

**Enantioselective Total Synthesis of (–)-Acetylaranotin, A Dihydrooxepine
Epidithiodiketopiperazine**

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Supporting Information 2 (NMR Spectra)

JAC6-67 CDCl3 indy

Sample Name:

JAC6-67

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-67

FidFile: PROTON02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jan 21 2011

Temp. 25.0 C / 298.1 K

Sample #33, Operator: jcodelli

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

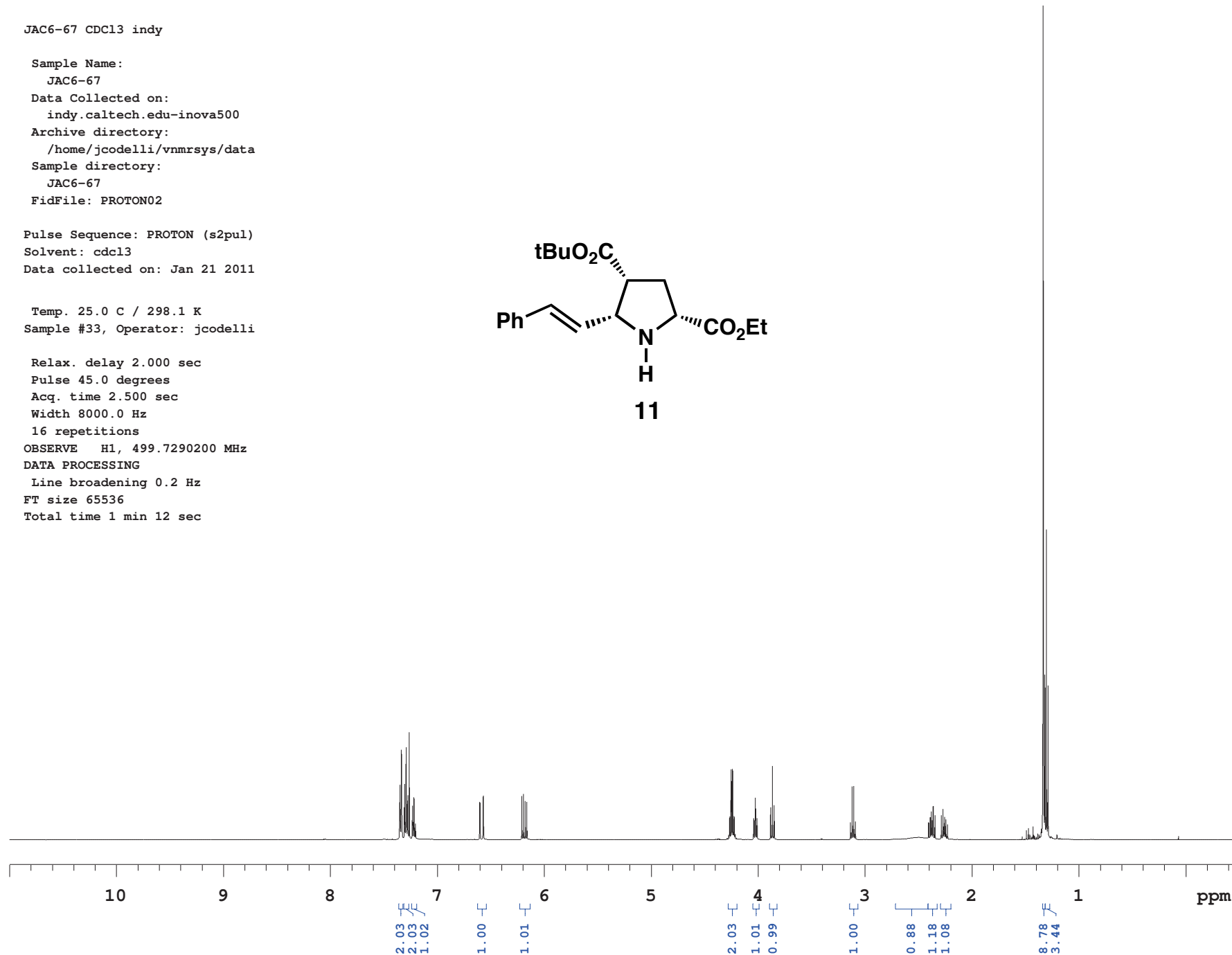
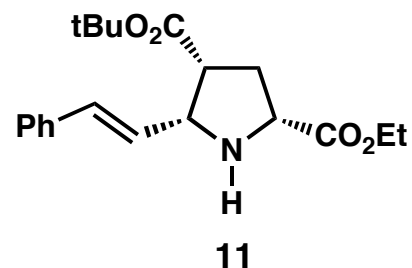
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



JAC6-67 CDC13 indy

Sample Name:

JAC6-67

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-67

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jan 18 2011

Temp. 25.0 C / 298.1 K

Sample #8, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

512 repetitions

OBSERVE C13, 125.6569681 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

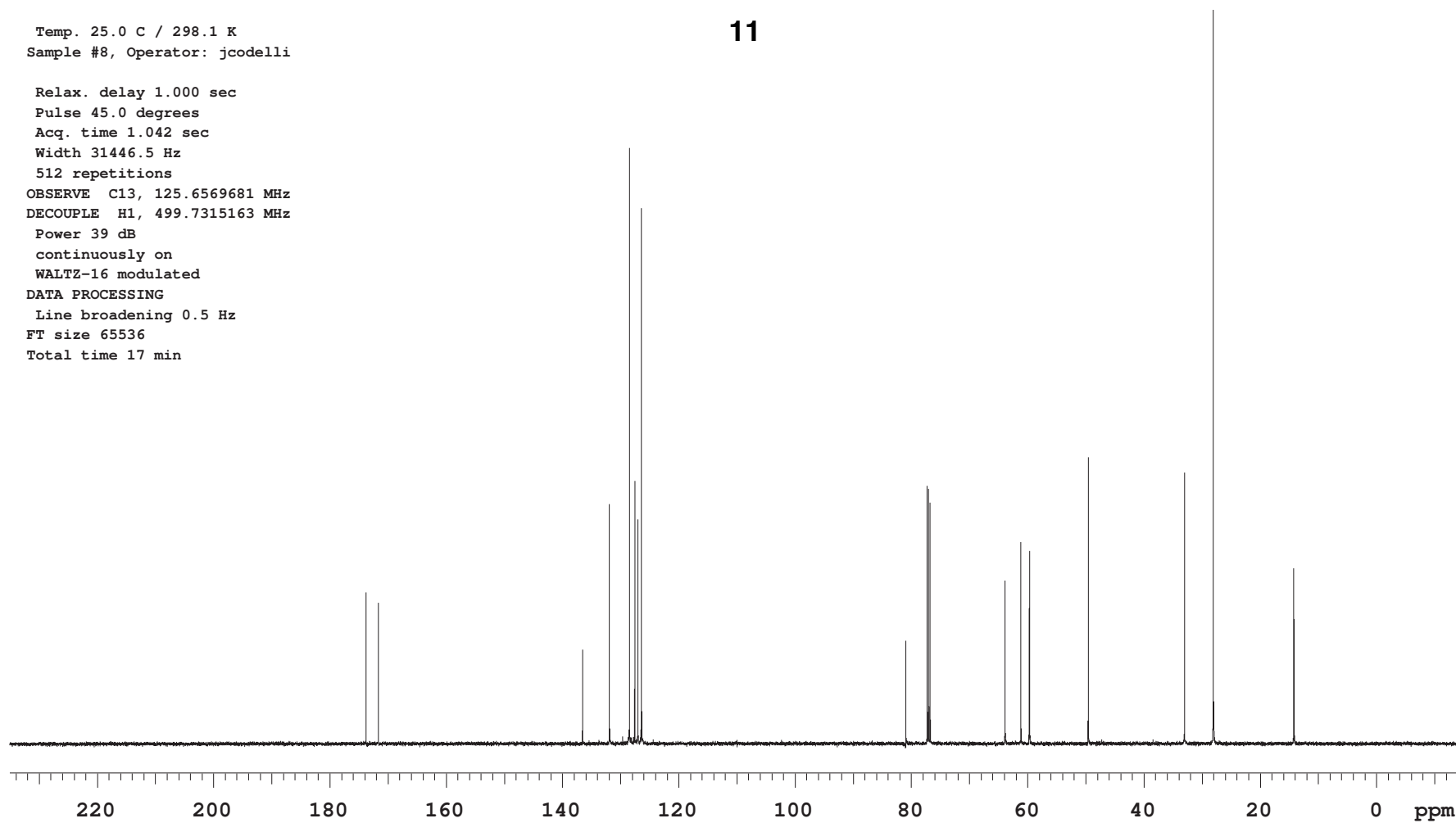
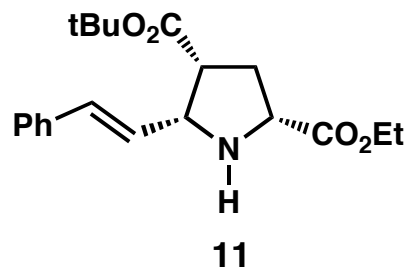
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 17 min



ALP-III-28characterize

Sample Name:

ALP-III-28characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-III-28characterize

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Aug 12 2011

Sample #46, Operator: apuchlop

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

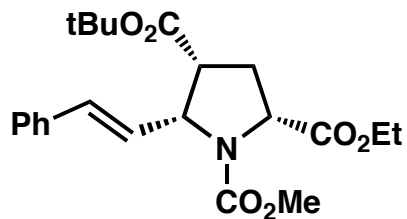
OBSERVE H1, 499.7225135 MHz

DATA PROCESSING

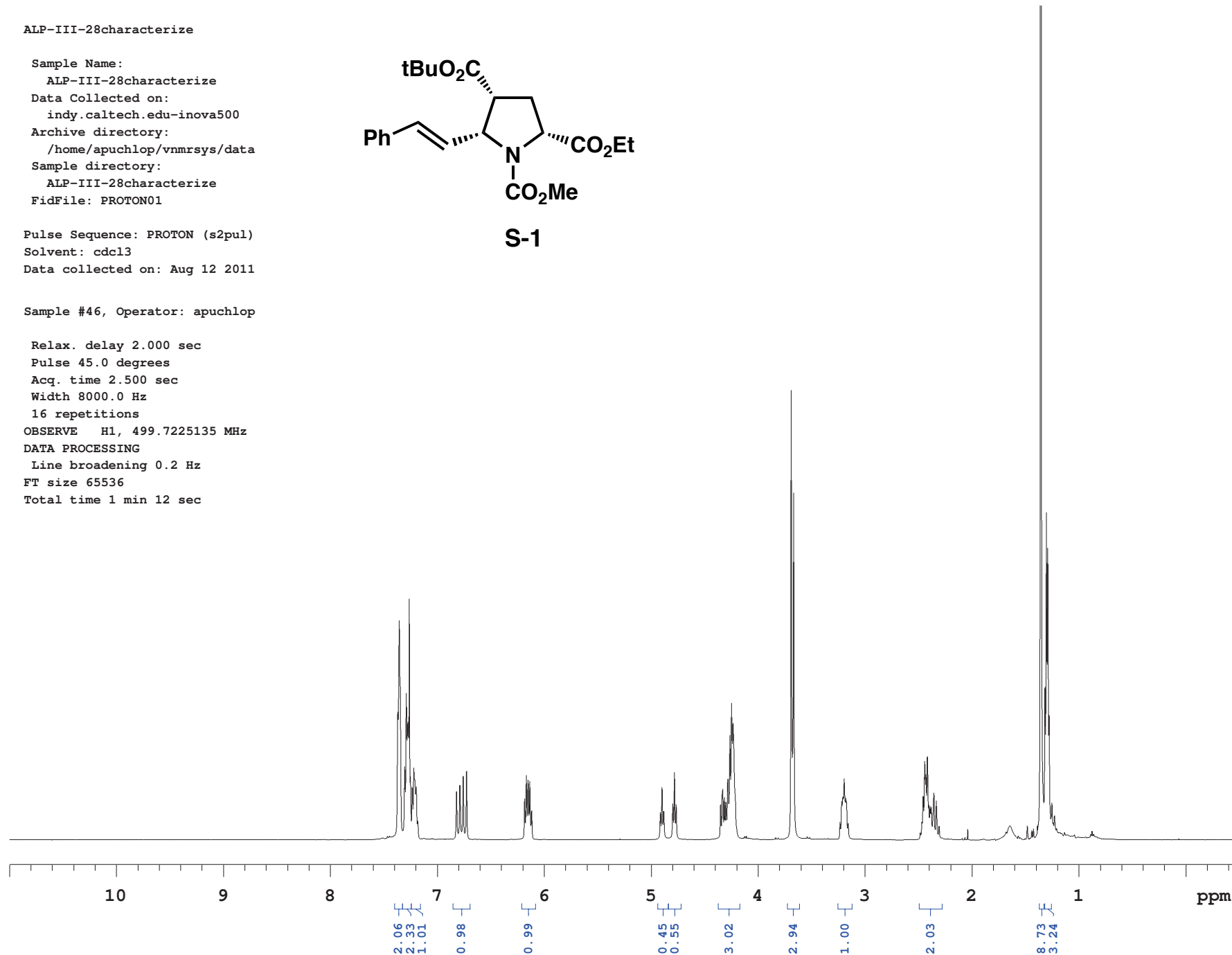
Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



S-1



ALP-II-157flash

Sample Name:

ALP-II-157flash

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-157flash

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Aug 1 2011

Sample #46, Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6553271 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

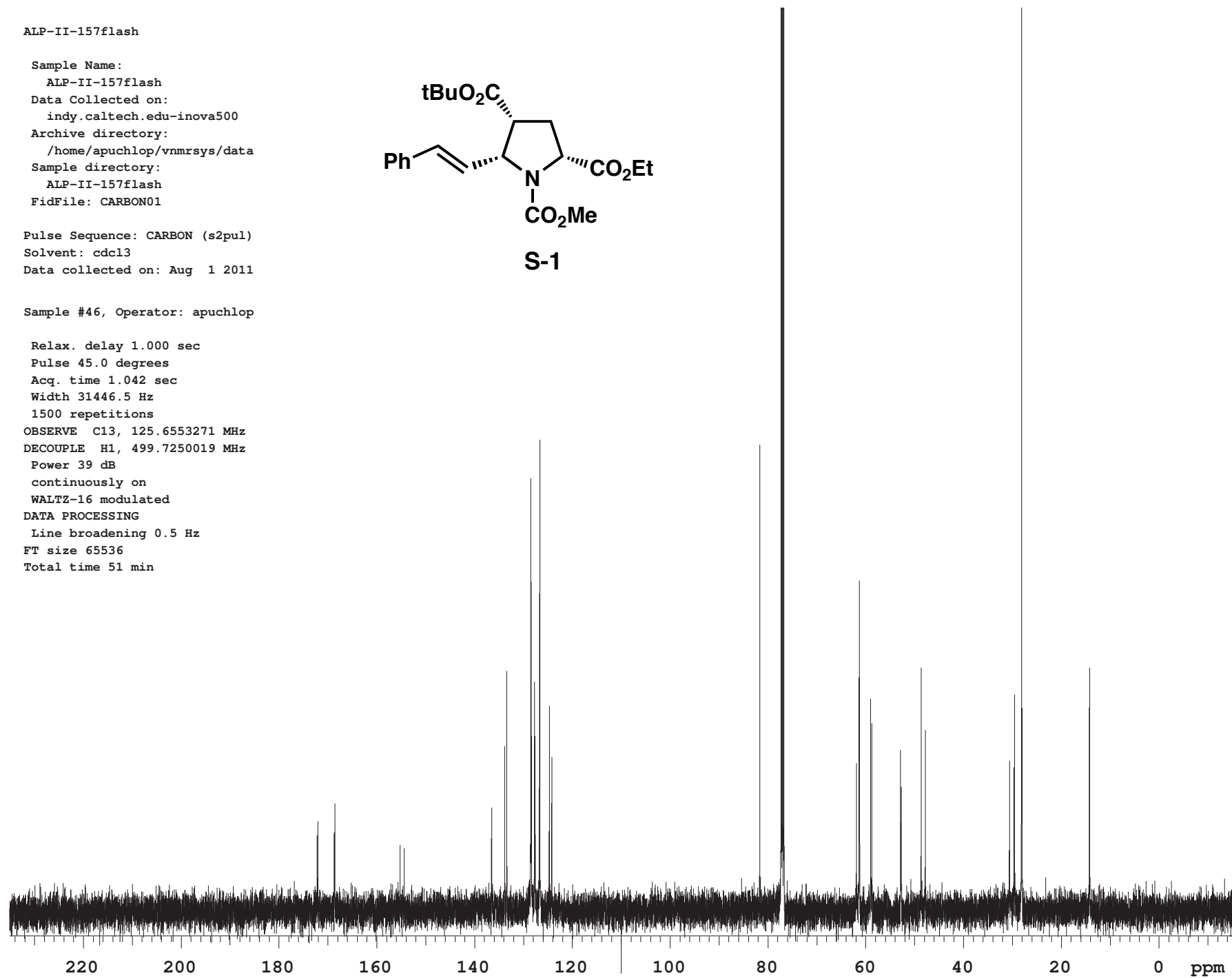
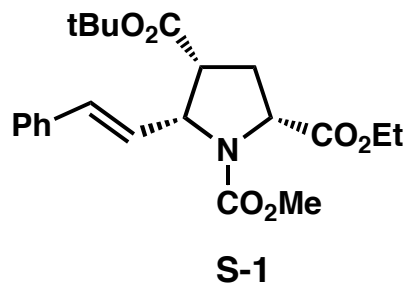
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



ALP-II-229

Sample Name:

ALP-II-229

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-229

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jun 7 2011

Temp. 25.0 C / 298.1 K

Sample #33, Operator: apuchlop

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

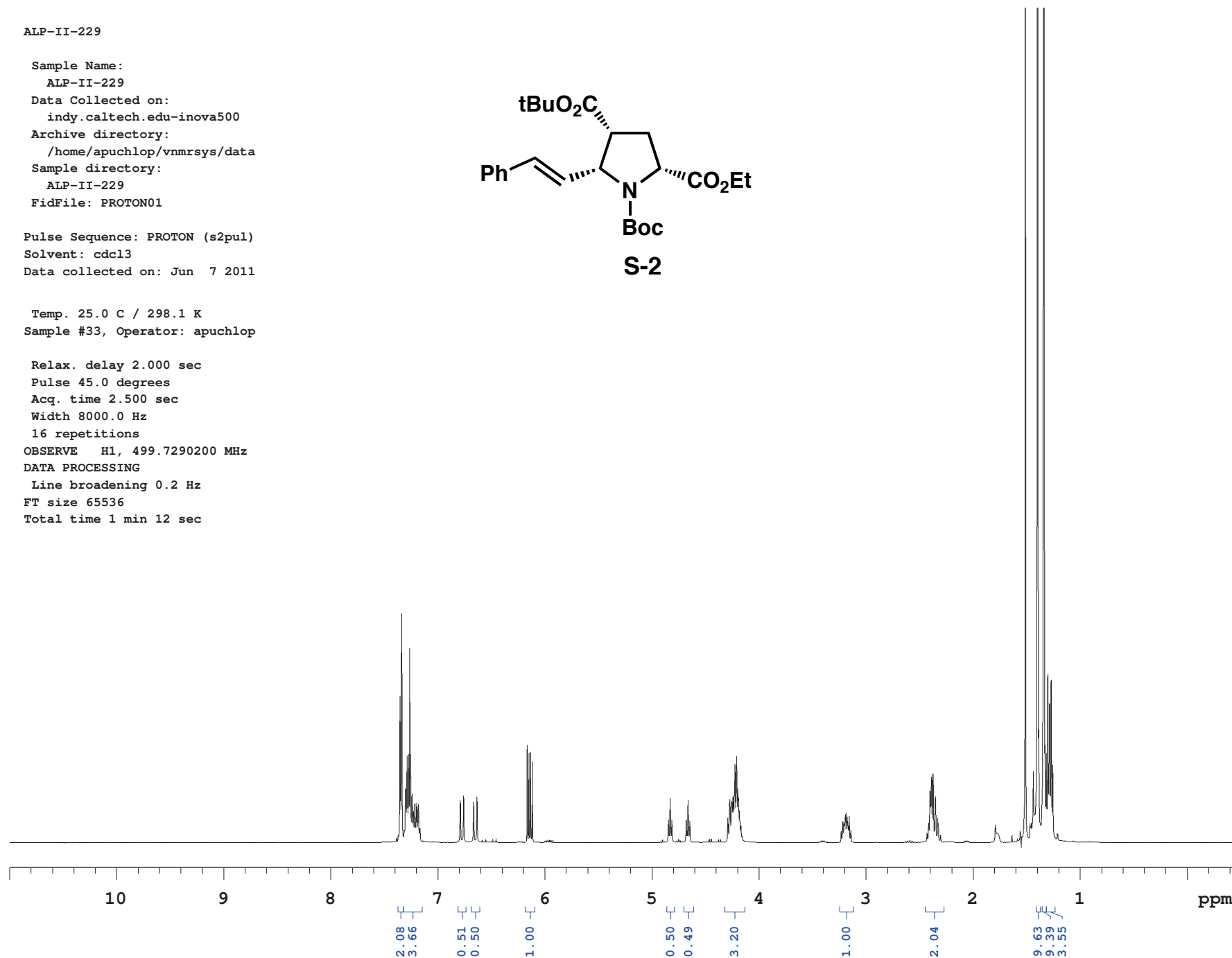
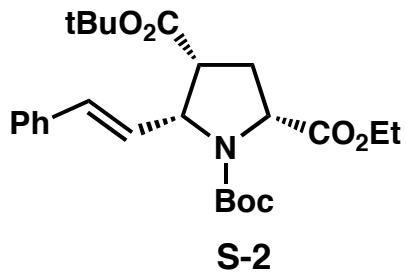
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



ALP-II-229

Sample Name:

ALP-II-229

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-229

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 7 2011

Temp. 25.0 C / 298.1 K

Sample #33, Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6569690 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

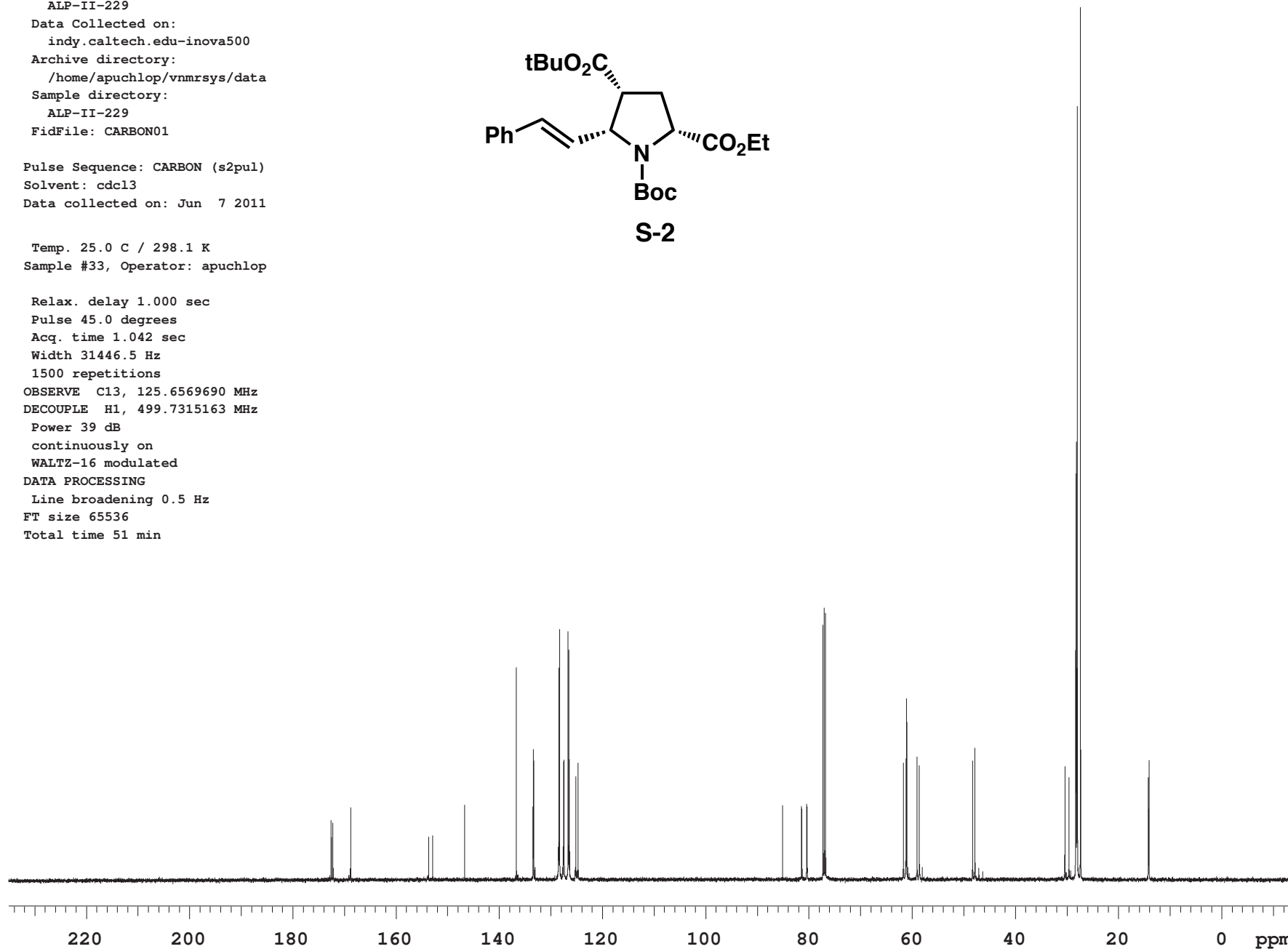
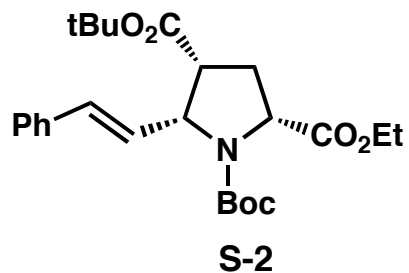
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



JAC6-79 CD3CN indy

Sample Name:

JAC6-79

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-79

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Feb 19 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

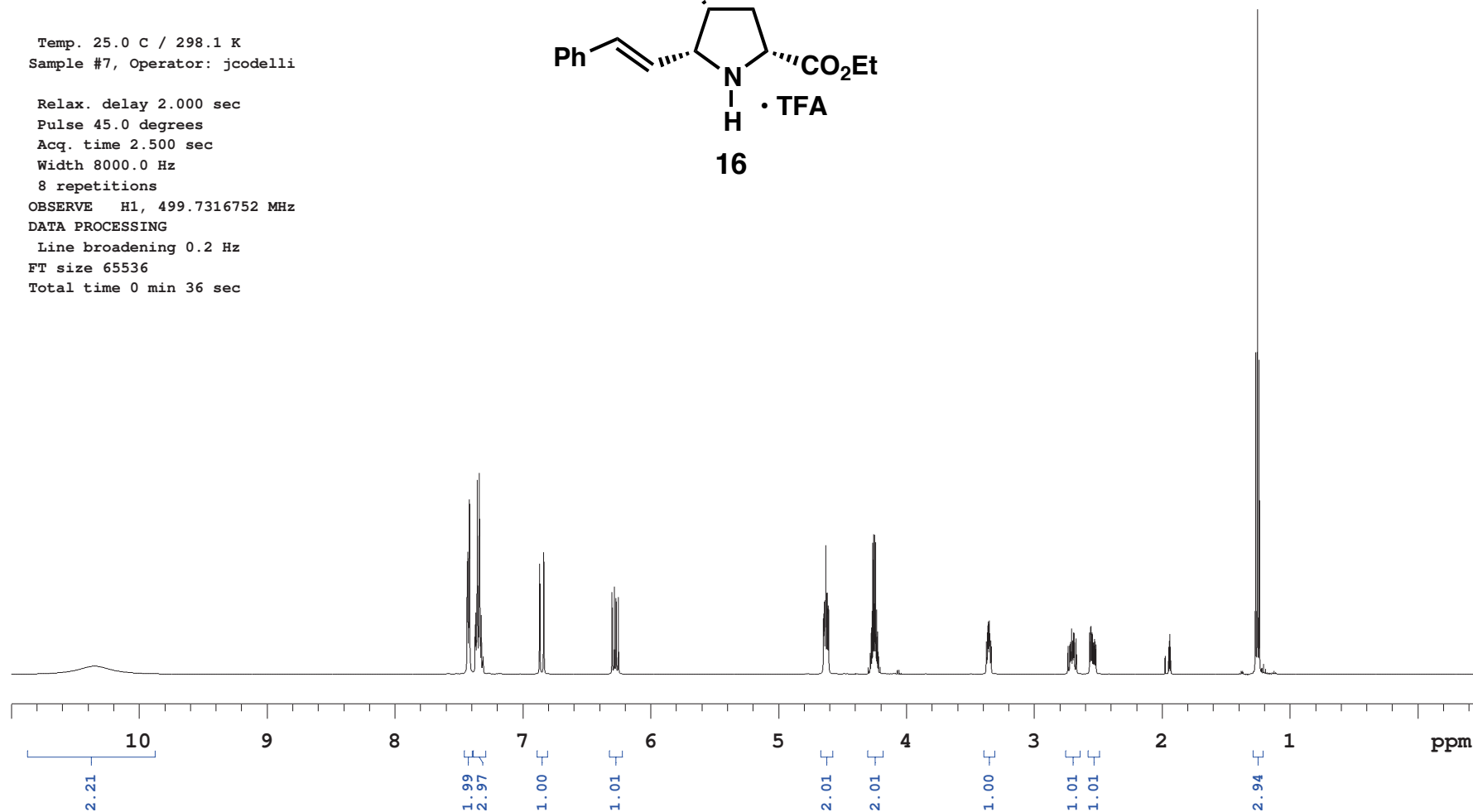
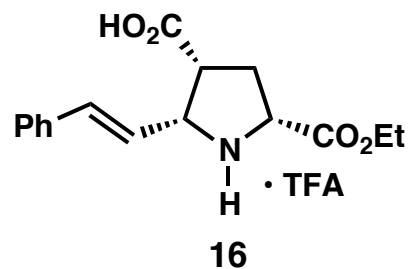
OBSERVE H1, 499.7316752 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 36 sec



