

ZK-530-245-C

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-incva400  
Archive directory:

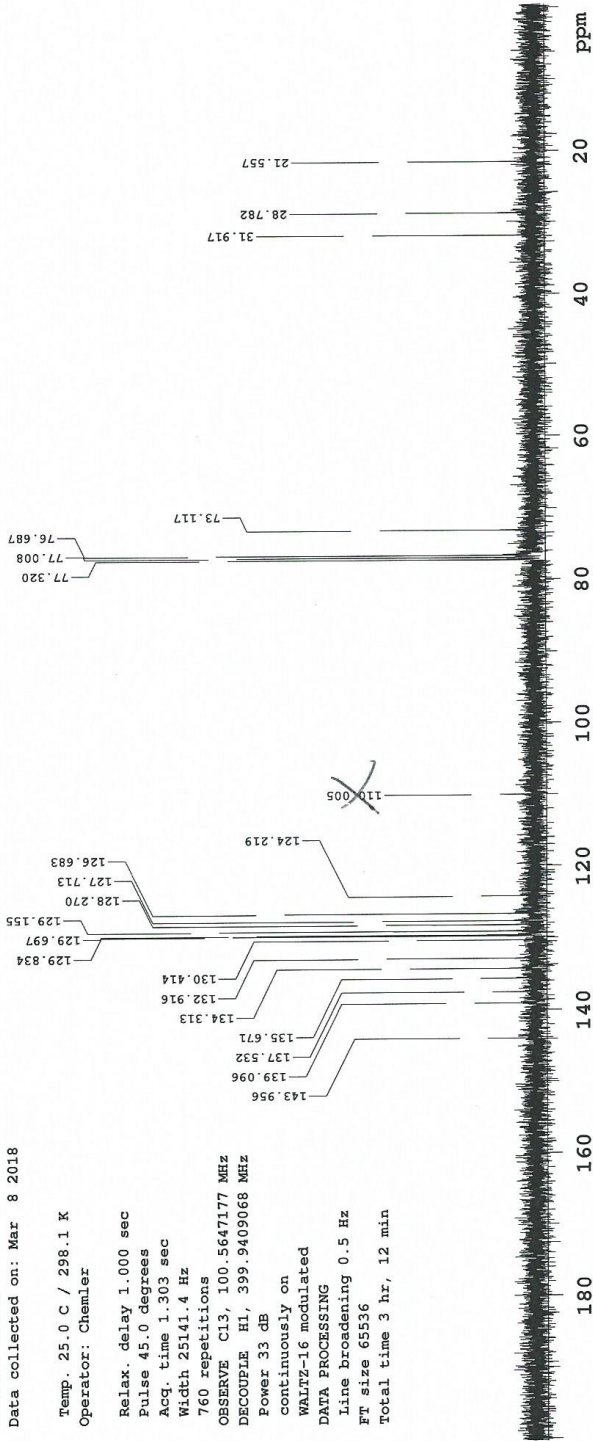
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 8 2018

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
760 repetitions  
OBSERVE C13, 100.5647177 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 12 min



JE\_1\_119\_011

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inoxa400  
Archive directory:

Sample directory:

File: js\_pg1525\_imine\_HNMR

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: 01/11/00

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degree

Acq. time 2.5600 sec

Width 6399.0 Hz

16 repetitions

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

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CPDPRG2

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CPDPRG2

CPDPRG2

CPDPRG2

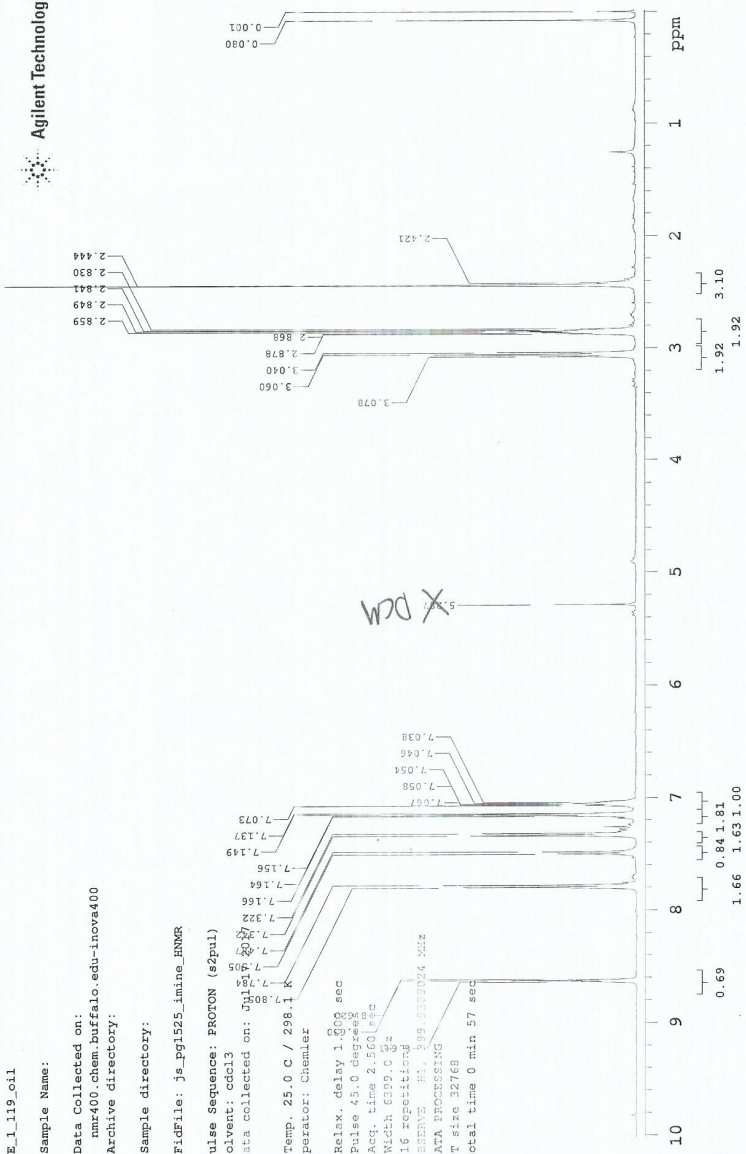
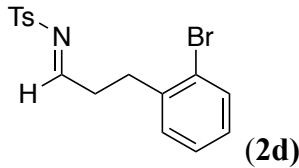
CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2

CPDPRG2



ASB-A93-PCF3-carbon

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu--inova400  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13

Data collected on: Jul 10 2017

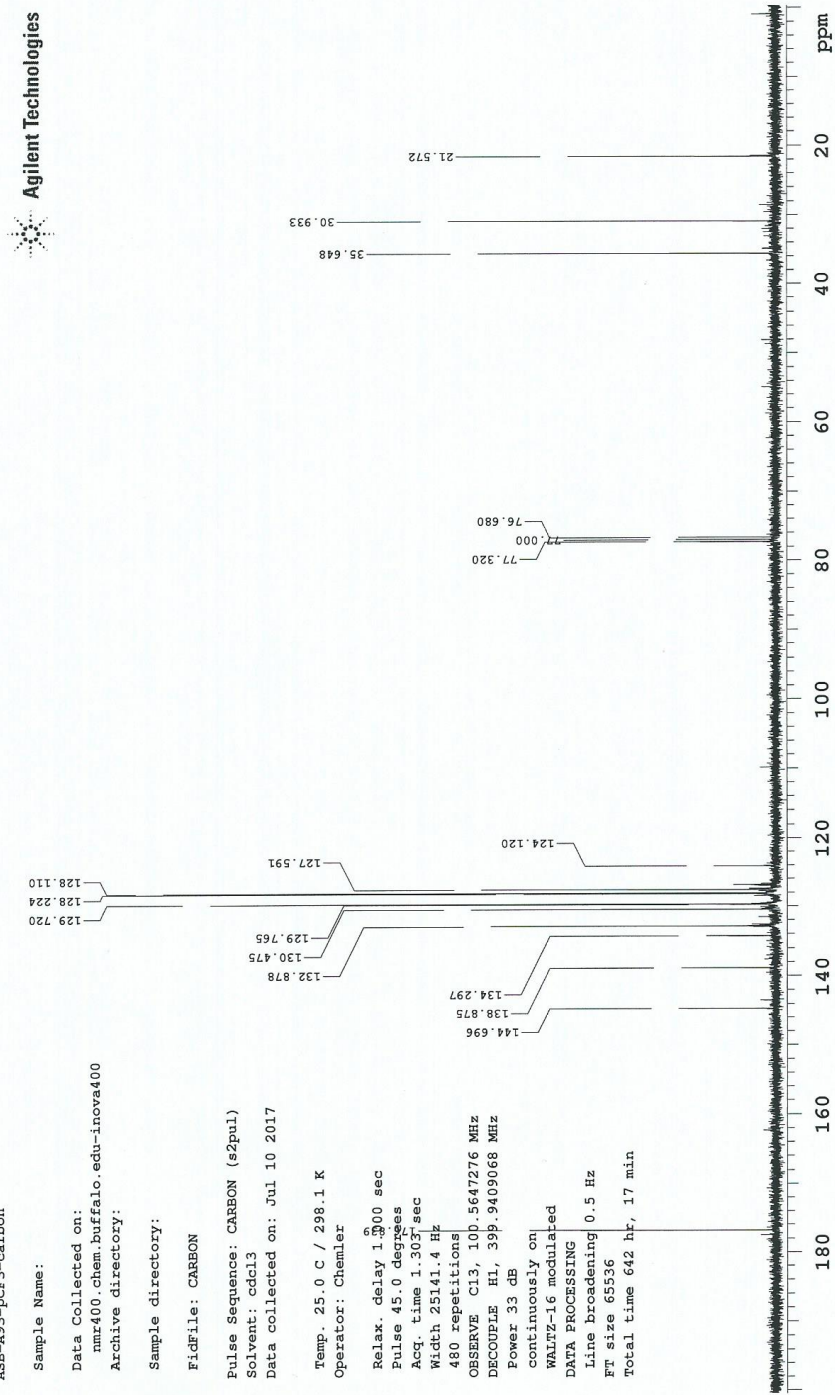
Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.500 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
480 repetitions

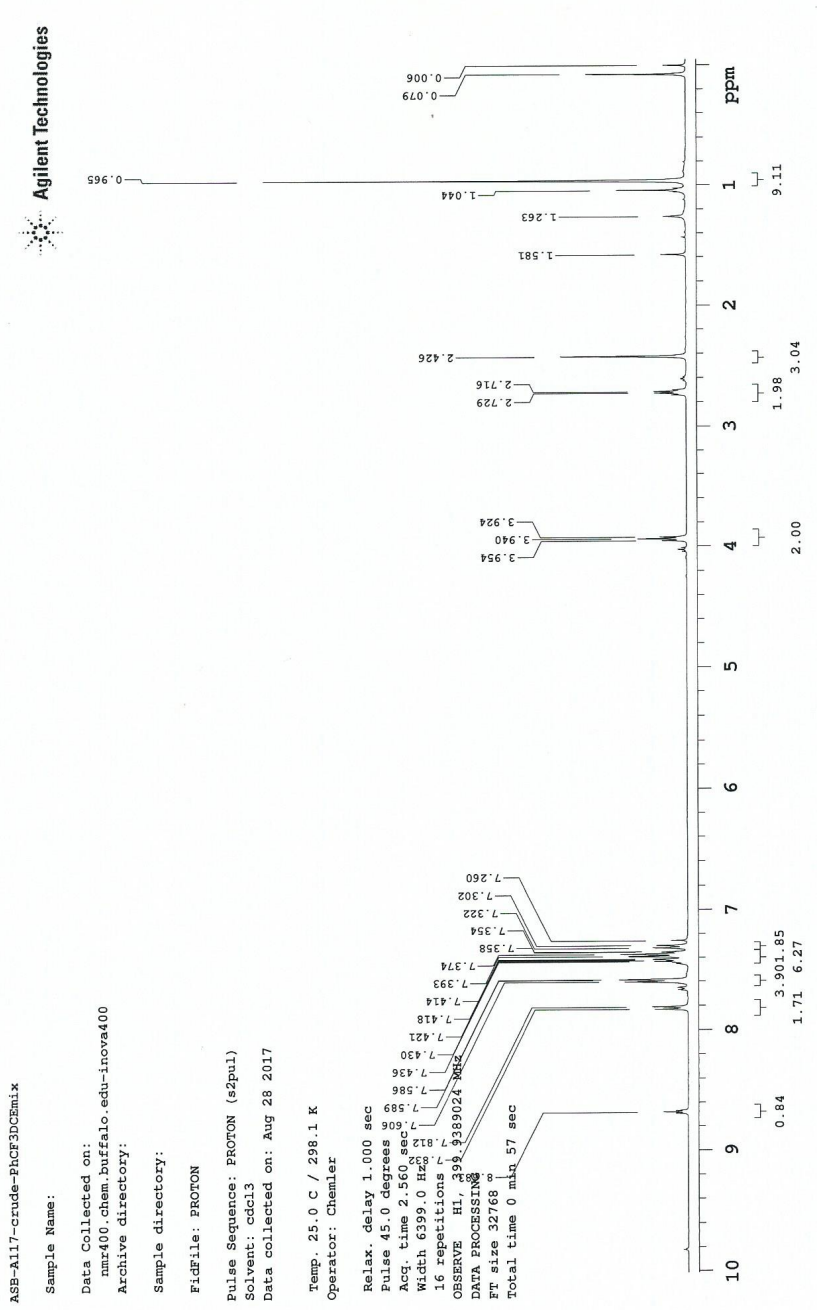
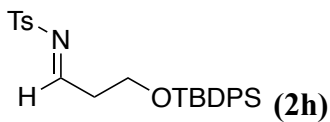
OBSERVE C13, 100.564726 MHz  
DECOUPLE H1, 399.9409068 MHz

Power 33 dB  
continuously on  
WALTZ-16 modulated

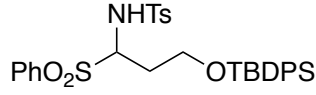
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 642 hr, 17 min







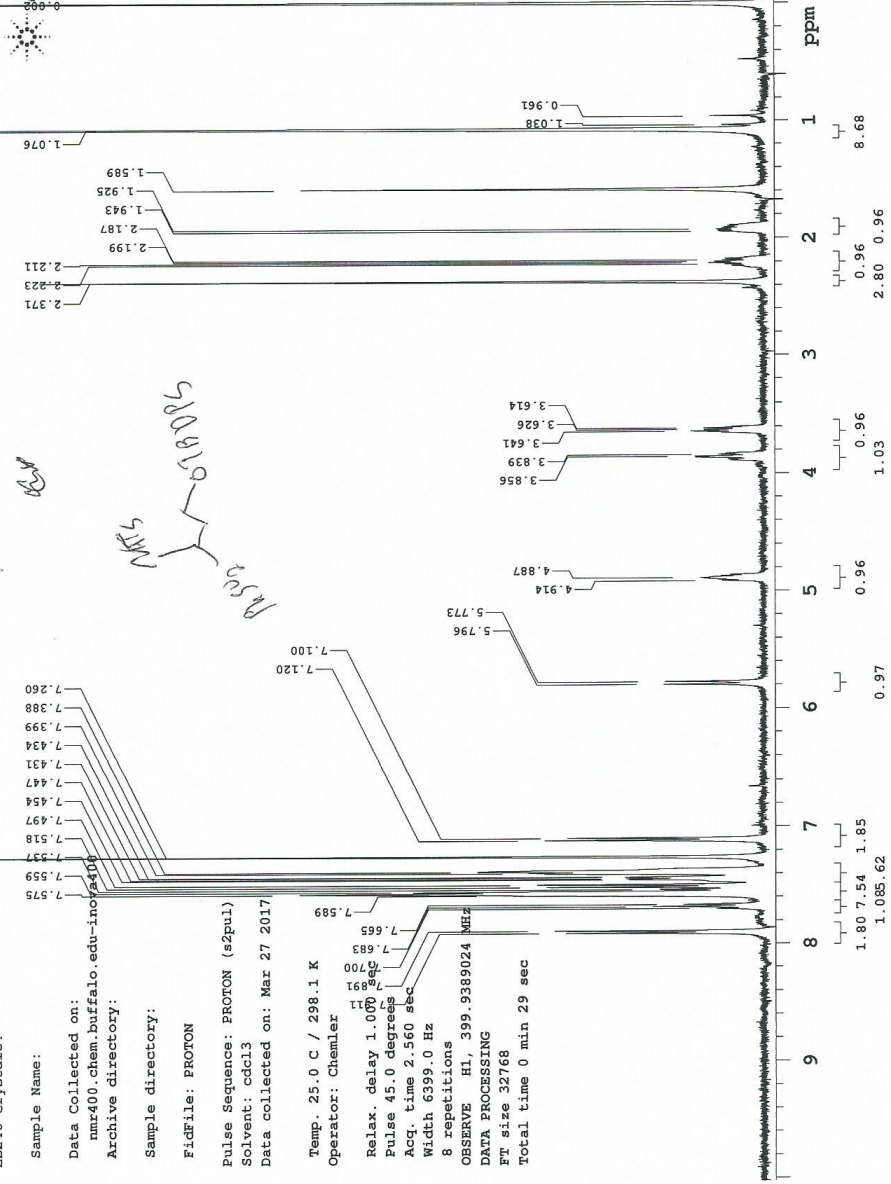




Agilent Technologies

1437

15



EB246-Crystals?

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inoxa400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 27 2017

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.00 sec

Pulse 45.0 degrees

Acq. time 2.560 sec

Width 6399.0 Hz

8 repetitions

OBSERVE H1, 399.9389024 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 29 sec

ZK-530-245-C

Sample Name:

Data Collected on: nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

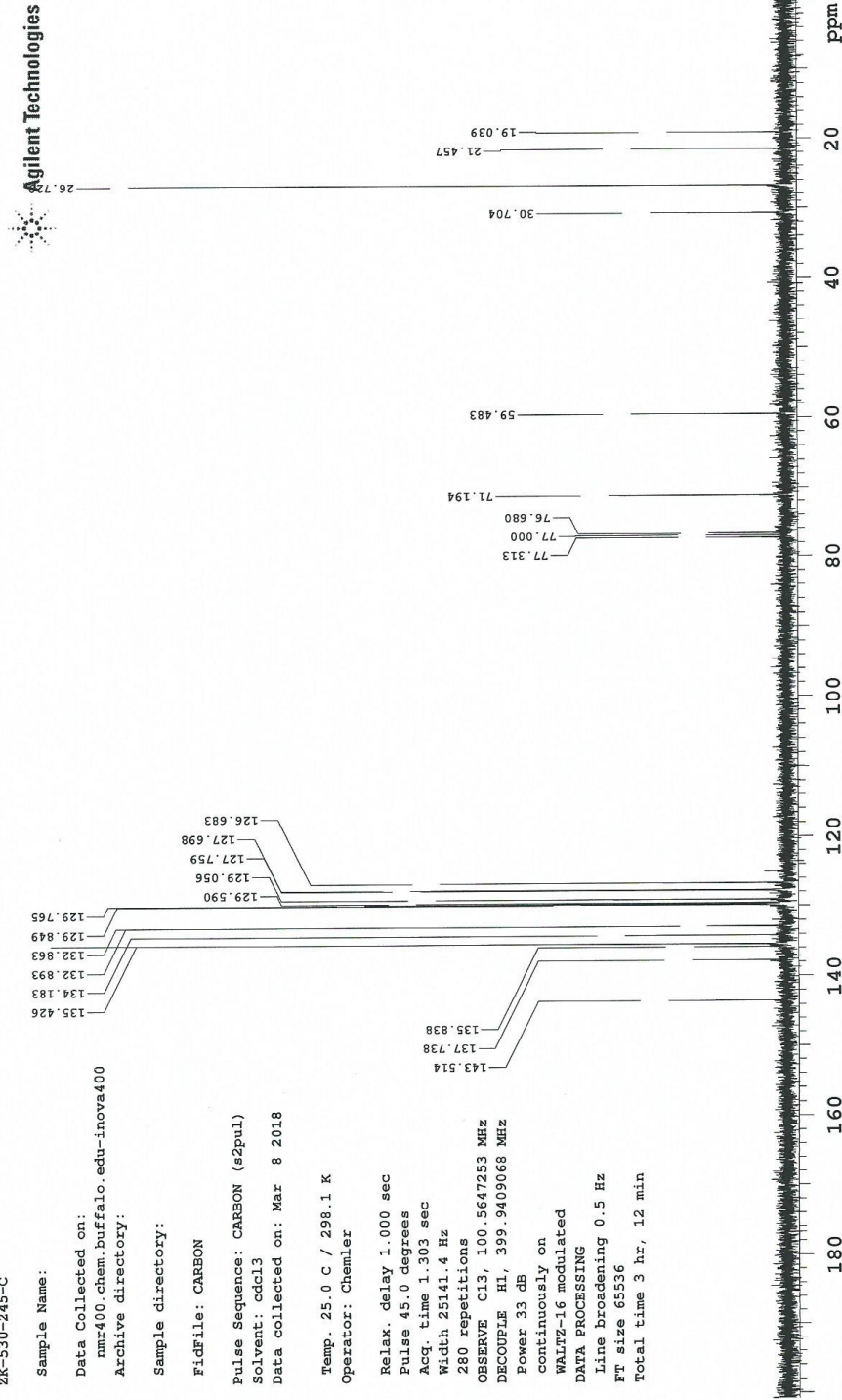
FidFile: CARBON

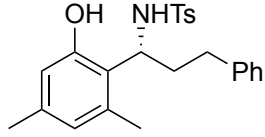
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 8 2018

Temp. 25.0 C / 298.1 K  
Operator: Chemler

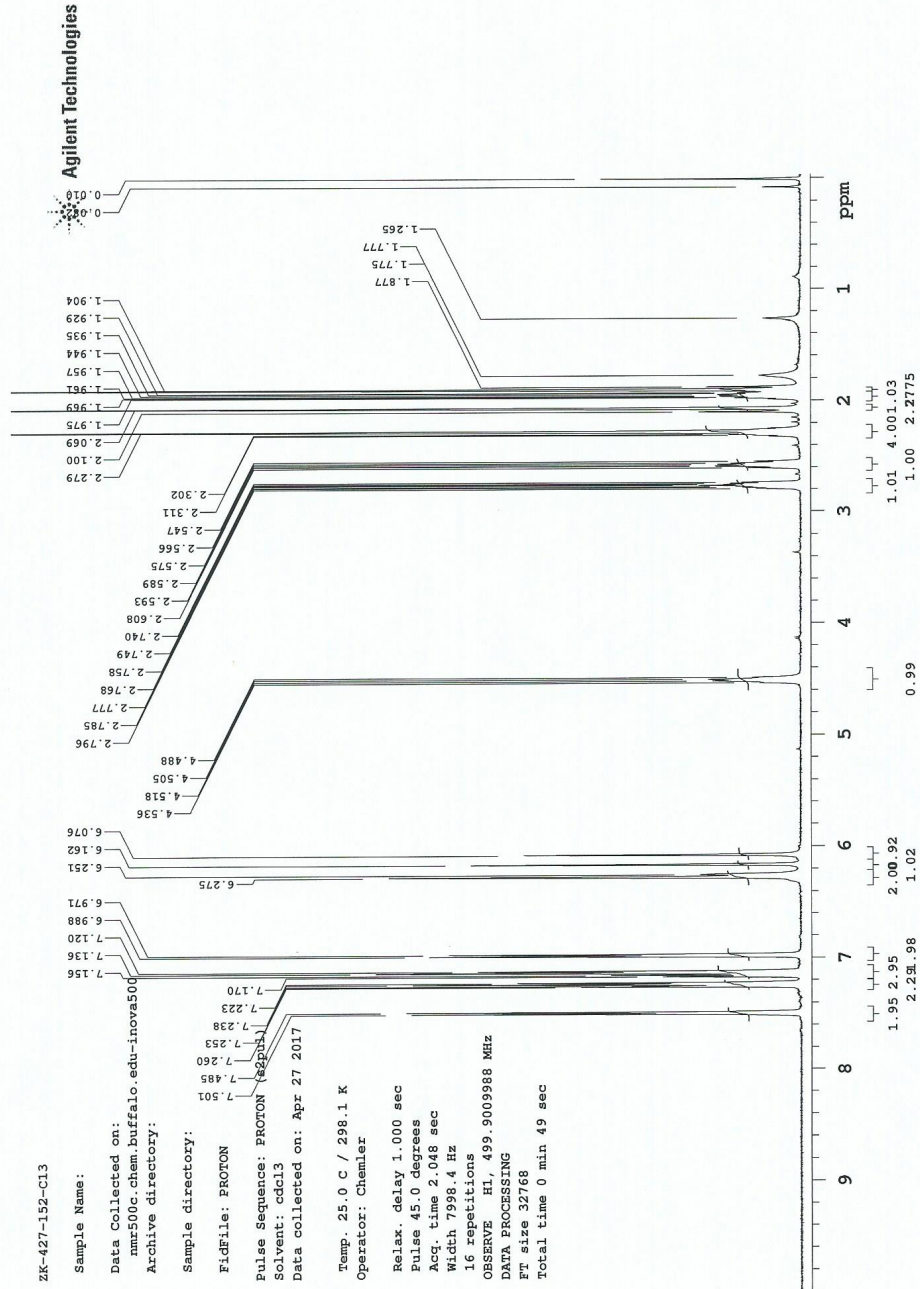
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
280 repetitions

OBSERVE C13, 100.5647253 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 3 hr, 12 min





(3a)





ZK-427-152-C13

Sample Name:

Data Collected on:  
nmr500c.chem.buffalo.edu-inova500

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Apr 27 2017

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.043 sec

Width 31421.8 Hz

336 repetitions

OBSERVE C13, 125.7002092 MHz

DECOUPLE H1, 499.9034960 MHz

Power 40 dB

continuously on

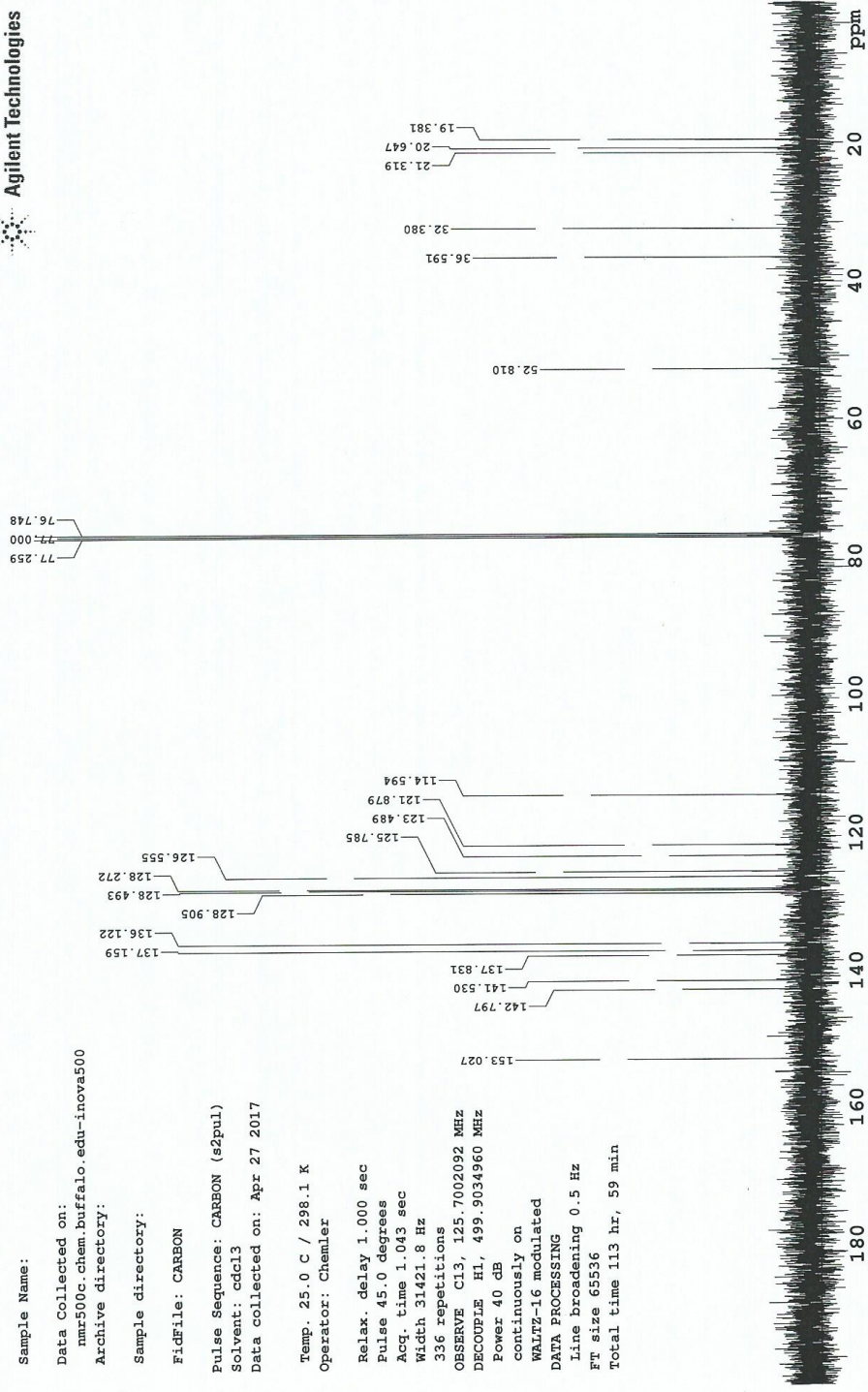
WALTZ-16 modulated

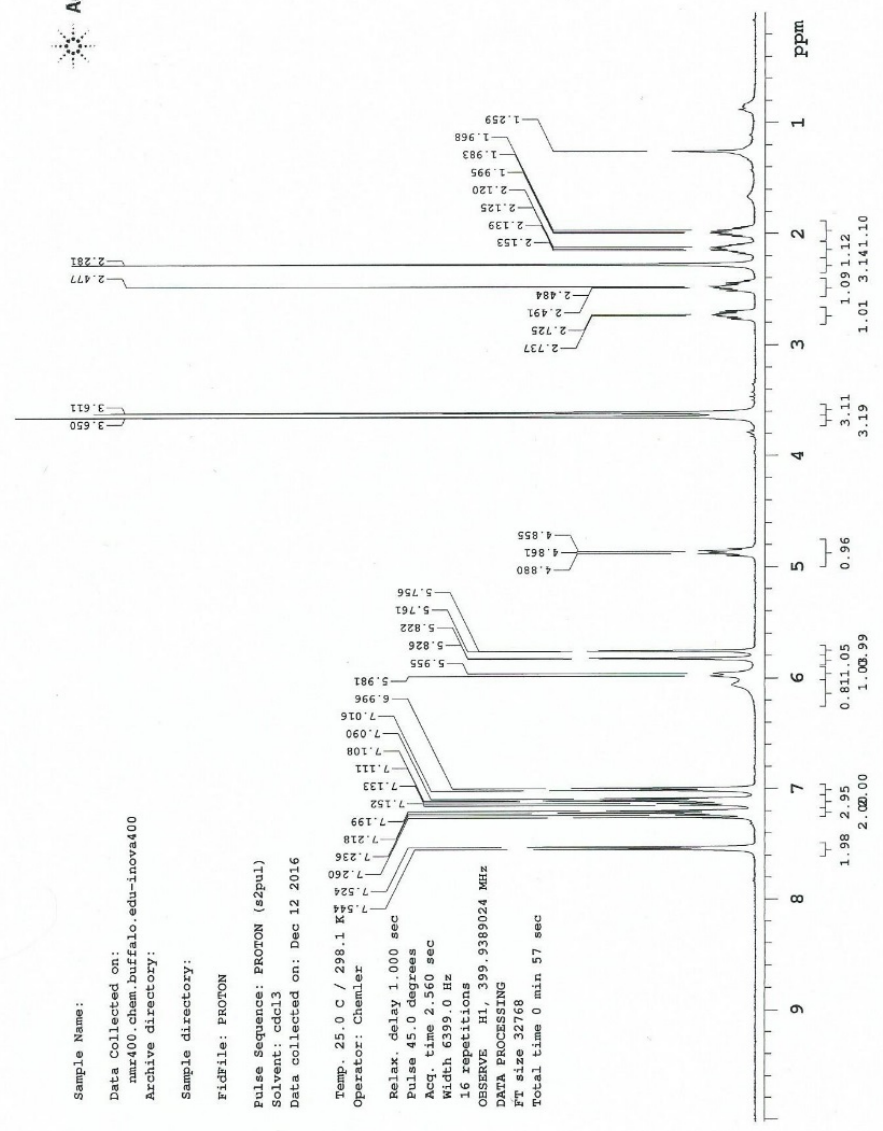
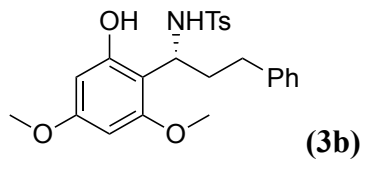
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 113 hr, 59 min





Sample Name:  
 Data Collected on:  
 nmr400.chem.buffalo.edu-inova400  
 Archive directory:  
 Sample directory:  
 FIDFile: PROTON  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Dec 12 2016

Temp. 25.0 C / 298.1 K  
 Operator: ChemLer  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.560 sec  
 Width 6399.0 Hz  
 16 repetitions  
 OBSERVE H1, 399.9389024 MHz  
 DATA PROCESSING  
 FT size 32768  
 Total time 0 min 57 sec

76.680  
77.000  
77.198  
77.313

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 12 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
20000 repetitions

OBSERVE c13, 100.5647184 MHz  
DECOUPLE h1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 12 hr, 50 min

128.827  
128.354  
128.171

126.744  
125.615

142.659  
141.919  
137.212

154.340  
158.025  
160.140

107.541

93.815  
91.099

55.317  
55.225

49.763

37.067

32.574

21.320

ppm

20

40

60

80

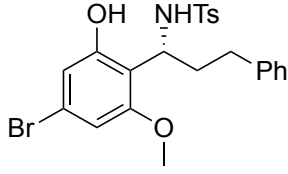
100

120

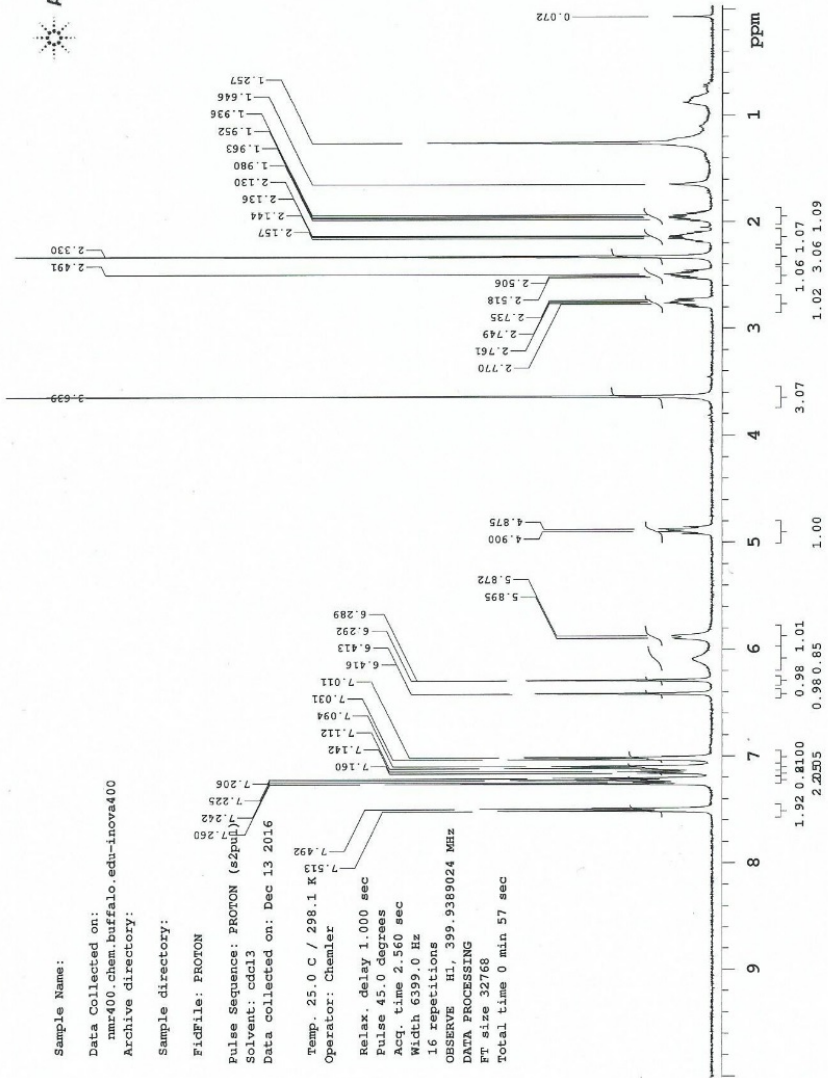
140

160

180



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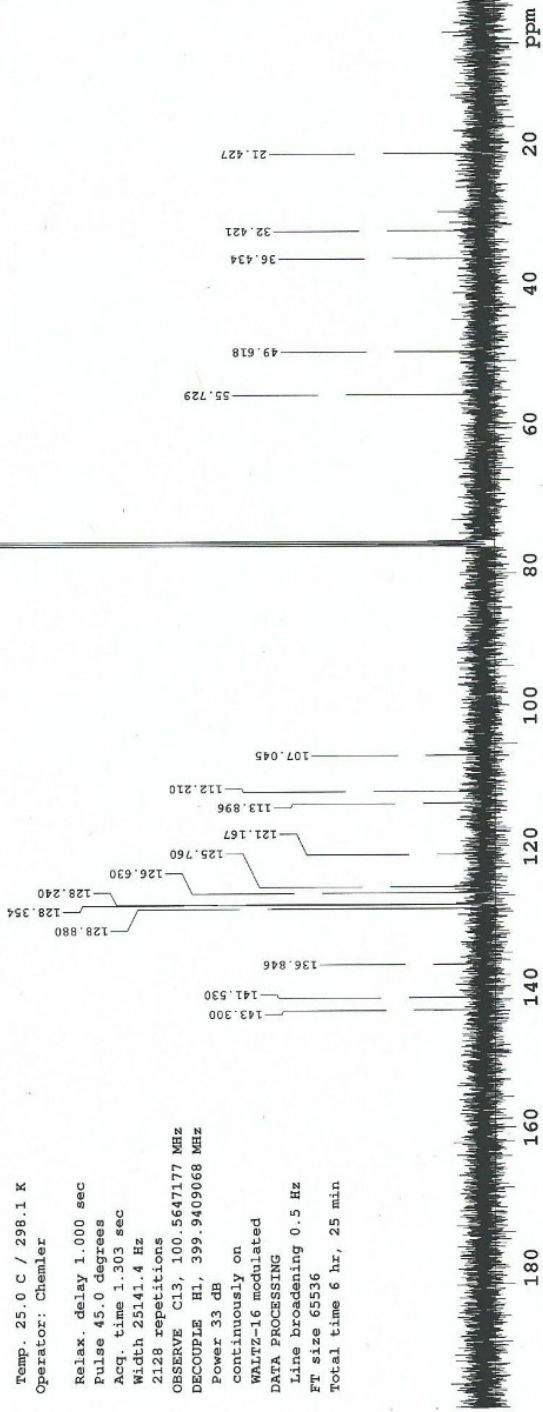


76.680  
77.000  
77.213

Sample Name:  
Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:  
FidFile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 13 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
2128 repetitions  
OBSERVE C13, 100.5647177 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 6 hr, 25 min





ZK-369-94-P

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Dec 13 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

