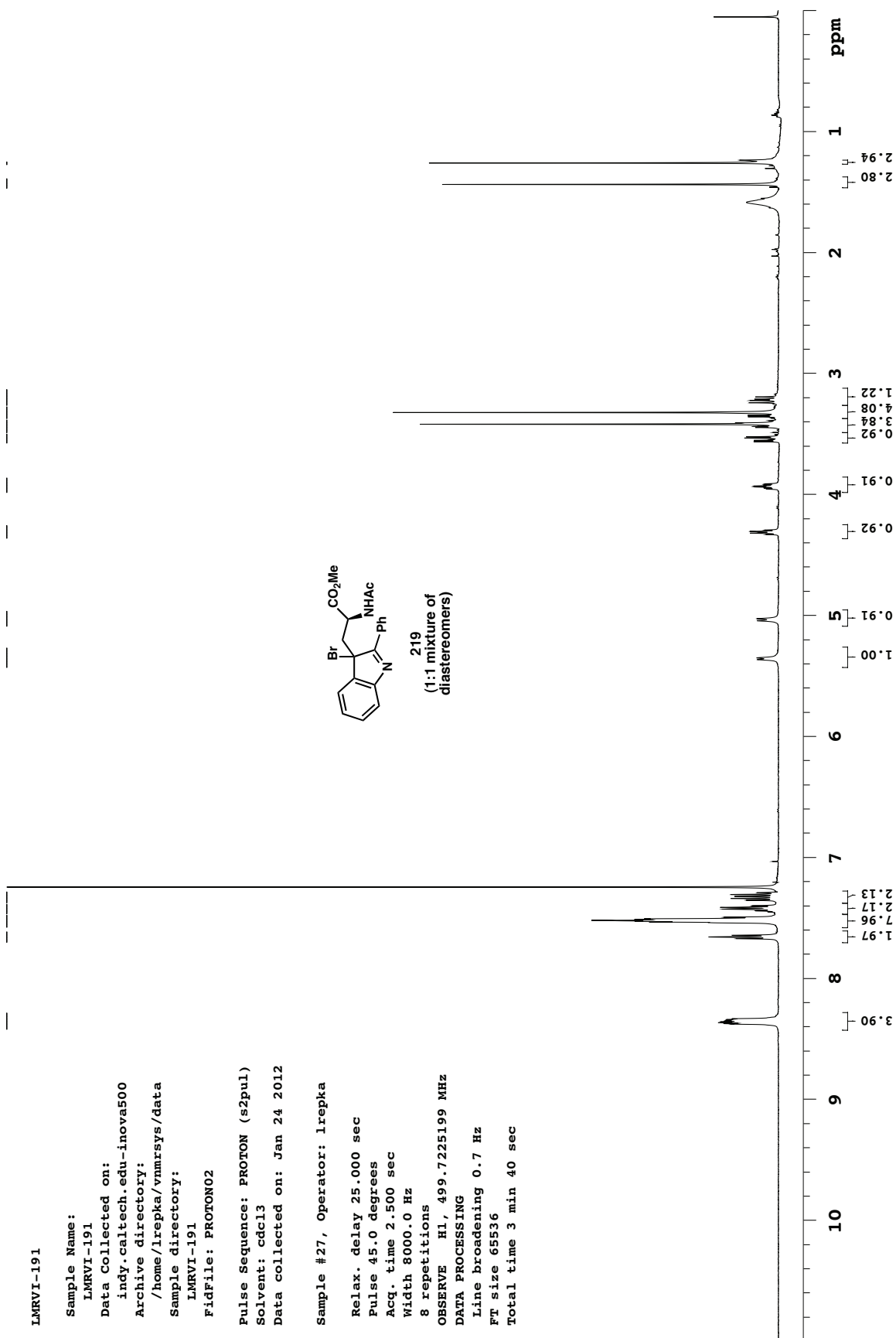


APPENDIX 4

Spectra Relevant to Chapter 4:

*Access to 2a-Phenylpyrroloindolines
by an Oxidative Cyclization Reaction*



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

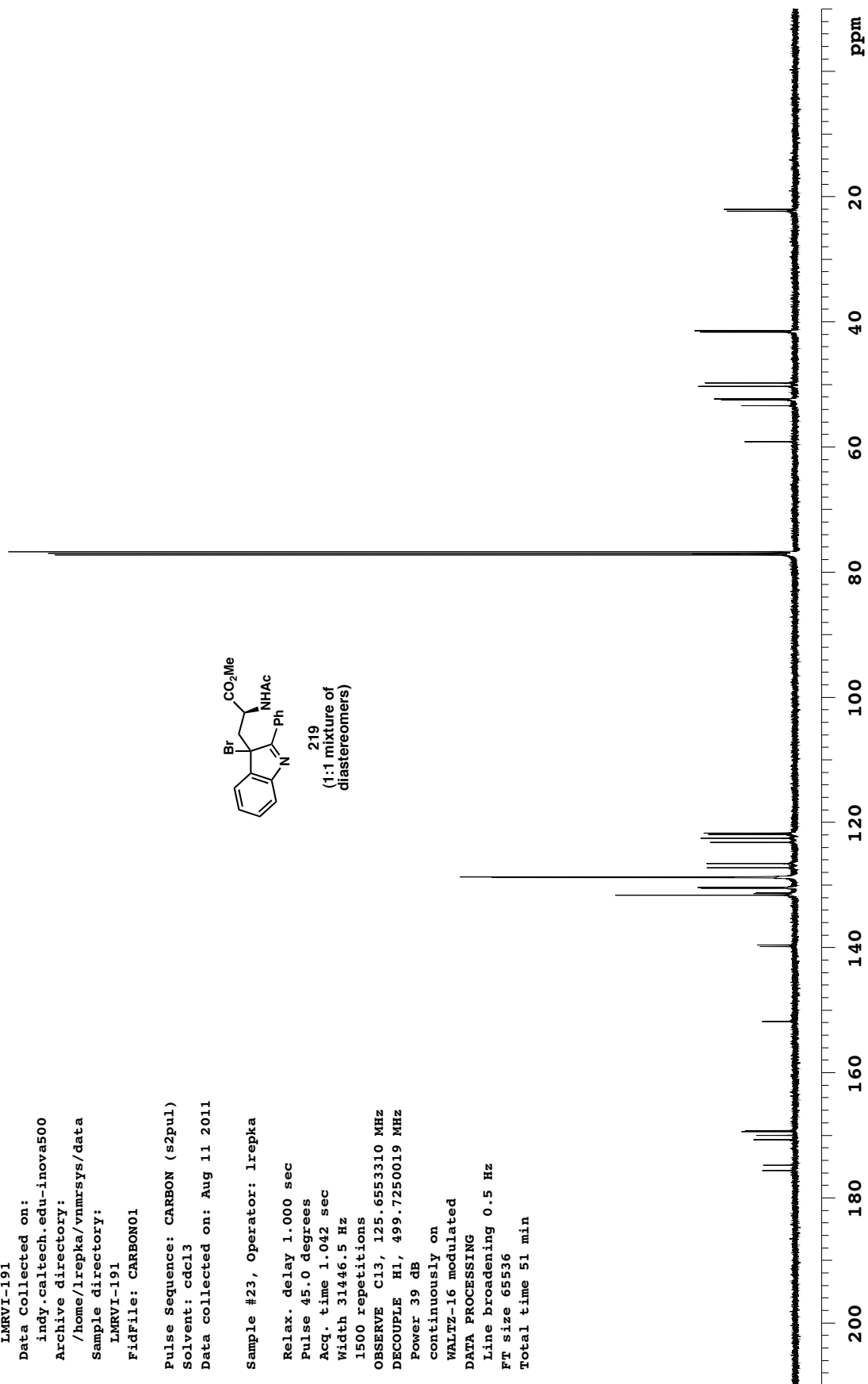
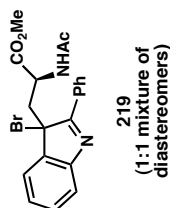
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 51 min



LMRVII-31

Sample Name:

LMRVII-31

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVII-31

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 19 2012

Sample #27, Operator: lrepka

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

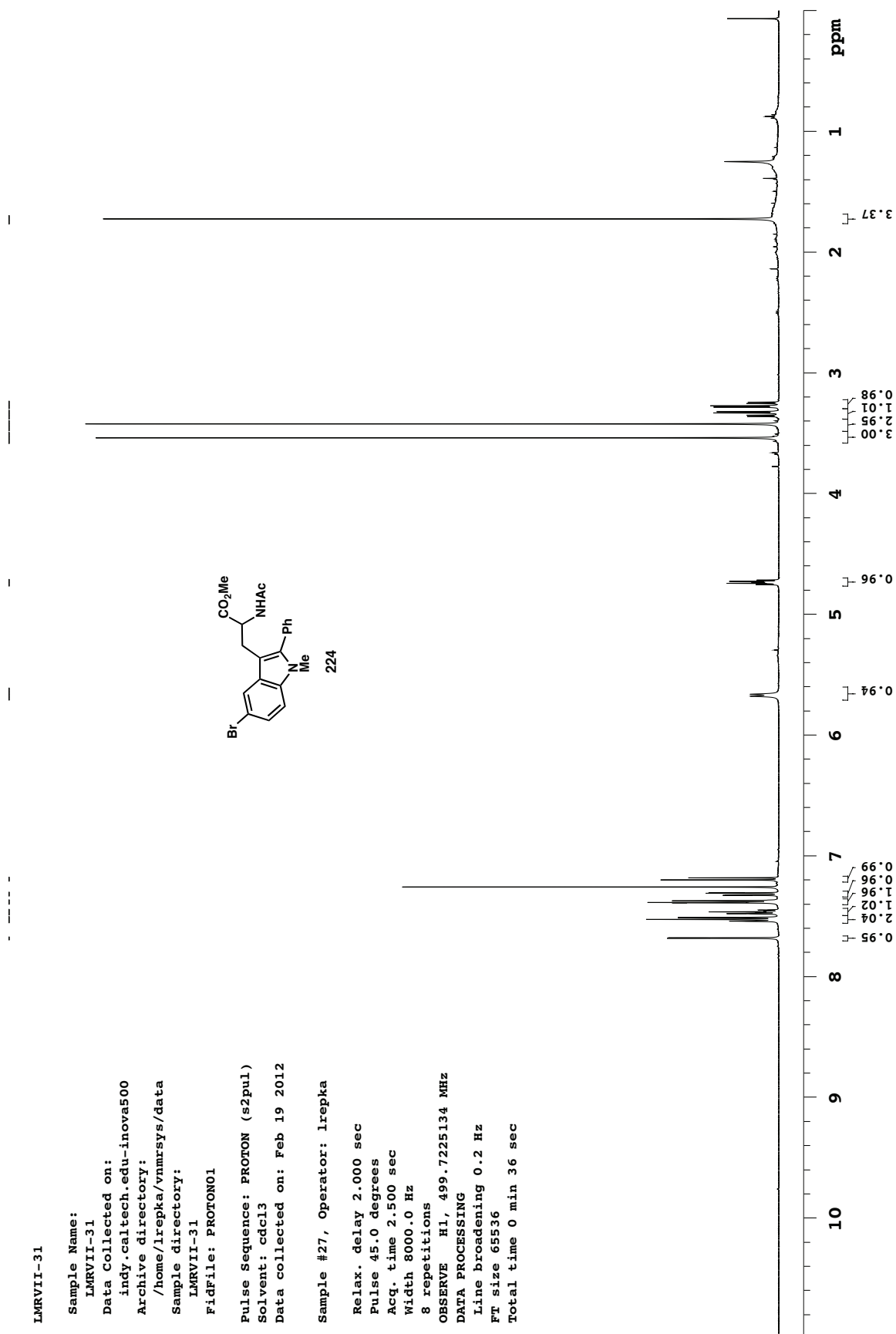
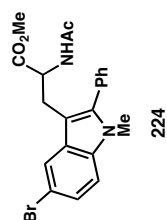
OBSERVE H1, 499.7225134 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 36 sec



LMRVII-31

Sample Name:

LMRVII-31
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-31
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

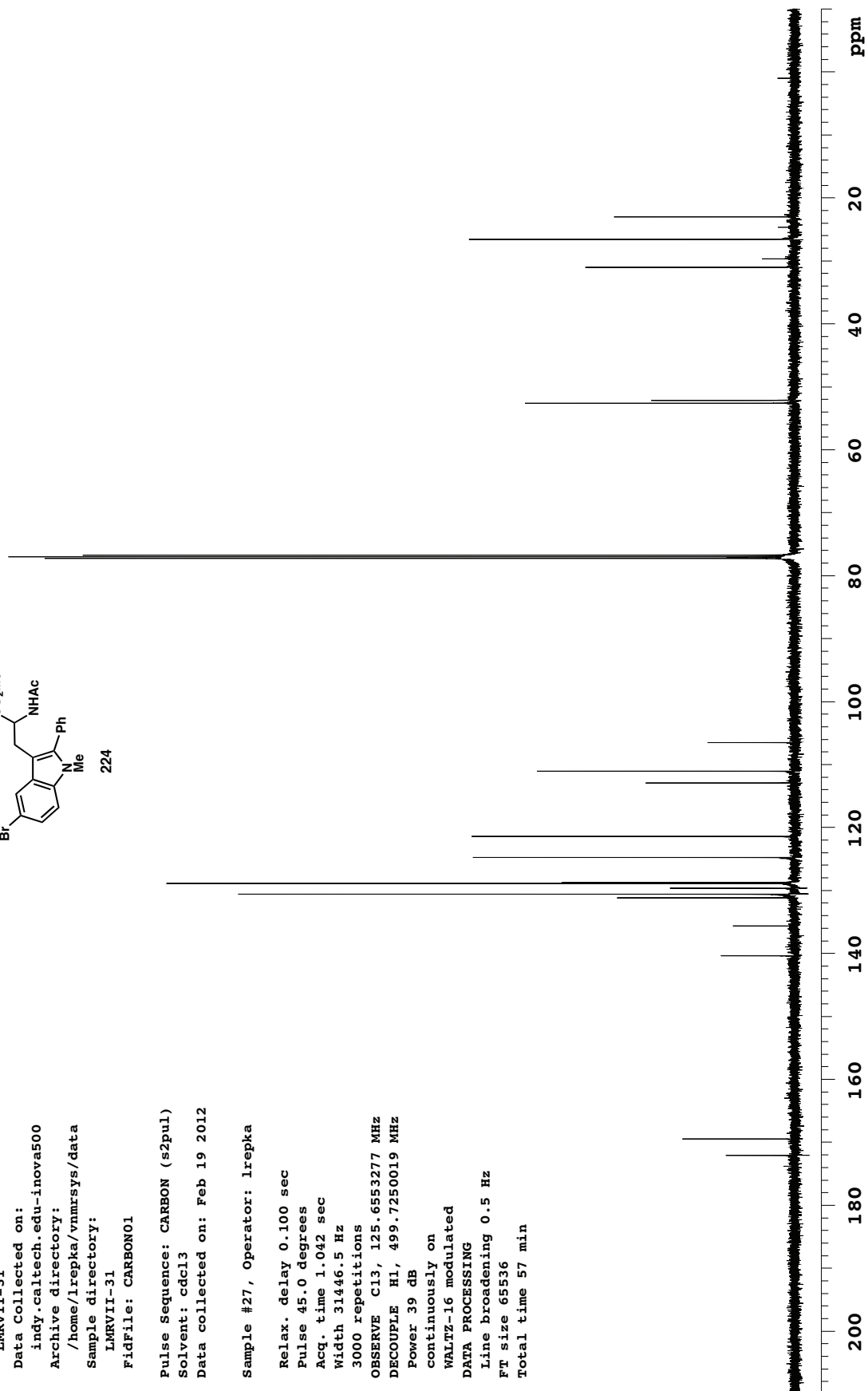
Solvent: cdcl3
Data collected on: Feb 19 2012

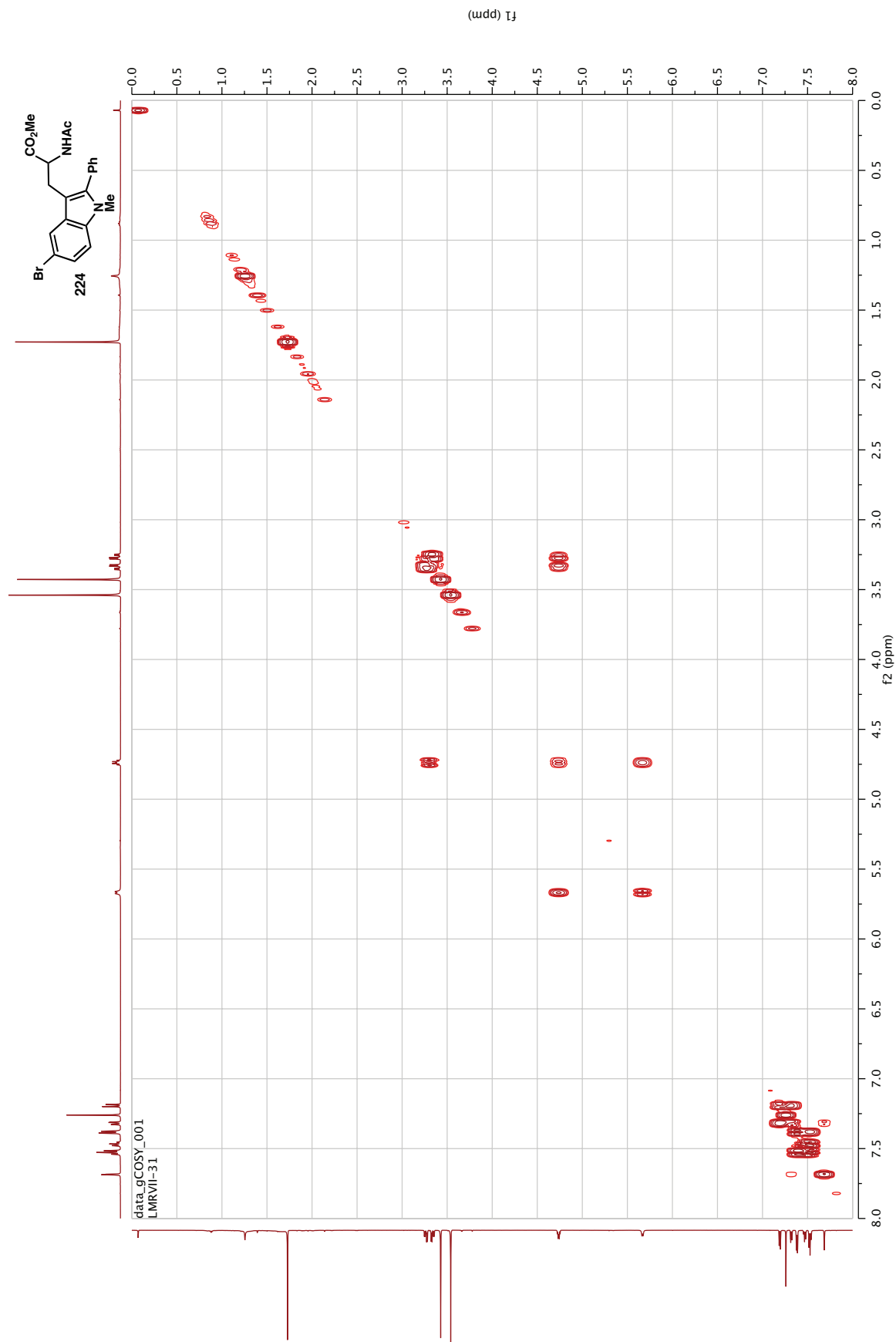
Sample #27, Operator: lrepka

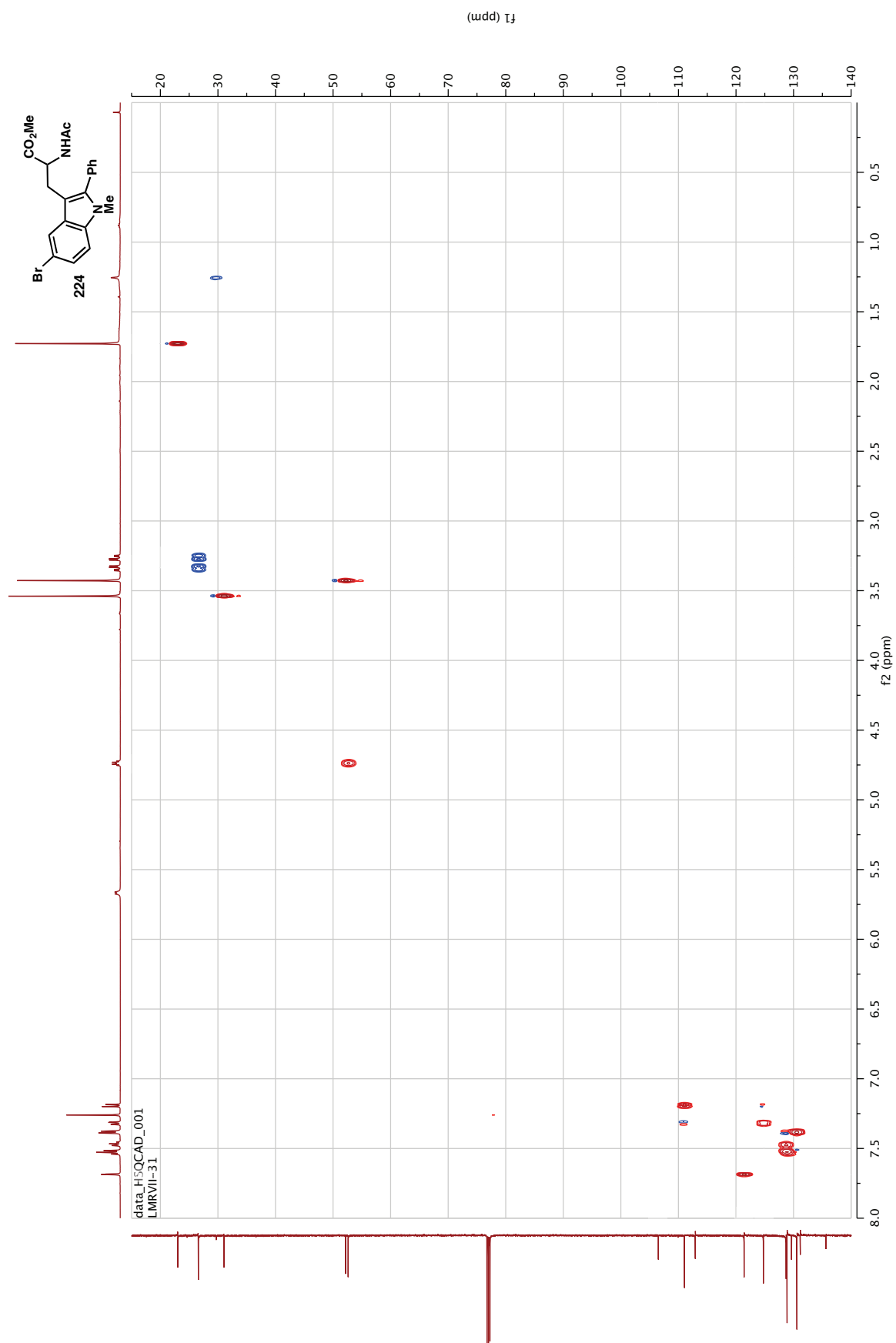
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
3000 repetitions
OBSERVE C13, 125.6553277 MHz
DECOUPLE H1, 499.7250019 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 57 min

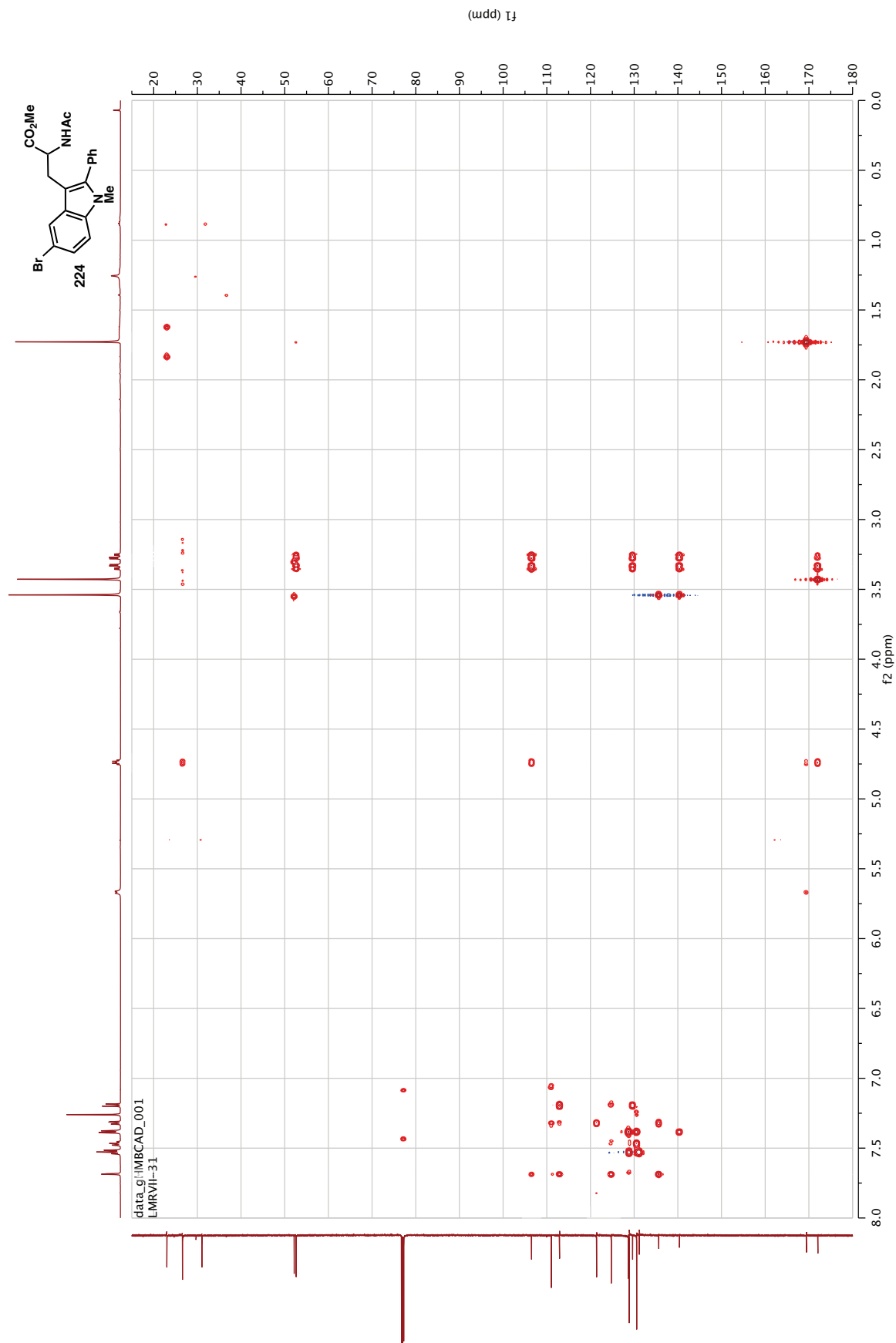


224









LMRVII-35-majordr

Sample Name:

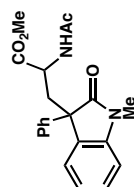
LMRVII-35-majordr
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-35-majordr
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 20 2012

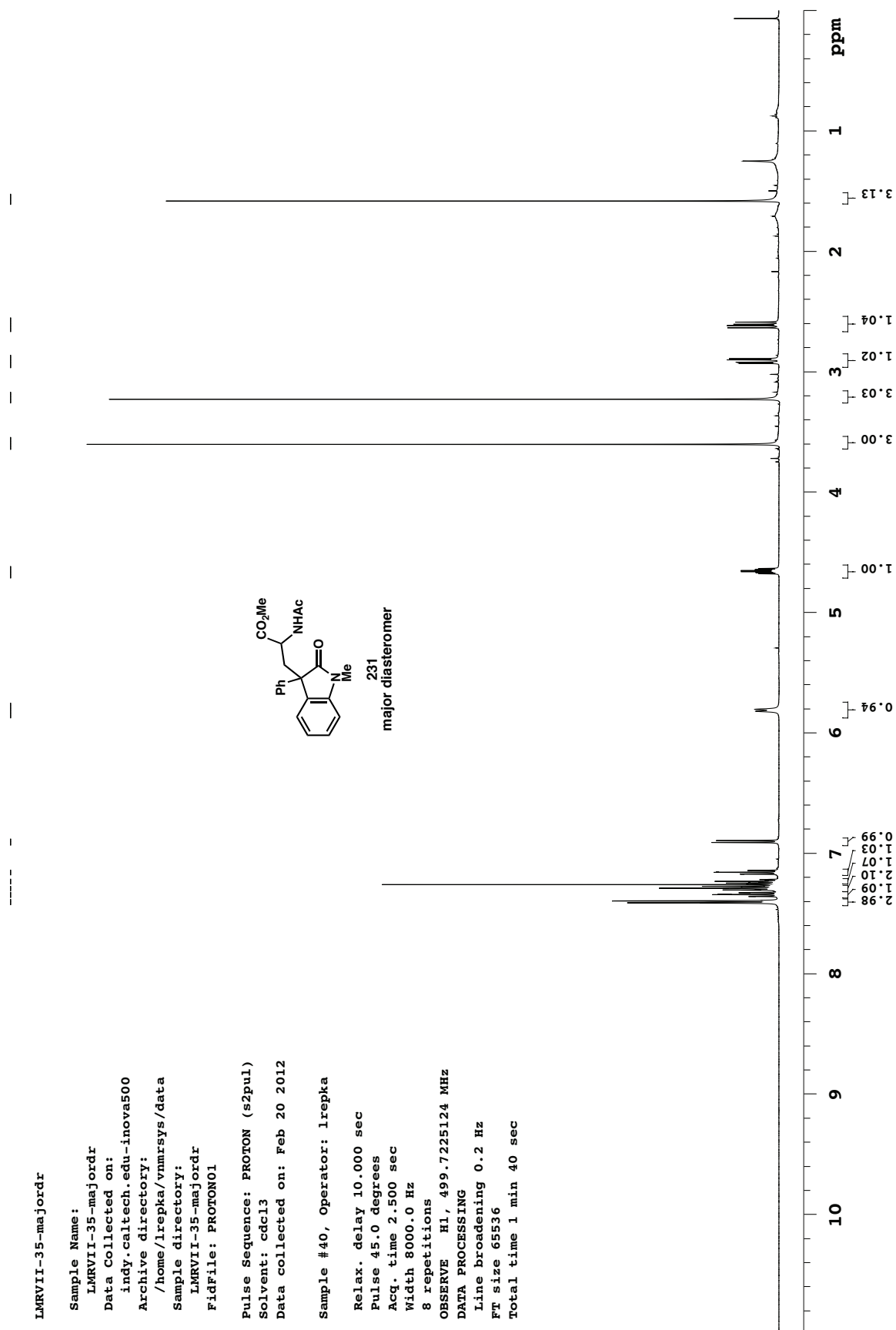
Sample #40, Operator: lrepka

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 8000.0 Hz
8 repetitions

OBSERVE H1, 499.7225124 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 1 min 40 sec