JAC6-79 CD3CN indy

Sample Name:

JAC6-79

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-79

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Feb 19 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6575114 MHz

DECOUPLE H1, 499.7341599 MHz

Power 39 dB

continuously on

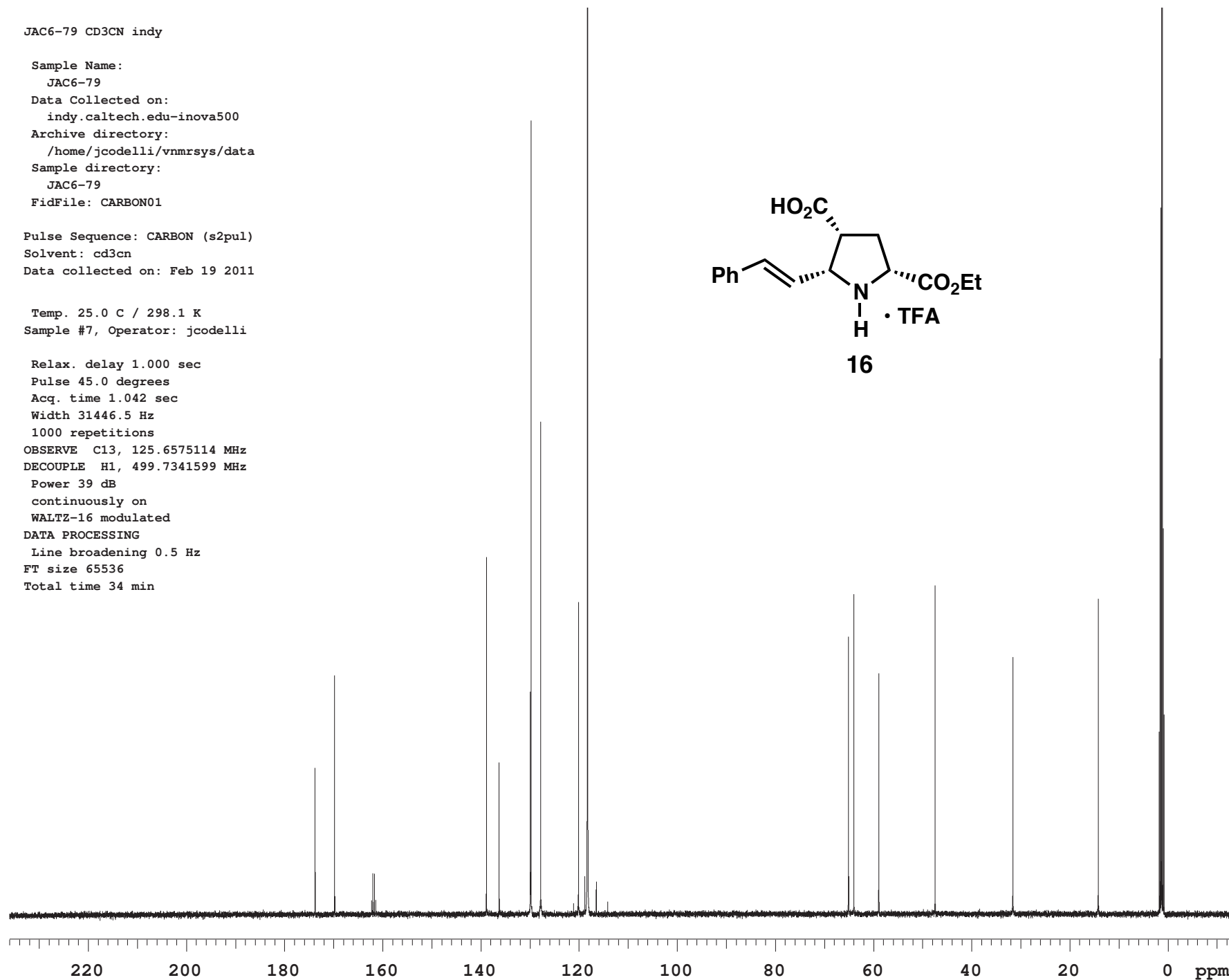
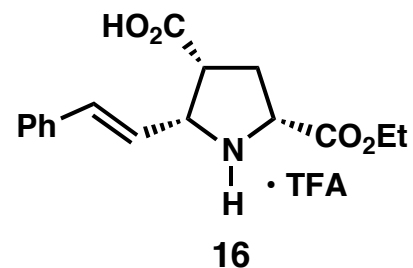
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



JAC6-85 CD3CN indy

Sample Name:

JAC6-85

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-85

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Feb 20 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

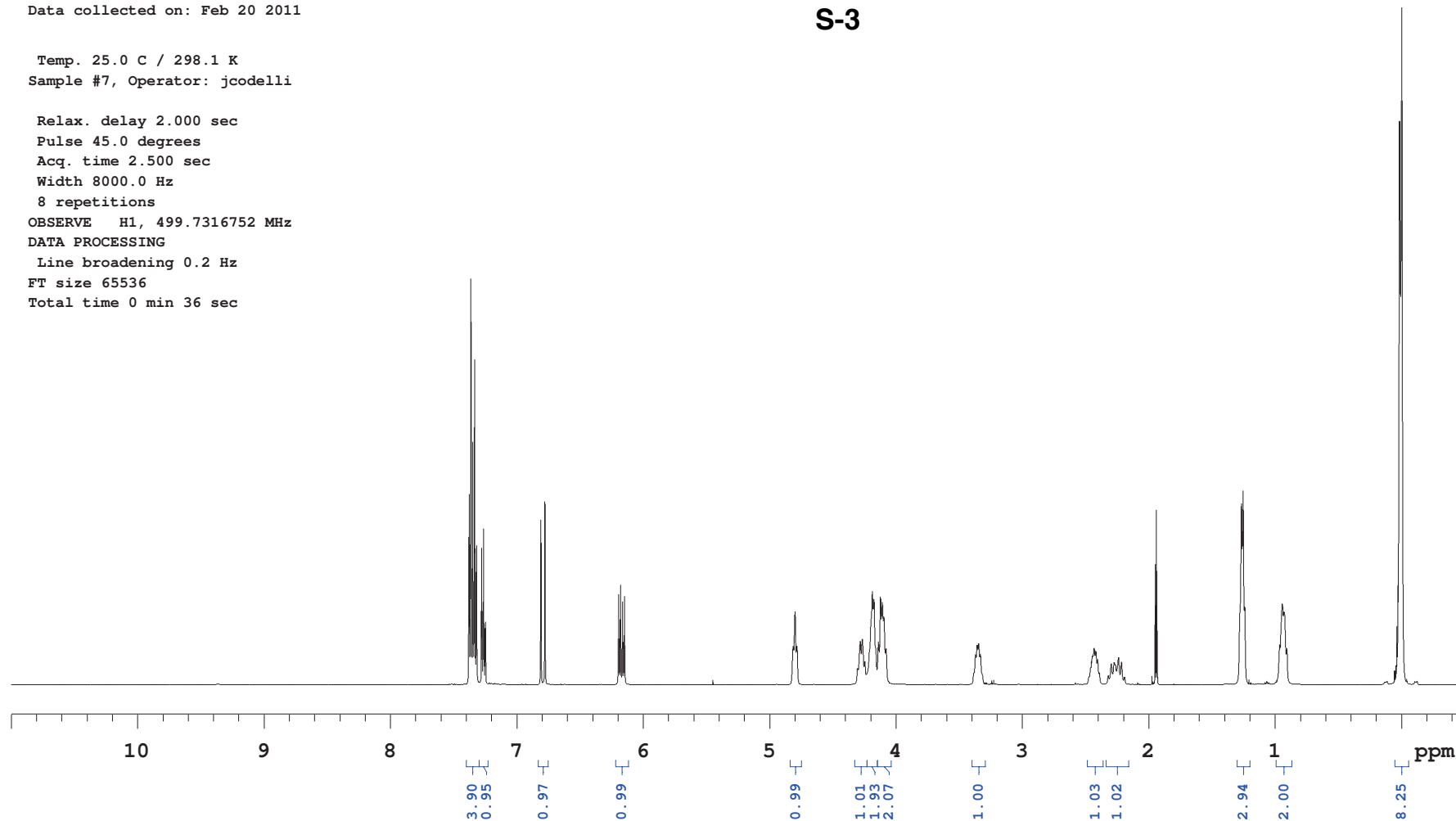
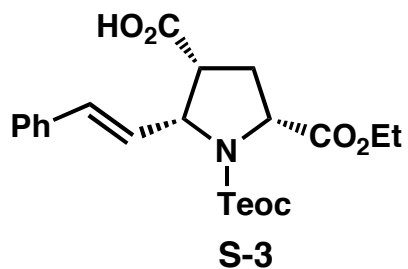
OBSERVE H1, 499.7316752 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 36 sec



JAC6-85 CD3CN indy

Sample Name:

JAC6-85

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-85

FidFile: CARBON02

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Feb 20 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

5000 repetitions

OBSERVE C13, 125.6575066 MHz

DECOUPLE H1, 499.7341599 MHz

Power 39 dB

continuously on

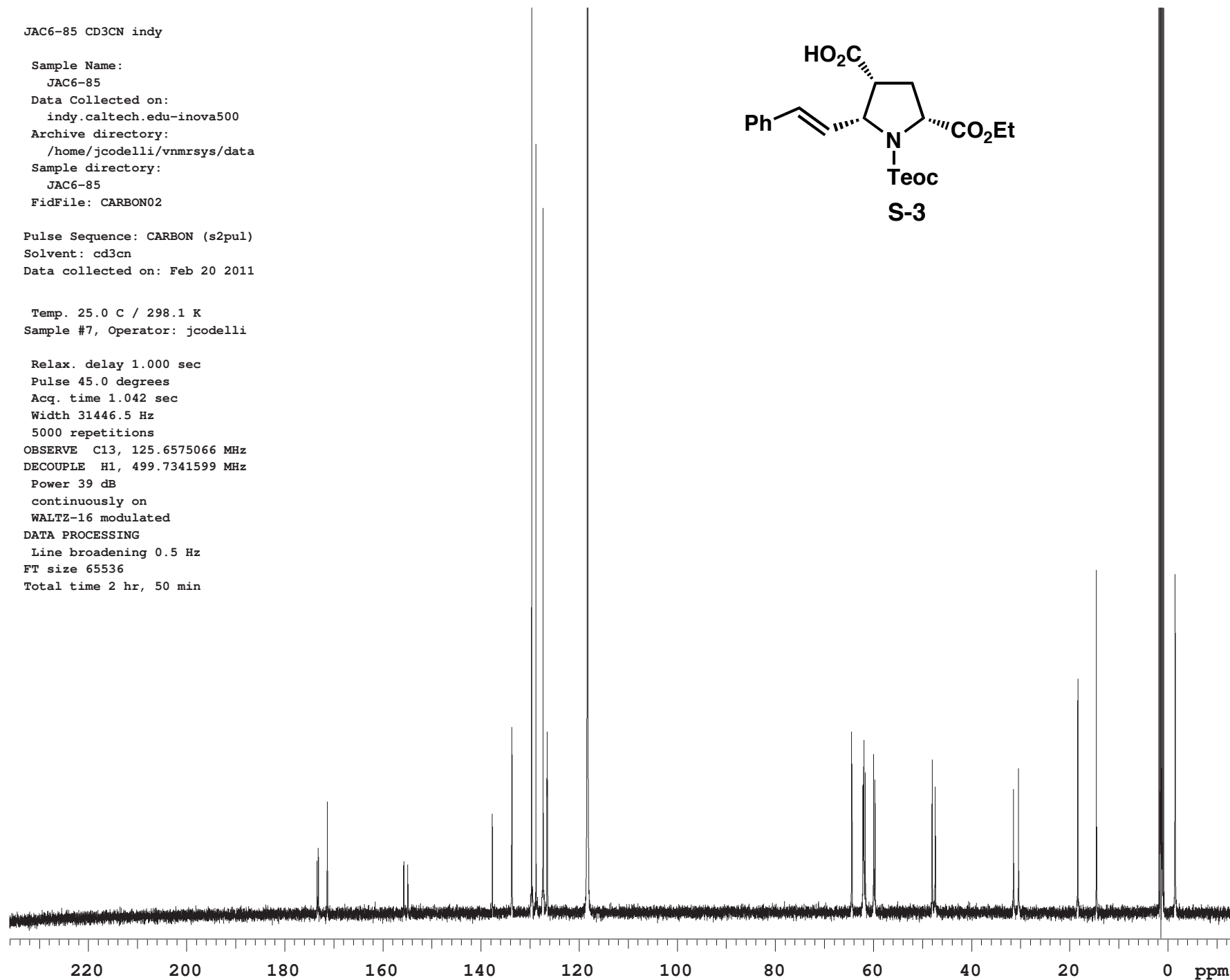
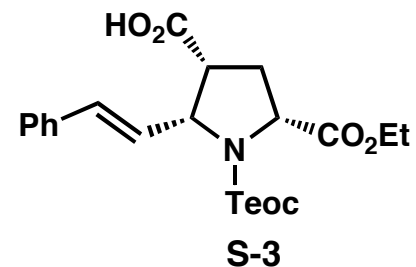
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 2 hr, 50 min



ALP-II-175characterize

Sample Name:

ALP-II-175characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-175characterize

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jun 14 2011

Temp. 25.0 C / 298.1 K

Sample #46, Operator: apuchlop

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

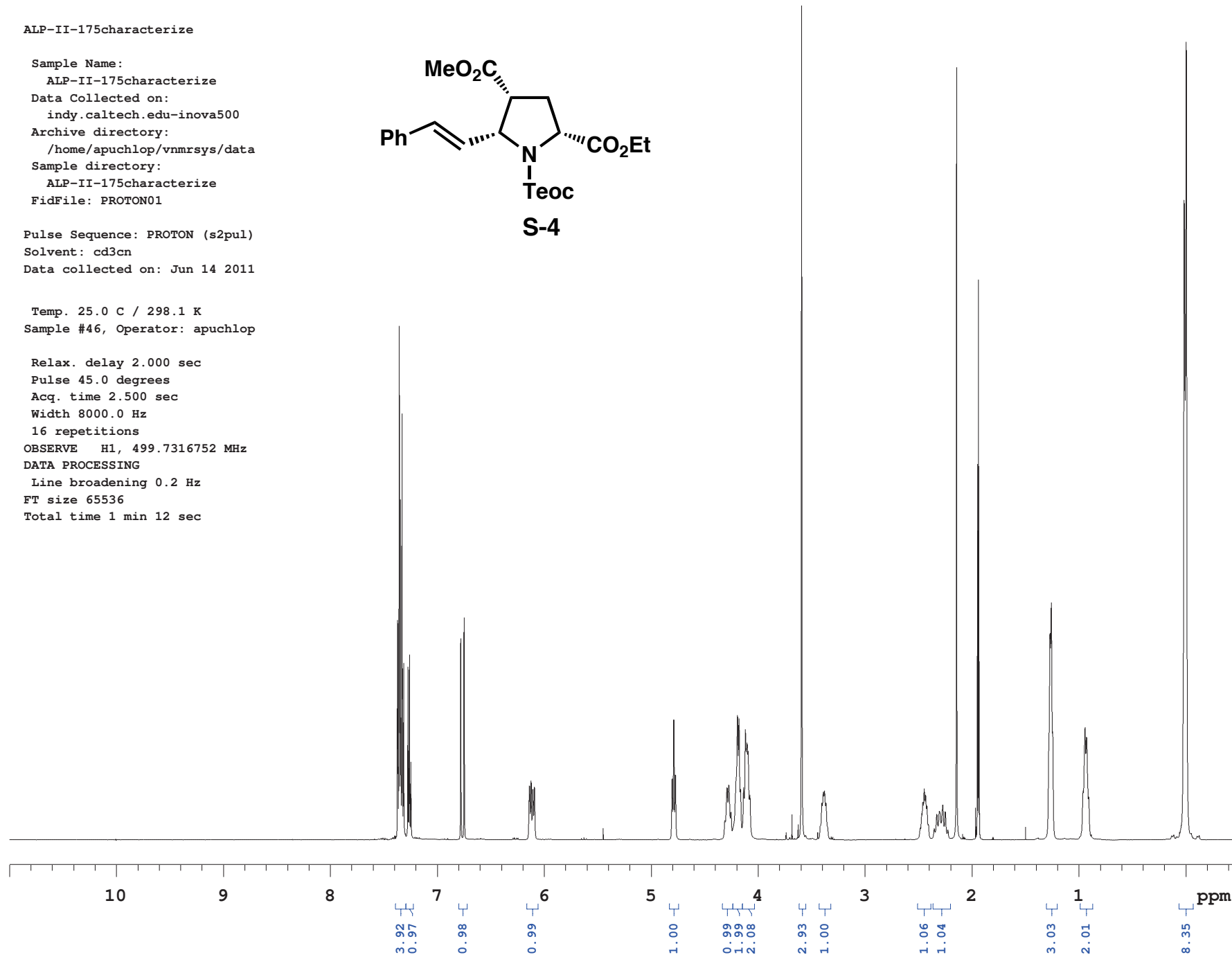
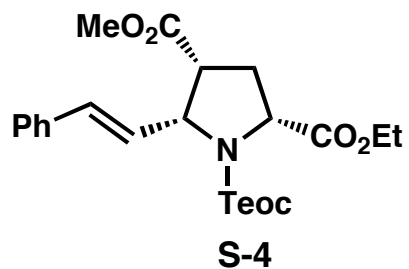
OBSERVE H1, 499.7316752 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



ALP-II-175characterize

Sample Name:

ALP-II-175characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-175characterize

FidFile: CARBON02

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Jun 15 2011

Temp. 25.0 C / 298.1 K

Sample #46, Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

7000 repetitions

OBSERVE C13, 125.6575066 MHz

DECOUPLE H1, 499.7341599 MHz

Power 39 dB

continuously on

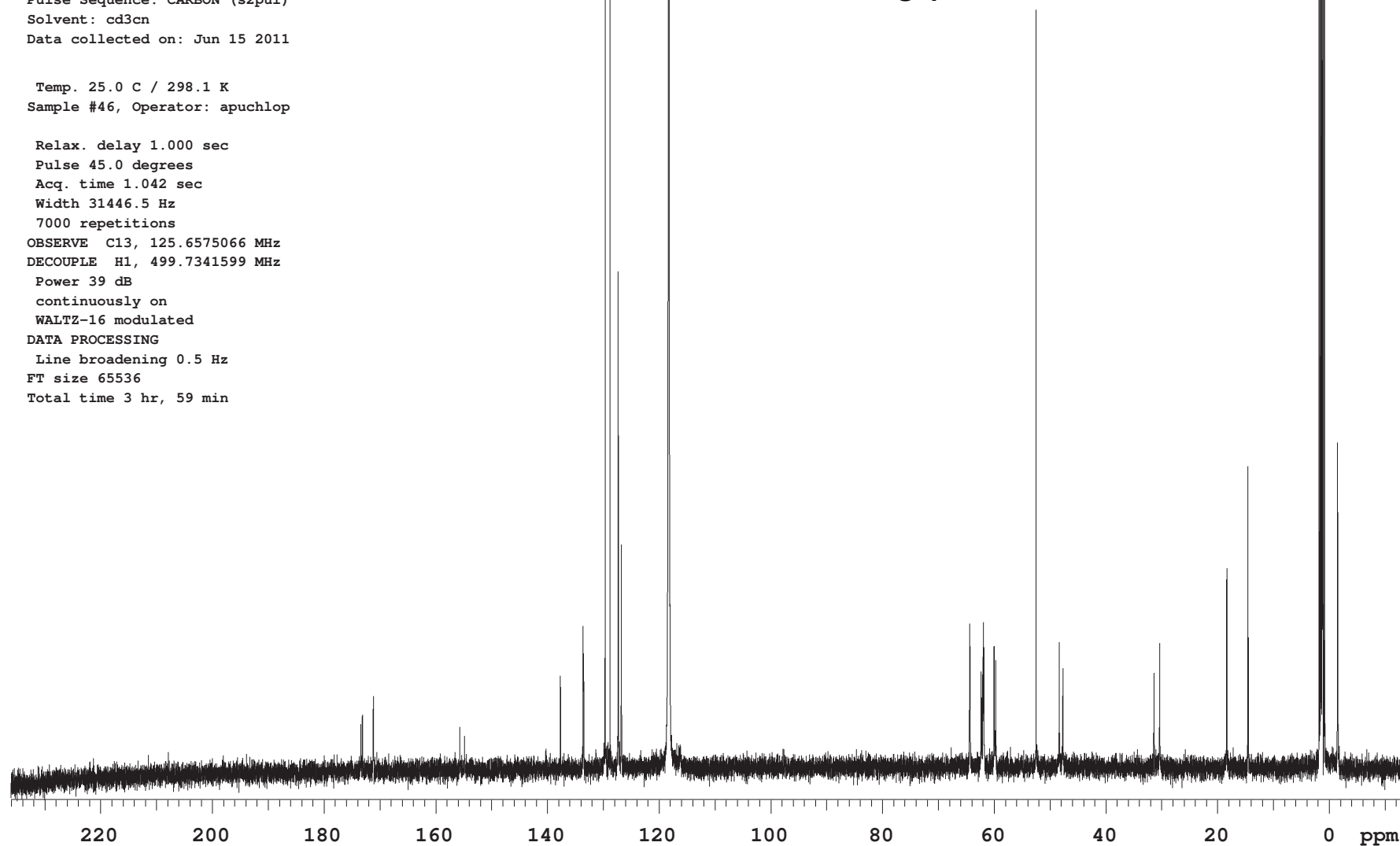
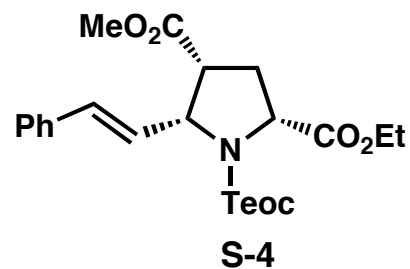
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 59 min



JAC6-113_115 60 _C DMSO siena

Sample Name:

JAC6-113_115

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-113_115

FidFile: PROTON02

Pulse Sequence: PROTON (s2pul)

Solvent: dmsd

Data collected on: Apr 27 2011

Temp. 60.0 C / 333.1 K

Sample #9, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

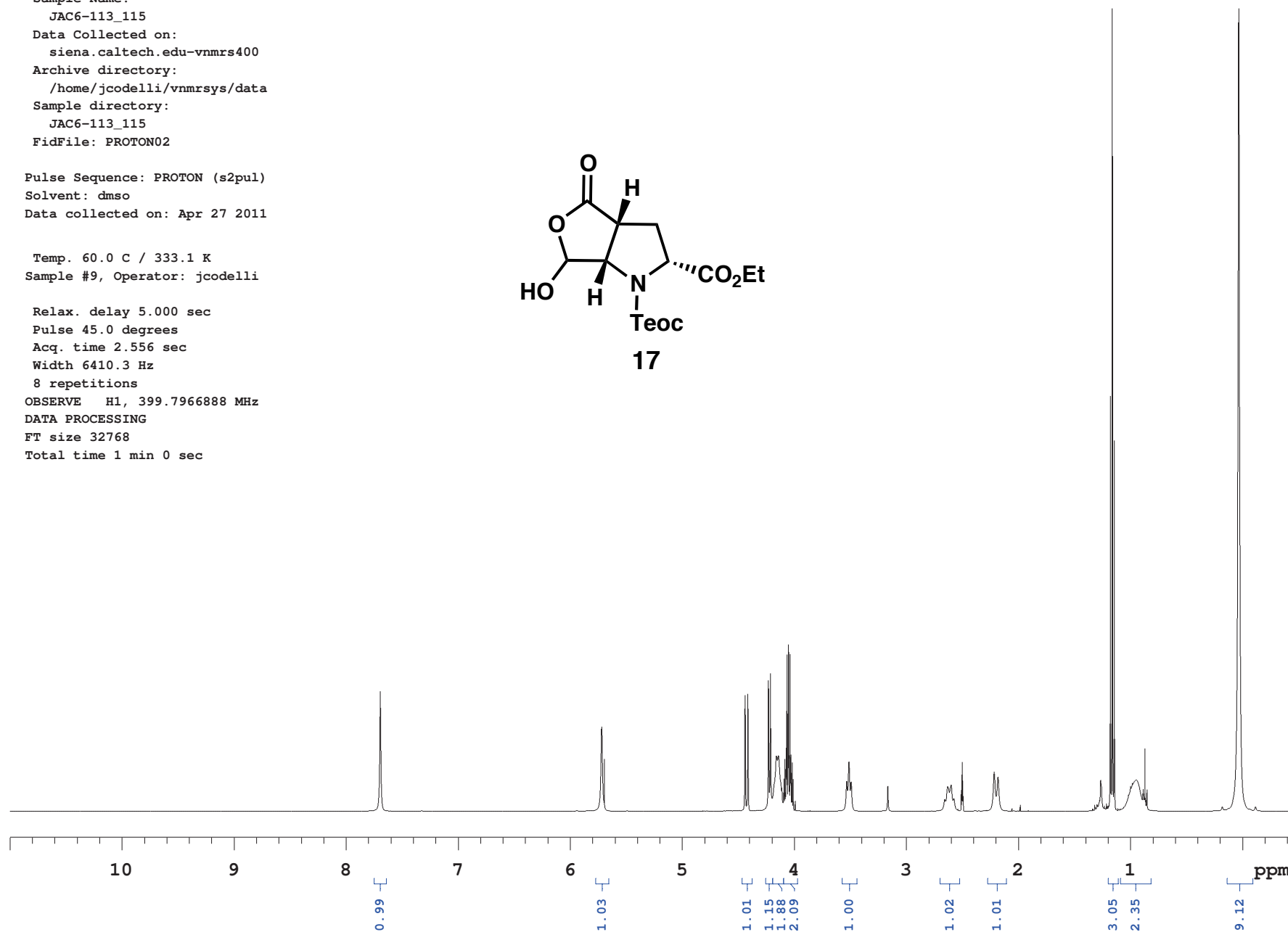
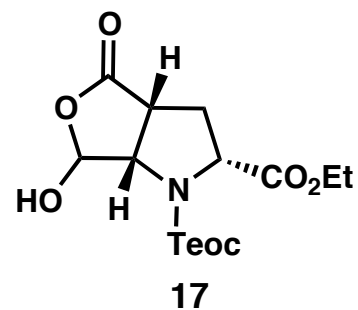
8 repetitions

OBSERVE H1, 399.7966888 MHz

DATA PROCESSING

FT size 32768

Total time 1 min 0 sec



JAC6-113_115 60 _C DMSO siena

Sample Name:

JAC6-113_115

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-113_115

FidFile: CARBON02

Pulse Sequence: CARBON (s2pul)