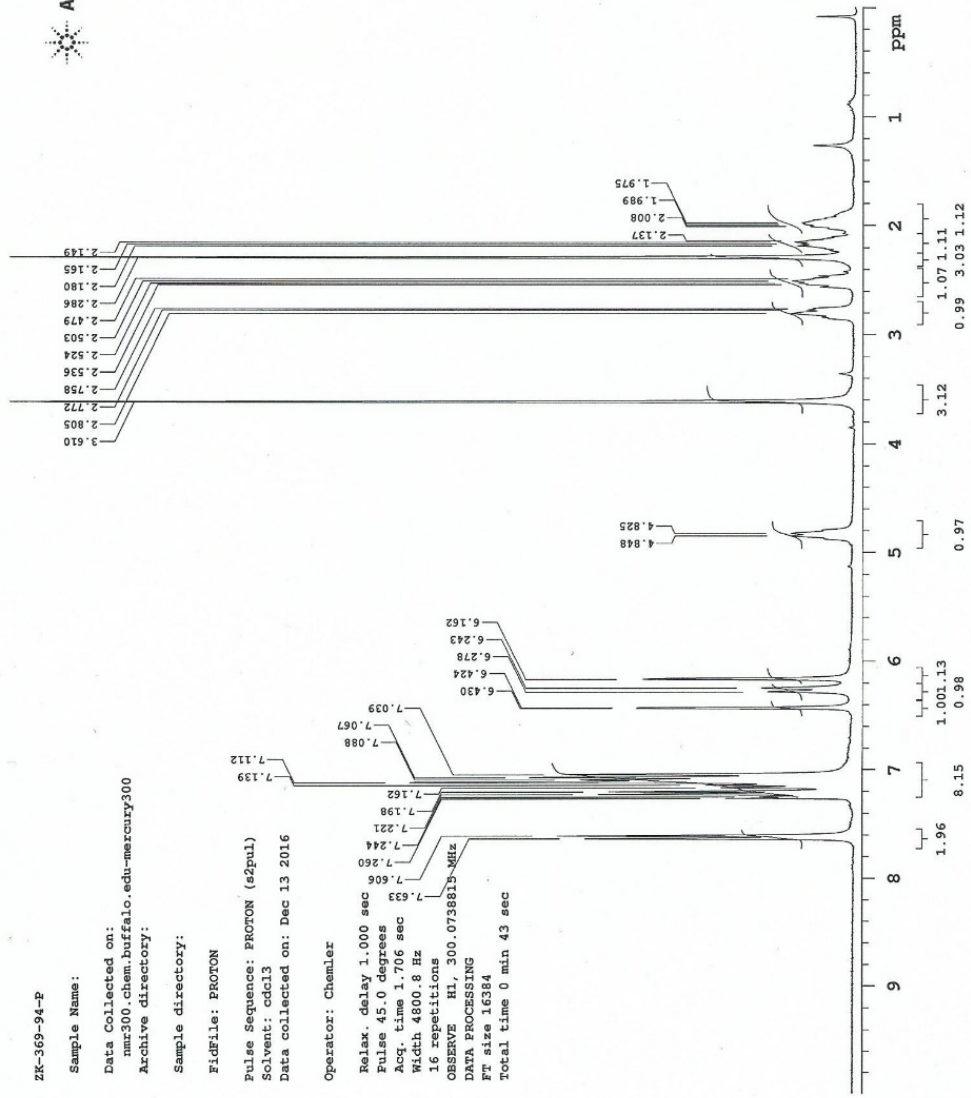
16 repetitions

OBSERVE H1, 300.0738813-MHz

DATA PROCESSING

FT size 16384

Total time 0 min 43 sec



ZK-369-94-P

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3  
Data collected on: Dec 13 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

896 repetitions

OBSERVE C13, 75.4536400 MHz

DECOUPLE H1, 300.0754430 MHz

Power 37 dB

continuously on

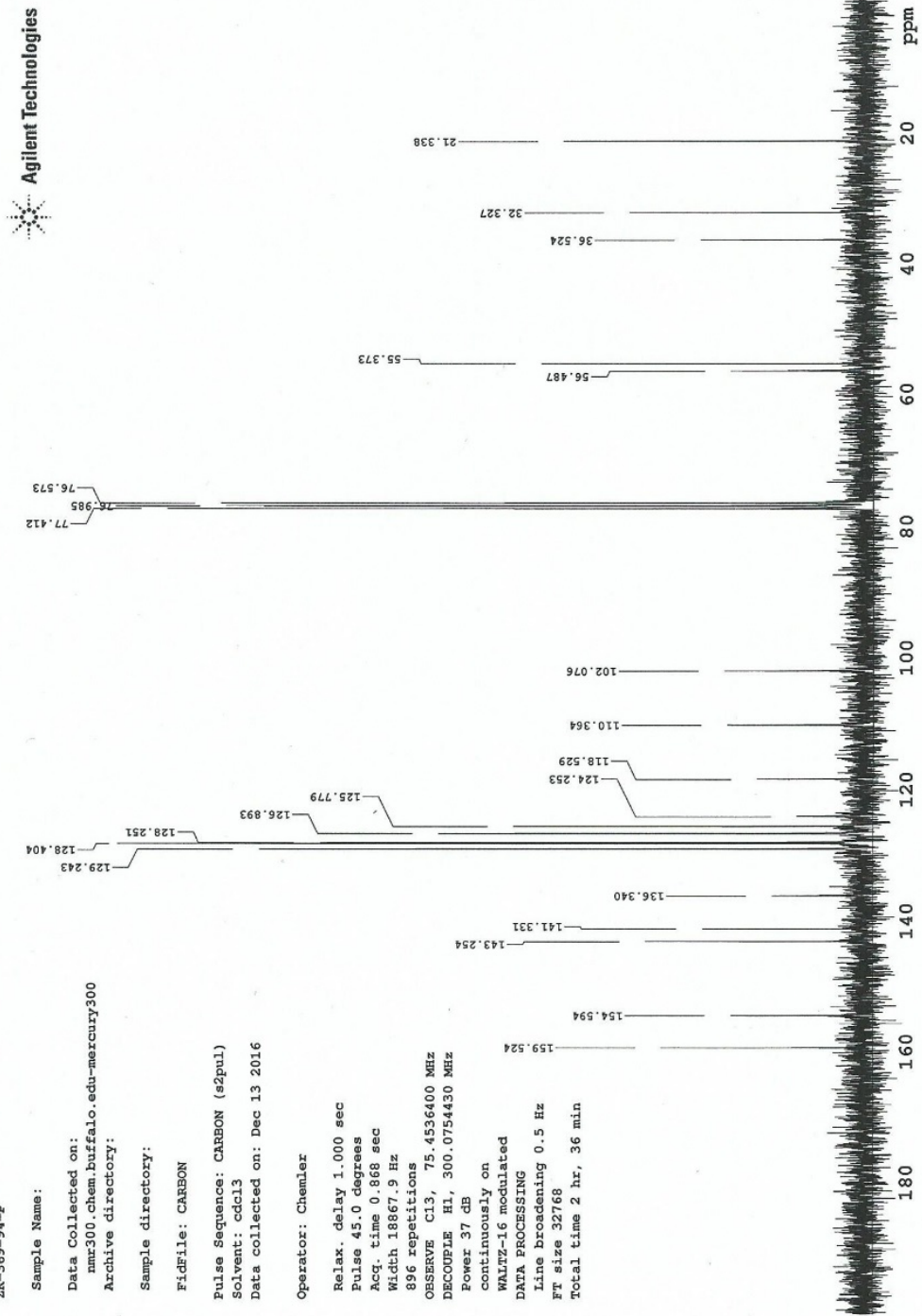
WALTZ-16 modulated

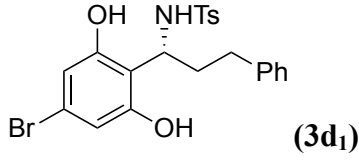
DATA PROCESSING

Line broadening 0.5 Hz

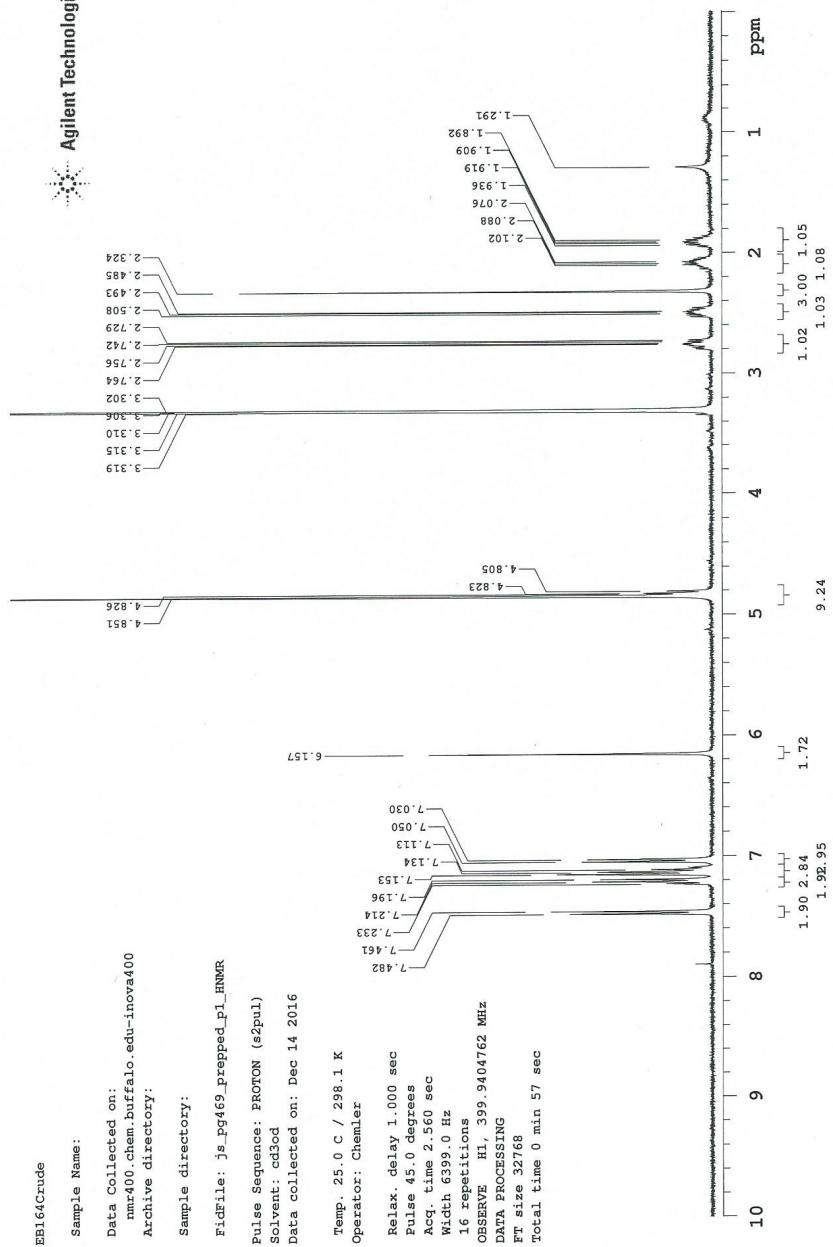
FT size 32768

Total time 2 hr, 36 min





Agilent Technologies



EB164Crude  
 Sample Name:  
 Data Collected on:  
 nmr400.chem.buffalo.edu-inova400  
 Archive directory:  
 Sample directory:  
 FIDFile: js\_pg469\_prepped\_pl\_HNMR  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cd3od  
 Data collected on: Dec 14 2016  
 Temp. 25.0 C / 298.1 K  
 Operator: Chemler  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.560 sec  
 Width 6399.0 Hz  
 16 repetitions  
 OBSERVE H1, 399.9404762 MHz  
 DATA PROCESSING  
 FT size 32768  
 Total time 0 min 57 sec

EB164Crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

F1dFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3od  
Data collected on: Dec 14 2016

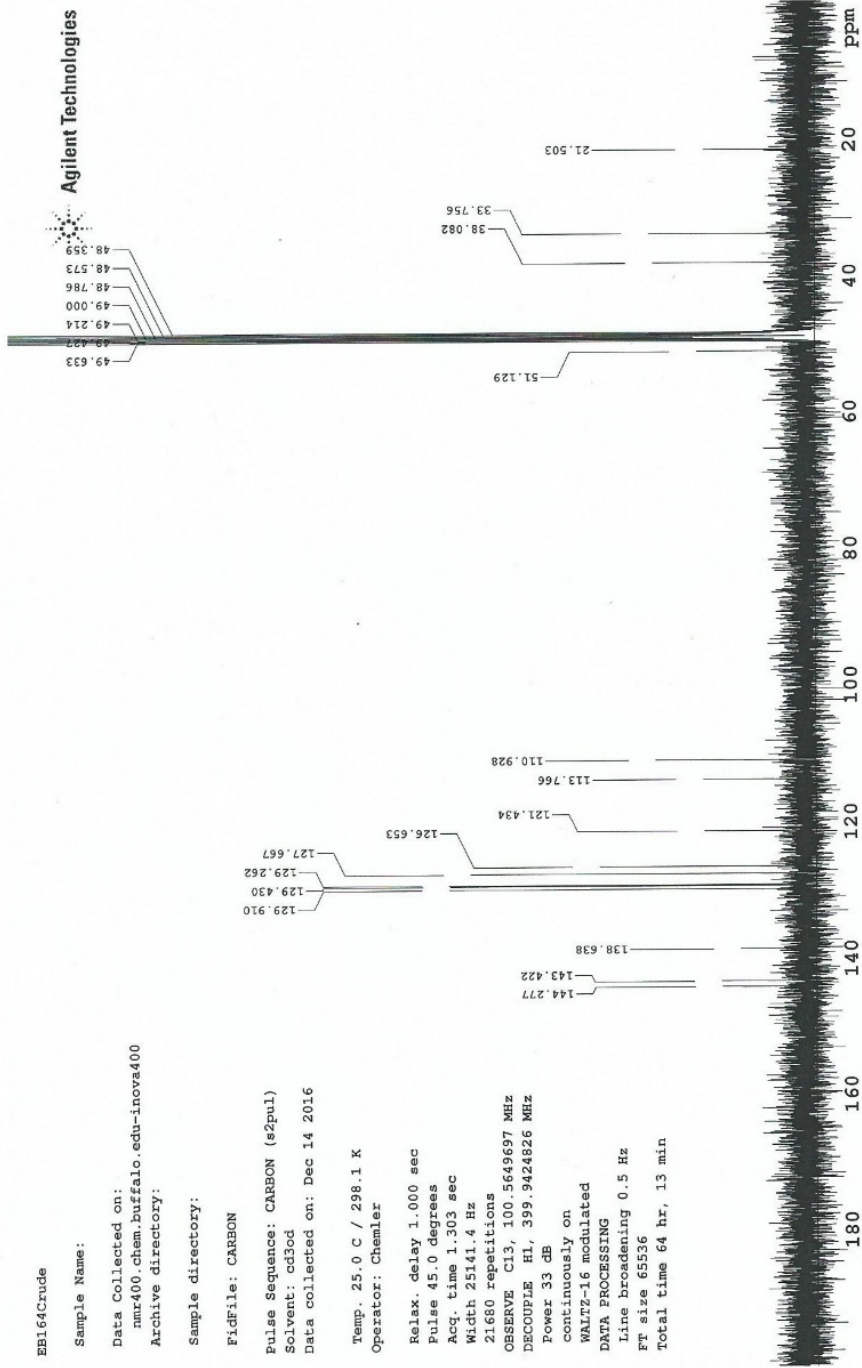
Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz

21680 repetitions  
OBSERVE C13, 100.5649697 MHz  
DECOUPLE H1, 399.9424826 MHz

Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 64 hr, 13 min

Agilent Technologies



RP\_Copper\_Recovered\_Stilla\_2

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

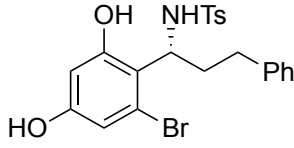
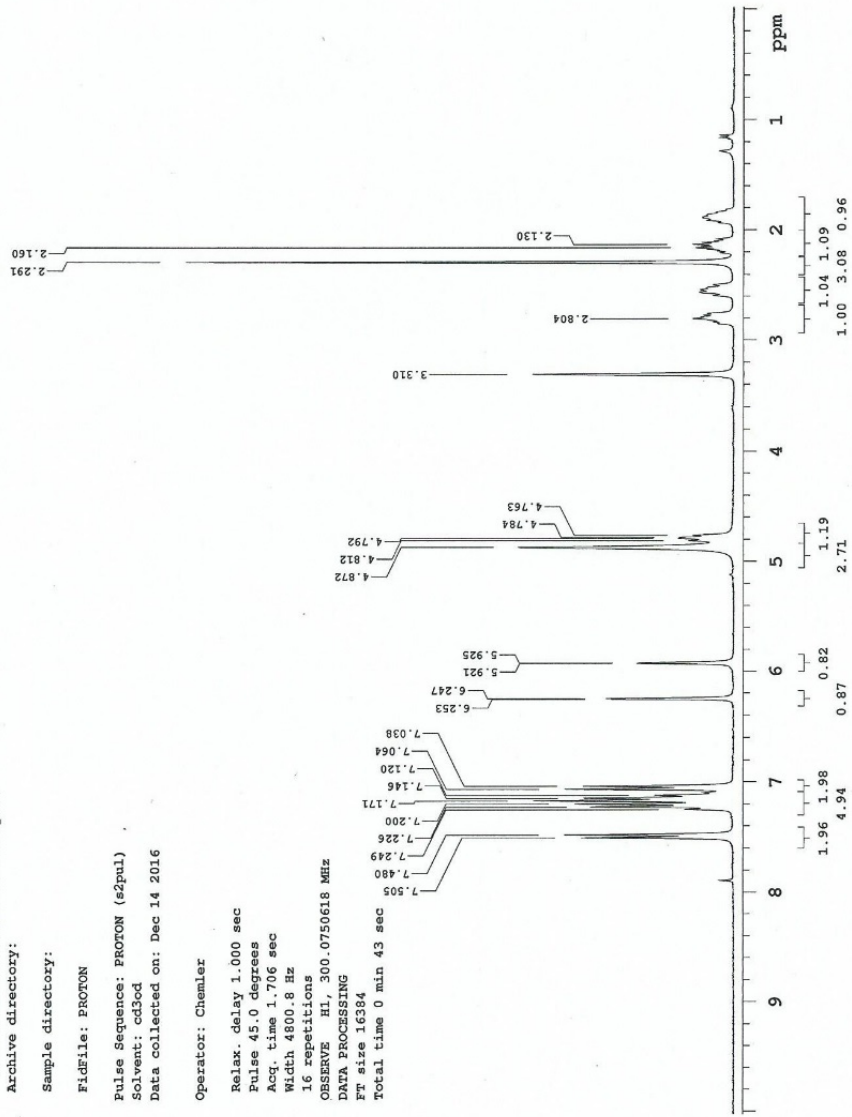
Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cd3od  
Data collected on: Dec 14 2016

Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.706 sec  
Width 4800.8 Hz  
16 repetitions

OBSERVE HL, 300.0750618 MHz  
DATA PROCESSING  
Ft size 16384  
Total time 0 min 43 sec





RP\_Copper\_Recovered\_Stille\_2

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

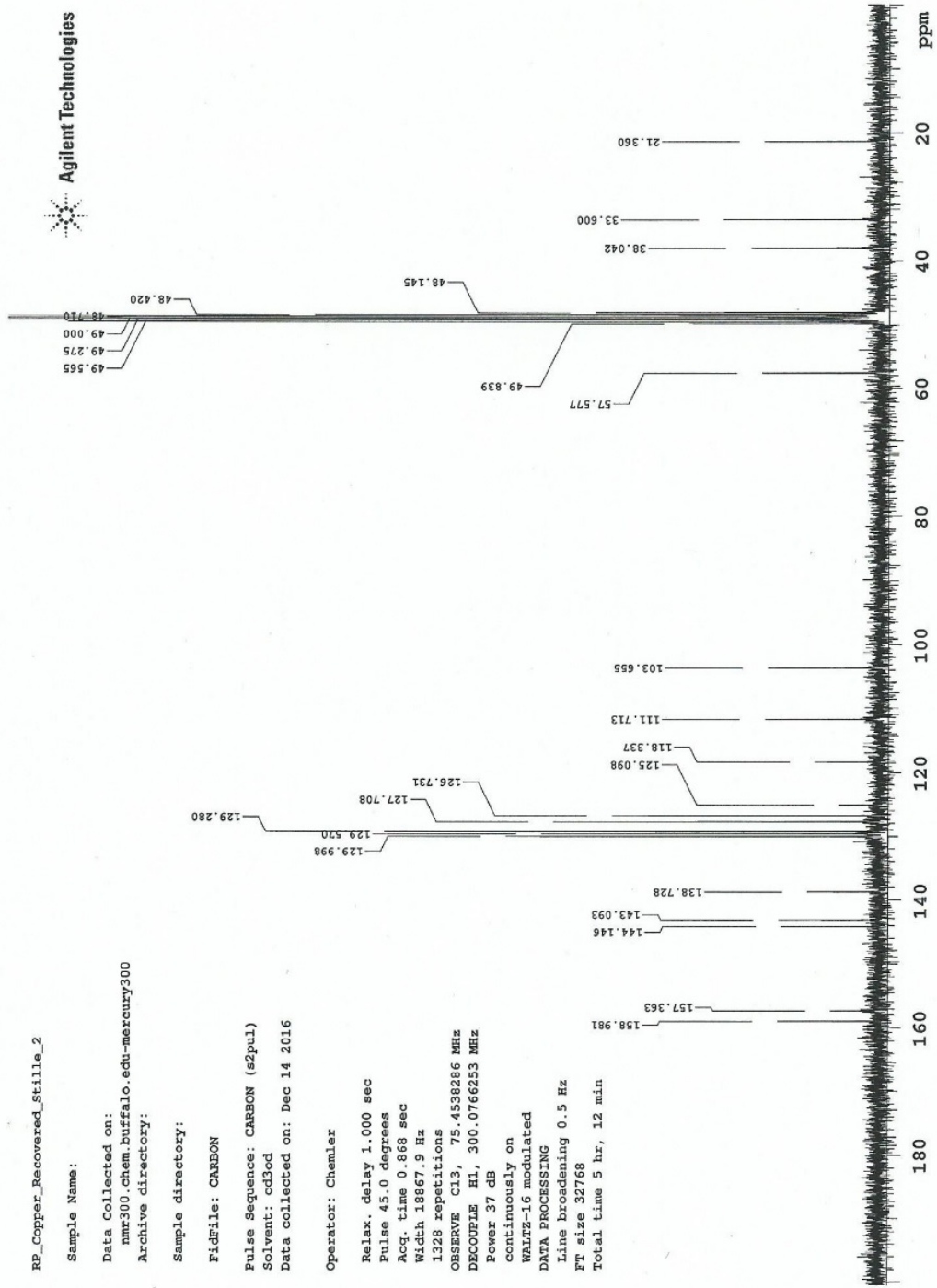
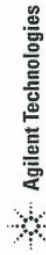
FidFile: CARBON

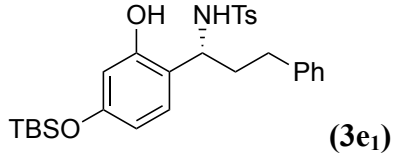
Pulse Sequence: CARBON (s2pul)

Solvent: cd3cd  
Data collected on: Dec 14 2016

Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
1328 repetitions  
OBSERVE C13, 75.4538286 MHz  
DECOUPLE H1, 300.0766253 MHz  
Power 37 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 32768  
Total time 5 hr, 12 min





Agilent Technologies

cdk-b2-r354-product

Sample Name:

Data Collected on:  
 nmr300.chem.buffalo.edu-mercury300  
 Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
 Solvent: cdc13  
 Data collected on: Dec 12 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

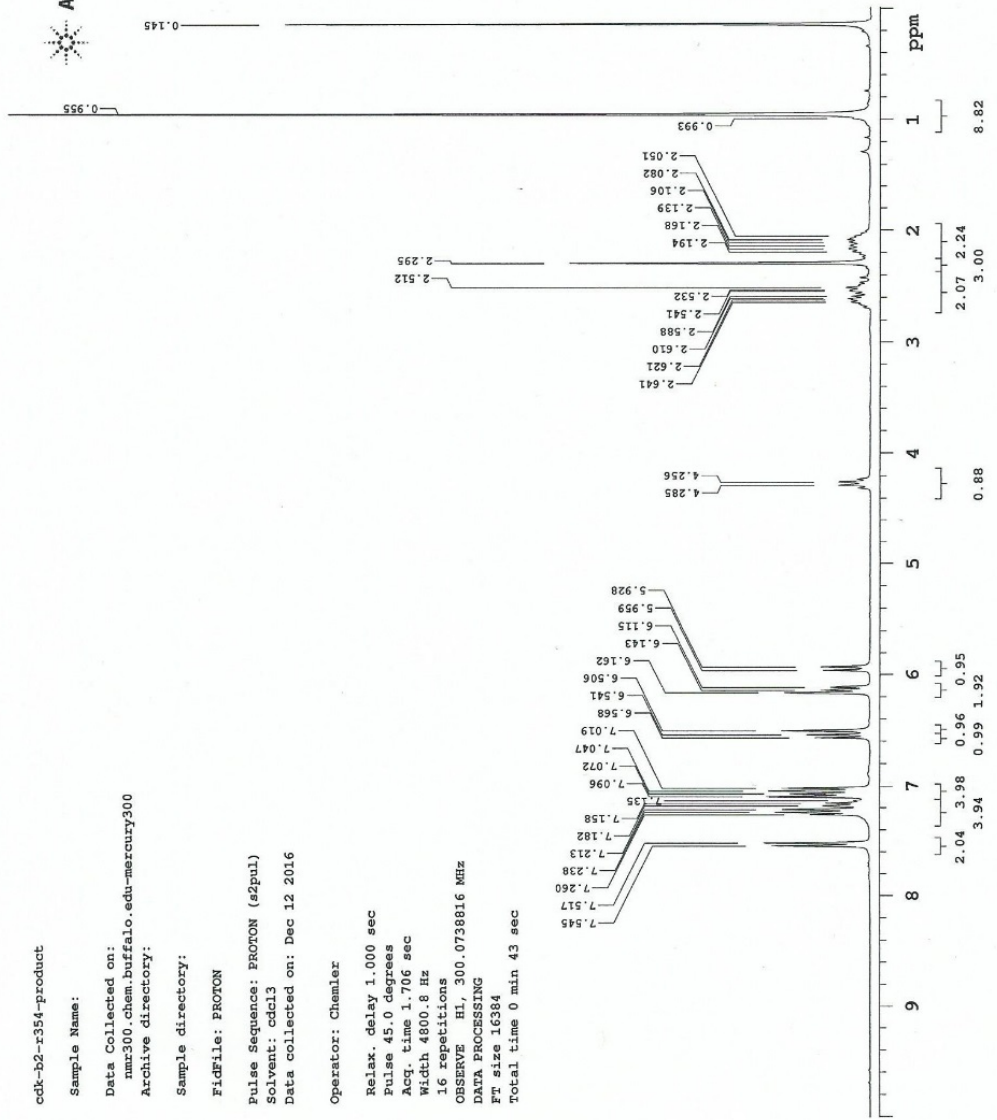
16 repetitions

OBSERVE H1, 300.0738816 MHz

DATA PROCESSING

FT size 16384

Total time 0 min 43 sec

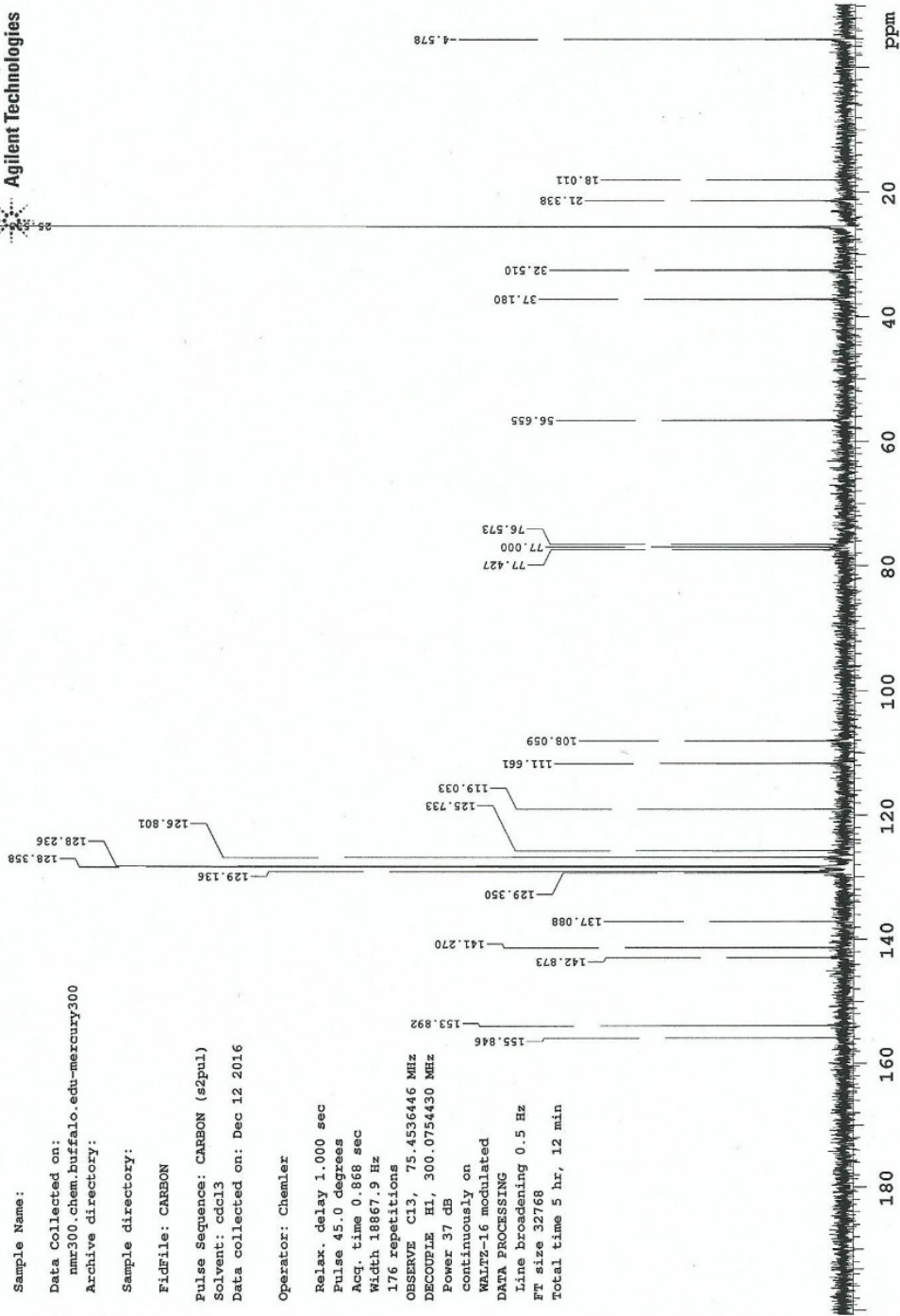


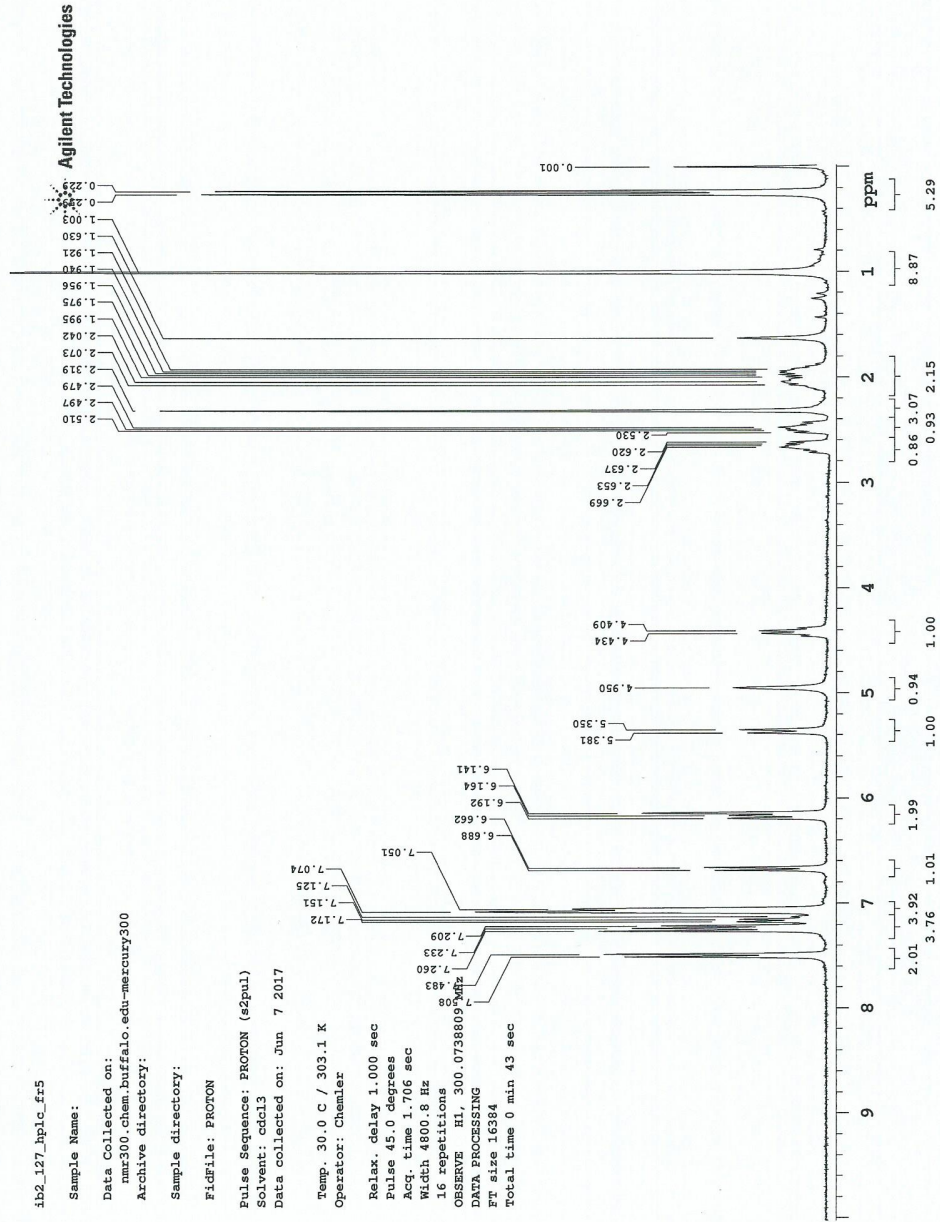
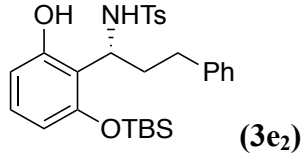
cdk-b2-r354-product

Sample Name:  
 Data Collected on:  
 nmr300.chem.buffalo.edu-mercury300  
 Archive directory:  
 Sample directory:  
 FidFile: CARBON  
 Pulse Sequence: CARBON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Dec 12 2016

Operator: Chemler

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 0.868 sec  
 Width 18867.9 Hz  
 176 repetitions  
 OBSERVE C13, 75.4536446 MHz  
 DECOUPLE H1, 300.0754430 MHz  
 Power 37 dB  
 continuously on  
 WALTZ-16 modulated  
 DATA PROCESSING  
 Line broadening 0.5 Hz  
 F1 size 32768  
 Total time 5 hr, 12 min







ib2\_127\_hp1c\_fr5

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

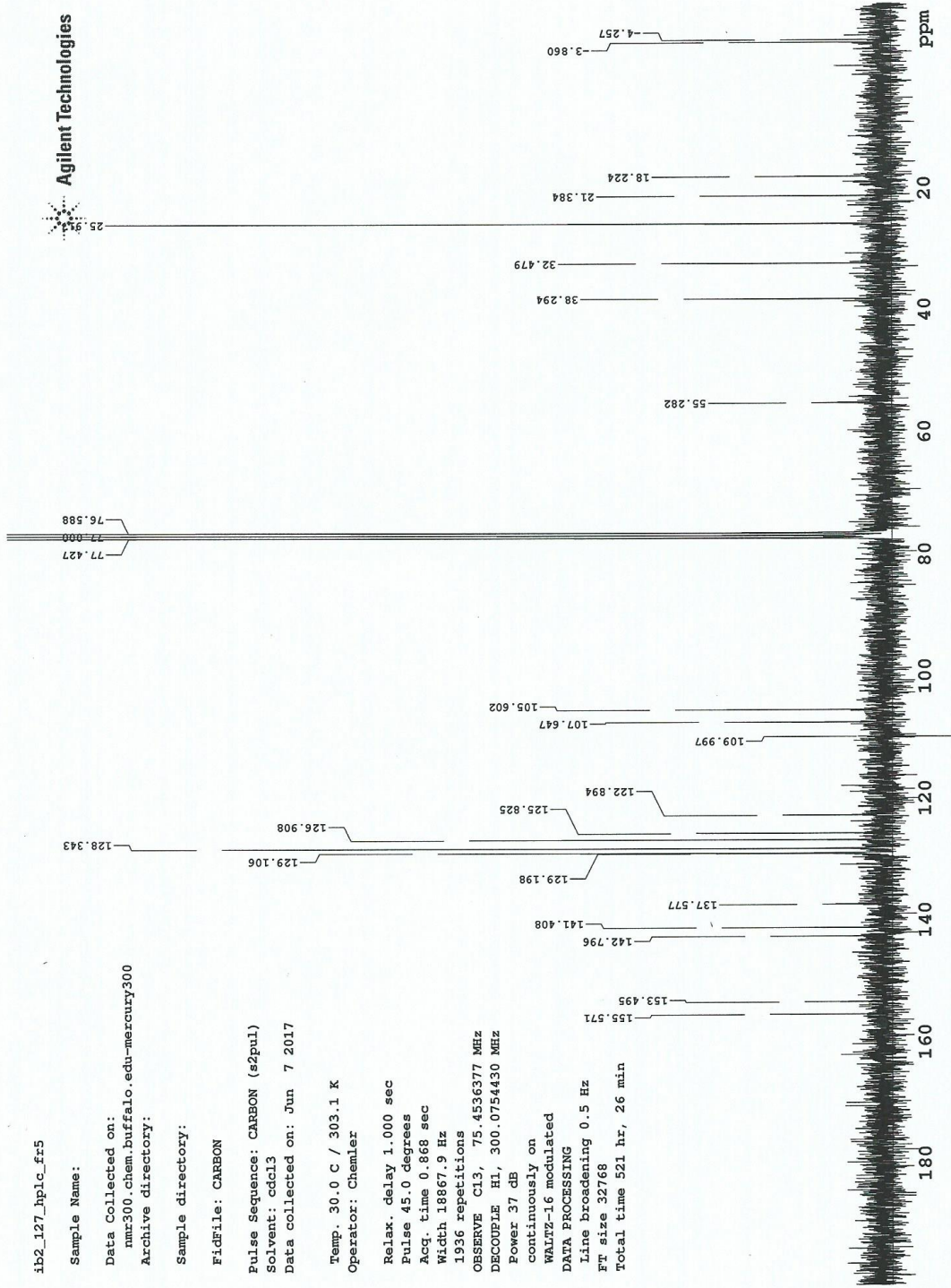
Fidfile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 7 2017

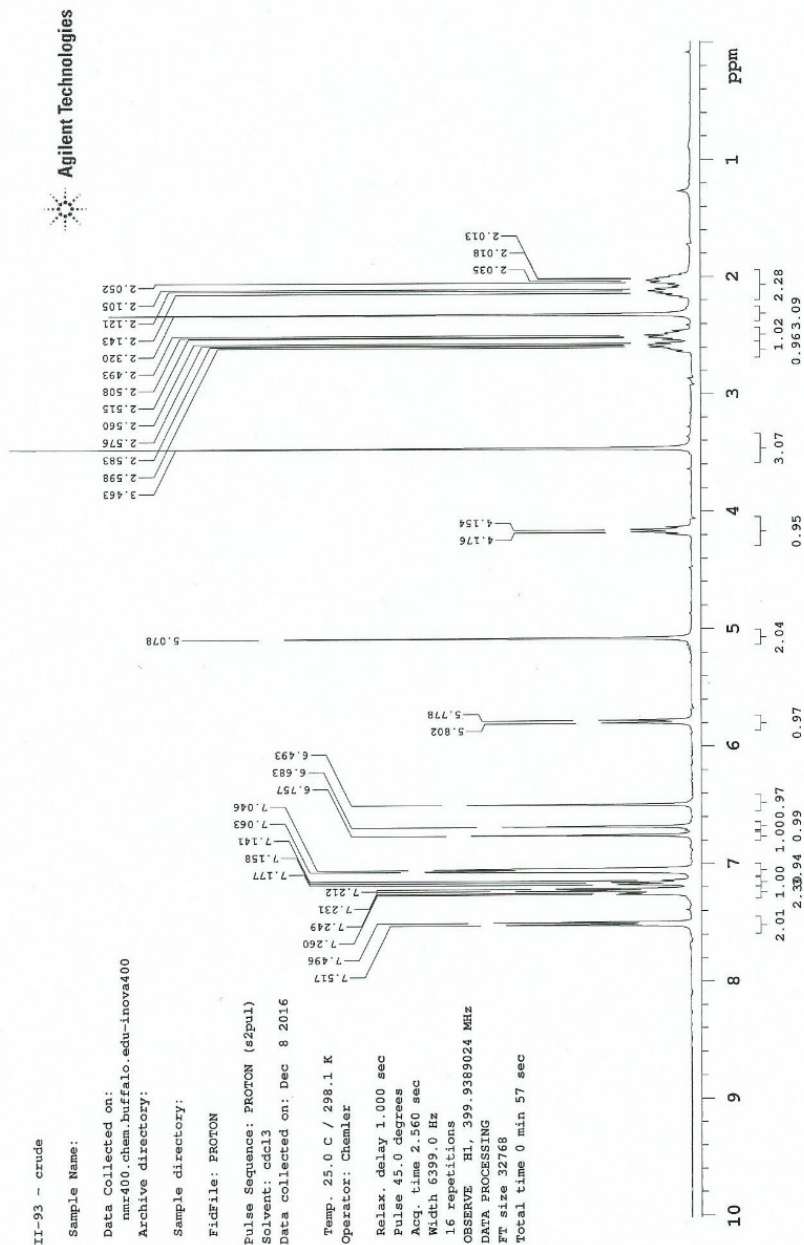
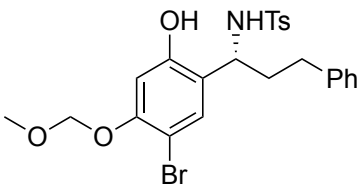
Temp. 30.0 C / 303.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
1936 repetitions

