

APPENDIX 1

Spectra Relevant to Chapter 2:

*Formal (3 + 2) Cycloaddition Approach
to Pyrroloindolines*

JN-1-197-col

Sample Name:

JN-1-197-col

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/jni/vnmrsys/data

Sample directory:

JN-1-197-col

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 19 2010

Temp. 25.0 C / 298.1 K

Sample #22, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4810.0 Hz

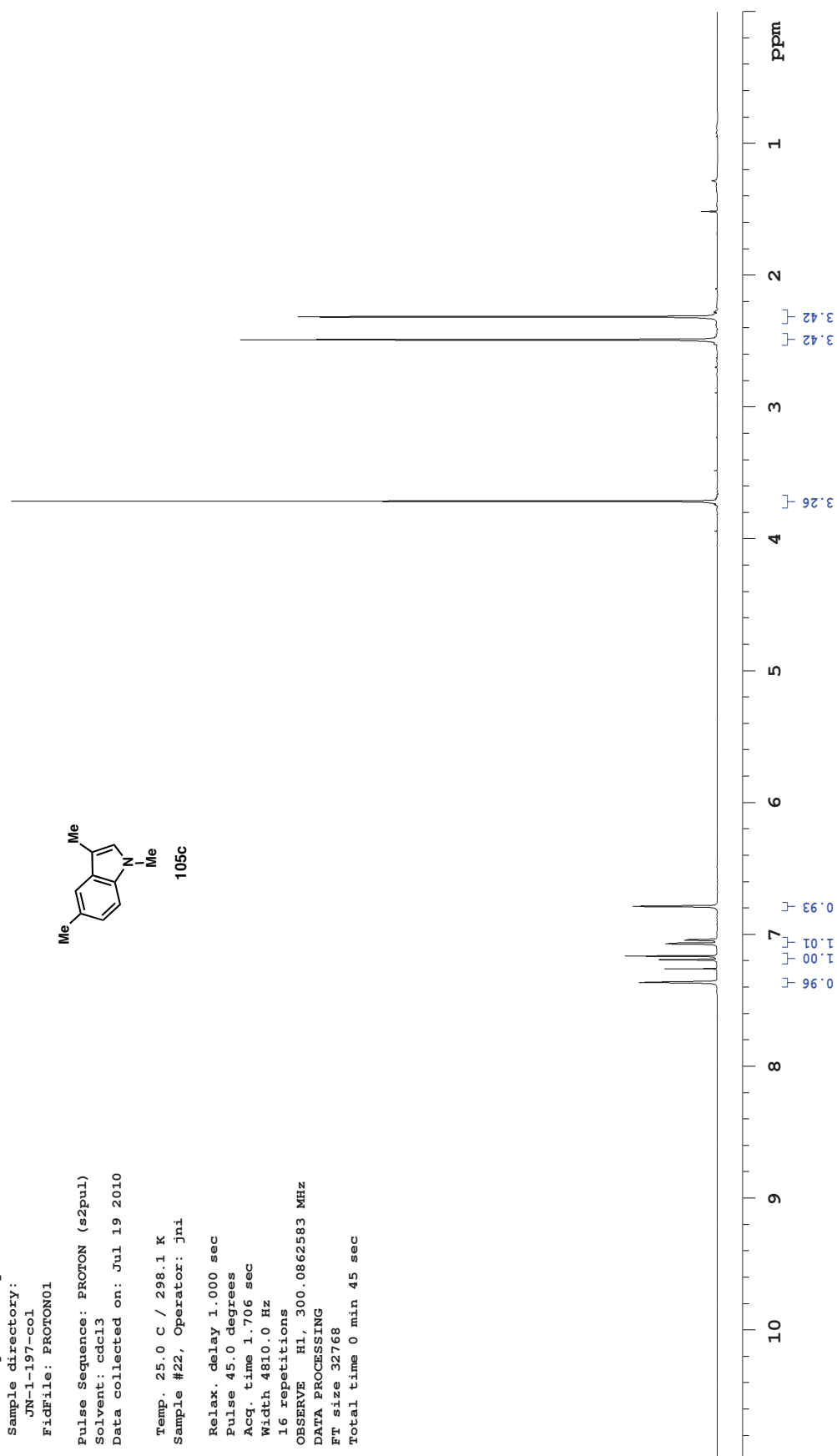
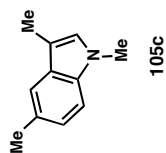
16 repetitions

OBSERVE H1, 300.0862583 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 45 sec



JN-1-197

Sample Name:

JN-1-197

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-197

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 19 2010

Temp. 25.0 C / 298.1 K

Operator: janeni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

3200 repetitions

OBSERVE C13, 125.6602406 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

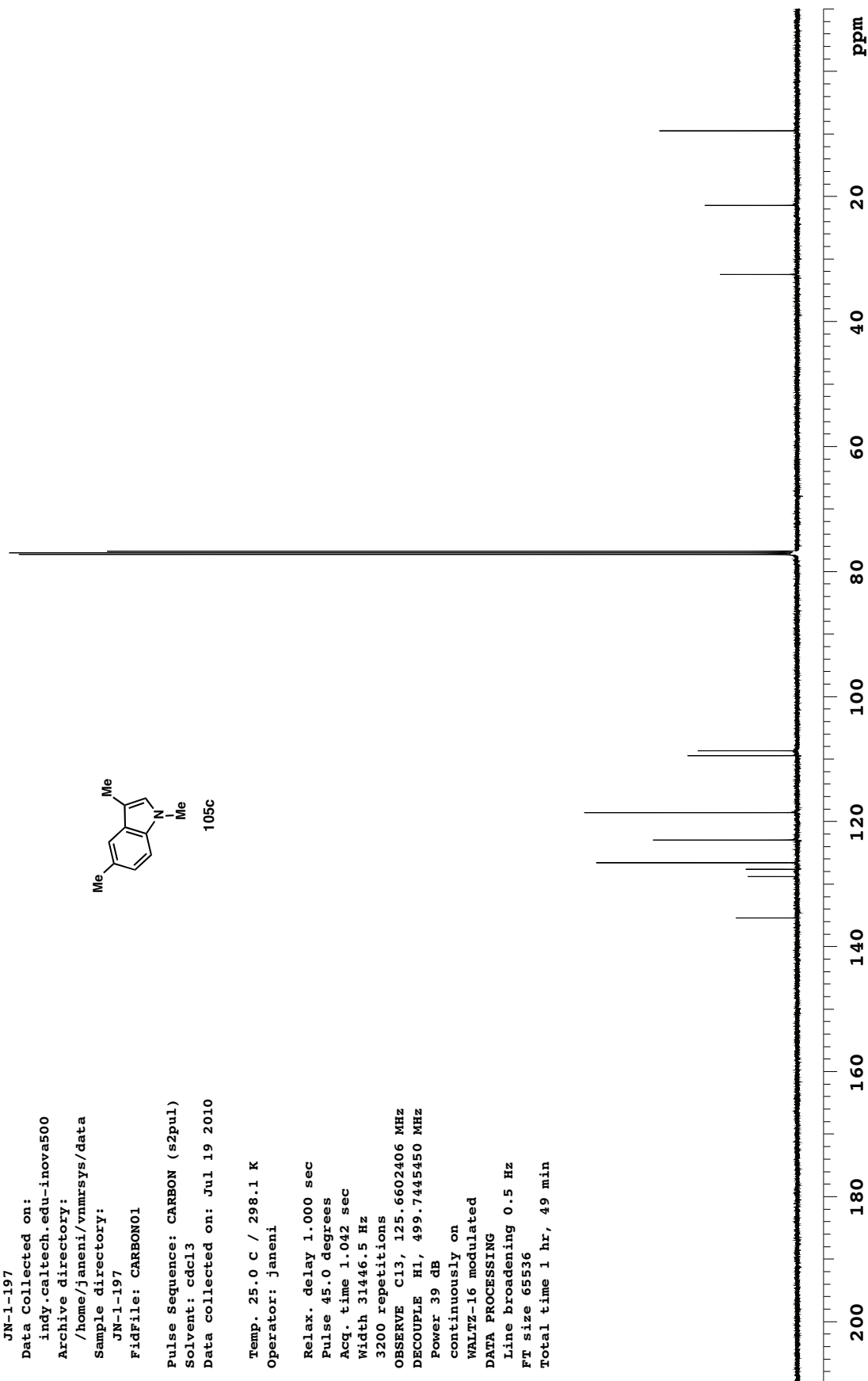
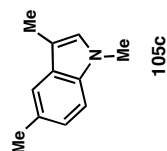
WALTZ-16 modulated

DATA PROCESSING

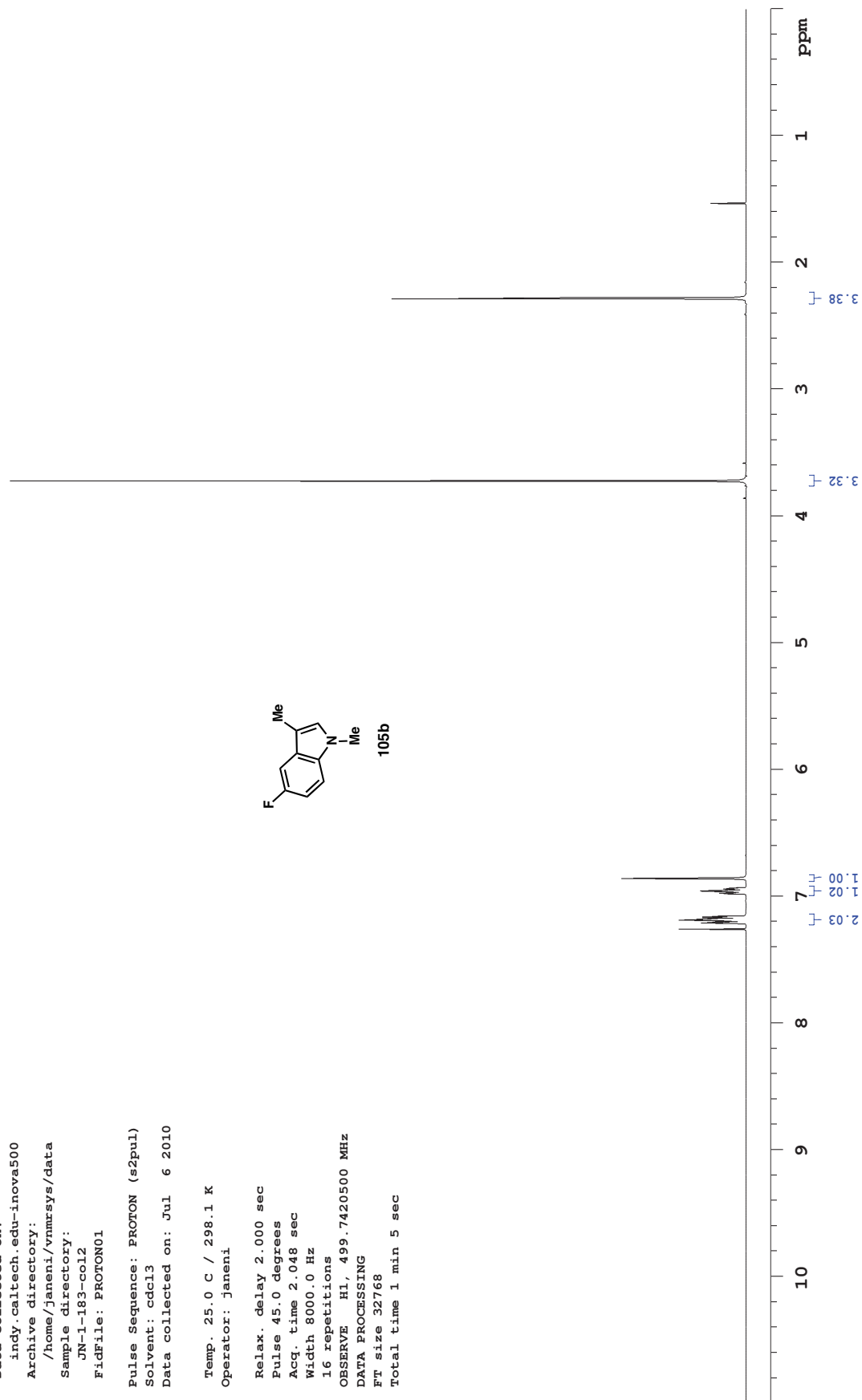
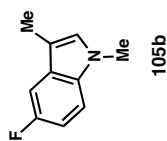
Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 49 min



Total time 1 min 5 sec



JN-1-183-col2

Sample Name:

JN-1-183-col2

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrSYS/data

Sample directory:

JN-1-183-col2

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 6 2010

Temp. 25.0 C / 298.1 K

Operator: janeni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

3200 repetitions

OBSERVE C13, 125.6602397 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

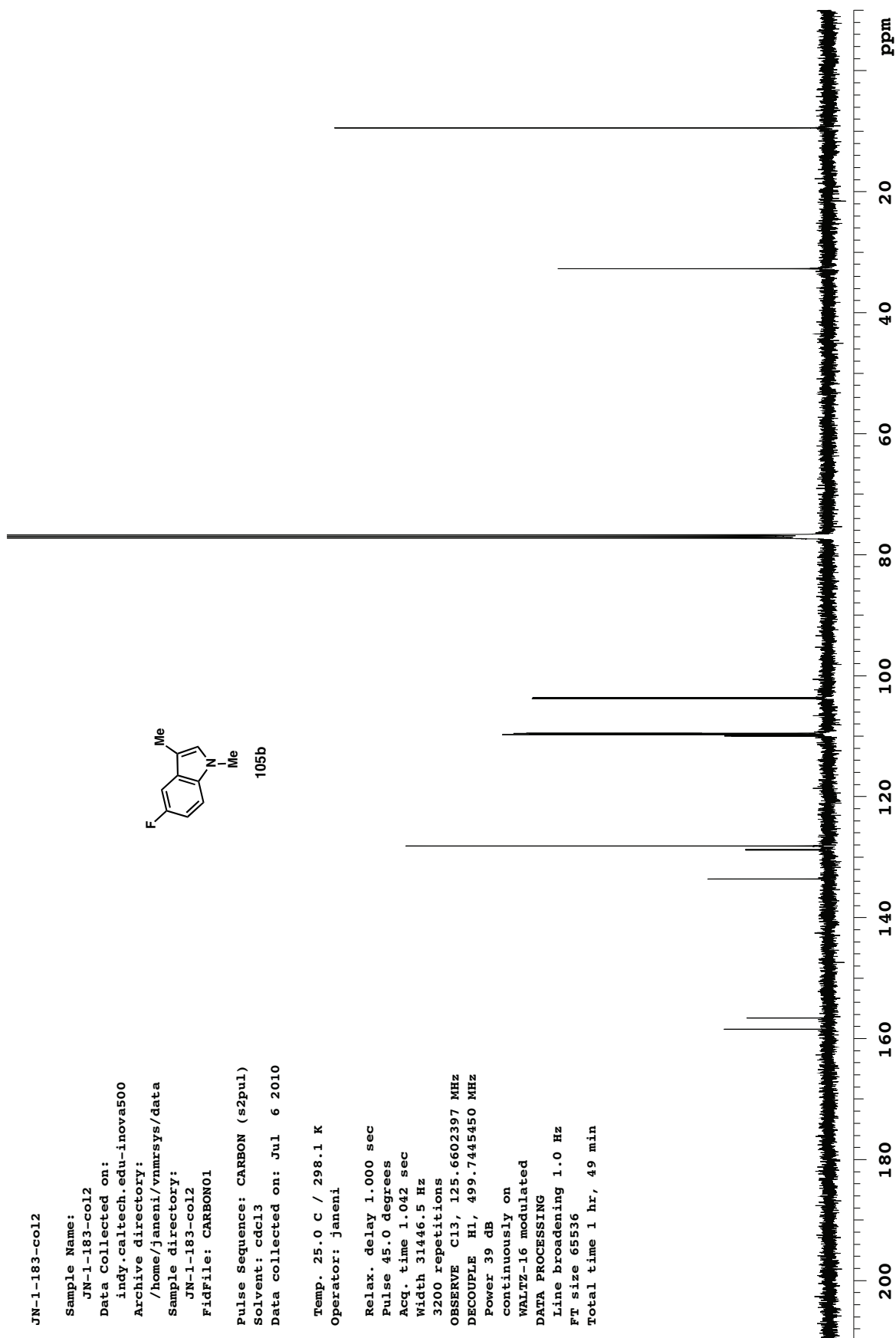
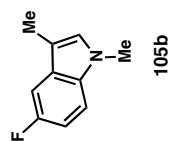
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1 hr, 49 min



JN-1-181-col

Sample Name:

JN-1-181-col

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-181-col

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 27 2010

Temp. 25.0 C / 298.1 K

Operator: janeni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8000.0 Hz

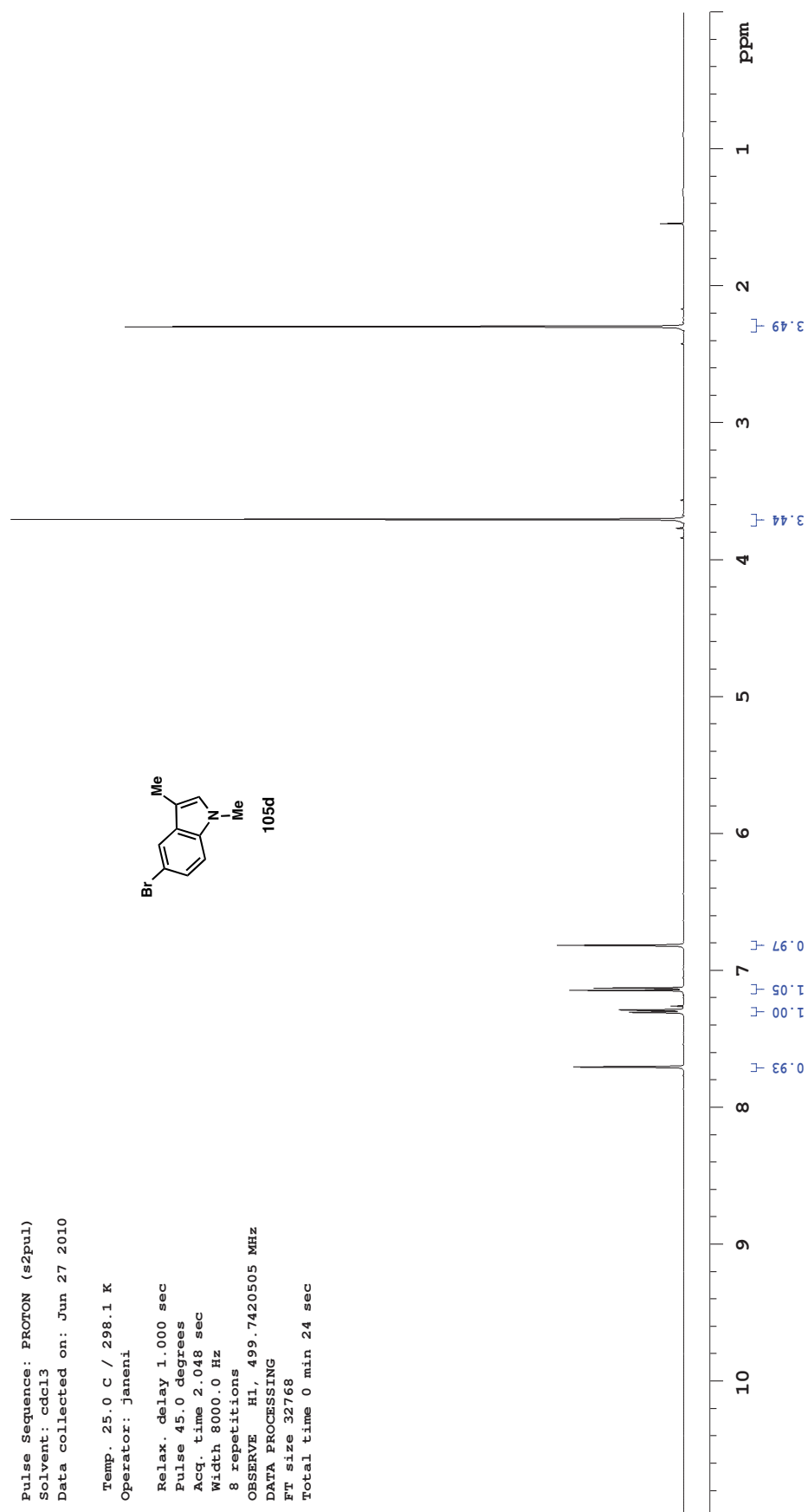
8 repetitions

OBSERVE H1, 499.7420505 MHz

DATA PROCESSING

Ft size 32768

Total time 0 min 24 sec



JN-1-181-col

Sample Name:

JN-1-181-col

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-181-col

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 27 2010

Temp. 25.0 C / 298.1 K

Operator: janeni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

3200 repetitions

OBSERVE C13, 125.6602458 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

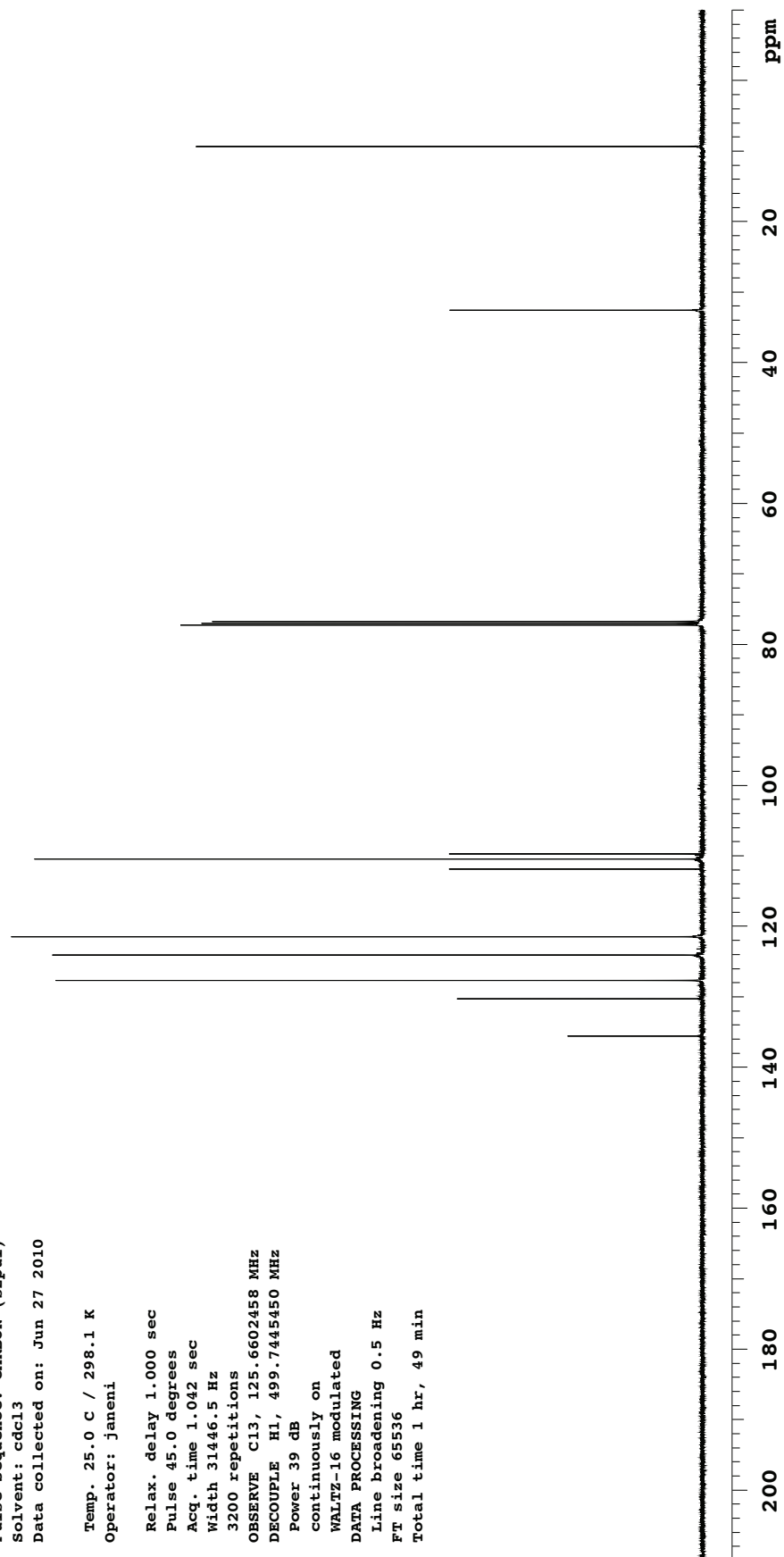
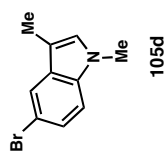
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 49 min



JN-1-199-col

Sample Name:

JN-1-199-col

Data Collected on:

sienna.caltech.edu-vnmrs400

Archive directory:

/home/jni/vnmrsys/data

Sample directory:

JN-1-199-col

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 24 2010

Temp. 26.0 C / 299.1 K

Sample #11, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

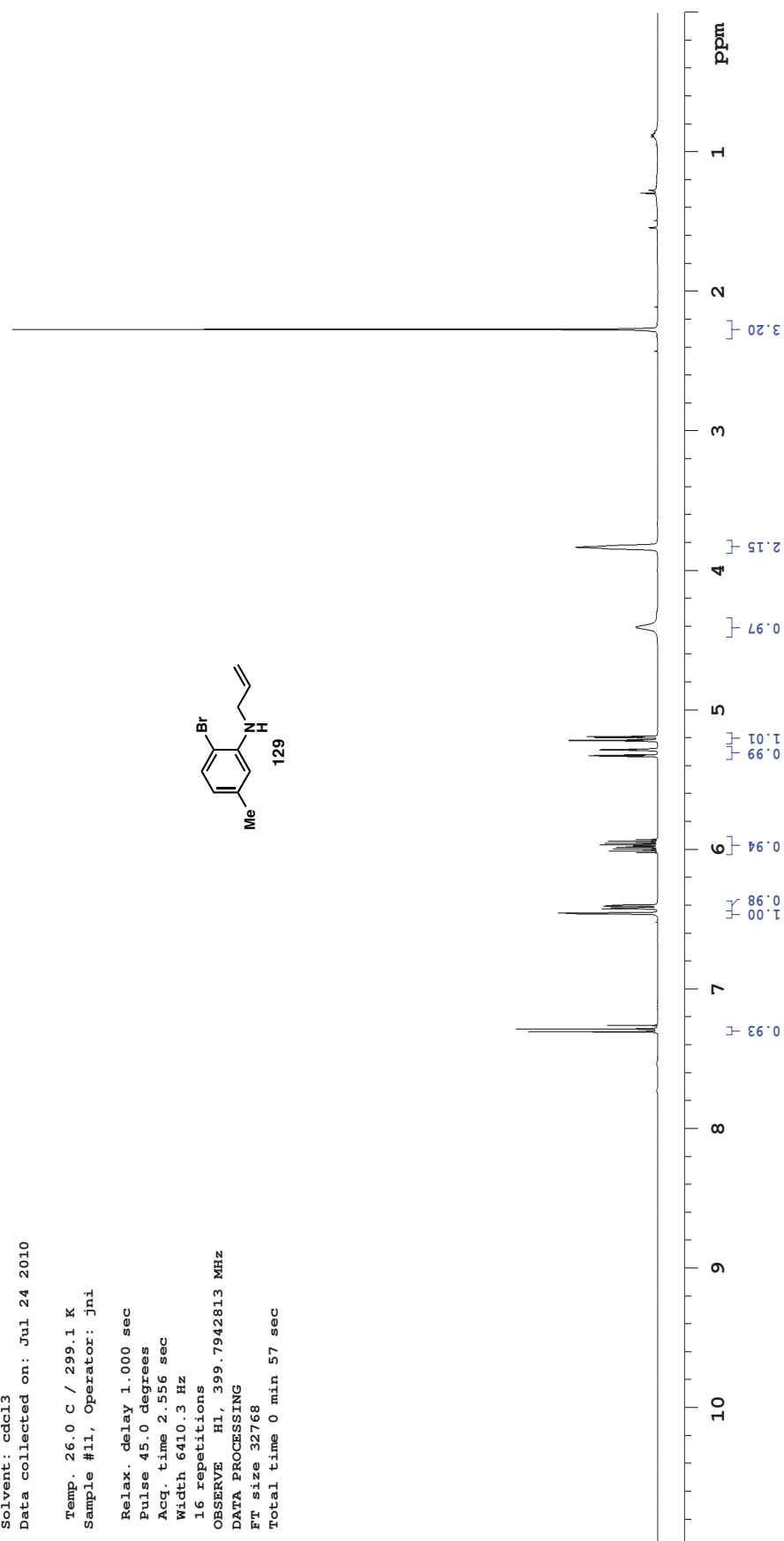
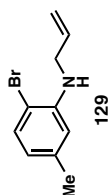
16 repetitions

OBSERVE H1, 399.7942813 MHz

DATA PROCESSING

Ft size 32768

Total time 0 min 57 sec



JN-1-199-col

Sample Name:

JN-1-199-col

Data Collected on:

siena.caltech.edu-vmrs400

Archive directory:

/home/jni/vmrsys/data

Sample directory:

JN-1-199-col

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 24 2010

Temp. 26.0 C / 299.1 K

Sample #11, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

2000 repetitions

OBSERVE C13, 100.5283540 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

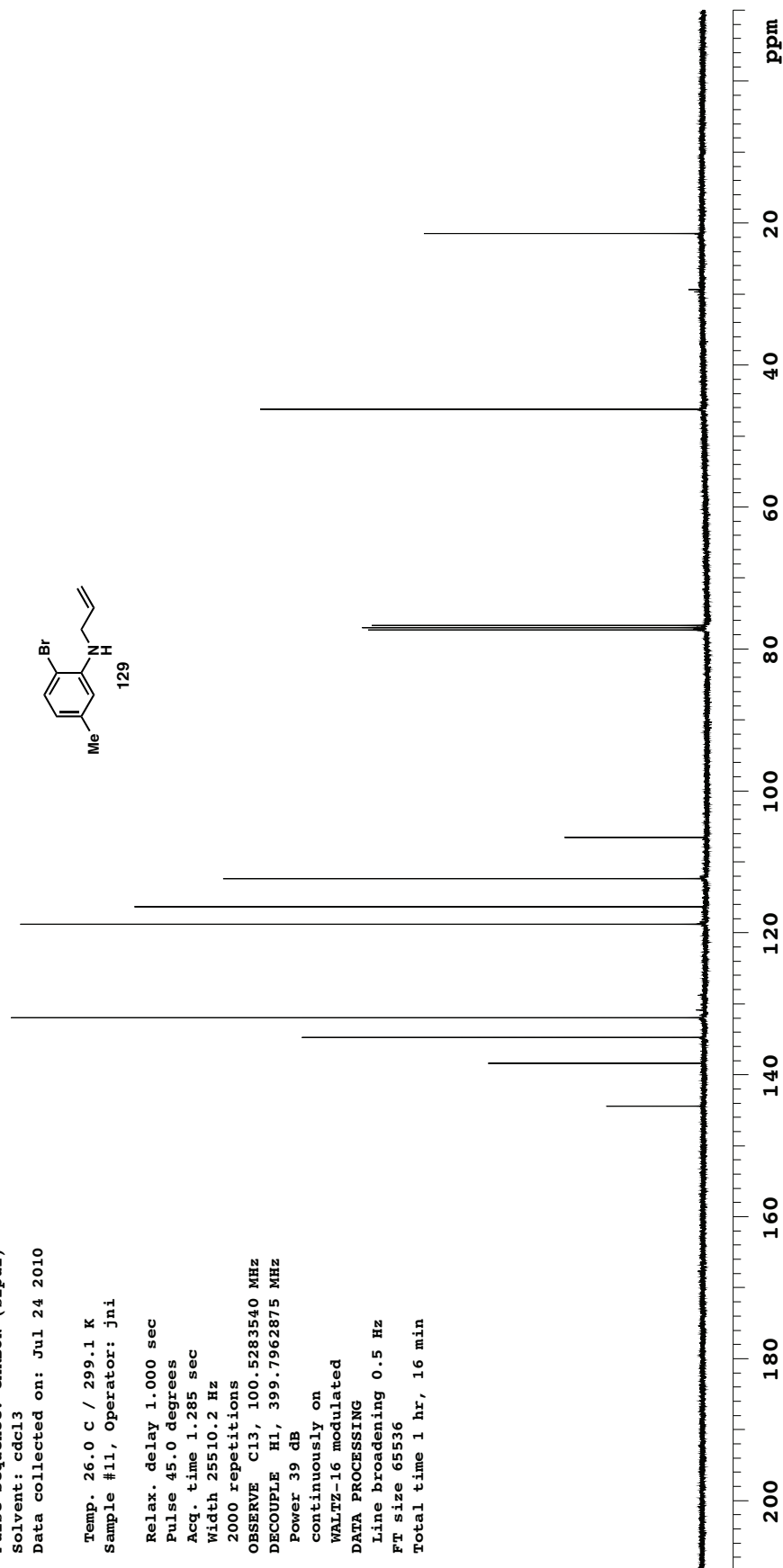
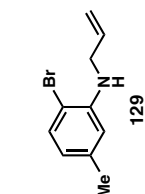
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

Ft size 65536

Total time 1 hr, 16 min



JN-1-201-col

Sample Name:

JN-1-201-col

Data Collected on:

sienna.caltech.edu-vnmrs400

Archive directory:

/home/jni/vnmrsys/data

Sample directory:

JN-1-201-col

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdd13

Data collected on: Jul 24 2010

Temp. 26.0 C / 299.1 K

Sample #12, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

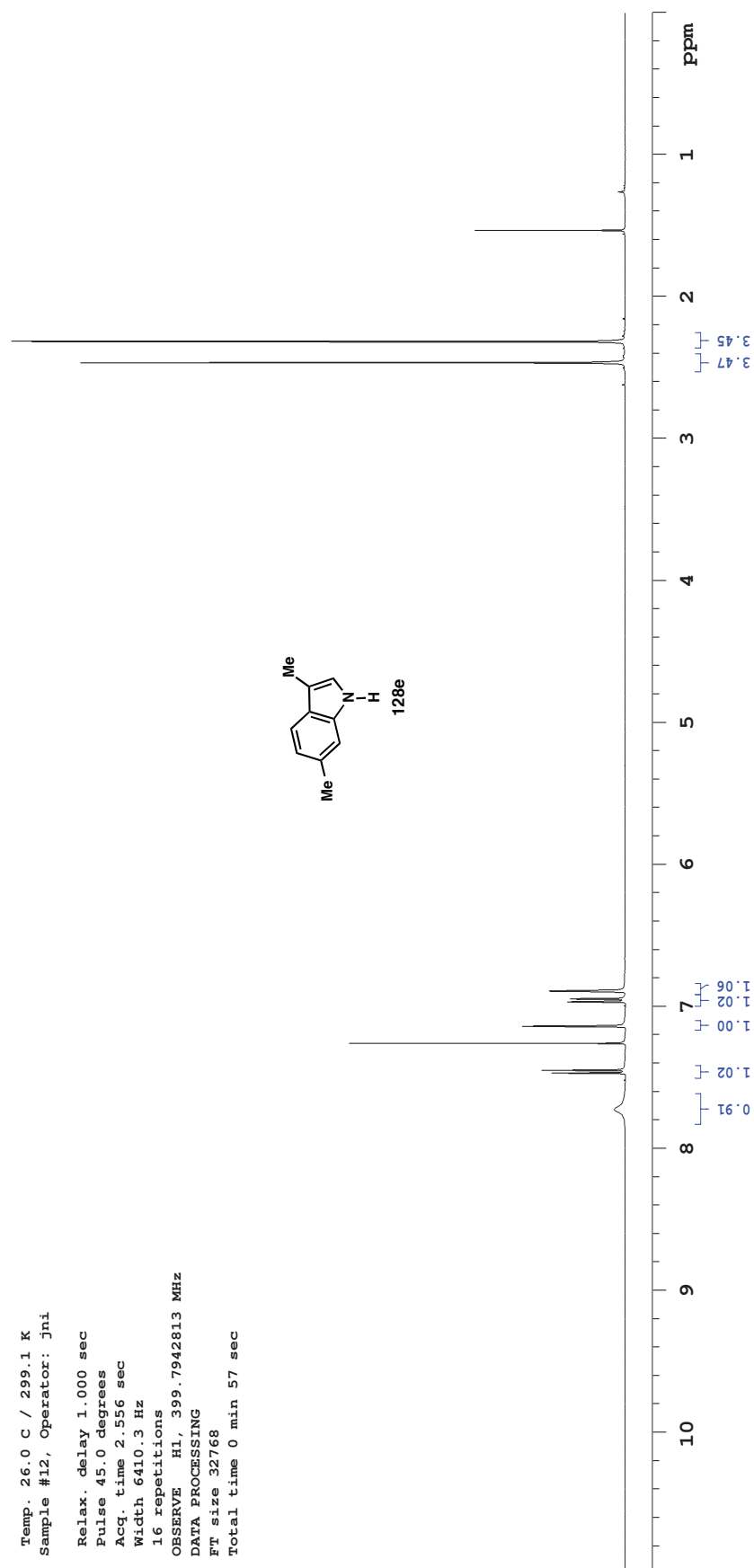
16 repetitions

OBSERVE H1, 399.7942813 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 57 sec