Solvent: dmsd

Data collected on: Apr 27 2011

Temp. 60.0 C / 333.1 K

Sample #9, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

256 repetitions

OBSERVE C13, 100.5289808 MHz

DECOUPLE H1, 399.7987005 MHz

Power 39 dB

continuously on

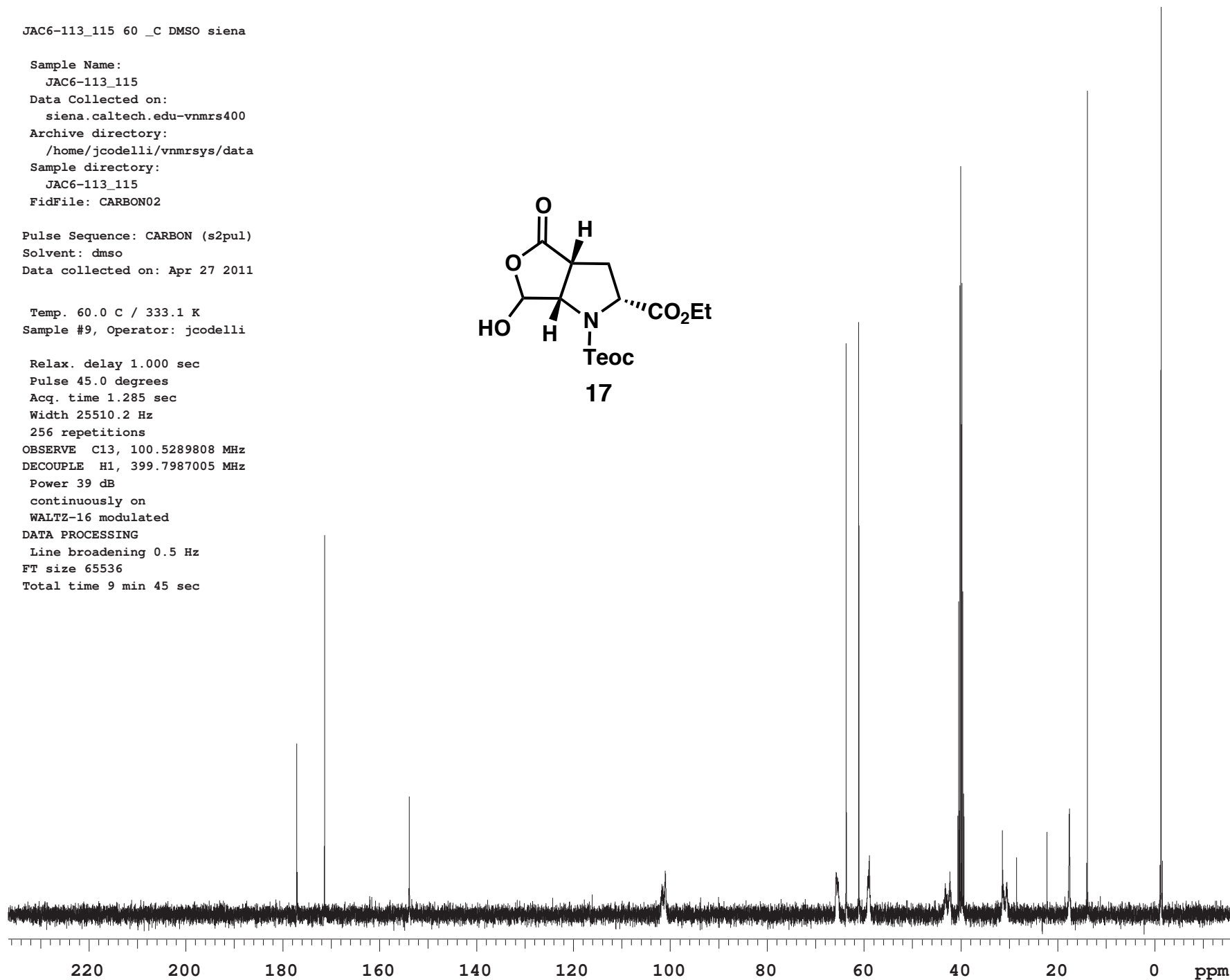
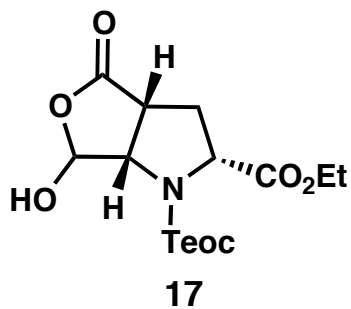
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 min 45 sec



JAC7-93 CDC13 indy

Sample Name:

JAC7-93

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-93

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Apr 29 2011

Temp. 25.0 C / 298.1 K

Sample #14, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

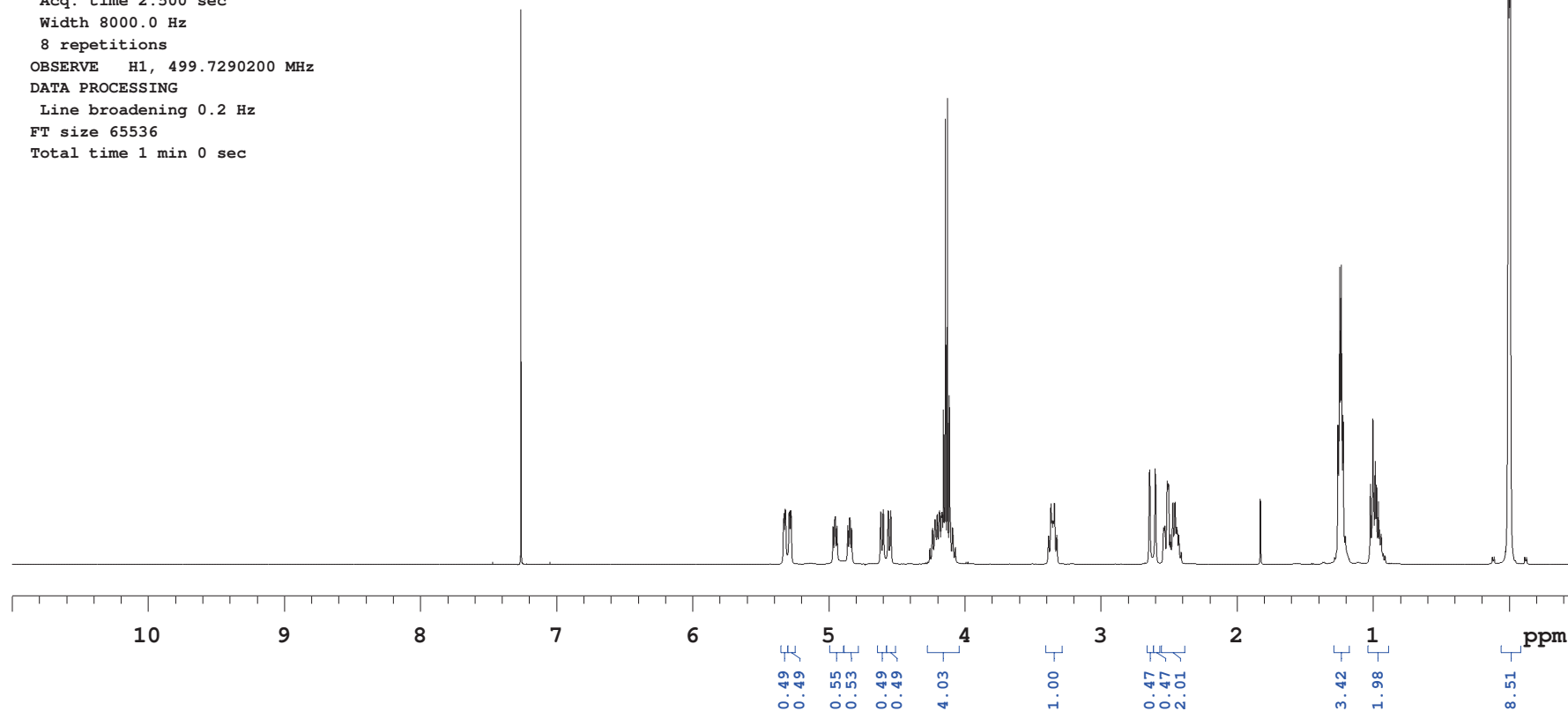
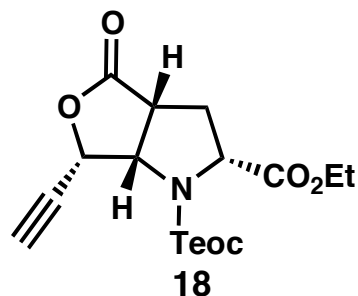
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 0 sec



JAC7-93 CDCl3 indy

Sample Name:

JAC7-93

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-93

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Apr 29 2011

Temp. 25.0 C / 298.1 K

Sample #14, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6569729 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

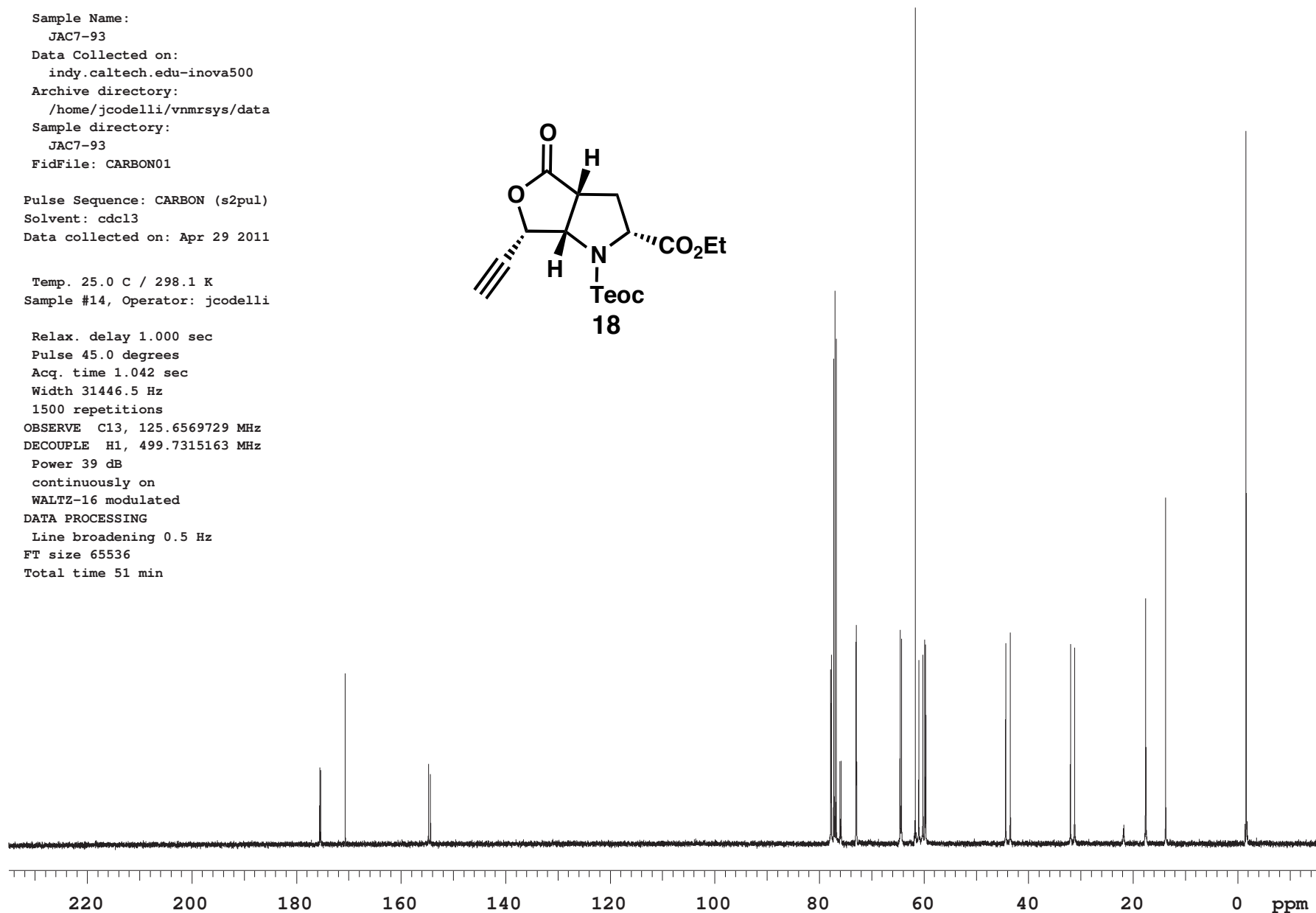
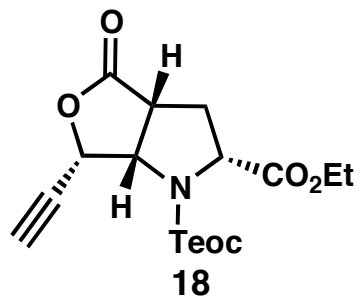
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



ALP-III-17characterize

Sample Name:

ALP-III-17characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-III-17characterize

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 27 2011

Sample #47, Operator: apuchlop

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

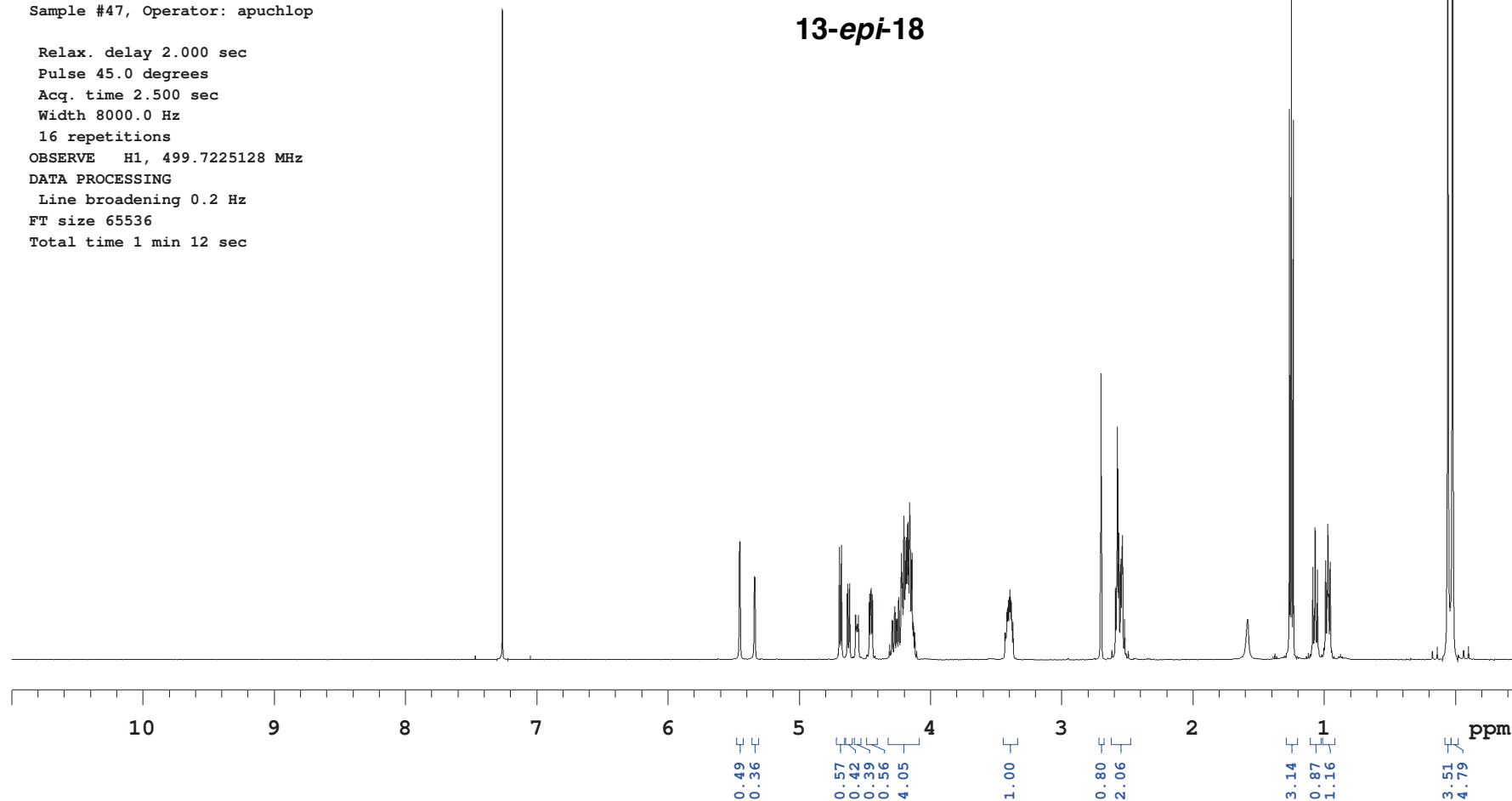
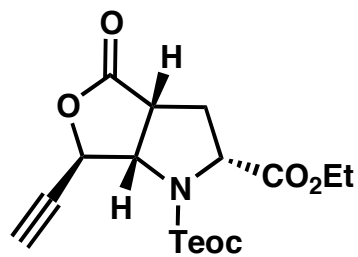
OBSERVE H1, 499.7225128 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



ALP-III-17characterize

Sample Name:

ALP-III-17characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-III-17characterize

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jul 27 2011

Sample #47, Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6553271 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

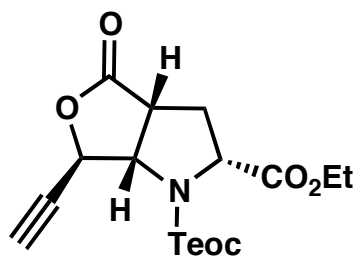
WALTZ-16 modulated

DATA PROCESSING

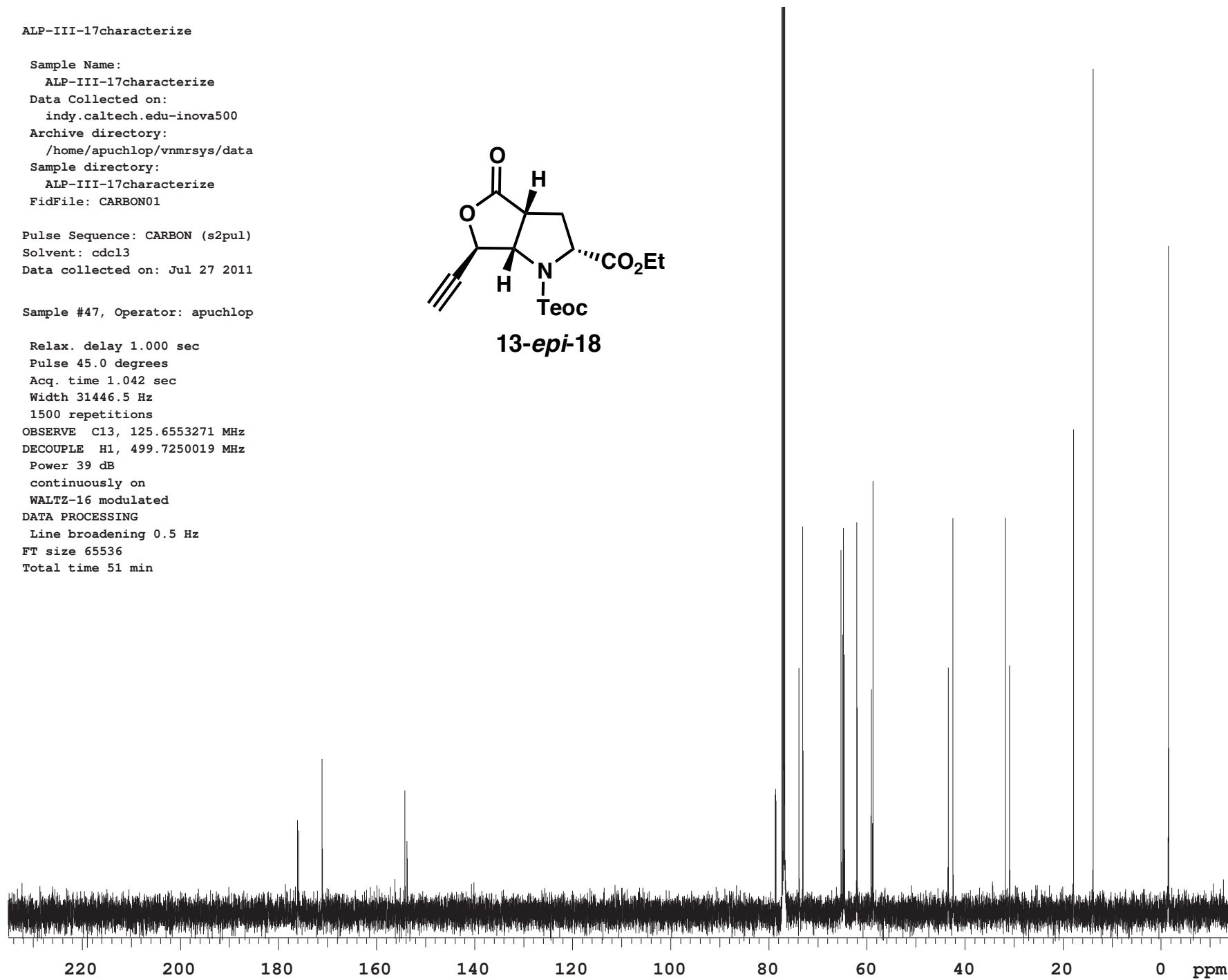
Line broadening 0.5 Hz

FT size 65536

Total time 51 min



13-*epi*-18



JAC3-215A CDC13 indy

Sample Name:

JAC3-215A

Data Collected on:

indy.caltech.edu-inova500

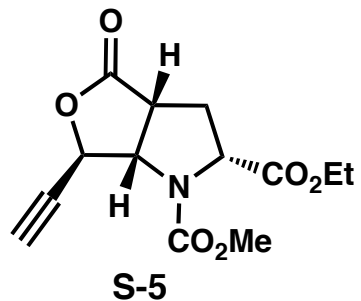
Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC3-215A

FidFile: PROTON01



Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Mar 21 2010

Temp. 25.0 C / 298.1 K

Sample #8, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8000.0 Hz

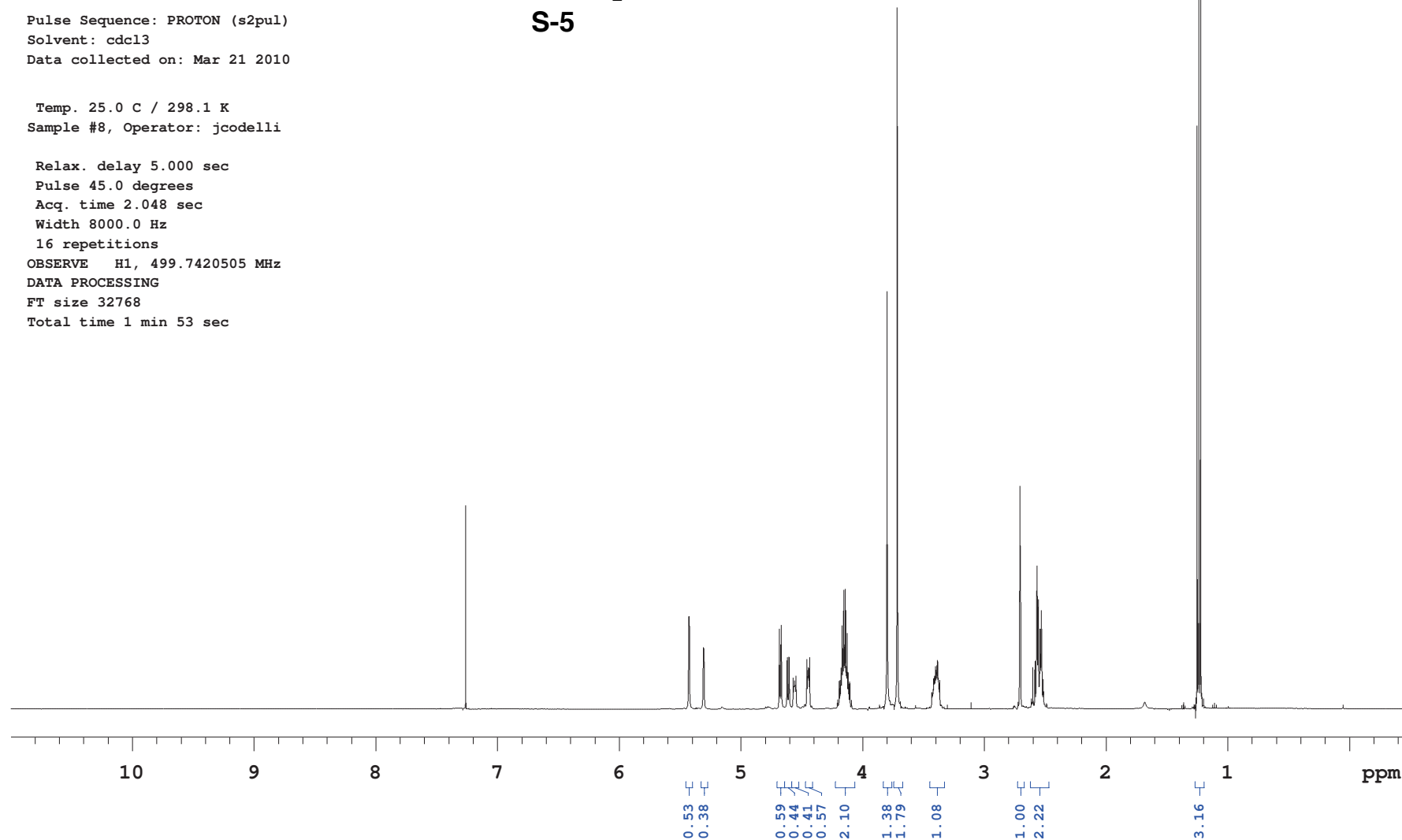
16 repetitions

OBSERVE H1, 499.7420505 MHz

DATA PROCESSING

FT size 32768

Total time 1 min 53 sec



JAC3-215A CDC13 indy

Sample Name:

JAC3-215A

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC3-215A

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Mar 21 2010

Temp. 25.0 C / 298.1 K

Sample #8, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1600 repetitions

OBSERVE C13, 125.6602433 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

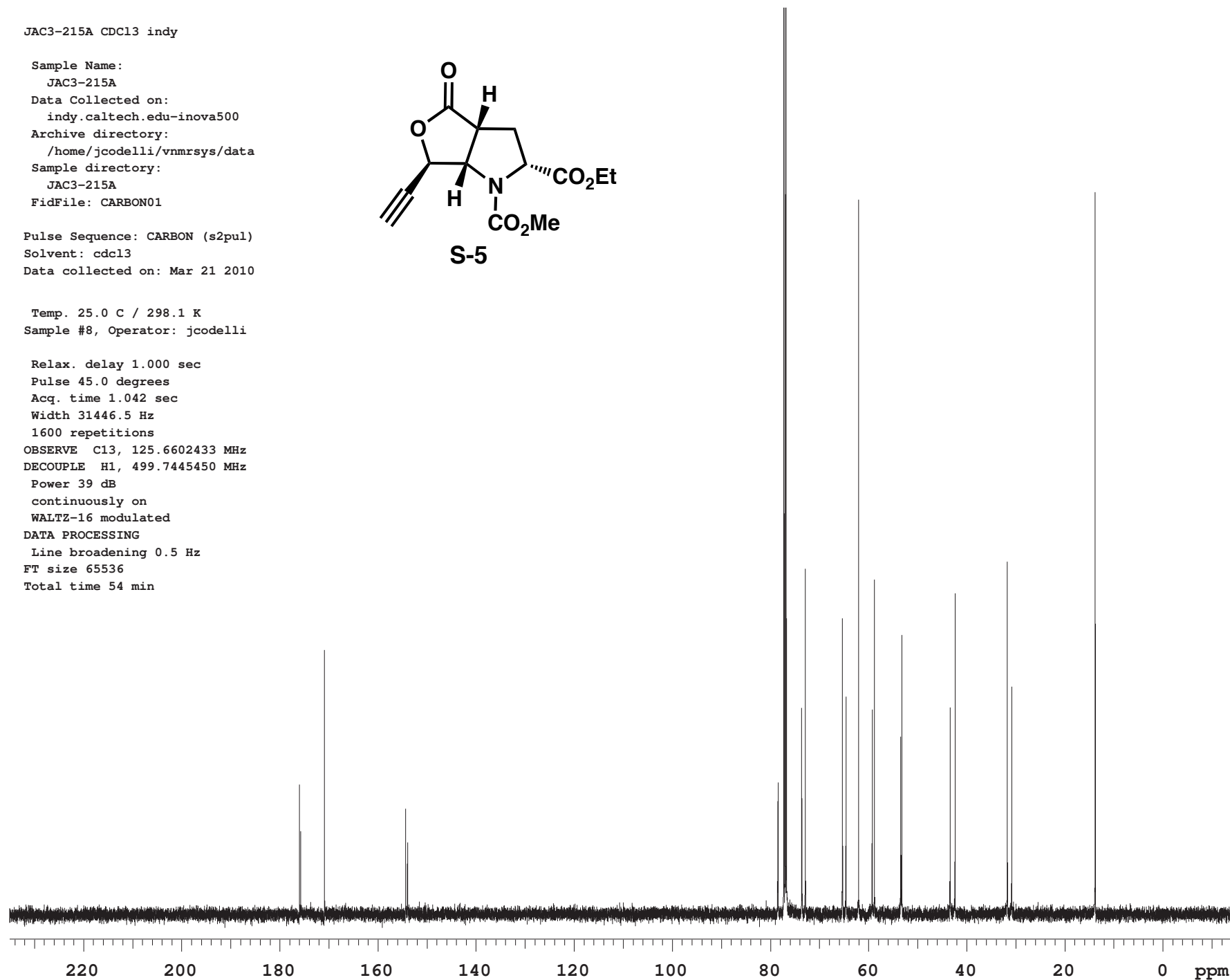
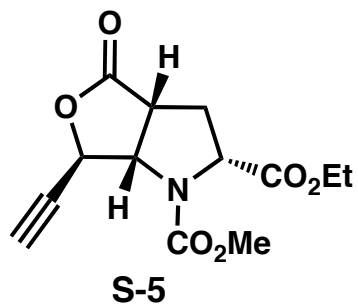
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 54 min



JAC7-97 CD3CN indy

Sample Name:

JAC7-97

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-97

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: May 1 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