OBSERVE C13, 75.4536377 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 37 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 521 hr, 26 min







II-93 - crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

File: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Dec 8 2016

Temp. 25.0 C / 298.1 K

Operator: Chemlar

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

768 repetitions

OBSERVE C13, 100.5647215 MHz

DECOUPLE H1, 399.9409068 MHz

Power 33 dB

continuously on

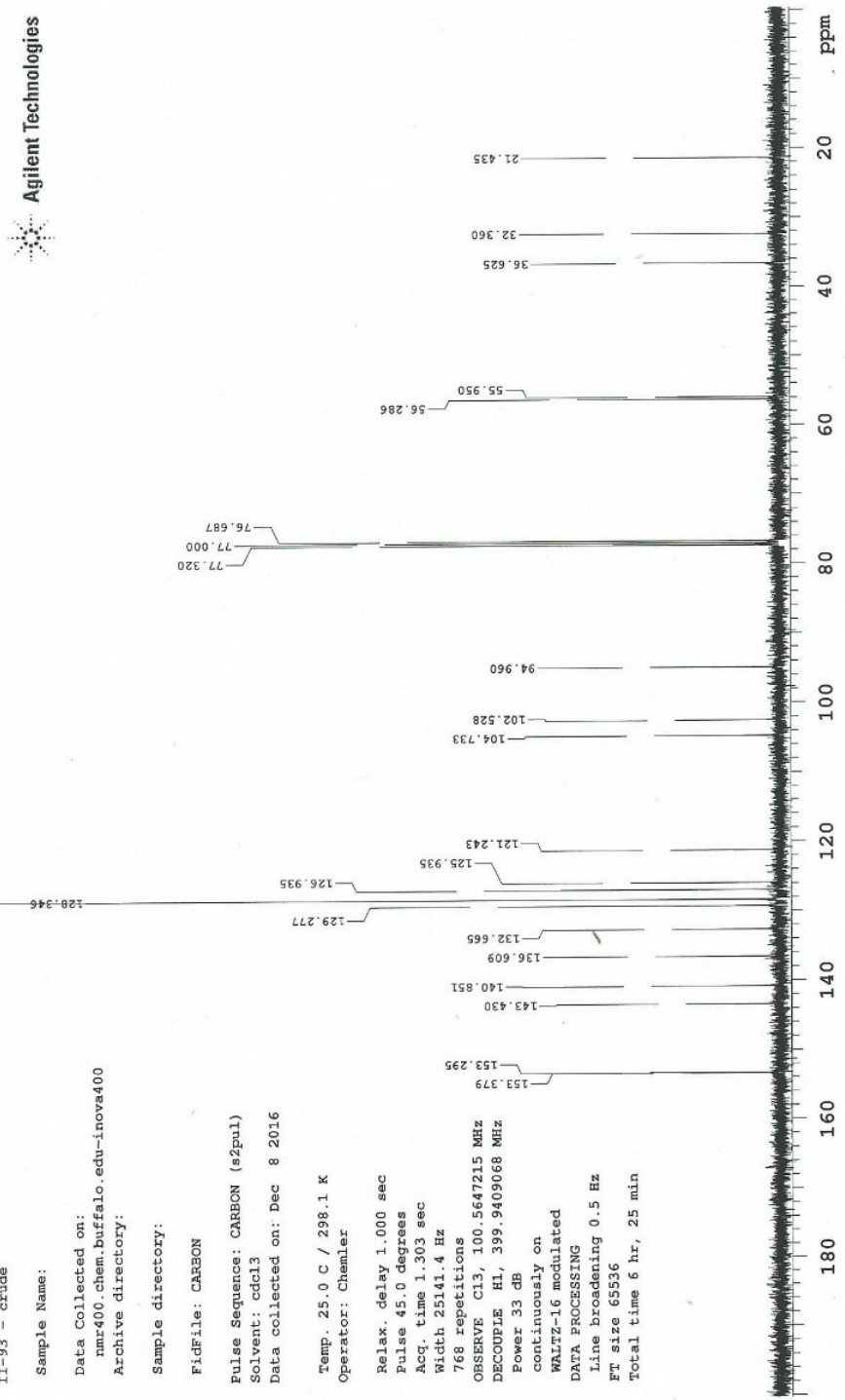
WALTZ-16 modulated

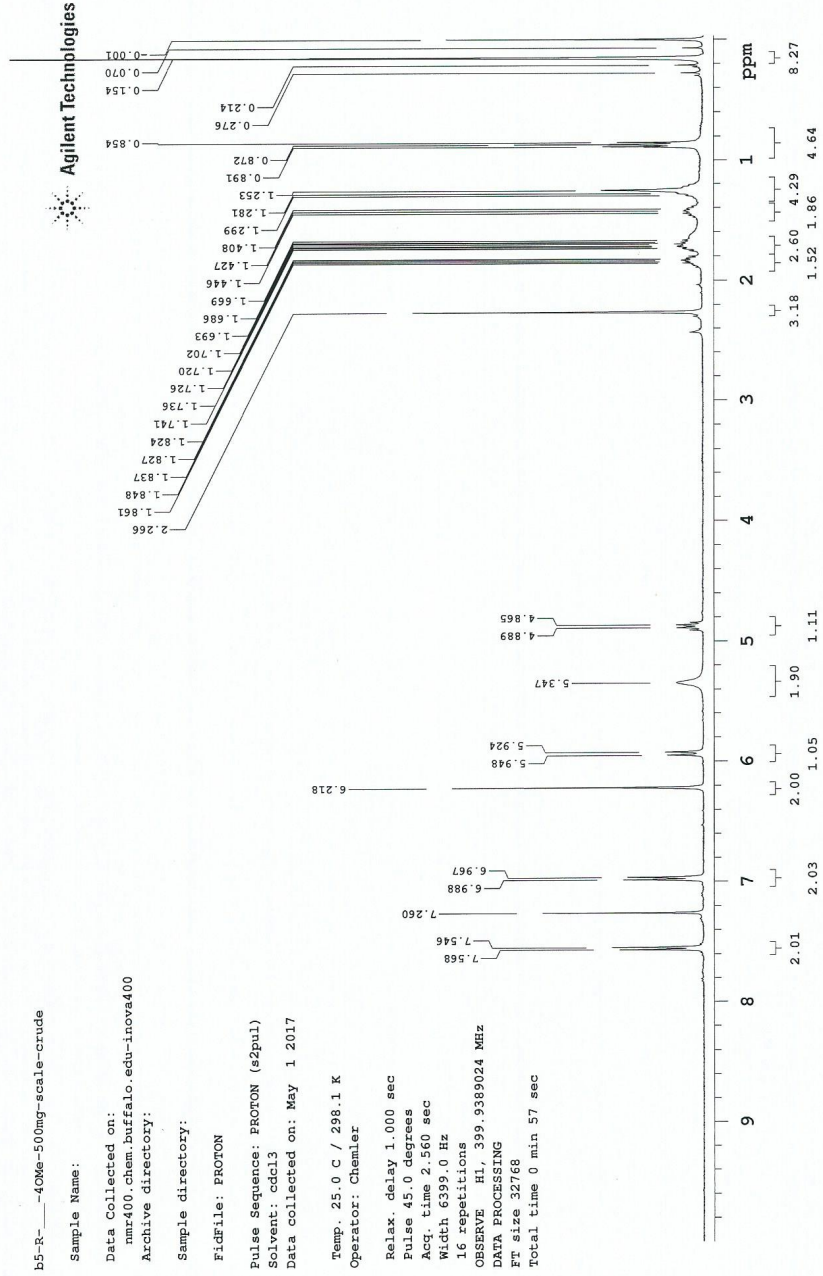
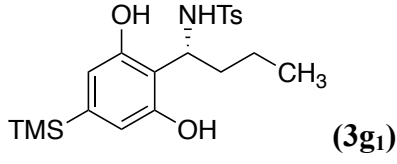
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 6 hr, 25 min





b5-R--40Me-500mg-scale-crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

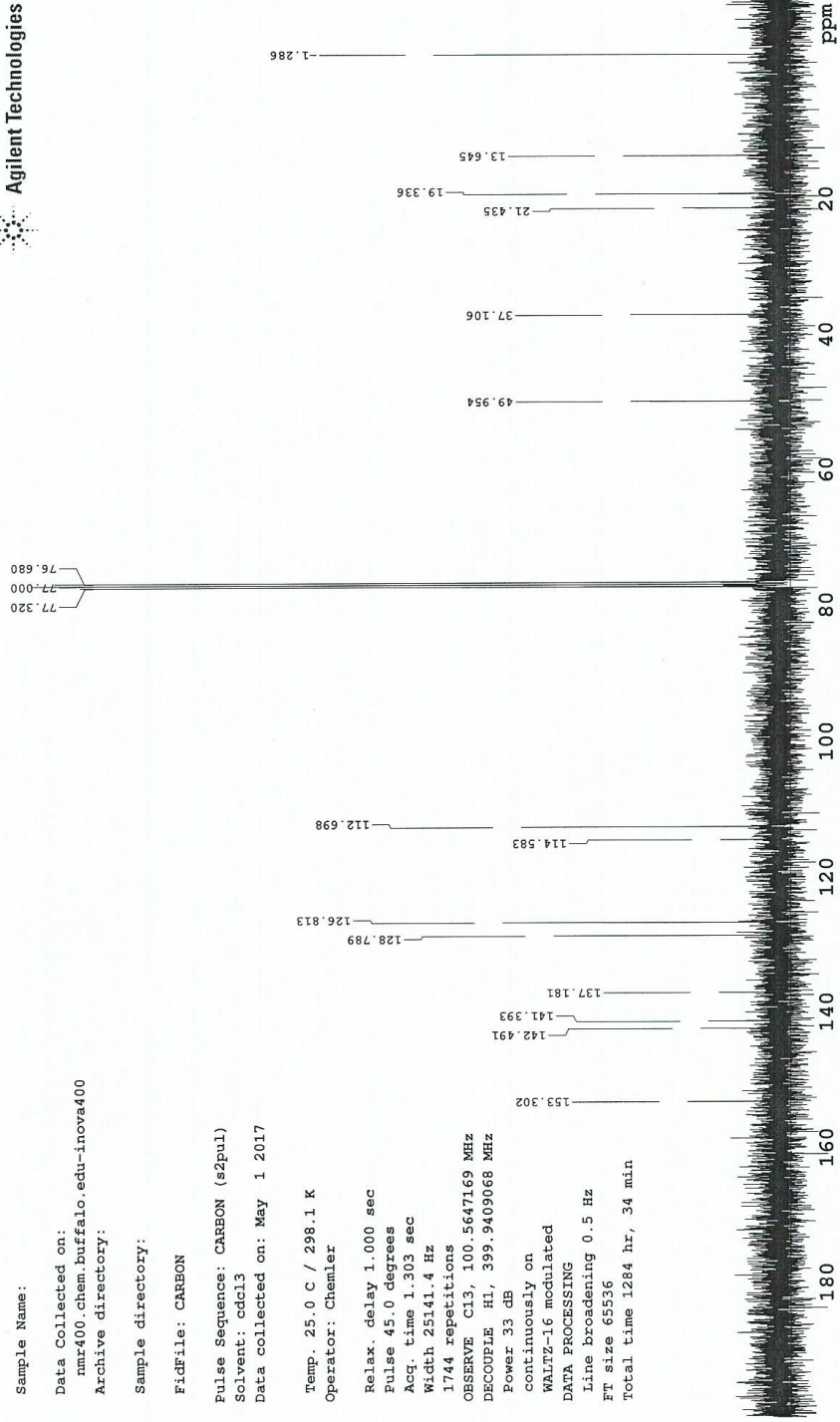
FidFile: CARBON

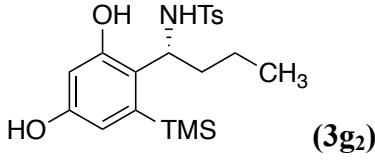
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: May 1 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

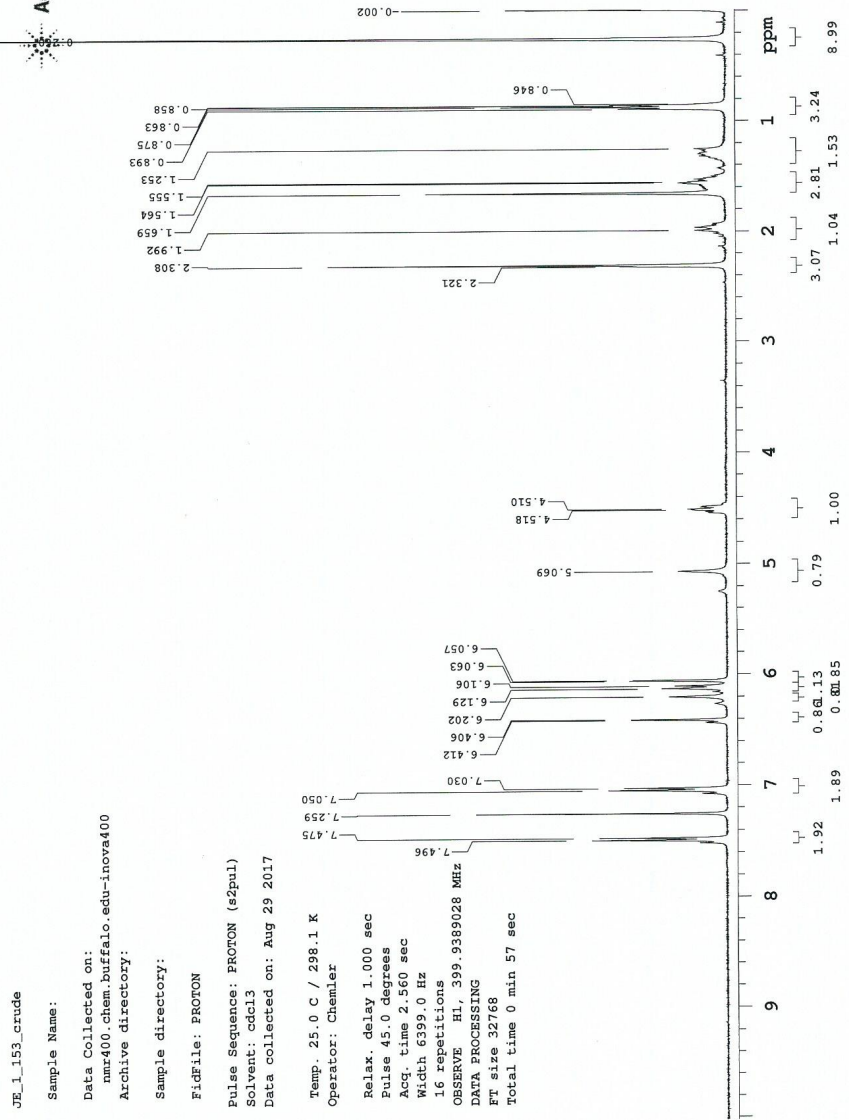
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
1744 repetitions

OBSERVE C13, 100.5647169 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 1284 hr, 34 min





Agilent Technologies



JE\_1\_153\_crude

Sample Name:

Data Collected on:

nmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

File: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 29 2017

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.560 sec

Width 6399.0 Hz

16 repetitions

OBSERVE H1, 399.9389028 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 57 sec



JE\_1\_153\_crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 29 2017

Temp.: 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

1984 repetitions

OBSERVE C13, 100.5647169 MHz

DECOUPLE H1, 399.9409068 MHz

Power 33 dB

continuously on

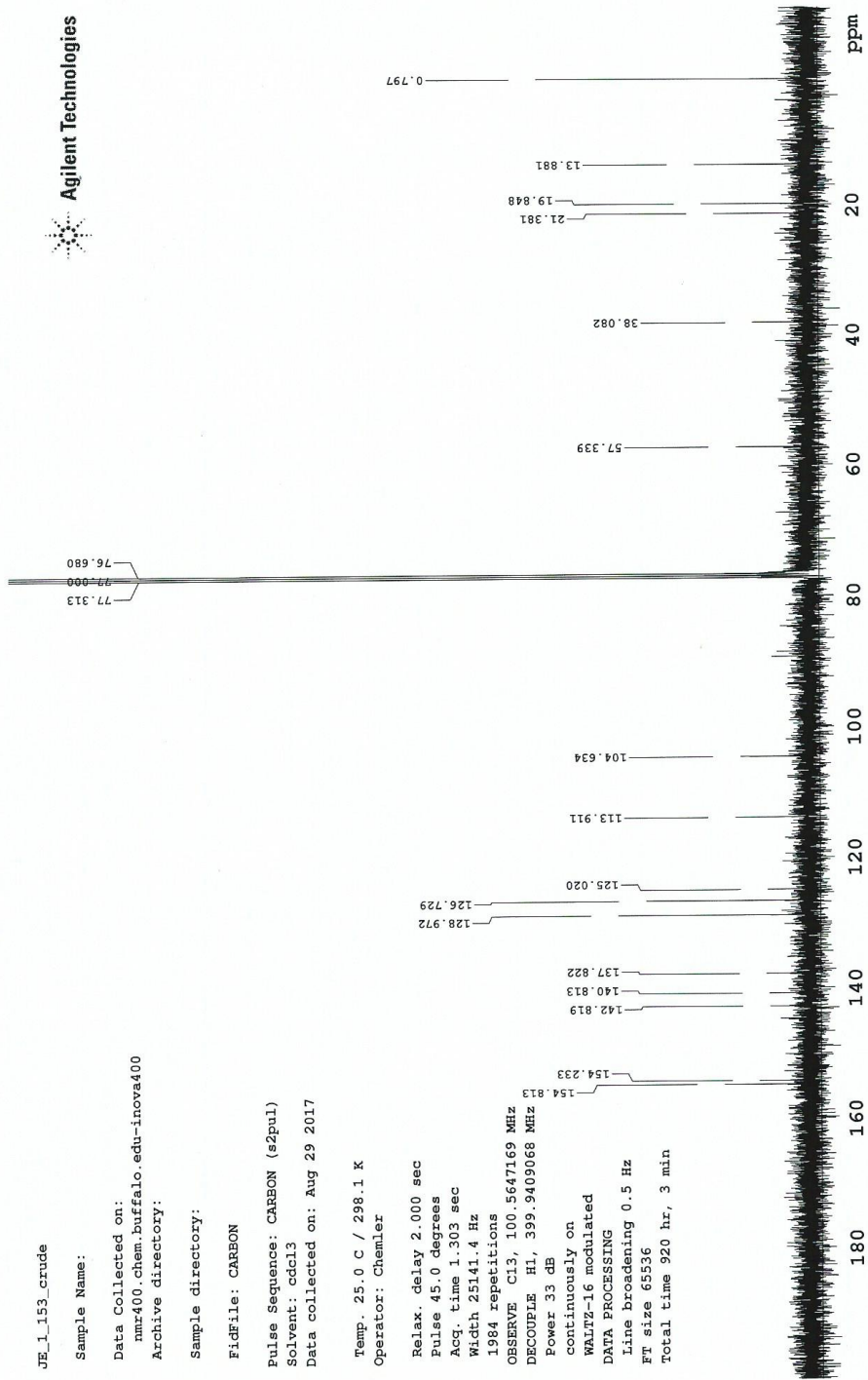
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 920 hr, 3 min



cdk-52-r454-crude

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Aug 28 2017

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

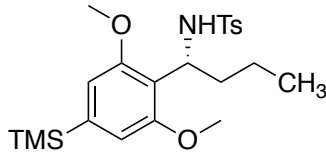
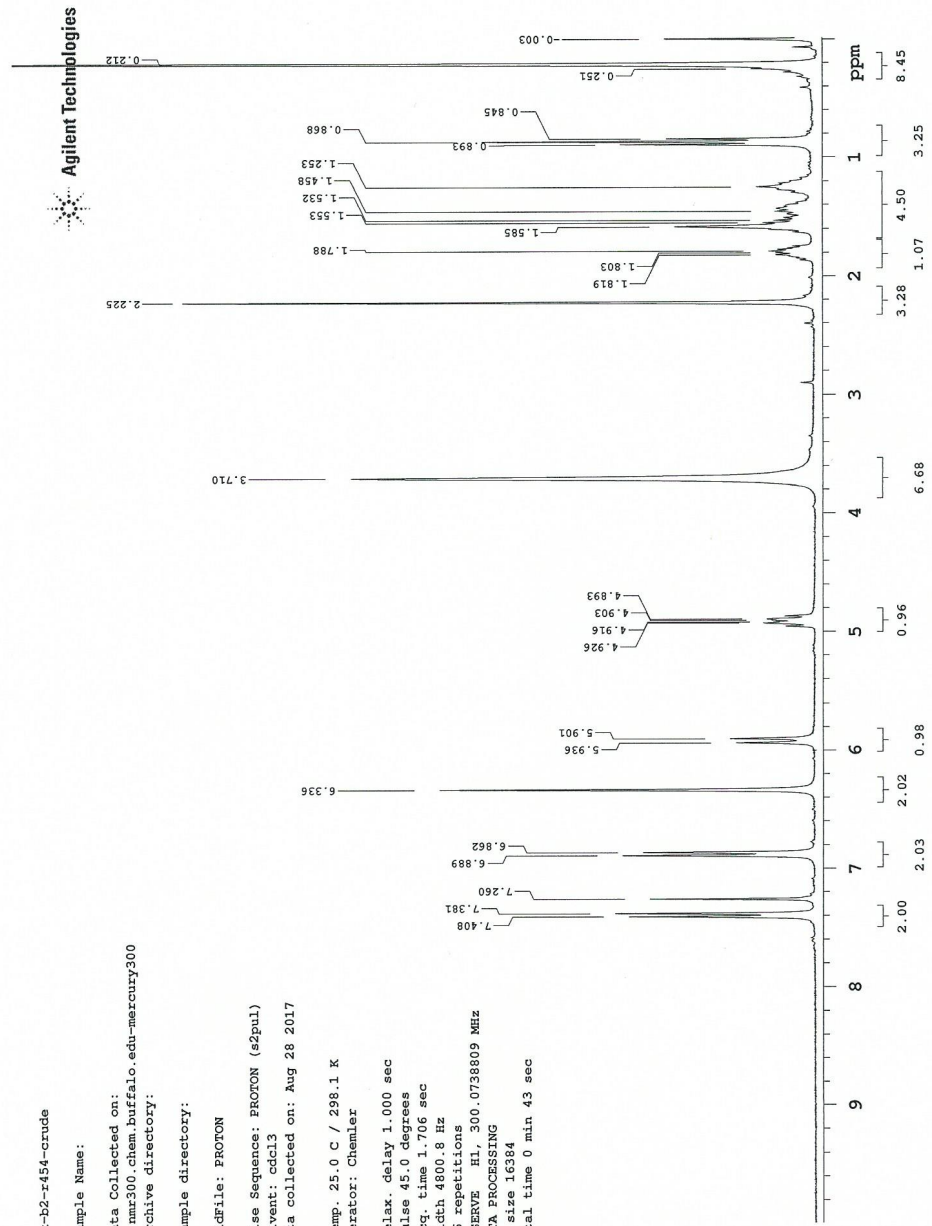
16 repetitions

OBSERVE HL, 300.0738809 MHz

DATA PROCESSING

FT size 16384

Total time 0 min 43 sec



cdk-b2-r454-crude

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FIDFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Aug 28 2017

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

2272 repetitions

OBSERVE C13, 75.4536377 MHZ

DECOUPLE H1, 300.0754430 MHZ

Power 37 dB

continuously on

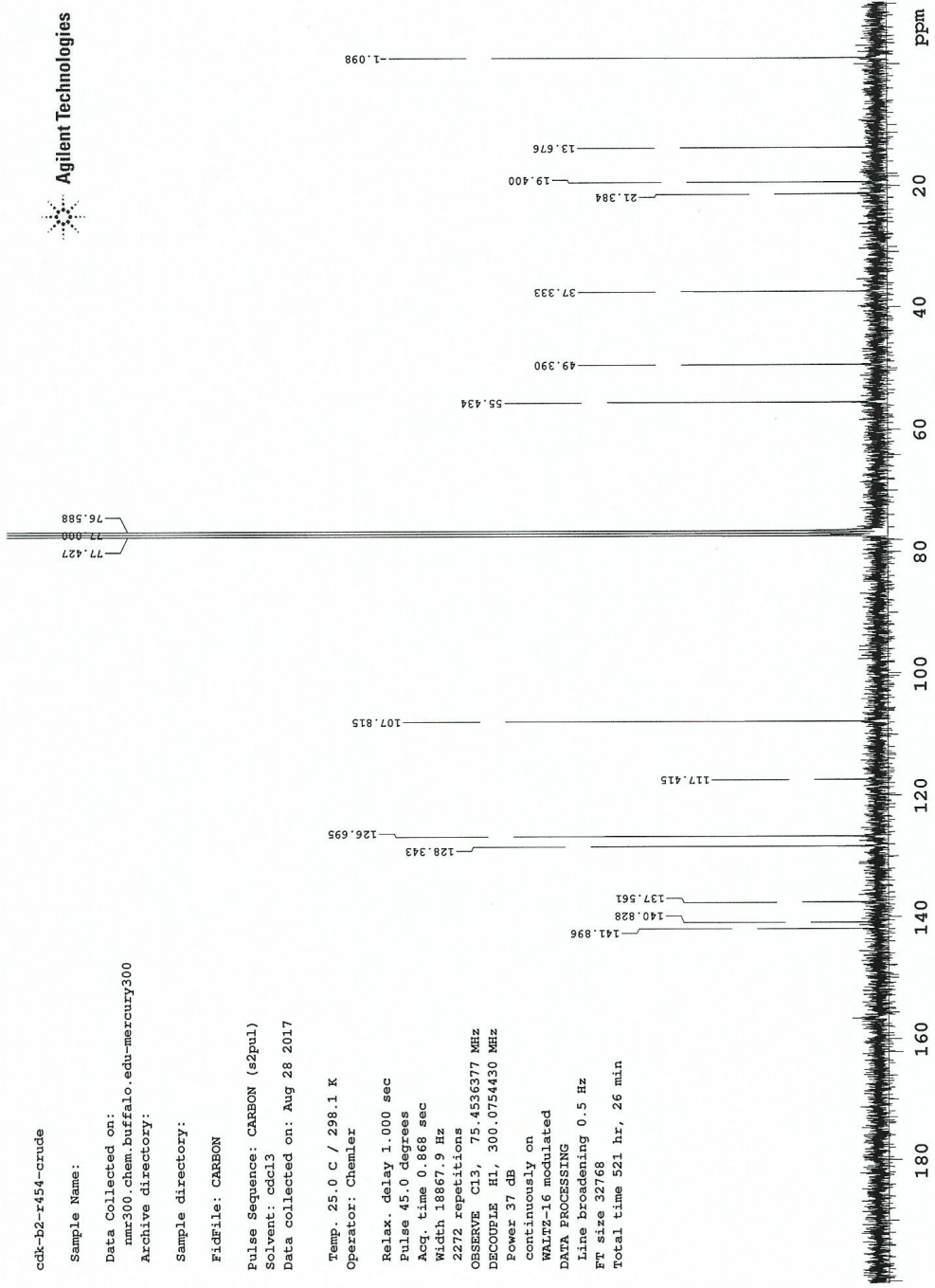
WALTZ-16 modulated

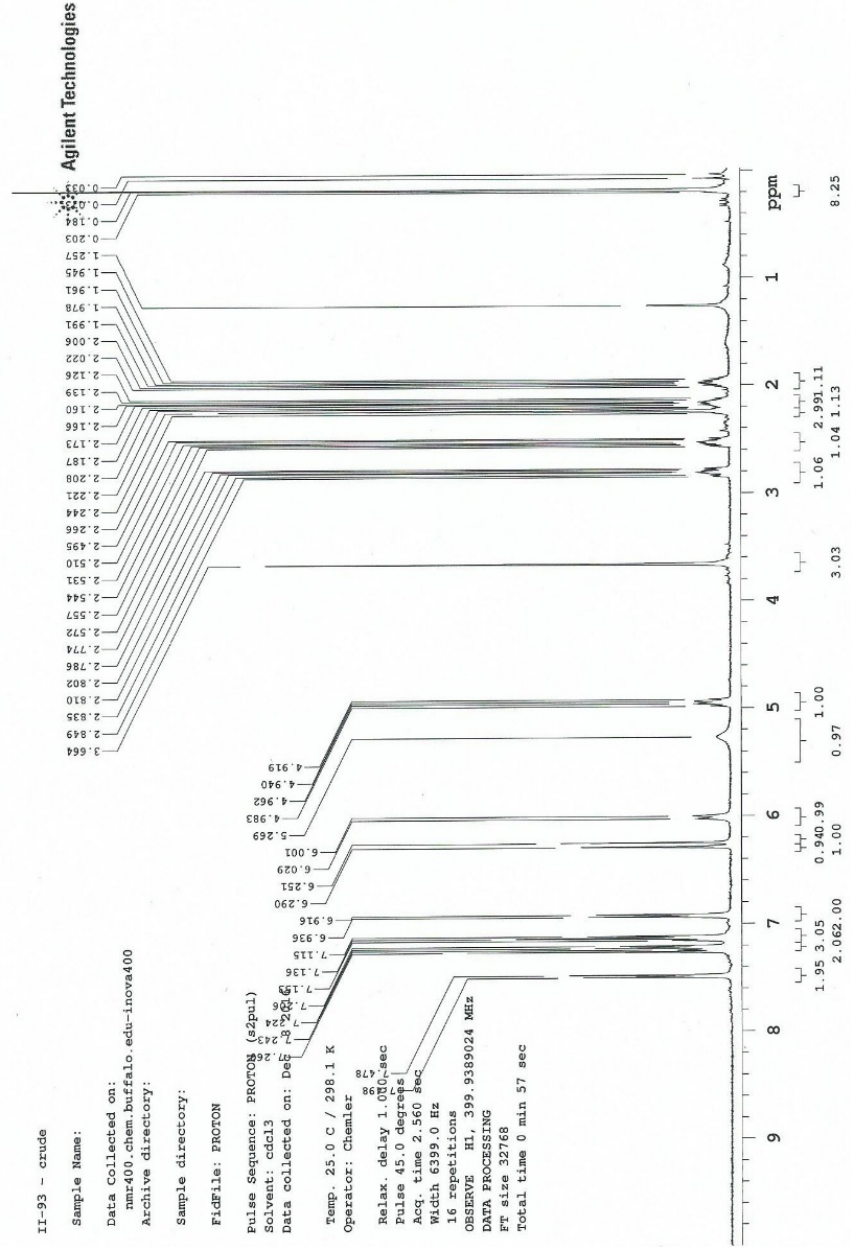
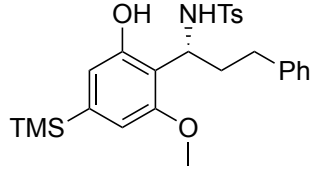
DATA PROCESSING

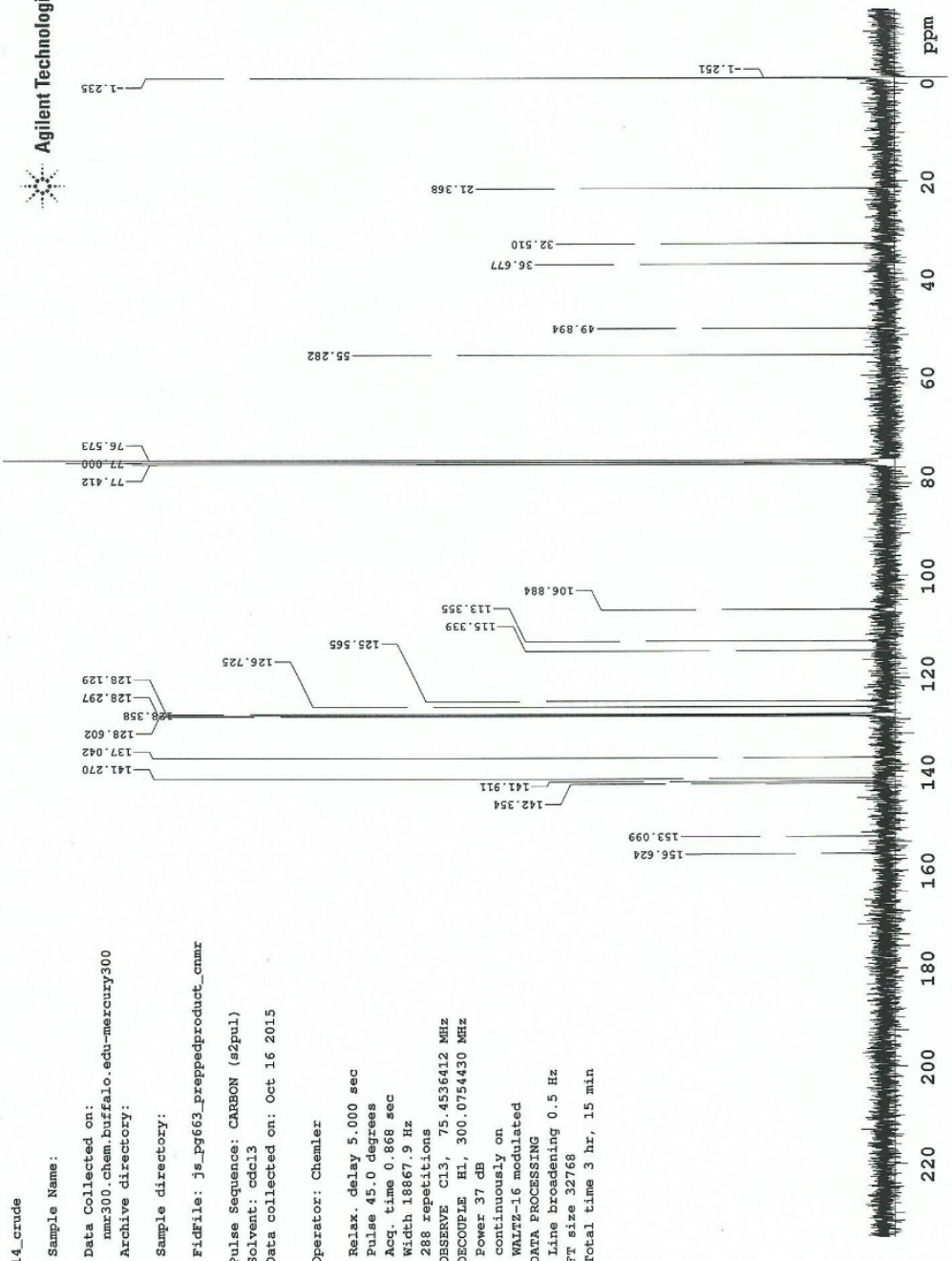
Line broadening 0.5 Hz

FT size 32768

Total time 521 hr, 26 min







14\_crude

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

Fidfile: js\_p9663\_preppedproduct\_cnmr

Pulse Sequence: CARBON (s2pul)

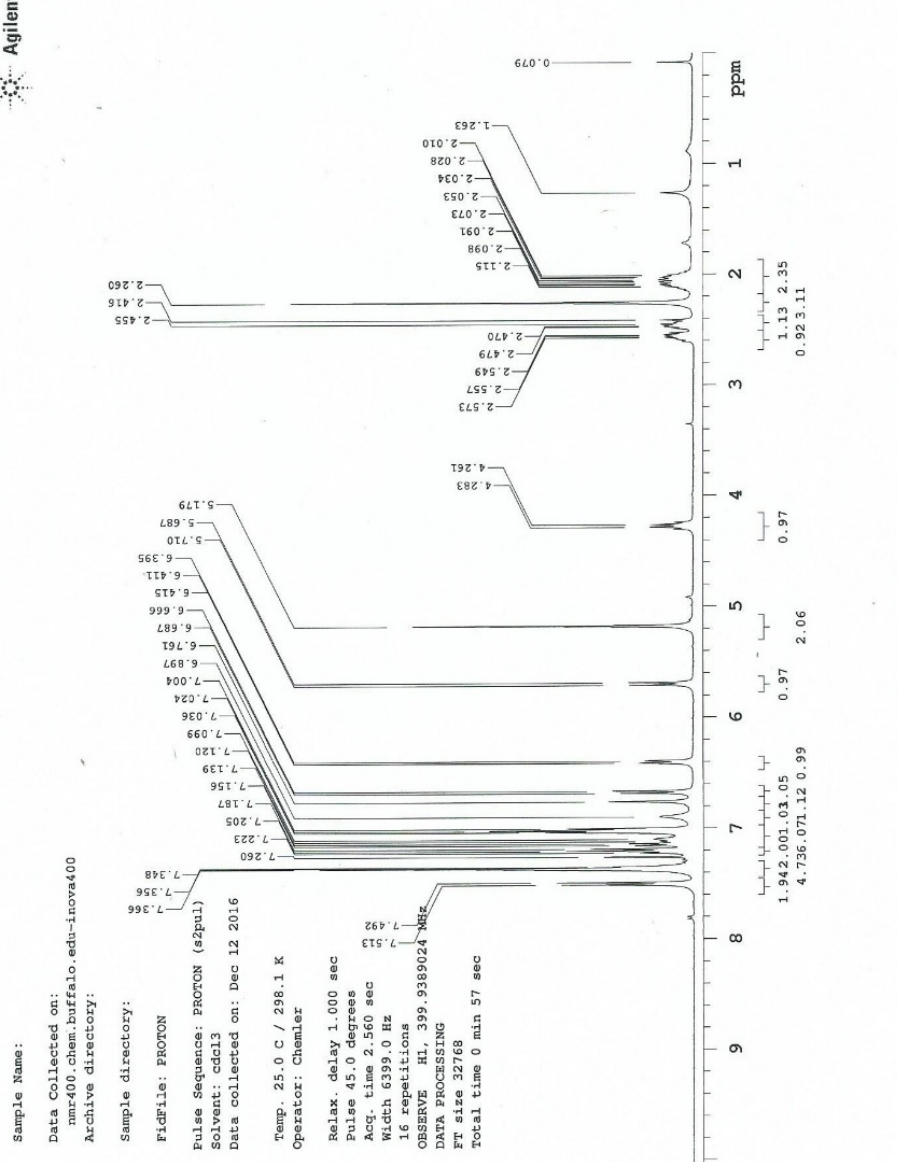
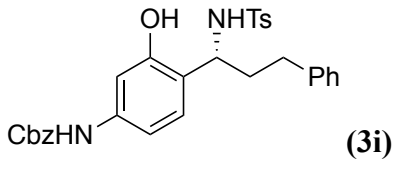
Solvent: cdcl3

Data collected on: Oct 16 2015

Operator: Chemler

Relax. delay 5.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
288 repetitions  
OBSERVE C13, 75.4536412 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 37 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 32768  
Total time 3 hr, 15 min





Sample Name:  
 Data Collected on:  
 nmr400.chem.buffalo.edu-inova400  
 Archive directory:  
 Sample directory:  
 F1: PROTON  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Dec 12 2016  
 Temp. 25.0 C / 298.1 K  
 Operator: Chemler  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.560 sec  
 Width 6399.0 Hz  
 16 repetitions  
 OBSERVE F1 399.9389024 MHz  
 DATA PROCESSING  
 FT size 32768  
 Total time 0 min 57 sec