JN-1-201-col

Sample Name:

JN-1-201-col
Data Collected on:
siena.caltech.edu-vmrs400
Archive directory:
/home/jni/vmrsys/data
Sample directory:
JN-1-201-col
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3
Data collected on: Jul 24 2010

Temp. 26.0 C / 299.1 K

Sample #12, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

4000 repetitions

OBSERVE C13, 100.5283515 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

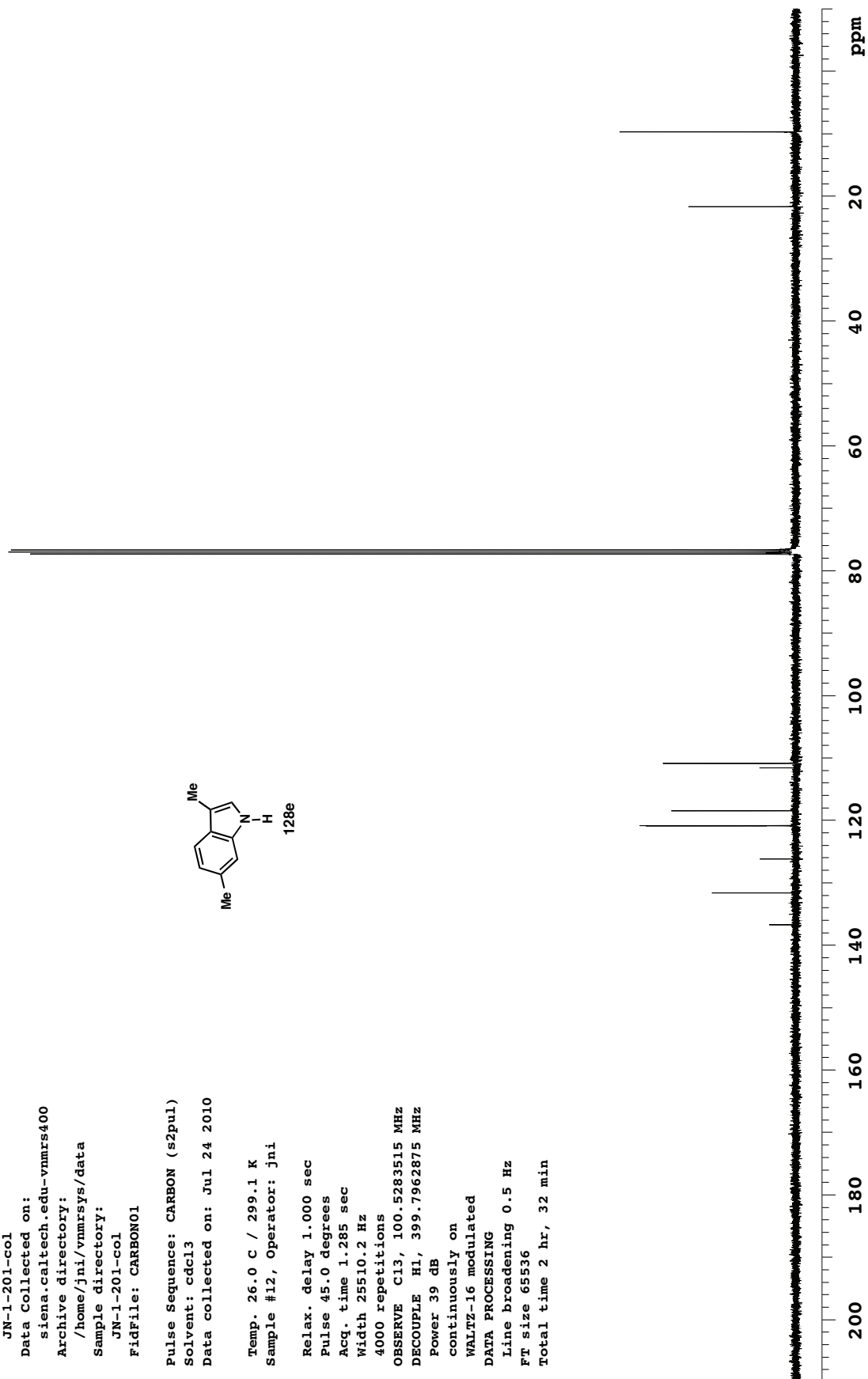
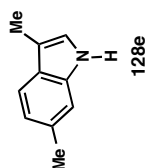
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 2 hr, 32 min



JN-1-203-col

Sample Name:

JN-1-203-col

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/jni/vnmrsys/data

Sample directory:

JN-1-203-col

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 19 2010

Temp. 25.0 C / 298.1 K

Sample #21, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4810.0 Hz

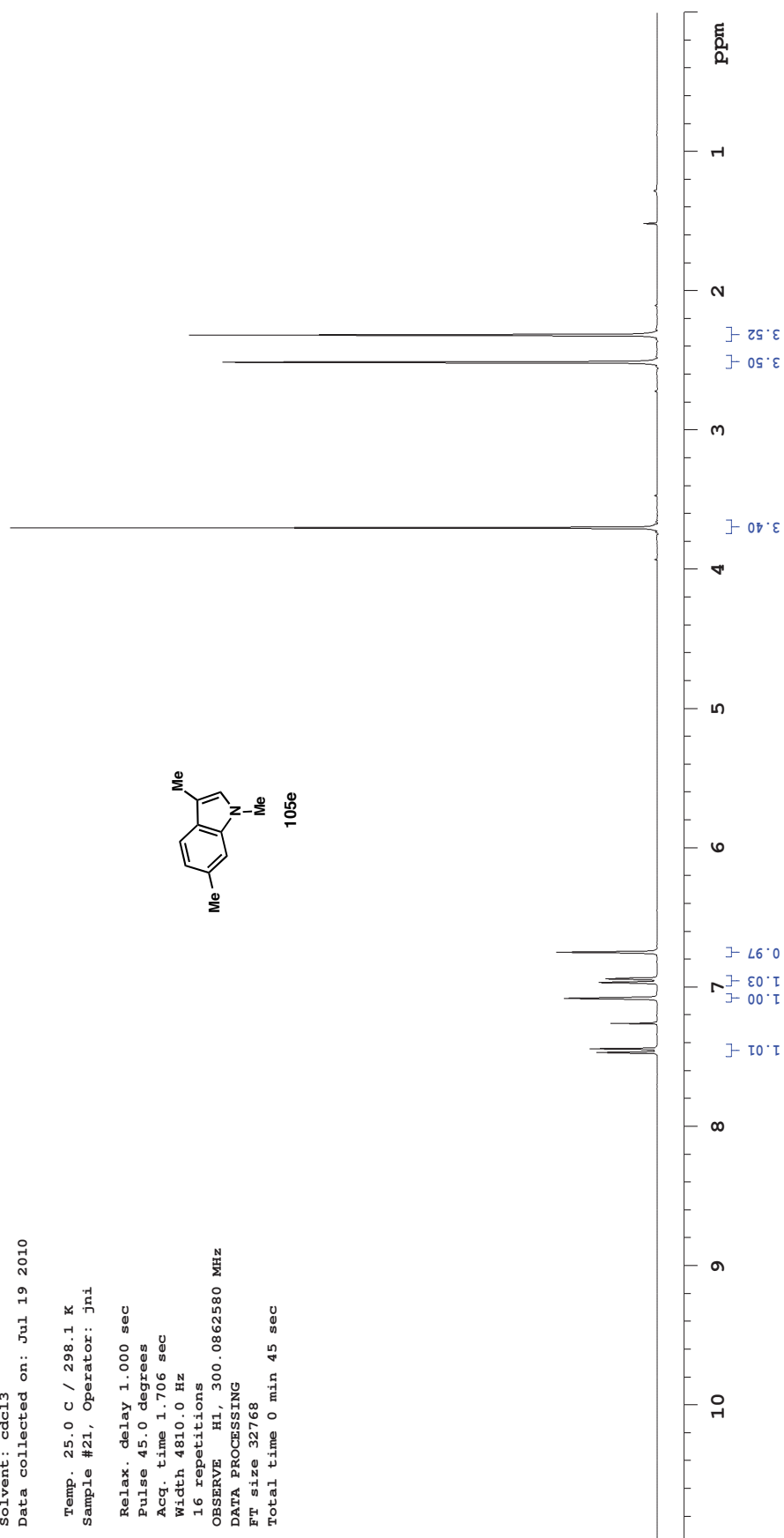
16 repetitions

OBSERVE H1, 300.0862580 MHz

DATA PROCESSING

Ft size 32768

Total time 0 min 45 sec



JN-1-203

Sample Name:

JN-1-203

Data Collected on:

siena.caltech.edu-vmrs400

Archive directory:

/home/jni/vmrsys/data

Sample directory:

JN-1-203

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 19 2010

Temp. 25.0 C / 298.1 K

Sample #3, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

5000 repetitions

OBSERVE C13, 100.5283529 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

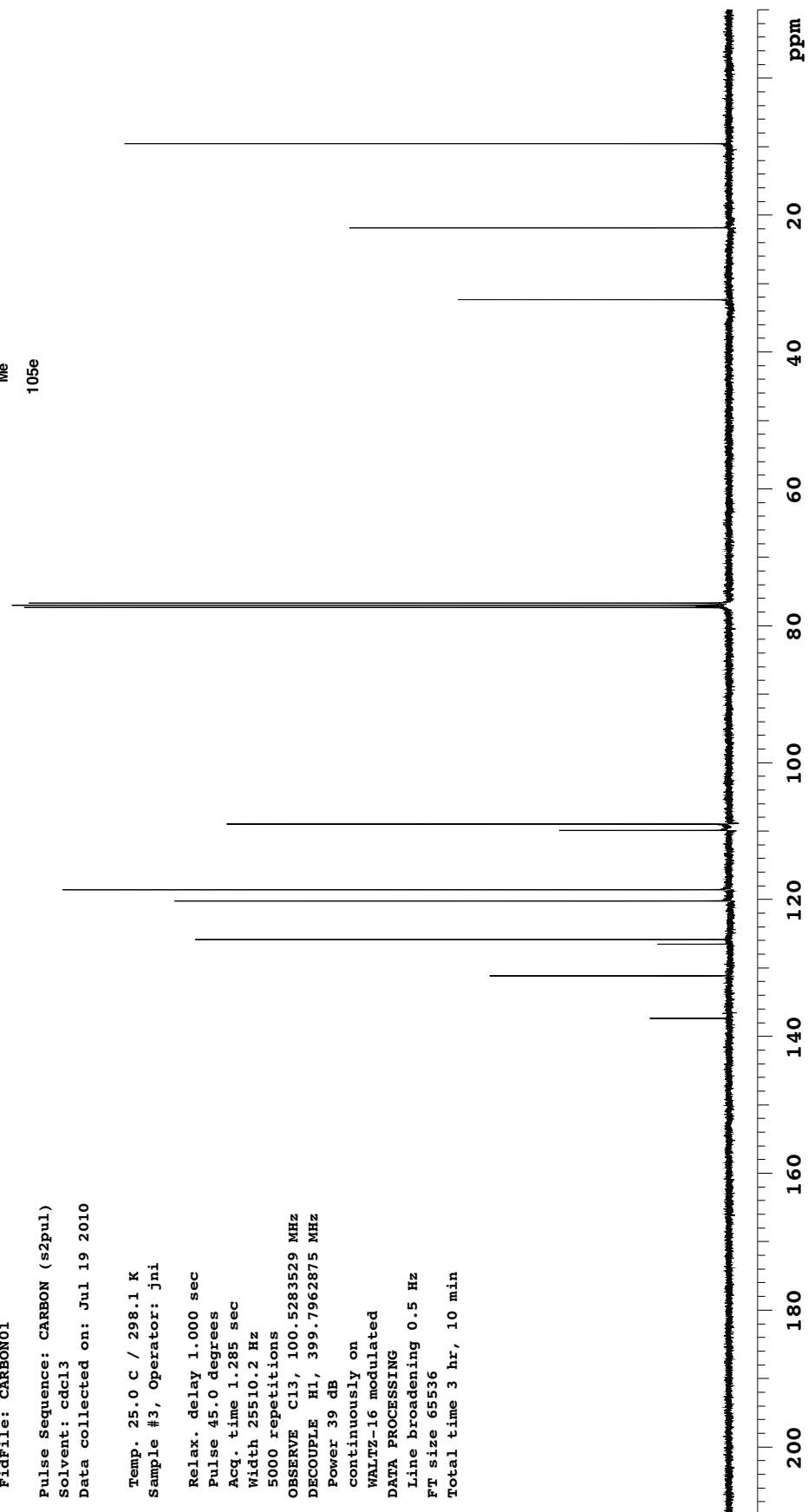
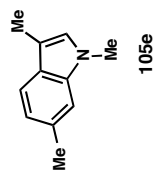
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 3 hr, 10 min



LMRIV-N-me-TBStryptophol

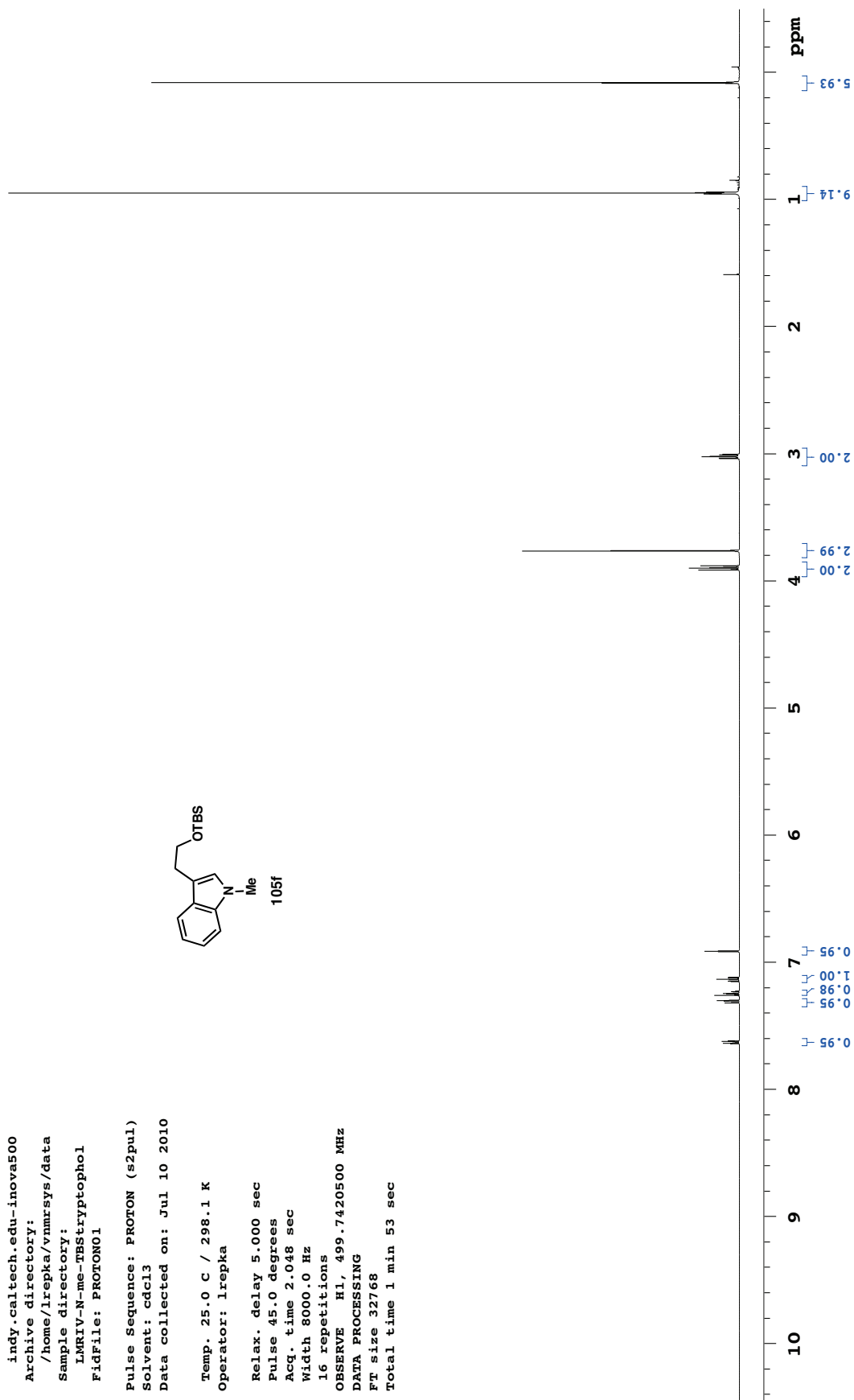
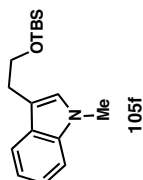
Sample Name:
LMRIV-N-me-TBStryptophol
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRIV-N-me-TBStryptophol
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 10 2010

Temp. 25.0 C / 298.1 K
Operator: lrepka

Relax. delay 5.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
16 repetitions

OBSERVE H1, 499.7420500 MHz
DATA PROCESSING
FT size 32768
Total time 1 min 53 sec



LMRIV-N-me-TBstryptophol2

Sample Name:

LMRIV-N-me-TBstryptophol2

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-N-me-TBstryptophol2

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 10 2010

Temp. 25.0 C / 298.1 K

Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

3500 repetitions

OBSERVE C13, 125.6602422 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

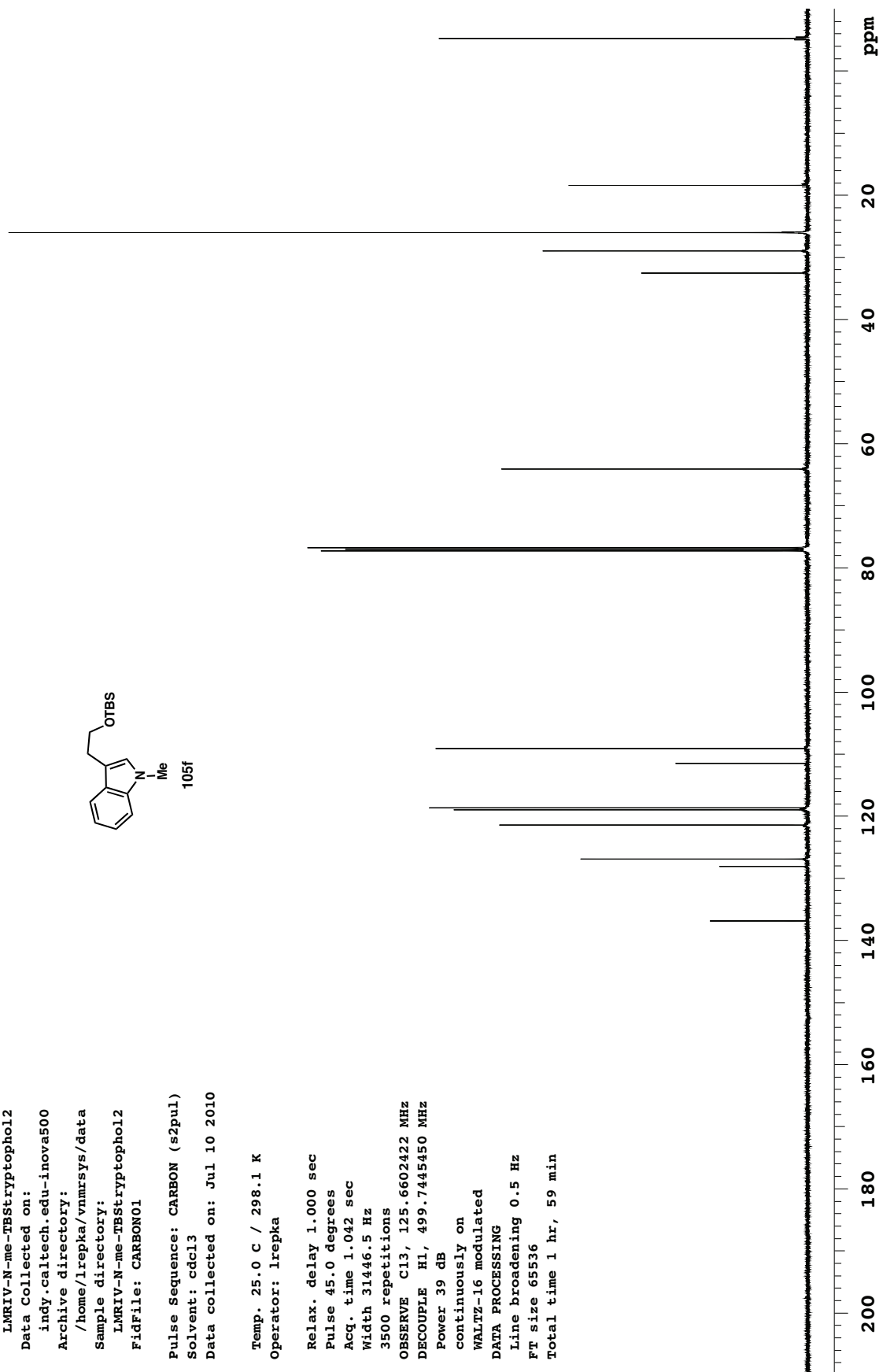
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

Ft size 65536

Total time 1 hr, 59 min



LMRIV-057-fxns2-11

Sample Name:

LMRIV-057-fxns2-11

Archive directory:

Sample directory:

FidFile: LMRIV-057-fxns16-20

Pulse Sequence: Proton (s2pul)

Solvent: cdcl3

Data collected on: Mar 1 2010

Operator: lrepka

VNMRS-400 "erice.caltech.edu"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.998 sec

Width 4796.2 Hz

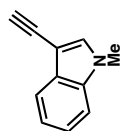
8 repetitions

OBSERVE H1, 299.8165711 MHz

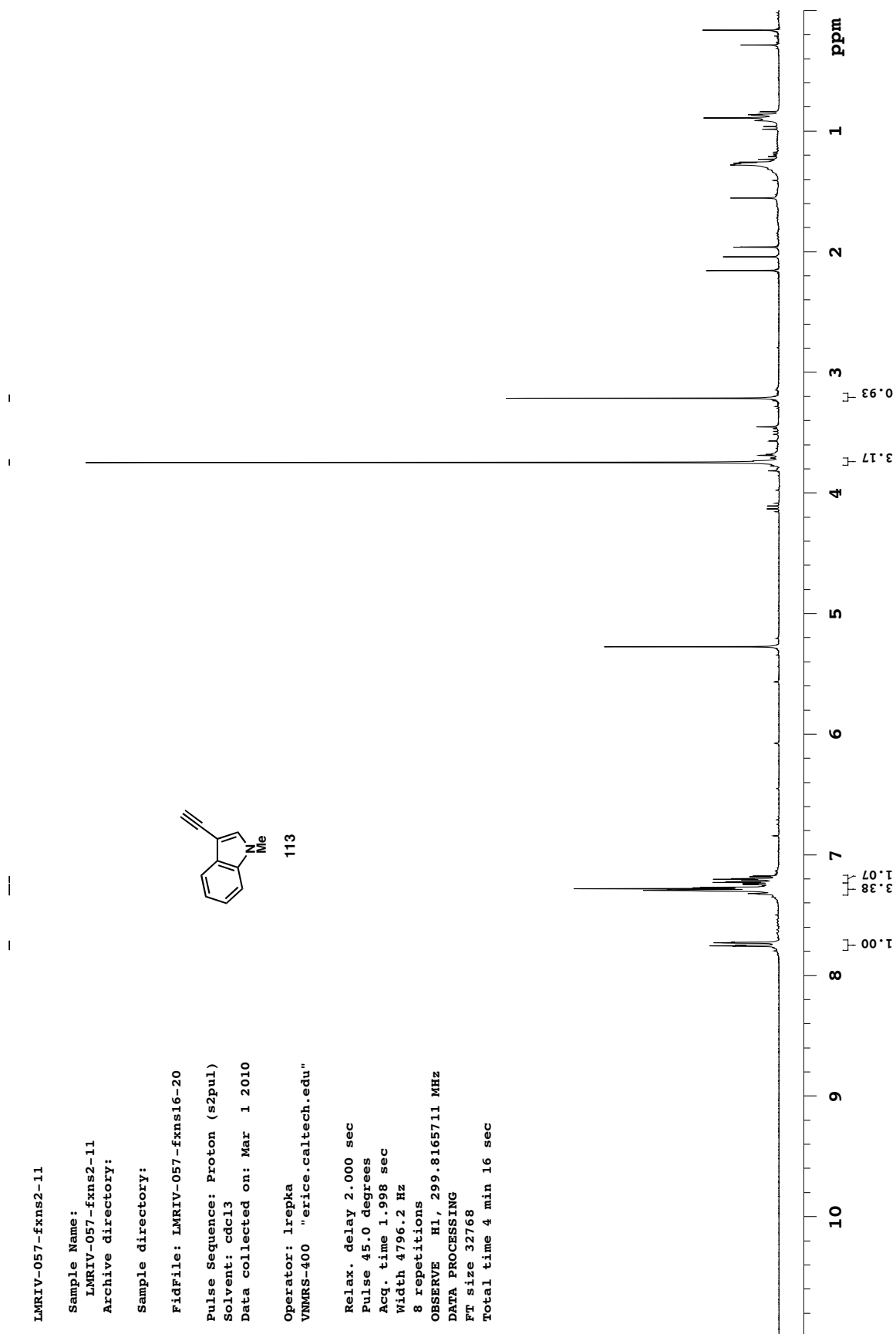
DATA PROCESSING

FT size 32768

Total time 4 min 16 sec



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PR4_F1

Sample Name:

PR4_F1

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/jchal/vnmrsys/data

Sample directory:

PR4_F1

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 14 2011

Sample #2, Operator: jchal

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4798.5 Hz

16 repetitions

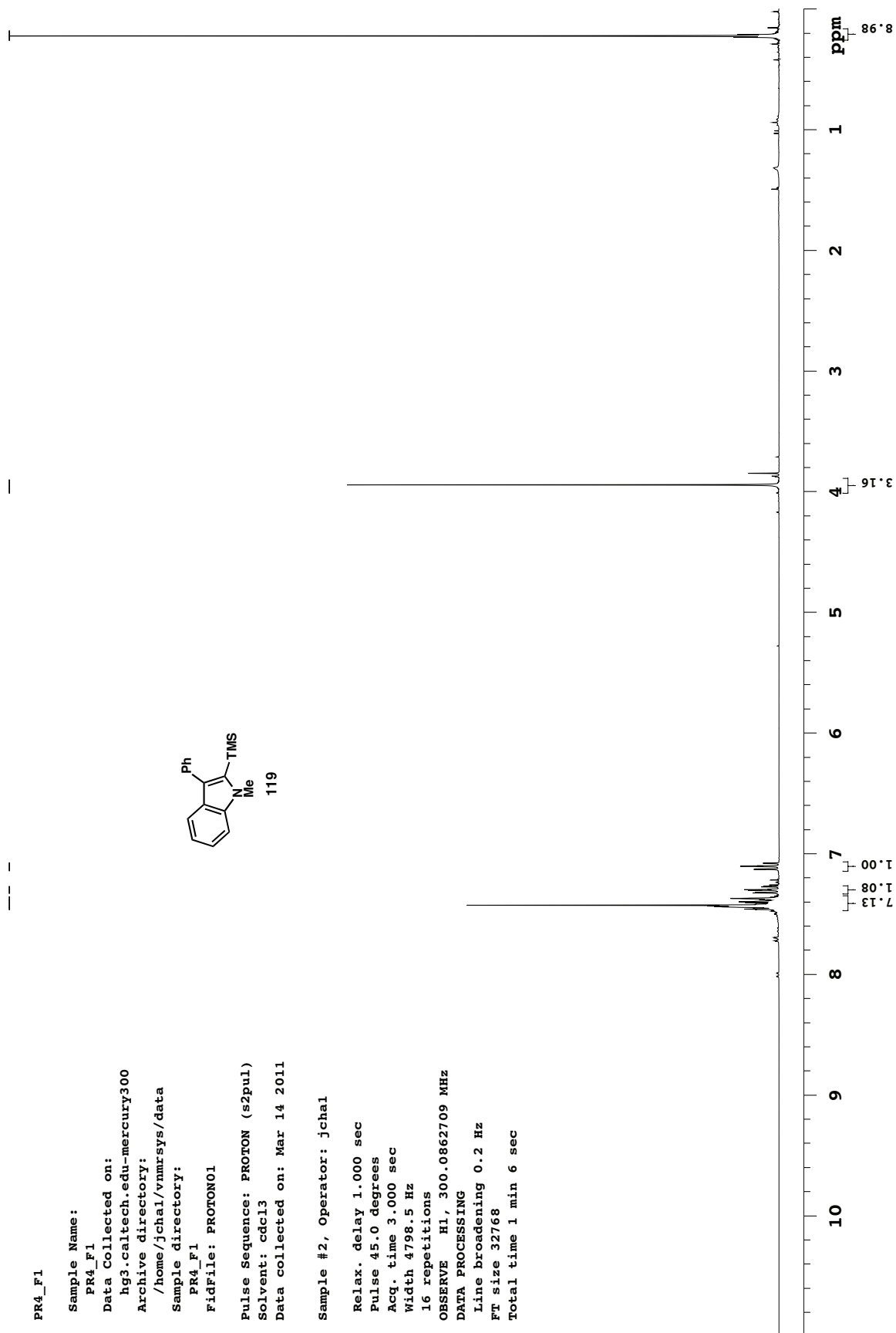
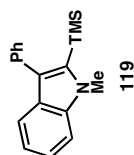
OBSERVE H1, 300.0862709 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min 6 sec



LMRIV-291-major-dr-hs qc

Sample Name:

LMRIV-291-major-dr-hs qc

Data Collected on:

sienna.caltech.edu-vnmrs400

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-291-major-dr-hs qc

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 1 2010

Temp. 25.0 C / 298.1 K

Sample #2, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

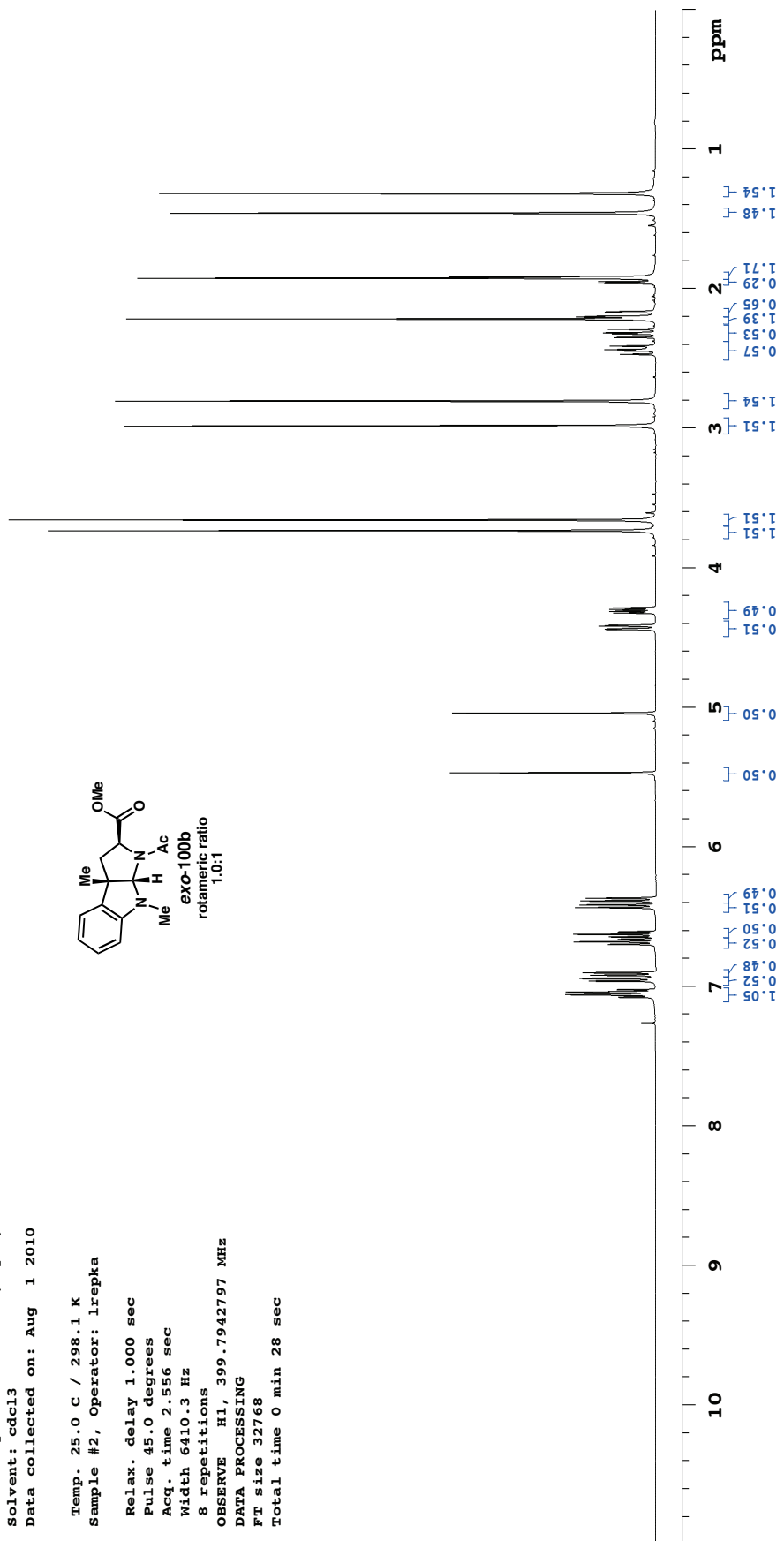
8 repetitions

OBSERVE H1, 399.7942797 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



LMRIV-291-major-dr-conc

Sample Name:

LMRIV-291-major-dr-conc

Data Collected on:

siena.caltech.edu-vmrs400

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-291-major-dr-conc

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 31 2010

Temp. 25.0 C / 298.1 K

Sample #11, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.468 sec

Width 22321.4 Hz

3000 repetitions

OBSERVE C13, 100.5283980 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

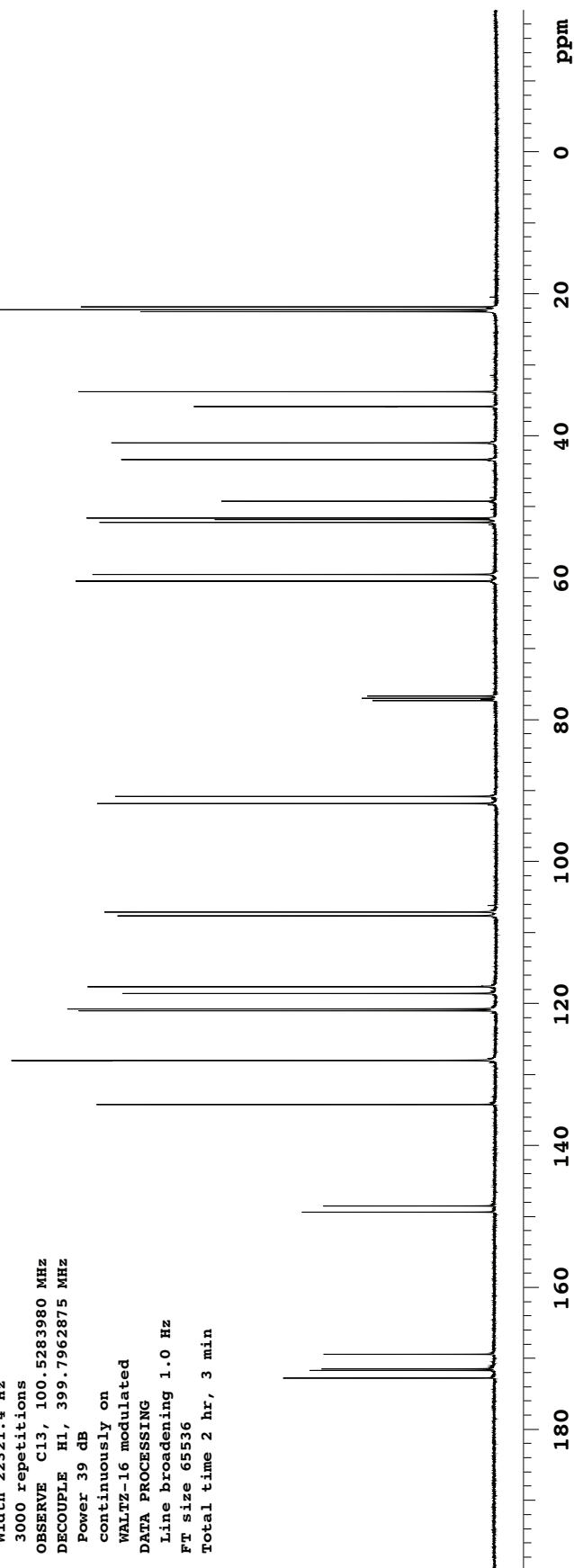
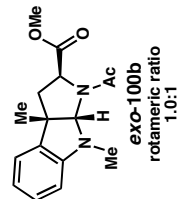
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2 hr, 3 min