231
major diastomer



LMRVII-35-majordr

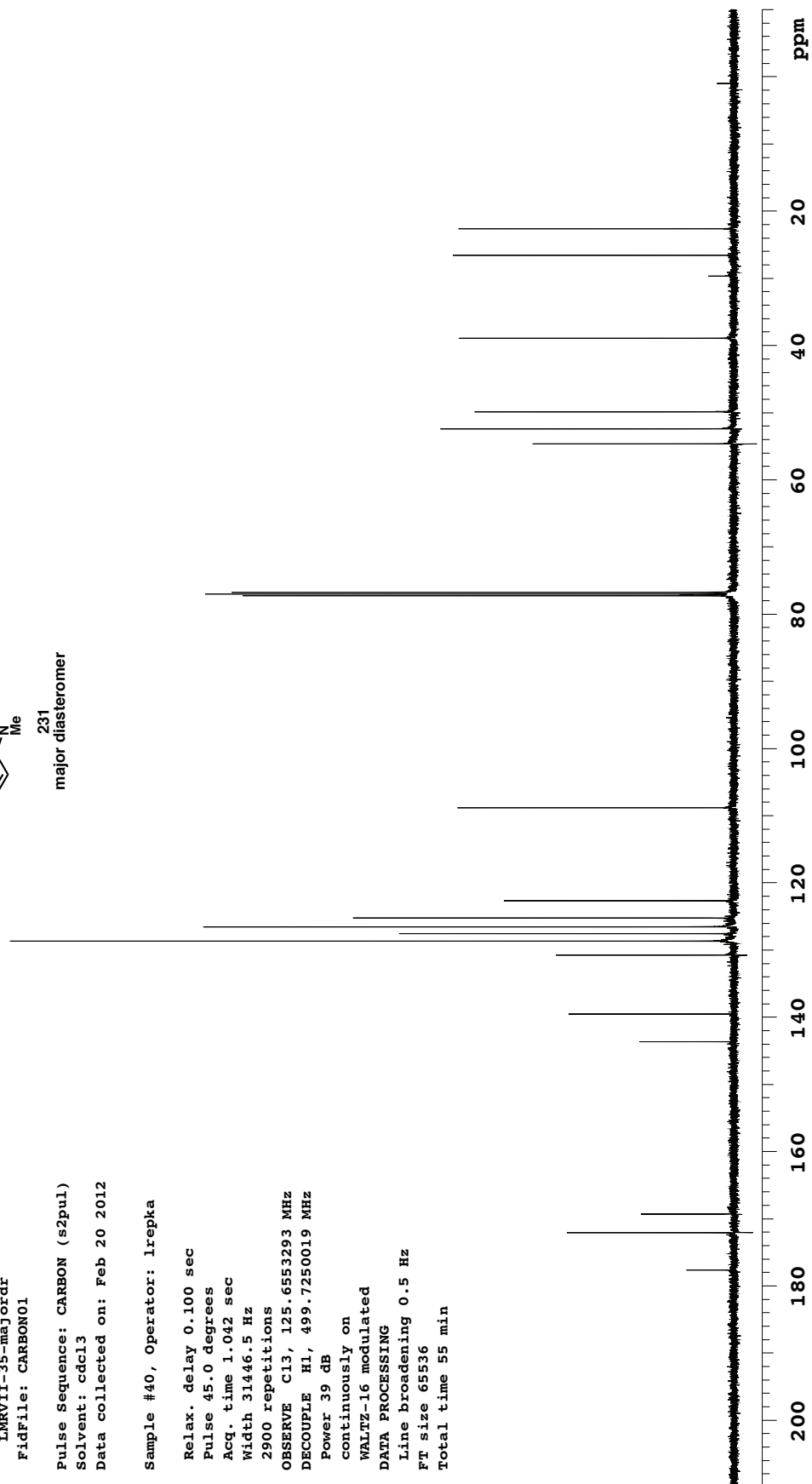
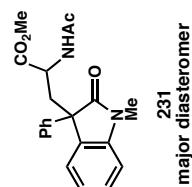
Sample Name:

LMRVII-35-majordr
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-35-majordr
FidFile: CARBON01

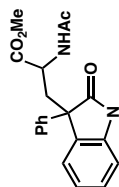
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 20 2012

Sample #40, Operator: lrepka

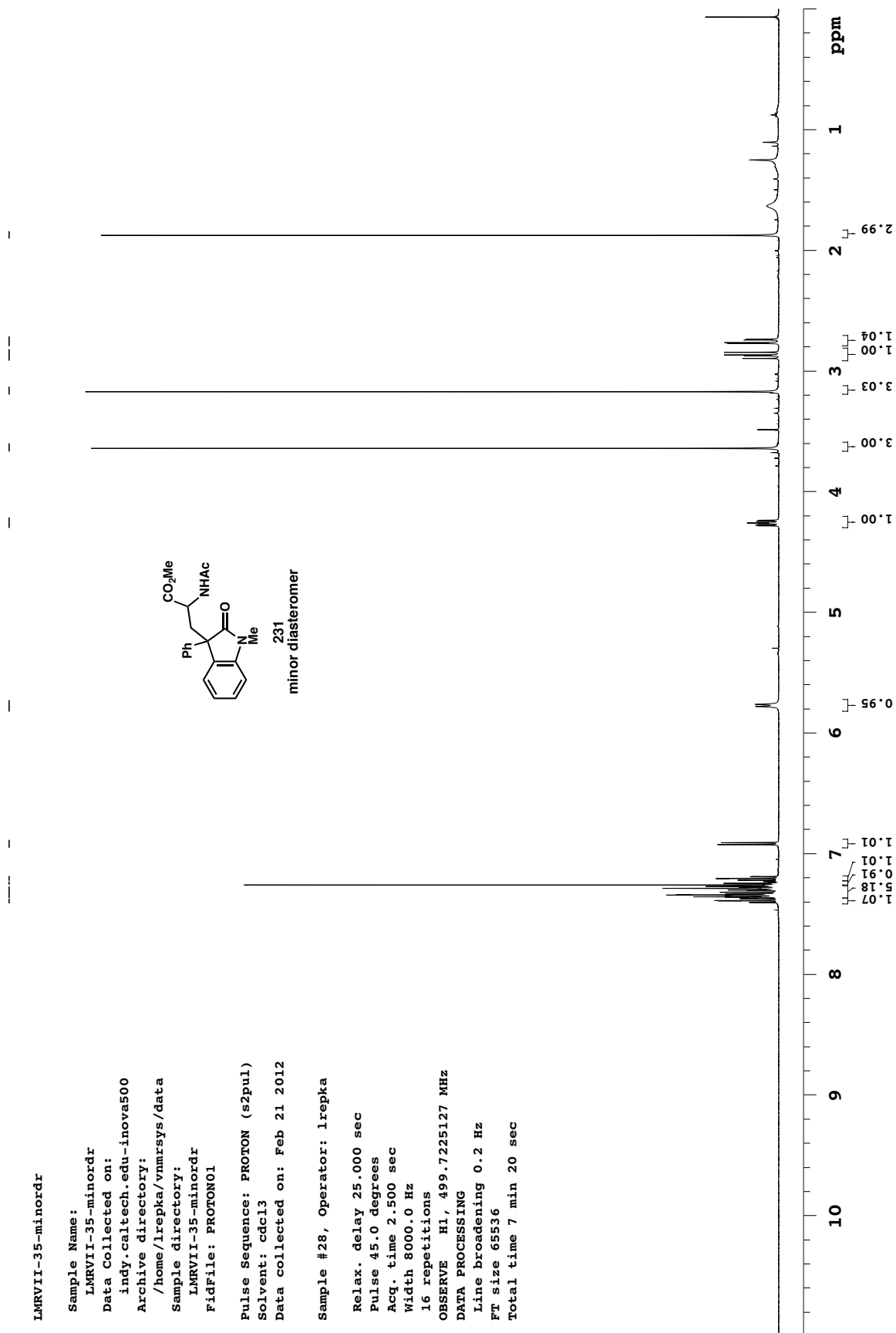
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
2900 repetitions
OBSERVE C13, 125.6553293 MHz
DECOUPLE H1, 499.7250019 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 55 min



Total time 7 min 20 sec



231
minor diastereomer



LMRVII-35-minordr

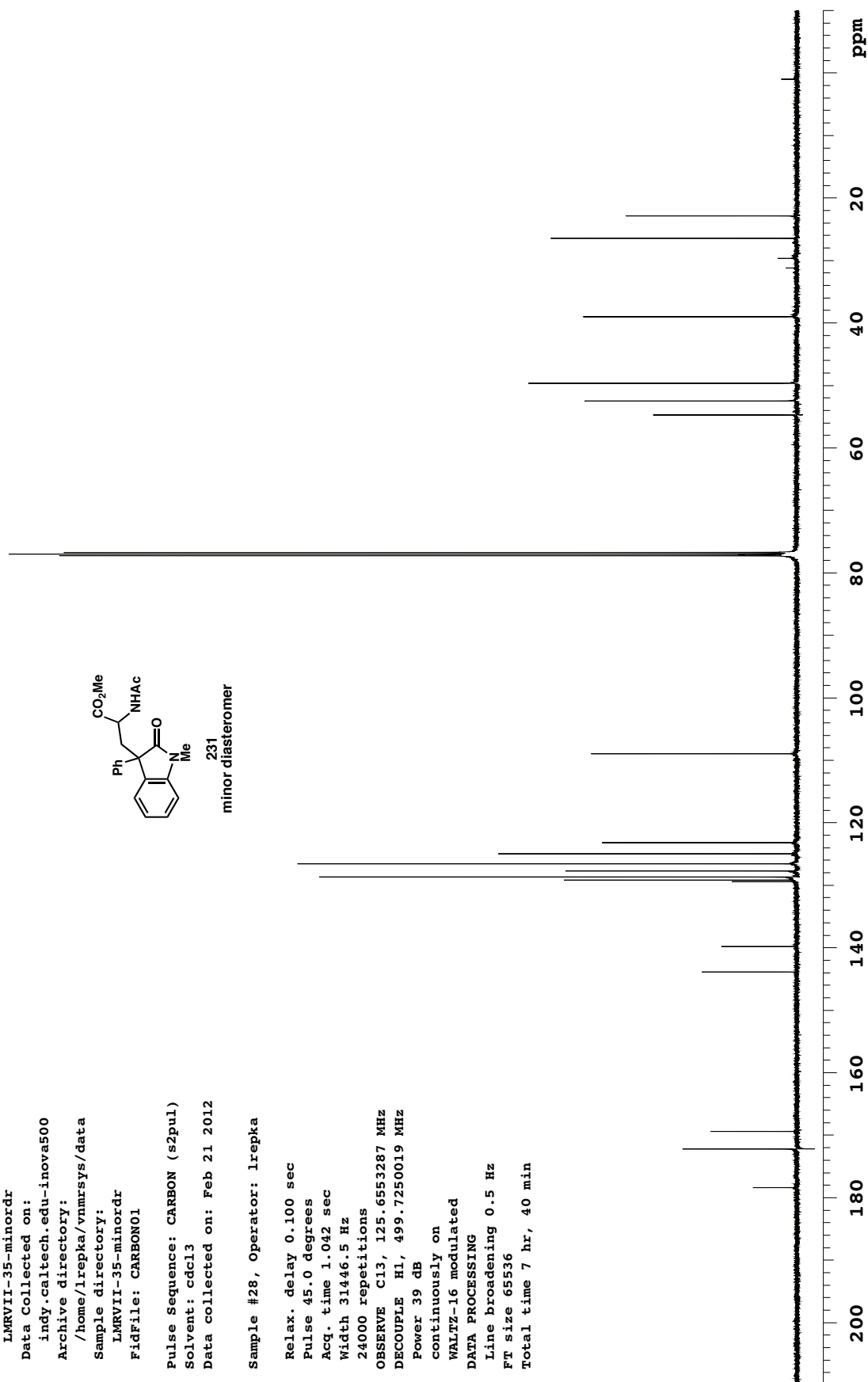
Sample Name:

LMRVII-35-minordr
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-35-minordr
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 21 2012

Sample #28, Operator: lrepka

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
24000 repetitions
OBSERVE C13, 125.6553287 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 7 hr, 40 min



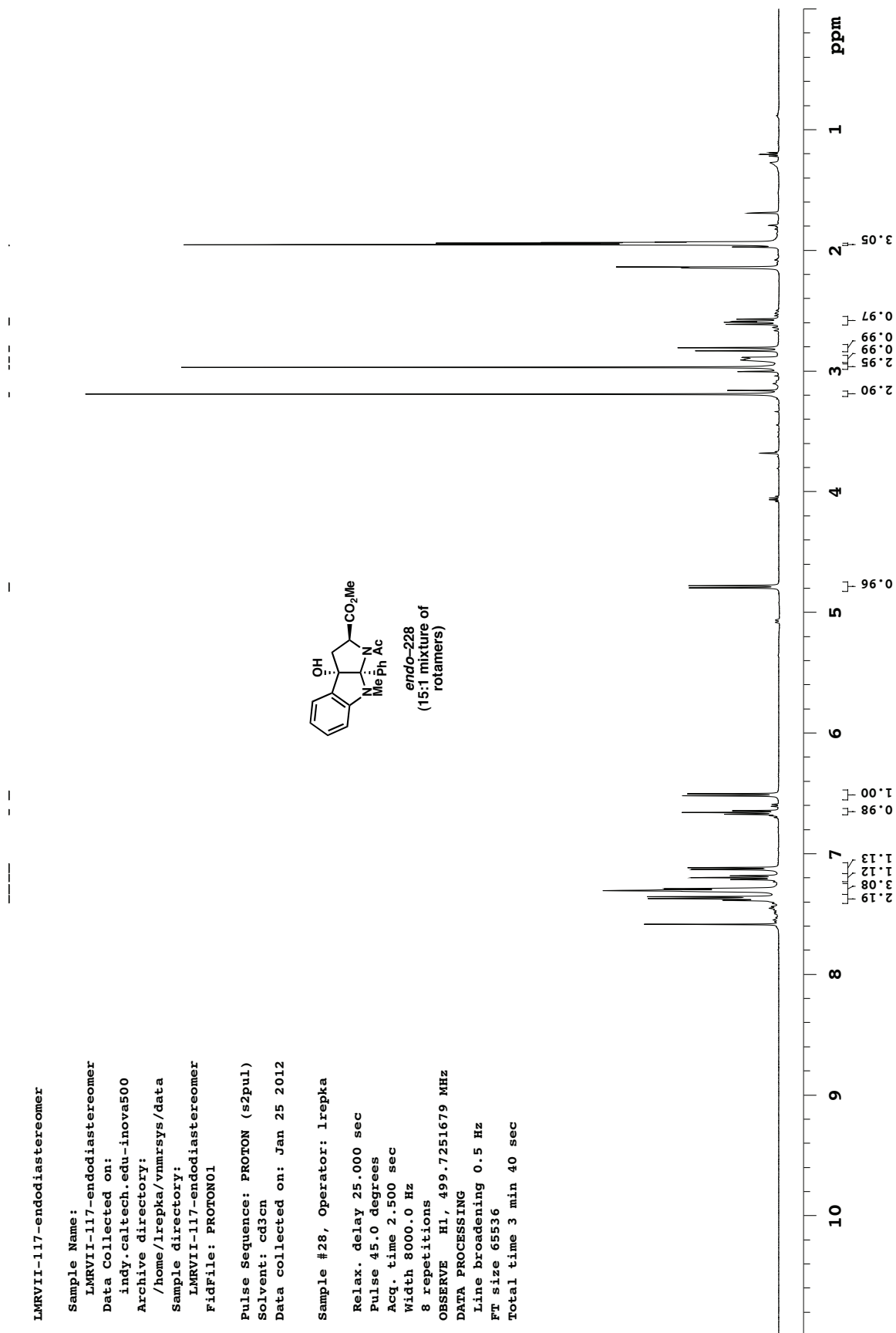
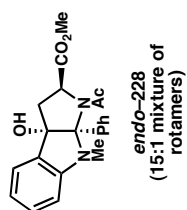
LMRVII-117-endodiastereomer

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, 499.7251679 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 min 40 sec



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, 125.6558756 MHz

DECOUPLE H1, 499.7276454 MHz

Power 39 dB

continuously on

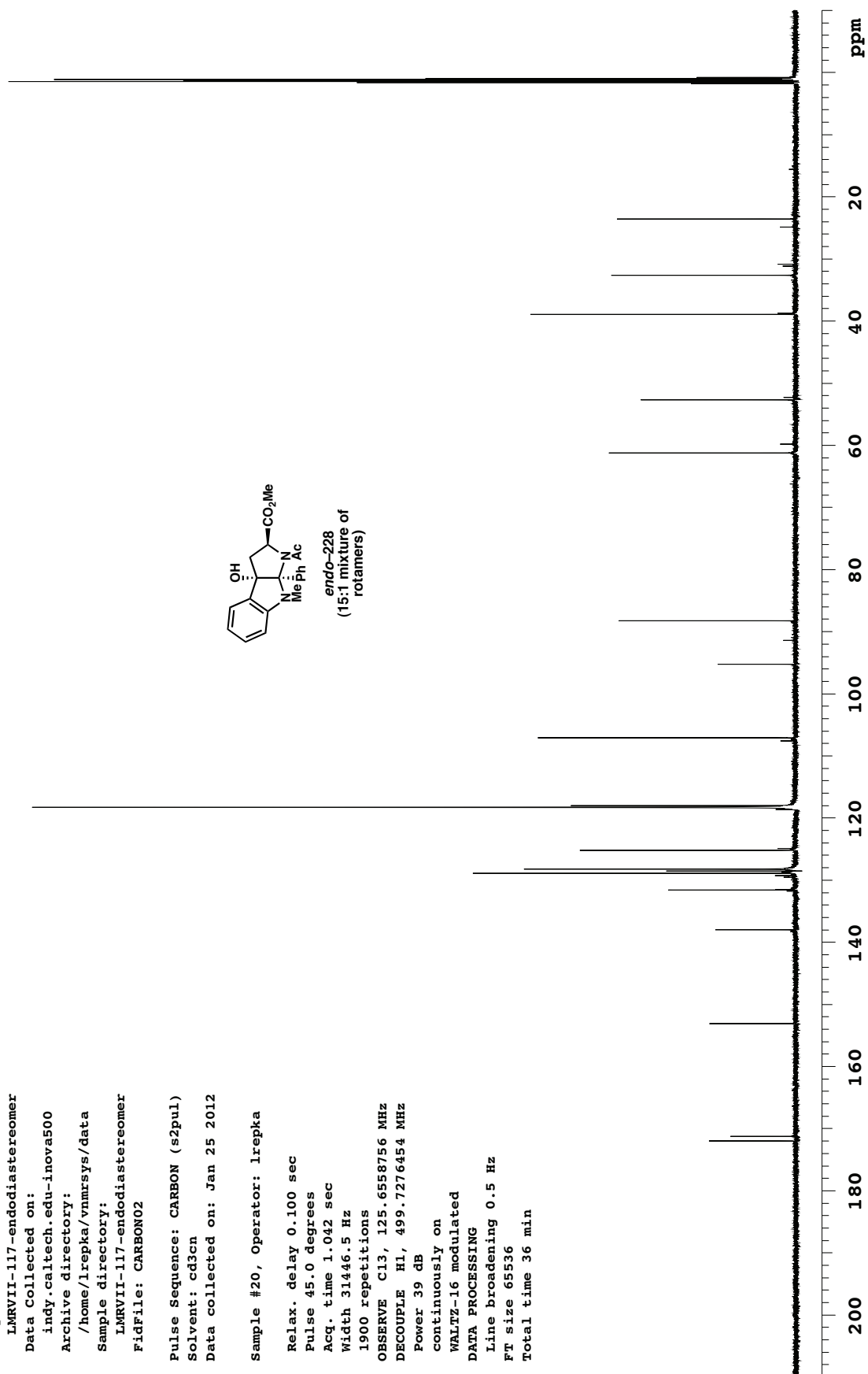
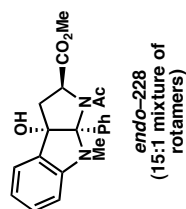
WALTZ-16 modulated

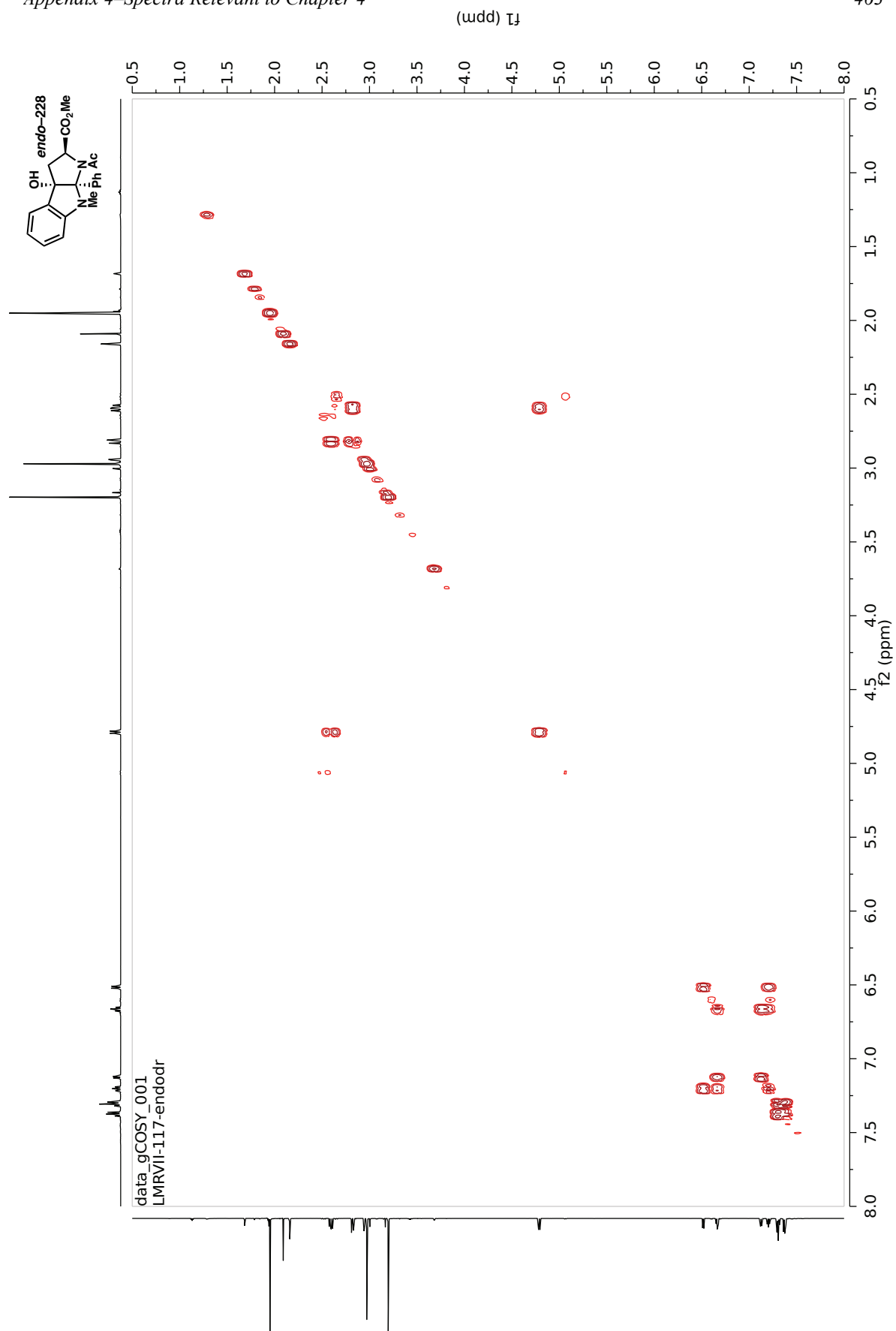
DATA PROCESSING

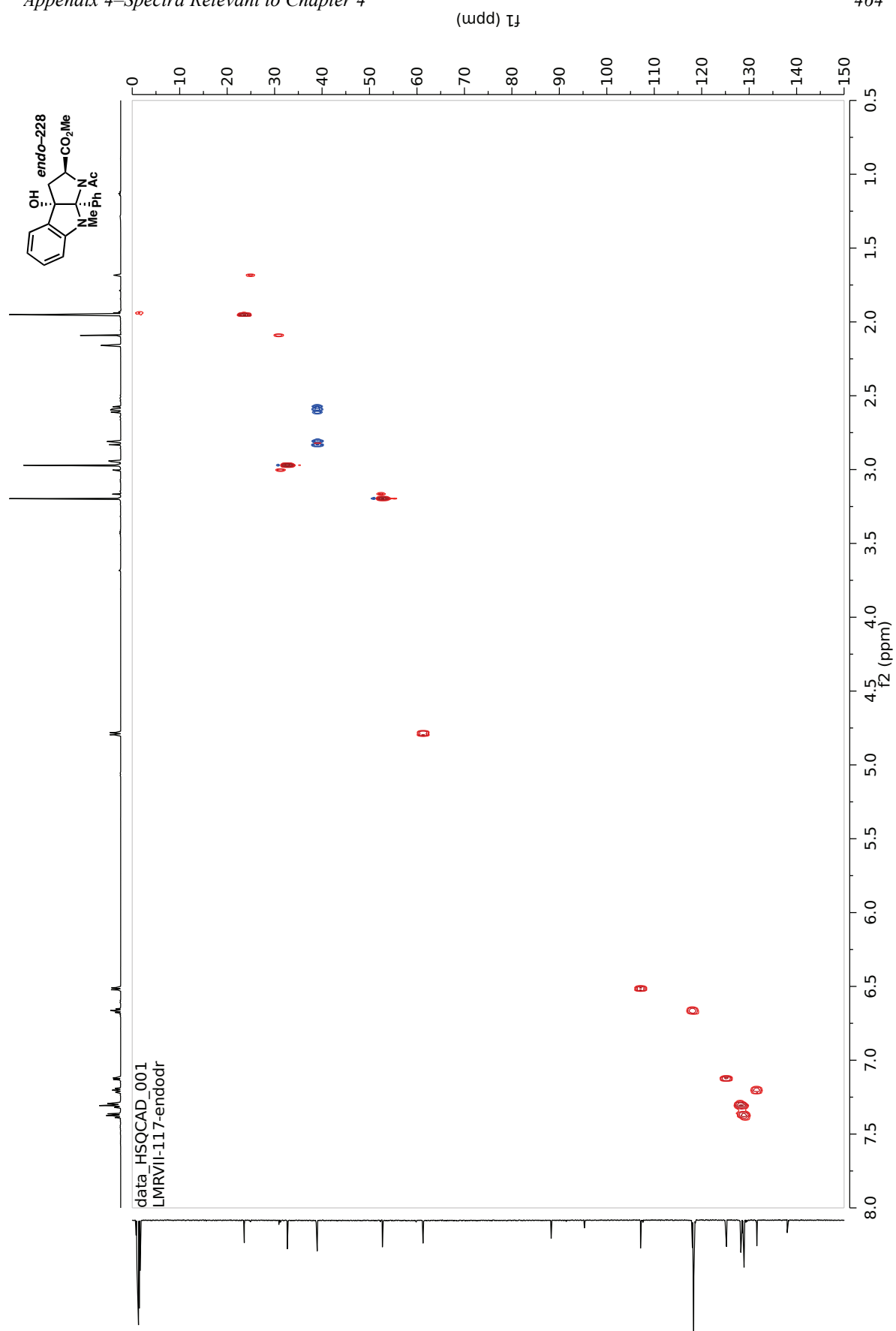
Line broadening 0.5 Hz

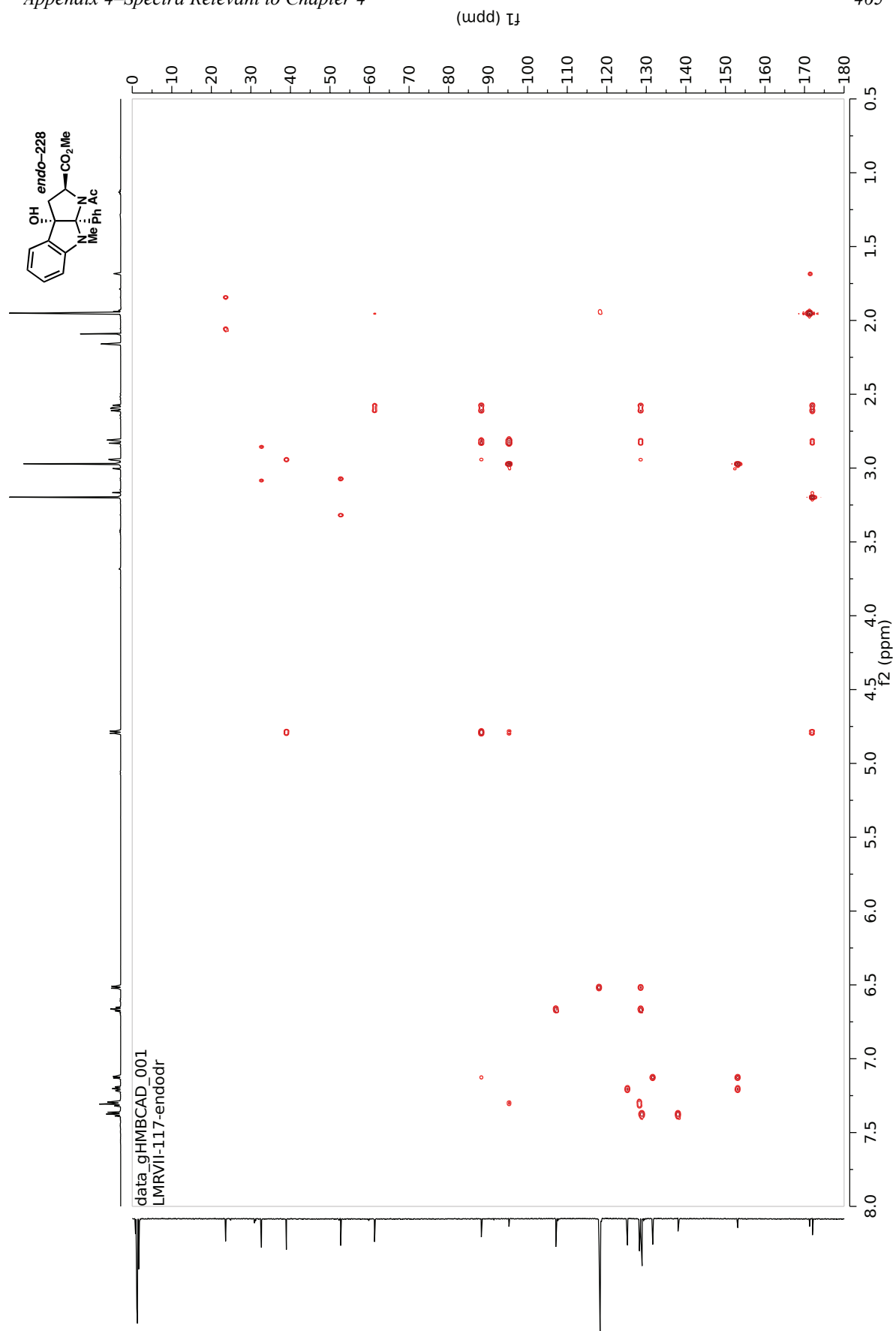
FT size 65536

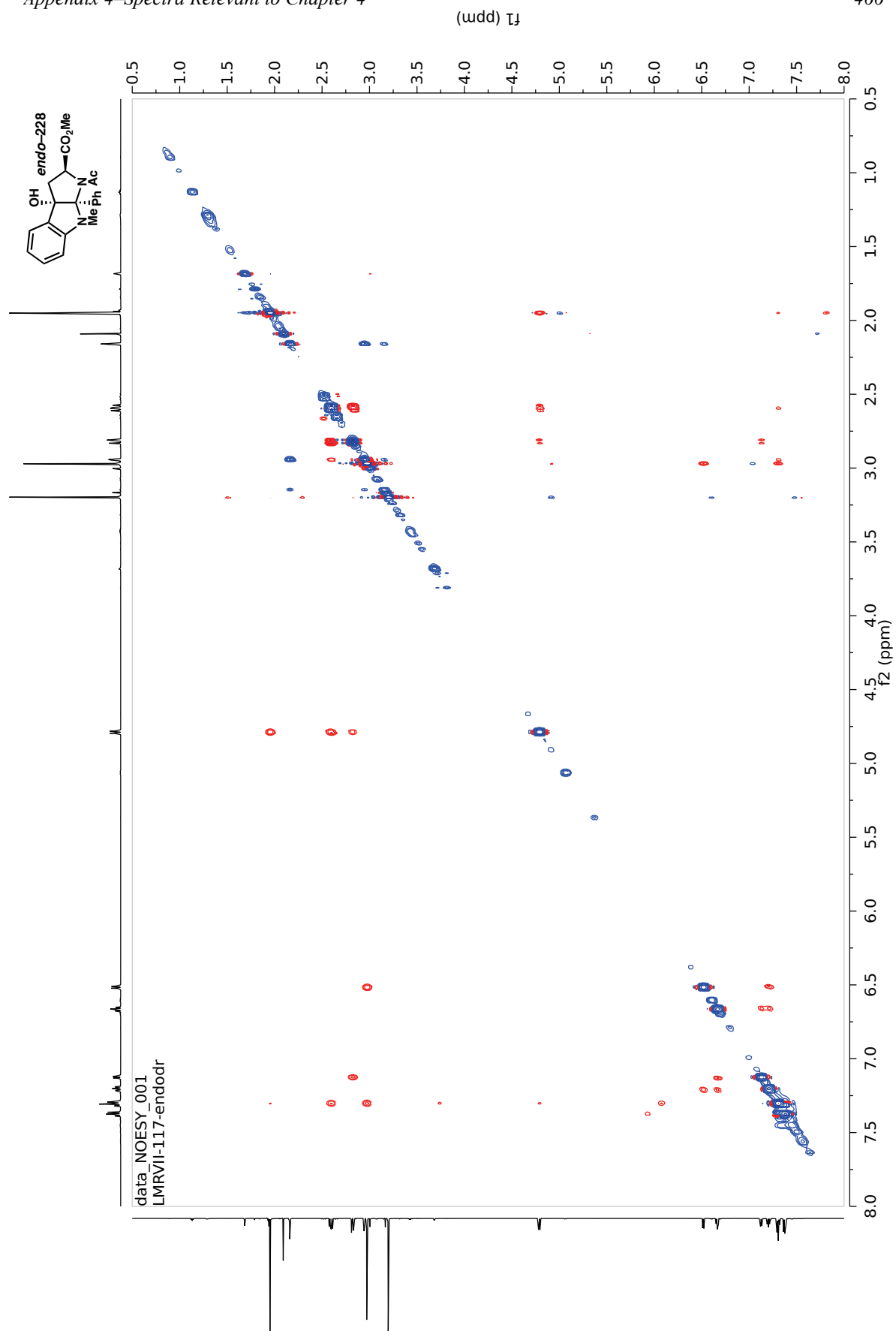
Total time 36 min











LMRVII-117-exodiastereomer

ErrorLog:

auto_20120127_01 loc:20 (night)

