.9642702315
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H	-2.9029598391	-1.8484827571	0.5345495435
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C	-2.7619666921	0.5343427228	-1.3246379813
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N	-0.805668764	-0.7544797669	0.5750551221
C	-0.498683353	0.4608158209	-0.2303193115
C	-1.2384536186	0.5018629726	-1.5709663129
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C	1.586019469	-1.3214107126	1.172881432
C	1.6322204909	0.193879829	0.9871457807
C	1.0148042659	0.5446059592	-0.3450490024
O	2.9480591599	0.7303892827	0.8727454544
C	2.8643648616	1.8591376431	-0.0380566446
O	1.5331035595	1.8480016791	-0.5878933087
C	3.903111336	1.6554603465	-1.135797372
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O	-3.4872317557	-0.1820868398	-2.3280040191
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C	-2.6533931843	-1.6537159137	1.926826135
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H	-3.0996541511	1.5829409757	-1.3155629949
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H	-0.9118564669	1.3729415865	-2.1519806305
H	-0.9882355678	-0.3935022637	-2.1521428223
H	-0.1500427581	-2.6272134662	1.2094083679
H	0.4468512317	-2.2330625533	-0.3969970034
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H	1.0832641222	0.6877081038	1.7998890749
H	1.3820365167	-0.1547187497	-1.1110683047
H	3.8789158527	2.491803207	-1.8396291548
H	4.9053674642	1.5900612093	-0.7026169644
H	3.6992304138	0.7302666164	-1.6807585444
H	4.0437240047	3.2100914344	1.1691291478
H	2.9057189781	4.0157615229	0.065326565
H	2.3026749075	3.2213336793	1.5341100058
H	-3.2456242743	0.1910470371	-3.1863541304
H	3.3921495382	-1.3741126431	0.5132419628
H	-2.5578753762	-0.8074898098	2.6131895445
H	-2.0382057316	-2.4720258466	2.3146779228
H	-3.6944494426	-1.9952474365	1.9332725873
H	-1.8550125352	-3.330998535	-0.1010185388
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H	-2.1205151082	-2.2312670216	-1.4682292045

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C	-3.0845690648	0.6385412574	-0.0235252839
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C	-0.8653087876	-0.4153218716	0.4427803749
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C	-3.8021877051	-0.572084904	0.6752321791
C	-2.8427930884	-1.7129551505	0.3126138965
O	-2.3699566776	-1.2951394426	-0.9952640466
C	0.4212835081	-0.8200133997	-0.2751015085
C	-3.9000601203	1.1520208772	-1.2175284213
C	-2.7620290716	1.798936873	0.923172672
C	1.3837602162	0.2632761776	-0.7983867265
O	2.6241149502	-0.4579043244	-0.8655018327
C	2.5505023063	-1.6076690502	0.0047839246
O	1.2727102797	-1.5401240888	0.6260235571
C	1.5674100398	1.5046307072	0.0856724619
C	2.8186581116	2.2923791944	-0.301319316
O	0.4311477528	2.345114968	-0.0721589414
O	2.7763404615	3.4907398836	0.483235778
C	3.6175148376	-1.5185304188	1.089043153
C	2.688509102	-2.8674748982	-0.8525638073
H	-0.6693529852	0.4169481179	1.1155373481
H	-1.7505559942	-1.4373894097	2.2104363959
H	-0.9542092008	-2.5290678142	1.0677714811
H	-3.9061165765	-0.4359866146	1.7559417157
H	-4.7977294877	-0.7410620661	0.2549409701
H	-3.2866878553	-2.7064984738	0.2273456382
H	0.1366234501	-1.46376593	-1.118433582
H	-4.8791174156	1.5128785113	-0.8835893586
H	-3.3757360064	1.9739688277	-1.7140082613
H	-4.05258875	0.3505185353	-1.9434557242
H	-2.0381897715	2.4765953265	0.4646574659
H	-3.6798461942	2.3553161764	1.1376952579
H	-2.3559730854	1.4613087491	1.8812299024
H	1.1104722383	0.5892384046	-1.8069702551
H	1.6730847252	1.1887981596	1.1370627253
H	3.7217603117	1.707097062	-0.1003150366
H	2.7815714467	2.5248956468	-1.375694724
H	0.715942182	3.2080746774	0.2692818927
H	3.4002899161	4.1238728358	0.1091510696
H	3.546372549	-2.3773311689	1.7624740369
H	4.6135245786	-1.5099300742	0.6382925665
H	3.4826319686	-0.6049863073	1.6722368215
H	1.8799926008	-2.9230098632	-1.5853268186
H	3.6384441678	-2.8508208257	-1.3939722902
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2a