LMRIV-291-minordr-hs qc

Sample Name:

LMRIV-291-minordr-hs qc

Data Collected on:

Siena.caltech.edu-vnmrs400

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-291-minordr-hs qc

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 1 2010

Temp. 25.0 C / 298.1 K

Sample #3, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

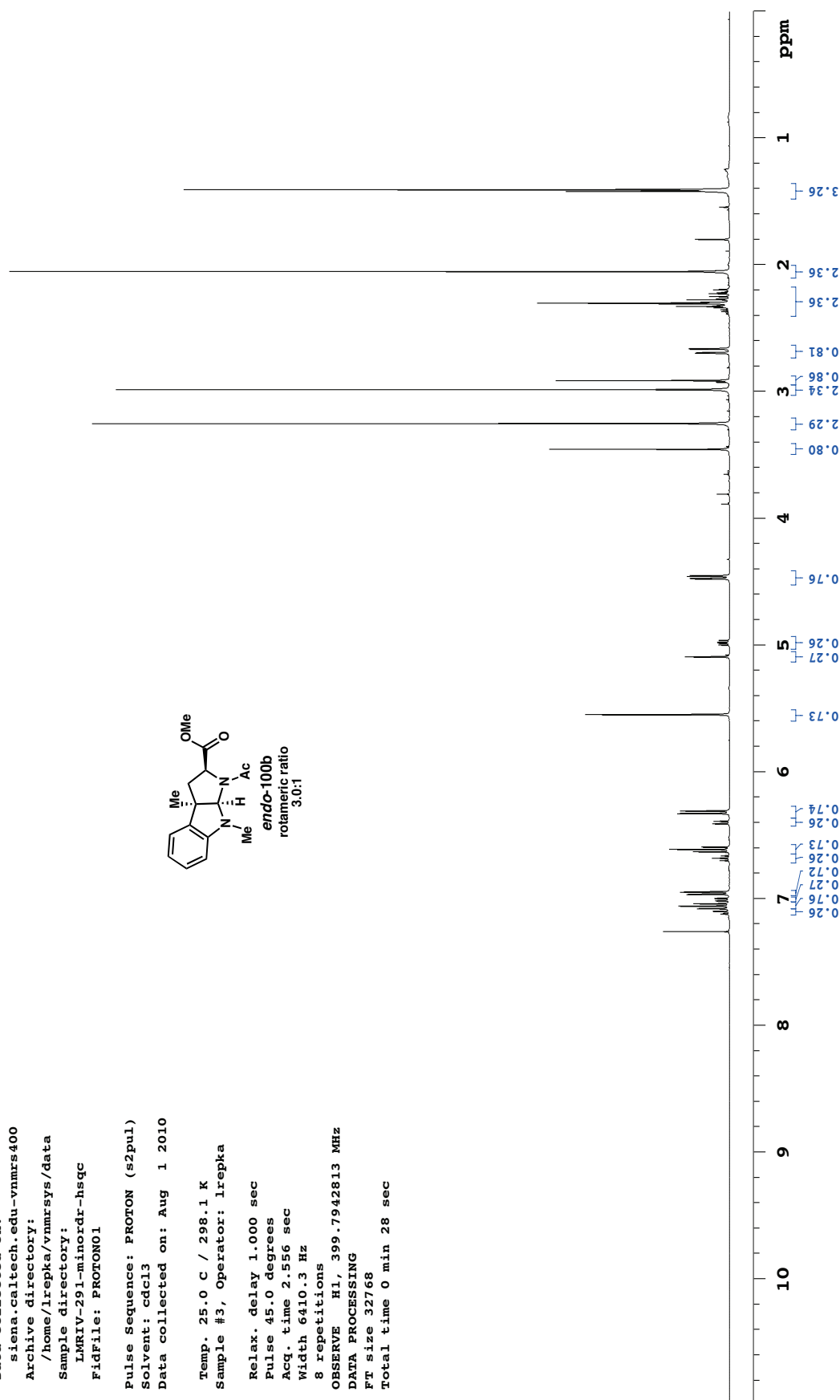
8 repetitions

OBSERVE H1, 399.7942813 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



LMRIV-291-minordr

Sample Name:

LMRIV-291-minordr

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-291-minordr

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 31 2010

Temp. 25.0 C / 298.1 K

Sample #12, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.258 sec

Width 26041.7 Hz

14500 repetitions

OBSERVE C13, 100.5283574 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

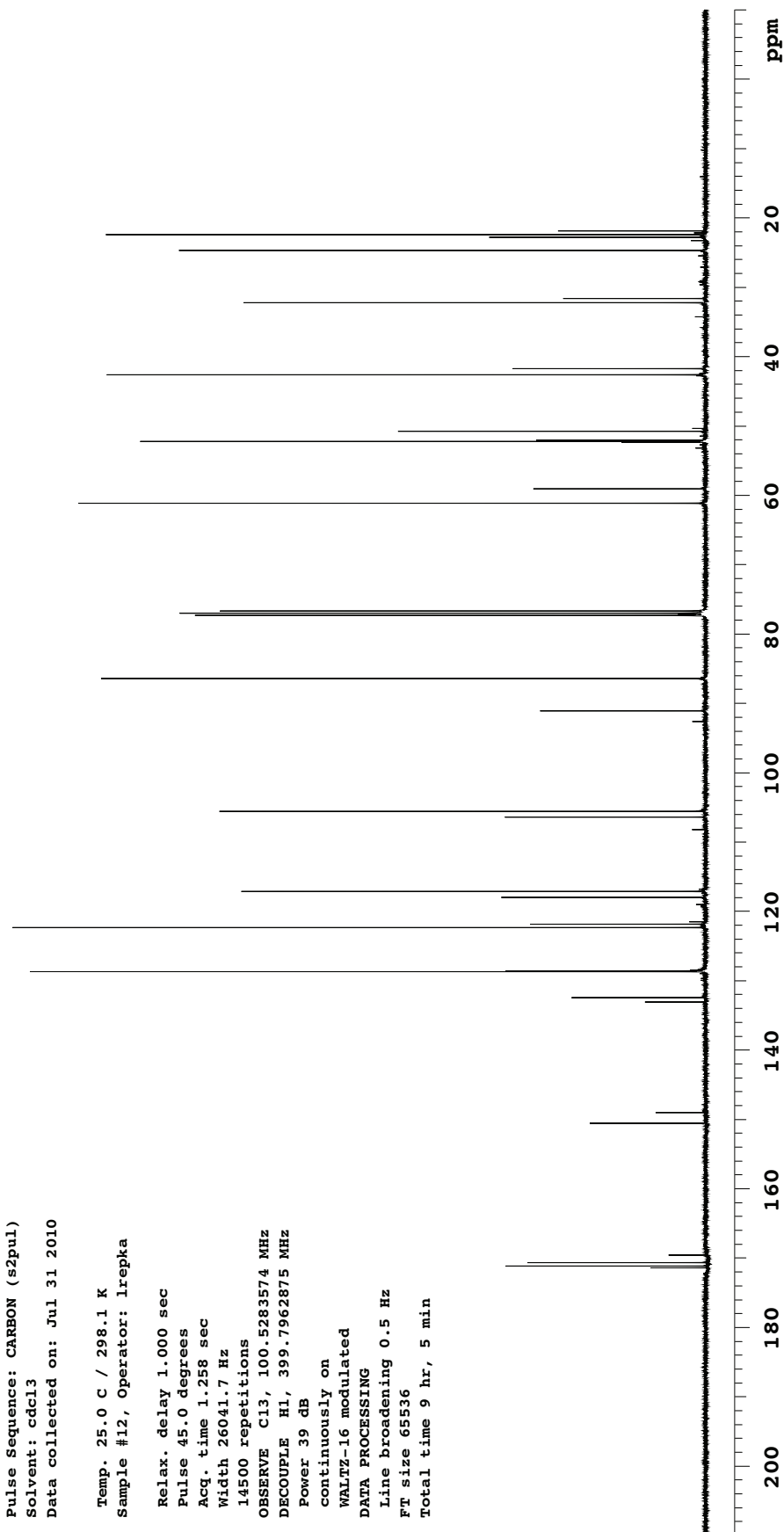
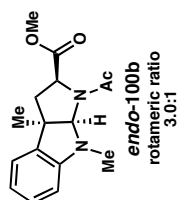
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 9 hr, 5 min



JN-1-131-majordiast

Sample Name:

JN-1-131-majordiast

Data Collected on:

sienna.caltech.edu-vmrs400

Archive directory:

/home/jni/vmrsys/data

Sample directory:

JN-1-131-majordiast

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: ccd13

Data collected on: Aug 5 2010

Temp. 25.0 C / 298.1 K

Sample #1, Operator: jni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

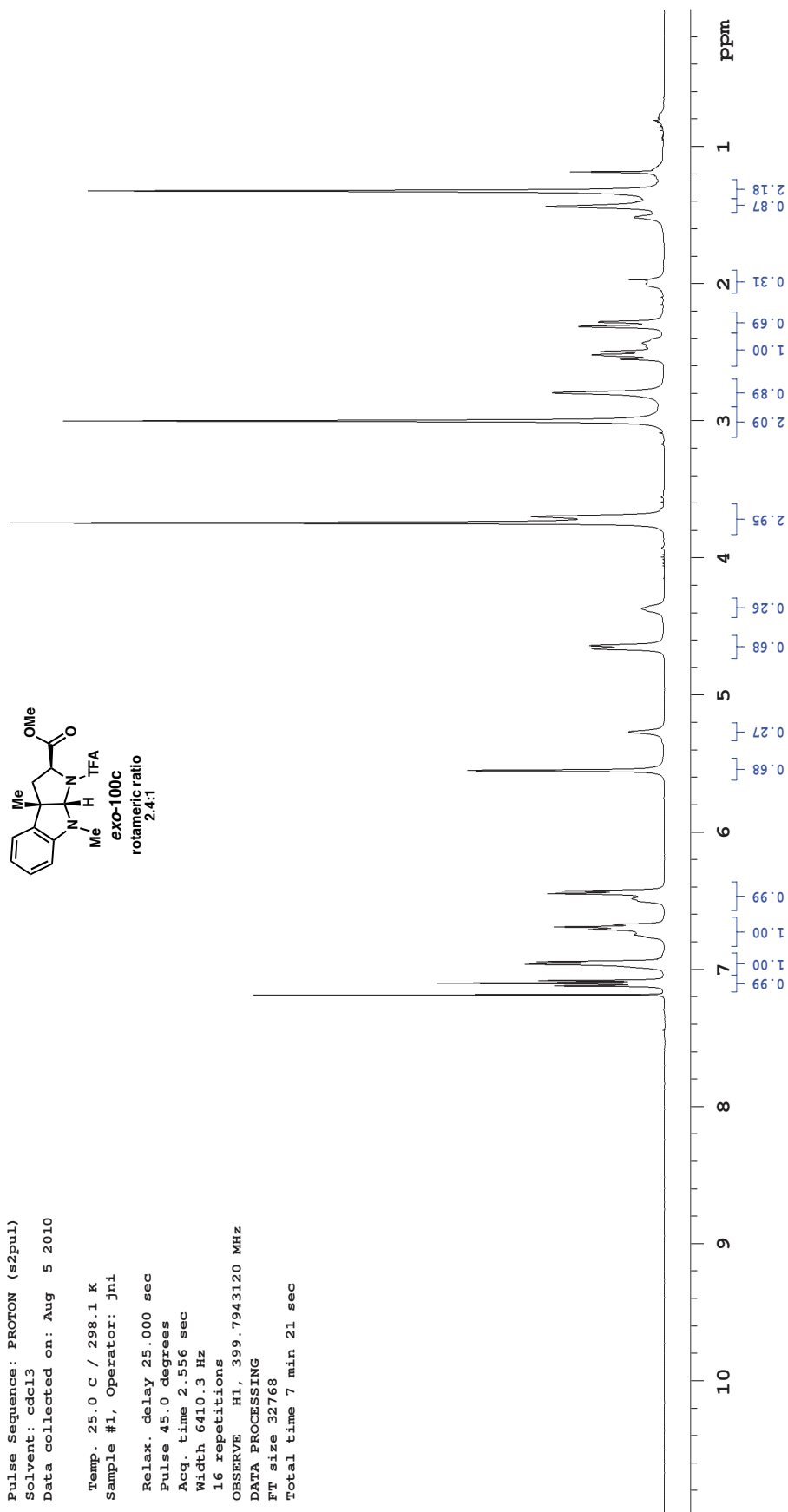
16 repetitions

OBSERVE H1, 399.7943120 MHz

DATA PROCESSING

Ft size 32768

Total time 7 min 21 sec



JN-1-131-majordiast

Sample Name:

JN-1-131-majordiast
Data Collected on:
siena.caltech.edu-vmrs400
Archive directory:
/home/jni/vmrsys/data
Sample directory:
JN-1-131-majordiast
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 5 2010

Temp. 25.0 C / 298.1 K
Sample #1, Operator: jni

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
9700 repetitions

OBSERVE C13, 100.5283531 MHz
DECOUPLE H1, 399.7962875 MHz
Power 39 dB

continuously on

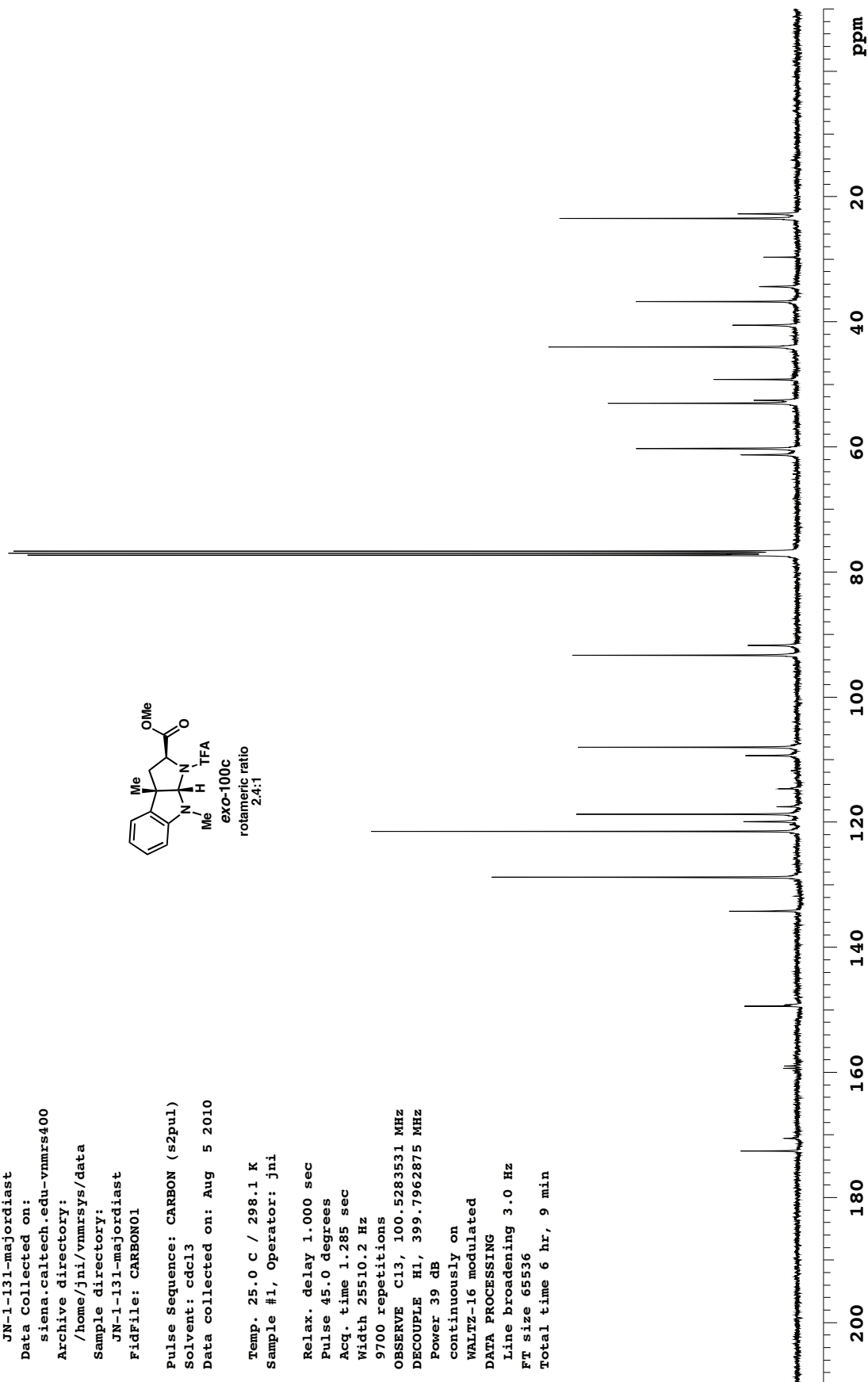
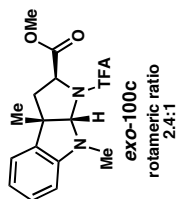
WALTZ-16 modulated

DATA PROCESSING

Line broadening 3.0 Hz

FT size 65536

Total time 6 hr, 9 min



JN-1-131-minordiast3

Sample Name:

JN-1-131-minordiast3

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vmrsys/data

Sample directory:

JN-1-131-minordiast3

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 5 2010

Operator: Janeni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

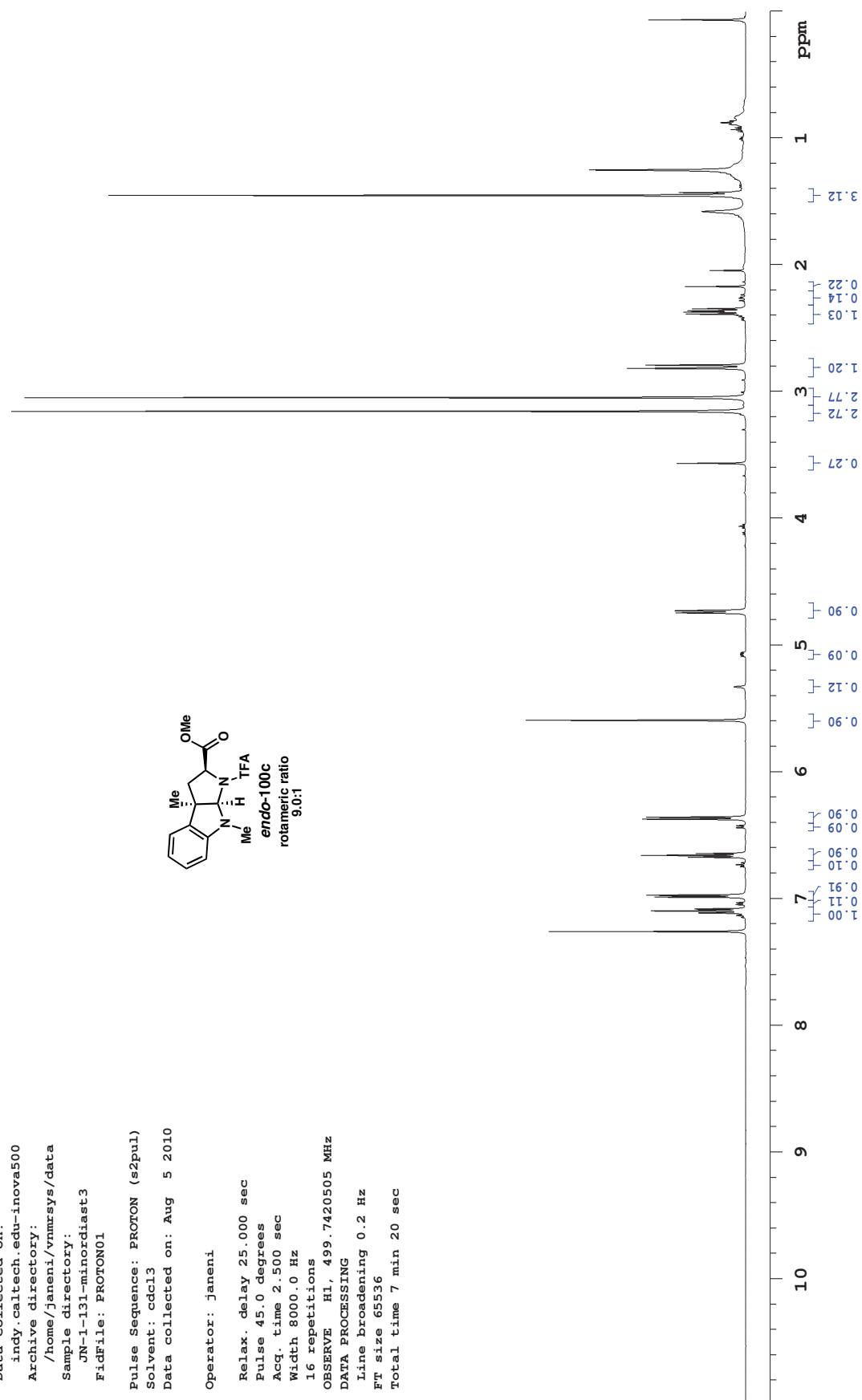
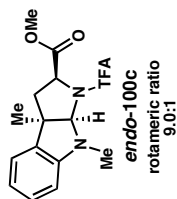
OBSERVE H1, 499.7420505 MHz

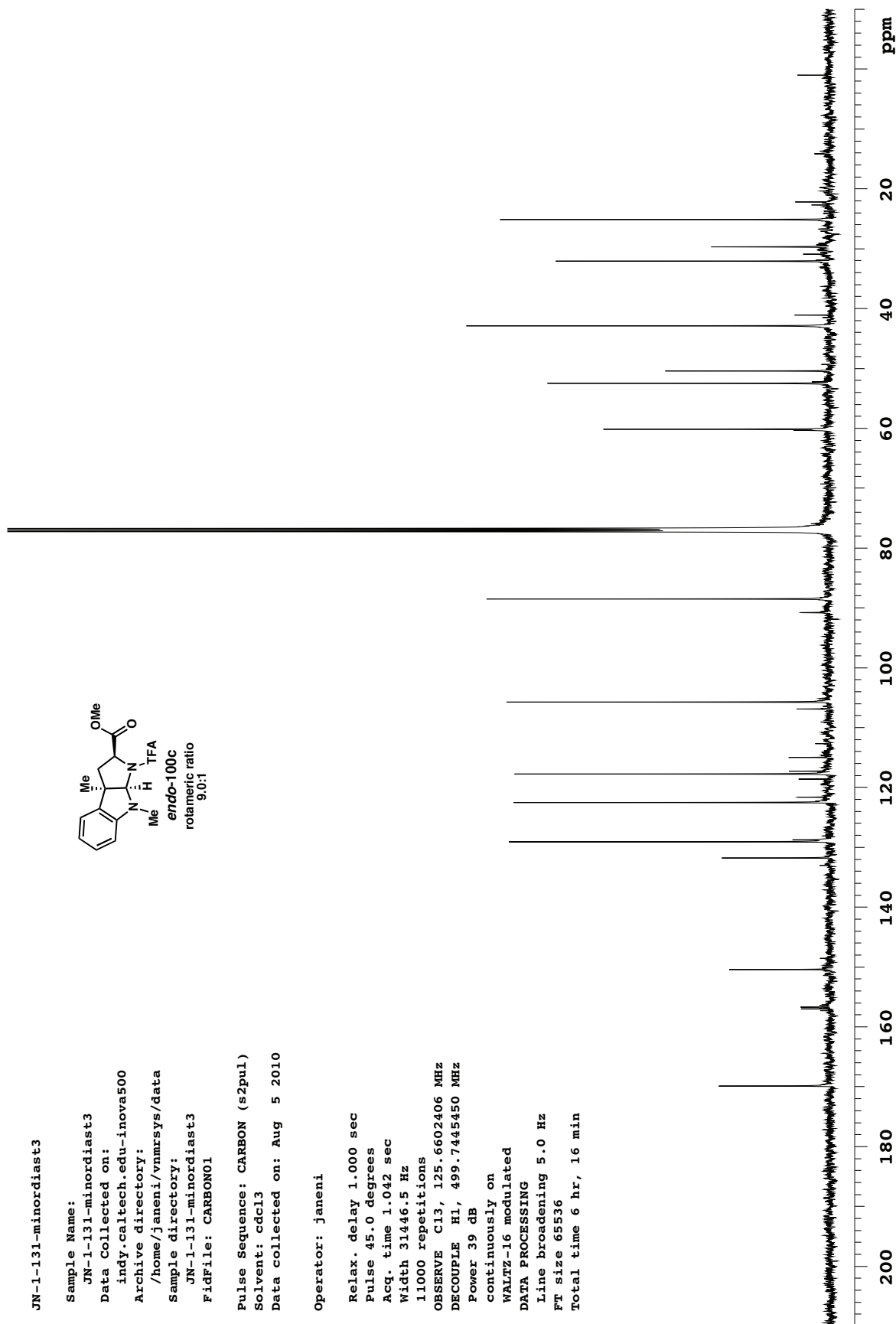
DATA PROCESSING

Line broadening 0.2 Hz

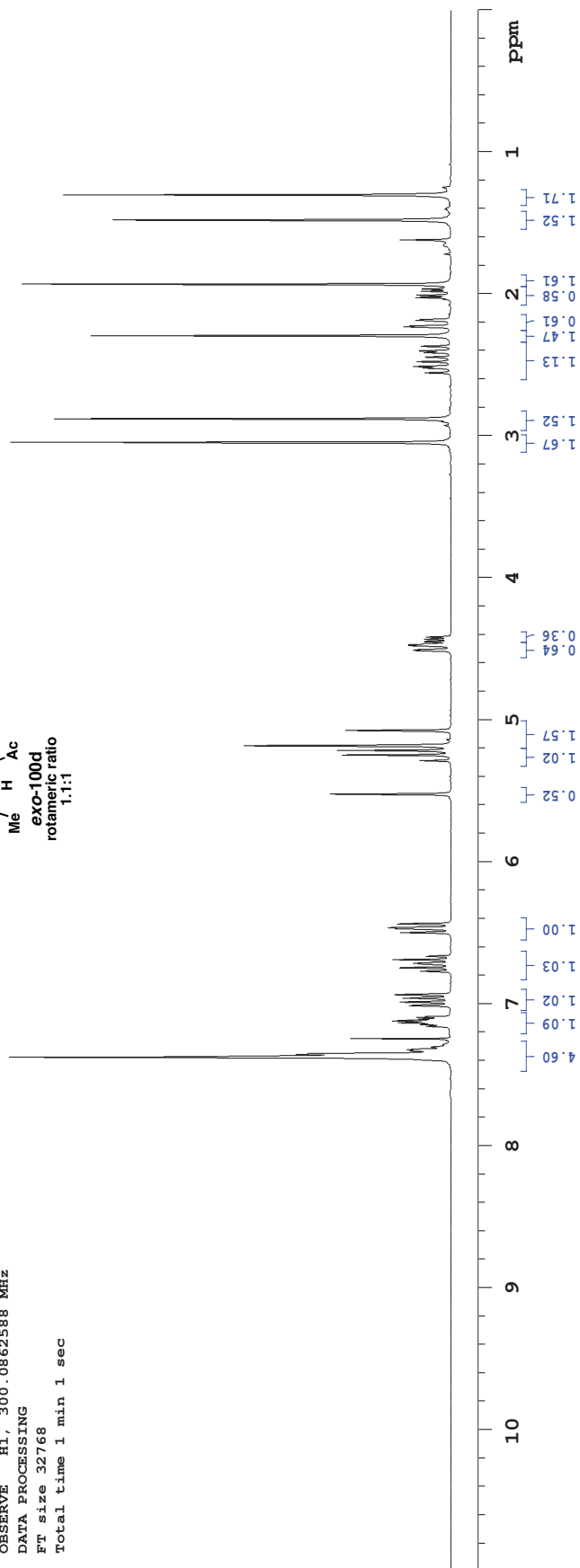
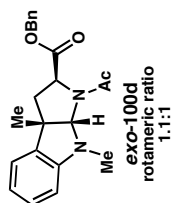
Ft size 65536

Total time 7 min 20 sec





Total time 1 min 1 sec



JN-1-151

Sample Name:

JN-1-151

Data Collected on:

siena.caltech.edu-vmrs400

Archive directory:

/home/jni/vmrsys/data

Sample directory:

JN-1-151

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 26 2010

Sample #1, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

8500 repetitions

OBSERVE C13, 100.5283573 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

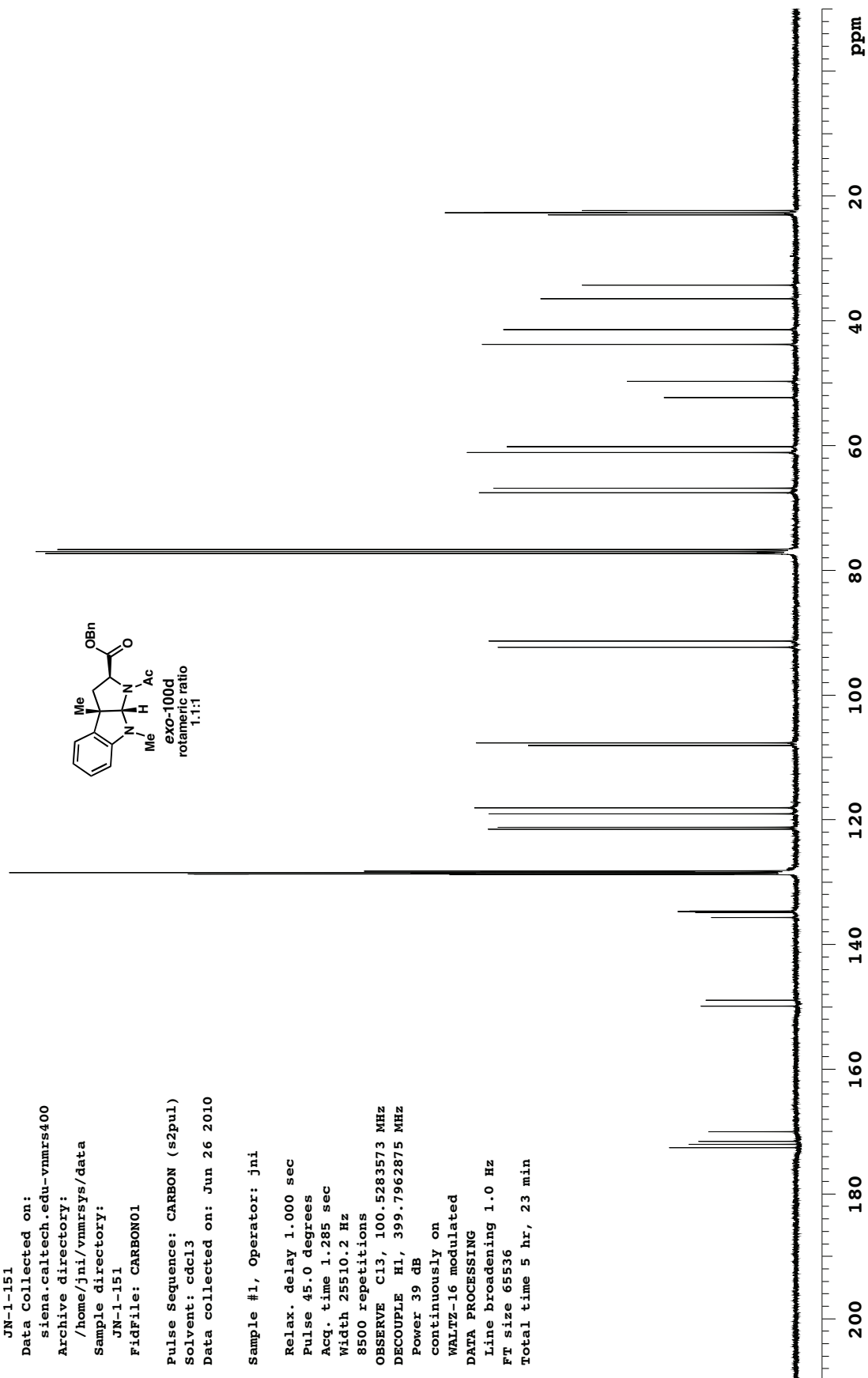
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 5 hr, 23 min



JN-1-151-minordiast3

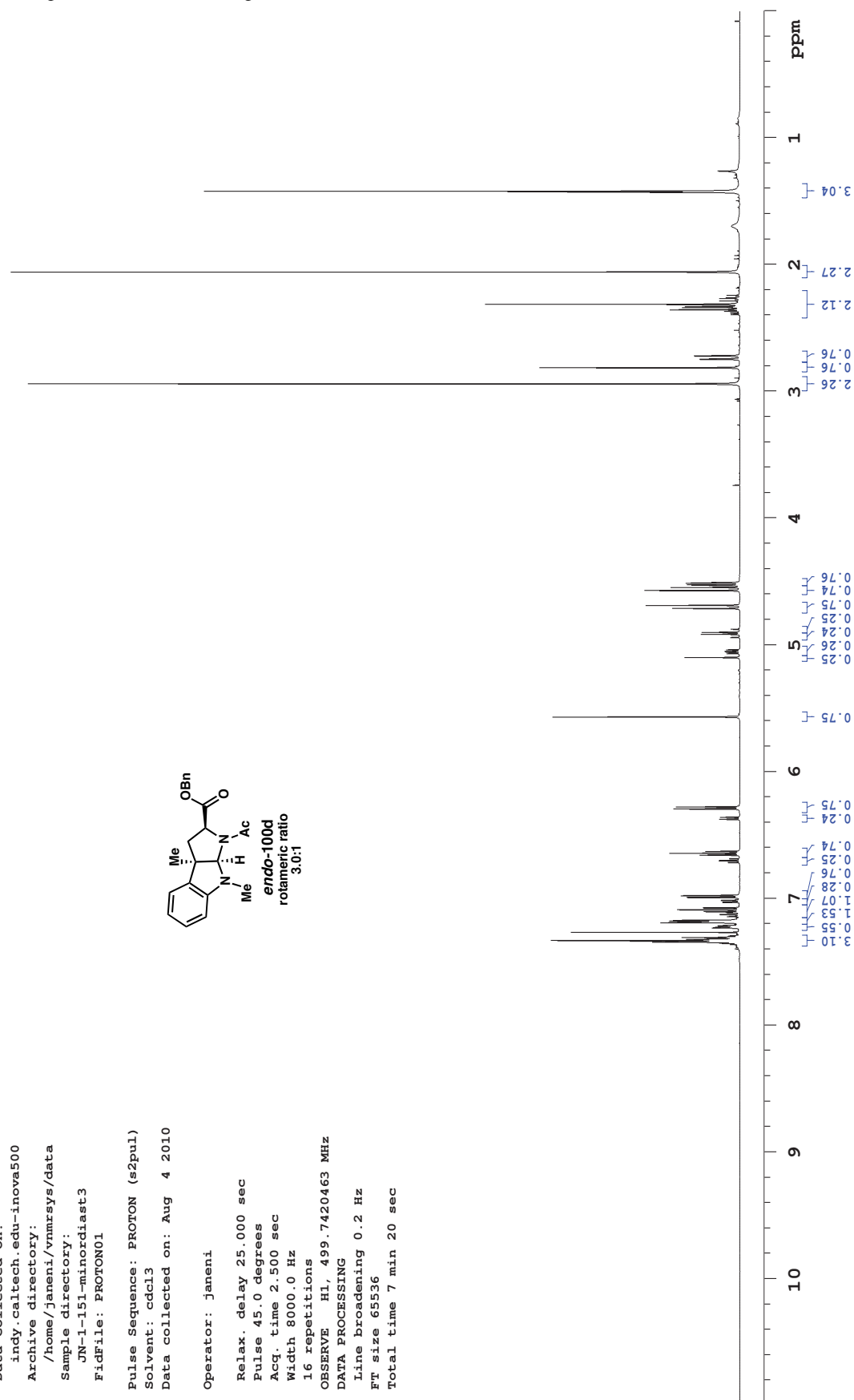
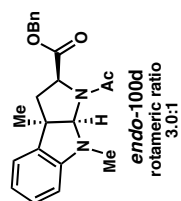
Sample Name:
 JN-1-151-minordiast3
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/janeni/vmrsys/data
 Sample directory:
 JN-1-151-minordiast3
 FIDFile: PROTON01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 4 2010

Operator: janeni

Relax. delay 25.000 sec
 Pulse 45.0 degrees
 Acq. time 2.500 sec
 Width 8000.0 Hz
 16 repetitions

OBSERVE H1, 499.7420463 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 7 min 20 sec