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

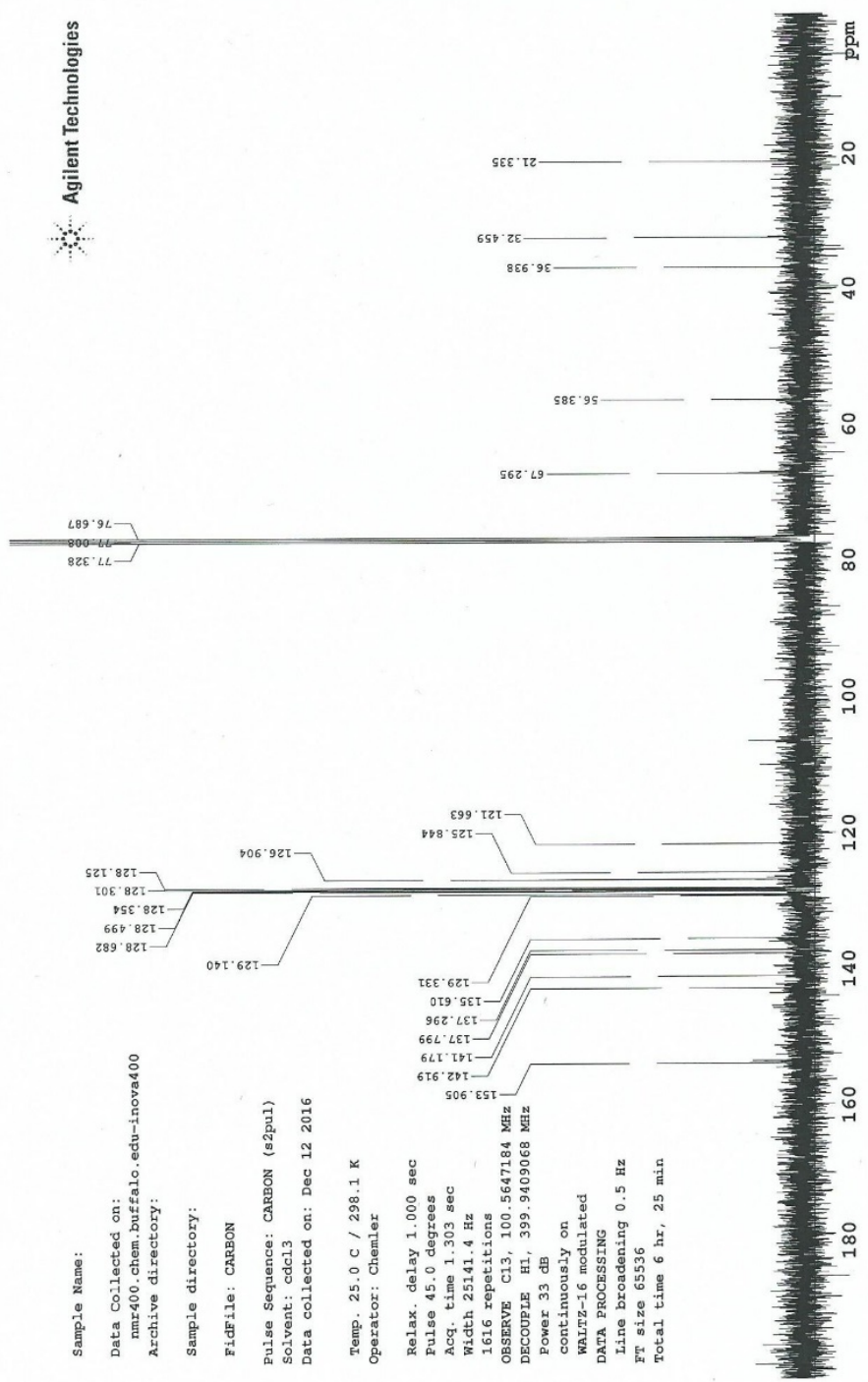
Sample directory:

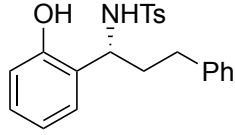
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 12 2016

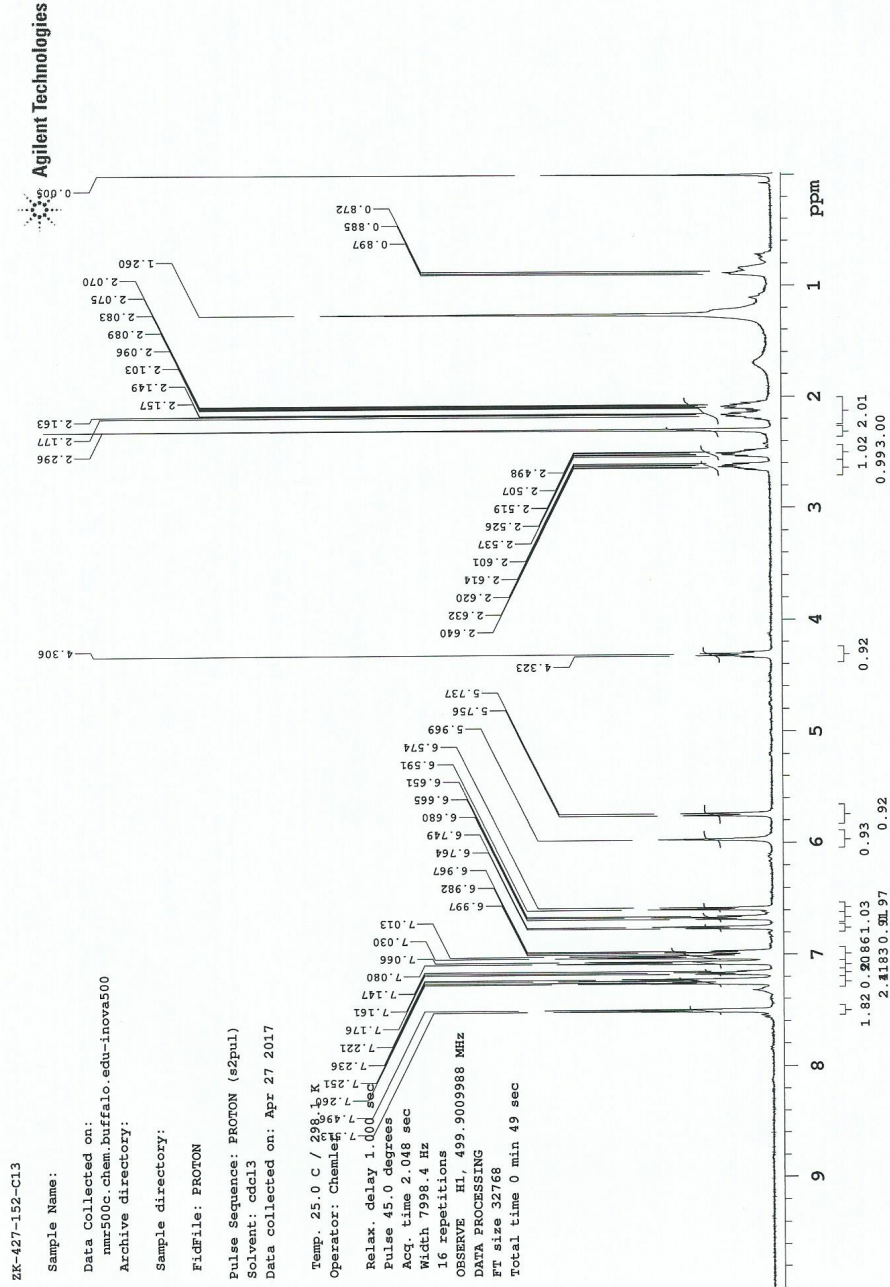
Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
1616 repetitions  
OBSERVE C13, 100.5647184 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 6 hr, 25 min





(3j)

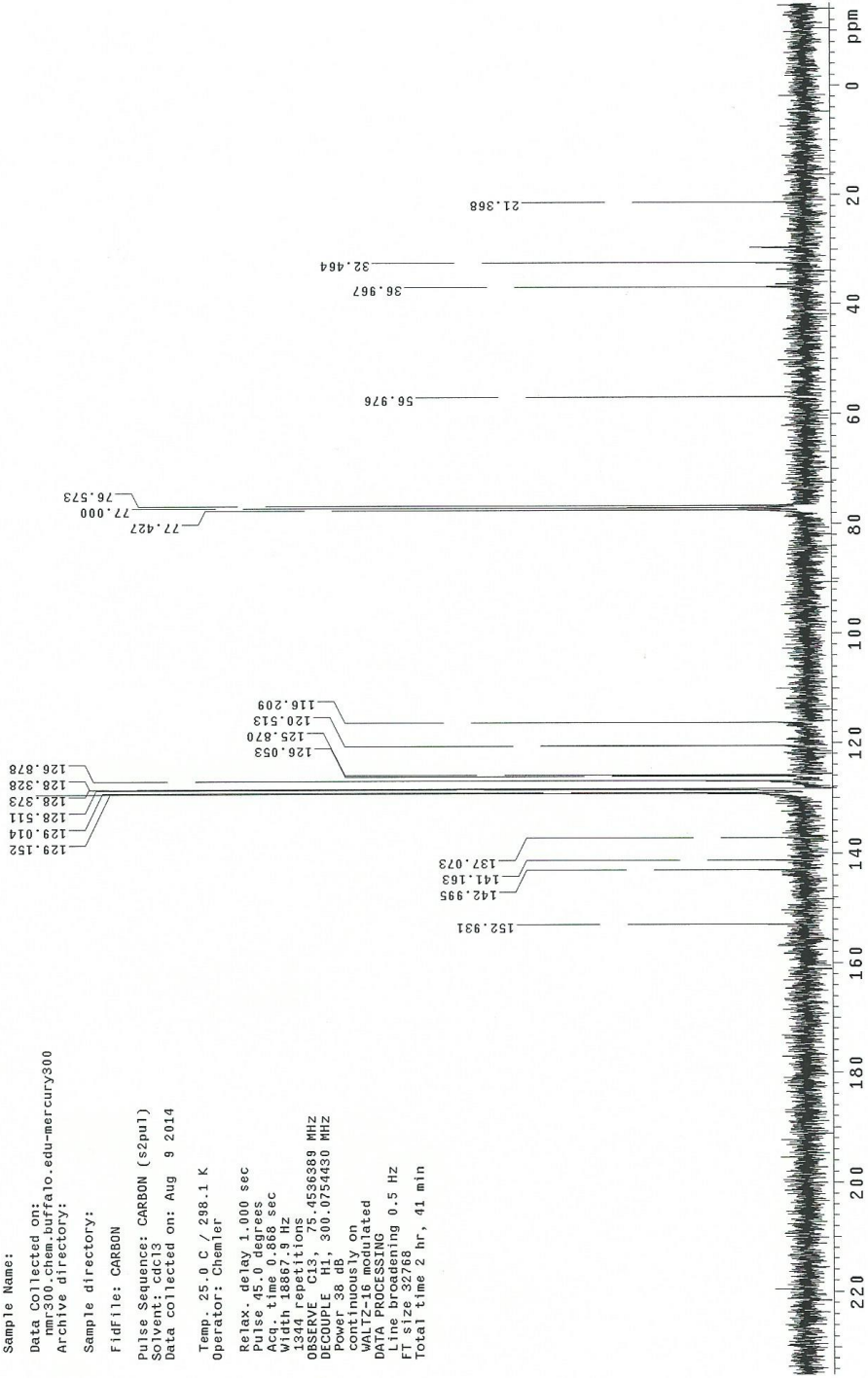


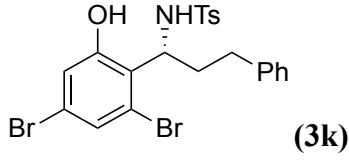
Dimethylphenol product

Sample Name:  
Data Collected on:  
Solvent:  
Archive directory:  
Sample directory:

FidFile: CARBON  
Pulse Sequence: CARBON (s2pul)  
Solvent: CCl3  
Data collected on: Aug 9 2014

Temp. 25.0 C / 298.1 K  
Operator: Chemier  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18897.9 Hz  
F1 - 101.625 MHz  
OBSERVE C13, 75.4536389 MHZ  
DECOUPLE H1, 300.0754430 MHZ  
Power 38 dB  
Continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
F1 - 101.625 MHz  
Total time 2 hr, 41 min





Agilent Technologies

cdk-b2-r354-product

Sample Name:

Data Collected on:  
 nmr300.chem.buffalo.edu-mercury300  
 Archive directory:

Sample directory:

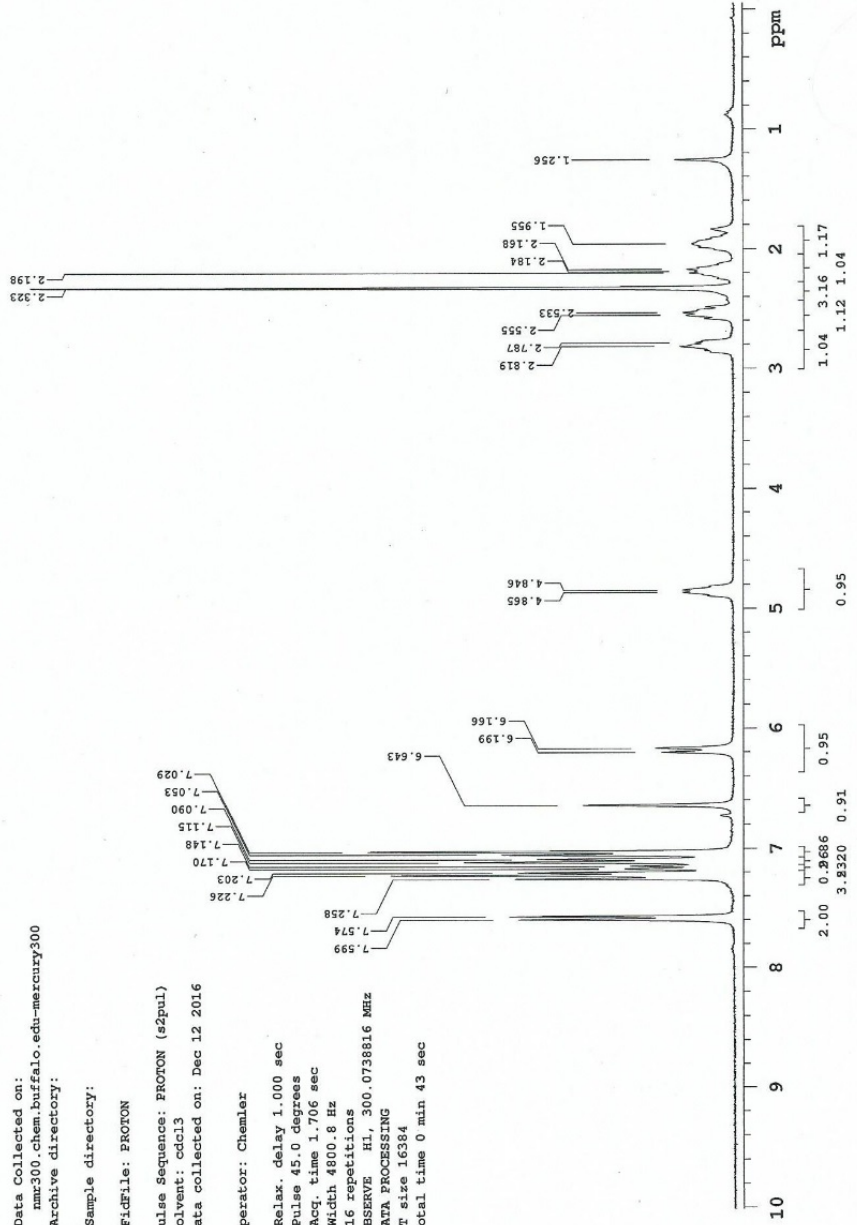
File: PROTON

Pulse Sequence: PROTON (s2pul)  
 Solvent: cdc13  
 Data collected on: Dec 12 2016

Operator: Chemler

Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.706 sec  
 Width 4800.8 Hz  
 16 repetitions

OBSERVE H1, 300.0738816 MHz  
 DATA PROCESSING  
 FT size 16384  
 Total time 0 min 43 sec





cdk-b2-r354-product

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Dec 12 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

2224 repetitions

OBSERVE C13, 75.4536377 MHz

DECOUPLE H1, 300.0754430 MHz

Power 37 dB

continuously on

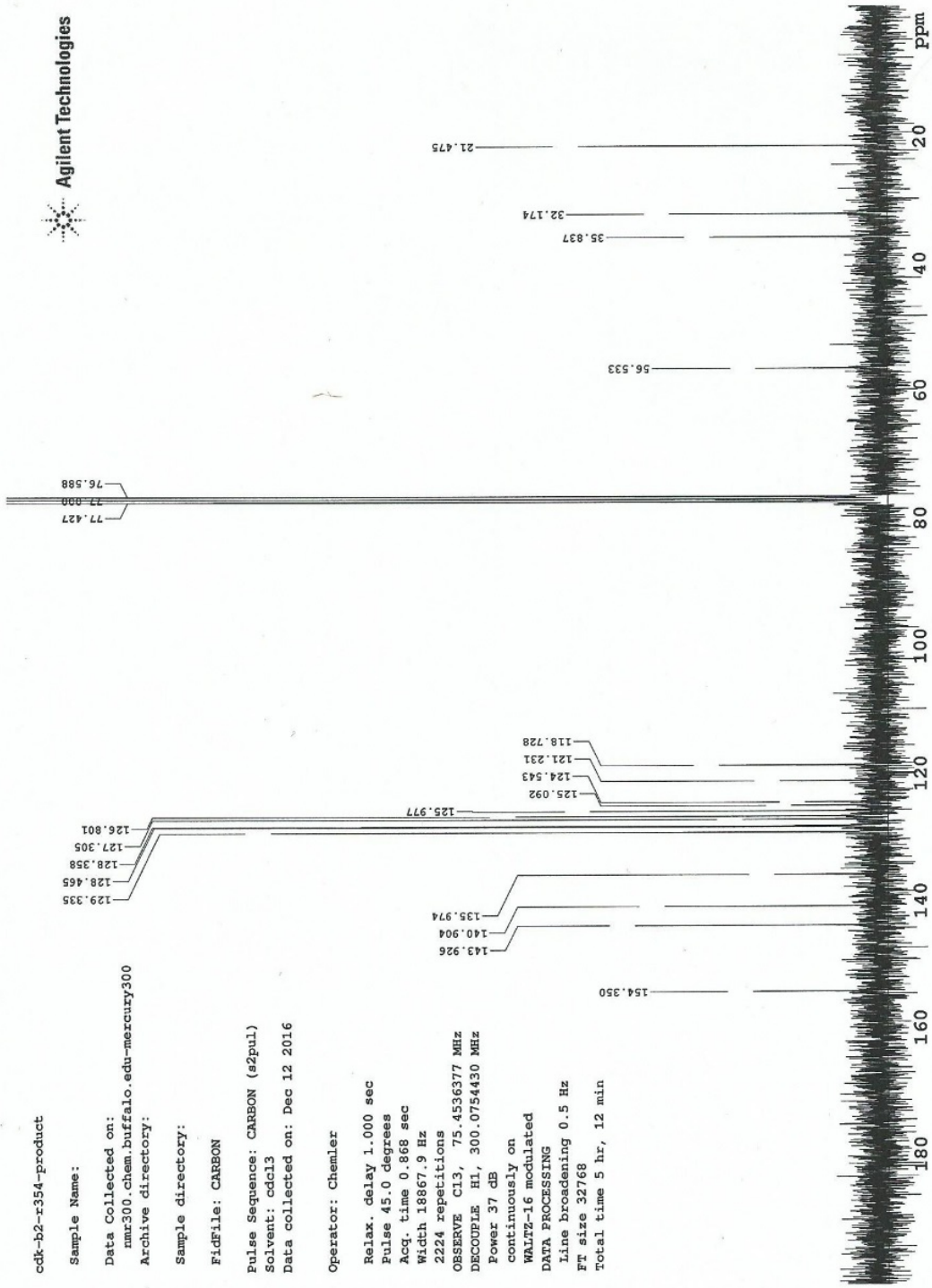
WALTZ-16 modulated

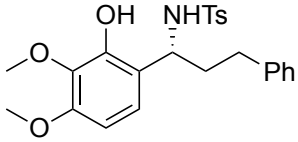
DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 5 hr, 12 min





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Agilent Technologies

RP\_Copper\_Recovered\_Stille\_2

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury-000

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 4 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

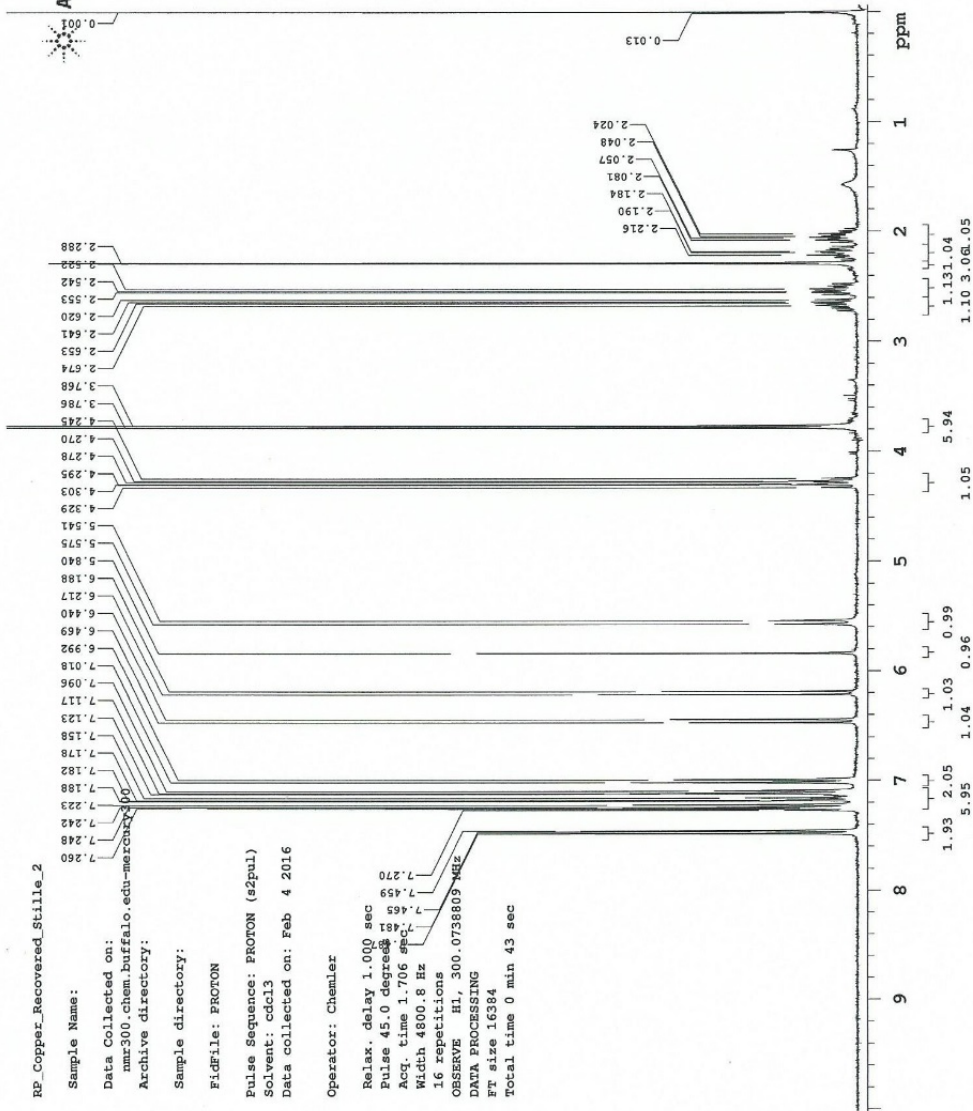
16 repetitions

OBSERVE H1, 300.0738809 MHz

DATA PROCESSING

Ff size 16384

Total time 0 min 43 sec



RP\_Copper\_Recovered\_Stille\_2

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

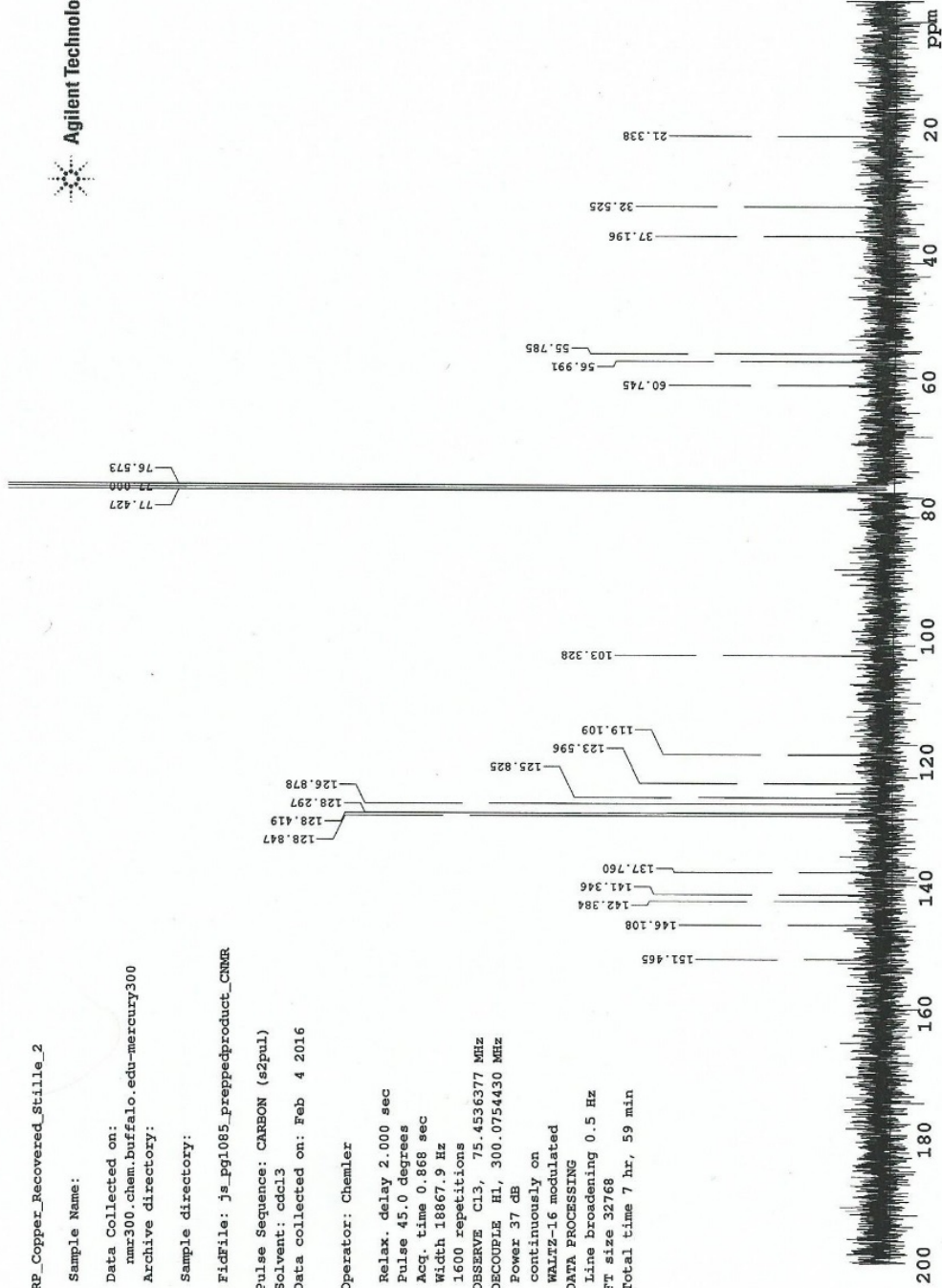
Fidfile: js\_pg1065\_preppedproduct\_CNMR

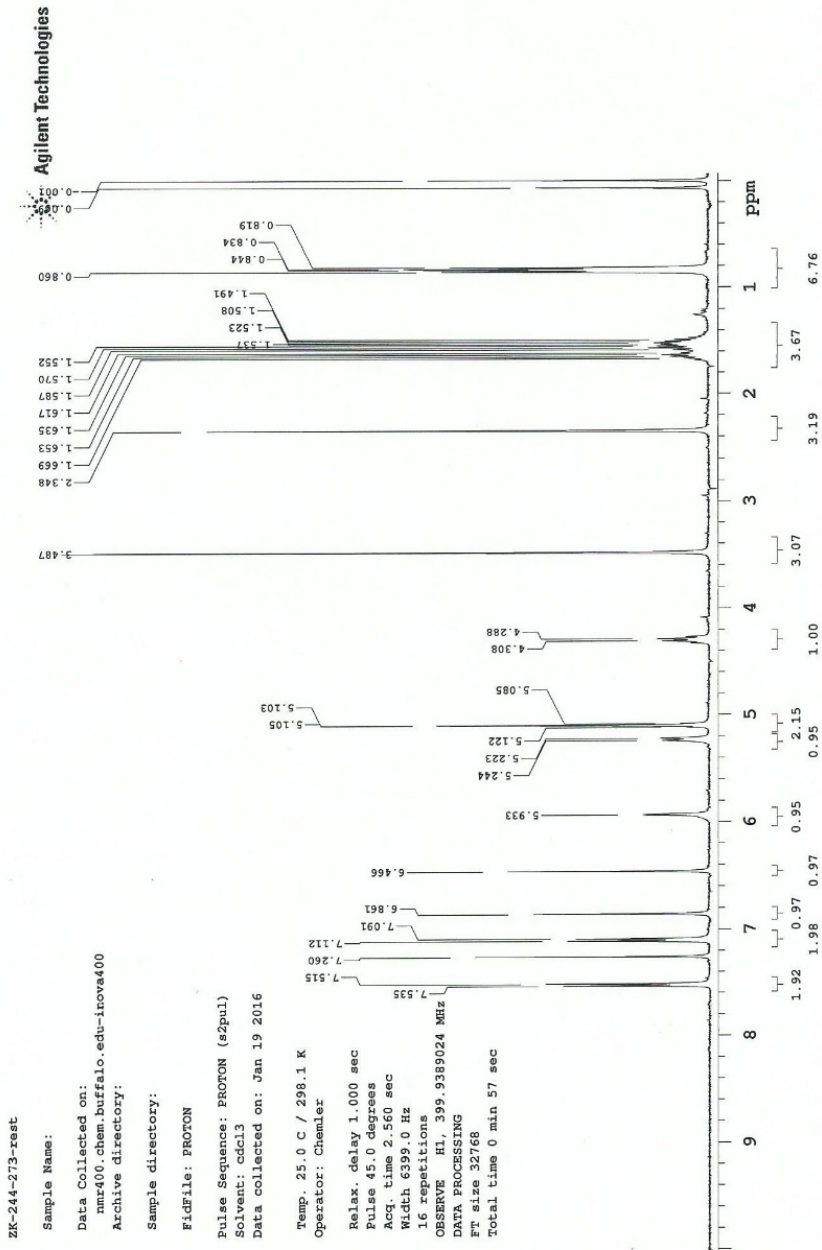
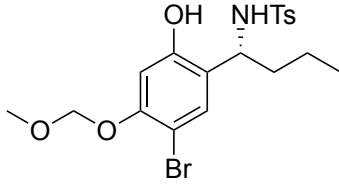
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 4 2016

Operator: Chemler

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 0.866 sec  
Width 18867.9 Hz  
1600 repetitions  
OBSERVE C13, 75.4536377 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 37 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 7 hr, 59 min

Agilent Technologies





SD-BI-p-279--stille-NHSO2Ar--gramscale-crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

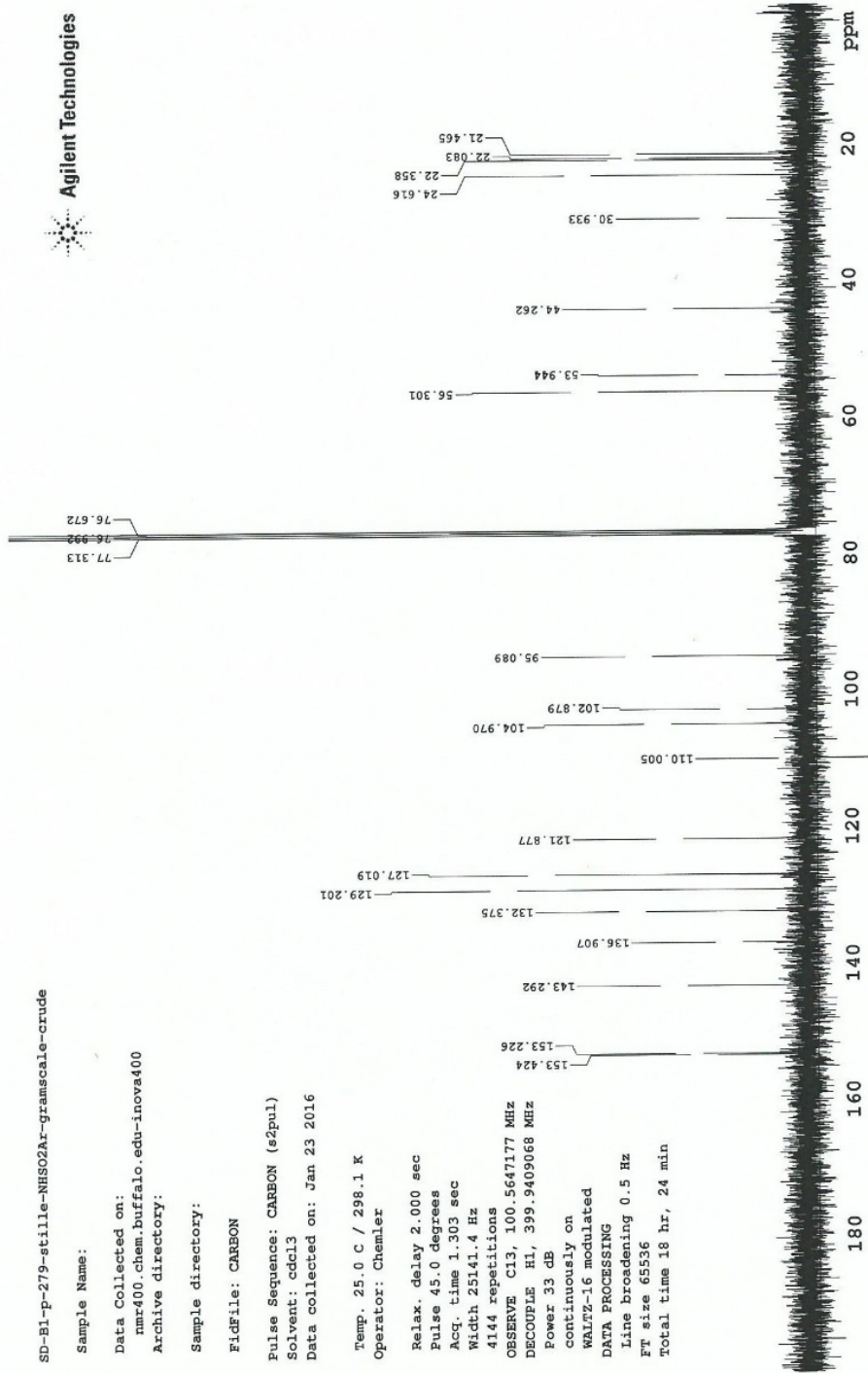
FIDFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 23 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
4144 repetitions  
OBSERVE C13, 100.5647177 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 18 hr, 24 min

Agilent Technologies







EB161-39

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3

Data collected on: Dec 15 2016

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

704 repetitions

OBSERVE c13, 100.5647207 MHz

DECOUPLE h1, 399.9409068 MHz

Power 33 dB

continuously on

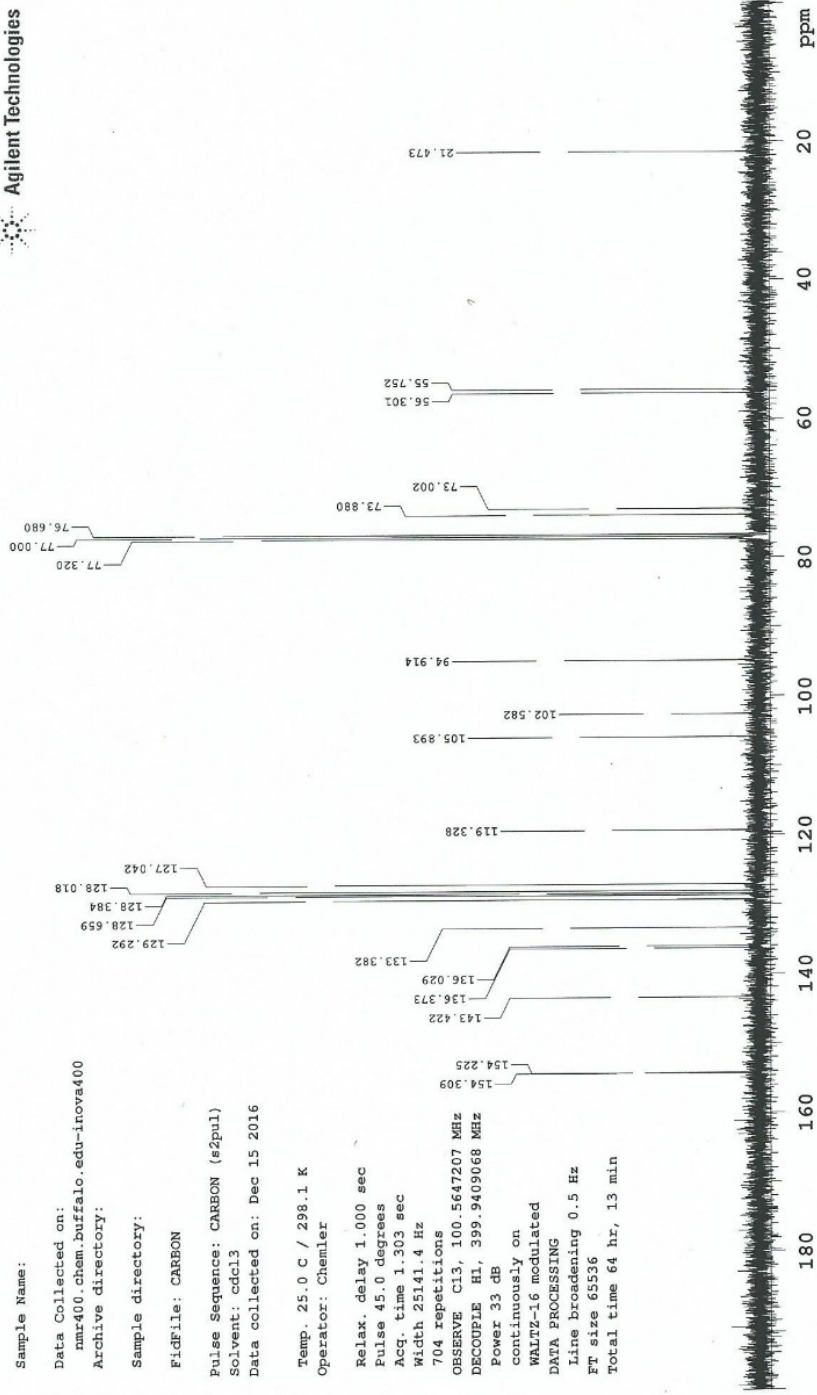
WALTZ-16 modulated

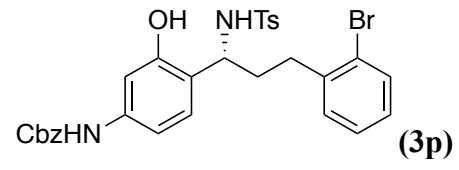
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 64 hr, 13 min