PROTON_003 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: PROTON02

Pulse Sequence: PROTON (s2pul)

Solvent: cd3cn

Data collected on: Jan 27 2012

Temp. 25.0 C / 298.1 K

Sample #20, Operator: lrepka

Relax. delay 25.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 8000.0 Hz

8 repetitions

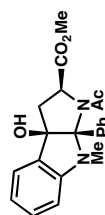
OBSERVE H1, 499.7251677 MHz

DATA PROCESSING

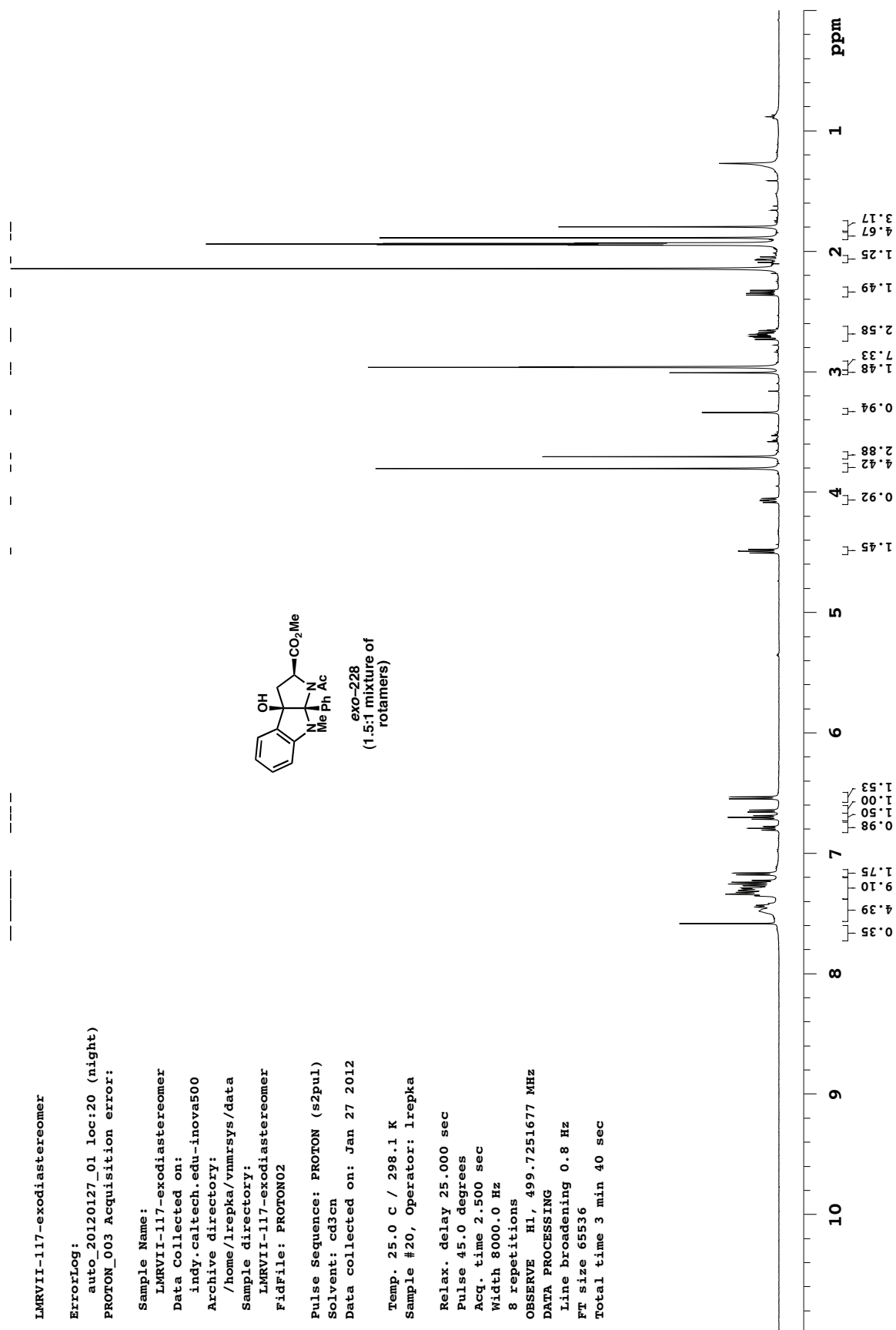
Line broadening 0.8 Hz

FT size 65536

Total time 3 min 40 sec



exo-228
(1.5:1 mixture of
rotamers)



LMRVII-117-exodiastereomer

ErrorLog:

auto_20120127_01_loc:20 (night)
 PROTON_003 Acquisition error:
 CARBON_001 Acquisition error:

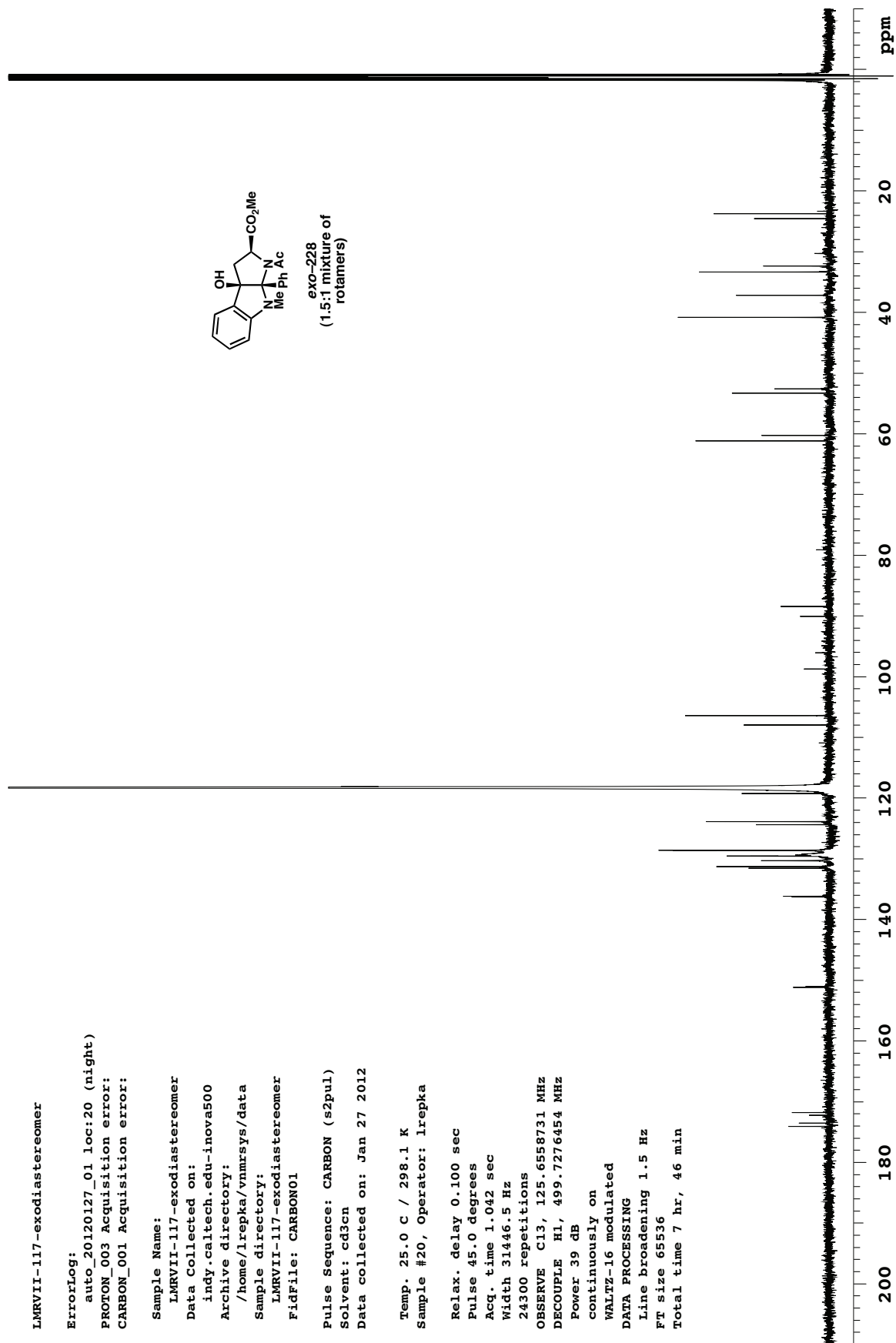
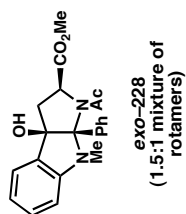
Sample Name:

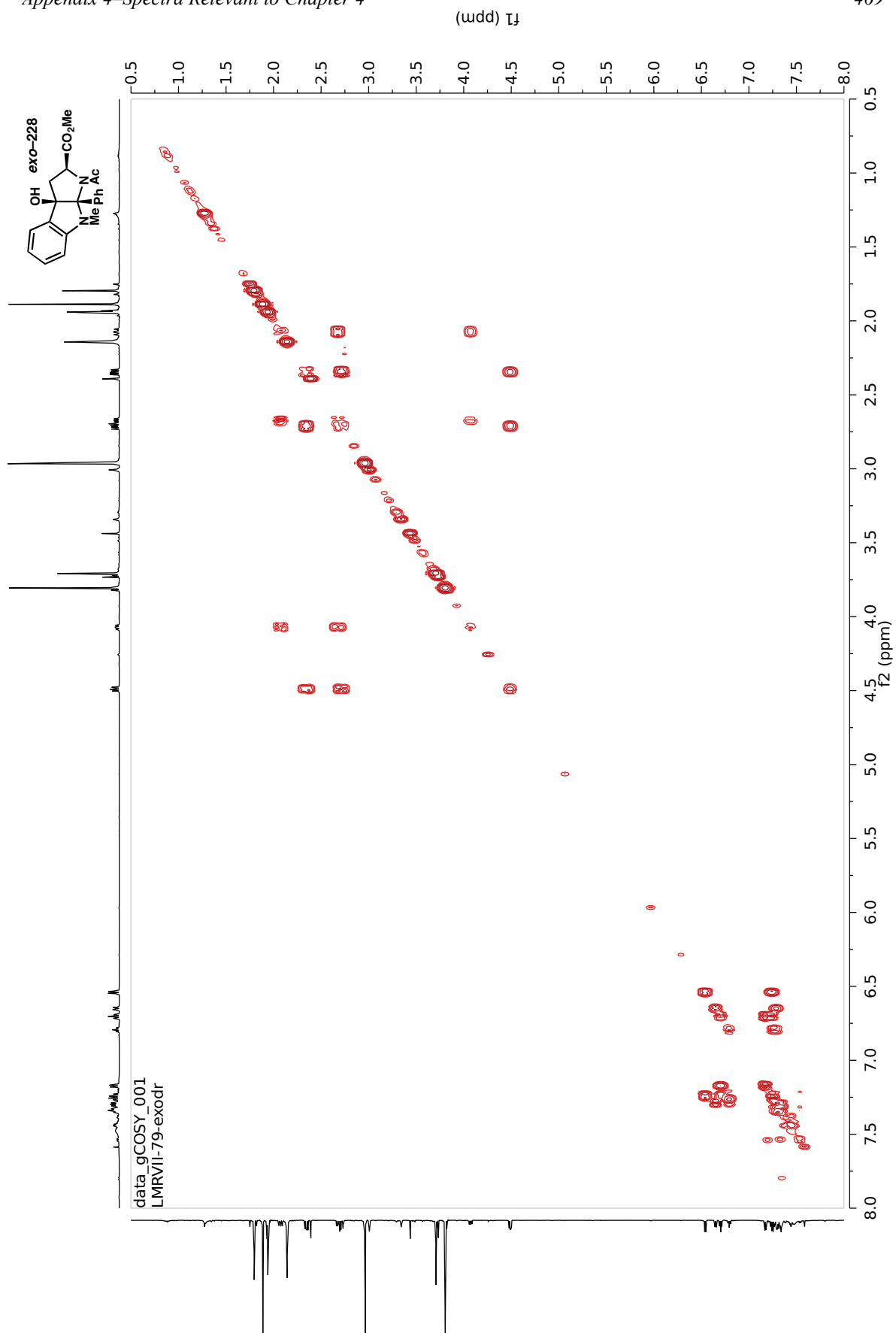
LMRVII-117-exodiastereomer
 Data Collected on:
 indy.caltech.edu-inova500
 Archive directory:
 /home/lrepka/vnmrsys/data
 Sample directory:
 LMRVII-117-exodiastereomer
 FIDFile: CARBON01

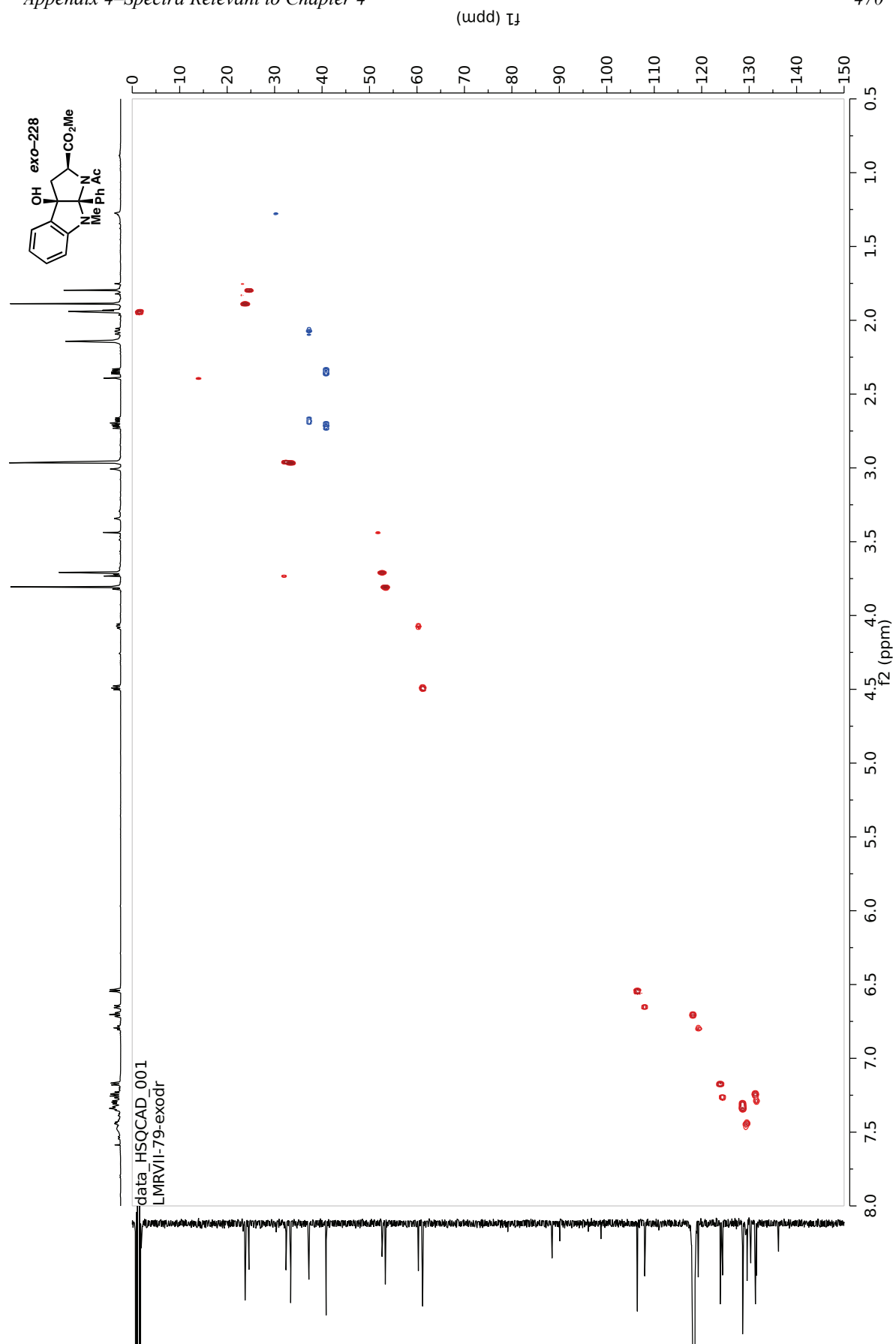
Pulse Sequence: CARBON (s2pul)
 Solvent: cd3cn
 Data collected on: Jan 27 2012

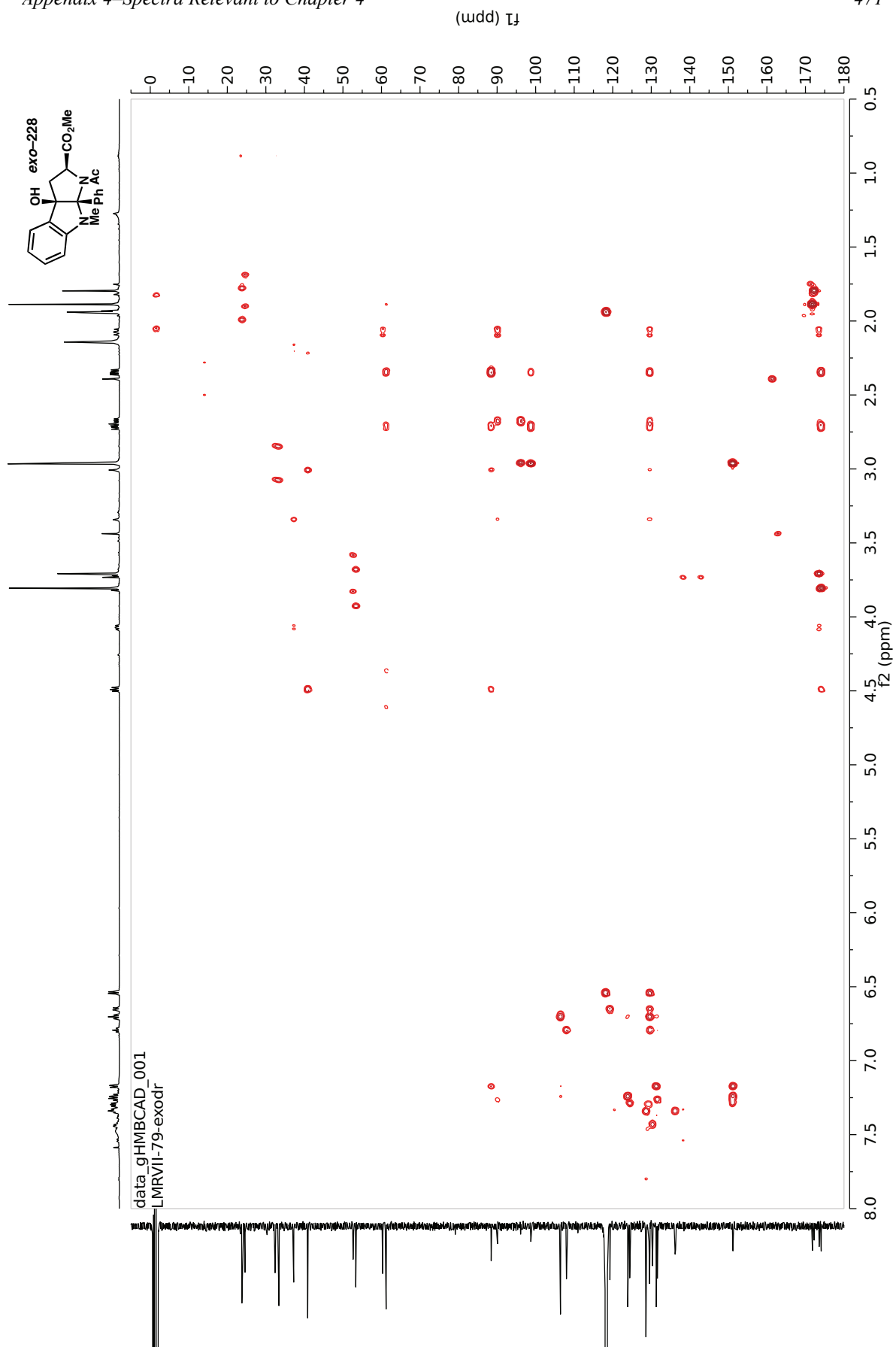
Temp. 25.0 C / 298.1 K
 Sample #20, Operator: lrepka

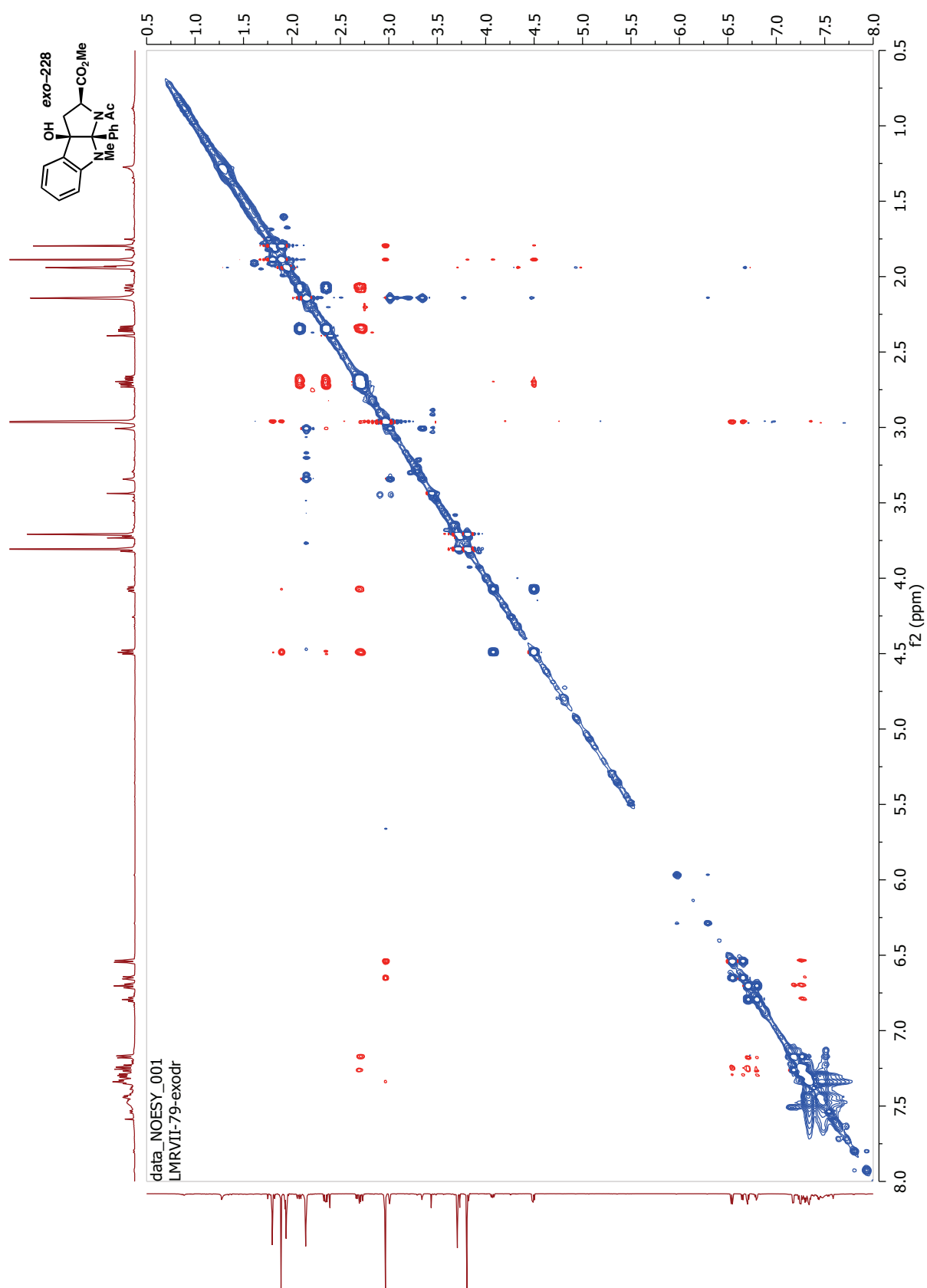
Relax. delay 0.100 sec
 Pulse 45.0 degrees
 Acq. time 1.042 sec
 Width 31446.5 Hz
 24300 repetitions
 OBSERVE C13, 125.6558731 MHz
 DECOUPLE H1, 499.7276454 MHz
 Power 39 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 65536
 Total time 7 hr, 46 min











LMRVII-205-f25-33

Sample Name:

LMRVII-205-f25-33

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/lrepka/vnmrSYS/data

Sample directory:

LMRVII-205-f25-33

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Apr 22 2012

Sample #40, Operator: lrepka

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4798.5 Hz

16 repetitions

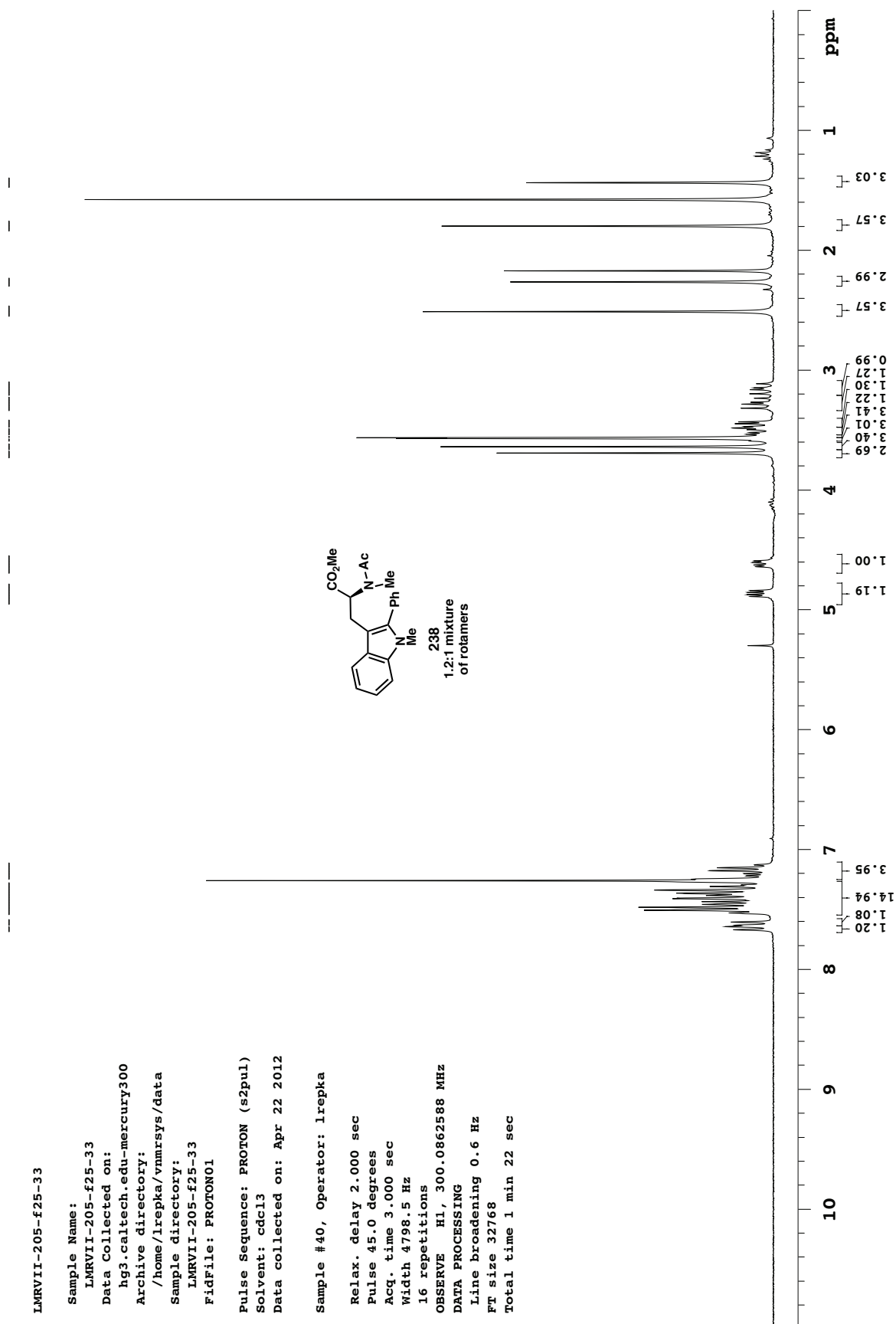
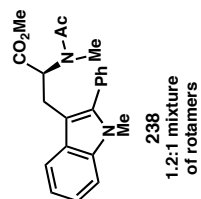
OBSERVE H1, 300.0862588 MHz