JN-1-151-minordiast3

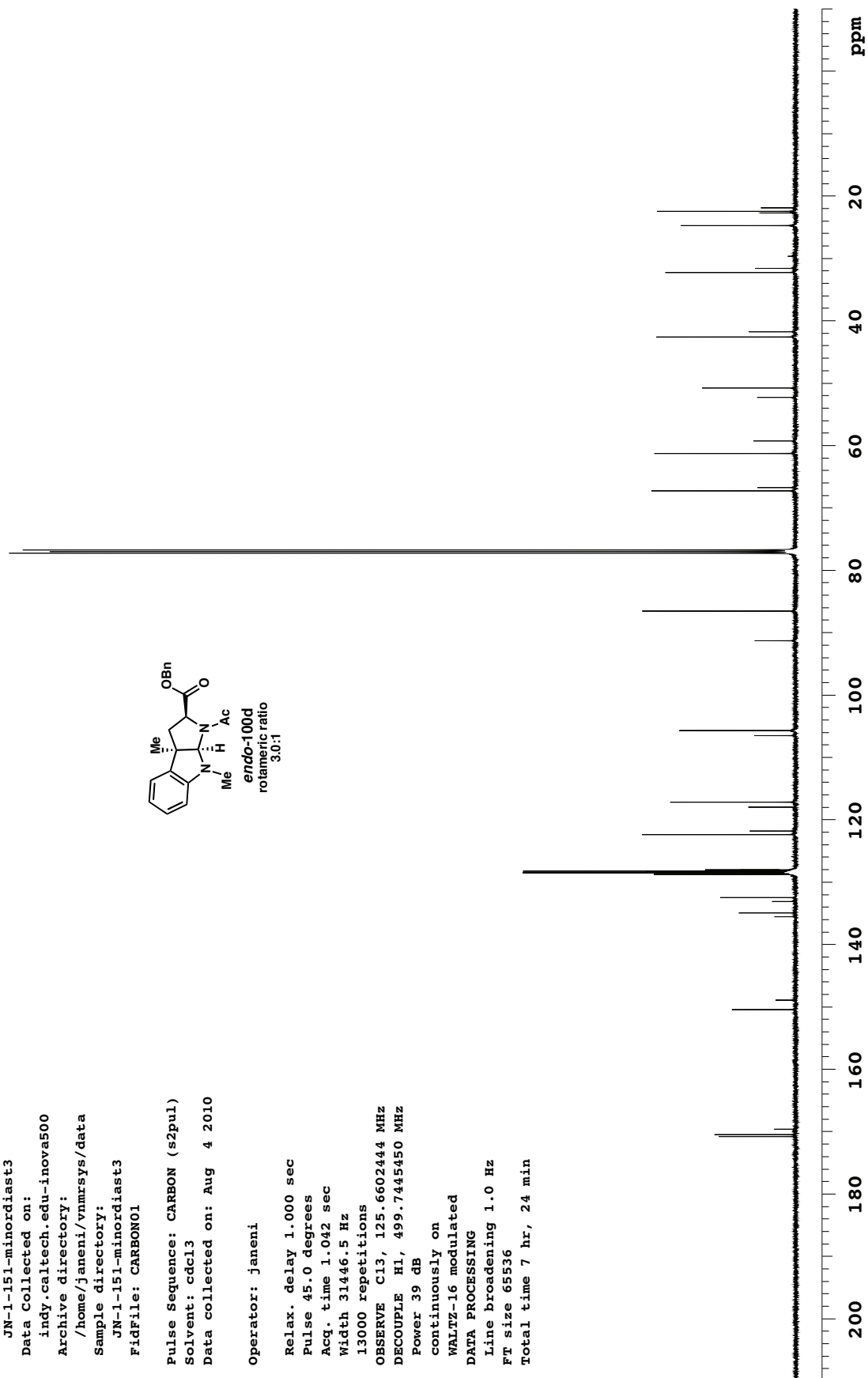
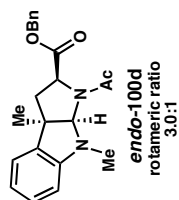
Sample Name:

JN-1-151-minordiast3
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/janeni/vnmrsys/data
Sample directory:
JN-1-151-minordiast3
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 4 2010

Operator: janeni

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
13000 repetitions
OBSERVE C13, 125.6602444 MHz
DECOUPLE H1, 499.7445450 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 7 hr, 24 min



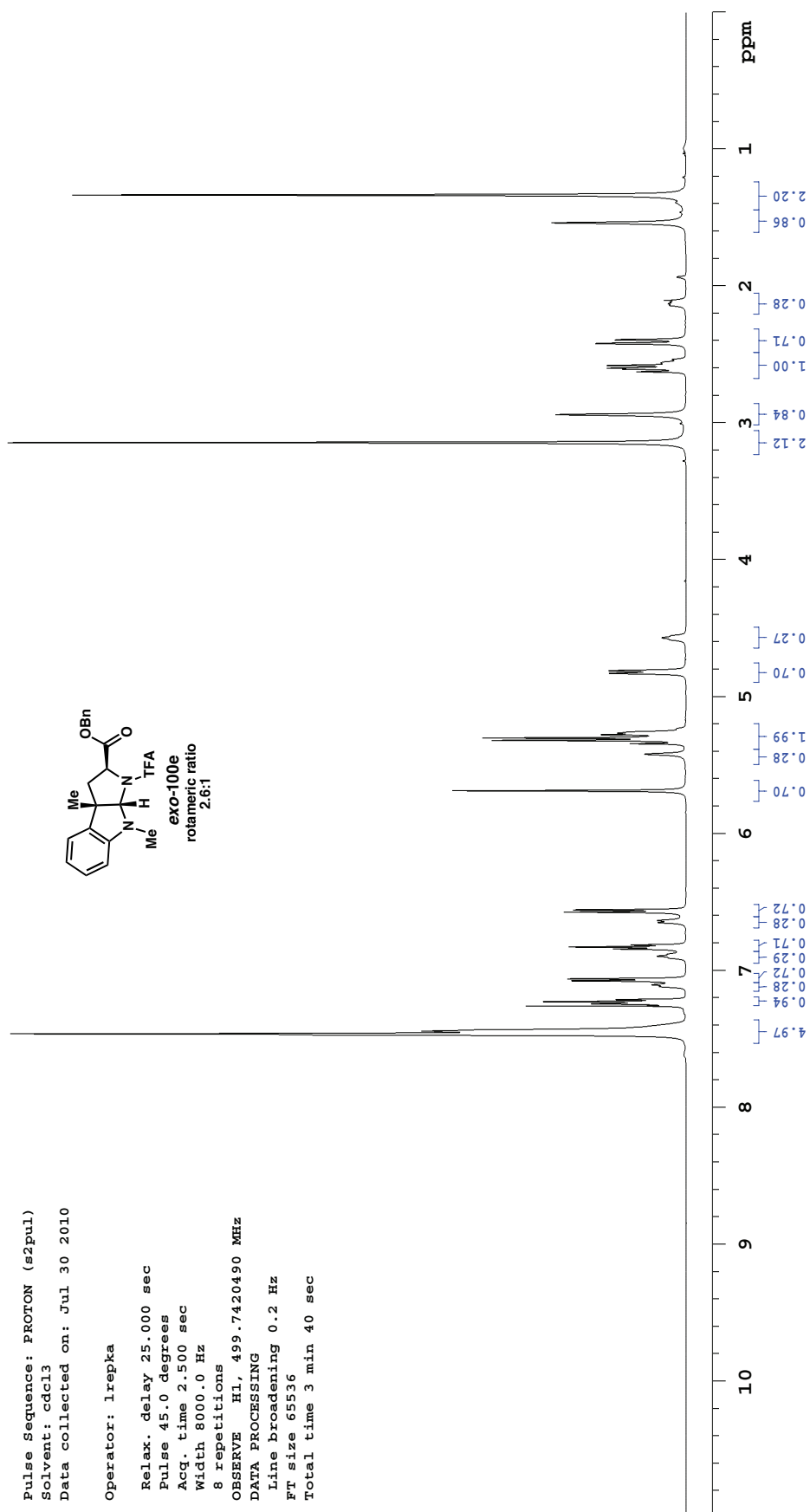
LMRIV-287-majordr-rd25

Sample Name:
 LMRIV-287-majordr-rd25
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/lrepka/vnmrsys/data
 Sample directory:
 LMRIV-287-majordr-rd25
 FIDFile: PROTON01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jul 30 2010

Operator: lrepka

Relax. delay 25.000 sec
 Pulse 45.0 degrees
 Acq. time 2.500 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.7420490 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 3 min 40 sec



LMRIV-scale-up-12h-major

Sample Name:

LMRIV-scale-up-12h-major

Data Collected on:

siena.caltech.edu-vmrs400

Archive directory:

/home/lrepka/vmrsys/data

Sample directory:

LMRIV-scale-up-12h-major

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 29 2010

Temp. 25.0 C / 298.1 K

Sample #1, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

11500 repetitions

OBSERVE C13, 100.5283829 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

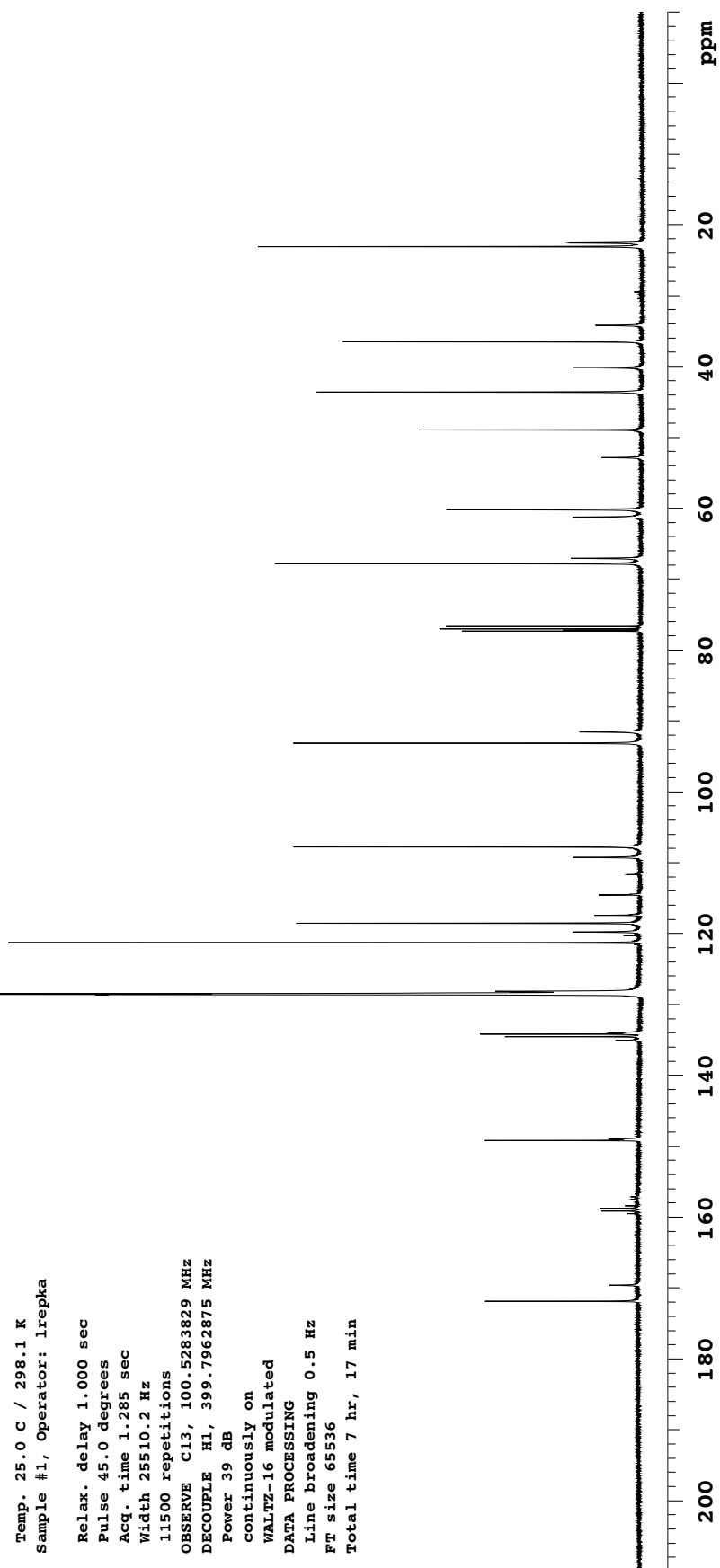
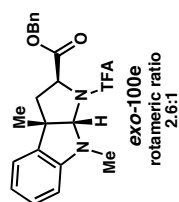
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 7 hr, 17 min



LMRIV-287-minor-8-5-10

Sample Name:

LMRIV-287-minor-8-5-10

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-287-minor-8-5-10

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 5 2010

Temp. 25.0 C / 298.1 K

Sample #46, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4810.0 Hz

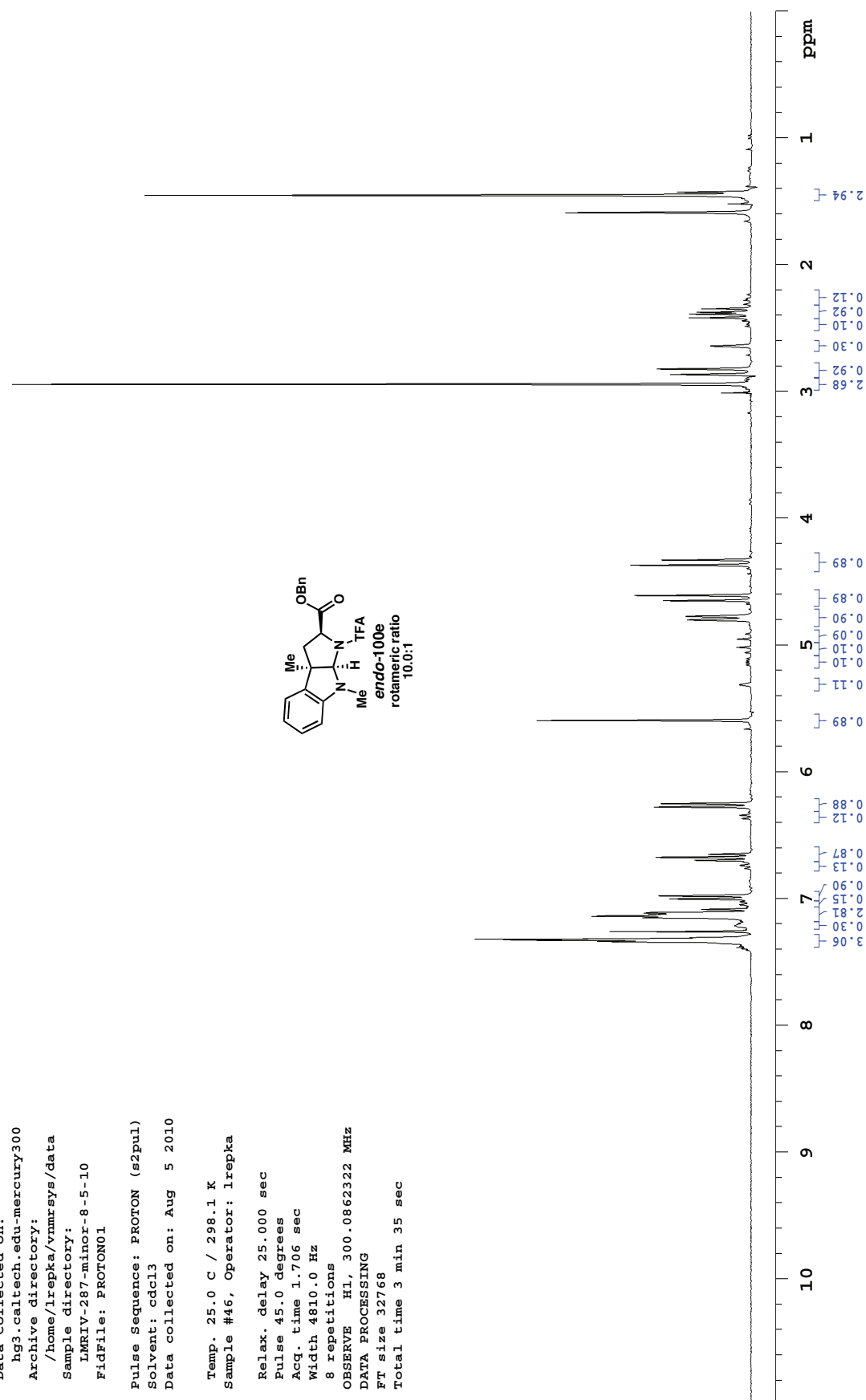
8 repetitions

OBSERVE H1, 300.0862322 MHz

DATA PROCESSING

FT size 32768

Total time 3 min 35 sec



LMRIV-scale-up-12h-minordr

Sample Name:

LMRIV-scale-up-12h-minordr

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-scale-up-12h-minordr

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 29 2010

Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

13500 repetitions

OBSERVE C13, 125.6602412 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

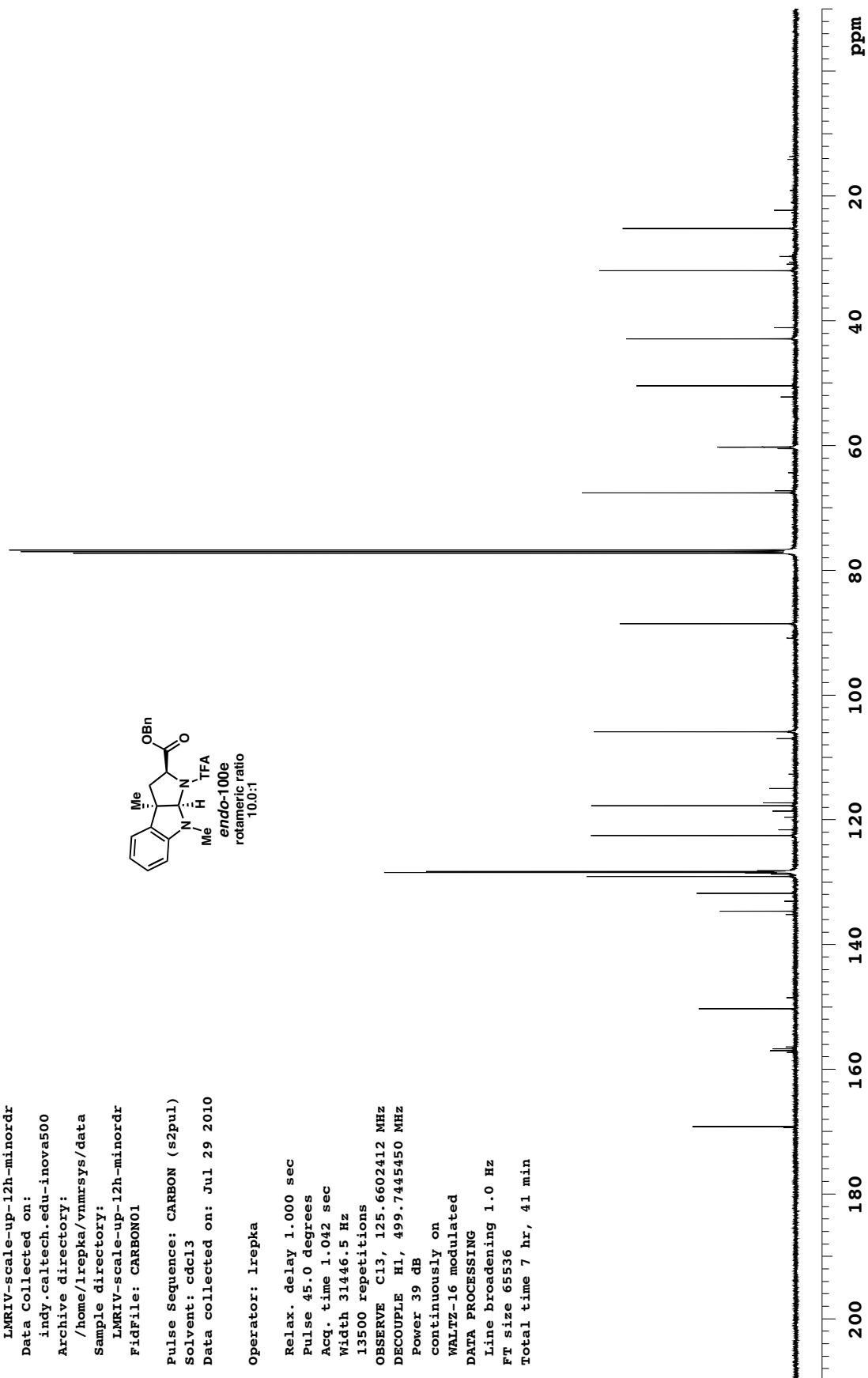
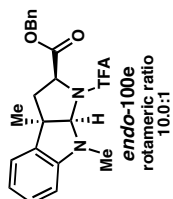
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 7 hr, 41 min



JN-1-191-majordiast

Sample Name:

JN-1-191-majordiast

Data Collected on:

sienna.caltech.edu—vnmrs400

Archive directory:

/home/jni/vnmrsys/data

Sample directory:

JN-1-191-majordiast

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 19 2010

Temp. 25.0 C / 298.1 K

Sample #5, Operator: jni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

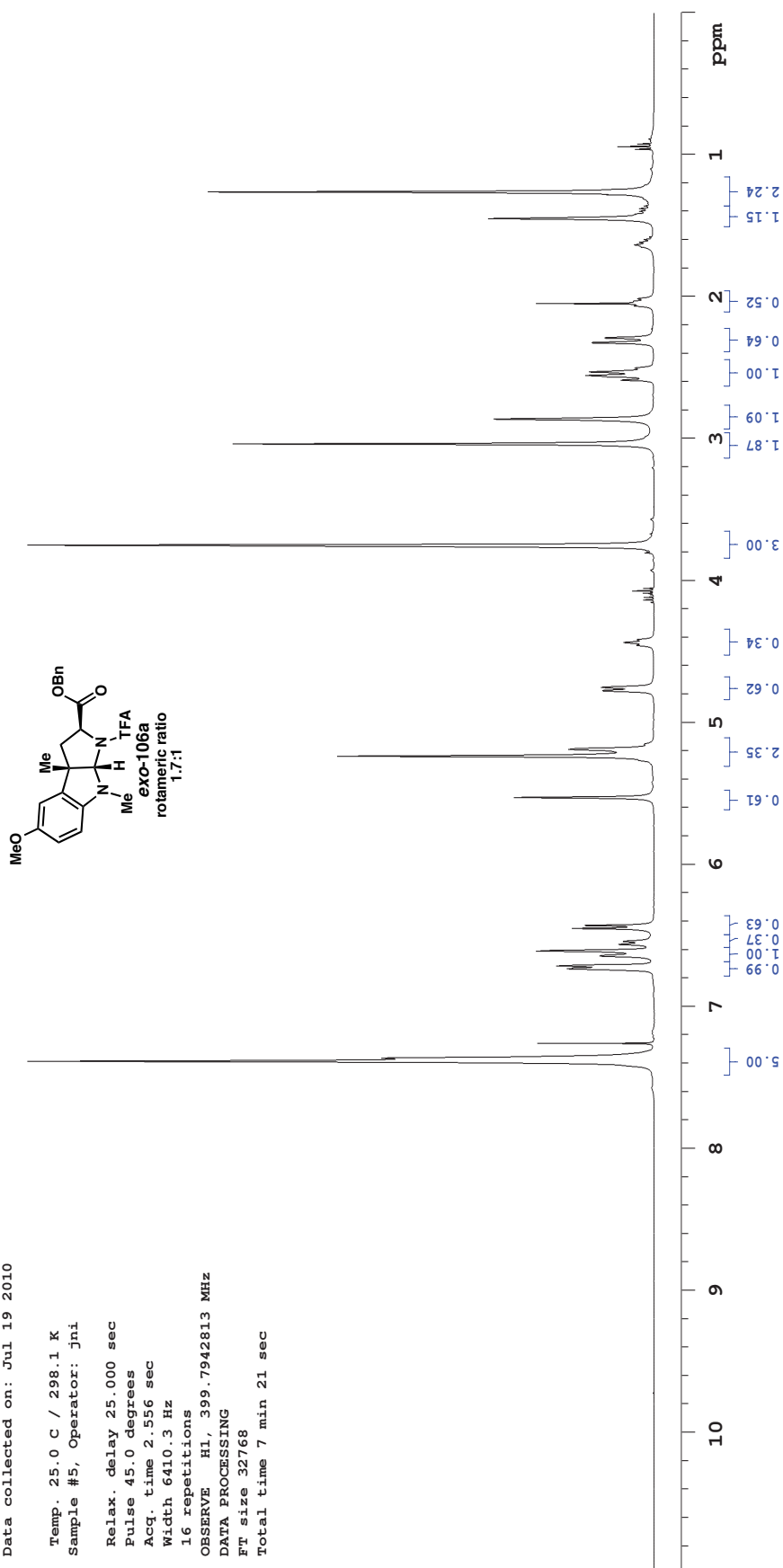
16 repetitions

OBSERVE H1, 399.7942813 MHz

DATA PROCESSING

Ft size 32768

Total time 7 min 21 sec



JN-1-191-majordiast

Sample Name:

JN-1-191-majordiast
Data Collected on:
siena.caltech.edu-vmrs400
Archive directory:
/home/jni/vmrsys/data
Sample directory:
JN-1-191-majordiast
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 19 2010

Temp. 25.0 C / 298.1 K
Sample #5, Operator: jni

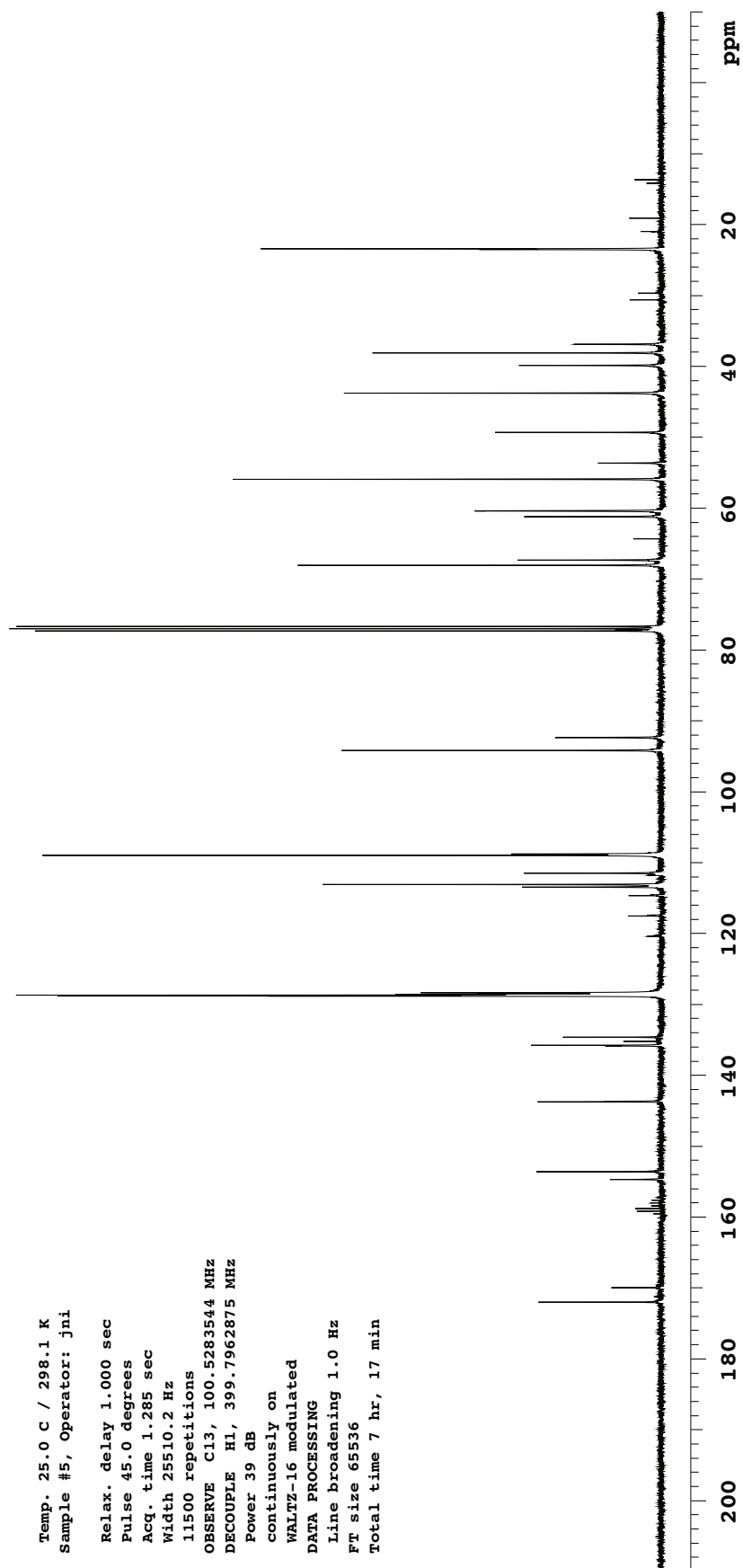
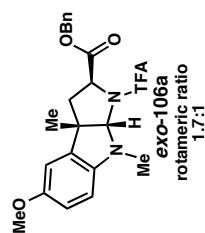
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
11500 repetitions

OBSERVE C13, 100.5283544 MHz
DECOUPLE H1, 399.7962875 MHz

Power 39 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz
FT size 65536
Total time 7 hr, 17 min



JN-1-191-minordiast

Sample Name:

JN-1-191-minordiast

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-191-minordiast

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 18 2010

Temp. 25.0 C / 298.1 K

Operator: janeni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

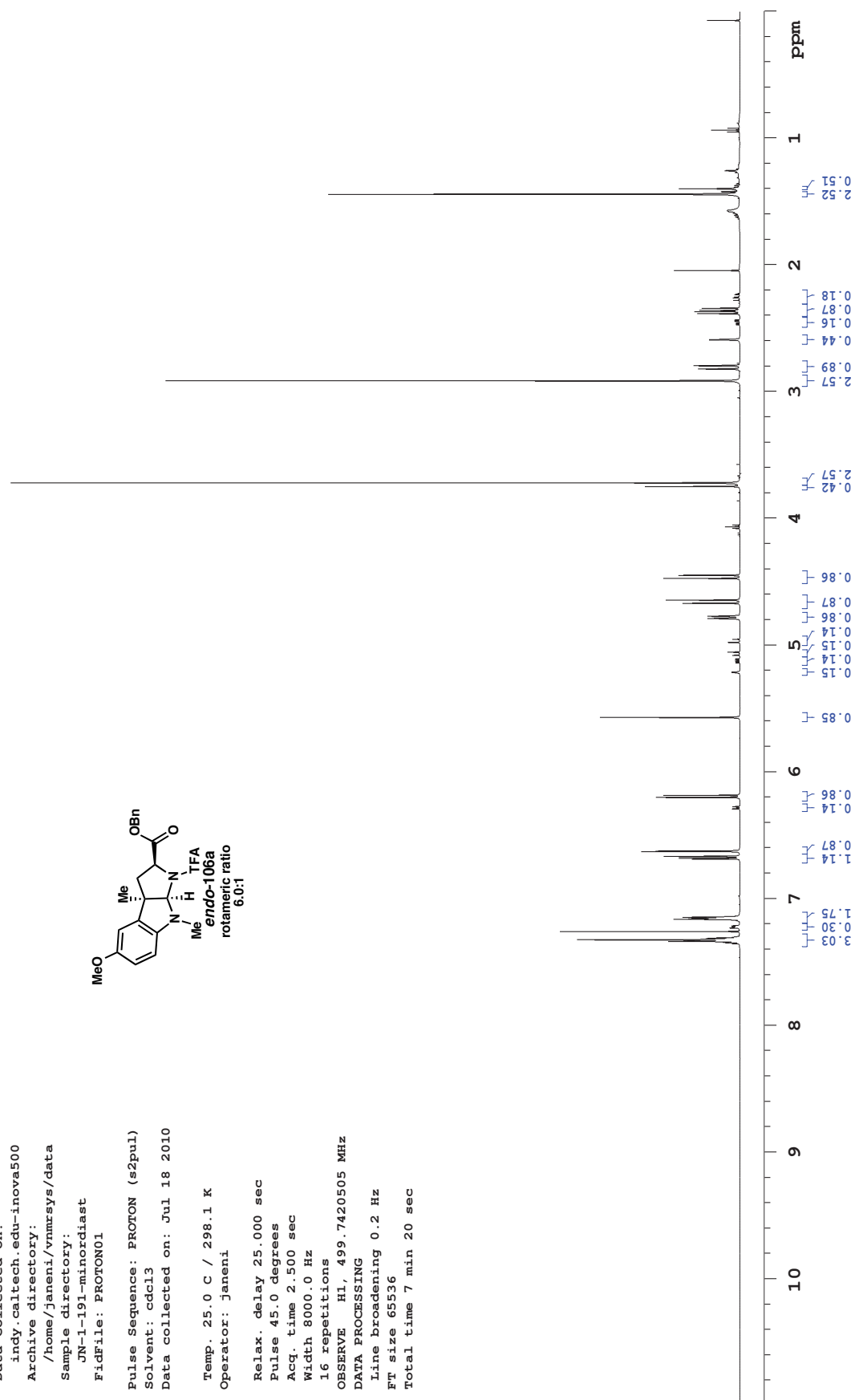
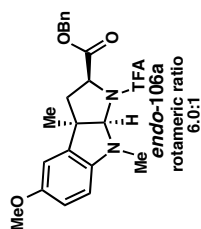
OBSERVE H1, 499.7420505 MHz

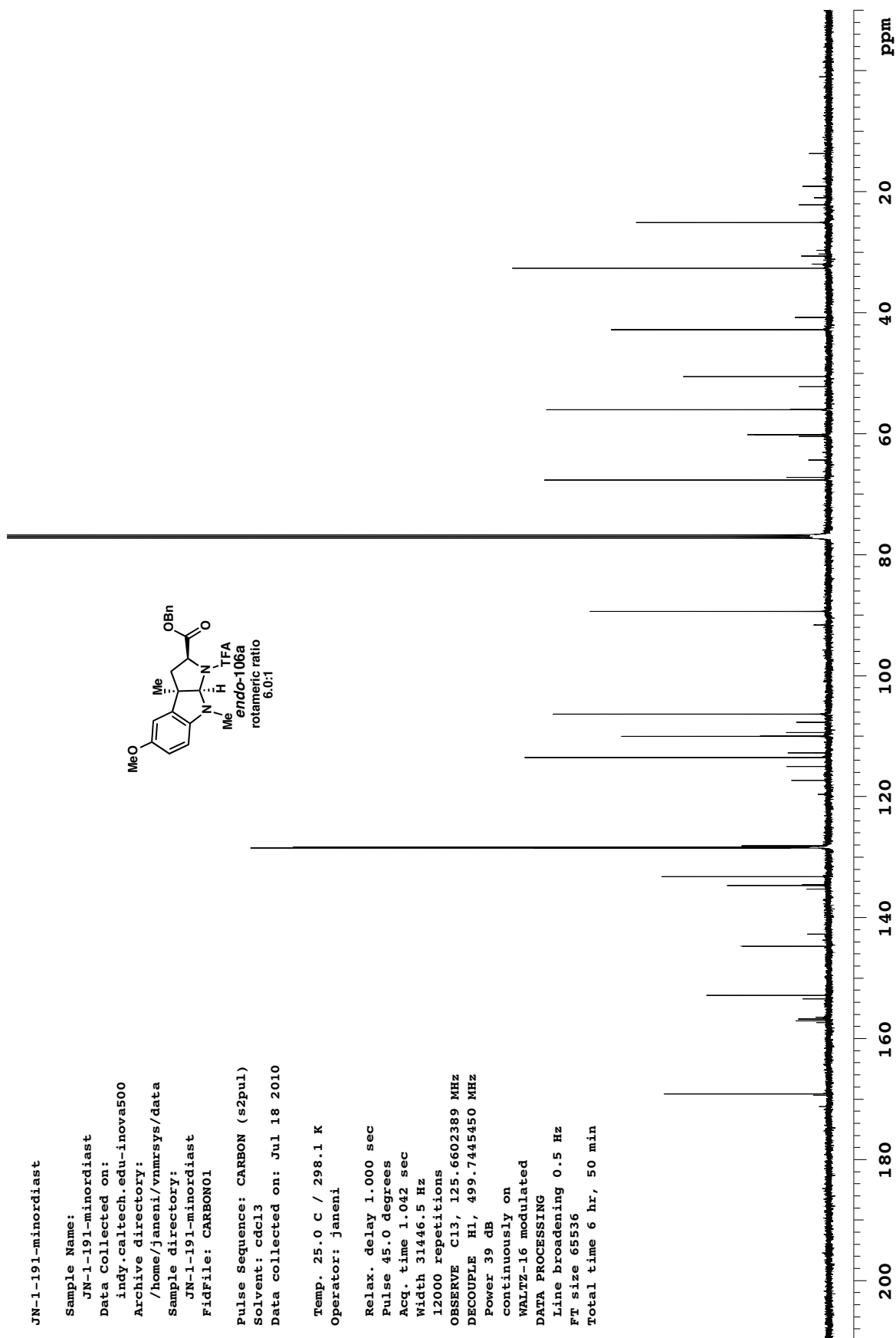
DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 7 min 20 sec





