

**Enantioselective Synthesis of Tryptophan Derivatives by a Tandem  
Friedel–Crafts Conjugate Addition/Asymmetric Protonation Reaction**

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**Supporting Information 2 (NMR spectra):**

LMRVI-067-3-C1-2,2'-MOM-R-BINOL

Sample Name:

LMRVI-067-3-C1-2\_2-MOM-R-BINOL

Data Collected on:

indy.caltech.edu-inova500

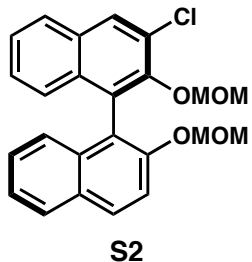
Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-067-3-C1-2\_2-MOM-R-BINOL

FidFile: PROTON01



Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 11 2011

Sample #33, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

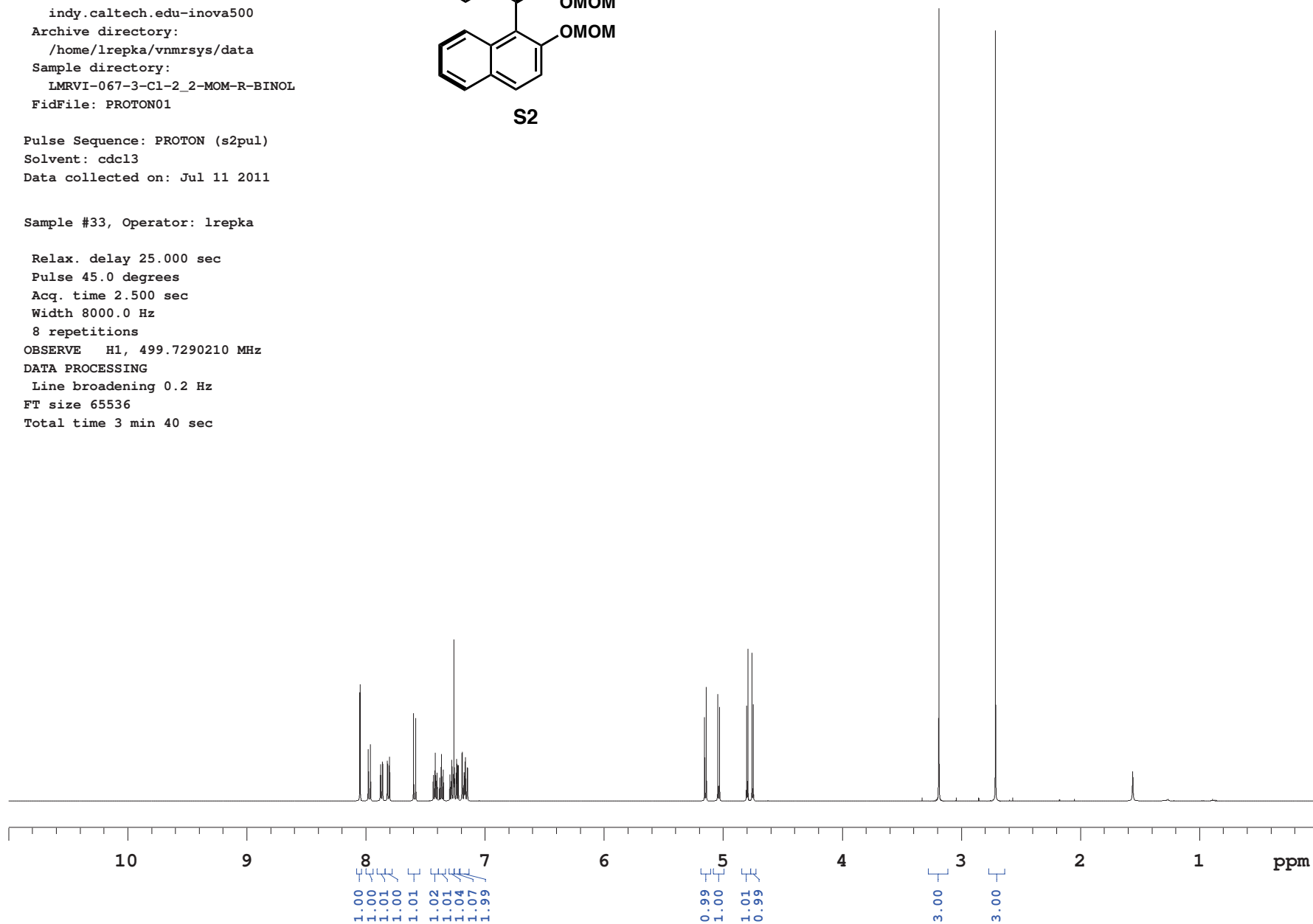
OBSERVE H1, 499.7290210 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



LMRVI-067-3-C1-2, 2'-MOM-R-BINOL

Sample Name:

LMRVI-067-3-C1-2\_2-MOM-R-BINOL

Data Collected on:

indy.caltech.edu-inova500

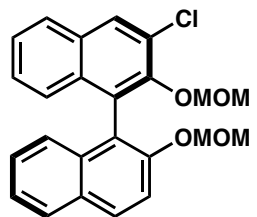
Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-067-3-C1-2\_2-MOM-R-BINOL

FidFile: CARBON01



S2

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 11 2011

Sample #33, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1590 repetitions

OBSERVE C13, 125.6569667 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

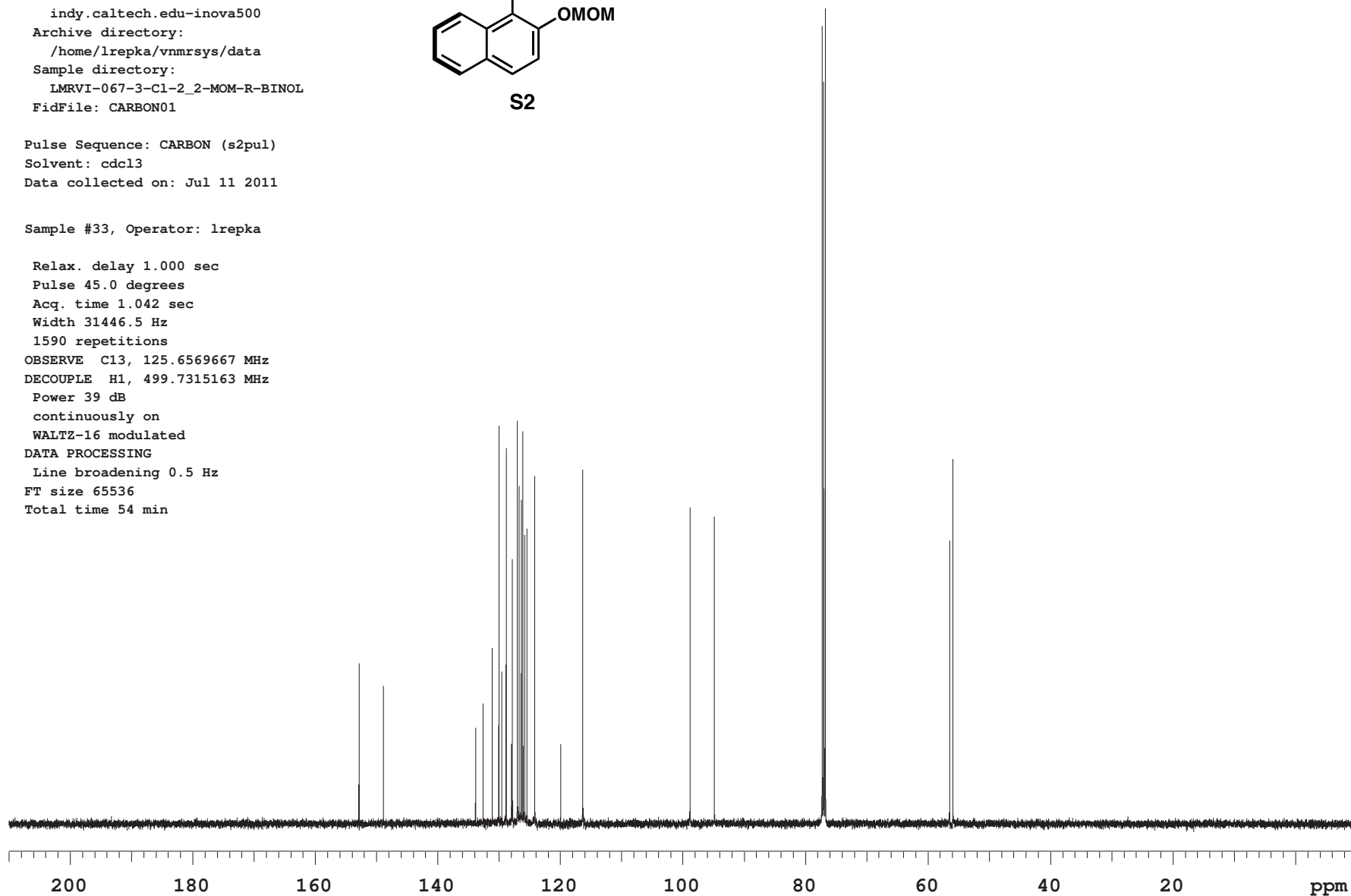
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 54 min



S83

LMRVI-093-3-C1-R-BINOL

Sample Name:

LMRVI-093-3-C1-R-BINOL

Data Collected on:

indy.caltech.edu-inova500

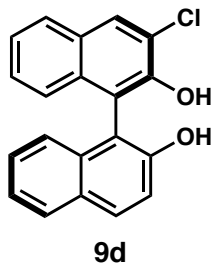
Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-093-3-C1-R-BINOL

FidFile: PROTON01



Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 11 2011

Sample #34, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

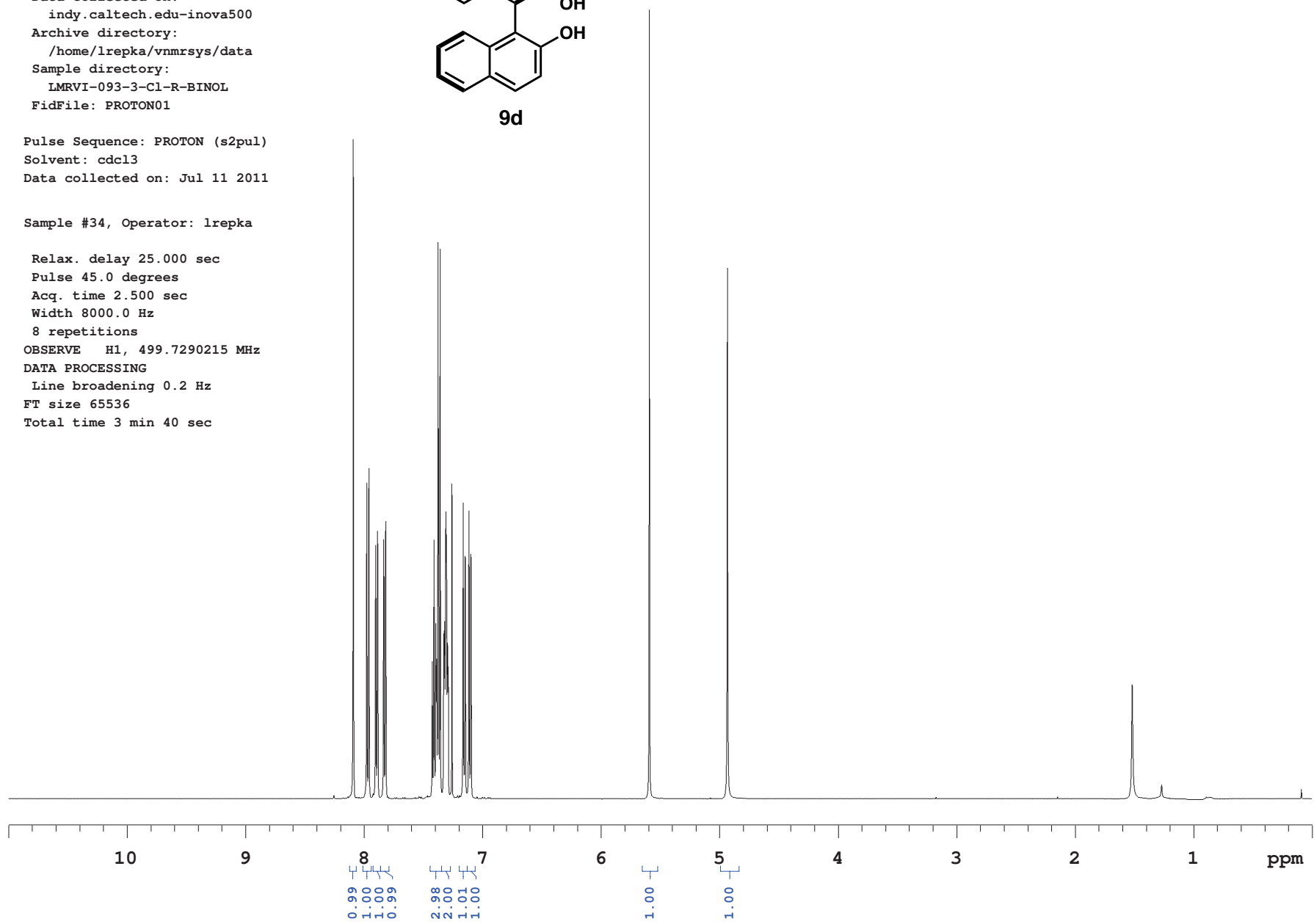
OBSERVE H1, 499.7290215 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



LMRVI-093-3-C1-R-BINOL

Sample Name:

LMRVI-093-3-C1-R-BINOL

Data Collected on:

indy.caltech.edu-inova500

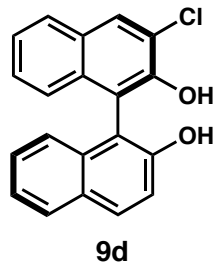
Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-093-3-C1-R-BINOL

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 11 2011

Sample #34, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

2000 repetitions

OBSERVE C13, 125.6569690 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

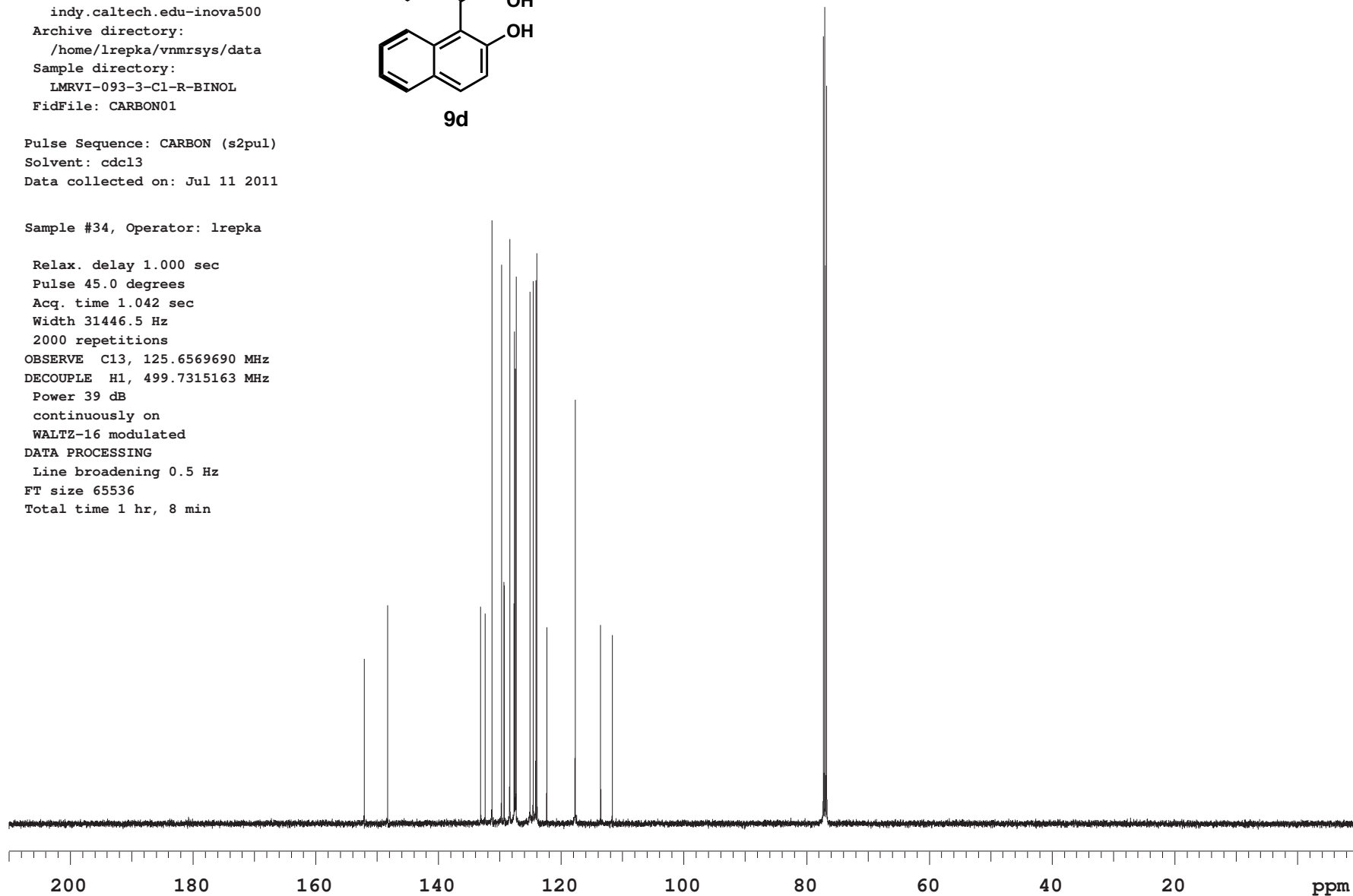
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 8 min



LMRVI-279-6,6'-hydroxy-MOM BINOL

Sample Name:

LMRVI-279

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-279

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Dec 20 2011

Sample #42, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

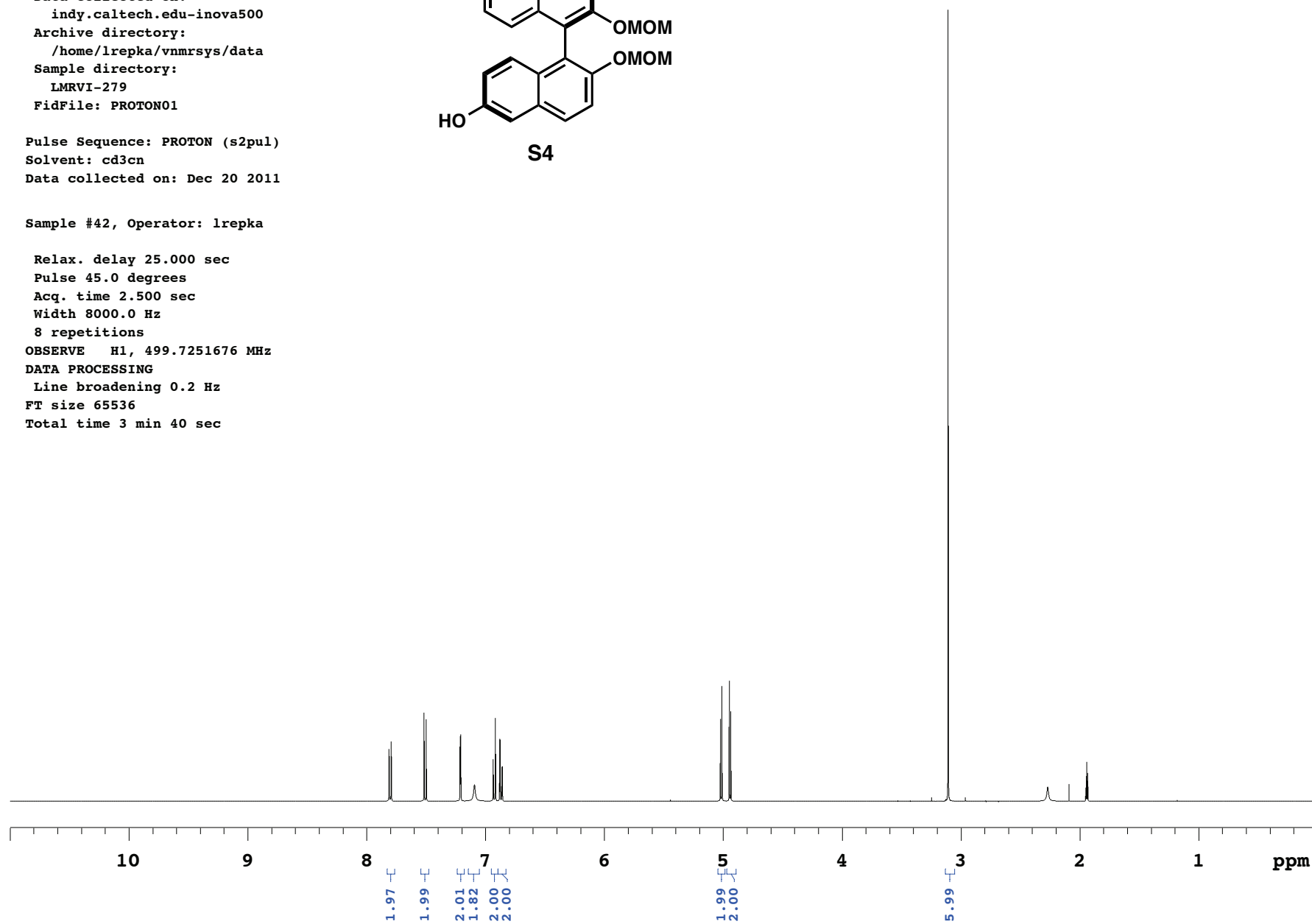
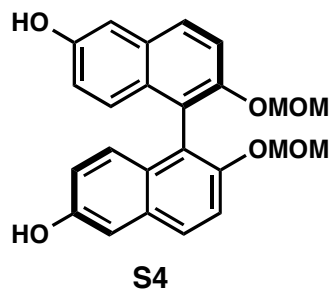
OBSERVE H1, 499.7251676 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



Sample Name:

LMRVI-279

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

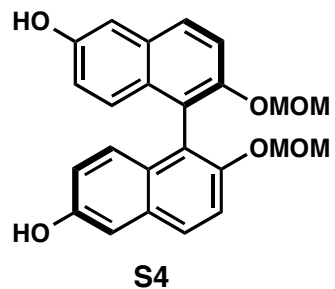
LMRVI-279

Fidfile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Dec 20 2011



Sample #42, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6558710 MHz

DECOUPLE H1, 499.7276454 MHz

Power 39 dB

continuously on

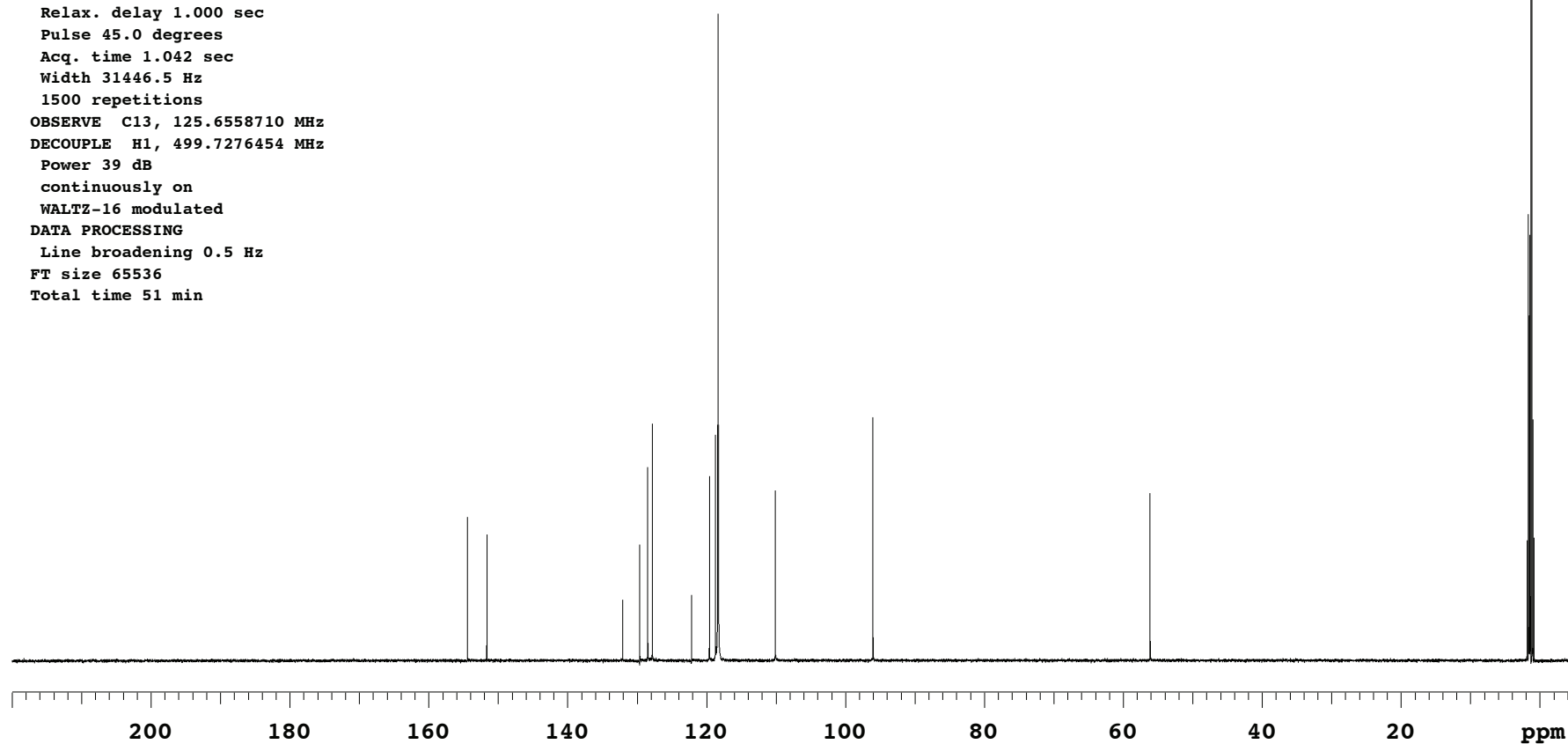
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



LMRVI-273-2-1-allyl-2-phenylindole

Sample Name:

LMRVI-273-2-1-allyl-2-phenylindole

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-273-2-1-allyl-2-phenylindole

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 4 2011

Sample #33, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

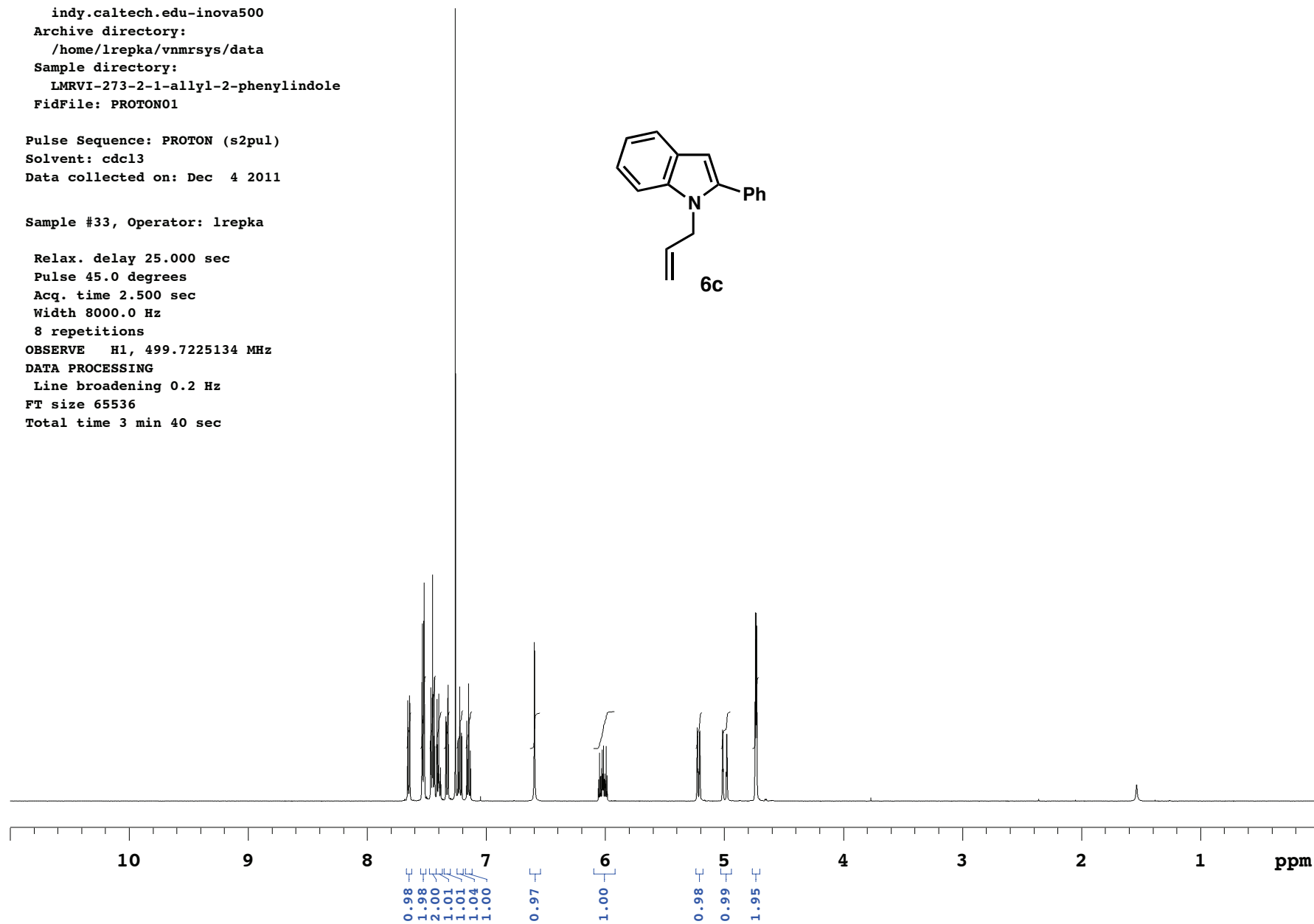
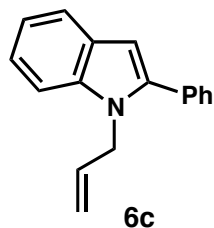
OBSERVE H1, 499.7225134 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec





LMRVI-273-1-allyl-2-phenylindole

Sample Name:

LMRVI-273-1-allyl-2-phenylindole

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-273-1-allyl-2-phenylindole

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Dec 4 2011

Sample #33, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6553343 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

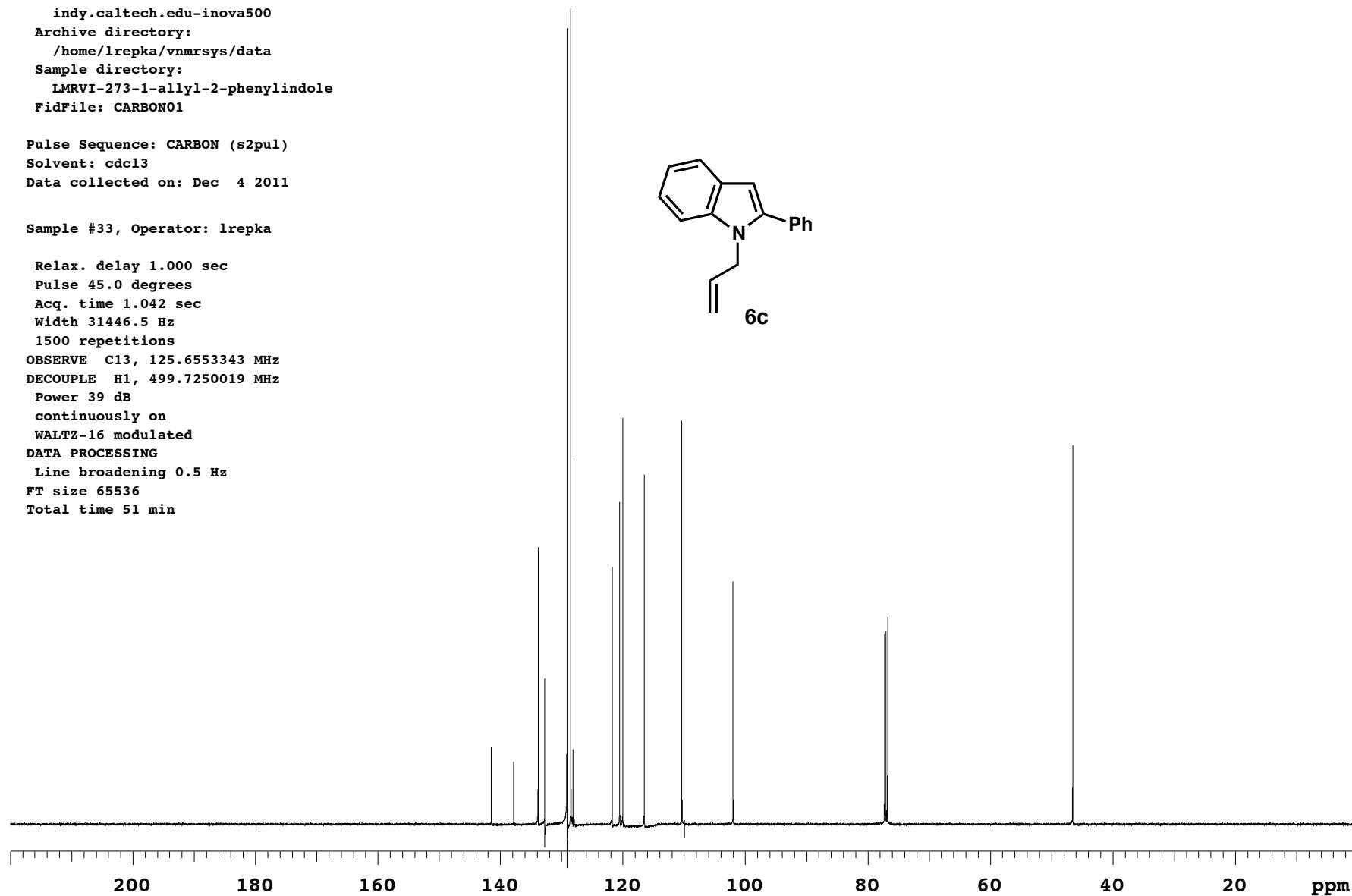
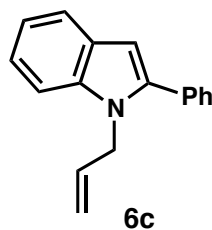
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



LMRVI-273-1,3-diallyl-2-phenylindole

Sample Name:

LMRVI-273-1\_3-diallyl-2-phenylindole

Data Collected on:

indy.caltech.edu-inova500

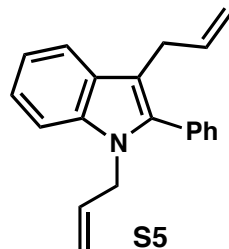
Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-273-1\_3-diallyl-2-phenylindole

FidFile: PROTON01



Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 11 2011

Sample #27, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

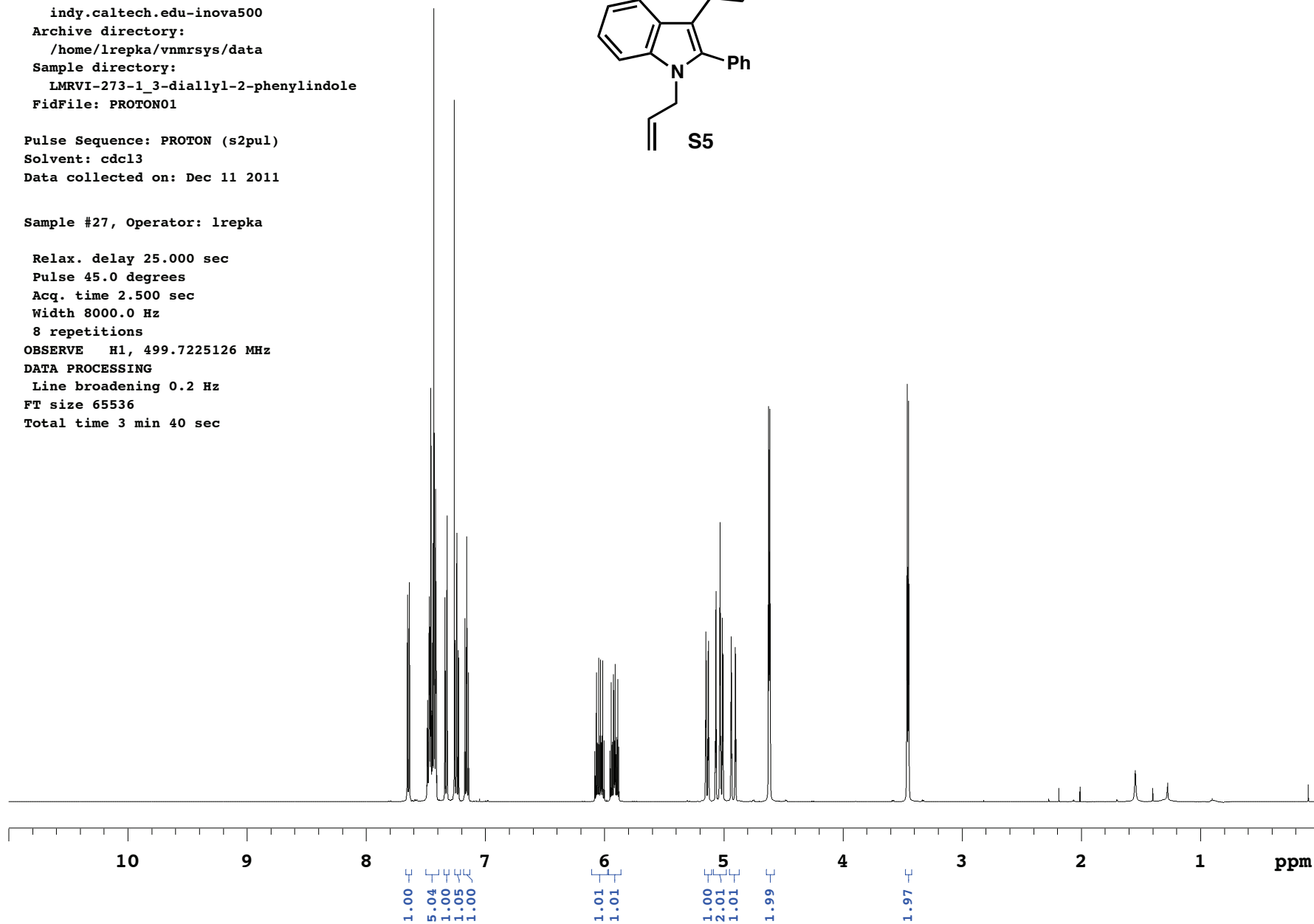
OBSERVE H1, 499.7225126 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