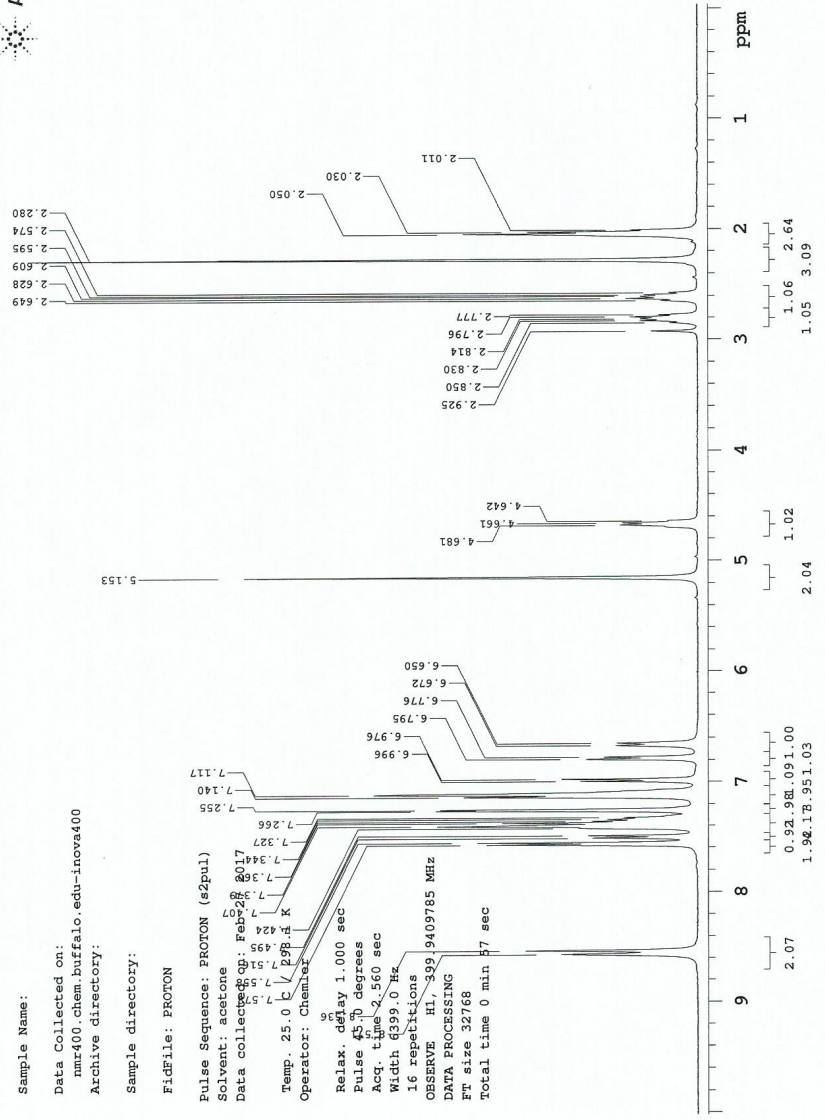


b5-R--4Br-s-tBuBox-110-crude

Sample Name:  
 Data Collected on:  
 nmr400.chem.buffalo.edu-inova400  
 Archive directory:

Sample directory:  
 FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
 Solvent: acetone  
 Data collected on: Feb 20 2007  
 Time: 12:45  
 Temp: 25.0 C / 77.0 K  
 Operator: Chemist  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.560 sec  
 Width 6399.0 Hz  
 16 repetitions  
 OBSERVE H1 399.9409785 MHz  
 DATA PROCESSING  
 Ft size 32768  
 Total time 0 min 57 sec



b5-R-4Br-s-tBuBox-110-crude

Sample Name:

Data Collected on:

nmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: acetone

Data collected on: Feb 27 2017

Temp. 25.0 C / 298.1 K

Operator: Chemlet

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

768 repetitions

OBSERVE C13, 100.5651464 MHz

DECOUPLE H1, 399.9429825 MHz

Power 33 dB

continuously on

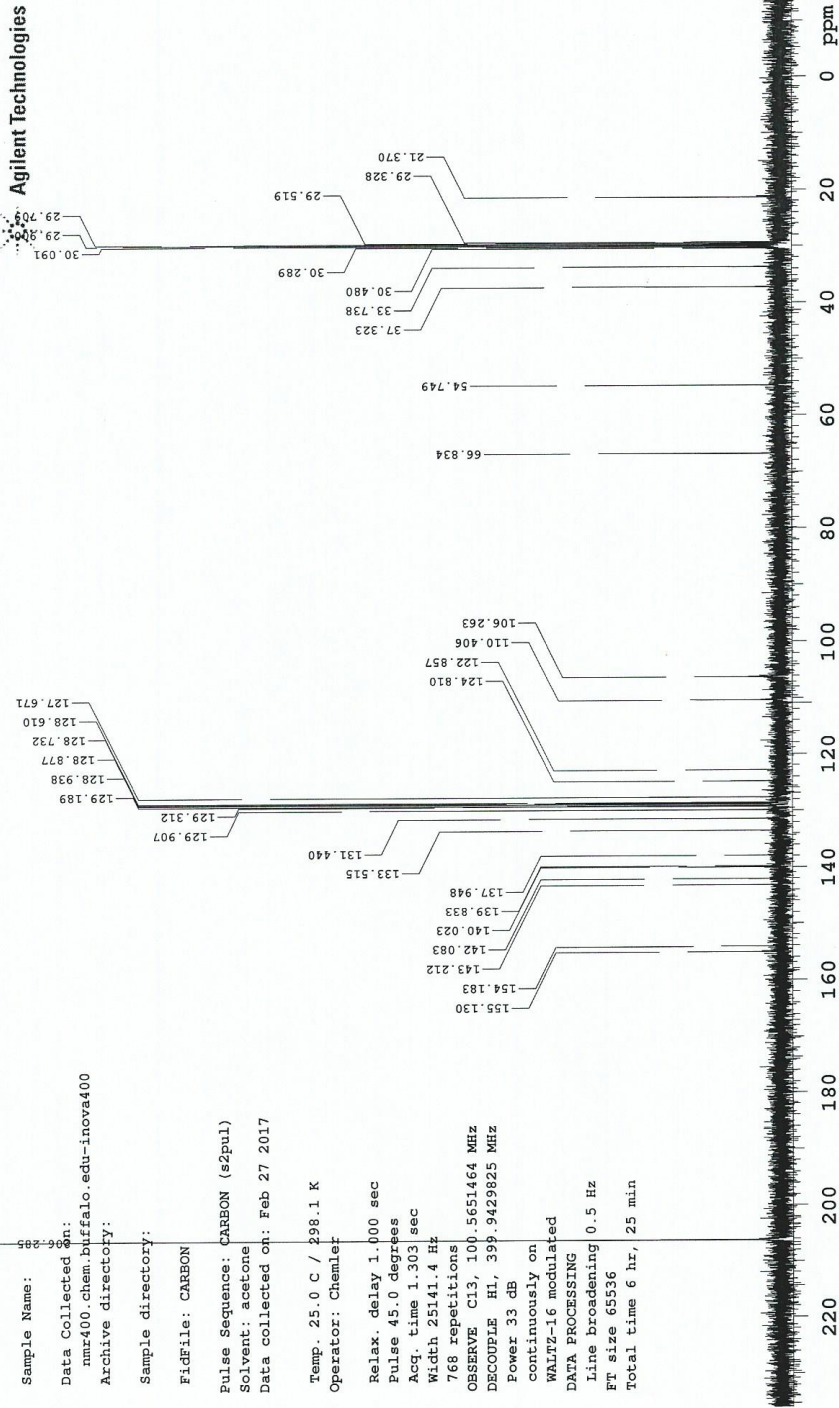
WALTZ-16 modulated

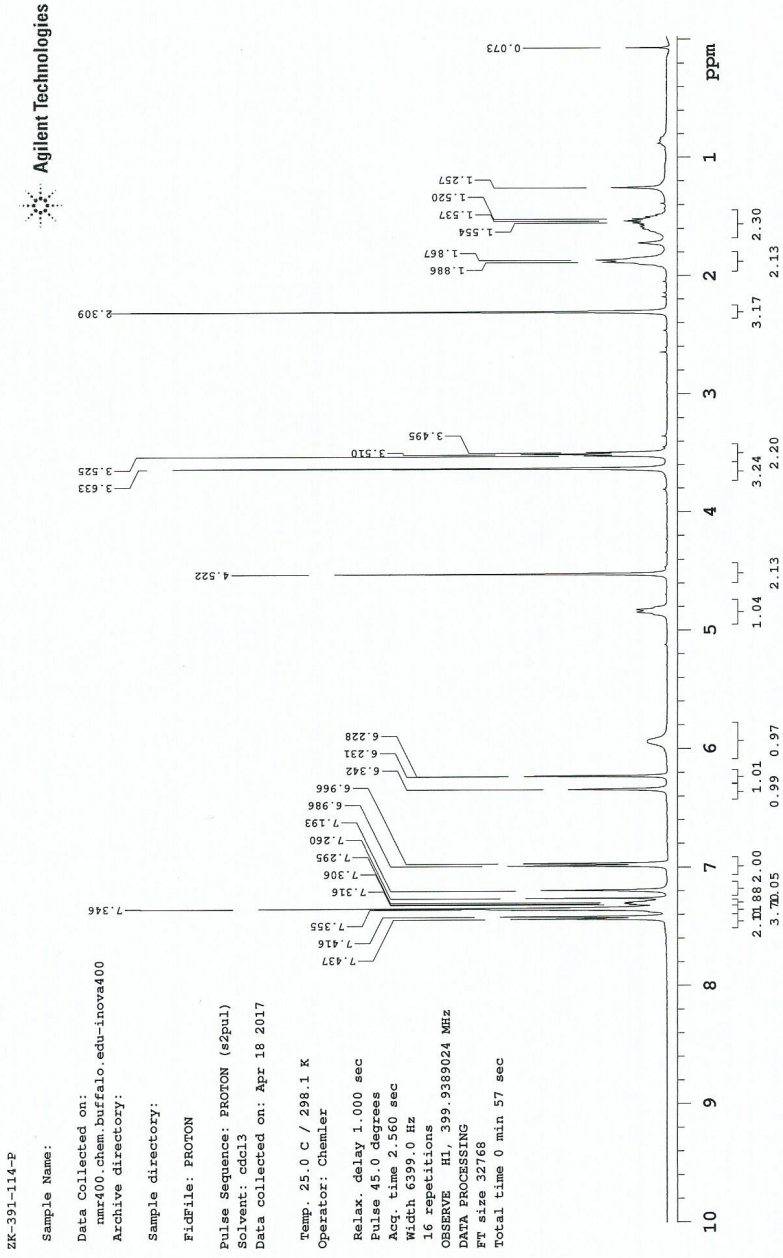
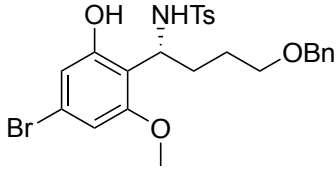
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 6 hr, 25 min







ZK-391-114-P

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

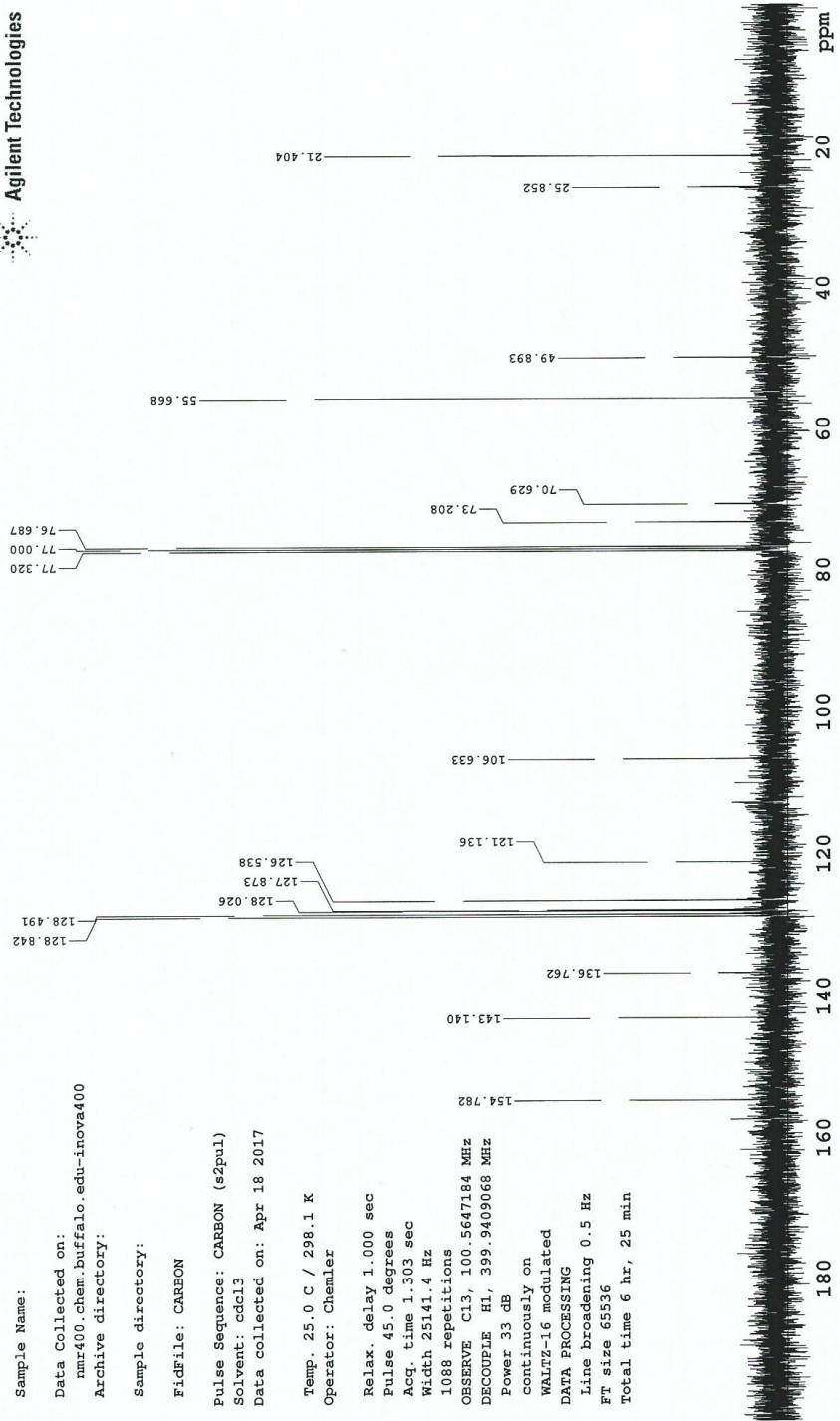
Fidfile: CARBON

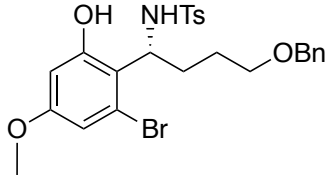
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 18 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz

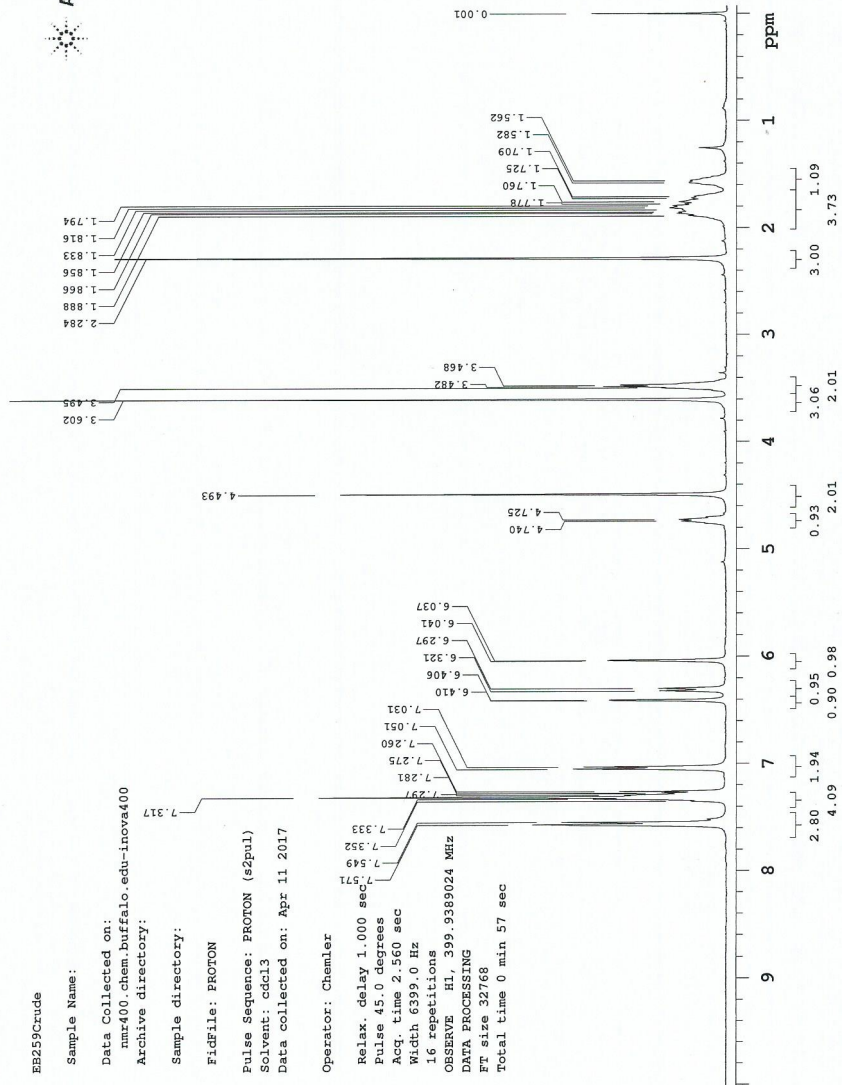
1088 repetitions  
OBSERVE CL3, 100.5647184 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 6 hr, 25 min





(3q<sub>2</sub>)

Agilent Technologies



EB259Crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

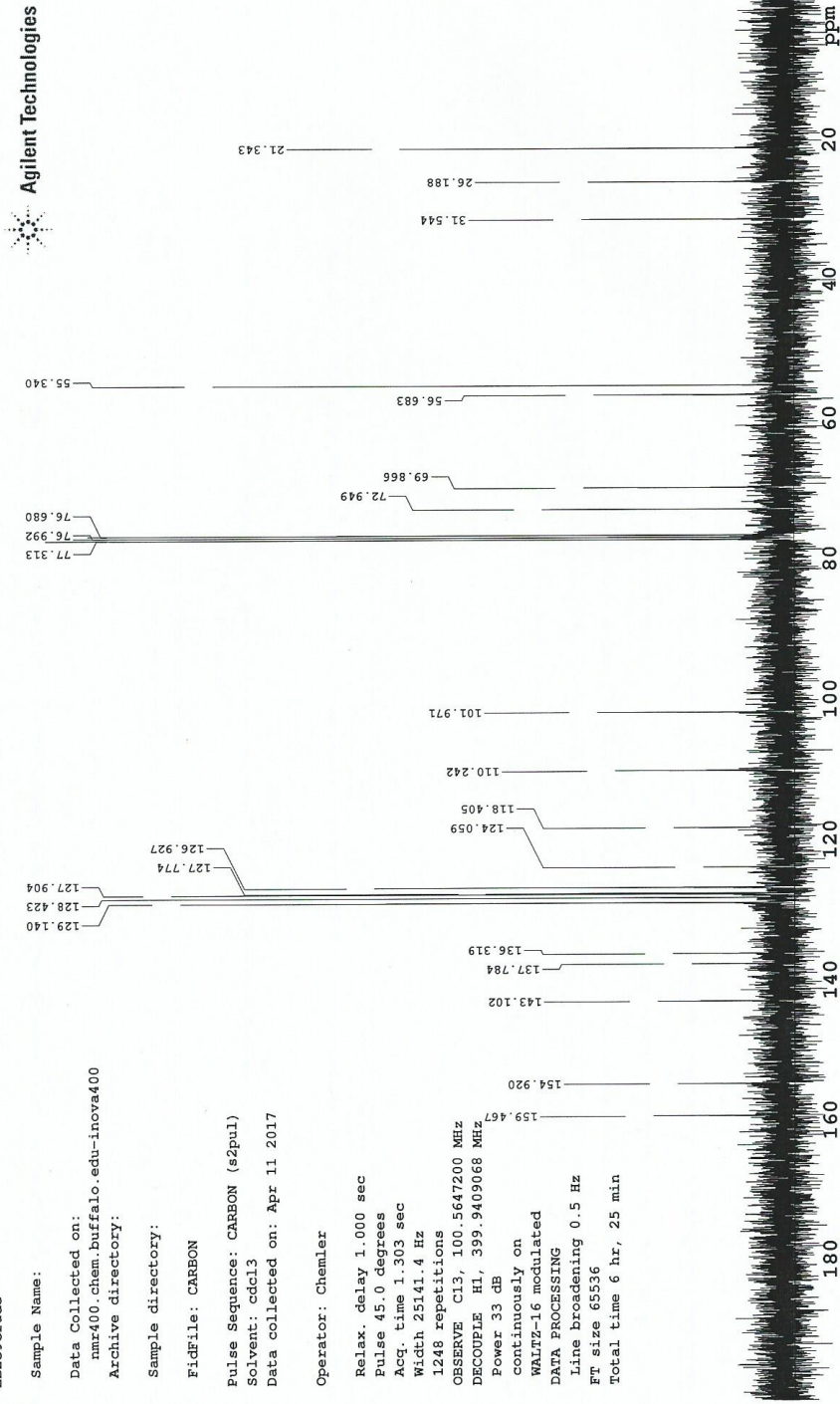
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 11 2017

Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
1248 repetitions  
OBSERVE C13, 100.5647200 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 6 hr, 25 min



ZK-575-100-C

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

Ficfile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 14 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

16 repetitions

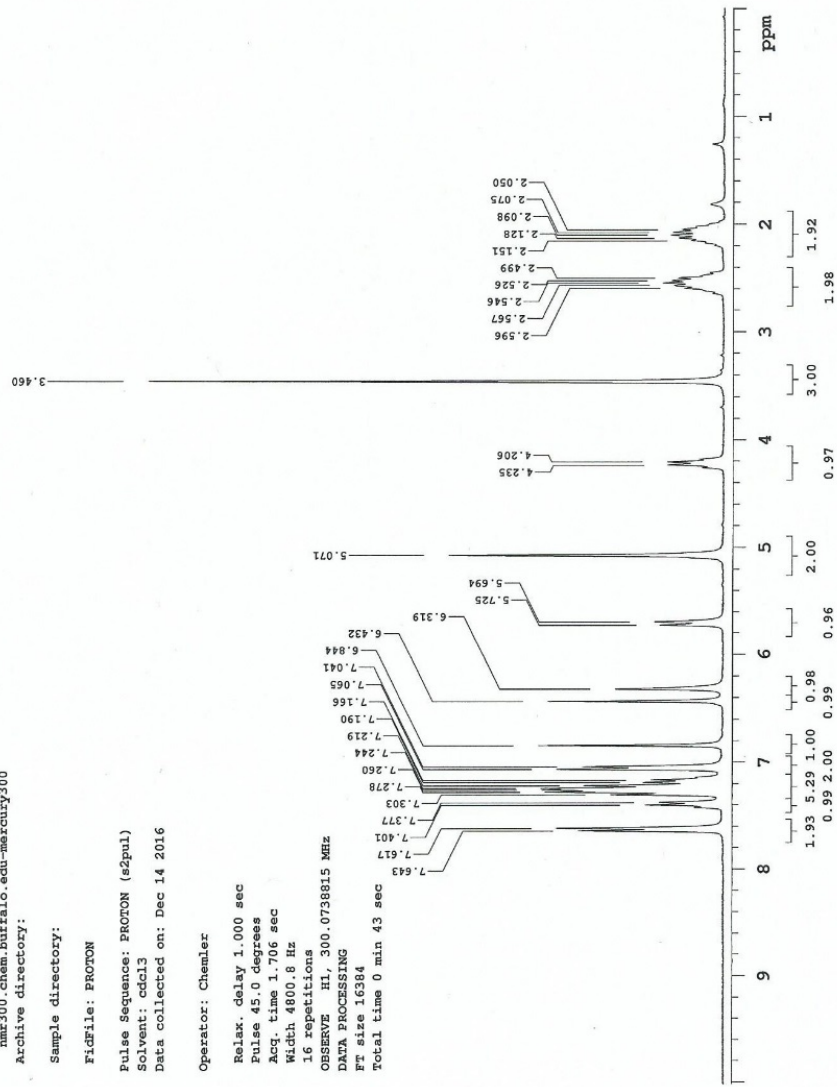
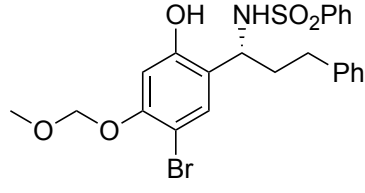
OSERVE HI, 300.0738815 MHz

DATA PROCESSING

FF size 16384

Total time 0 min 43 sec

Agilent Technologies



ZK-375-100-C

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Dec 14 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

832 repetitions

OBSERVE C13, 75.4536389 MHz

DECOUPLE H1, 300.0754430 MHz

Power 37 dB

continuously on

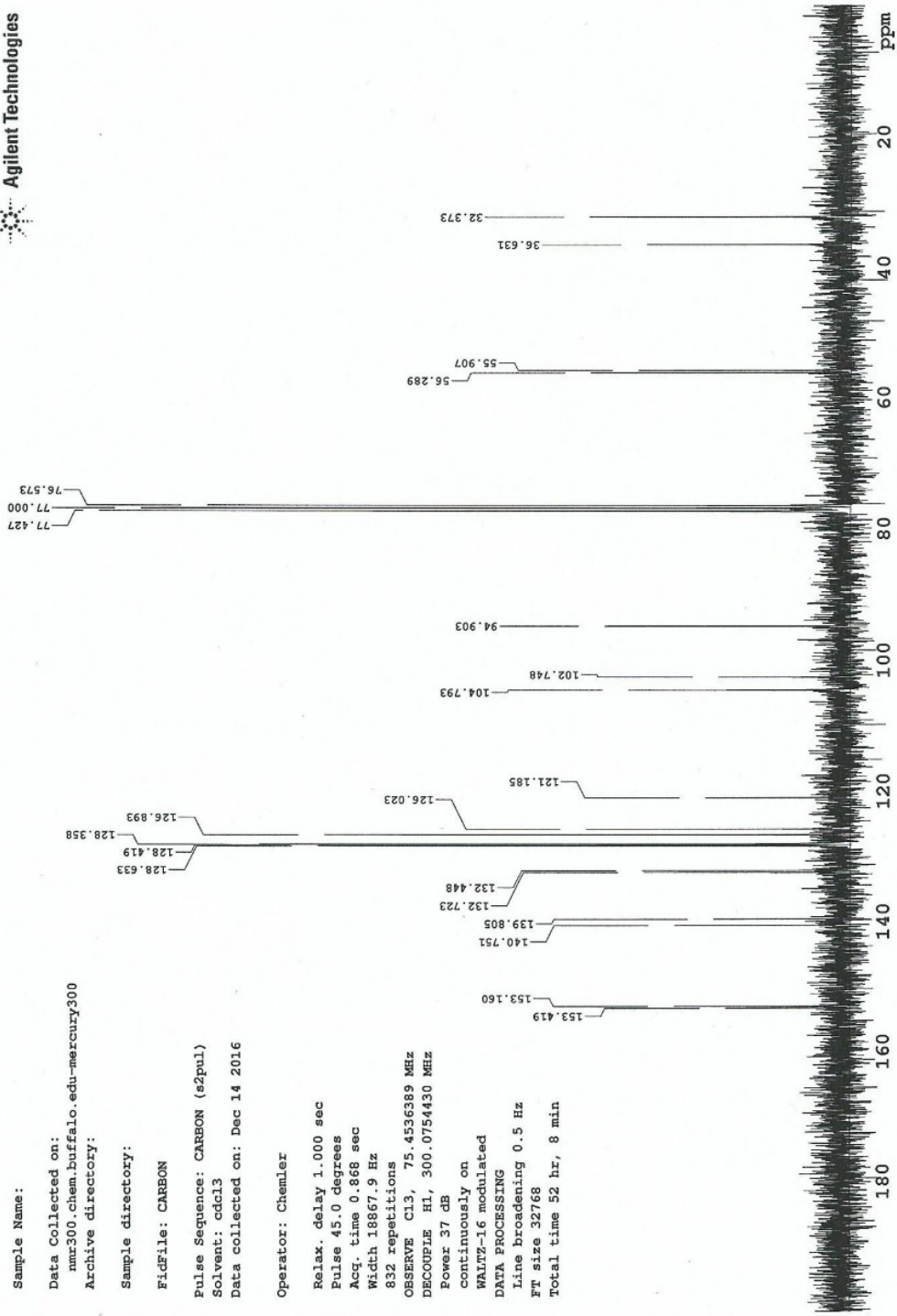
WALTZ-16 modulated

DATA PROCESSING

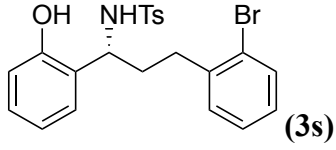
Line broadening 0.5 Hz

Ft size 32768

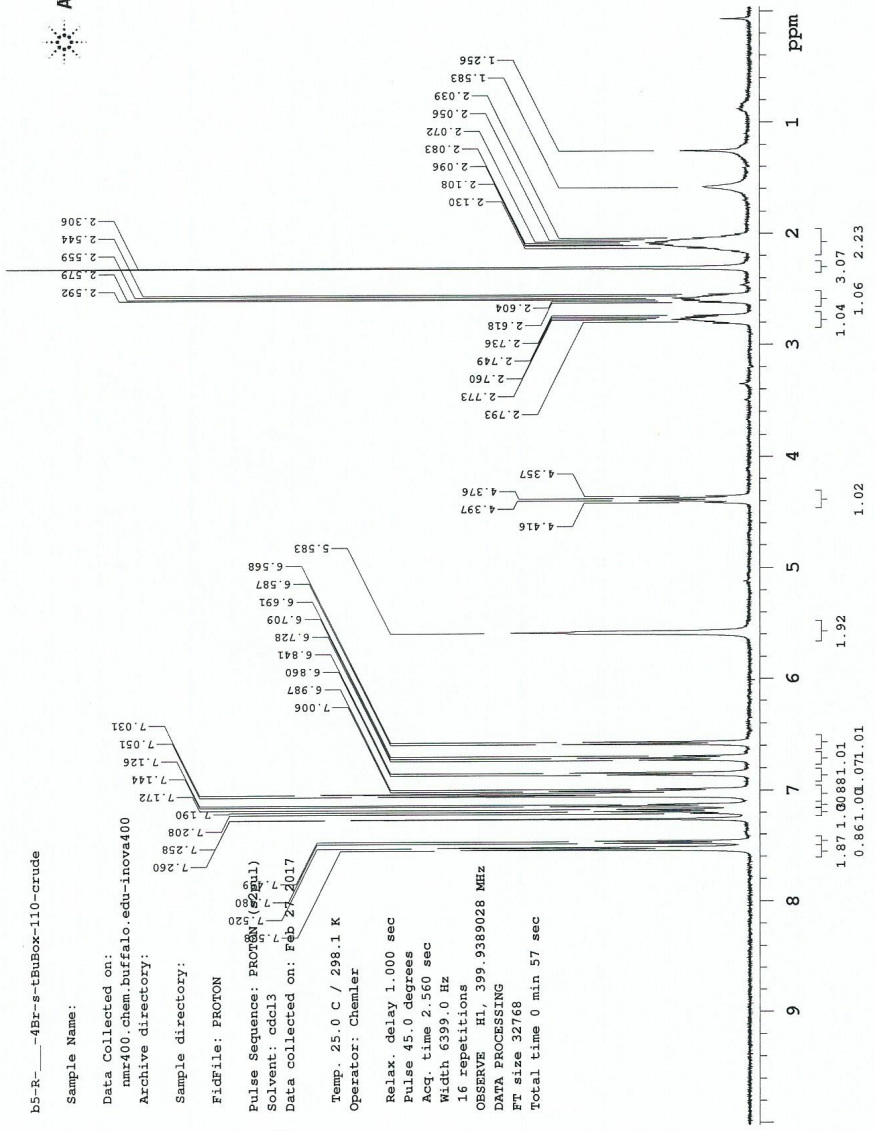
Total time 52 hr, 8 min







Agilent Technologies



b5-R-4Br-s-tBuBox-110-crude  
 Sample Name:  
 Data Collected on: nmr400.chem.buffalo.edu-incova400  
 Archive directory:  
 Sample directory:  
 File: PROTON  
 Pulse Sequence: PROTON (zgpg30)  
 Solvent: cdcl3  
 Data collected on: Feb 27 2017  
 Temp. 25.0 C / 298.1 K  
 Operator: Chemler  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.560 sec  
 Width 6399.0 Hz  
 16 repetitions  
 OBSERVE H1 399.9389028 MHz  
 DATA PROCESSING  
 F1 size 32768  
 Total time 0 min 57 sec

b5-R-4Br-s-tBuBox-110-crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

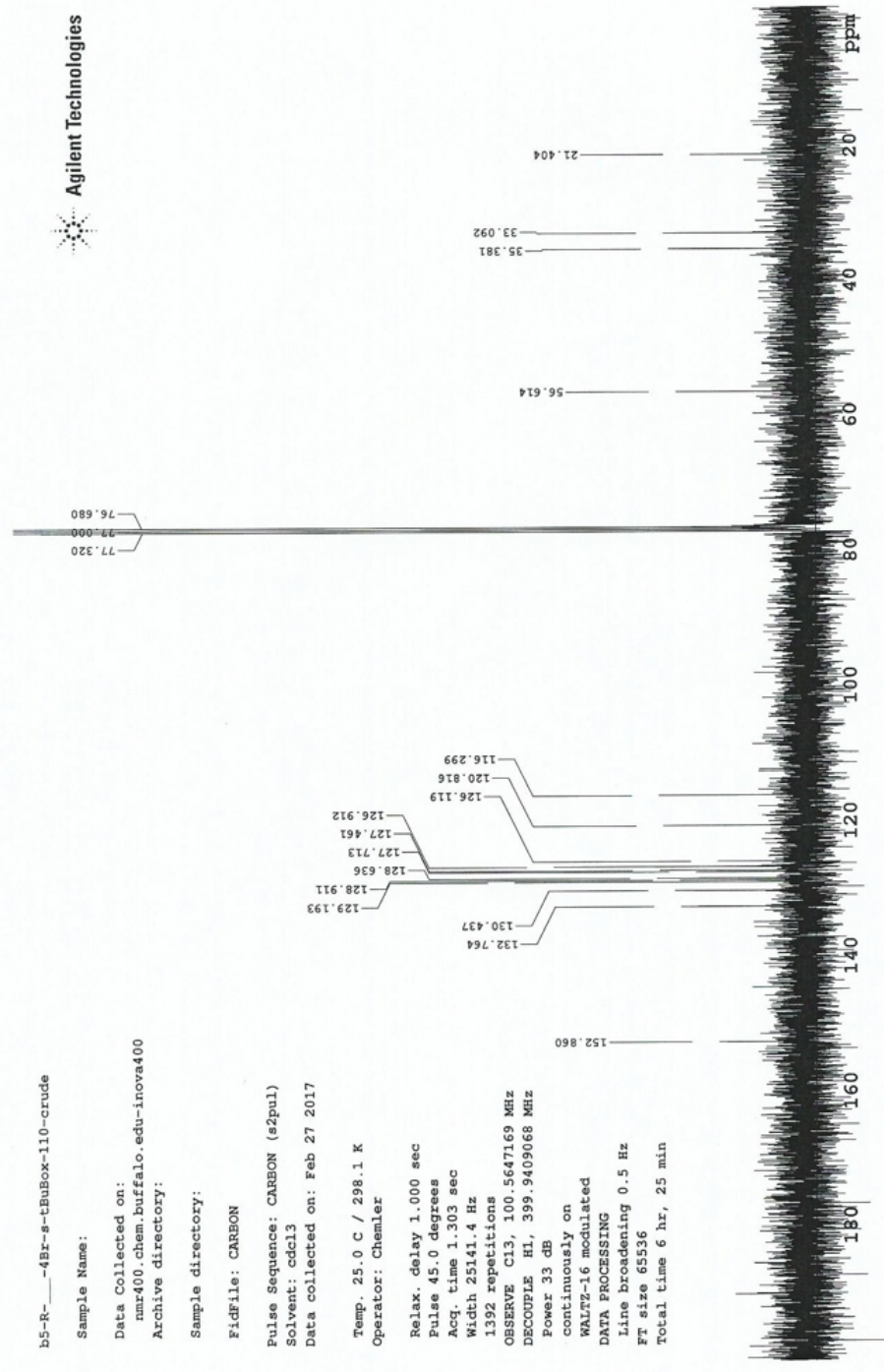
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 27 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
1392 repetitions  
OBSERVE C13, 100.5647169 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB

continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 6 hr, 25 min



EE161-39

Sample Name:

Data Collected on:  
nmr-400.chem.buffalo.edu-inova400  
Archive directory:

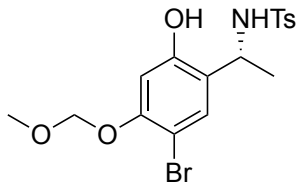
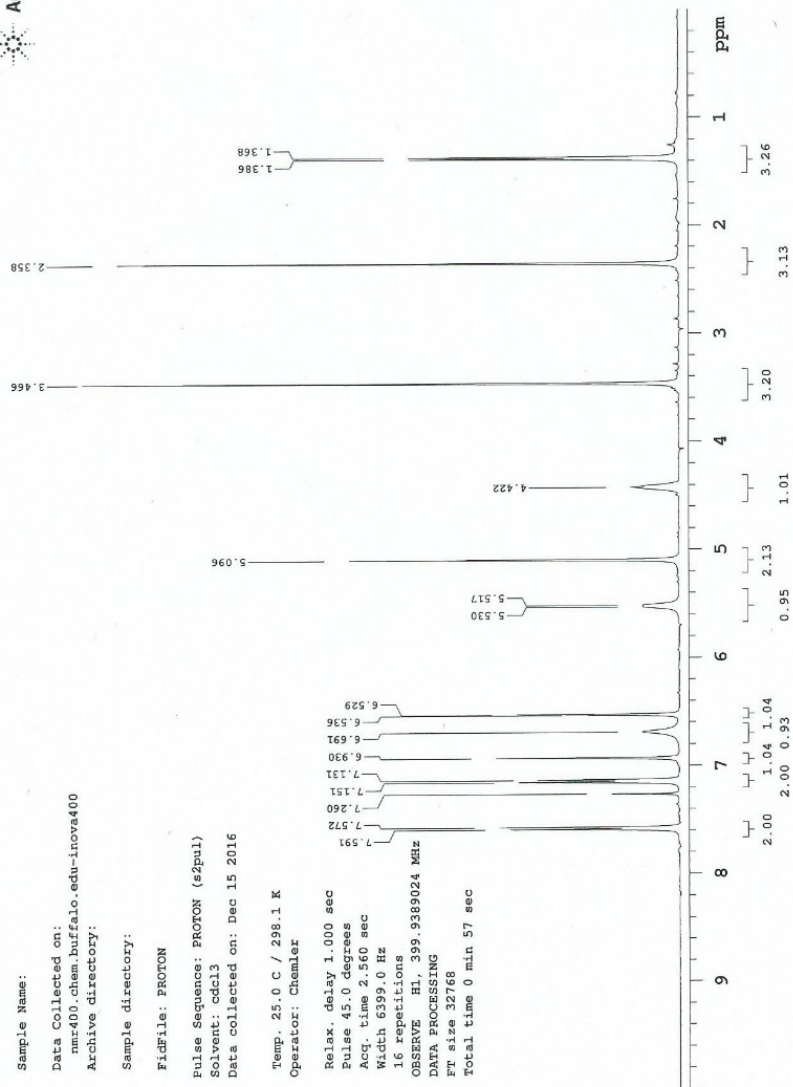
Sample directory:

File: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 15 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.560 sec  
Width 6399.0 Hz  
16 repetitions  
OBSERVE H1, 399.9389024 MHz  
DATA PROCESSING  
Ft size 32768  
Total time 0 min 57 sec