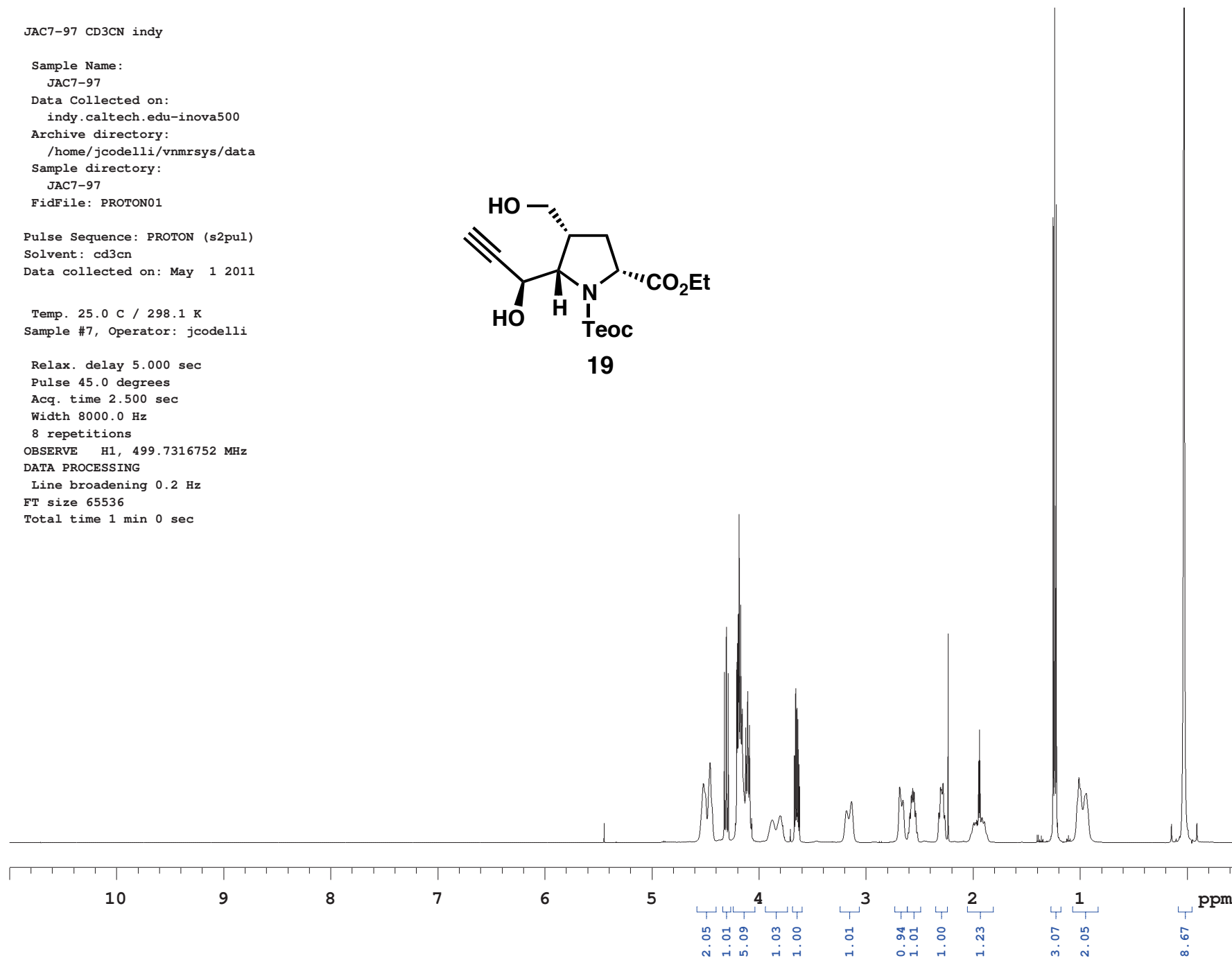
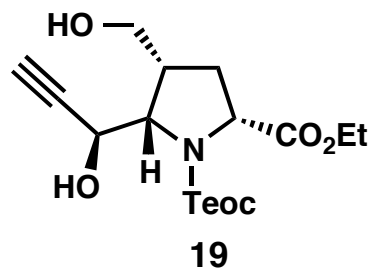
OBSERVE H1, 499.7316752 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 0 sec



JAC7-97 CD3CN indy

Sample Name:

JAC7-97

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-97

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: May 1 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1400 repetitions

OBSERVE C13, 125.6575076 MHz

DECOUPLE H1, 499.7341599 MHz

Power 39 dB

continuously on

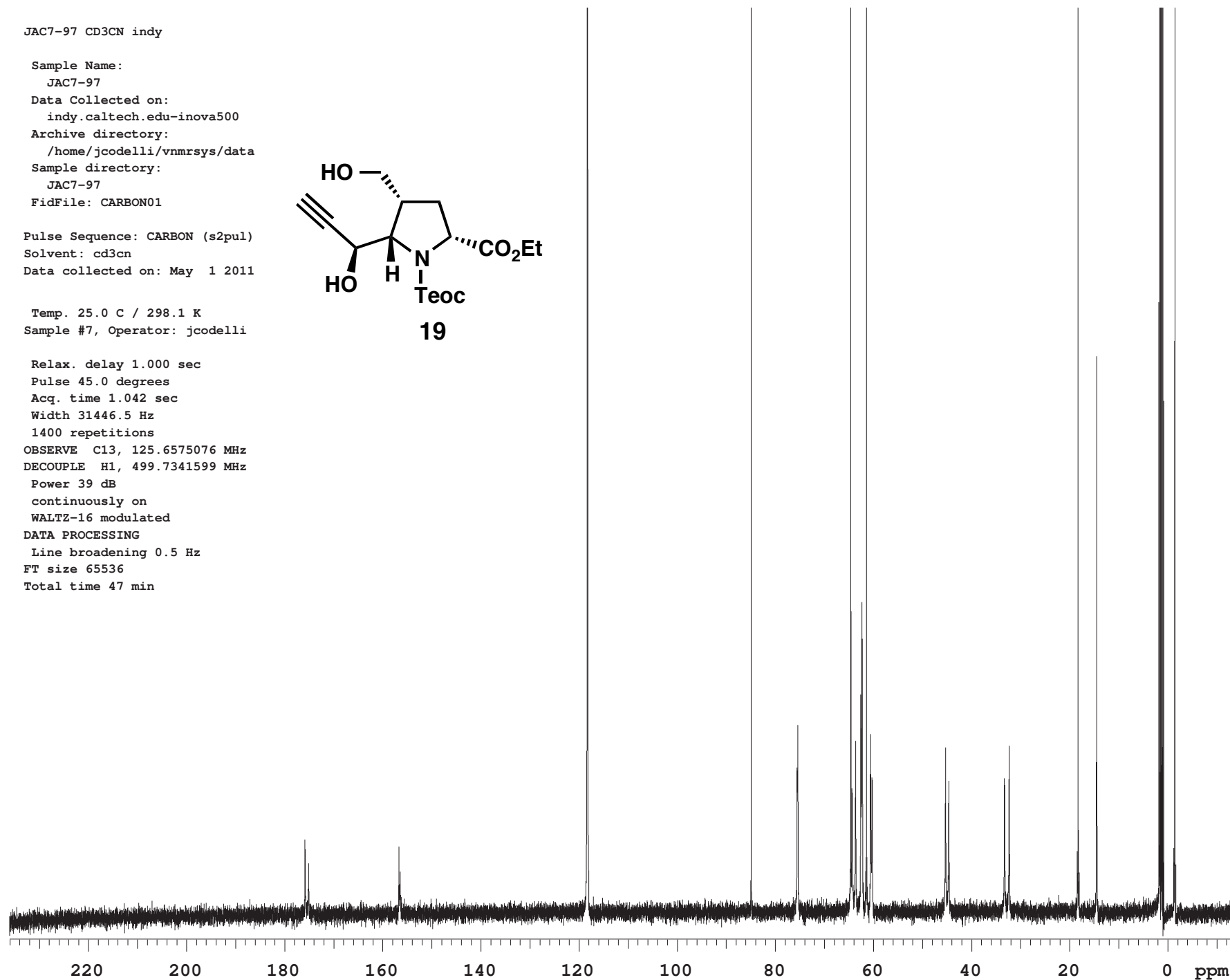
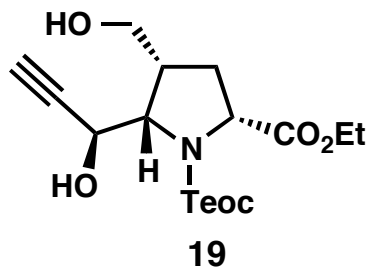
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 47 min



JAC7-99 CD3CN indy

Sample Name:

JAC7-99

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-99

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: May 6 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

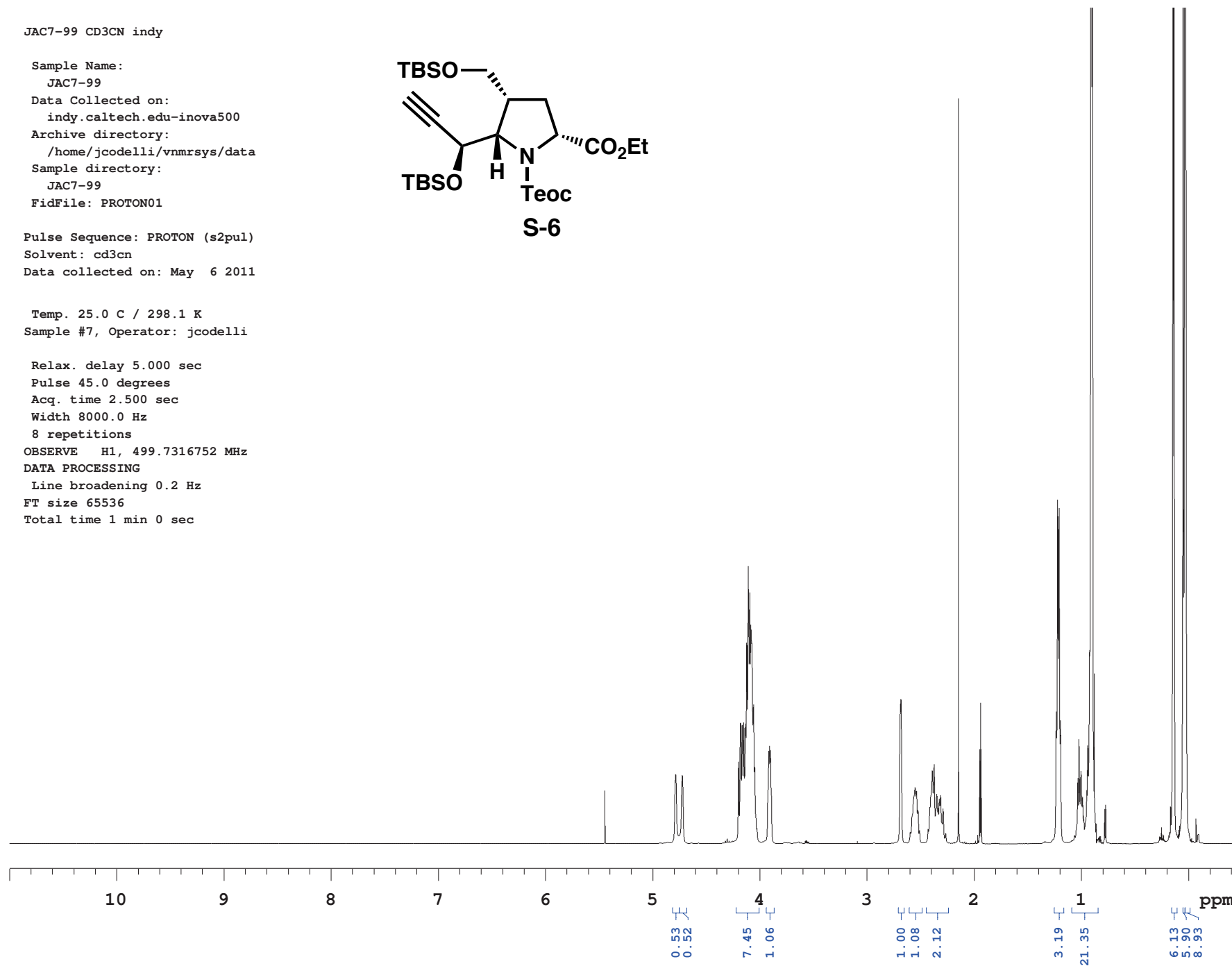
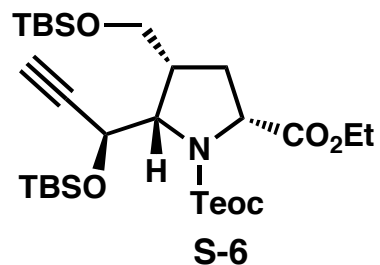
OBSERVE H1, 499.7316752 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 0 sec



JAC7-99 CD3CN indy

Sample Name:

JAC7-99

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-99

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: May 6 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1400 repetitions

OBSERVE C13, 125.6574961 MHz

DECOUPLE H1, 499.7341599 MHz

Power 39 dB

continuously on

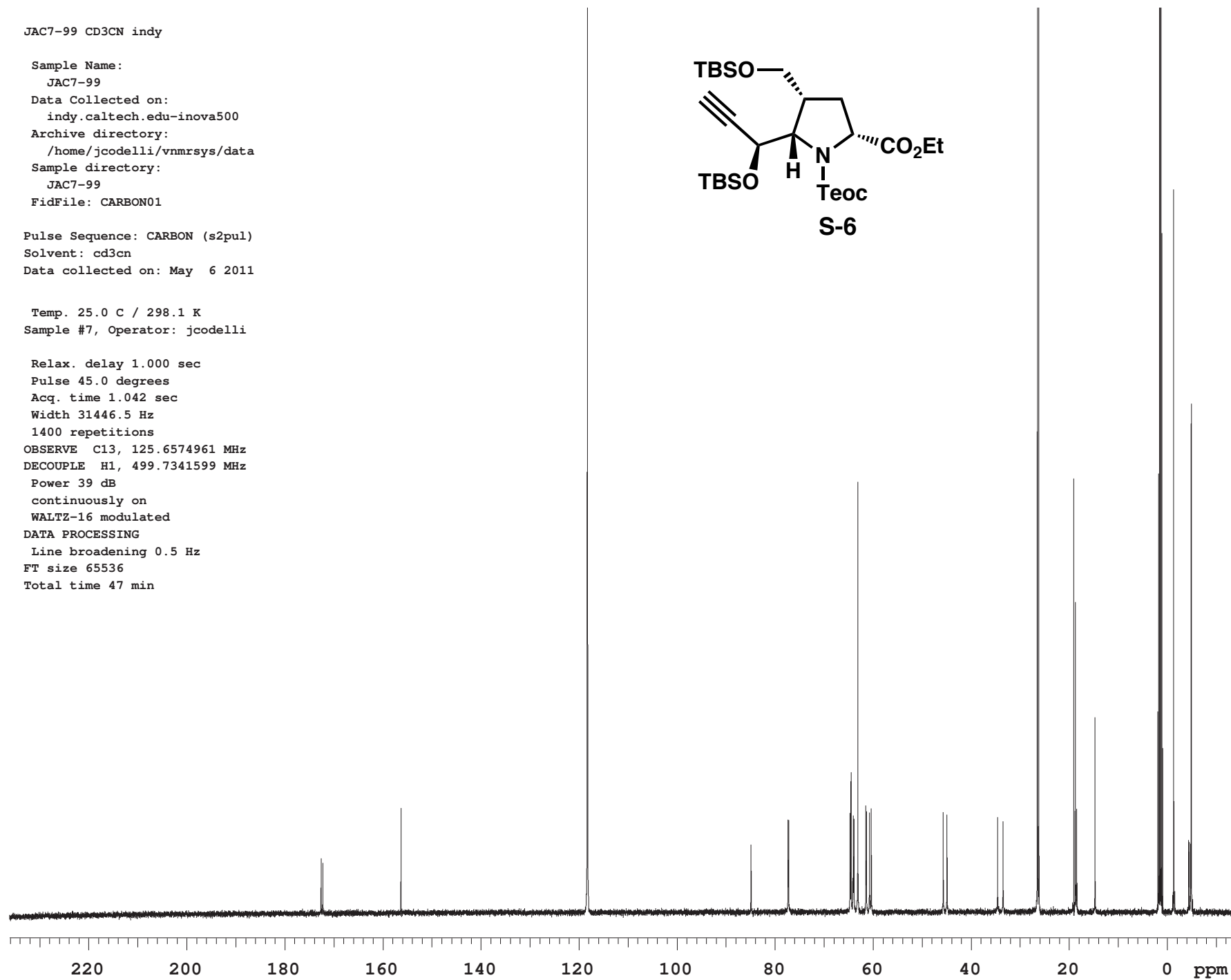
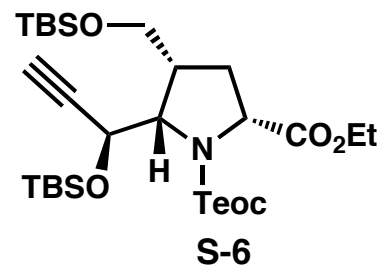
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 47 min



ALP-II-263characterize?

Sample Name:

ALP-II-263characterize_

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-263characterize_

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jun 13 2011

Temp. 25.0 C / 298.1 K

Sample #40, Operator: apuchlop

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

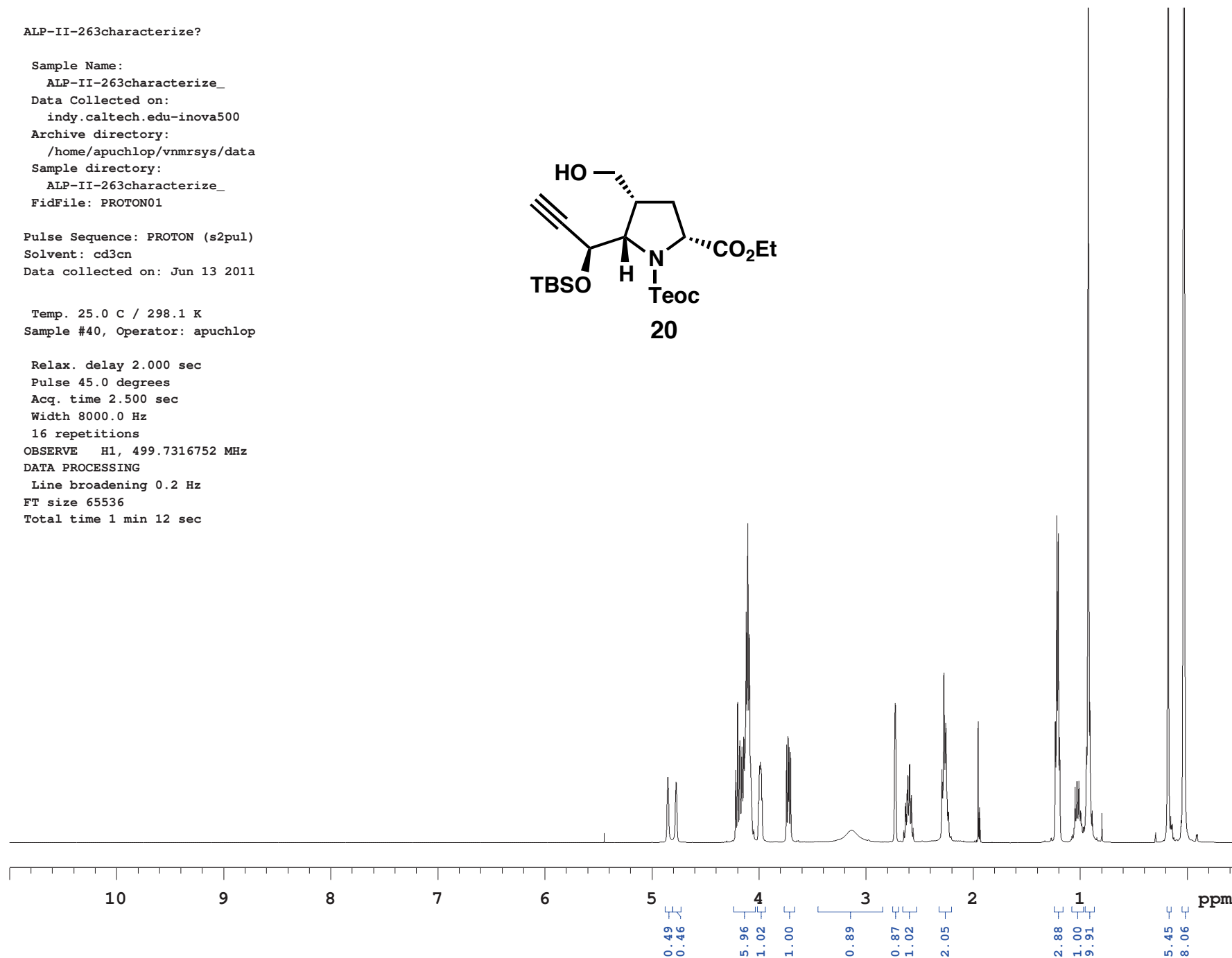
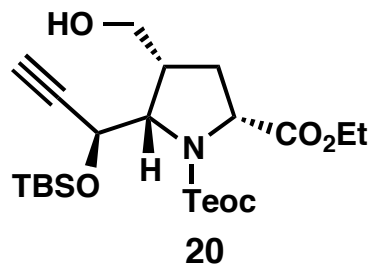
OBSERVE H1, 499.7316752 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



ALP-II-263characterize

Sample Name:

ALP-II-263characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-263characterize

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Jun 13 2011

Temp. 25.0 C / 298.1 K

Sample #40, Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6574951 MHz

DECOUPLE H1, 499.7341599 MHz

Power 39 dB

continuously on

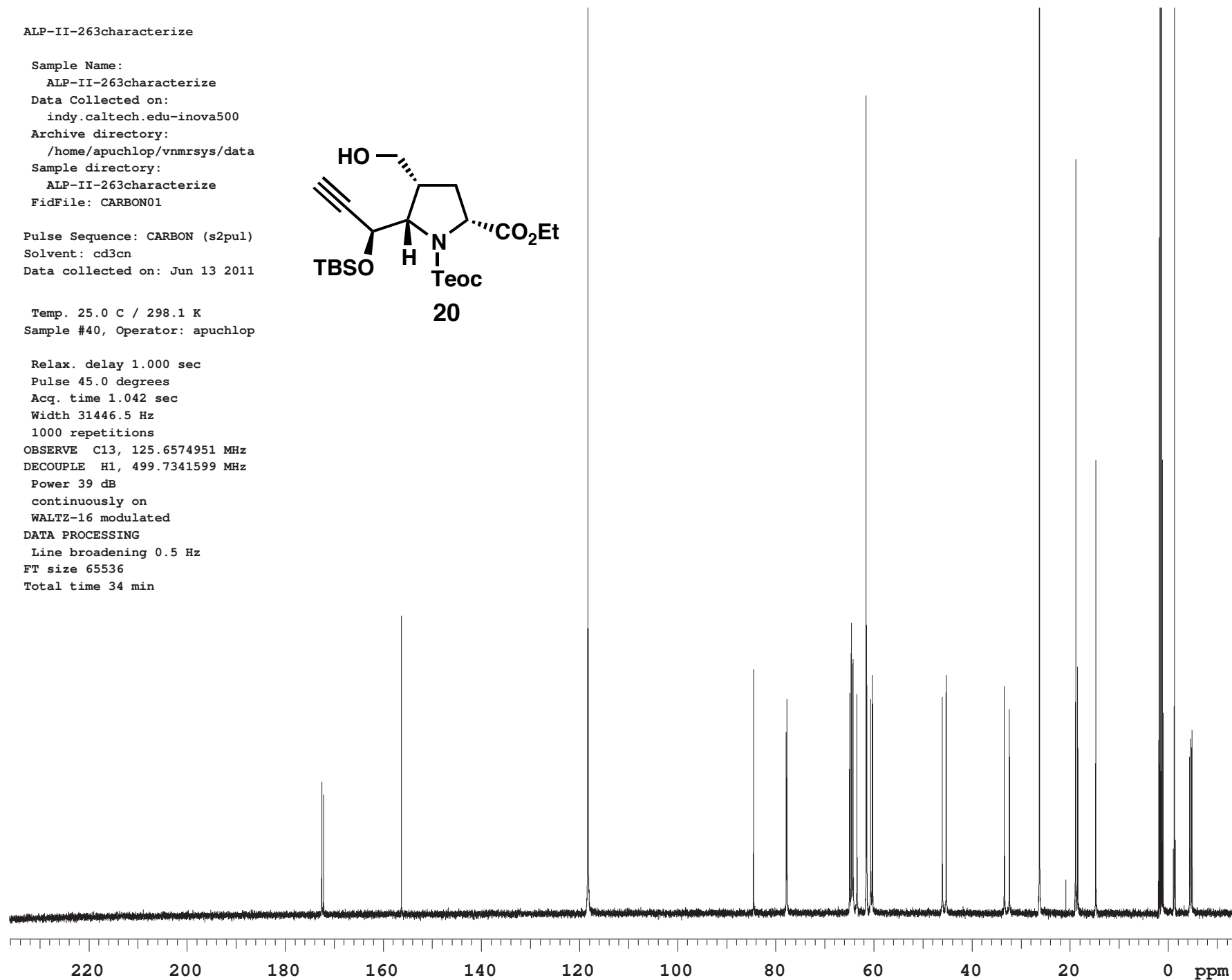
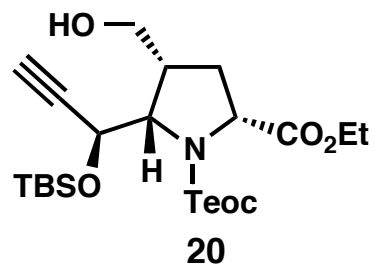
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



ALP-II-265characterize

Sample Name:

ALP-II-265characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-265characterize

FidFile: PROTON03

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jun 14 2011

Temp. 25.0 C / 298.1 K

Sample #46, Operator: apuchlop

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

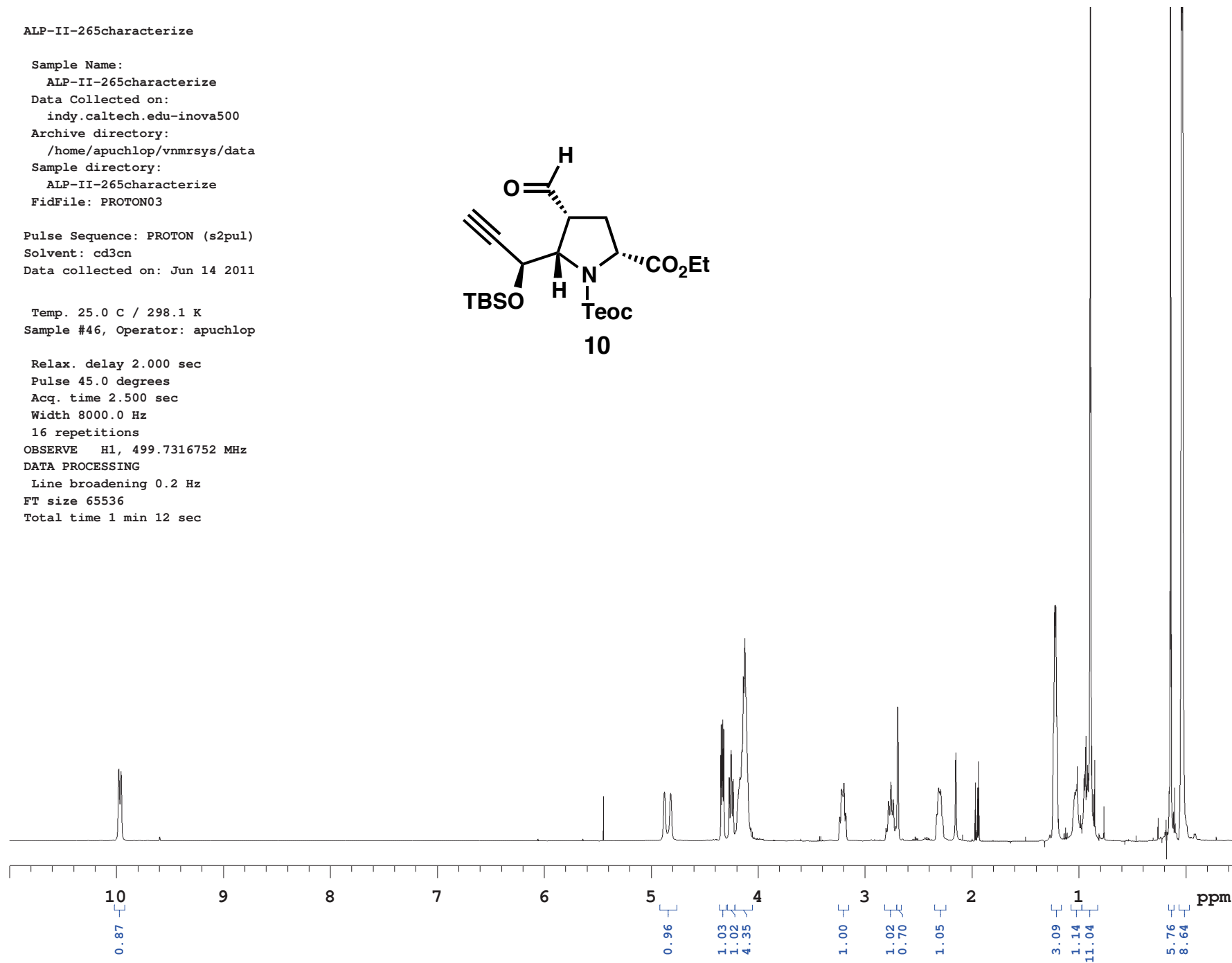
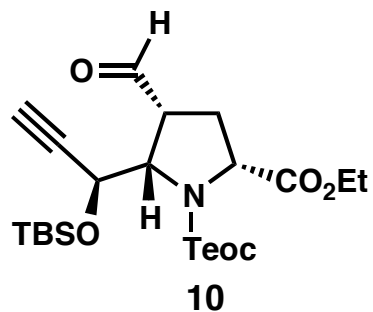
OBSERVE H1, 499.7316752 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



ALP-II-265characterize

Sample Name:

ALP-II-265characterize

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

ALP-II-265characterize

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Jun 14 2011

Temp. 25.0 C / 298.1 K

Sample #46, Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6575019 MHz

DECOUPLE H1, 499.7341599 MHz

Power 39 dB

continuously on

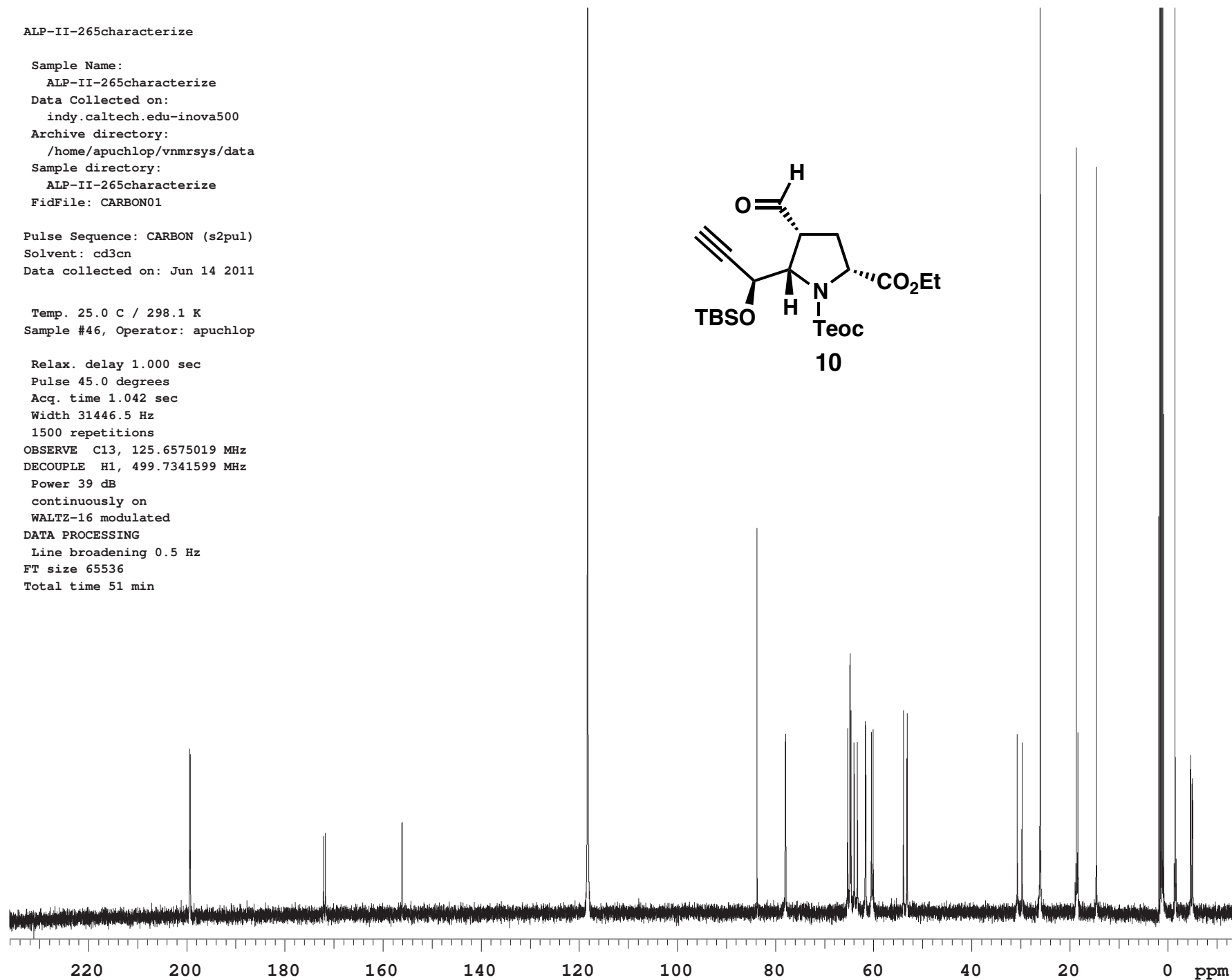
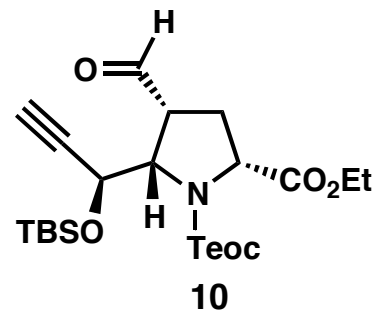
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



JAC6-203 CDC13 indy

Sample Name:

JAC6-203

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-203

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Feb 18 2011

Temp. 25.0 C / 298.1 K

Sample #8, Operator: jcodelli

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

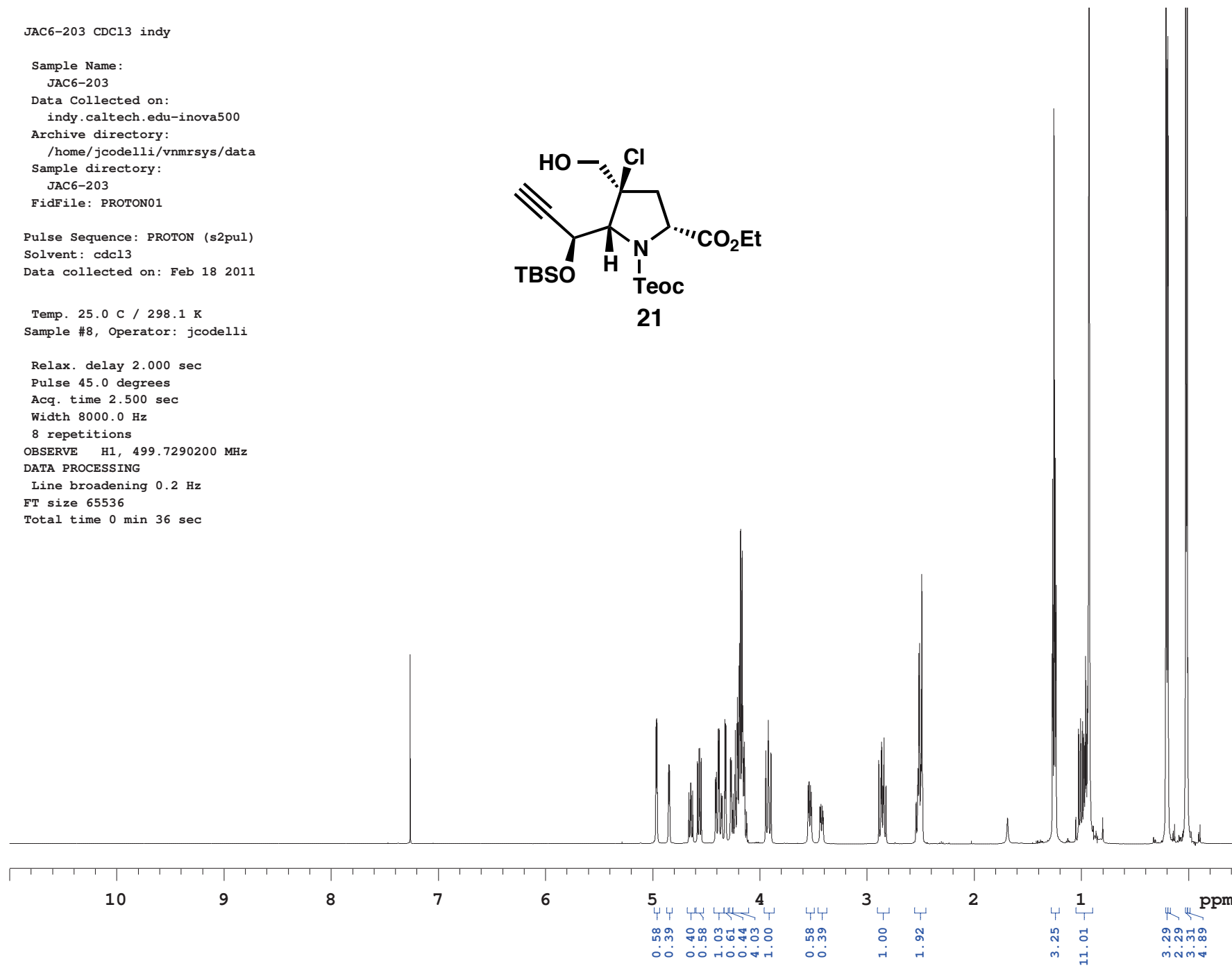
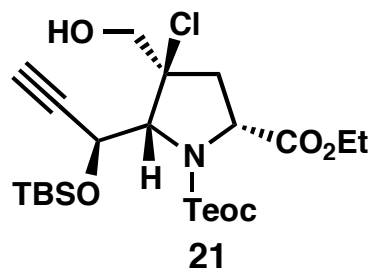
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 36 sec



JAC6-201 CDC13 indy

Sample Name:

JAC6-201

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC6-201

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Feb 18 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6569662 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

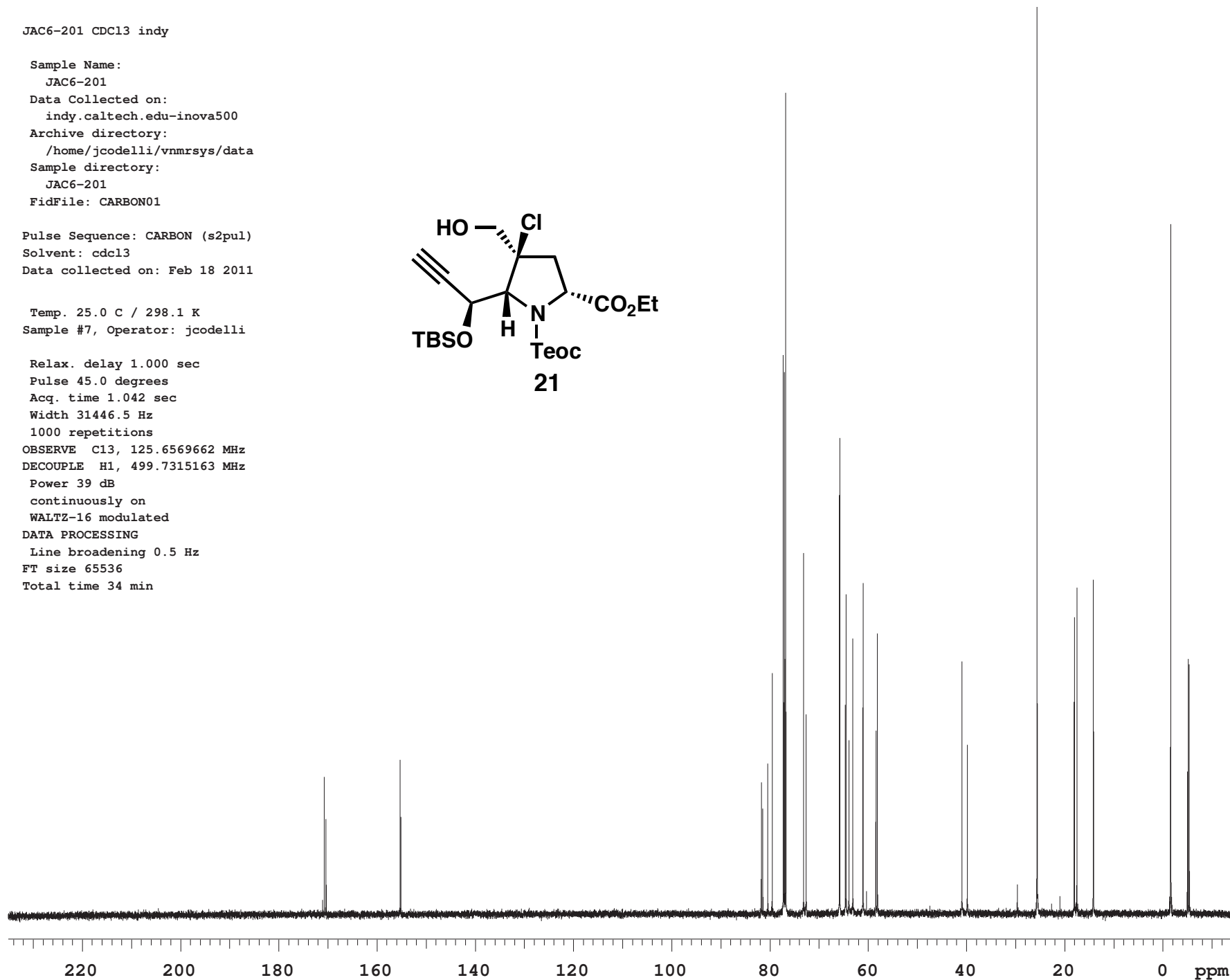
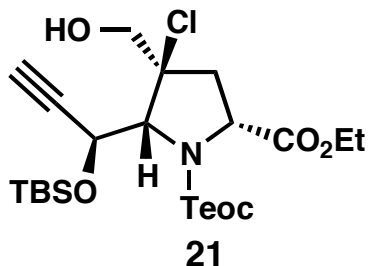
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



JAC7-237 60degreesC CD3CN siena

Sample Name:

JAC7-237

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-237

FidFile: PROTON04

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jul 1 2011

Temp. 60.0 C / 333.1 K

Sample #6, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

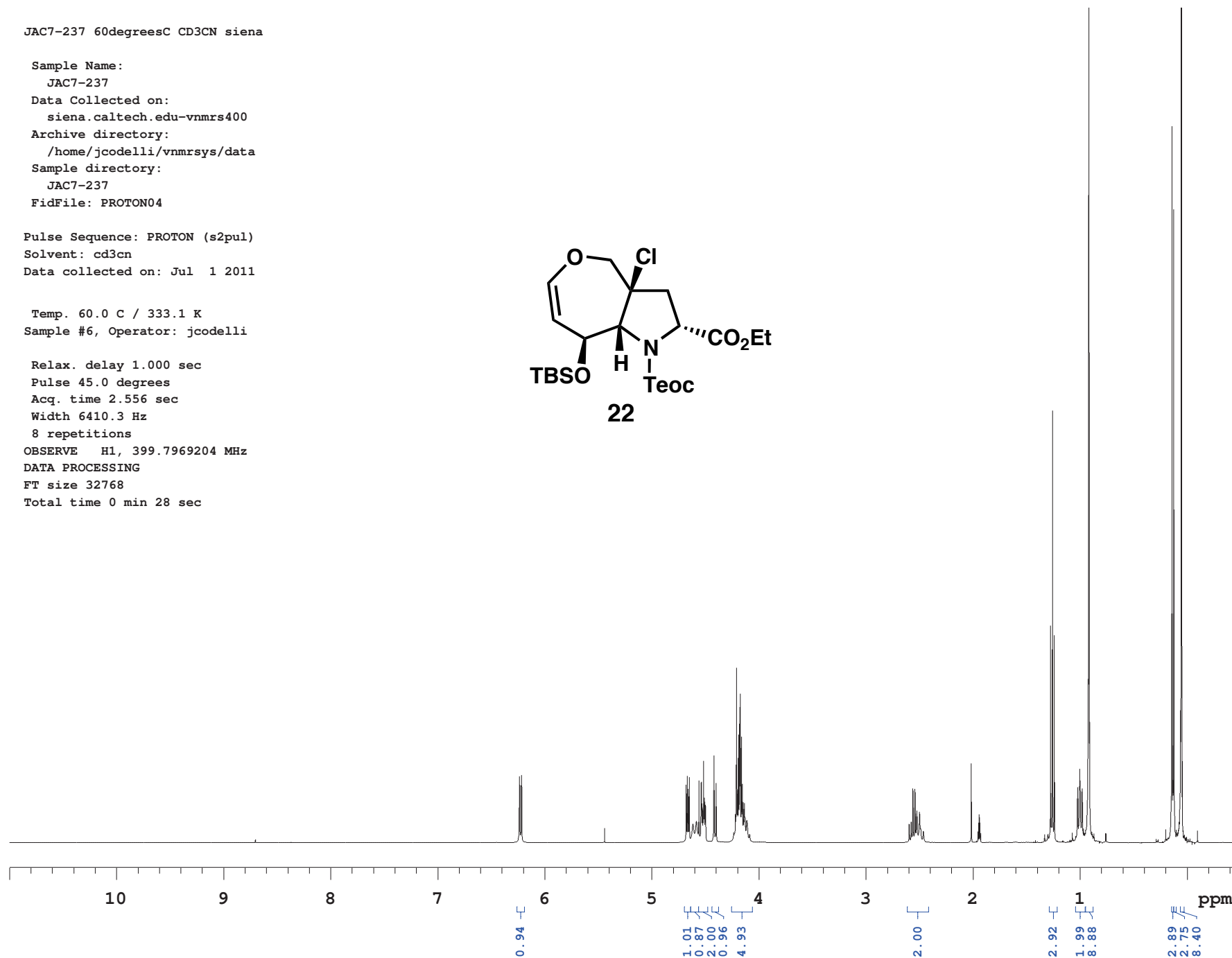
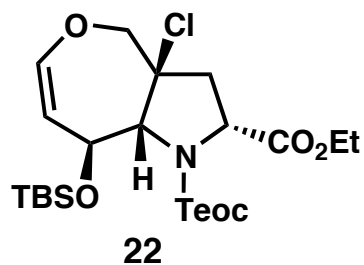
8 repetitions

OBSERVE H1, 399.7969204 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



ALP-III-25 60degreesC CD3CN siena

Sample Name:

ALP-III-25

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: alp-III-25

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Jul 29 2011

Temp. 60.0 C / 333.1 K

Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

2500 repetitions

OBSERVE C13, 100.528812 MHz

DECOUPLE H1, 399.7989164 MHz

Power 39 dB

continuously on

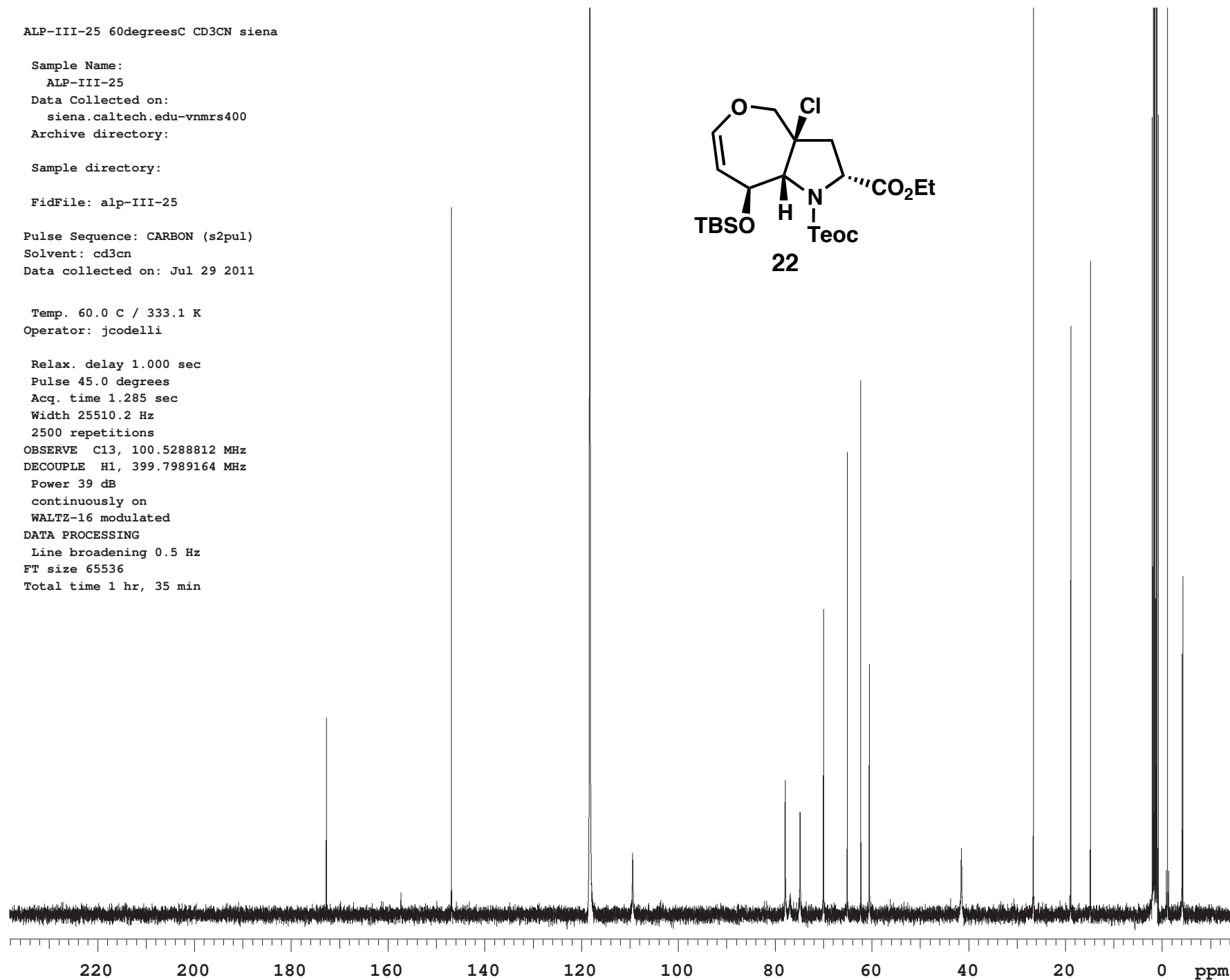
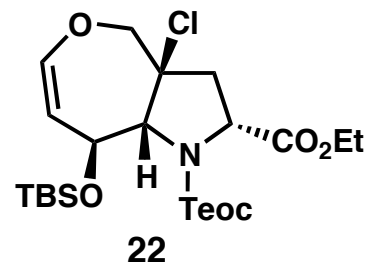
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 35 min



JAC7-245hplc 50degreesC CDC13 siena

Sample Name:

JAC7-245hplc

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-245hplc

FidFile: PROTON03

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 10 2011

Temp. 50.0 C / 323.1 K

Sample #8, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

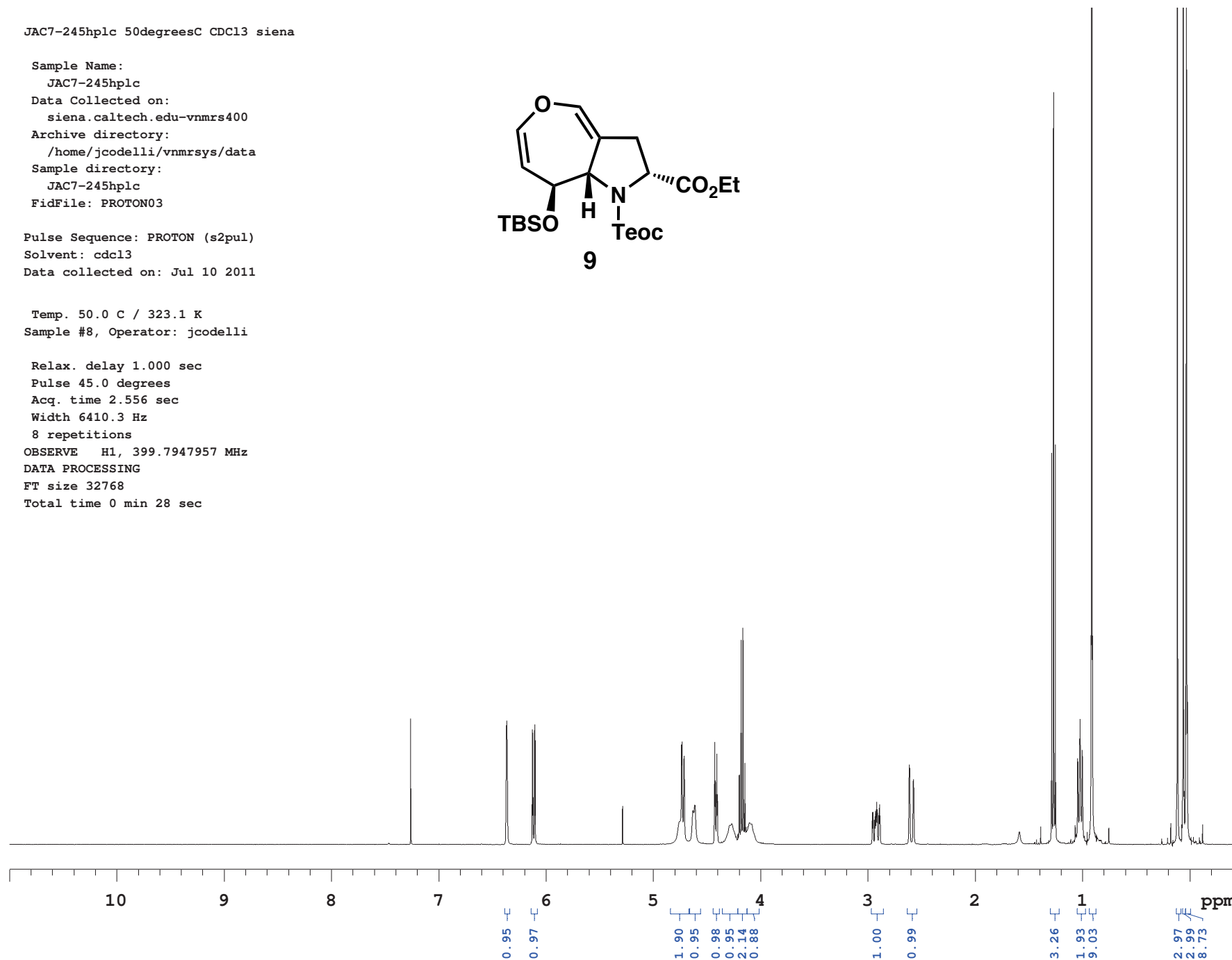
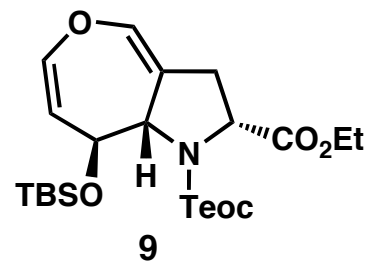
8 repetitions

OBSERVE H1, 399.7947957 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



JAC7-245hplc CDC13 siena

Sample Name:

JAC7-245hplc

Data Collected on:

siena.caltech.edu-vnmrs400

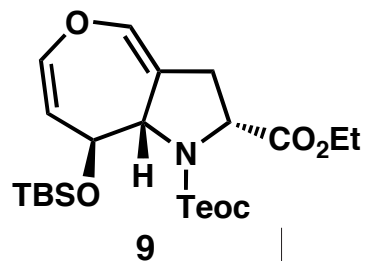
Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-245hplc

