Synthesis and Properties of Heavy Chalcogen Analogues of the Texas Reds and Related Rhodamines

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Supporting Information

Contents:

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}H), an Inova 400 (126 MHz for ^{125}Te), or a Mercury 300 (75.5 MHz for ^{13}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. Alkyllithiums (*s*-butyllithium and *t*-butyllithium) were titrated immediately prior to use with anhydrous diphenylacetic acid.

II-MK-120dry

Sample Name:

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

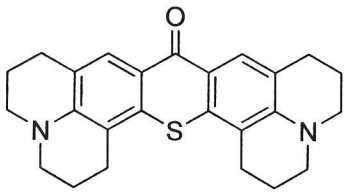
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Feb 12 2014

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



2-S

II-MK-120carbon

Sample Name:

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

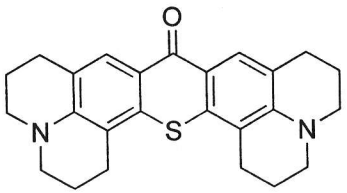
Sample directory:

FidFile: II-MK-120carbon

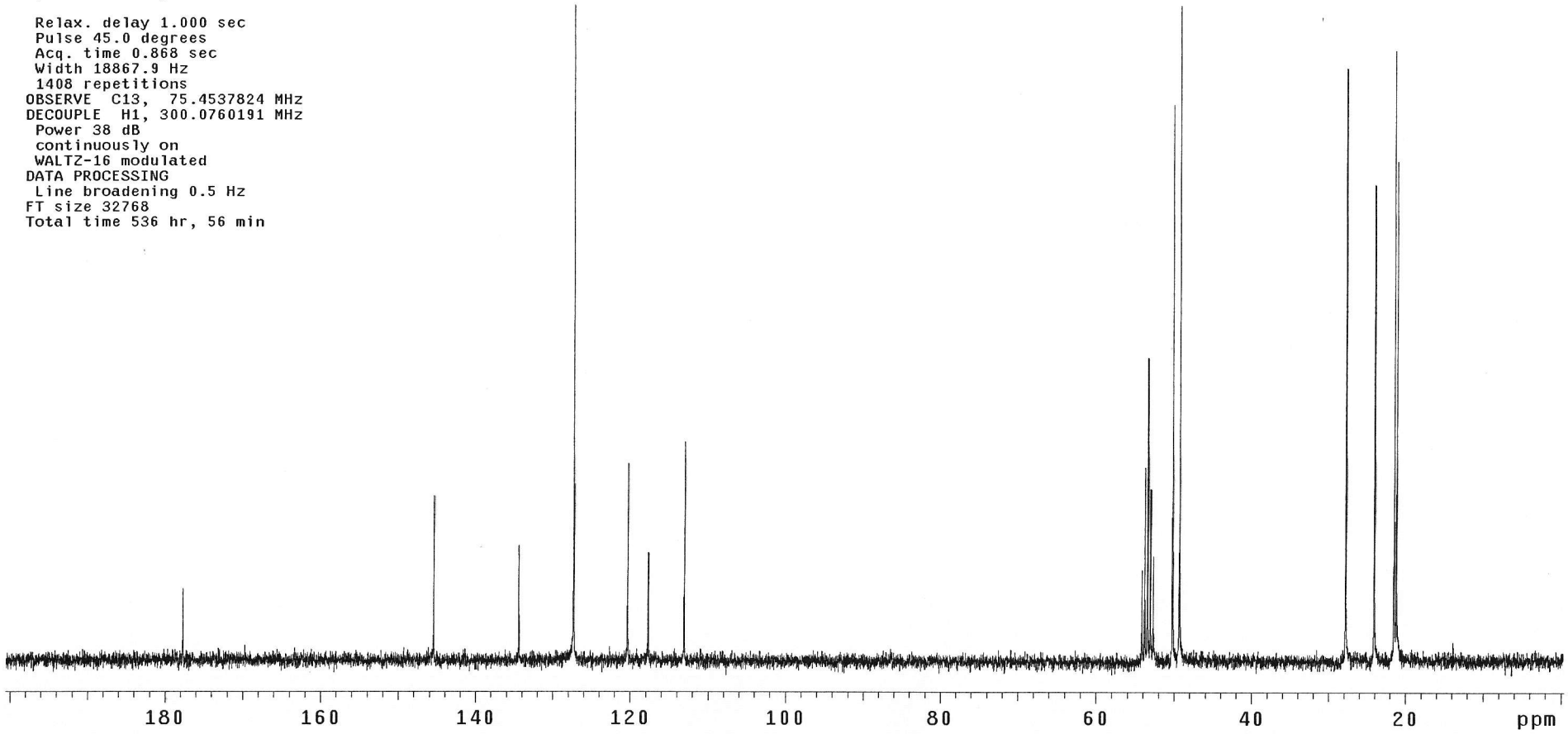
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 24 2013

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
1408 repetitions
OBSERVE C13, 75.4537824 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



2-S



II-MK-093dry

Sample Name:

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

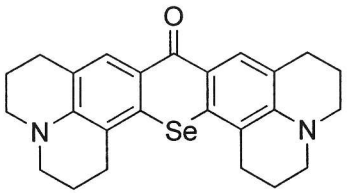
Sample directory:

FidFile: II-MK-093dried

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



2-Se

II-MK-093carbon

Sample Name:

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

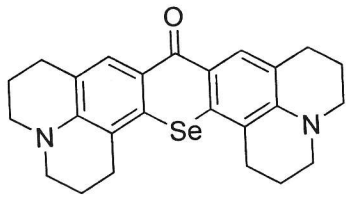
Sample directory:

FidFile: II-MK-093carbon

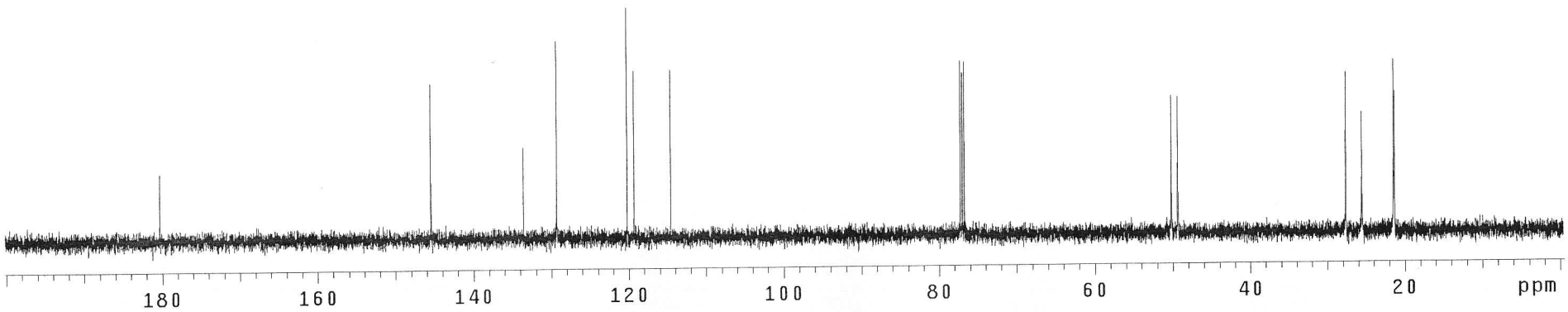
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 13 2013