C	1.6178715717	1.3482414522	2.207525331
N	1.3696156615	0.5510412554	0.9409027333
C	0.2893774692	-0.4748246682	1.1034493137
C	0.9409305375	-1.5617450402	2.0108552923
C	2.2450193671	0.2706010814	3.1597614511
C	2.3281182002	-0.9382826323	2.2136902121
O	2.5445320033	-0.2977017626	0.9259744293
C	-0.1073819866	-0.9886942742	-0.2807364705
C	2.6402305783	2.4330275403	1.8424001899
C	0.3369638854	2.0011558503	2.735604191
C	-0.9686717664	-0.054158279	-1.1483264665
O	-1.6737602613	-0.9936669	-1.9628837694
C	-1.8729855728	-2.1897903636	-1.2097325036
O	-0.9673352348	-2.1139958969	-0.0953801138
C	-0.2305832021	0.9265945144	-2.0687021357
C	-1.1996163007	1.6912774141	-2.9748167917
O	0.443114868	1.9265923225	-1.3177723318
O	-2.0257864647	2.5545072331	-2.2100208816
C	-1.5180128647	-3.3760766864	-2.0999462702
C	-3.2959437919	-2.2538239057	-0.6600932256
H	-0.5873181729	-0.0189728636	1.5645492027
H	0.3958473844	-1.7122512269	2.9460578556
H	0.9989662098	-2.5201251898	1.49141983
H	1.6249789187	0.0705877523	4.03847969
H	3.2359336314	0.5777922193	3.5044135492
H	3.1449037072	-1.6375621719	2.397106807
H	0.8025288392	-1.2823787902	-0.8271151545
H	2.9590249012	2.9673011218	2.7433459423
H	2.204756883	3.157658307	1.1474139421
H	3.5190138729	1.986303501	1.3731824048
H	-0.1766480832	2.5428624092	1.9345708191
H	-0.360757075	1.2839262698	3.1759271355
H	0.5953006757	2.7235904767	3.5153296626
H	-1.6684022707	0.5185673947	-0.5208574284
H	0.466284062	0.3474715501	-2.6972075475
H	-1.8494725113	0.9944308106	-3.5090549142
H	-0.6071843443	2.2556018388	-3.7121494567
H	0.9588881321	1.4986595118	-0.5980488577
H	-1.4081141556	3.0122646132	-1.6184521919
H	-1.6516208778	-4.3146474661	-1.5552262283
H	-2.1586643694	-3.3890934751	-2.9860981867
H	-0.4773034359	-3.2980970081	-2.4236358857
H	-3.5135380033	-1.3531158855	-0.080734636
H	-4.0161237367	-2.3263768622	-1.4794906014
H	-3.4135328775	-3.1245710916	-0.0087379349

IXa

C	-0.3682117394	1.4024155488	-2.6993305971
C	-1.8620771015	1.4506178504	-2.3945276226
C	-2.3616156459	0.207383586	-1.6291870842
N	-1.5129140965	0.0266071651	-0.4243615012
C	-0.0694653402	-0.0722547769	-0.6572450596
C	0.4188816213	1.1766201987	-1.4069878577
C	0.6336878208	-0.1646714121	0.70120273
O	-0.0286983082	2.6460543141	-3.3133322496
C	-3.7897415432	0.4634718584	-1.1234301867
C	-2.3709291773	-1.0452755394	-2.5373270795
C	0.3530328857	-1.3987500911	1.6111435221
C	-0.016652615	-2.6783009452	0.8690750605
O	-1.1307322587	-2.9034668358	0.4441472303
O	2.0405307673	-0.2726519002	0.5030857337
C	2.6095482404	-0.7823731832	1.7018400642
O	1.5737027688	-1.5885024469	2.309853178
C	2.9856048766	0.3423960692	2.6666279657
C	3.78932813	-1.6695316164	1.3331016245
H	-0.1600004156	0.5759560827	-3.3986294346
H	-2.0451443222	2.3436946277	-1.7854908551
H	-2.4255881214	1.5696461514	-3.3261449798
H	-1.8253379319	-0.8242767834	0.041491872
H	0.2212482575	-0.9659738975	-1.2399379323
H	0.27659514	2.057355863	-0.7681672713
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H	0.3843085143	0.7388955355	1.2759868047
H	0.9156882492	2.623469007	-3.5177159164
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H	-3.8072259492	1.3274720884	-0.4534719848
H	-4.472485892	0.6507470668	-1.9587082164
H	-3.0303671925	-0.8983047212	-3.3996425087
H	-1.3772092146	-1.2916931279	-2.9219780169
H	-2.7319969749	-1.9147570261	-1.9782449926
H	-0.4559293758	-1.1818075547	2.3188589432
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H	2.1200565547	0.97494366	2.8786914798
H	3.3408426082	-0.0771574548	3.611557617
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