LMRVI-273-1,3-diallyl-2-phenylindole

Sample Name:

LMRVI-273-1\_3-diallyl-2-phenylindole

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

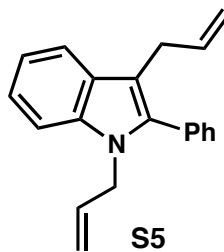
LMRVI-273-1\_3-diallyl-2-phenylindole

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Dec 11 2011



Sample #27, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6553307 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

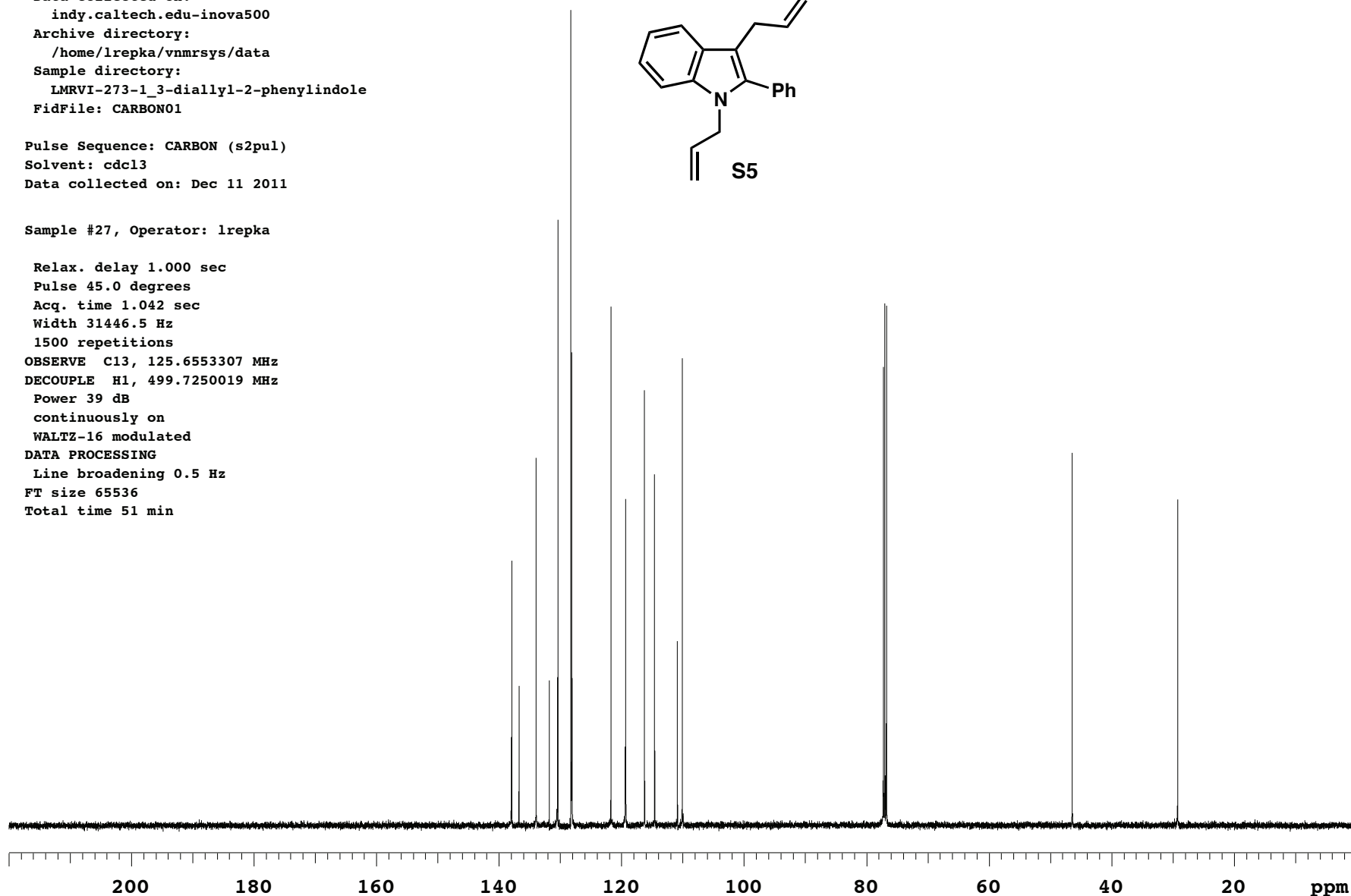
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



LMRVI-219

Sample Name:

LMRVI-219

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-219

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Sep 2 2011

Sample #33, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

6 repetitions

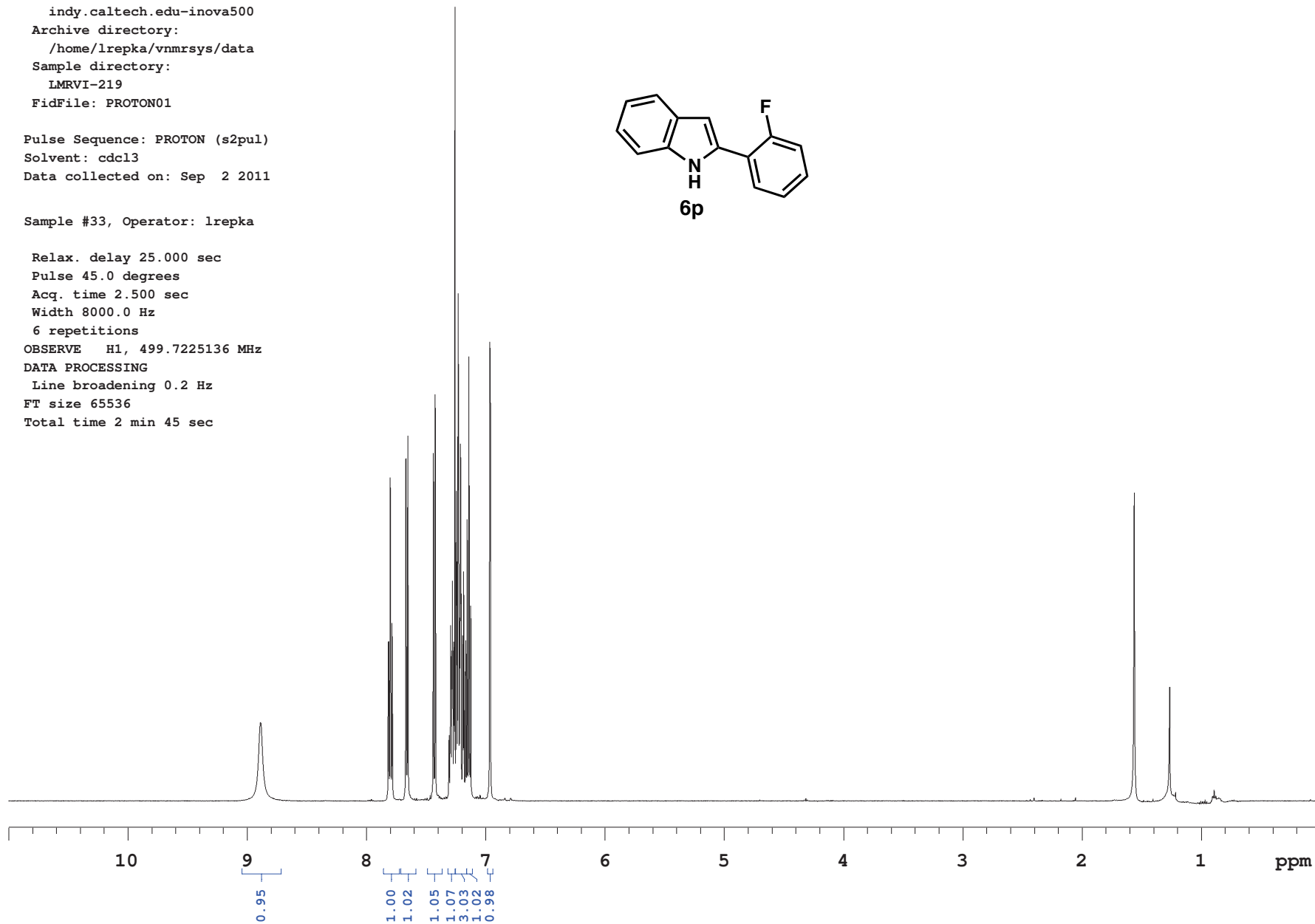
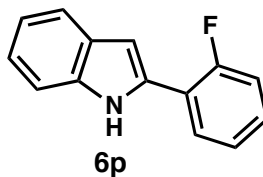
OBSERVE H1, 499.7225136 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 45 sec



LMRVI-219

Sample Name:

LMRVI-219

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

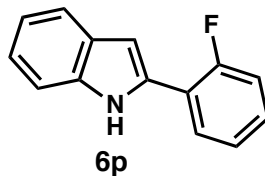
LMRVI-219

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Sep 2 2011



Sample #33, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1600 repetitions

OBSERVE C13, 125.6553281 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

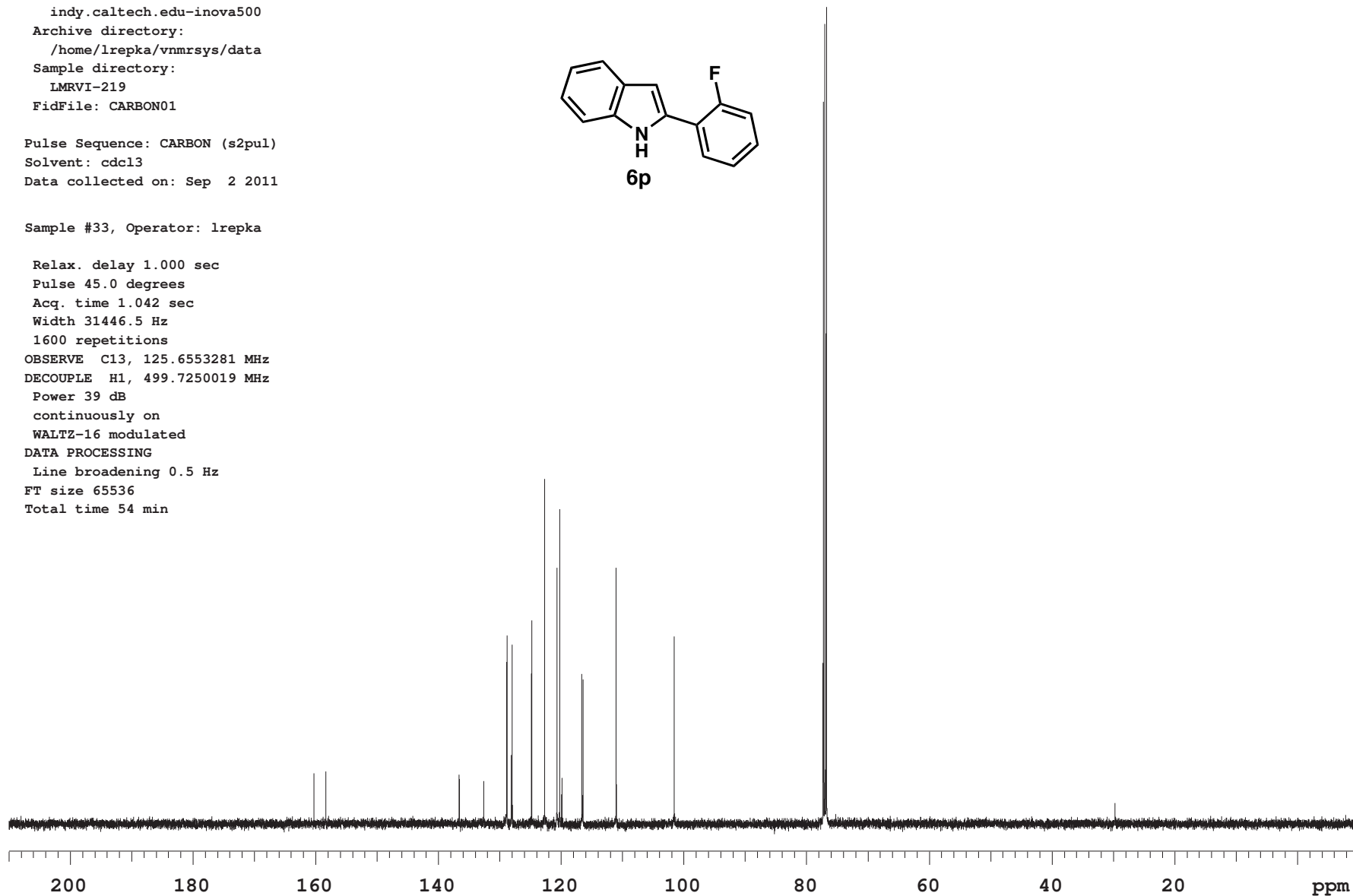
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 54 min



MEK-phthalimide-indole-final

Sample Name:

MEK-phthalimide-indole-final

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrSYS/data

Sample directory:

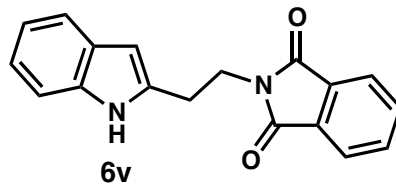
MEK-phthalimide-indole-final

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 2 2011



Sample #10, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

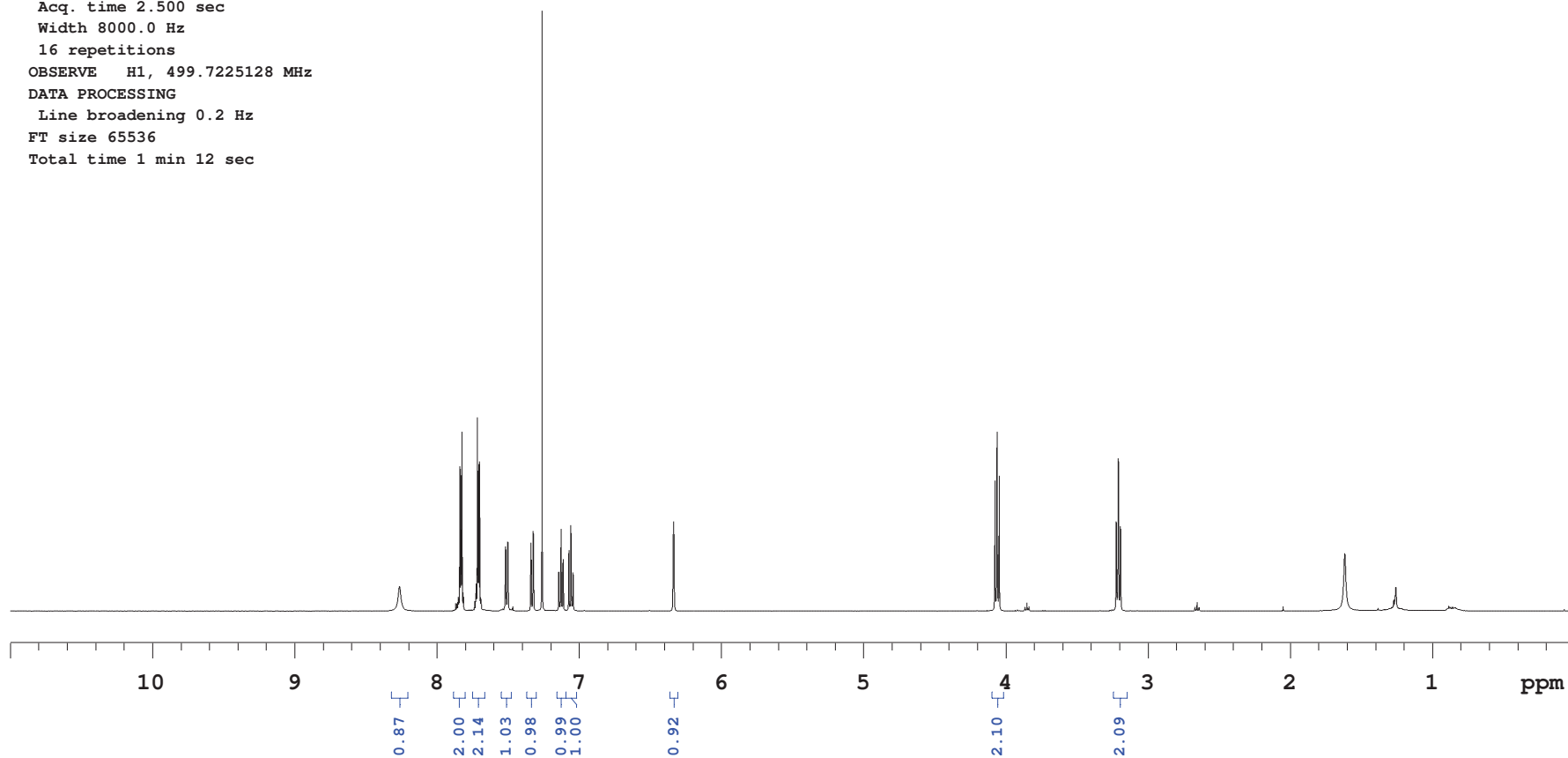
OBSERVE H1, 499.7225128 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



MEK-phthalimide-indole-final

Sample Name:

MEK-phthalimide-indole-final

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

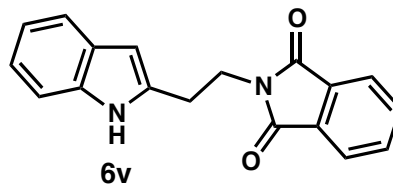
MEK-phthalimide-indole-final

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Sep 2 2011



Sample #10, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553271 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

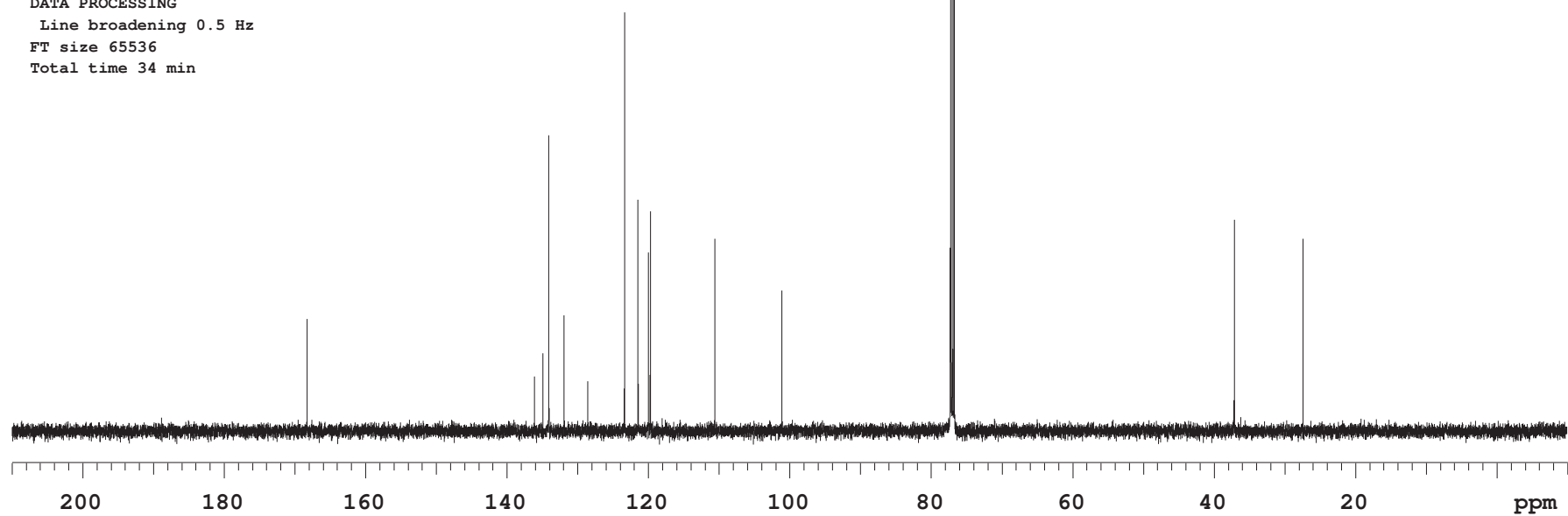
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



LMRVI-161

Sample Name:

LMRVI-161

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-161

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 27 2011

Sample #33, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

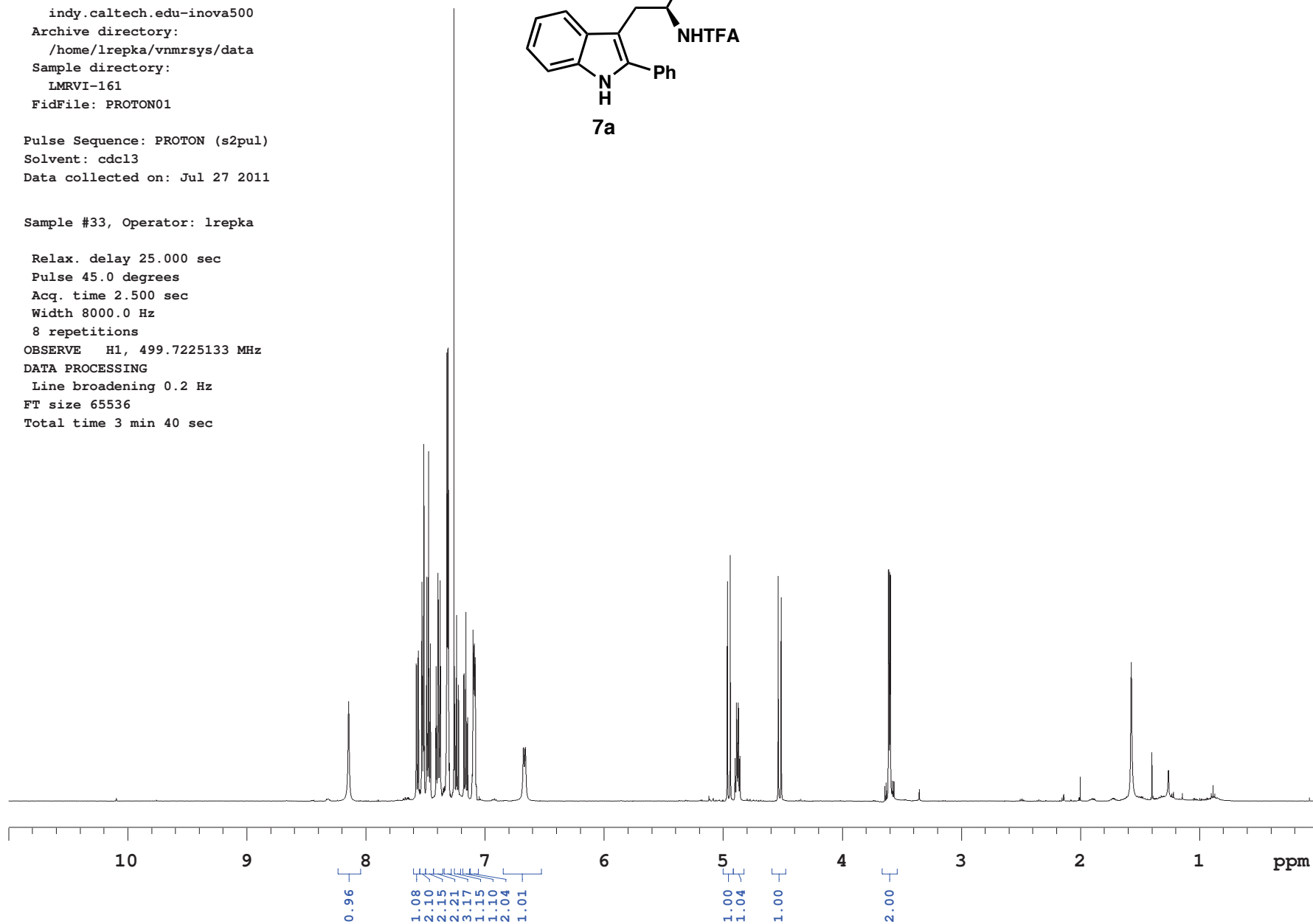
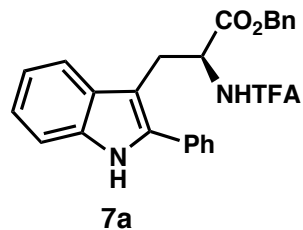
OBSERVE H1, 499.7225133 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec





LMRVI-161

Sample Name:

LMRVI-161

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-161

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 27 2011

Sample #33, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

10000 repetitions

OBSERVE C13, 125.6553284 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

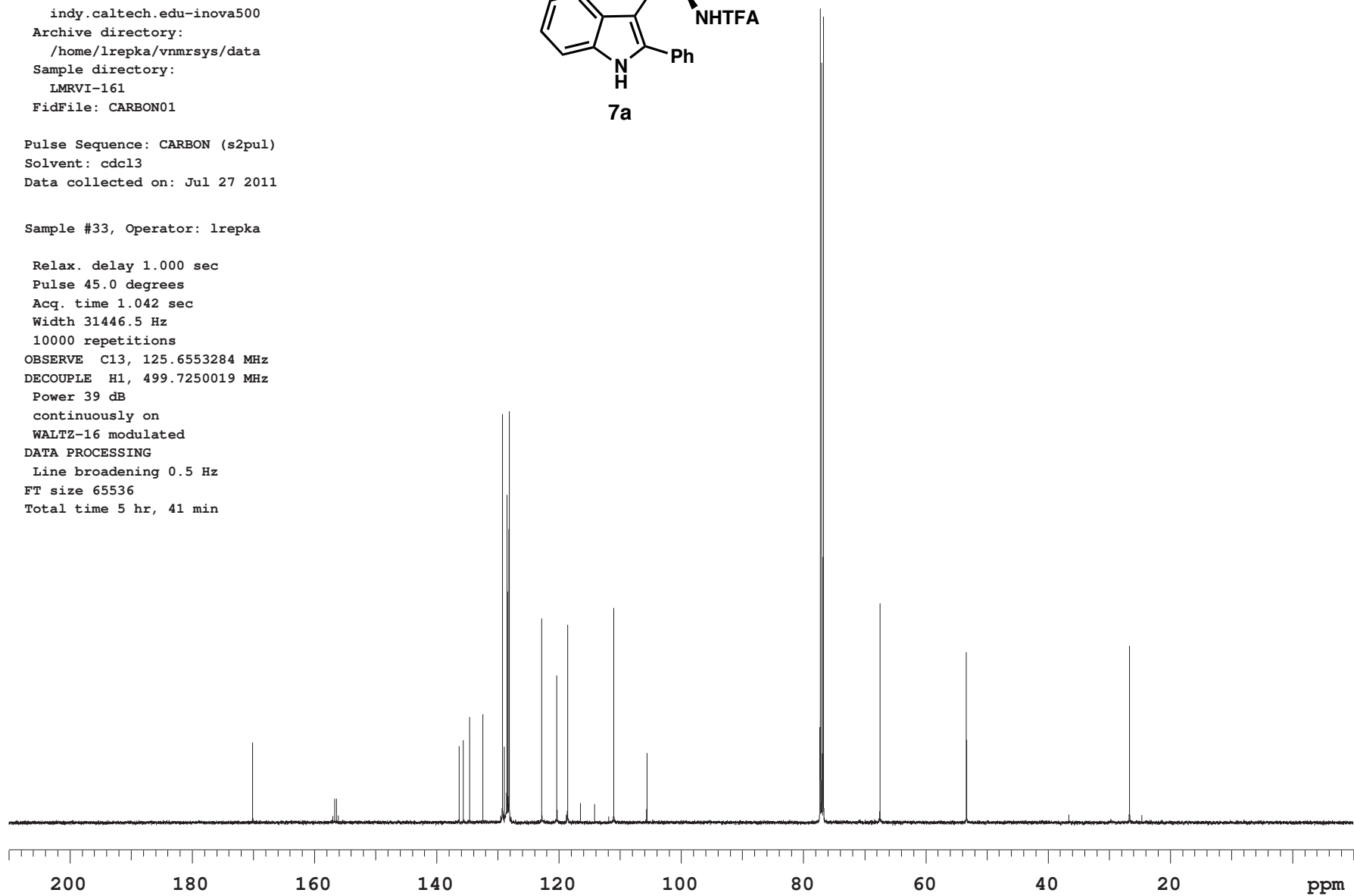
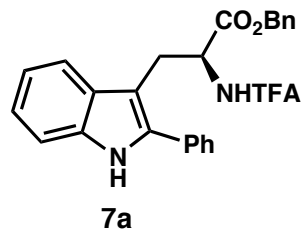
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 5 hr, 41 min



LMRVI-205-1

Sample Name:

LMRVI-205-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-205-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Aug 23 2011

Sample #33, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

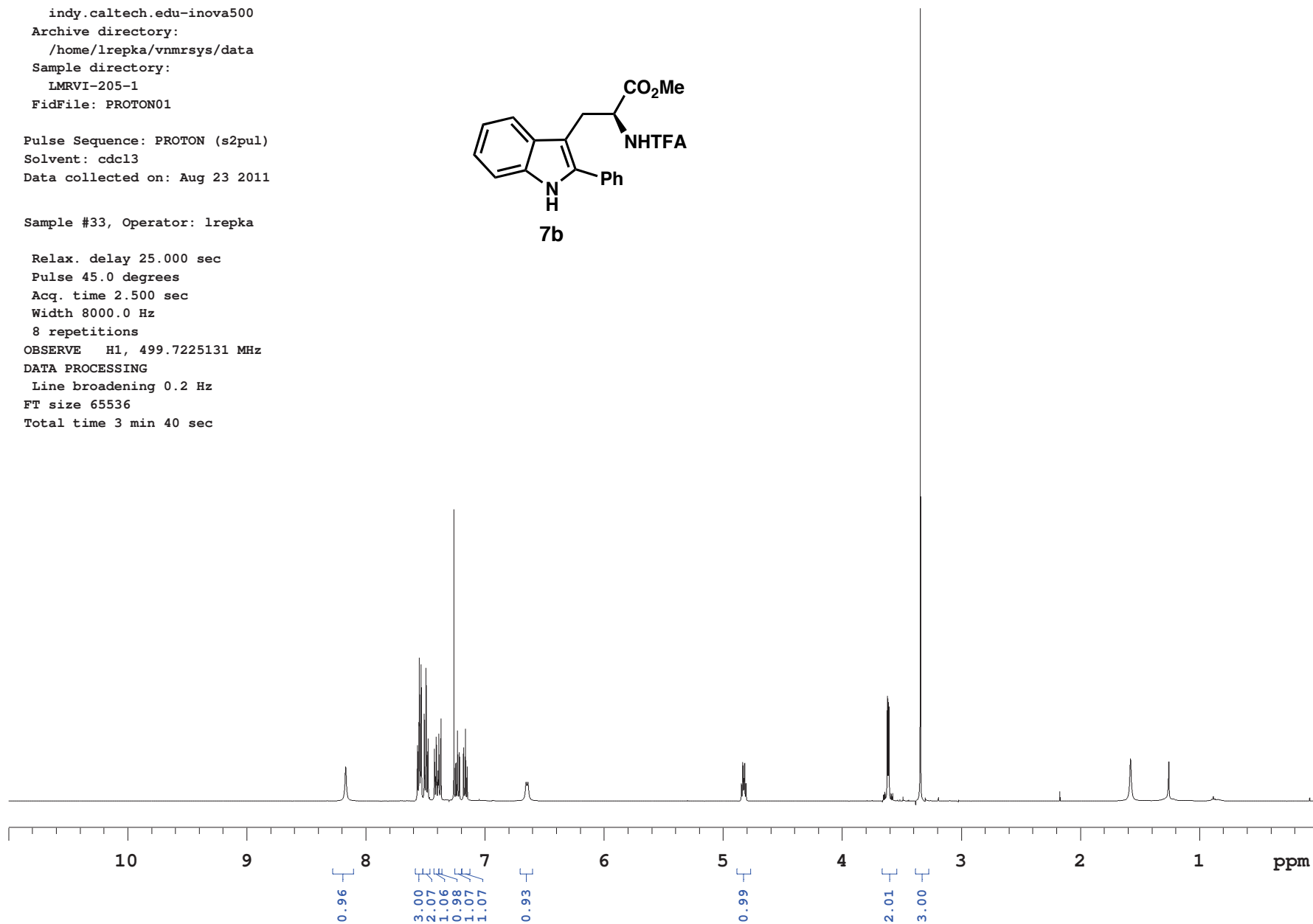
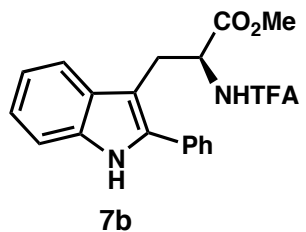
OBSERVE H1, 499.7225131 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



LMRVI-205-1

Sample Name:

LMRVI-205-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

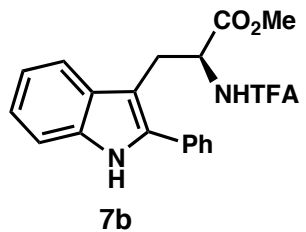
LMRVI-205-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Aug 23 2011



Sample #33, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

10000 repetitions

OBSERVE C13, 125.6553292 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

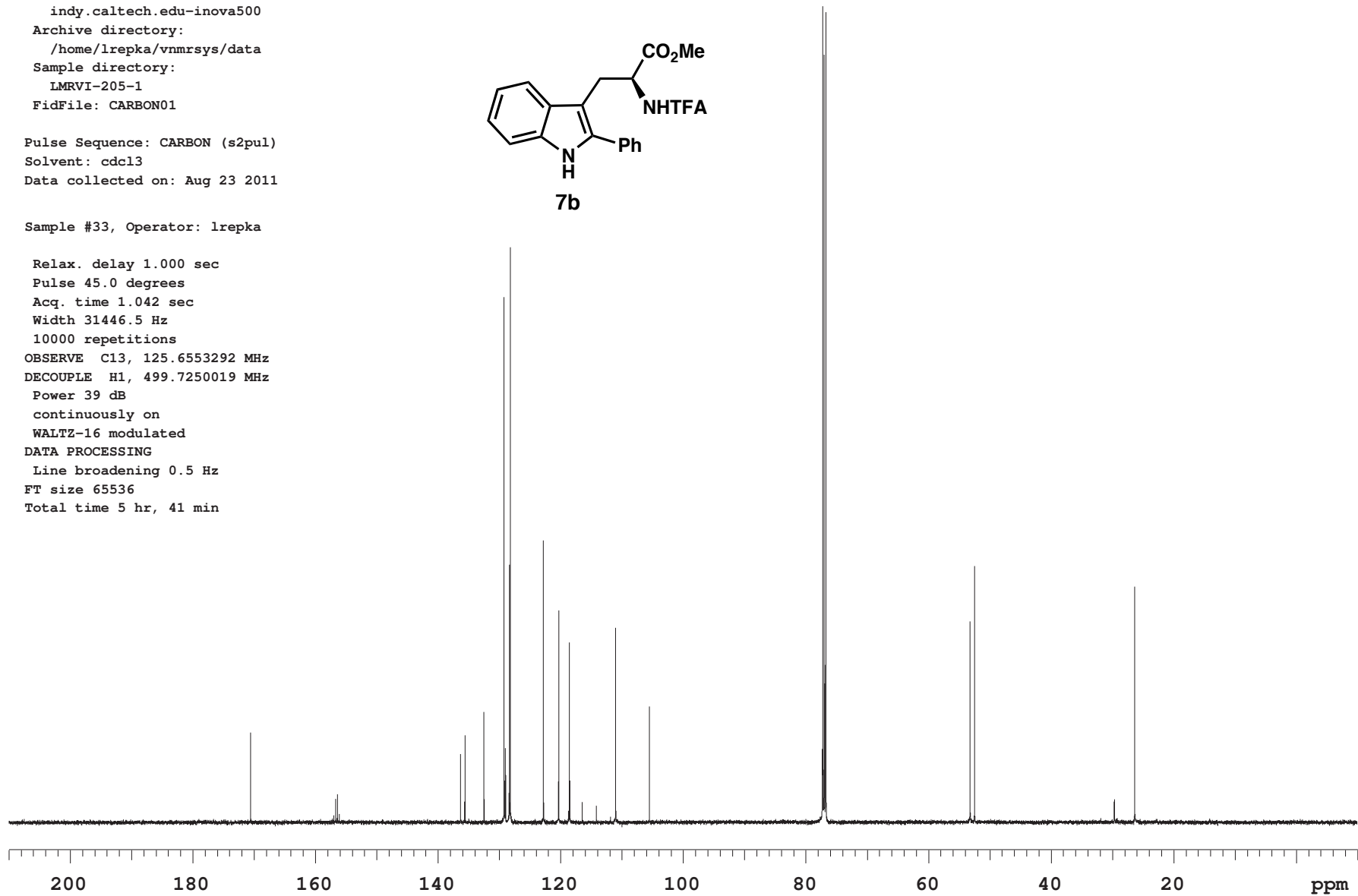
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 5 hr, 41 min



LMRVI-171

Sample Name:

LMRVI-171

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-171

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 25 2011

Sample #33, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

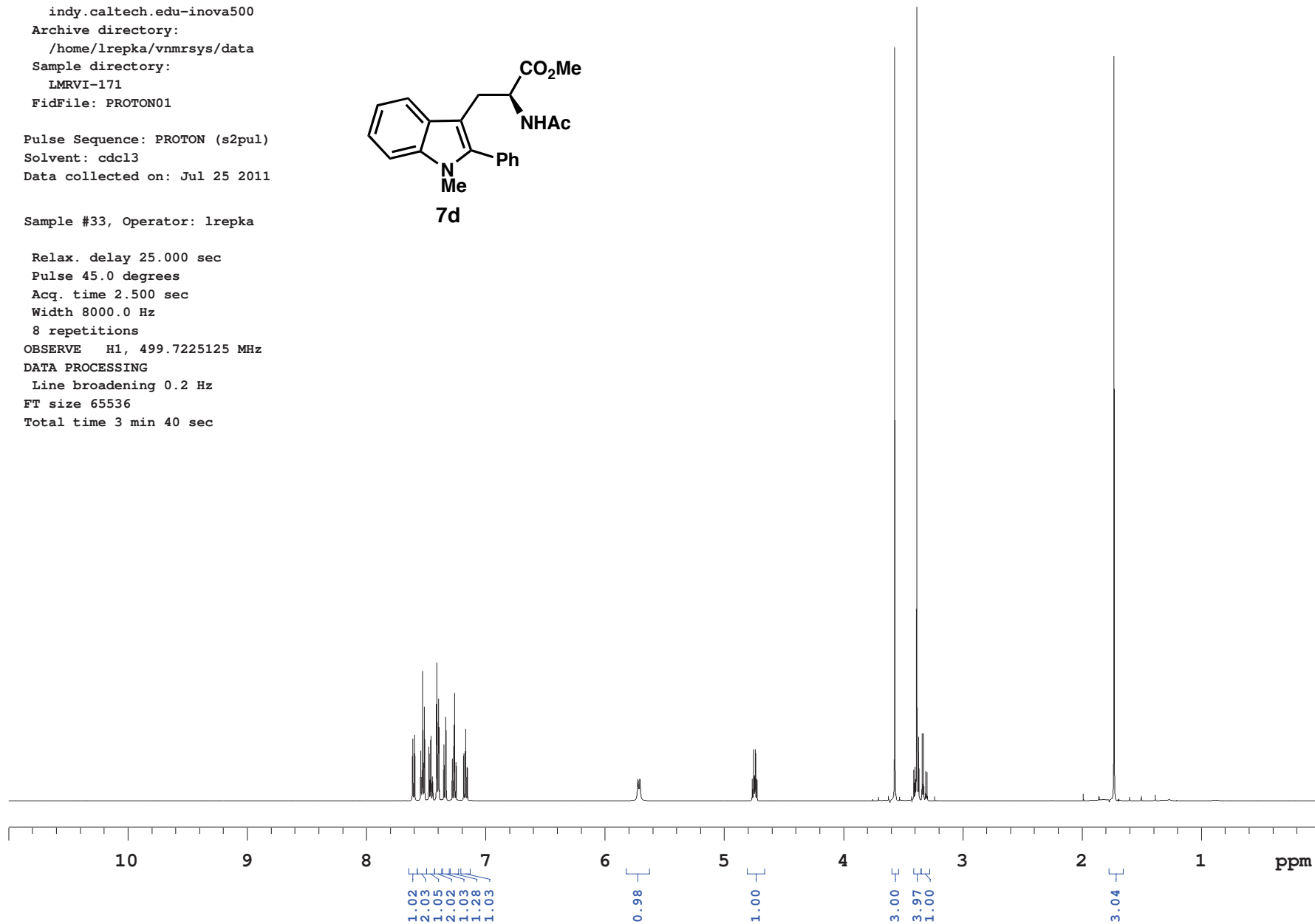
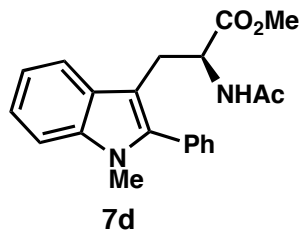
OBSERVE H1, 499.7225125 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



LMRVI-171

Sample Name:

LMRVI-171

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-171

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jul 25 2011

Sample #33, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6553354 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

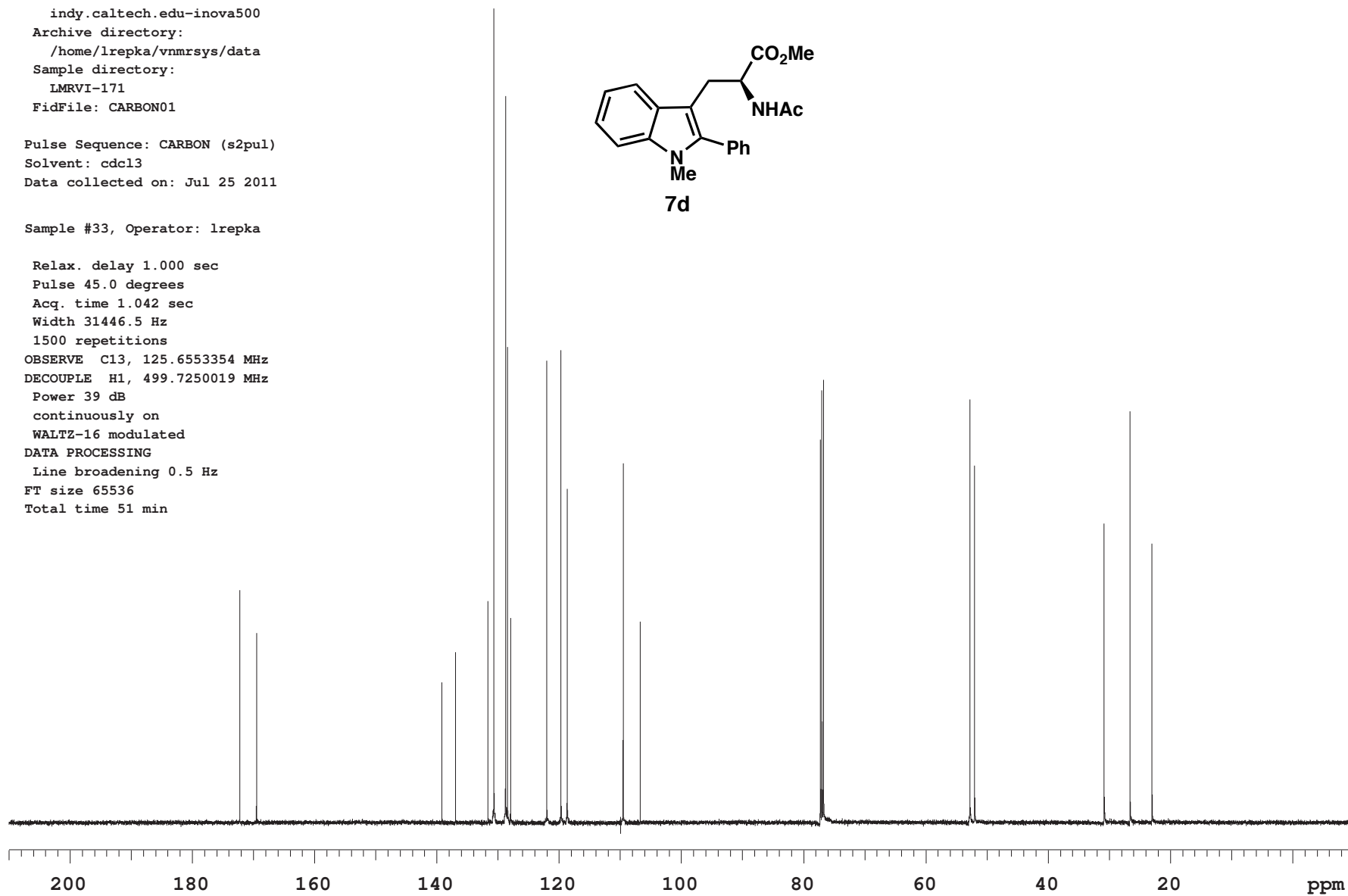
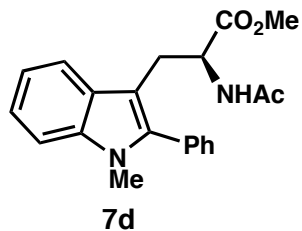
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min

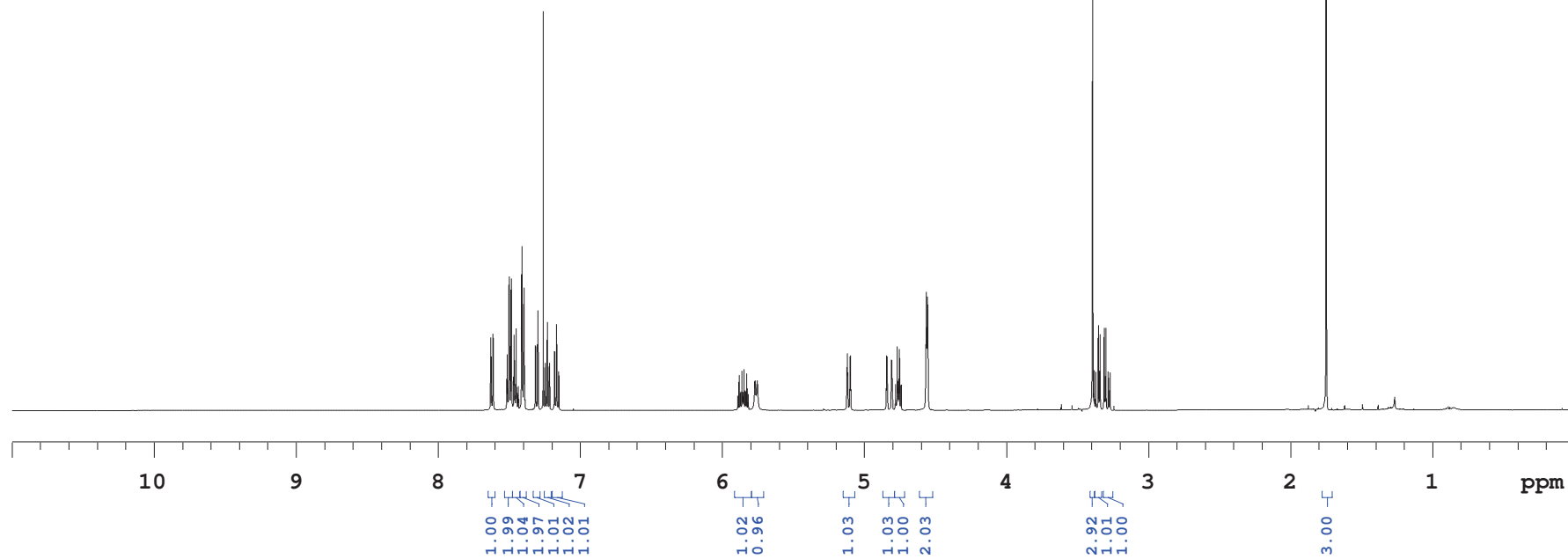
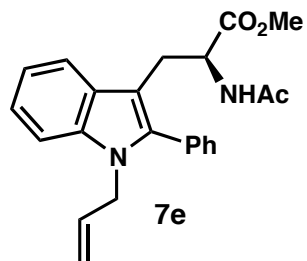


Sample Name:  
LMR-allyl  
Data Collected on:  
indy.caltech.edu-inova500  
Archive directory:  
/home/mkieffer/vnmrsys/data  
Sample directory:  
LMR-allyl  
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 14 2012

Sample #20, Operator: mkieffer

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 2.500 sec  
Width 8000.0 Hz  
32 repetitions  
OBSERVE H1, 499.7225125 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 2 min 24 sec

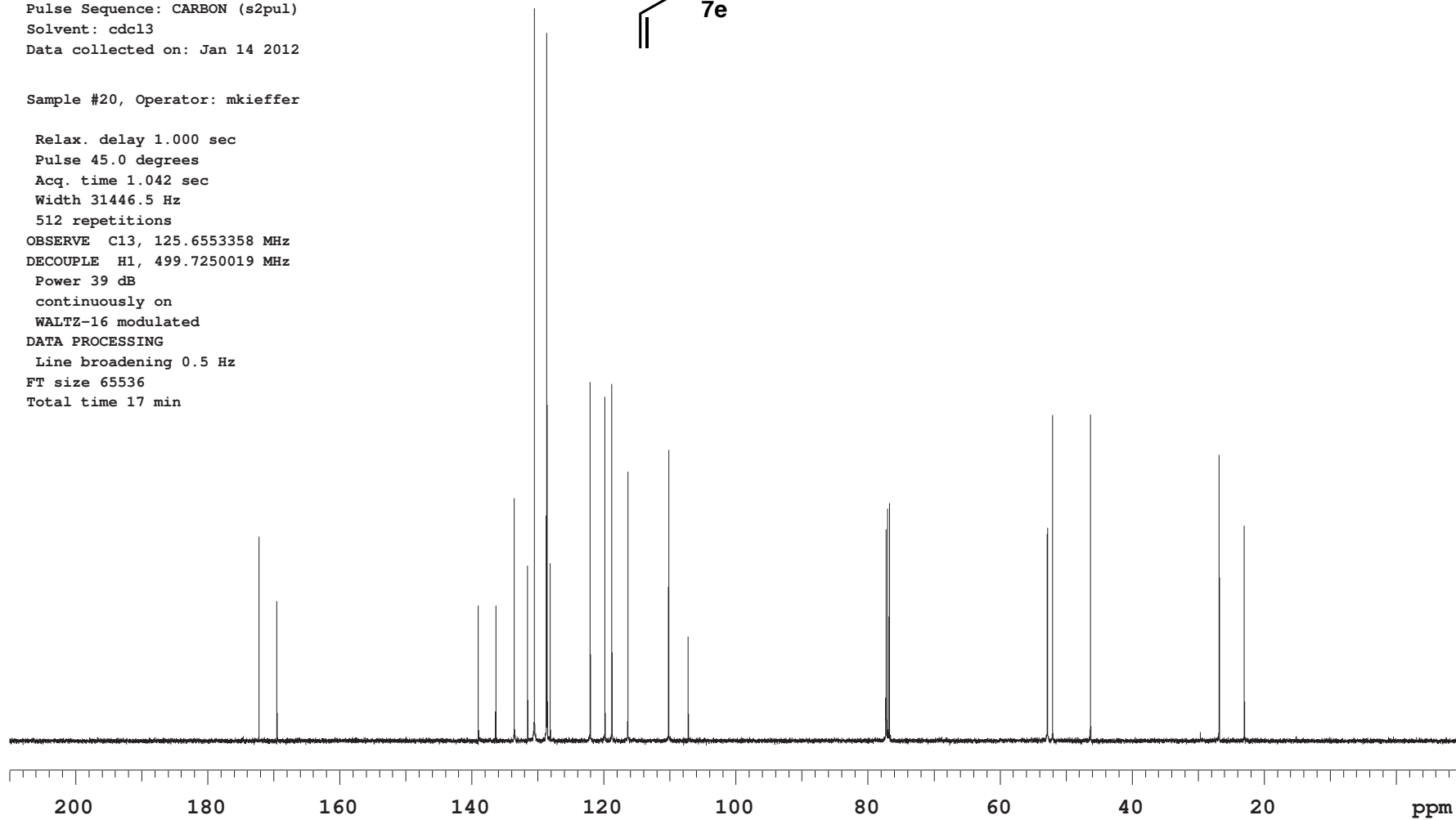
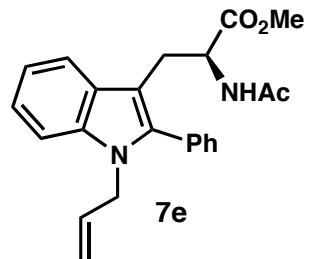


Sample Name:  
LMR-allyl  
Data Collected on:  
indy.caltech.edu-inova500  
Archive directory:  
/home/mkieffer/vnmrSYS/data  
Sample directory:  
LMR-allyl  
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Jan 14 2012

Sample #20, Operator: mkieffer

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.042 sec  
Width 31446.5 Hz  
512 repetitions  
OBSERVE C13, 125.6553358 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 17 min



MEK3186-1

Sample Name:

MEK3186-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3186-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 15 2011

Sample #15, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

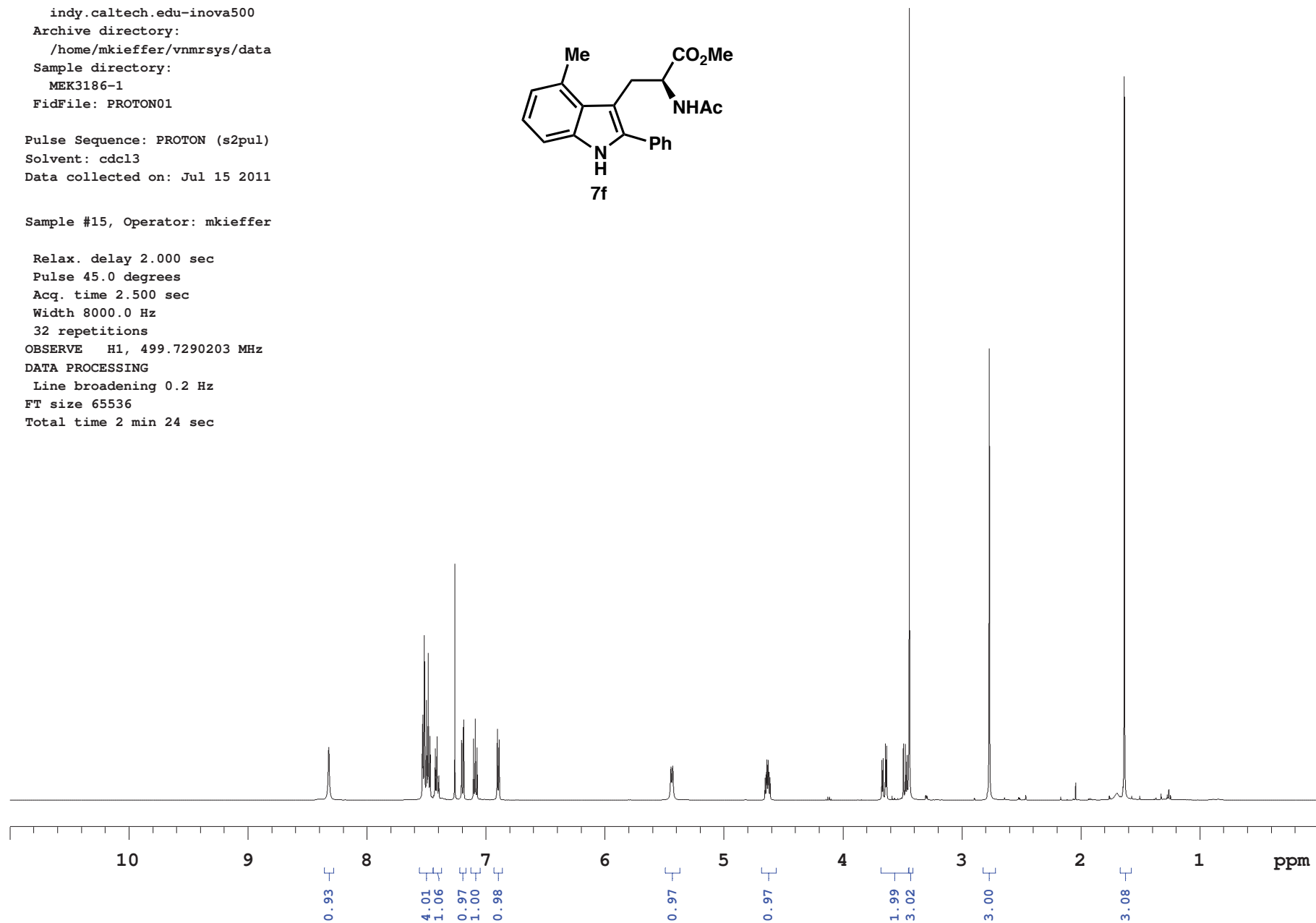
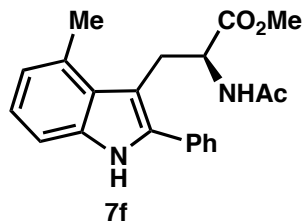
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



S104



MEK3186-1

Sample Name:

MEK3186-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3186-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 15 2011

Sample #15, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553310 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

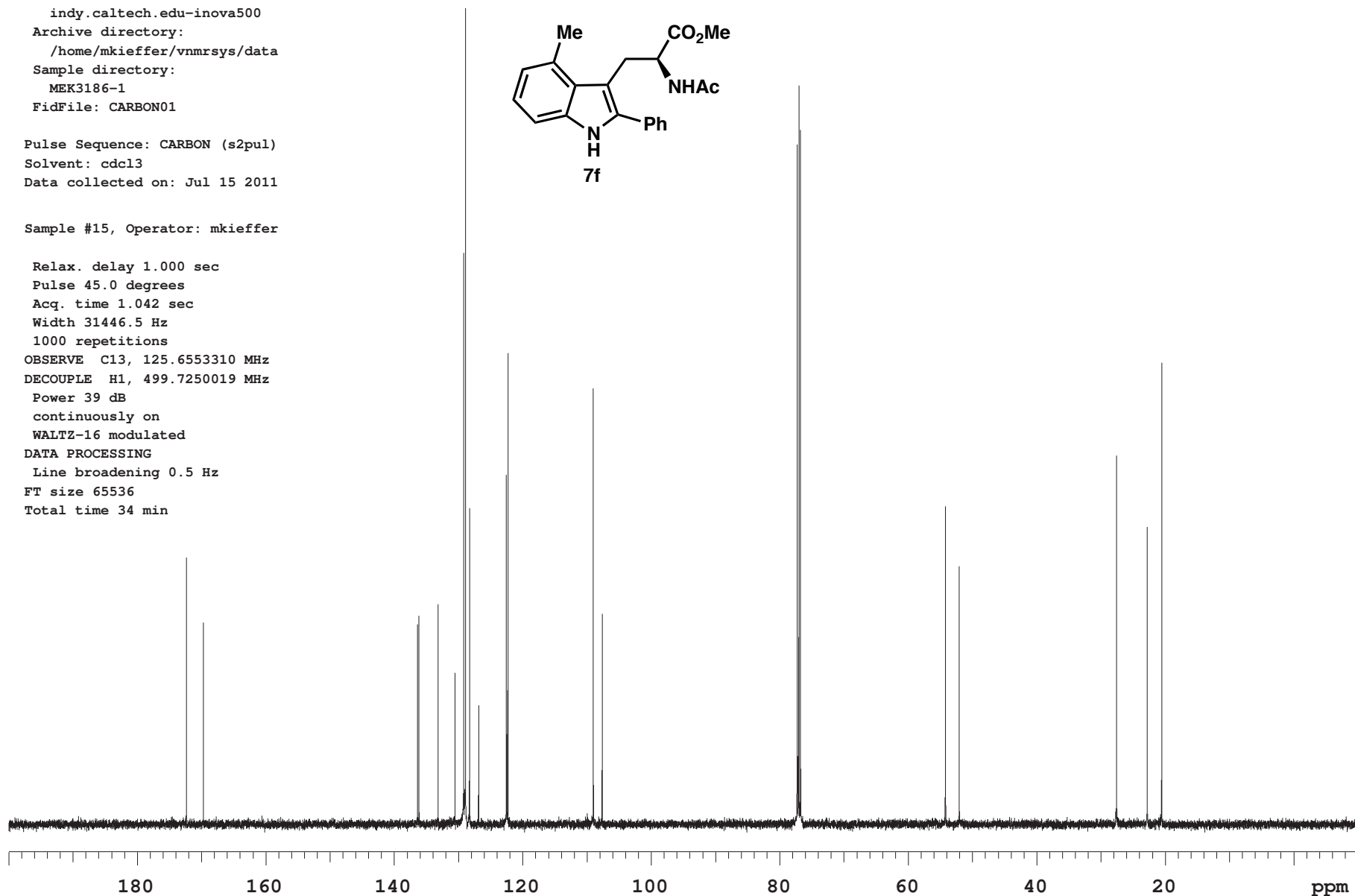
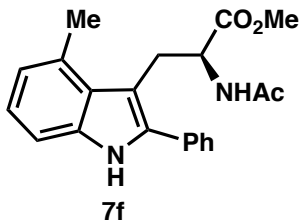
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



MEK3084-1

Sample Name:

MEK3084-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3084-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 9 2011

Temp. 25.0 C / 298.1 K

Sample #39, Operator: mkieffer

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

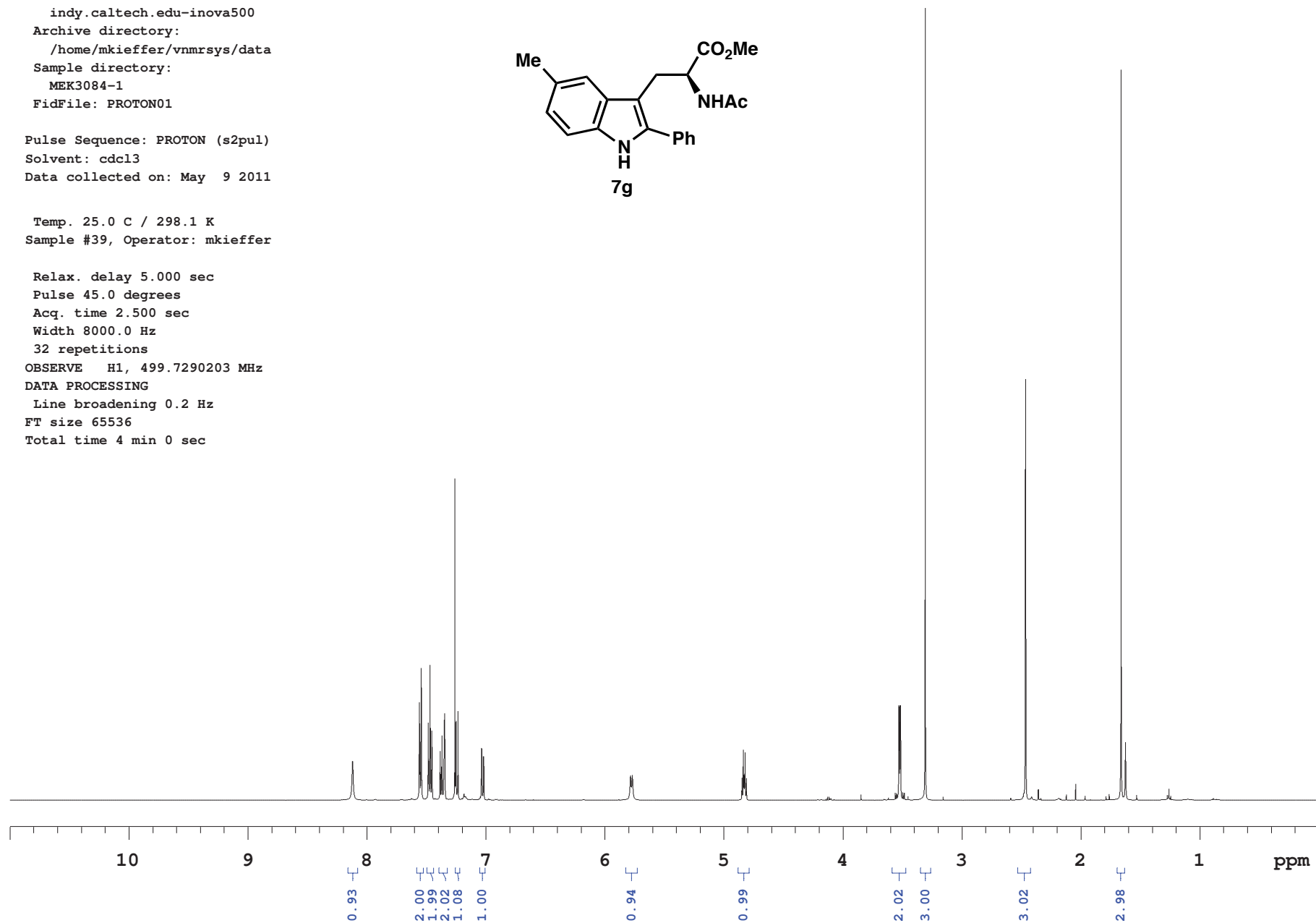
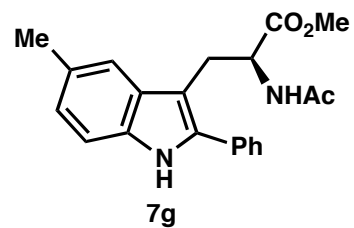
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 4 min 0 sec



MEK3084-1

Sample Name:

MEK3084-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3084-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 9 2011

Temp. 25.0 C / 298.1 K

Sample #39, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

512 repetitions

OBSERVE C13, 125.6569642 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

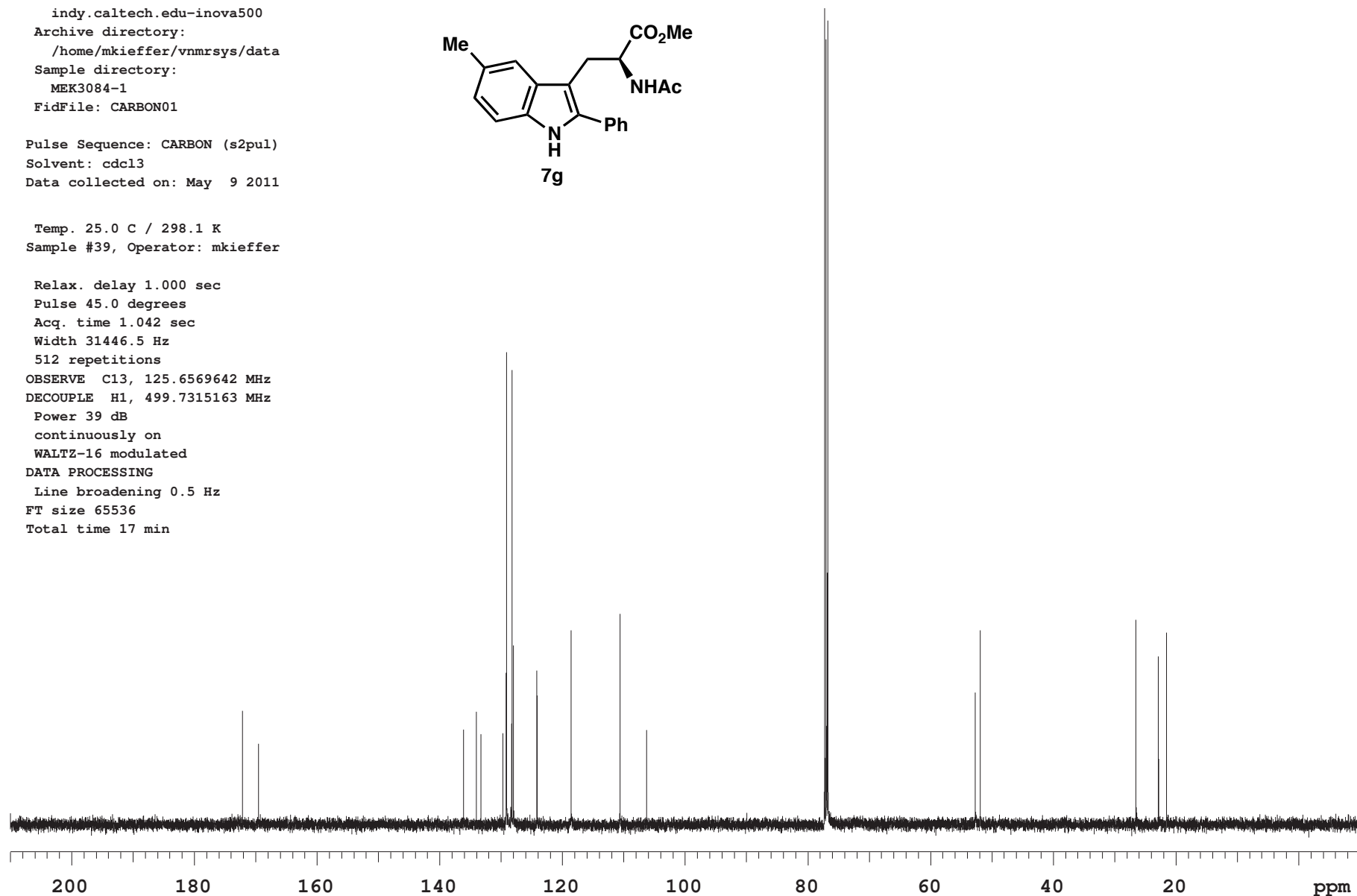
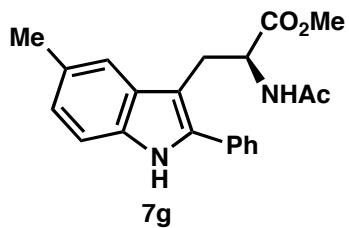
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 17 min



MEK3193-1

Sample Name:

MEK3193-1

Data Collected on:

indy.caltech.edu-inova500

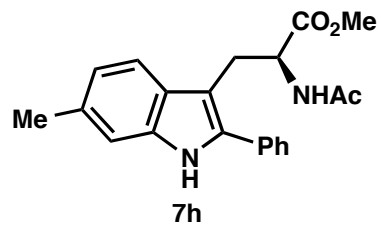
Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3193-1

FidFile: PROTON01



Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 21 2011

Sample #33, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

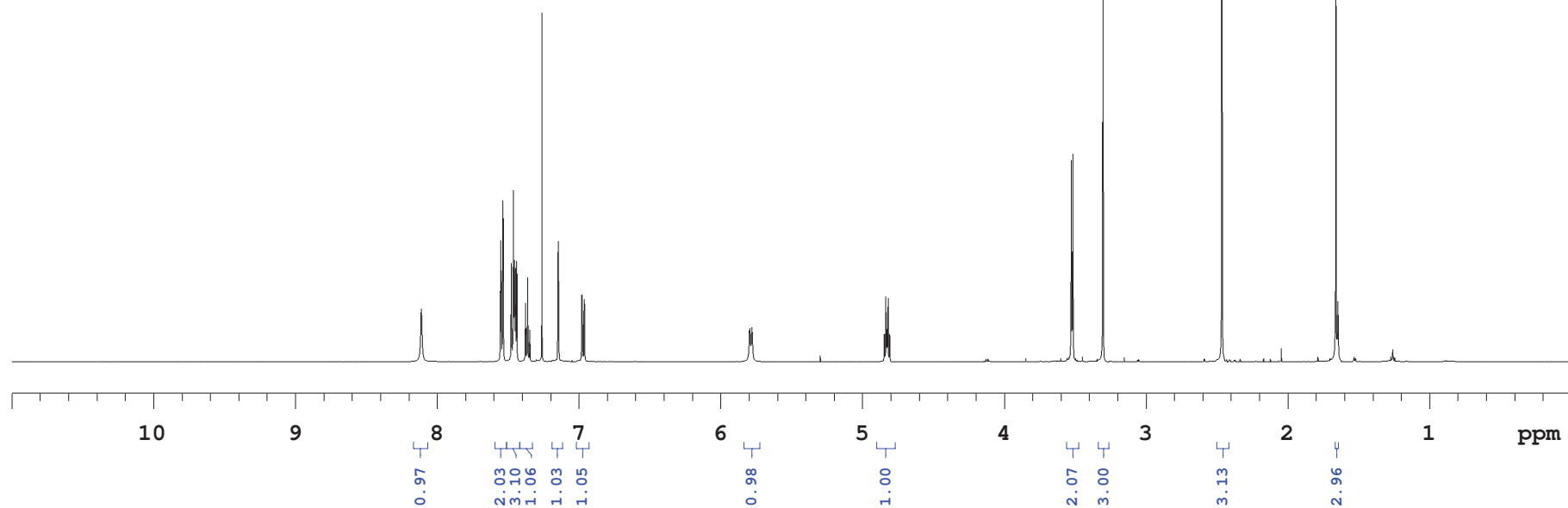
OBSERVE H1, 499.7225125 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



S108

MEK3193-1

Sample Name:

MEK3193-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3193-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 21 2011

Sample #33, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553291 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

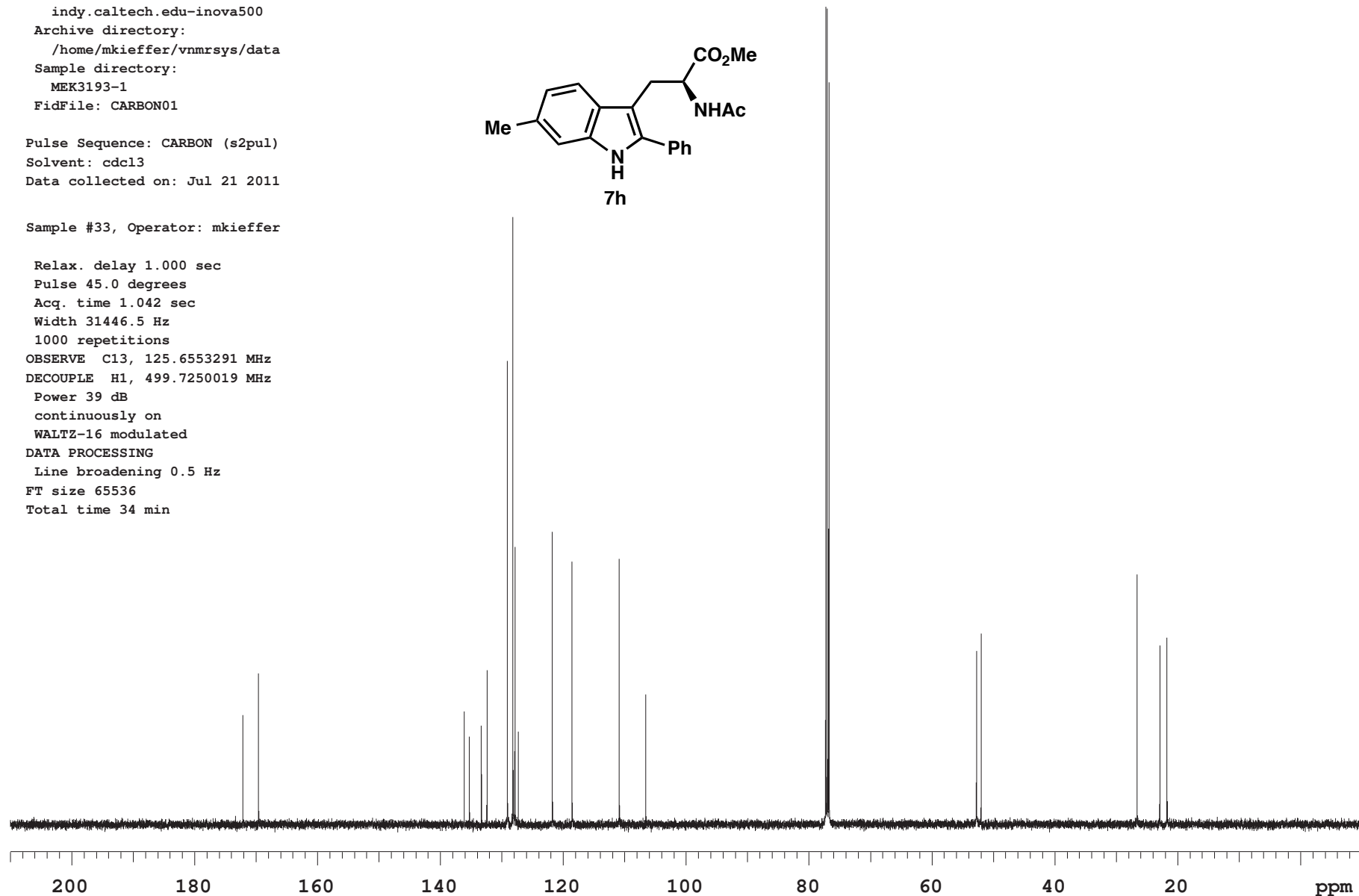
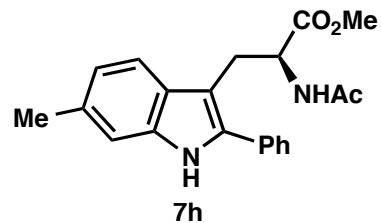
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