DATA PROCESSING

Line broadening 0.6 Hz

FT size 32768

Total time 1 min 22 sec



LMRVII-219-f17-23

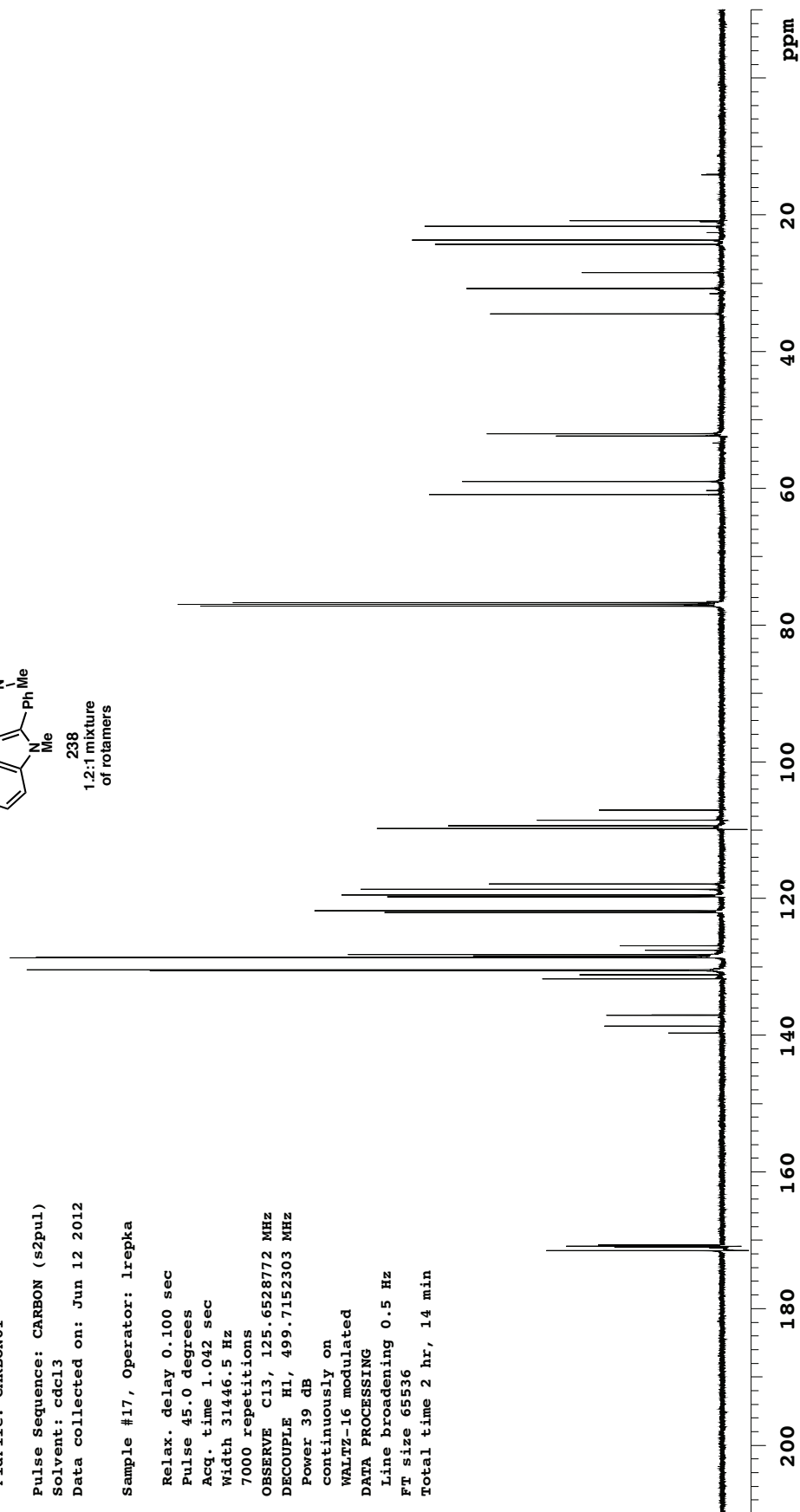
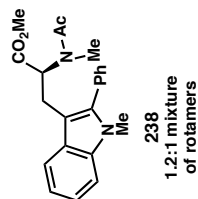
Sample Name:

LMRVII-219-f17-23
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrSYS/data
Sample directory:
LMRVII-219-f17-23
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 12 2012

Sample #17, Operator: lrepka

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
7000 repetitions
OBSERVE C13, 125.6528772 MHz
DECOUPLE H1, 499.7152303 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 2 hr, 14 min



LMRVII-215-pdt-1f56-2f31

Sample Name:

LMRVII-215-pdt-1f56-2f31

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVII-215-pdt-1f56-2f31

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 2 2012

Sample #41, Operator: lrepka

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 4798.5 Hz

16 repetitions

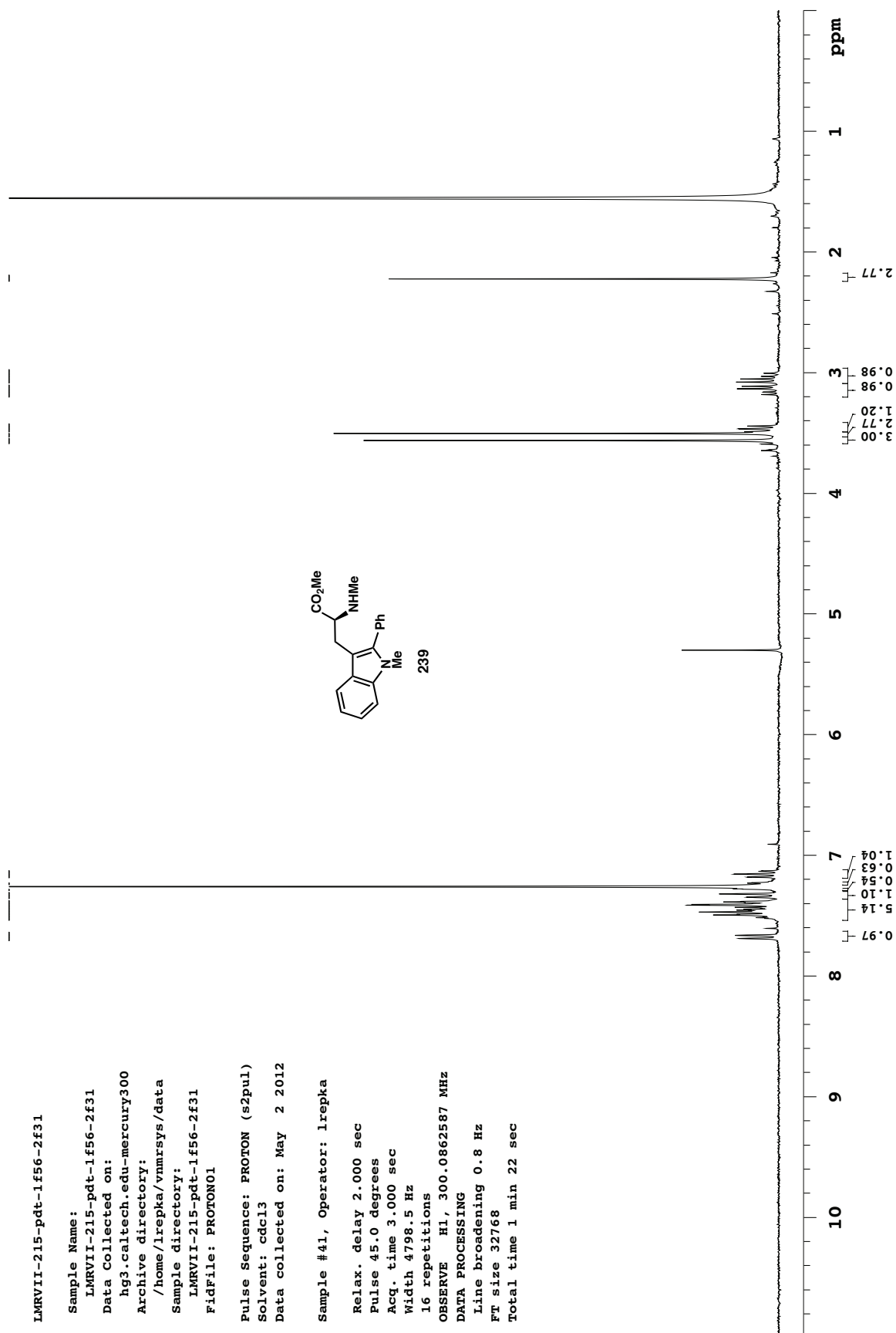
OBSERVE H1, 300.0862587 MHz

DATA PROCESSING

Line broadening 0.8 Hz

FT size 32768

Total time 1 min 22 sec



LMRVII-219-f25-42

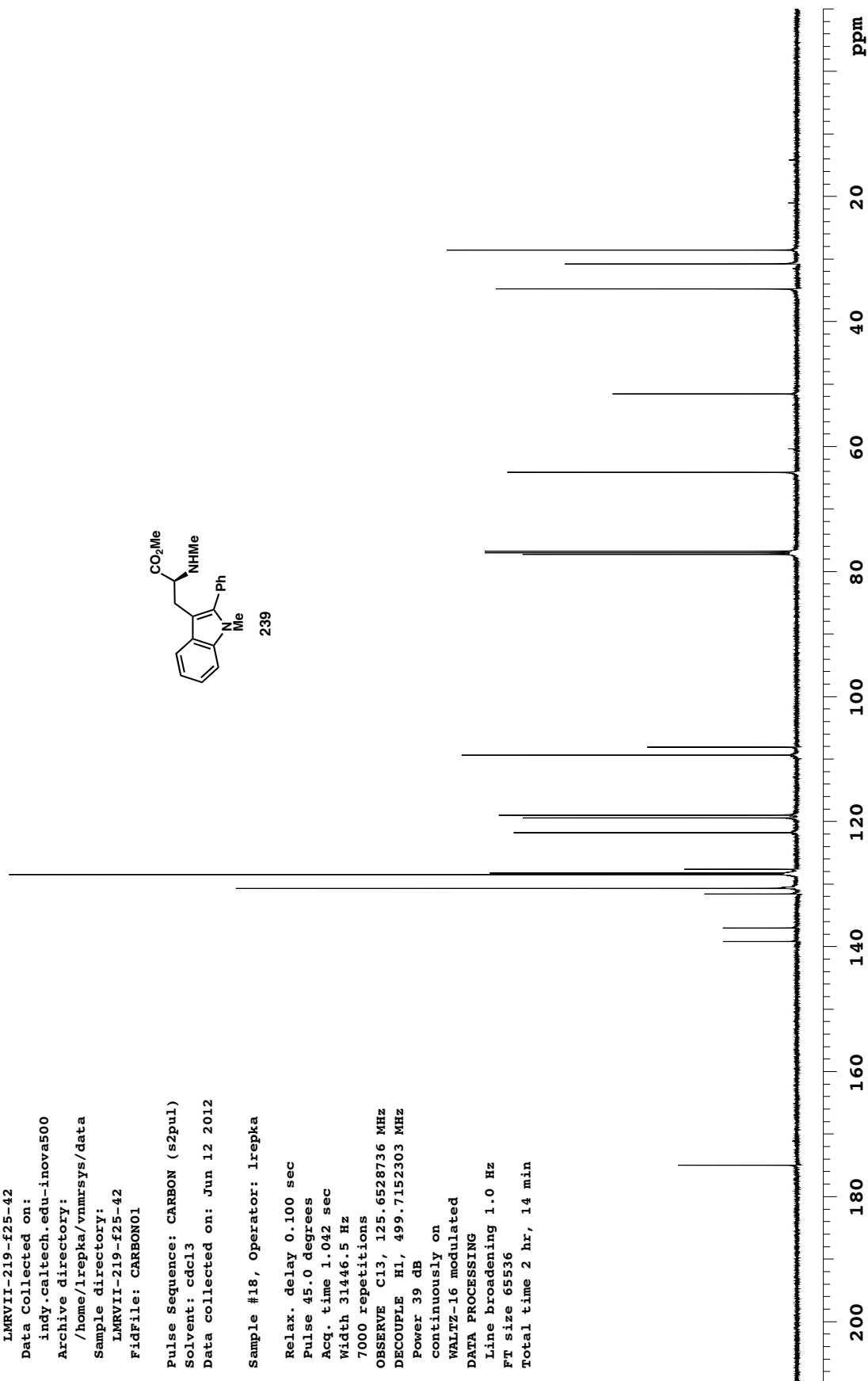
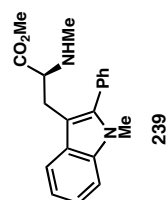
Sample Name:

LMRVII-219-f25-42
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-219-f25-42
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 12 2012

Sample #18, Operator: lrepka

Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
7000 repetitions
OBSERVE C13, 125.6528736 MHz
DECOUPLE H1, 499.7152303 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
Ft size 65536
Total time 2 hr, 14 min



LMRVII-225-phplc-f1

Sample Name:
LMRVII-225-phplc-f1
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-225-phplc-f1
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: May 11 2012

Sample #37, Operator: lrepka

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 8000.0 Hz

16 repetitions

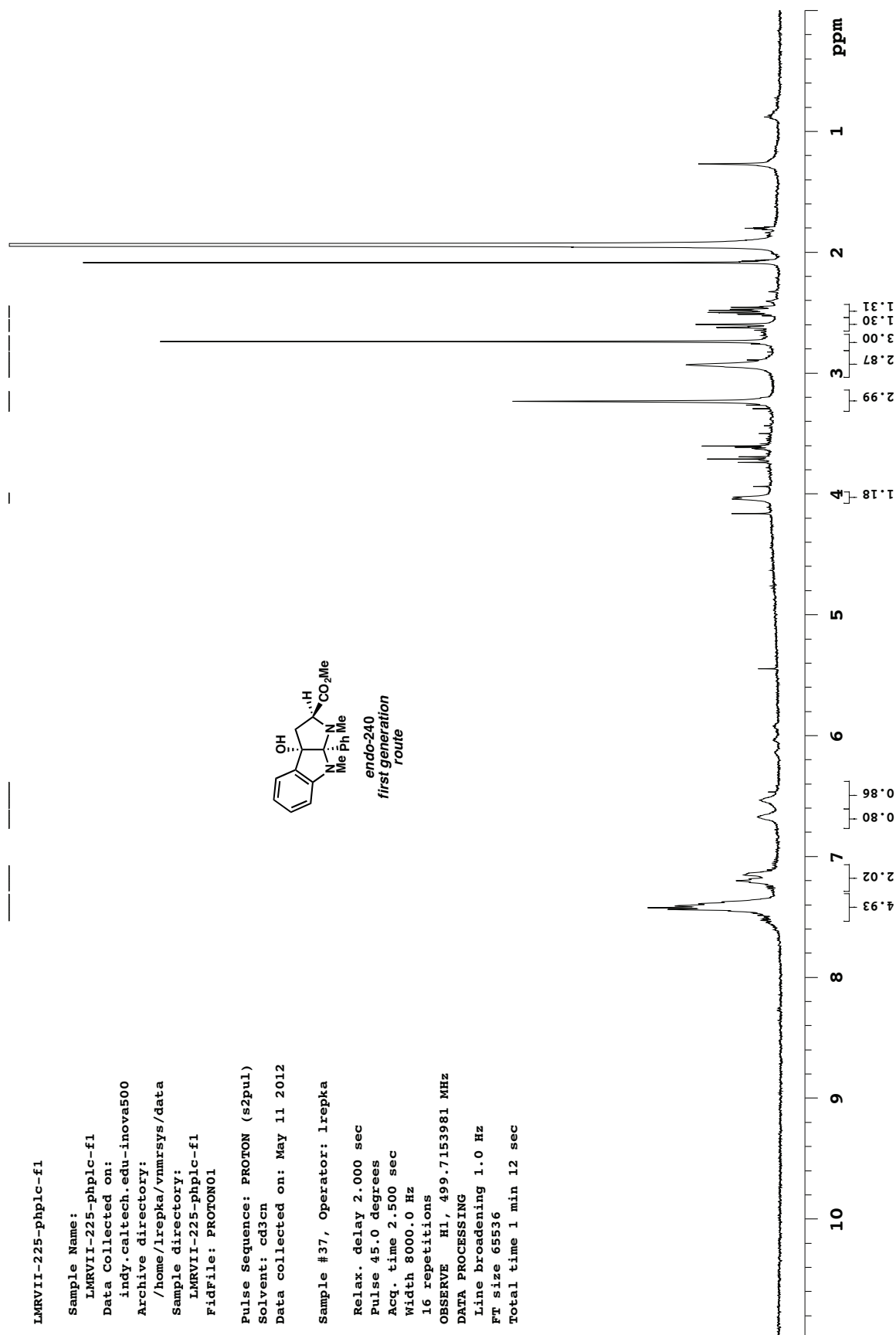
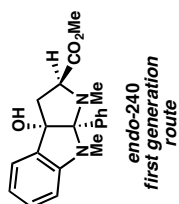
OBSERVE H1, 499.7153981 MHz

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1 min 12 sec



LMRVII-225-phplc-f2

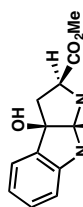
Sample Name:
LMRVII-225-phplc-f2
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-225-phplc-f2
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: May 11 2012

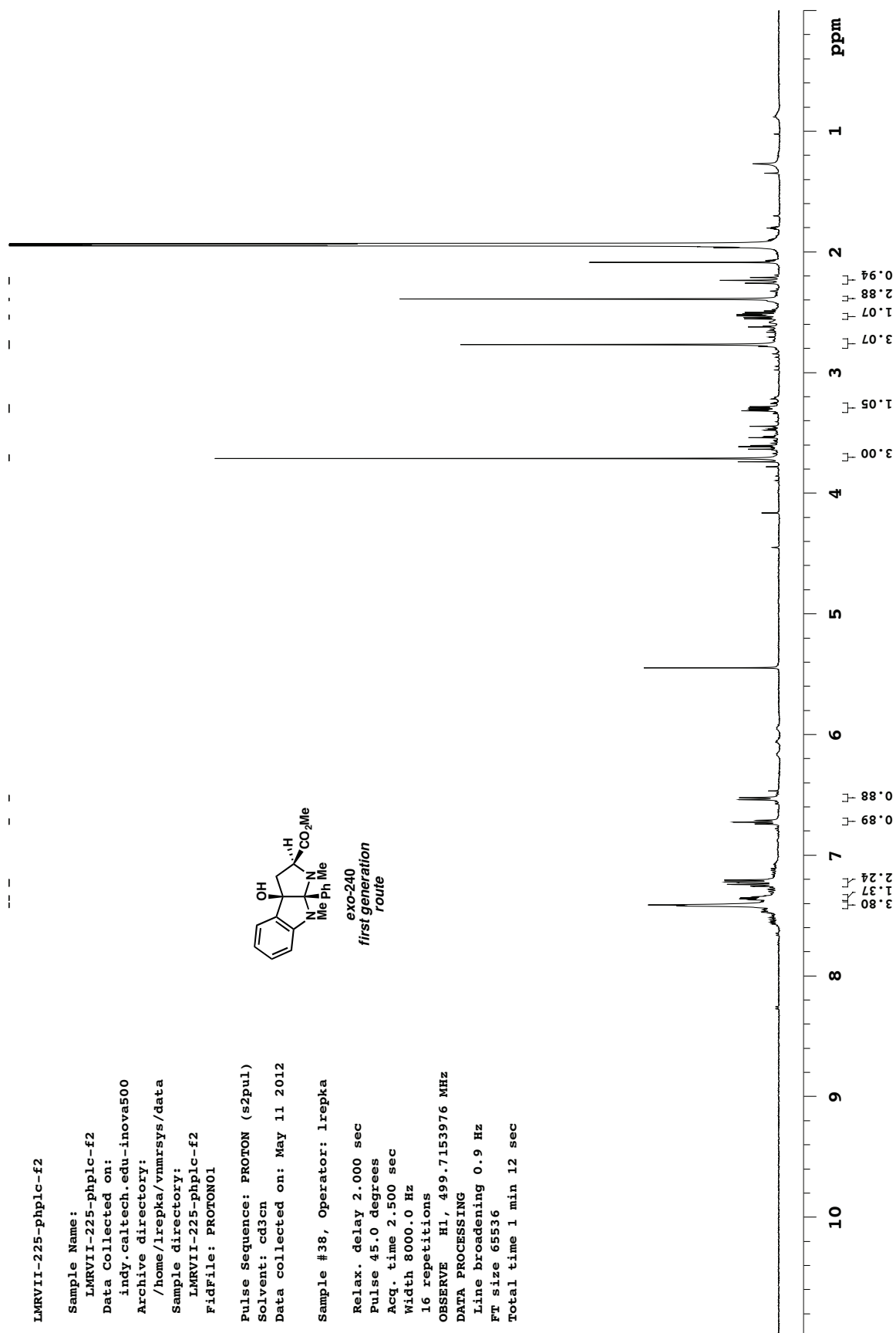
Sample #38, Operator: lrepka

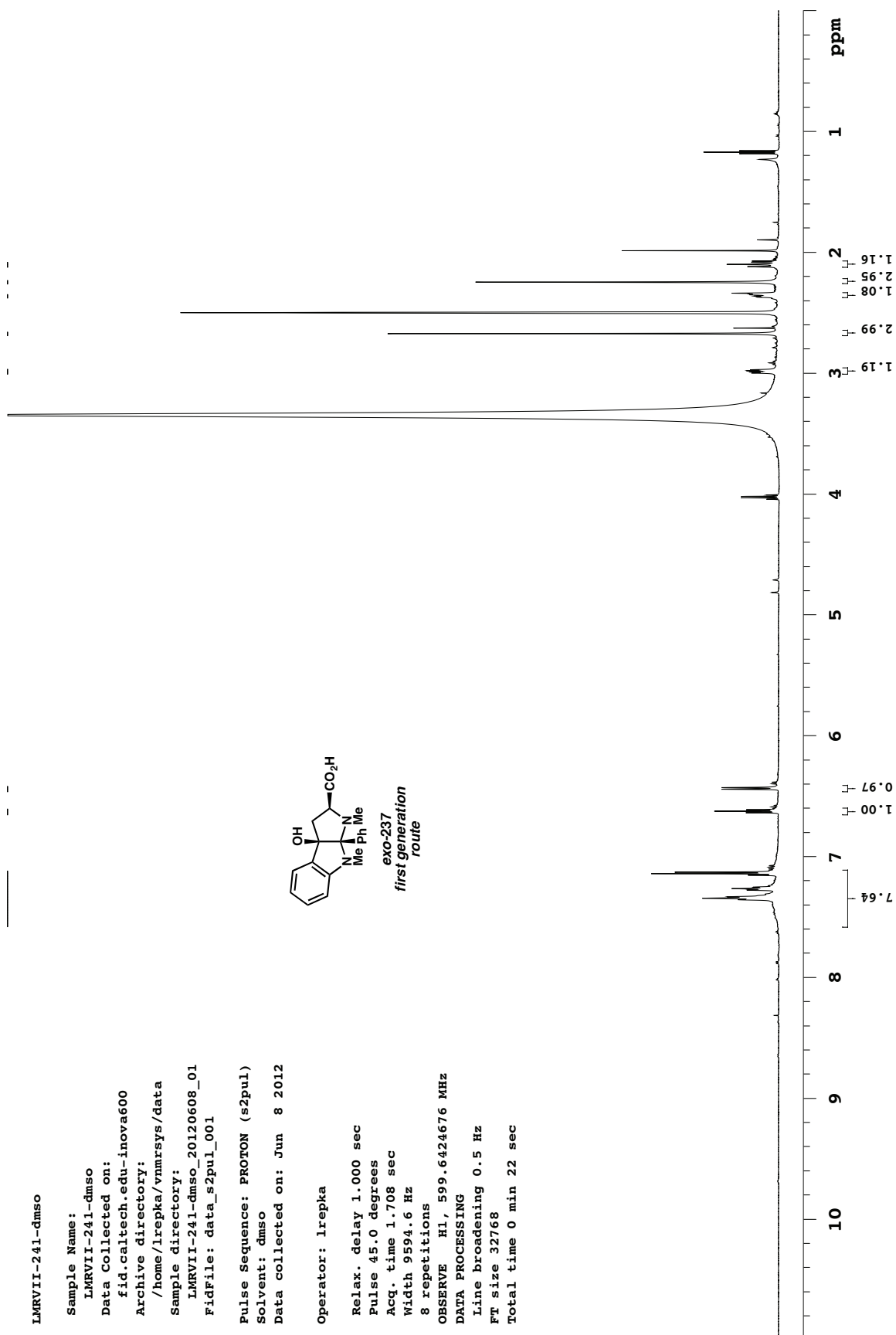
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 8000.0 Hz

16 repetitions
OBSERVE H1, 499.7153976 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 65536
Total time 1 min 12 sec



exo-240
first generation
route





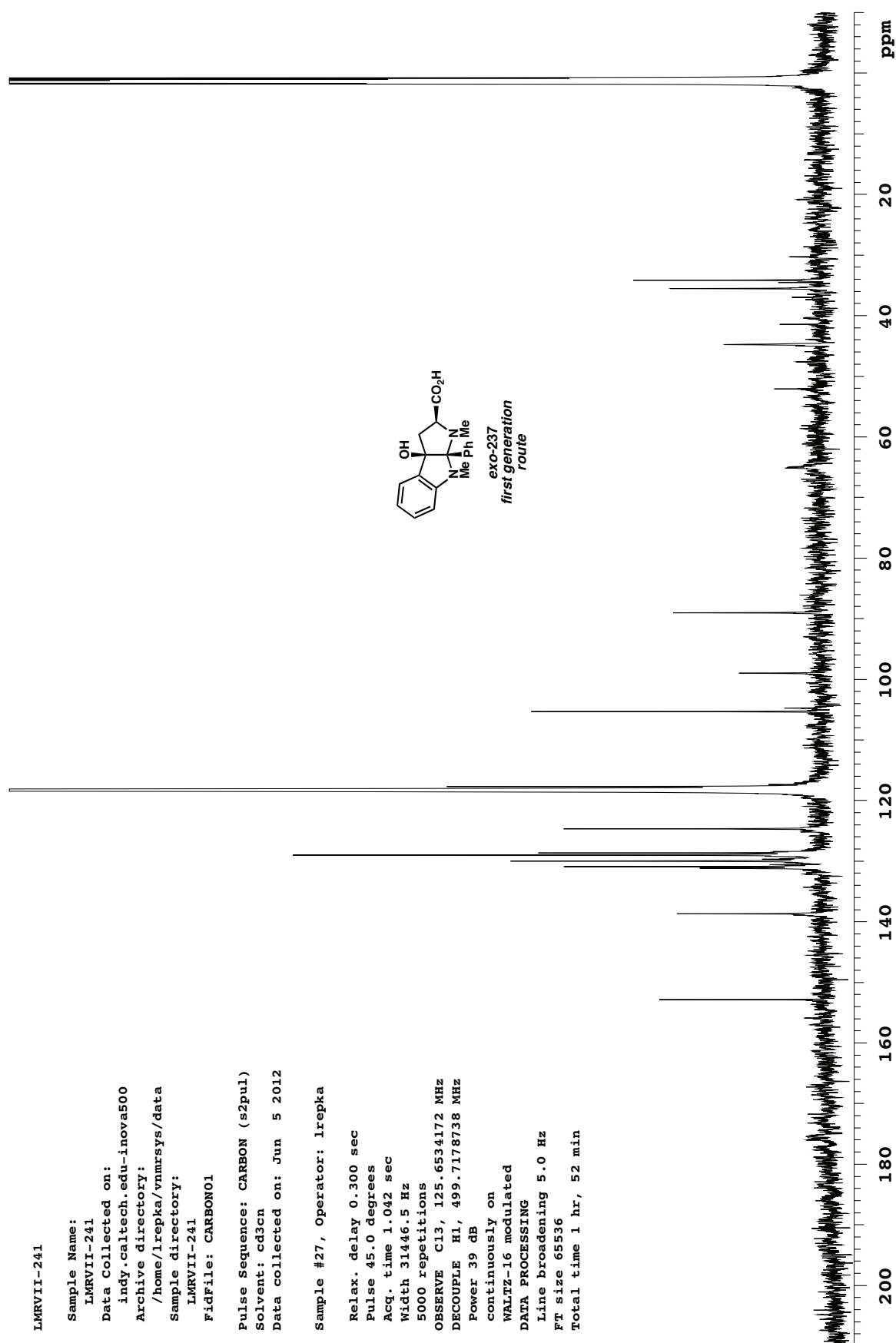
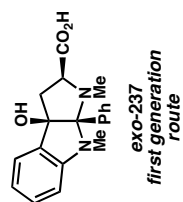
LMRVII-241

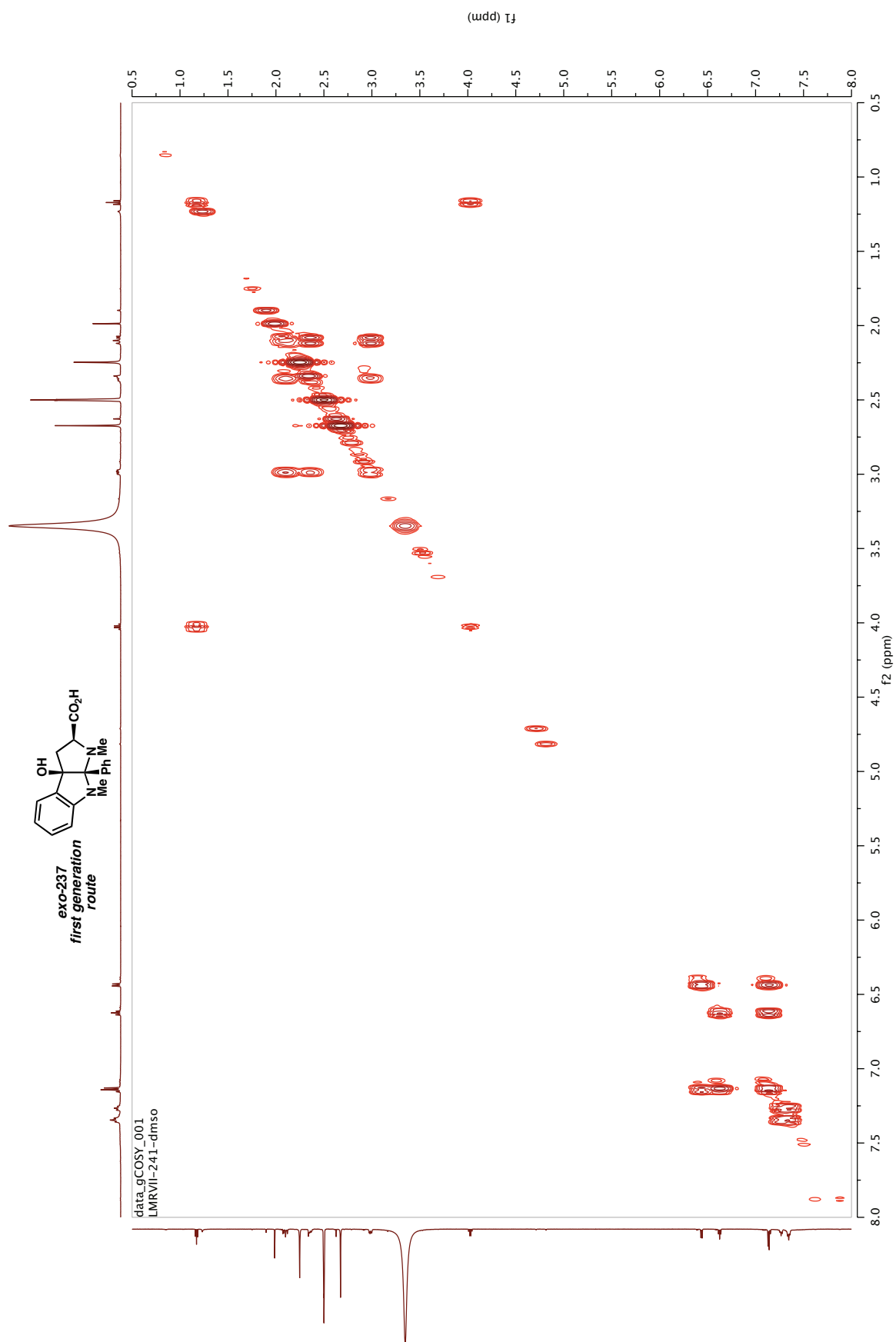
Sample Name:
LMRVII-241
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVII-241
FidFile: CARBON01