EB161-39

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

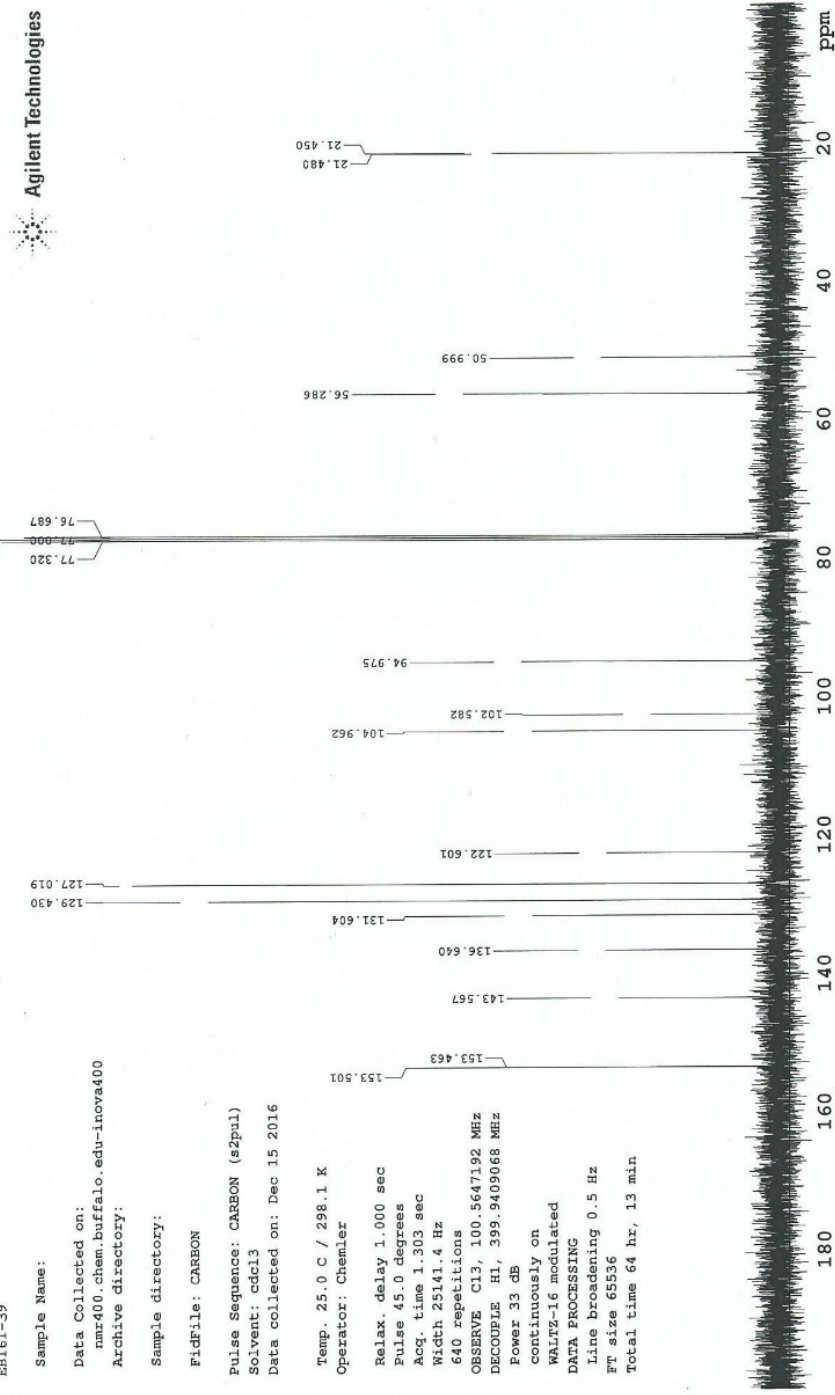
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 15 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
640 repetitions  
OBSERVE C13, 100.5647192 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 64 hr, 13 min







ZK-423-148-P

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

File: CARBON

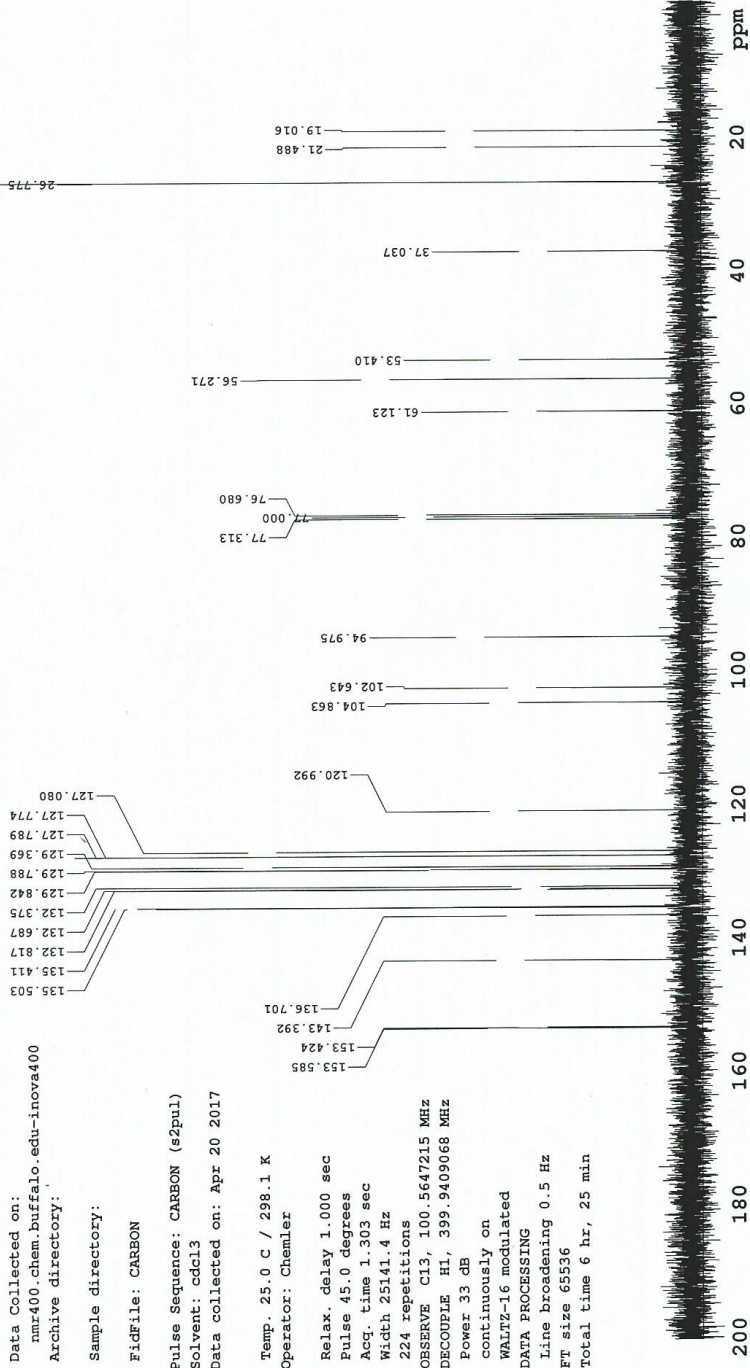
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 20 2017

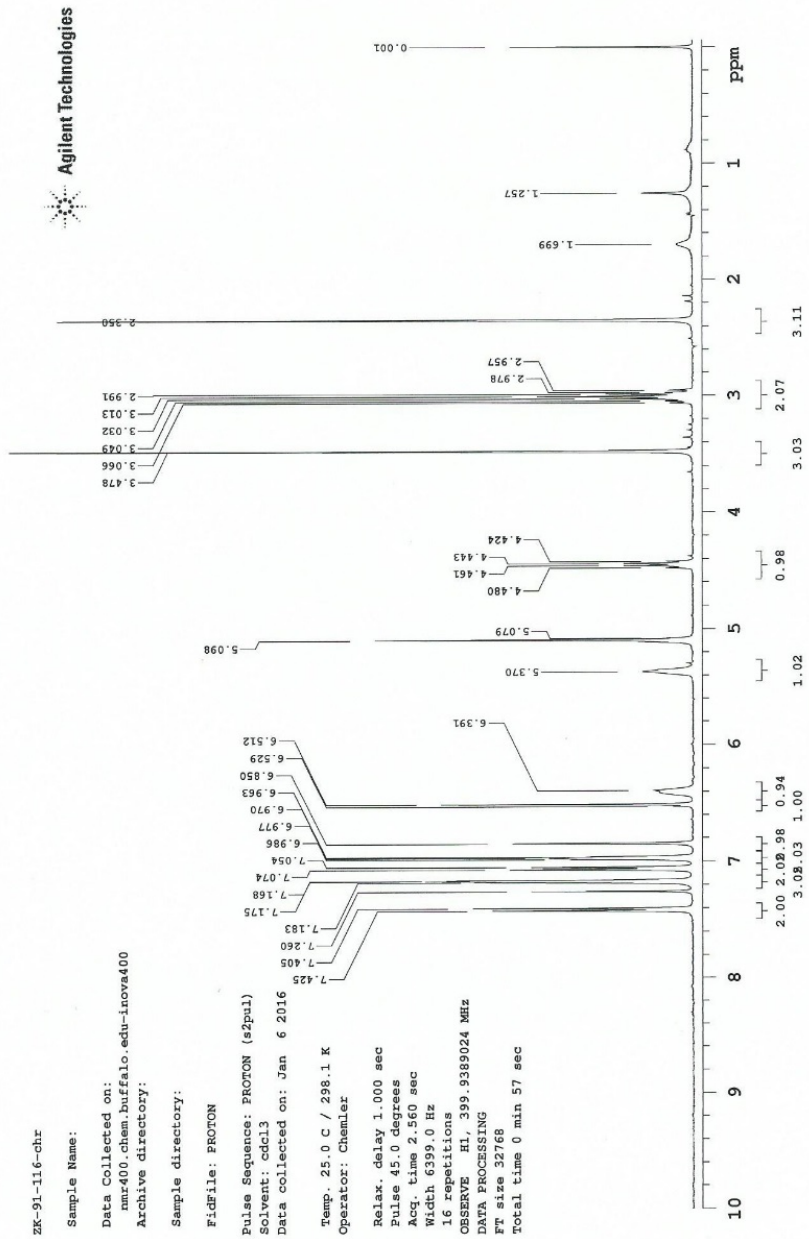
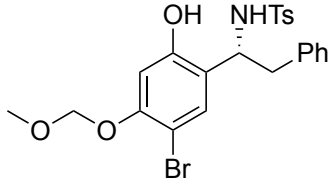
Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
224 repetitions

OBSERVE C13, 100.5647215 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 6 hr, 25 min

Agilent Technologies





ZK-91-116-chr

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

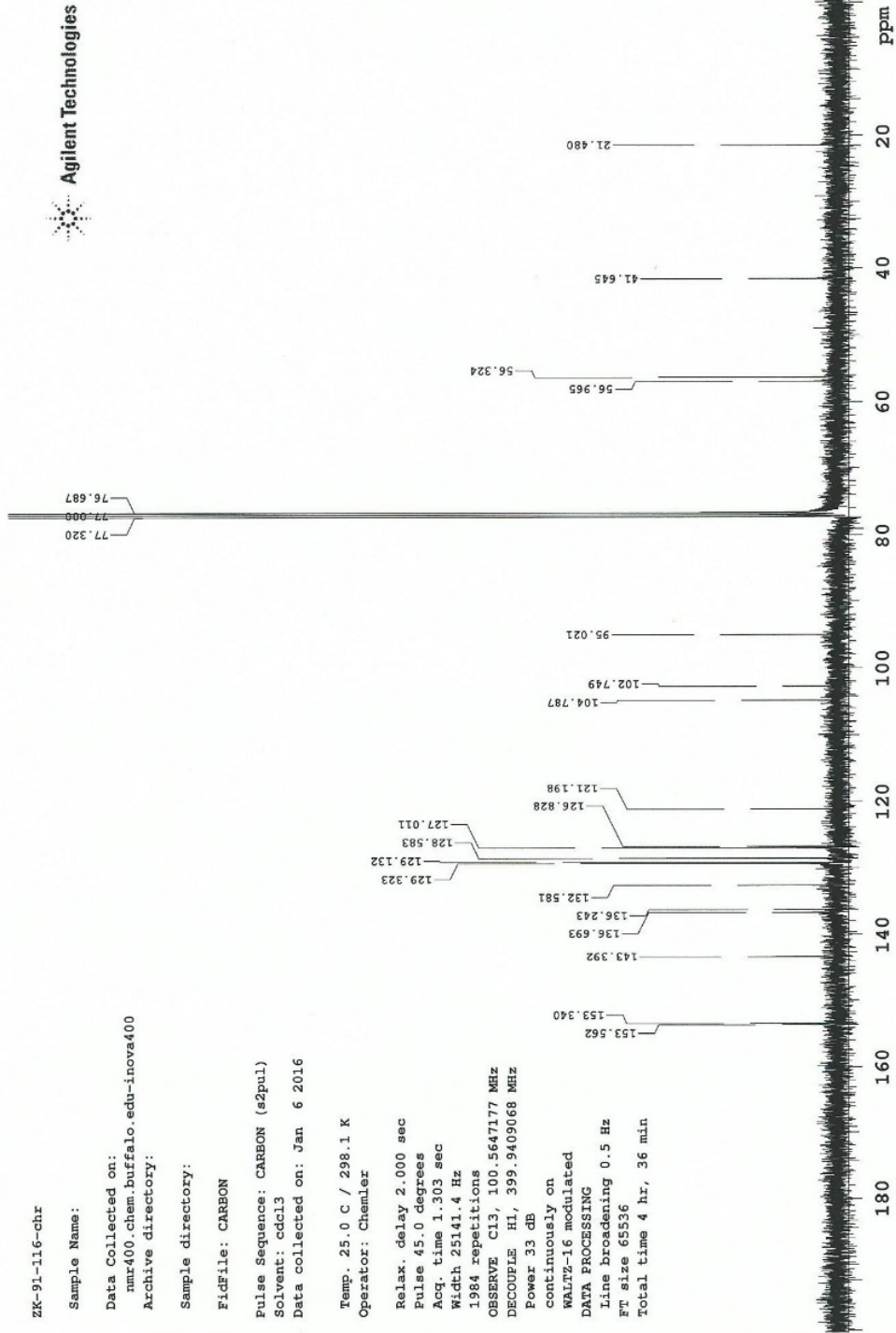
Fidfile: CARBON

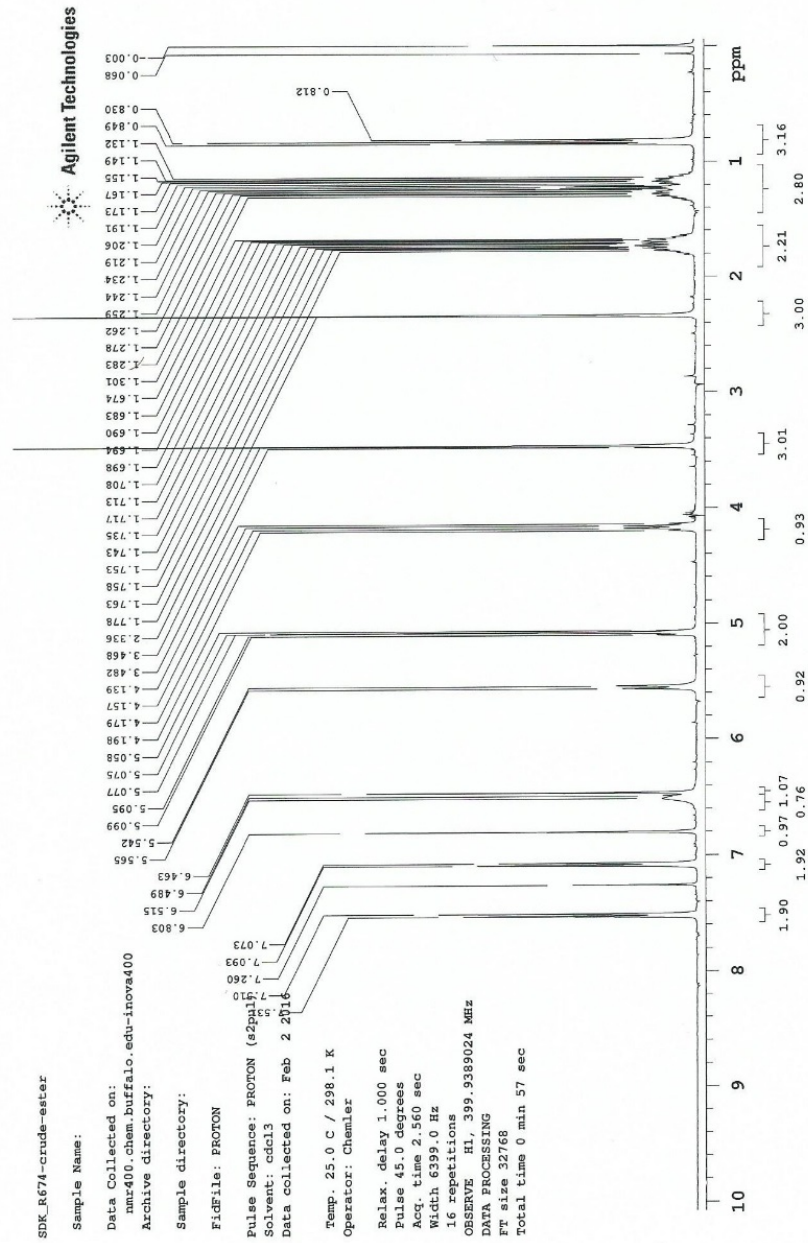
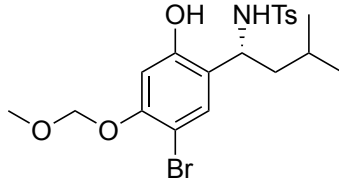
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 6 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
1984 repetitions  
OBSERVE C13, 100.5647177 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 4 hr, 36 min

Agilent Technologies







ib\_251\_HPLC\_product

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jan 28 2016

Operator: Chemler

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

768 repetitions

OBSERVE C13, 75.4536377 MHZ

DECOUPLE H1, 300.0754430 MHZ

Power 37 dB

continuously on

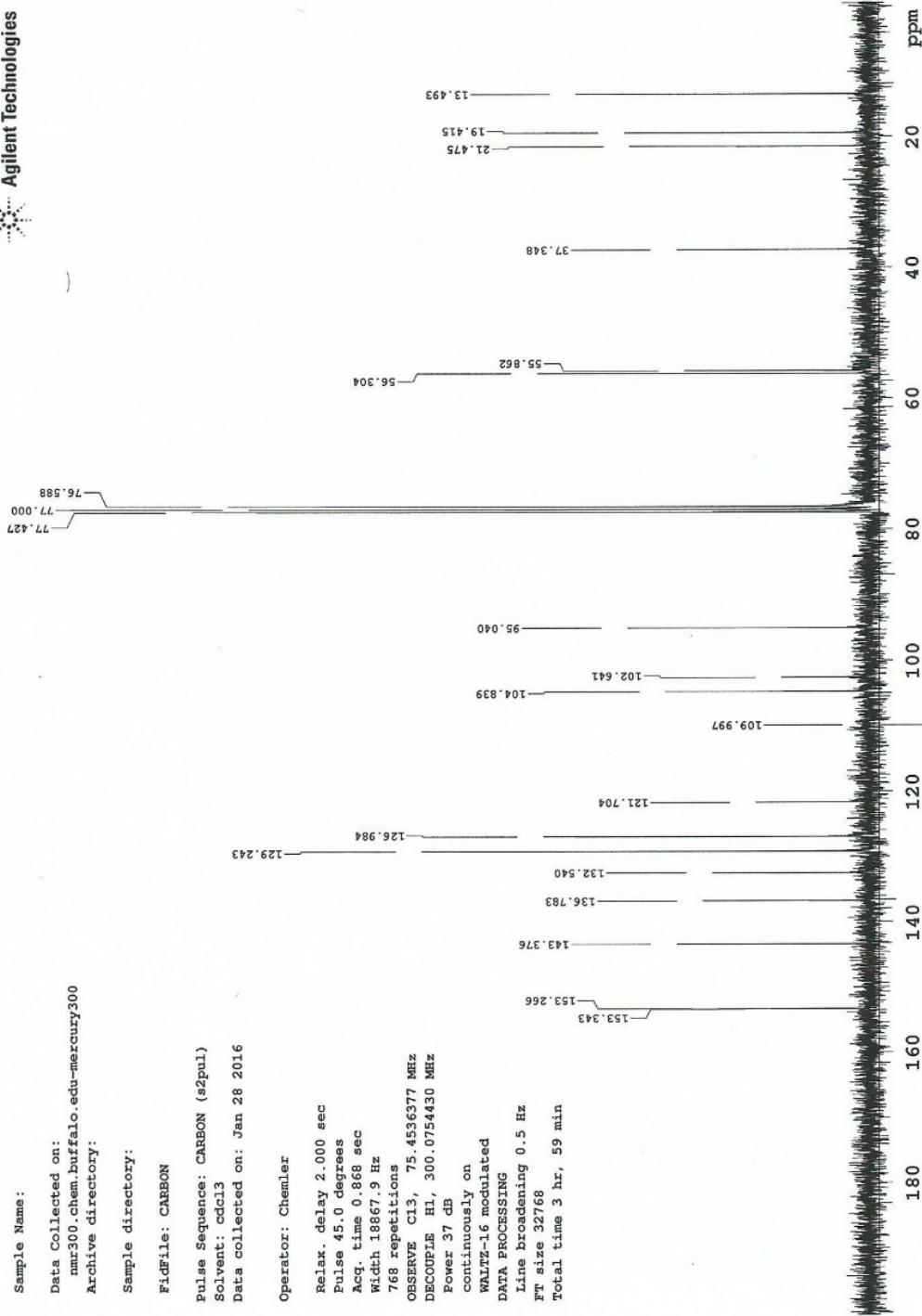
WALTZ-16 modulated

DATA PROCESSING

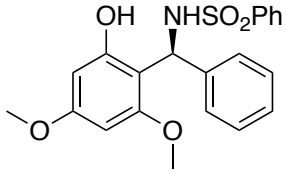
Line broadening 0.5 Hz

FT size 32768

Total time 3 hr, 59 min







(5b)

Agilent Technologies

n5-P--Shuk-Spir-J-Claisen-of-5Br-pentyl-alkene-prd-1H

Sample Name:

Data Collected on:  
nmz400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 6 2016

Temp: 25.0 C / 298.1 K

Operator: Chemlar

Relax. delay 1.000 sec

Pulse 45.0 degree

Acq. time 2.560 sec

Width 6399.0 Hz

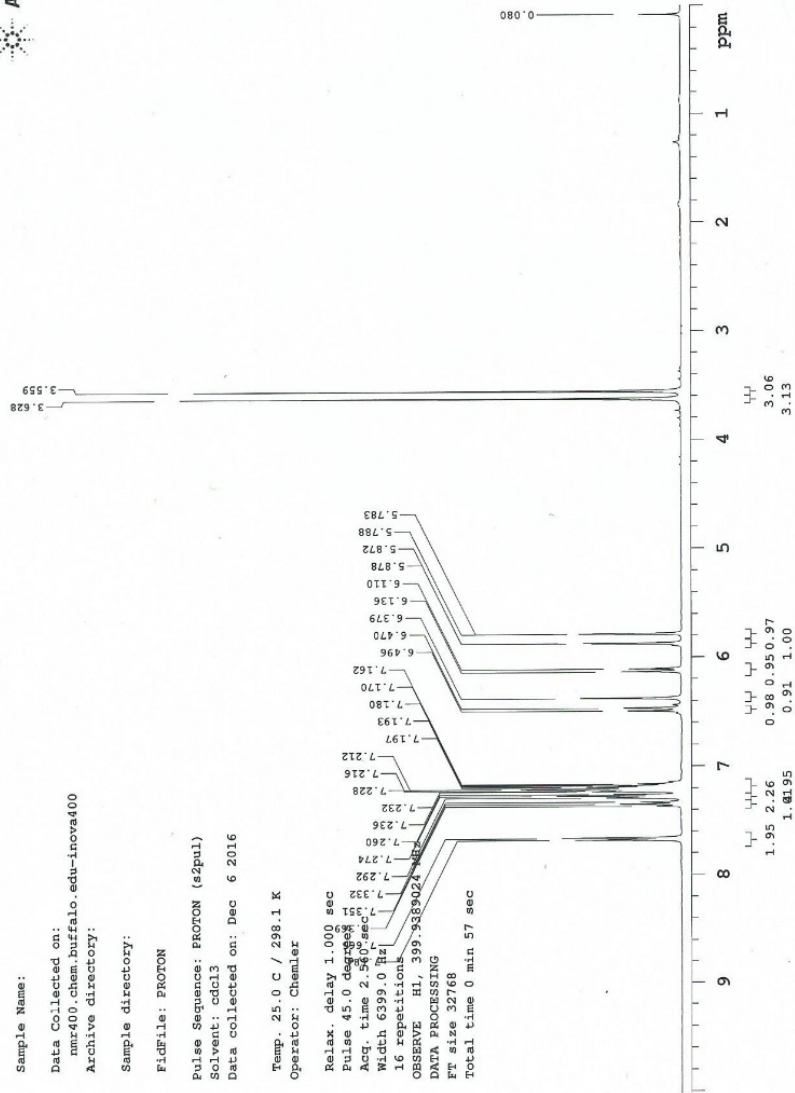
16 repetitions

OBSERVE H1, 399.938902 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 57 sec



n5-R\_--Shuk-Spir-J-Claisen-of-5Br-pentyl-alkene-prd-1H

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

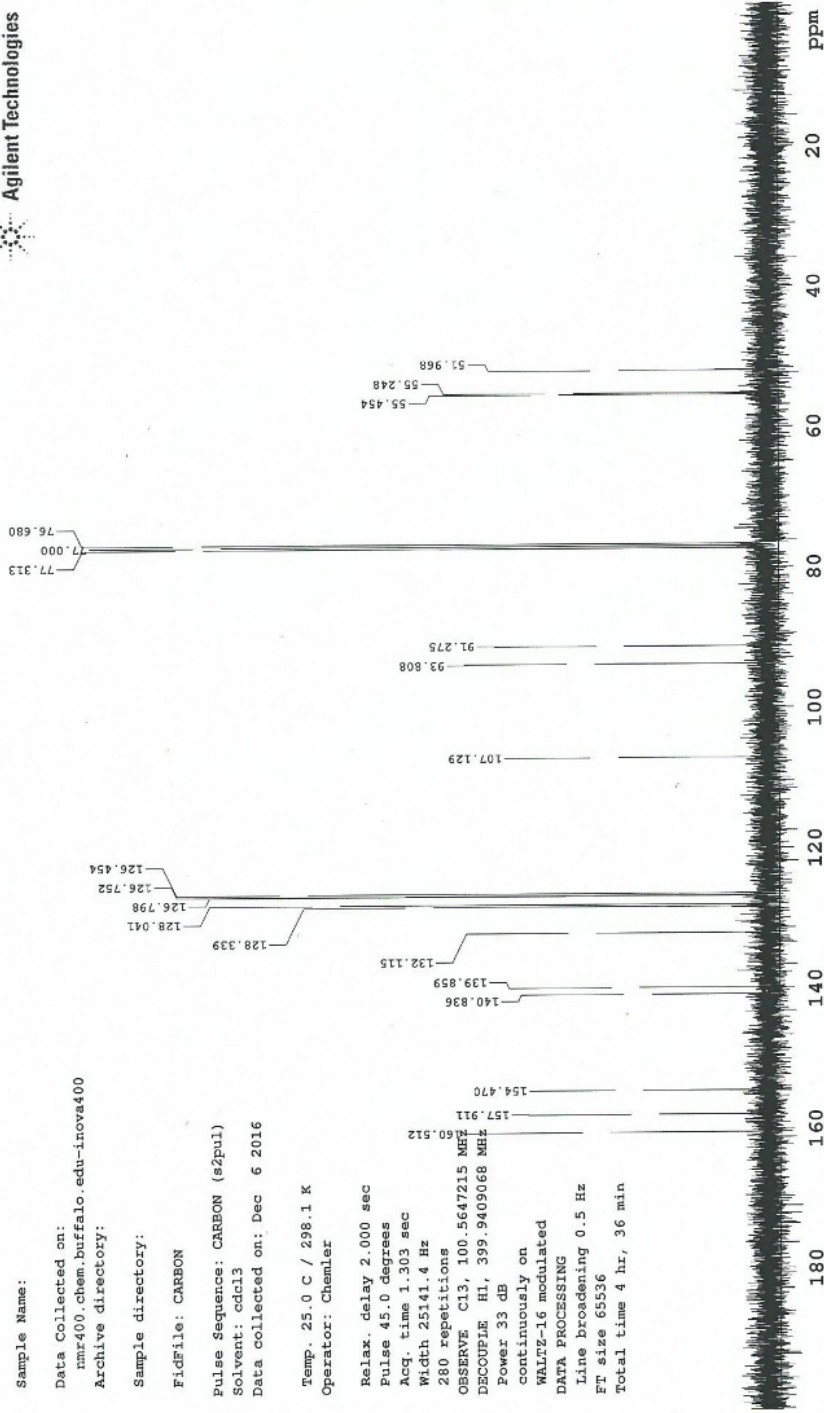
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 6 2016

Temp.: 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
280 repetitions  
OBSERVE C13, 100.5647215 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 4 hr, 36 min



ib2\_63\_crude

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

F1CFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 6 2016

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

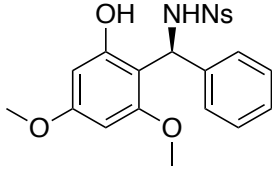
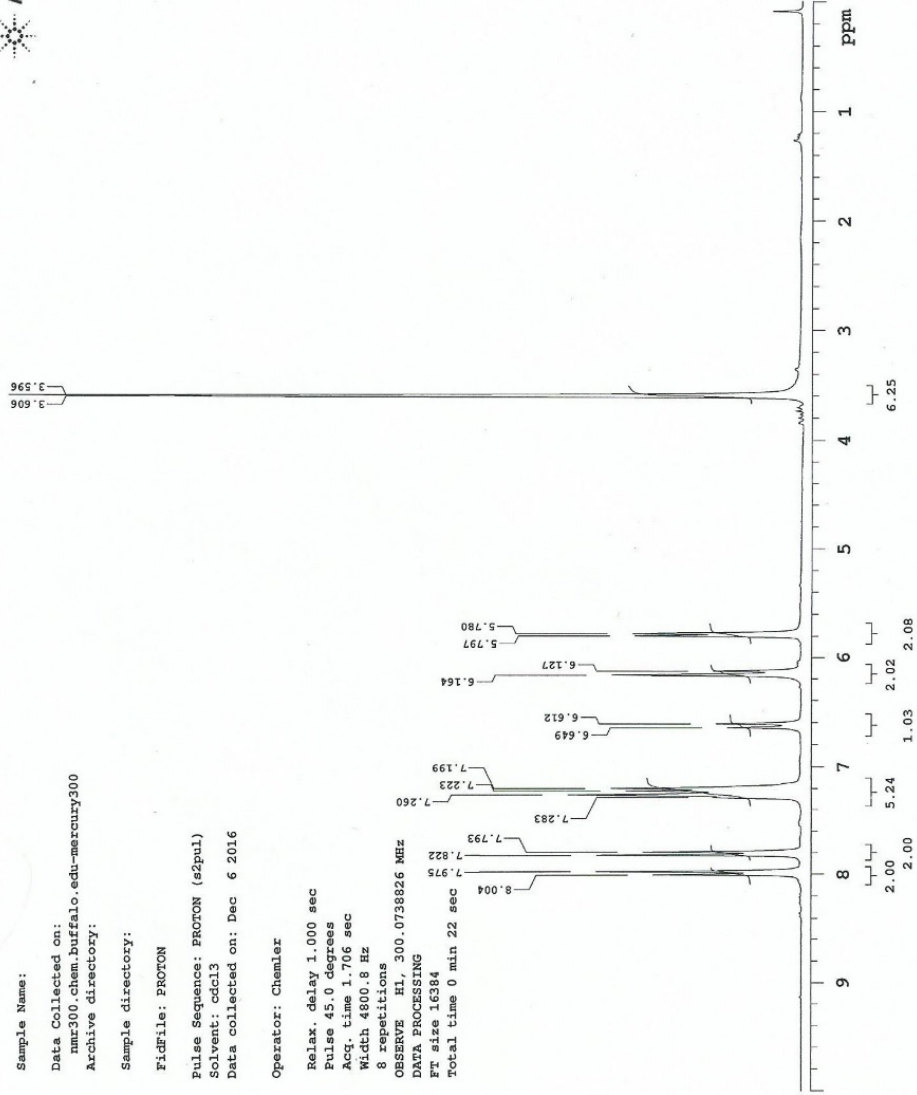
8 repetitions

OBSERVE HL, 300.0738826 MHz

DATA PROCESSING

FT size 16384

Total time 0 min 22 sec



ib2\_63\_crude

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

File: CARBON

Pulse Sequence: CARBON (s2Pul)

Solvent: cdcl3

Data collected on: Dec 6 2016

Operator: Chemler

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

320 repetitions

OBSERVE C13, 75.4536423 MHz

DECOUPLE H1, 300.0754430 MHz

Power 37 dB

continuously on

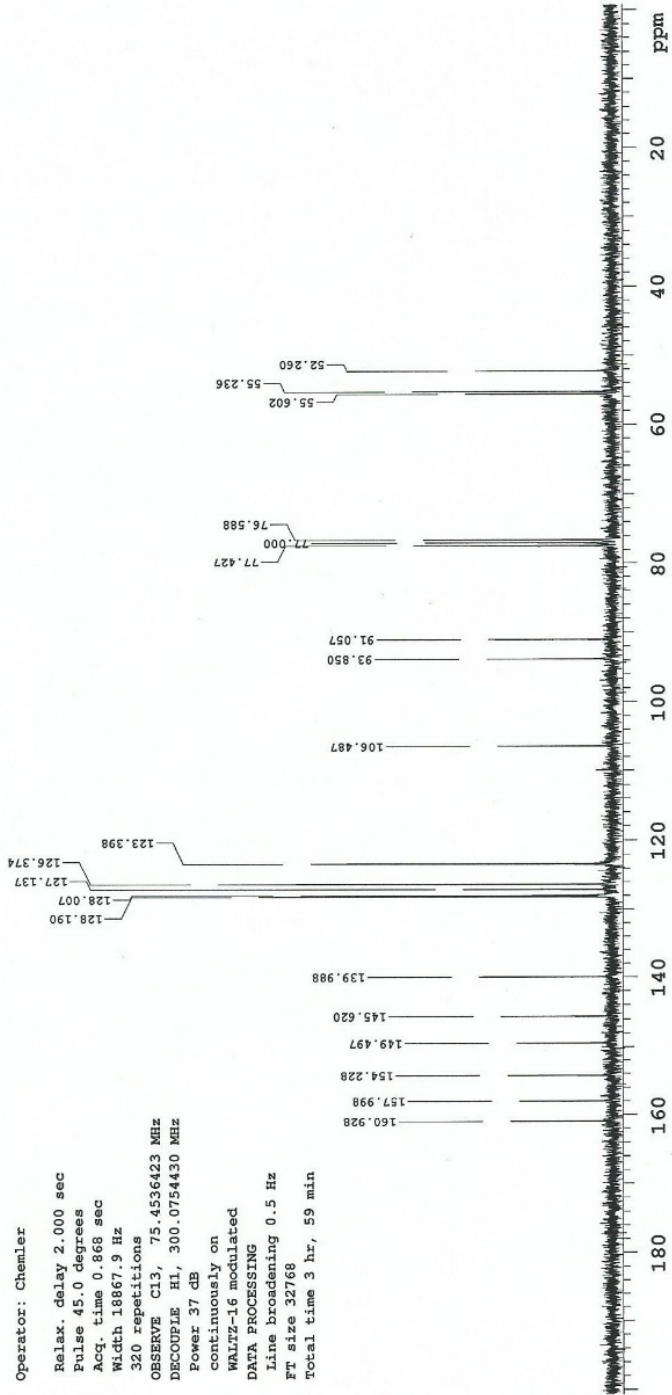
WALTZ-16 modulated

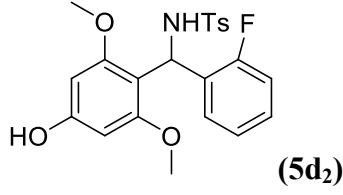
DATA PROCESSING

Line broadening 0.5 Hz

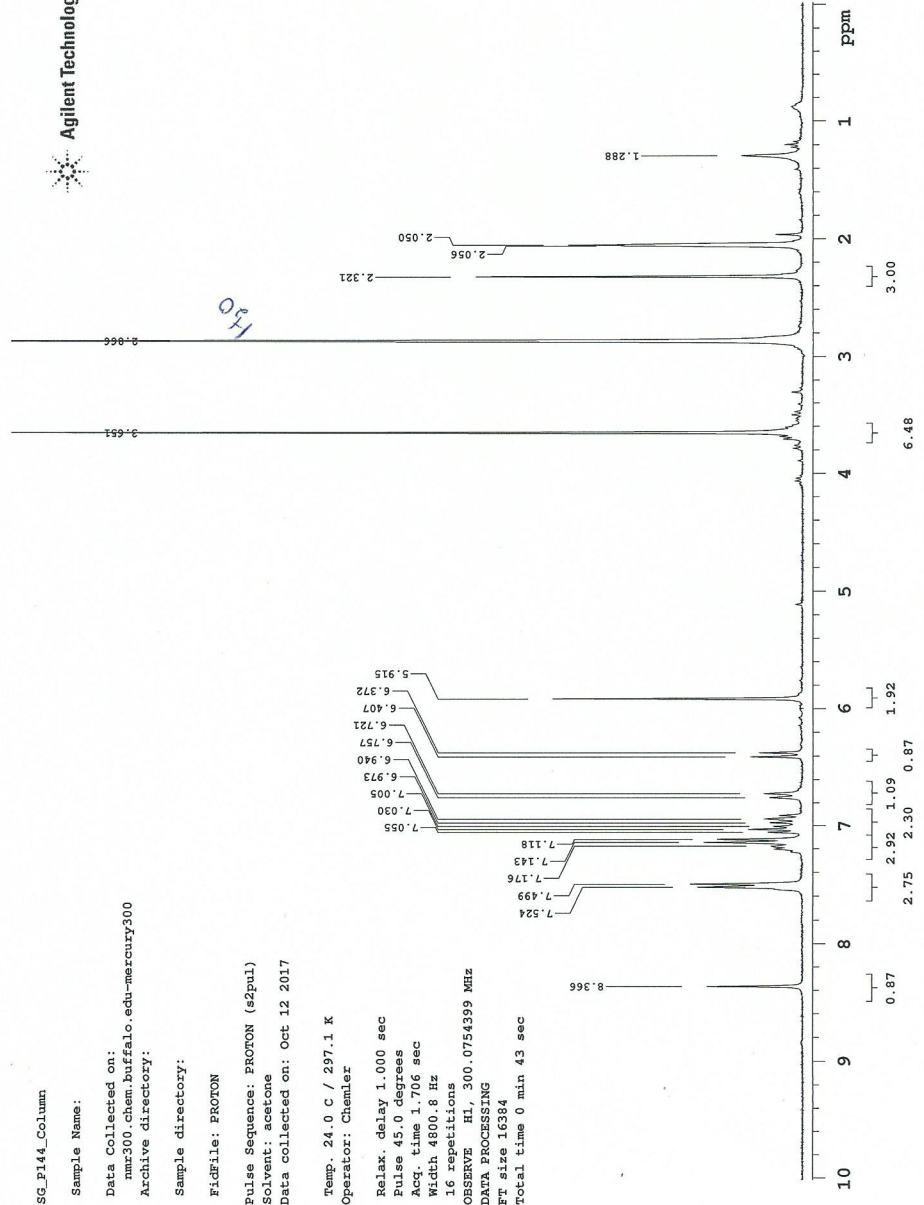
FT size 32768

Total time 3 hr, 59 min





Agilent Technologies



SG\_P144\_Column

Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pull)

Solvent: acetone

Data collected on: Oct 12 2017

Temp. 24.0 C / 297.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

16 repetitions

OBSERVE H1, 500.0754399 MHz

DATA PROCESSING

FT size 16384

Total time 0 min 43 sec



cdk-b2-r397-product1

Sample Name:

Data Collected on: 10/13/2017  
mmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

File: 13C-Oct14

Pulse Sequence: CARBON (s2pul)