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jul 10 2011

Temp. 50.0 C / 323.1 K

Sample #4, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

2000 repetitions

OBSERVE C13, 100.5284739 MHz

DECOUPLE H1, 399.7968015 MHz

Power 39 dB

continuously on

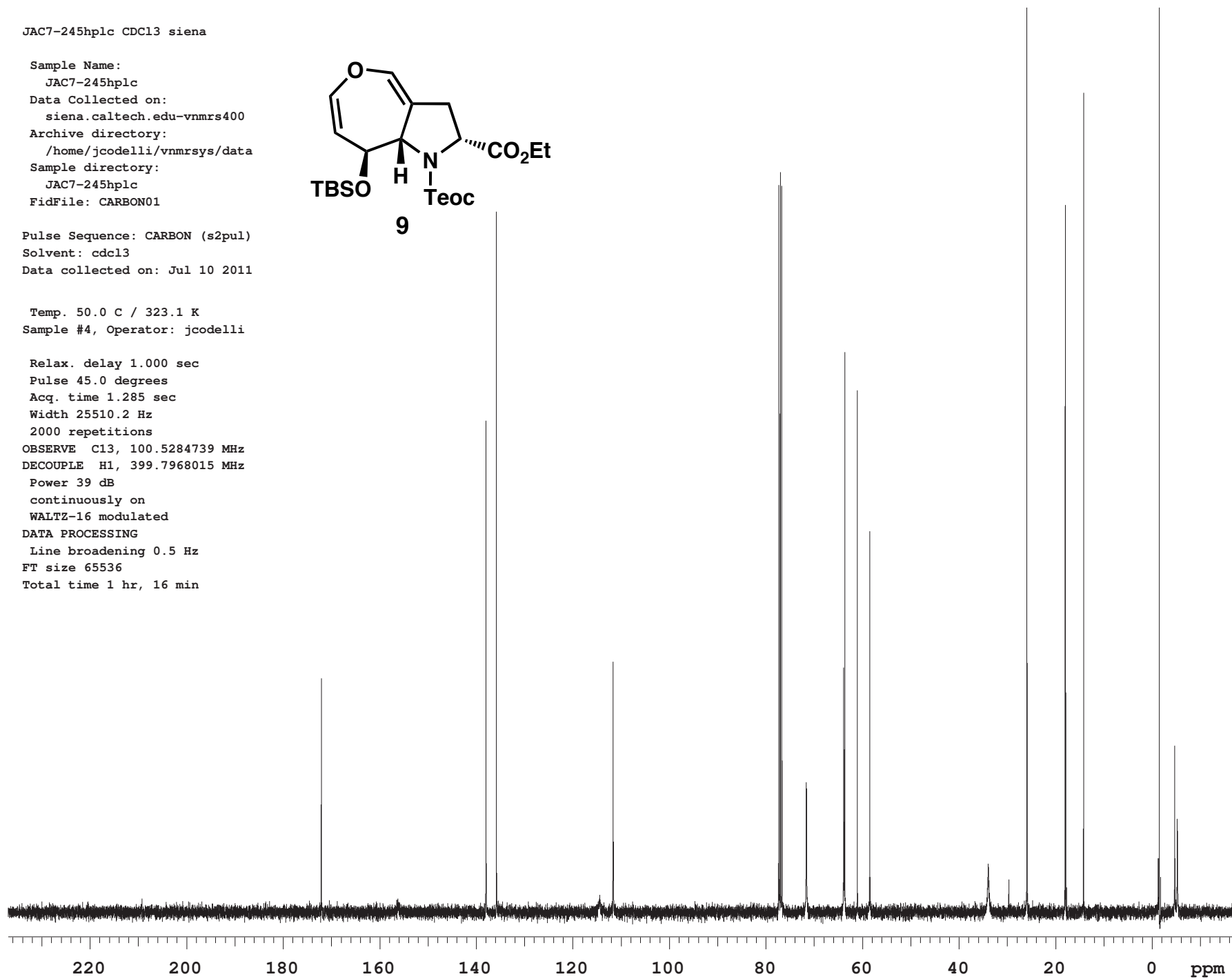
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 16 min



alp-iii-29b CD3CN 60degreesC siena

Sample Name:

alp-iii-29b

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/apuchlop/vnmrsys/data

Sample directory:

alp-iii-29b

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Aug 9 2011

Temp. 60.0 C / 333.1 K

Sample #6, Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

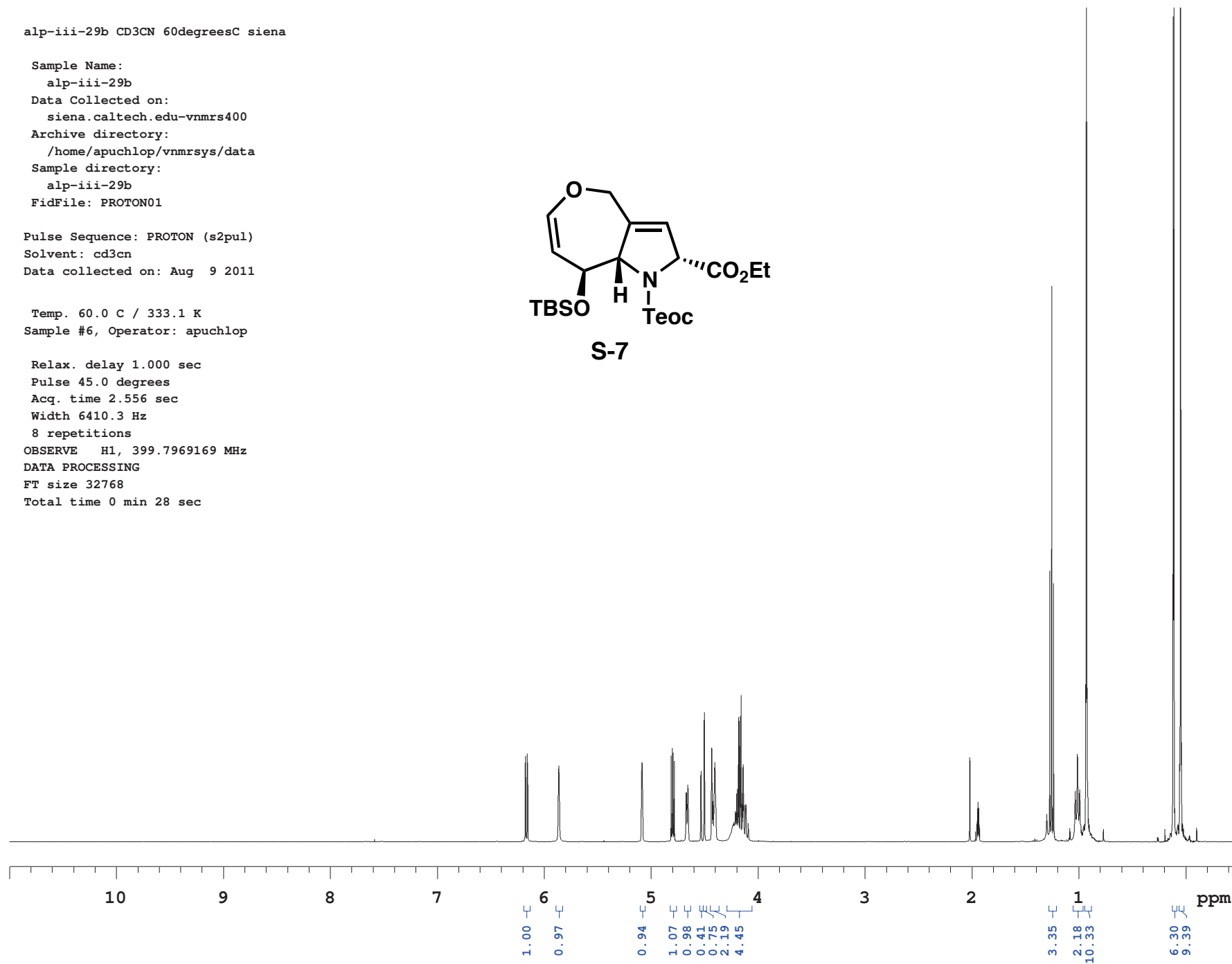
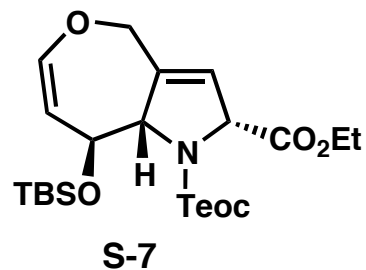
8 repetitions

OBSERVE H1, 399.7969169 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



alp-iii-29b CD3CN 60degreesC siena

Sample Name:

alp-iii-29b

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

Sample directory:

FidFile: ALP-III-29B13C60degreesCsiena

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Aug 9 2011

Temp. 60.0 C / 333.1 K

Operator: apuchlop

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

512 repetitions

OBSERVE C13, 100.5288789 MHz

DECOUPLE H1, 399.7989164 MHz

Power 39 dB

continuously on

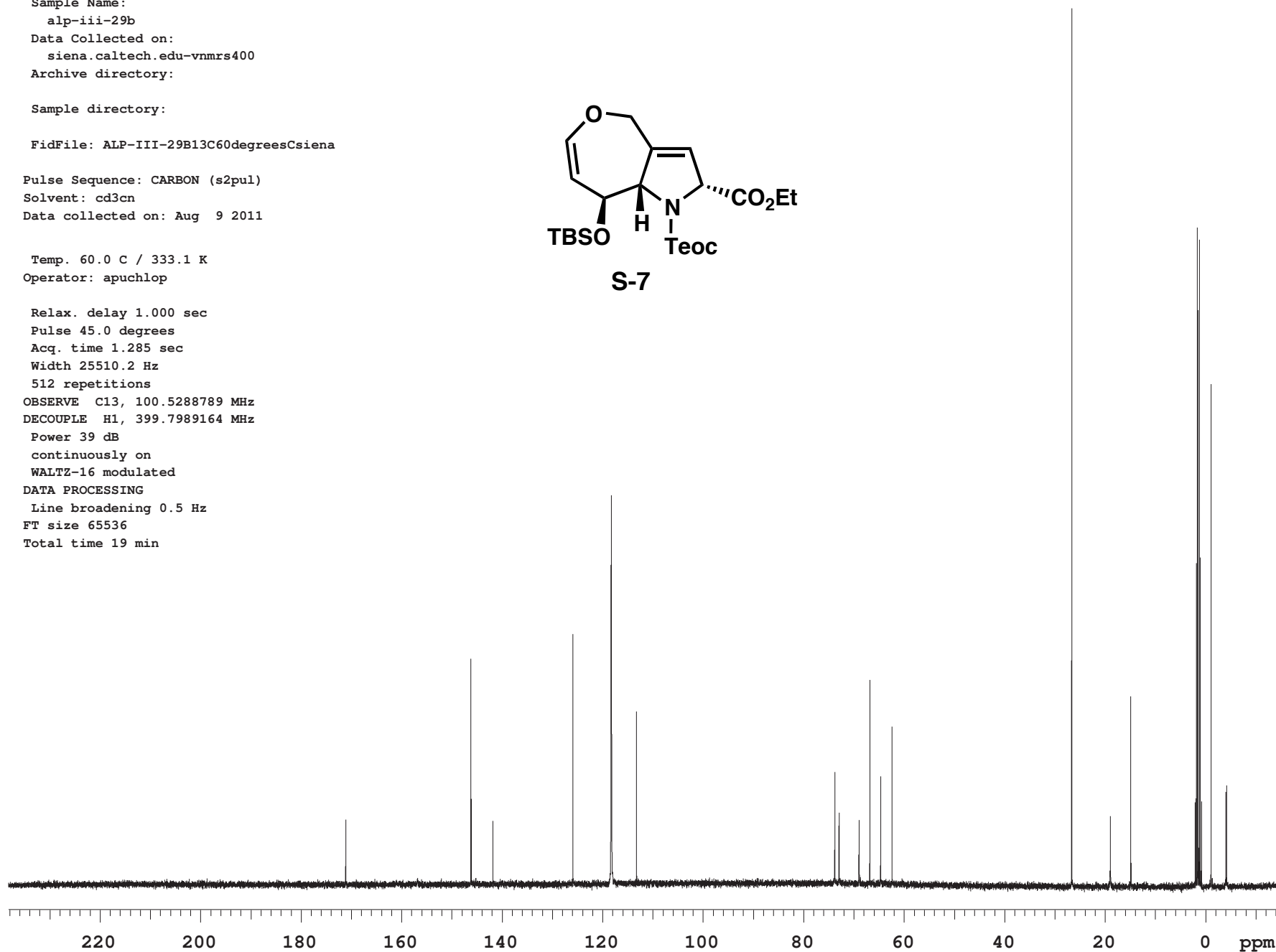
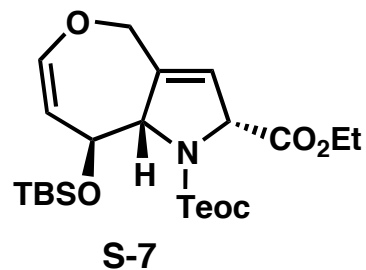
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 19 min



JAC7-251 50degreesC CDC13 siena

Sample Name:

JAC7-251

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-251

FidFile: PROTON03

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 16 2011

Temp. 50.0 C / 323.1 K

Sample #8, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

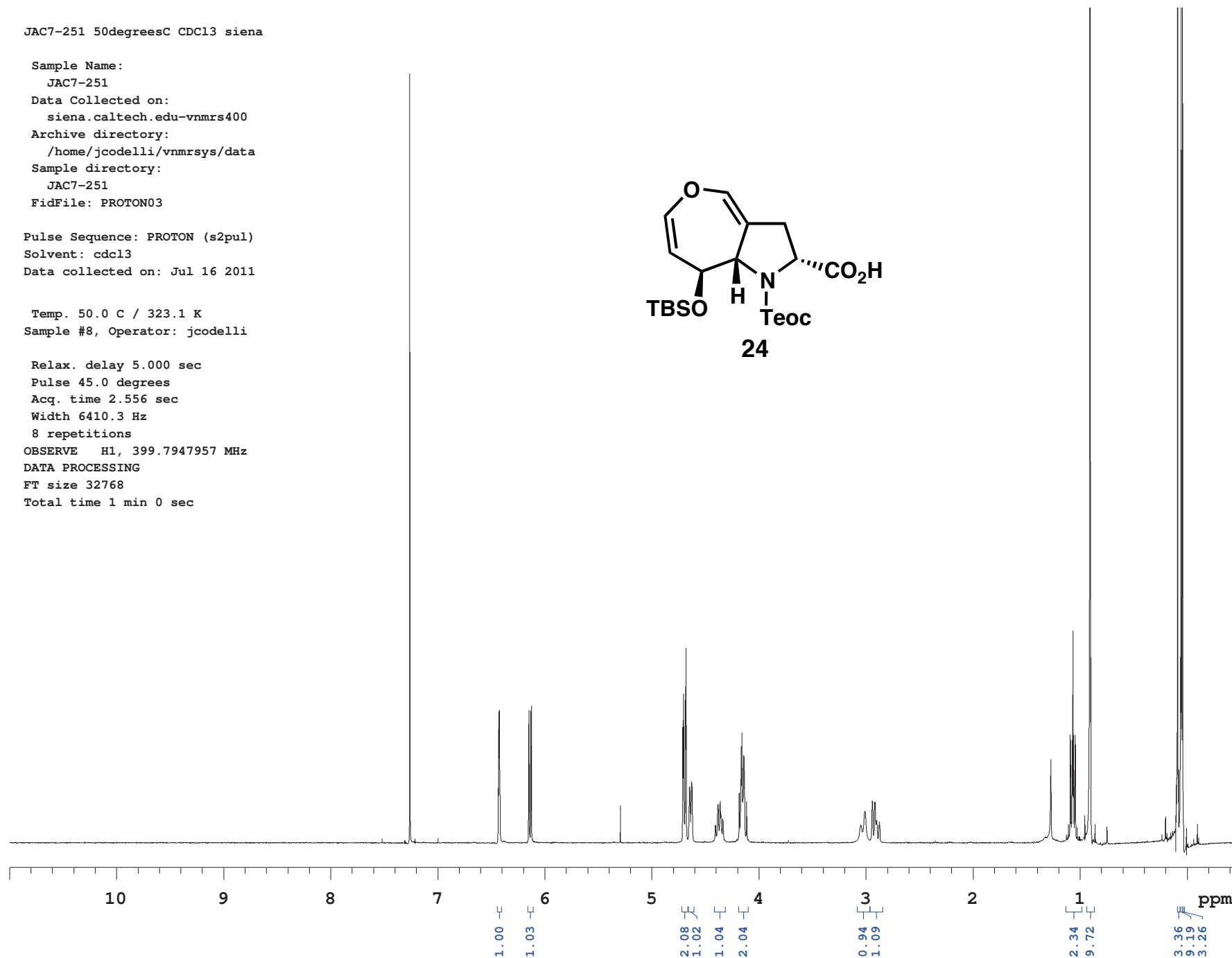
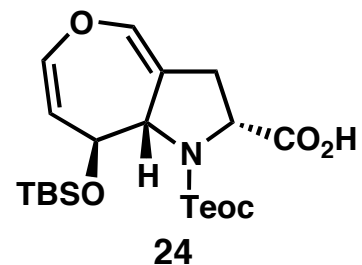
8 repetitions

OBSERVE H1, 399.7947957 MHz

DATA PROCESSING

FT size 32768

Total time 1 min 0 sec



JAC7-251 50degreesC CDC13 siena

Sample Name:

JAC7-237

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

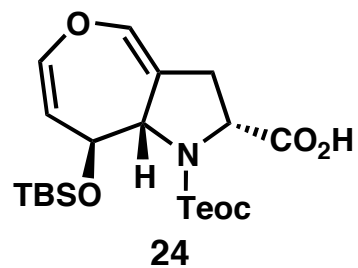
JAC7-237

FidFile: jac7-251-50degrees-13C

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jul 14 2011



Temp. 50.0 C / 323.1 K

Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

4000 repetitions

OBSERVE C13, 100.5284739 MHz

DECOUPLE H1, 399.7968015 MHz

Power 39 dB

continuously on

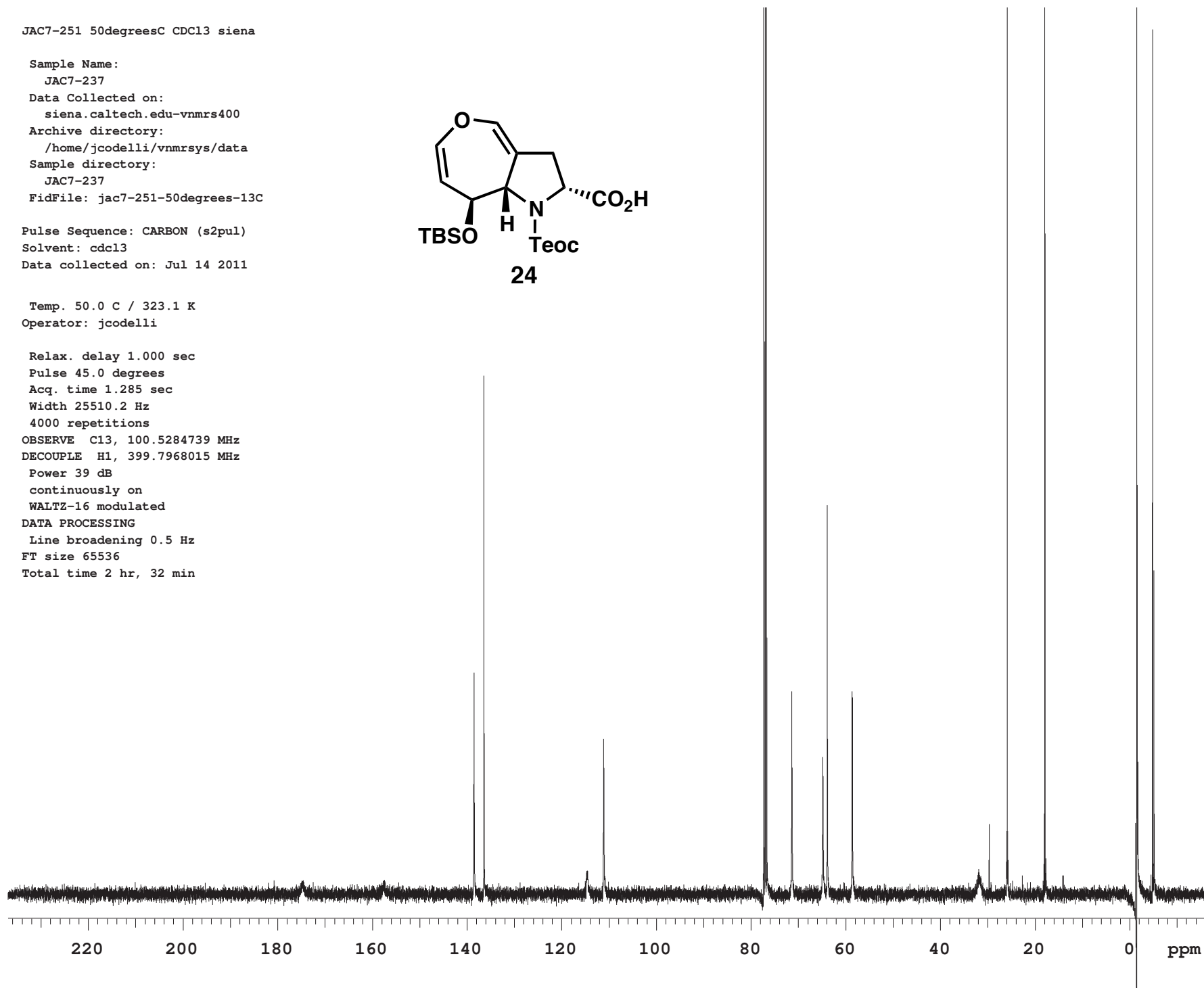
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 2 hr, 32 min



S85

JAC7-133 CDC13 indy

Sample Name:

JAC7-133

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-133

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: May 15 2011

Temp. 25.0 C / 298.1 K

Sample #8, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

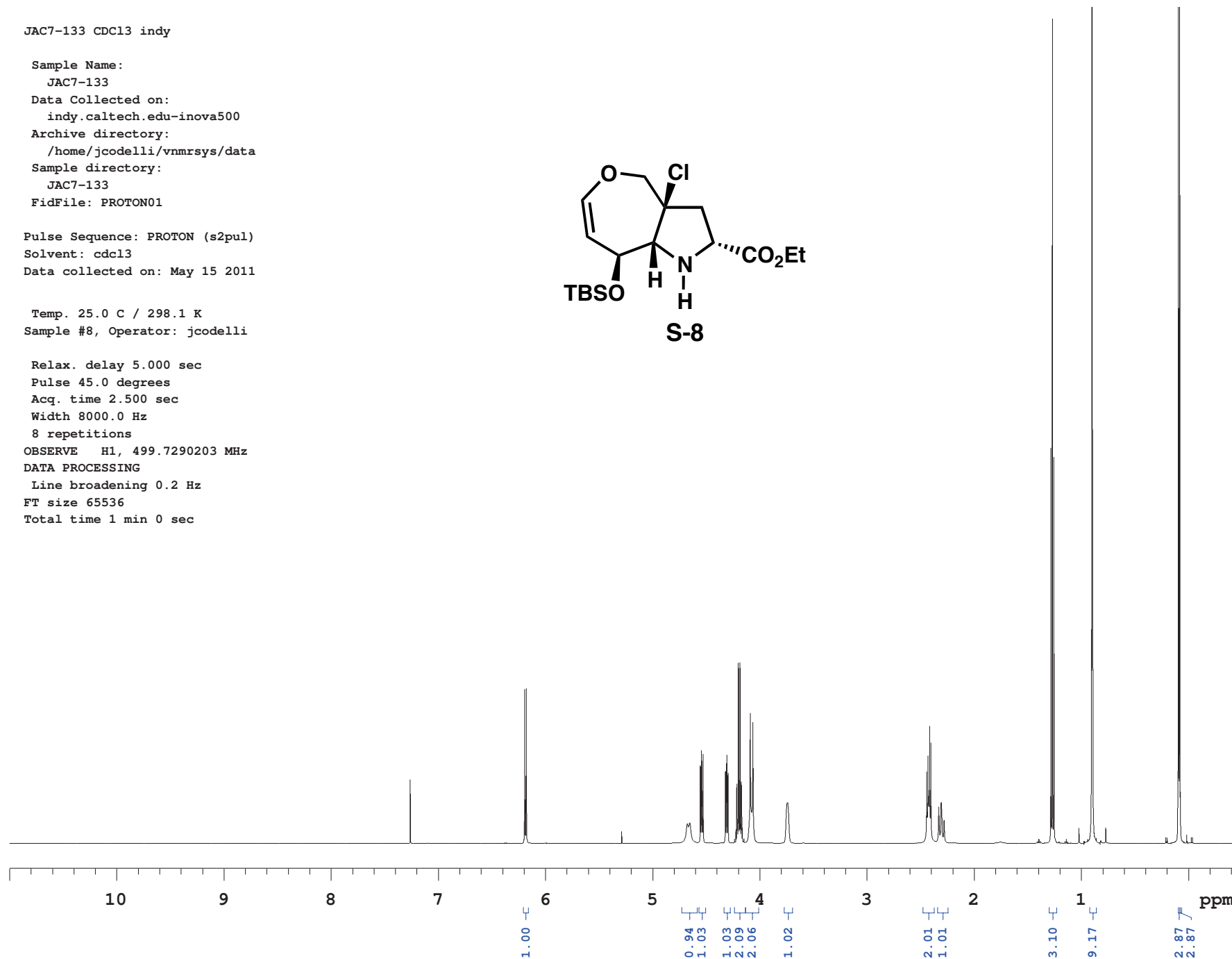
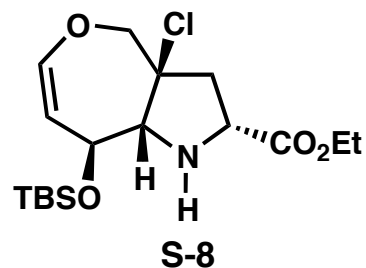
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 0 sec



JAC7-133 CDCl3 indy

Sample Name:

JAC7-133

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-133

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 15 2011

Temp. 25.0 C / 298.1 K

Sample #8, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1400 repetitions

OBSERVE C13, 125.6569642 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

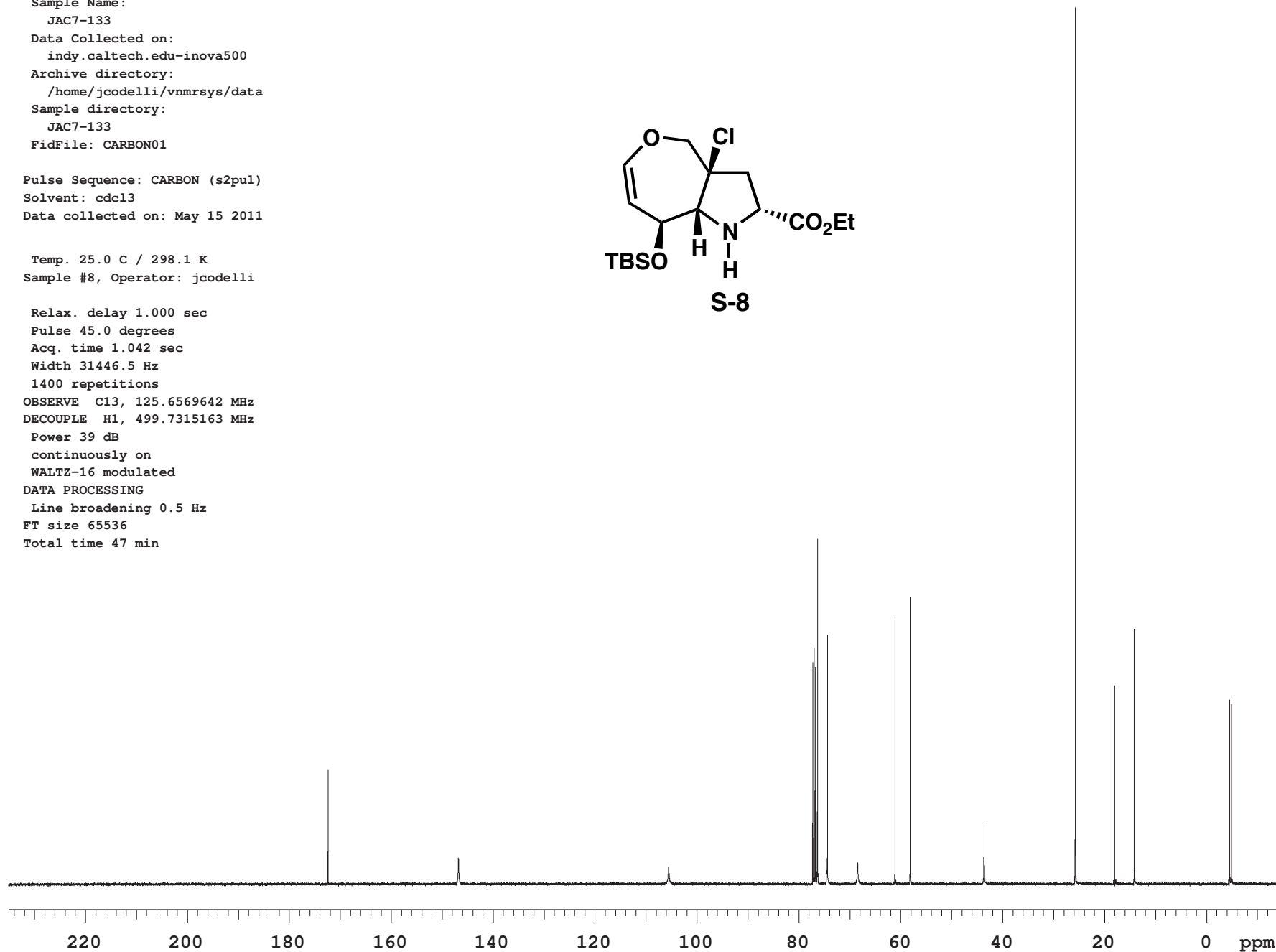
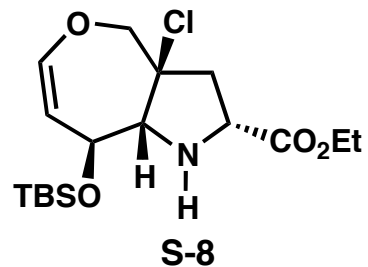
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 47 min



JAC7-249 CDCl3 indy

Sample Name:

JAC7-249

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-249

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 10 2011

Sample #14, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

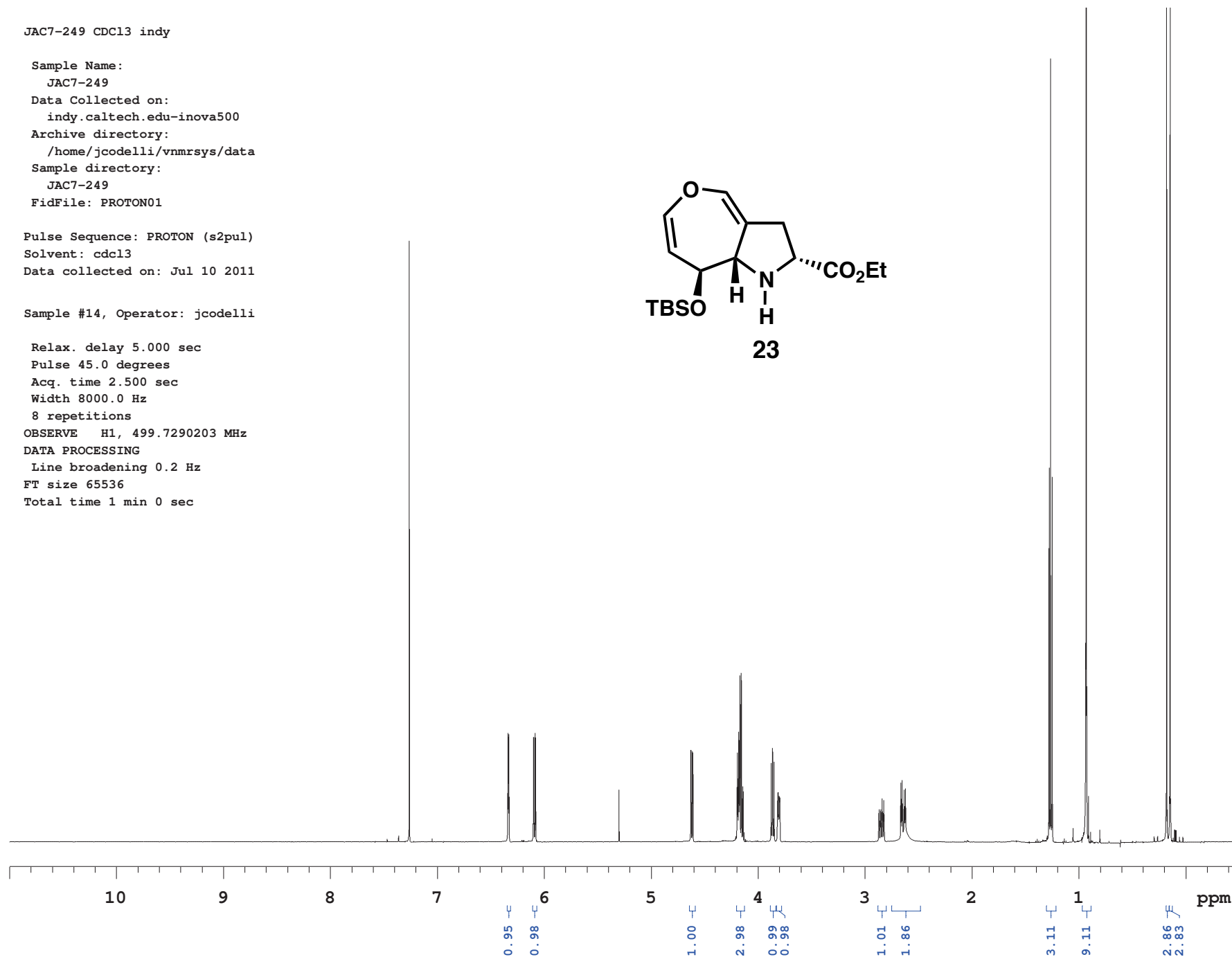
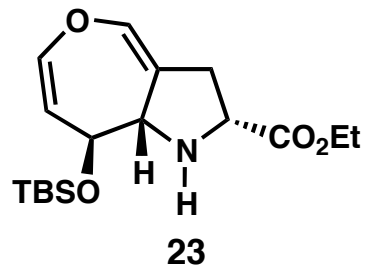
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 0 sec



