

## Supporting Information for:

### Longer-Wavelength-Absorbing, Extended Chalcogenorhodamine Dyes

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## General Methods

Reactions conducted under an inert atmosphere were conducted under argon. All reagents were purchased from commercial sources and were used without further purification unless otherwise stated. Tetrahydrofuran (THF) was distilled from sodium benzophenone ketyl prior to use. All other solvents were dried over activated molecular sieves prior to use. Solutions were concentrated in vacuo on a Heidolph rotary evaporator. NMR spectra were recorded on an Inova 500 (500 MHz for  $^1\text{H}$ ), an Inova 400 (400 MHz for  $^1\text{H}$ ), or a Mercury 300 (75.5 MHz for  $^{13}\text{C}$ ) instrument referenced to residual solvent signal, or for chloroform, to TMS. Electronic absorption spectra were recorded on a Perkin-Elmer Lambda 12 spectrophotometer in 1-cm quartz cuvettes. Melting points were determined with a Mel-Temp capillary melting point apparatus and are uncorrected. Magnesium was washed copiously with 1 M HCl, followed by ethanol, followed by diethyl ether, and dried for several hours at 110 °C prior to use. *N,N,N',N'*-Tetramethylethylenediamine (TMEDA) was distilled from potassium hydroxide pellets and stored over activated molecular sieves prior to use. Alkylolithiums (*n*-butyllithium, *s*-butyllithium and *t*-butyllithium) were titrated immediately prior to use with anhydrous diphenylacetic acid.

III-MK-054-dry

Sample Name:

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

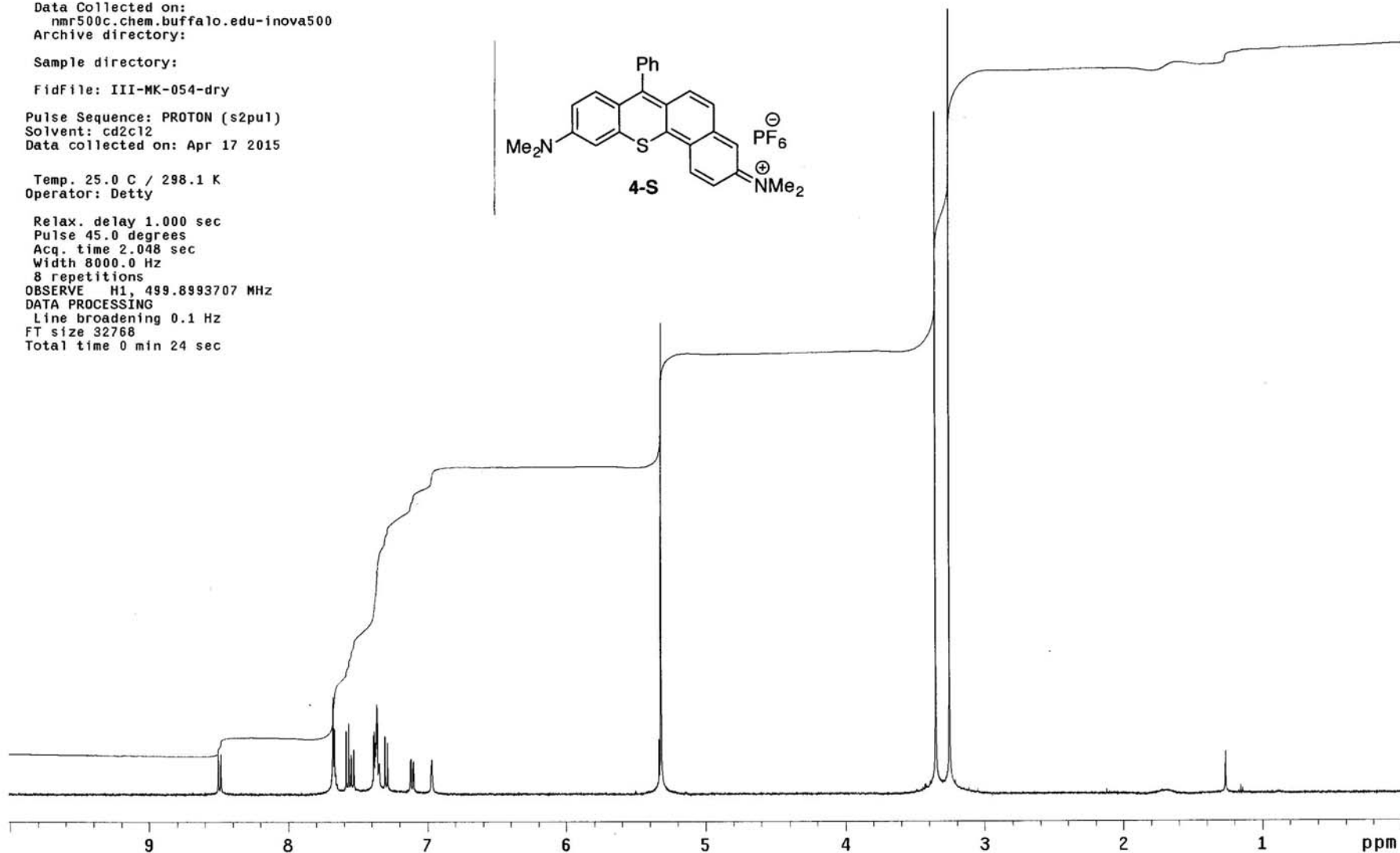
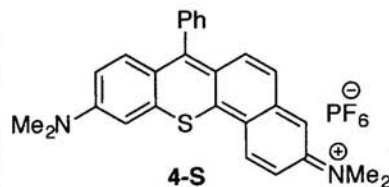
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FidFile: III-MK-054-dry

Pulse Sequence: PROTON (s2pu1)  
Solvent: cd2c12  
Data collected on: Apr 17 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993707 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



III-MK-054carbon

Sample Name:

Data Collected on:  
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Archive directory:

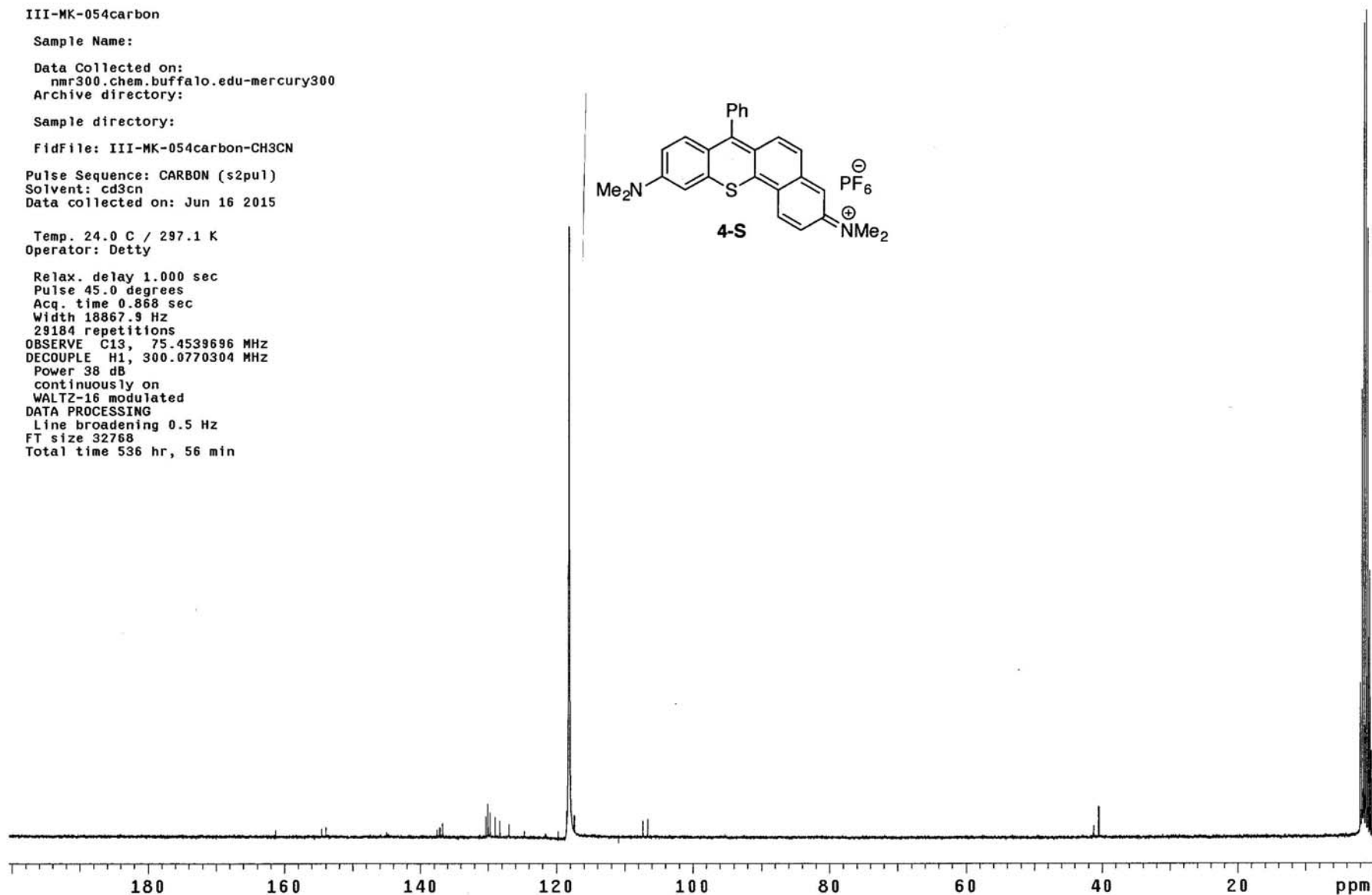
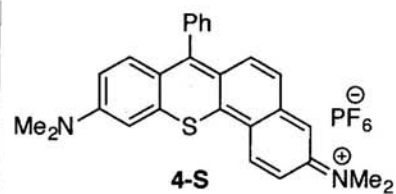
Sample directory:

FidFile: III-MK-054carbon-CH3CN

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3cn  
Data collected on: Jun 16 2015

Temp. 24.0 C / 297.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
29184 repetitions  
OBSERVE C13, 75.4539696 MHz  
DECOUPLE H1, 300.0770304 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



III-MK-054carbon

Sample Name:

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

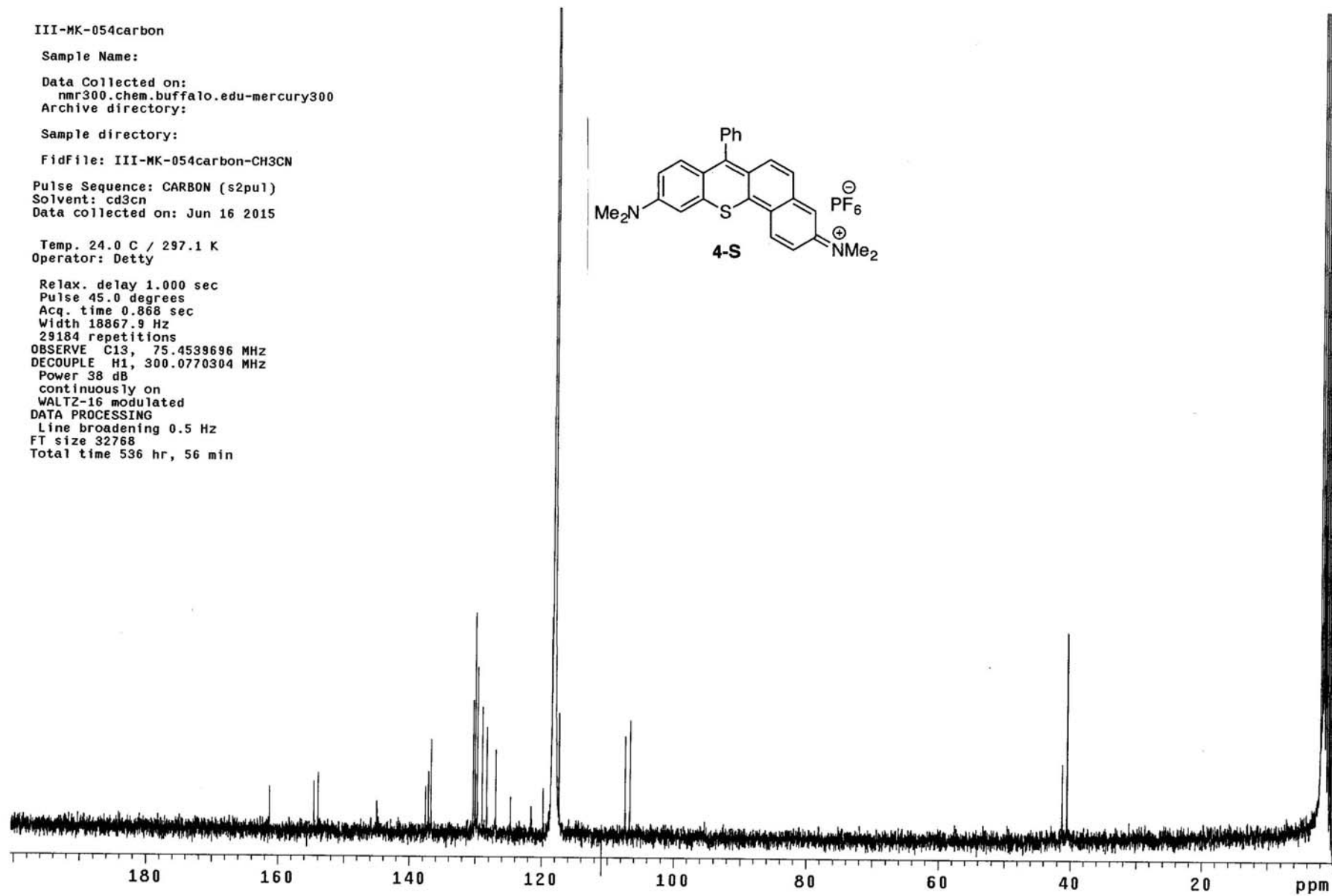
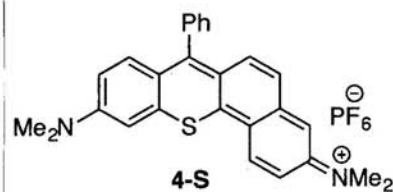
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FidFile: III-MK-054carbon-CH3CN

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3cn  
Data collected on: Jun 16 2015

Temp. 24.0 C / 297.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
29184 repetitions  
OBSERVE C13, 75.4539696 MHz  
DECOUPLE H1, 300.0770304 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



Sample Name: II-MK-207

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

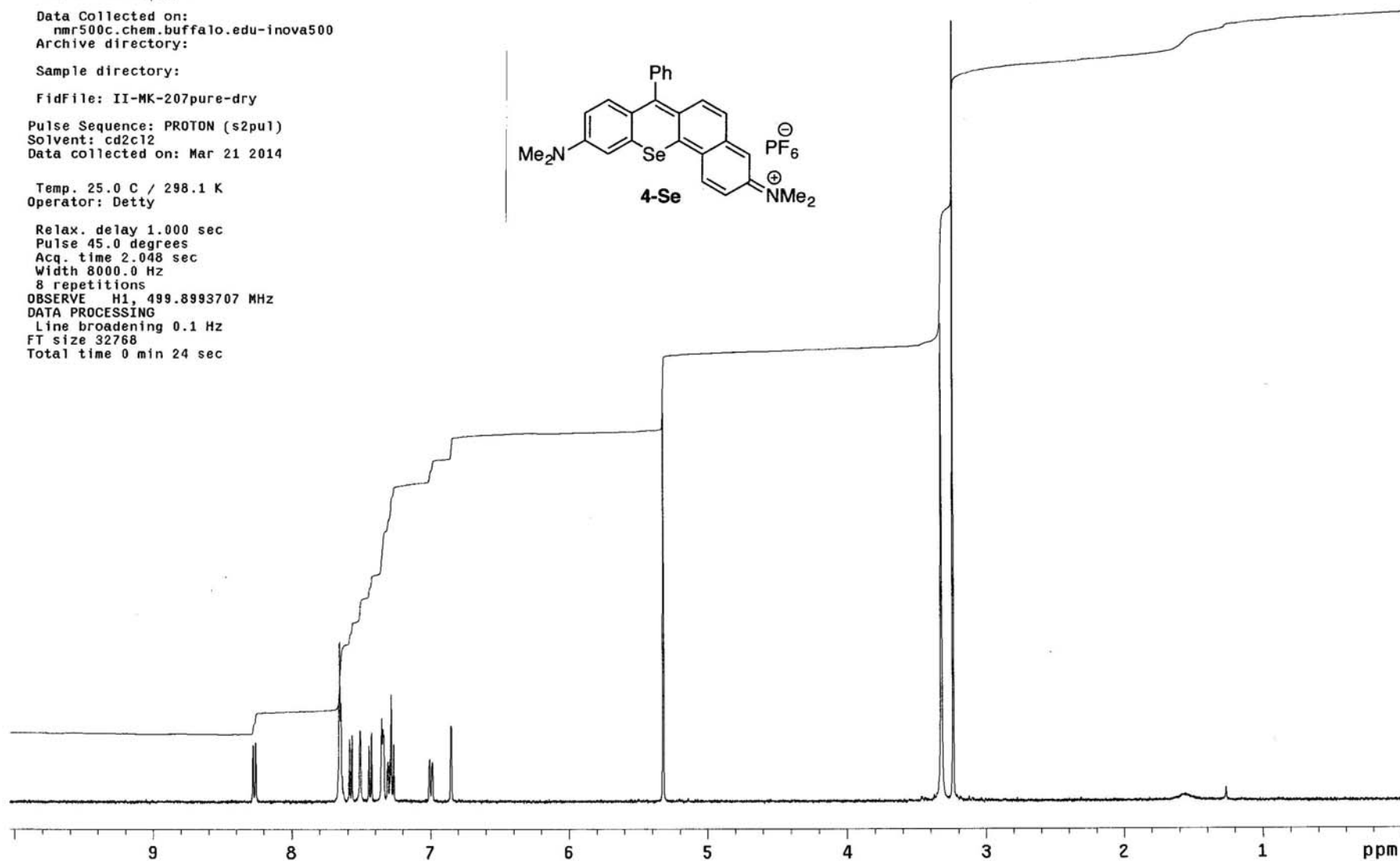
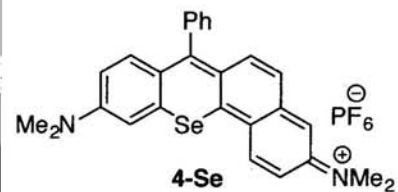
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Pulse Sequence: PROTON (s2pu1)  
Solvent: cd2cl2  
Data collected on: Mar 21 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993707 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



II-MK-207carbon

Sample Name:

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

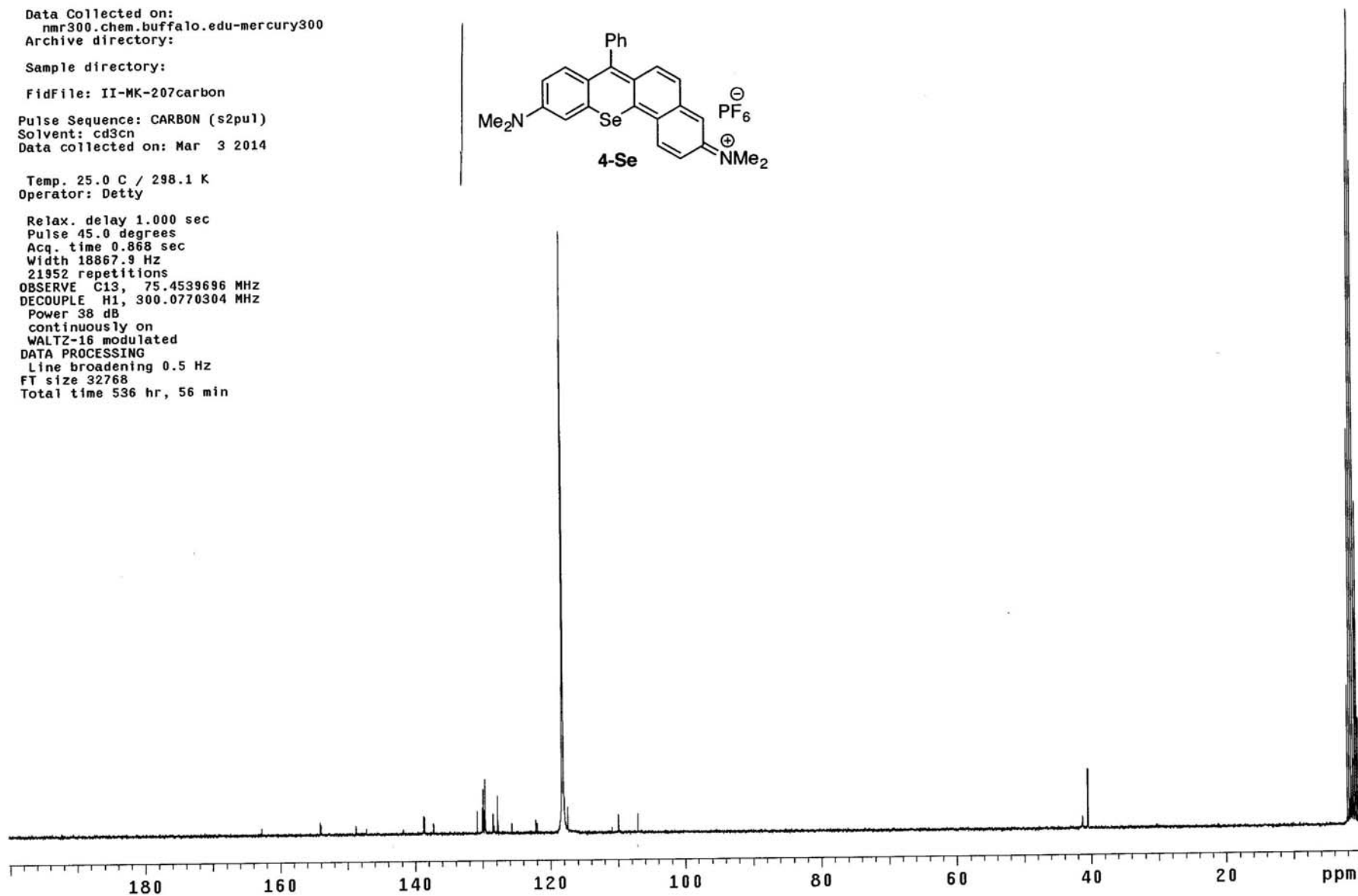
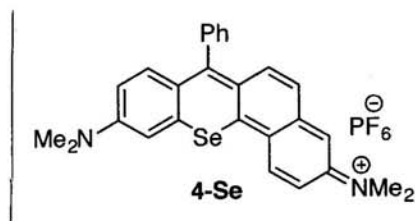
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FidFile: II-MK-207carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3cn  
Data collected on: Mar 3 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
21952 repetitions  
OBSERVE C13, 75.4539696 MHz  
DECOUPLE H1, 300.0770304 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



II-MK-207carbon

Sample Name:

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

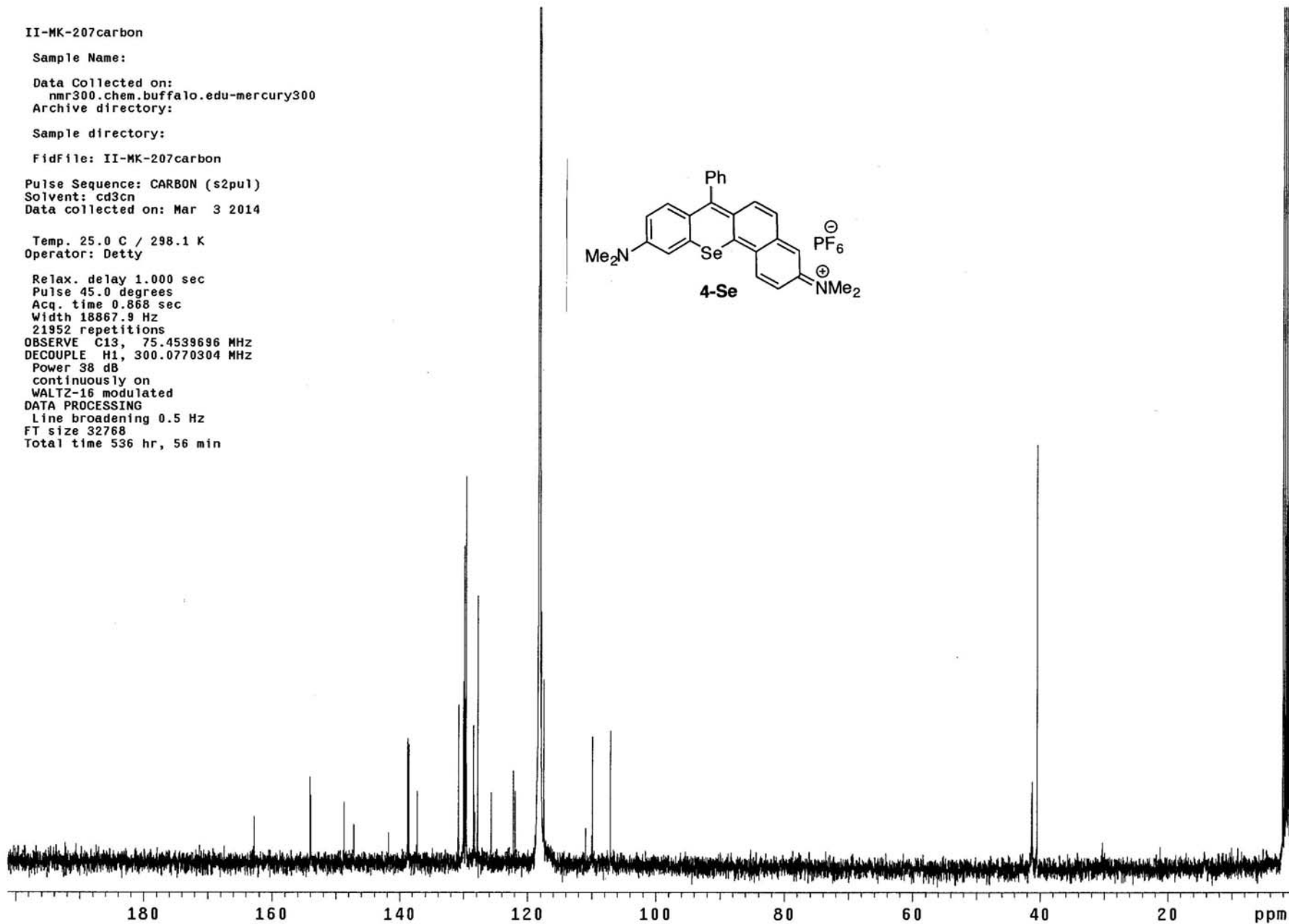
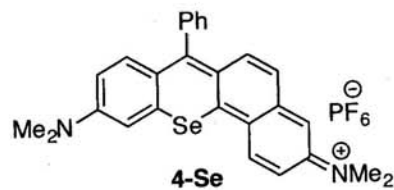
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Pulse Sequence: CARBON (s2pul)  
Solvent: cd3cn  
Data collected on: Mar 3 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
21952 repetitions  
OBSERVE C13, 75.4539696 MHz  
DECOUPLE H1, 300.0770304 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S8



II-MK-231

Sample Name:

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

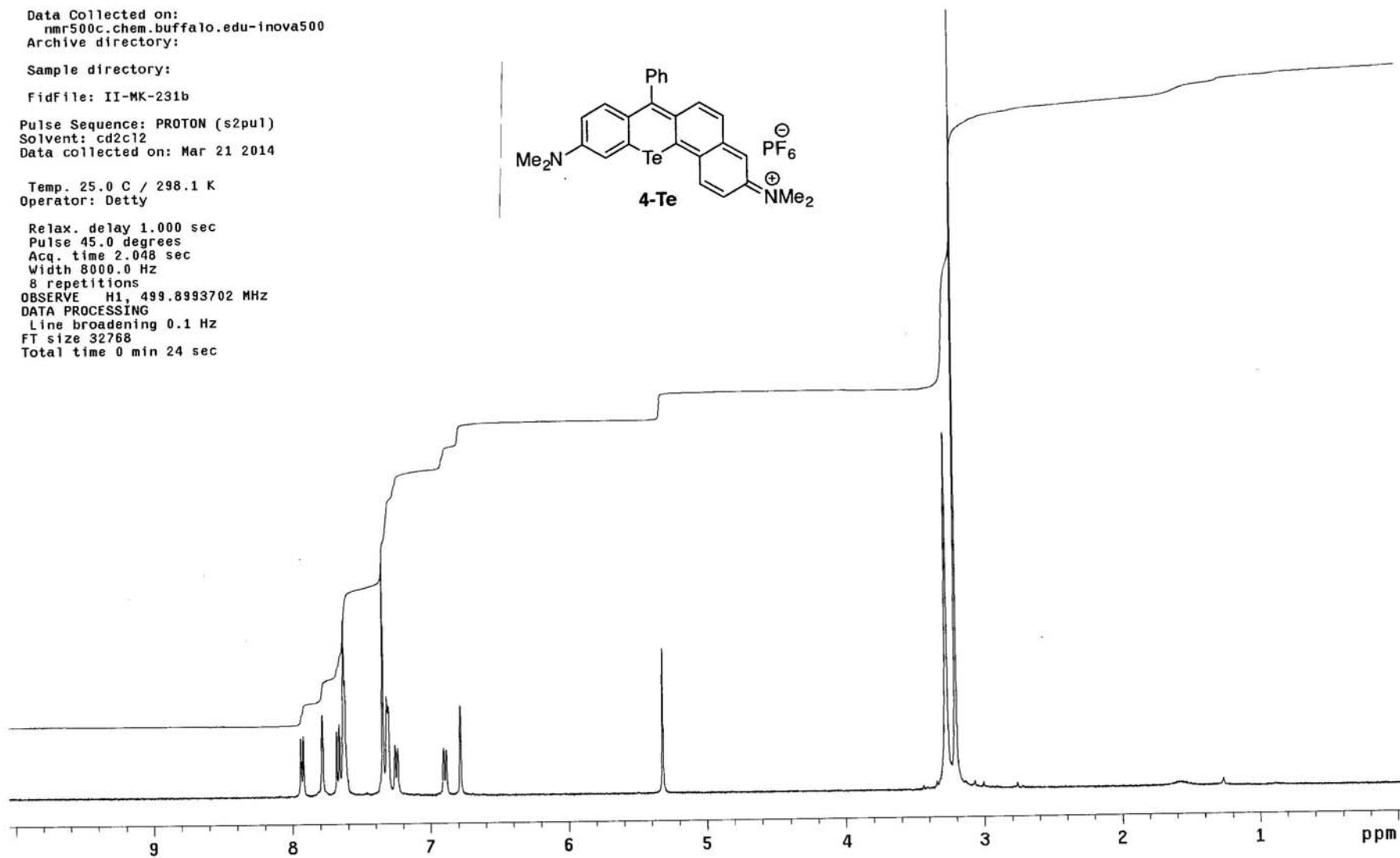
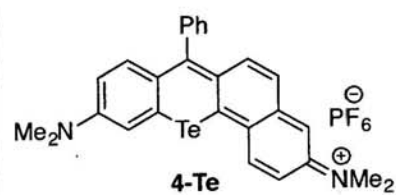
Sample directory:

FidFile: II-MK-231b

Pulse Sequence: PROTON (s2pul)  
Solvent: cd2cl2  
Data collected on: Mar 21 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993702 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



III-MK-056-dry-2

Sample Name:

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

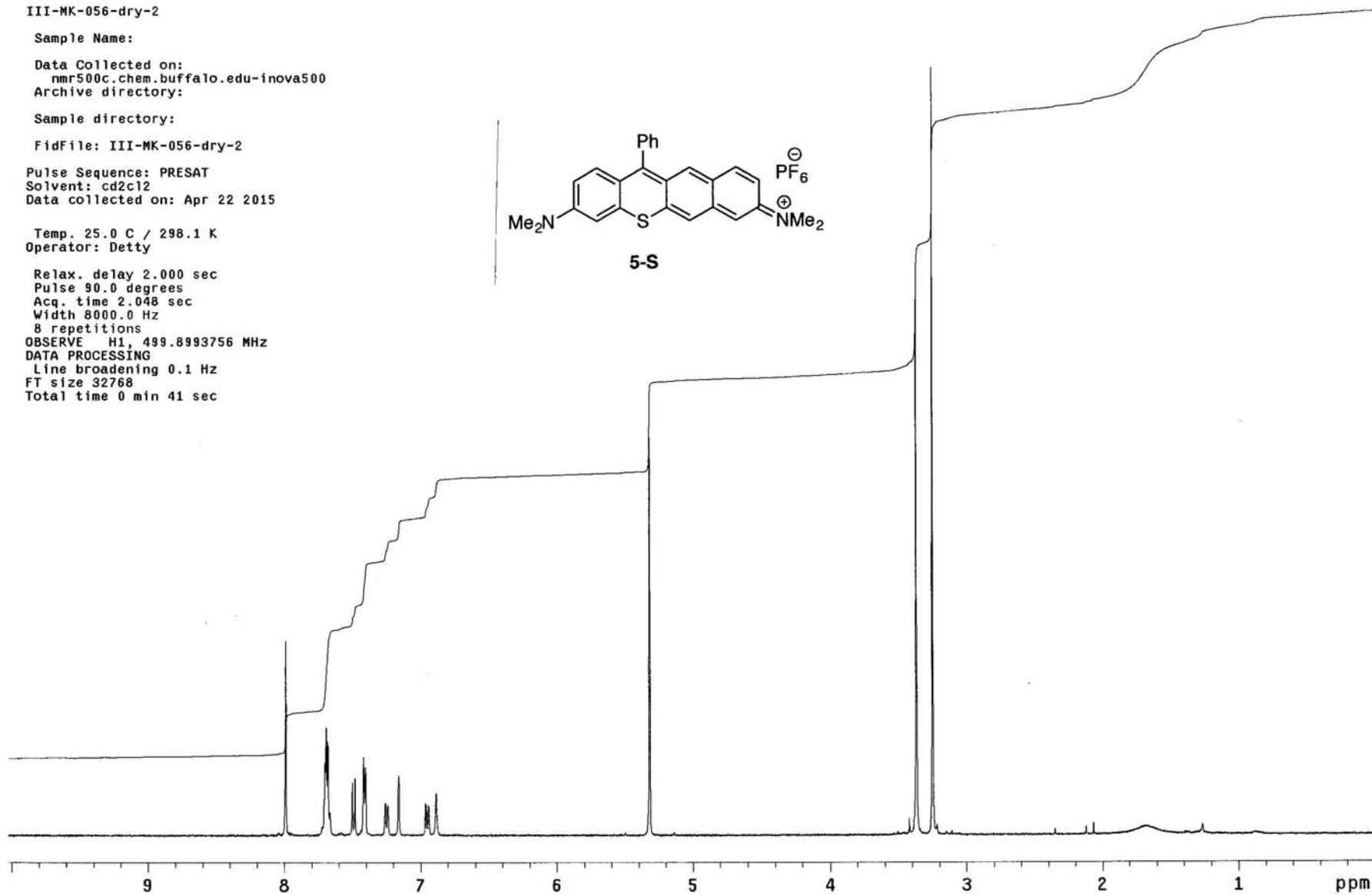
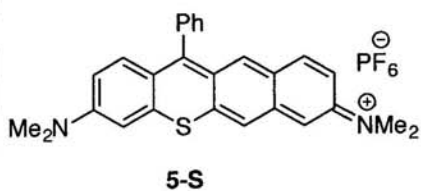
Sample directory:

FidFile: III-MK-056-dry-2

Pulse Sequence: PRESAT  
Solvent: cd2cl2  
Data collected on: Apr 22 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 2.000 sec  
Pulse 90.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993756 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 41 sec



III-MK-056carbon

Sample Name:

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

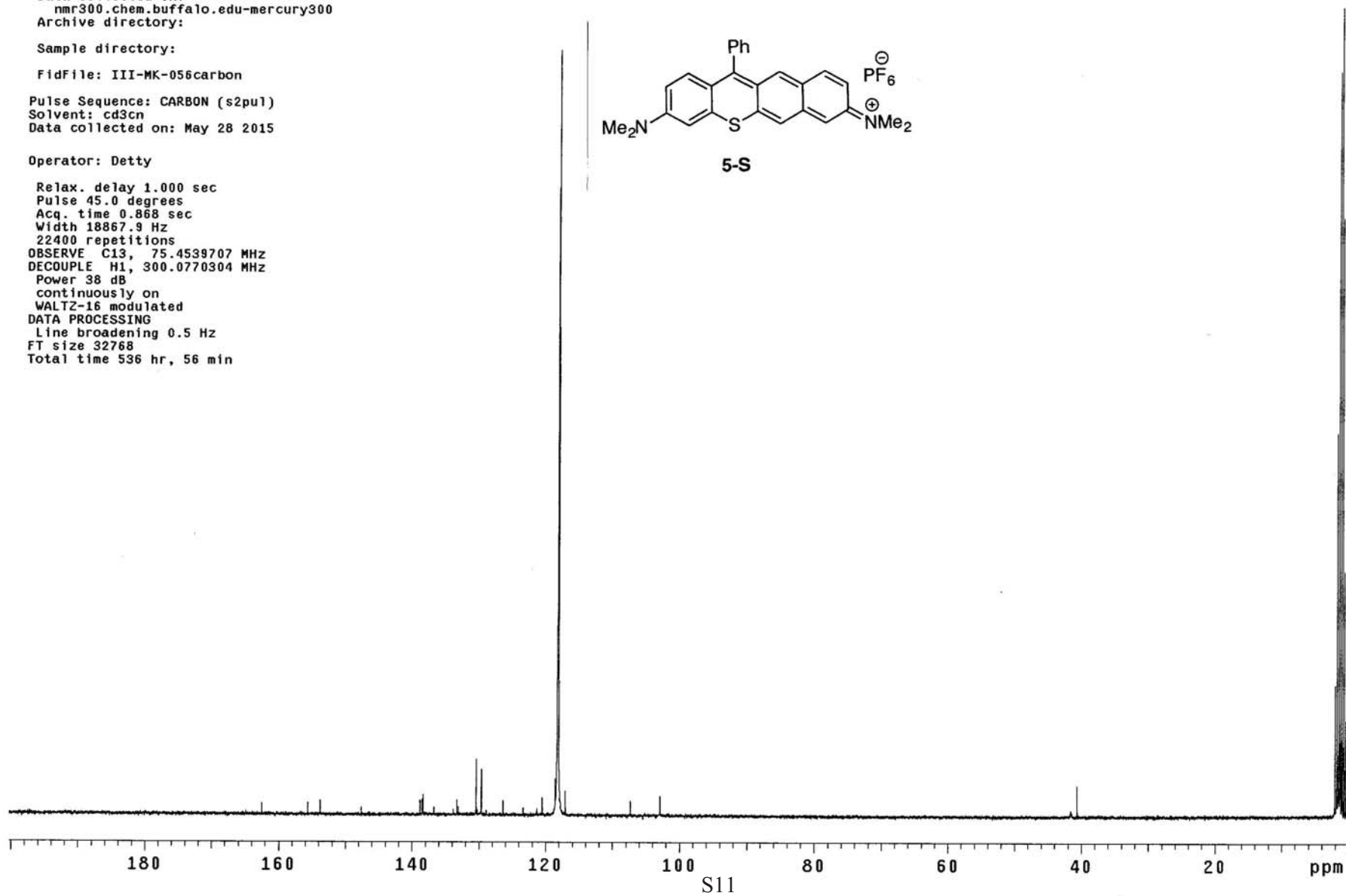
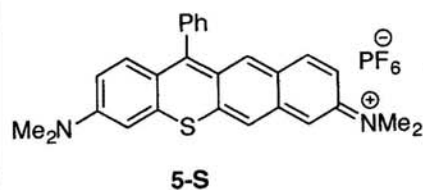
Sample directory:

FidFile: III-MK-056carbon

Pulse Sequence: CARBON (s2pu1)  
Solvent: cd3cn  
Data collected on: May 28 2015

Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
22400 repetitions  
OBSERVE C13, 75.4539707 MHz  
DECOUPLE H1, 300.0770304 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



III-MK-056carbon

Sample Name:

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

Archive directory:

Sample directory:

FidFile: III-MK-056carbon

Pulse Sequence: CARBON (s2pu1)

Solvent: cd3cn

Data collected on: May 28 2015

Operator: Detty

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

22400 repetitions

OBSERVE C13, 75.4539707 MHz

DECOUPLE H1, 300.0770304 MHz

Power 38 dB

continuously on

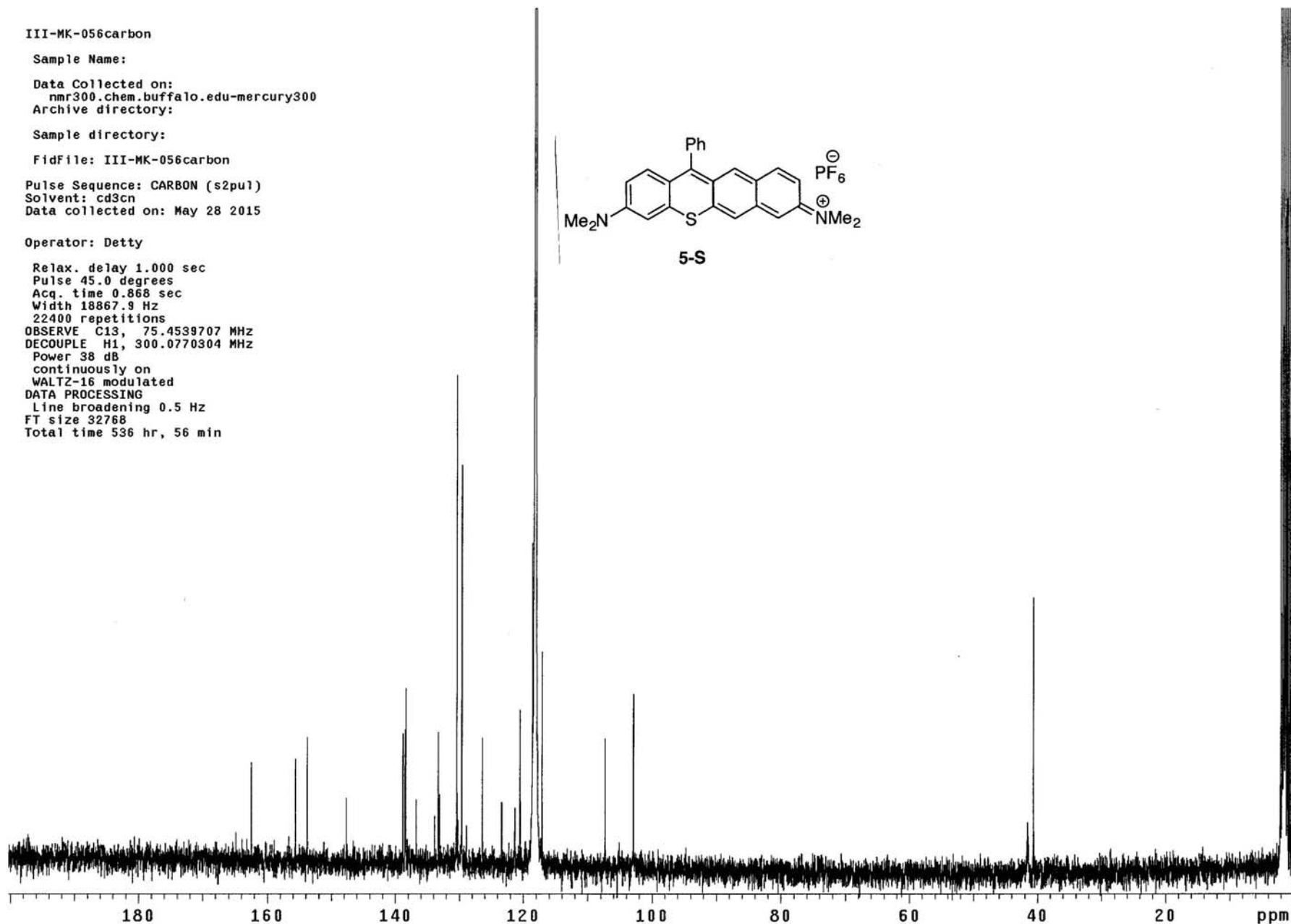
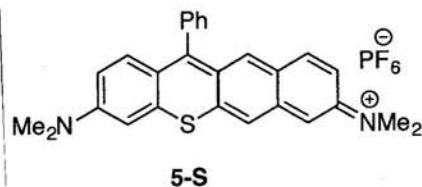
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 536 hr, 56 min



S12

III-MK-050-dry

Sample Name:

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

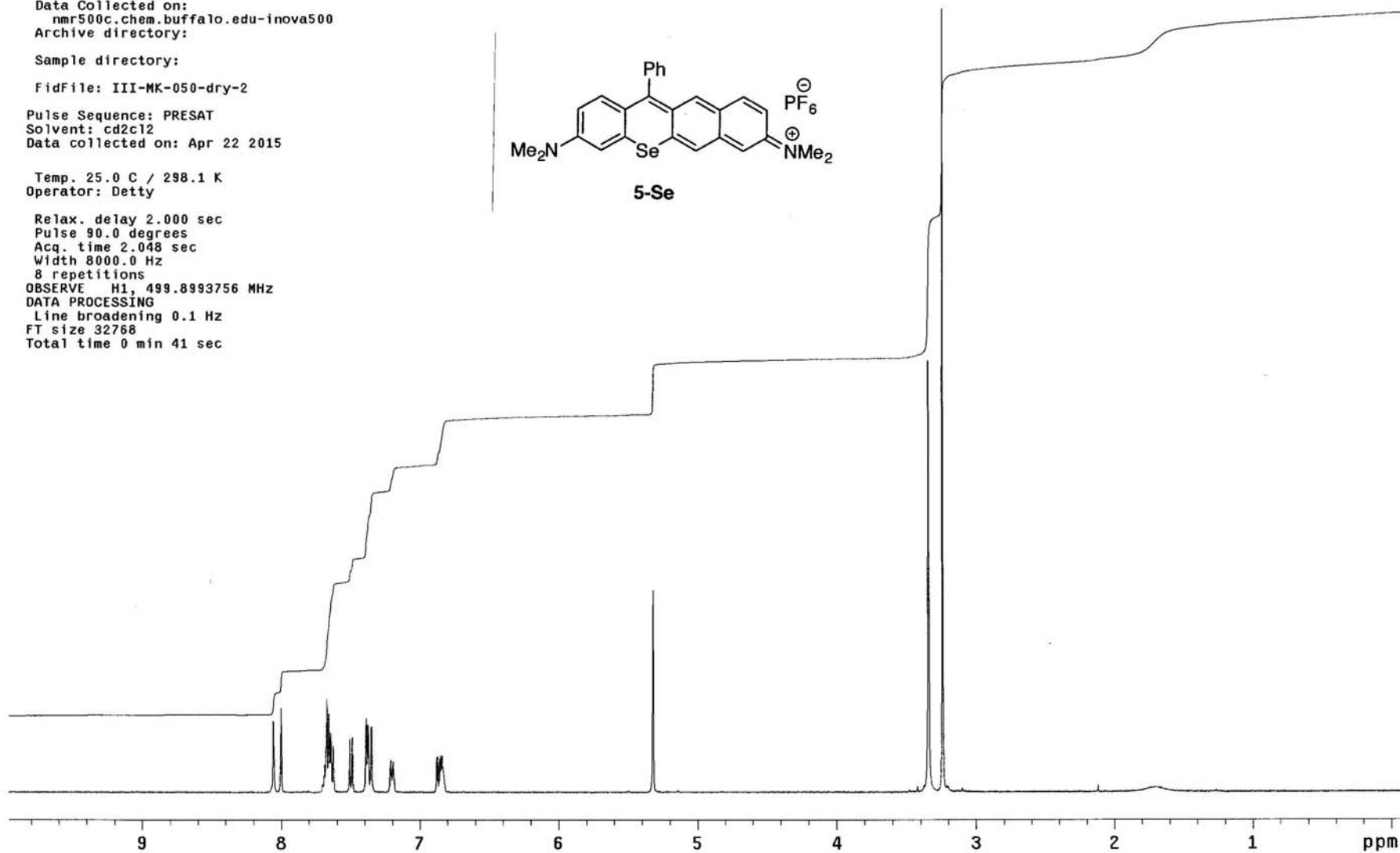
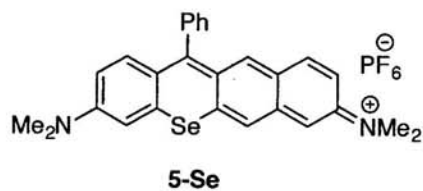
Sample directory:

FidFile: III-MK-050-dry-2

Pulse Sequence: PRESAT  
Solvent: cd2cl2  
Data collected on: Apr 22 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 2.000 sec  
Pulse 90.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993756 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 41 sec



III-MK-050carbon

Sample Name:

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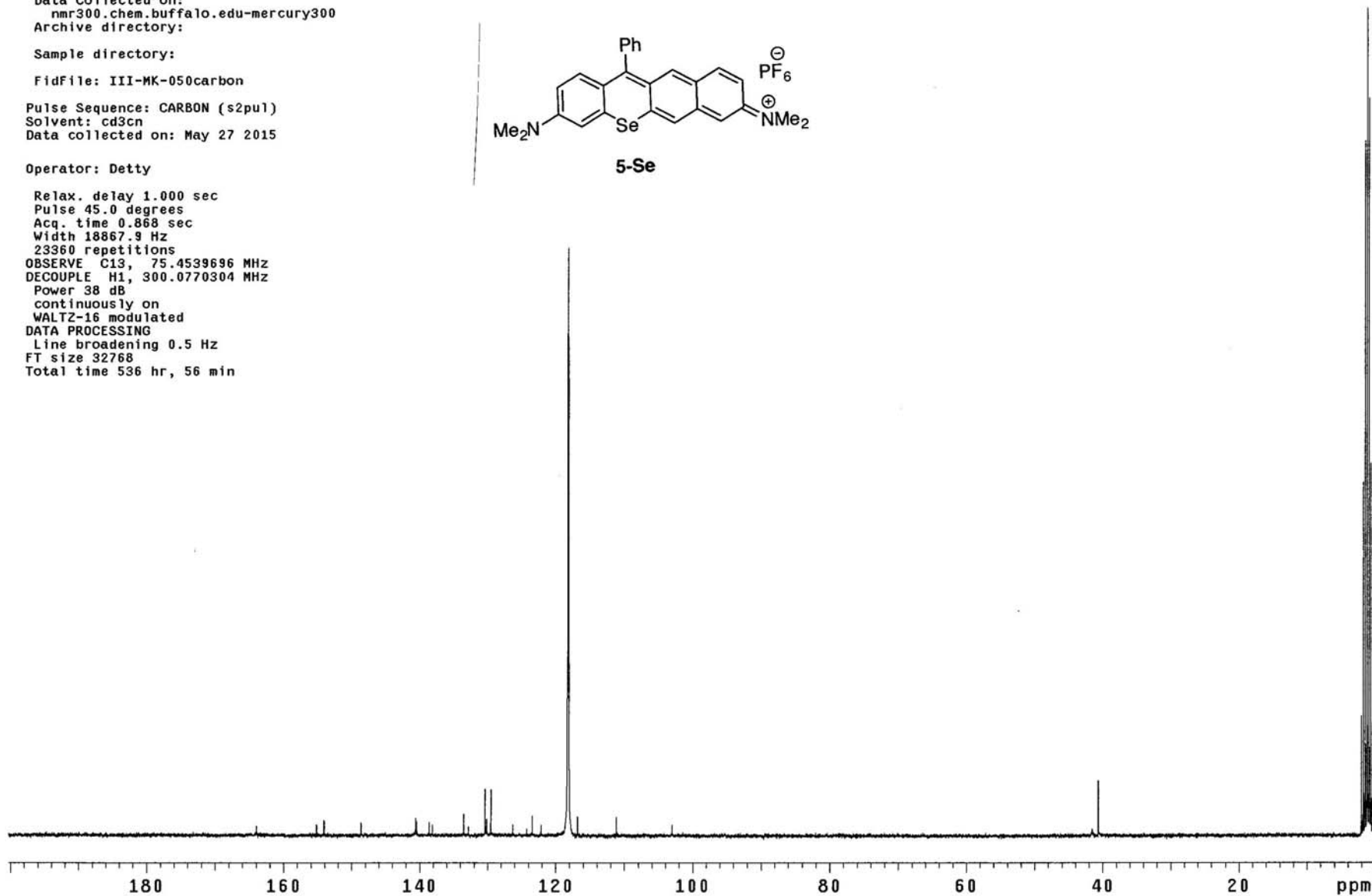
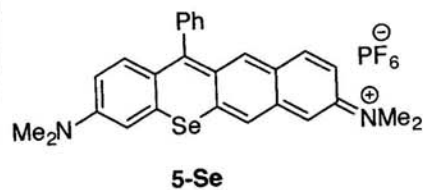
Sample directory:

FidFile: III-MK-050carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3cn  
Data collected on: May 27 2015

Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
23360 repetitions  
OBSERVE C13, 75.4539696 MHz  
DECOUPLE H1, 300.0770304 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S14

III-MK-050carbon

Sample Name:

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

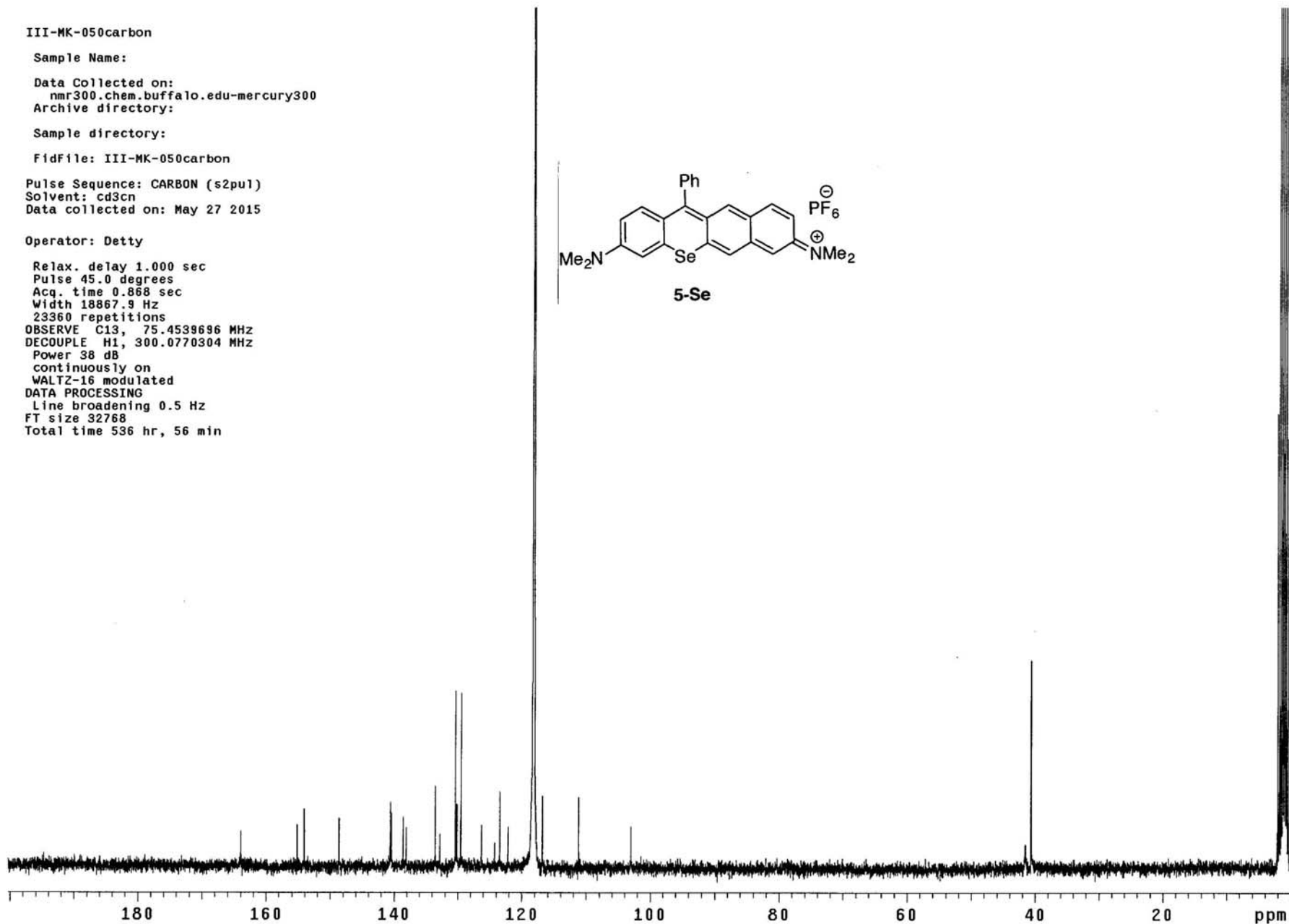
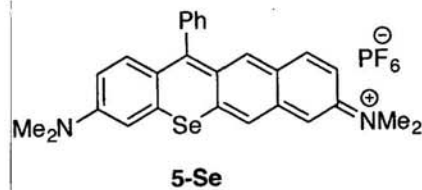
Sample directory:

FidFile: III-MK-050carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cd3cn  
Data collected on: May 27 2015

Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
23360 repetitions  
OBSERVE C13, 75.4539696 MHz  
DECOUPLE H1, 300.0770304 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S15

II-MK-230recryst

Sample Name:

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

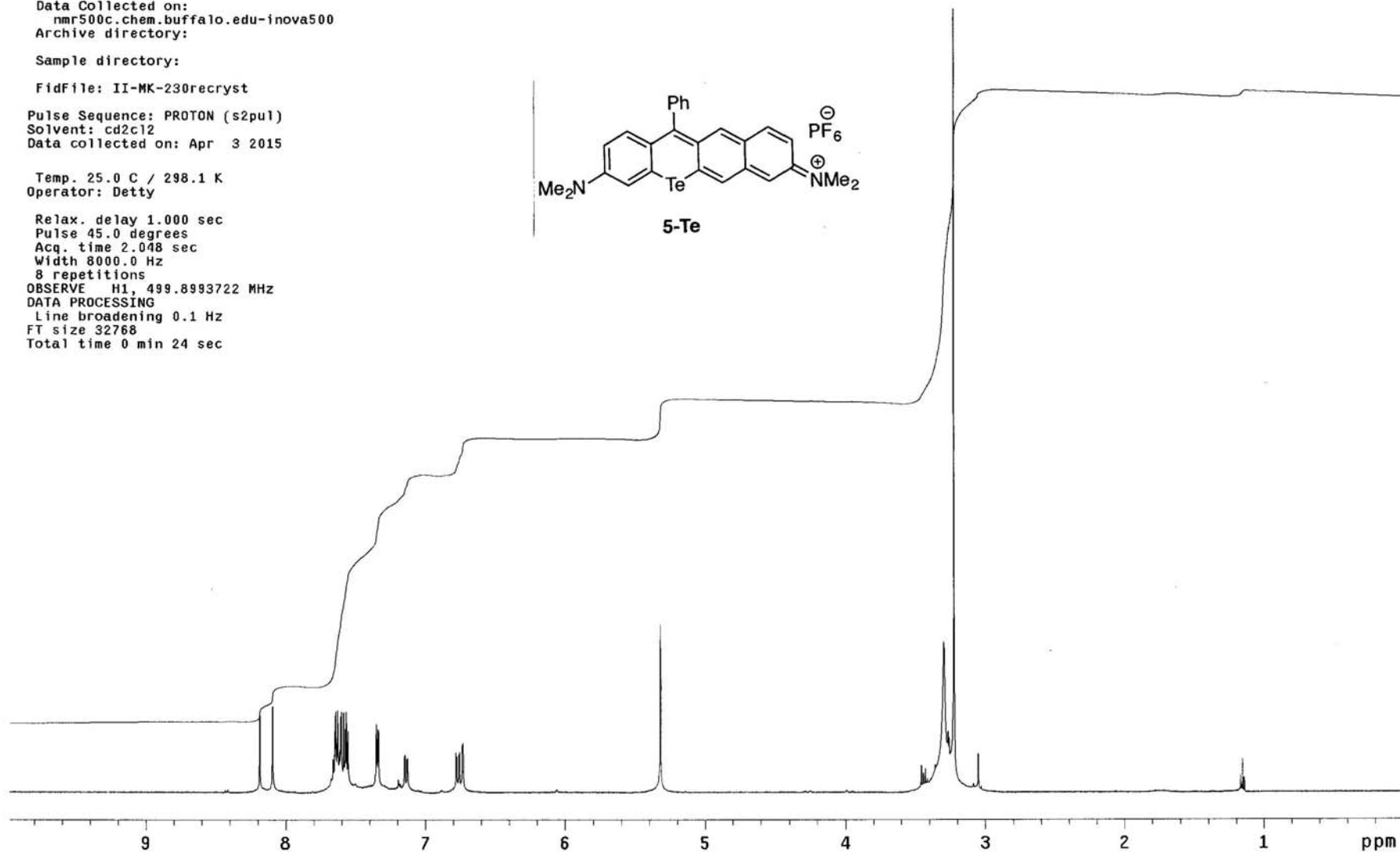
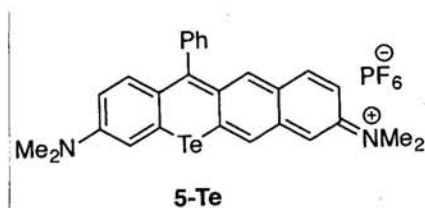
Sample directory:

FidFile: II-MK-230recryst

Pulse Sequence: PROTON (s2pul)  
Solvent: cd2cl2  
Data collected on: Apr 3 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993722 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec





Bent S Xan

Sample Name:

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

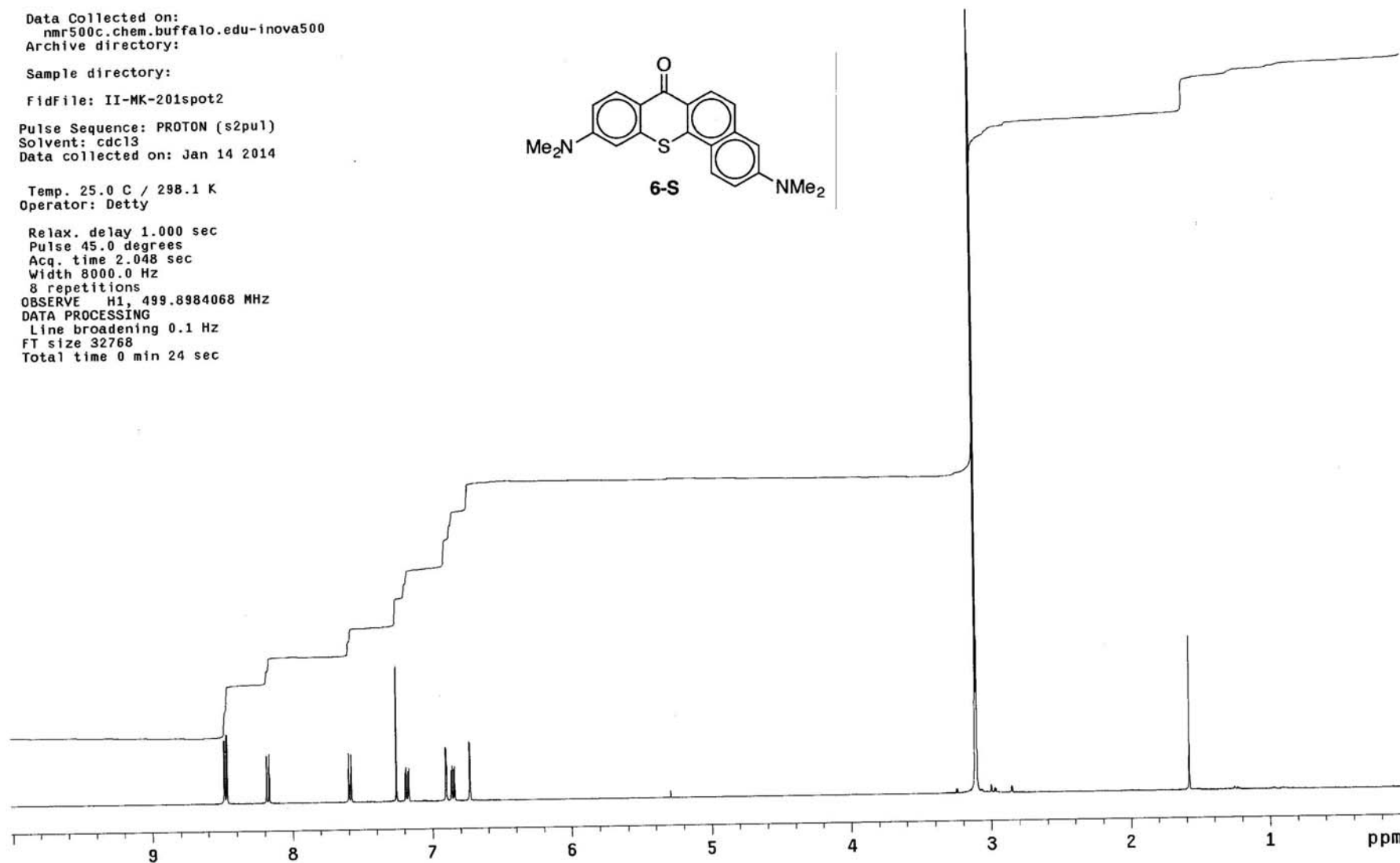
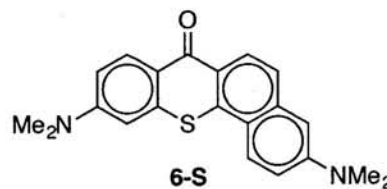
Sample directory:

FidFile: II-MK-201spot2

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Jan 14 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984068 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



Bent S xan

Sample Name:

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

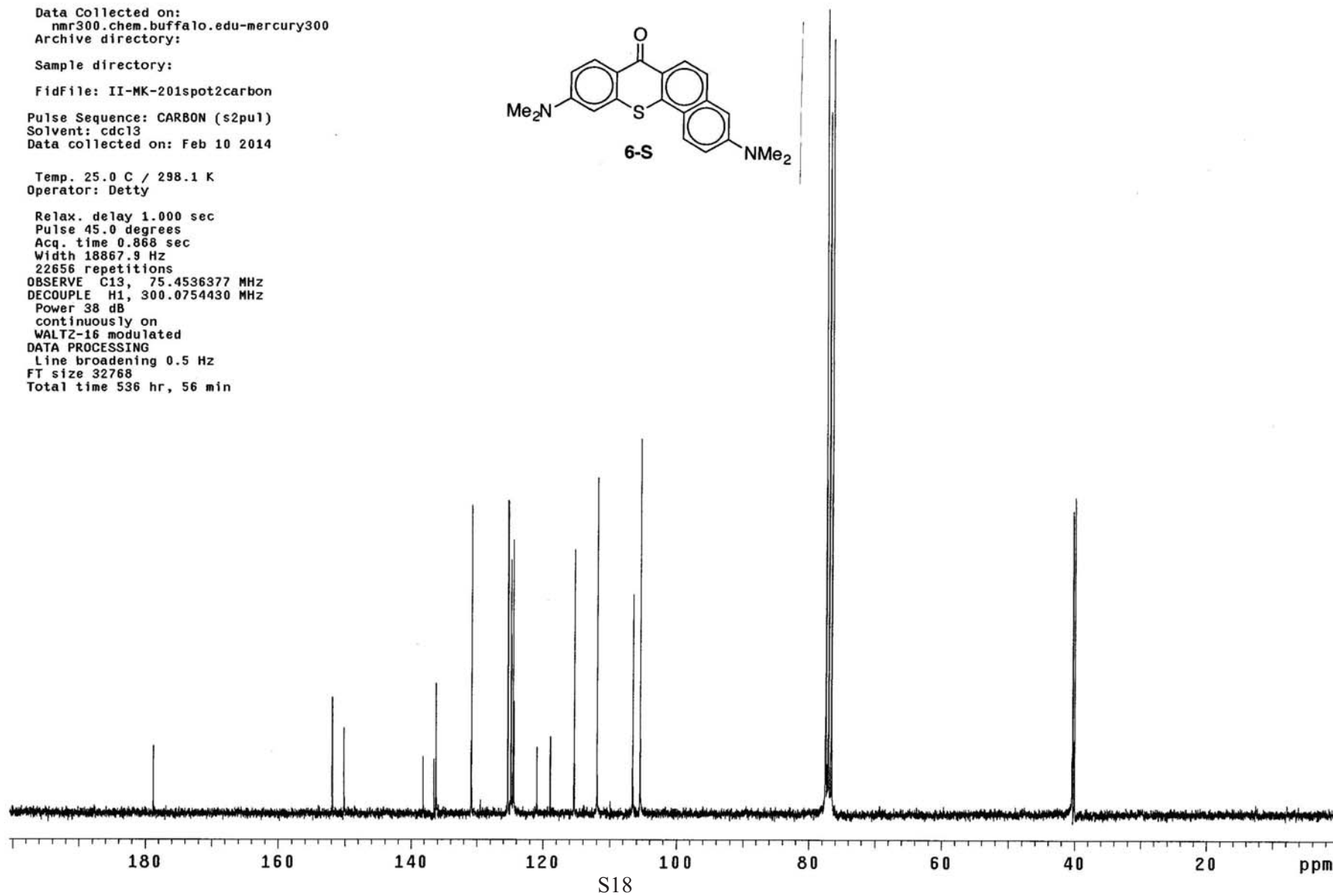
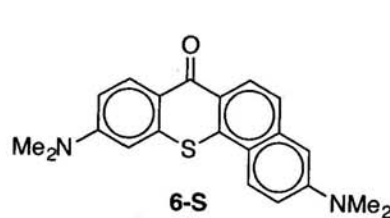
Sample directory:

FidFile: II-MK-201spot2carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Feb 10 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
22656 repetitions  
OBSERVE C13, 75.4536377 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



Se bent xan

Sample Name:

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

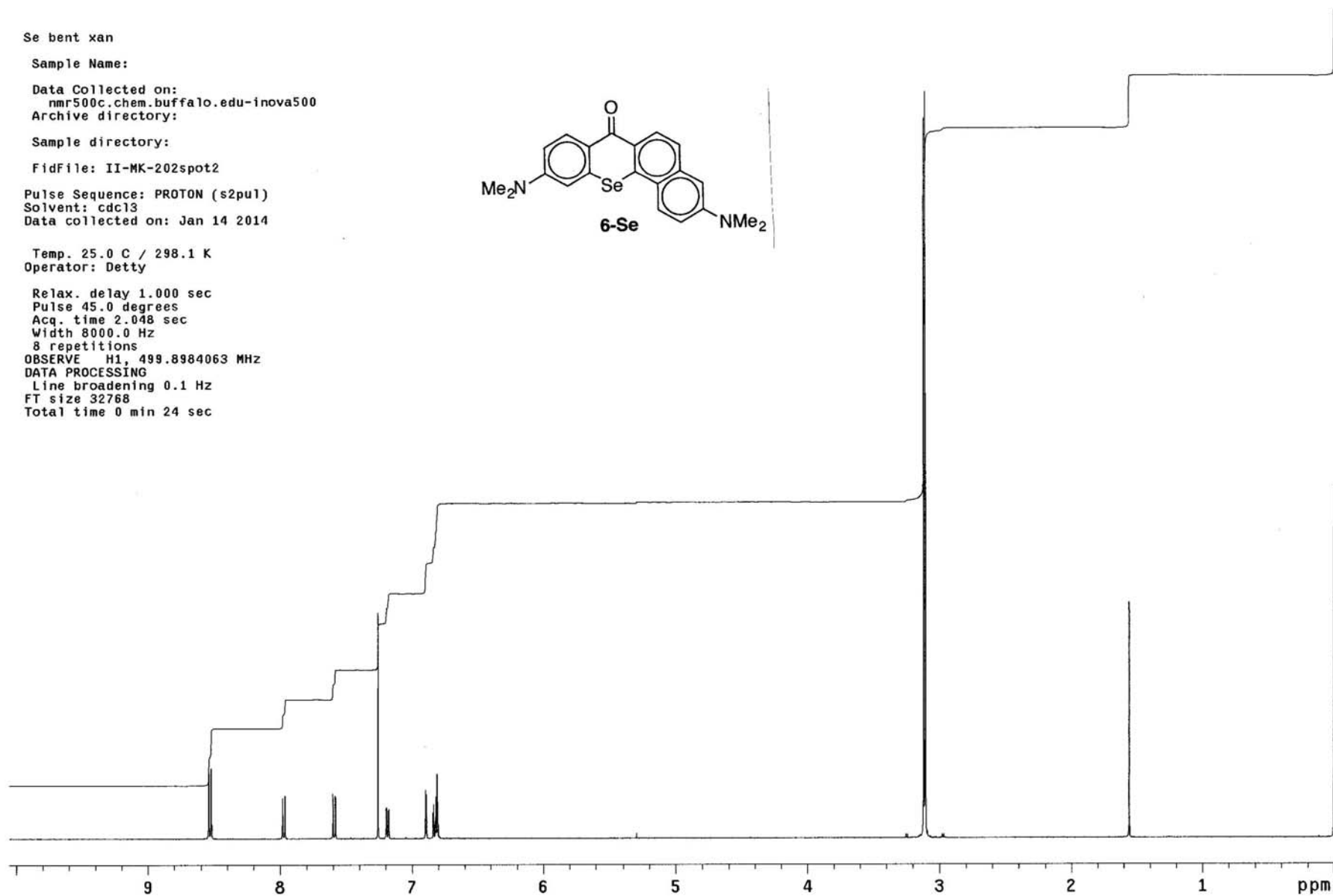
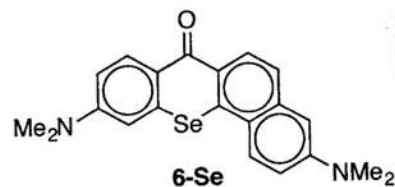
Sample directory:

FidFile: II-MK-202spot2

Pulse Sequence: PROTON (s2pu1)  
Solvent: cdc13  
Data collected on: Jan 14 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984063 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



Bent Se xan Carbon

Sample Name:

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

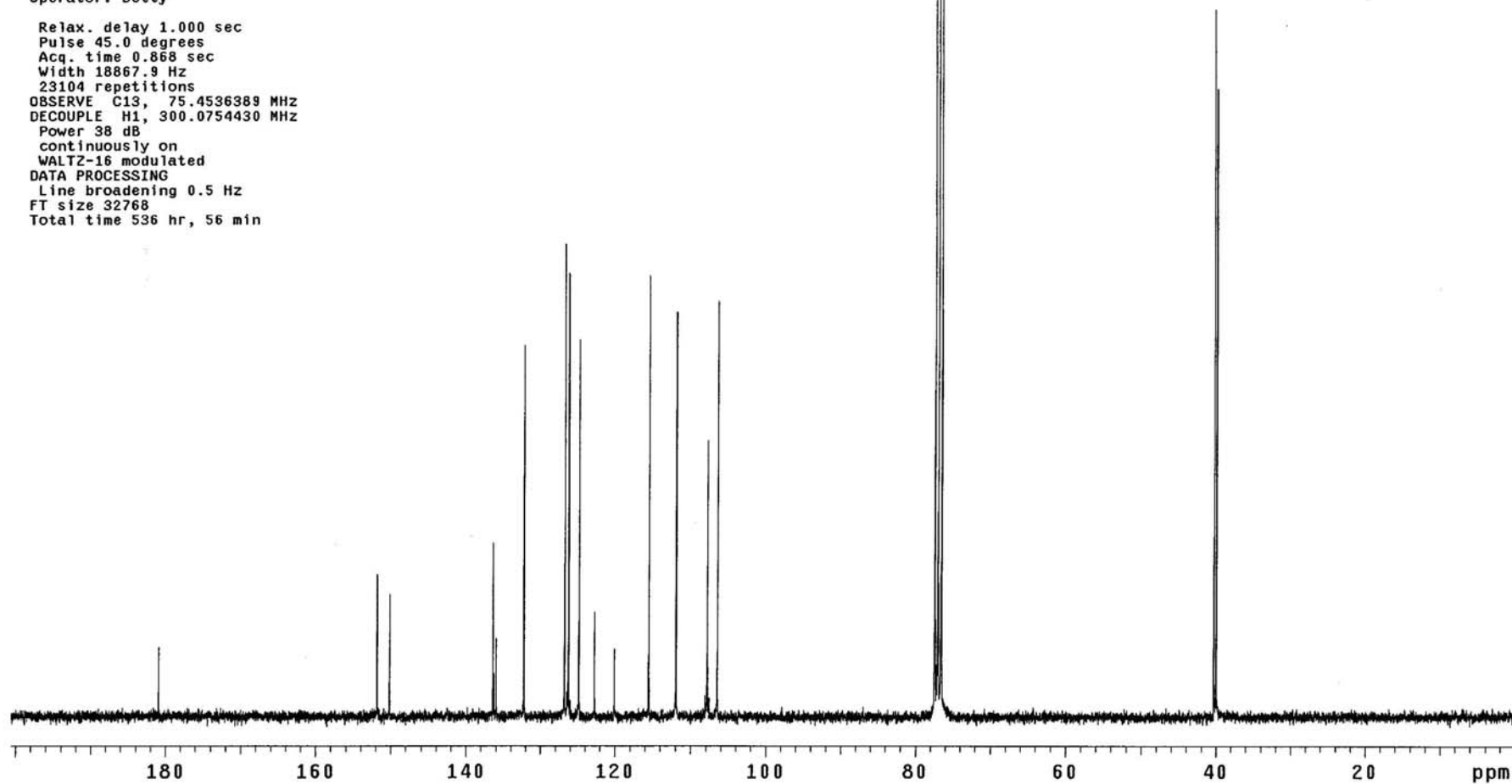
Sample directory:

FidFile: II-MK-202spot2carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 13 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
23104 repetitions  
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  
FT size 32768  
Total time 536 hr, 56 min



S20

Bent Te Xan

Sample Name:

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

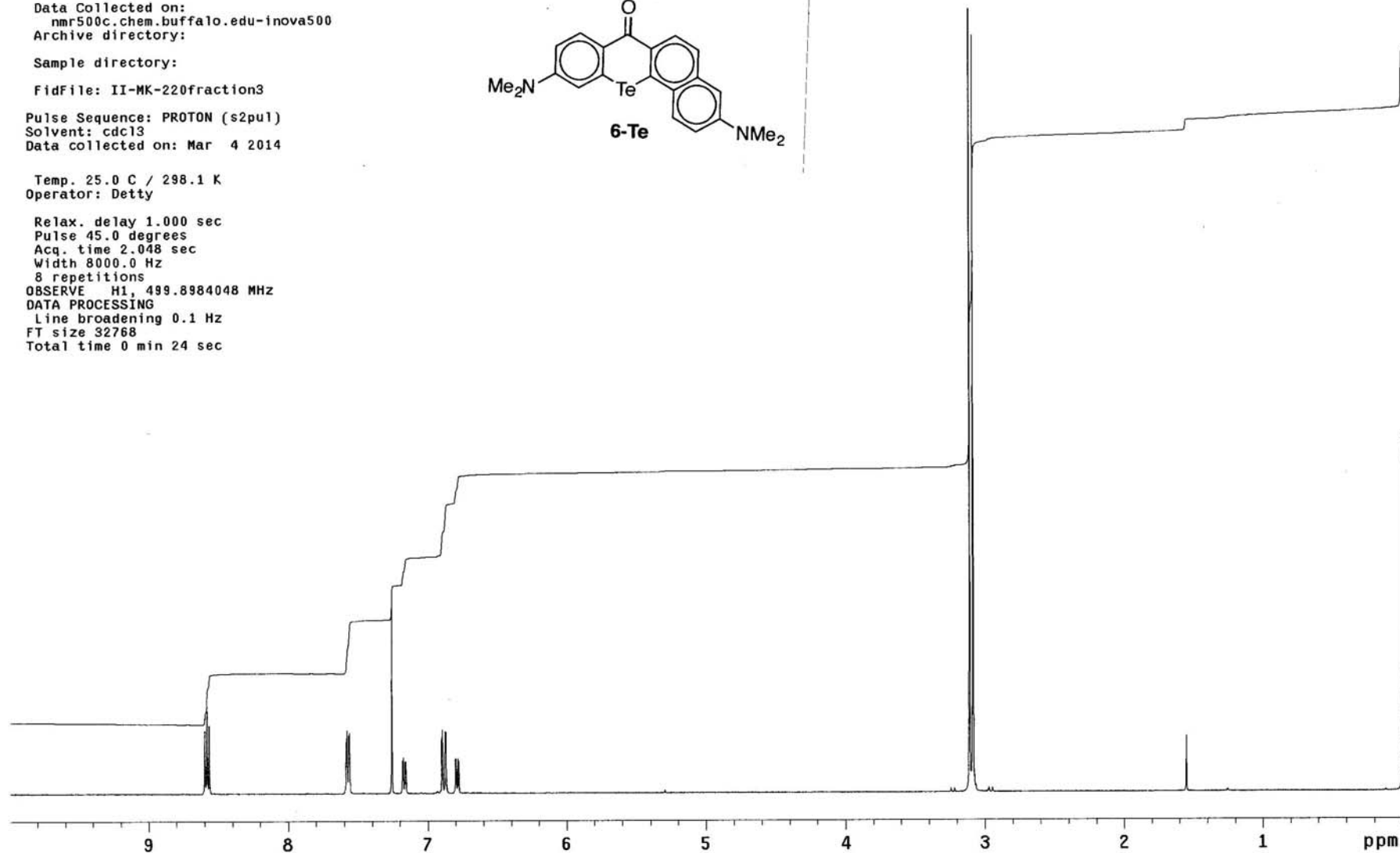
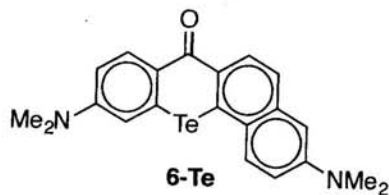
Sample directory:

FidFile: II-MK-220fraction3

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 4 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984048 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



II-MK-220carbon

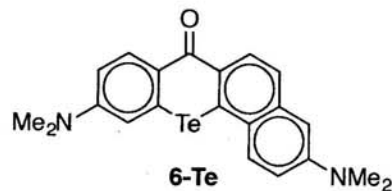
Sample Name:

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

Sample directory:

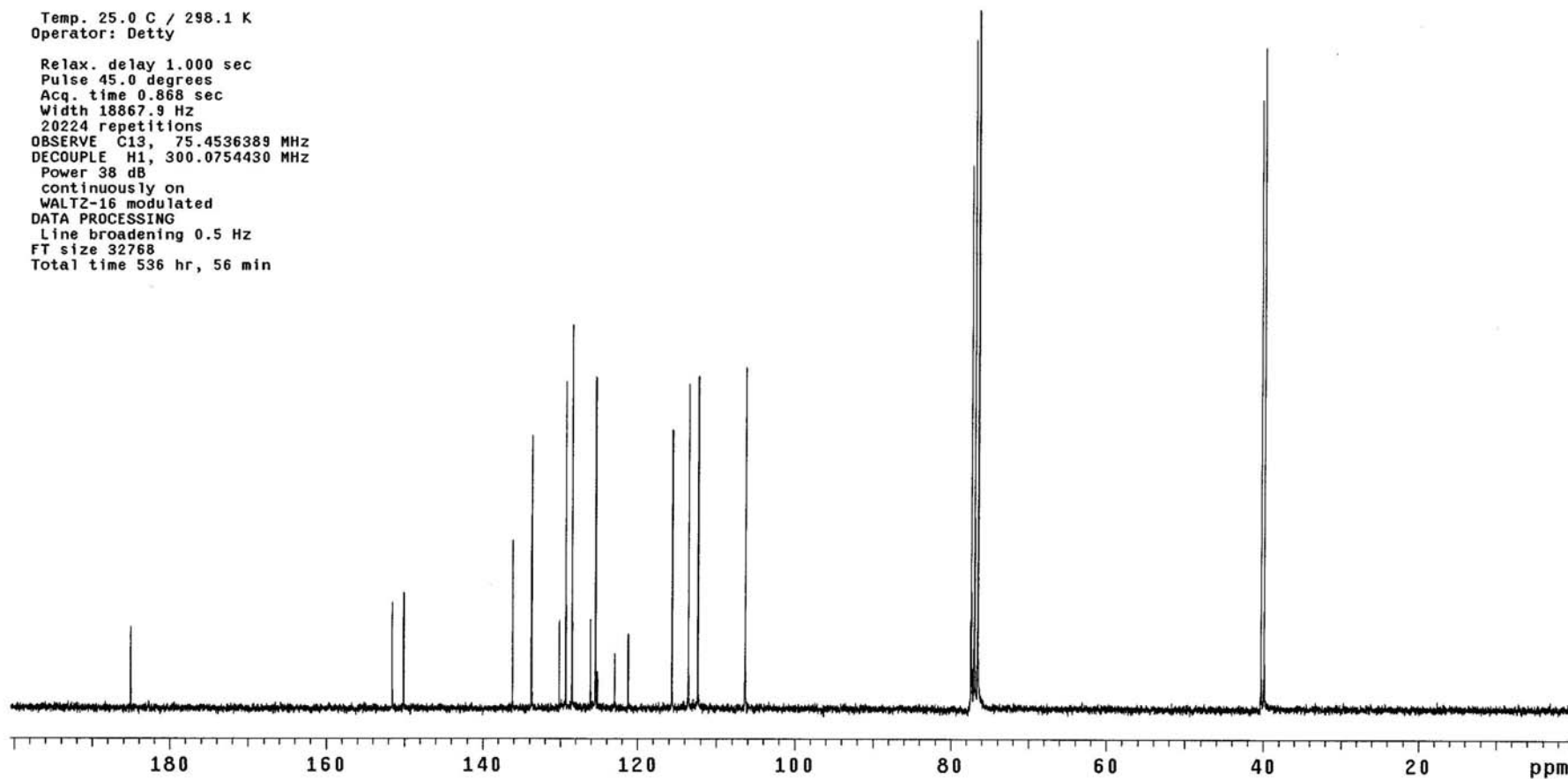
FidFile: II-MK-220carbon

Pulse Sequence: CARBON (s2pu1)  
Solvent: cdc13  
Data collected on: Mar 17 2014



Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
20224 repetitions  
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  
FT size 32768  
Total time 536 hr, 56 min



Linear S Xan

Sample Name:

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

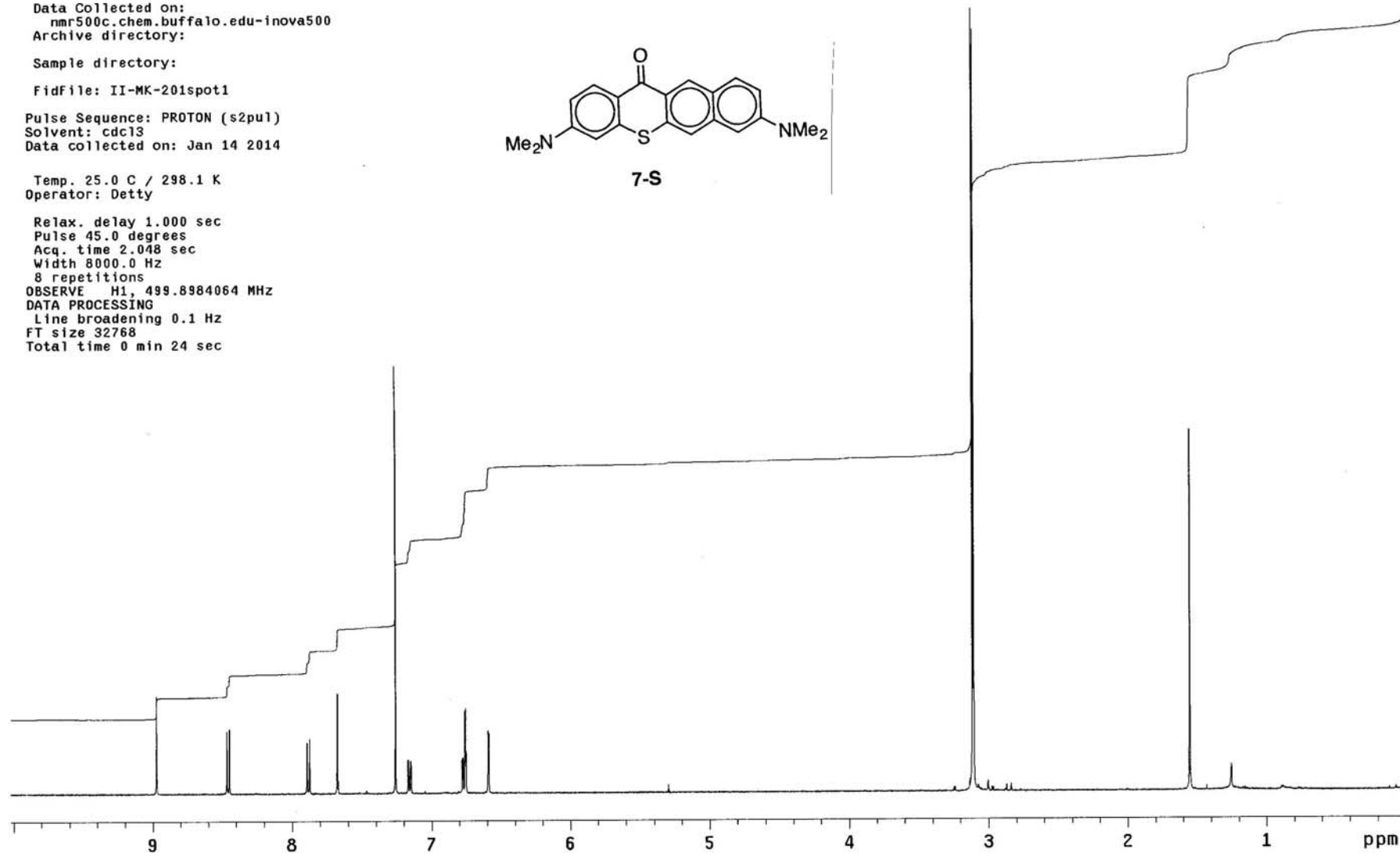
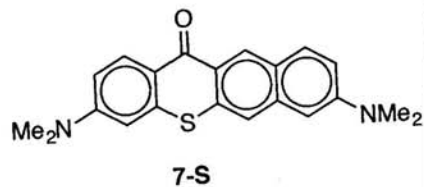
Sample directory:

FidFile: II-MK-201spot1

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Jan 14 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984064 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



Linear S xan

Sample Name:

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

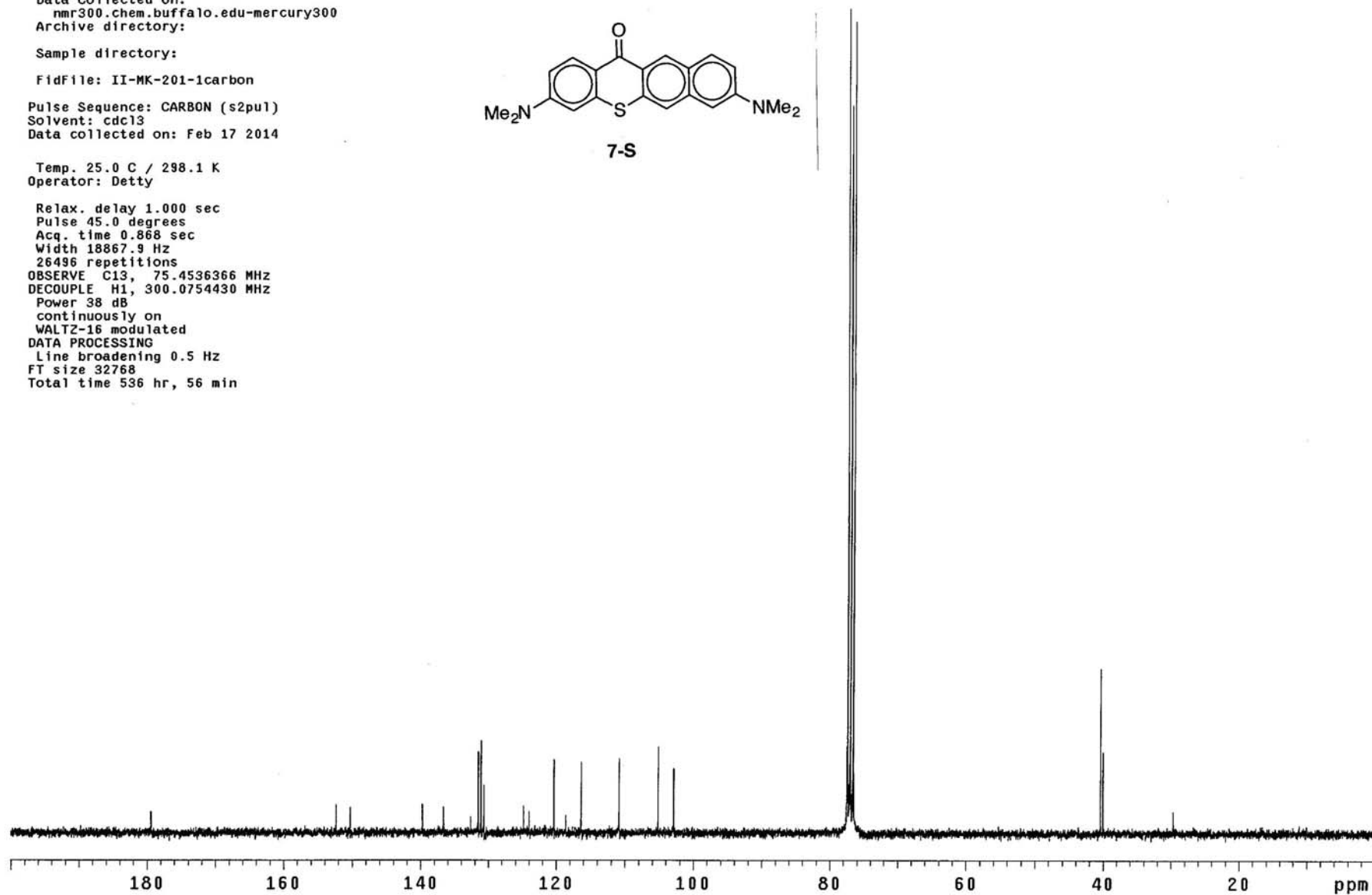
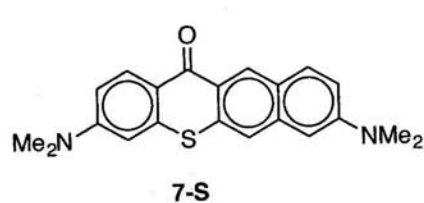
Sample directory:

FidFile: II-MK-201-1carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Feb 17 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
26496 repetitions  
OBSERVE C13, 75.4536366 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S24



Linear Se Xan

Sample Name:

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

Archive directory:

Sample directory:

FidFile: II-MK-215spot1b

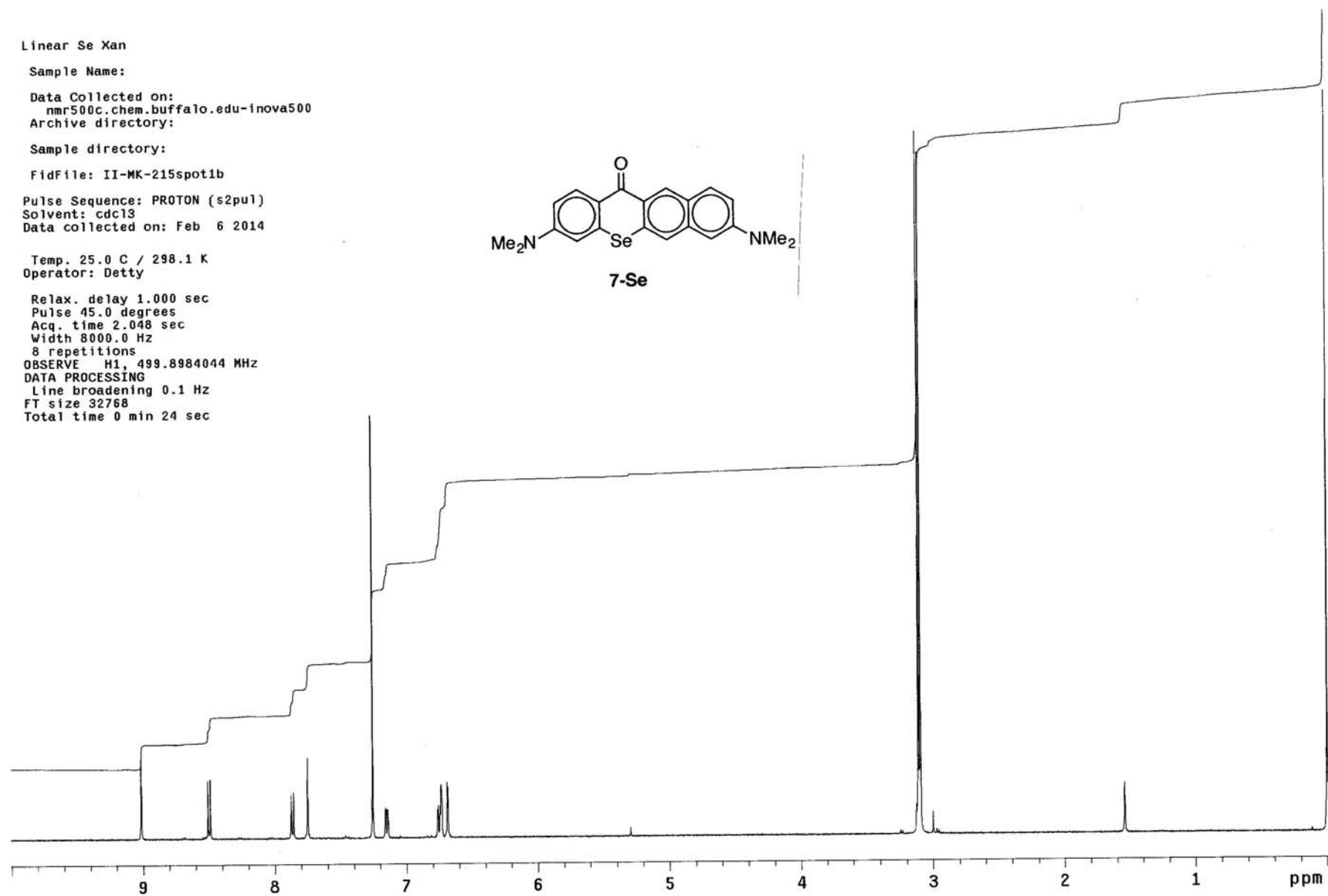
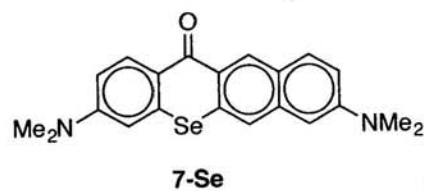
Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Feb 6 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984044 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



Liner Se xan Carbon

Sample Name:

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

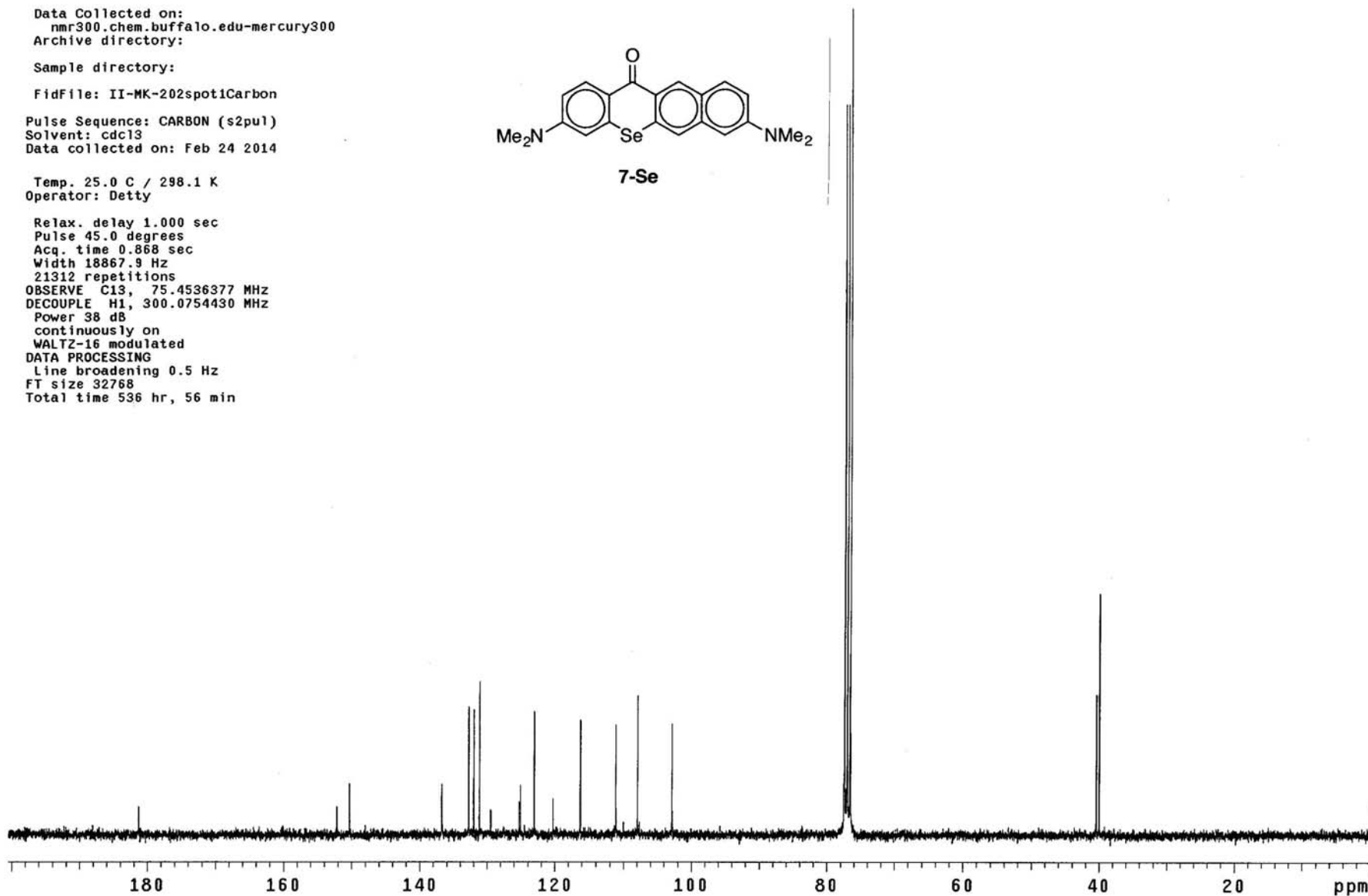
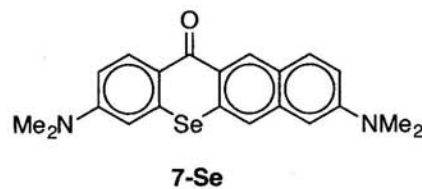
Sample directory:

FidFile: II-MK-202spot1Carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 24 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
21312 repetitions  
OBSERVE C13, 75.4536377 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S26

II-MK-219

Sample Name:

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

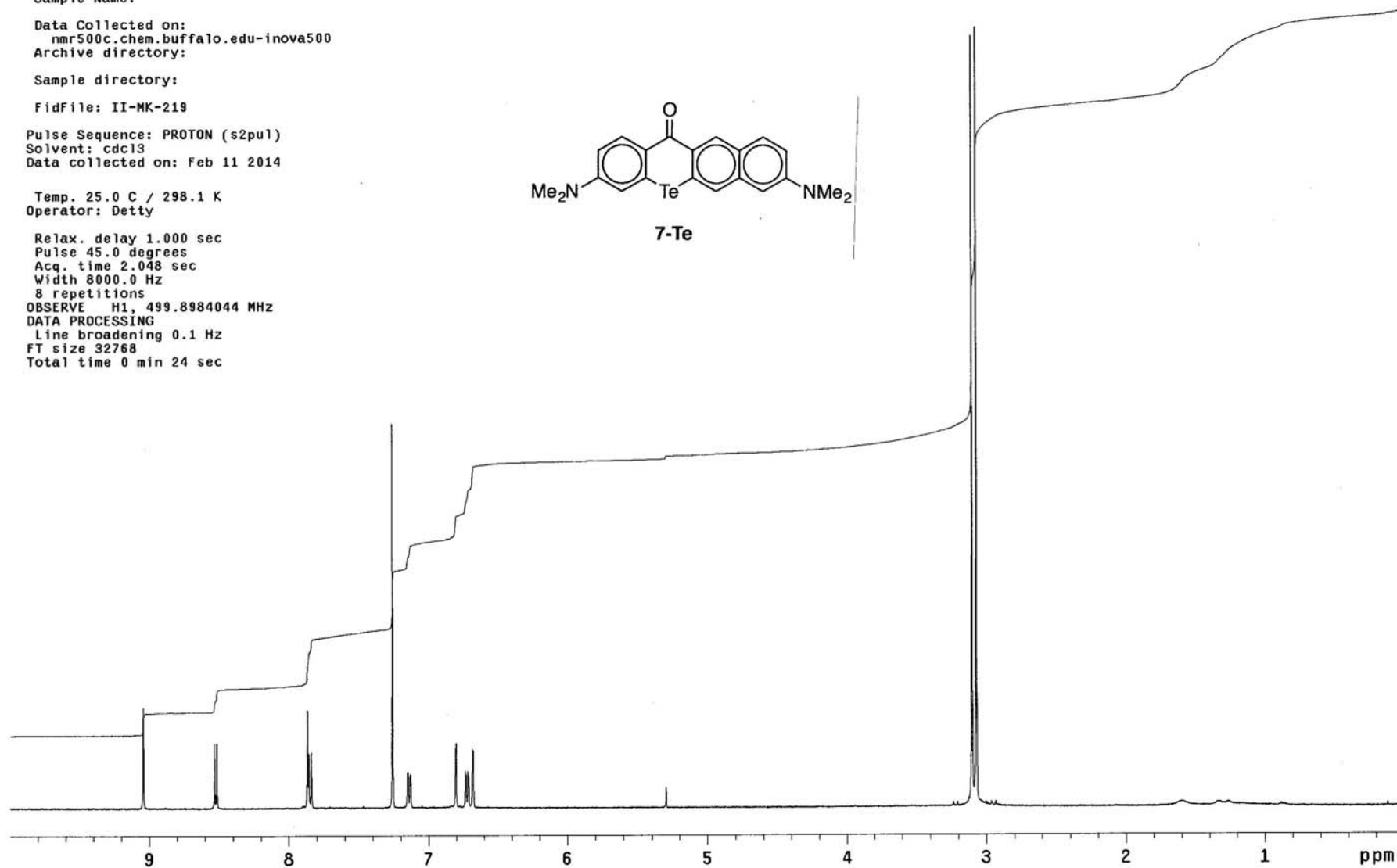
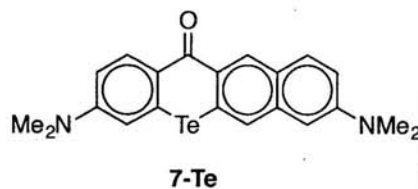
Sample directory:

FidFile: II-MK-219

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 11 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984044 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



## II-MK-219Carbon

Sample Name:

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

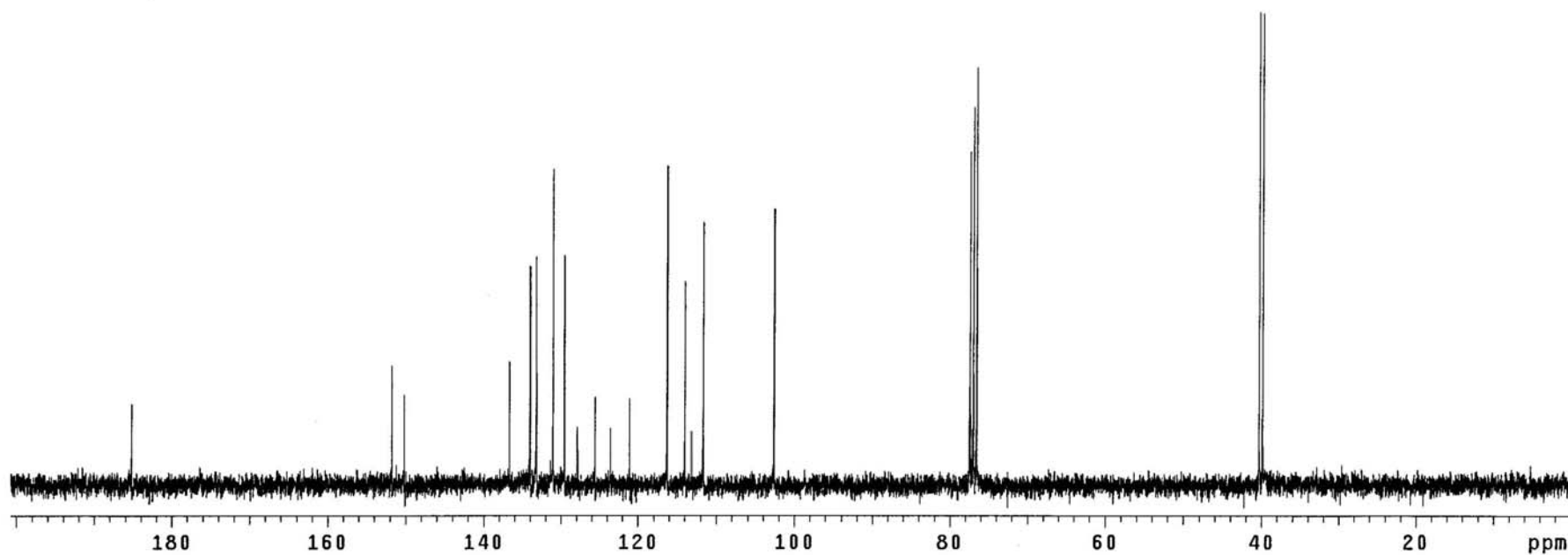
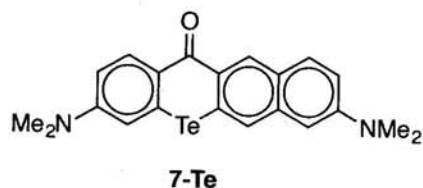
Sample directory:

FidFile: II-MK-219Carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 25 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
768 repetitions  
OBSERVE C13, 75.4536412 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S28

## Nap Diethyl Amide

Sample Name:

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

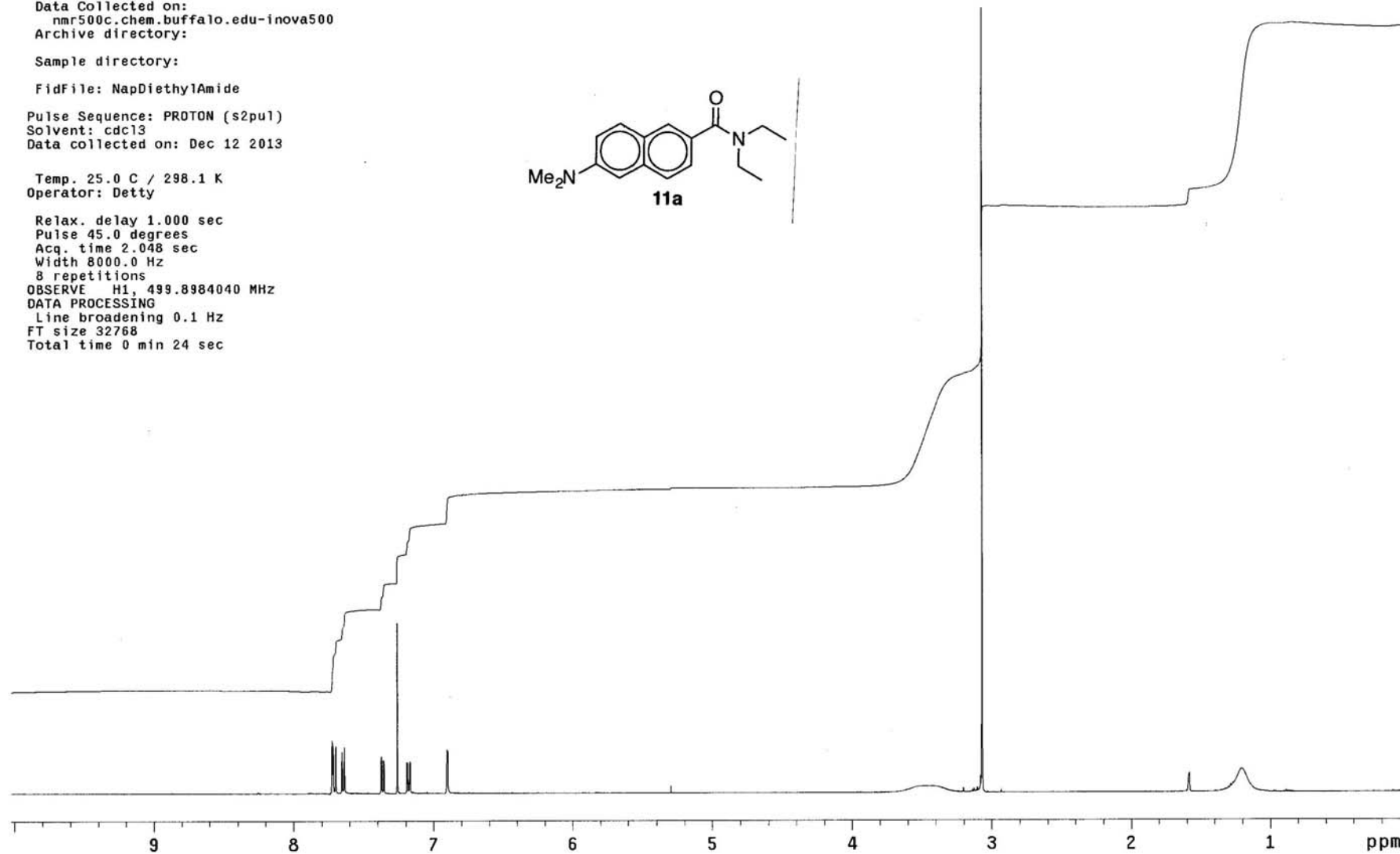
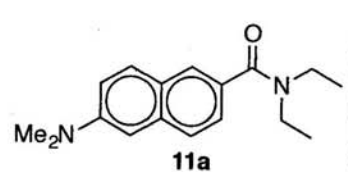
Sample directory:

FidFile: NapDiethylAmide

Pulse Sequence: PROTON (s2pu1)  
Solvent: cdcl3  
Data collected on: Dec 12 2013

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984040 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



II-MK-180carbon

Sample Name:

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

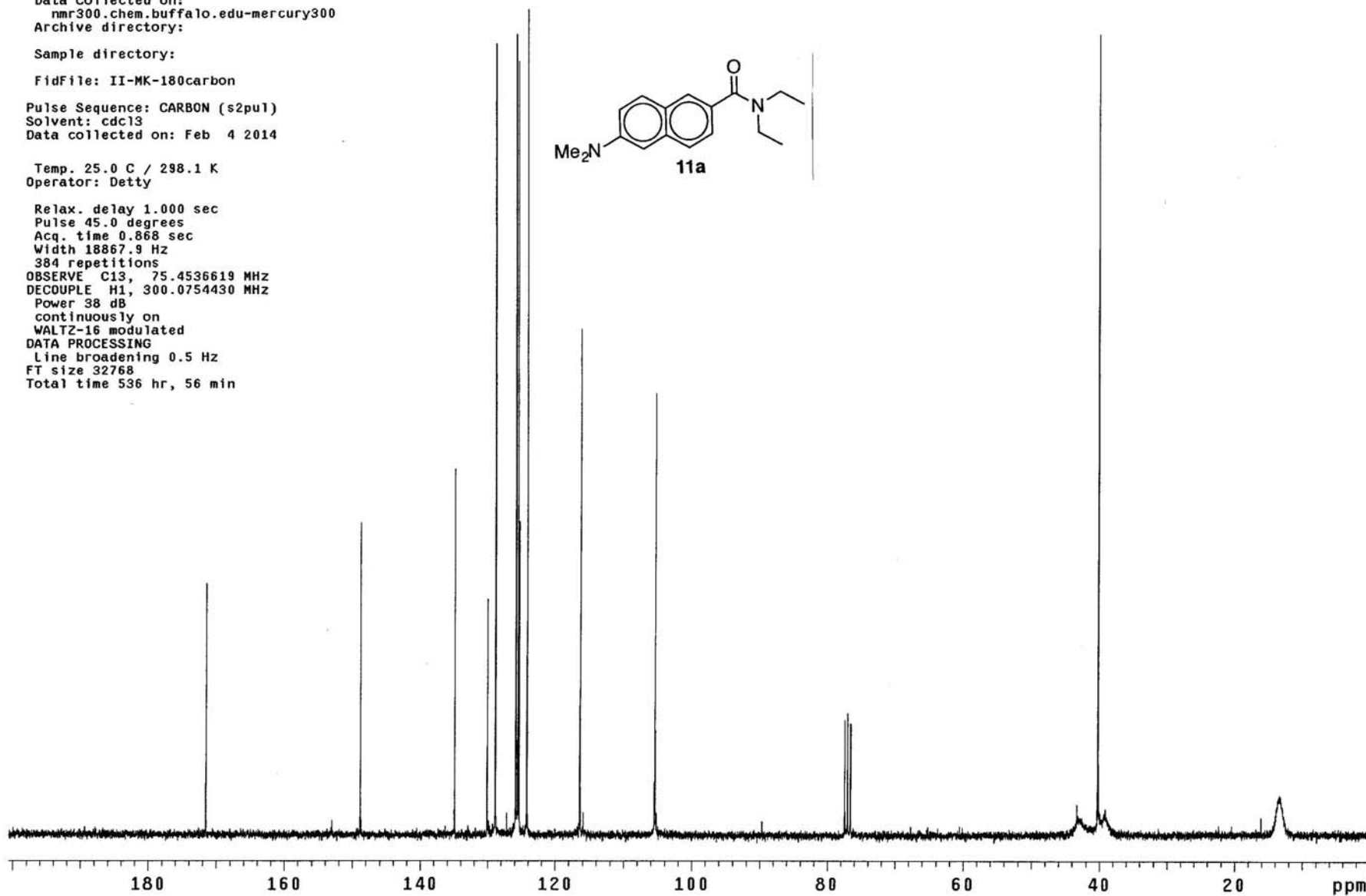
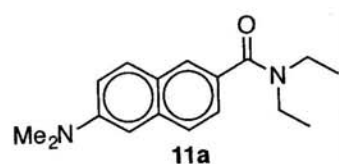
Sample directory:

FidFile: II-MK-180carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Feb 4 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
384 repetitions  
OBSERVE C13, 75.4536619 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S30

## Diisopropyl Amide

Sample Name:

Data Collected on:  
chemnmr500.chem.buffalo.edu-inova500  
Archive directory:

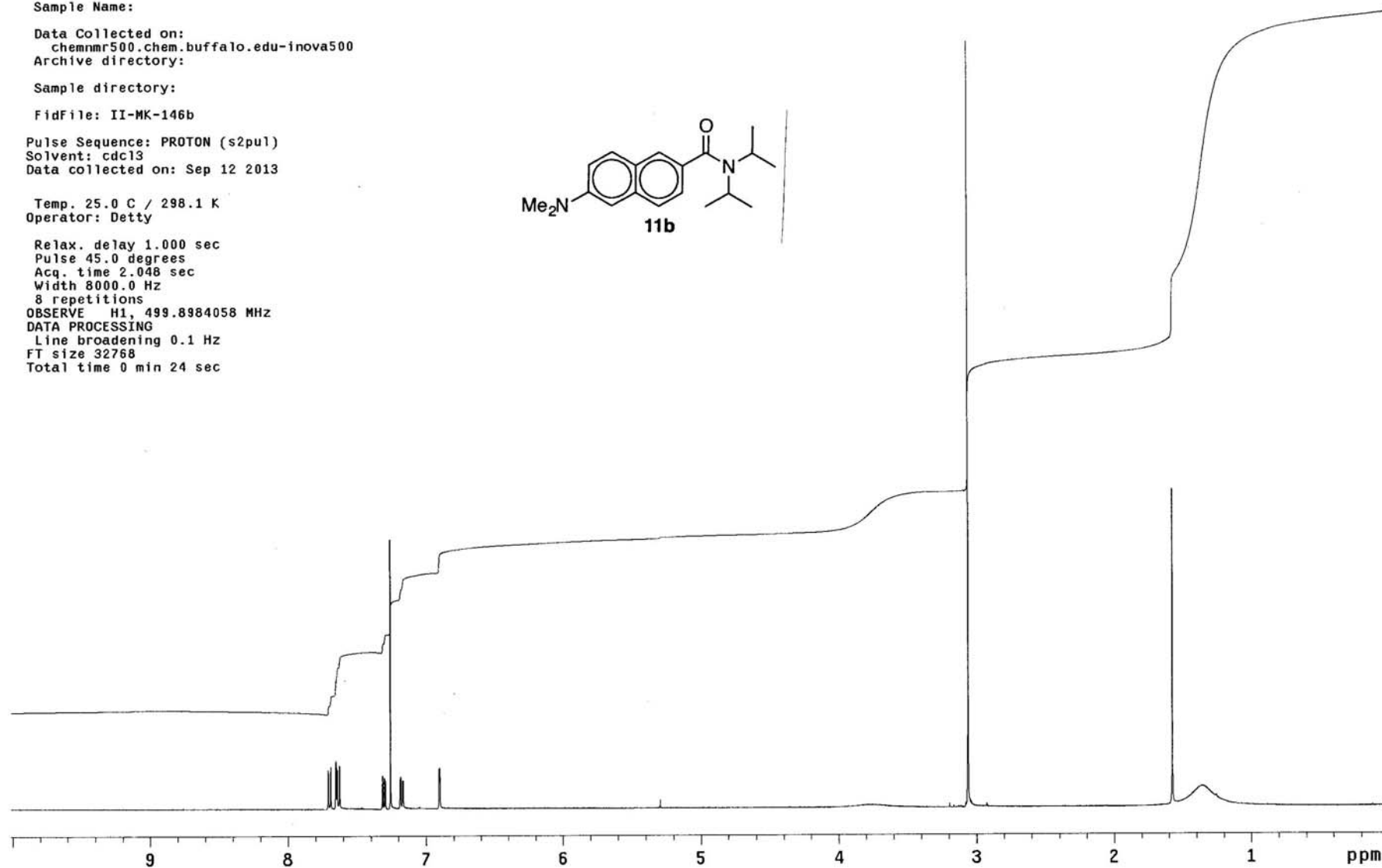
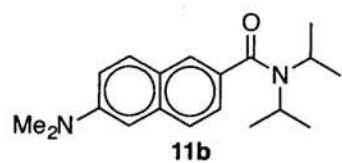
Sample directory:

FidFile: II-MK-146b

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 12 2013

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984058 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



## Diisopropyl Amide Carbon

Sample Name:

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

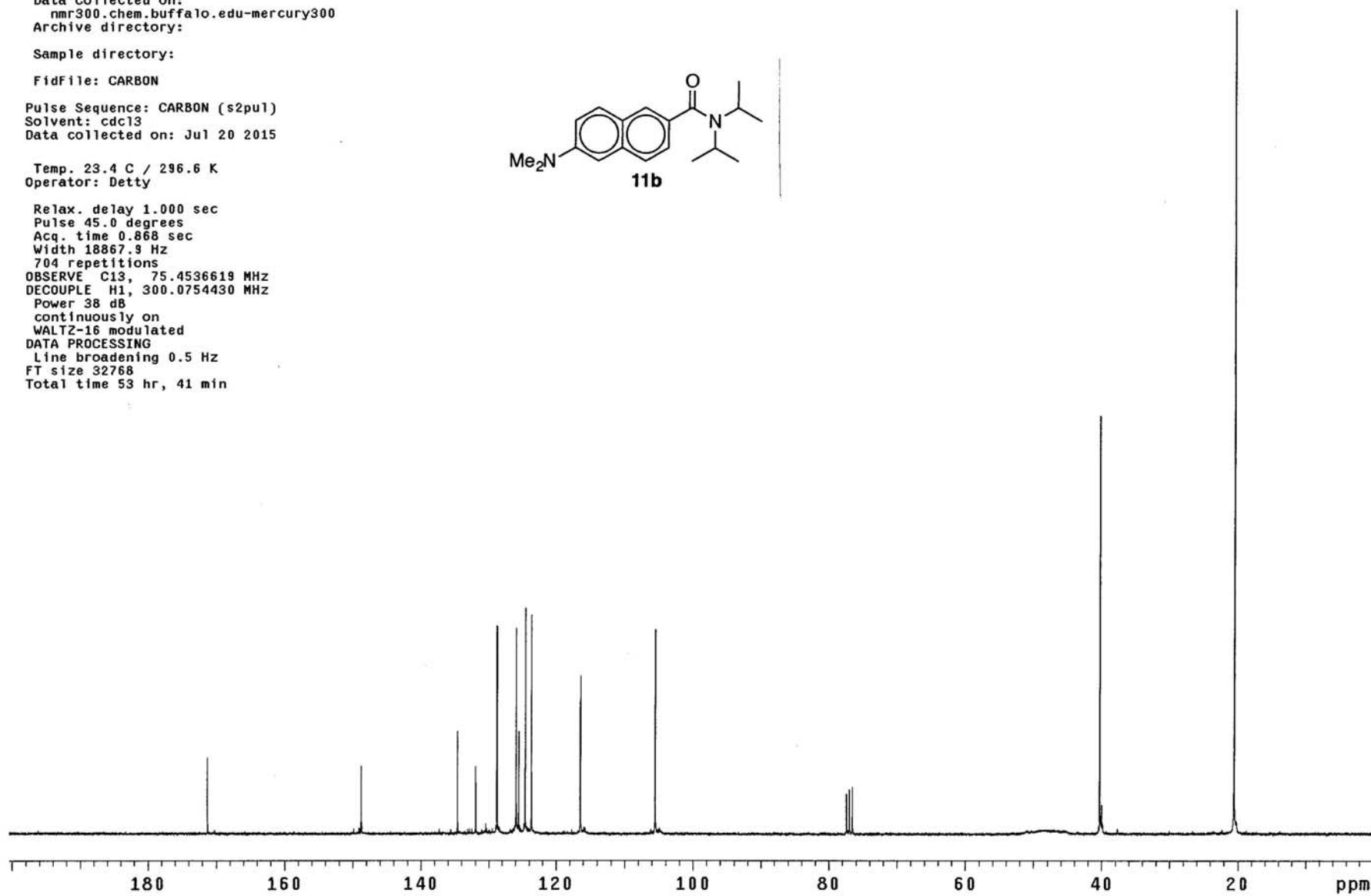
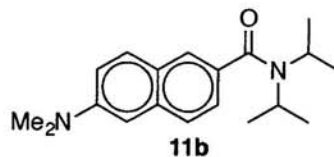
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)  
Solvent: cdc13  
Data collected on: Jul 20 2015

Temp. 23.4 C / 296.6 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
704 repetitions  
OBSERVE C13, 75.4536619 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 53 hr, 41 min





II-MK-152

Sample Name:

Data Collected on:  
chemnmr500.chem.buffalo.edu-inova500  
Archive directory:

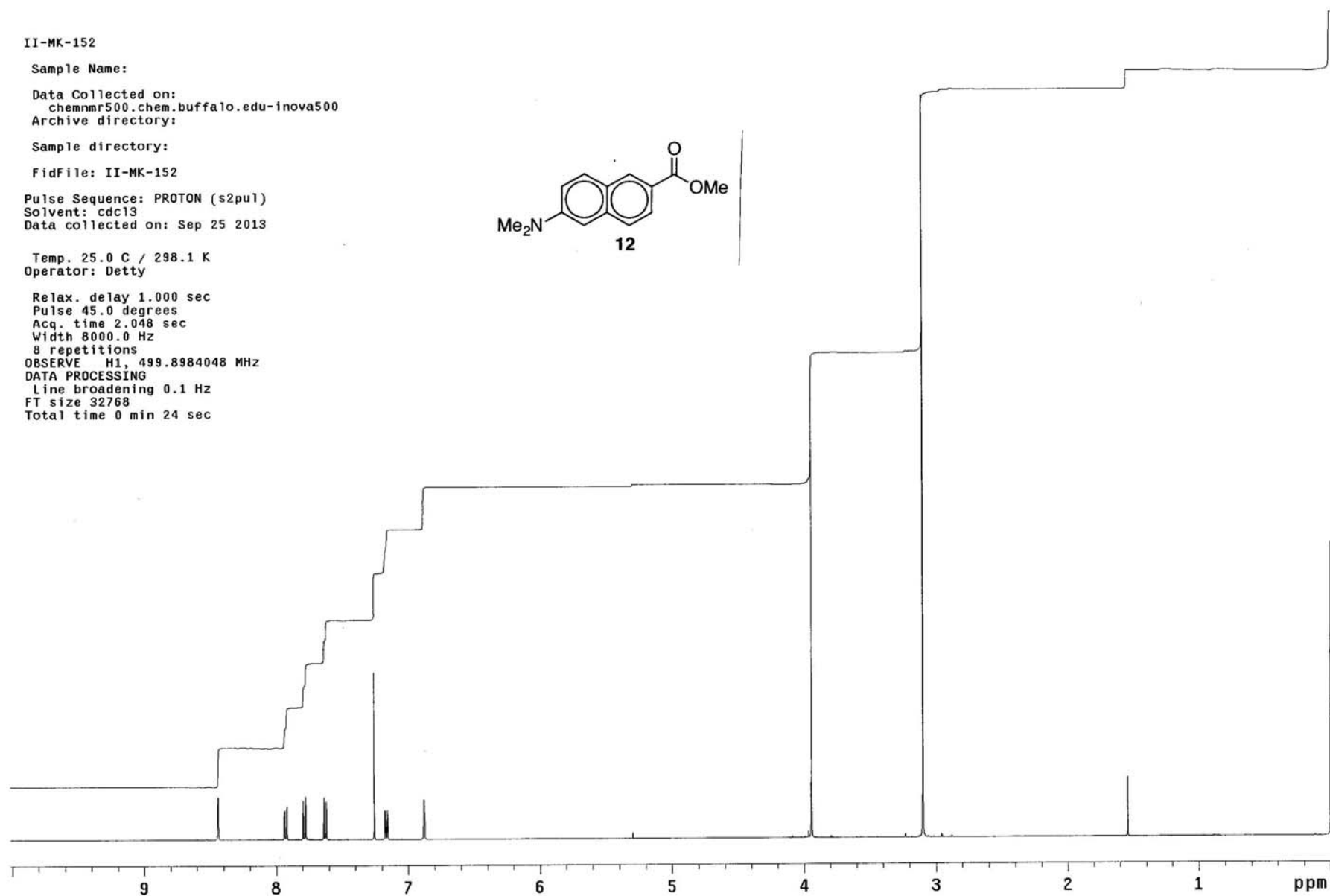
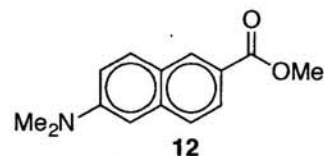
Sample directory:

FidFile: II-MK-152

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Sep 25 2013

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984048 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



## Methyl Ester Carbon

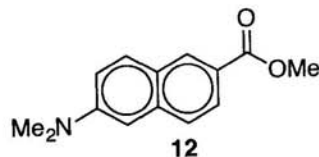
Sample Name:

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

Sample directory:

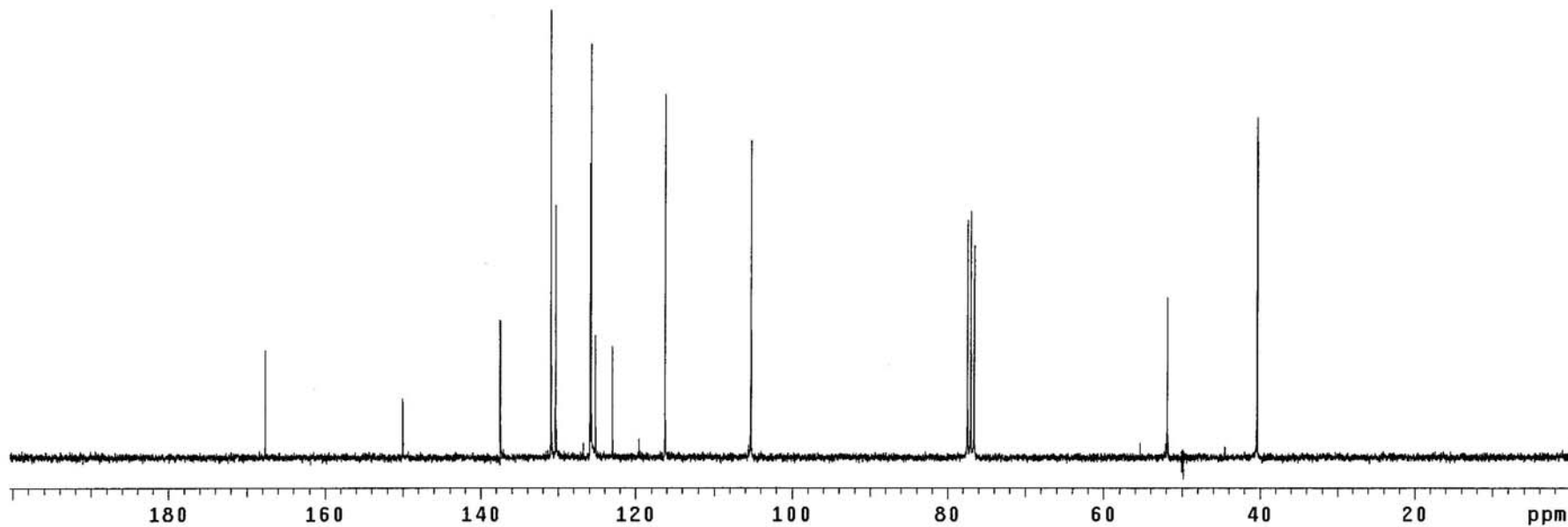
FidFile: 2-bdc-118-afterplug

Pulse Sequence: CARBON (s2pu1)  
Solvent: cdc13  
Data collected on: Dec 17 2010



Temp. 21.0 C / 294.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
2432 repetitions  
OBSERVE C13, 75.4536412 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 42 hr, 57 min