Solvent: acetone

Data collected on: Oct 13 2017

Temp. 24.0 C / 297.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

30448 repetitions

OBSERVE C13, 75.459629 MHz

DECOUPLE H1, 300.077004 MHz

Power 37 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 5214 hr, 29 min



30.583  
30.324  
30.079  
29.820  
29.561  
29.301  
29.042

55.751

92.609

129.529  
129.193  
129.086  
127.530

129.193

21.304

47.433  
47.402

124.141  
124.096  
115.793  
115.503  
107.277

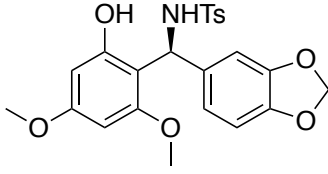
130.353  
130.307  
130.170  
130.002

143.174  
139.480

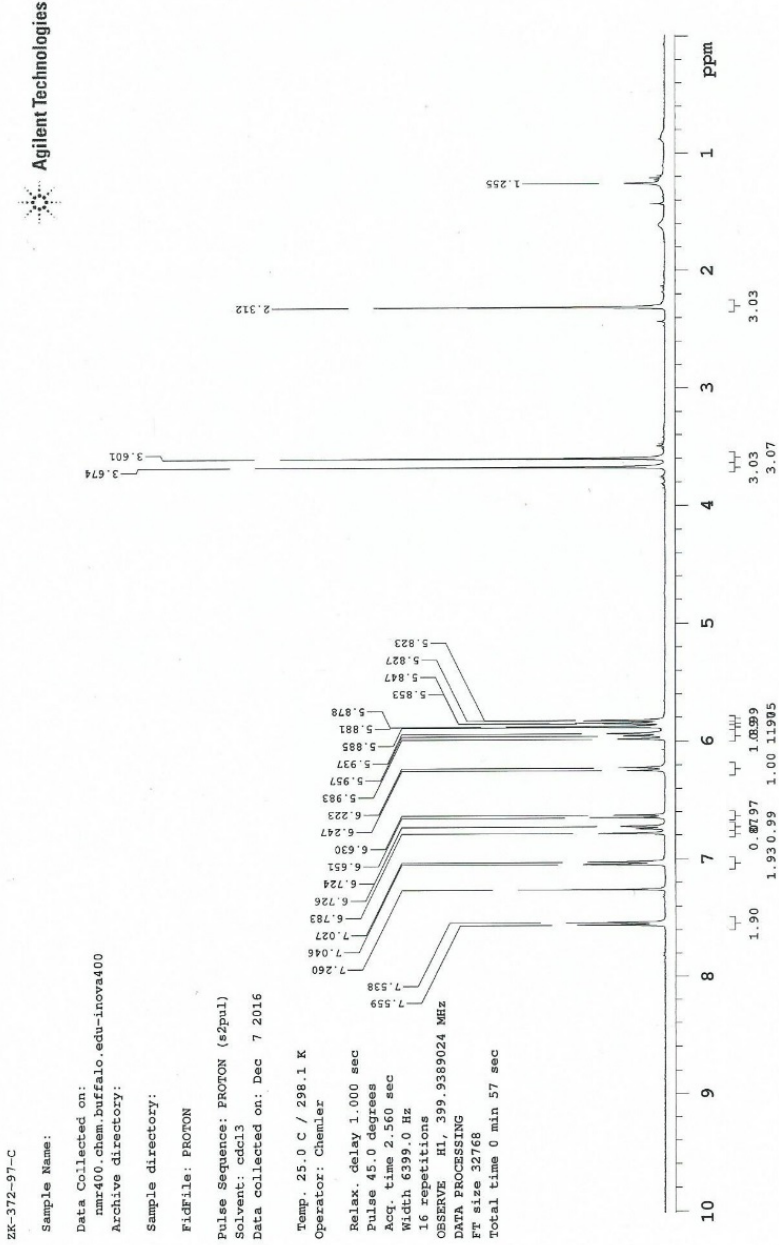
159.016  
159.138  
159.779

162.420

220 200 180 160 140 120 100 80 60 40 20 0 ppm



(5e)



ZK-372-97-C

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 7 2016

Temp. 25.0 C / 298.1 K

Operator: Chealer

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

1584 repetitions

OBSERVE C13, 100.5647169 MHz

DECOUPLE H1, 399.9409068 MHz

Power 33 dB

continuously on

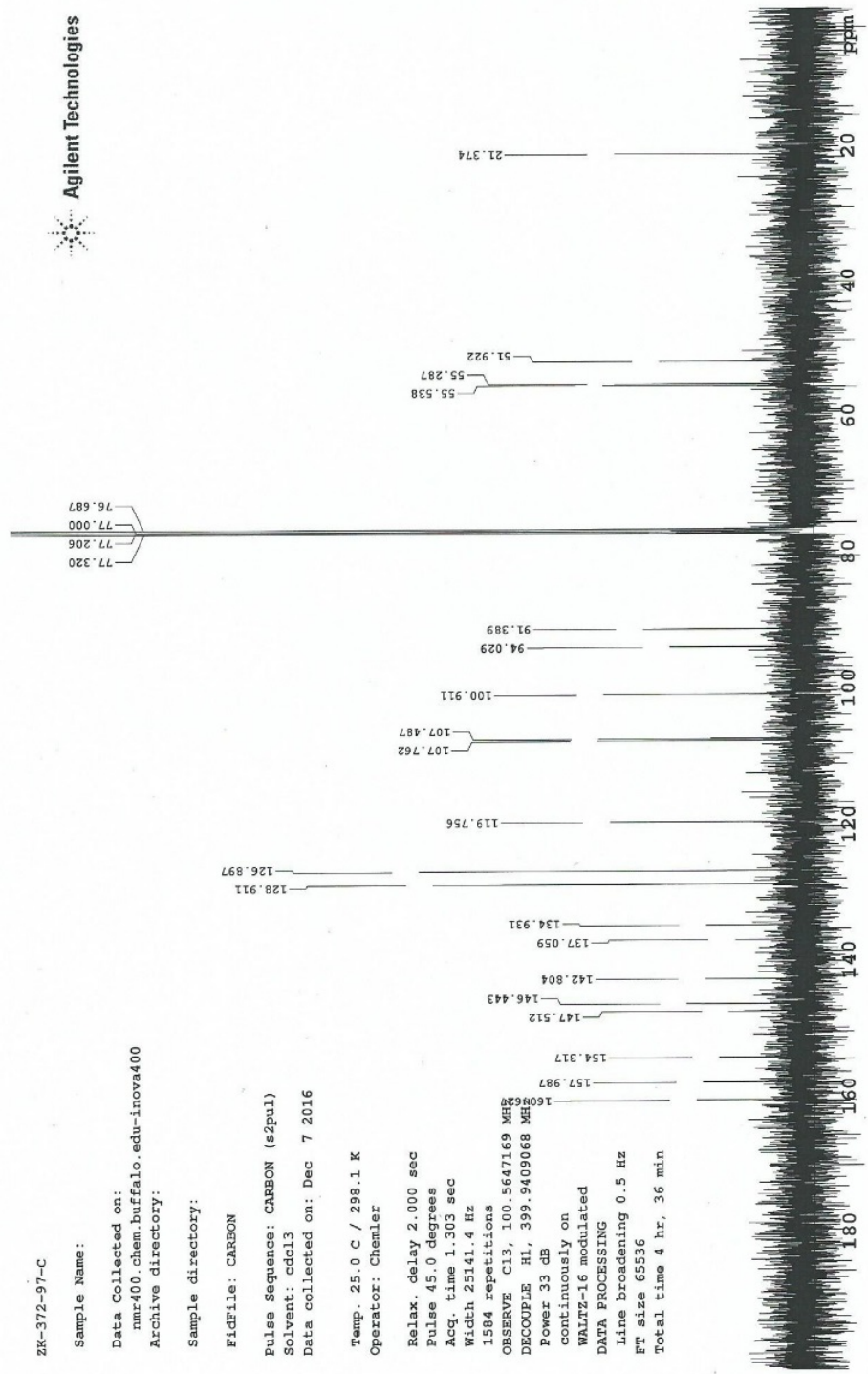
WALTZ-16 modulated

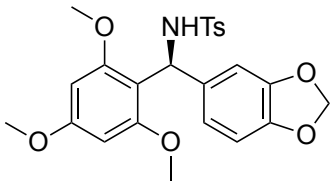
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 4 hr, 36 min





b5-R-156-Shuk-SFIR-alkene-J-claisen-Cl3-1

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 6 2016

Operator: Chemier

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.706 sec

Width 4800.8 Hz

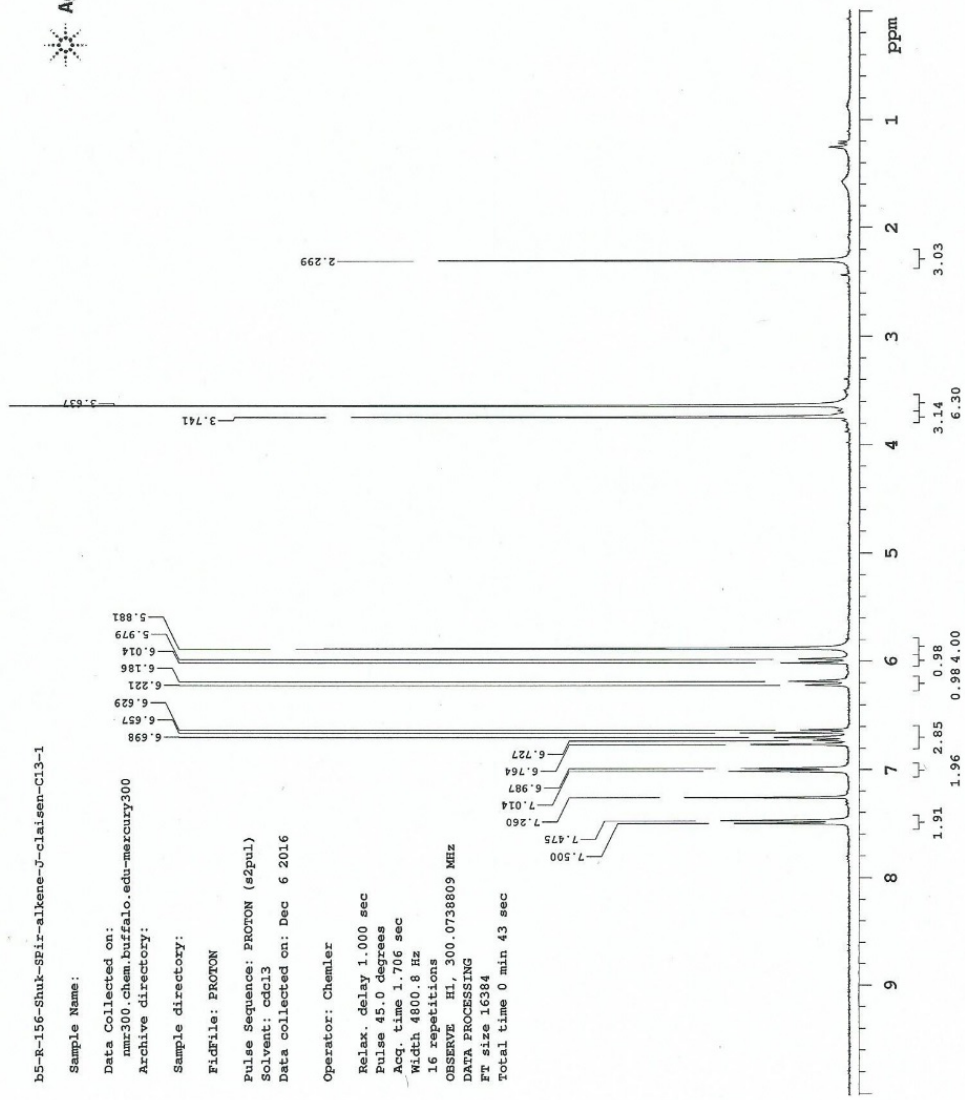
16 repetitions

OBSERVE H1, 300.0738809 MHz

DATA PROCESSING

FT size 16384

Total time 0 min 43 sec



b5-R-156-Shuk-SFIR-alkene-J-claisen-Cl3-1



Sample Name:

Data Collected on:  
nmr300.chem.buffalo.edu-mercury300  
Archive directory:

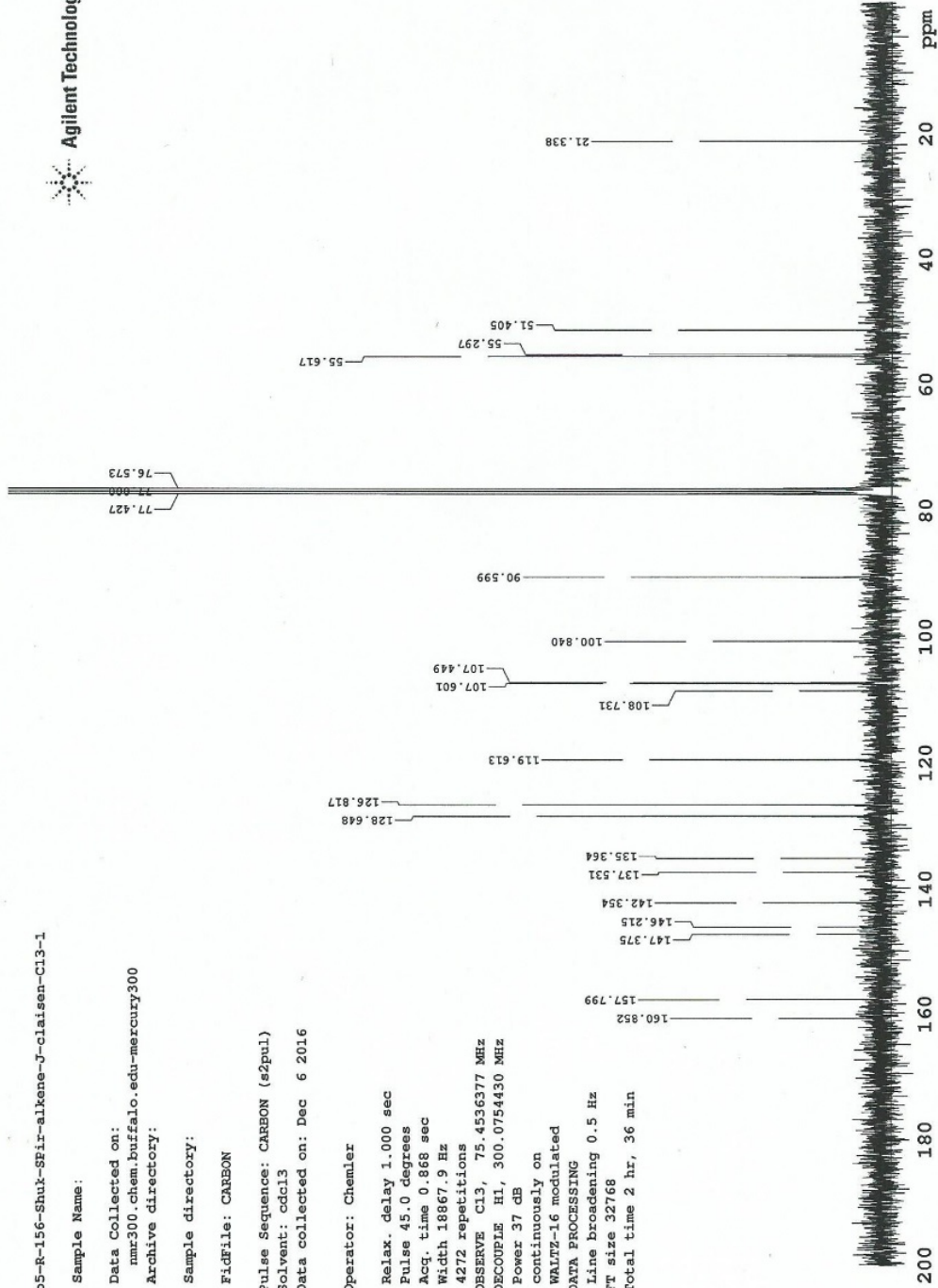
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 6 2016

Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
4272 repetitions  
OBSERVE C13, 75.4536377 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 37 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 32768  
Total time 2 hr, 36 min





n5-R---Shuk-Spir-J-Claissen-of-5Br-pentyl-alkene-prd-1H

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

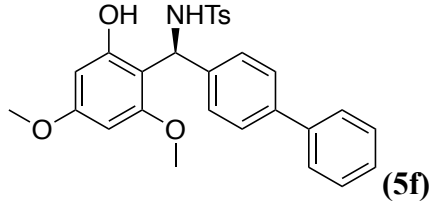
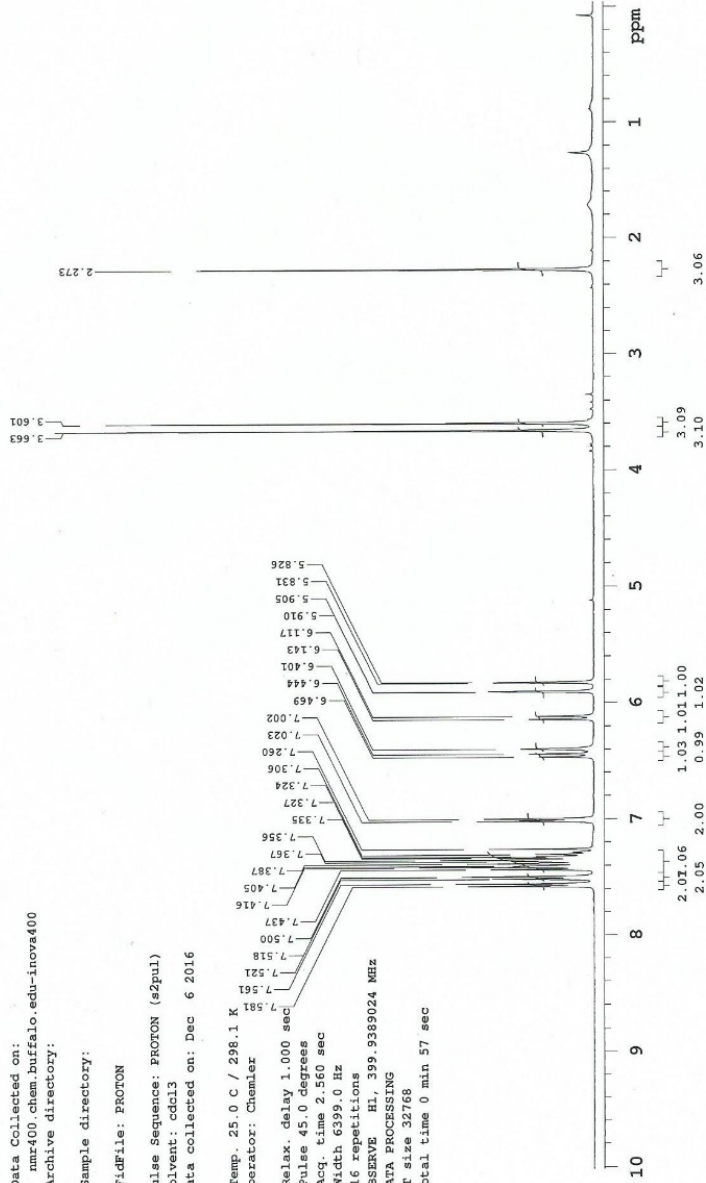
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Dec 6 2016

Temp: 25.0 C / 298.1 K  
Operator: Chemtaz

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.560 sec  
Width 6399.0 Hz  
16 repetitions

OBSERVE H1, 399.9389024 MHz  
DATA PROCESSING  
Ft size 32768  
Total time 0 min 57 sec



n5-R-\_\_\_-Shuk-Spir-J-Claisen-of-5Br-pentyl-alkene-prd-1H

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

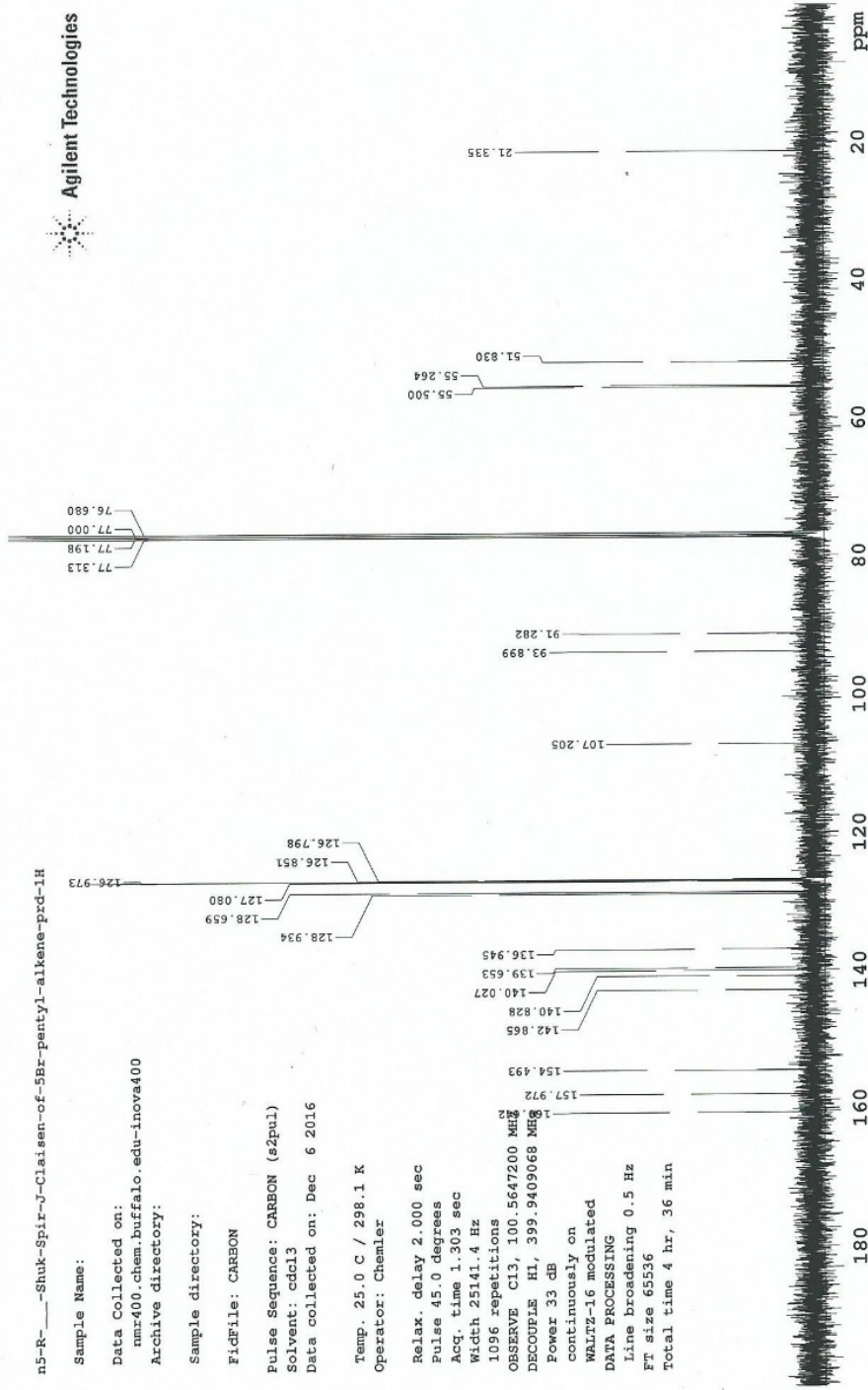
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 6 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
1096 repetitions

OBSERVE C13, 100.5647200 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 4 hr, 36 min



n5-R\_--Shuk-Spir--J-Claisen-of-5Br-pentyl-alkene-prd-1H

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

File: PROTON

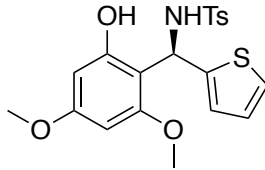
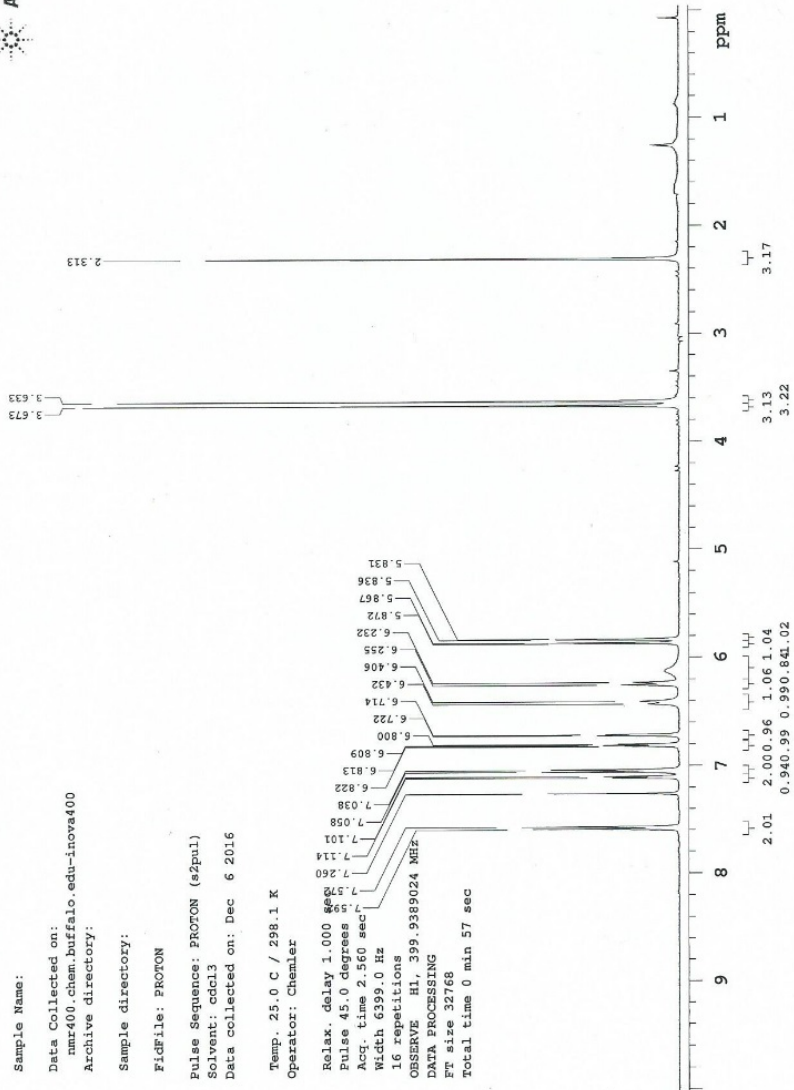
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 6 2016

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.560 sec  
Width 6399.0 Hz  
16 Repetitions  
OBSERVE H1, 399.9389024 MHz  
DATA PROCESSING  
Ft size 32768  
Total time 0 min 57 sec

Agilent Technologies



n5-R-\_\_\_-Shuk-Spir-J-Claisen-of-5Br-pentyl-alkene-prod-1H

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

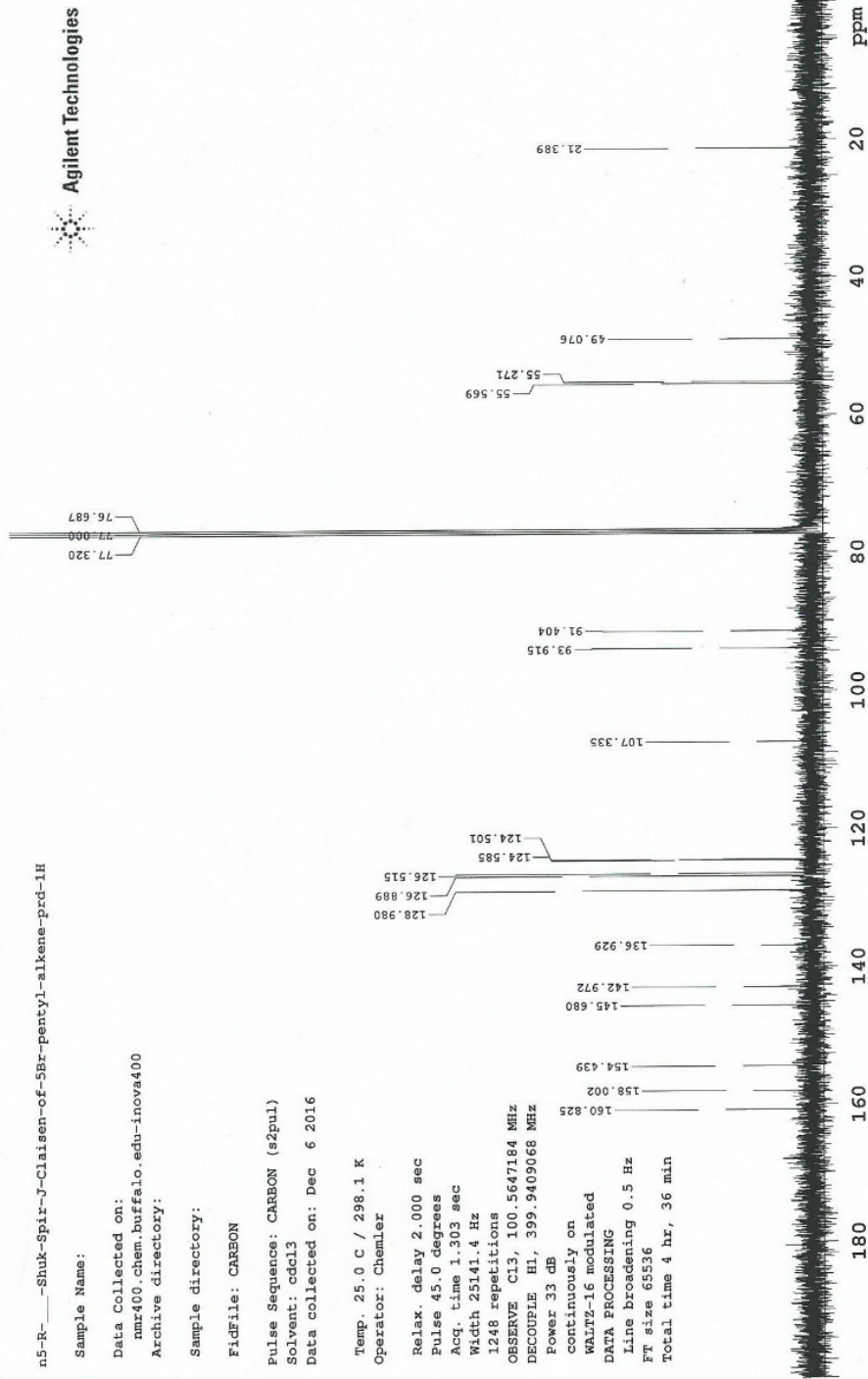
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Dec 6 2016

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 2.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz

1248 repetitions  
OBSERVE C13, 100.5647184 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 4 hr, 36 min



ZK-427-152-C13

Sample Name:

Data Collected on:  
nmr500c.chem.buffalo.edu-inova500  
Archive directory:

Sample directory:

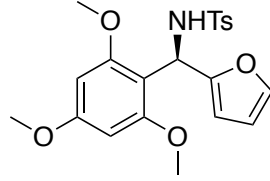
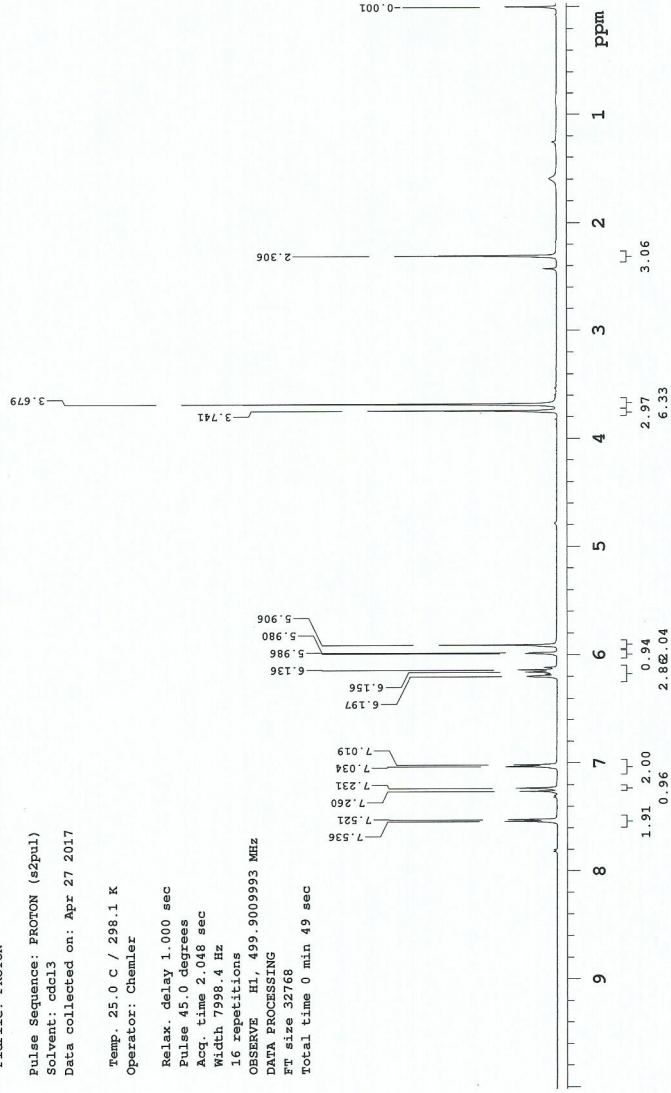
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 27 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 7998.4 Hz  
16 repetitions

OBSERVE H1 499.9009993 MHz  
DATA PROCESSING  
Ft size 32768  
Total time 0 min 49 sec





ZK-427-152-C13

Sample Name:

Data Collected on:  
nmr500c.chem.buffalo.edu-inova500  
Archive directory:

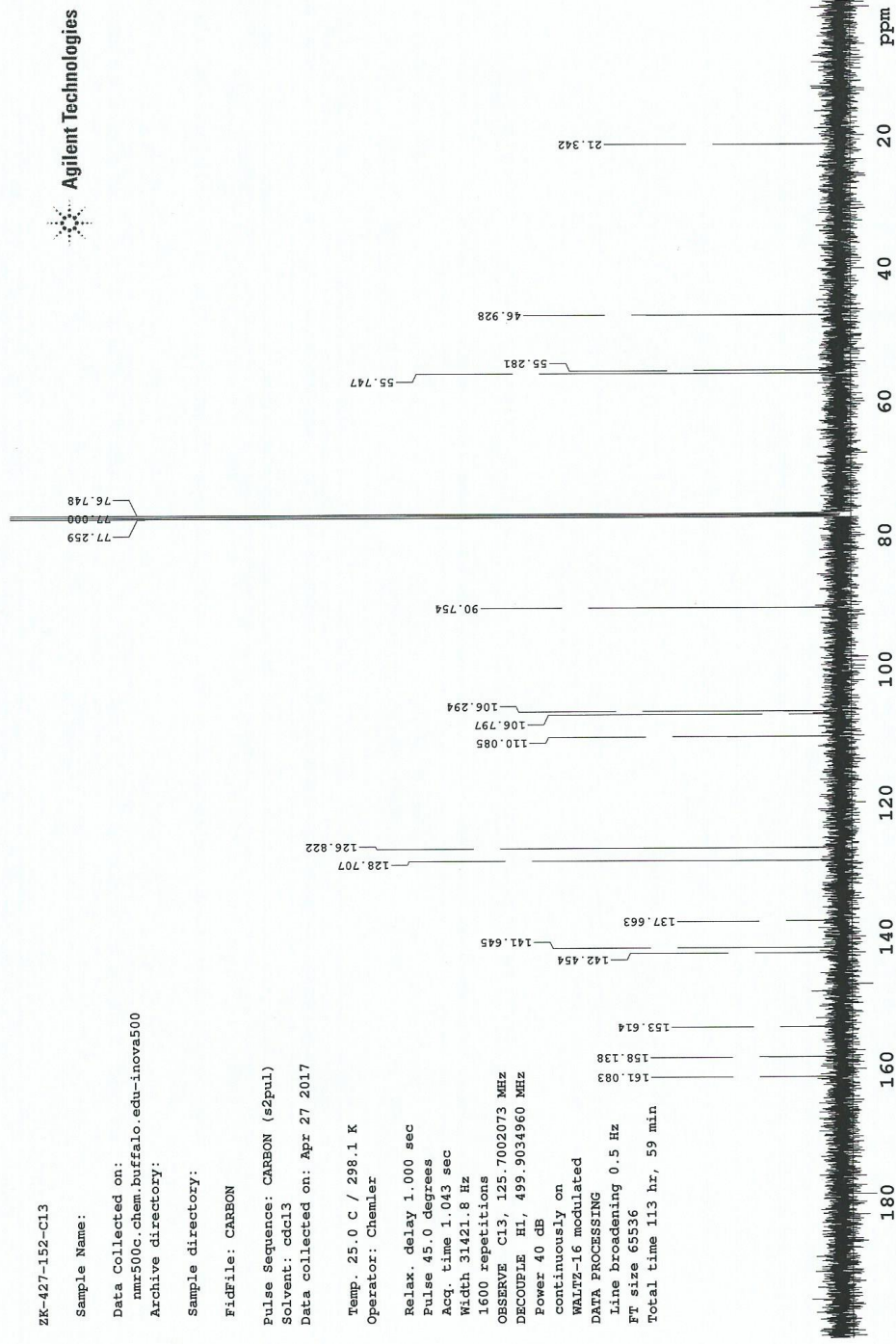
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 27 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.043 sec  
Width 31421.8 Hz  
1600 repetitions  
OBSERVE C13, 125.7002073 MHz  
DECOUPLE H1, 499.9034960 MHz  
Power 40 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 113 hr, 59 min



ZK-457-182-C

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

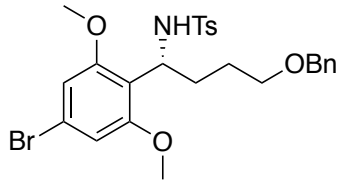
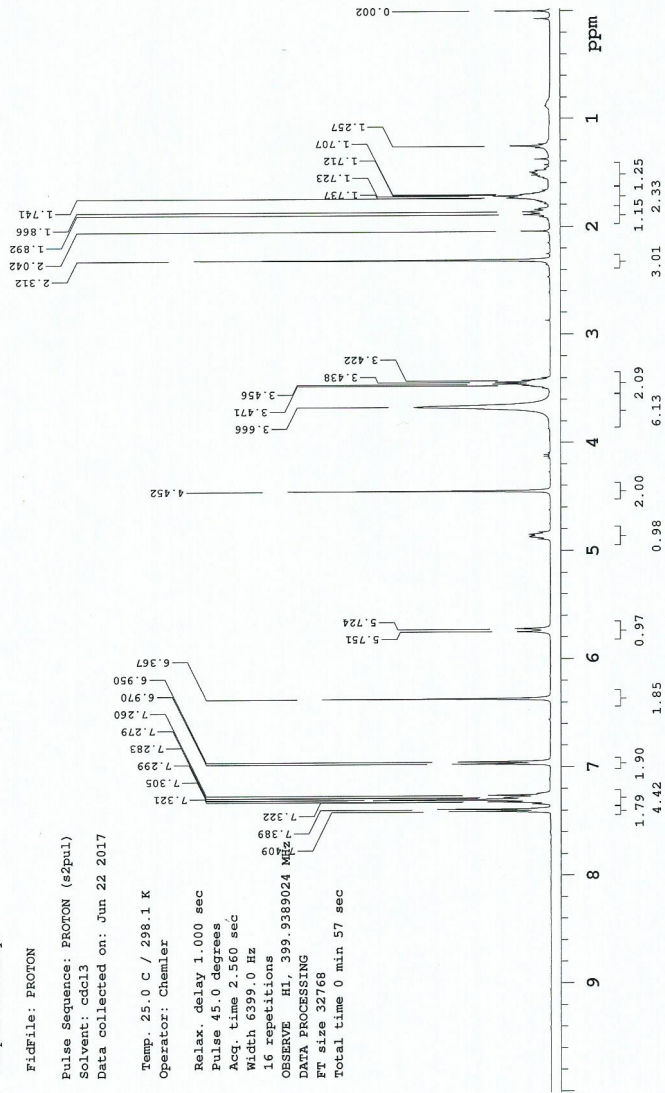
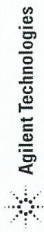
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 22 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.560 sec  
Width 6399.0 Hz  
16 repetitions  
ORSERVE H1\_399.9389024 MHz  
DATA PROCESSING  
Ft size 32768  
Total time 0 min 57 sec



(6)