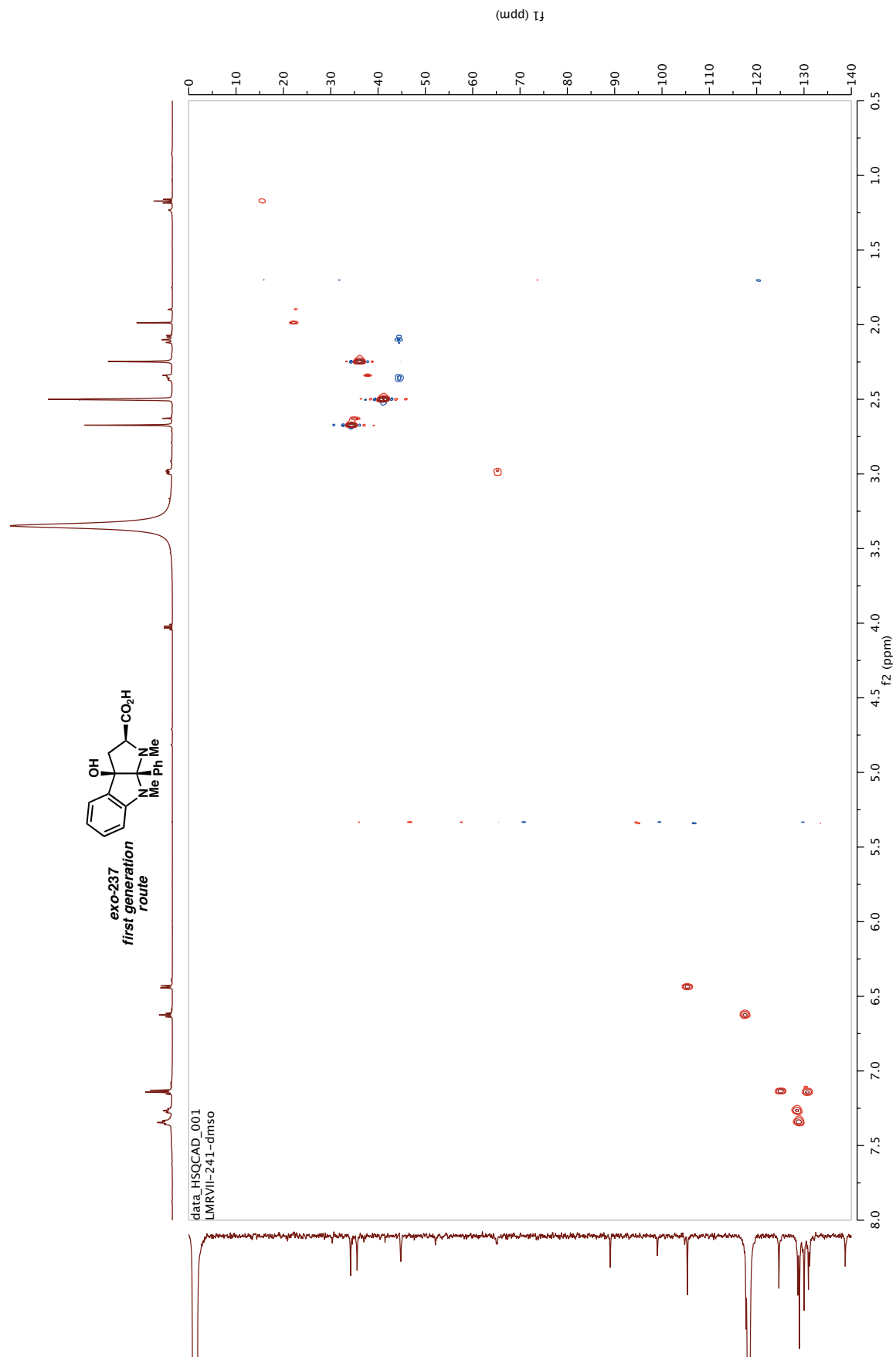
Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: Jun 5 2012

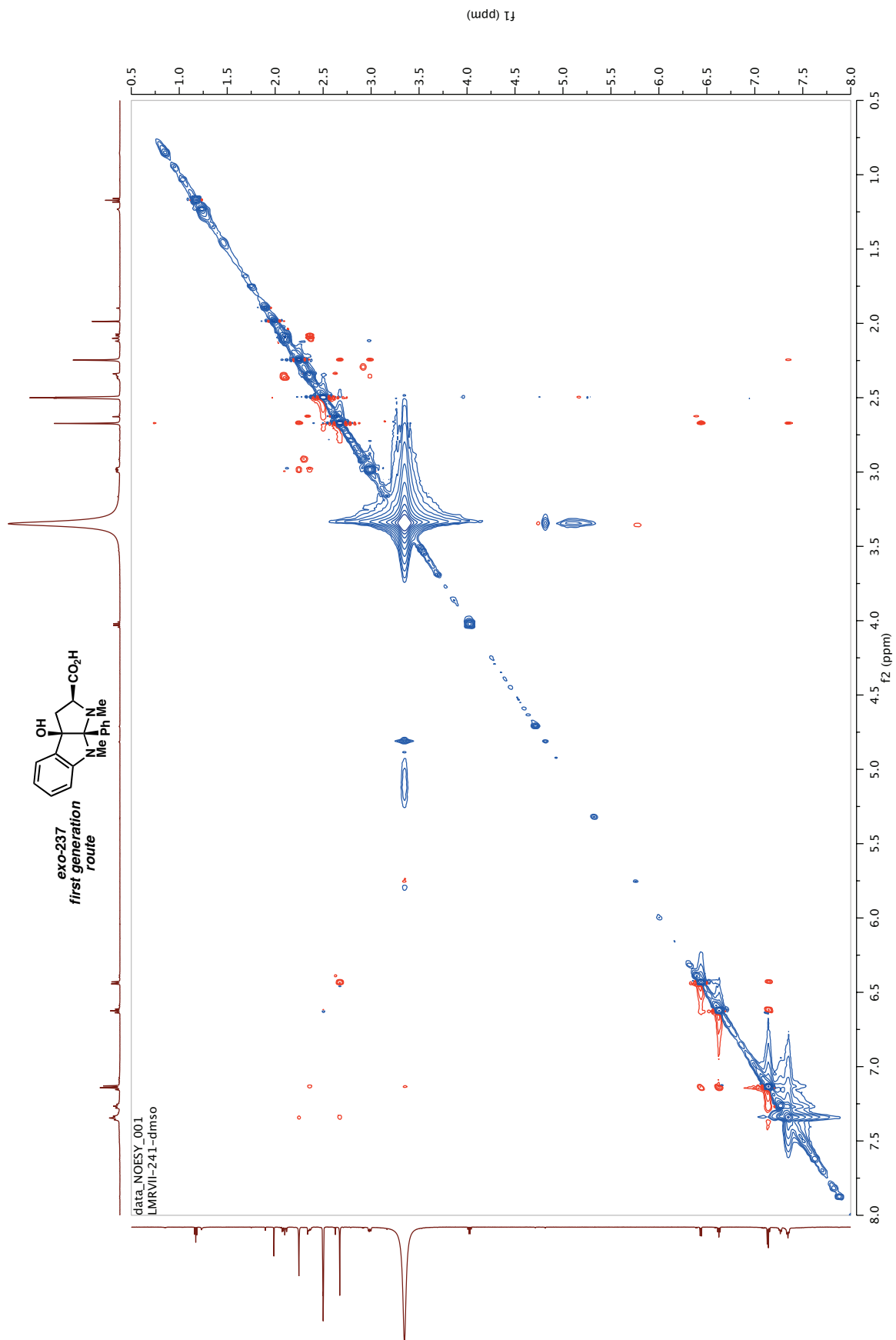
Sample #27, Operator: lrepka

Relax. delay 0.300 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
5000 repetitions
OBSERVE C13, 125.6534172 MHz
DECOUPLE H1, 499.7178738 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 5.0 Hz
FT size 65536
Total time 1 hr, 52 min







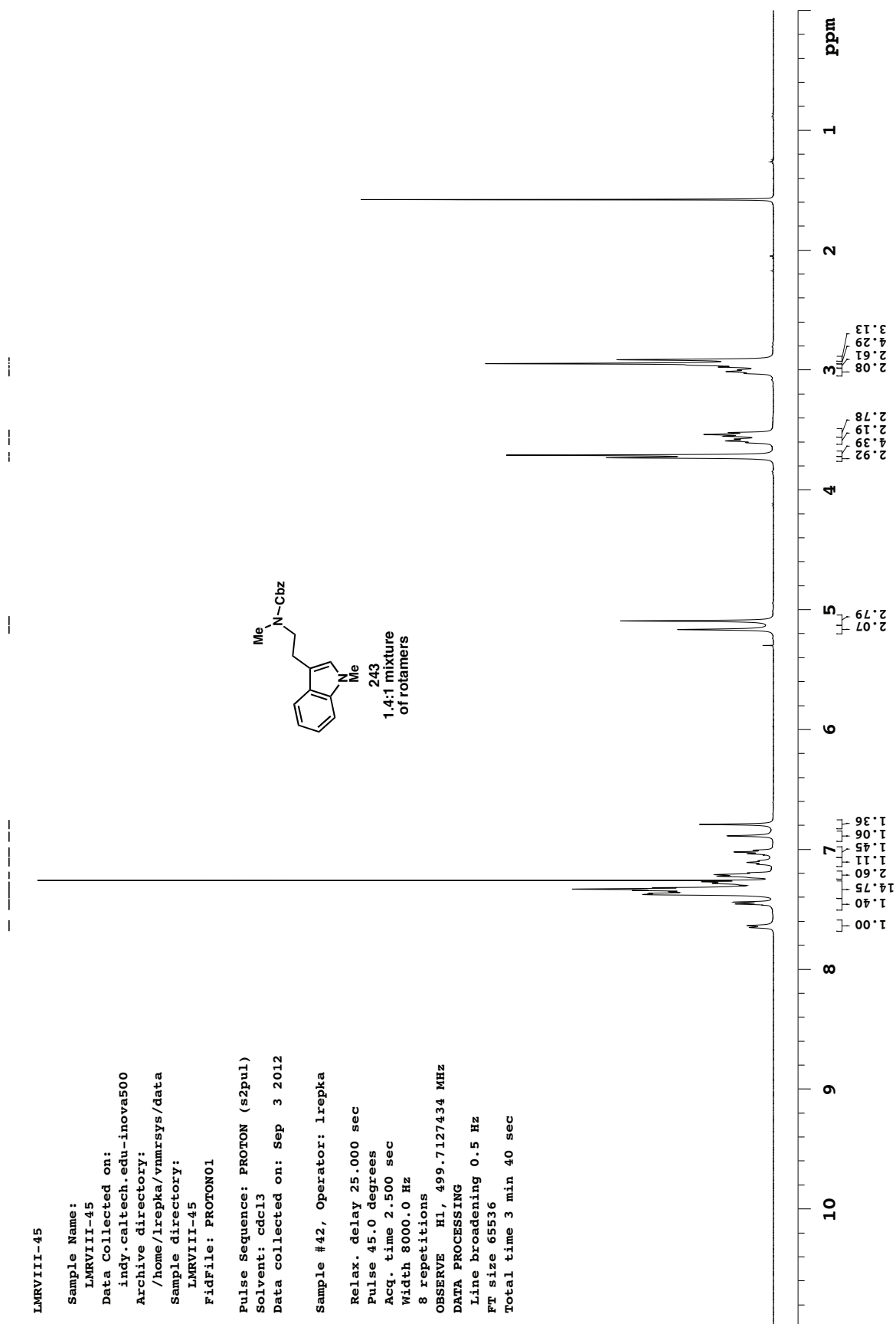
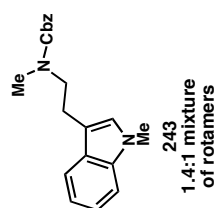


LMRVIII-45

Sample Name:
LMRVIII-45
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVIII-45
FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2012

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, 499.7127434 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 3 min 40 sec



LMRVIII-45-carbon

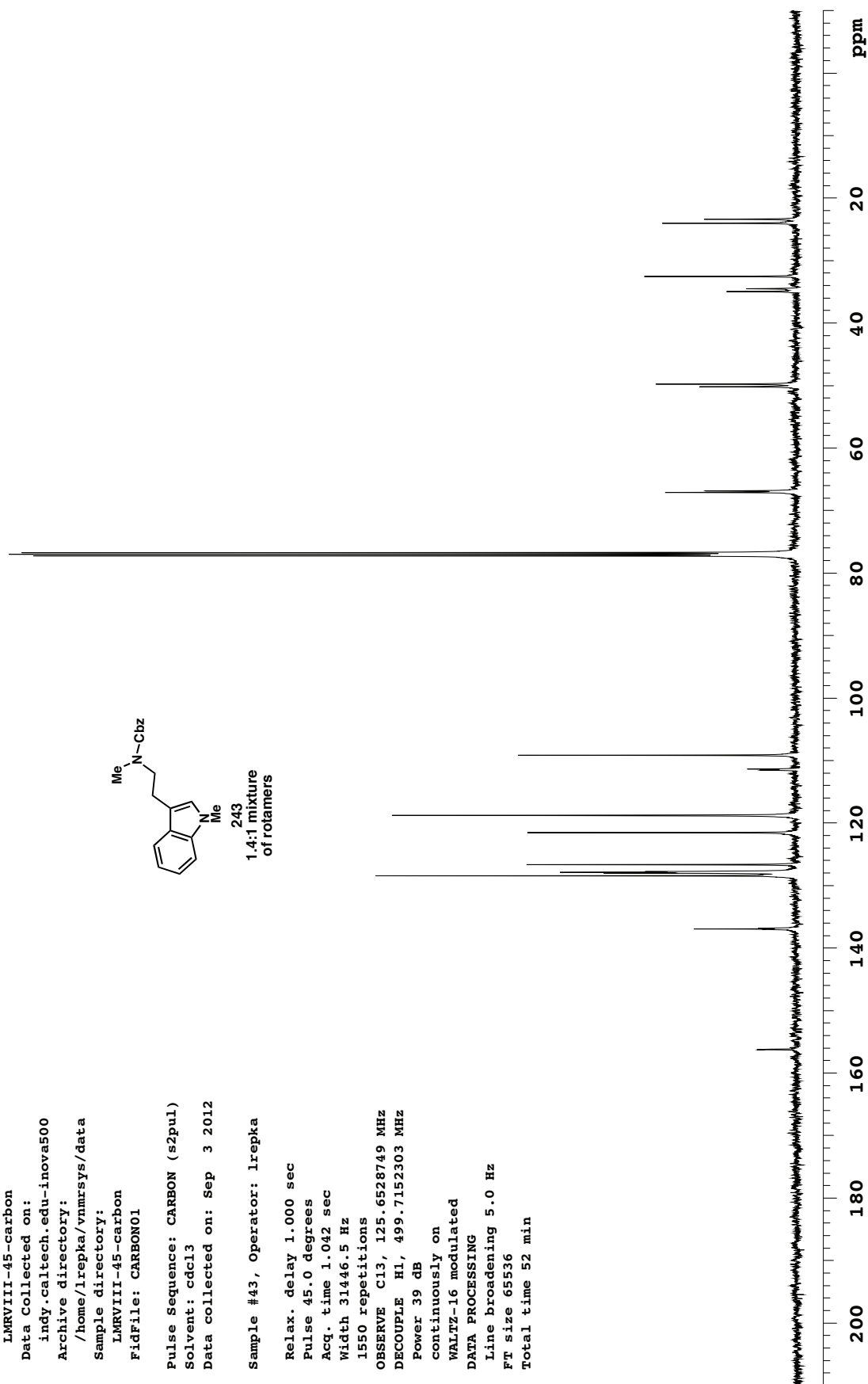
Sample Name:

LMRVIII-45-carbon
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrSYS/data
Sample directory:
LMRVIII-45-carbon
FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 3 2012

Sample #43, Operator: lrepka

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
1550 repetitions
OBSERVE C13, 125.6528749 MHz
DECOUPLE H1, 499.7152303 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 5.0 Hz
FT size 65536
Total time 52 min



AMAO-1-75

Sample Name:

AMAO-1-75

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsvs/data

Sample directory:

AMAO-1-75

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 12 2013

Sample #10, Operator: amao

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.273 sec

Width 5006.3 Hz

16 repetitions

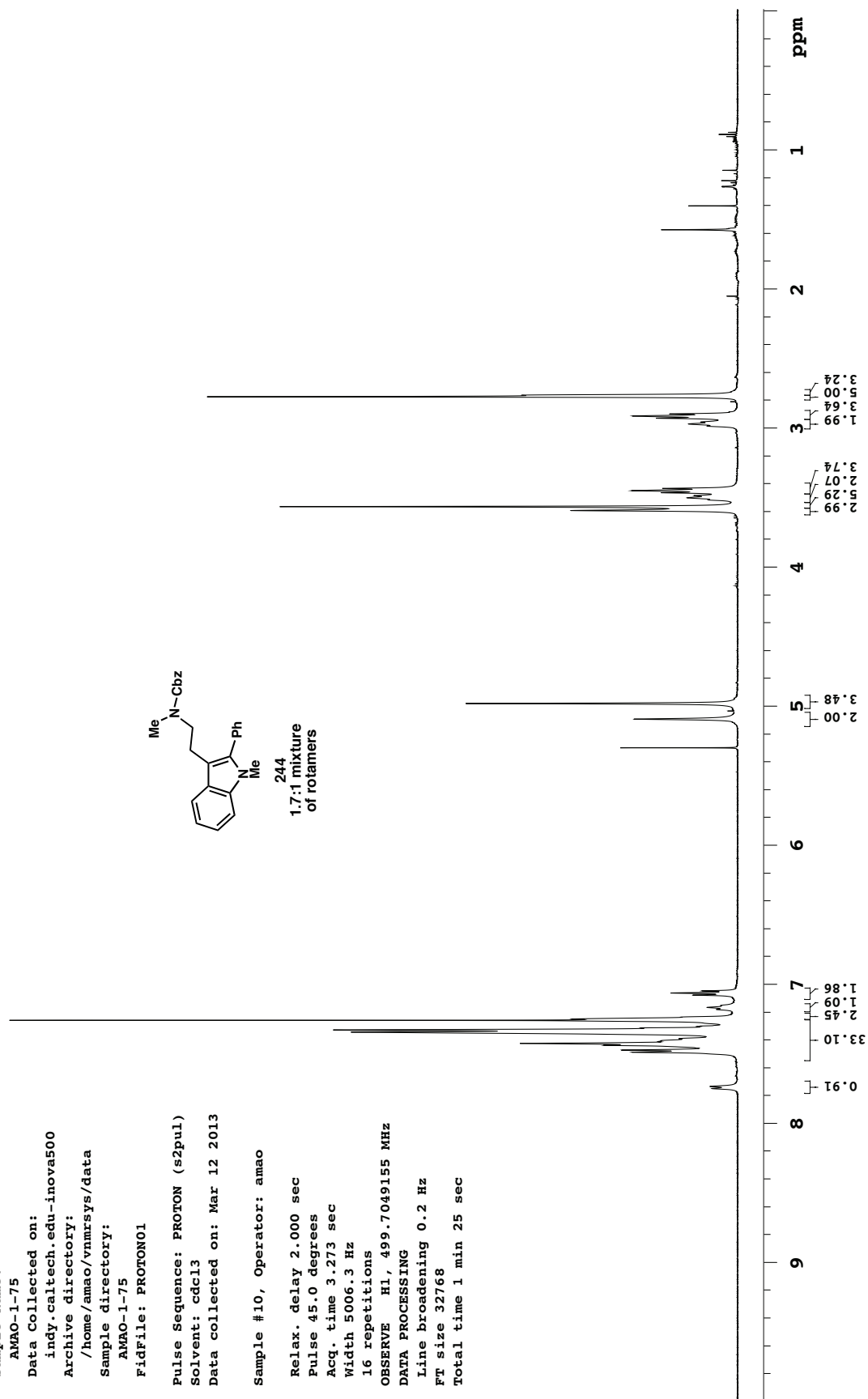
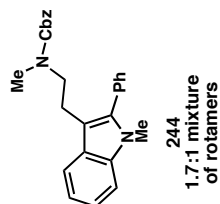
OBSERVE H1, 499.7049155 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 32768

Total time 1 min 25 sec



AMAO-1-51

Sample Name:

AMAO-1-51

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-51

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 12 2013

Sample #8, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6509065 MHz

DECOUPLE H1, 499.7074131 MHz

Power 39 dB

continuously on

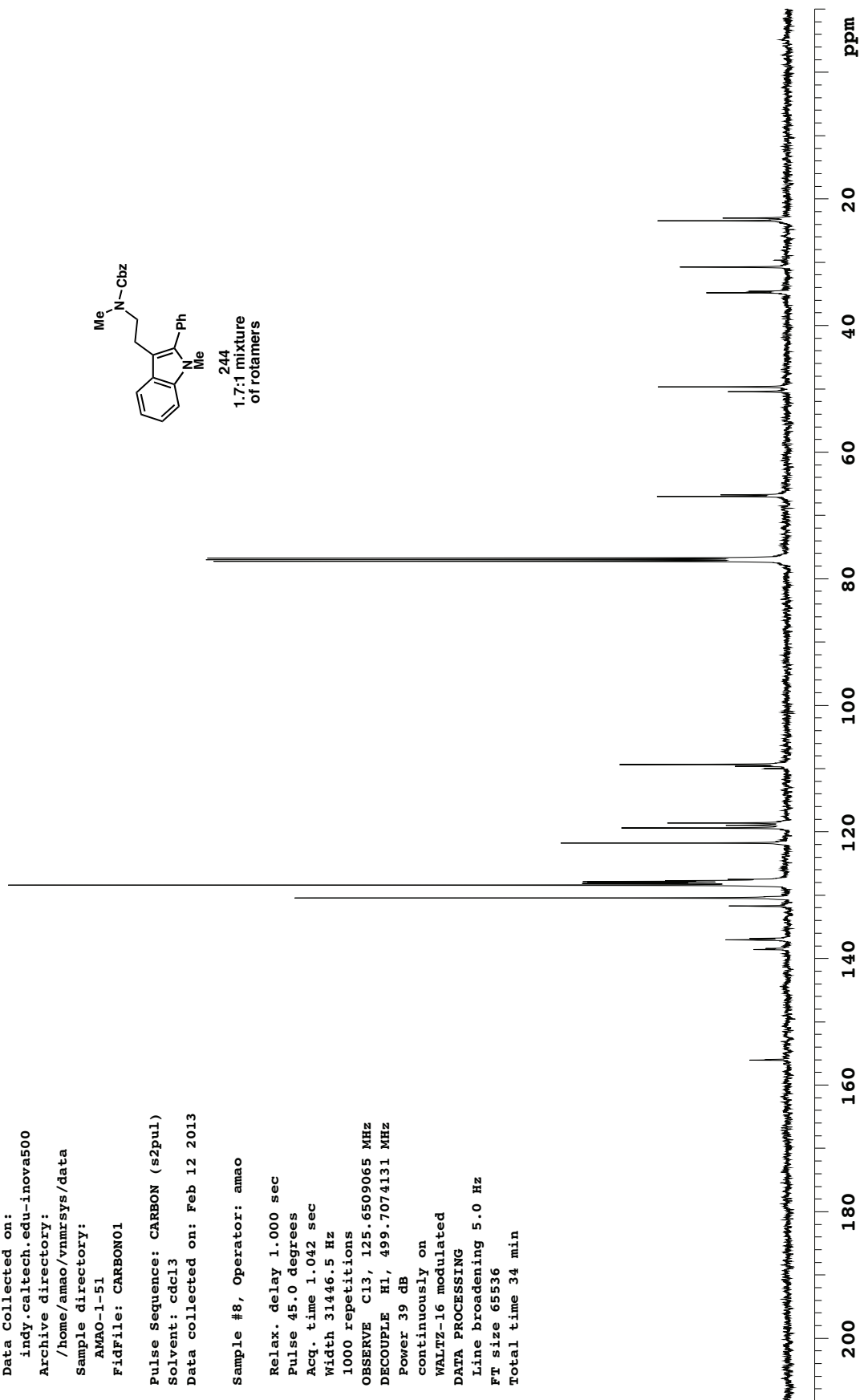
WALTZ-16 modulated

DATA PROCESSING

Line broadening 5.0 Hz

FT size 65536

Total time 34 min



AMAO-1-82

Sample Name:

AMAO-1-82

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-82

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 15 2013

Sample #15, Operator: amao

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 3.273 sec

Width 5006.3 Hz

16 repetitions

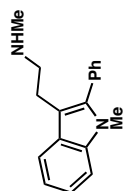
OBSERVE H1, 499.7049157 MHz

DATA PROCESSING

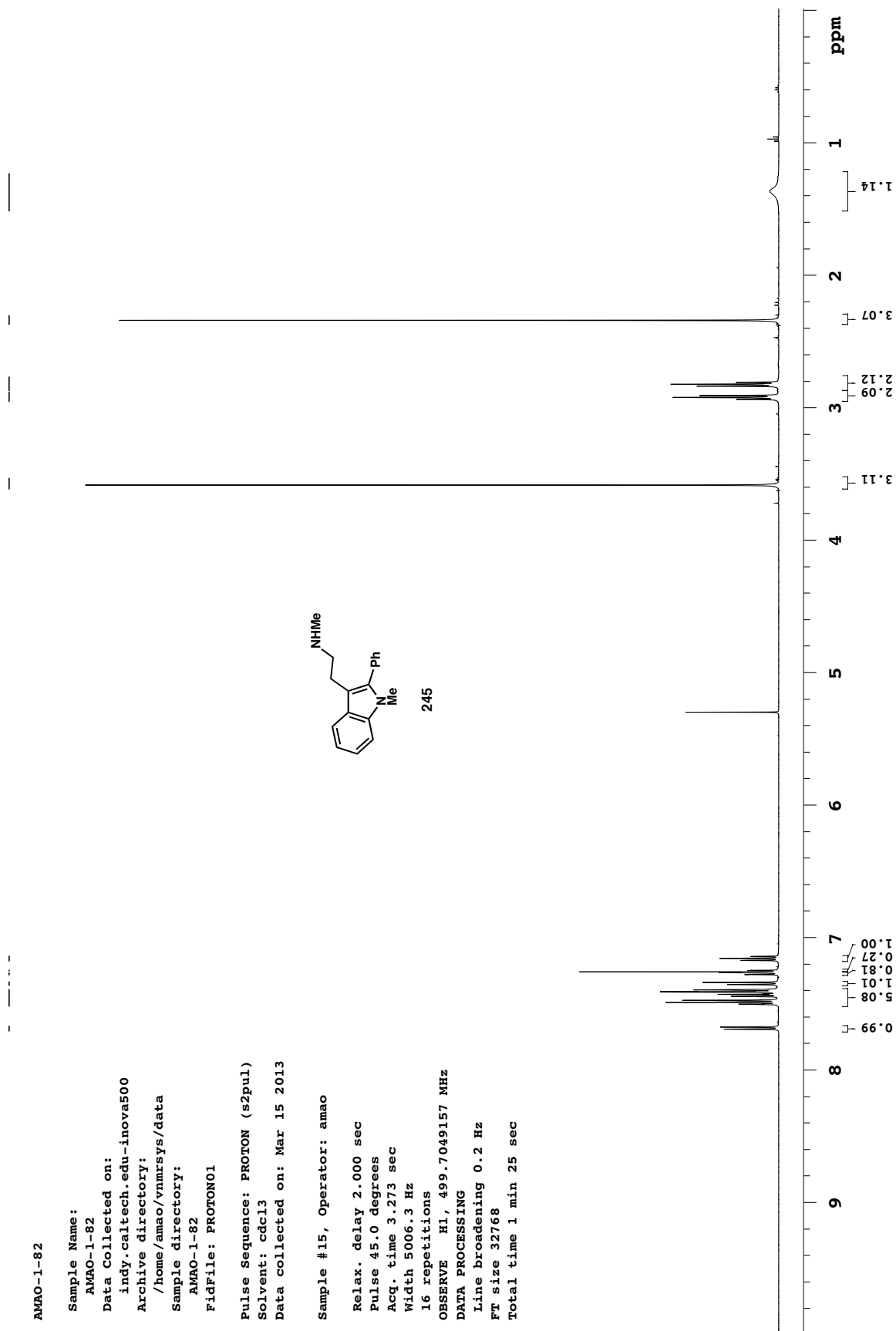
Line broadening 0.2 Hz

FT size 32768

Total time 1 min 25 sec



245



AMAO-1-15-F69-75B

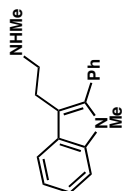
Sample Name:

AMAO-1-15-F69-75B
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/amao/vnmrsys/data
Sample directory:
AMAO-1-15-F69-75B
FidFile: CARBON01

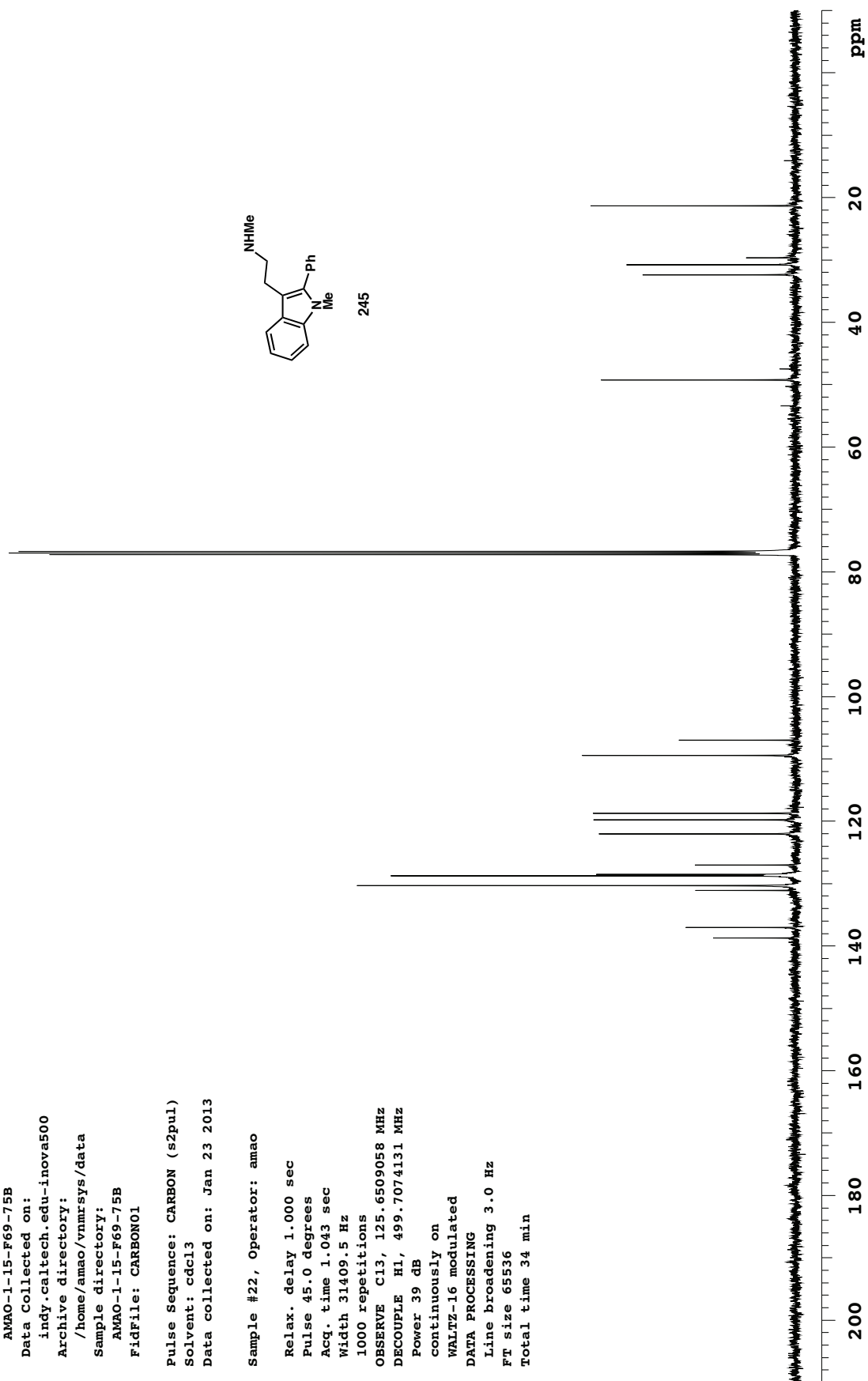
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 23 2013