JN-1-195-majordiast4

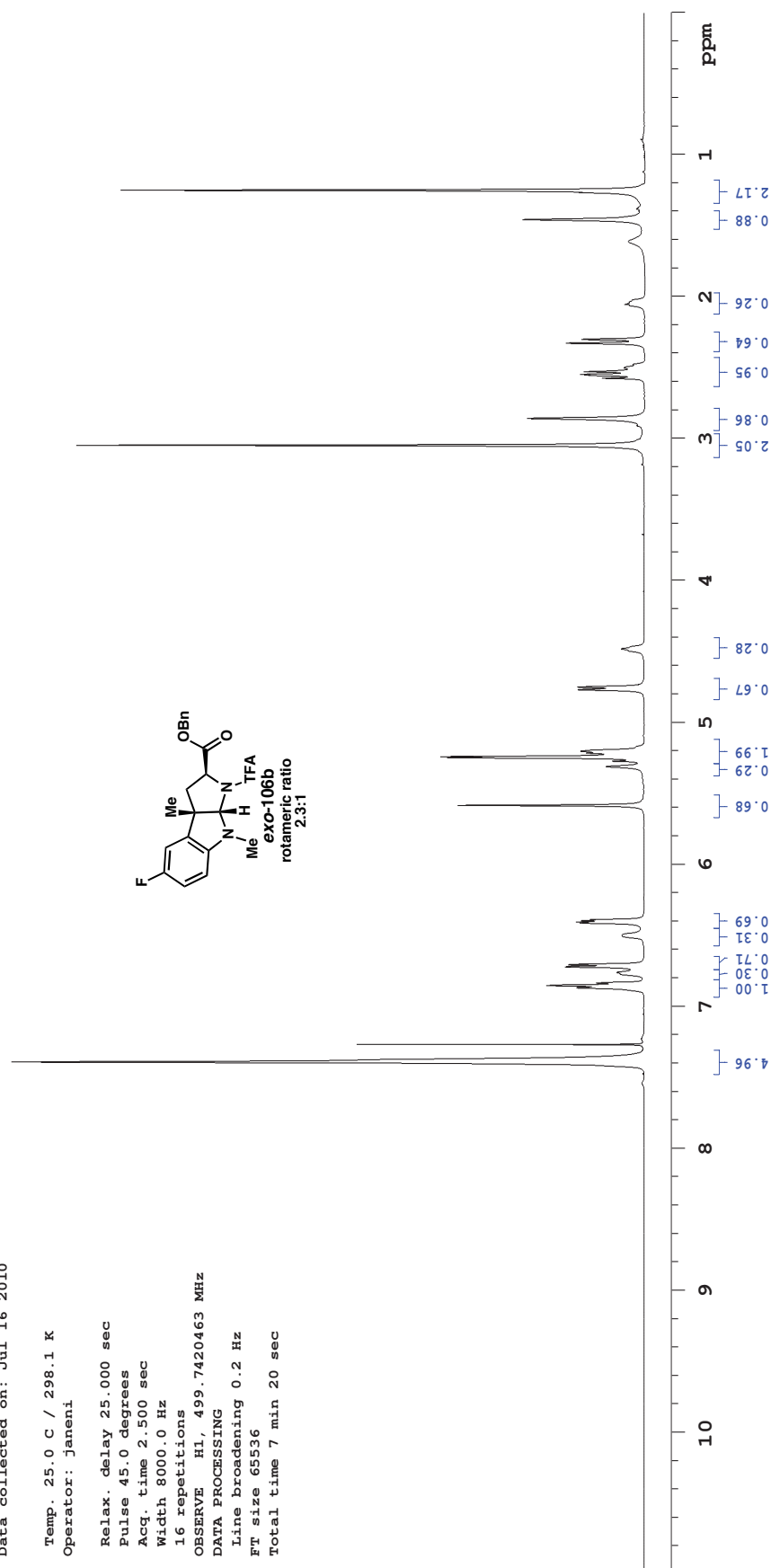
Sample Name:
JN-1-195-majordiast4
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/janeni/vnmrsys/data
Sample directory:
JN-1-195-majordiast4
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cdl3
Data collected on: Jul 16 2010

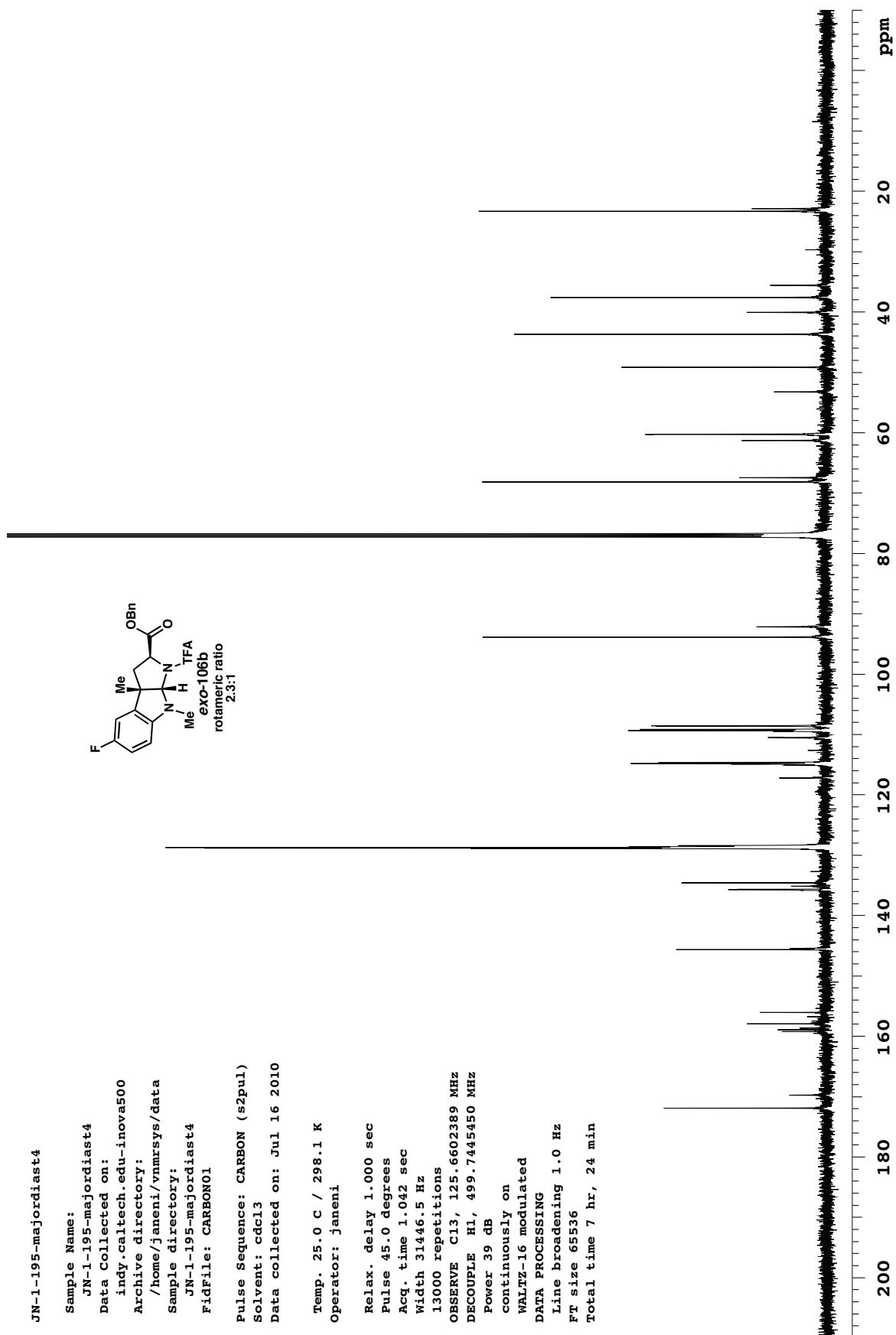
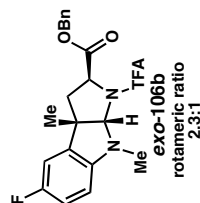
Temp. 25.0 C / 298.1 K
Operator: janeni

Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 8000.0 Hz
16 repetitions

OBSERVE H1, 499.7420463 MHz
DATA PROCESSING
Line broadening 0.2 Hz
Ft size 65536
Total time 7 min 20 sec



OBSERVE C13, 125.6602389 MHz
 DECOUPLE H1, 499.7445450 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FFT size 65536
 Total time 7 hr, 24 min



JN-1-195-minordiast

Sample Name:

JN-1-195-minordiast

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-195-minordiast

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 15 2010

Temp. 25.0 C / 298.1 K

Operator: janeni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

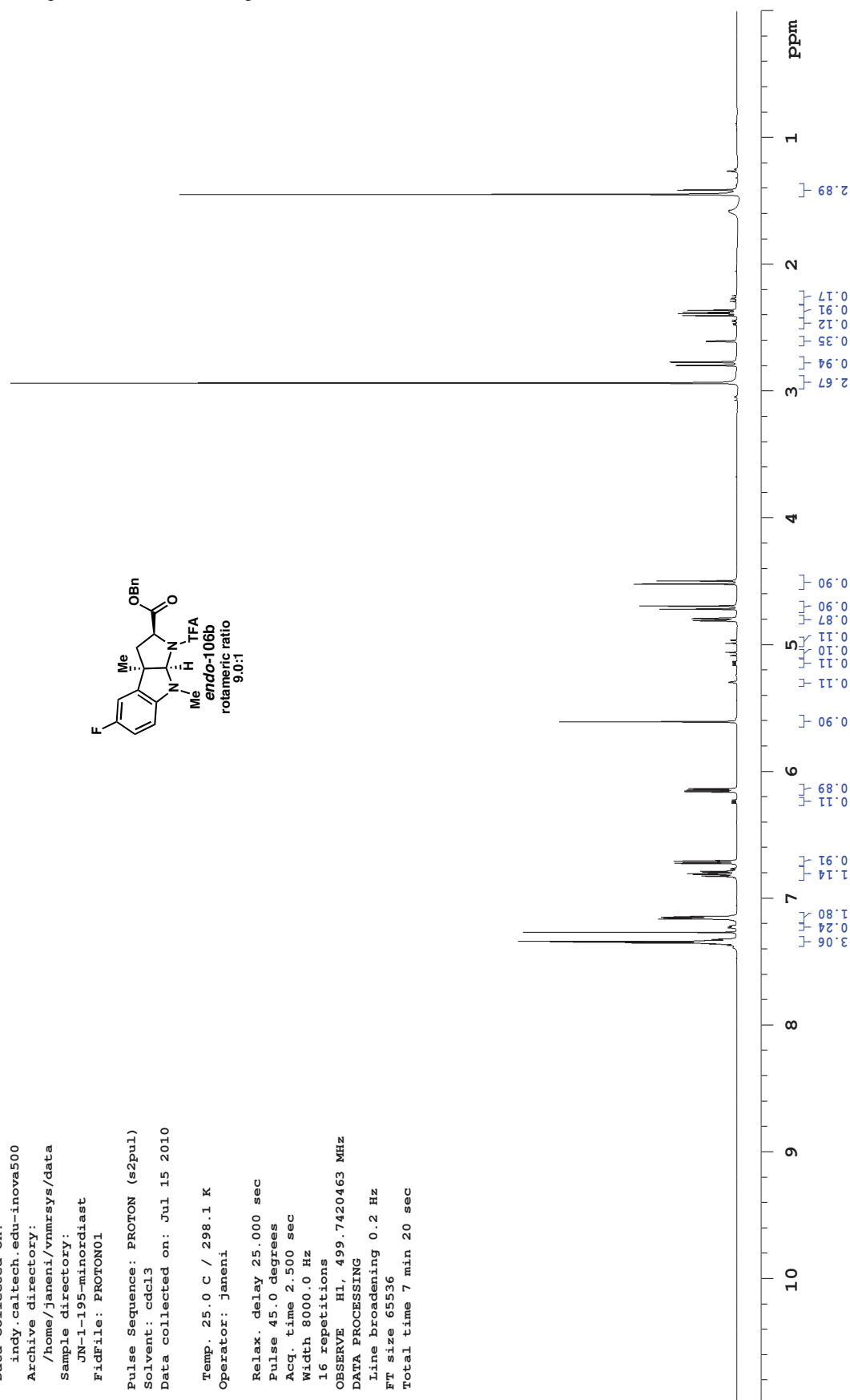
OBSERVE H1, 499.7420463 MHz

DATA PROCESSING

Line broadening 0.2 Hz

Ft size 65536

Total time 7 min 20 sec



JN-1-195-minordiast

Sample Name:

JN-1-195-minordiast
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/janeni/vnmrSYS/data
Sample directory:
JN-1-195-minordiast
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 15 2010

Temp. 25.0 C / 298.1 K
Operator: janeni

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
13000 repetitions

OBSERVE C13, 125.6602387 MHz
DECOUPLE H1, 499.7445450 MHz
Power 39 dB

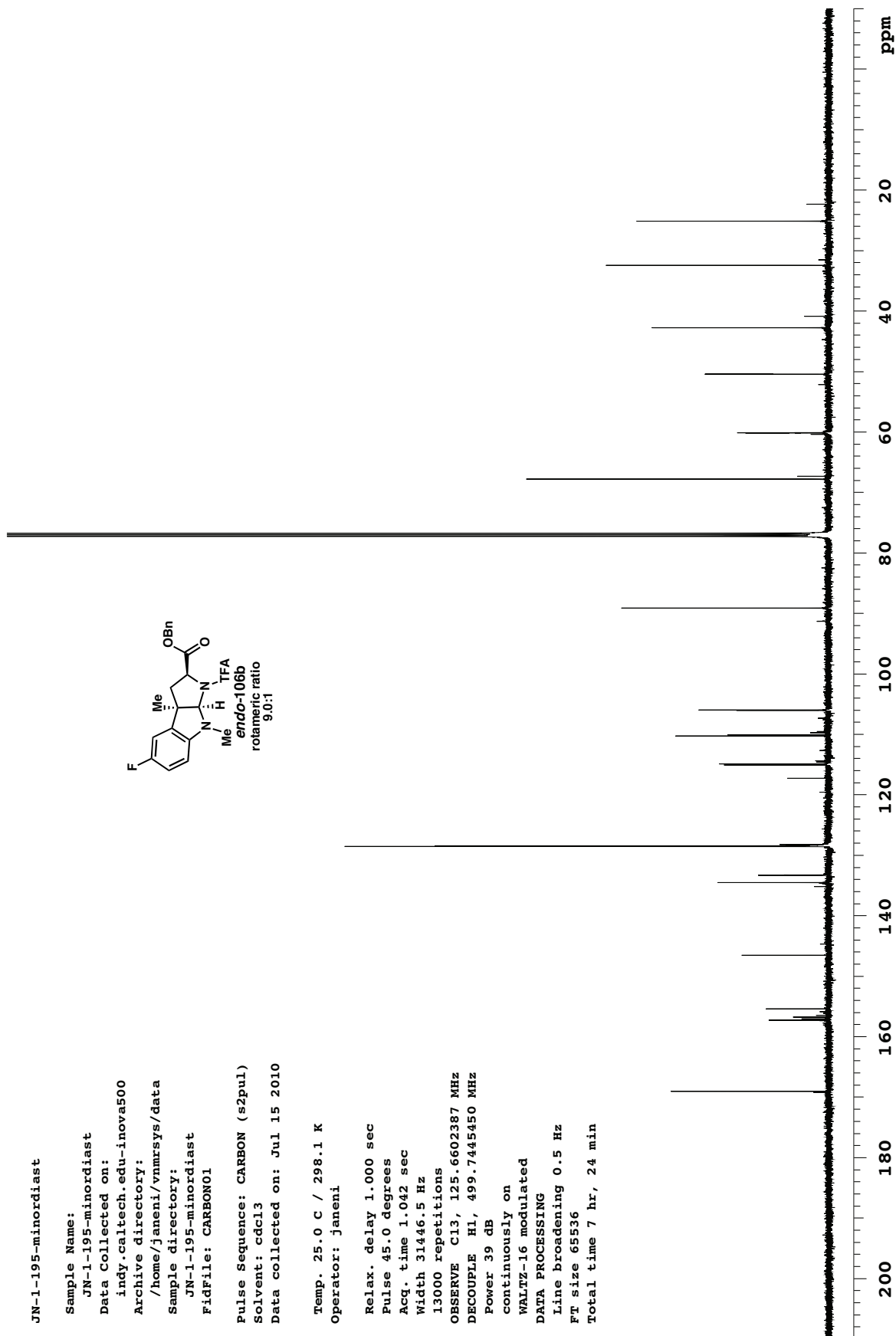
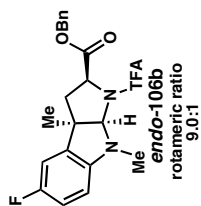
continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz
FT size 65536

Total time 7 hr, 24 min

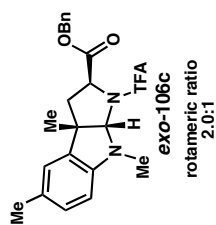


JN-1-171-majdiast

Sample Name:
JN-1-171-majdiast
Data Collected on:
sienna.caltech.edu-vnmrs400
Archive directory:
/home/jni/vnmrsys/data
Sample directory:
JN-1-171-majdiast
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2010

Temp. 25.0 C / 298.1 K
Sample #4, Operator: jni
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.7942813 MHz
DATA PROCESSING
Ft size 32768
Total time 7 min 21 sec



JN-1-171-majdiast

Sample Name:

JN-1-171-majdiast
Data Collected on:
siena.caltech.edu-vmrs400
Archive directory:
/home/jni/vmrsys/data
Sample directory:
JN-1-171-majdiast
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2010

Temp. 25.0 C / 298.1 K
Sample #4, Operator: jni

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
11000 repetitions

OBSERVE C13, 100.5283542 MHz
DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

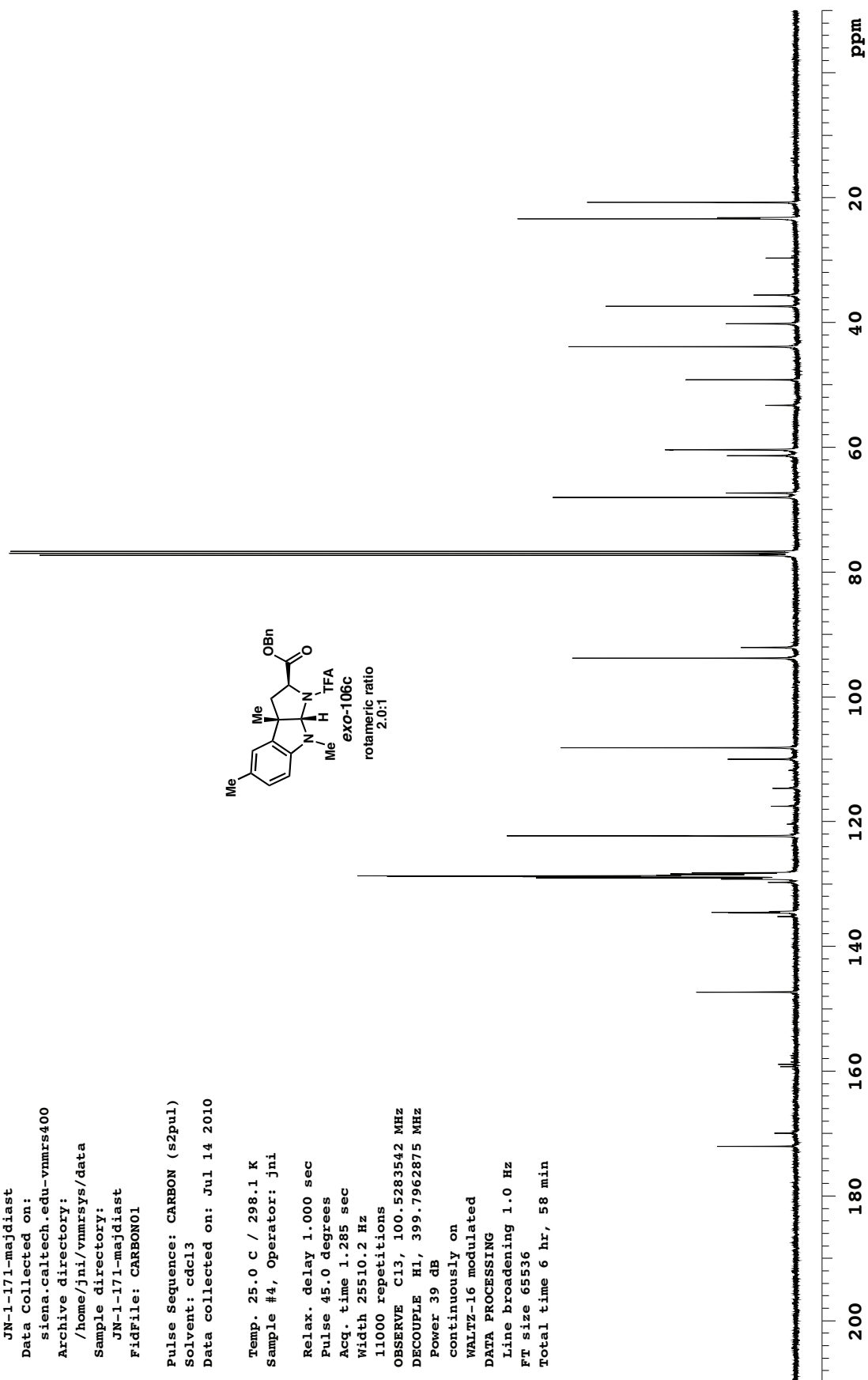
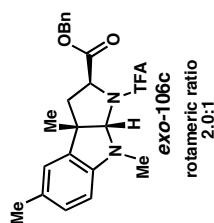
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 6 hr, 58 min



JN-1-171-mindiast2

Sample Name:

JN-1-171-mindiast2

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/jni/vnmrsys/data

Sample directory:

JN-1-171-mindiast2

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 13 2010

Temp. 25.0 C / 298.1 K

Sample #17, Operator: jni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4810.0 Hz

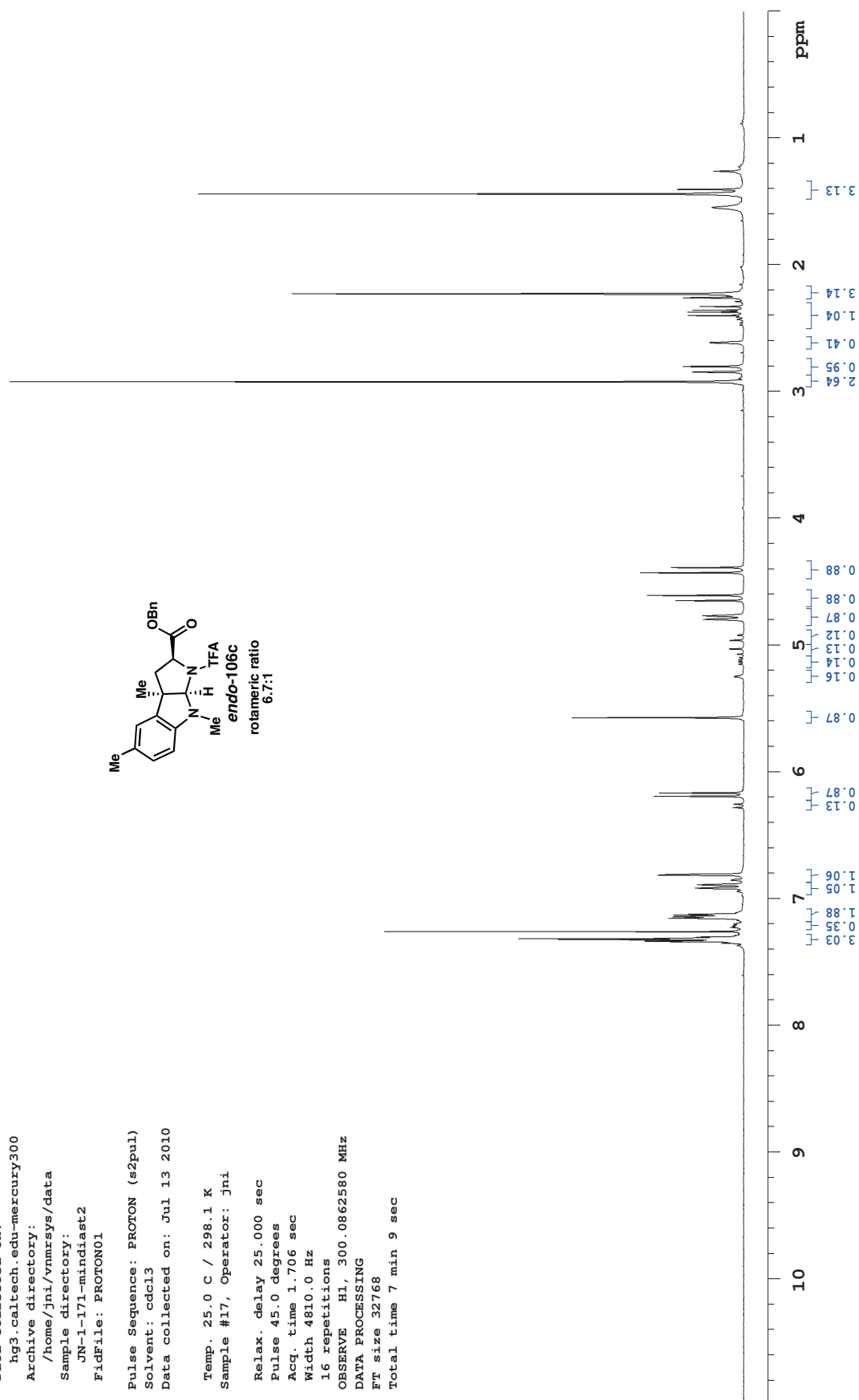
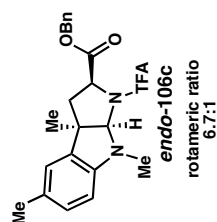
16 repetitions

OBSERVE H1, 300.0862580 MHz

DATA PROCESSING

Ft size 32768

Total time 7 min 9 sec



JN-1-171-minordiast2

Sample Name:
 JN-1-171-minordiast2
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/janeni/vnmrsys/data
 Sample directory:
 JN-1-171-minordiast2
 FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jul 14 2010

Temp. 25.0 C / 298.1 K
 Operator: janeni

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.042 sec
 Width 31446.5 Hz

13000 repetitions
 OBSERVE C13, 125.6602382 MHz
 DECOUPLE H1, 499.7445450 MHz
 Power 39 dB

continuously on

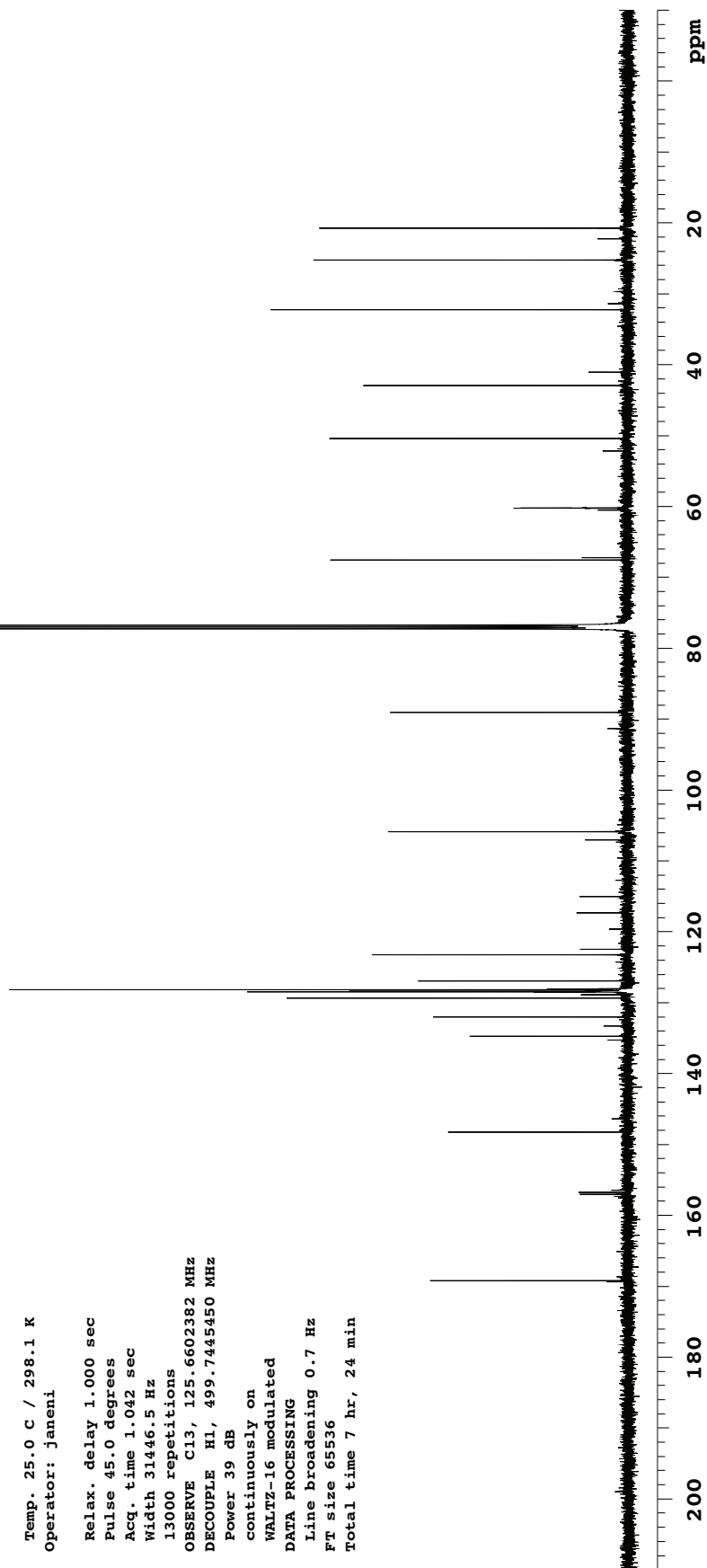
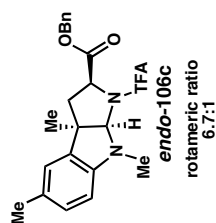
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.7 Hz

FT size 65536

Total time 7 hr, 24 min



LMRIV-177-major-dr-hsqc2

Sample Name:

LMRIV-177-major-dr-hsqc2

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-177-major-dr-hsqc2

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 31 2010

Operator: lrepka

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

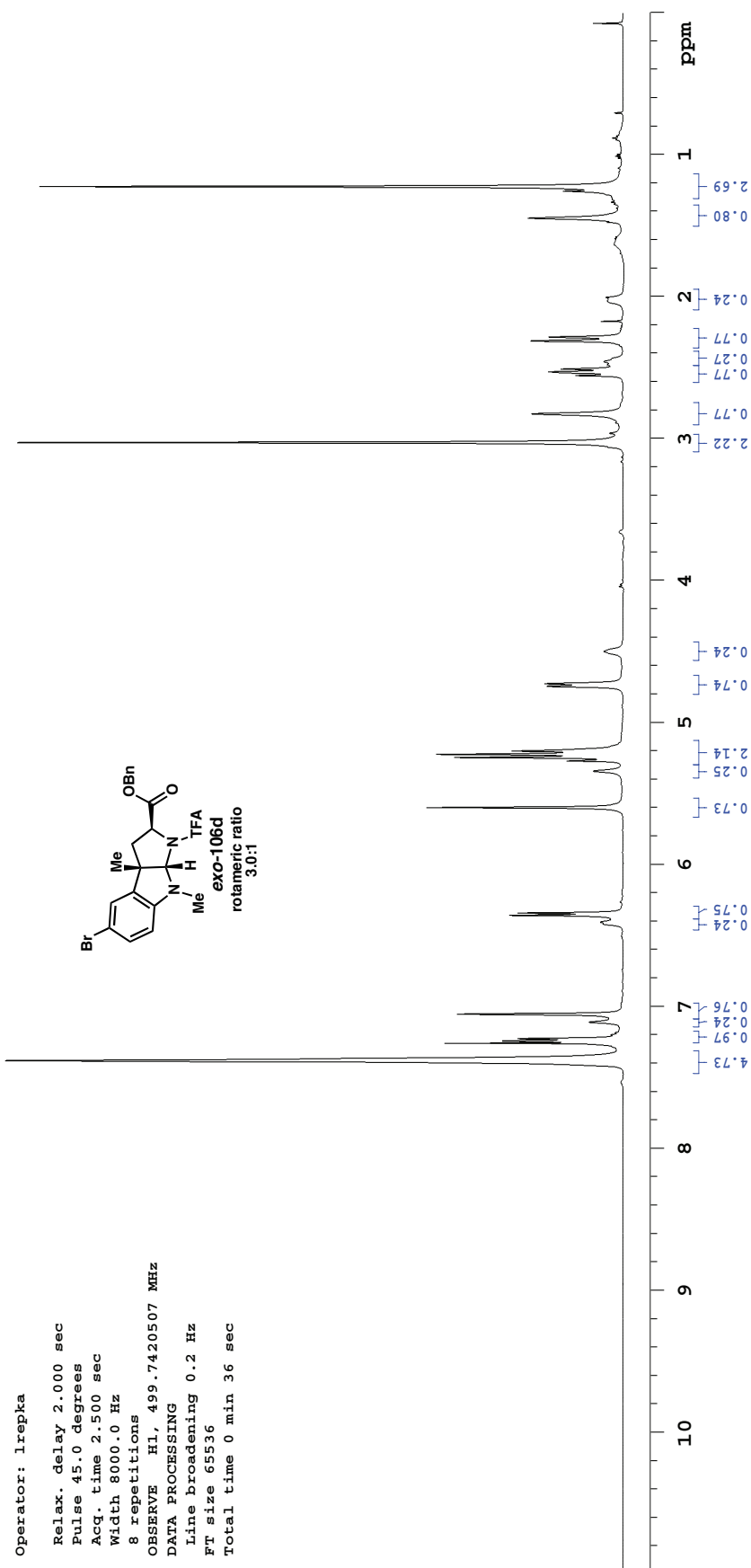
OBSERVE H1, 499.7420507 MHz

DATA PROCESSING

Line broadening 0.2 Hz

Ft size 65536

Total time 0 min 36 sec



LMRIV-177-major-dr-7-31-10

Sample Name:

LMRIV-177-major-dr-7-31-10

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-177-major-dr-7-31-10

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 31 2010

Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.022 sec

Width 32051.3 Hz

13250 repetitions

OBSERVE C13, 125.6602418 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

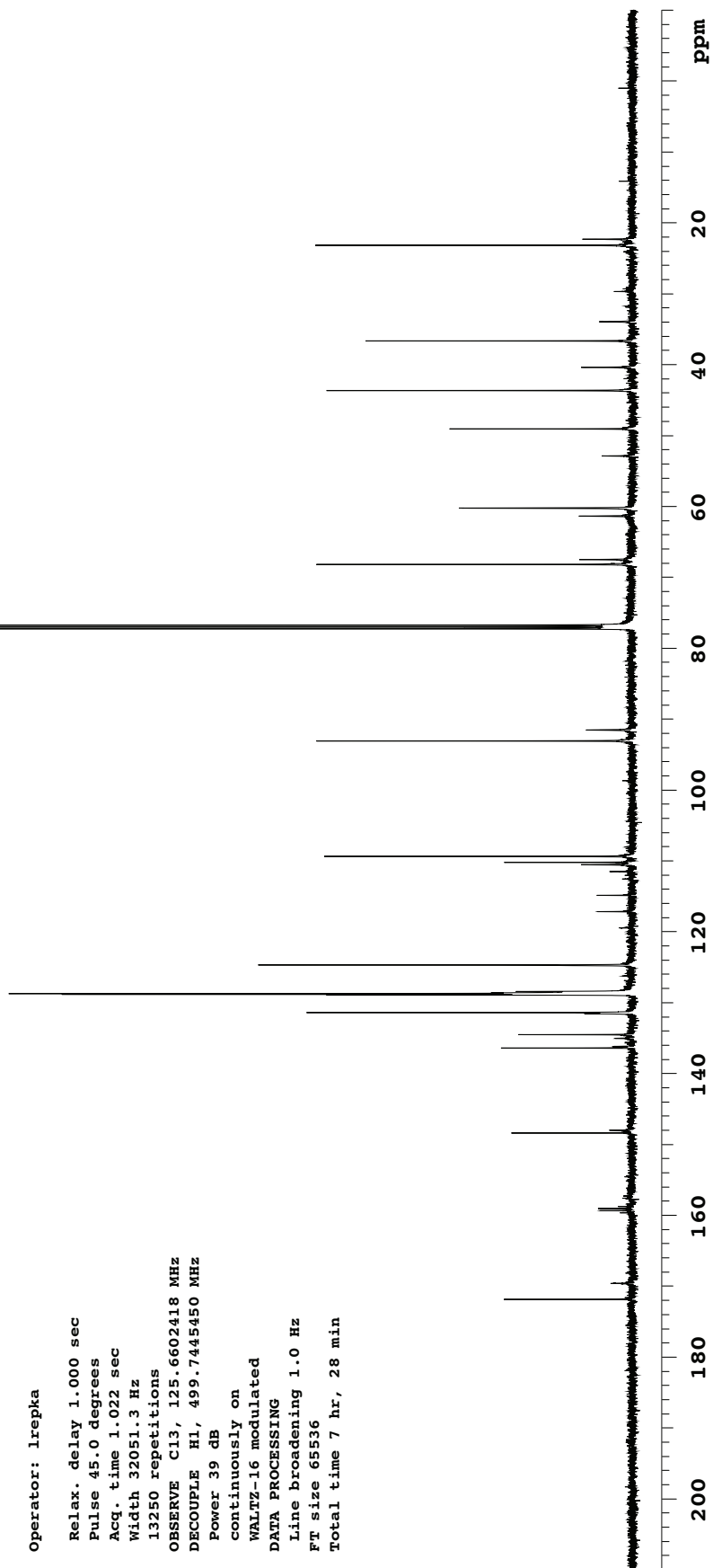
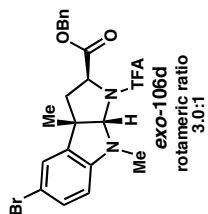
WALTZ-16 modulated