JAC7-249 CDC13 indy

Sample Name:

JAC7-249

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-249

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jul 10 2011

Sample #15, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1400 repetitions

OBSERVE C13, 125.6569662 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

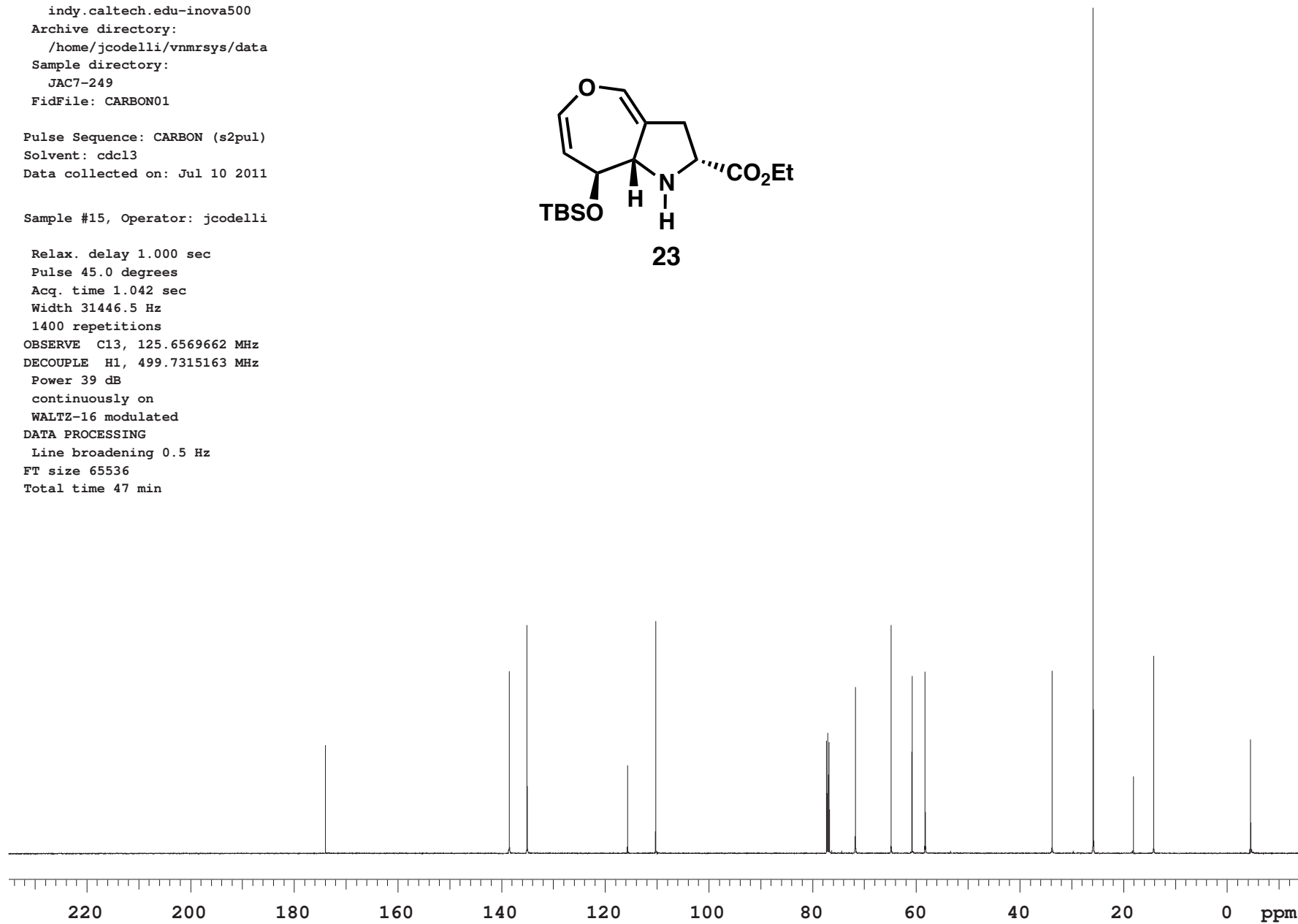
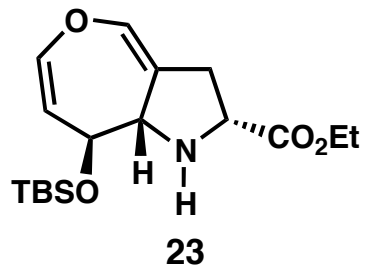
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 47 min



JAC7-143 temp=50 CDC13 siena

Sample Name:

JAC7-143temp=50

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-143temp=50

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jun 13 2011

Temp. 50.0 C / 323.1 K

Sample #7, Operator: jcodelli

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

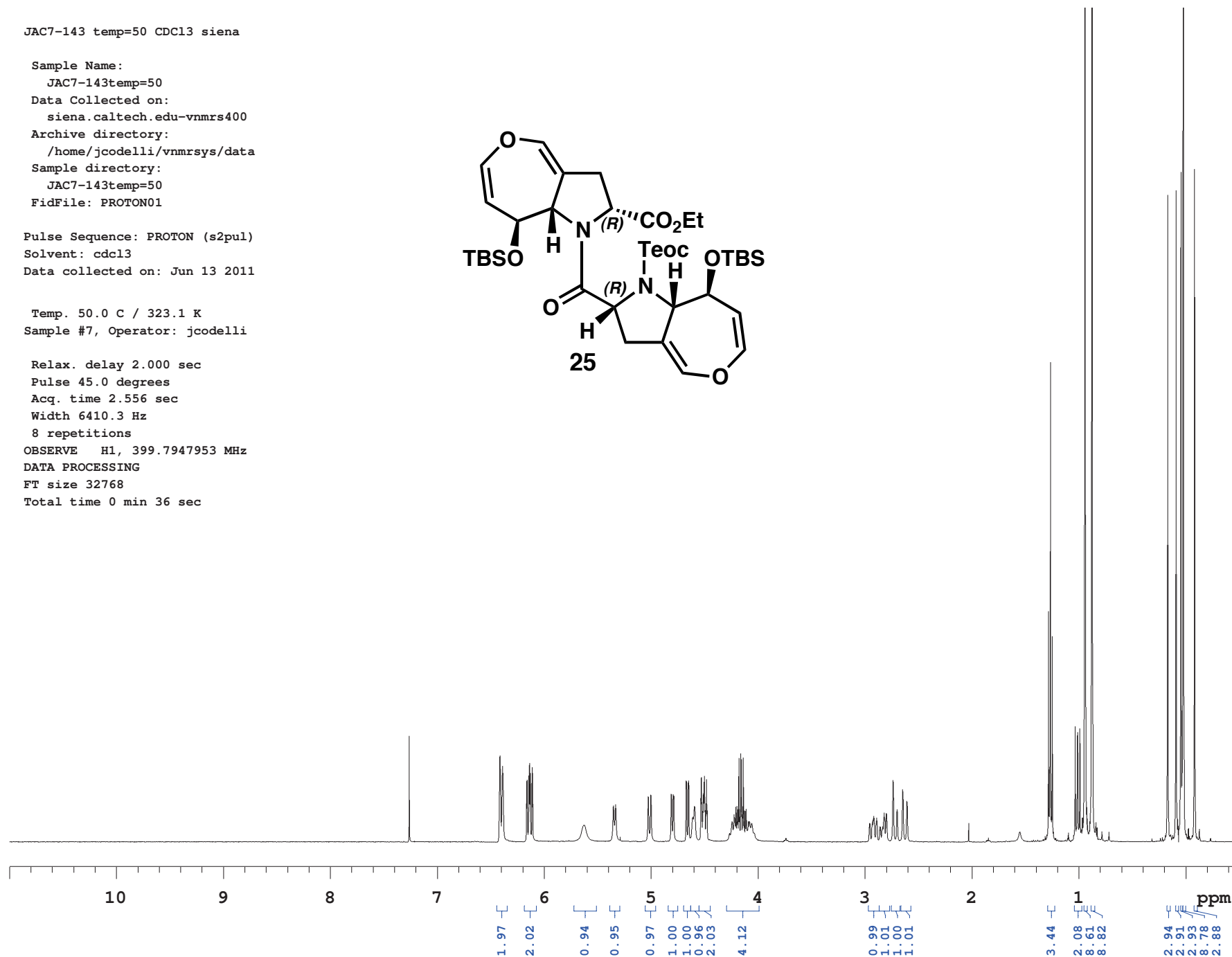
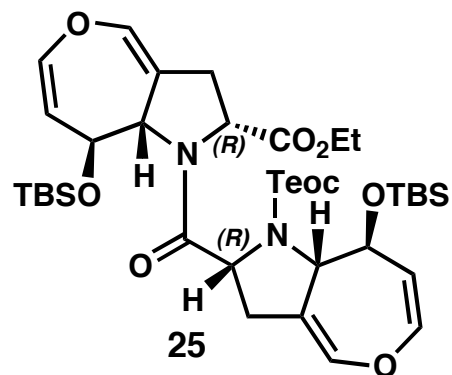
8 repetitions

OBSERVE H1, 399.7947953 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 36 sec



JAC7-143 50degreesC CDC13 siena

Sample Name:

JAC7-143

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-143

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jul 17 2011

Temp. 50.0 C / 323.1 K

Sample #1, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

5000 repetitions

OBSERVE C13, 100.5284739 MHz

DECOUPLE H1, 399.7968015 MHz

Power 39 dB

continuously on

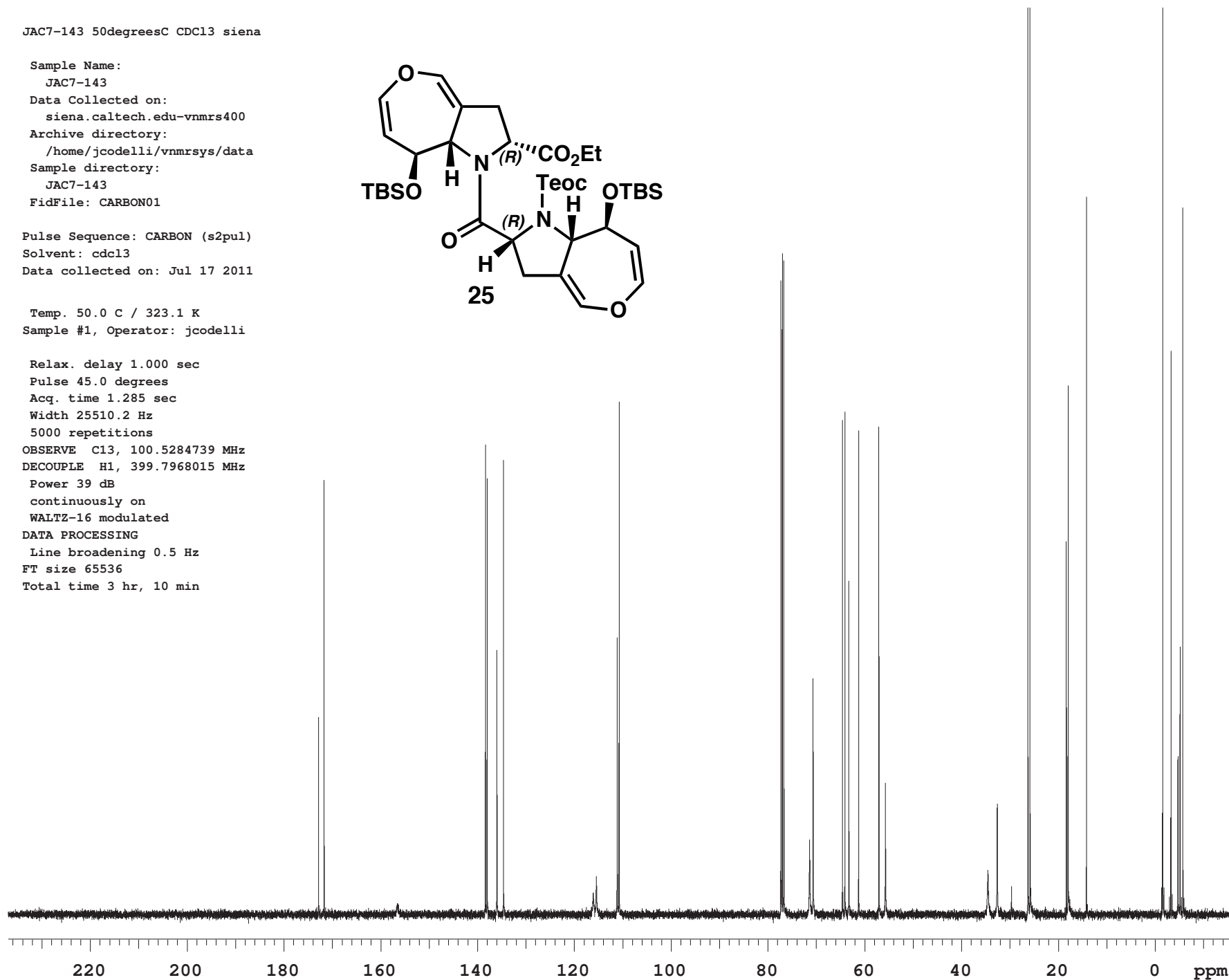
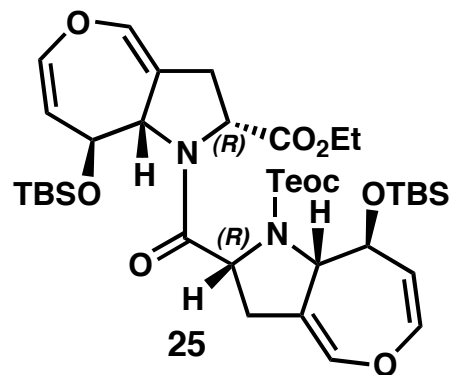
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 10 min



JAC7-211 CD3CN indy

Sample Name:

JAC7-211

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-211

FidFile: PROTON05

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Aug 13 2011

Sample #10, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

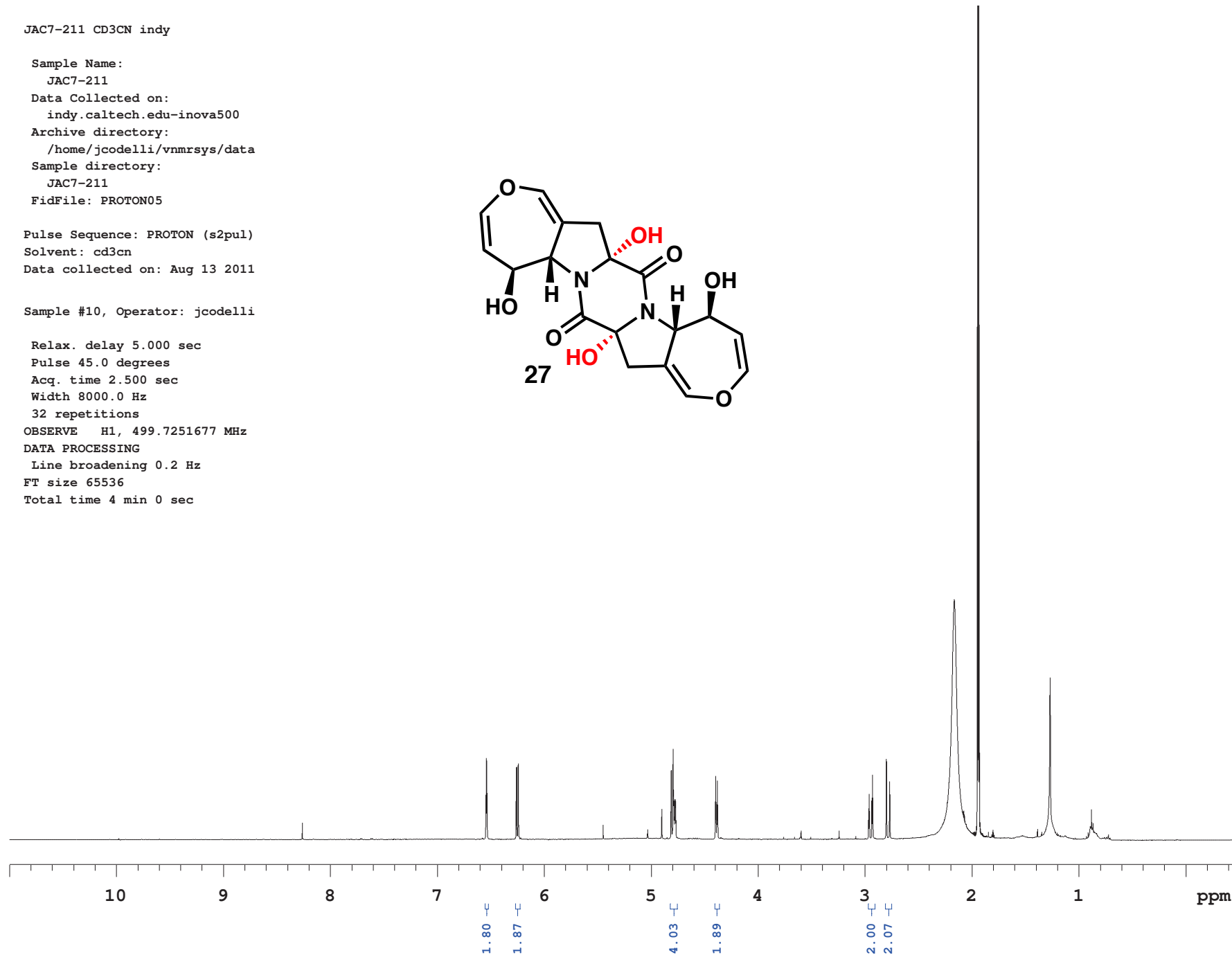
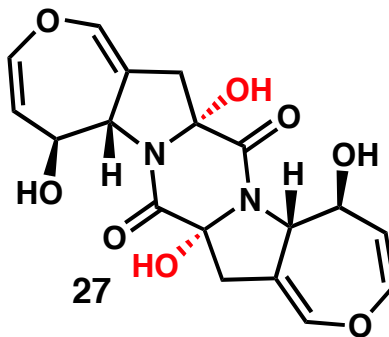
OBSERVE H1, 499.7251677 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 4 min 0 sec



JAC7-211 CD3CN indy

Sample Name:

JAC7-211

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-211

FidFile: CARBON02

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Aug 14 2011

Sample #10, Operator: jcodelli

Relax. delay 0.050 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

10000 repetitions

OBSERVE C13, 125.6558744 MHz

DECOUPLE H1, 499.7276454 MHz

Power 39 dB

continuously on

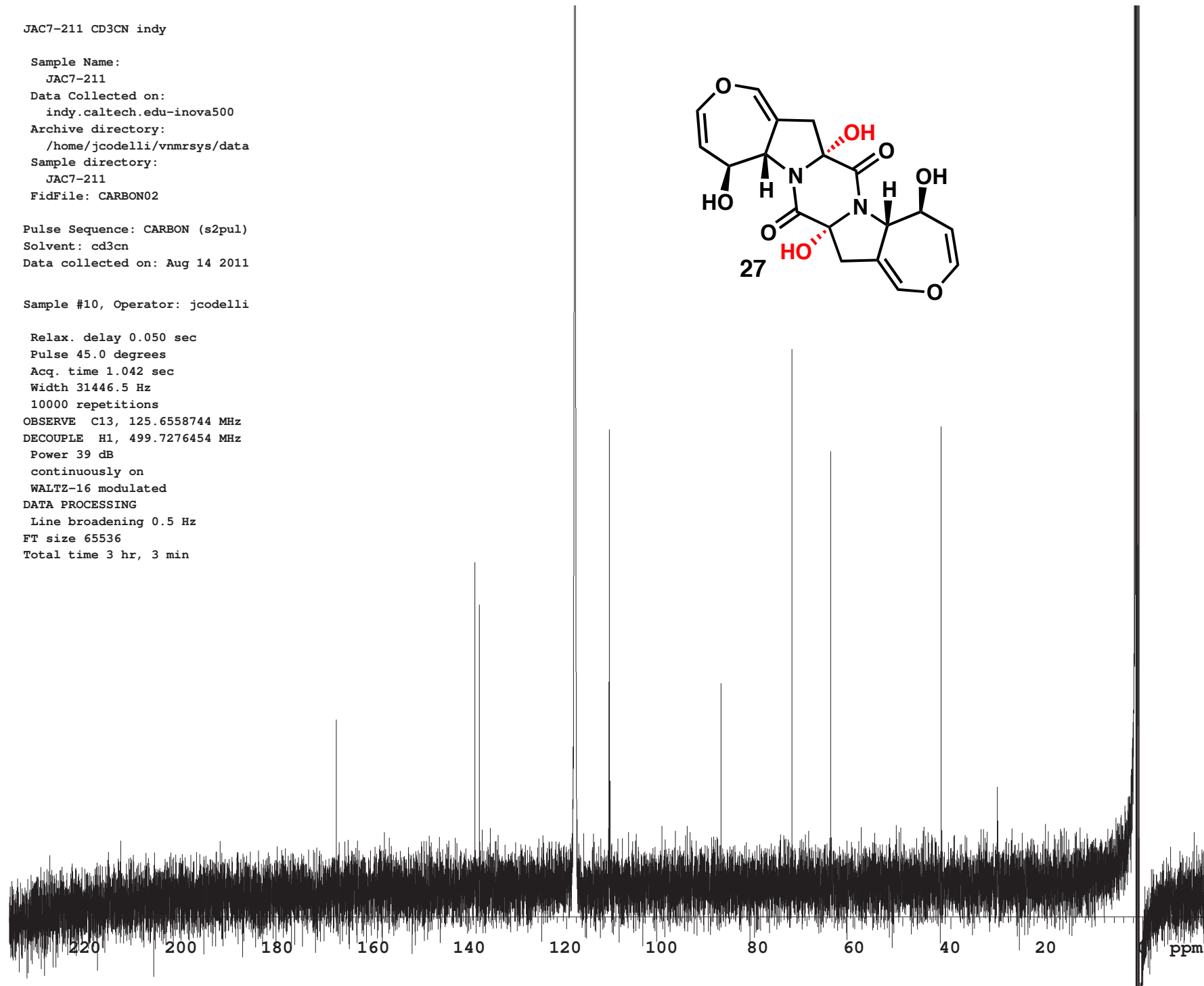
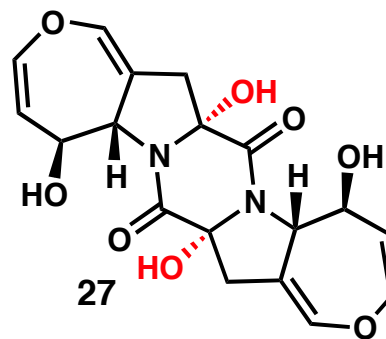
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 3 min



JAC7-209 CDCl3 indy

Sample Name:

JAC7-209

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-209

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 15 2011

Temp. 25.0 C / 298.1 K

Sample #14, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

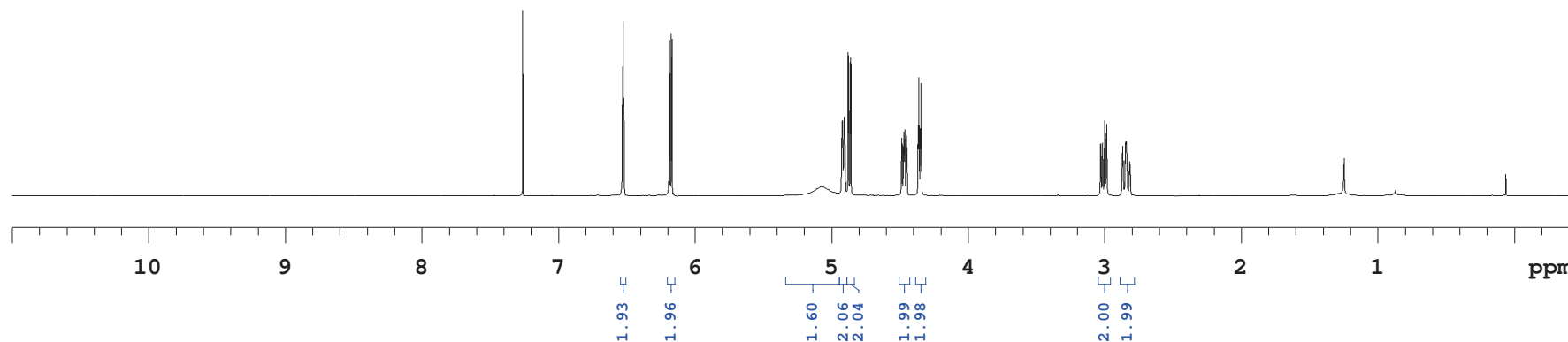
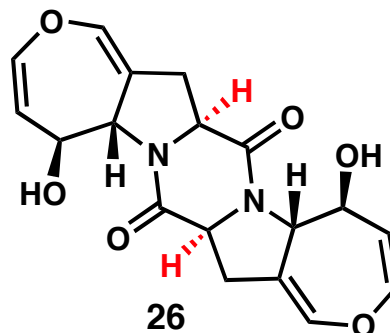
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 0 sec



JAC7-209 CDCl3 indy

Sample Name:

JAC7-209

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-209

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 15 2011

Temp. 25.0 C / 298.1 K

Sample #14, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6569642 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

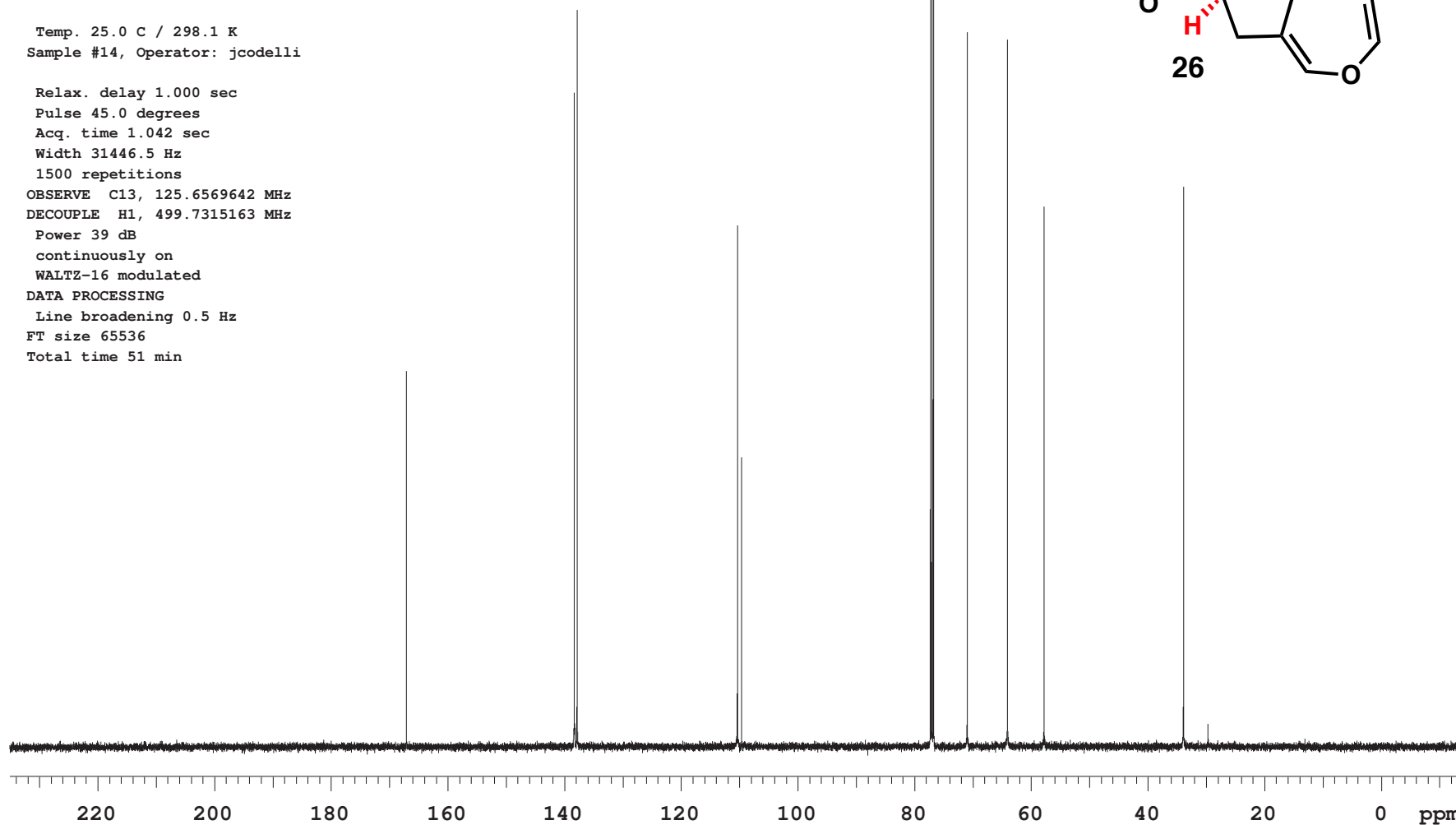
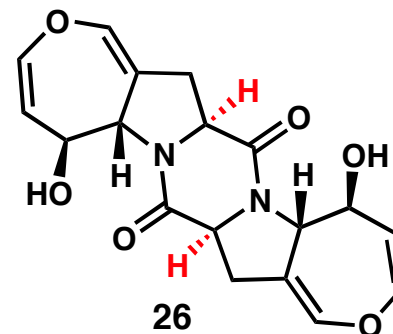
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