Sample #22, Operator: amao

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.043 sec
Width 31409.5 Hz
1000 repetitions
OBSERVE C13, 125.6509058 MHz
DECOUPLE H1, 499.7074131 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 3.0 Hz
FT size 65536
Total time 34 min



245

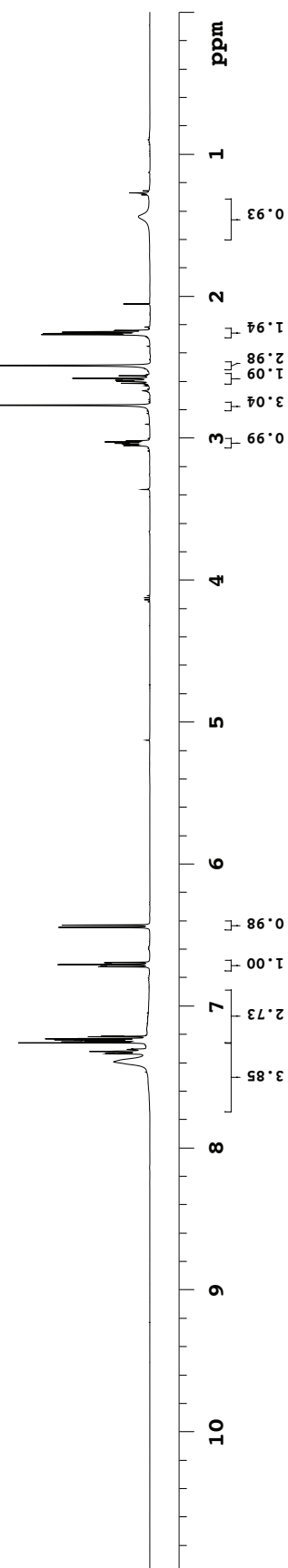
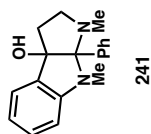


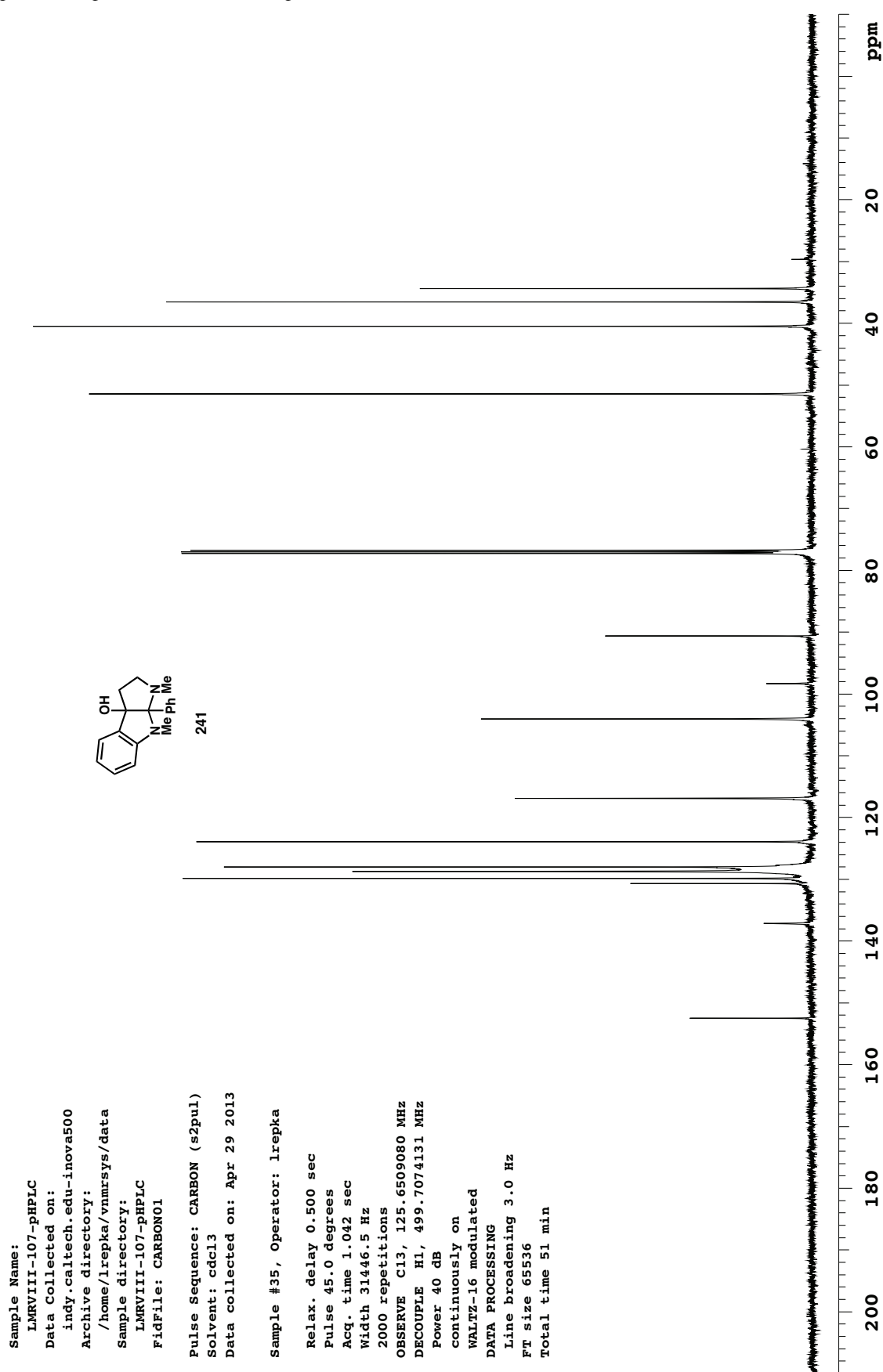
Sample Name:
LMRVIII-107-pHPLC
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVIII-107-pHPLC
FidFile: PROTON02

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 29 2013

Sample #35, Operator: lrepka

Relax. delay 5.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7049150 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 2 min 8 sec





LMRVIII-109-proton

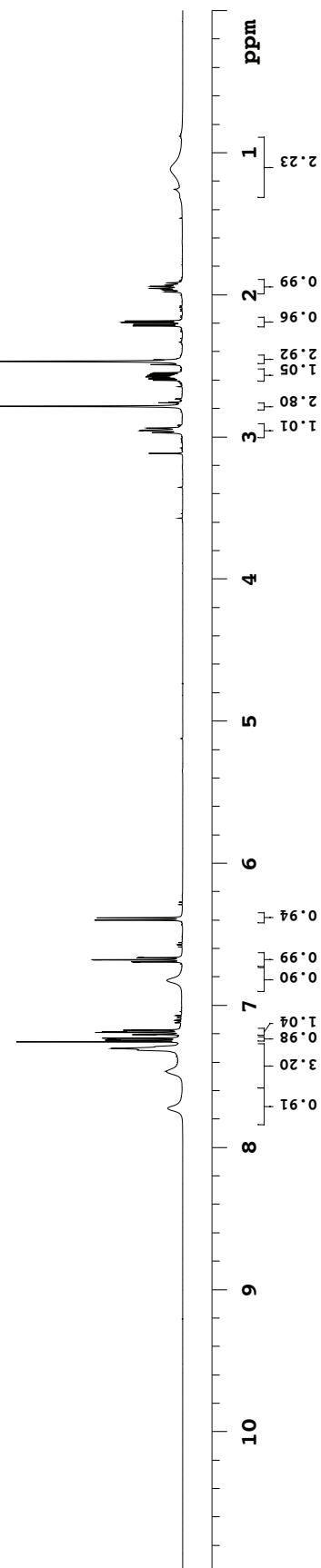
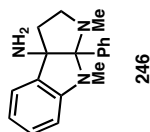
Sample Name:

LMRVIII-109-proton
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVIII-109-proton
FidFile: PROTON01

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

Sample #18, Operator: lrepka

Relax. delay 5.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.7049166 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 2 min 8 sec



LMRVIII-109-carbon

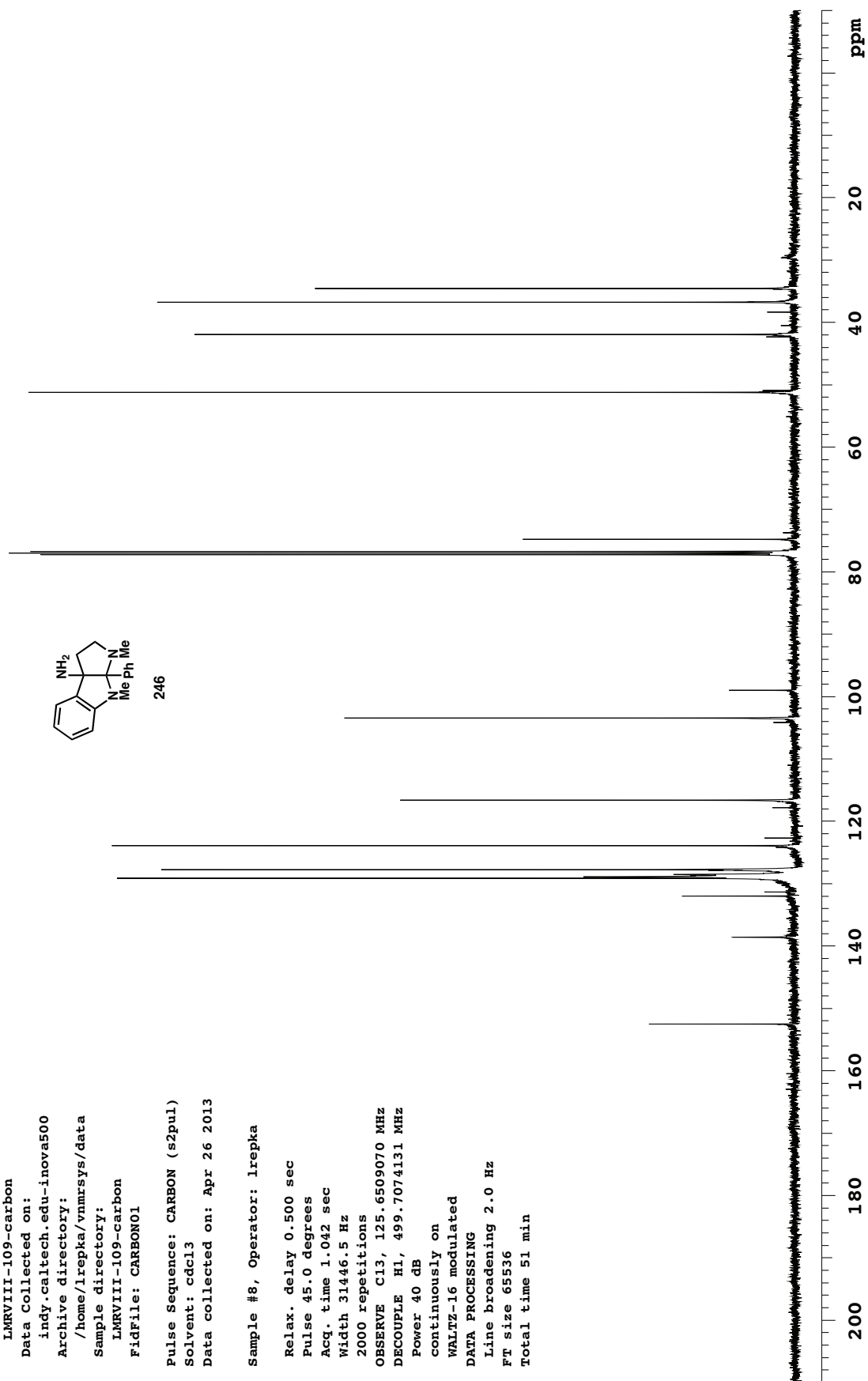
Sample Name:

LMRVIII-109-carbon
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVIII-109-carbon
FidFile: CARBON01

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

Sample #8, Operator: lrepka

Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
2000 repetitions
OBSERVE C13, 125.6509070 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 51 min



AMAO-1-62

Sample Name:

AMAO-1-62

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-62

FidFile: PROTON03

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 26 2013

Sample #28, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 8000.0 Hz

8 repetitions

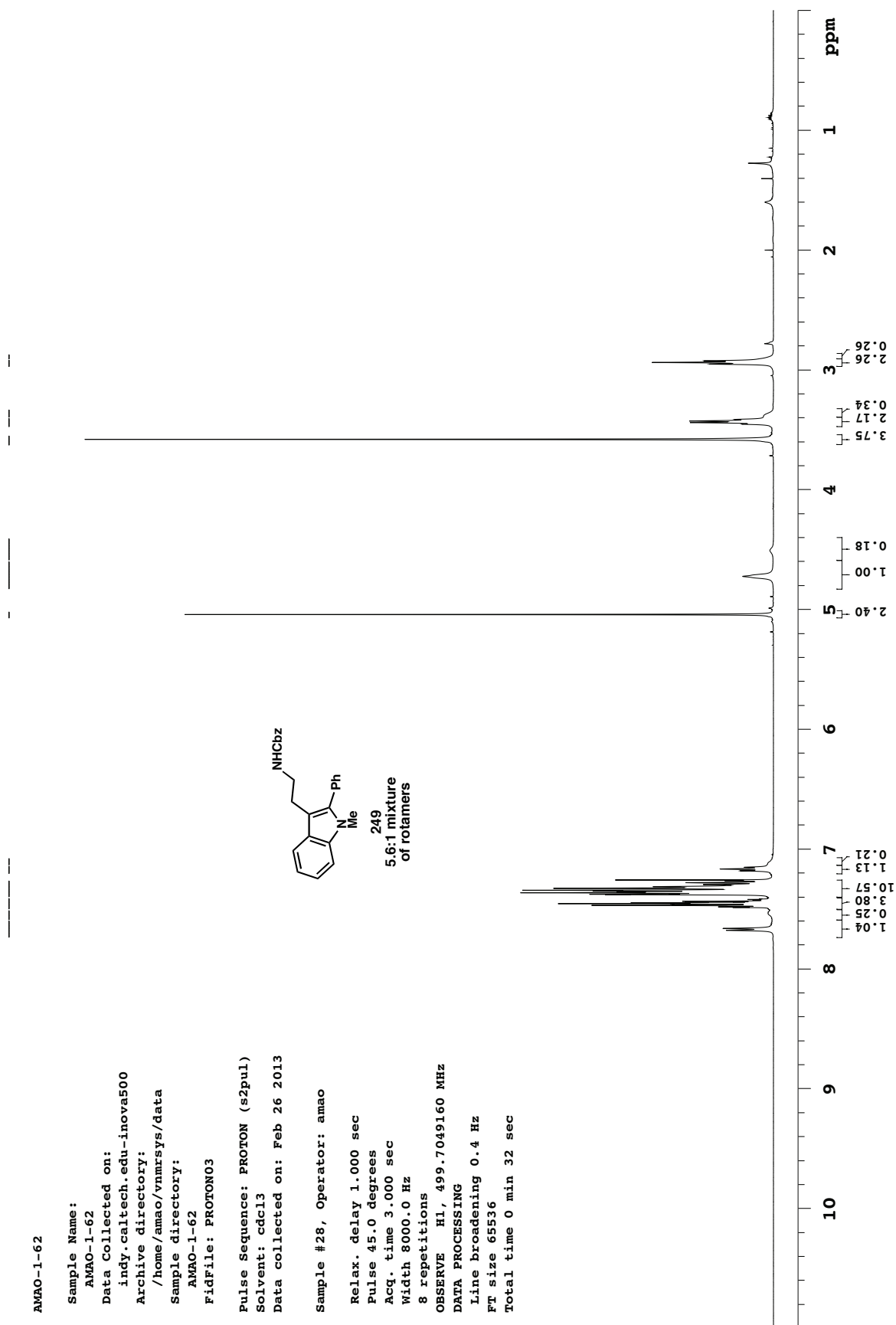
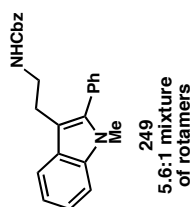
OBSERVE H1, 499.7049160 MHz

DATA PROCESSING

Line broadening 0.4 Hz

FT size 65536

Total time 0 min 32 sec



AMAO-1-62

Sample Name:

AMAO-1-62

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-62

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 26 2013

Sample #28, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6509073 MHz

DECOUPLE H1, 499.7074131 MHz

Power 39 dB

continuously on

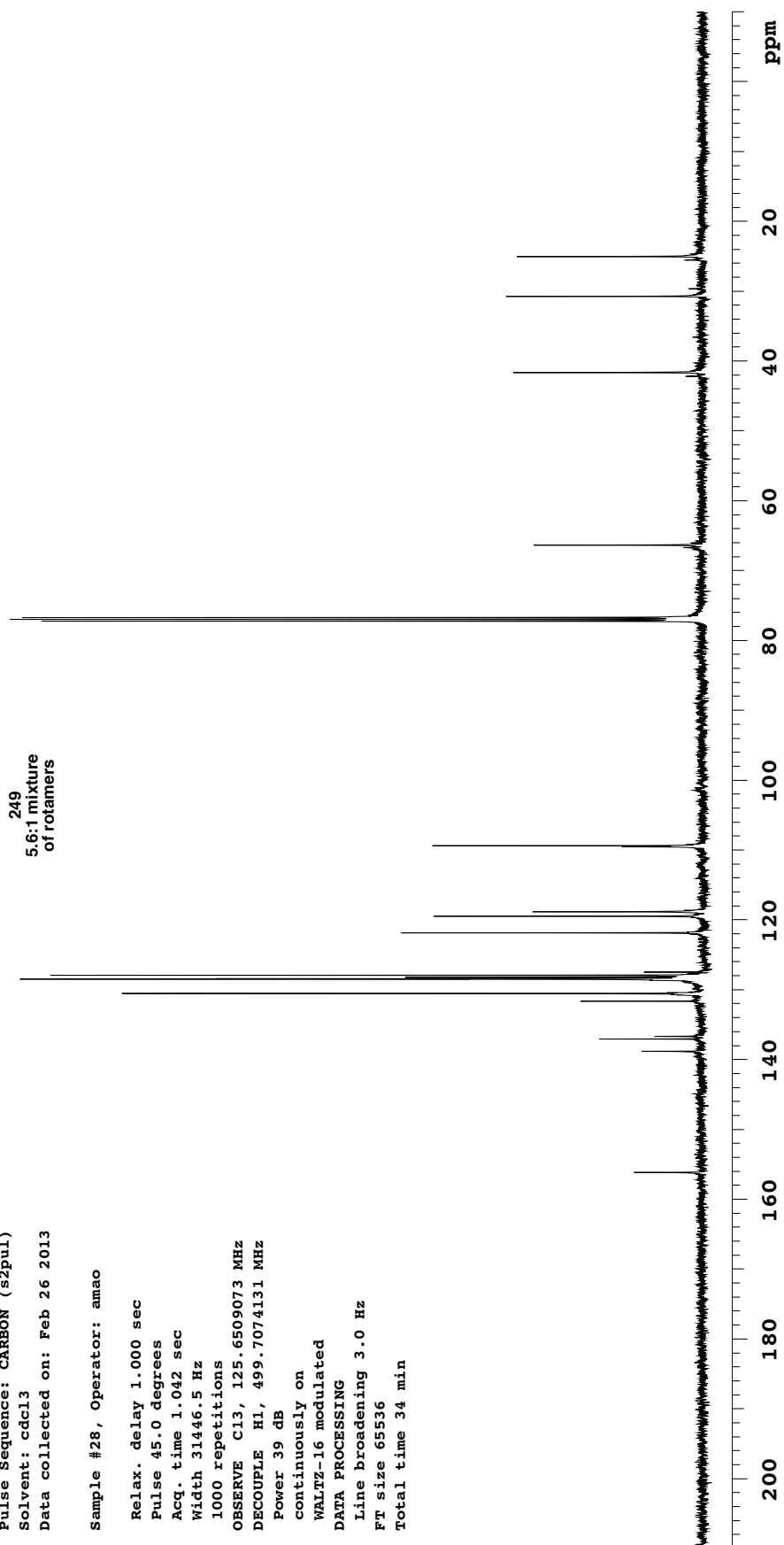
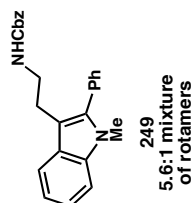
WALTZ-16 modulated

DATA PROCESSING

Line broadening 3.0 Hz

FT size 65536

Total time 34 min



LMRVIII-111-PHPLC

Sample Name:

LMRVIII-111-PHPLC

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrsys/data

Sample directory:

LMRVIII-111-PHPLC

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Apr 30 2013

Sample #34, Operator: lrepka

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 8000.0 Hz

16 repetitions

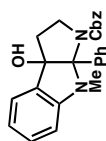
OBSERVE H1, 499.7049152 MHz

DATA PROCESSING

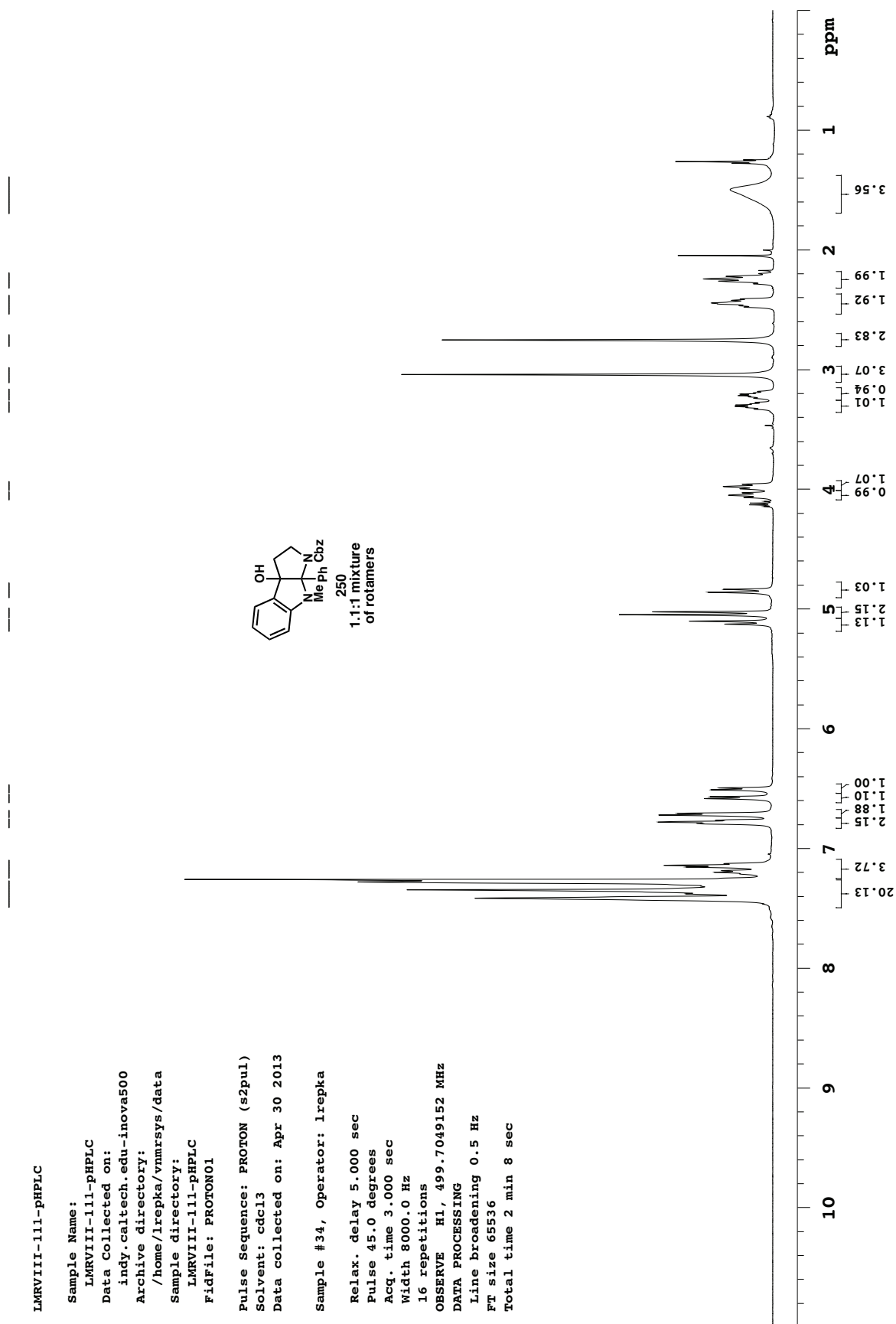
Line broadening 0.5 Hz

FT size 65536

Total time 2 min 8 sec



250
1:1:1 mixture
of rotamers



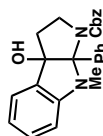
LMRVIII-111-PHPLC

Sample Name:
LMRVIII-111-PHPLC
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/lrepka/vnmrsys/data
Sample directory:
LMRVIII-111-PHPLC
FidFile: CARBON01

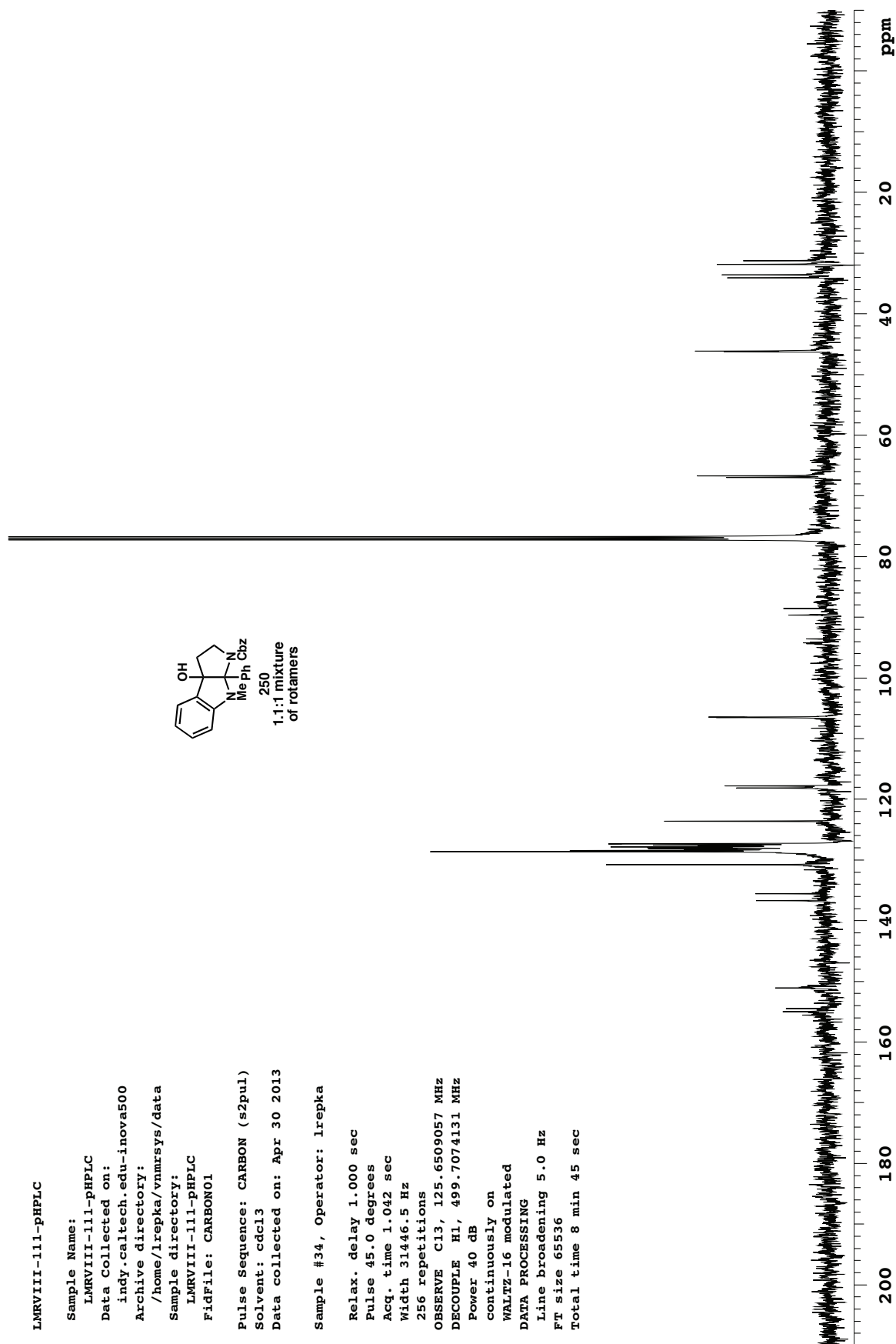
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 30 2013

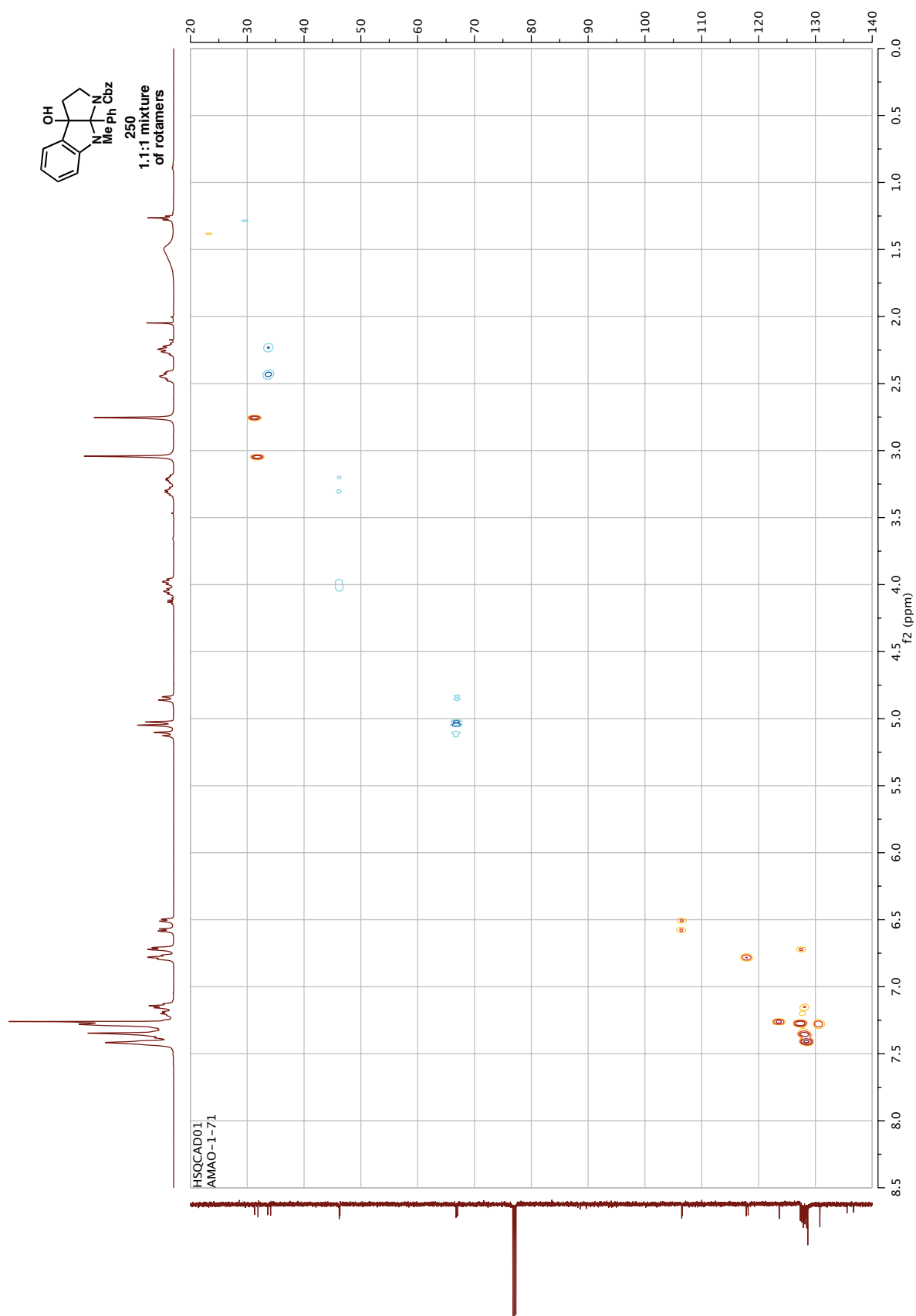
Sample #34, Operator: lrepka

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
256 repetitions
OBSERVE C13, 125.6509057 MHz
DECOUPLE H1, 499.7074131 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 5.0 Hz
FT size 65536
Total time 8 min 45 sec