MEK3148-1

Sample Name:

MEK3148-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3148-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 20 2011

Temp. 25.0 C / 298.1 K

Sample #14, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

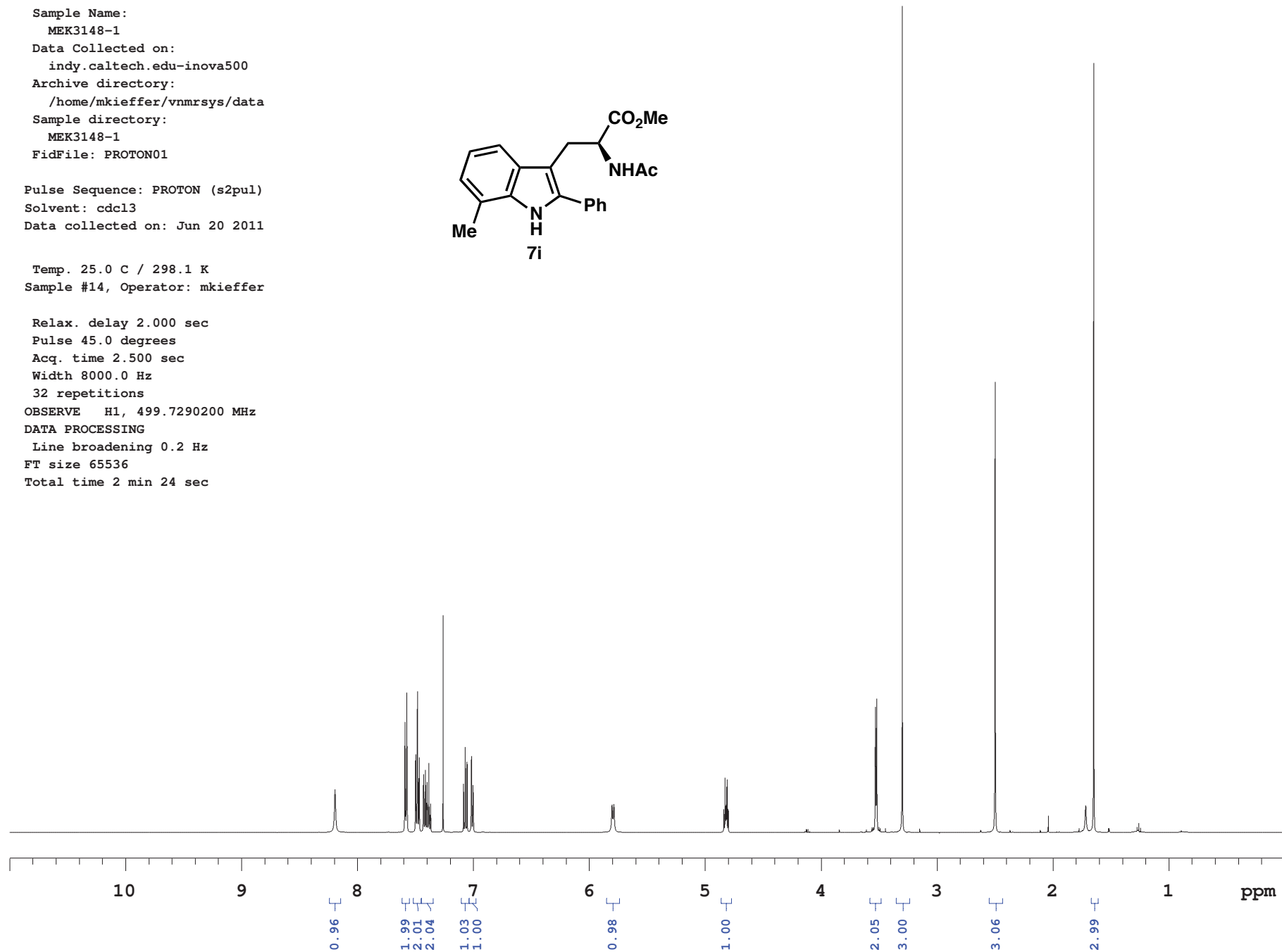
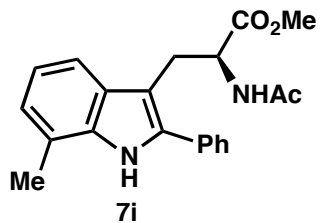
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



MEK3130-1

Sample Name:

MEK3130-1

Data Collected on:

indy.caltech.edu-inova500

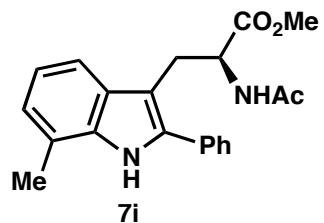
Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3130-1

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 7 2011

Temp. 25.0 C / 298.1 K

Sample #15, Operator: mkieffer

Relax. delay 2.000 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

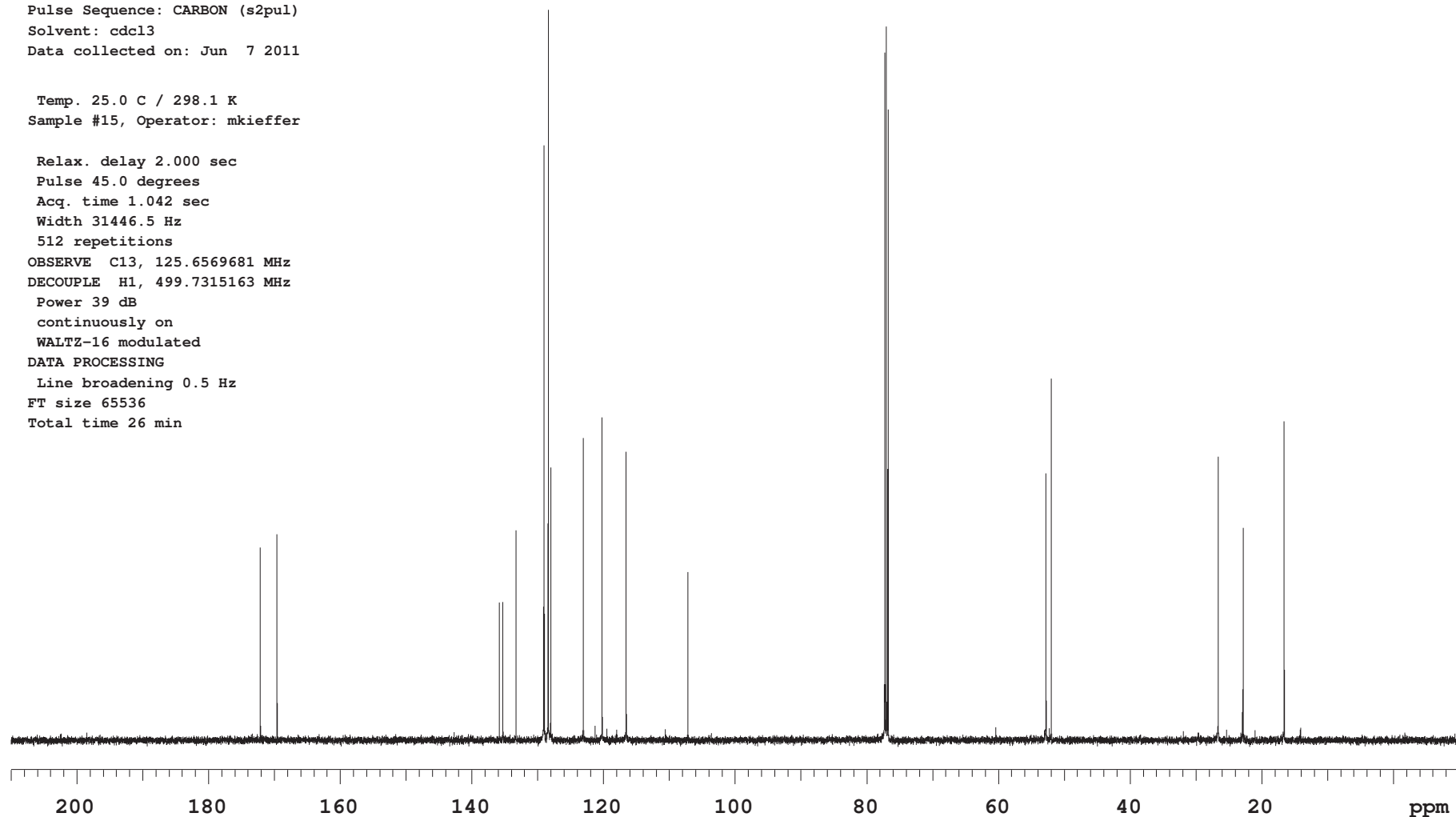
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 26 min



MEK3185-1

Sample Name:

MEK3185-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3185-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 15 2011

Sample #14, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

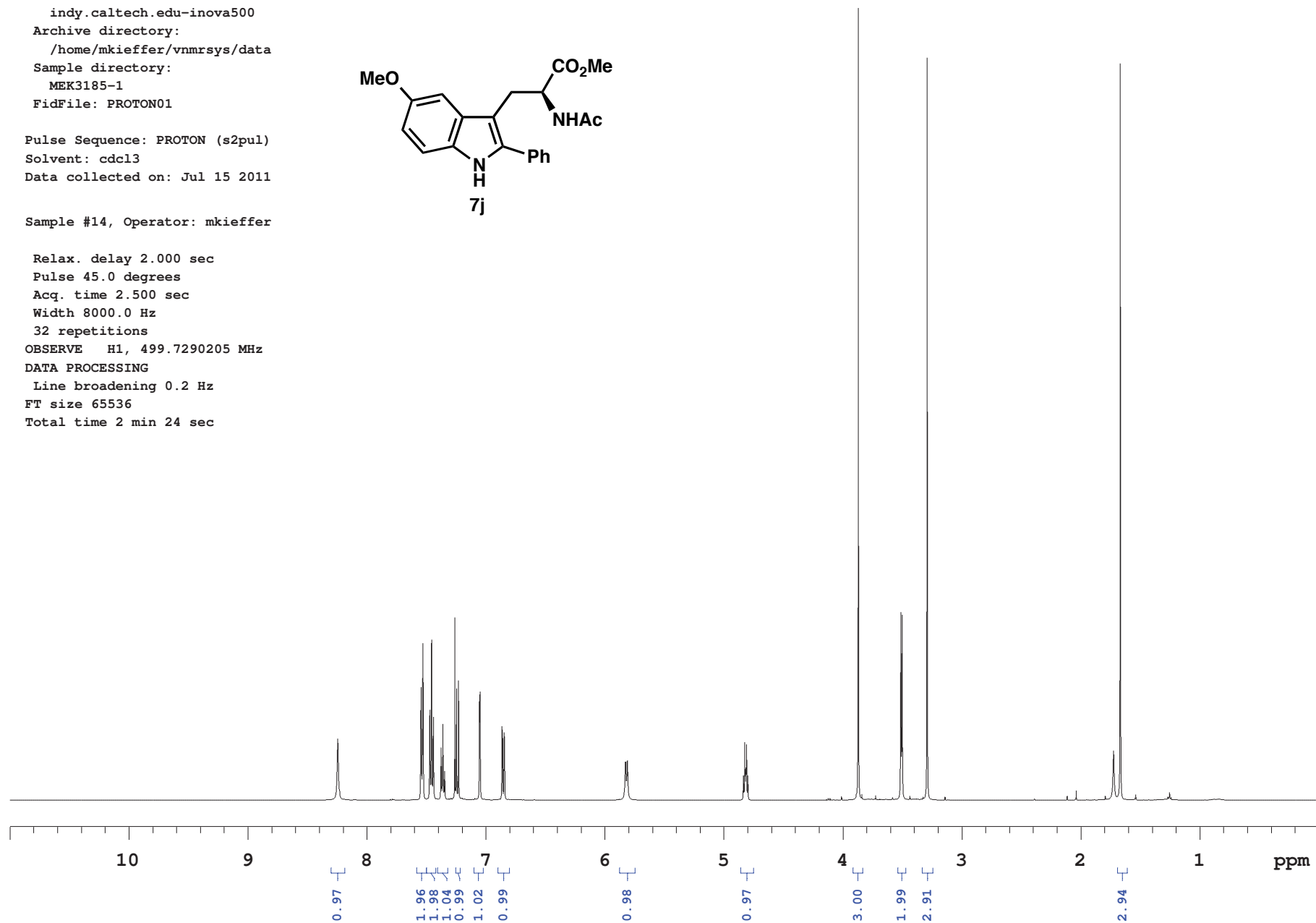
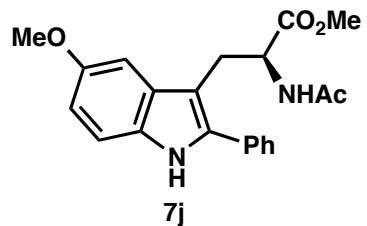
OBSERVE H1, 499.7290205 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec





MEK3185-1

Sample Name:

MEK3185-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3185-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 15 2011

Sample #14, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553300 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

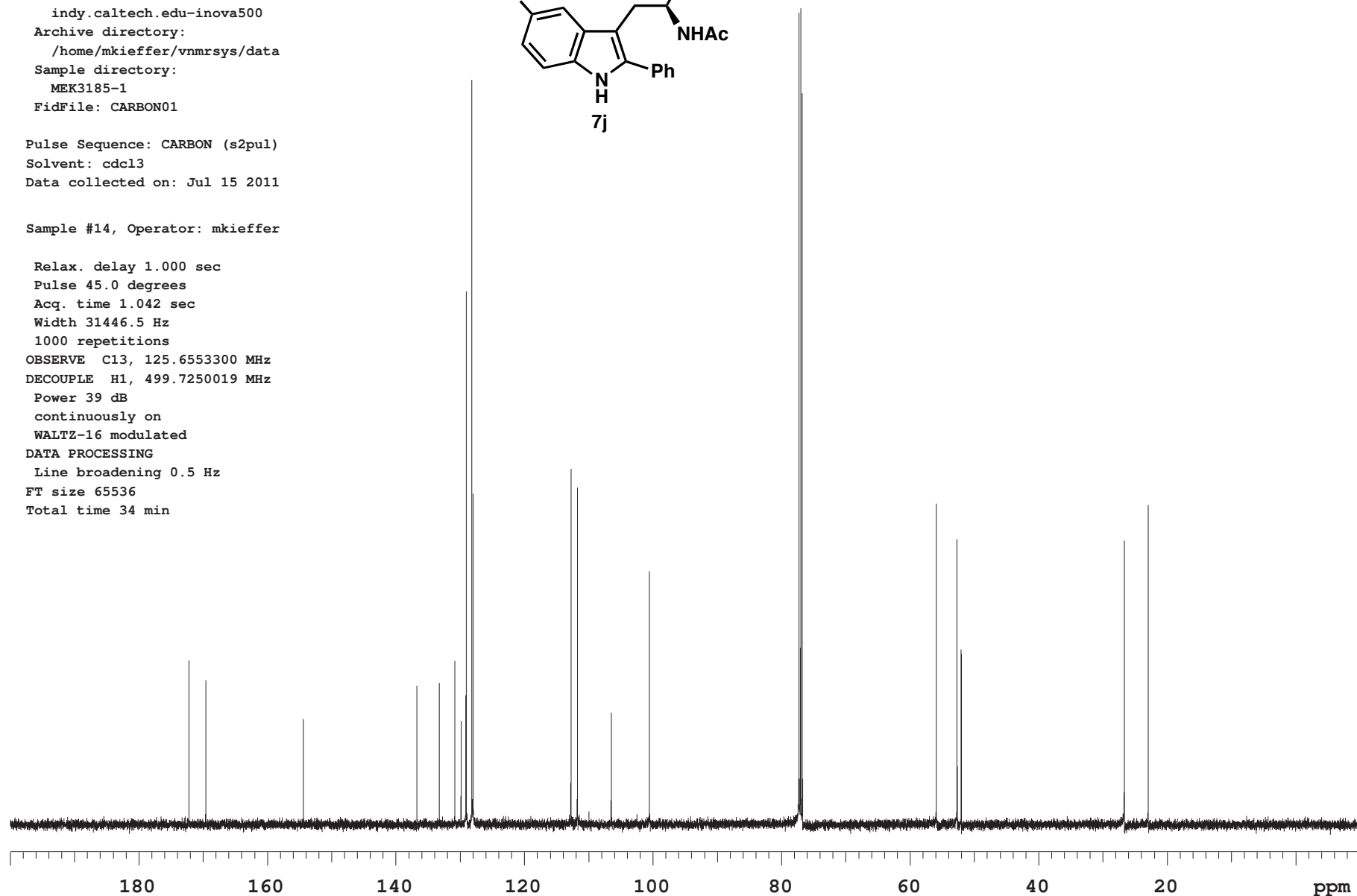
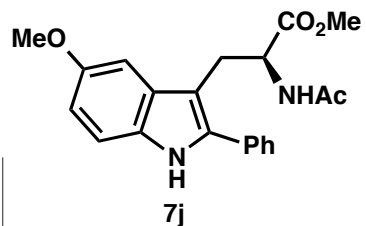
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



MEK-5-Br

Sample Name:

MEK-5-Br

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK-5-Br

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 25 2011

Sample #15, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

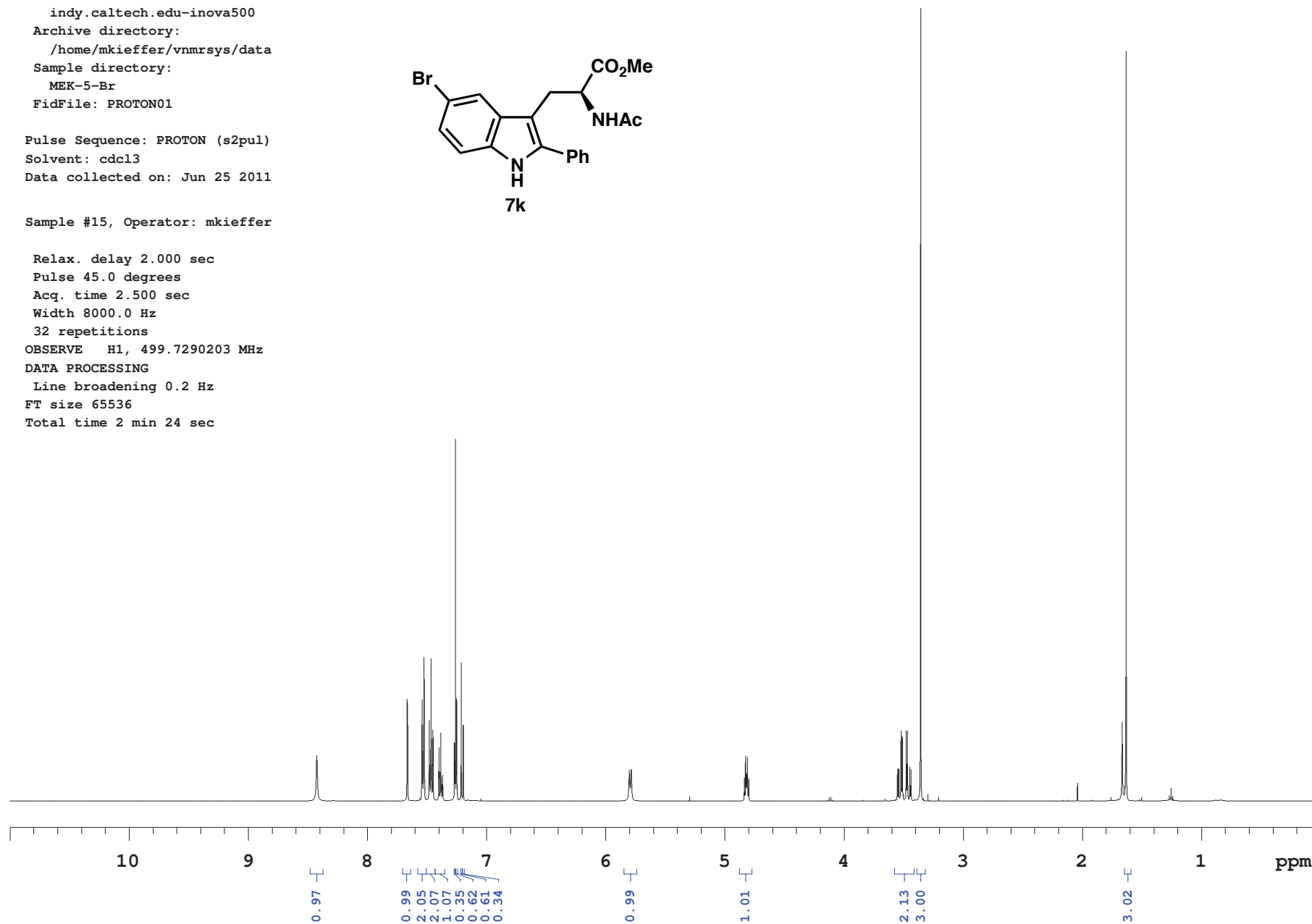
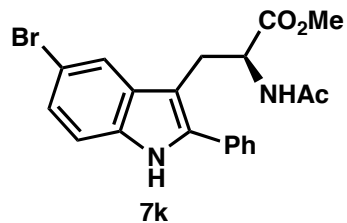
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



MEK-5-Br

Sample Name:

MEK-5-Br

Data Collected on:

indy.caltech.edu-inova500

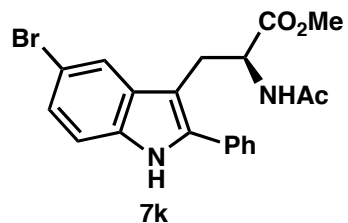
Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK-5-Br

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 25 2011

Sample #15, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6666408 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

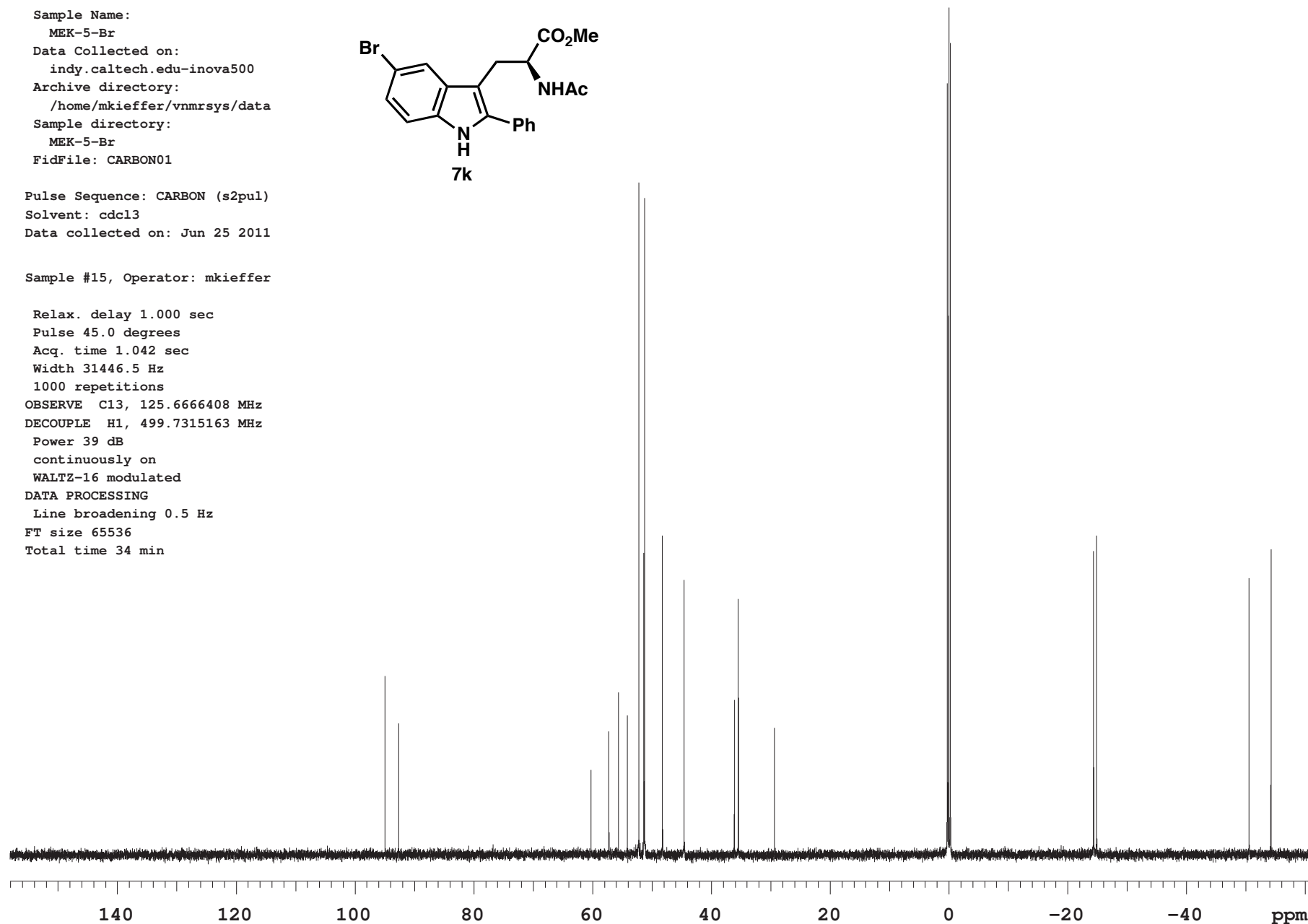
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



MEK3150-1

Sample Name:

MEK3150-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3150-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 20 2011

Temp. 25.0 C / 298.1 K

Sample #15, Operator: mkieffer

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

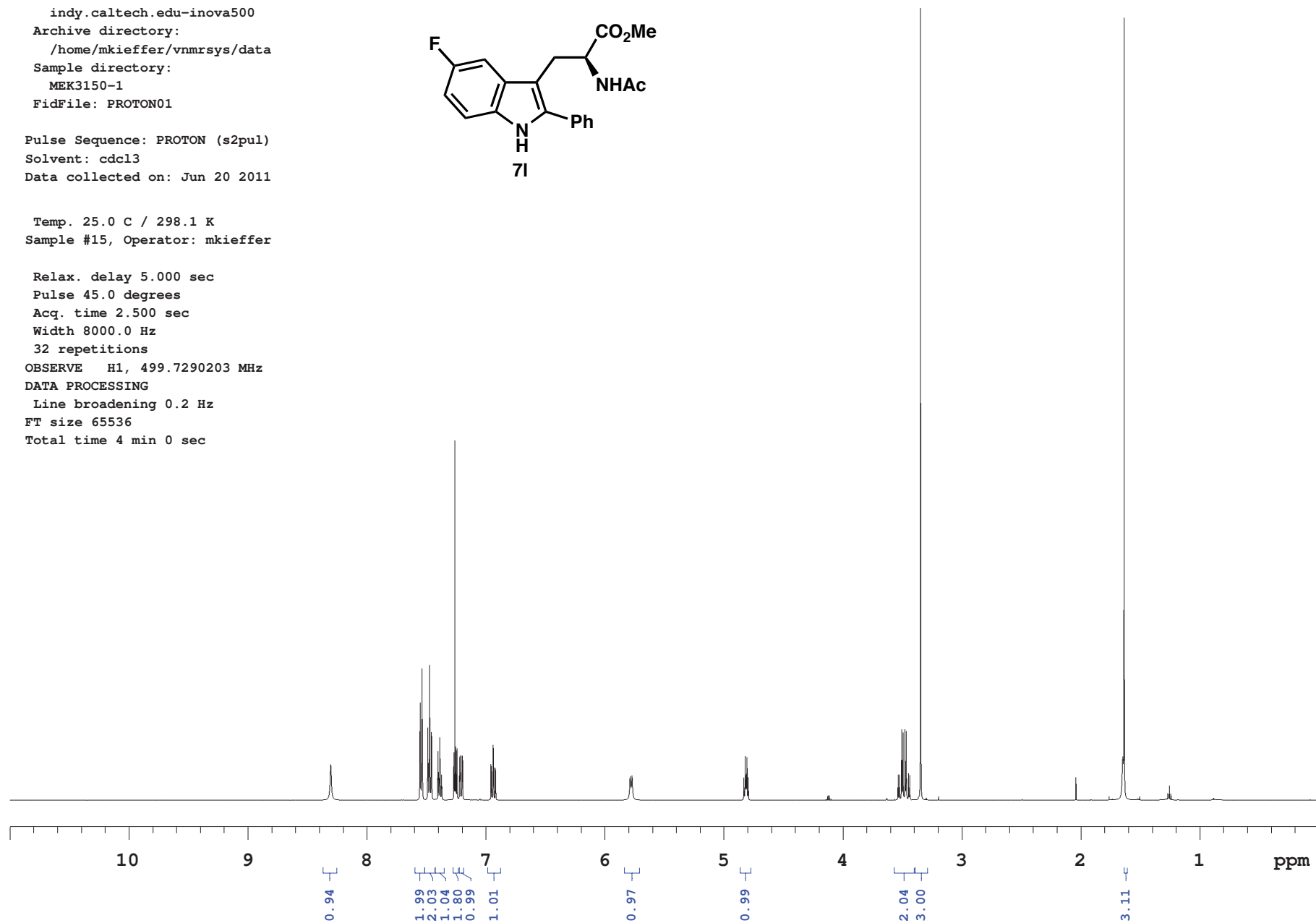
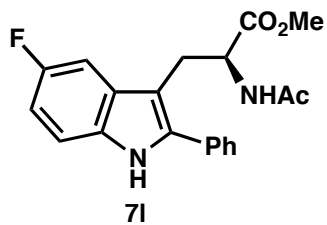
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 4 min 0 sec



MEK3150-1

Sample Name:

MEK3150-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3150-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Jun 20 2011

Temp. 25.0 C / 298.1 K

Sample #15, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6569633 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

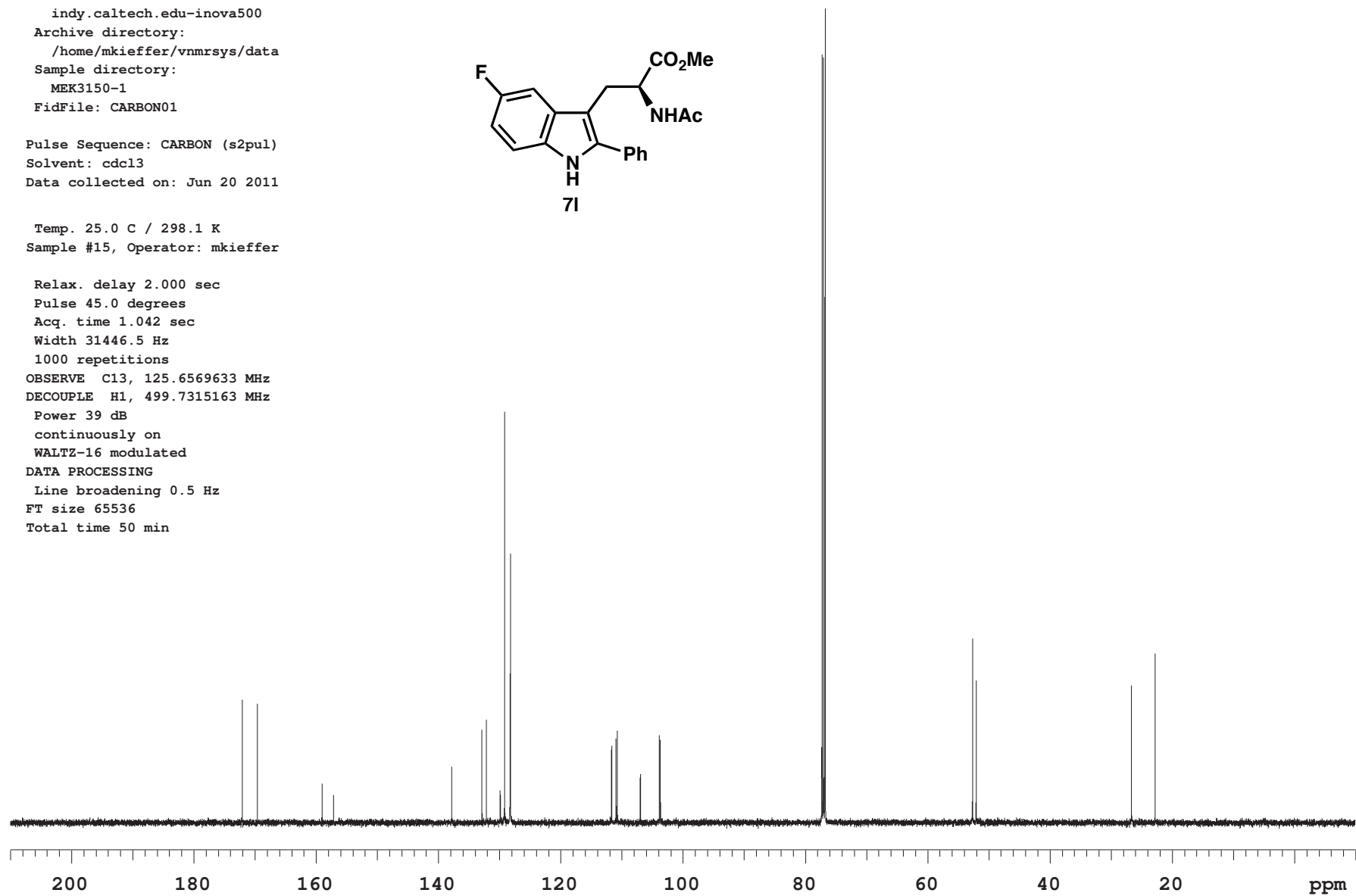
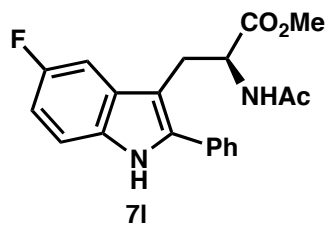
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 50 min



MEK3080-1

Sample Name:

MEK3080-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3080-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 8 2011

Temp. 25.0 C / 298.1 K

Sample #42, Operator: mkieffer

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

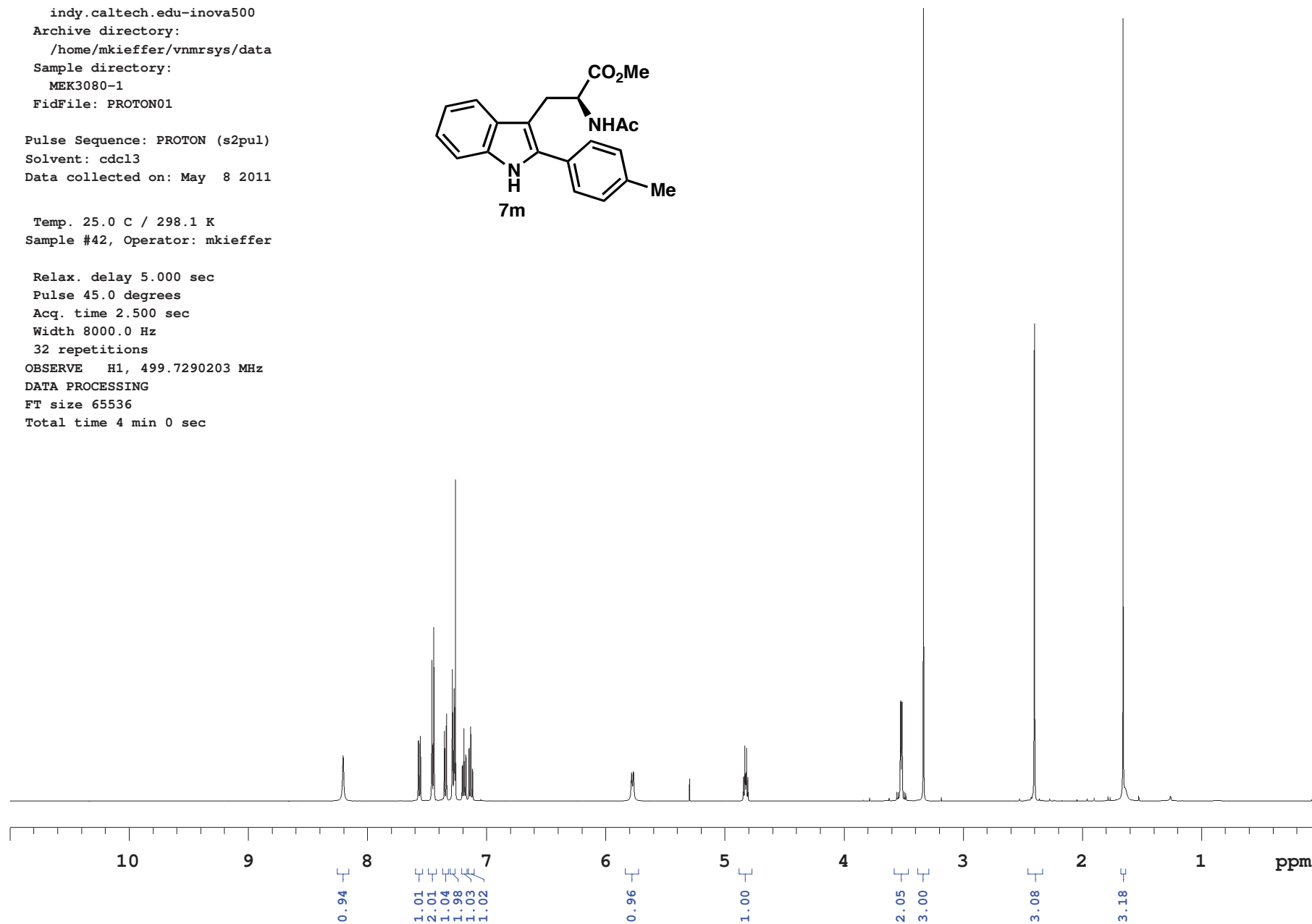
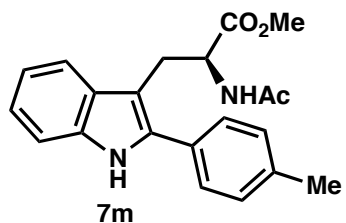
32 repetitions

OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

FT size 65536

Total time 4 min 0 sec



MEK3080-1

Sample Name:

MEK3080-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3080-1

FidFile: current

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 8 2011

Temp. 25.0 C / 298.1 K

Sample #42, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

384 repetitions

OBSERVE C13, 125.6569642 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

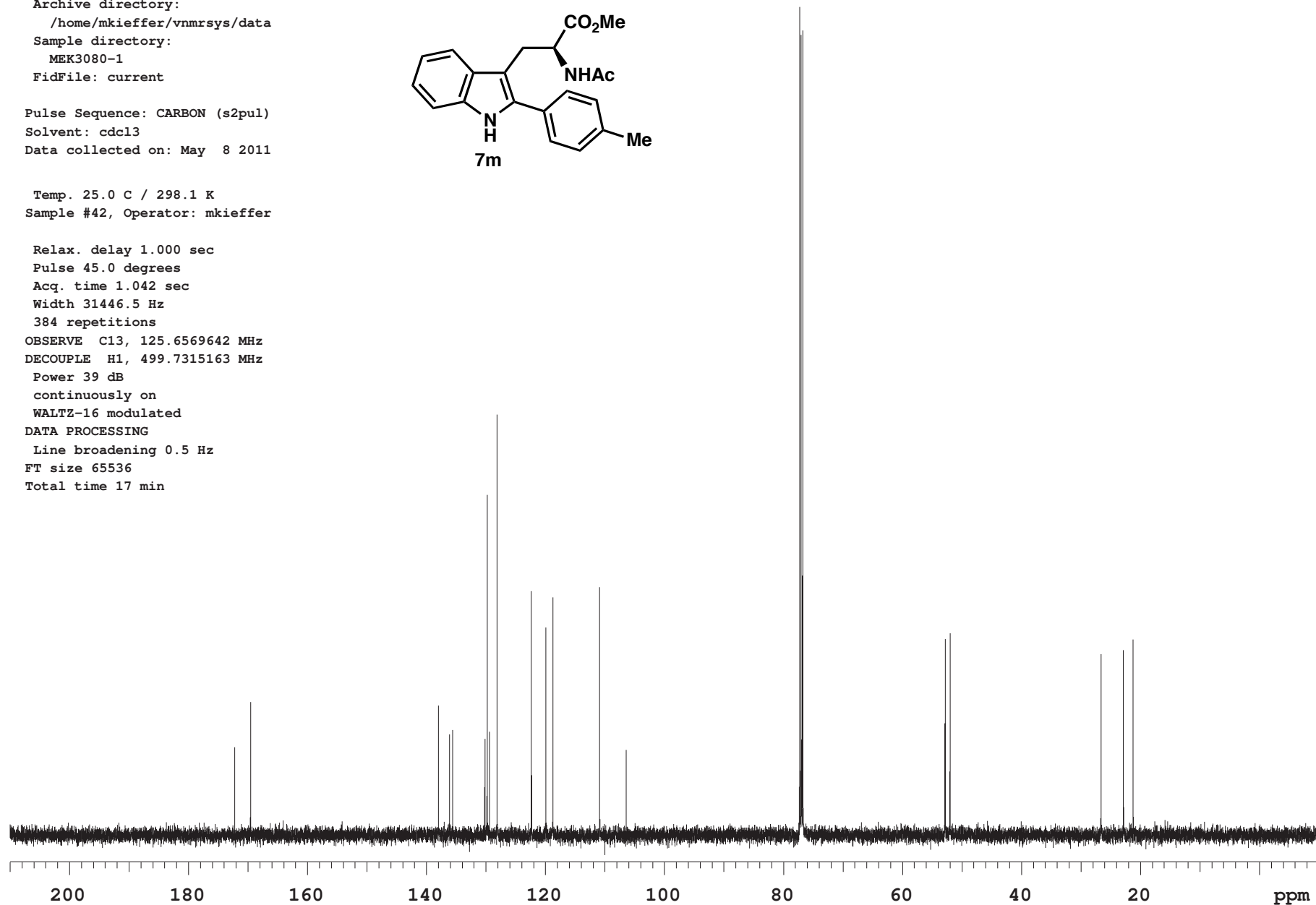
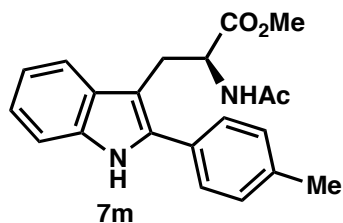
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 17 min



MEK3238-1

Sample Name:

MEK3238-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3238-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Aug 31 2011

Sample #20, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

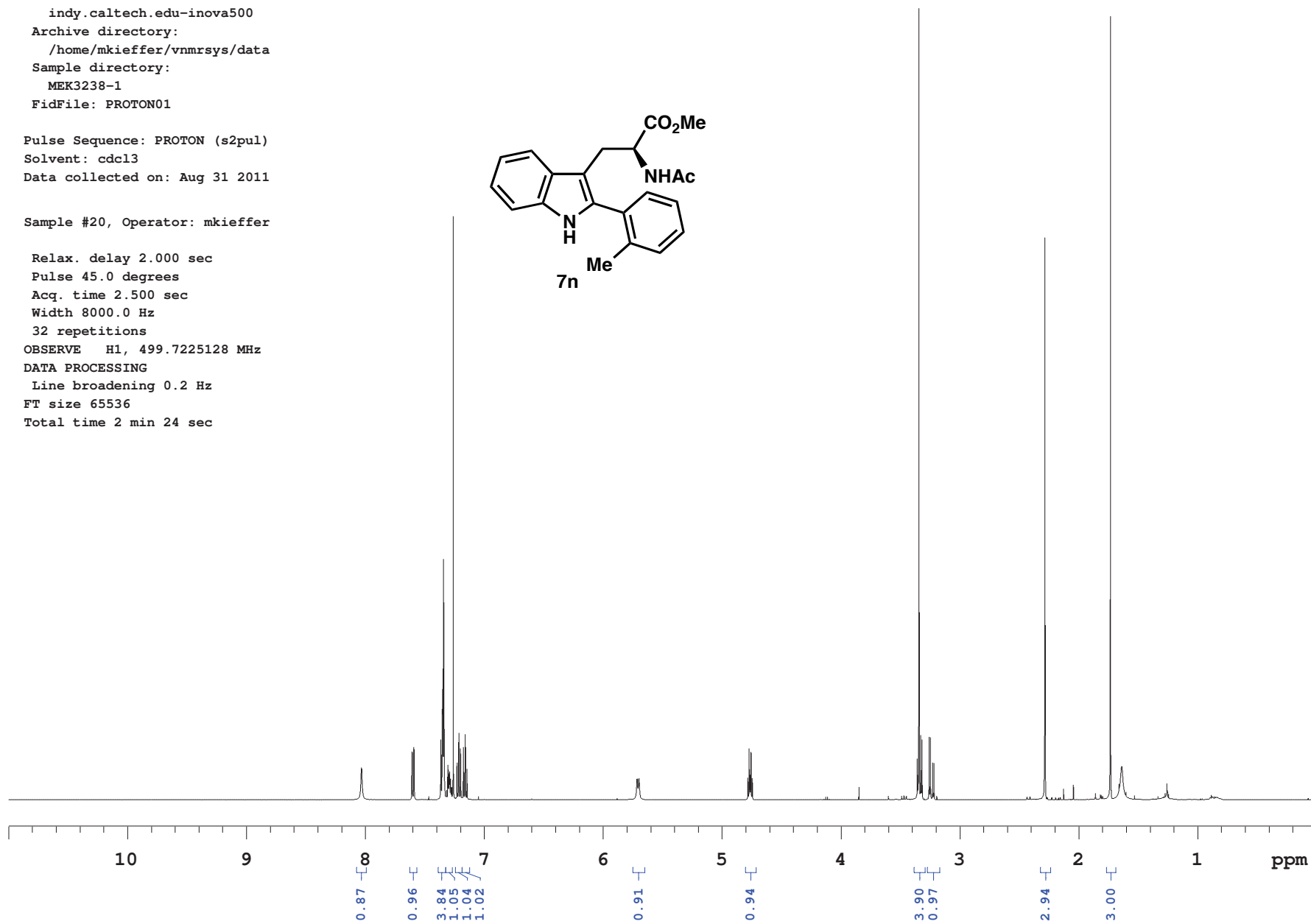
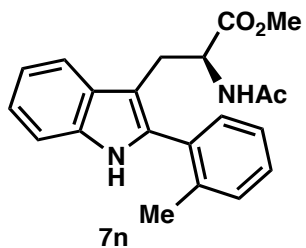
OBSERVE H1, 499.7225128 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec





MEK3238-1

Sample Name:

MEK3238-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3238-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Aug 31 2011

Sample #20, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553271 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

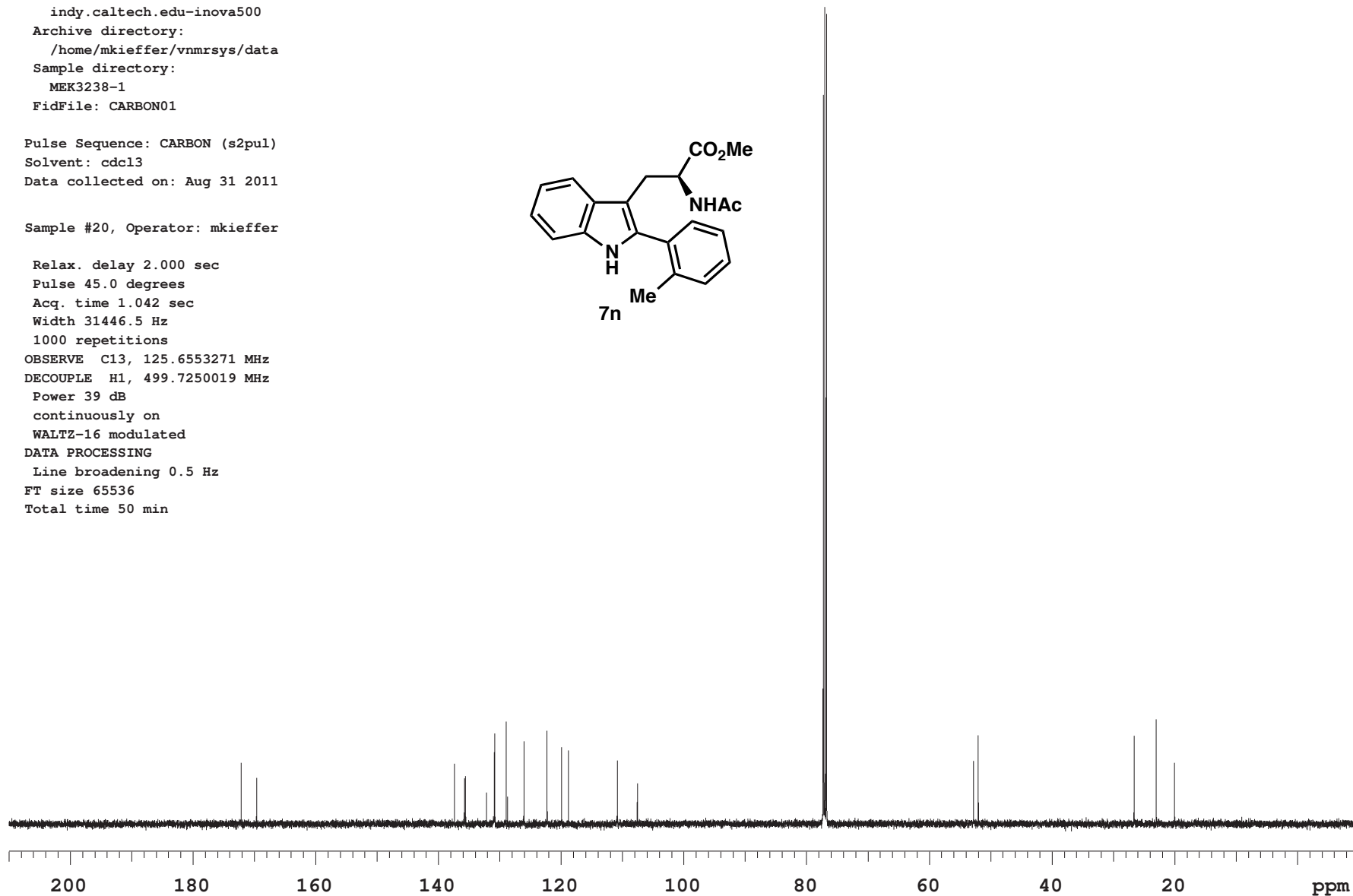
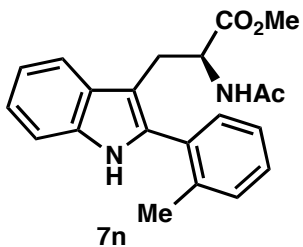
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 50 min



MEK3113-1

Sample Name:

MEK3113-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

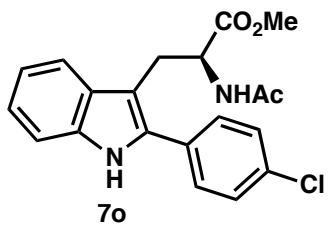
MEK3113-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 24 2011



Temp. 25.0 C / 298.1 K

Sample #35, Operator: mkieffer

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

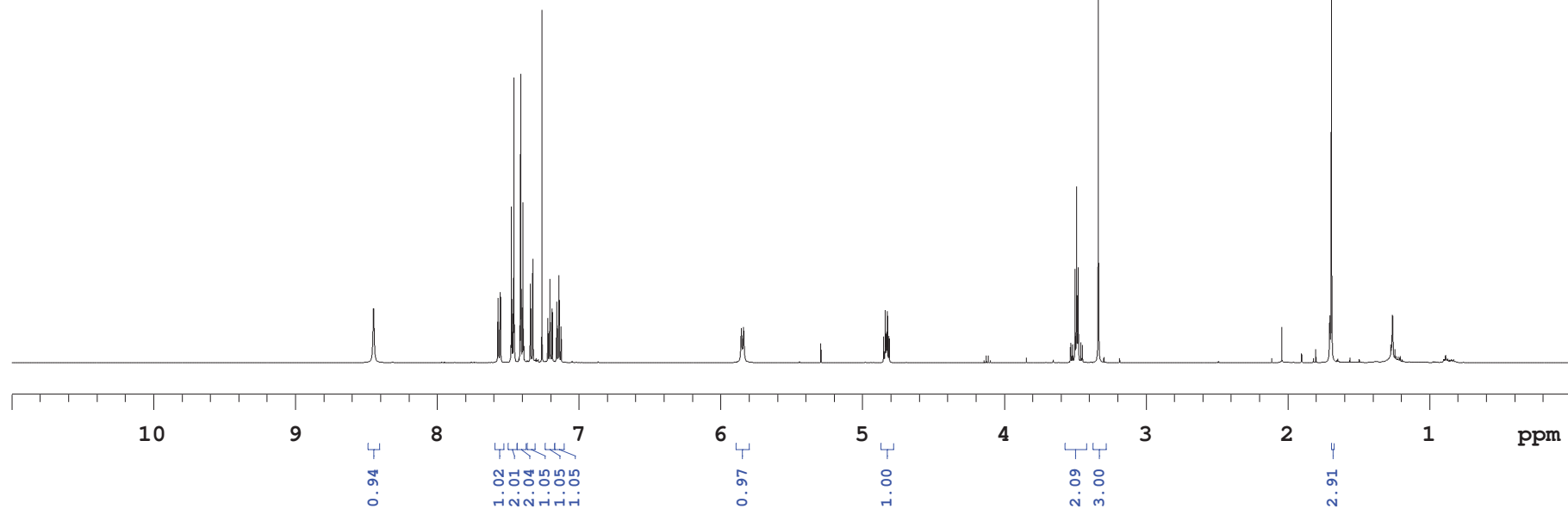
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 4 min 0 sec



MEK3113-1

Sample Name:

MEK3113-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3113-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 24 2011

Temp. 25.0 C / 298.1 K

Sample #35, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

2000 repetitions

OBSERVE C13, 125.6569662 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

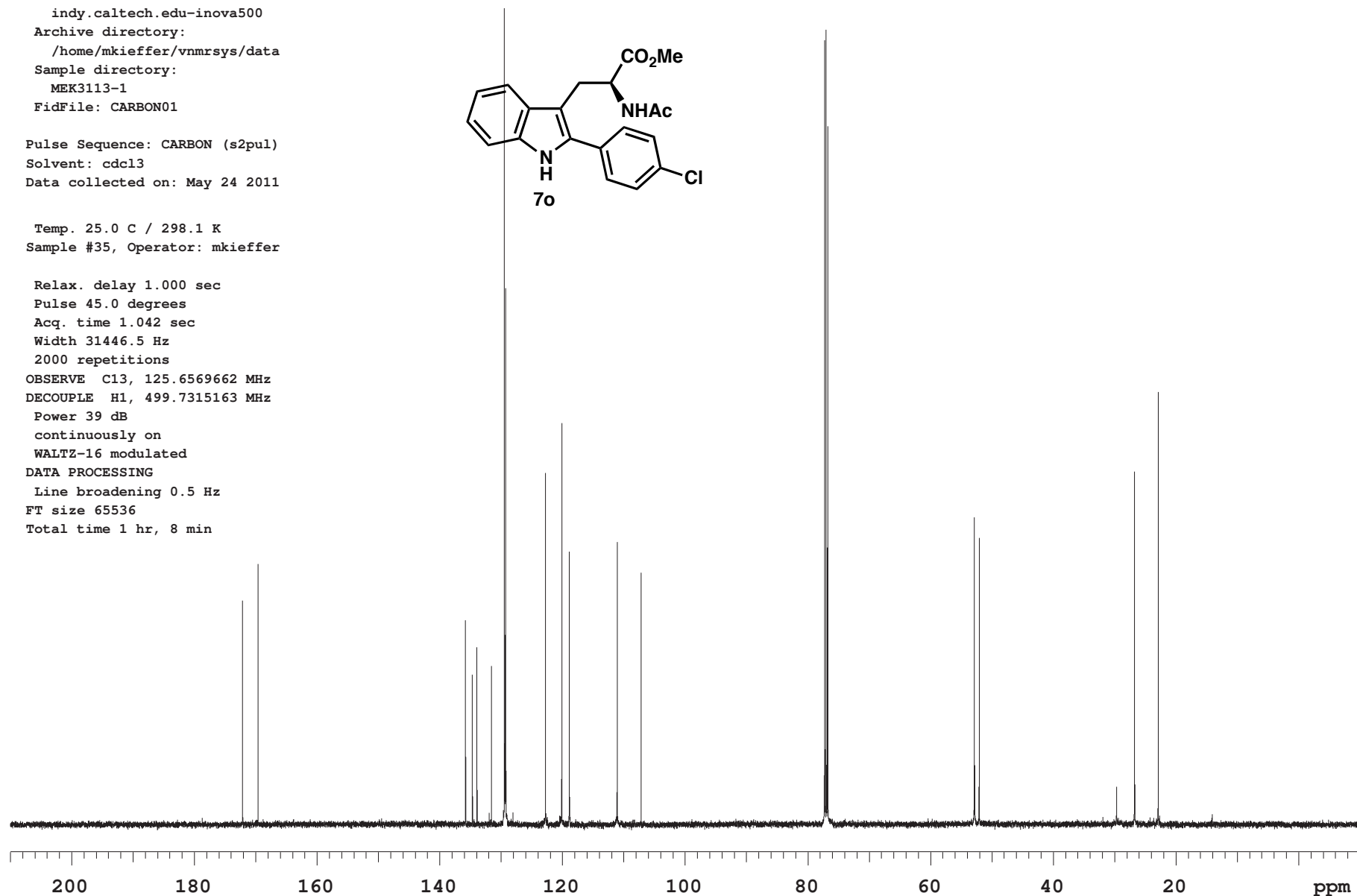
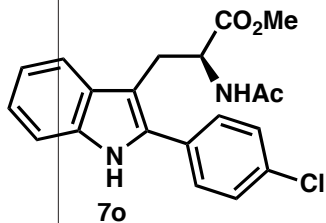
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 8 min



MEK-para-F

Sample Name:

MEK-para-F

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

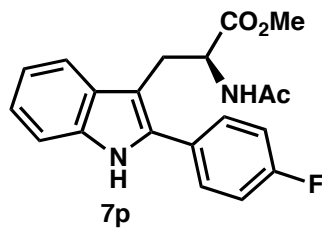
MEK-para-F

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 25 2011



Sample #14, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

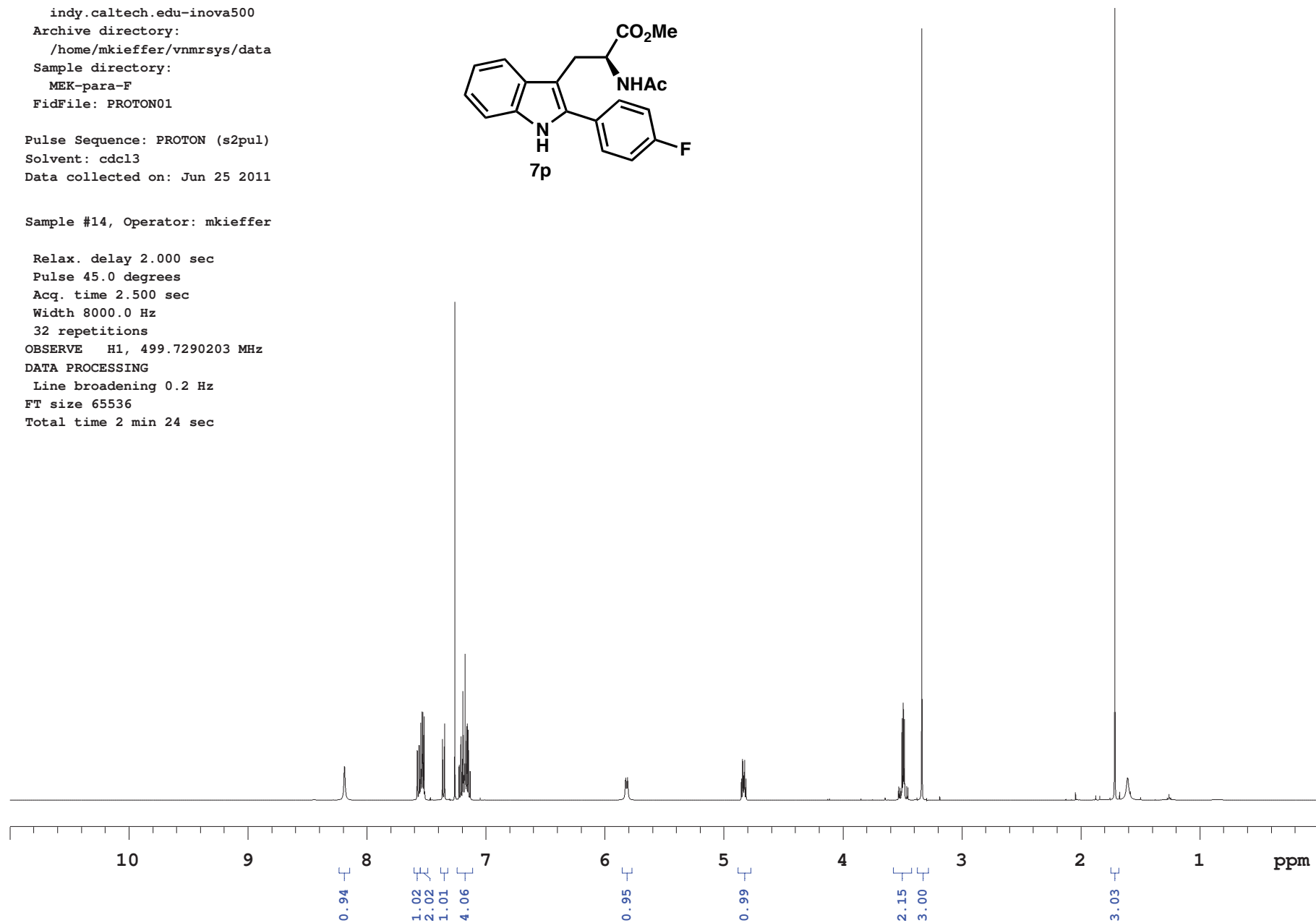
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



S124

MEK3086-1

Sample Name:

MEK3086-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3086-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 10 2011

Temp. 25.0 C / 298.1 K

Sample #39, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

512 repetitions

OBSERVE C13, 125.6569623 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

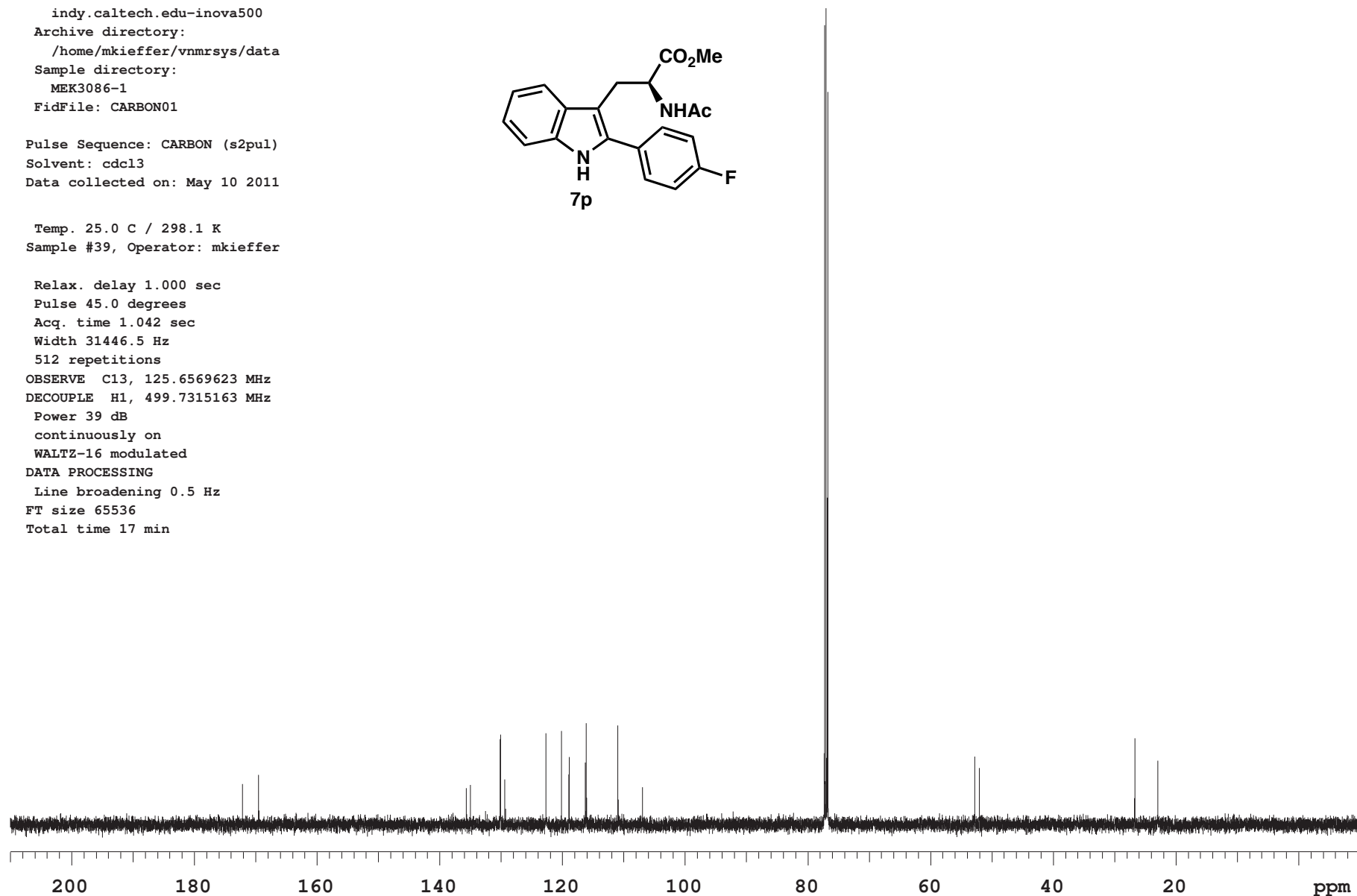
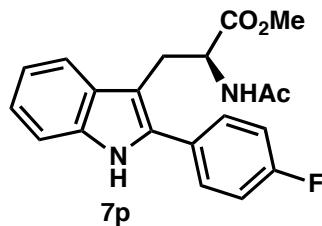
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 17 min



MEK3079-1

Sample Name:

MEK3079-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

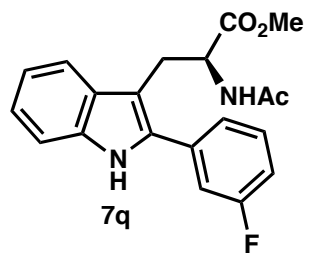
MEK3079-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: May 8 2011



Temp. 25.0 C / 298.1 K

Sample #41, Operator: mkieffer

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

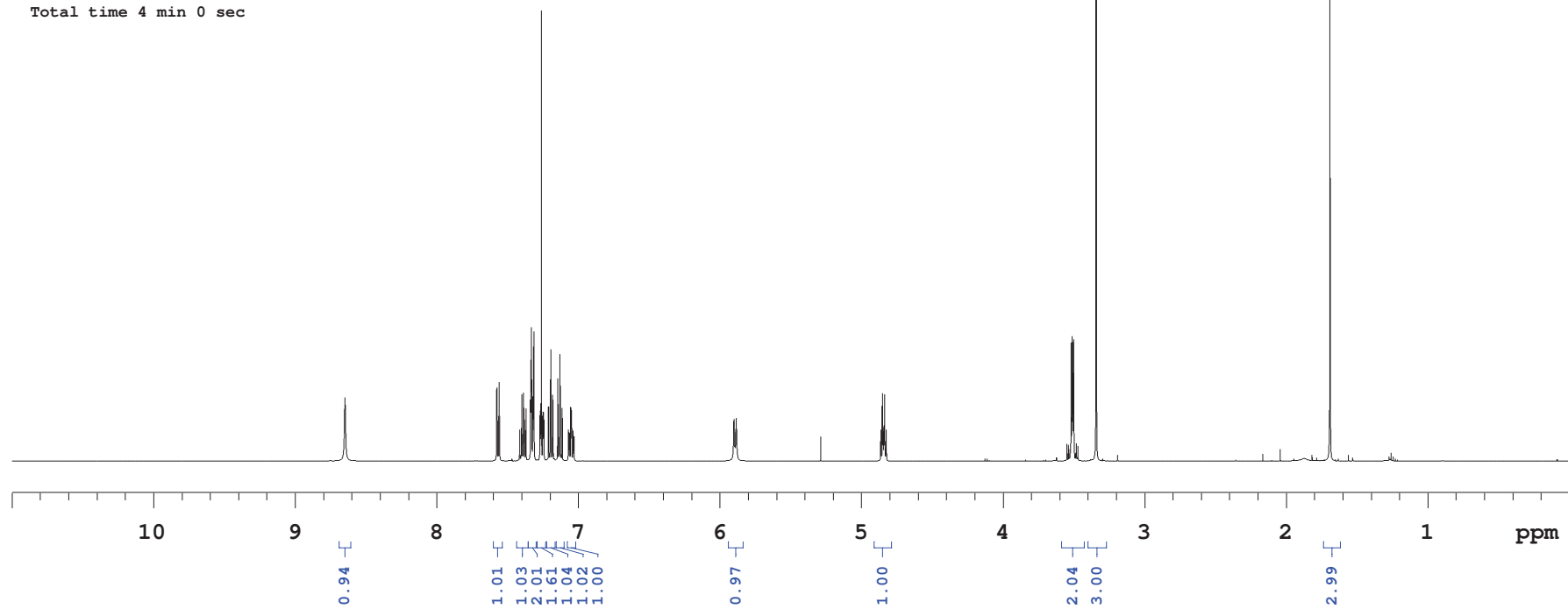
32 repetitions

OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

FT size 65536

Total time 4 min 0 sec



MEK3079-1

Sample Name:

MEK3079-1

Data Collected on:

indy.caltech.edu-inova500

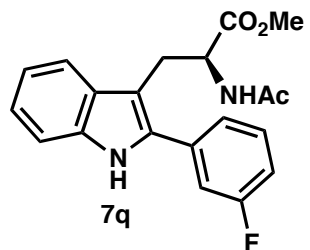
Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3079-1

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 8 2011

Temp. 25.0 C / 298.1 K

Sample #41, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

256 repetitions

OBSERVE C13, 125.6569690 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

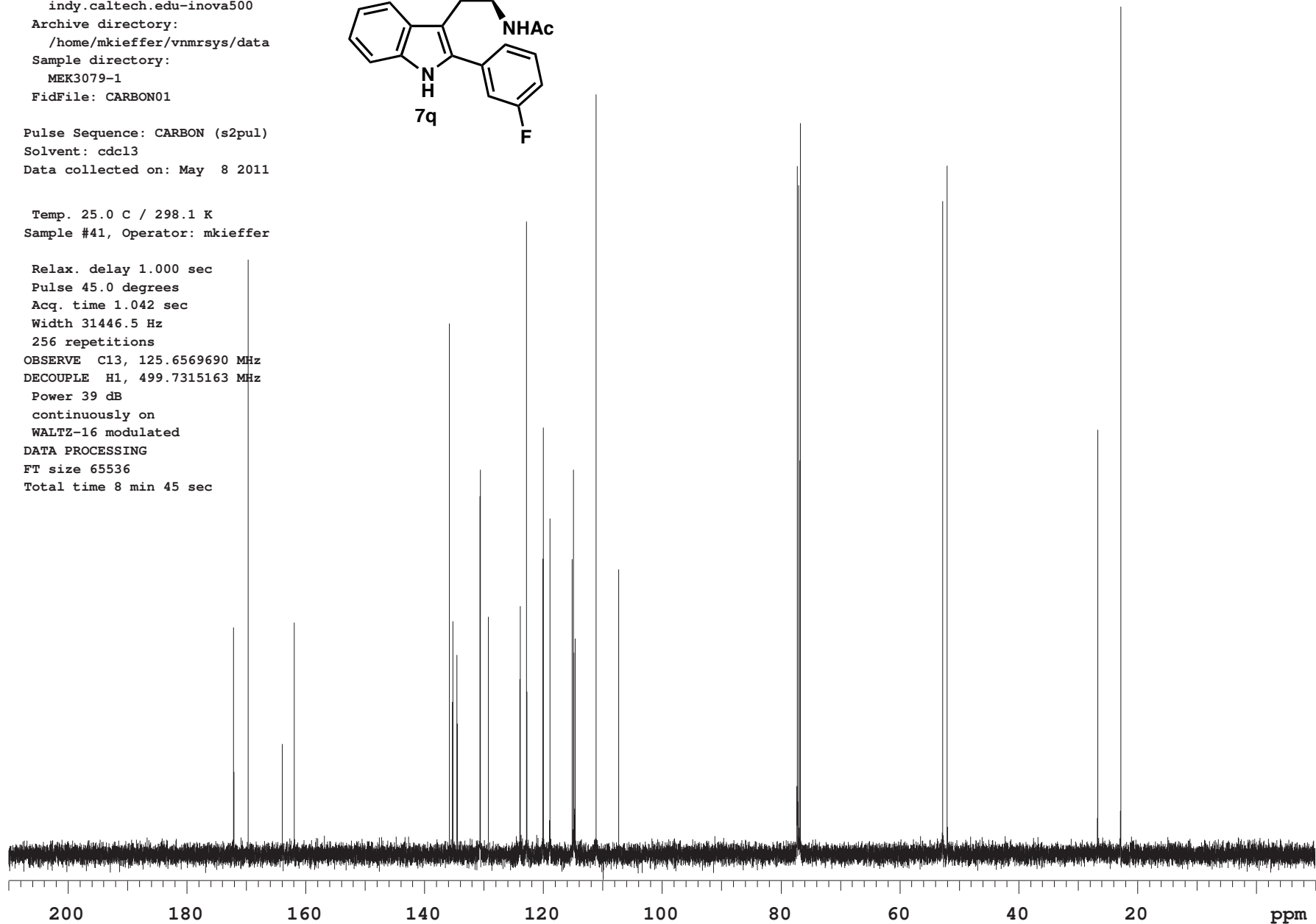
continuously on

WALTZ-16 modulated

DATA PROCESSING

FT size 65536

Total time 8 min 45 sec



MEK-ortho-fluoro-1

Sample Name:

MEK-ortho-fluoro-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK-ortho-fluoro-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 26 2011

Sample #33, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

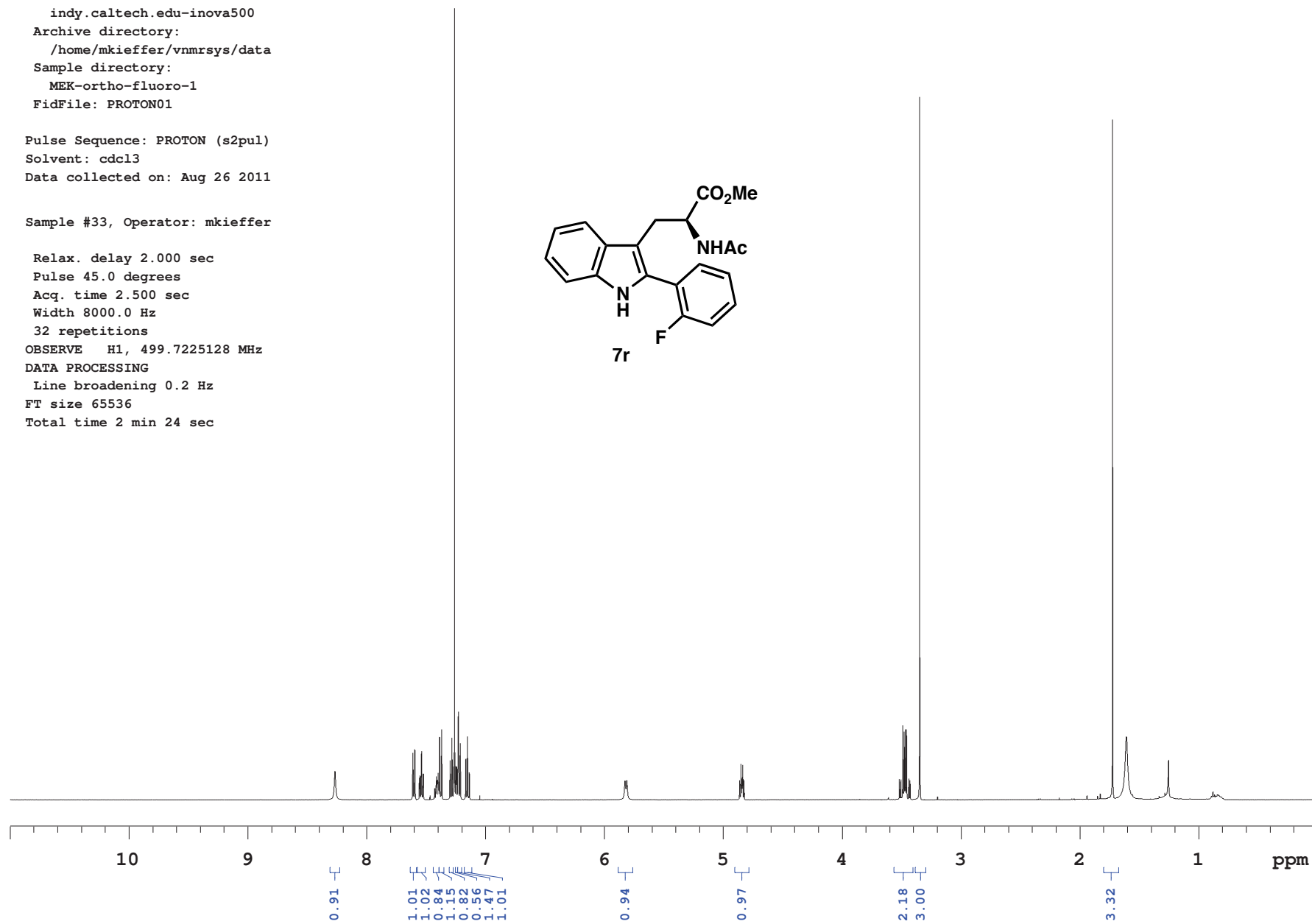
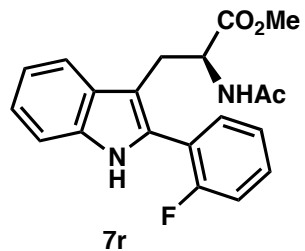
OBSERVE H1, 499.7225128 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec





MEK3219-2

Sample Name:

MEK3219-2

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3219-2

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Aug 17 2011

Sample #7, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553271 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

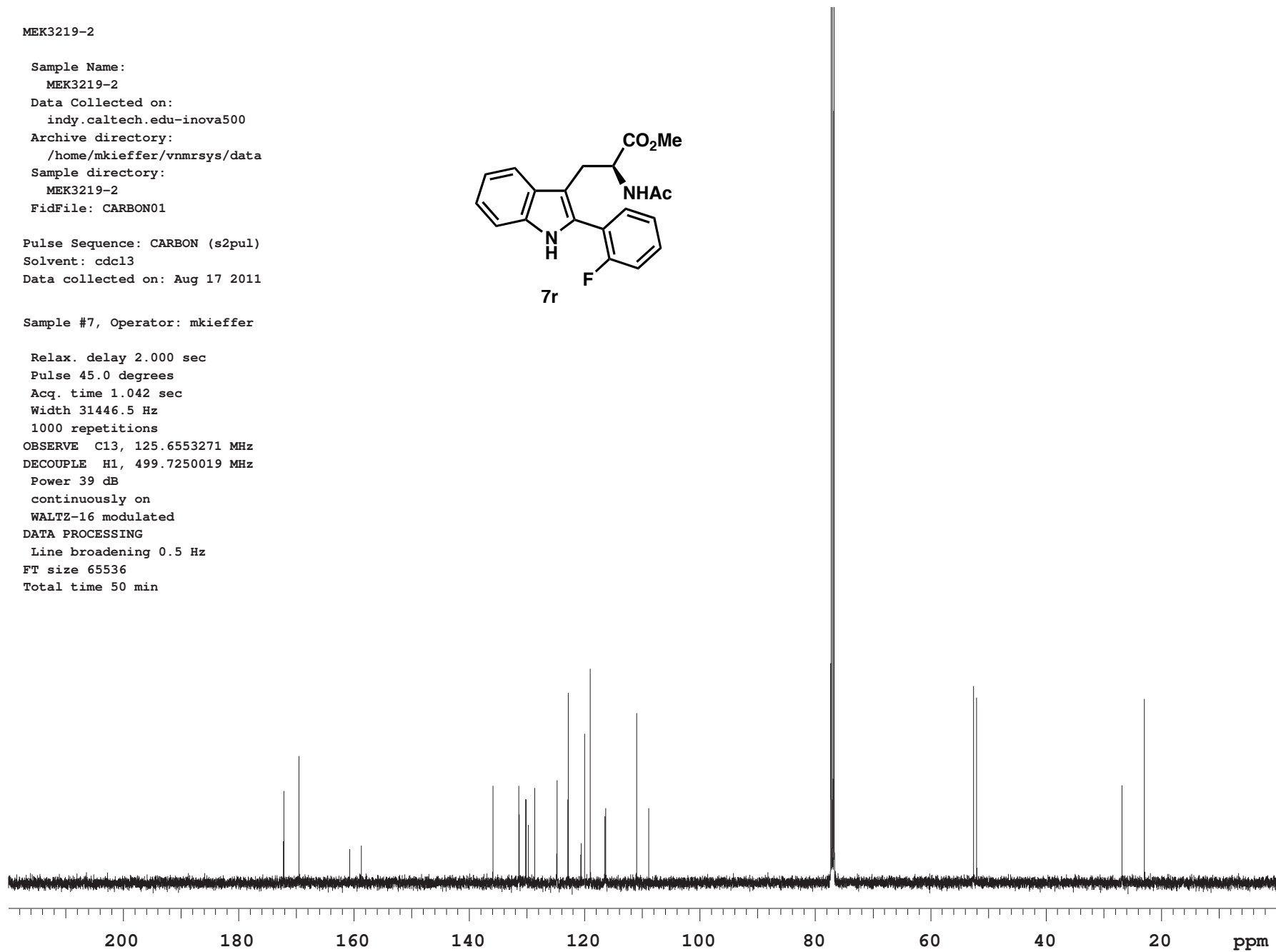
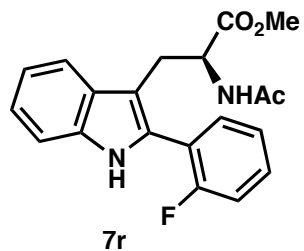
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 50 min



MEK-m-OMe

Sample Name:

MEK-m-OMe

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

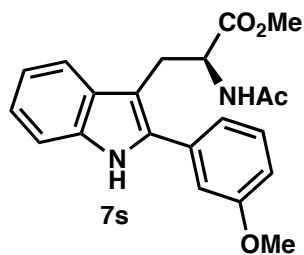
MEK-m-OMe

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 25 2011



Sample #16, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

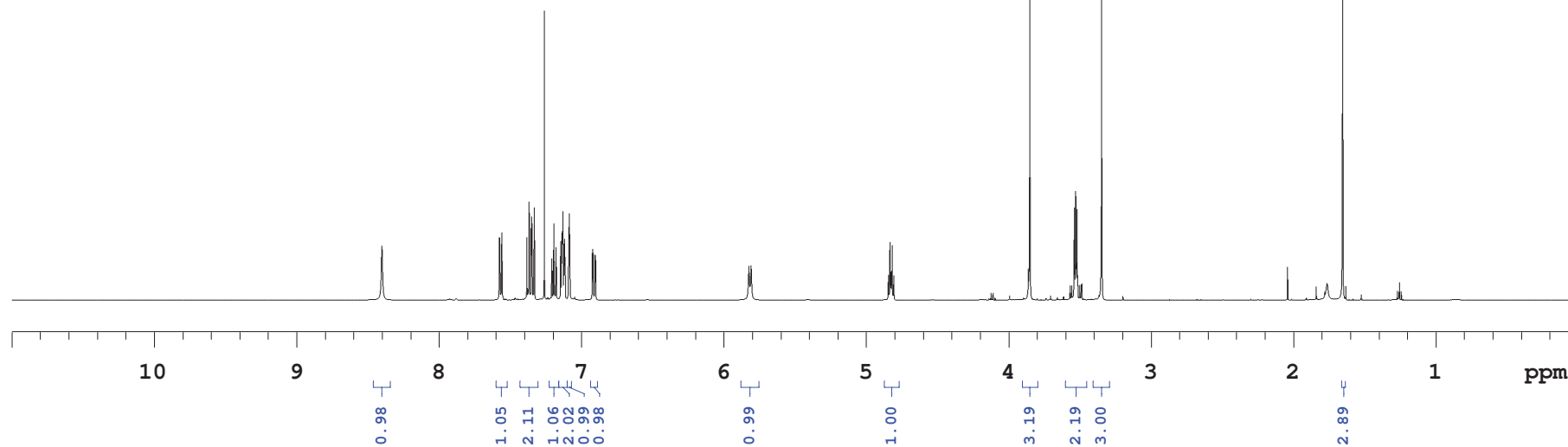
OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



MEK-m-OMe

Sample Name:

MEK-m-OMe

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

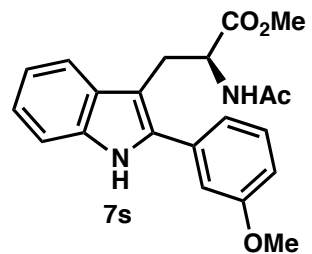
MEK-m-OMe

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 25 2011



Sample #16, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6569681 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

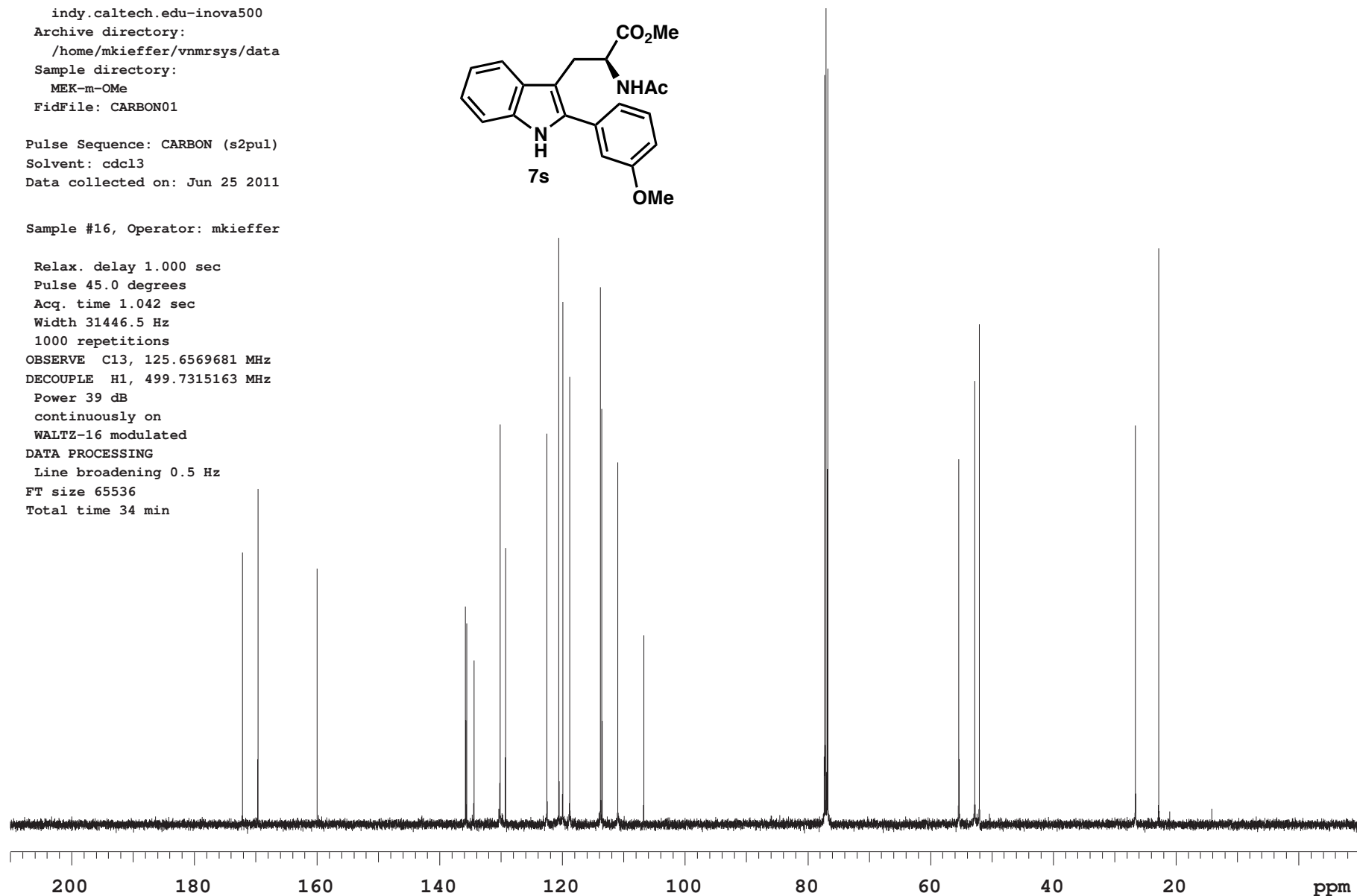
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



MEK3083-1

Sample Name:

MEK3083-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3083-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 9 2011

Temp. 25.0 C / 298.1 K

Sample #38, Operator: mkieffer

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

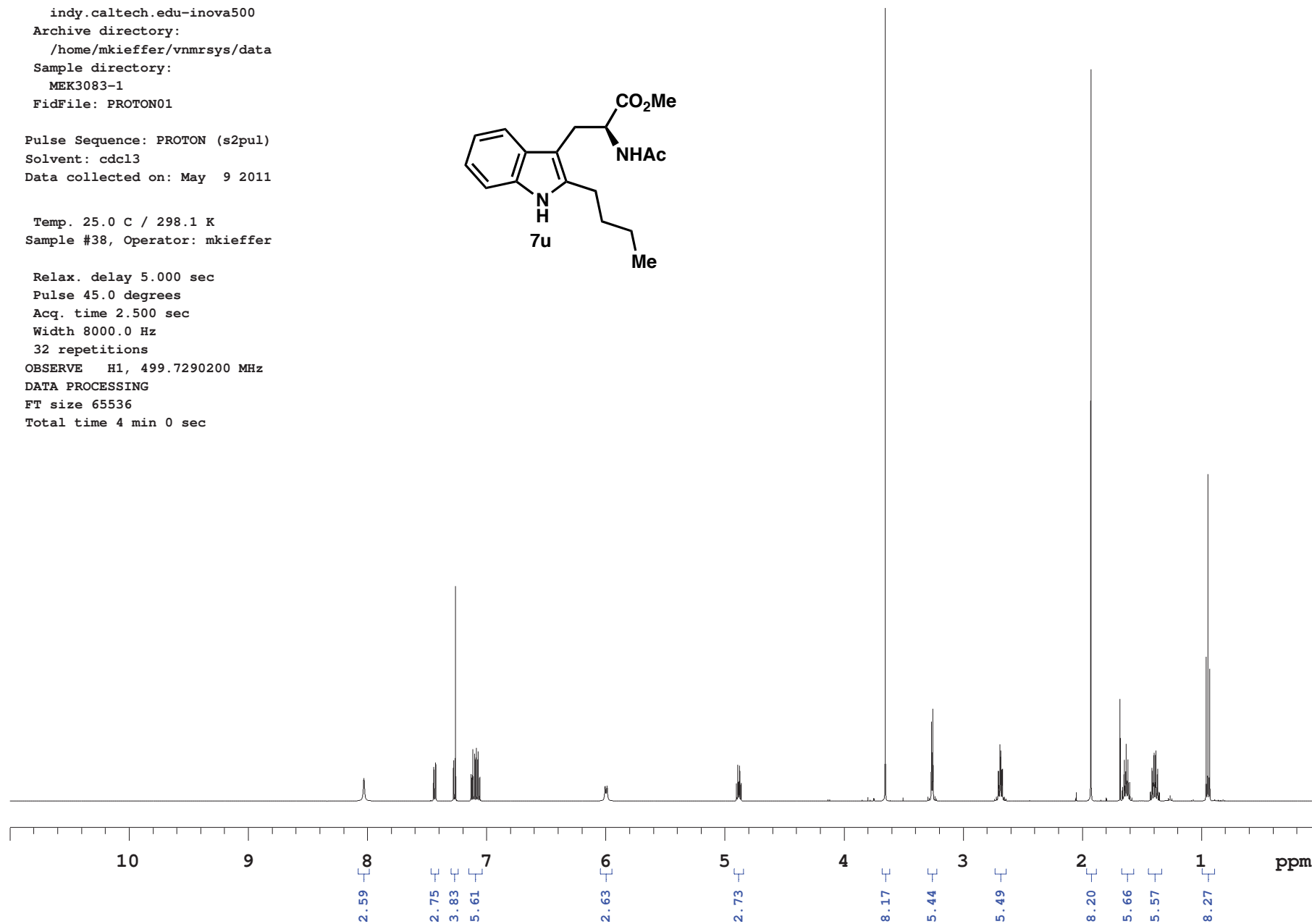
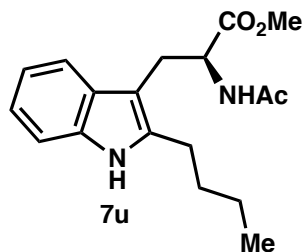
32 repetitions

OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

FT size 65536

Total time 4 min 0 sec



MEK3080-1

Sample Name:

MEK3080-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3080-1

FidFile: current

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 8 2011

Temp. 25.0 C / 298.1 K

Sample #42, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

384 repetitions

OBSERVE C13, 125.6569642 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

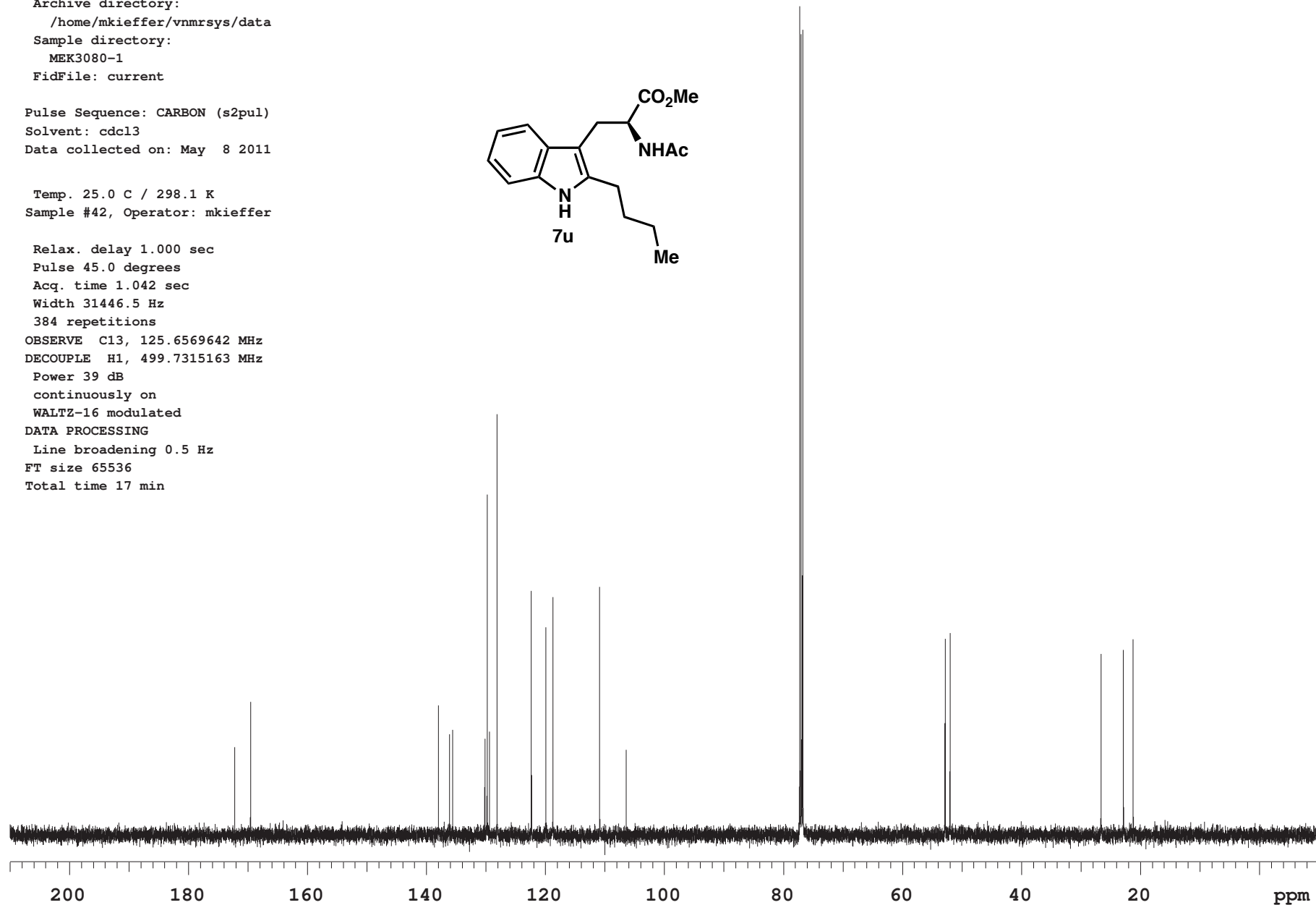
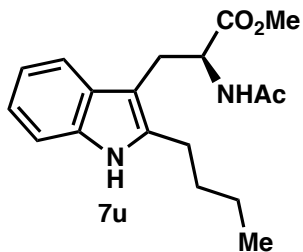
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 17 min



S133

MEK3129-1

Sample Name:

MEK3129-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

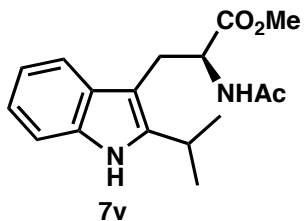
MEK3129-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 7 2011



Temp. 25.0 C / 298.1 K

Sample #14, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

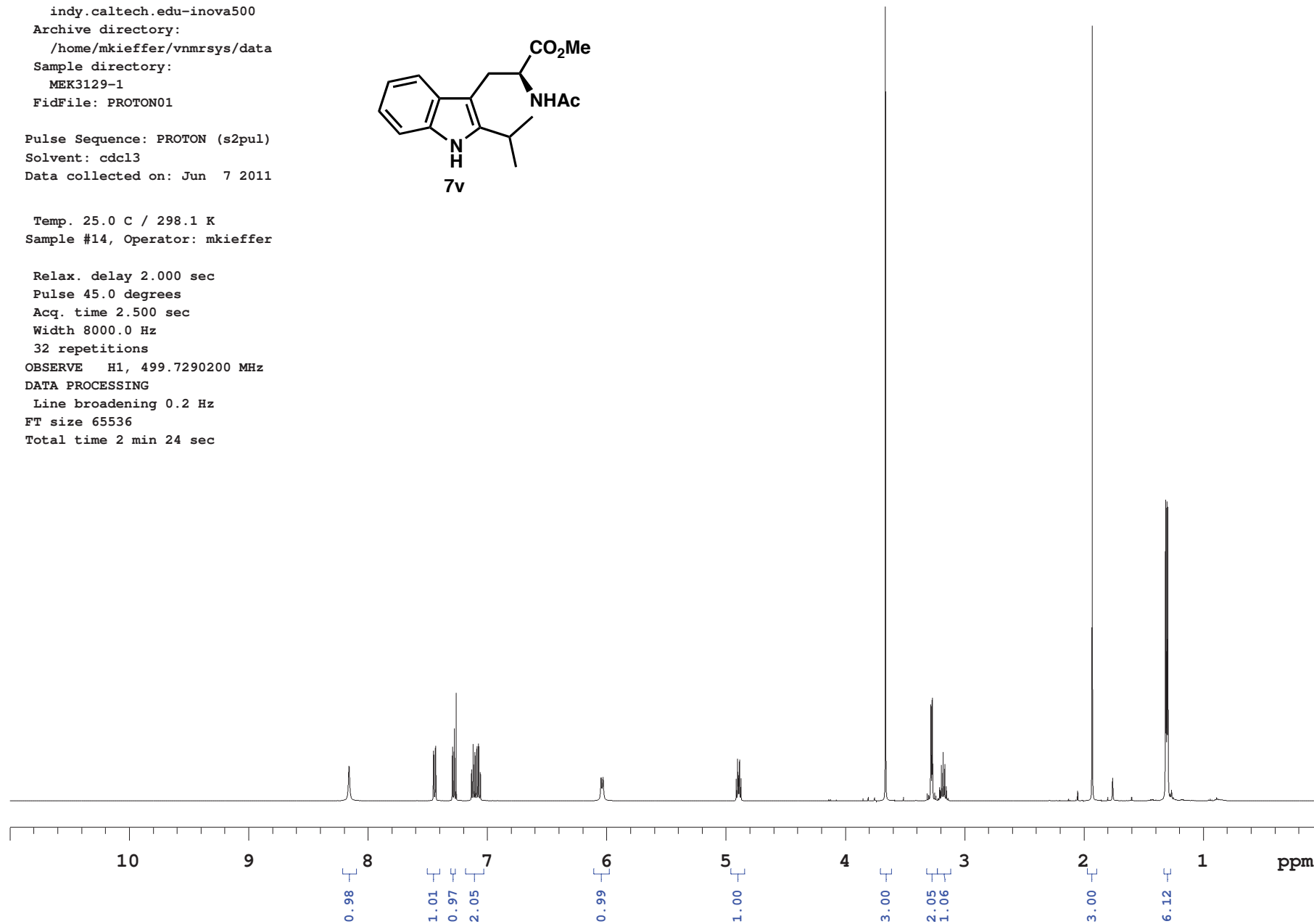
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



MEK3129-1

Sample Name:

MEK3129-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3129-1

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 7 2011

Temp. 25.0 C / 298.1 K

Sample #14, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

512 repetitions

OBSERVE C13, 125.6569671 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

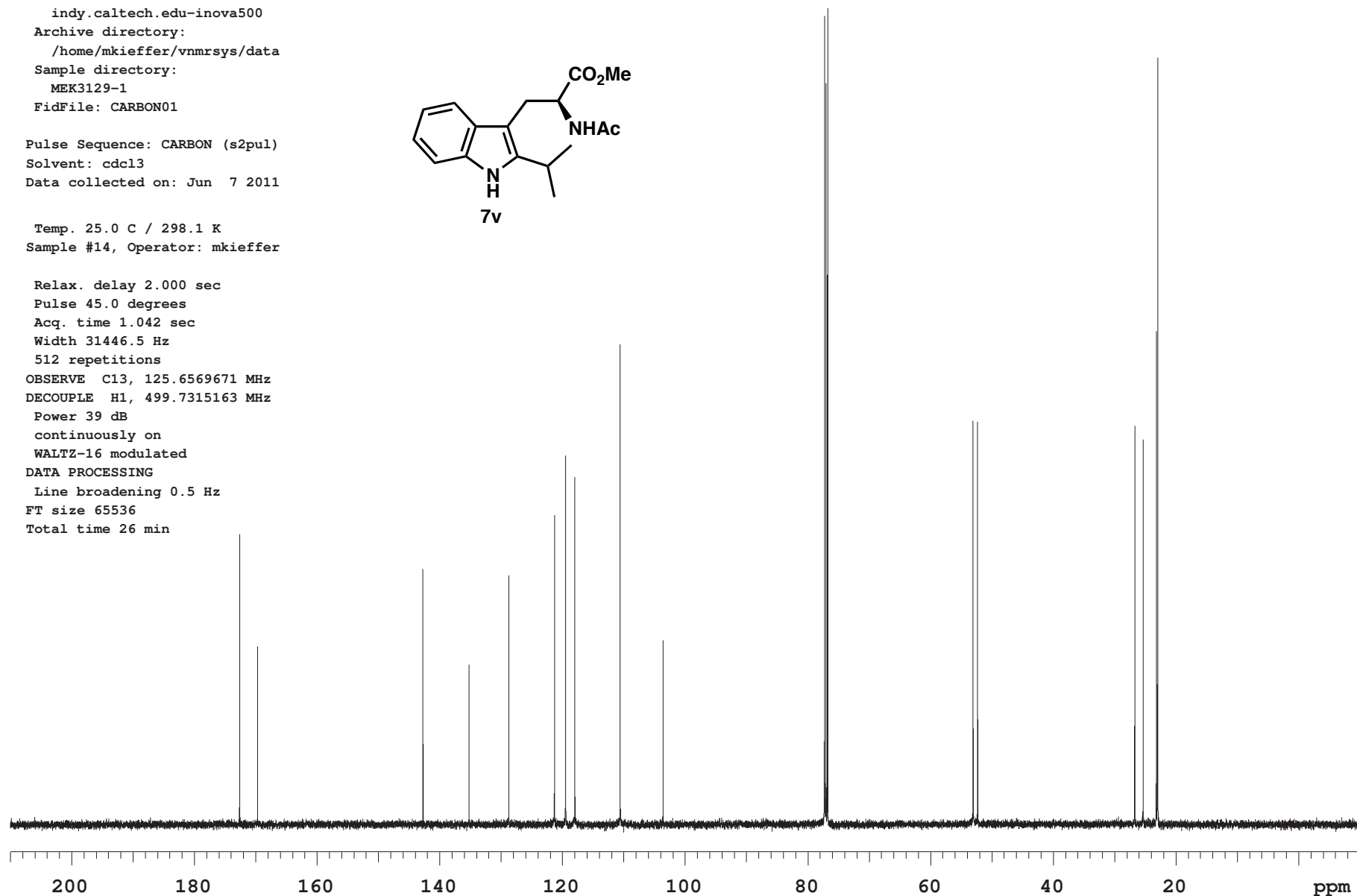
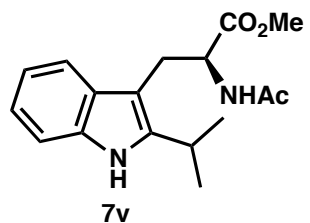
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 26 min



MEK-t-butyl-rac

Sample Name:

MEK-t-butyl-rac

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK-t-butyl-rac

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 5 2011

Temp. 25.0 C / 298.1 K

Sample #27, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

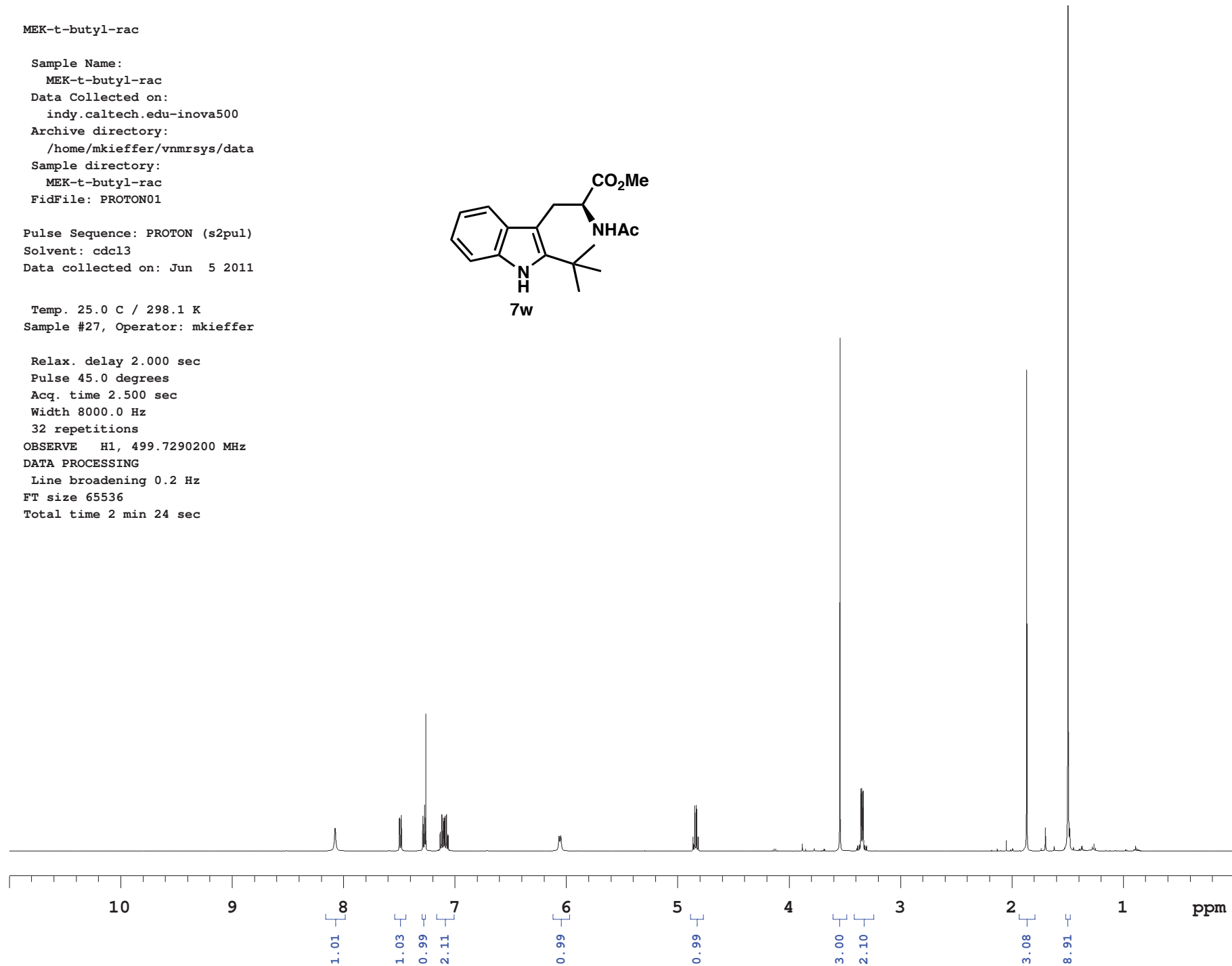
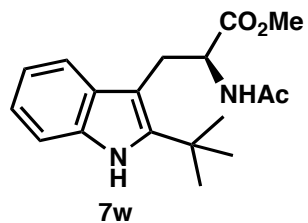
OBSERVE H1, 499.7290200 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec





MEK-t-butyl-rac

Sample Name:

MEK-t-butyl-rac

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

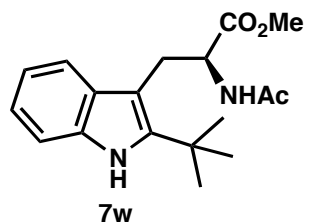
MEK-t-butyl-rac

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 5 2011



Temp. 25.0 C / 298.1 K

Sample #27, Operator: mkieffer

Relax. delay 2.000 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

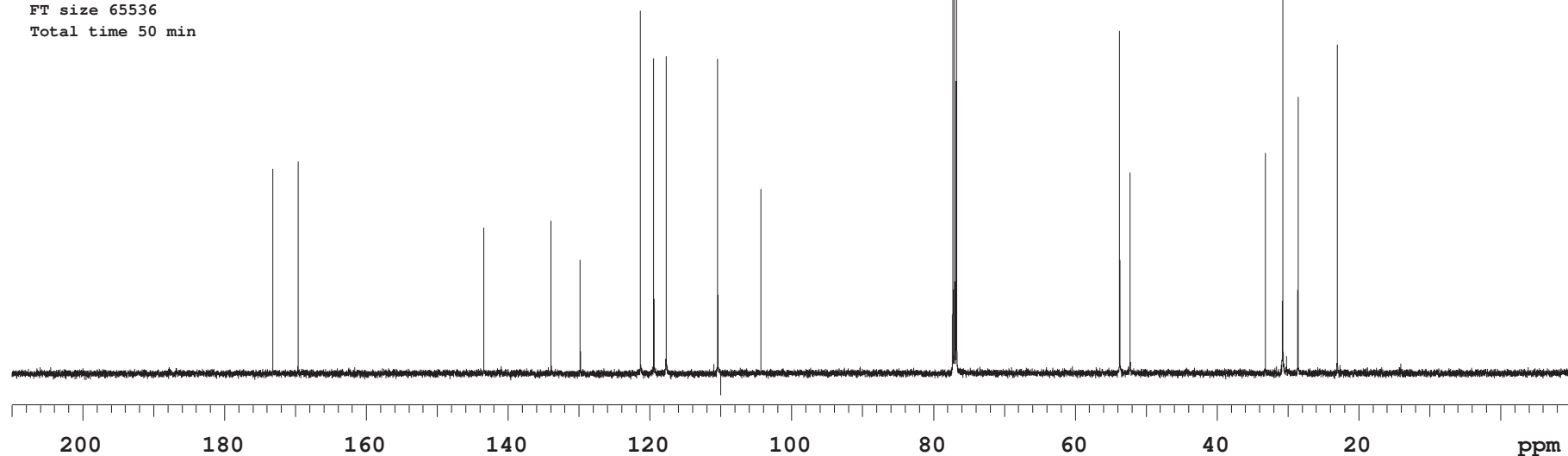
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 50 min