DATA PROCESSING

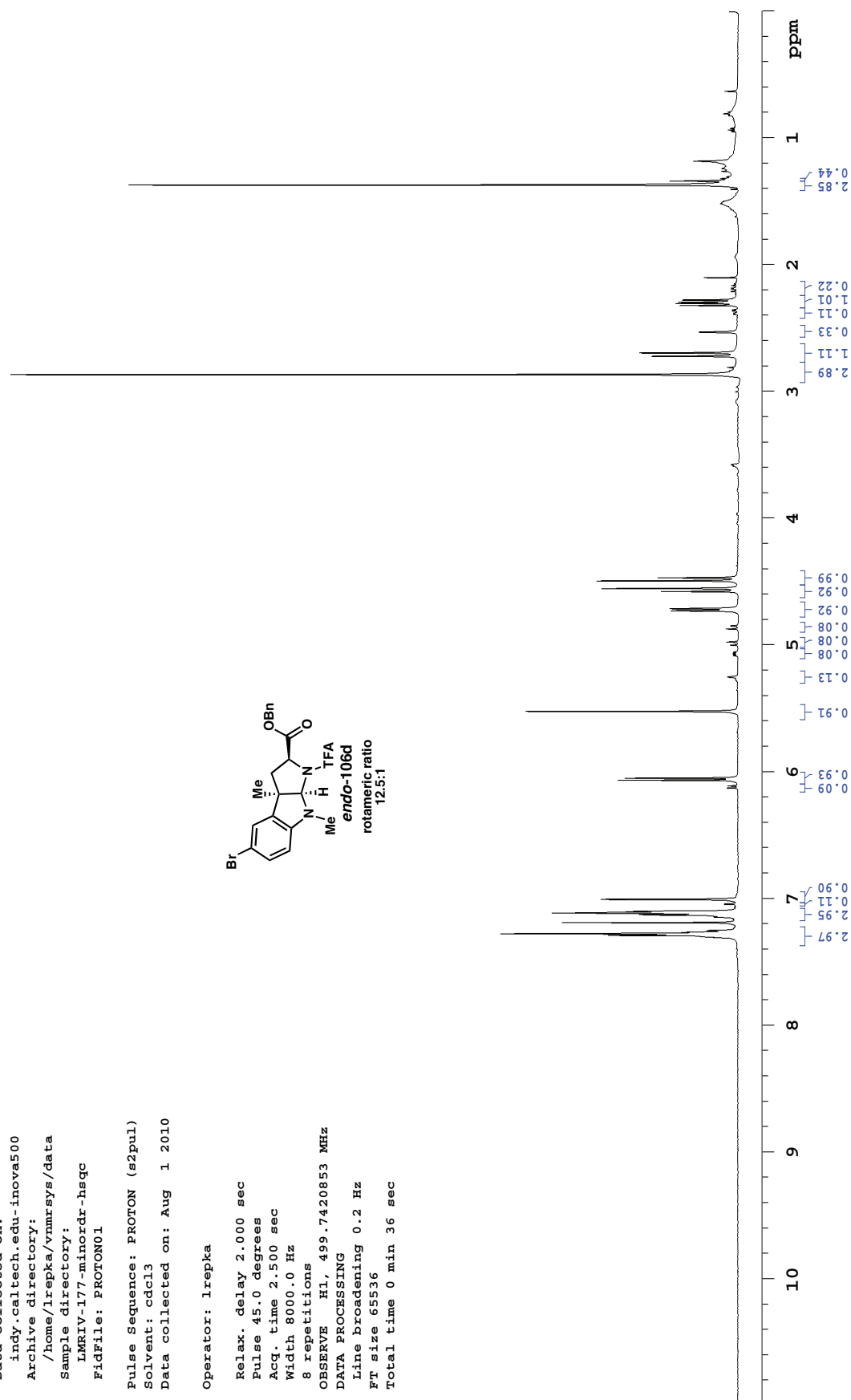
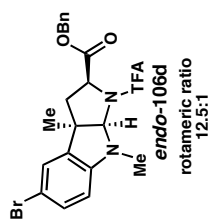
Line broadening 1.0 Hz

FT size 65536

Total time 7 hr, 28 min



Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.7420853 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 36 sec



LMRIV-177-minordr

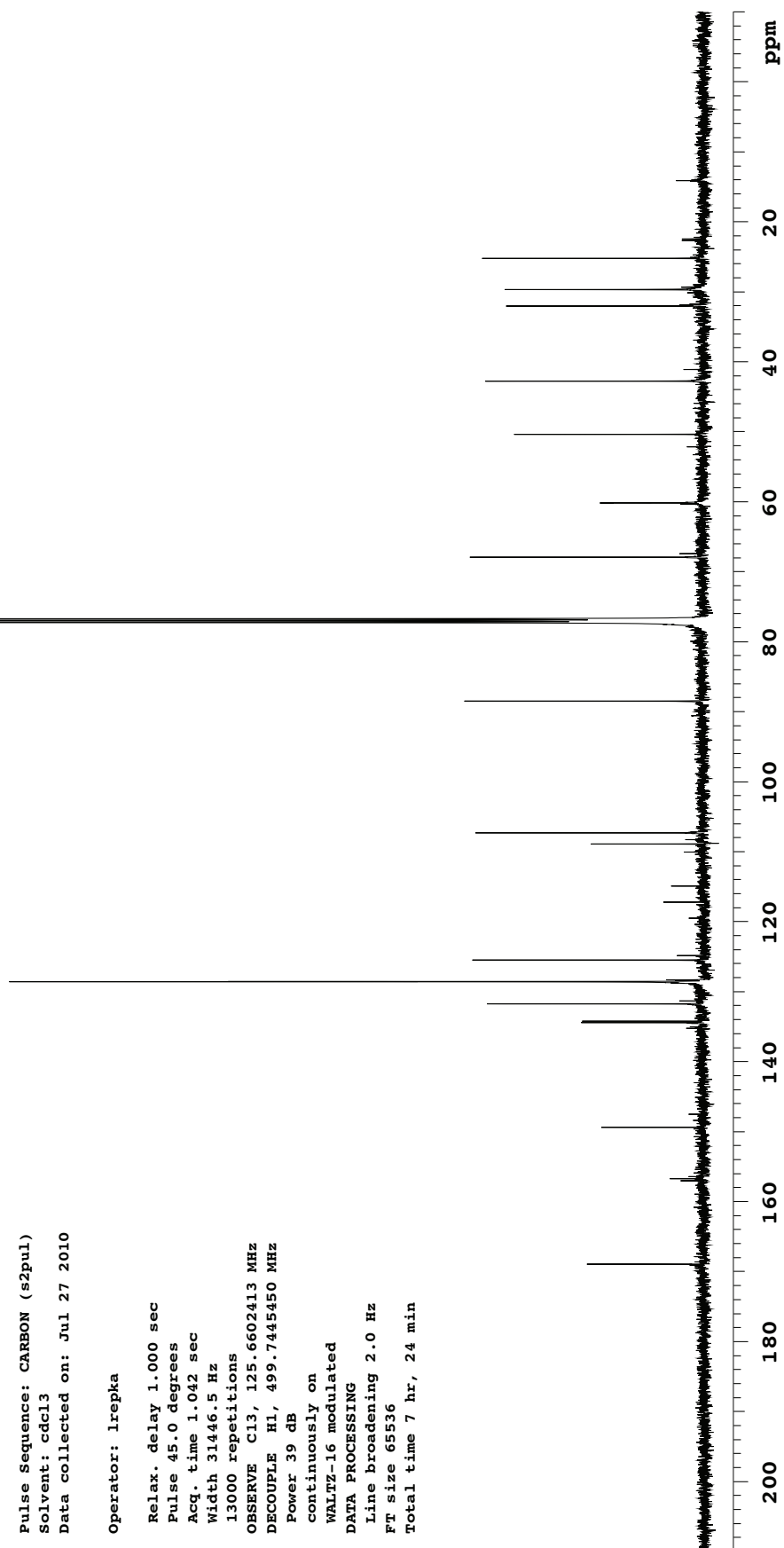
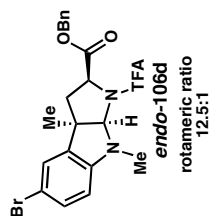
Sample Name:

LMRIV-177-minordr
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRIV-177-minordr
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 27 2010

Operator: lrepka

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
13000 repetitions
OBSERVE C13, 125.6602413 MHz
DECOUPLE H1, 499.7445450 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 7 hr, 24 min



JN-1-215-majoridiast2

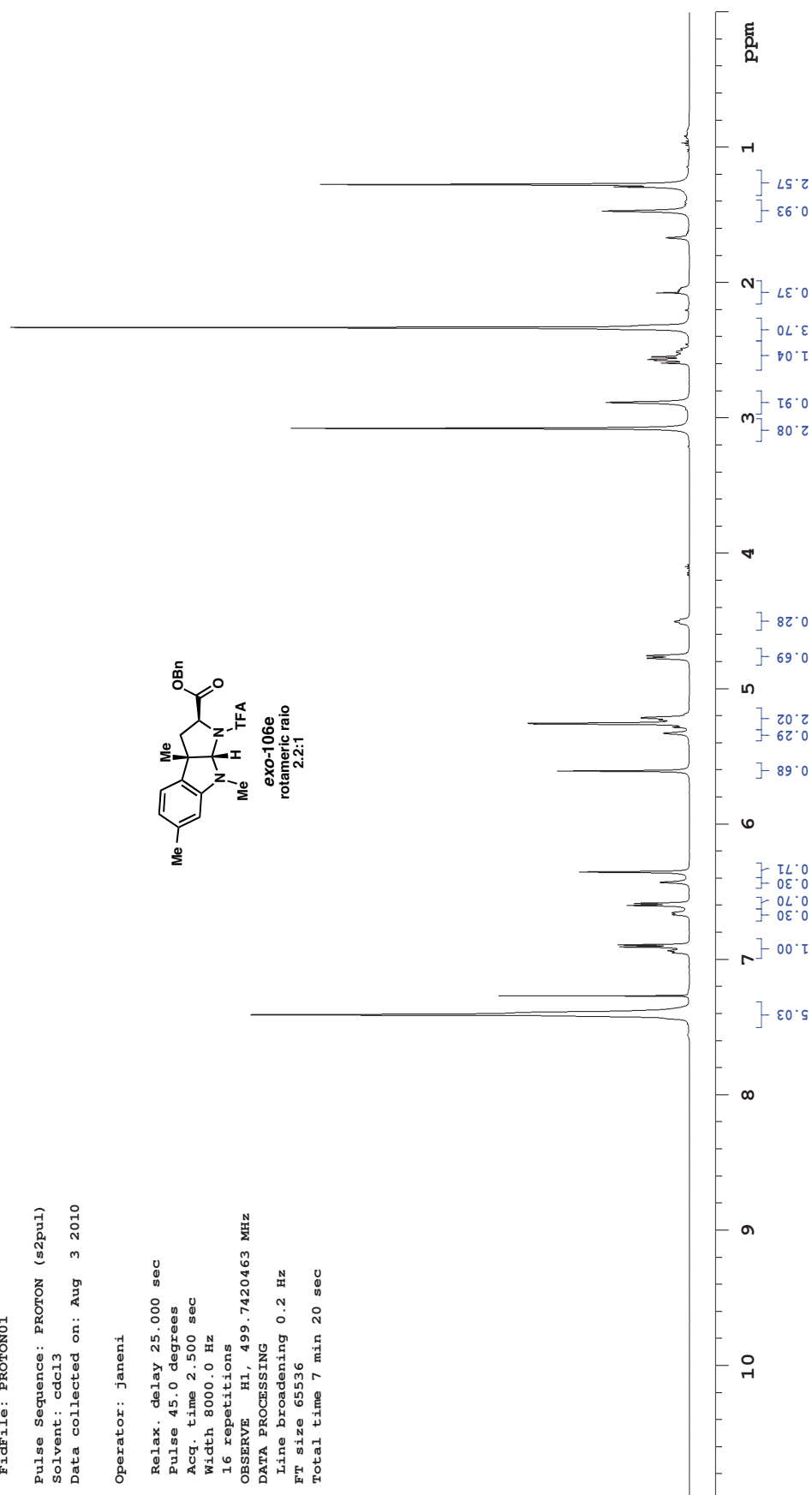
Sample Name:
 JN-1-215-majoridiast2
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/janeni/vnmrsys/data
 Sample directory:
 JN-1-215-majoridiast2
 FIDFile: PROTON01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Aug 3 2010

Operator: janeni

Relax. delay 25.000 sec
 Pulse 45.0 degrees
 Acq. time 2.500 sec
 Width 8000.0 Hz
 16 repetitions

OBSERVE H1, 499.7420463 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 7 min 20 sec



JN-1-215-majordiast2

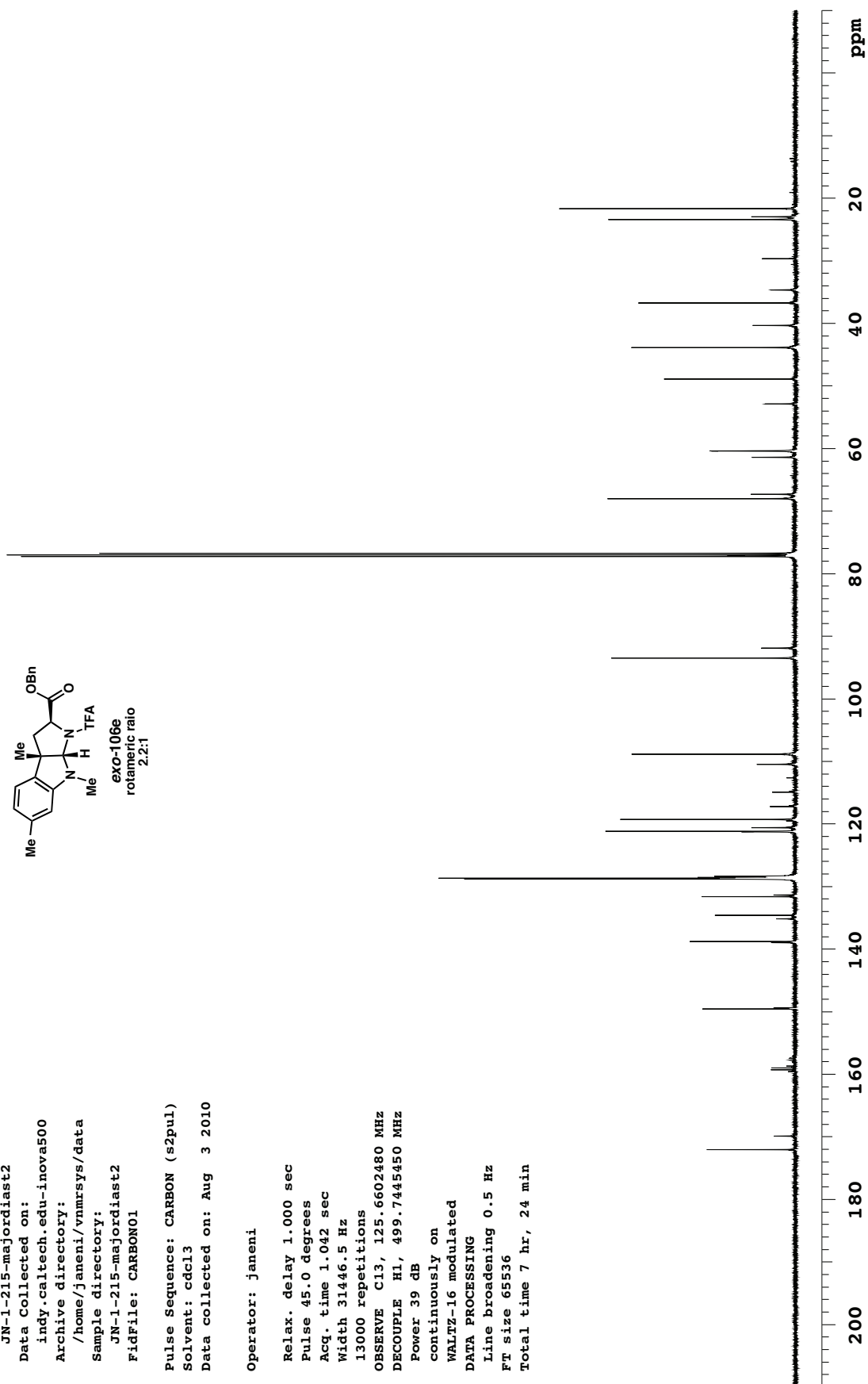
Sample Name:

JN-1-215-majordiast2
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/janeni/vnmrsys/data
Sample directory:
JN-1-215-majordiast2
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 3 2010

Operator: janeni

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
13000 repetitions
OBSERVE C13, 125.6602480 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 7 hr, 24 min



JN-1-215-minordiast2

Sample Name:

JN-1-215-minordiast2

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-215-minordiast2

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 2 2010

Operator: janeni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

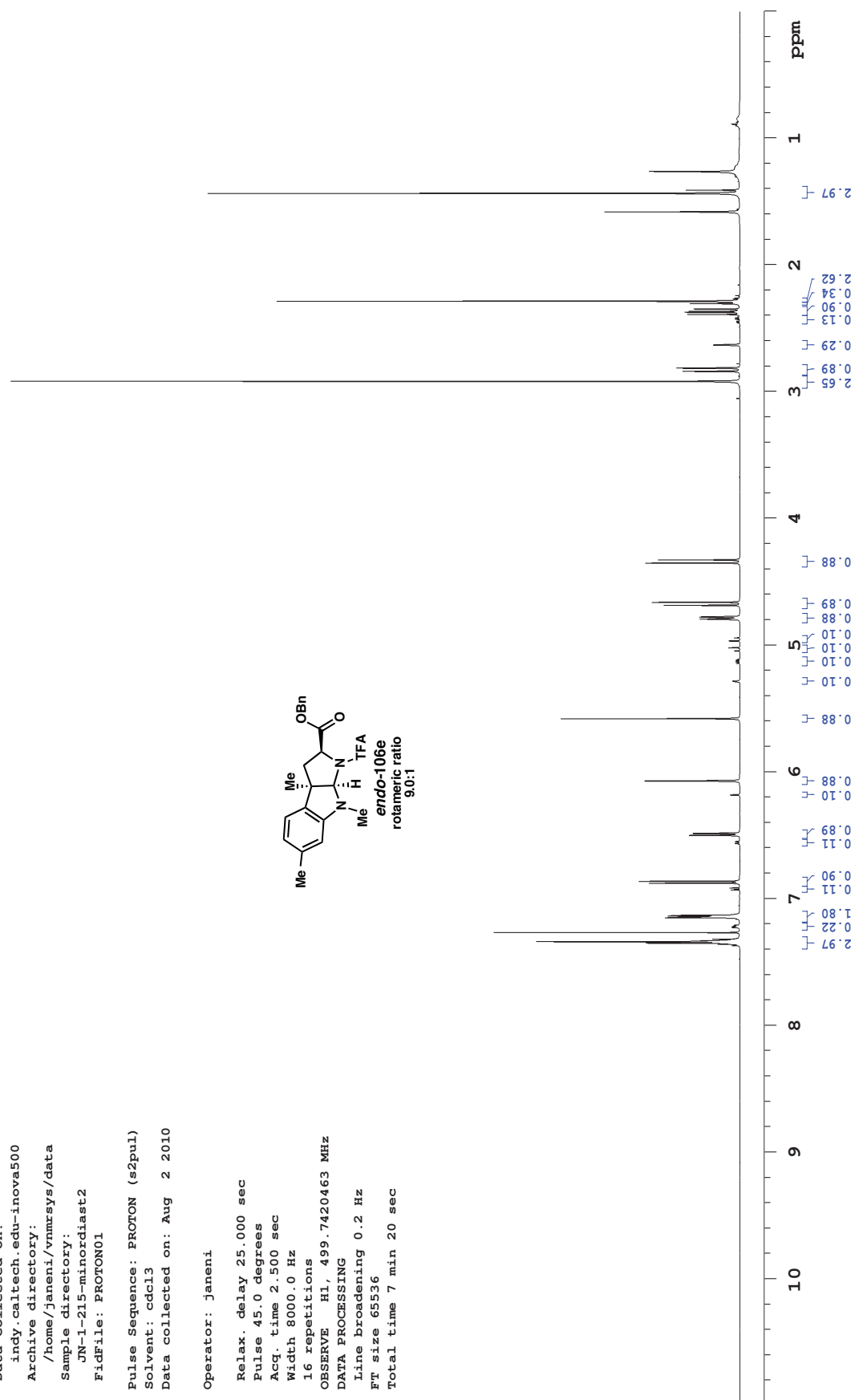
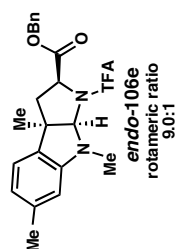
OBSERVE H1, 499.7420463 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 7 min 20 sec



JN-1-215-minordiast2

Sample Name:

JN-1-215-minordiast2

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-215-minordiast2

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 2 2010

Operator: janeni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

12500 repetitions

OBSERVE C13, 125.6602413 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

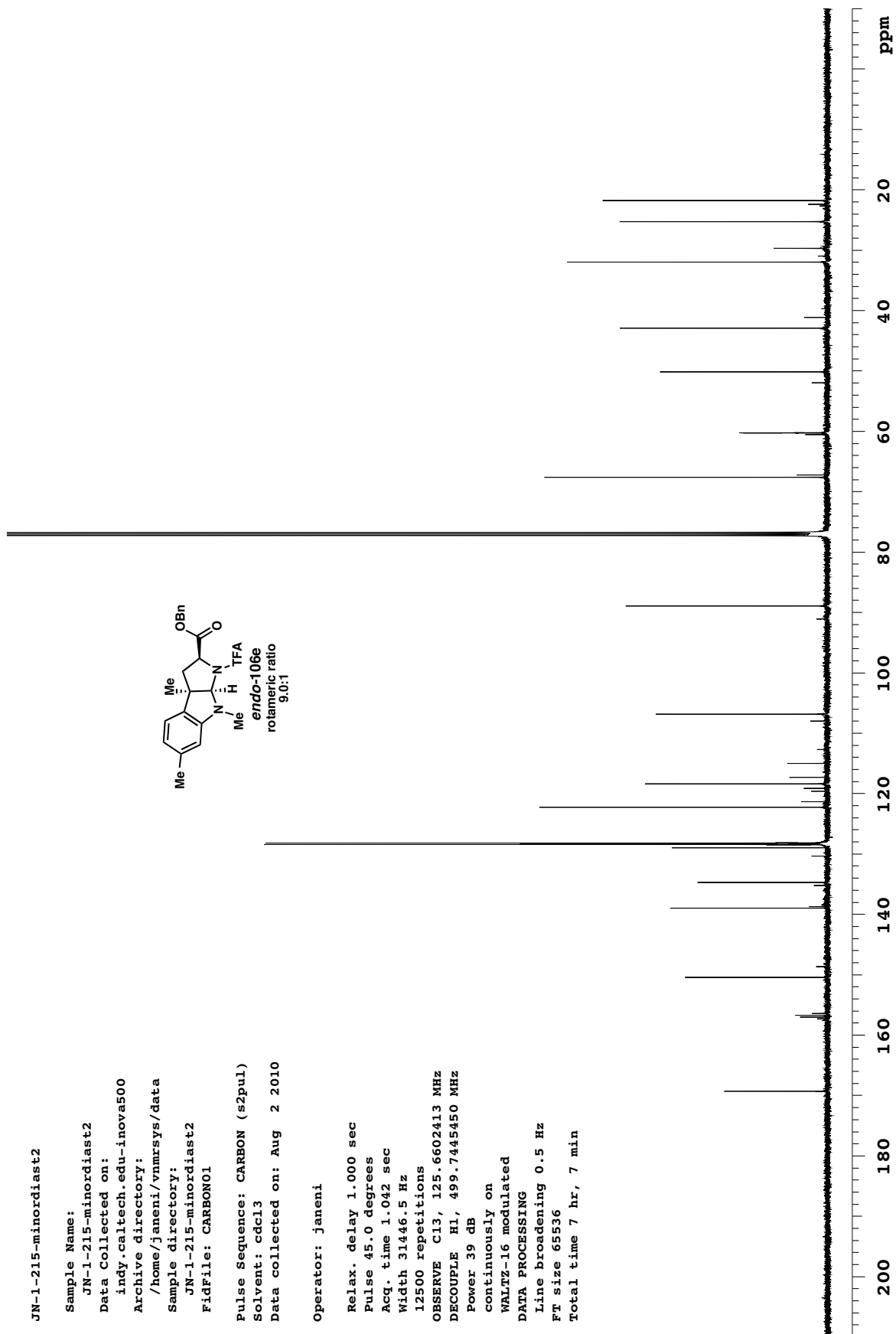
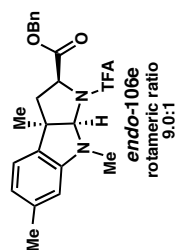
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 7 hr, 7 min



LMRIV-285-major-rd25

Sample Name:

LMRIV-285-major-rd25

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-285-major-rd25

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 30 2010

Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

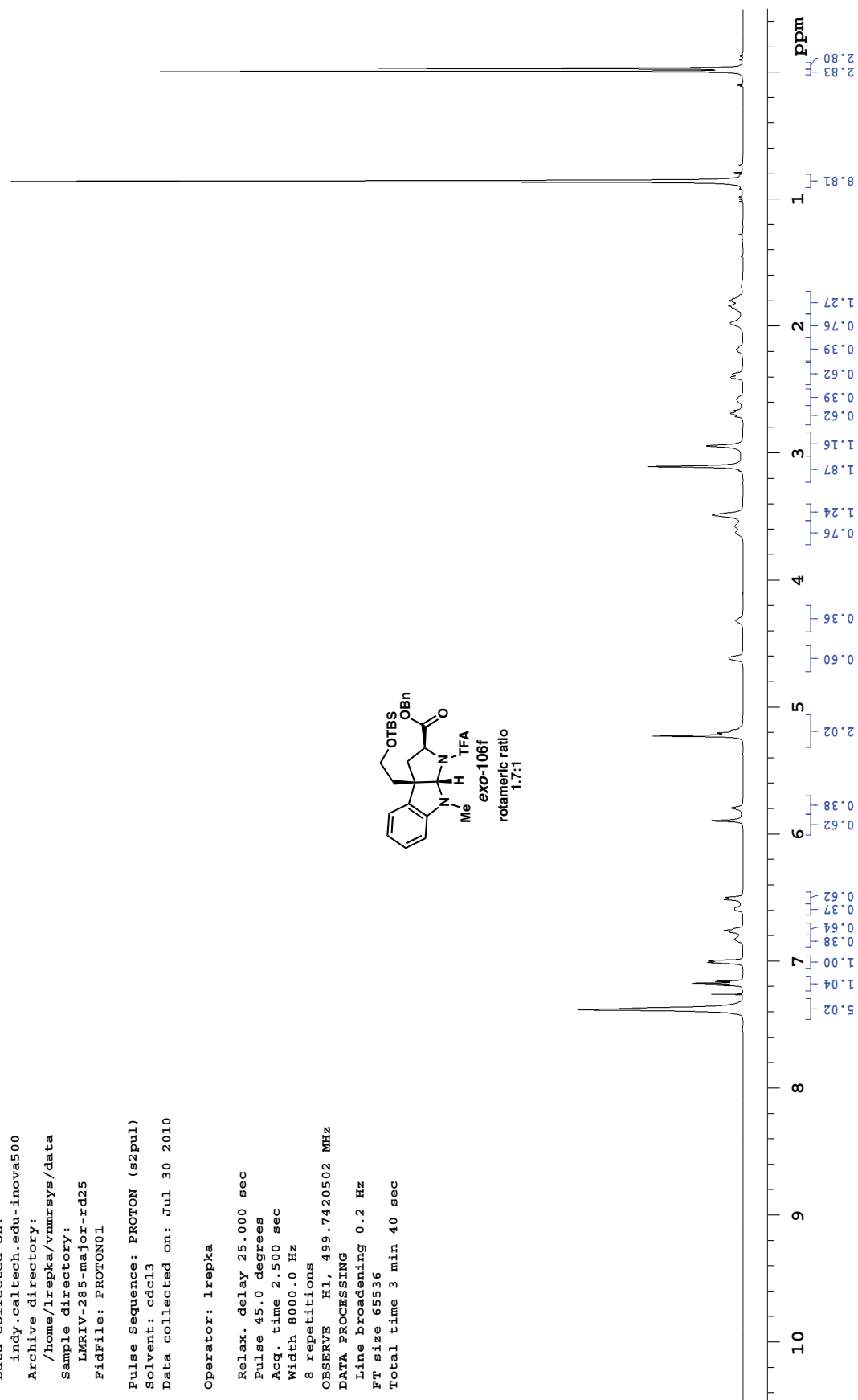
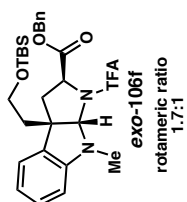
OBSERVE H1, 499.7420502 MHz

DATA PROCESSING

Line broadening 0.2 Hz

Ft size 65536

Total time 3 min 40 sec



LMRIV-285-major-dr-2-again

Sample Name:

LMRIV-285-major-dr-2-again

Data Collected on:

siena.caltech.edu-vnmrs400

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-285-major-dr-2-again

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 30 2010

Temp. 25.0 C / 298.1 K

Sample #2, Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.258 sec

Width 26041.7 Hz

10500 repetitions

OBSERVE C13, 100.5283569 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

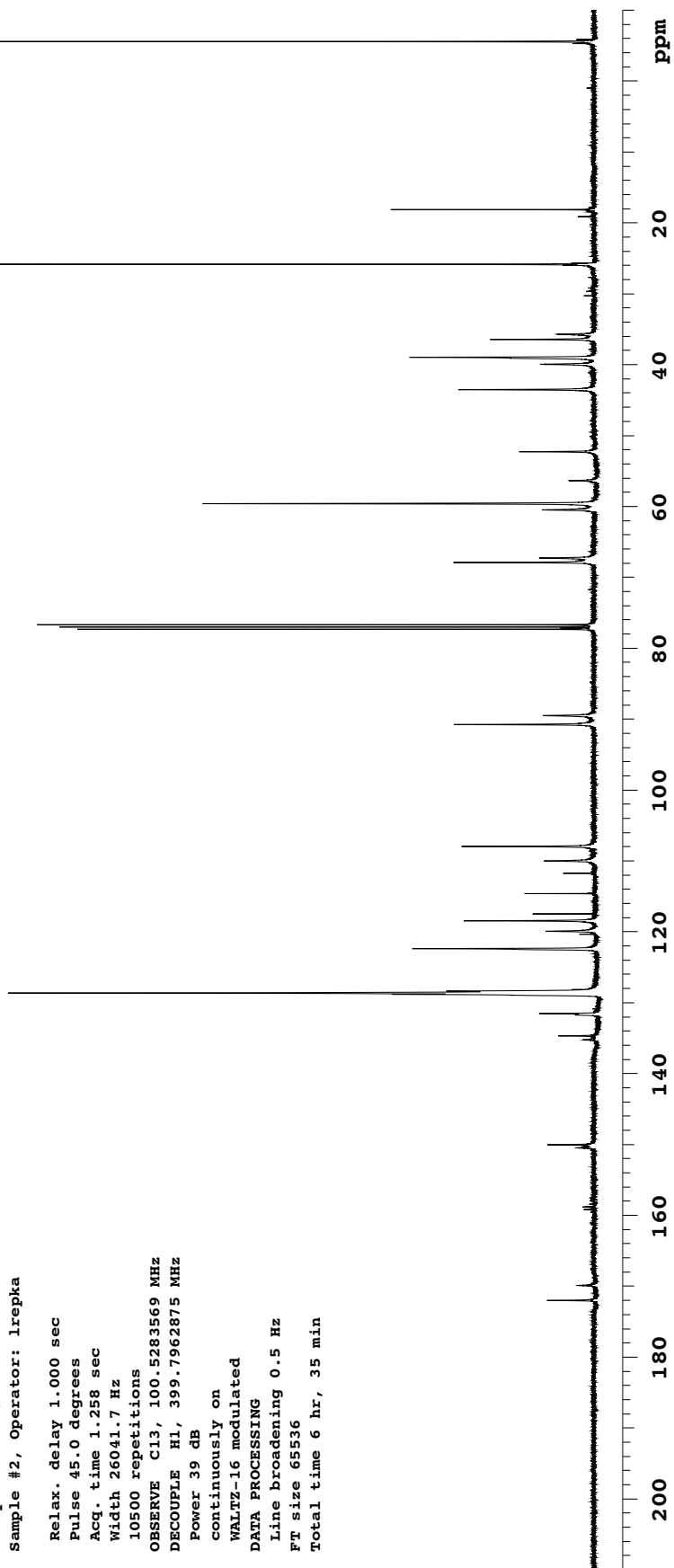
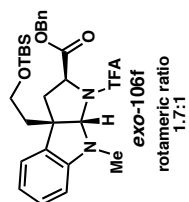
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 6 hr, 35 min



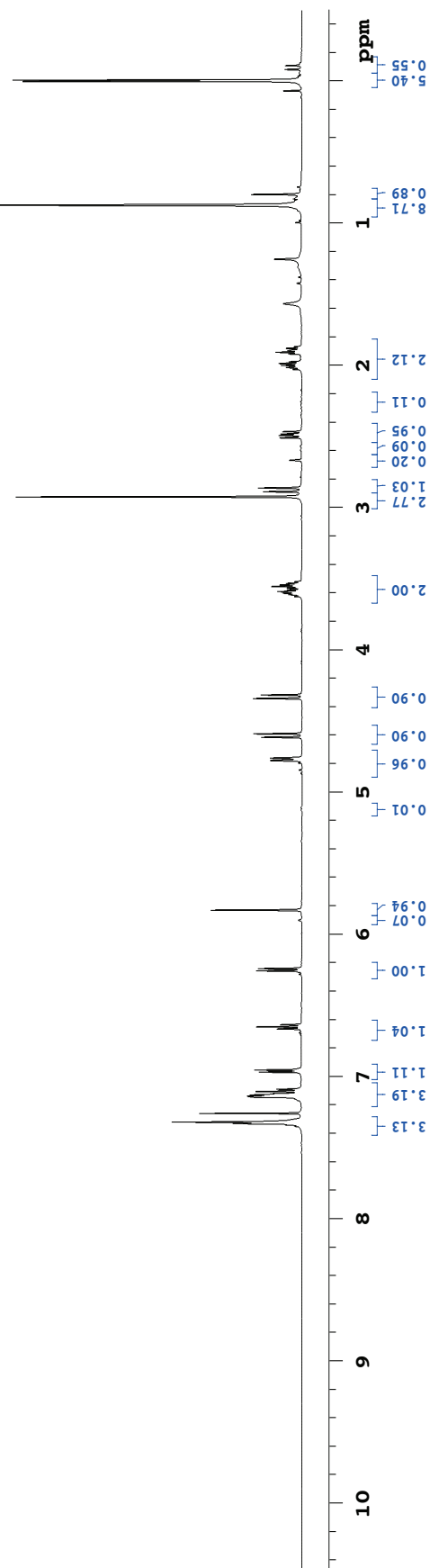
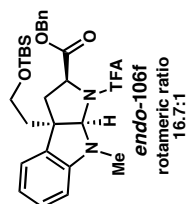
LMRIV-285-minor-rd25

Sample Name:
 LMRIV-285-minor-rd25
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/lrepka/vnmrsys/data
 Sample directory:
 LMRIV-285-minor-rd25
 FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jul 30 2010

Operator: lrepka

Relax. delay 25.000 sec
 Pulse 45.0 degrees
 Acq. time 2.500 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.7420512 MHz
 DATA PROCESSING
 Line broadening 0.2 Hz
 FT size 65536
 Total time 3 min 40 sec