ZK-457-182-C

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

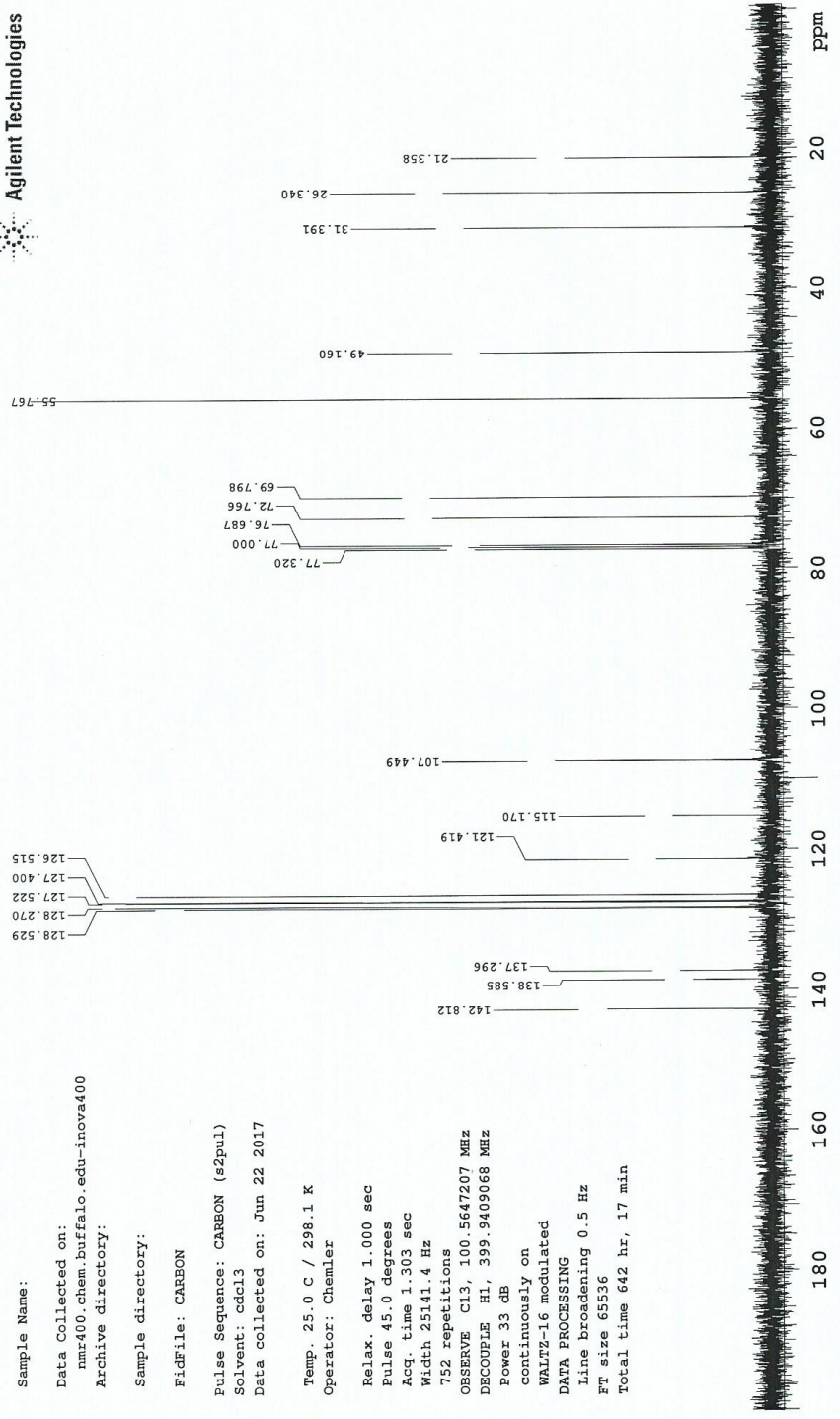
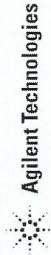
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 22 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
752 repetitions  
OBSERVE C13, 100.5647207 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 642 hr, 17 min



cdk-b2-r431-product3

Sample Name:

Data Collected on: nm-400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 26 2012

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.560 sec

Width 6399.0 Hz

16 repetitions

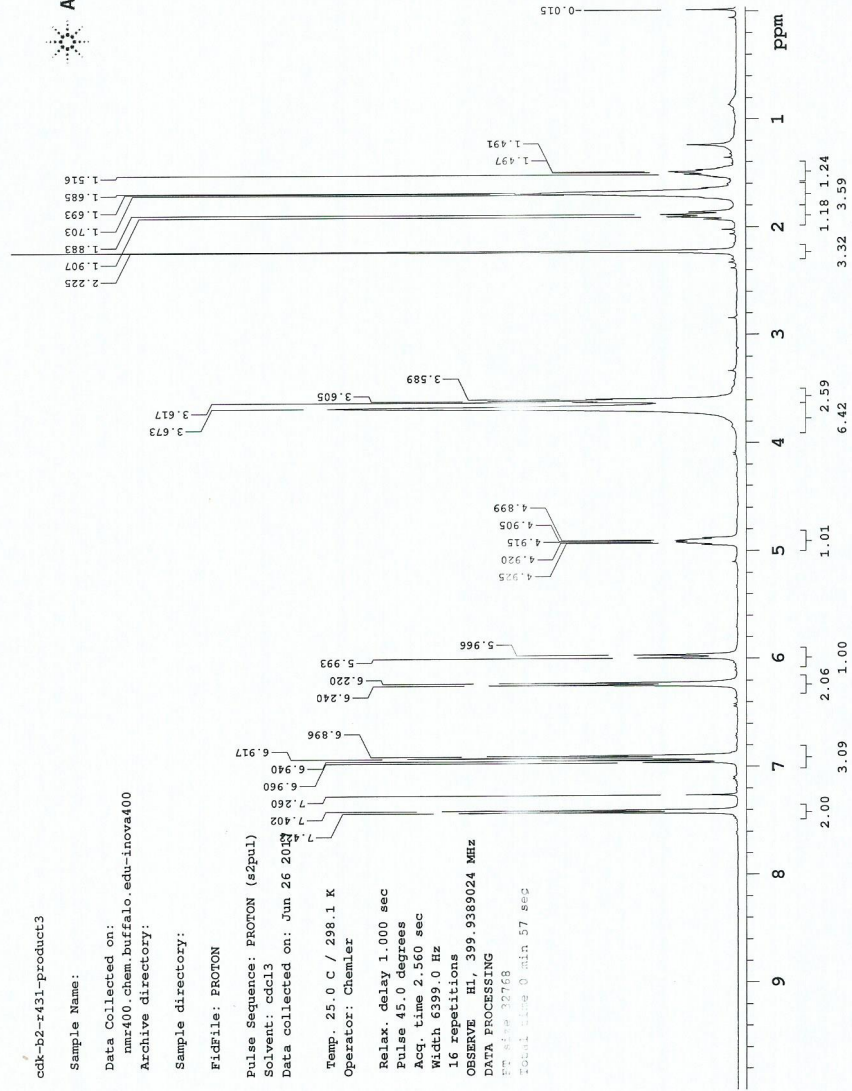
OBSERVE HL, 399.9389024 MHz

DATA PROCESSING

FT AVER 32768

Total time 0 min 57 sec

Agilent Technologies



(7)



cdh-b2-r431-product3

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

Sample directory:

FidFile: CARBON

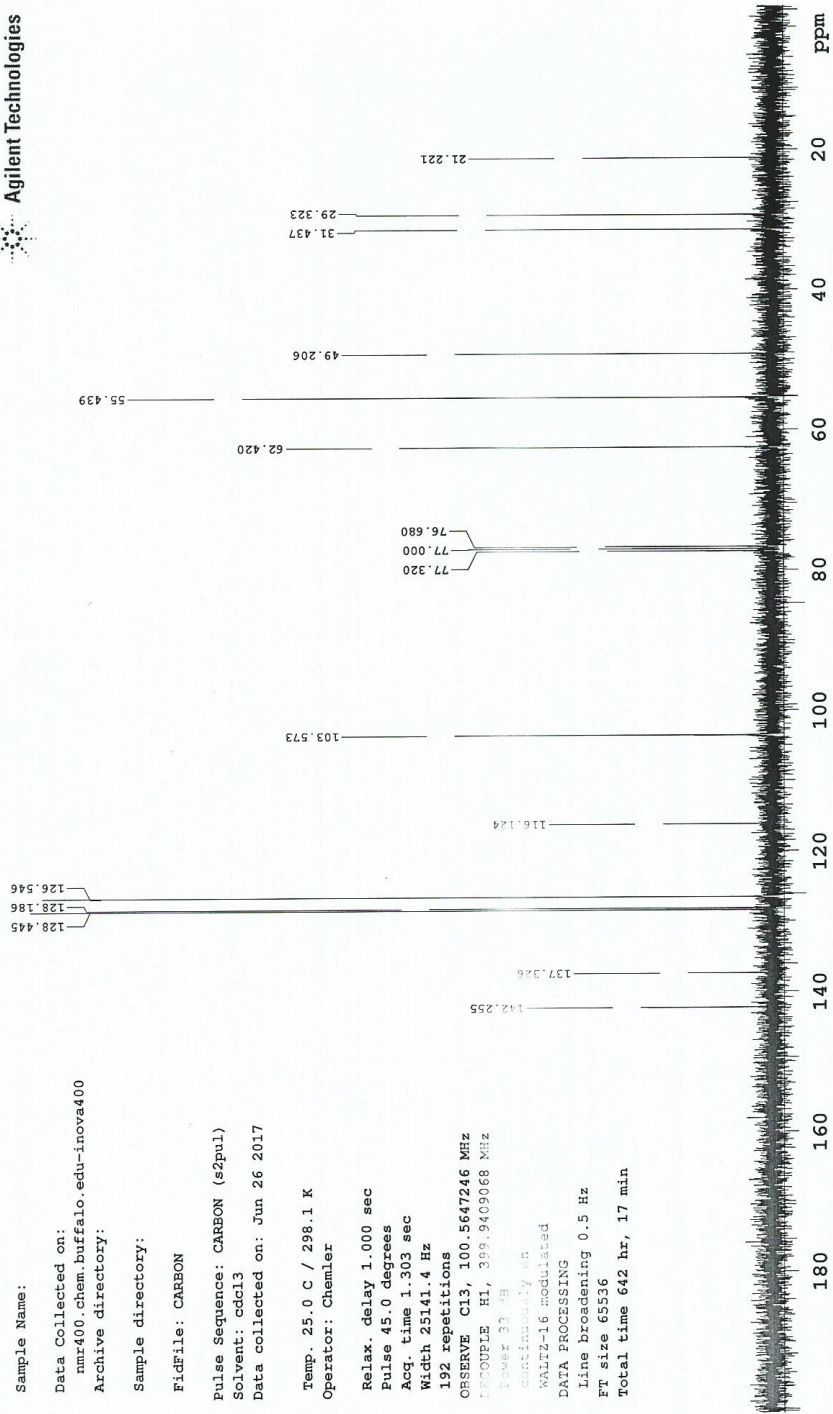
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Jun 26 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

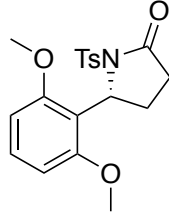
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
192 repetitions

OBSERVE C13, 100.5647246 MHz  
P1/2 399.9409068 MHz

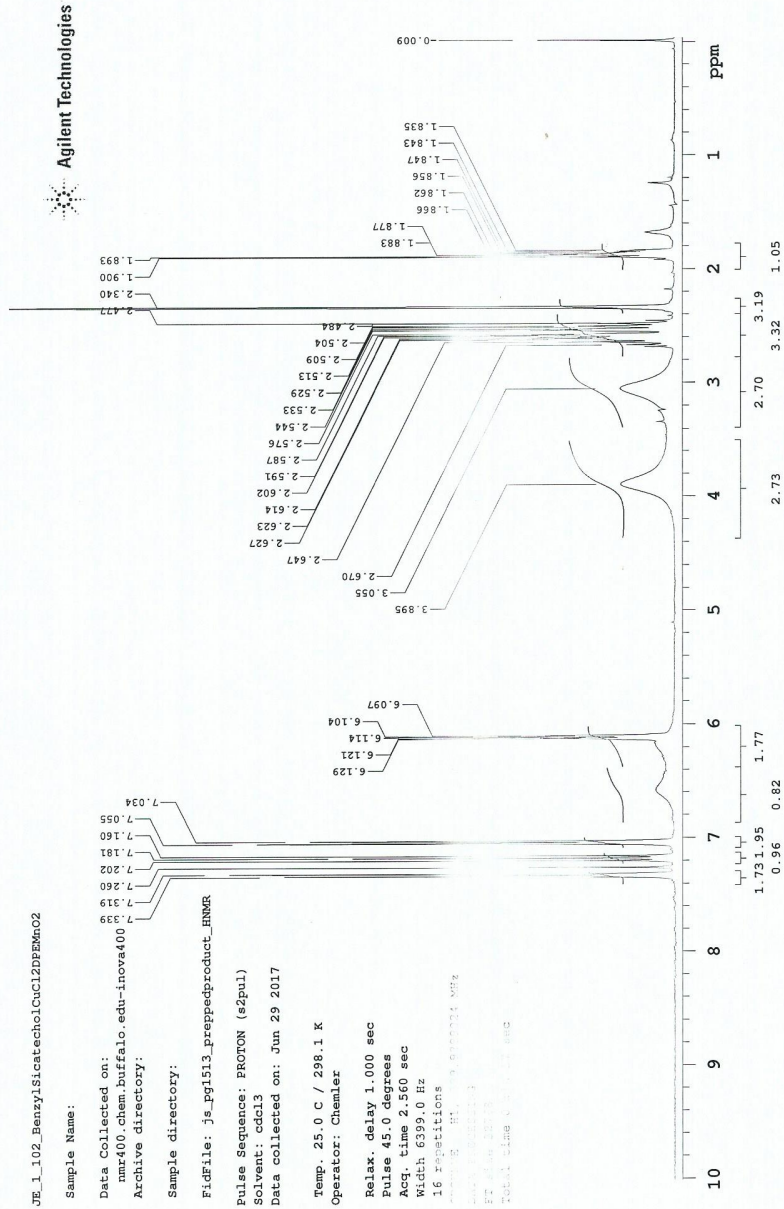
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 642 hr, 17 min



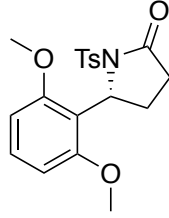




(8, 25°C)

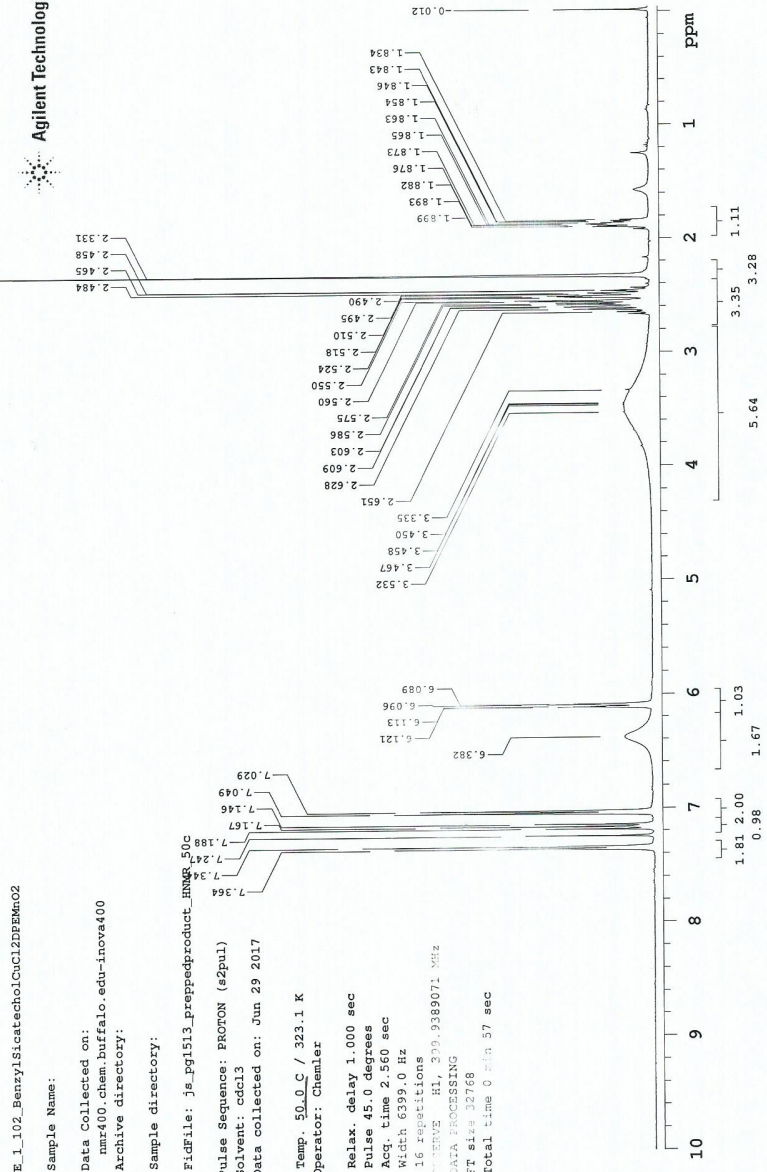






(8, 50°C)

Agilent Technologies



JE\_1\_102\_BenzylicatecholCuCl2DFEM02

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

Fidfile: js\_pg1513\_preppedproduct\_HMR\_50c

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Jun 29 2017

Temp. 50.0 C / 323.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.500 sec

Width 6399.0 Hz

16 repetitions

ORTEWO H1, 300.9389071 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 37 sec

JE\_1\_102\_BenzylSicstecholCuCl2DFEMnO2

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jun 29 2017

Temp. 50.0 C / 323.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

512 repetitions

NUC1: 13C, PULPROG: zgpg30

NUC2: 1H, PULPROG: zgpg30

NUC3: 13C, PULPROG: zgpg30

NUC4: 1H, PULPROG: zgpg30

NUC5: 13C, PULPROG: zgpg30

NUC6: 1H, PULPROG: zgpg30

NUC7: 13C, PULPROG: zgpg30

NUC8: 1H, PULPROG: zgpg30

NUC9: 13C, PULPROG: zgpg30

NUC10: 1H, PULPROG: zgpg30

NUC11: 13C, PULPROG: zgpg30

NUC12: 1H, PULPROG: zgpg30

NUC13: 13C, PULPROG: zgpg30

NUC14: 1H, PULPROG: zgpg30

NUC15: 13C, PULPROG: zgpg30

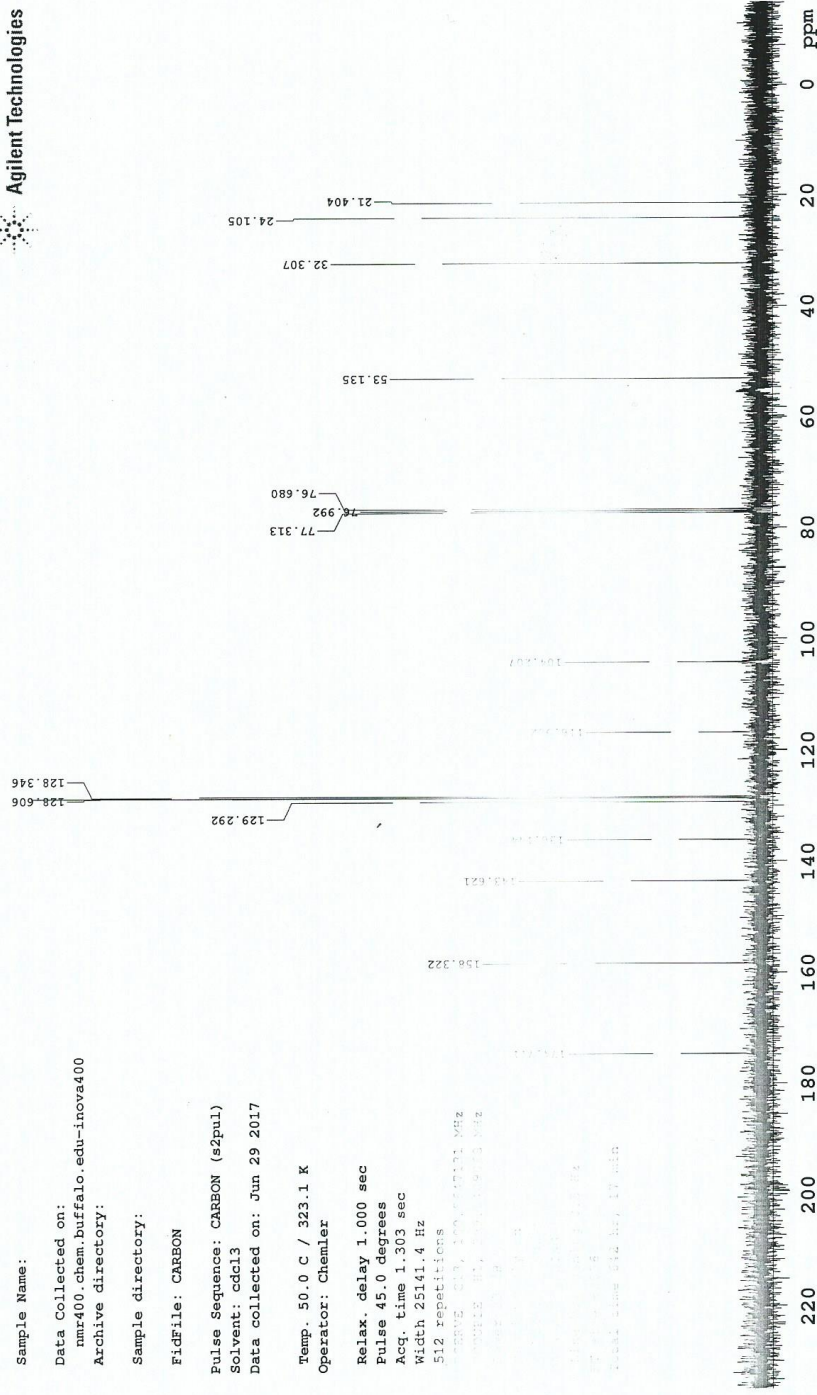
NUC16: 1H, PULPROG: zgpg30

NUC17: 13C, PULPROG: zgpg30

NUC18: 1H, PULPROG: zgpg30

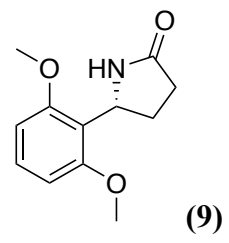
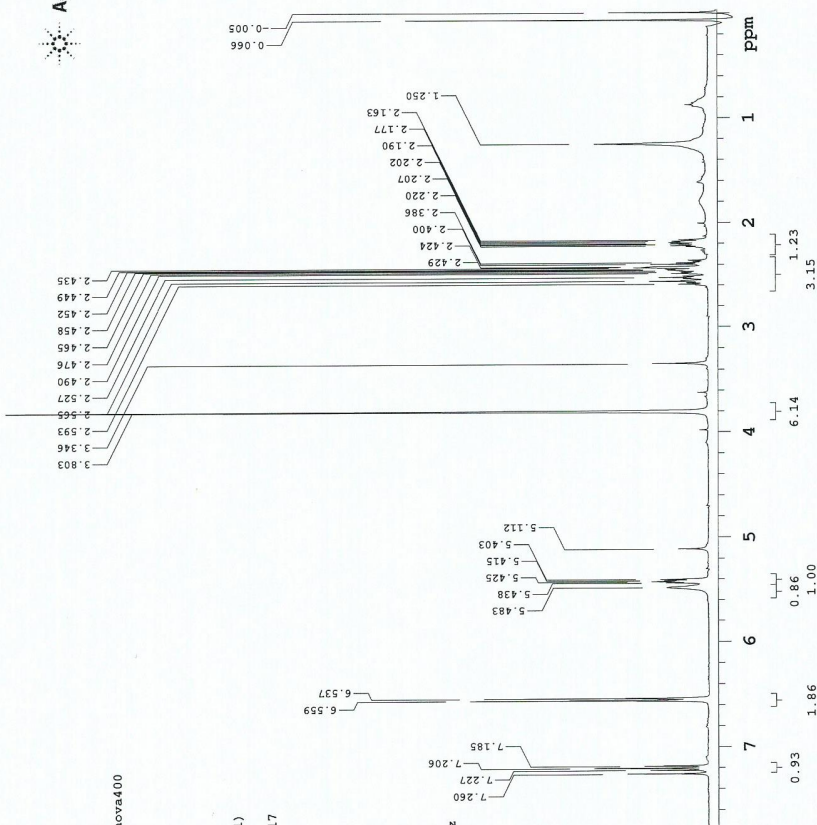
NUC19: 13C, PULPROG: zgpg30

NUC20: 1H, PULPROG: zgpg30





JE\_1\_117\_3benzylpropionicacid  
 Sample Name:  
 Data Collected on: nmr400.chem.buffalo.edu-inova400  
 Archive directory:  
 Sample directory:  
 FidFile: PROTON  
 Pulse Sequence: PROTON (s2pul)  
 Solvent: cdcl3  
 Data collected on: Jul 12 2017  
 Temp.: 25.0 C / 298.1 K  
 Operator: Chemler  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 2.560 sec  
 Width 6399.0 Hz  
 16 repetitions  
 OBSERVE H1, 399.9389024 MHz  
 DATA PROCESSING  
 FT size 32768  
 Total time 0 min 57 sec





JE\_1\_117\_3benzylpropionicacid

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

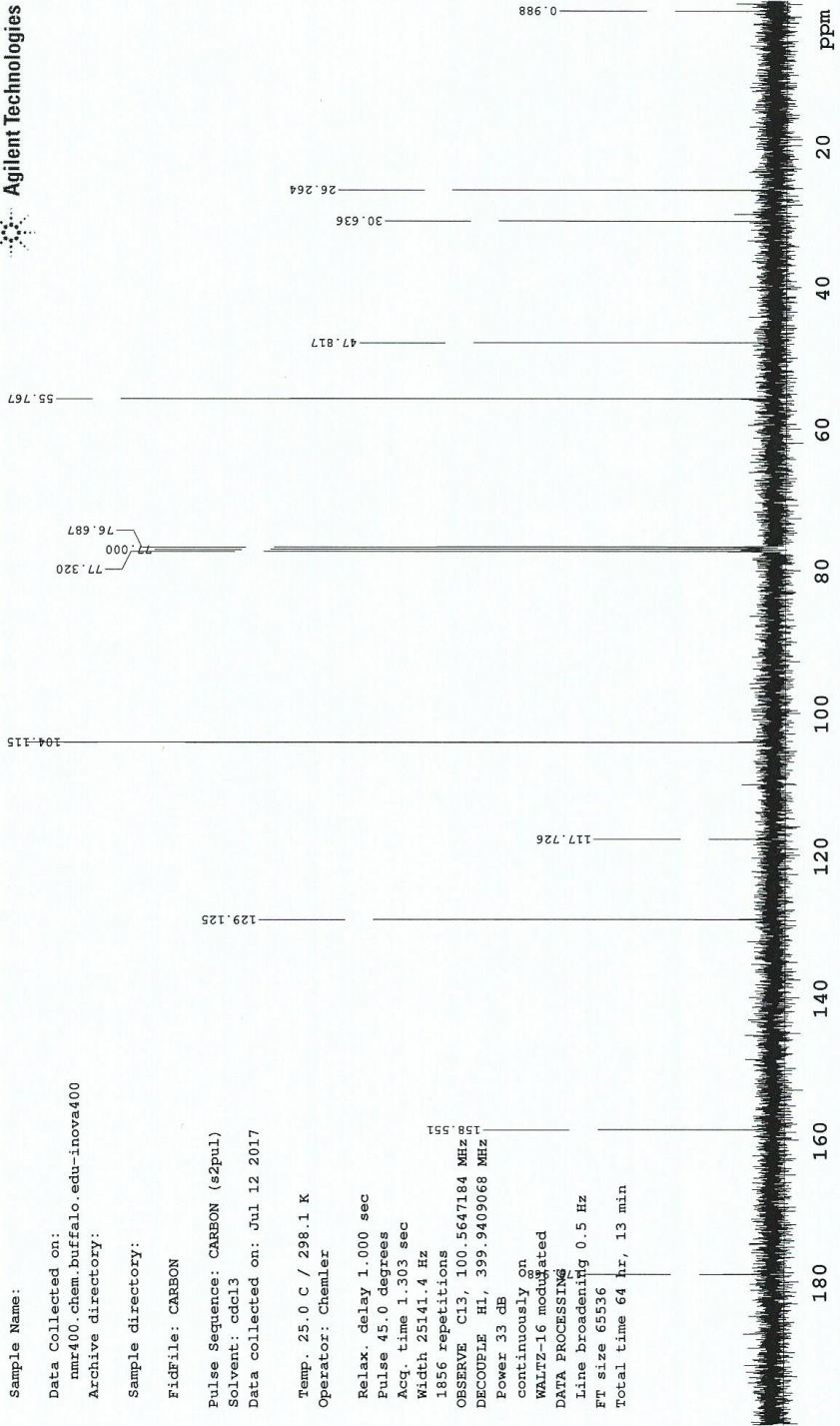
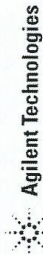
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Jul 12 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
1856 repetitions  
OBSERVE C13, 100.5647184 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 64 hr, 13 min





JE\_1\_129\_A



Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400  
Archive directory:

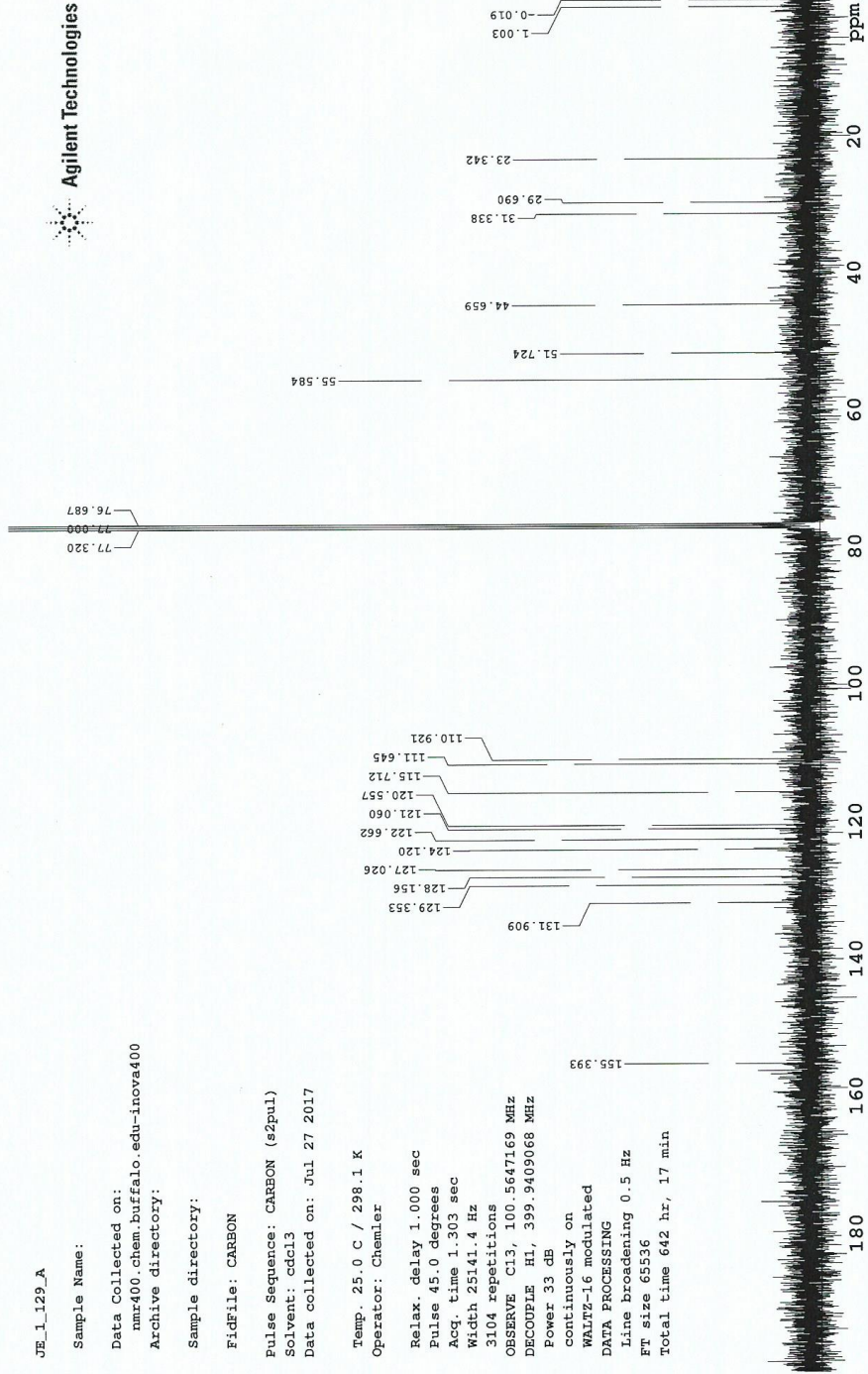
Sample directory:

FidFile: CARBON

Pulse Sequence: CAREON (s2Pul)  
Solvent: cdcl3  
Data collected on: Jul 27 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
3104 repetitions  
OBSERVE C13, 100.5647169 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 642 hr, 17 min







II-144\_crude

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-inova400

Archive directory:

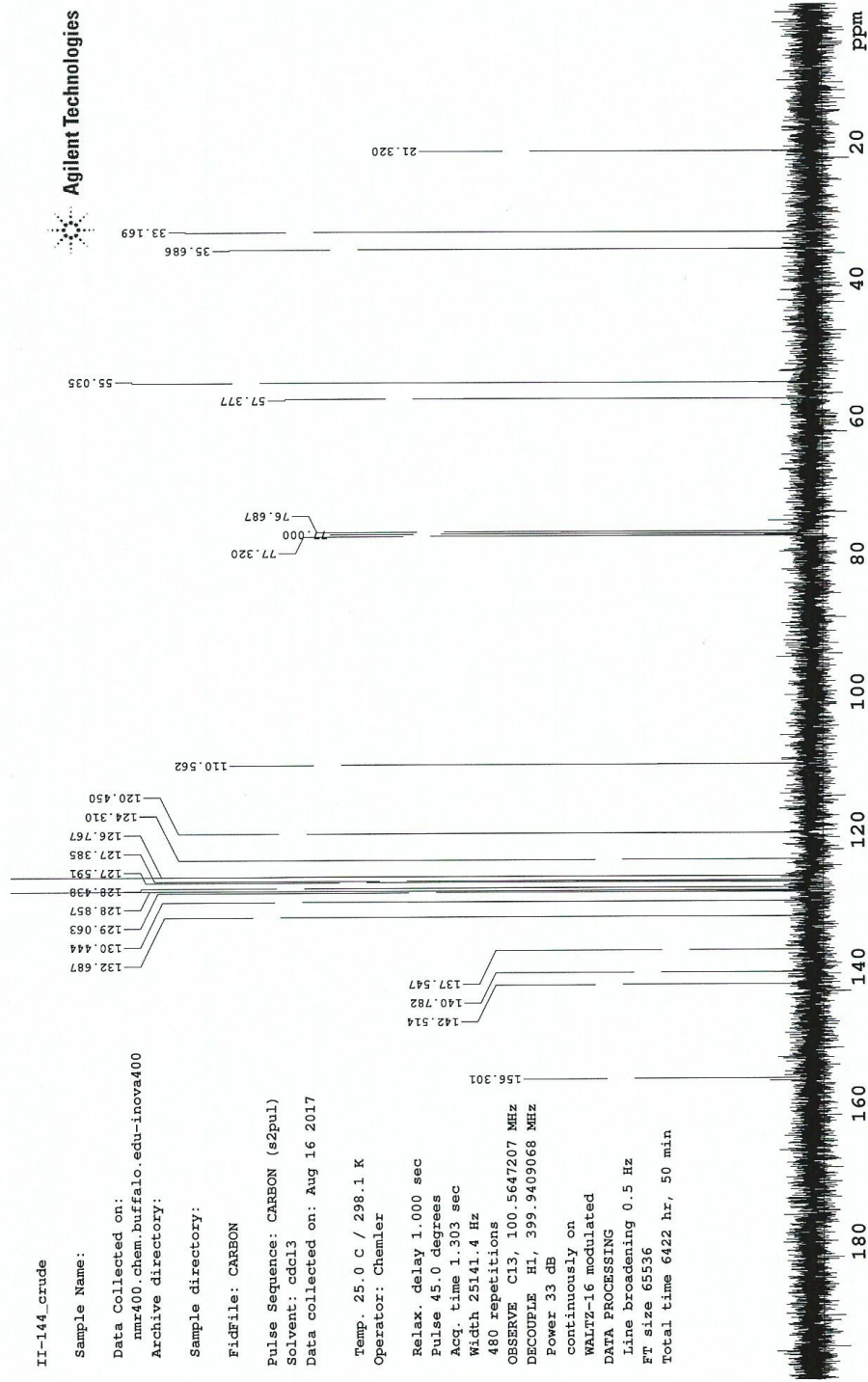
Sample directory:

FidFile: CARBON

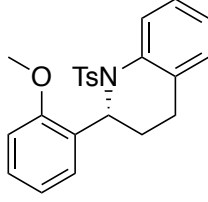
Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Aug 16 2017

Temp. 25.0 C / 298.1 K  
Operator: Chemler

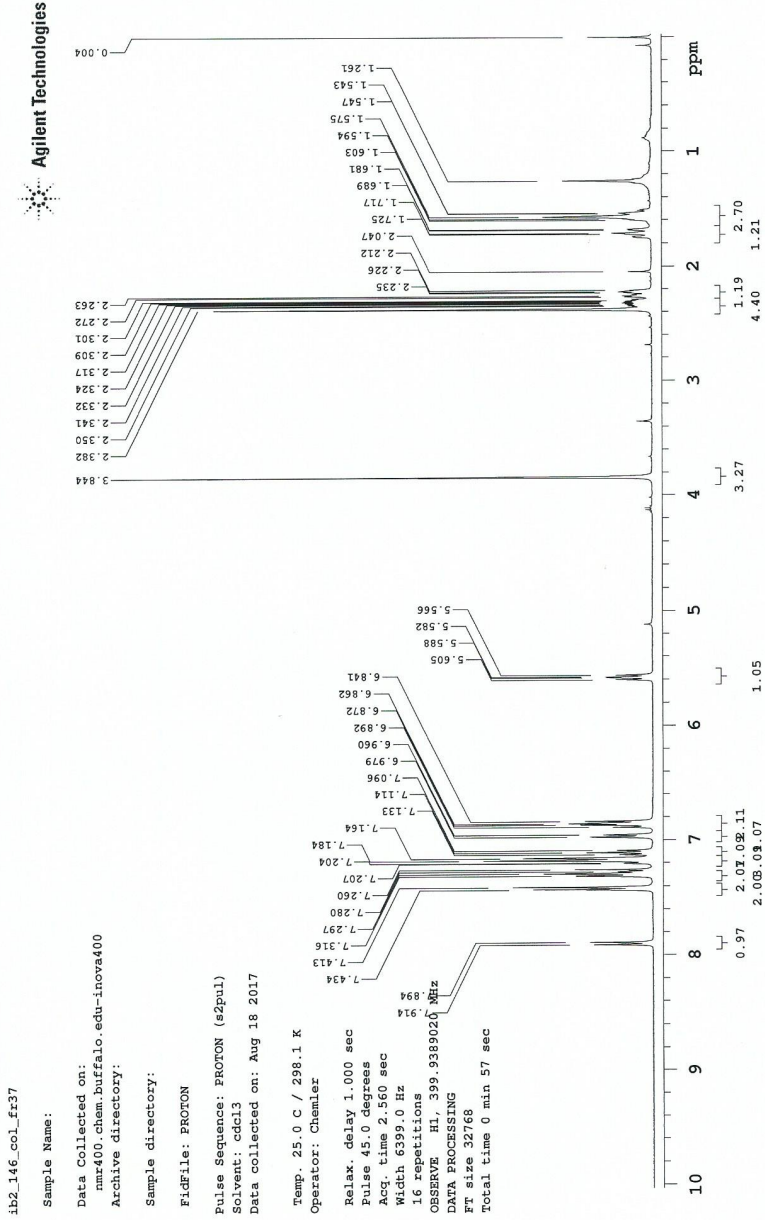
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.303 sec  
Width 25141.4 Hz  
480 repetitions  
OBSERVE C13, 100.5647207 MHz  
DECOUPLE H1, 399.9409068 MHz  
Power 33 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
Ft size 65536  
Total time 6422 hr, 50 min







(13)



ib2\_146\_col\_fr37

Sample Name:

Data Collected on:  
nmr400.chem.buffalo.edu-incova400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Aug 18 2017

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25141.4 Hz

1664 repetitions

OBSERVE C13, 100.5647184 MHz

DECOUPLE H1, 399.9409068 MHz

Power 33 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 642 hr, 17 min