MEK-phthalimide

Sample Name:

MEK-phthalimide

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK-phthalimide

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 6 2011

Temp. 25.0 C / 298.1 K

Sample #20, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

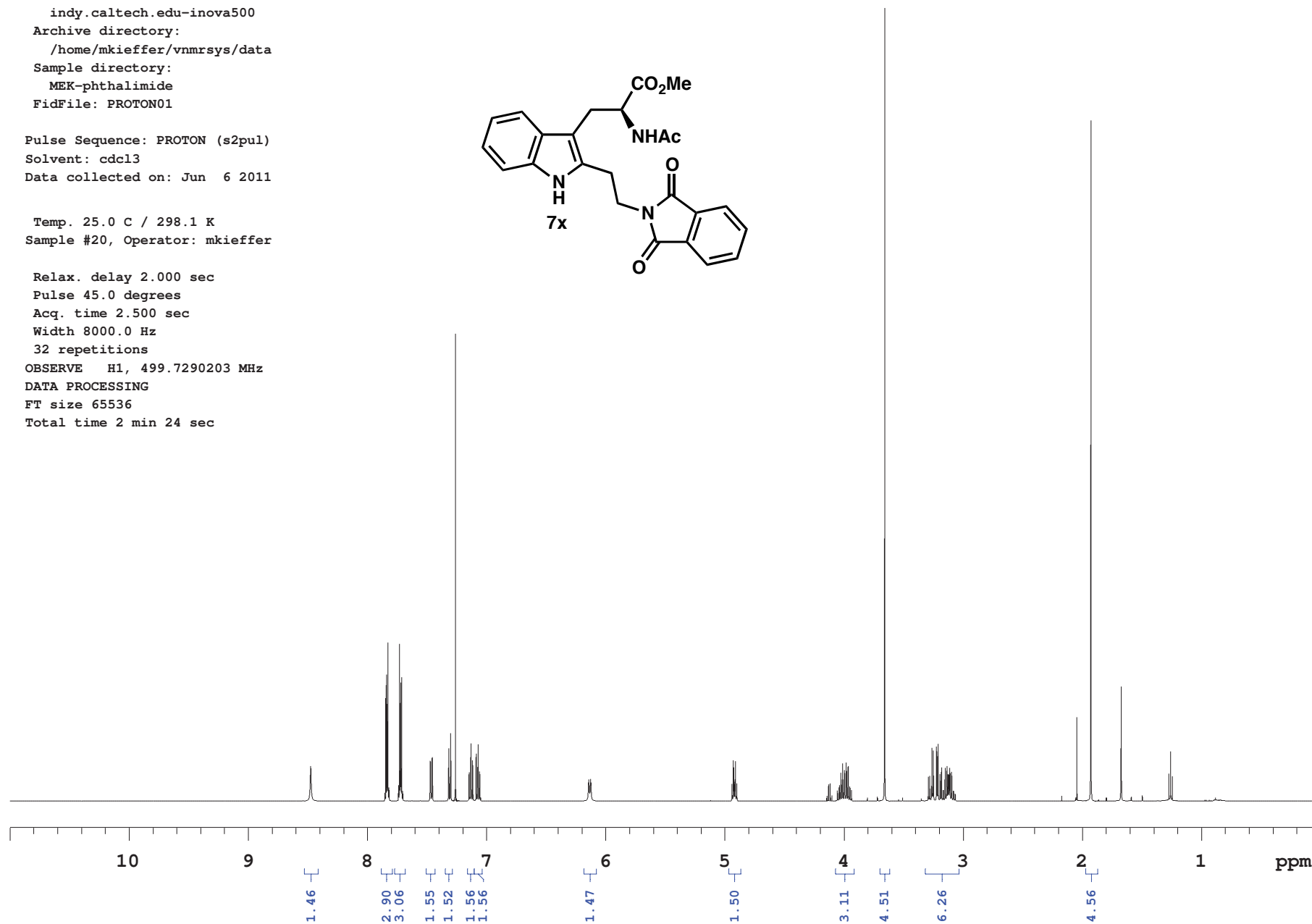
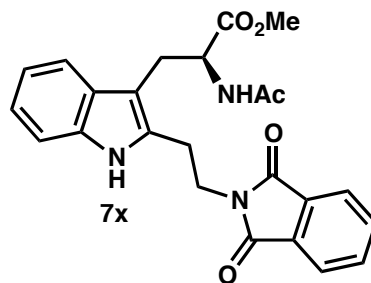
32 repetitions

OBSERVE H1, 499.7290203 MHz

DATA PROCESSING

FT size 65536

Total time 2 min 24 sec



MEK-phthalimide

Sample Name:

MEK-phthalimide

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK-phthalimide

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 6 2011

Temp. 25.0 C / 298.1 K

Sample #20, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6569633 MHz

DECOUPLE H1, 499.7315163 MHz

Power 39 dB

continuously on

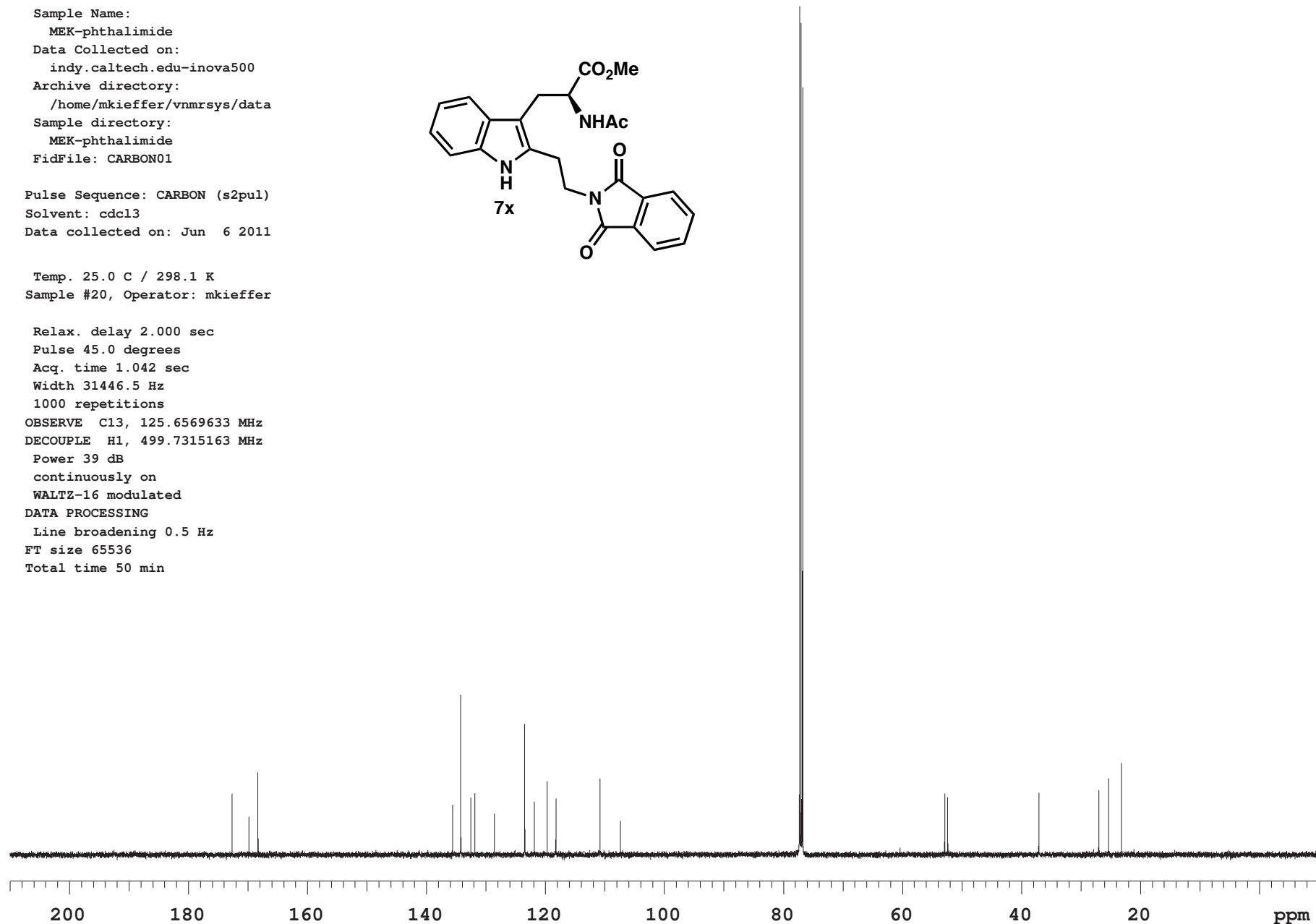
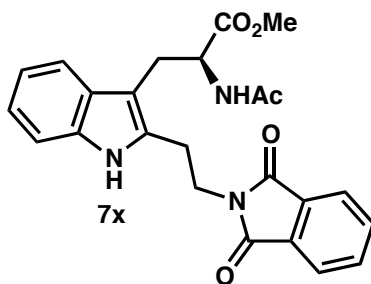
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 50 min



MEK2306-1

Sample Name:

MEK2306-1

Data Collected on:

indy.caltech.edu-inova500

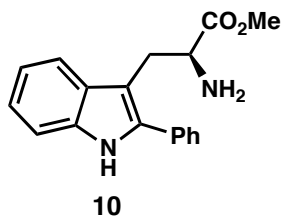
Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK2306-1

FidFile: PROTON01



Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 4 2011

Sample #14, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

32 repetitions

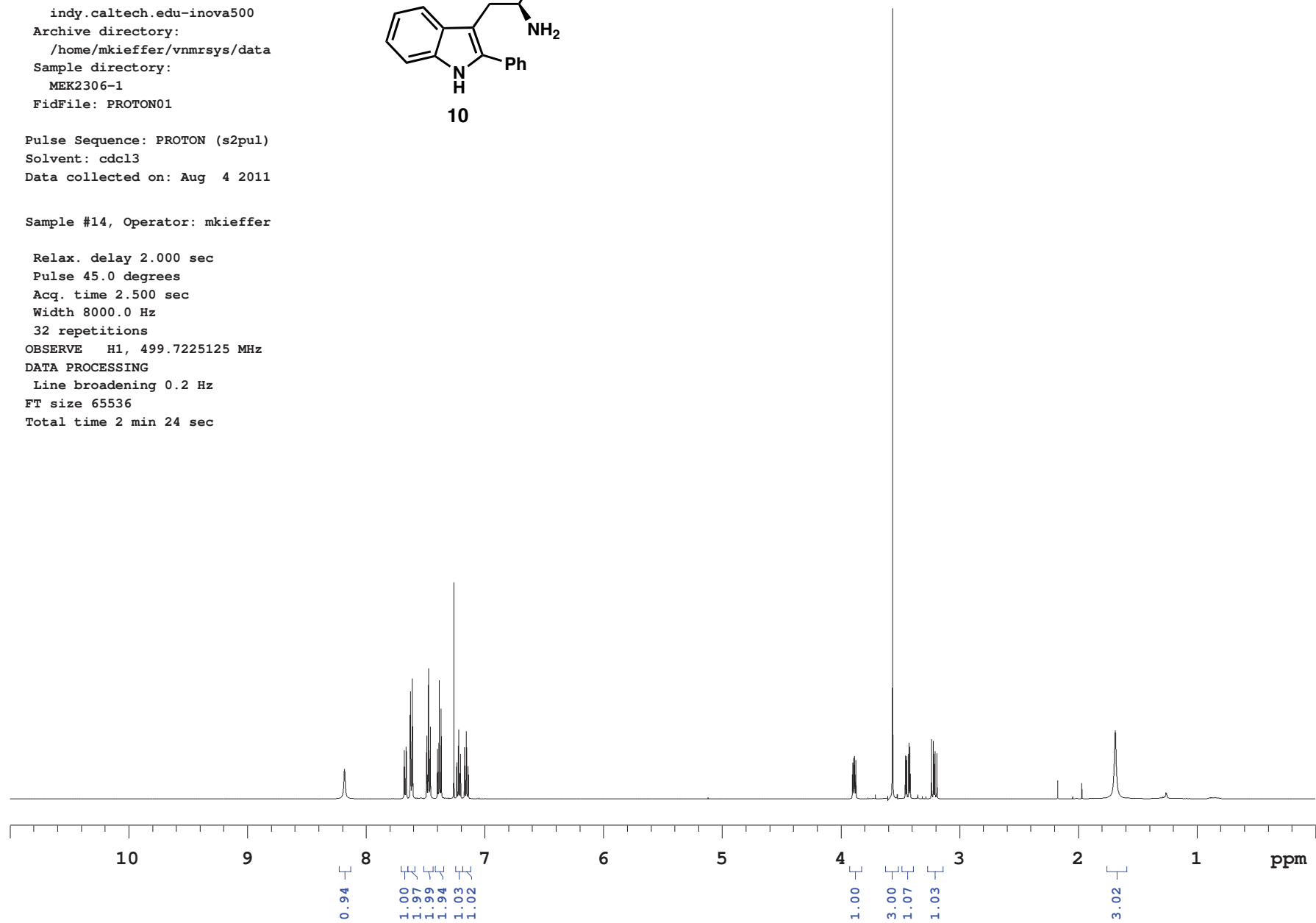
OBSERVE H1, 499.7225125 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 2 min 24 sec



MEK3206-1

Sample Name:

MEK3206-1

Data Collected on:

indy.caltech.edu-inova500

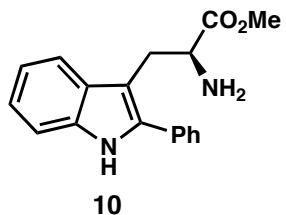
Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3206-1

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Aug 4 2011

Sample #14, Operator: mkieffer

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553281 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

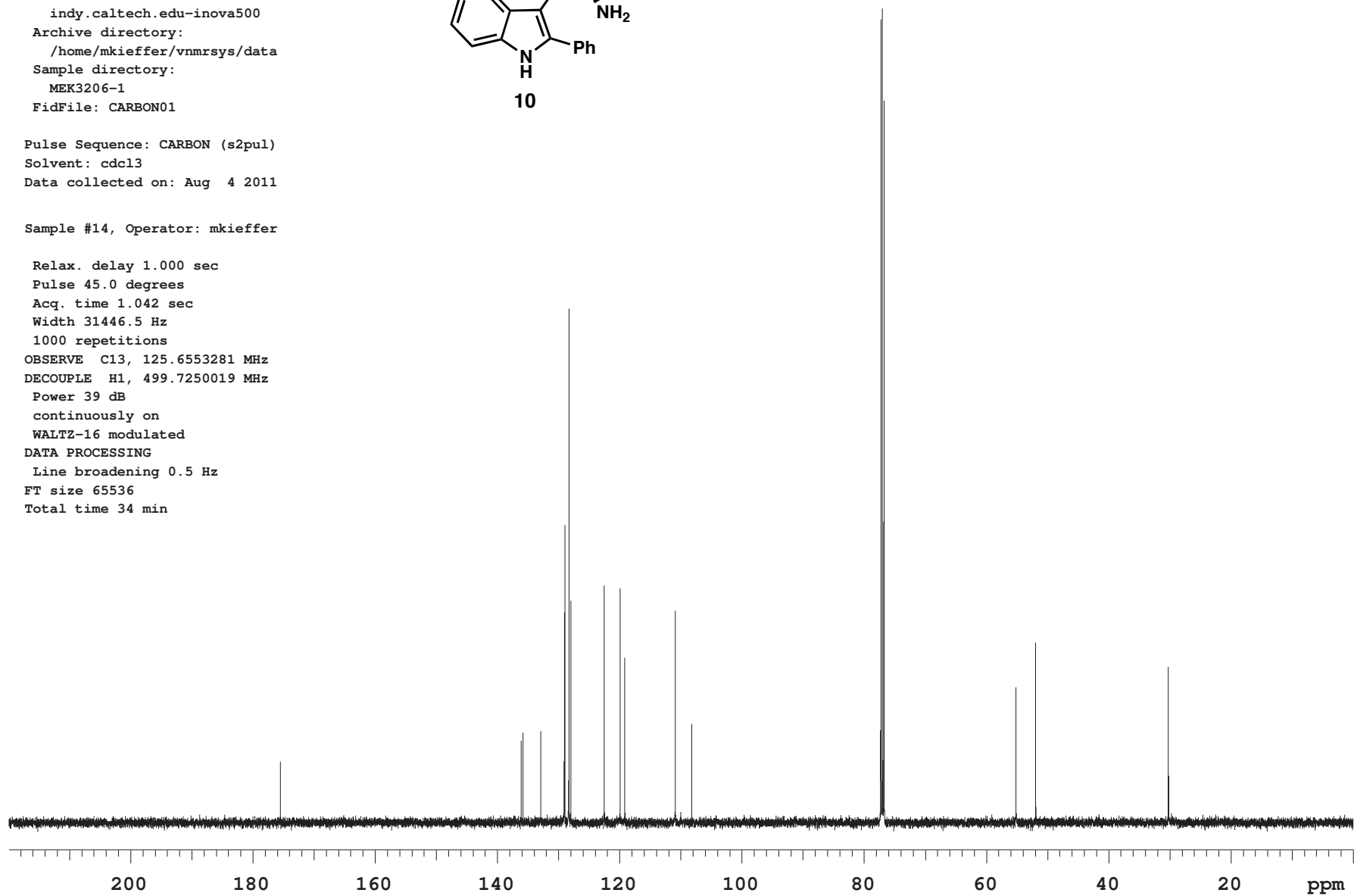
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 34 min



MEK-methylcarbamate-1

Sample Name:

MEK-methylcarbamate-1

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK-methylcarbamate-1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Aug 30 2011

Sample #22, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

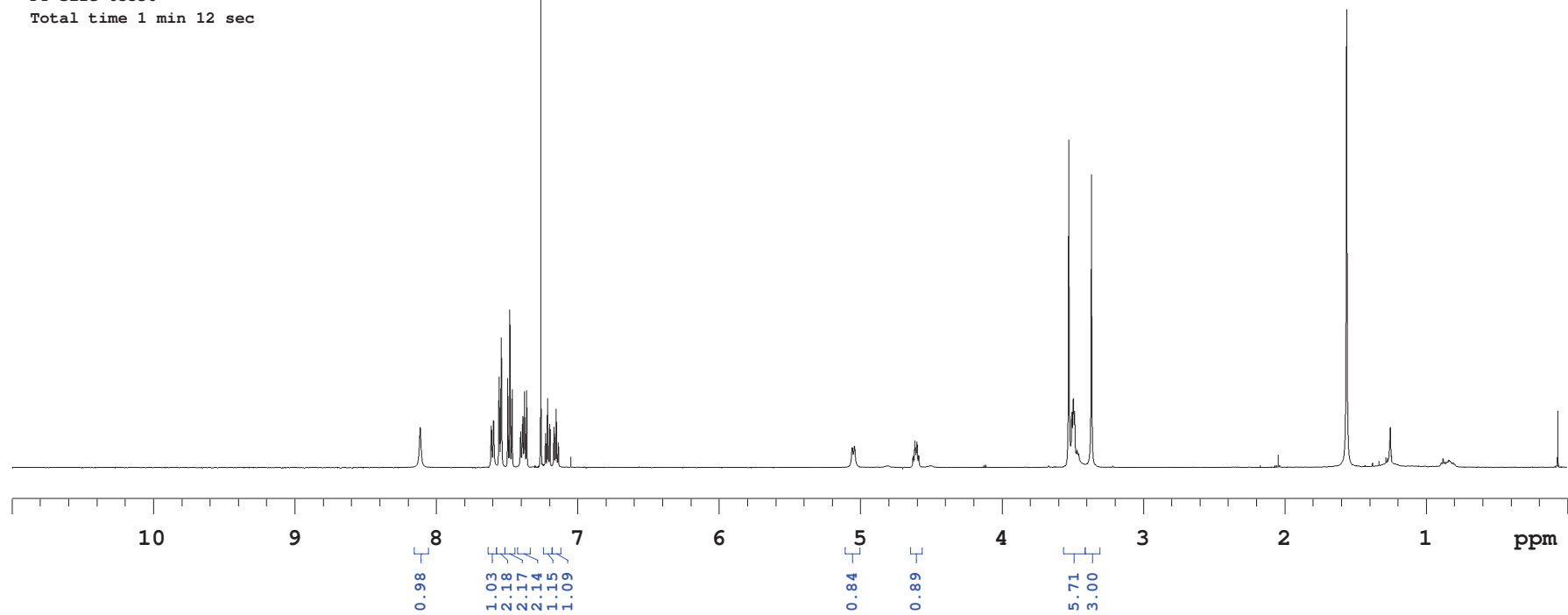
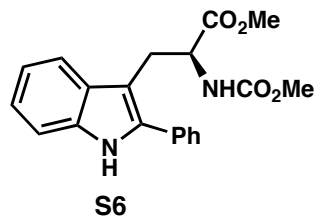
OBSERVE H1, 499.7225128 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 1 min 12 sec



MEK3233-X

Sample Name:

MEK3233-X

Data Collected on:

indy.caltech.edu-inova500

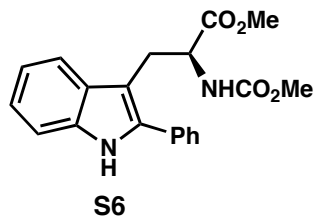
Archive directory:

/home/mkieffer/vnmrsys/data

Sample directory:

MEK3233-X

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 28 2011

Sample #20, Operator: mkieffer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6553271 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

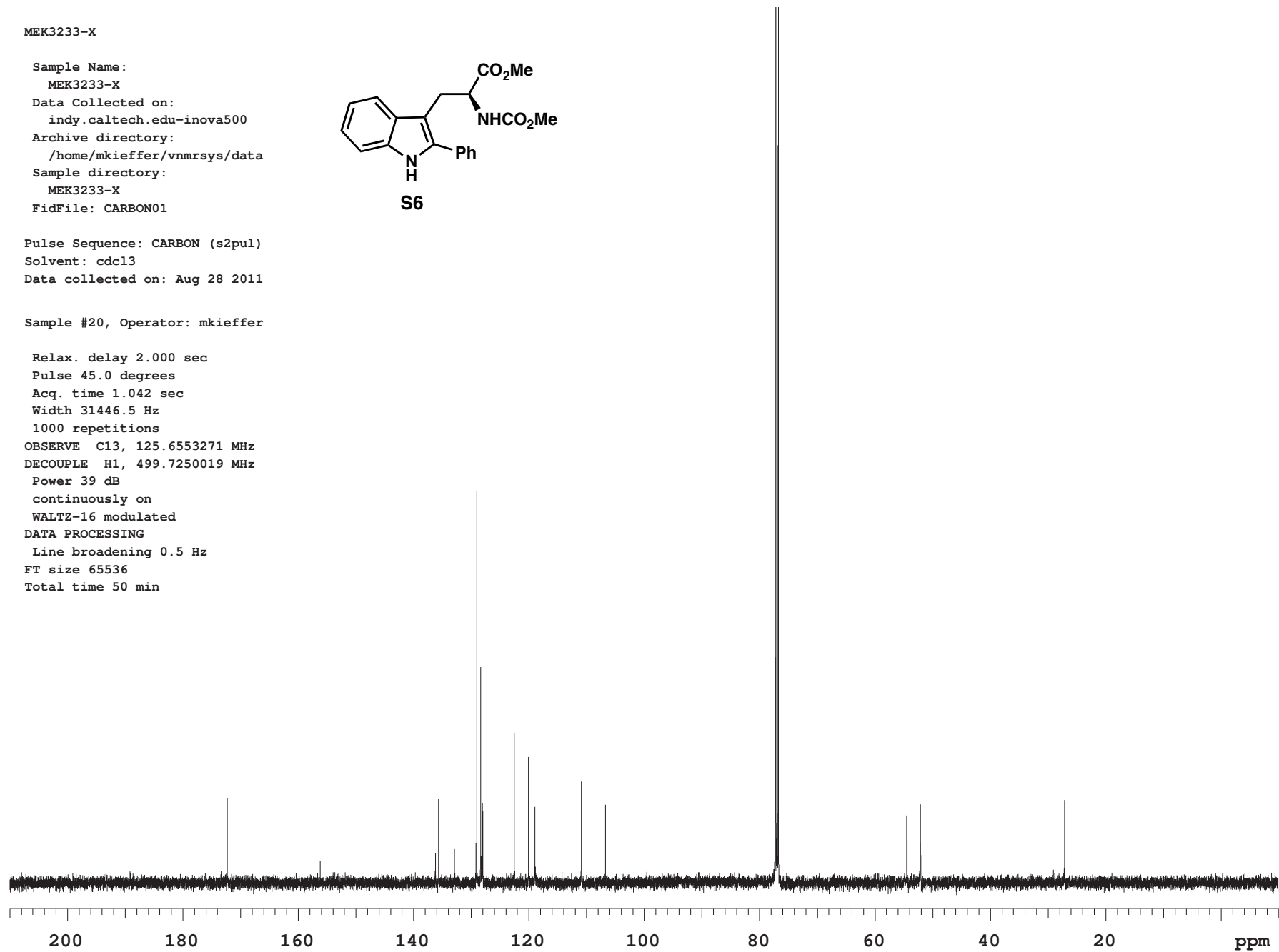
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 50 min



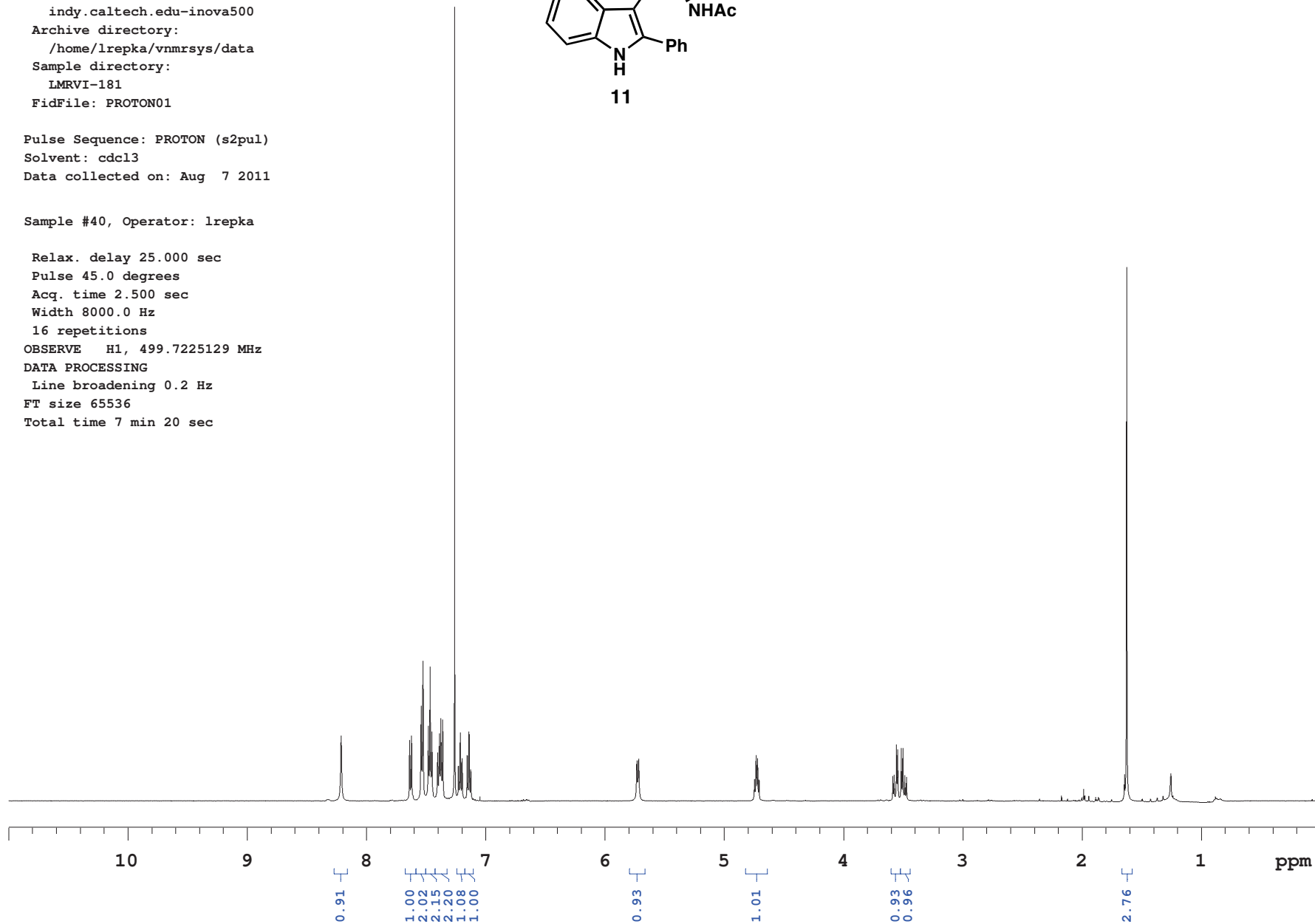
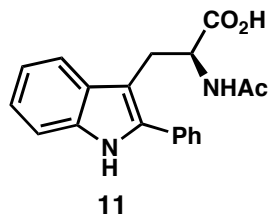
LMRVI-181

Sample Name:  
LMRVI-181  
Data Collected on:  
indy.caltech.edu-inova500  
Archive directory:  
/home/lrepka/vnmrsys/data  
Sample directory:  
LMRVI-181  
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Aug 7 2011

Sample #40, Operator: lrepka

Relax. delay 25.000 sec  
Pulse 45.0 degrees  
Acq. time 2.500 sec  
Width 8000.0 Hz  
16 repetitions  
OBSERVE H1, 499.7225129 MHz  
DATA PROCESSING  
Line broadening 0.2 Hz  
FT size 65536  
Total time 7 min 20 sec





LMRVI-179

Sample Name:

LMRVI-179

Data Collected on:

indy.caltech.edu-inova500

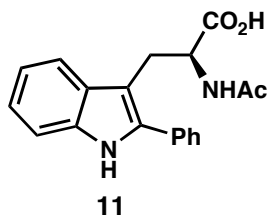
Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-179

FidFile: CARBON01



Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 2 2011

Sample #20, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6553305 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

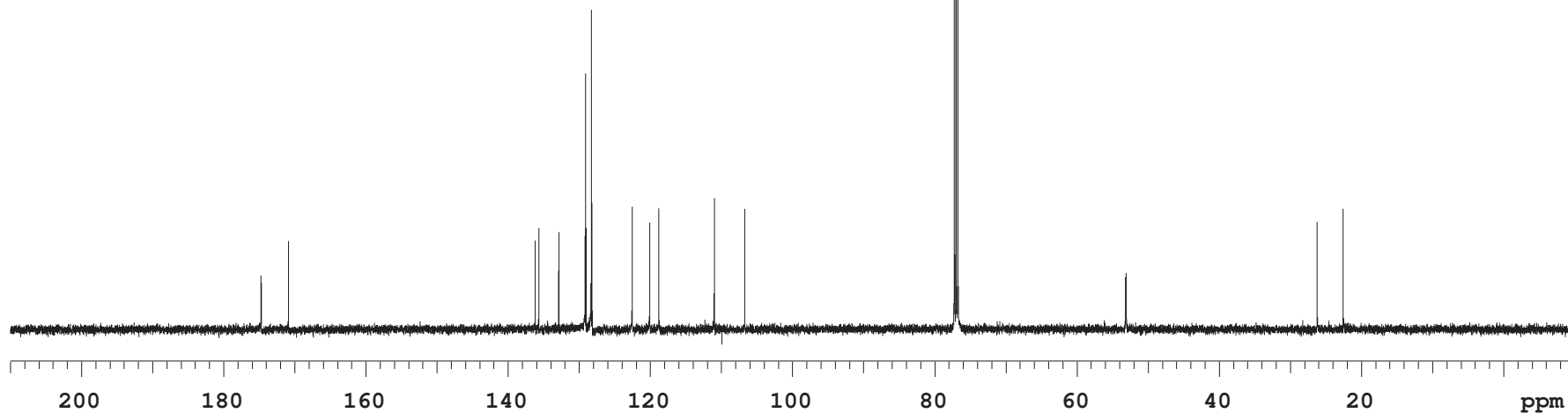
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



LMRVI-191

Sample Name:

LMRVI-191

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-191

FidFile: PROTON02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jan 24 2012

Sample #27, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

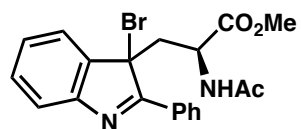
OBSERVE H1, 499.7225134 MHz

DATA PROCESSING

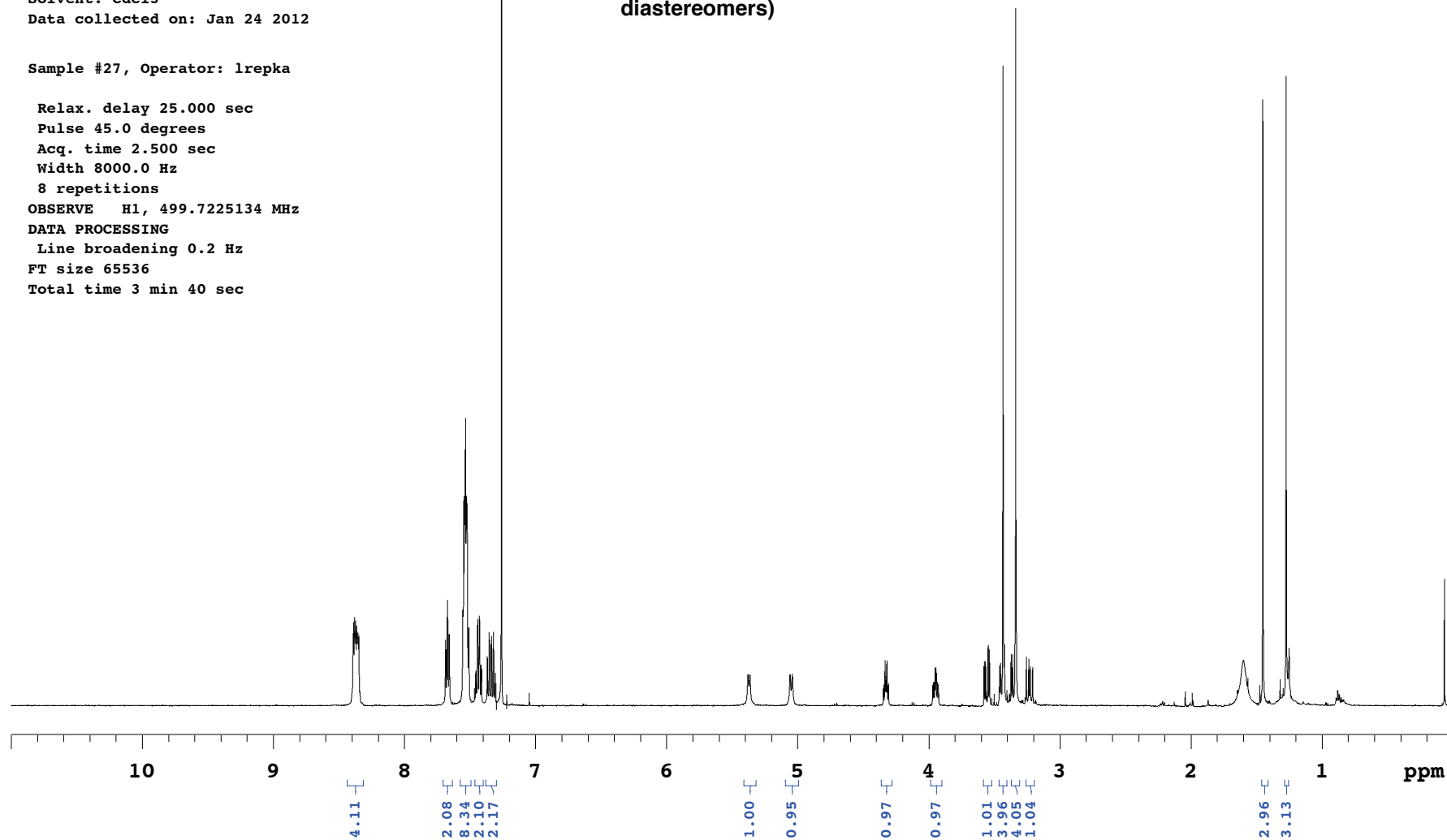
Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



12  
(1:1 mixture of diastereomers)



LMRVI-191

Sample Name:

LMRVI-191

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVI-191

Fidfile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 11 2011

Sample #23, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1500 repetitions

OBSERVE C13, 125.6553310 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

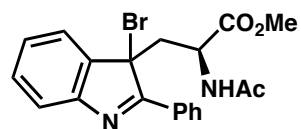
WALTZ-16 modulated

DATA PROCESSING

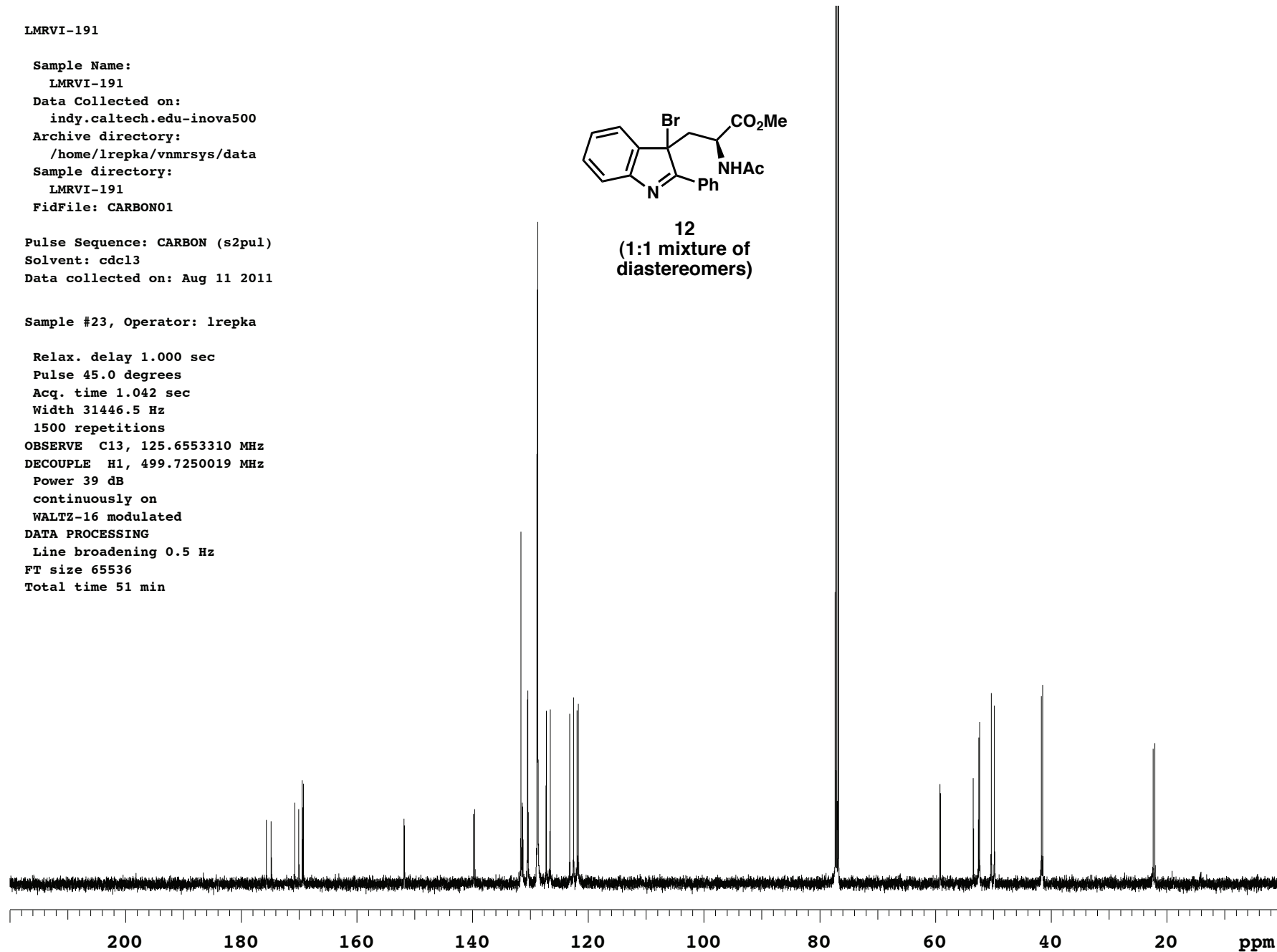
Line broadening 0.5 Hz

FT size 65536

Total time 51 min



12  
(1:1 mixture of  
diastereomers)



LMRVII-117-endodiastereomer

Sample Name:

LMRVII-117-endodiastereomer

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVII-117-endodiastereomer

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jan 25 2012

Sample #28, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

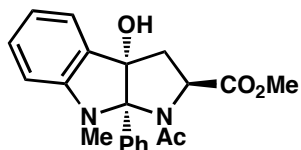
OBSERVE H1, 499.7251682 MHz

DATA PROCESSING

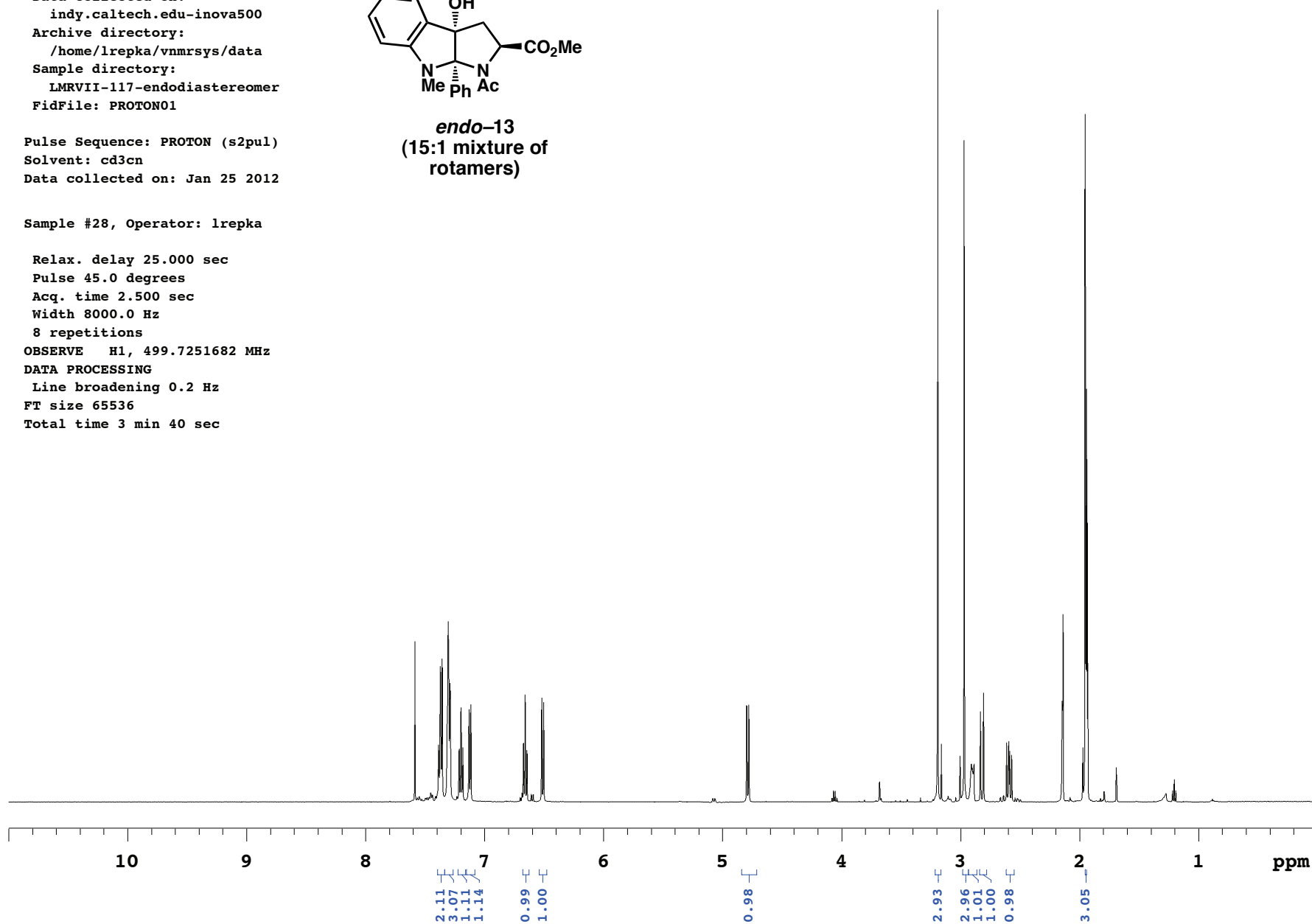
Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



*endo*-13  
(15:1 mixture of rotamers)



LMRVII-117-endodiastereomer

Sample Name:

LMRVII-117-endodiastereomer

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVII-117-endodiastereomer

Fidfile: CARBON02

Pulse Sequence: CARBON (s2pul)

Solvent: cd3cn

Data collected on: Jan 25 2012

Sample #20, Operator: lrepka

Relax. delay 0.100 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1900 repetitions

OBSERVE C13, 125.6558704 MHz

DECOUPLE H1, 499.7276454 MHz

Power 39 dB

continuously on

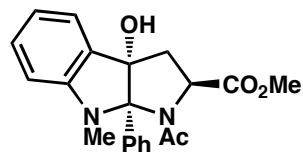
WALTZ-16 modulated

DATA PROCESSING

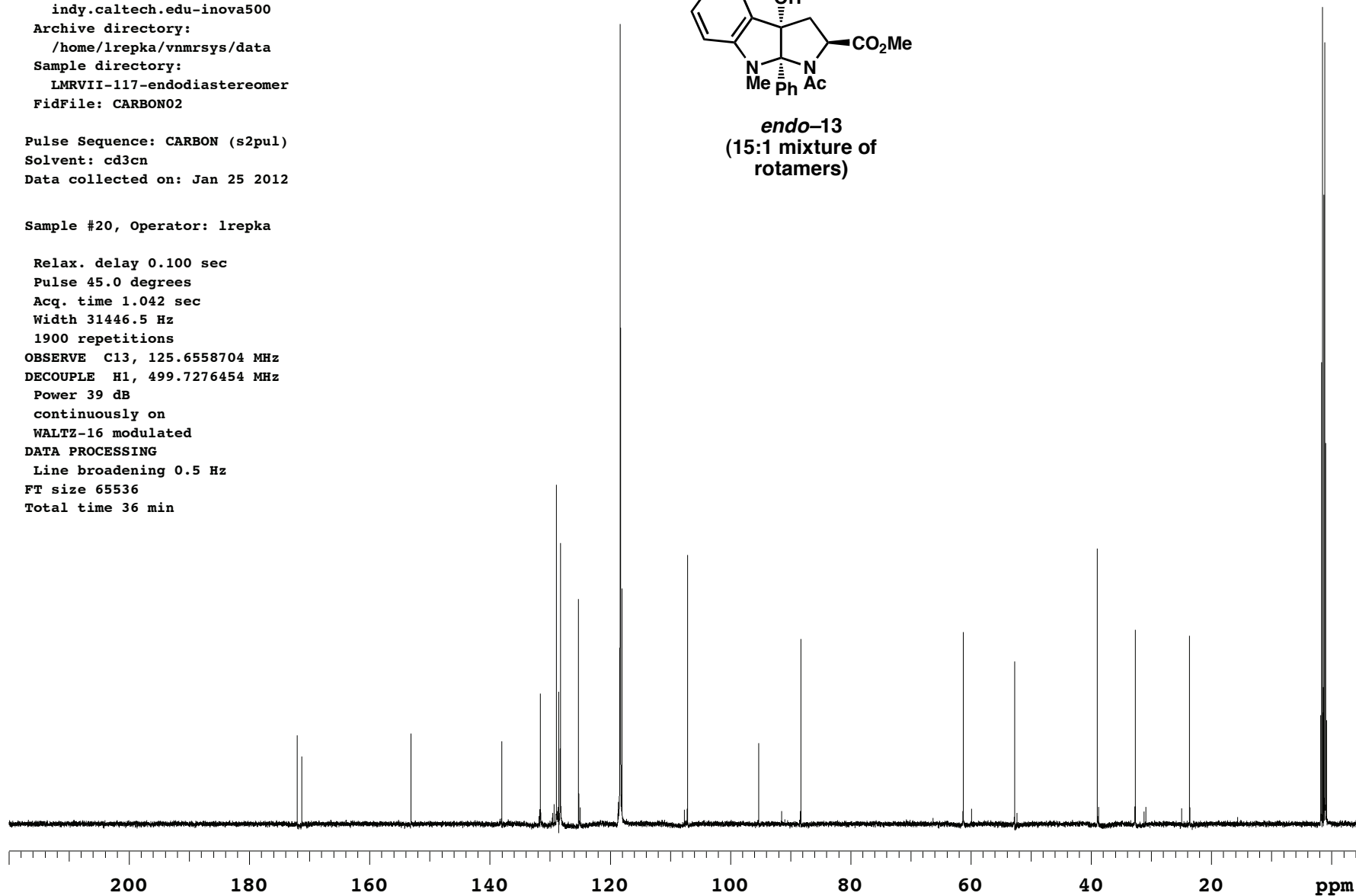
Line broadening 0.5 Hz

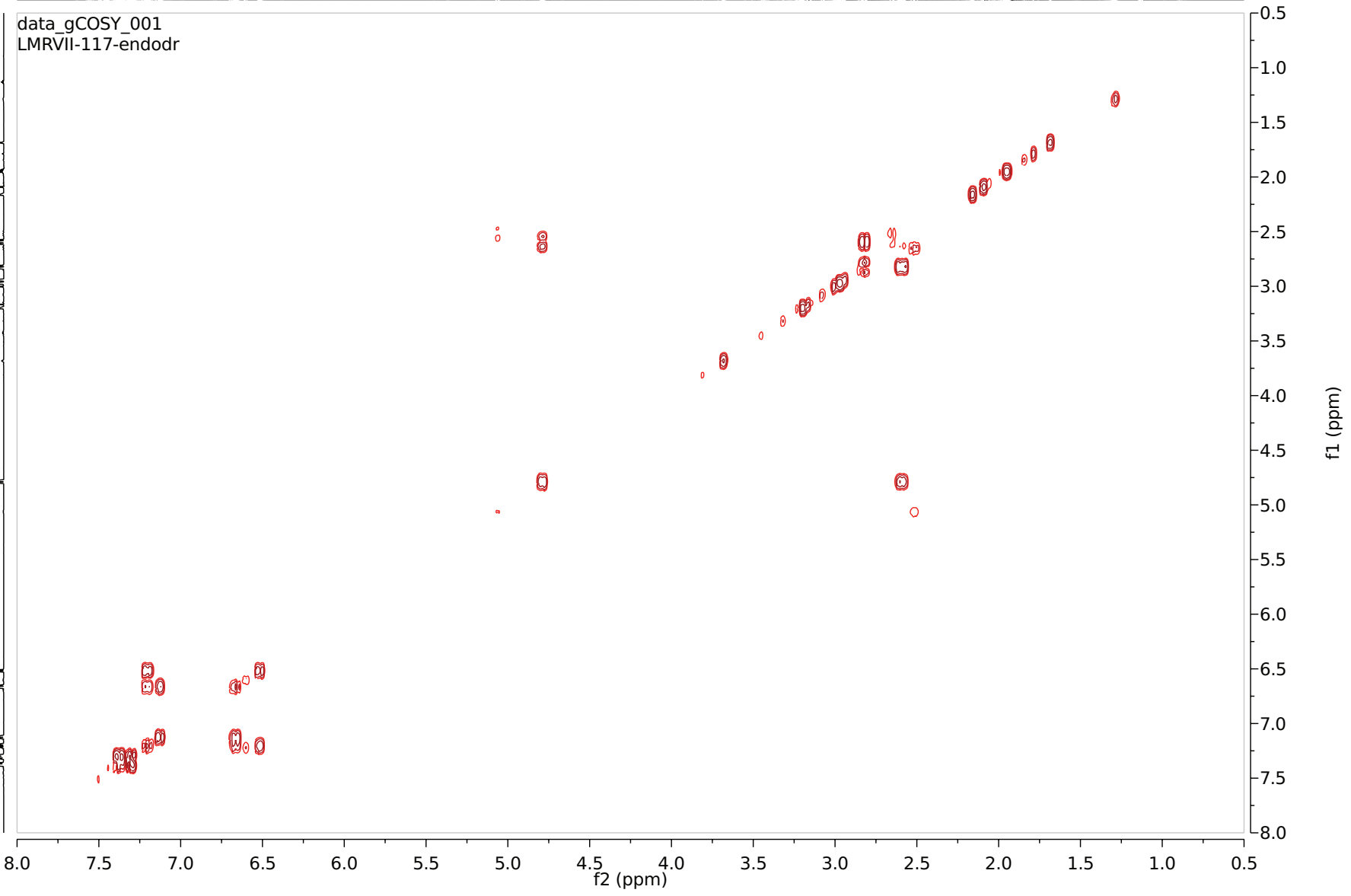
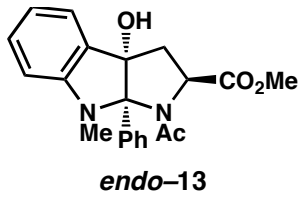
FT size 65536

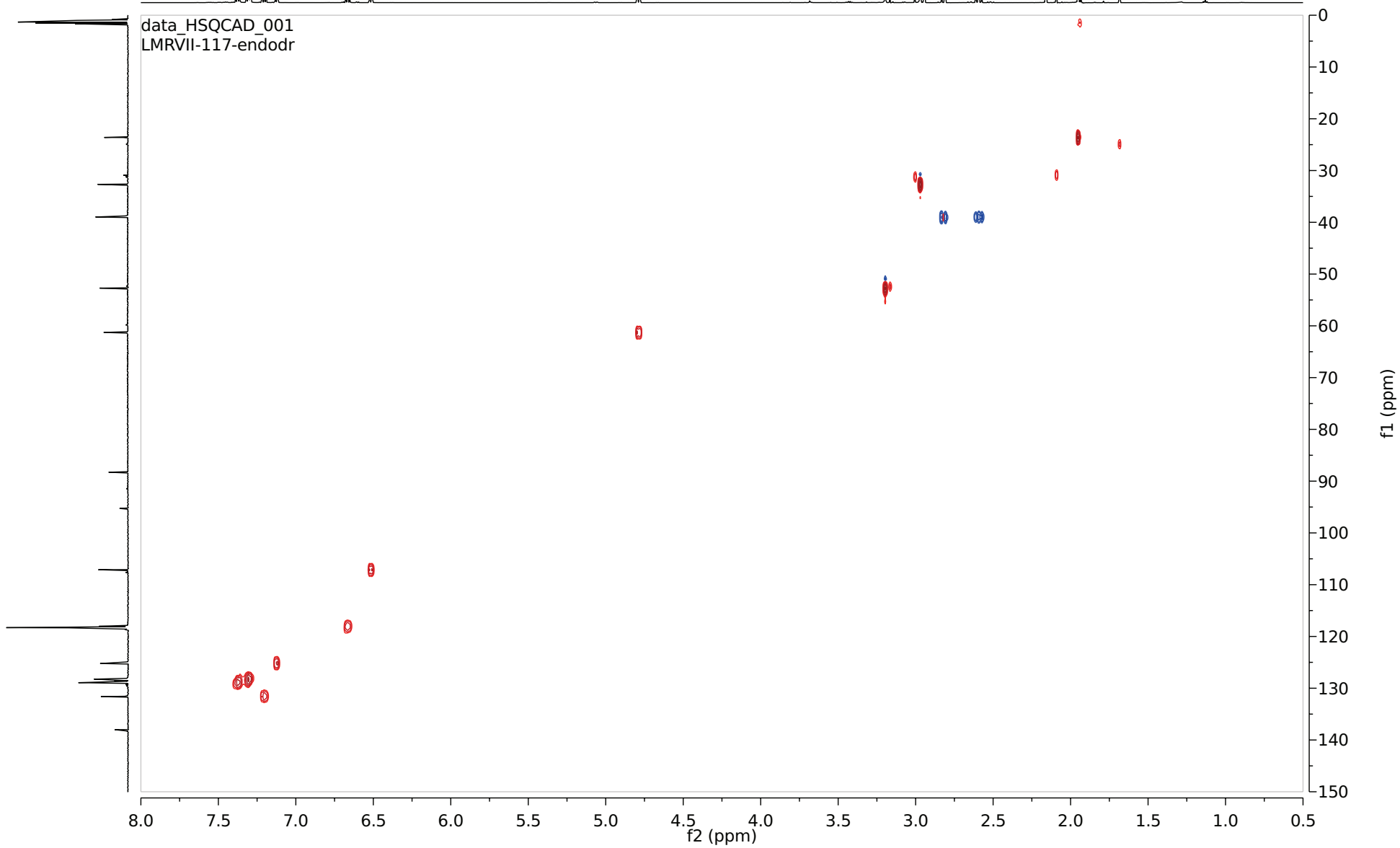
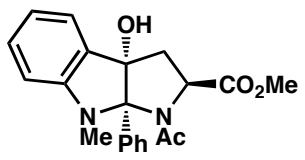
Total time 36 min

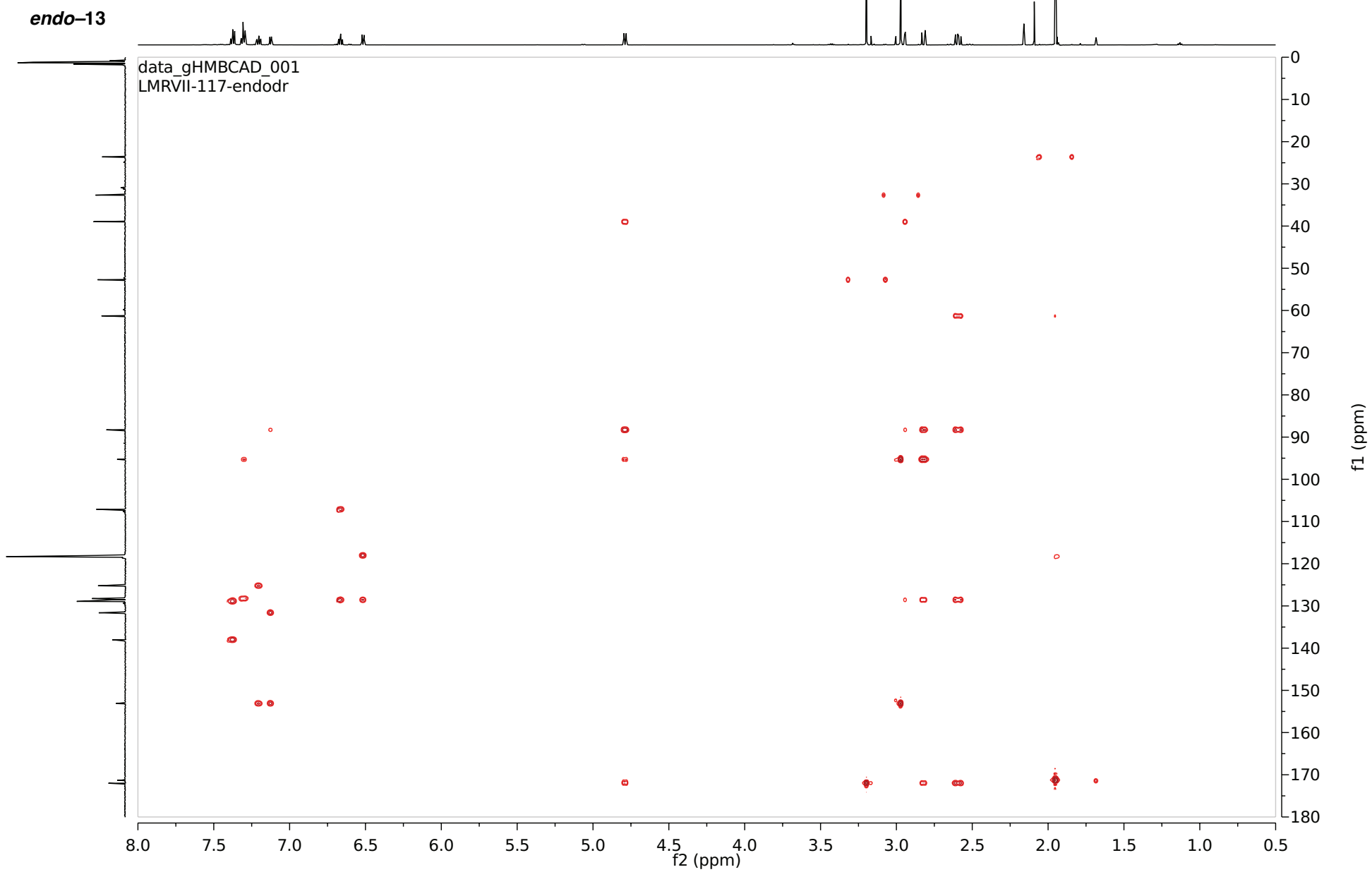
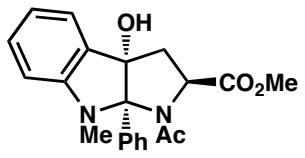


*endo*-13  
(15:1 mixture of rotamers)

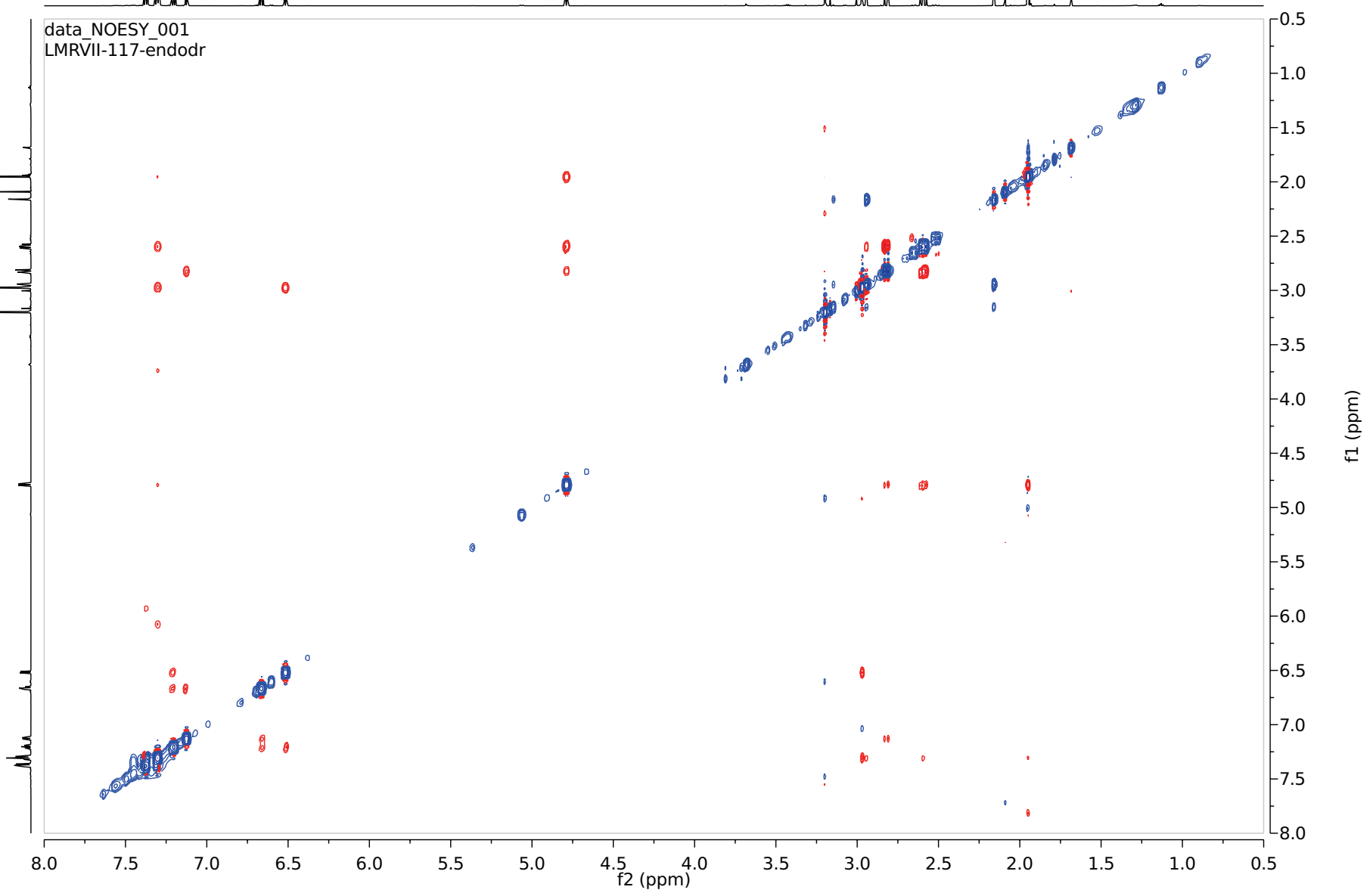
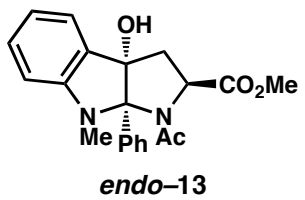












LMRVII-117-exodiastereomer

Sample Name:

LMRVII-117-exodiastereomer

Data Collected on:

indy.caltech.edu-inova500

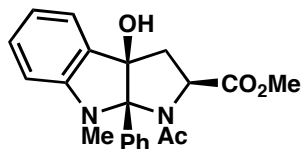
Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVII-117-exodiastereomer

FidFile: PROTON01



*exo*-13  
(1.5:1 mixture of rotamers)

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jan 25 2012

Sample #29, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

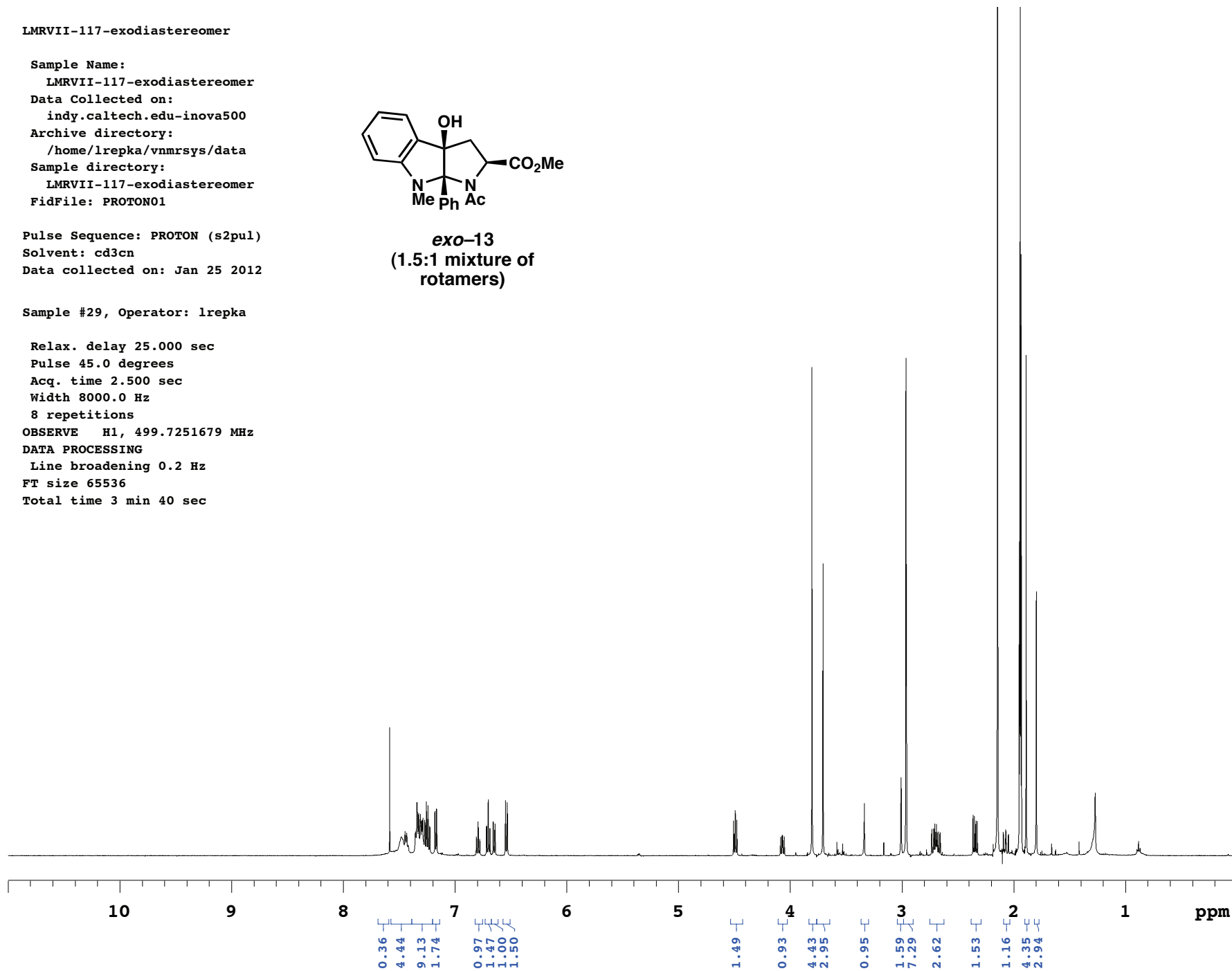
OBSERVE H1, 499.7251679 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 3 min 40 sec



LMRVII-117-exodiastereomer

ErrorLog:

auto\_20120127\_01 loc:20 (night)  
PROTON\_003 Acquisition error:  
CARBON\_001 Acquisition error:

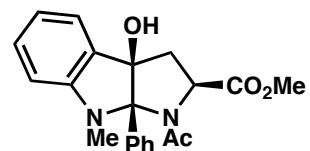
Sample Name:

LMRVII-117-exodiastereomer  
Data Collected on:  
indy.caltech.edu-inova500  
Archive directory:  
/home/lrepka/vnmrsys/data  
Sample directory:  
LMRVII-117-exodiastereomer  
FidFile: CARBON01

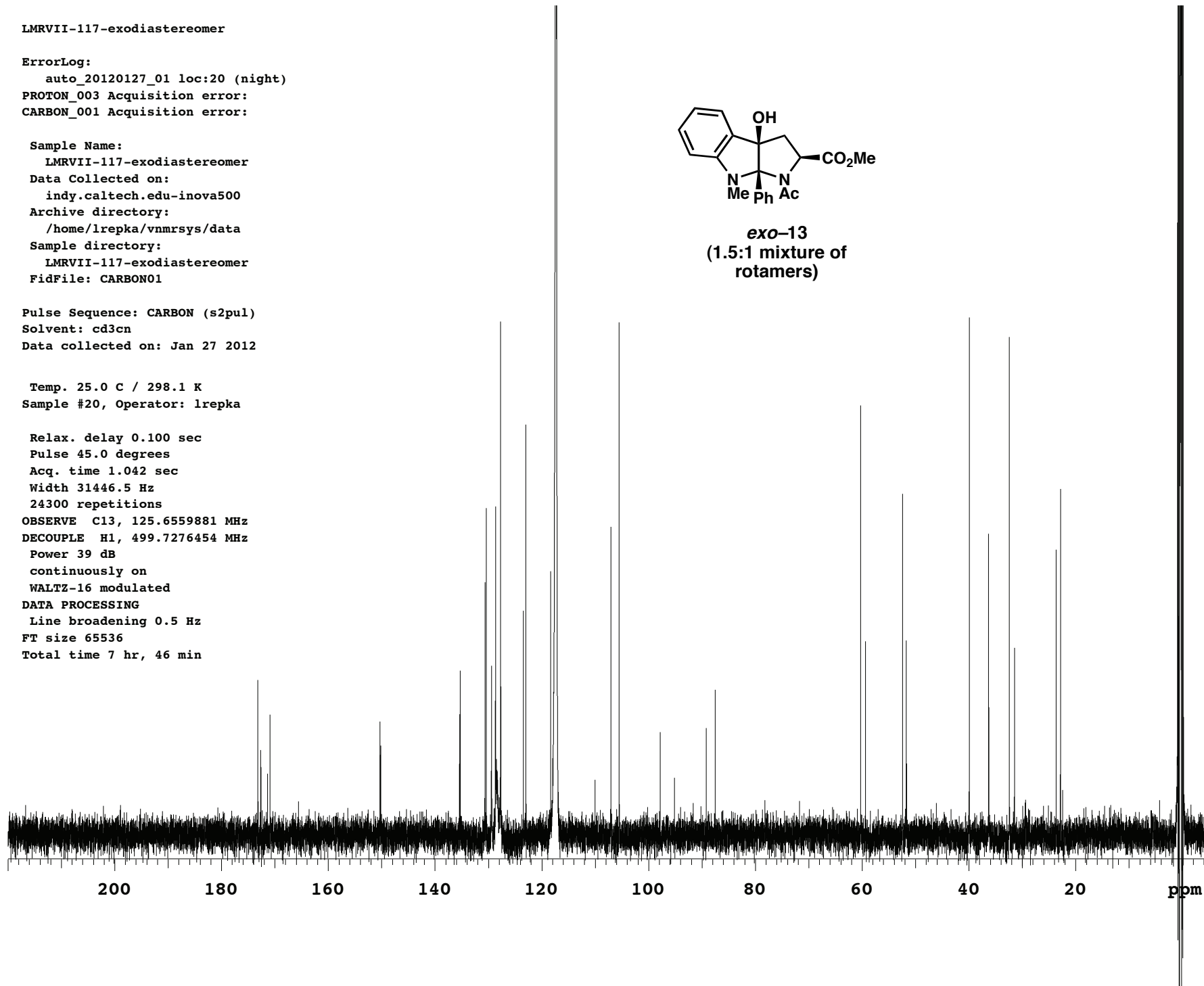
Pulse Sequence: CARBON (s2pul)  
Solvent: cd3cn  
Data collected on: Jan 27 2012

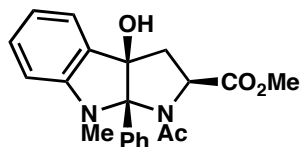
Temp. 25.0 C / 298.1 K  
Sample #20, Operator: lrepka

Relax. delay 0.100 sec  
Pulse 45.0 degrees  
Acq. time 1.042 sec  
Width 31446.5 Hz  
24300 repetitions  
OBSERVE C13, 125.6559881 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 7 hr, 46 min



*exo*-13  
(1.5:1 mixture of rotamers)





*exo-13*