LMRIV-285-minordr-2-carbon

Sample Name:

LMRIV-285-minordr-2-carbon

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRIV-285-minordr-2-carbon

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 30 2010

Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.022 sec

Width 32051.3 Hz

13000 repetitions

OBSERVE C13, 125.6602398 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

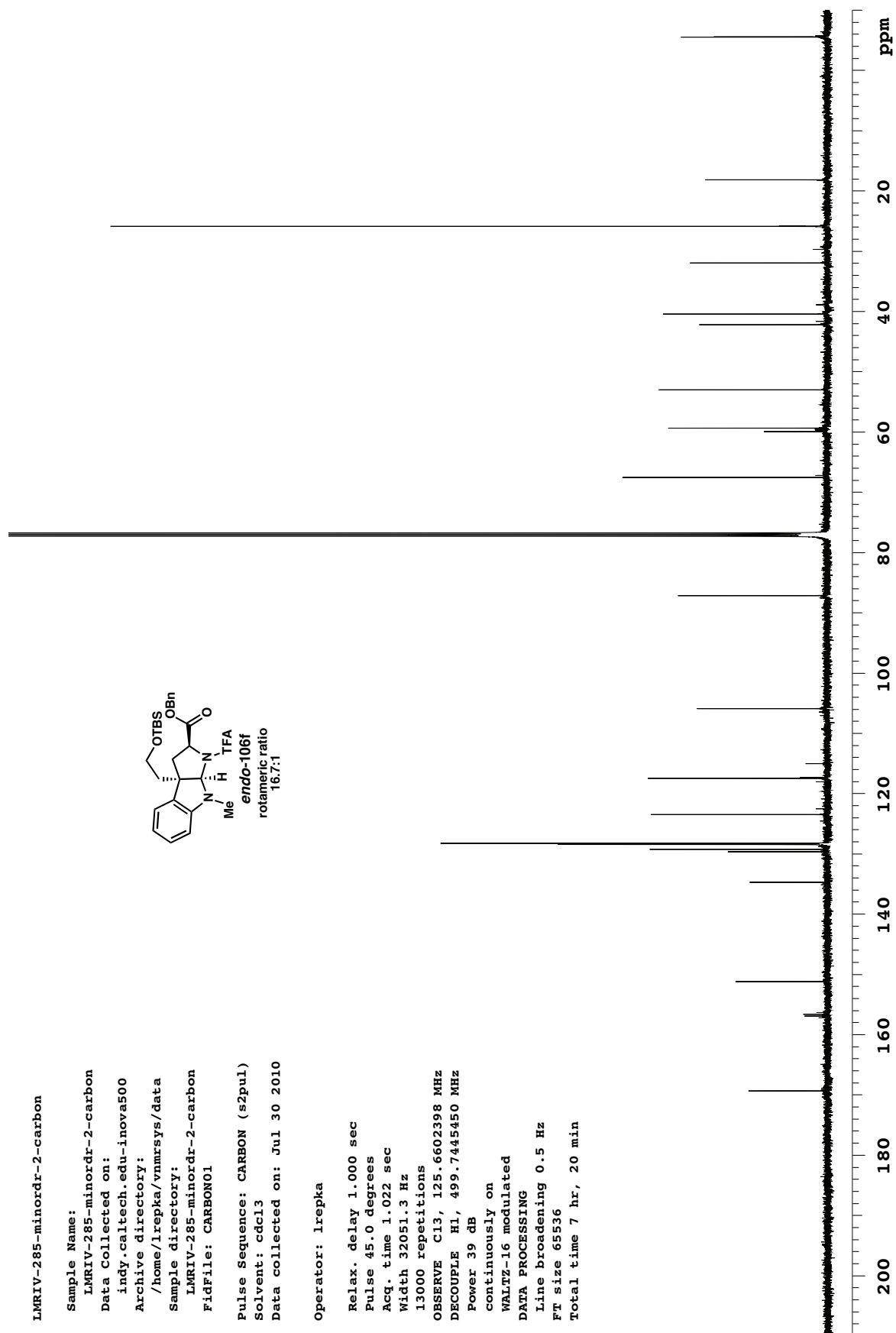
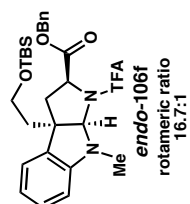
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 7 hr, 20 min



LMRIV-275-pentanewash

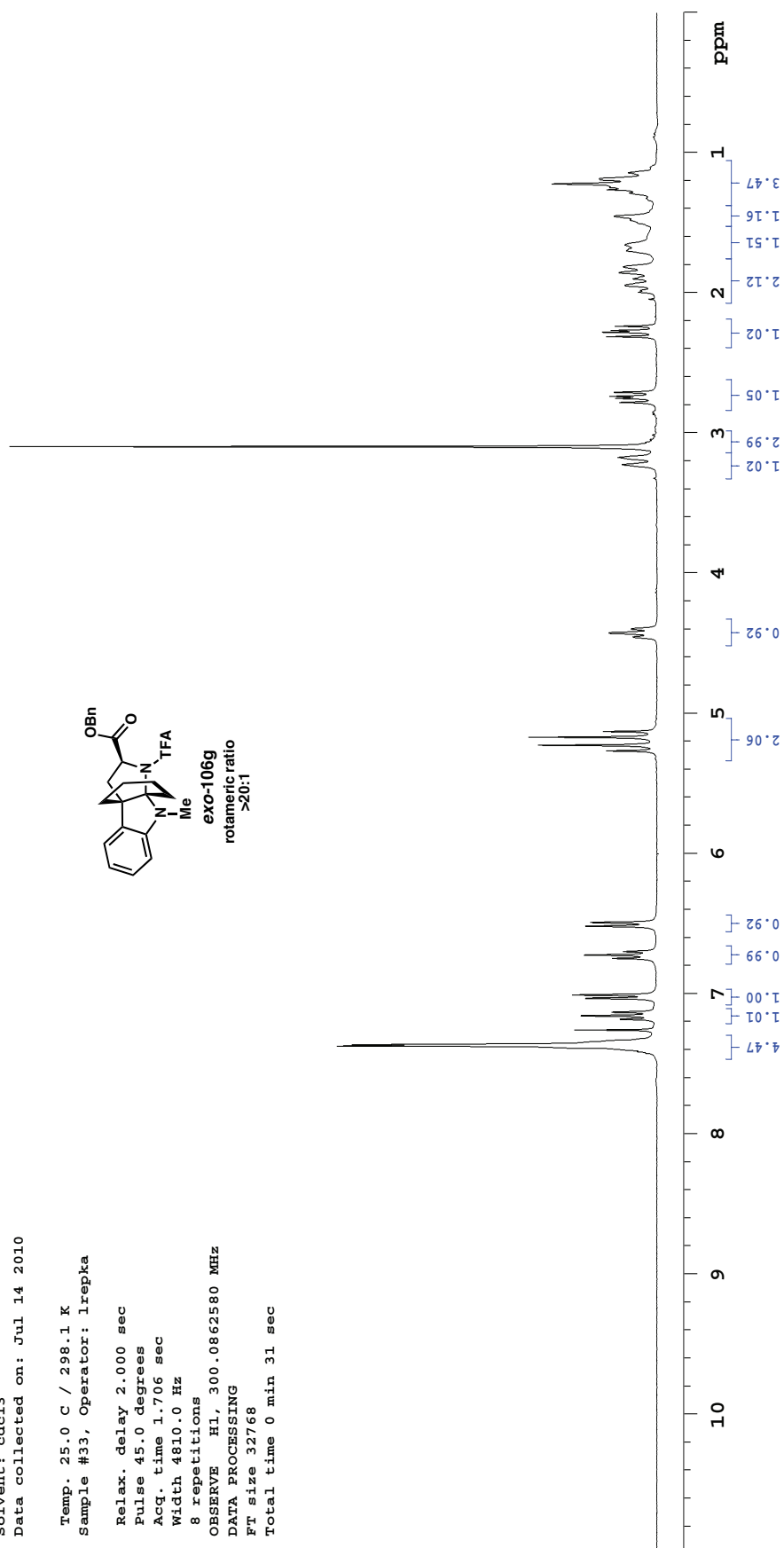
Sample Name:
LMRIV-275-pentanewash
Data Collected on:
hg3.caltech.edu-mercury300
Archive directory:
/home/lrepka/vnmrSYS/data
Sample directory:
LMRIV-275-pentanewash
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2010

Temp. 25.0 C / 298.1 K
Sample #33, Operator: lrepka

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.706 sec
Width 4810.0 Hz
8 repetitions

OBSERVE H1, 300.0862580 MHz
DATA PROCESSING
Ft size 32768
Total time 0 min 31 sec



LMRIV-275

Sample Name:

LMRIV-275

Data Collected on:

siena.caltech.edu-vmrs400

Archive directory:

/home/jni/vmrsys/data

Sample directory:

LMRIV-275

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 15 2010

Temp. 25.0 C / 298.1 K

Sample #8, Operator: jni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.285 sec

Width 25510.2 Hz

11500 repetitions

OBSERVE C13, 100.5283535 MHz

DECOUPLE H1, 399.7962875 MHz

Power 39 dB

continuously on

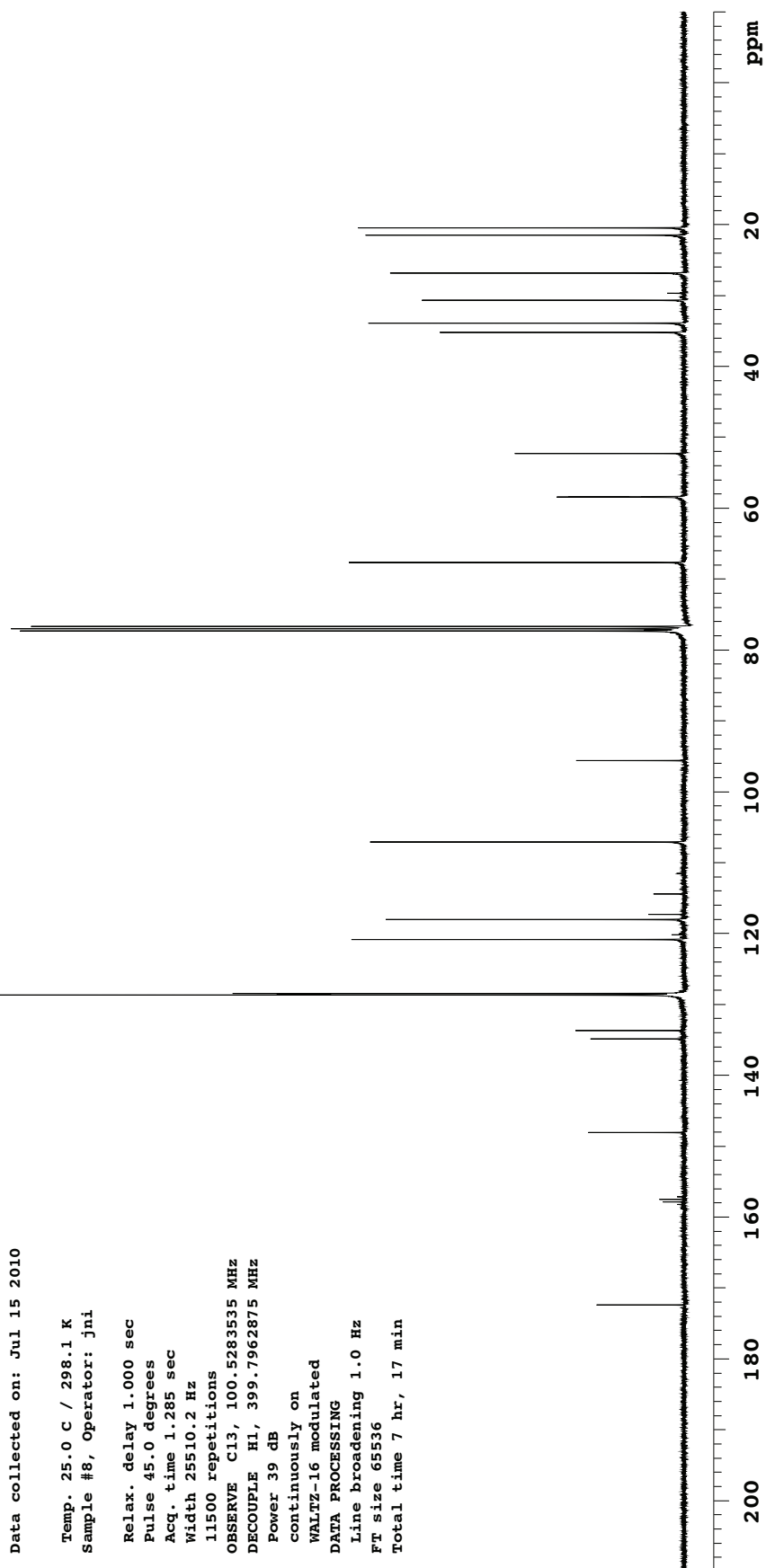
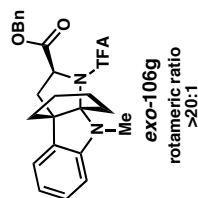
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 7 hr, 17 min



LMRIV-267-major diastereomer

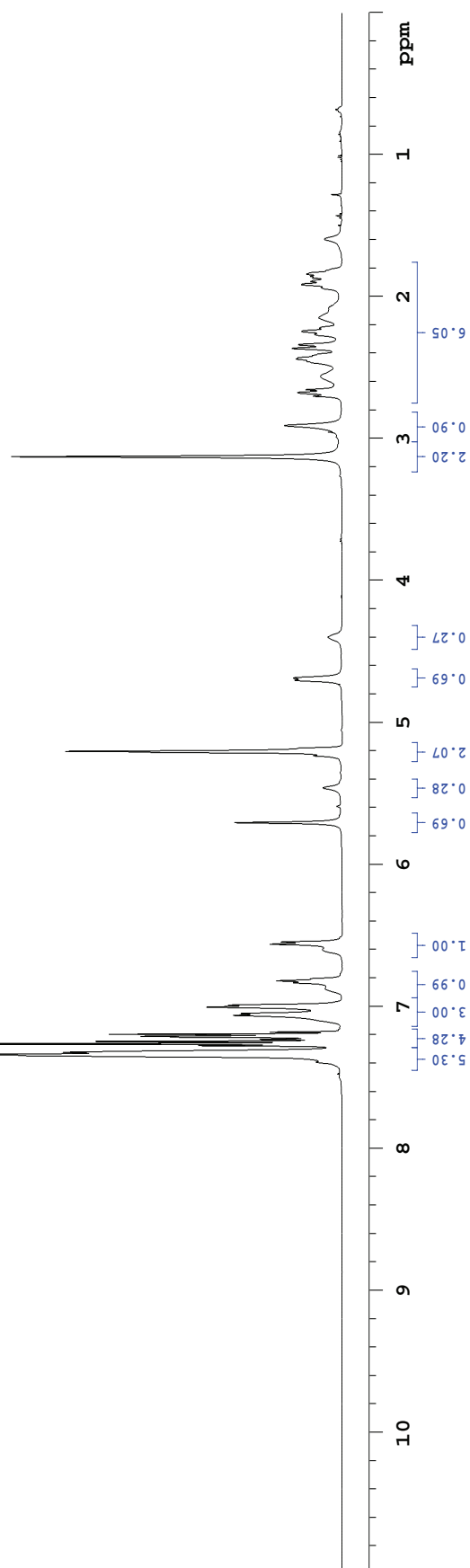
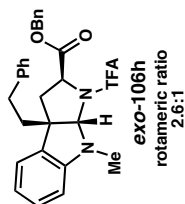
Sample Name:
LMRIV-267-majordr
Data Collected on:
indy.caltech.edu-incova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRIV-267-majordr
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 19 2010

Temp. 25.0 C / 298.1 K
Operator: lrepka

Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 8000.0 Hz
16 repetitions

OBSERVE H1, 499.7420463 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 7 min 20 sec



LMRIV-267-majorshigemi

Sample Name:

LMRIV-267-majorshigemi
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRIV-267-majorshigemi
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 20 2010

Temp. 25.0 C / 298.1 K
Operator: lrepka

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
12400 repetitions

OBSERVE C13, 125.6602469 MHz
DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

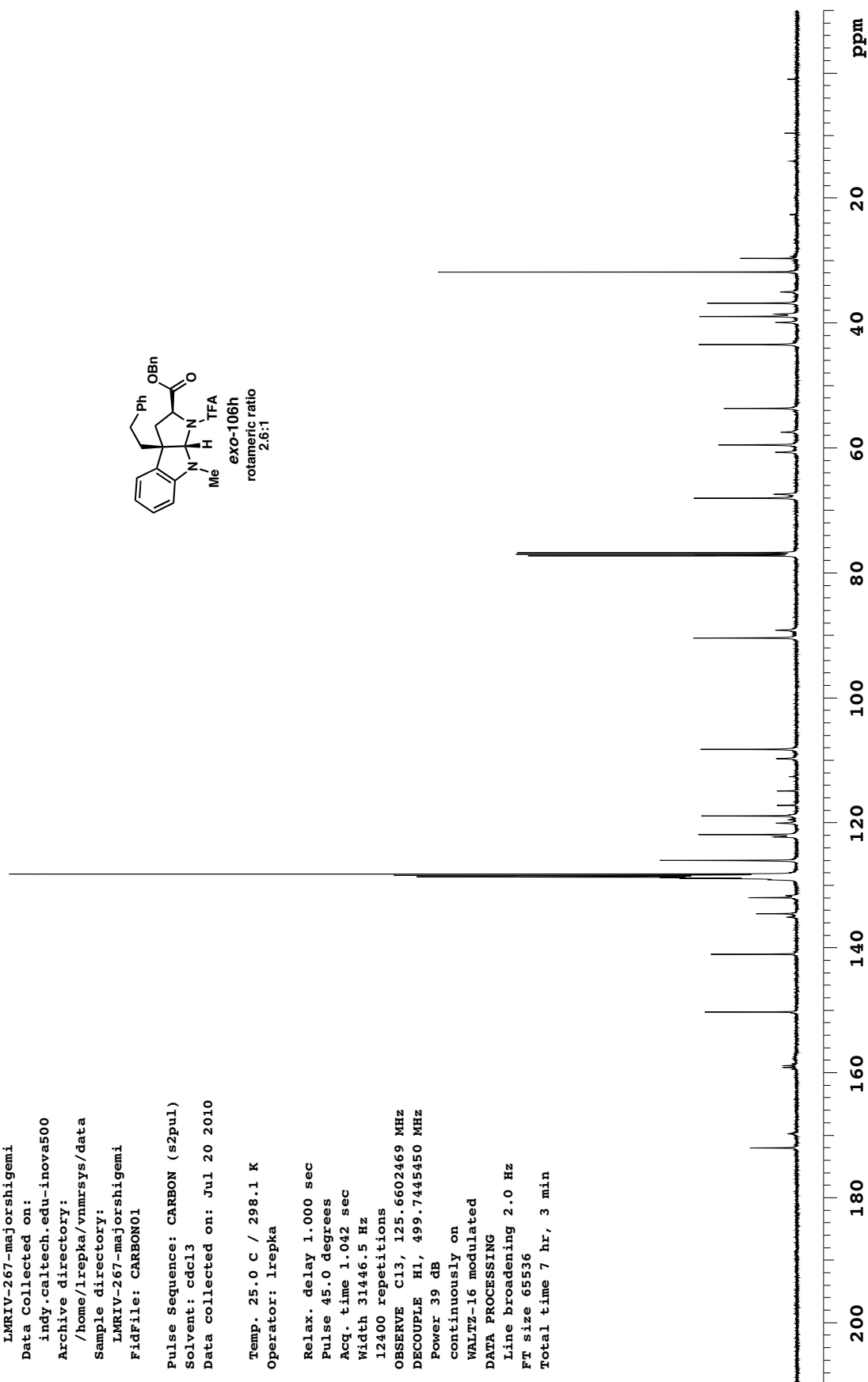
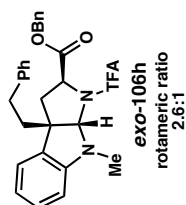
WALTZ-16 modulated

DATA PROCESSING

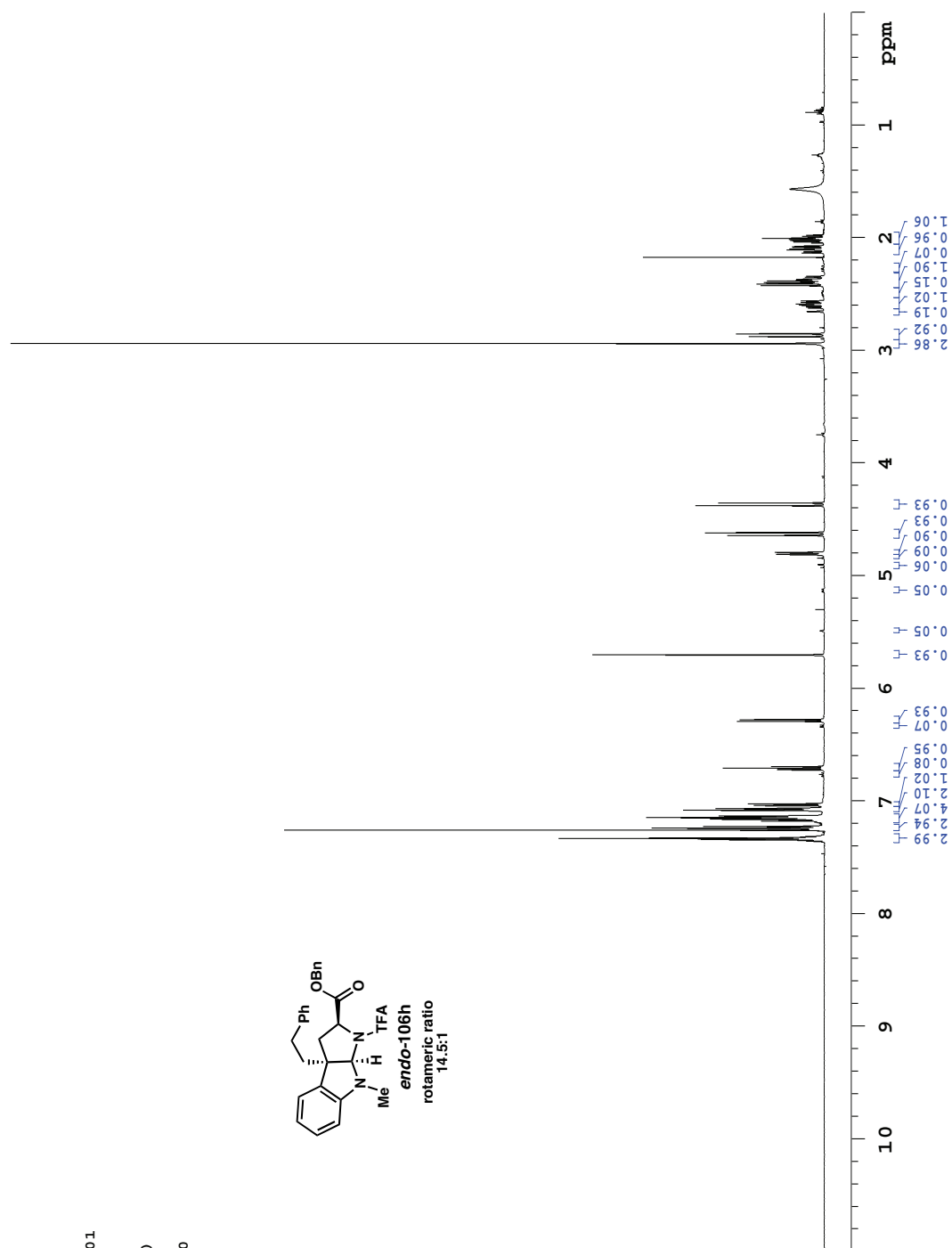
Line broadening 2.0 Hz

FT size 65536

Total time 7 hr, 3 min



endo-106h
rotameric ratio
14.5:1



LMRIV-267-minor3

Sample Name:

LMRIV-267-minor3

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrSYS/data

Sample directory:

LMRIV-267-minor3_20100717_01

FidFile: data_s2pul_002

Pulse Sequence: CARBON (s2pul)

Solvent: CDCl₃

Data collected on: Jul 17 2010

Temp. 25.0 C / 298.1 K

Operator: lrepka

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.043 sec

Width 31409.5 Hz

12000 repetitions

OBSERVE C13, 125.6602386 MHz

DECOUPLE H1, 499.7445450 MHz

Power 39 dB

continuously on

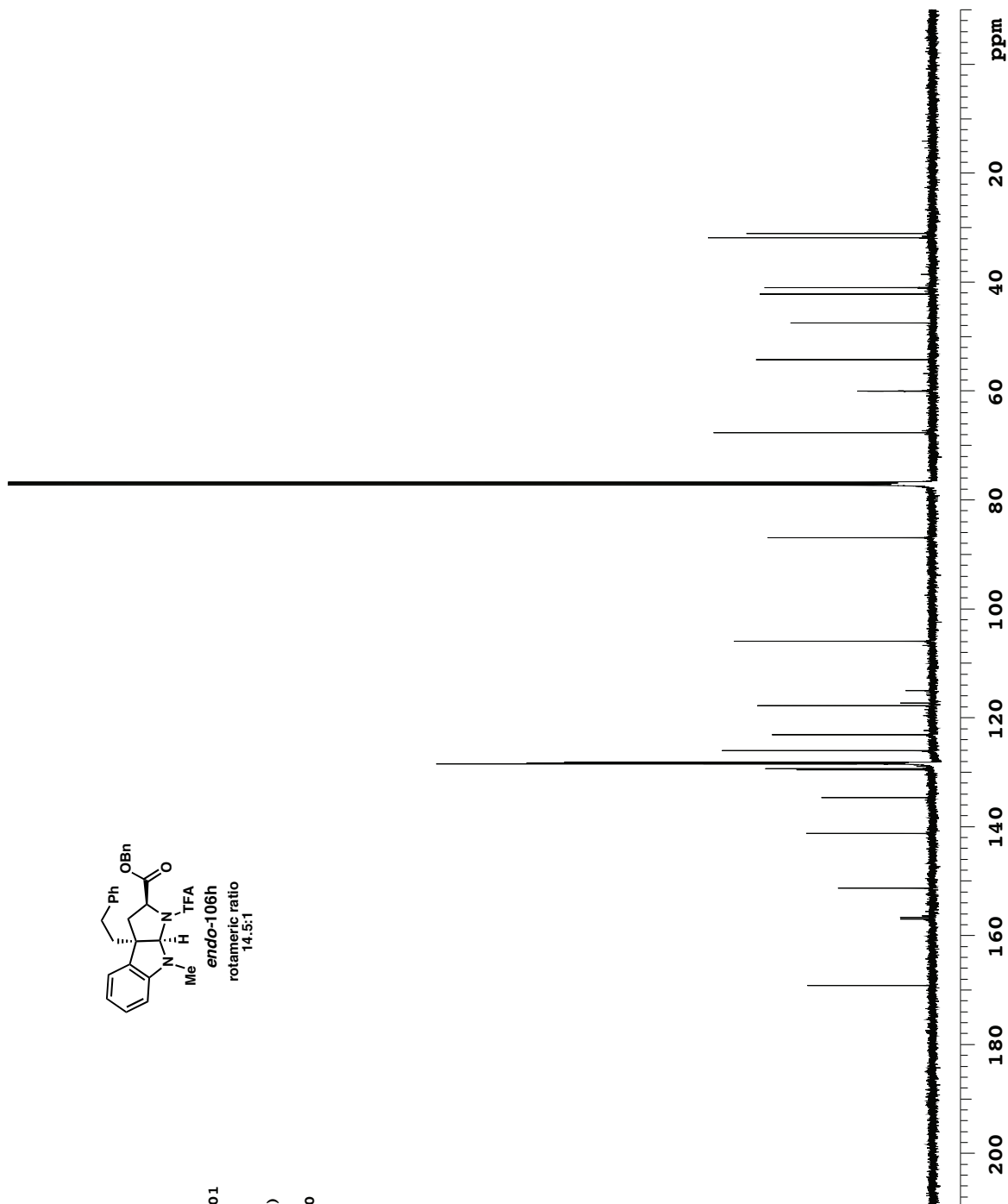
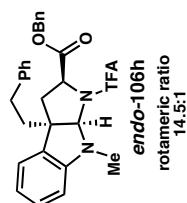
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 6 hr, 50 min



JN-1-211-majordiast

Sample Name:

JN-1-211-majordiast

Data Collected on:

sienna.caltech.edu—vnmrs400

Archive directory:

/home/jni/vnmrsys/data

Sample directory:

JN-1-211-majordiast

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 28 2010

Temp. 25.0 C / 298.1 K

Sample #6, Operator: jni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.556 sec

Width 6410.3 Hz

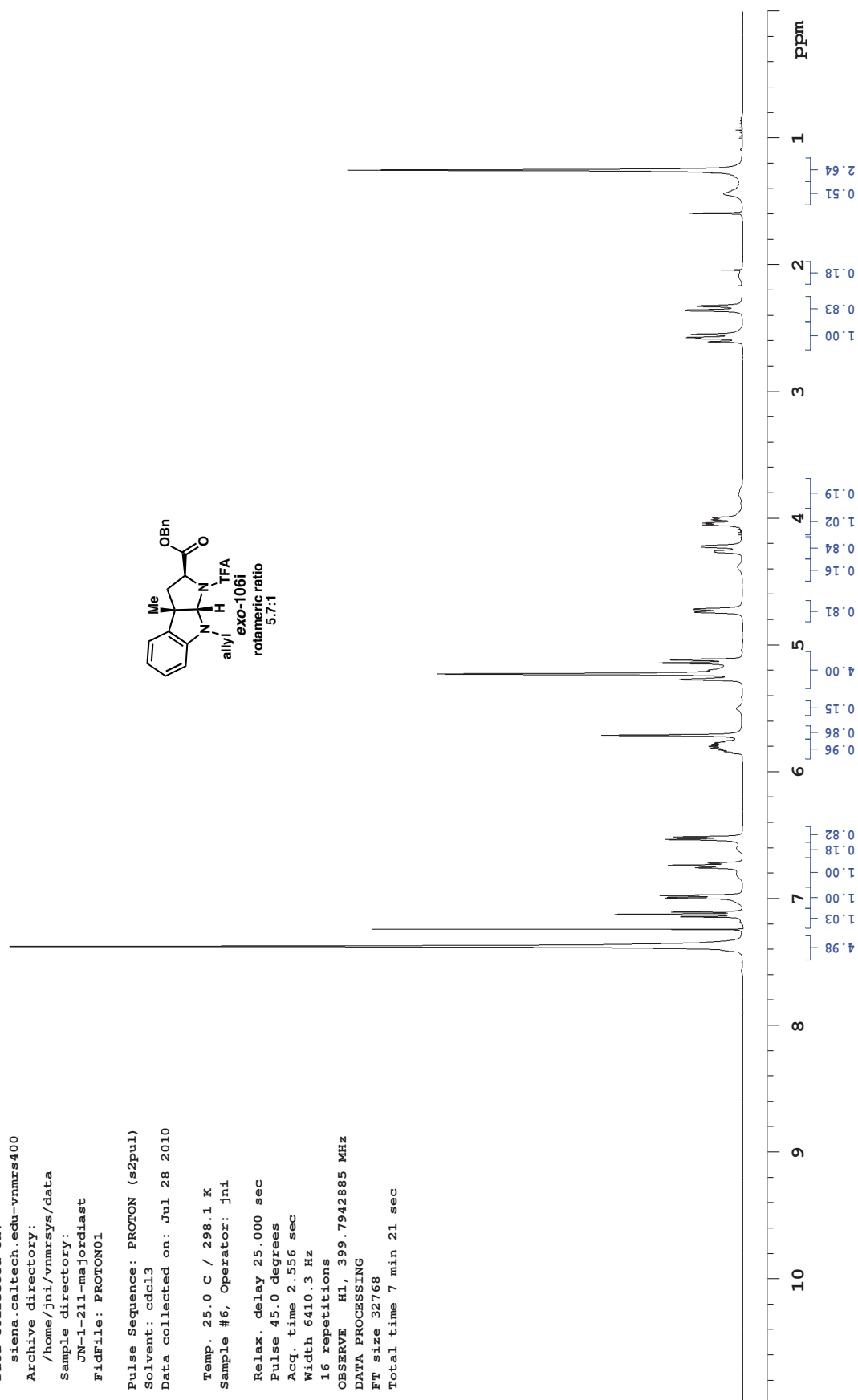
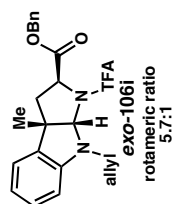
16 repetitions

OBSERVE H1, 399.7942885 MHz

DATA PROCESSING

FT size 32768

Total time 7 min 21 sec



JN-1-211-majordiast

Sample Name:

JN-1-211-majordiast
Data Collected on:
siena.caltech.edu-vmrs400
Archive directory:
/home/jni/vmrsys/data
Sample directory:
JN-1-211-majordiast
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 28 2010

Temp. 25.0 C / 298.1 K
Sample #6, Operator: jni

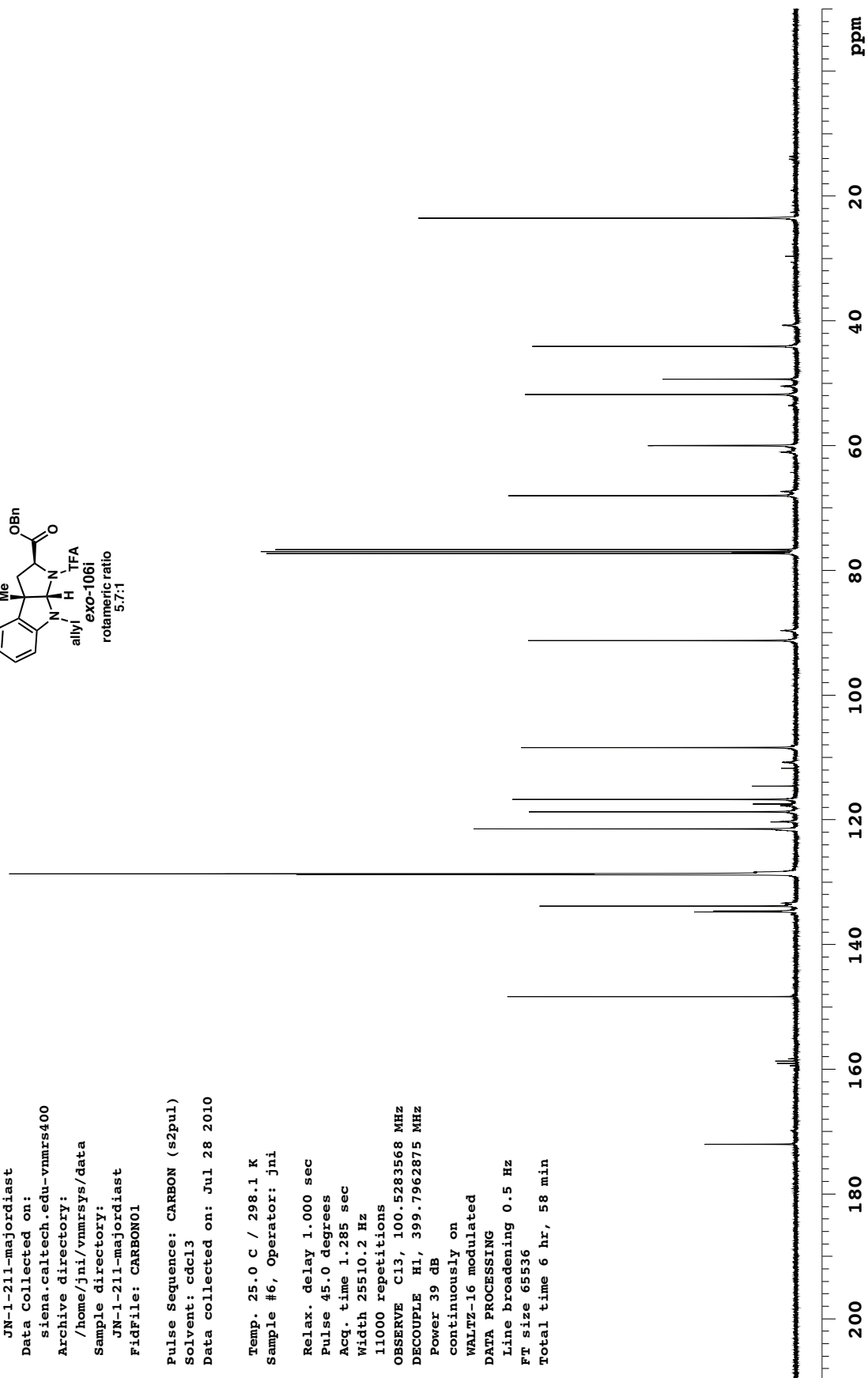
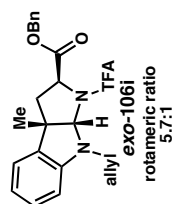
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.285 sec
Width 25510.2 Hz
11000 repetitions