JAC7-221 CDC13 indy

Sample Name:

JAC7-221

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-221

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jun 21 2011

Temp. 25.0 C / 298.1 K

Sample #7, Operator: jcodelli

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

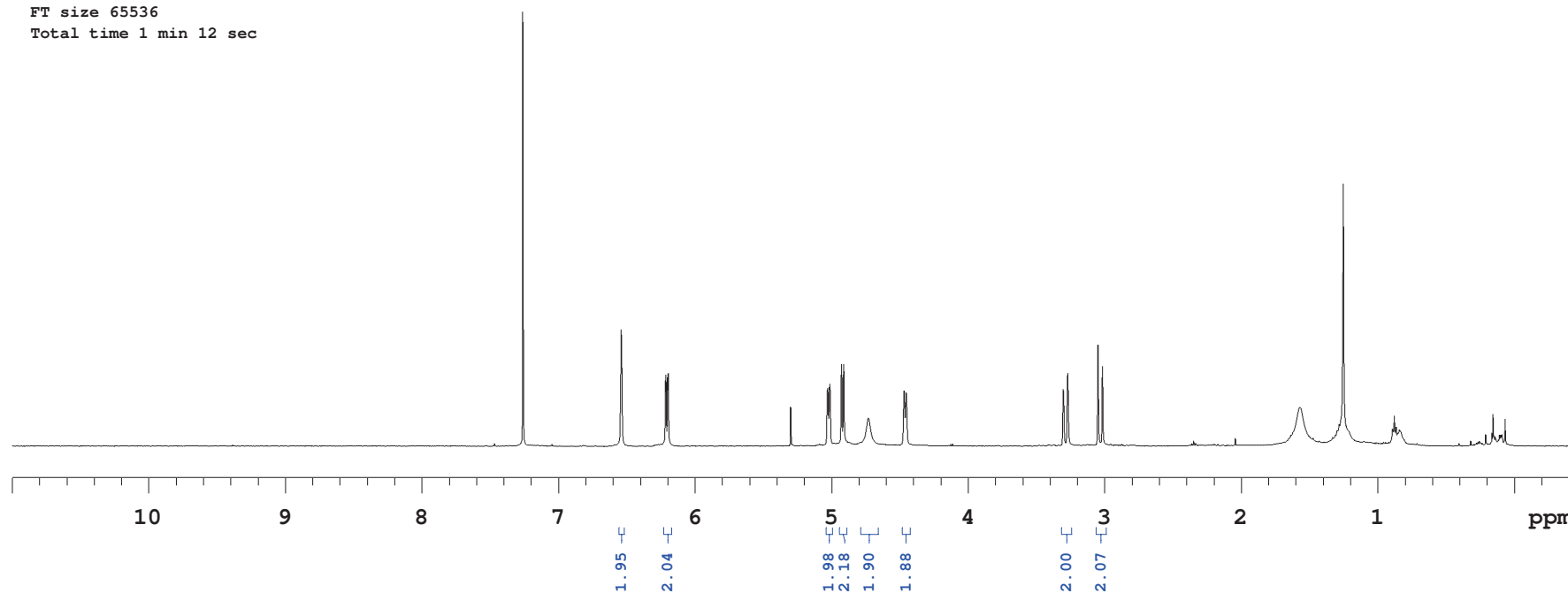
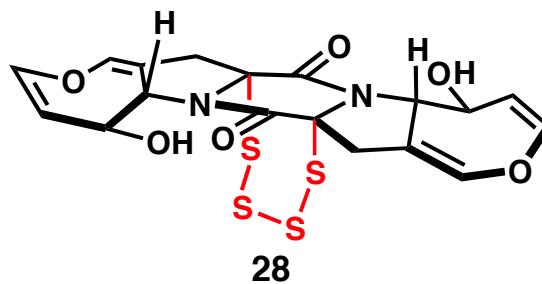
OBSERVE H1, 499.7290210 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



JAC7-239 CDC13 indy

Sample Name:

JAC7-239

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-239

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jun 29 2011

Sample #7, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1700 repetitions

OBSERVE C13, 125.6569633 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

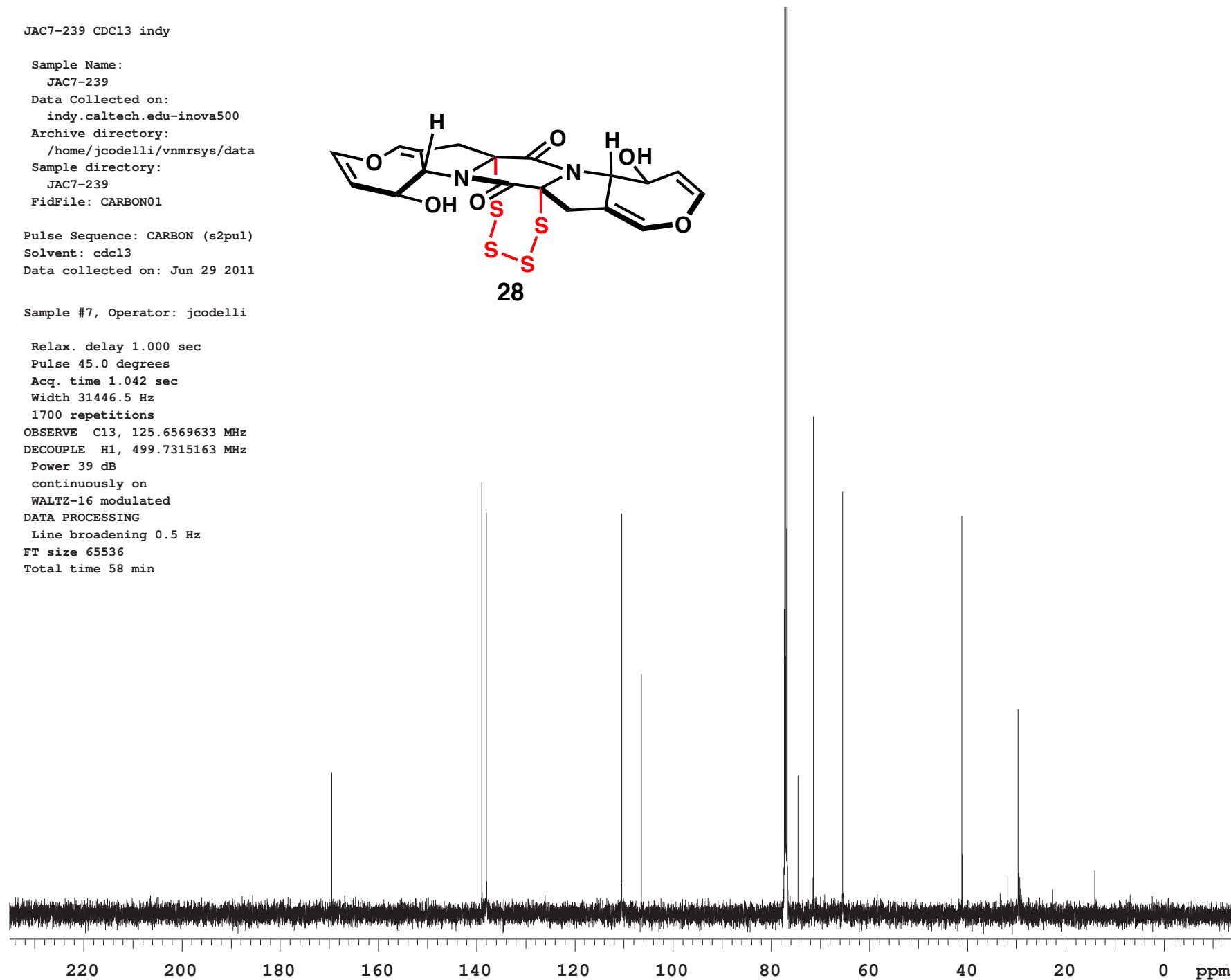
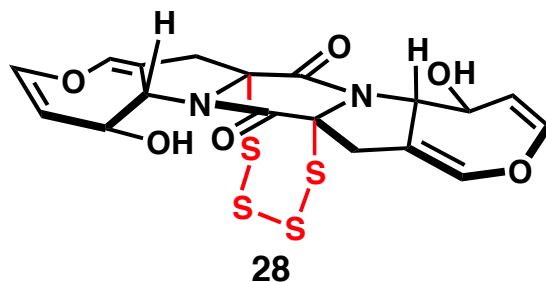
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 58 min



JAC7-243 CDC13 indy

Sample Name:

JAC7-243

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrSYS/data

Sample directory:

JAC7-243

FidFile: PROTON02

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 20 2011

Sample #7, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

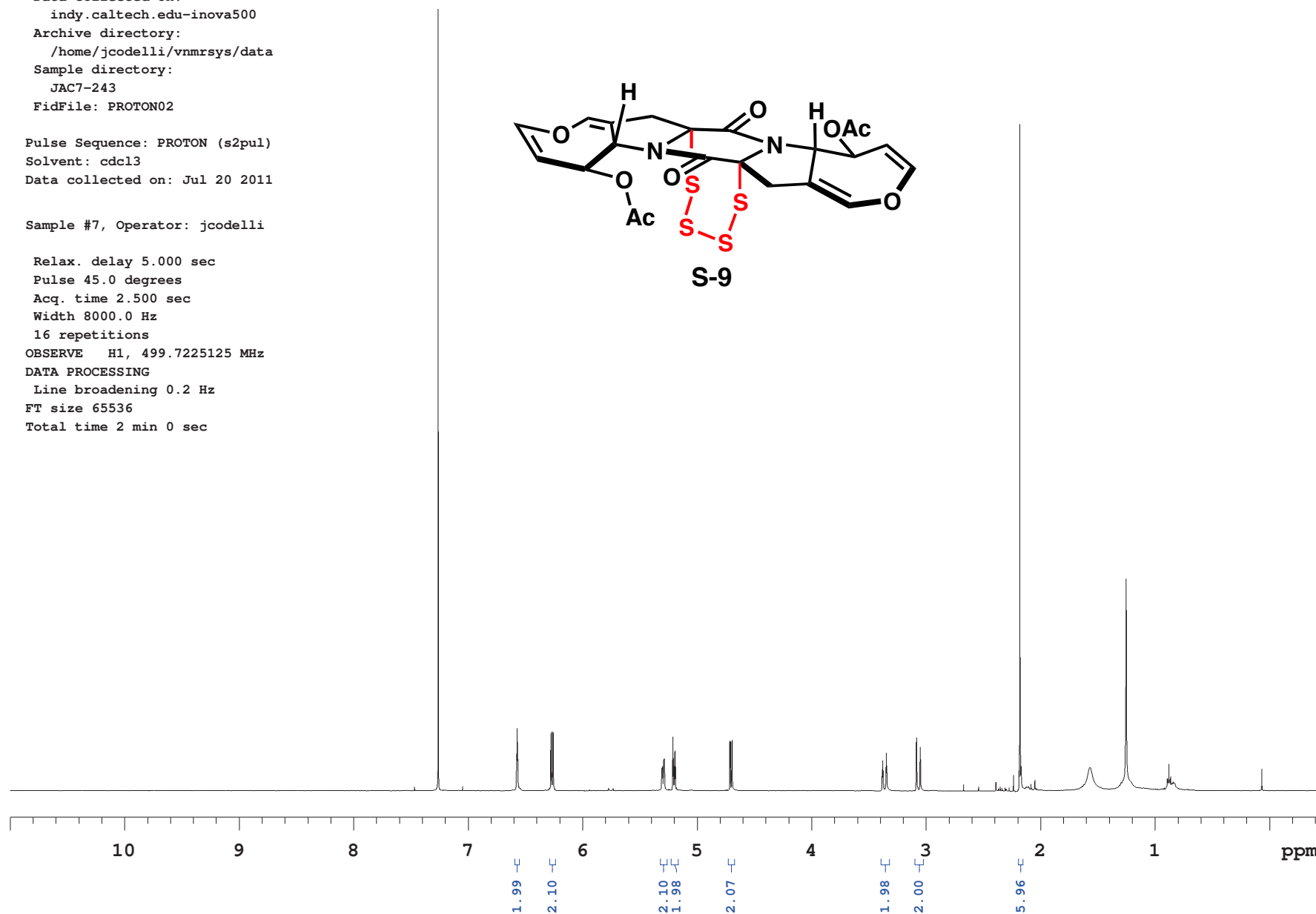
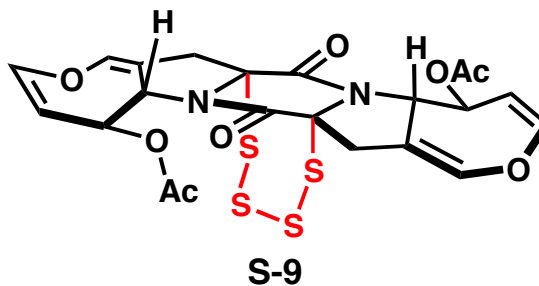
OBSERVE H1, 499.7225125 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 0 sec



JAC7-243 CDC13 indy

Sample Name:

JAC7-243

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-243

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jun 30 2011

Sample #7, Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

10000 repetitions

OBSERVE C13, 125.6569623 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

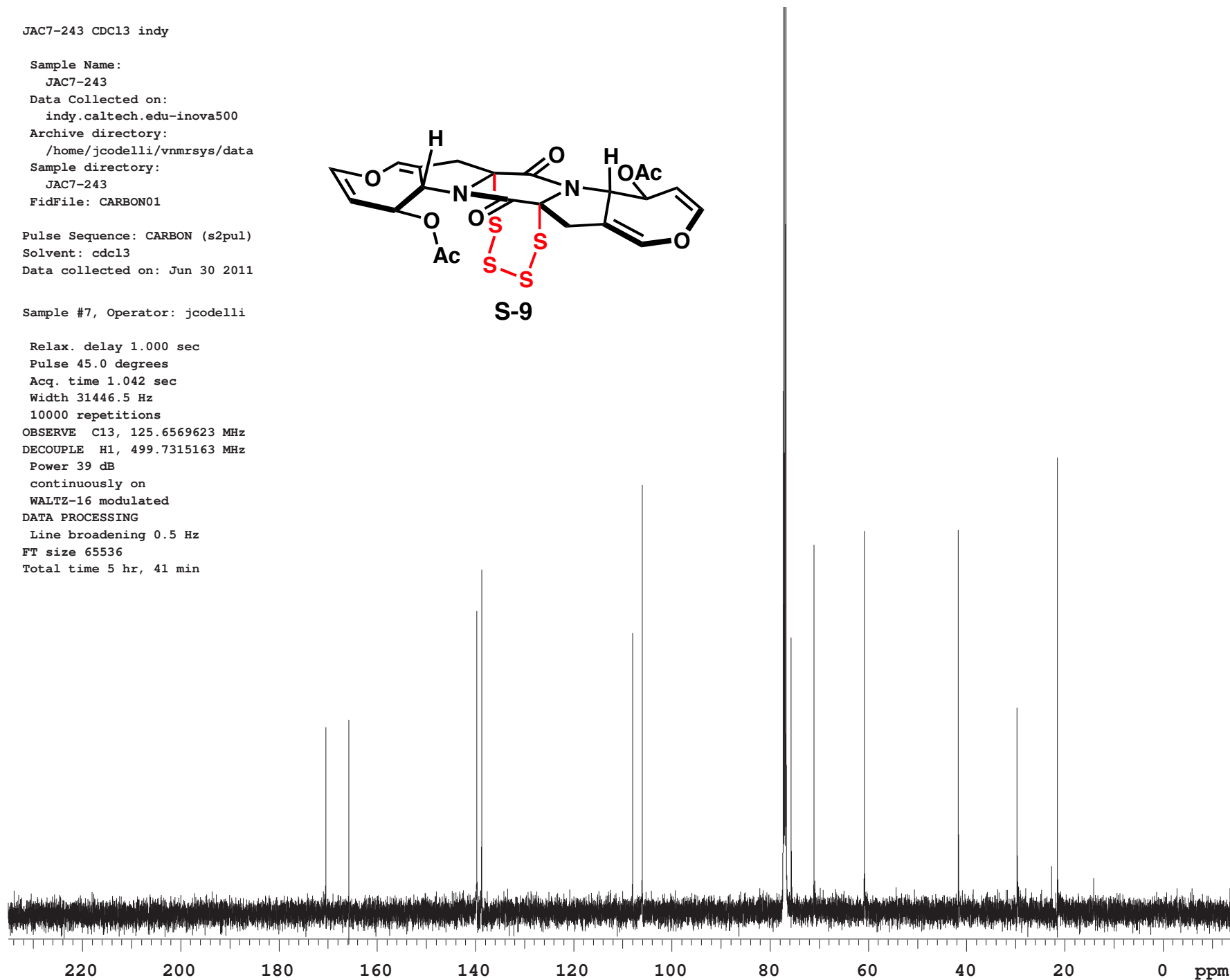
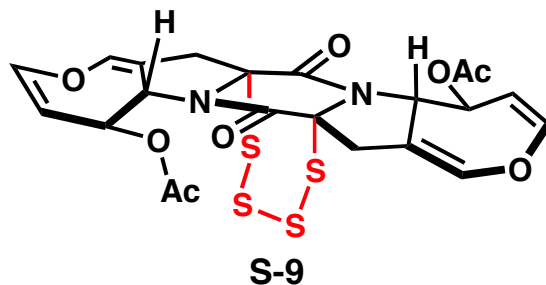
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 5 hr, 41 min



JAC7-301 CDC13 siena

Sample Name:

JAC7-301

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-301

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Aug 5 2011

Sample #9, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

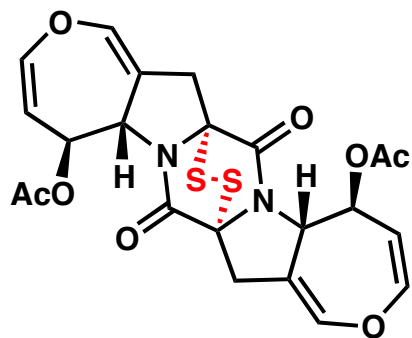
64 repetitions

OBSERVE H1, 399.7947965 MHz

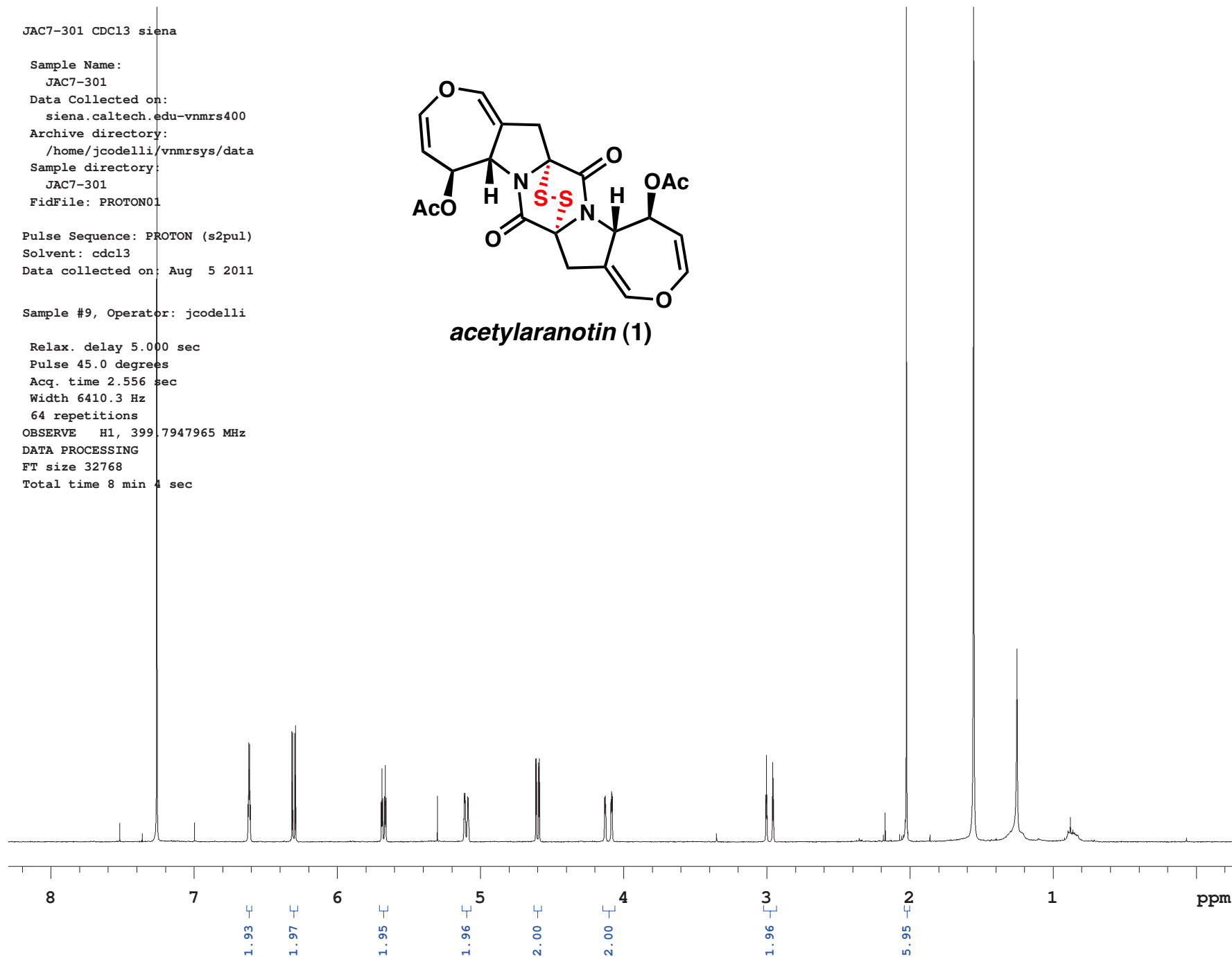
DATA PROCESSING

FT size 32768

Total time 8 min 4 sec



acetylaranotin (1)



JAC7-301 DMSO indy

Sample Name:

JAC7-301

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/jcodelli/vnmrsys/data

Sample directory:

JAC7-301

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: dmsd

Data collected on: Aug 6 2011

Sample #7, Operator: jcodelli

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

40 repetitions

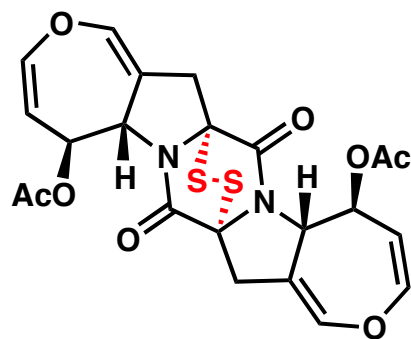
OBSERVE H1, 499.7248788 MHz

DATA PROCESSING

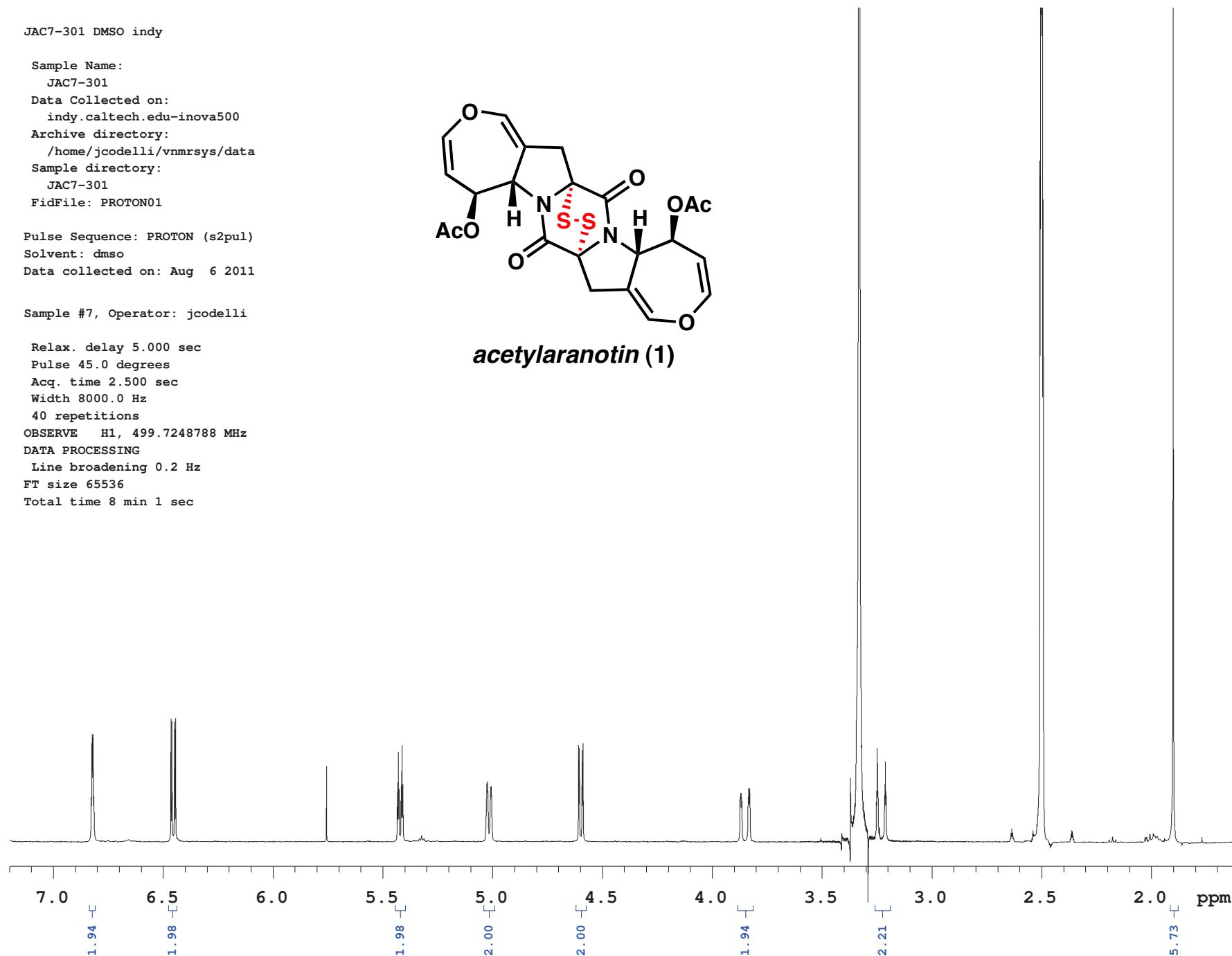
Line broadening 0.2 Hz

FT size 65536

Total time 8 min 1 sec



acetylaranotin (1)



JAC7-301 DMSO-d6 daytona

Sample Name:

JAC7-301

Data Collected on:

daytona.caltech.edu-inova500

Archive directory:

Sample directory:

FidFile: jac7-301carbon

Pulse Sequence: CARBON (s2pul)

Solvent: dmsc

Data collected on: Aug 6 2011

Temp. 25.0 C / 298.1 K

Operator: jcodelli

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.043 sec

Width 31421.8 Hz

26500 repetitions

OBSERVE C13, 125.6876974 MHz

DECOUPLE H1, 499.8537553 MHz

Power 39 dB

continuously on

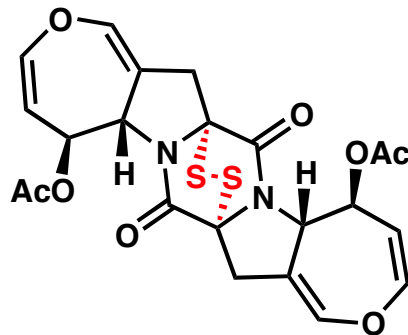
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 15 hr, 6 min



acetylaranotin (1)