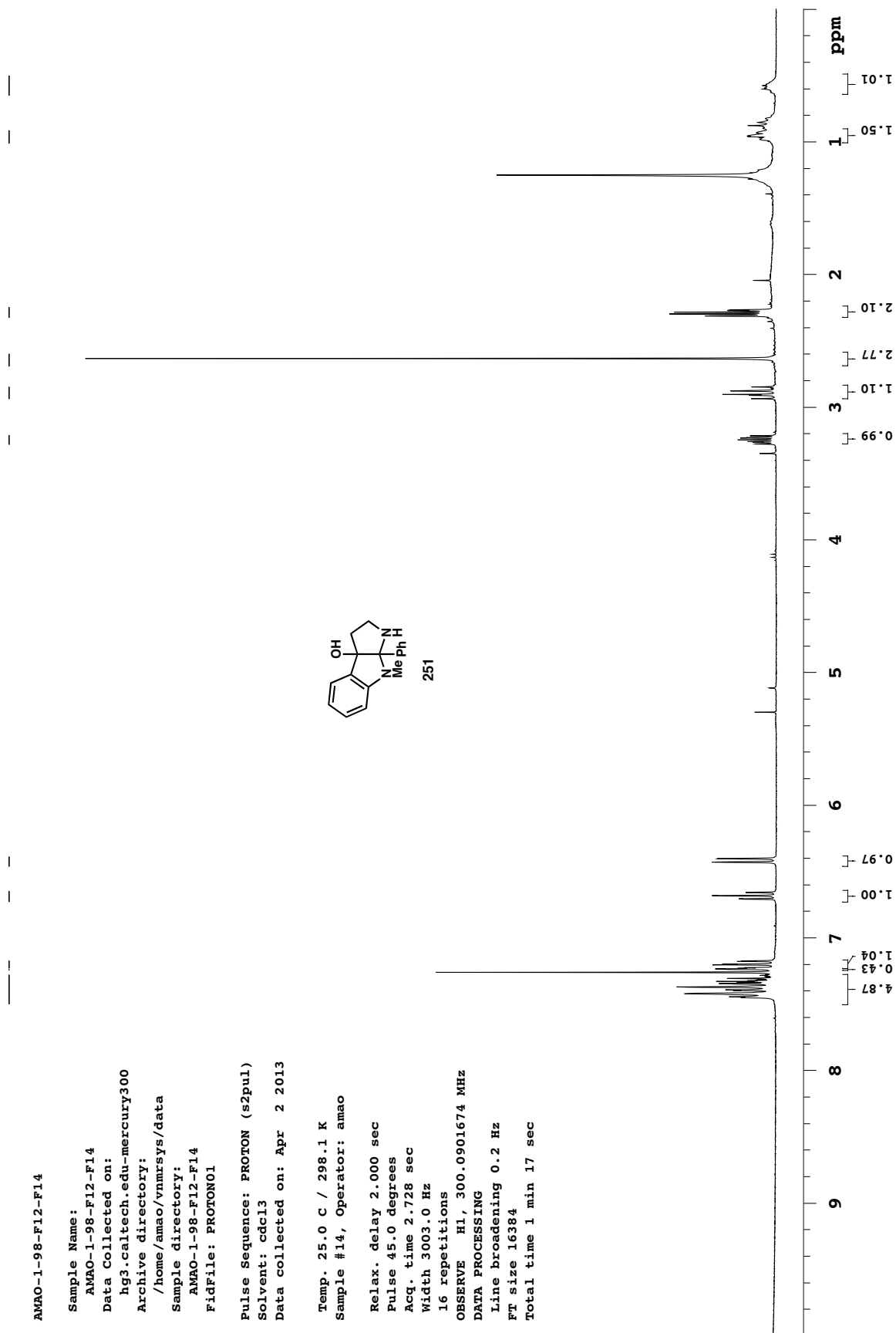
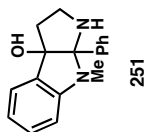


250
1:1:1 mixture
of rotamers





OBSERVE H1, 300.0901674 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 16384
Total time 1 min 17 sec



LMRVIII-113

Sample Name:

LMRVIII-113

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/lrepka/vnmrSYS/data

Sample directory:

LMRVIII-113

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: May 1 2013

Sample #34, Operator: lrepka

Relax. delay 0.200 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

3600 repetitions

OBSERVE C13, 125.6509034 MHz

DECOUPLE H1, 499.7074131 MHz

Power 40 dB

continuously on

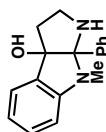
WALTZ-16 modulated

DATA PROCESSING

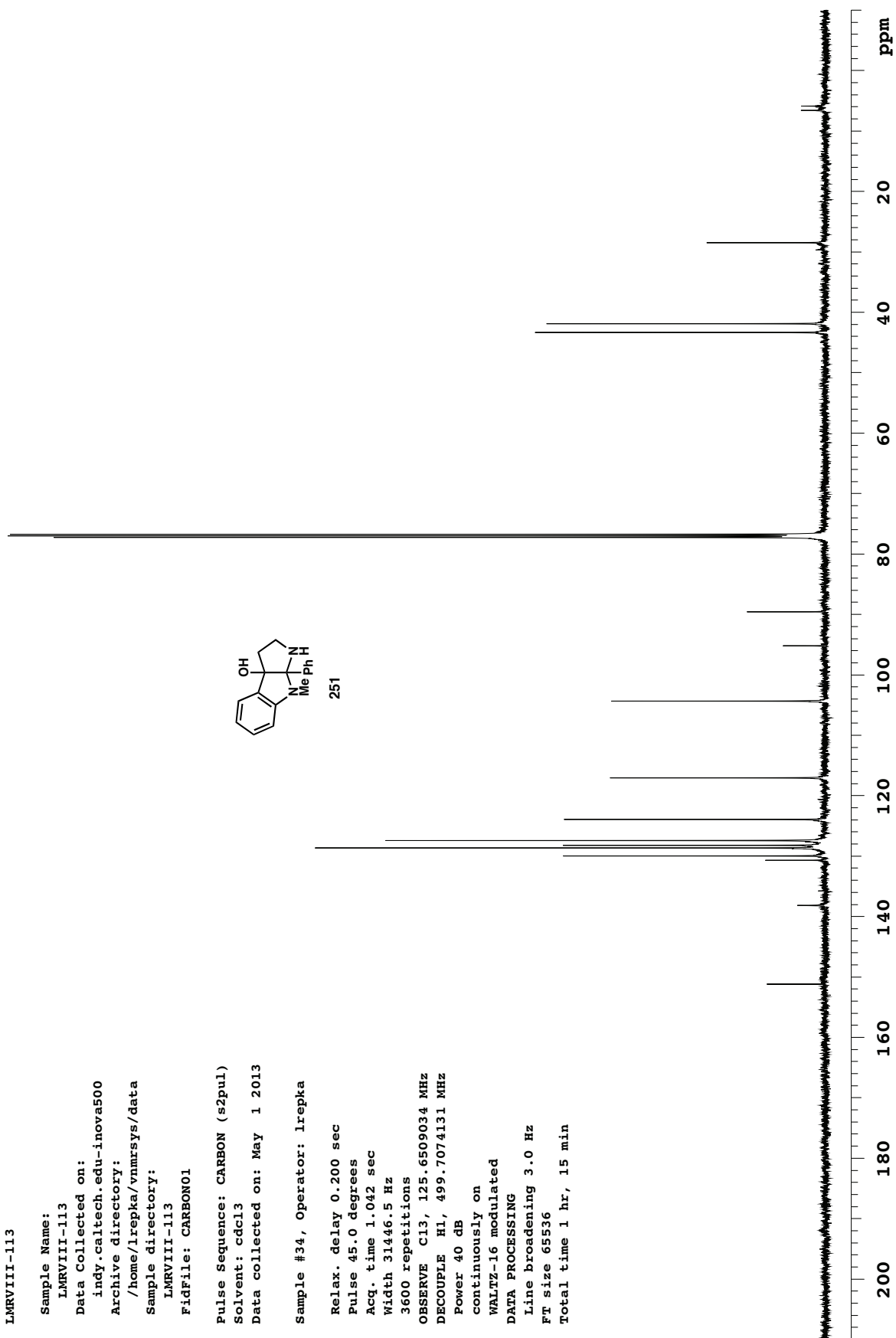
Line broadening 3.0 Hz

FT size 65536

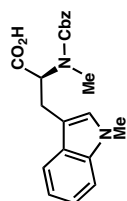
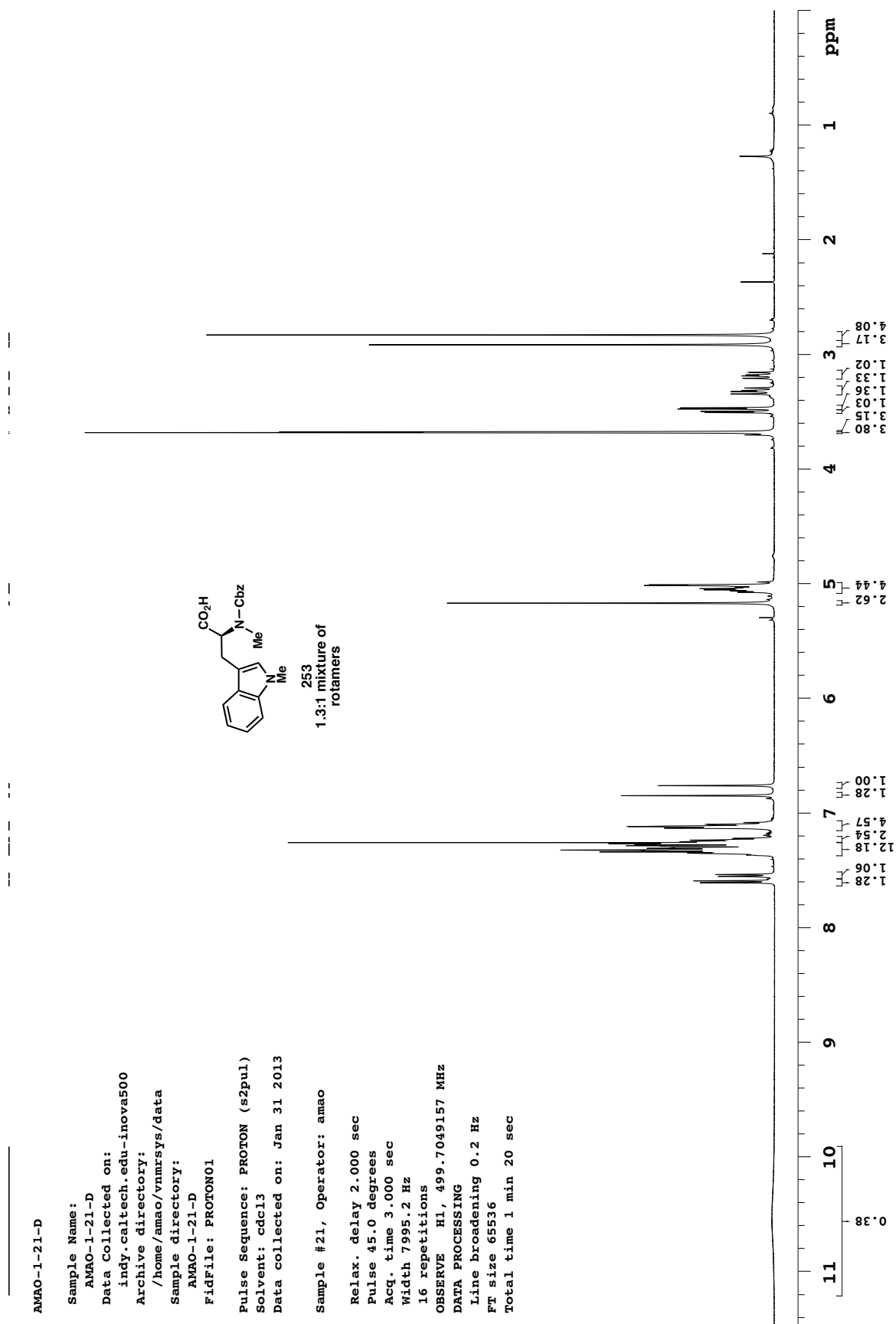
Total time 1 hr, 15 min



251



Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 7995.2 Hz
16 repetitions
OBSERVE H1, 499.704915
DATA PROCESSING
Line broadening 0.2 Hz
FFT size 65536
Total time 1 min 20 sec

253
1.3:1 mixture of
rotamers

AMAO-1-21E

Sample Name:

AMAO-1-21E

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-21E

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 4 2013

Sample #5, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.043 sec

Width 31409.5 Hz

1000 repetitions

OBSERVE C13, 125.6509118 MHz

DECOUPLE H1, 499.7074131 MHz

Power 39 dB

continuously on

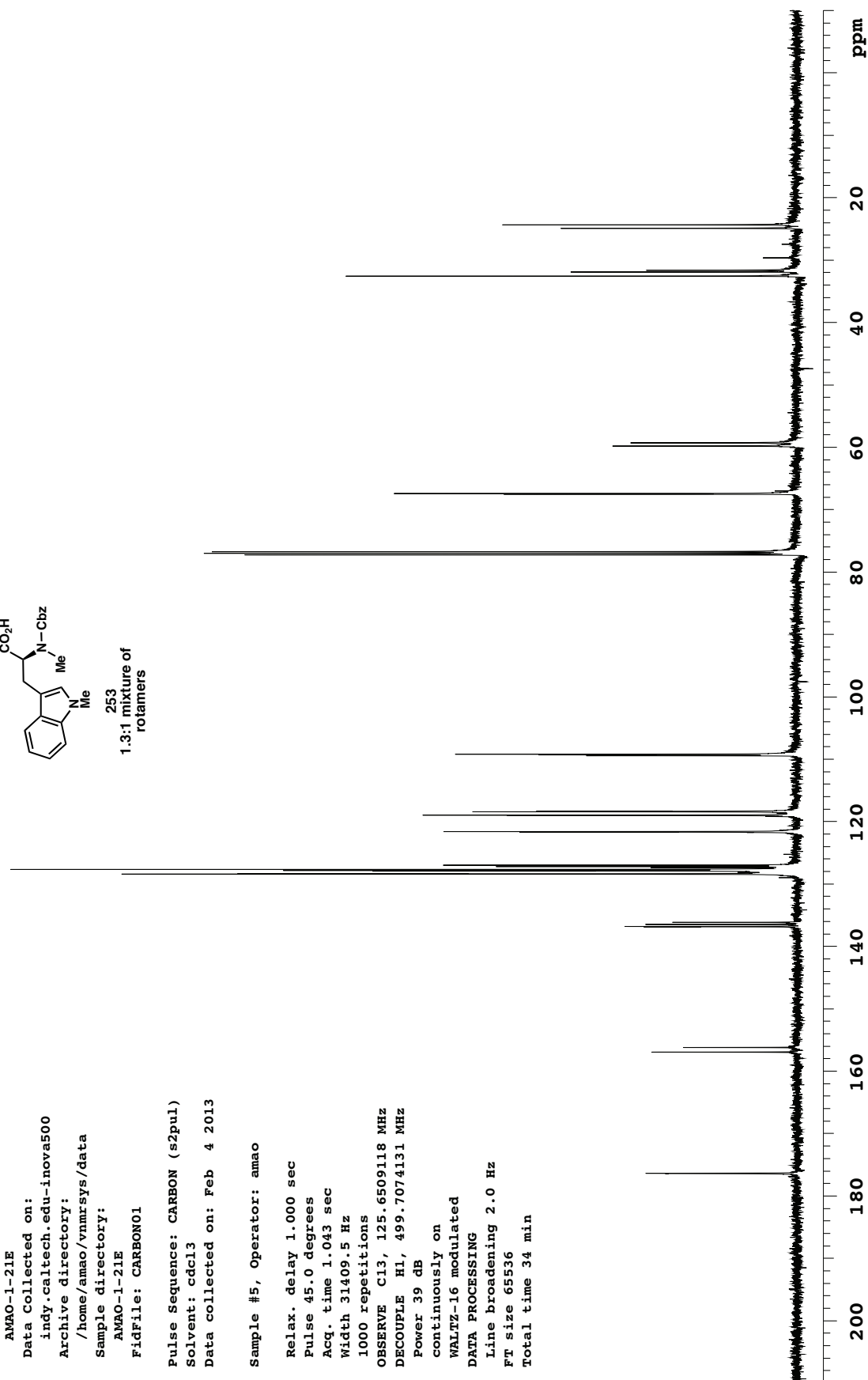
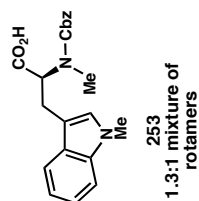
WALTZ-16 modulated

DATA PROCESSING

Line broadening 2.0 Hz

FT size 65536

Total time 34 min

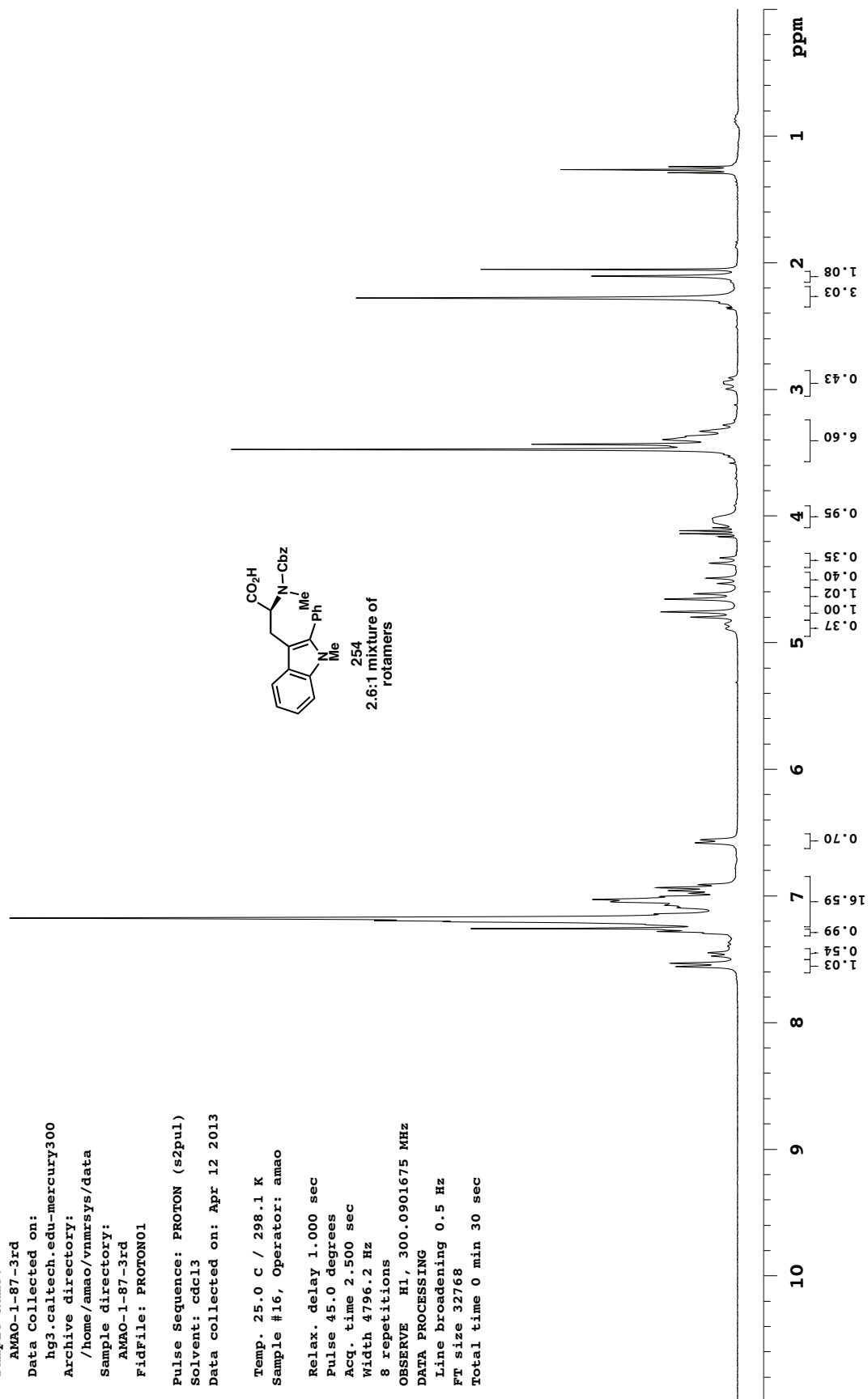
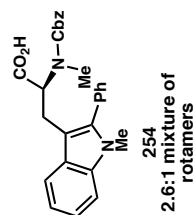


```

Temp. 25.0 C / 298.1 K
Sample #16, Operator: amao

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.500 sec
Width 4796.2 Hz
8 repetitions
OBSERVE H1, 300.0901675 MHz
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 0 min 30 sec

```



AMAO-1-41-42B

Sample Name:

AMAO-1-41-42B

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-41-42B

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Feb 10 2013

Sample #14, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.043 sec

Width 31409.5 Hz

1000 repetitions

OBSERVE C13, 125.6509097 MHz

DECOUPLE H1, 499.7074131 MHz

Power 39 dB

continuously on

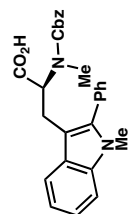
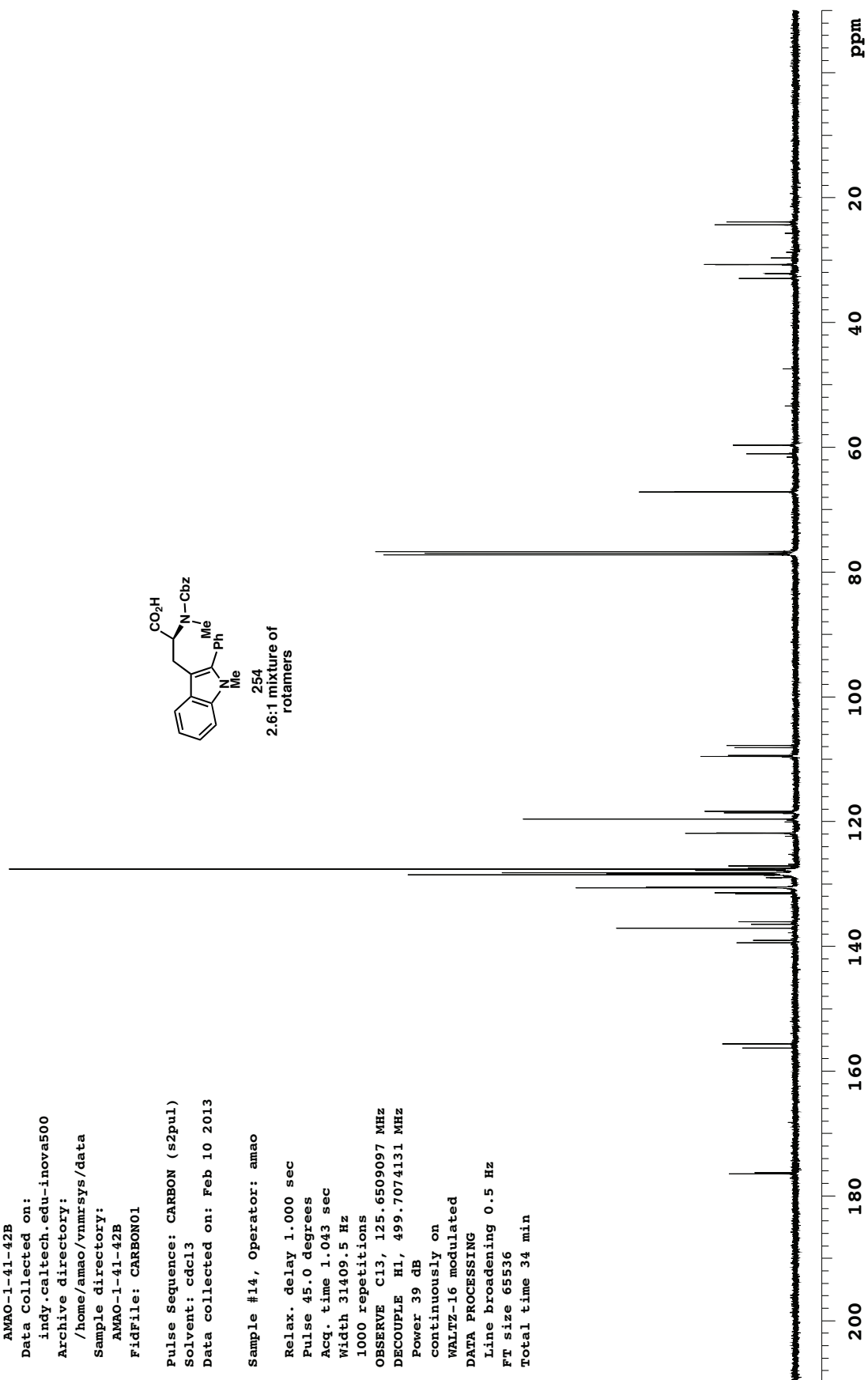
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

Ft size 65536

Total time 34 min

254
2.6:1 mixture of
rotamers

AMAO-1-74

Sample Name:

AMAO-1-74

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsvs/data

Sample directory:

AMAO-1-74

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 7 2013

Sample #30, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 8000.0 Hz

8 repetitions

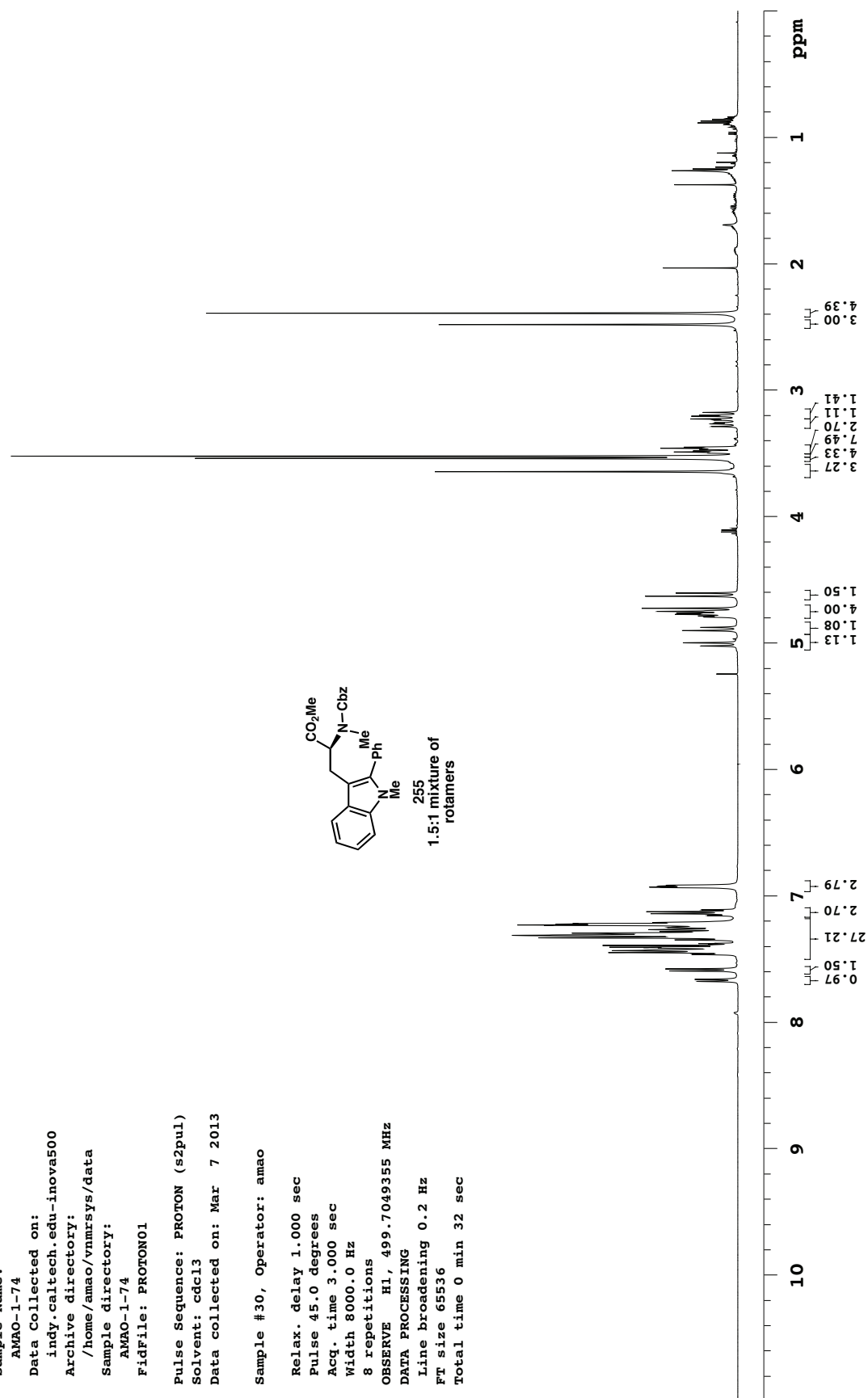
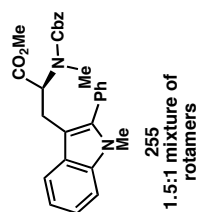
OBSERVE H1, 499.7049355 MHz

DATA PROCESSING

Line broadening 0.2 Hz

FT size 65536

Total time 0 min 32 sec



AMAO-1-74

Sample Name:

AMAO-1-74

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-74

FidFile: CARBON01

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 8 2013

Sample #30, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1000 repetitions

OBSERVE C13, 125.6509173 MHz

DECOUPLE H1, 499.7074131 MHz

Power 39 dB

continuously on

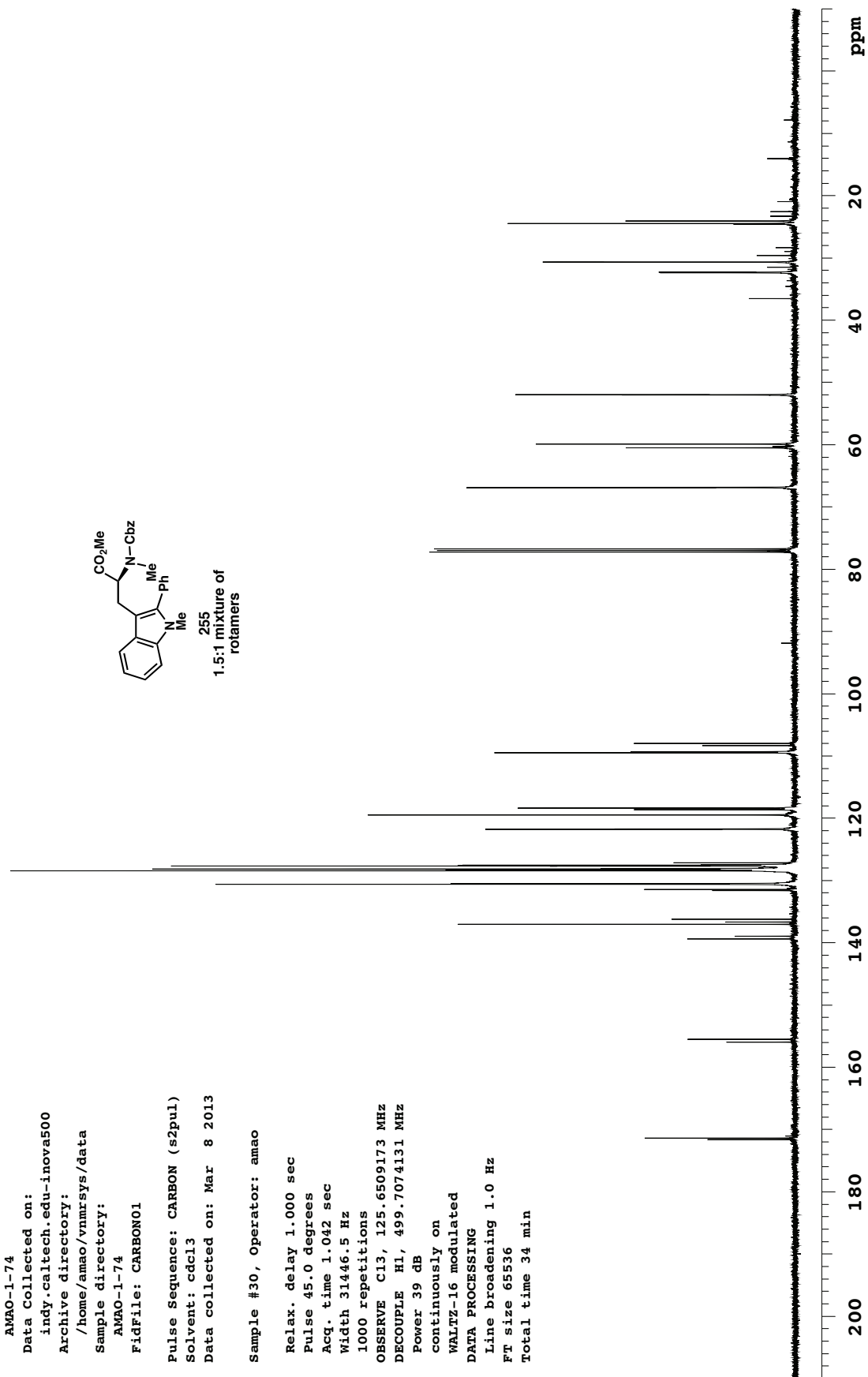
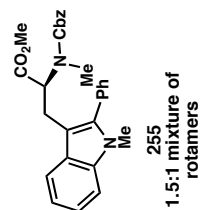
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 34 min



AMAO-1-103

Sample Name:

AMAO-1-103

Data Collected on:

indy.caltech.edu-inova500

Archive directory:

/home/amao/vnmrsvs/data

Sample directory:

AMAO-1-103

FidFile: PROTON02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 1 2013

Sample #1, Operator: amao

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 3.000 sec

Width 8000.0 Hz

8 repetitions

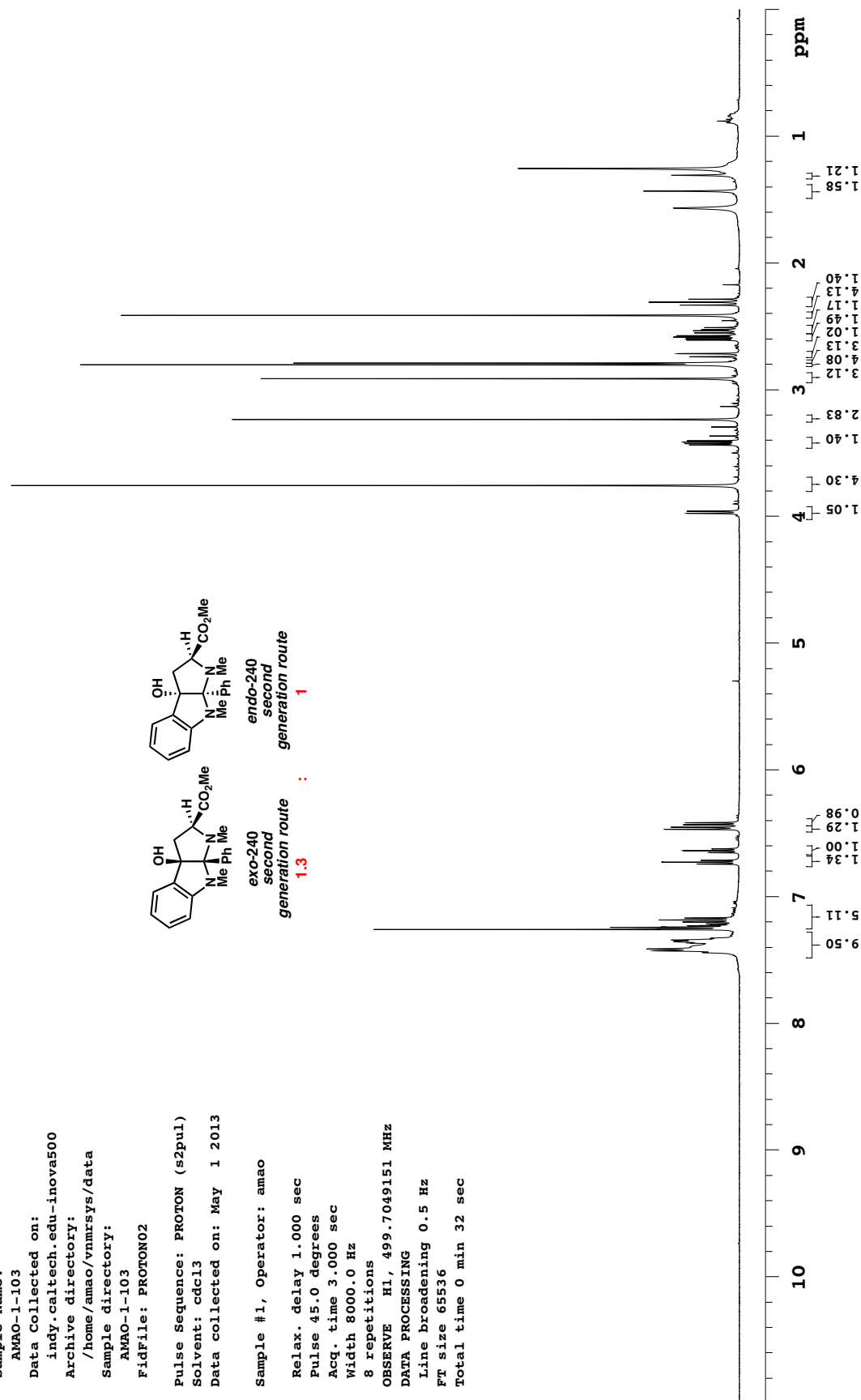
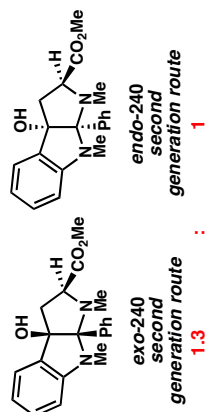
OBSERVE H1, 499.7049151 MHz

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 0 min 32 sec

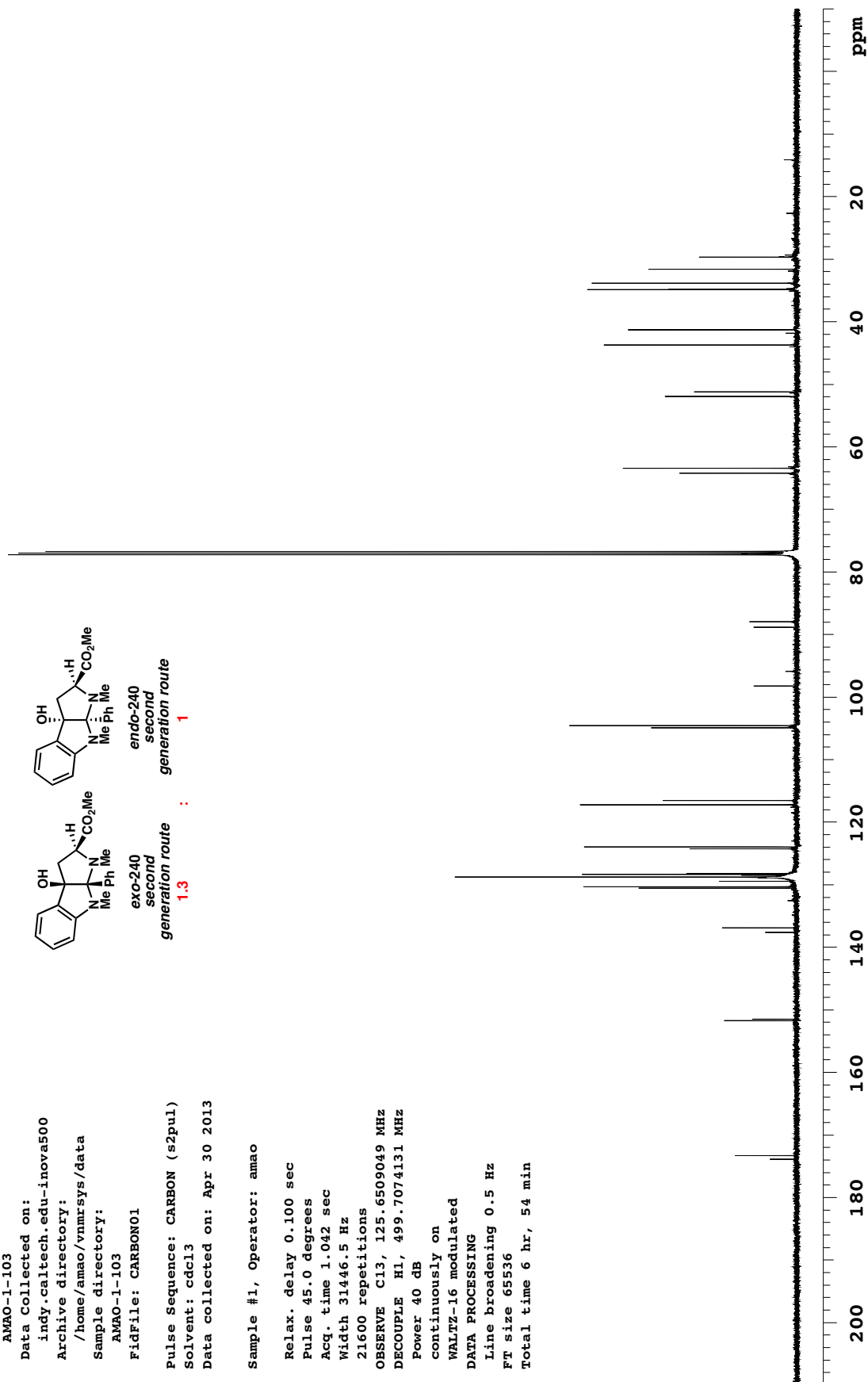


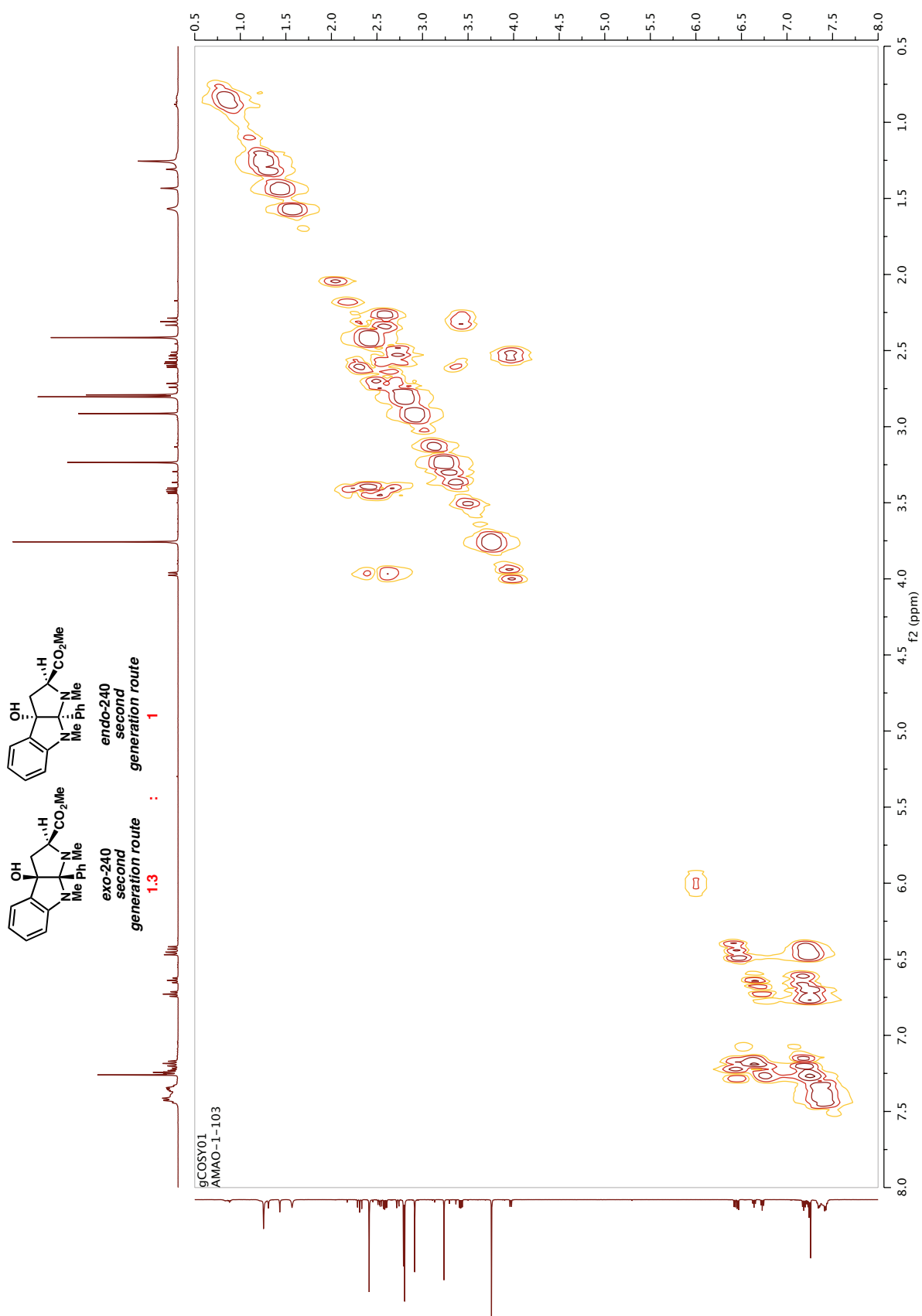
AMAO-1-103

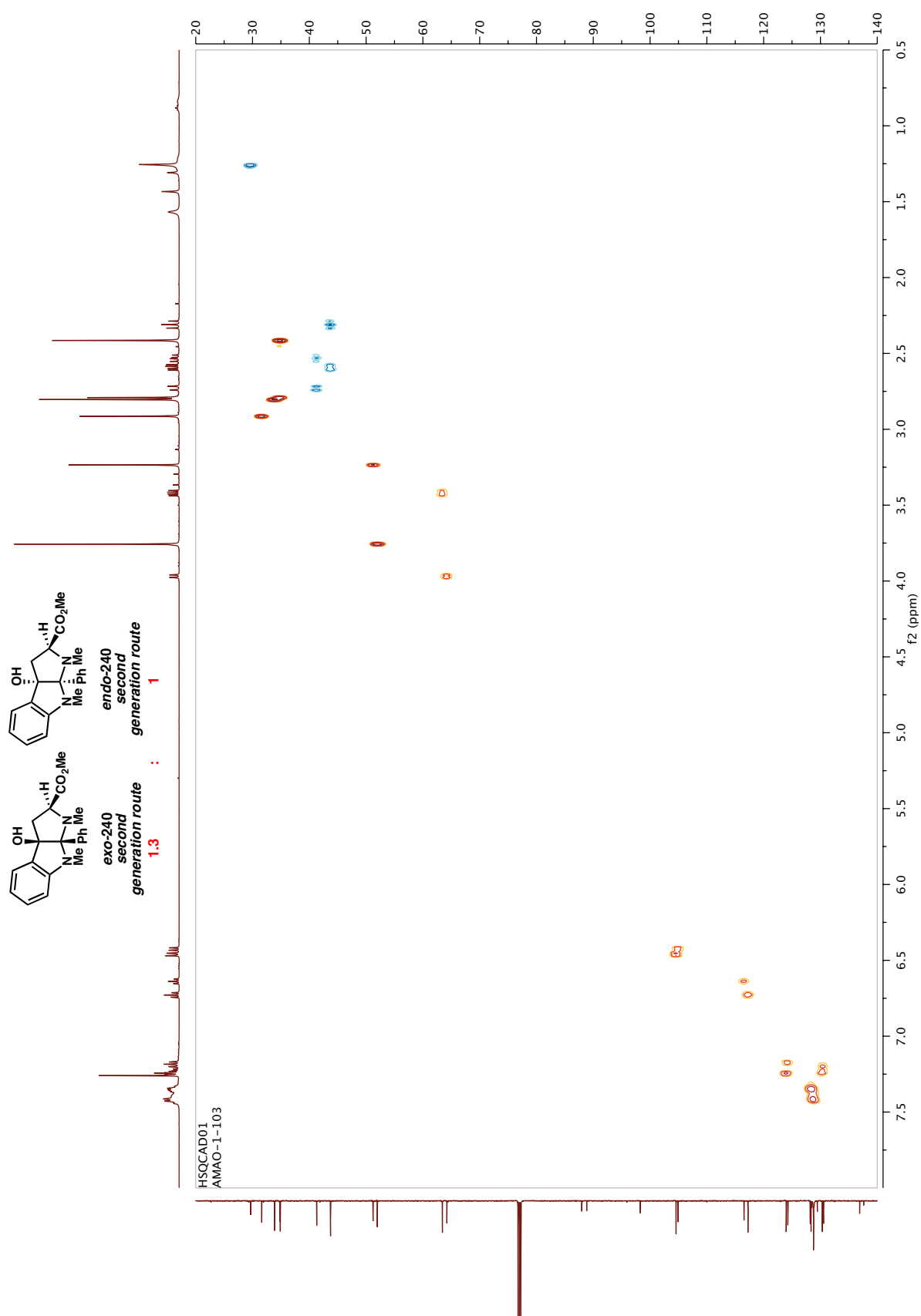
Sample Name:
AMAO-1-103
Data Collected on:
indy.caltech.edu-inova500
Archive directory:
/home/amao/vnmrsys/data
Sample directory:
AMAO-1-103
FidFile: CARBON01
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 30 2013

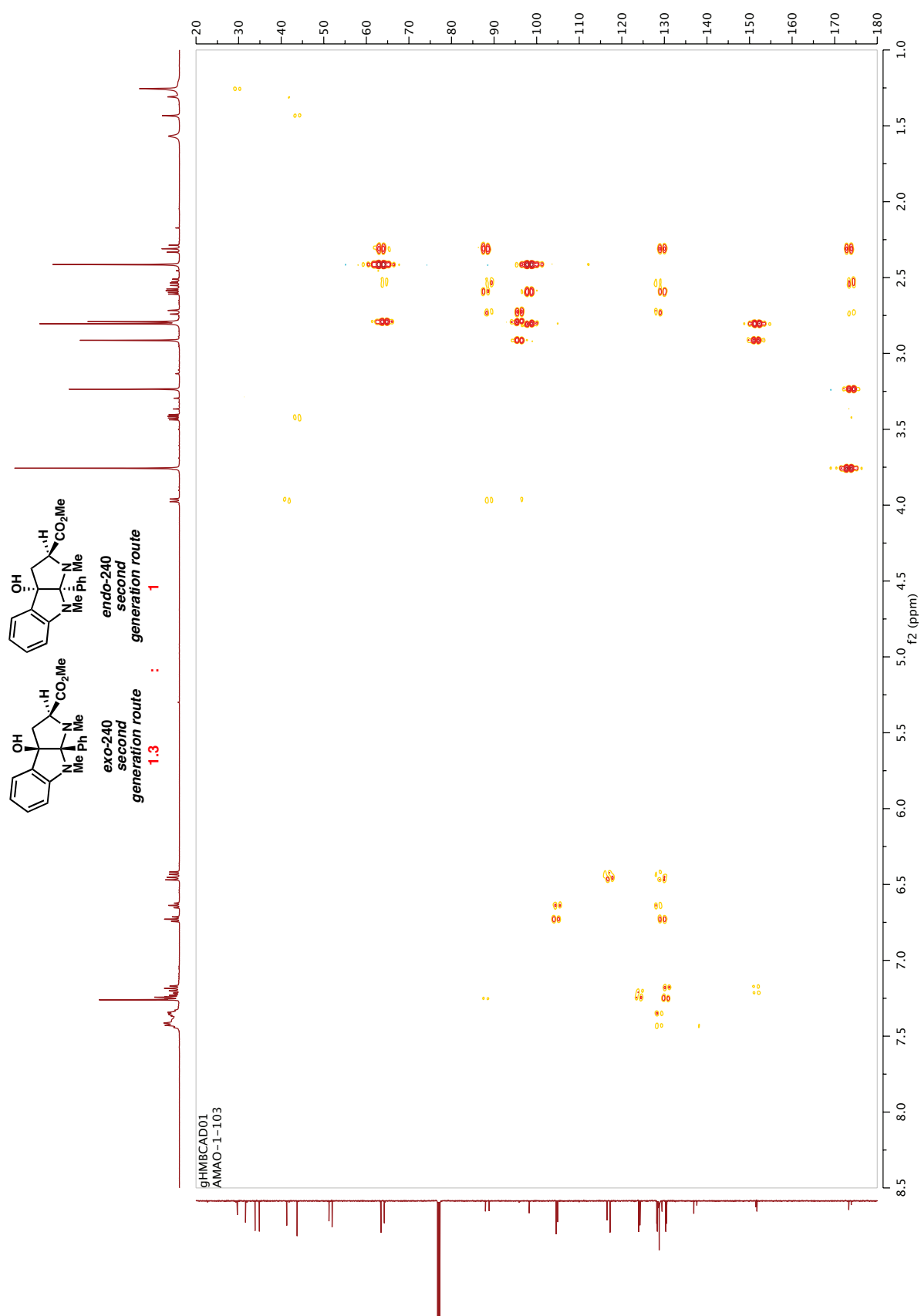
Sample #1, Operator: amao

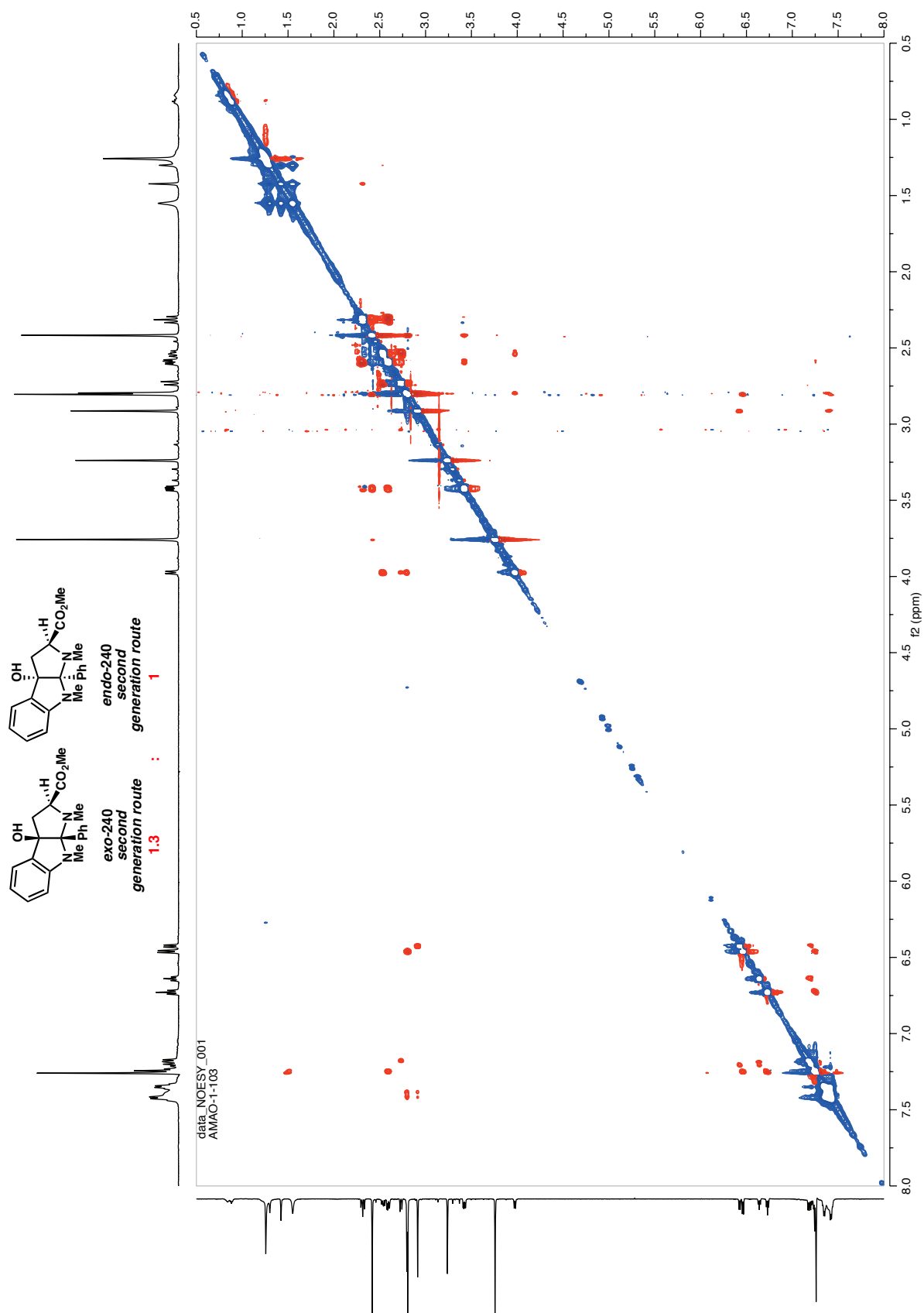
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
21600 repetitions
OBSERVE C13, 125.6509049 MHz
DECOUPLE H1, 499.7074131 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 6 hr, 54 min

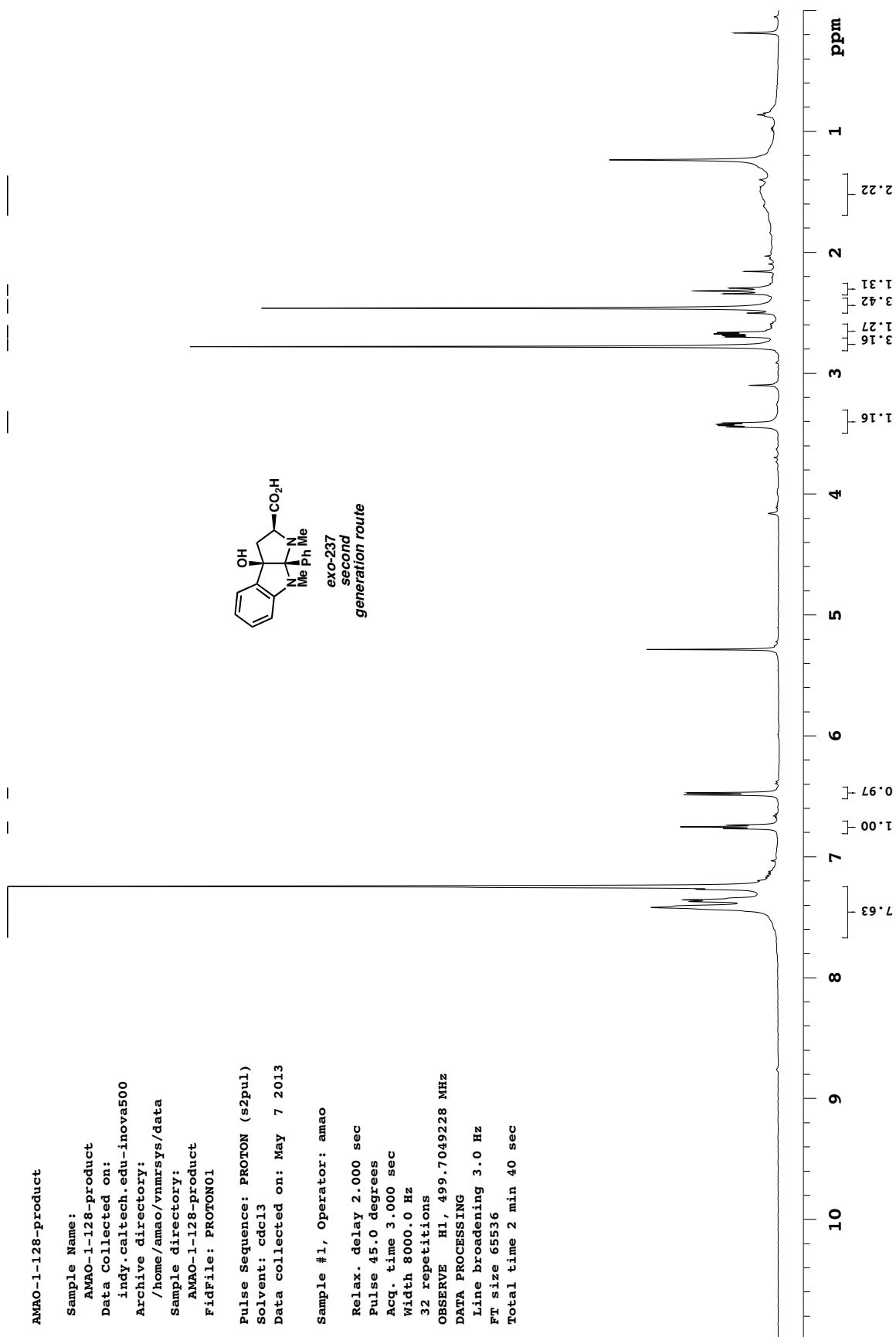












AMAO-1-128-F11-F14

Sample Name:

AMAO-1-128-F11-F14

Data Collected on:

hg3.caltech.edu-mercury300

Archive directory:

/home/amao/vnmrsys/data

Sample directory:

AMAO-1-128-F11-F14

FidFile: PROTON01

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 7 2013

Temp. 25.0 C / 298.1 K

Sample #2, Operator: amao

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 4796.2 Hz

32 repetitions

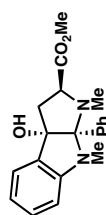
OBSERVE H1, 300.0901672 MHz

DATA PROCESSING

Line broadening 1.0 Hz

FT size 32768

Total time 2 min 27 sec



exo-240
second generation-post
exo-240 saponification