OBSERVE C13, 100.5283568 MHz
DECOUPLE H1, 399.7962875 MHz

Power 39 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz
FT size 65536
Total time 6 hr, 58 min



JN-1-211-minordiast

Sample Name:

JN-1-211-minordiast

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-1-211-minordiast

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jul 28 2010

Operator: janeni

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

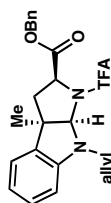
OBSERVE H1, 499.7420463 MHz

DATA PROCESSING

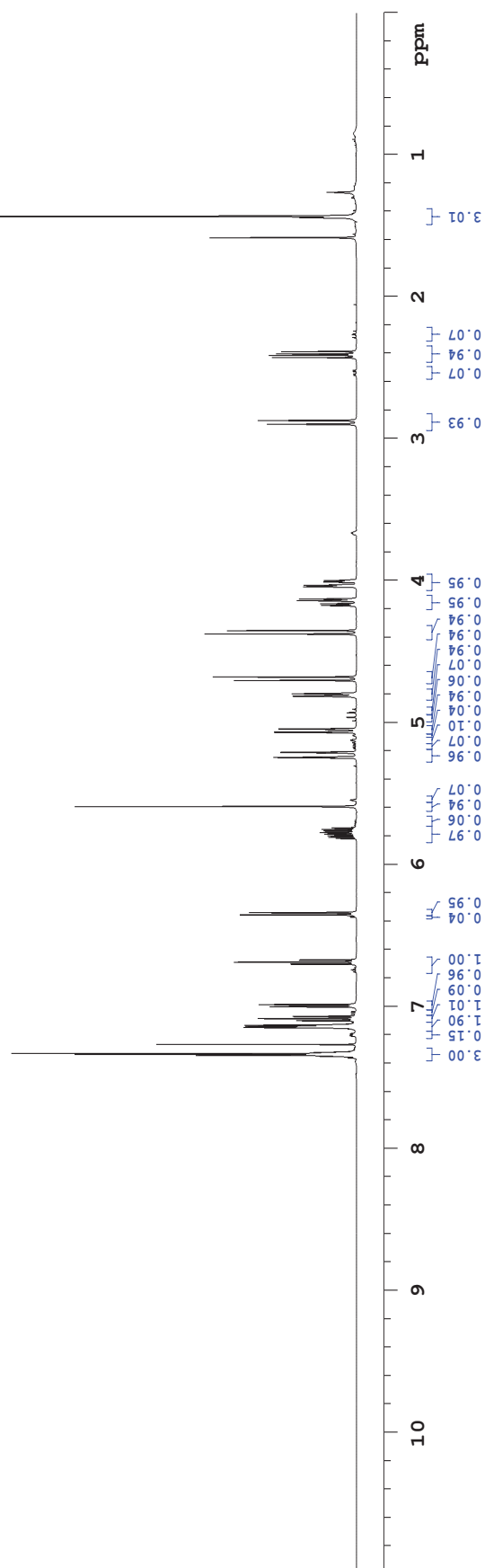
Line broadening 0.2 Hz

Ft size 65536

Total time 7 min 20 sec



endo-1061
rotameric ratio
15.7:1



JN-1-211-minordiast

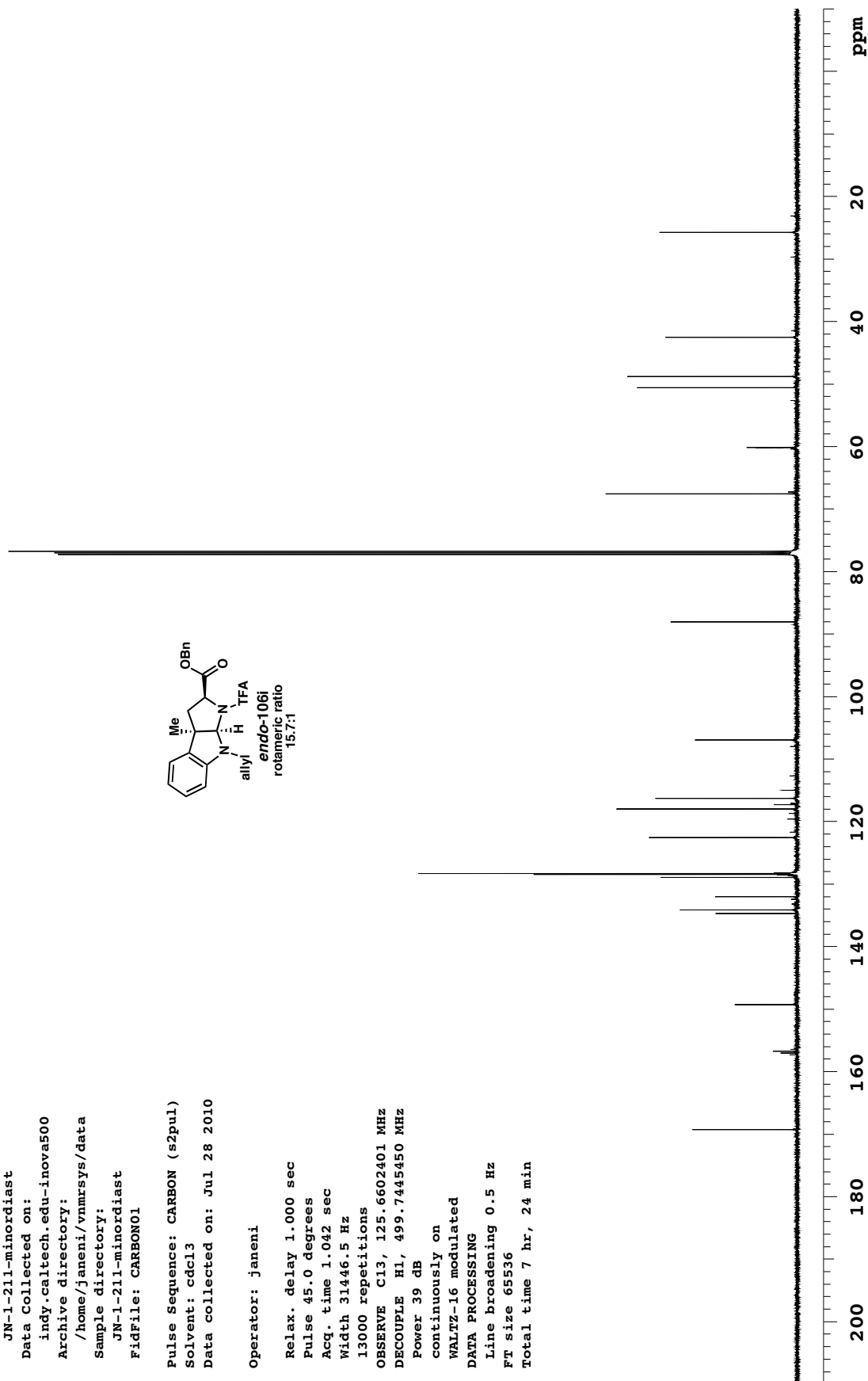
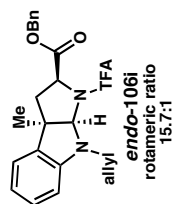
Sample Name:

JN-1-211-minordiast
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/janeni/vnmrsys/data
Sample directory:
JN-1-211-minordiast
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 28 2010

Operator: janeni

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
13000 repetitions
OBSERVE C13, 125.6602401 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 7 hr, 24 min



LMRV-047-major01r

Sample Name:

LMRV-047-major01r
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/lrepka/vnmrsys/data
 Sample directory:
 LMRV-047-major01r
 FIDFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 16 2010

Temp. 25.0 C / 298.1 K

Sample #35, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

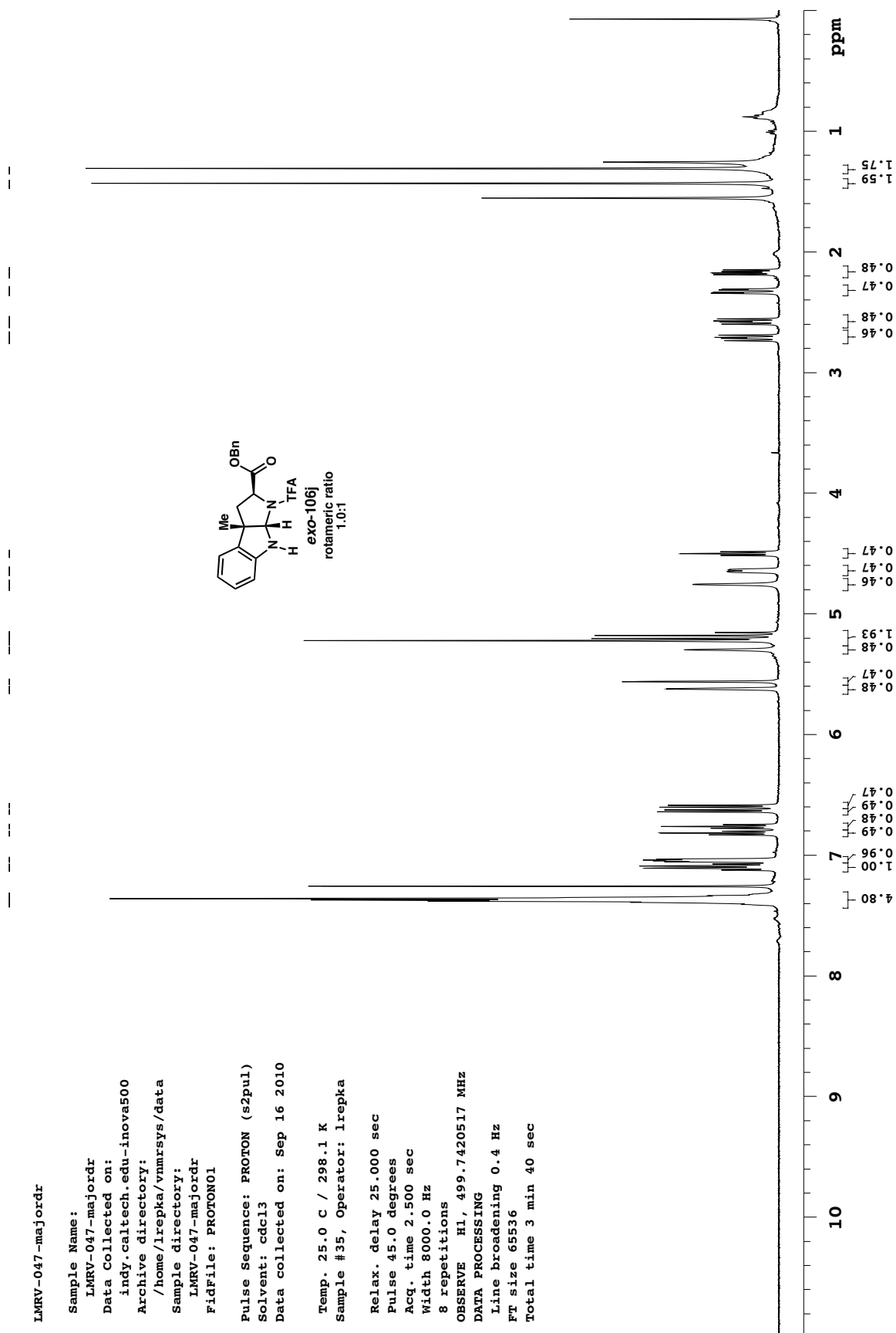
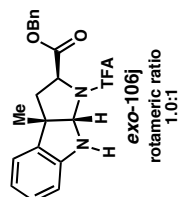
OBSERVE H1, 499.7420517 MHz

DATA PROCESSING

Line broadening 0.4 Hz

FT size 65536

Total time 3 min 40 sec



LMRV-047-majordr

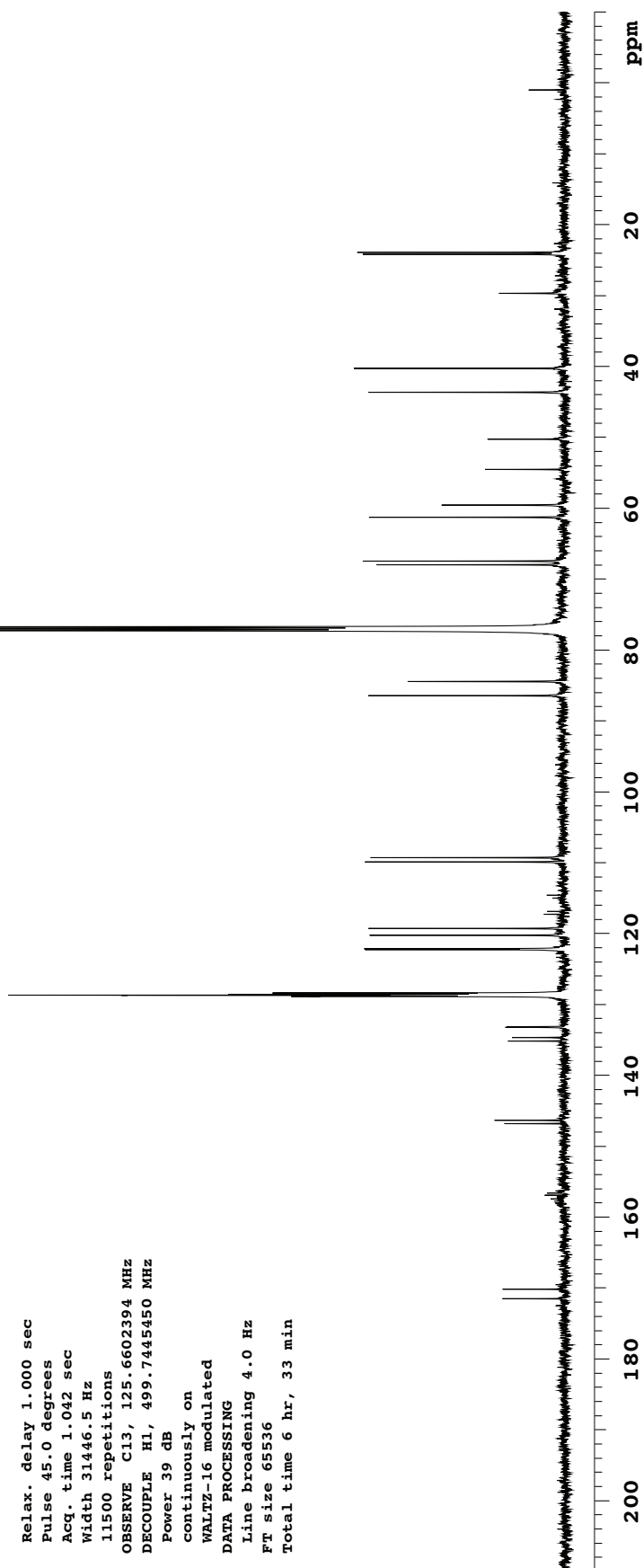
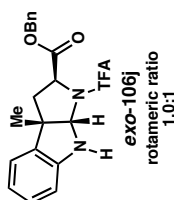
Sample Name:

LMRV-047-majordr
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRV-047-majordr
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 16 2010

Temp. 25.0 C / 298.1 K
Sample #35, Operator: lrepka

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
11500 repetitions
OBSERVE C13, 125.6602394 MHz
DECOUPLE H1, 499.7445450 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 4.0 Hz
FT size 65536
Total time 6 hr, 33 min



JN-3-101-carbon

Sample Name:

JN-3-101-carbon

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-3-101-carbon

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jan 25 2012

Sample #17, Operator: janeni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

16 repetitions

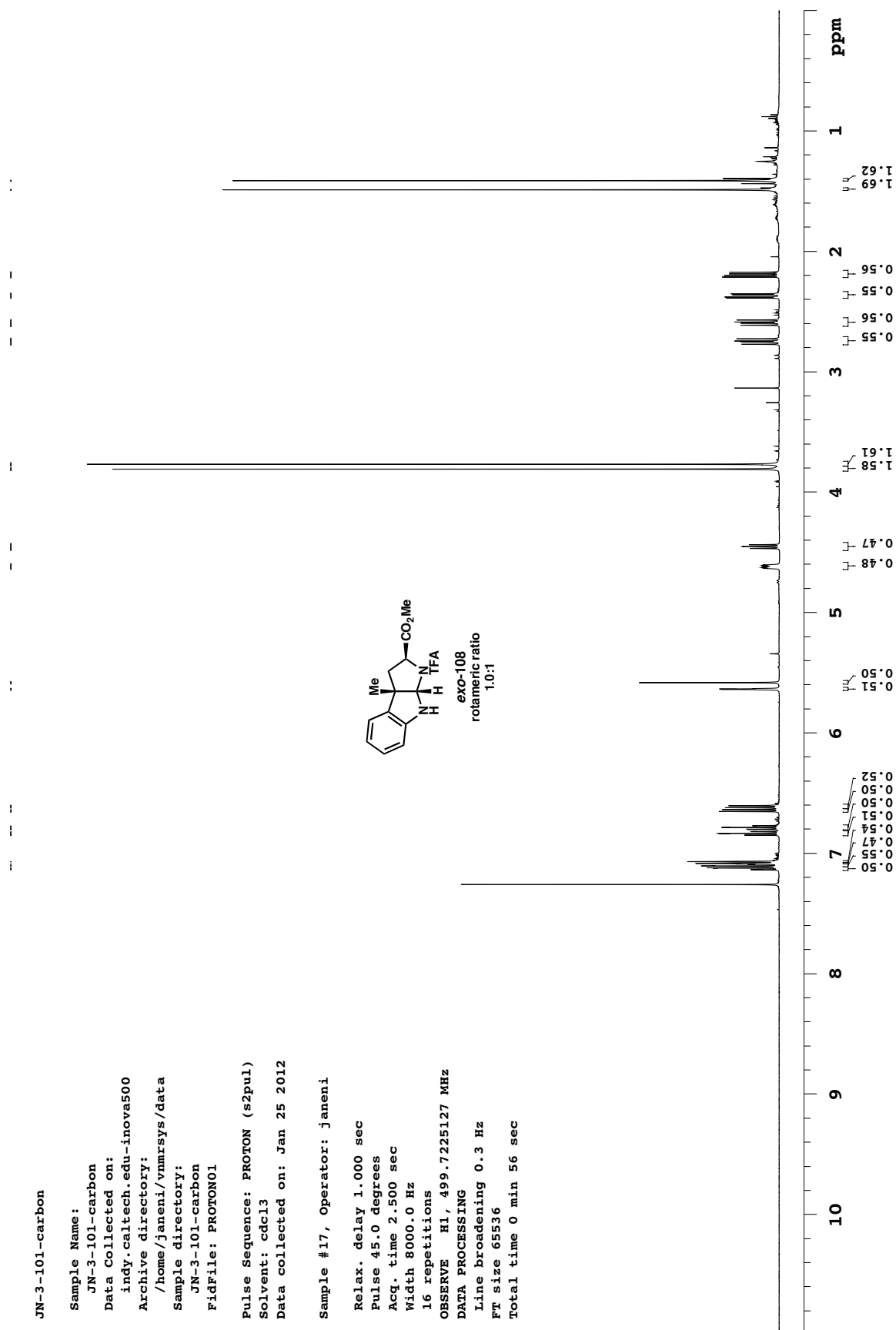
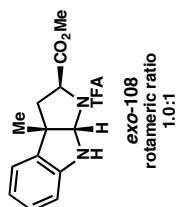
OBSERVE H1, 499.7225127 MHz

DATA PROCESSING

Line broadening 0.3 Hz

FT size 65536

Total time 0 min 56 sec



JN-3-101-carbon

Sample Name:

JN-3-101-carbon

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/janeni/vnmrsys/data

Sample directory:

JN-3-101-carbon

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jan 25 2012

Sample #17, Operator: janeni

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

10000 repetitions

OBSERVE C13, 125.6553277 MHz

DECOUPLE H1, 499.7250019 MHz

Power 39 dB

continuously on

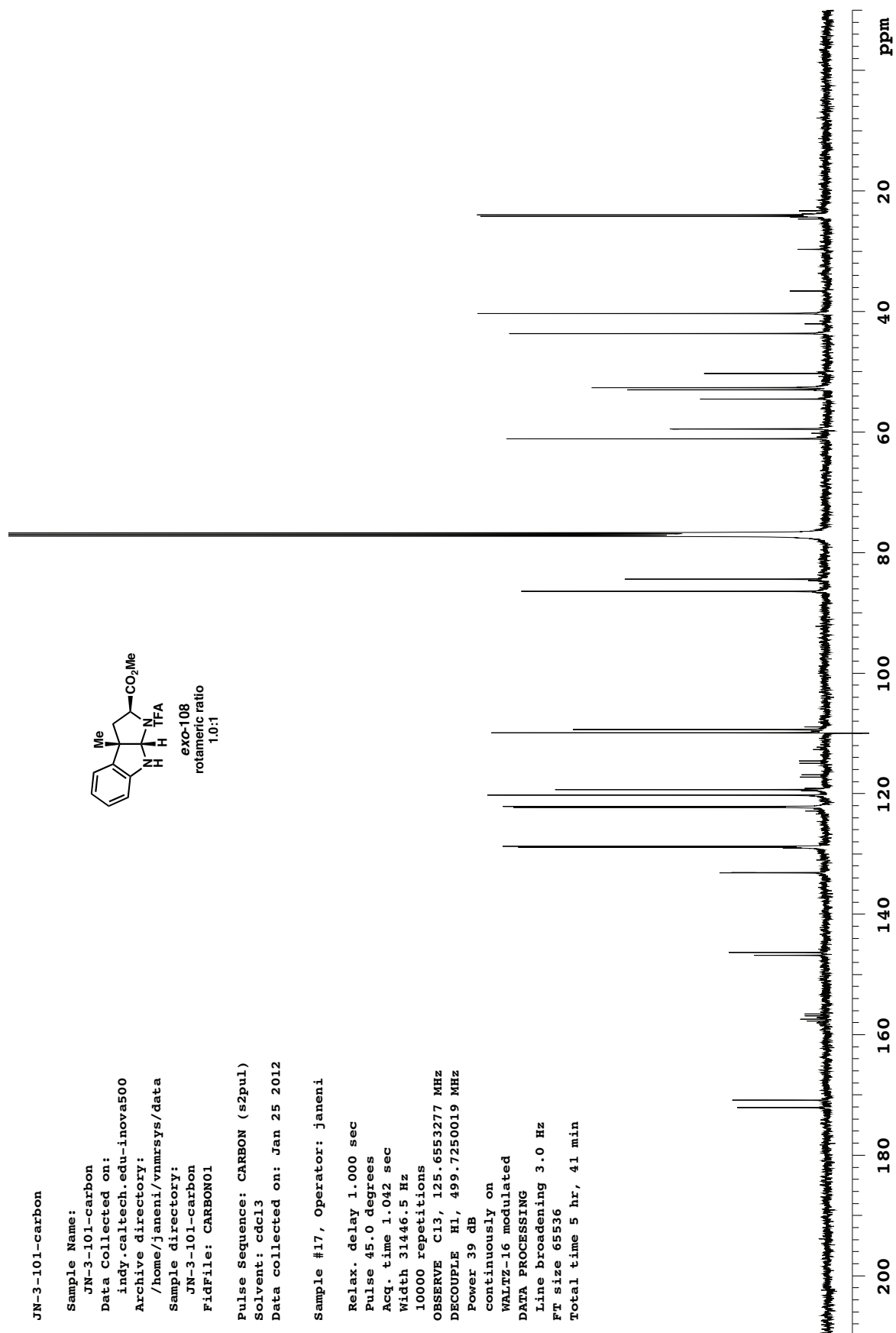
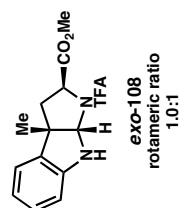
WALTZ-16 modulated

DATA PROCESSING

Line broadening 3.0 Hz

FT size 65536

Total time 5 hr, 41 min



LMRII-073-1.0workup

Sample Name:

LMRII-073-1.0workup

Archive directory:

Sample directory:

FidFile: LMRII-073-1.0workup

Pulse Sequence: Proton (s2pul)

Solvent: cdcl3

Data collected on: Sep 25 2009

Operator: lrepka

VNMRS-400 "erice.caltech.edu"

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.998 sec

Width 4796.2 Hz

2 repetitions

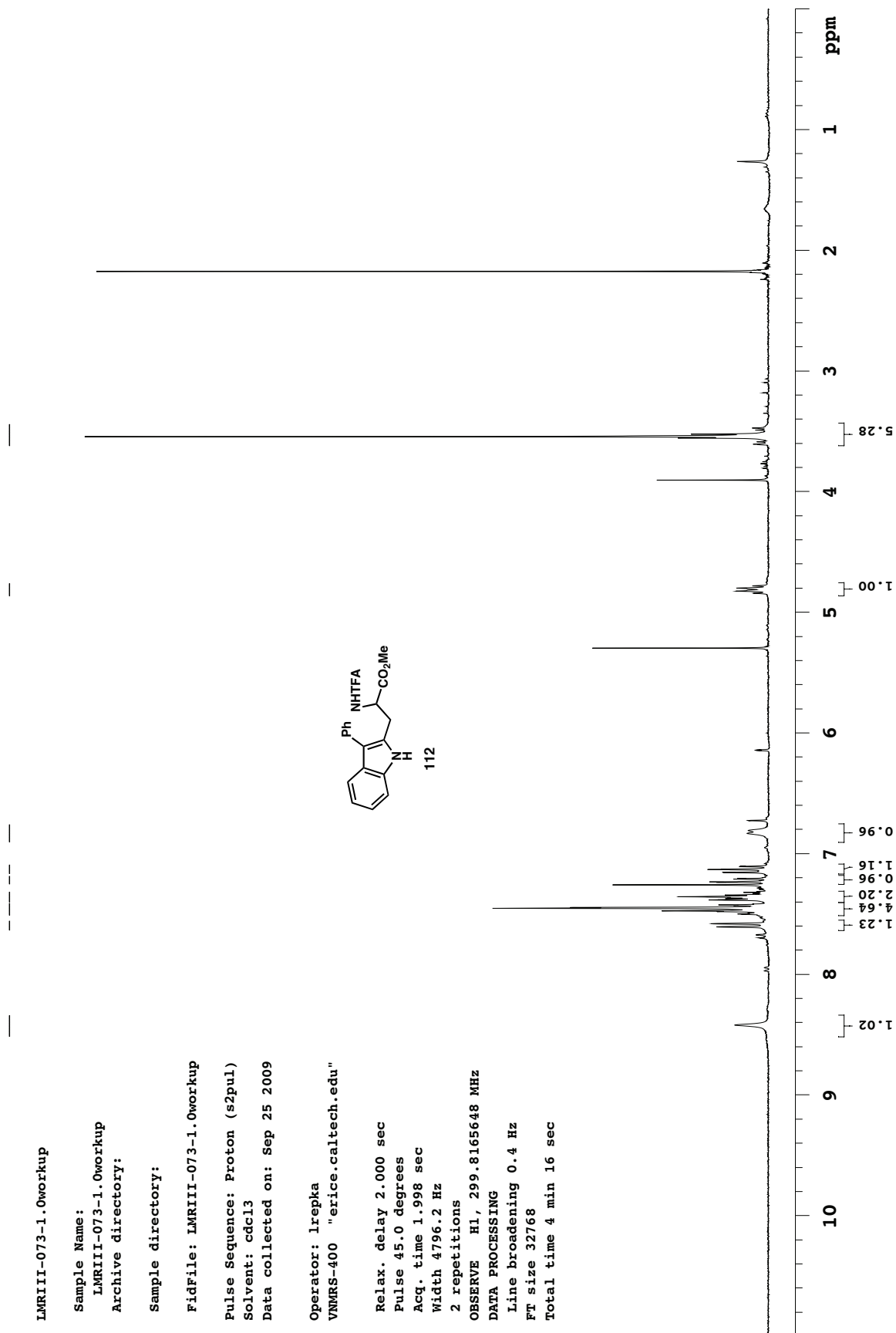
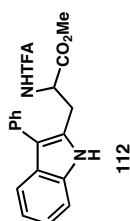
OBSERVE H1, 299.8165648 MHz

DATA PROCESSING

Line broadening 0.4 Hz

FT size 32768

Total time 4 min 16 sec



LMRIII-107

Sample Name:

LMRIII-107

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

Sample directory:

FidFile: Carbon_01

Pulse Sequence: Carbon (s2pul)

Solvent: cdcl3

Data collected on: Oct 7 2009

Sample #38, Operator: slevin

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.300 sec

Width 30165.9 Hz

800 repetitions

OBSERVE C13, 125.6635224 MHz

DECOUPLE H1, 499.7575738 MHz

Power 39 dB

continuously on

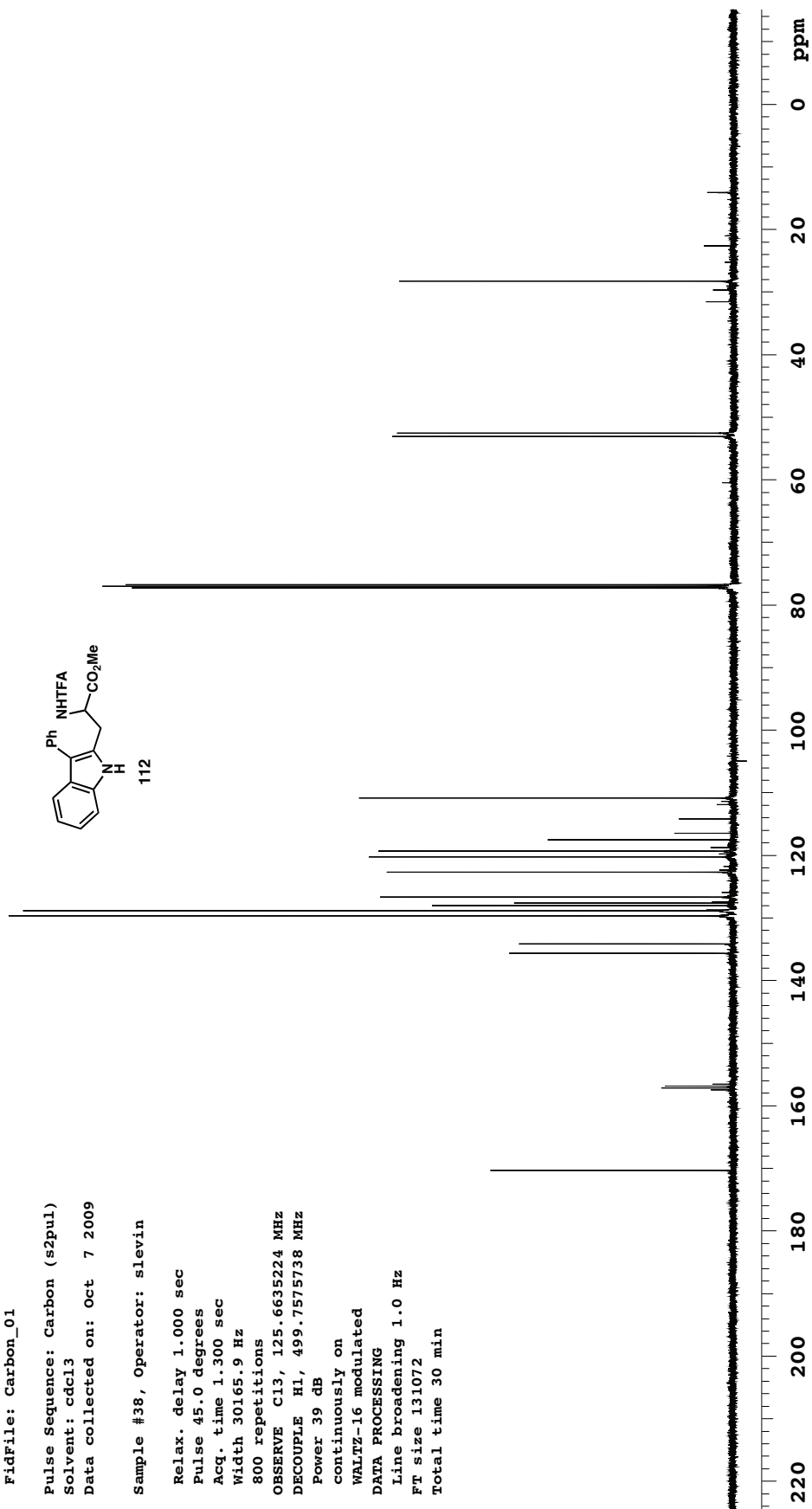
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

Ft size 131072

Total time 30 min



LMRV-229-column

Sample Name:

LMRV-229-column

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRV-229-column

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jan 28 2011

Sample #33, Operator: lrepka

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4798.5 Hz

16 repetitions

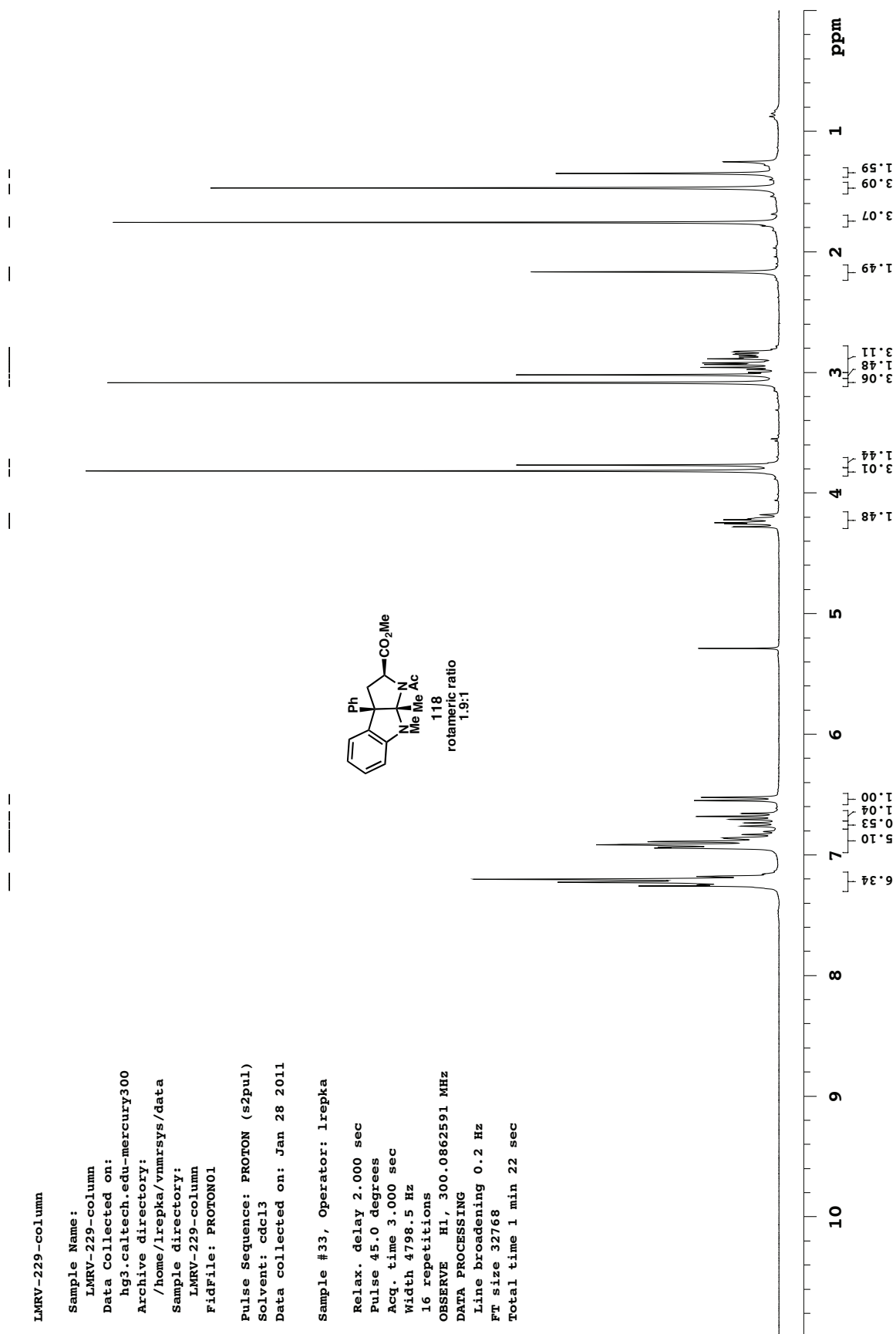
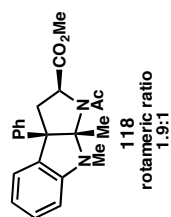
OBSERVE H1, 300.0862591 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min 22 sec



LMRV-233—carbon

Sample Name:

LMRV-233—carbon
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/lrepka/vnmrsys/data
 Sample directory:
 LMRV-233—carbon
 FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jun 3 2013

Sample #22, Operator: lrepka

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.042 sec
 Width 31446.5 Hz
 256 repetitions
 OBSERVE C13, 125.6509091 MHz
 DECOUPLE H1, 499.7074131 MHz
 Power 40 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 2.0 Hz
 FT size 65536
 Total time 8 min 45 sec