S34

III-MK-040 butyl ketone

Sample Name:

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

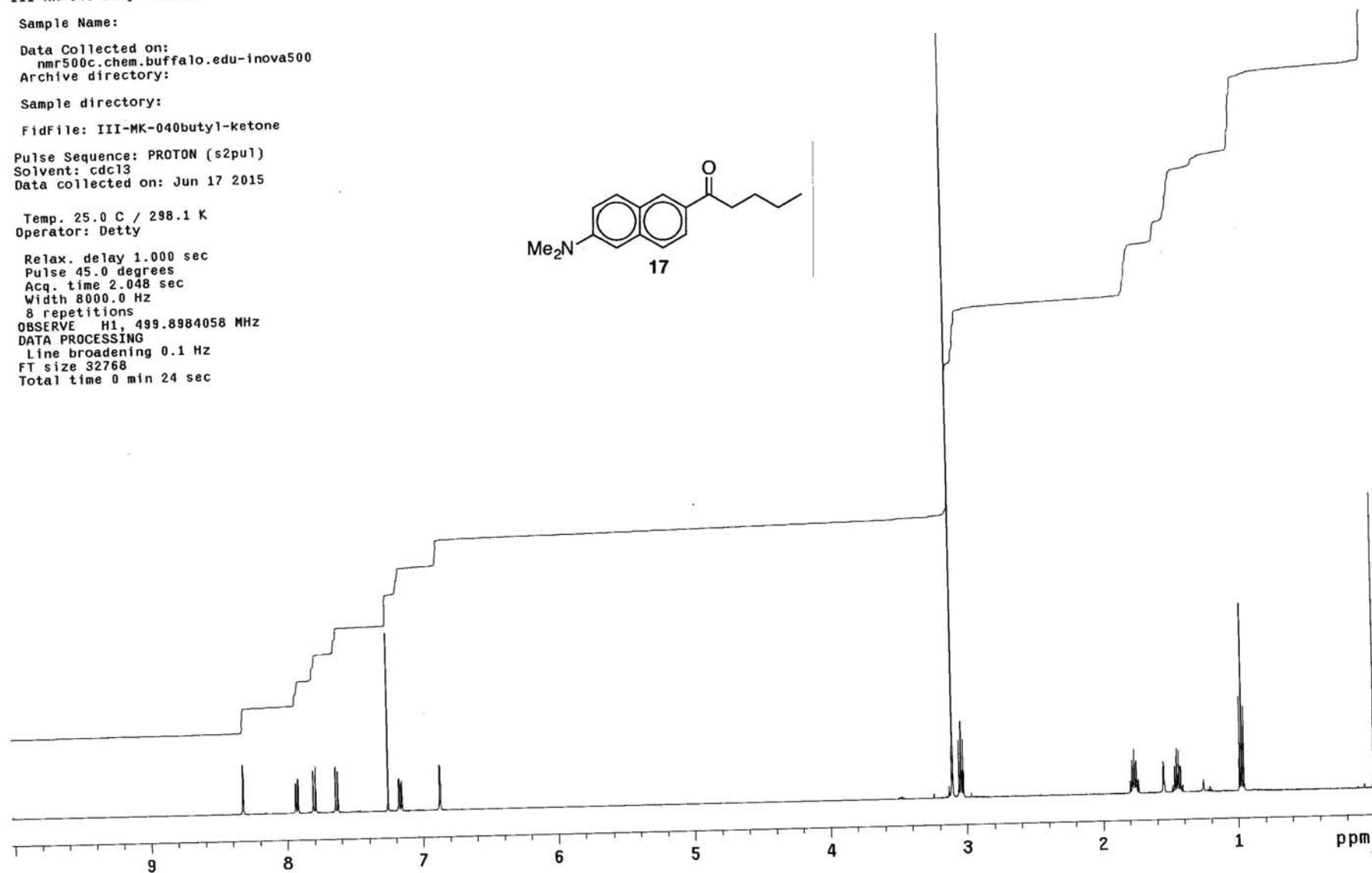
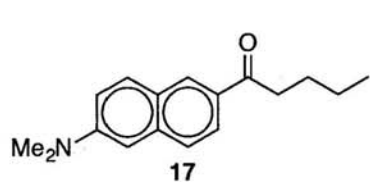
Sample directory:

FidFile: III-MK-040butyl-ketone

Pulse Sequence: PROTON (s2pu1)  
Solvent: cdc13  
Data collected on: Jun 17 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984058 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



III-MK-040 butyl ketone

Sample Name:

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

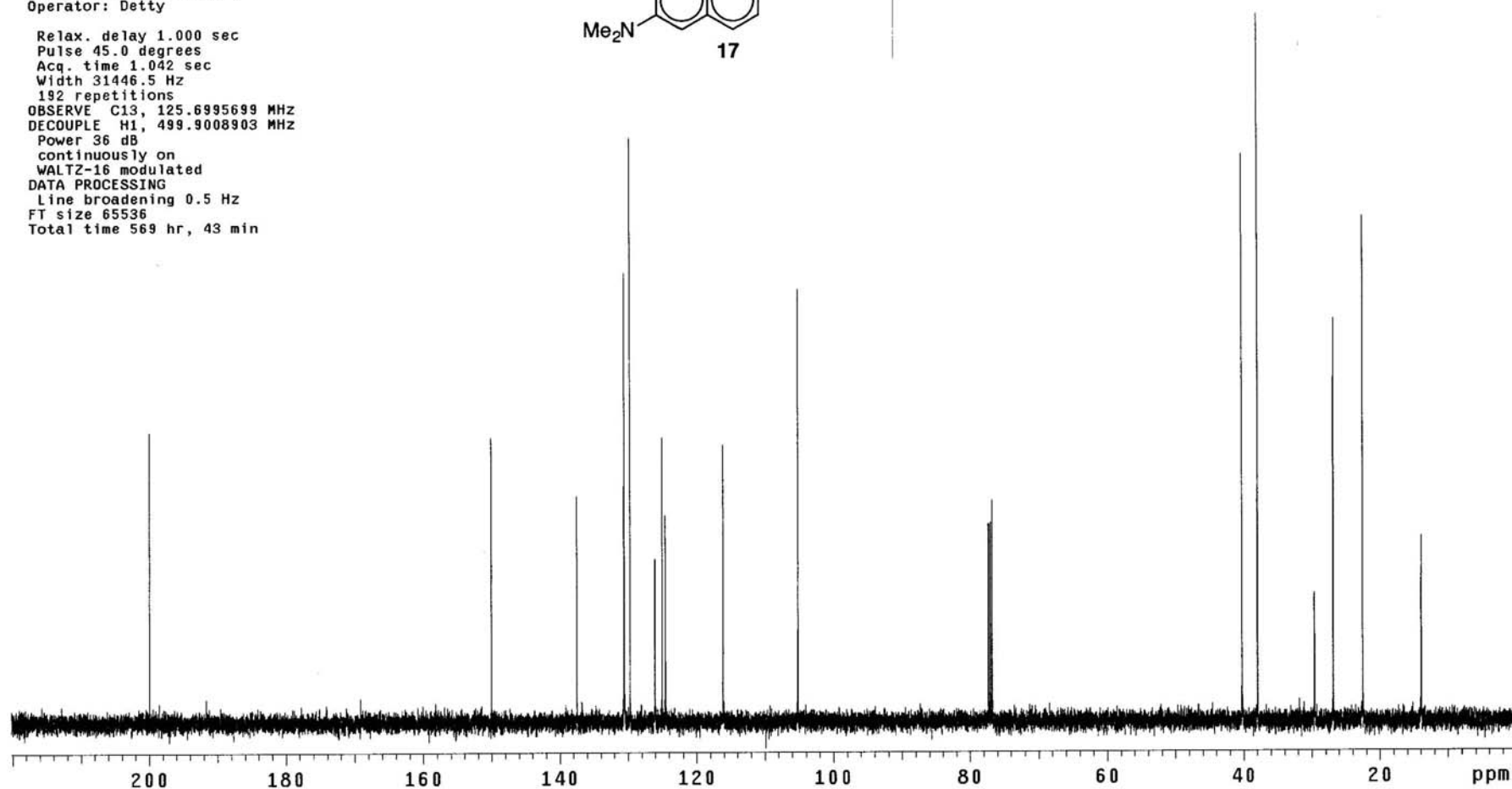
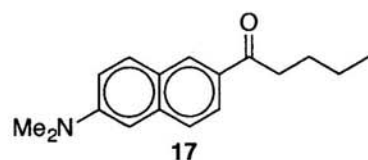
Sample directory:

FidFile: III-MK-040butyl-ketone-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Jun 17 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.042 sec  
Width 31446.5 Hz  
192 repetitions  
OBSERVE C13, 125.6995699 MHz  
DECOUPLE H1, 499.9008903 MHz  
Power 36 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 569 hr, 43 min



III-MK-040 Ketone

Sample Name:

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

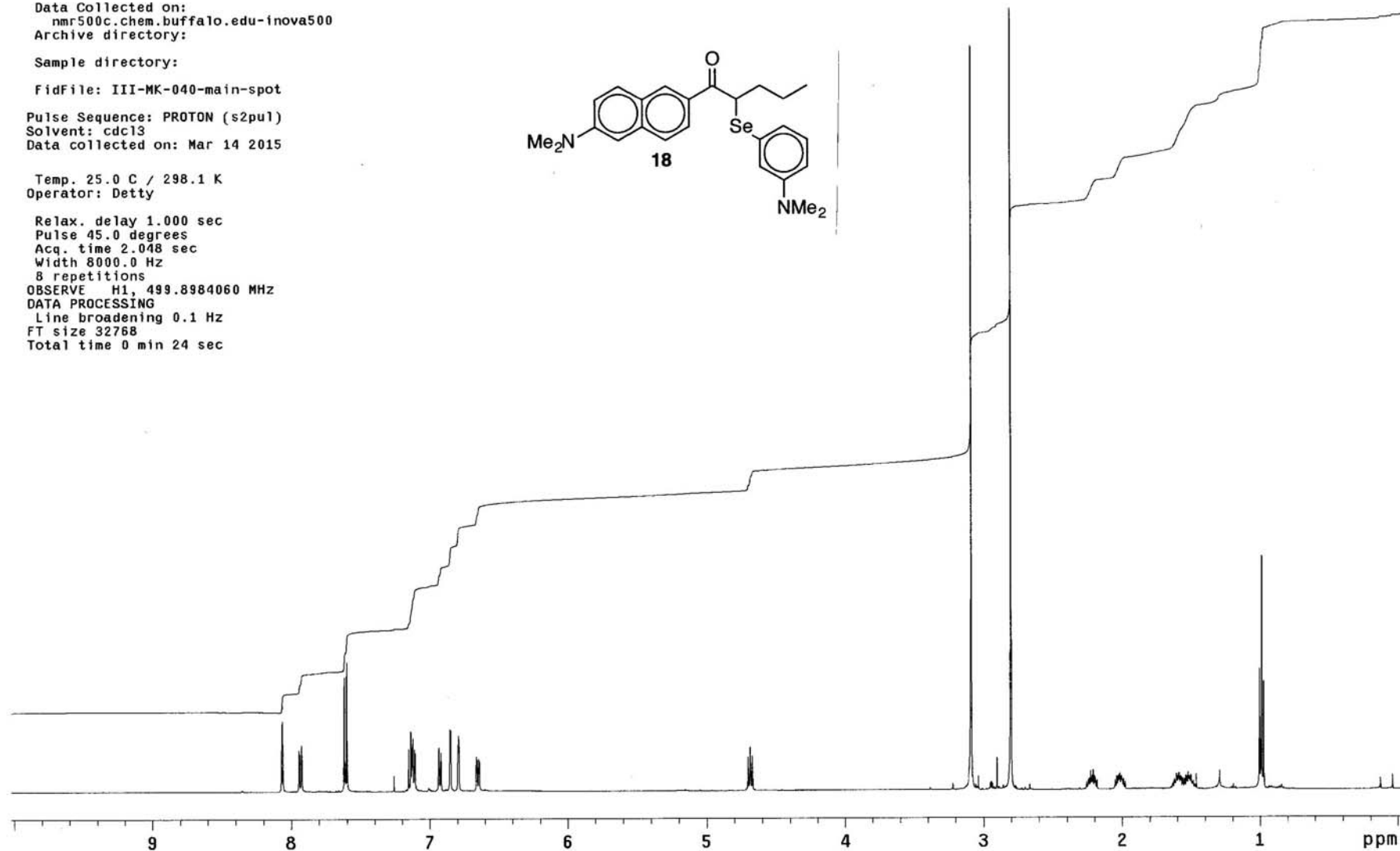
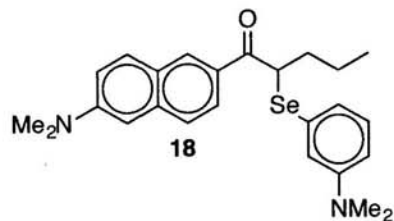
Sample directory:

FidFile: III-MK-040-main-spot

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Mar 14 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984060 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



## III-MK-040 Ketone Carbon

Sample Name:

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

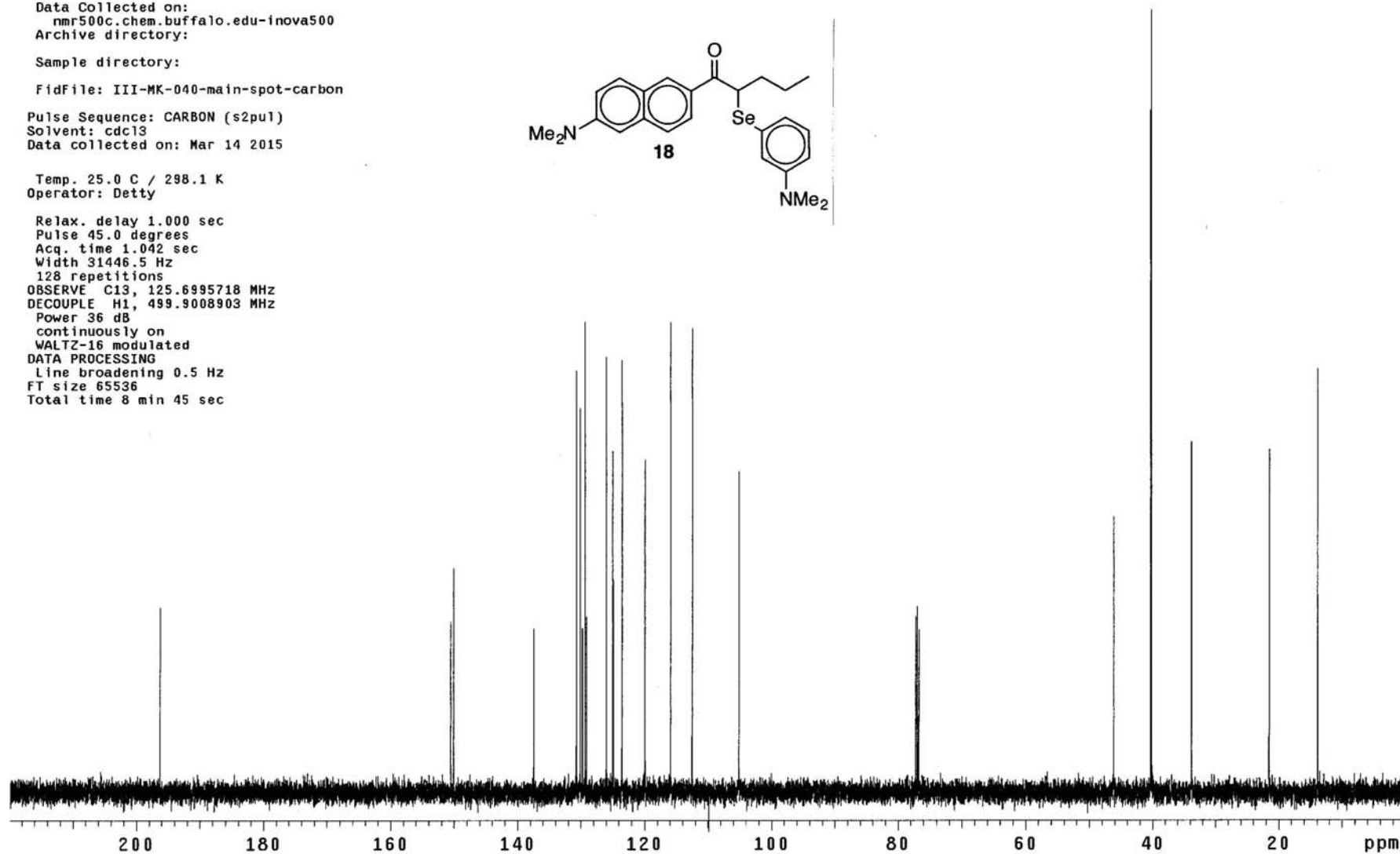
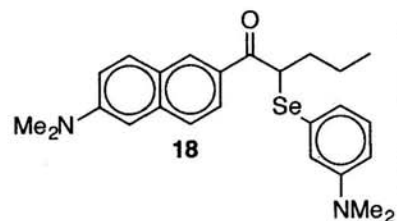
Sample directory:

FidFile: III-MK-040-main-spot-carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Mar 14 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.042 sec  
Width 31446.5 Hz  
128 repetitions  
OBSERVE C13, 125.6995718 MHz  
DECOUPLE H1, 499.9008903 MHz  
Power 36 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 8 min 45 sec



II-MK-158

Sample Name:

Data Collected on:  
chemnmr500.chem.buffalo.edu-inova500  
Archive directory:

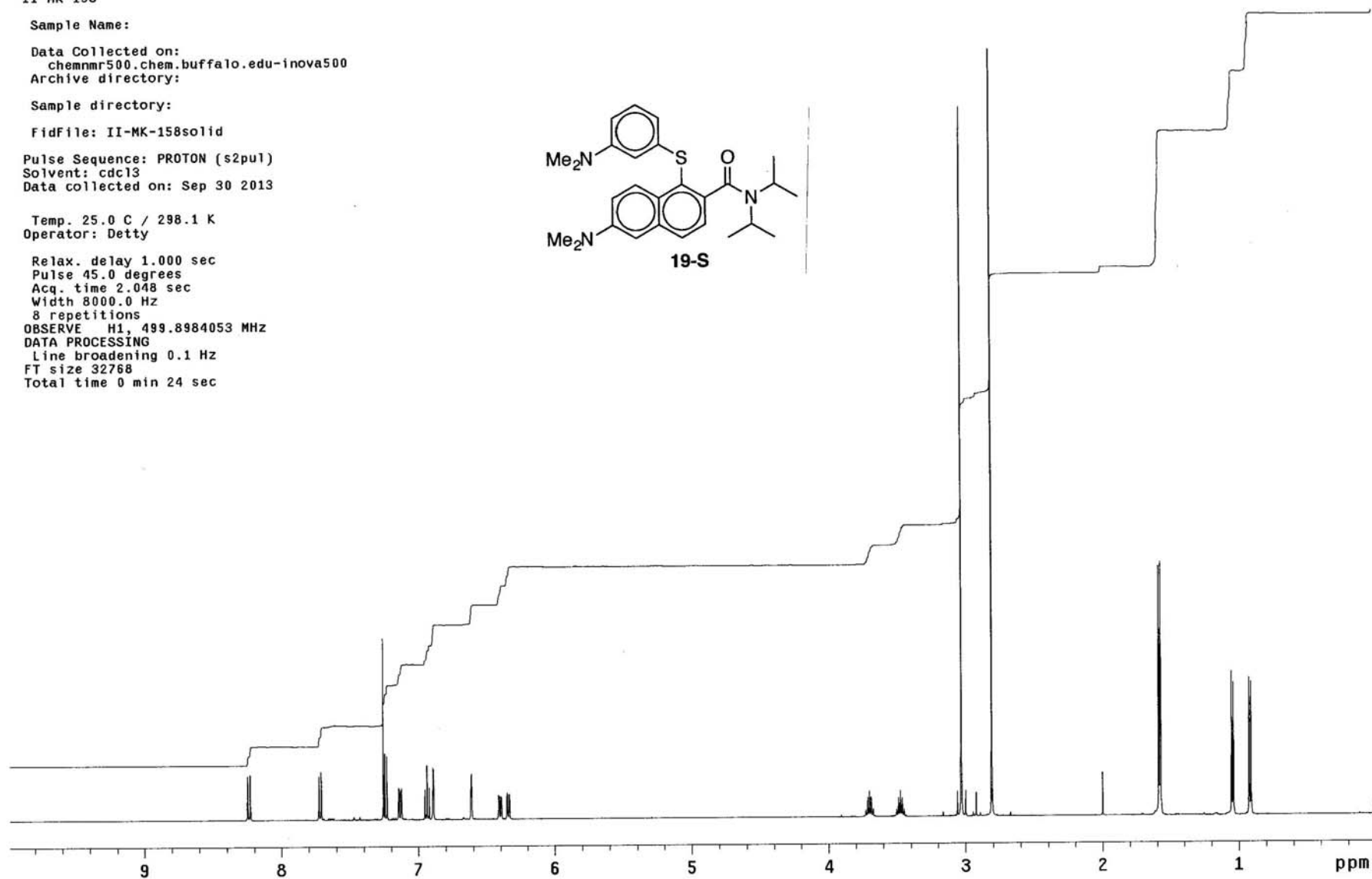
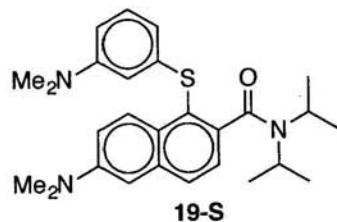
Sample directory:

FidFile: II-MK-158solid

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 30 2013

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984053 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



II-MK-158carbon

Sample Name:

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

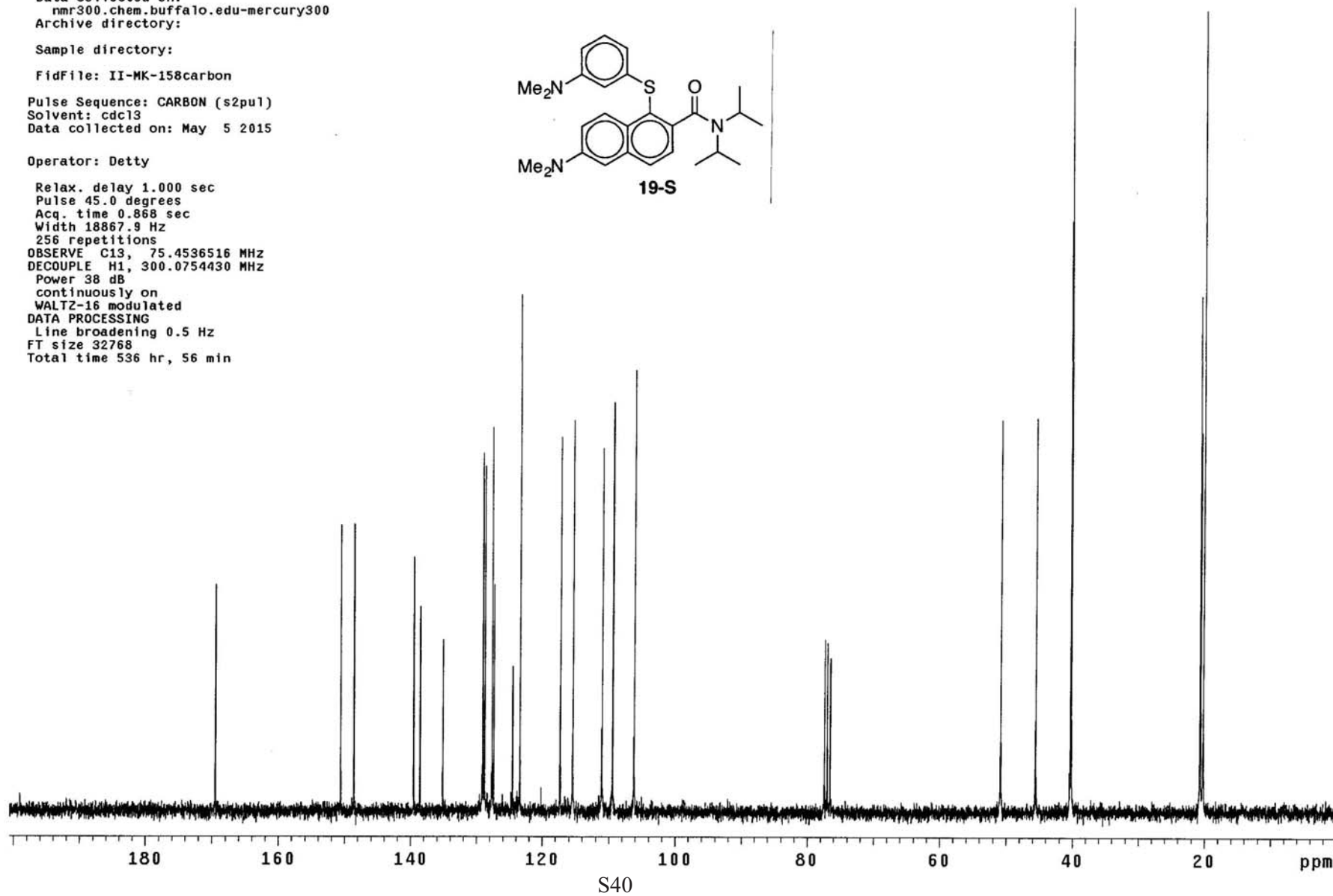
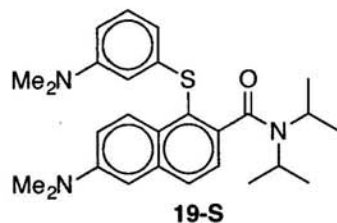
Sample directory:

FidFile: II-MK-158carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: May 5 2015

Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
256 repetitions  
OBSERVE C13, 75.4536516 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min





III-MK-030recryst

Sample Name:

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

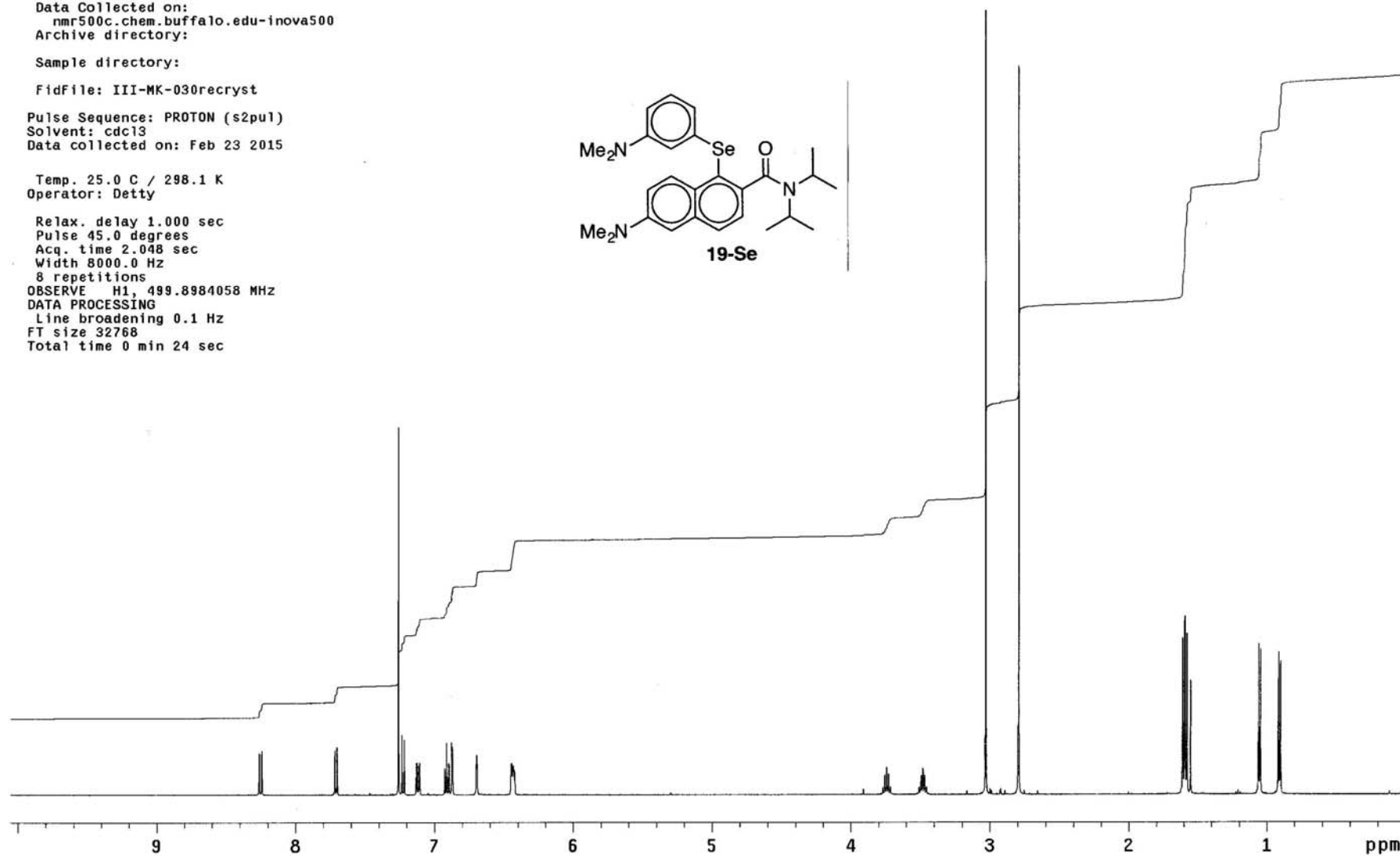
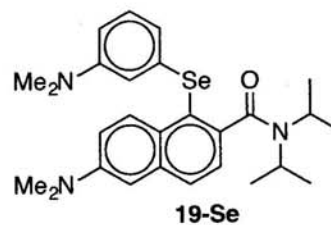
Sample directory:

FidFile: III-MK-030recryst

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Feb 23 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984058 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



III-MK-030carbon

Sample Name:

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

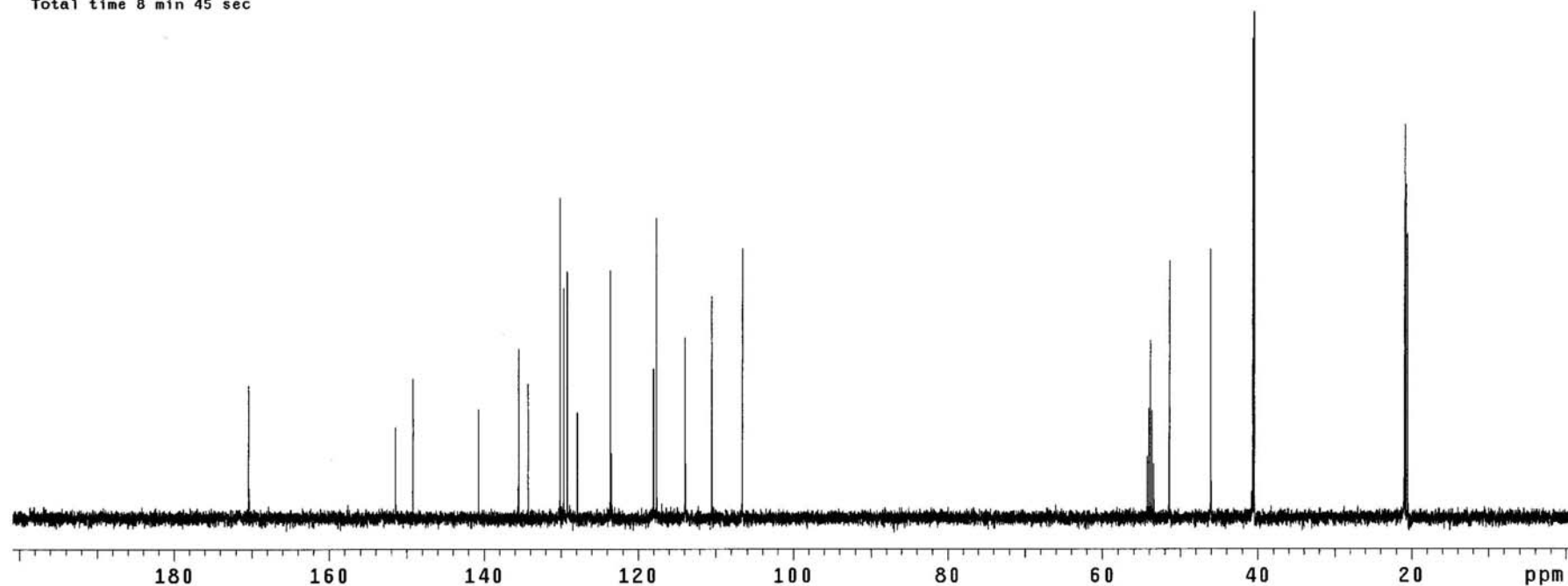
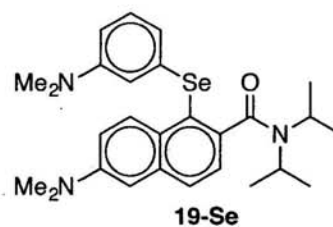
Sample directory:

FidFile: III-MK-030carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cd2cl2  
Data collected on: Feb 22 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.042 sec  
Width 31446.5 Hz  
128 repetitions  
OBSERVE C13, 125.6997545 MHz  
DECOUPLE H1, 499.9018501 MHz  
Power 36 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 8 min 45 sec



S42

III-MK-039dry

Sample Name:

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

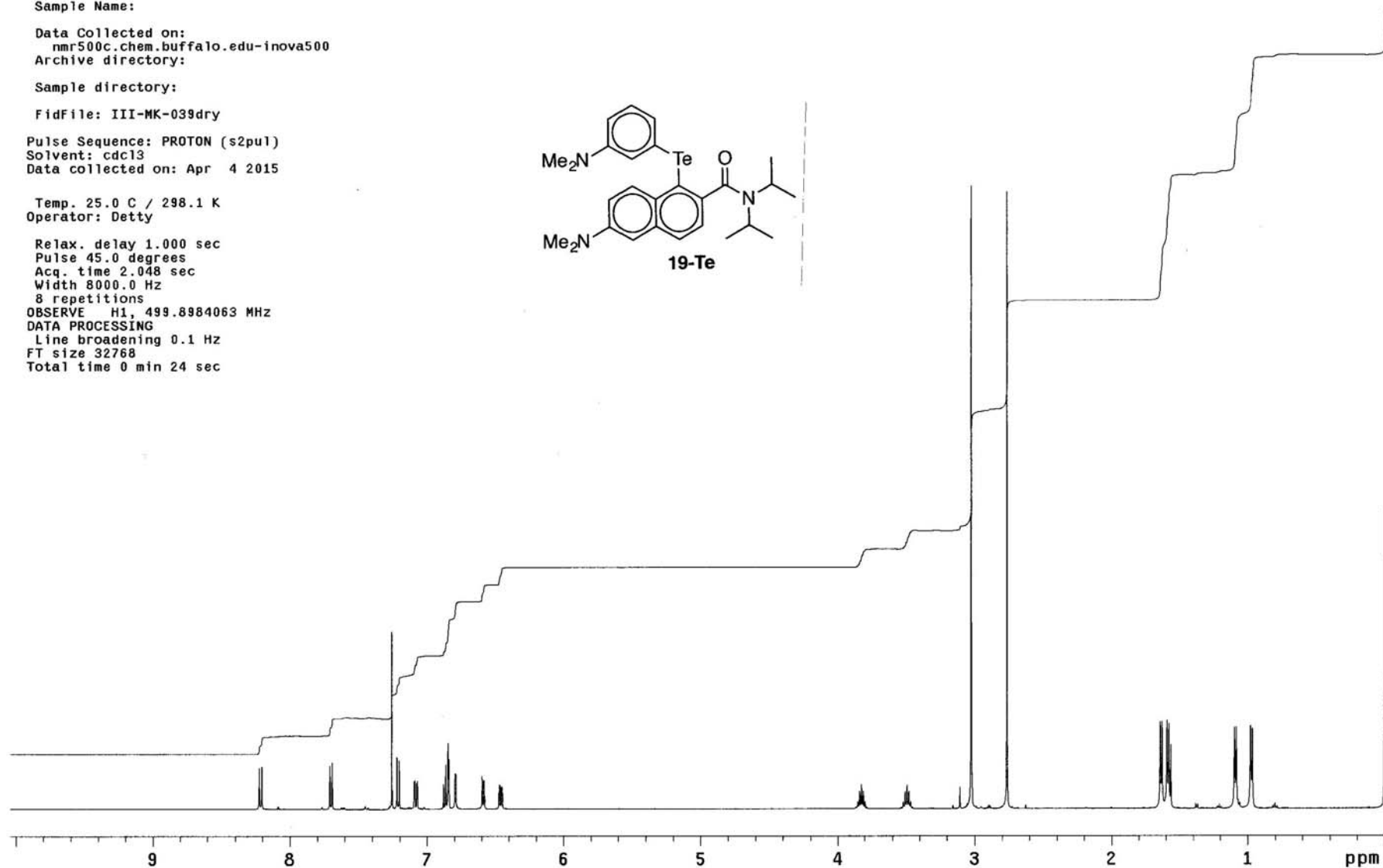
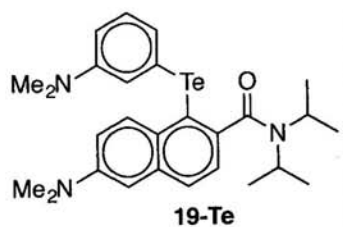
Sample directory:

FidFile: III-MK-039dry

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 4 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8984063 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



III-MK-039carbon

Sample Name:

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

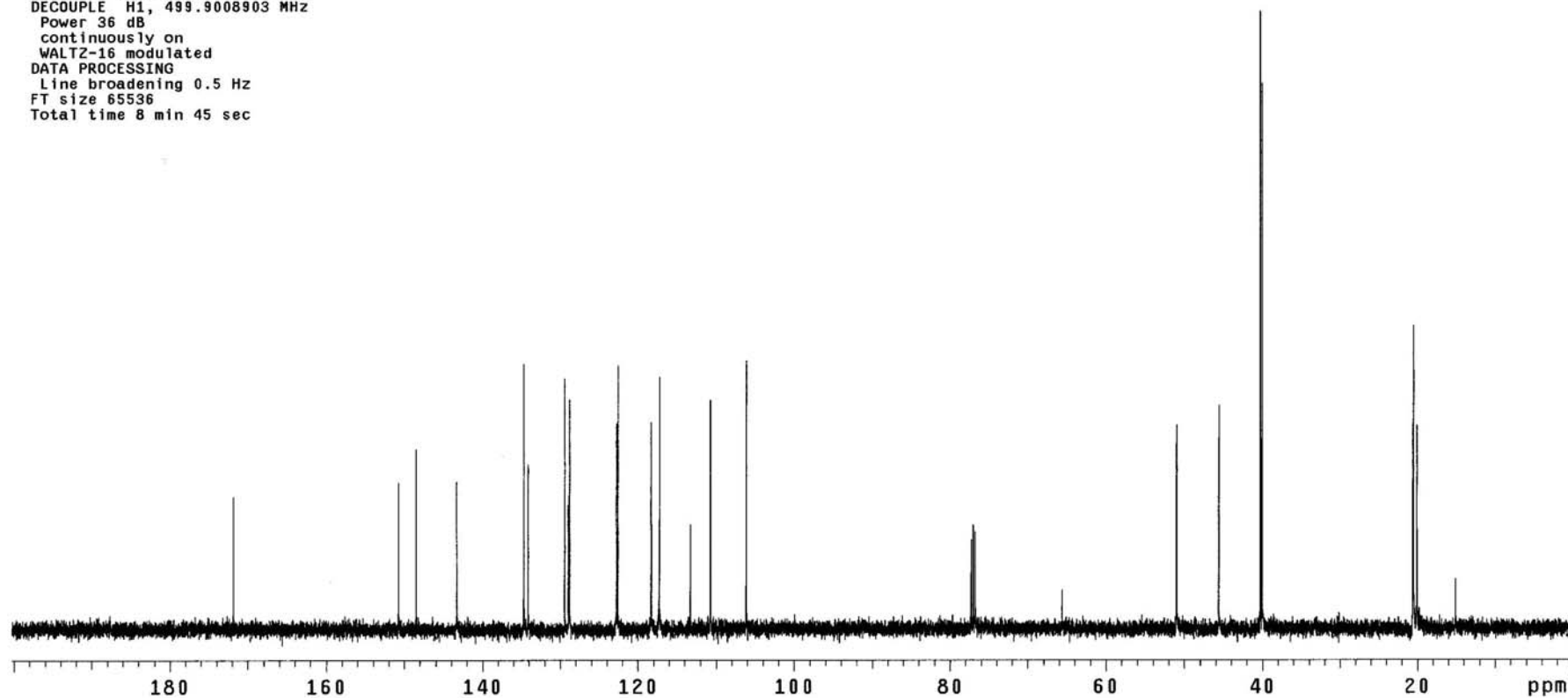
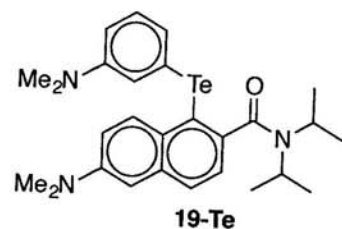
Sample directory:

FidFile: III-MK-039carbon

Pulse Sequence: CARBON (s2pu1)  
Solvent: cdc13  
Data collected on: Mar 12 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.042 sec  
Width 31446.5 Hz  
128 repetitions  
OBSERVE C13, 125.6995901 MHz  
DECOUPLE H1, 499.9008903 MHz  
Power 36 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 8 min 45 sec



III-MK-028dry

Sample Name:

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

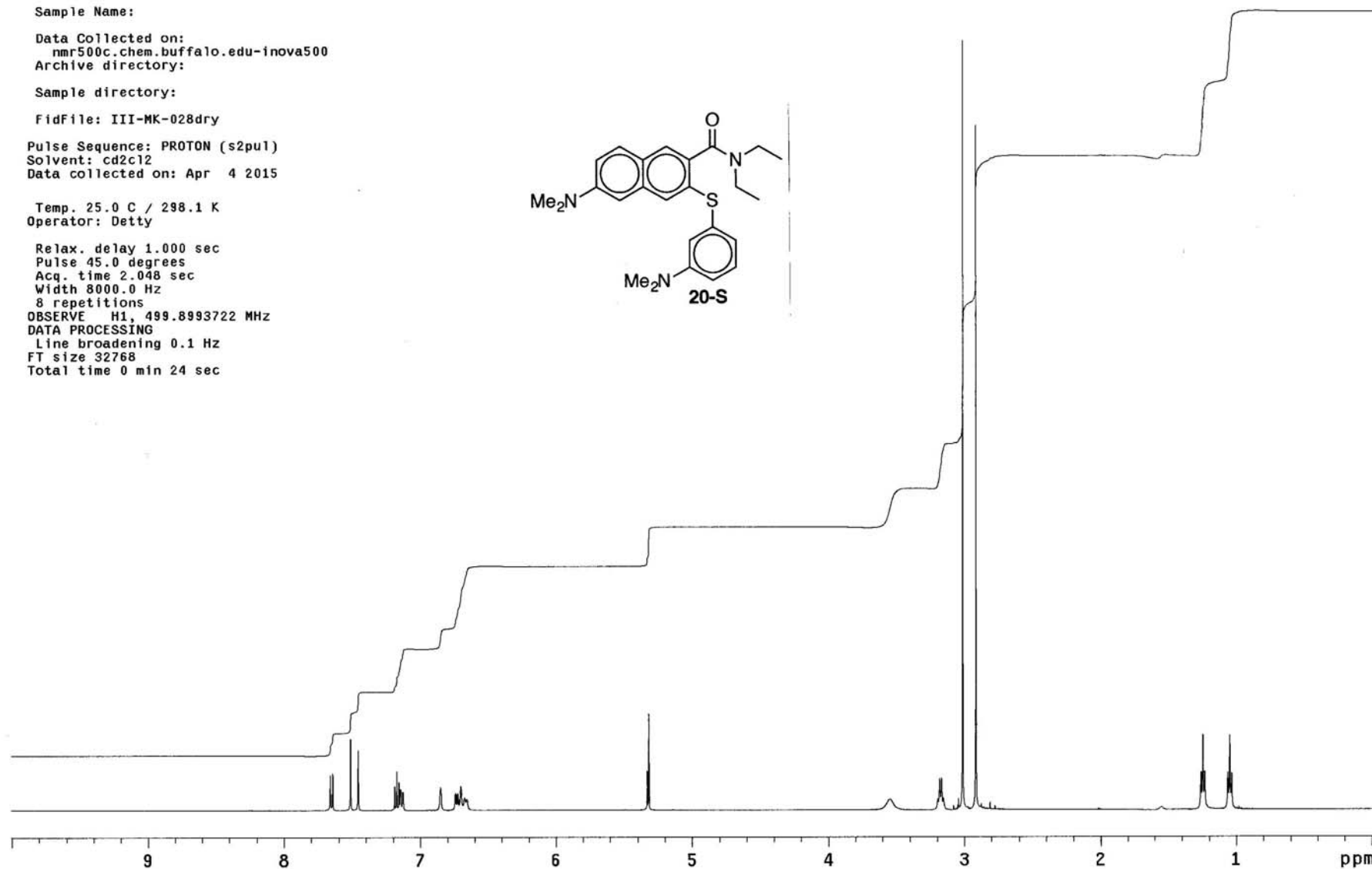
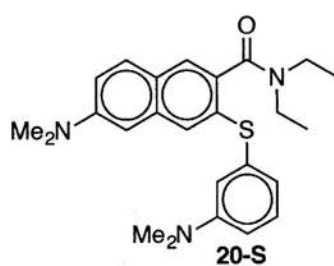
Sample directory:

FidFile: III-MK-028dry

Pulse Sequence: PROTON (s2pu1)  
Solvent: cd2cl2  
Data collected on: Apr 4 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993722 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



III-MK-028dry

Sample Name:

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

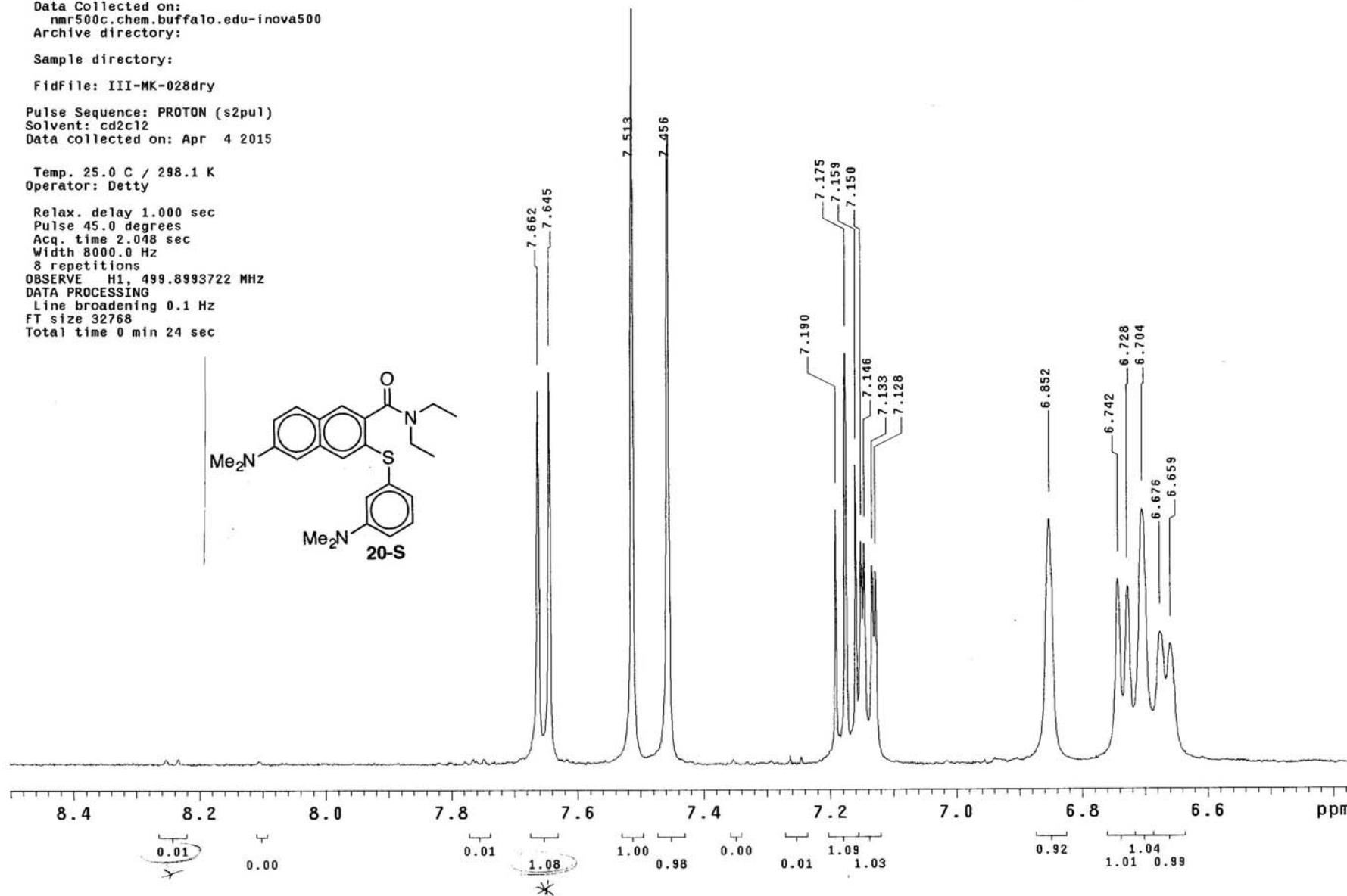
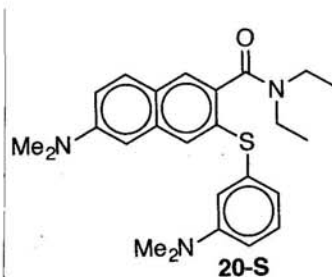
Sample directory:

FidFile: III-MK-028dry

Pulse Sequence: PROTON (s2pul)  
Solvent: cd2c12  
Data collected on: Apr 4 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8993722 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



III-MK-028dry

Sample Name:

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

Sample directory:

FidFile: III-MK-028dry

Pulse Sequence: PROTON (s2pul)  
Solvent: cd2c12  
Data collected on: Apr 4 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions

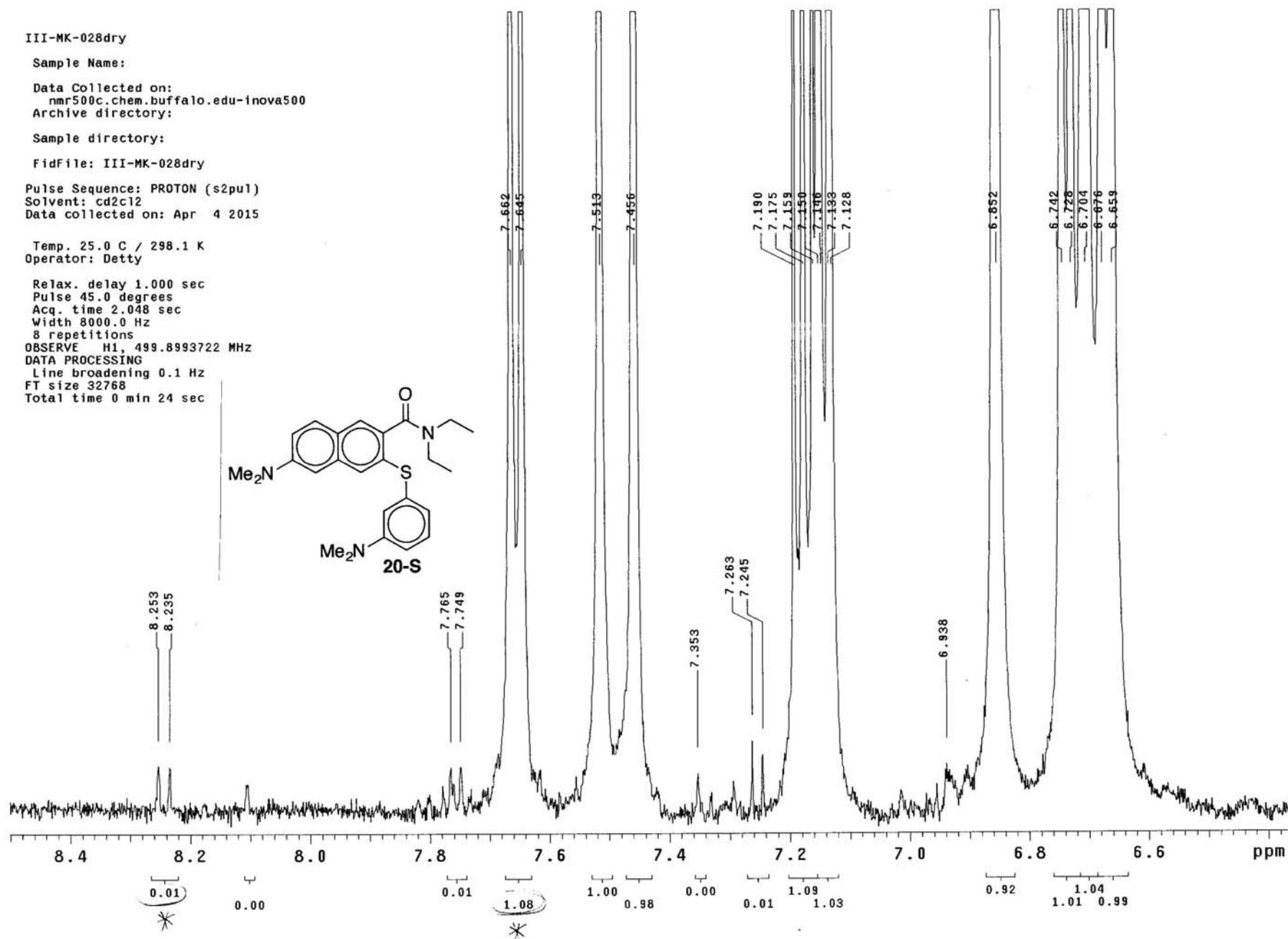
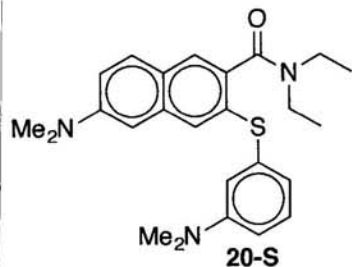
OBSERVE H1, 499.8993722 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 0 min 24 sec



III-MK-028carbon

Sample Name:

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

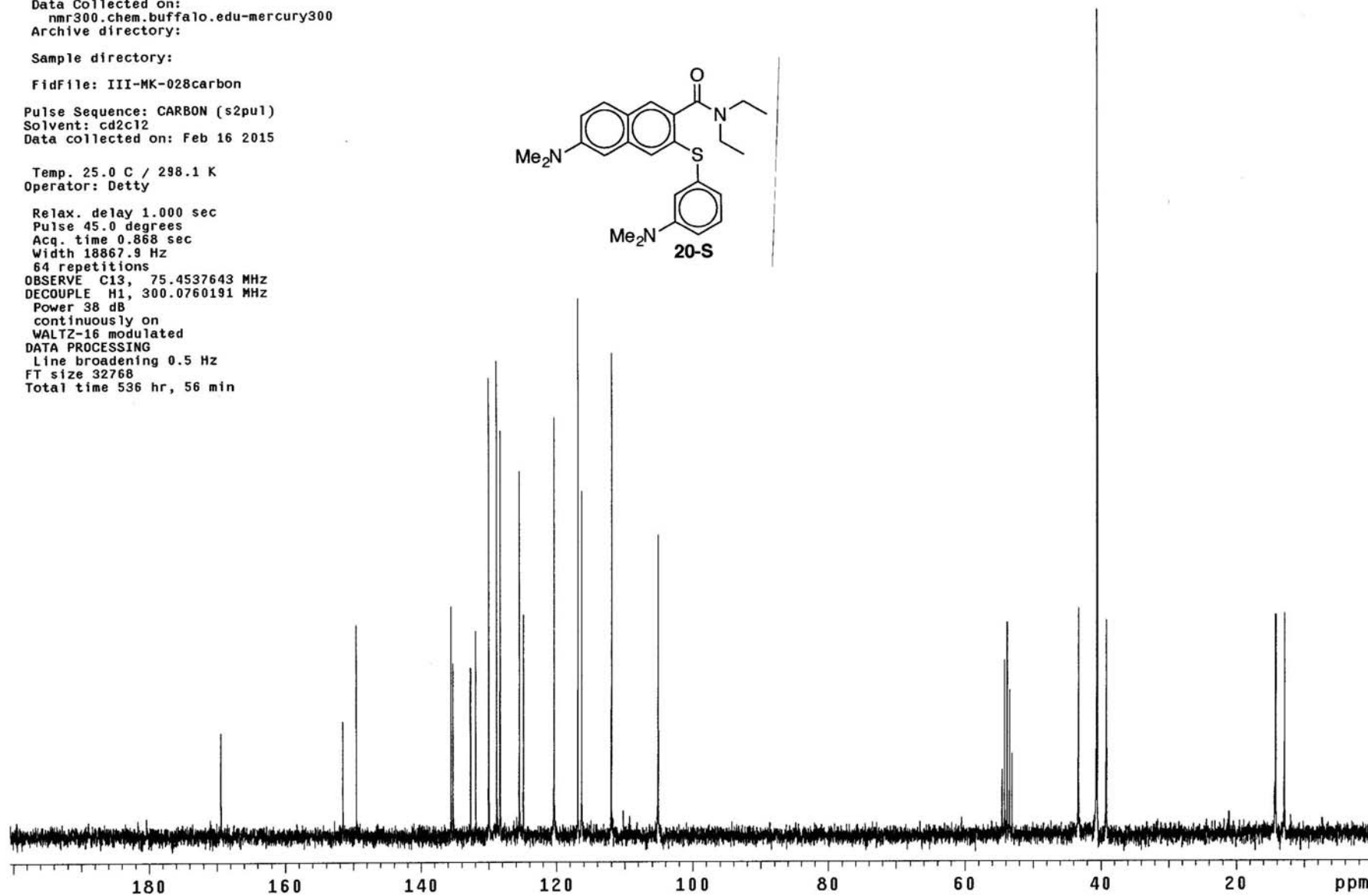
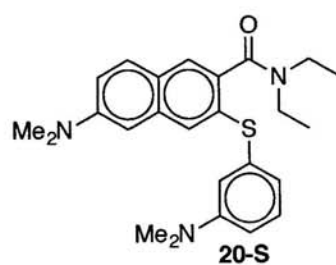
Sample directory:

FidFile: III-MK-028carbon

Pulse Sequence: CARBON (s2pu1)  
Solvent: cd2cl2  
Data collected on: Feb 16 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
64 repetitions  
OBSERVE C13, 75.4537643 MHz  
DECOUPLE H1, 300.0760191 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



S48



III-MK-032

Sample Name:

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

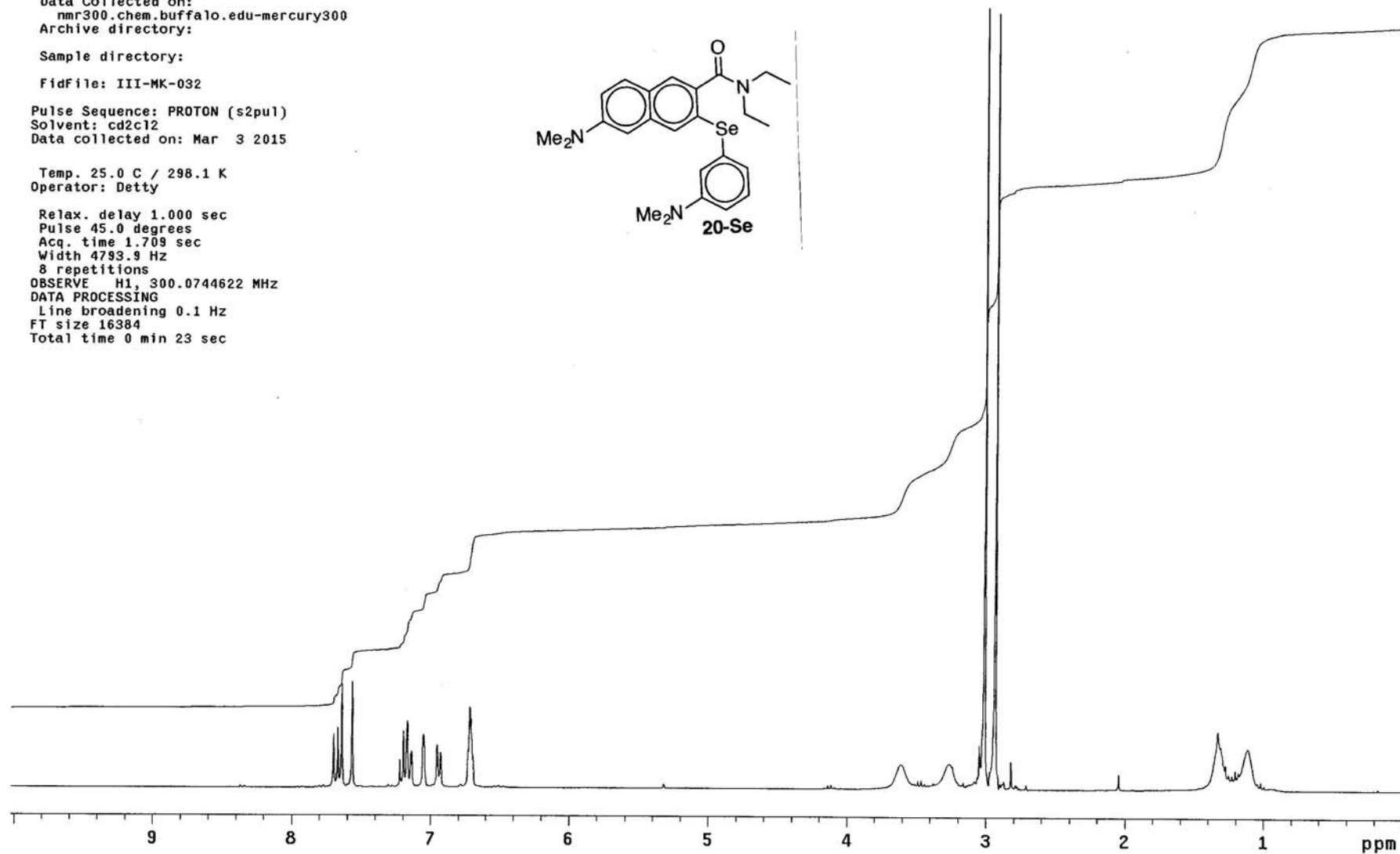
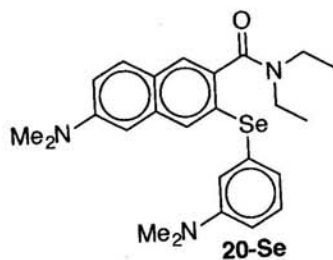
Sample directory:

FidFile: III-MK-032

Pulse Sequence: PROTON (s2pul)  
Solvent: cd2cl2  
Data collected on: Mar 3 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0744622 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec



III-MK-032

Sample Name:

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

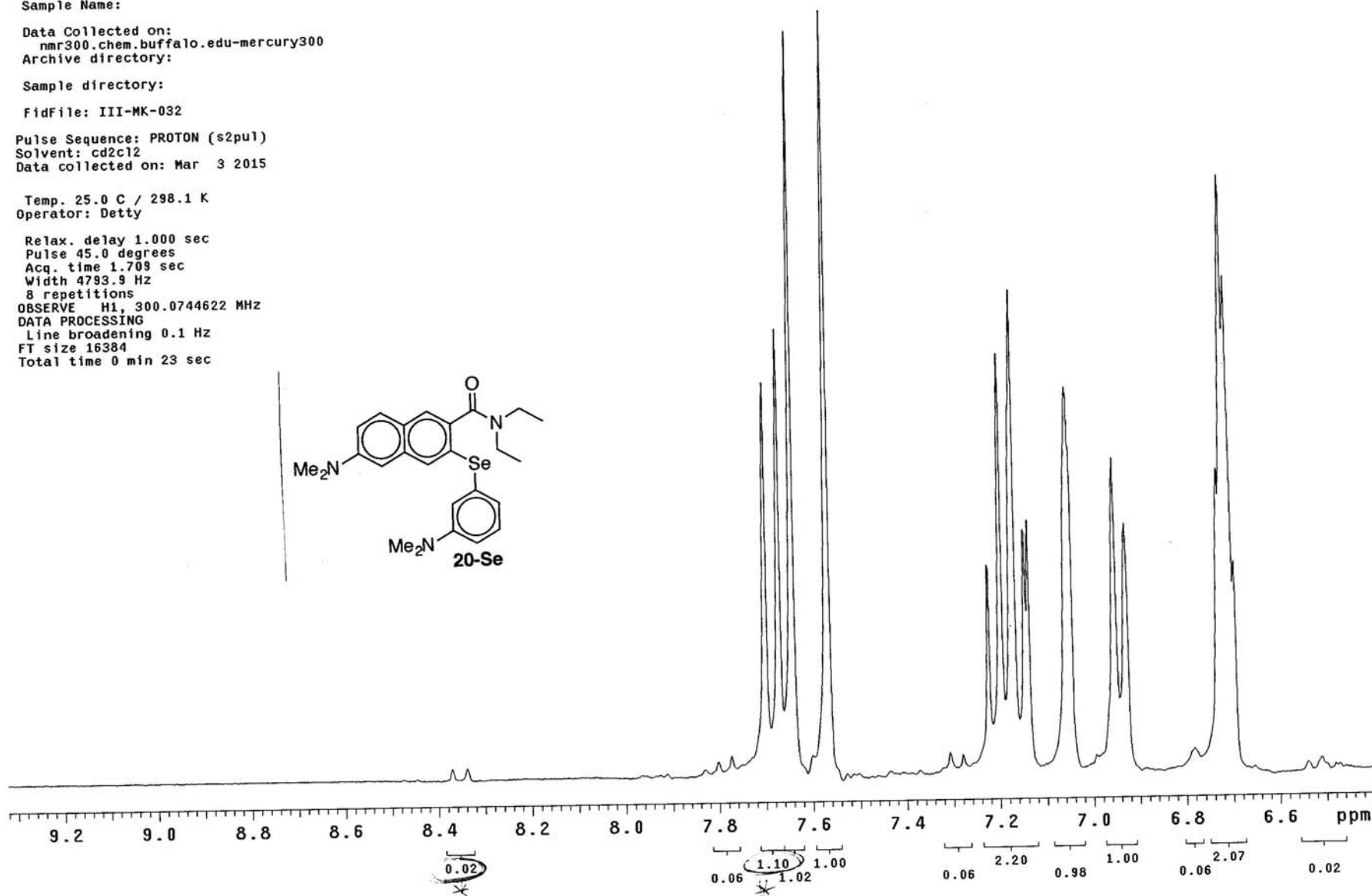
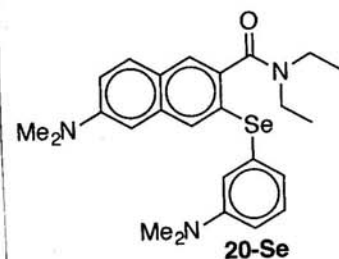
Sample directory:

FidFile: III-MK-032

Pulse Sequence: PROTON (s2pu1)  
Solvent: cd2c12  
Data collected on: Mar 3 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0744622 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec



S50

III-MK-032

Sample Name:

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

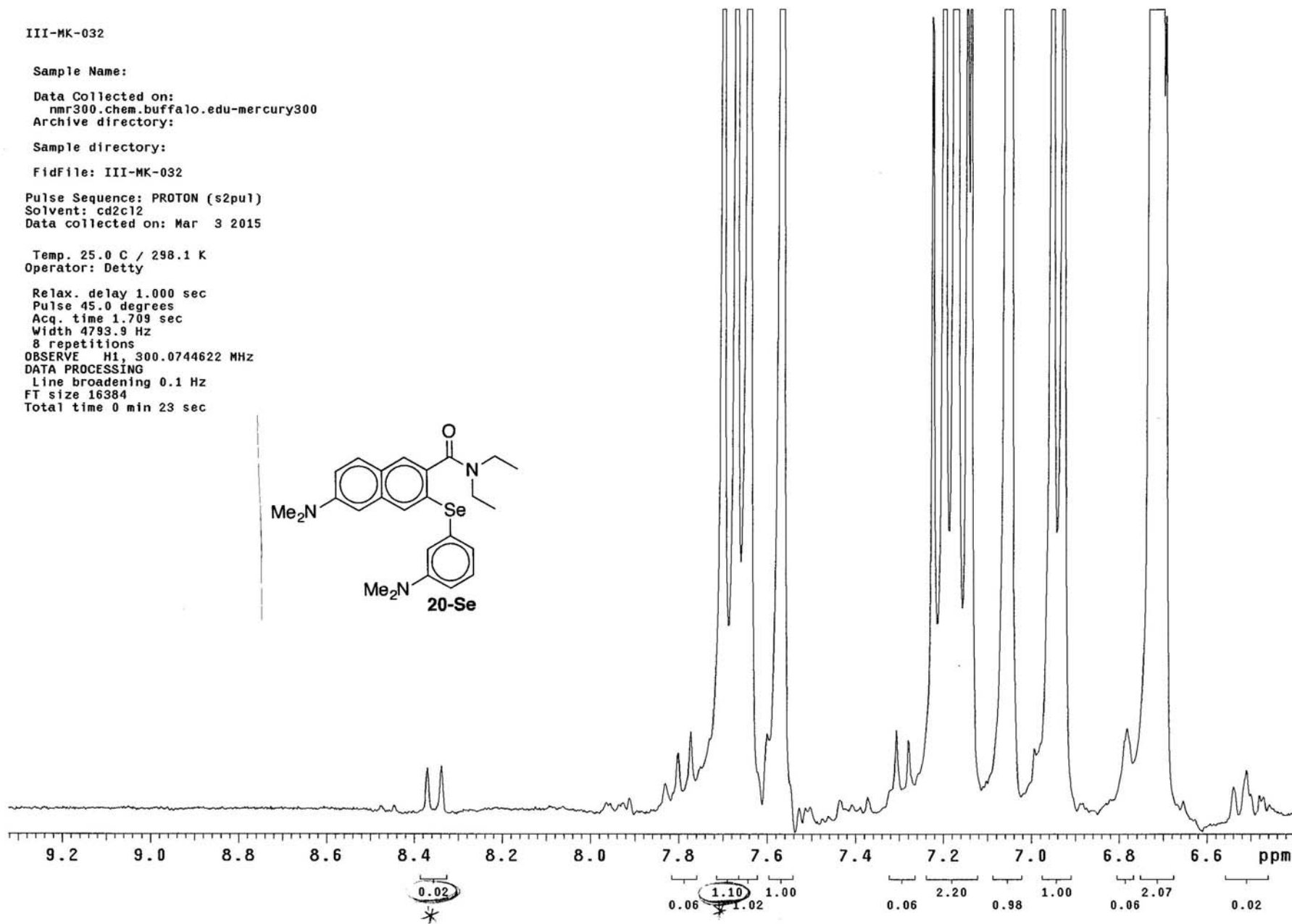
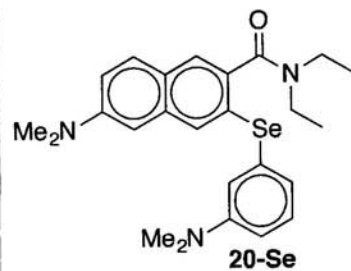
Sample directory:

FidFile: III-MK-032

Pulse Sequence: PROTON (s2pul)  
Solvent: cd2cl2  
Data collected on: Mar 3 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0744622 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec



III-MK-032carbon

Sample Name:

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

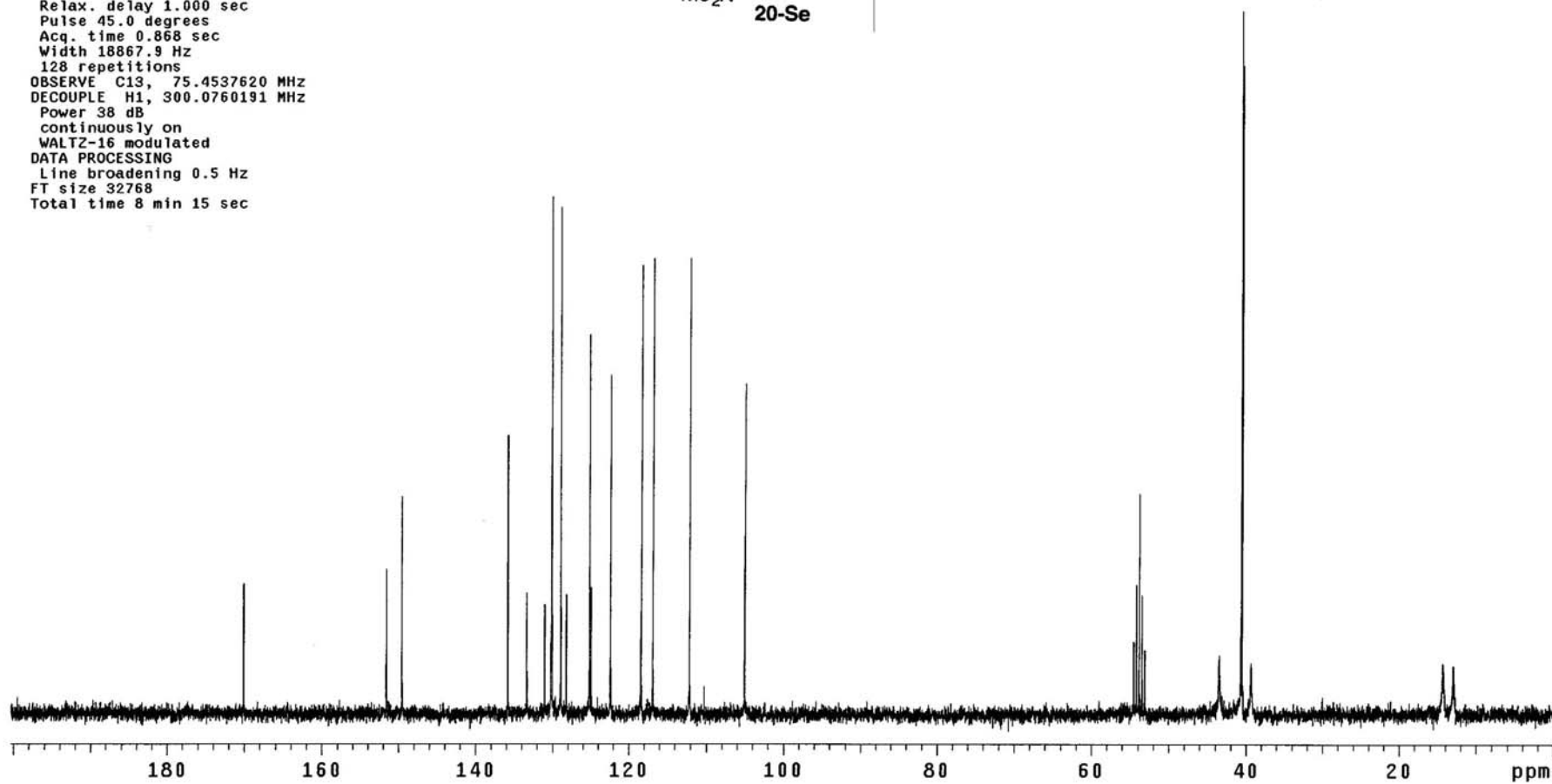
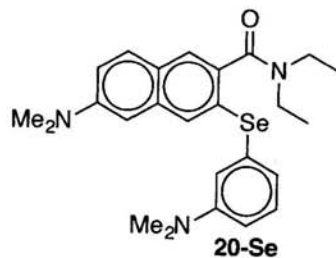
Sample directory:

FidFile: III-MK-032carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cd2c12  
Data collected on: Mar 3 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
128 repetitions  
OBSERVE C13, 75.4537620 MHz  
DECOUPLE H1, 300.0760191 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 8 min 15 sec



S52

III-MK-031

Sample Name:

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

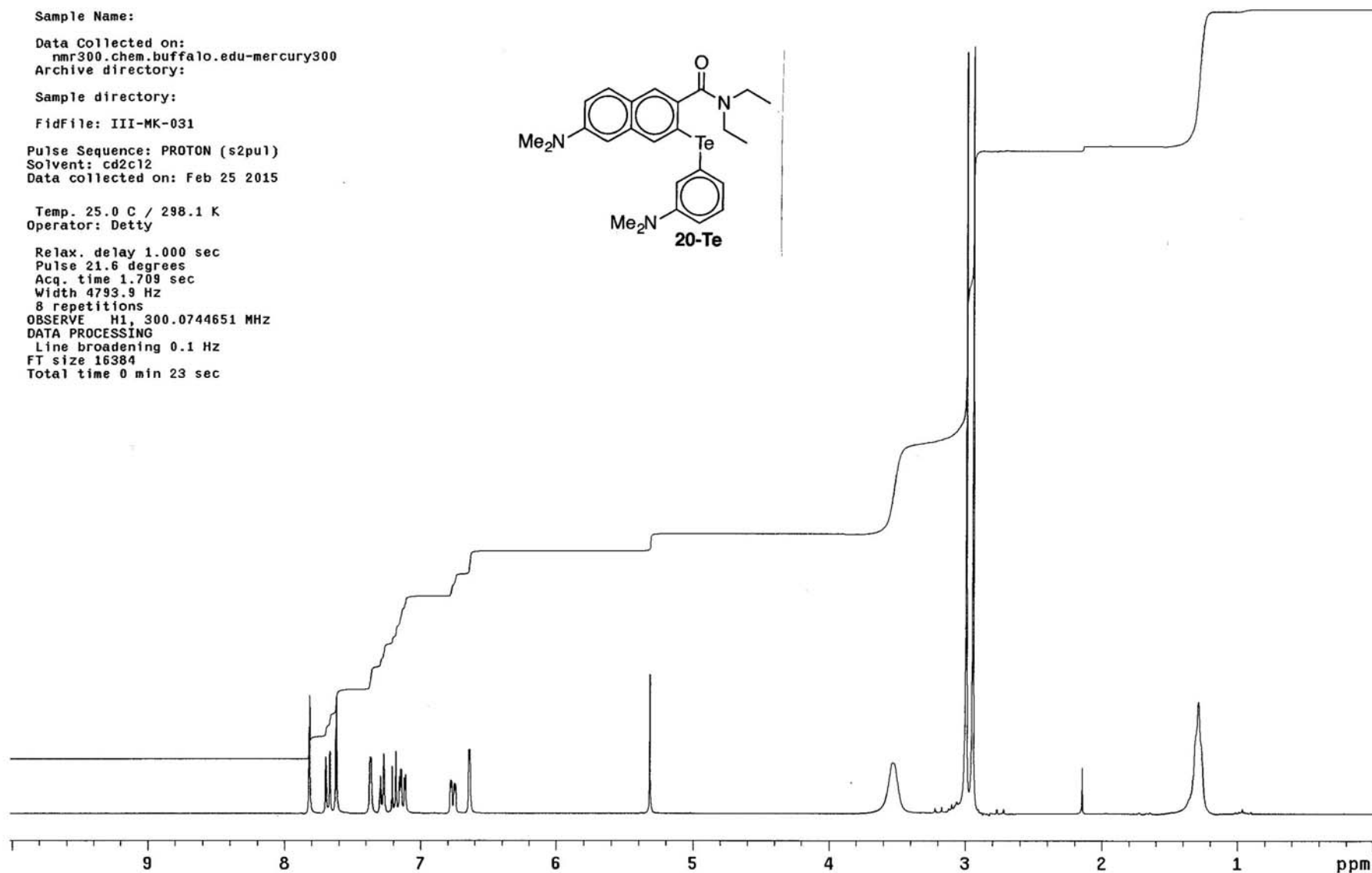
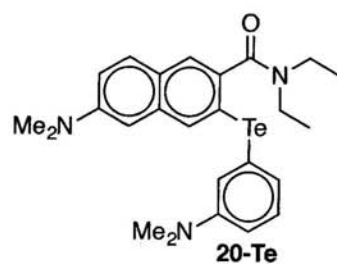
Sample directory:

FidFile: III-MK-031

Pulse Sequence: PROTON (s2pul)  
Solvent: cd2cl2  
Data collected on: Feb 25 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 21.6 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0744651 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec



III-MK-031

Sample Name:

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

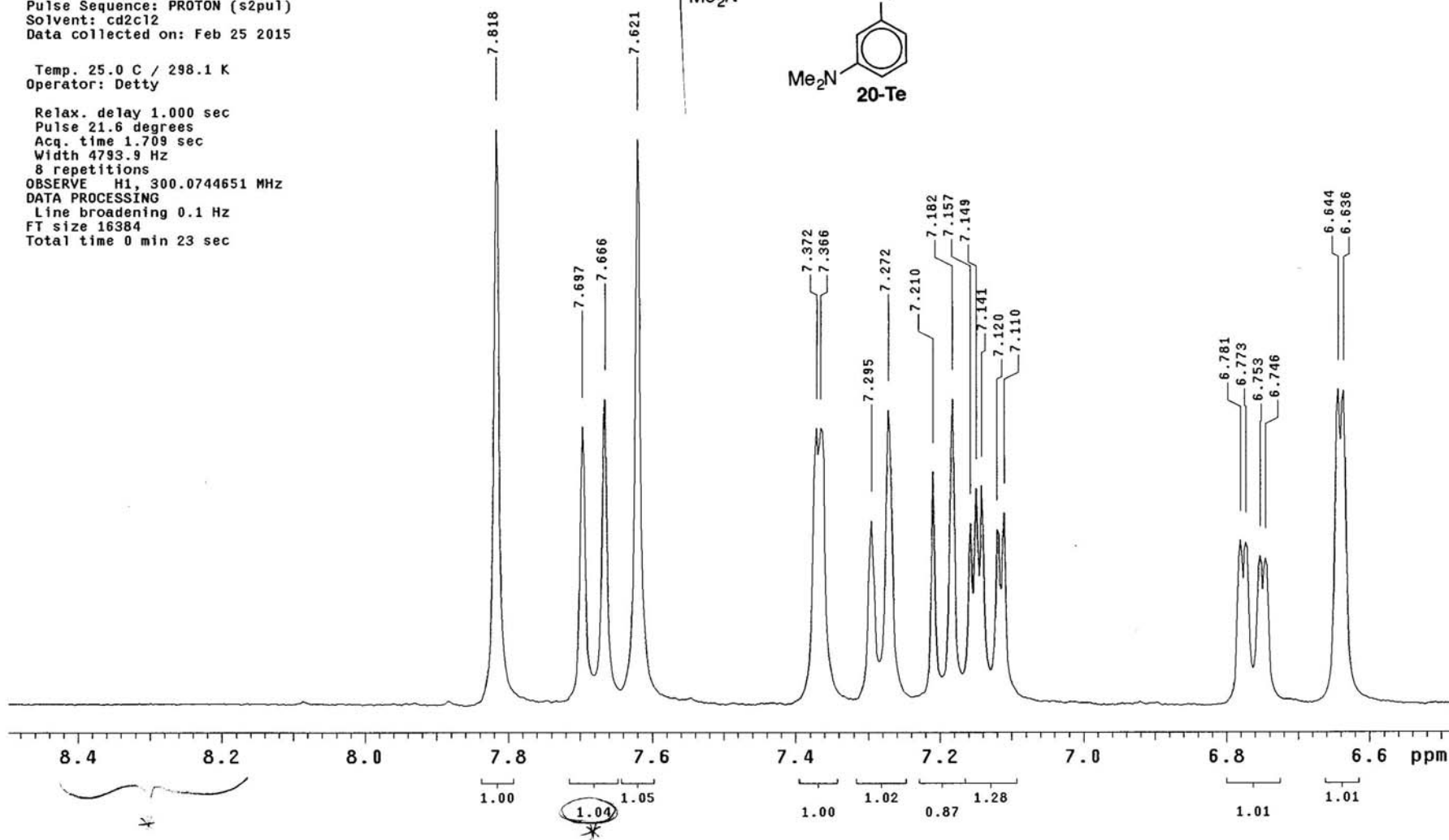
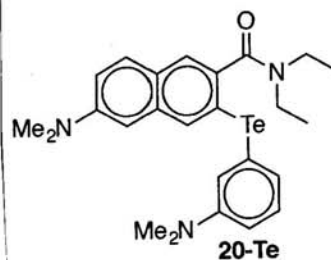
Sample directory:

FidFile: III-MK-031

Pulse Sequence: PROTON (s2pu1)  
Solvent: cd2c12  
Data collected on: Feb 25 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 21.6 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0744651 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec



III-MK-031carbon

Sample Name:

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

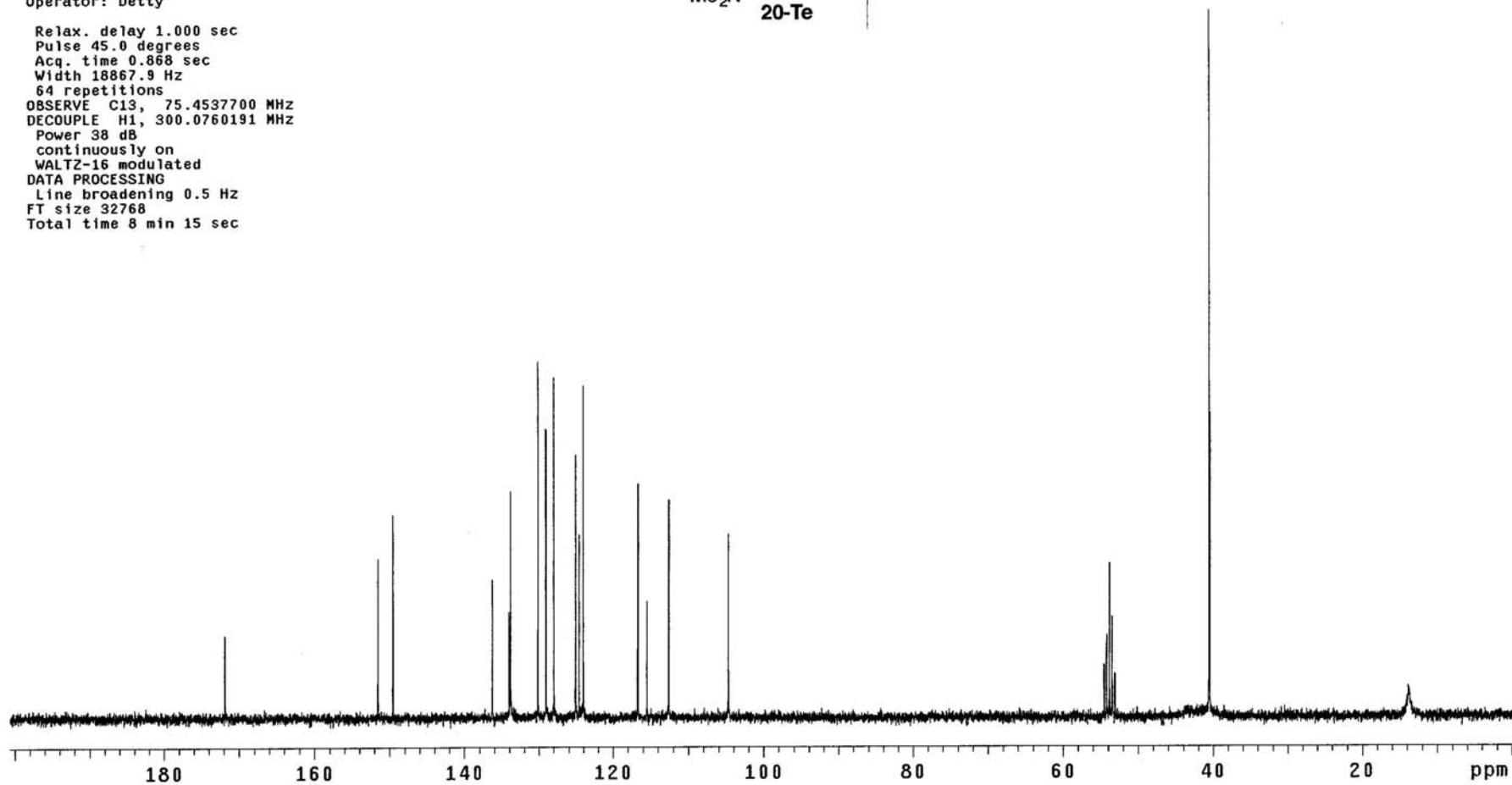
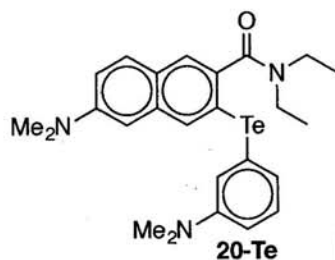
Sample directory:

FidFile: III-MK-031carbon

Pulse Sequence: CARBON (s2pul)  
Solvent: cd2c12  
Data collected on: Feb 25 2015

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
64 repetitions  
OBSERVE C13, 75.4537700 MHz  
DECOUPLE H1, 300.0760191 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 8 min 15 sec



S55

III-MK-062 secondary amide

Sample Name:

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

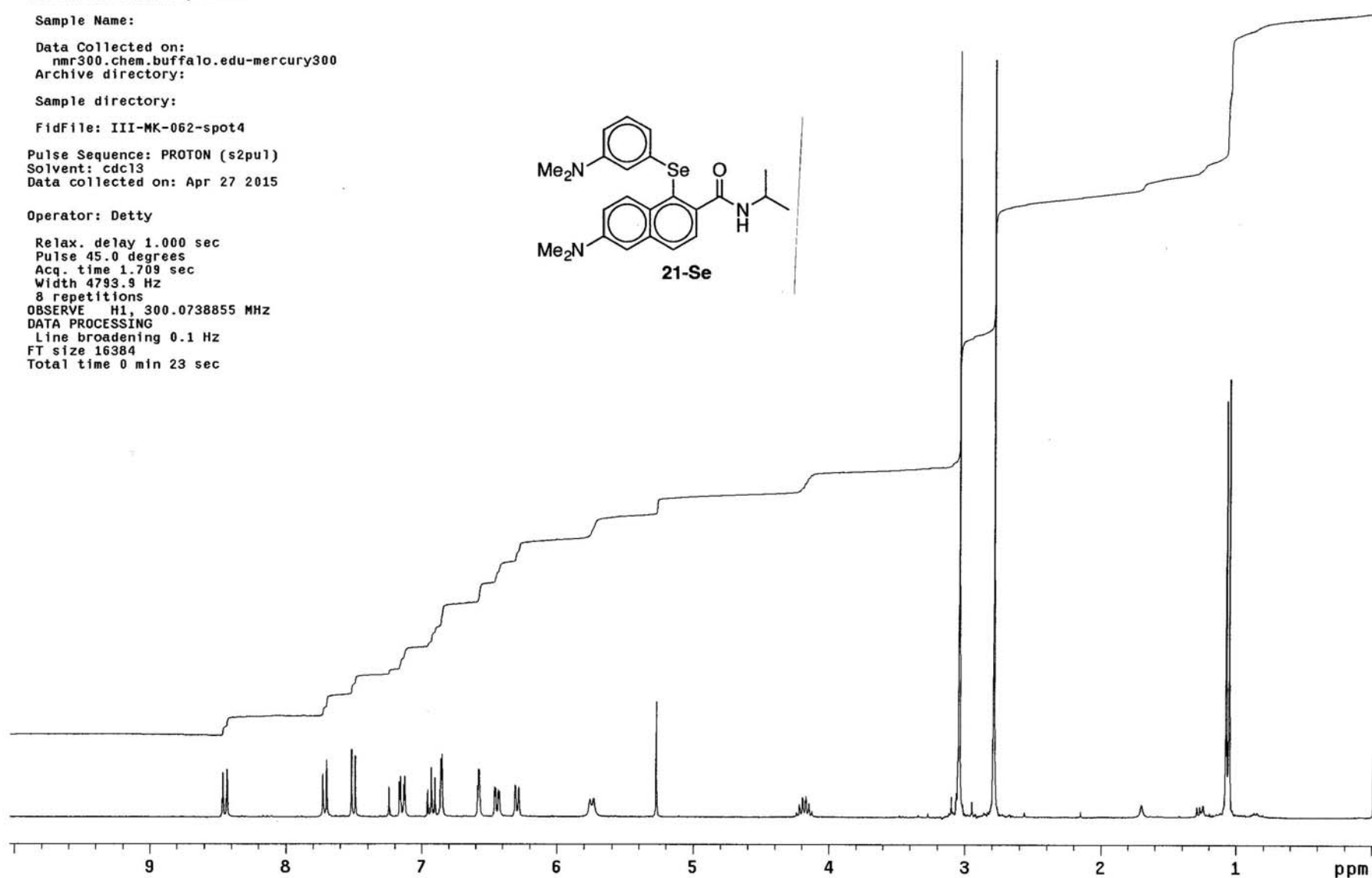
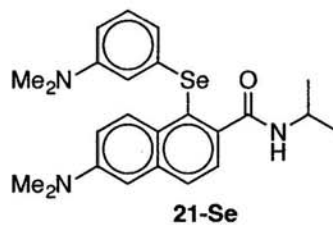
Sample directory:

FidFile: III-MK-062-spot4

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 27 2015

Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0738855 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec





III-MK-062 secondary amide carbon

Sample Name:

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

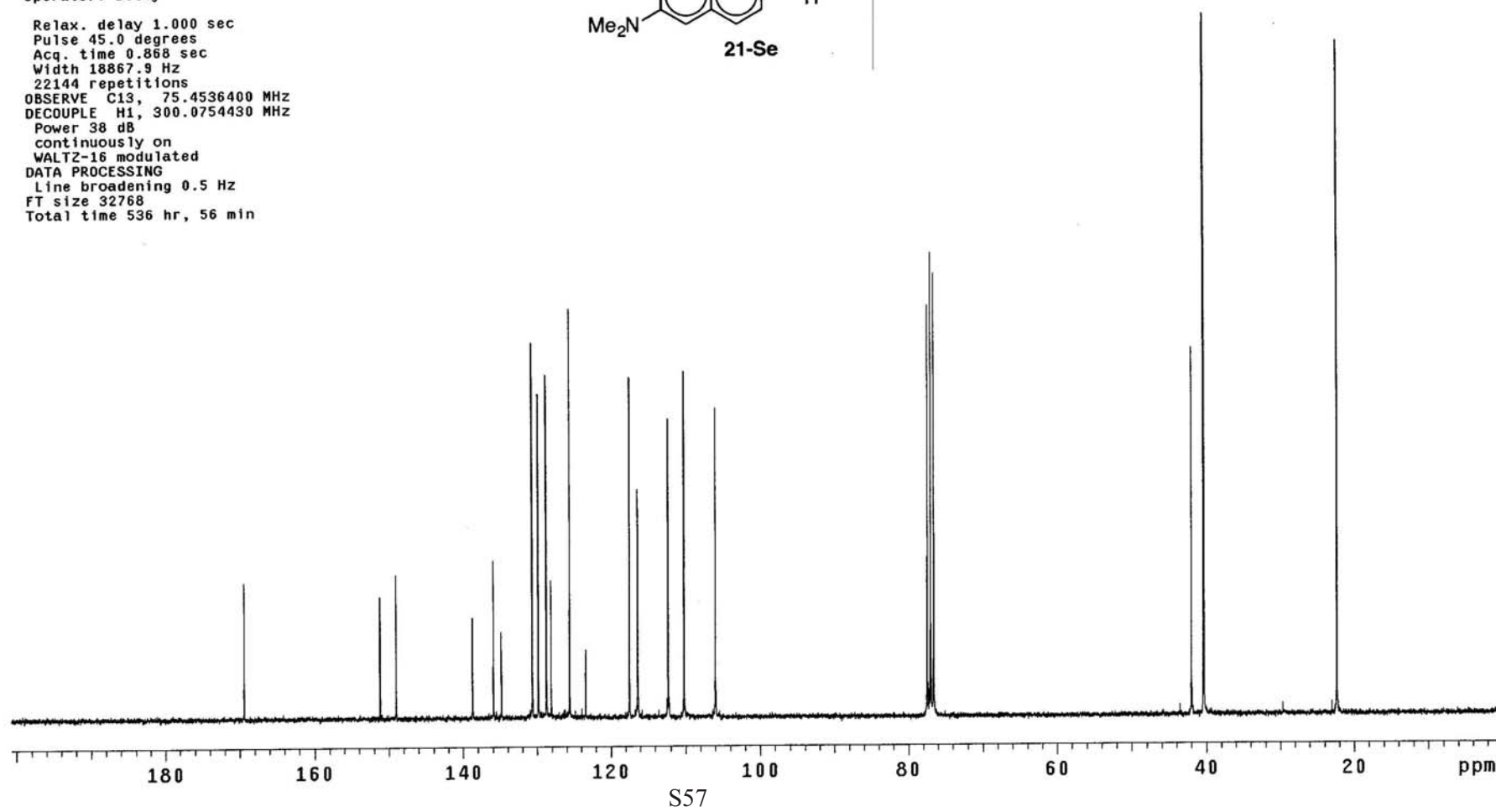
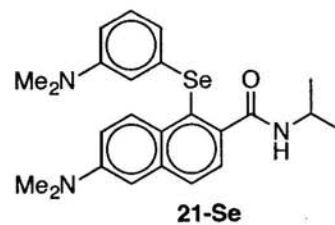
Sample directory:

FidFile: III-MK-062-spot4-carbon2

Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Apr 27 2015

Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 0.868 sec  
Width 18867.9 Hz  
22144 repetitions  
OBSERVE C13, 75.4536400 MHz  
DECOUPLE H1, 300.0754430 MHz  
Power 38 dB  
continuously on  
WALTZ-16 modulated  
DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 32768  
Total time 536 hr, 56 min



Diethyl S Mix II-MK-186

Sample Name:

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

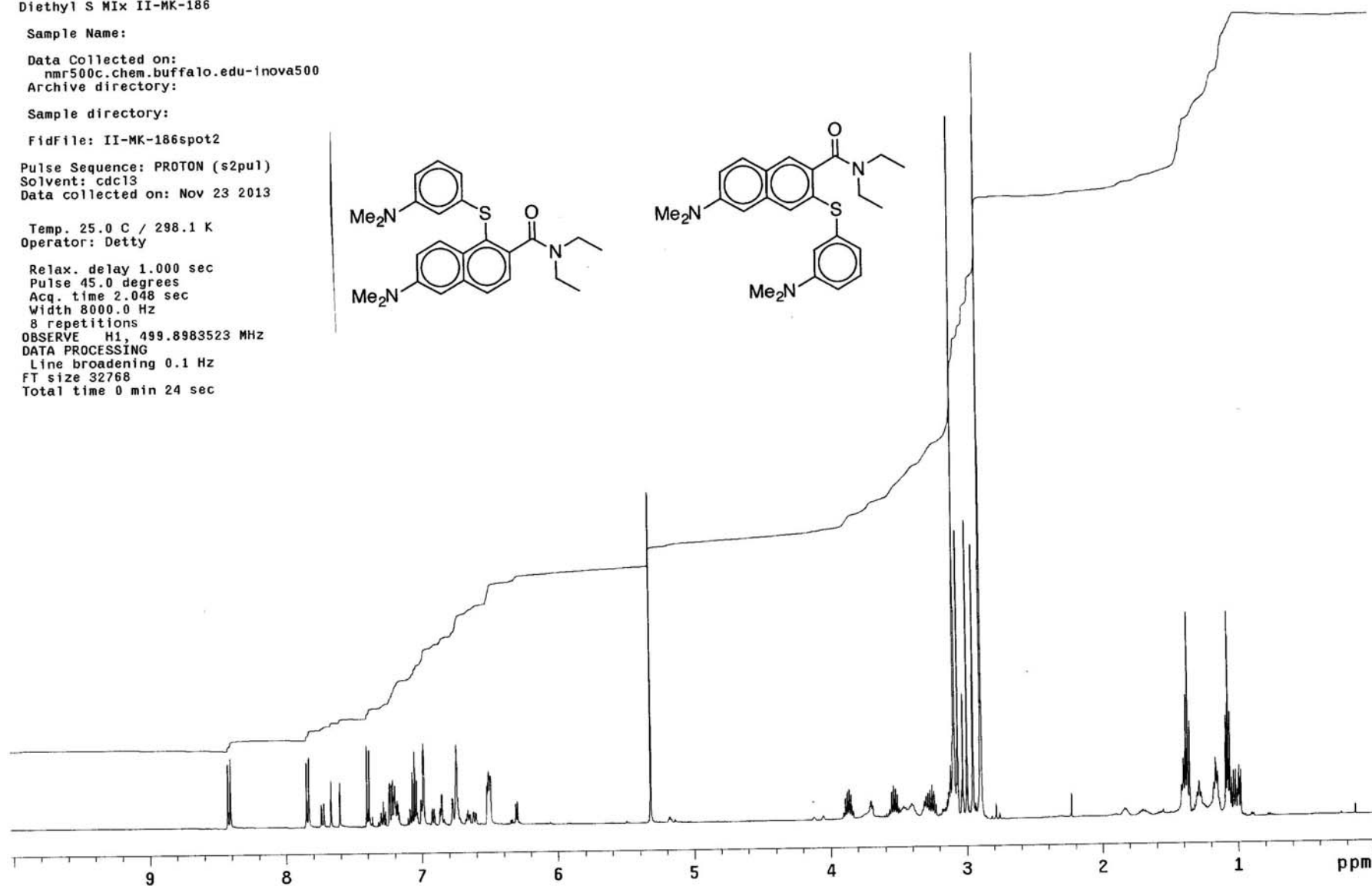
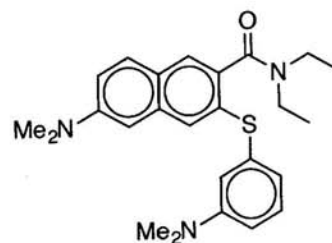
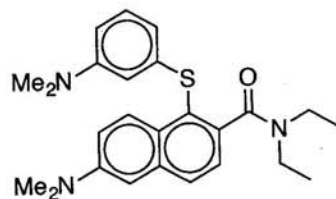
Sample directory:

FidFile: II-MK-186spot2

Pulse Sequence: PROTON (s2pu1)  
Solvent: cdc13  
Data collected on: Nov 23 2013

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8983523 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



Diethyl S Mix II-MK-186

Sample Name:

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

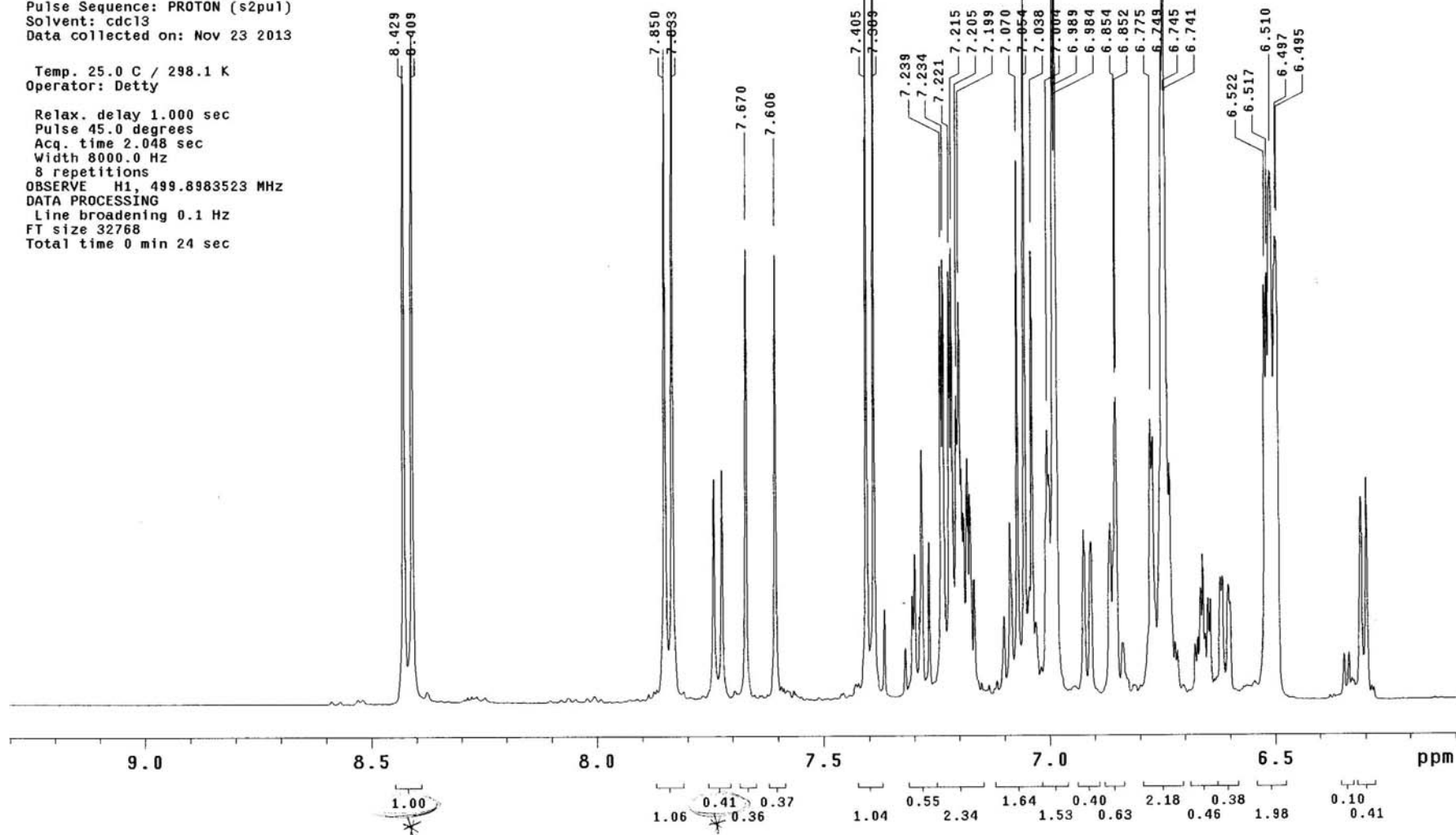
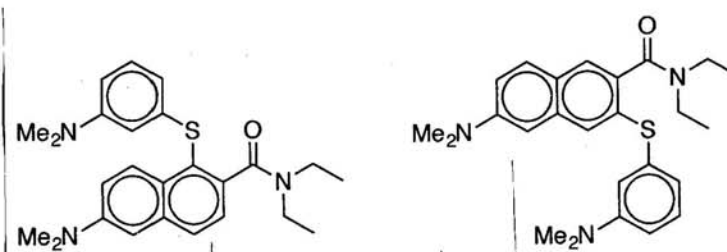
Sample directory:

FidFile: II-MK-186spot2

Pulse Sequence: PROTON (s2pu1)  
Solvent: cdc13  
Data collected on: Nov 23 2013

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8983523 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



Diethyl Se Mix II-MK-200

Sample Name:

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

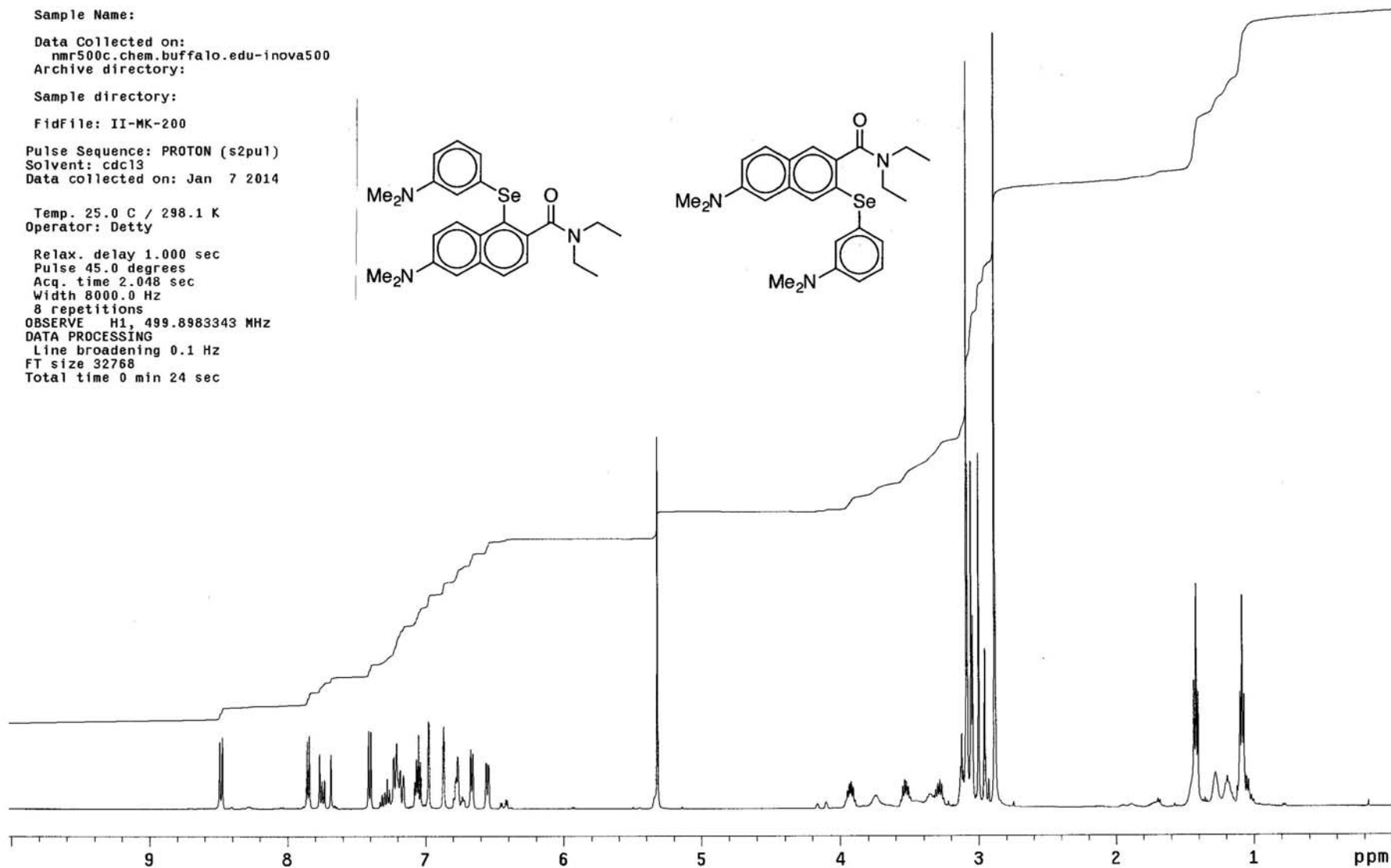
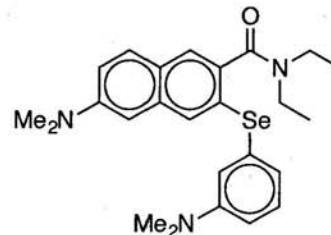
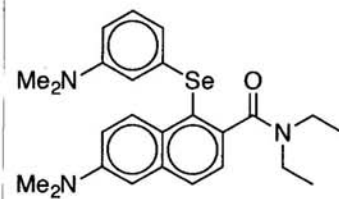
Sample directory:

FidFile: II-MK-200

Pulse Sequence: PROTON (s2pu1)  
Solvent: cdc13  
Data collected on: Jan 7 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8983343 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



Diethyl Se Mix II-MK-200

Sample Name:

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

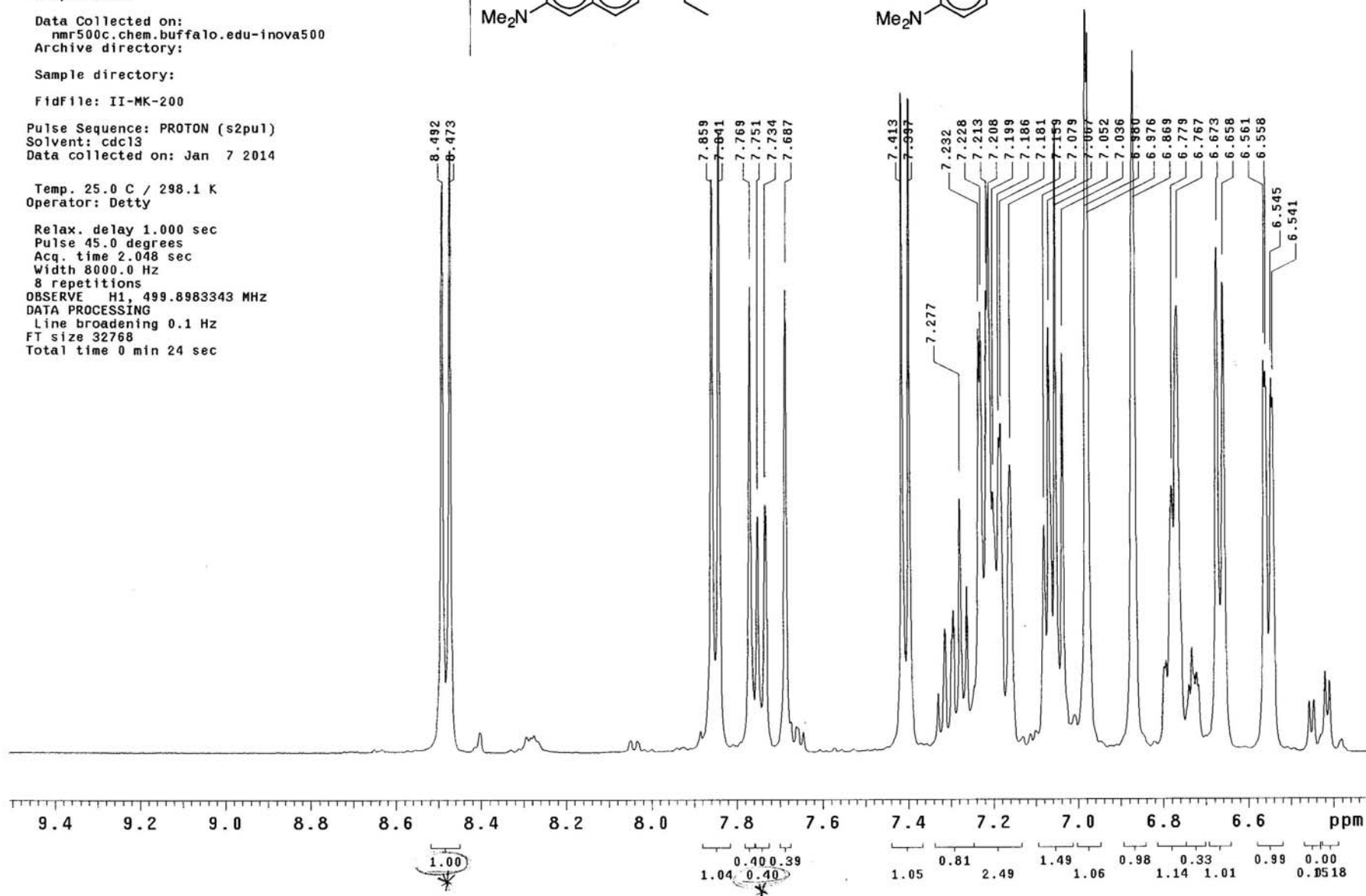
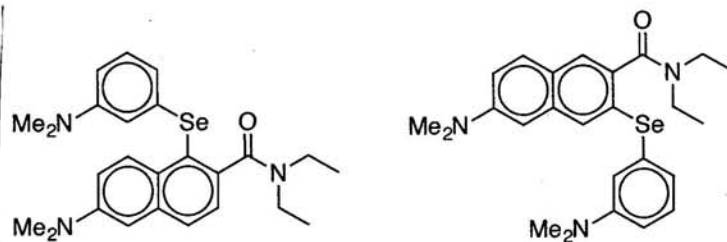
Sample directory:

FidFile: II-MK-200

Pulse Sequence: PROTON (s2pul)  
Solvent: cdc13  
Data collected on: Jan 7 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.048 sec  
Width 8000.0 Hz  
8 repetitions  
OBSERVE H1, 499.8983343 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 32768  
Total time 0 min 24 sec



II-MK-213

Sample Name:

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

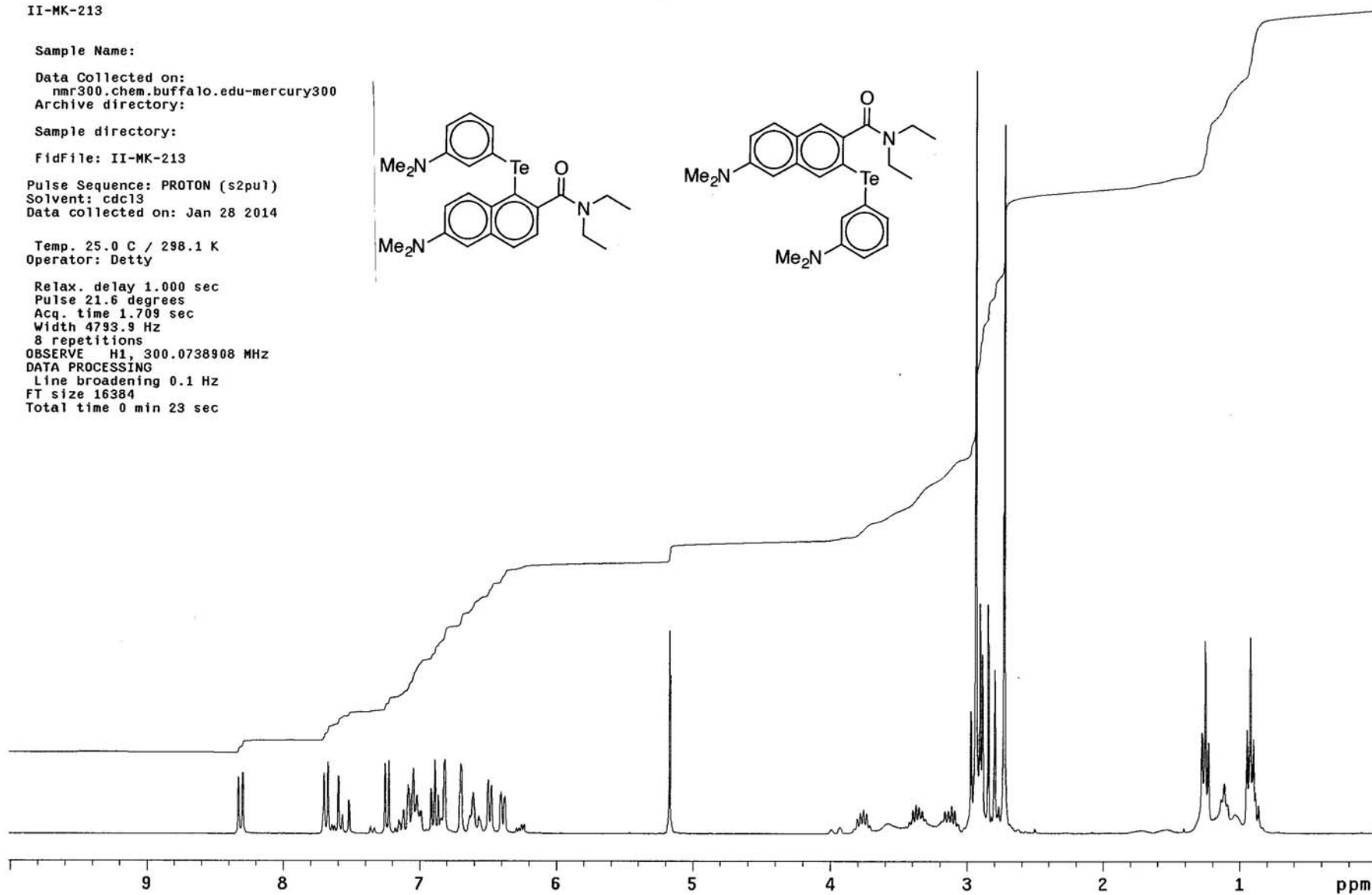
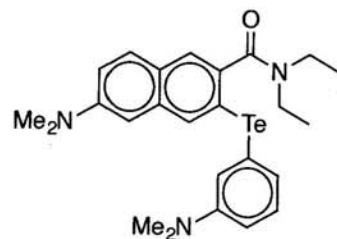
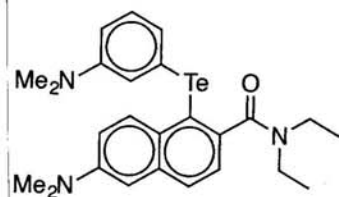
Sample directory:

FidFile: II-MK-213

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 28 2014

Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 21.6 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0738908 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec





II-MK-213

Sample Name:

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

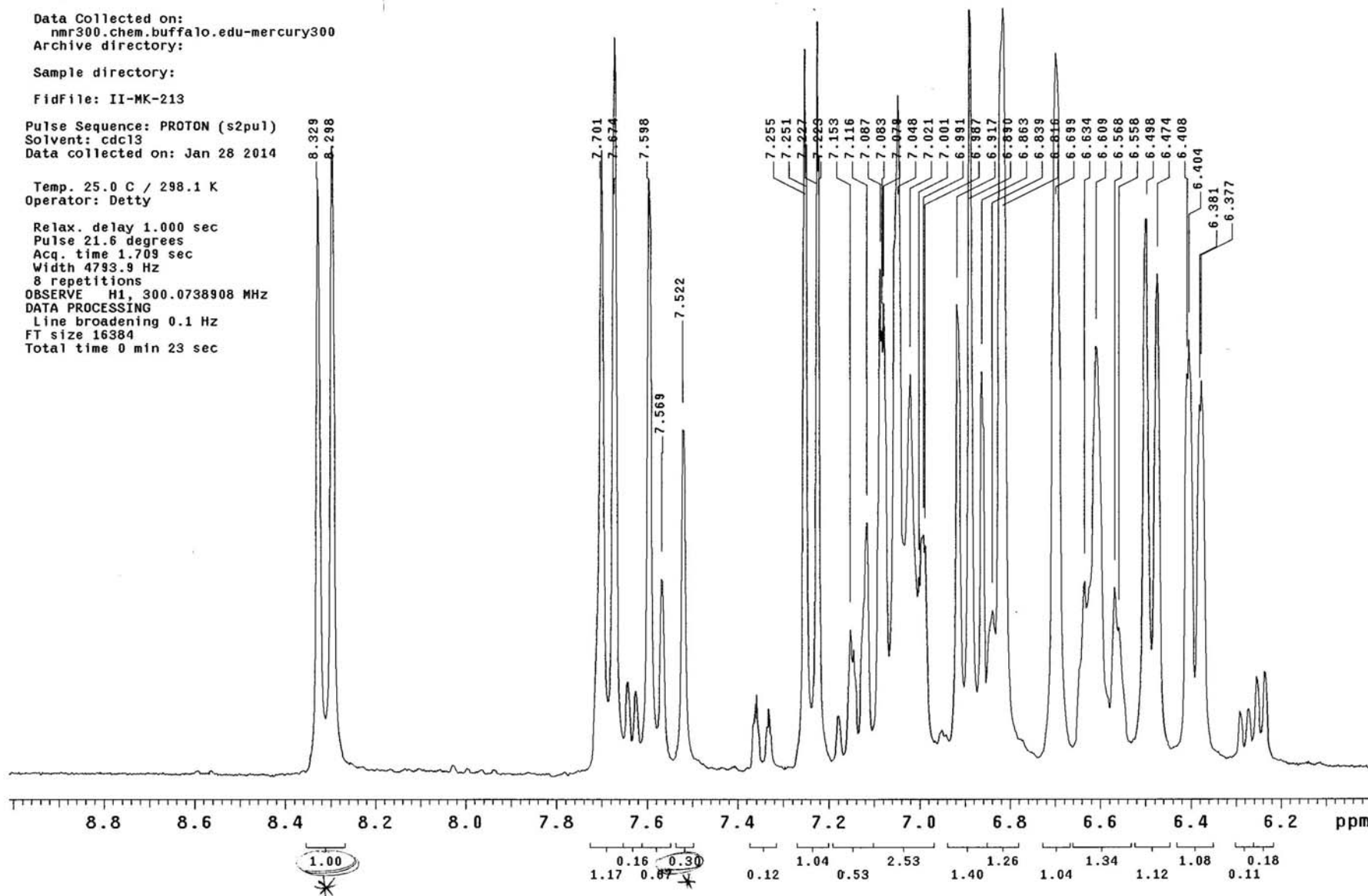
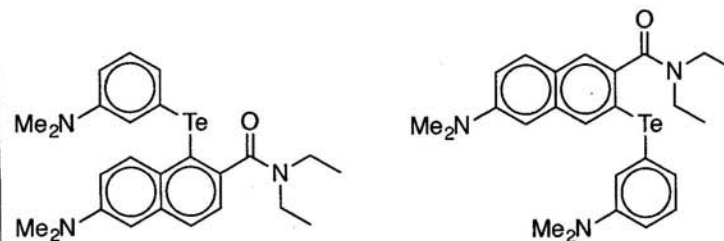
Sample directory:

FidFile: II-MK-213

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Jan 28 2014

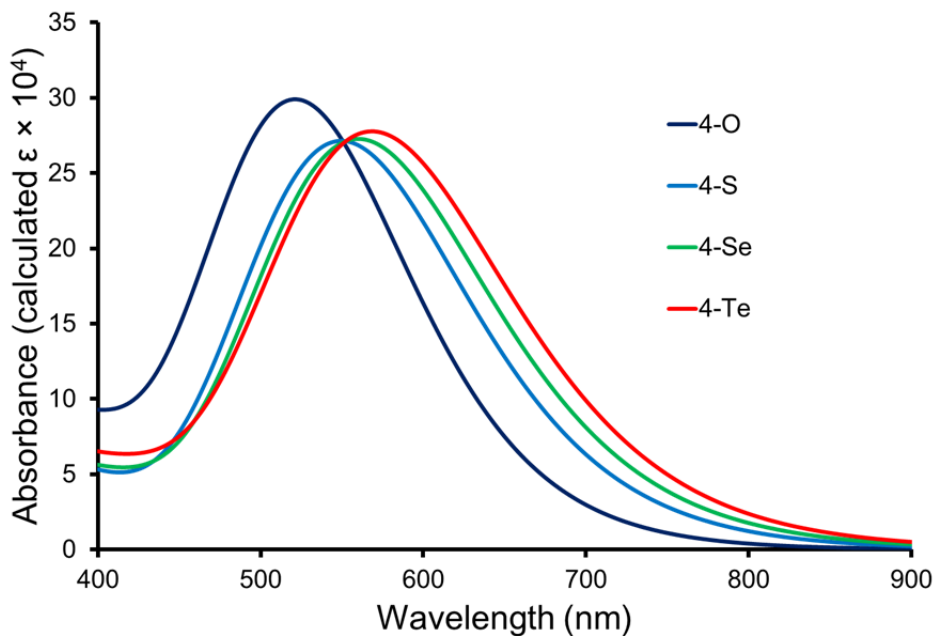
Temp. 25.0 C / 298.1 K  
Operator: Detty

Relax. delay 1.000 sec  
Pulse 21.6 degrees  
Acq. time 1.709 sec  
Width 4793.9 Hz  
8 repetitions  
OBSERVE H1, 300.0738908 MHz  
DATA PROCESSING  
Line broadening 0.1 Hz  
FT size 16384  
Total time 0 min 23 sec

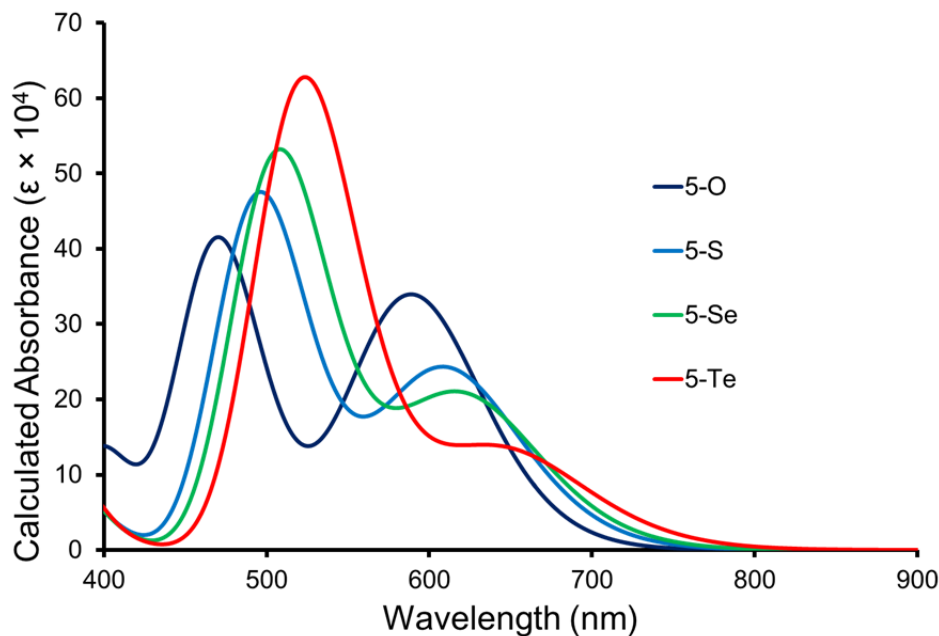


S63

deprotection

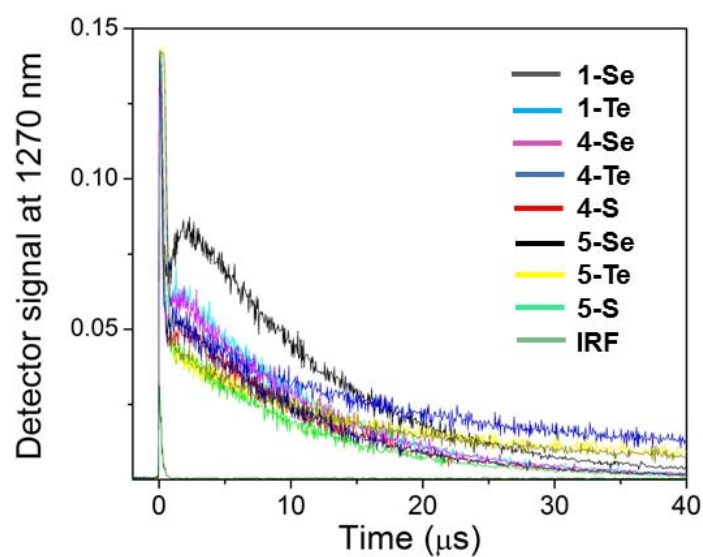


**Figure S1.** The calculated absorption spectra of **4-E** dyes. Generated from the 20 lowest energy excitations from a TD-DFT calculation (B3LYP/6-311+G(d)/LanL2DZ) with a Gaussian function with FRHM 0.17 eV on each excitation.

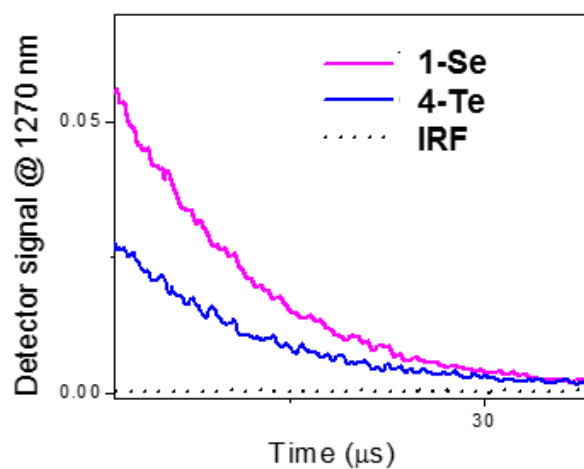


**Figure S2.** The calculated absorption spectra of **5-E** dyes. Generated from the 20 lowest energy excitations from a TD-DFT calculation (B3LYP/6-311+G(d)/LanL2DZ) with a Gaussian function with FRHM 0.17 eV on each excitation.





**Figure S3.** Decays of phosphorescence from  $^1\text{O}_2$  sensitized by compounds **1-Se**, **1-Te**, **4-S**, **4-Se**, **4-Te**, **5-S**, **5-Se**, and **5-Te** used for determination of  $^1\text{O}_2$  quantum yields. Signal obtained from air-saturated MeOH in the cuvette was used as the instrument response function (IRF).



**Figure S4.** Decays from phosphorescence from  $^1\text{O}_2$  sensitized by compounds **1-Se** [standard with  $\Phi(^1\text{O}_2) = 0.87$ ] and **4-Te** [ $\Phi(^1\text{O}_2) = 0.43$ ].