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, 125.6995673 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, 42 min



2-Se



II-MK-103

Sample Name:

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

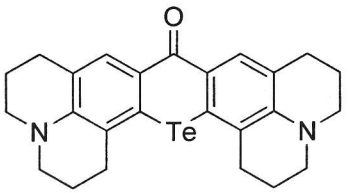
Sample directory:

FidFile: II-MK-103

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 10 2013

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



2-Te

II-MK-103carbon

Sample Name:

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

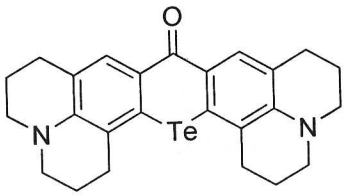
Sample directory:

FidFile: II-MK-103carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 10 2013

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
26112 repetitions
OBSERVE C13, 75.4537824 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



2-Te

II-GS-269-recrystallization

Sample Name:

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

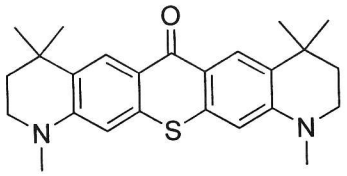
Sample directory:

FidFile: II-GS-267-recrystallization

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



3-S

II-GS-267-13C

Sample Name:

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

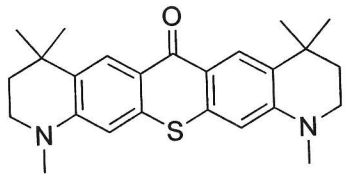
Sample directory:

FidFile: II-GS-267-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jul 22 2013

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, 75.4536582 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 53 hr, 41 min



3-S

II-GS-176-recrystallization

Sample Name:

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

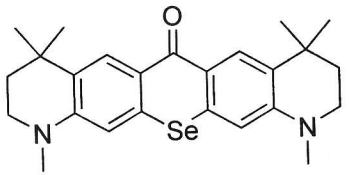
Sample directory:

FidFile: II-GS-176-recrystallization

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 6 2013

Temp. 19.0 C / 292.1 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



3-Se

II-GS-176-recrystallization-13C

Sample Name:

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

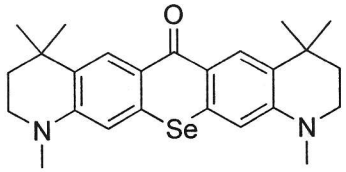
Sample directory:

FidFile: II-GS-176-recrystallization-13C

Pulse Sequence: CARBON (s2pul)
Solvent: D2O
Data collected on: Feb 6 2013

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
1024 repetitions
OBSERVE C13, 75.4536532 MHz
DECOUPLE H1, 300.0762142 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



3-Se

II-GS-246-recrystallization

Sample Name:

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

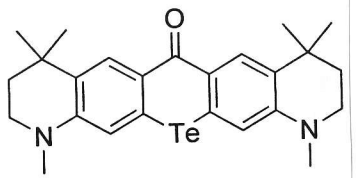
Sample directory:

FidFile: II-GS-245-recrystallization

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 11 2013

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



3-Te

II-GS-246-13C

Sample Name:

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

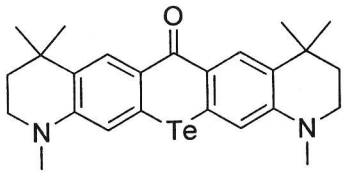
Sample directory:

FidFile: II-GS-246-13C

Pulse Sequence: CARBON (s2pul)
Solvent: D2O
Data collected on: Jun 11 2013

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
640 repetitions
OBSERVE C13, 75.4536566 MHz
DECOUPLE H1, 300.0762142 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



3-Te

II-GS-275-recrystallization

Sample Name:

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

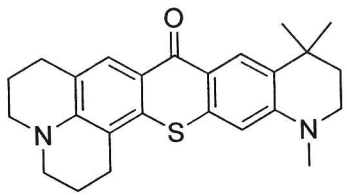
Sample directory:

FidFile: II-GS-275-recrystallization

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 5 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, 499.8984068 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



4-S

II-GS-275-13C

Sample Name:

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

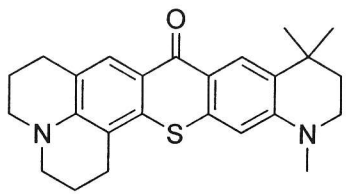
Sample directory:

FidFile: II-GS-275-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 5 2013

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, 75.4536677 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 536 hr, 56 min



4-S

II-GS-172-spot2

Sample Name:

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

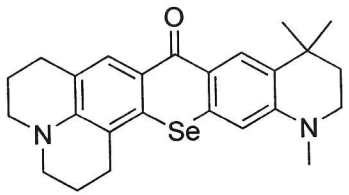
Sample directory:

FidFile: II-GS-172-spot2

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 5 2013

Temp. 19.0 C / 292.1 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



4-Se

II-GS-172-spot2-13C

Sample Name:

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

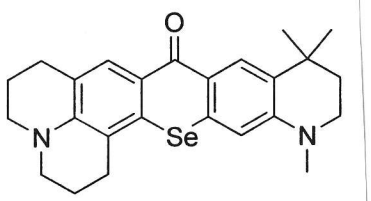
Sample directory:

FidFile: II-GS-172-spot2-13C

Pulse Sequence: CARBON (s2pul)
Solvent: D2O
Data collected on: Feb 5 2013

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
3328 repetitions
OBSERVE C13, 75.4536532 MHz
DECOUPLE H1, 300.0762142 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



4-Se

II-MK-104dry

Sample Name:

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

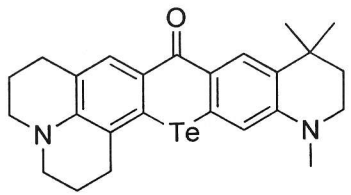
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Feb 12 2014

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, 300.0746296 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 16384
Total time 0 min 23 sec



4-Te

II-MK-104carbon-dcm

Sample Name:

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

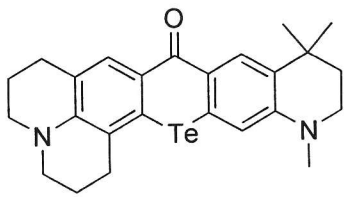
Sample directory:

FidFile: II-MK-104carbon-dcm

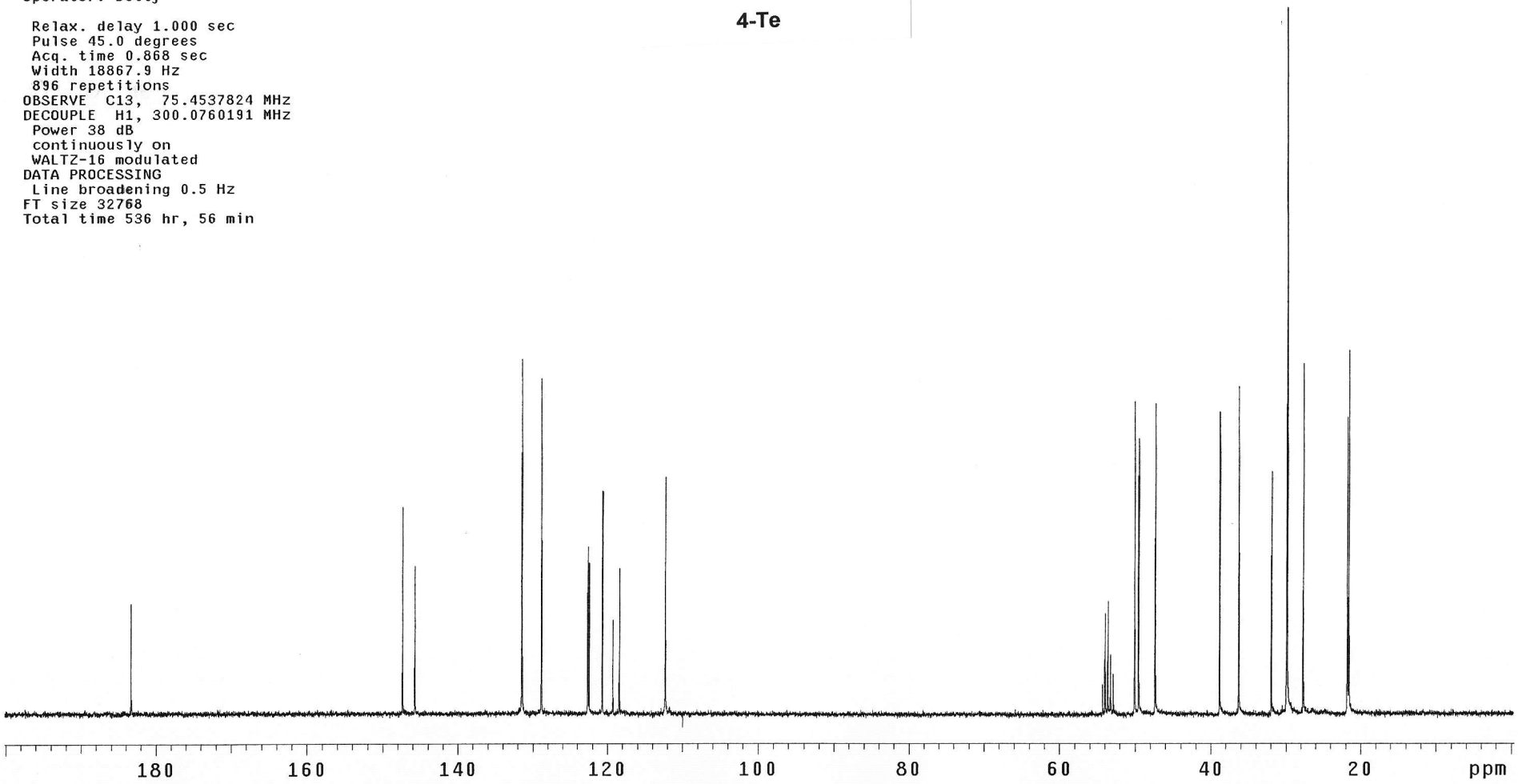
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 7 2013

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
896 repetitions
OBSERVE C13, 75.4537824 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



4-Te



II-MK-133

Sample Name:

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

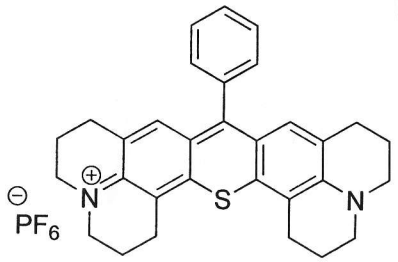
Sample directory:

FidFile: II-MK-133

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 28 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993717 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



5-S

II-MK-133carbon

Sample Name:

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

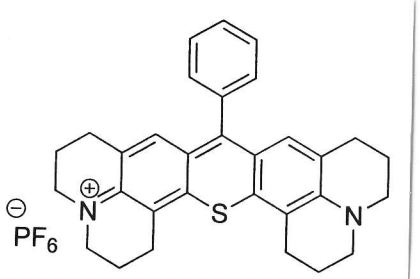
Sample directory:

FidFile: II-Mk-133carbon

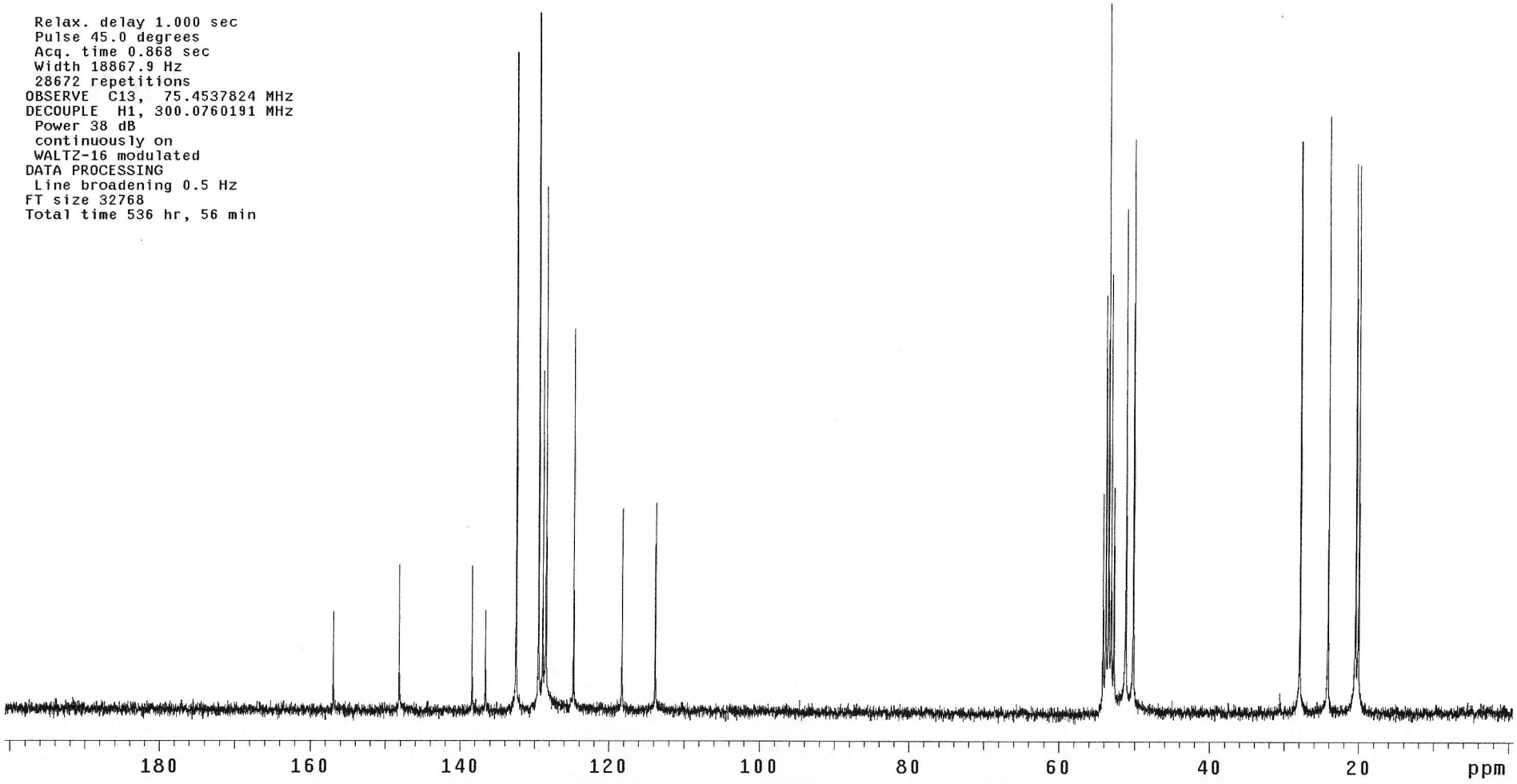
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 30 2013

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
28672 repetitions
OBSERVE C13, 75.4537824 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



5-S



II-MK-095

Sample Name:

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

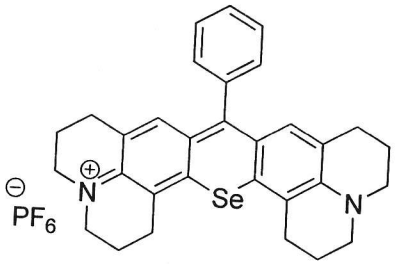
Sample directory:

FidFile: II-MK-095

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: May 20 2013

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



5-Se

II-MK-095carbon

Sample Name:

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

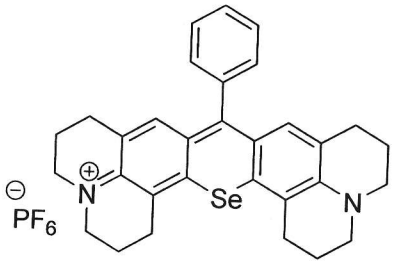
Sample directory:

FidFile: II-MK-095carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jul 22 2013

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
26880 repetitions
OBSERVE C13, 75.4537824 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



5-Se

II-MK-130

Sample Name:

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

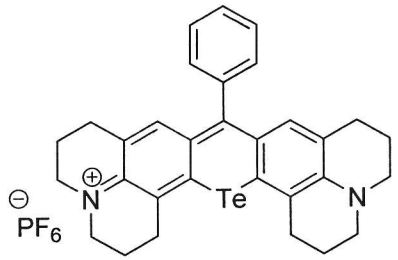
Sample directory:

FidFile: II-MK-130

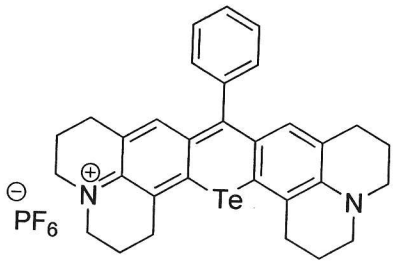
Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 28 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993717 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec

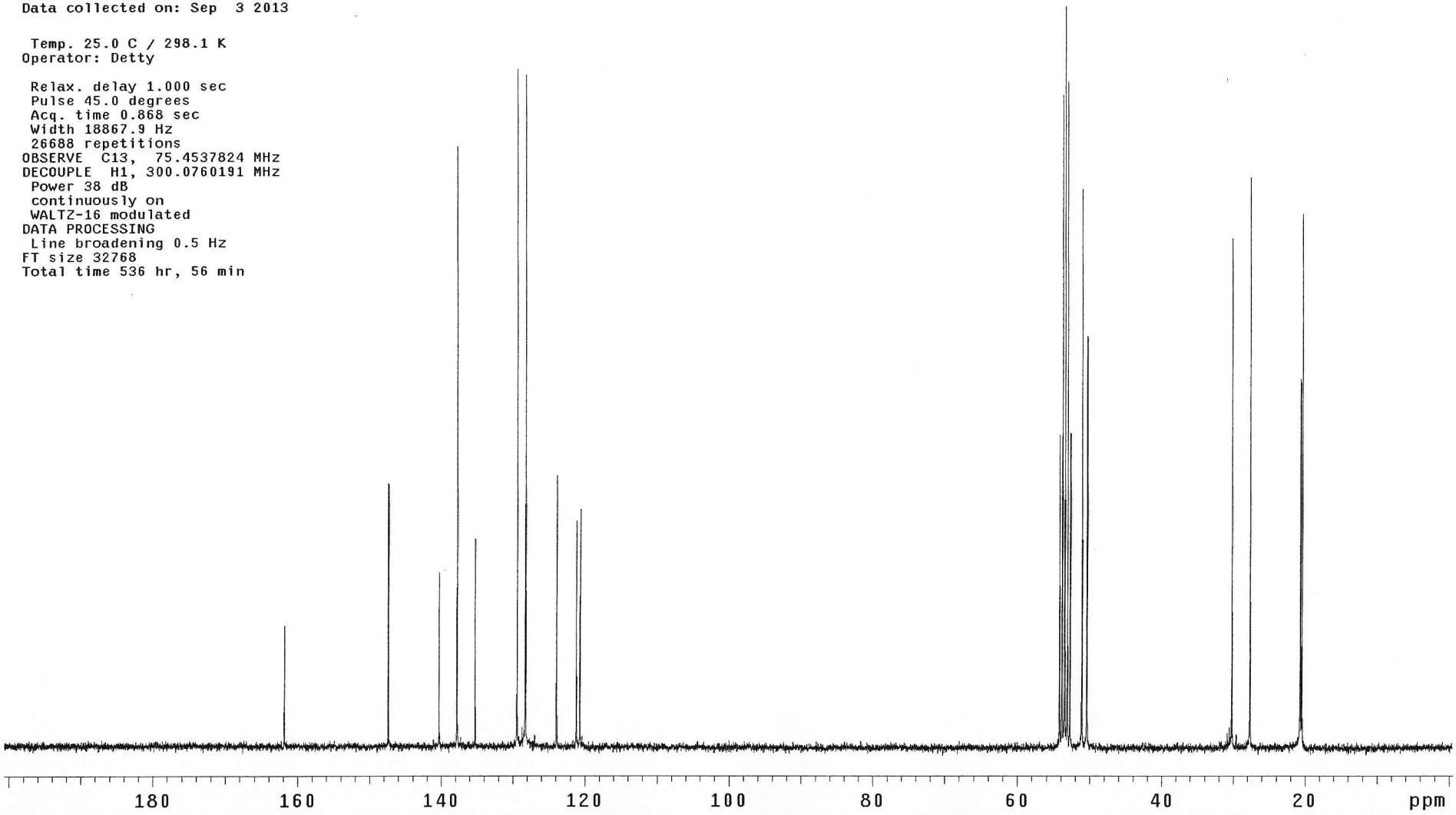


5-Te



5-Te

```
II-MK-130carbon

 Sample Name:

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

 Sample directory:

 FidFile: II-MK-130carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep  3 2013

 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
 26688 repetitions
OBSERVE  C13,  75.4537824 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
```



II-GS-289-crude

Sample Name:

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

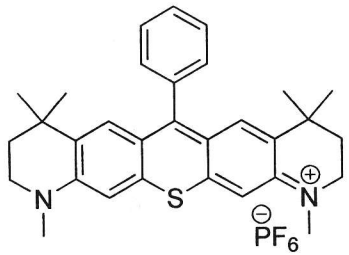
Sample directory:

FidFile: II-GS-289-crude

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 16 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, 499.8993727 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



6-S

II-GS-289-13C

Sample Name:

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

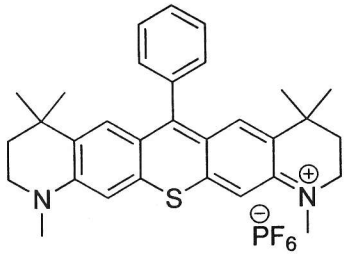
Sample directory:

FidFile: II-GS-289-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 13 2013

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
1856 repetitions
OBSERVE C13, 75.4537597 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 5369 hr, 21 min



6-S

II-GS-177-crude

Sample Name:

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

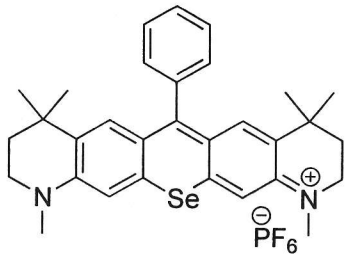
Sample directory:

FidFile: II-GS-177-crude

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Feb 11 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, 499.8993732 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



6-Se

II-GS-177-13C-3

Sample Name:

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

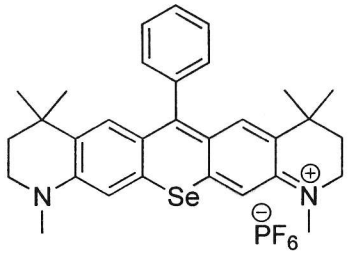
Sample directory:

FidFile: II-GS-177-13C-3

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 19 2013

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
30336 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 5369 hr, 21 min



6-Se

II-GS-290-recrystallization

Sample Name:

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

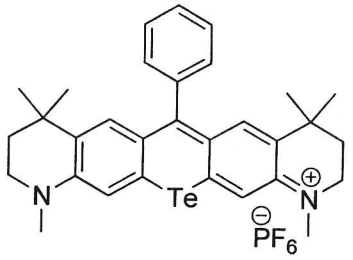
Sample directory:

FidFile: II-GS-290-recrystallization

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 20 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, 499.8984034 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



6-Te

II-GS-290-13C

Sample Name:

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

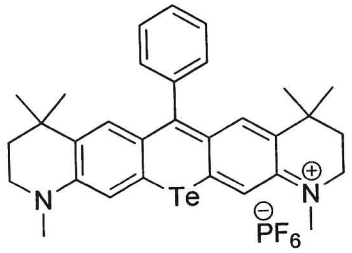
Sample directory:

FidFile: II-GS-290-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 15 2013

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, 75.4537597 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 5369 hr, 21 min



6-Te

II-GS-288-crude

Sample Name:

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

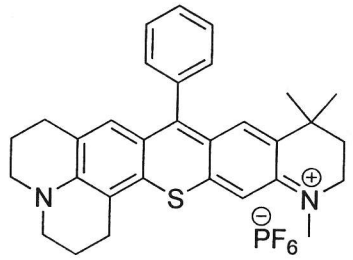
Sample directory:

FidFile: II-GS-288-crude

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 16 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, 499.8993712 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



7-S

II-GS-288-13C

Sample Name:

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

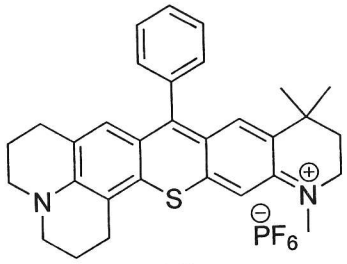
Sample directory:

FidFile: II-GS-288-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 13 2013

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
28544 repetitions
OBSERVE C13, 75.4537608 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 5369 hr, 21 min



7-S

II-GS-179-crude

Sample Name:

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

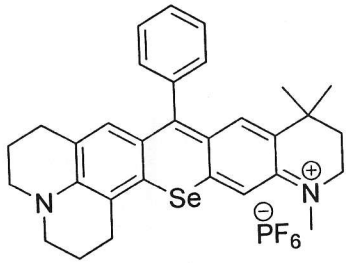
Sample directory:

FidFile: II-GS-179-crude

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Feb 12 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993697 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



7-Se

II-GS-179-13C

Sample Name:

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

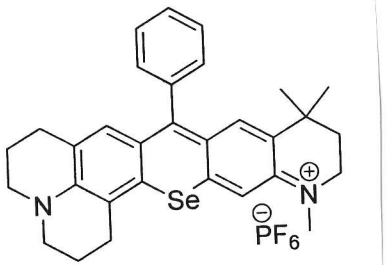
Sample directory:

FidFile: II-GS-179-13C

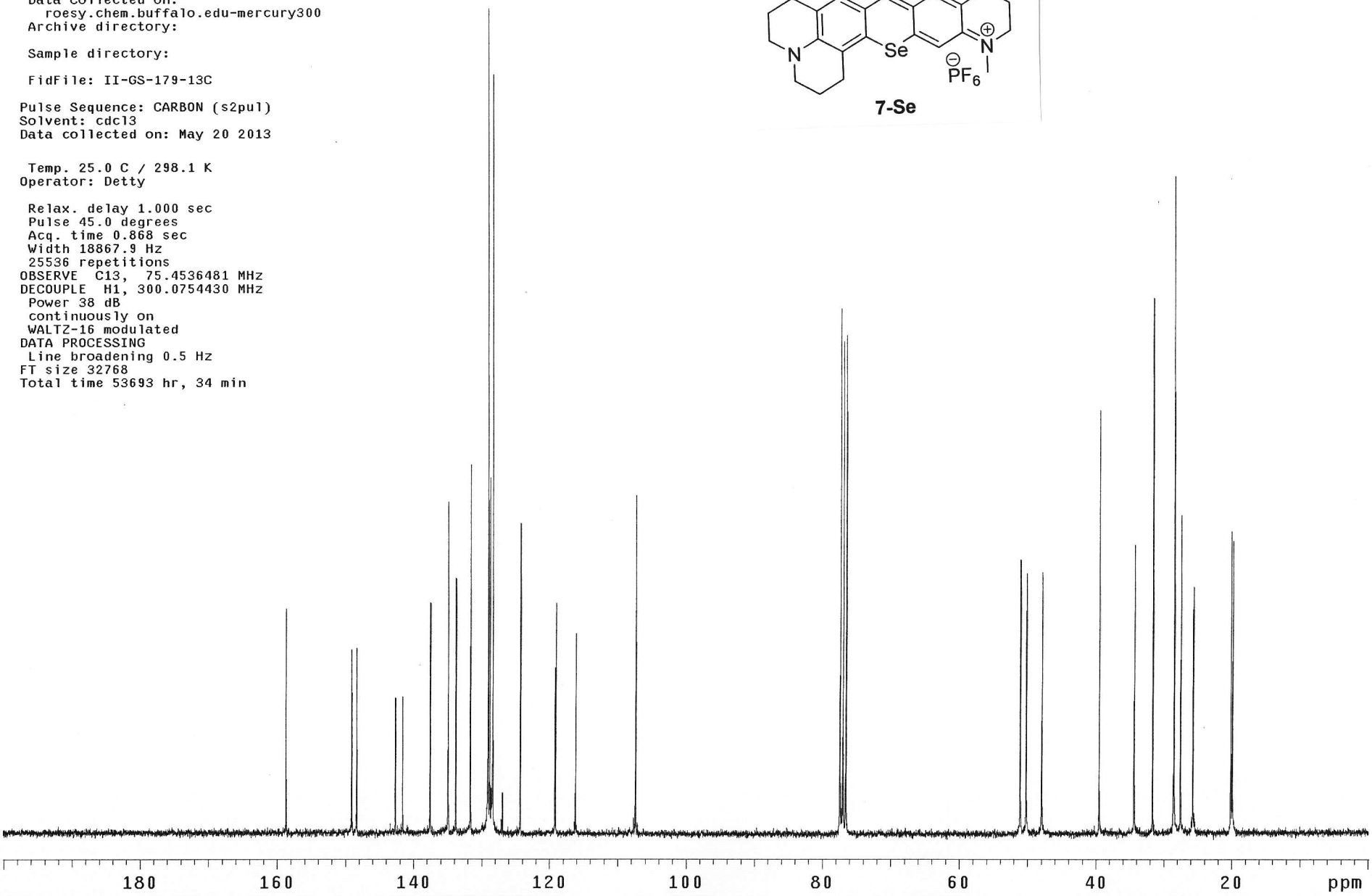
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: May 20 2013

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
25536 repetitions
OBSERVE C13, 75.4536481 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 53693 hr, 34 min



7-Se



II-MK-131

Sample Name:

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

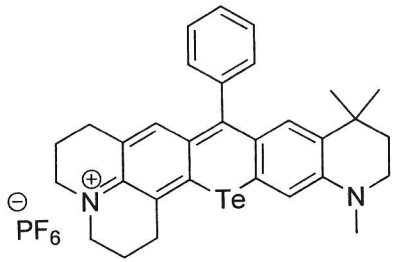
Sample directory:

FidFile: II-MK-131

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 28 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993717 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



7-Te

II-MK-131carbon

Sample Name:

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

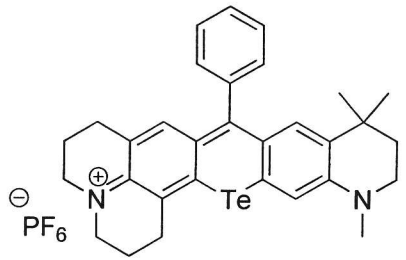
Sample directory:

FidFile: II-MK-131carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
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 0.868 sec
Width 18867.9 Hz
27200 repetitions
OBSERVE C13, 75.4537824 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



7-Te

II-MK-054

Sample Name:

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

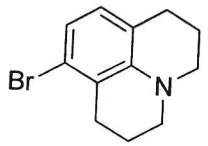
Sample directory:

FidFile: II-MK-054b

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Mar 26 2013

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



9

II-MK-054carbon

Sample Name:

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

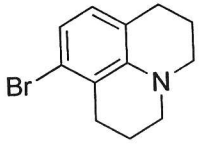
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 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
192 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



9

II-MK-114dry

Sample Name:

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

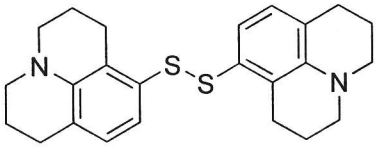
Sample directory:

FidFile: II-MK-114b

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Jul 11 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, 499.8993712 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



10-S

II-MK-113carbon

Sample Name:

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

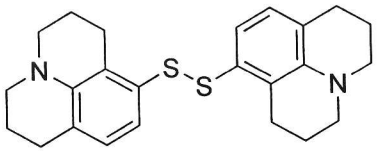
Sample directory:

FidFile: II-MK-113carbon

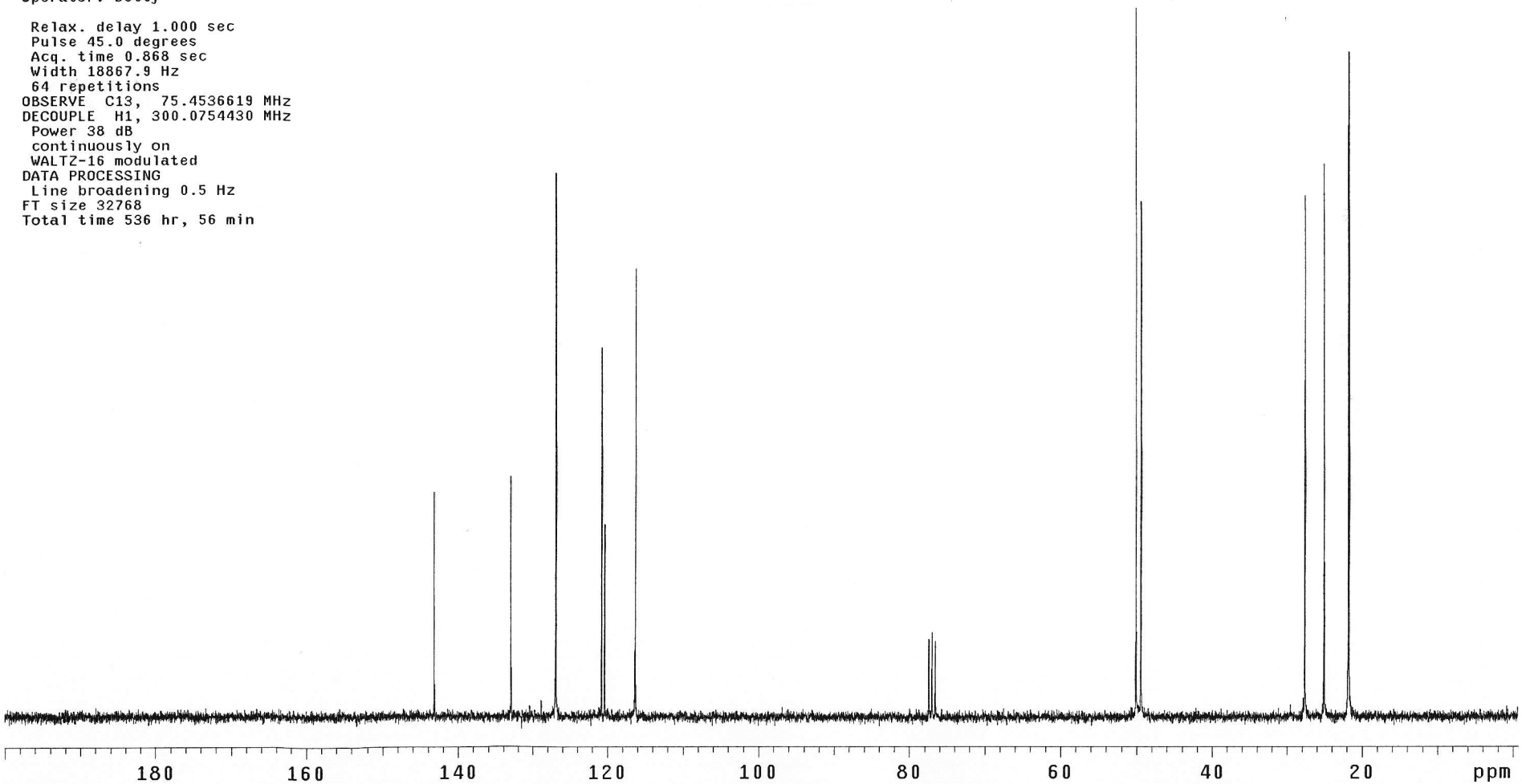
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 9 2013

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, 75.4536619 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



10-S



II-MK-068spot3

Sample Name:

Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:

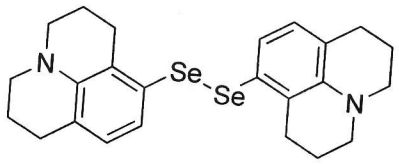
Sample directory:

FidFile: II-MK-068spot3

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Mar 20 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.560 sec
Width 6399.0 Hz
8 repetitions
OBSERVE H1, 399.9389017 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 29 sec



10-Se

II-MK-068carbon

Sample Name:

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

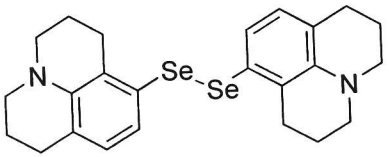
Sample directory:

FidFile: II-MK-068carbon

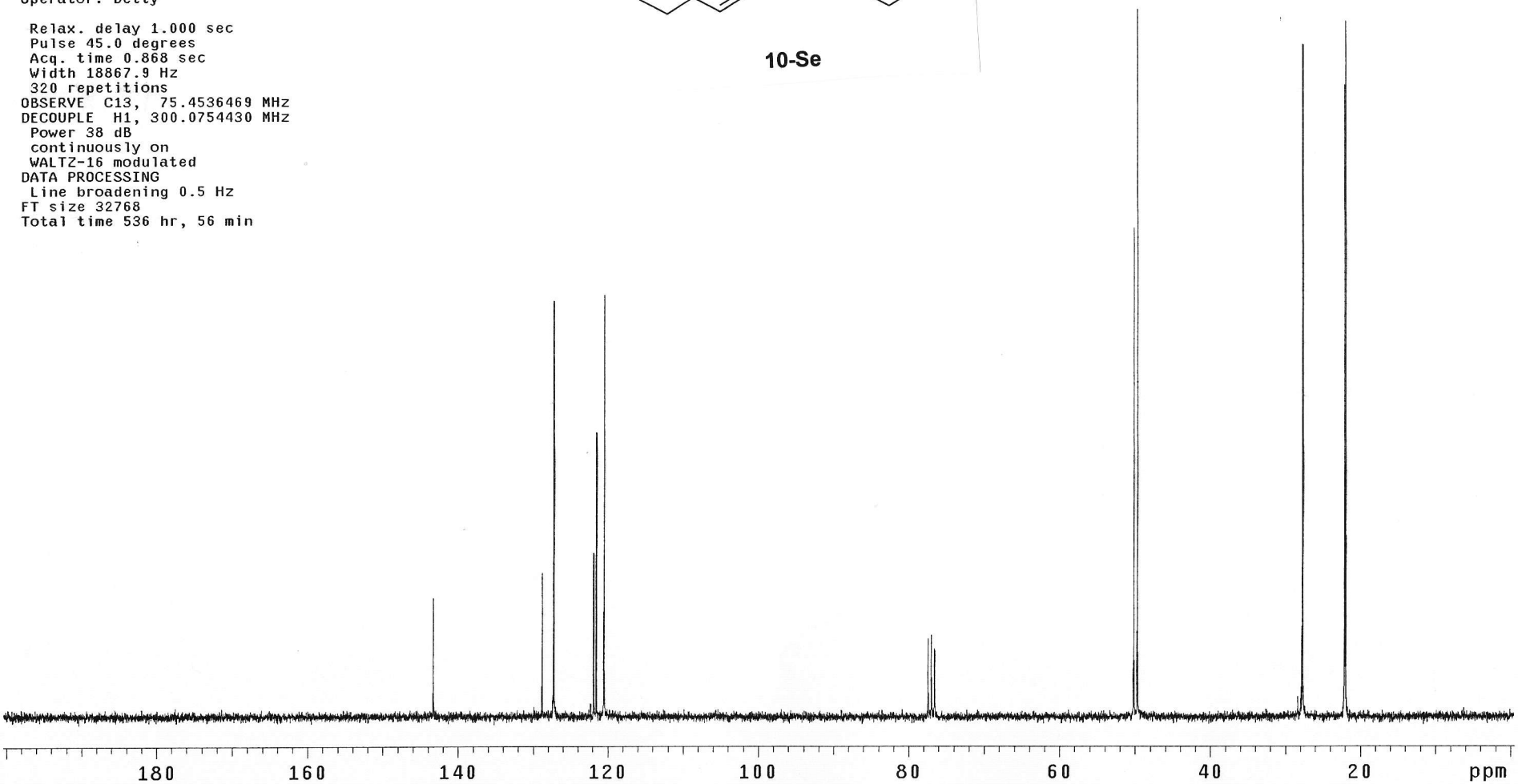
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Mar 20 2013

Temp. 40.0 C / 313.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
320 repetitions
OBSERVE C13, 75.4536469 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



10-Se



II-MK-094

Sample Name:

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

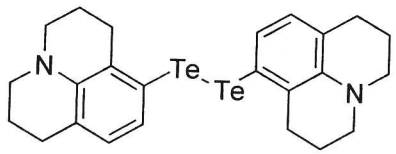
Sample directory:

FidFile: II-MK-094dcm

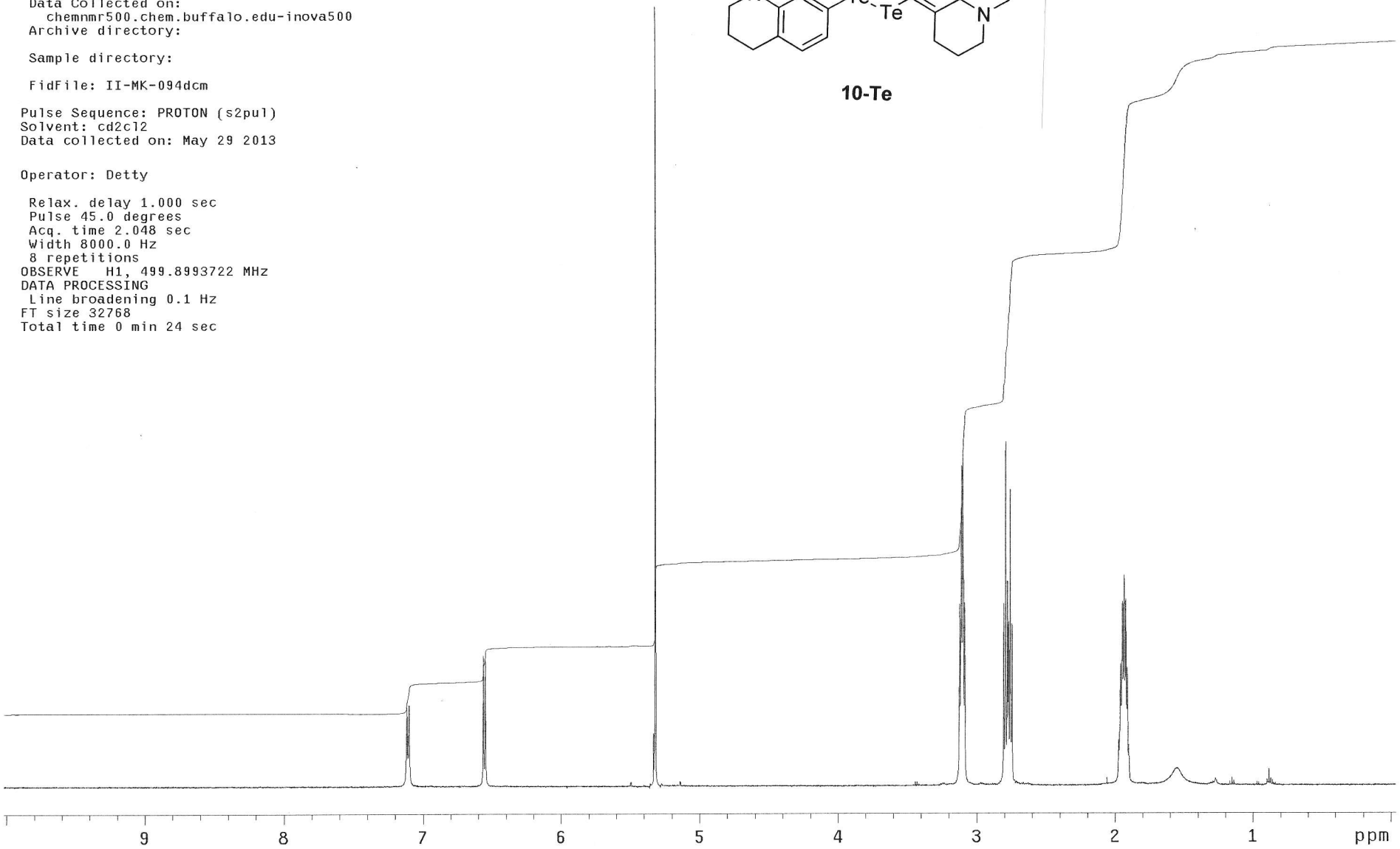
Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: May 29 2013

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



10-Te



II-MK-100carbon

Sample Name:

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

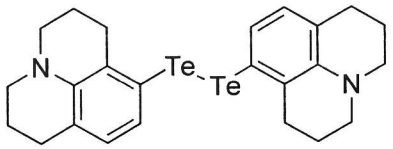
Sample directory:

FidFile: II-MK-110carbon

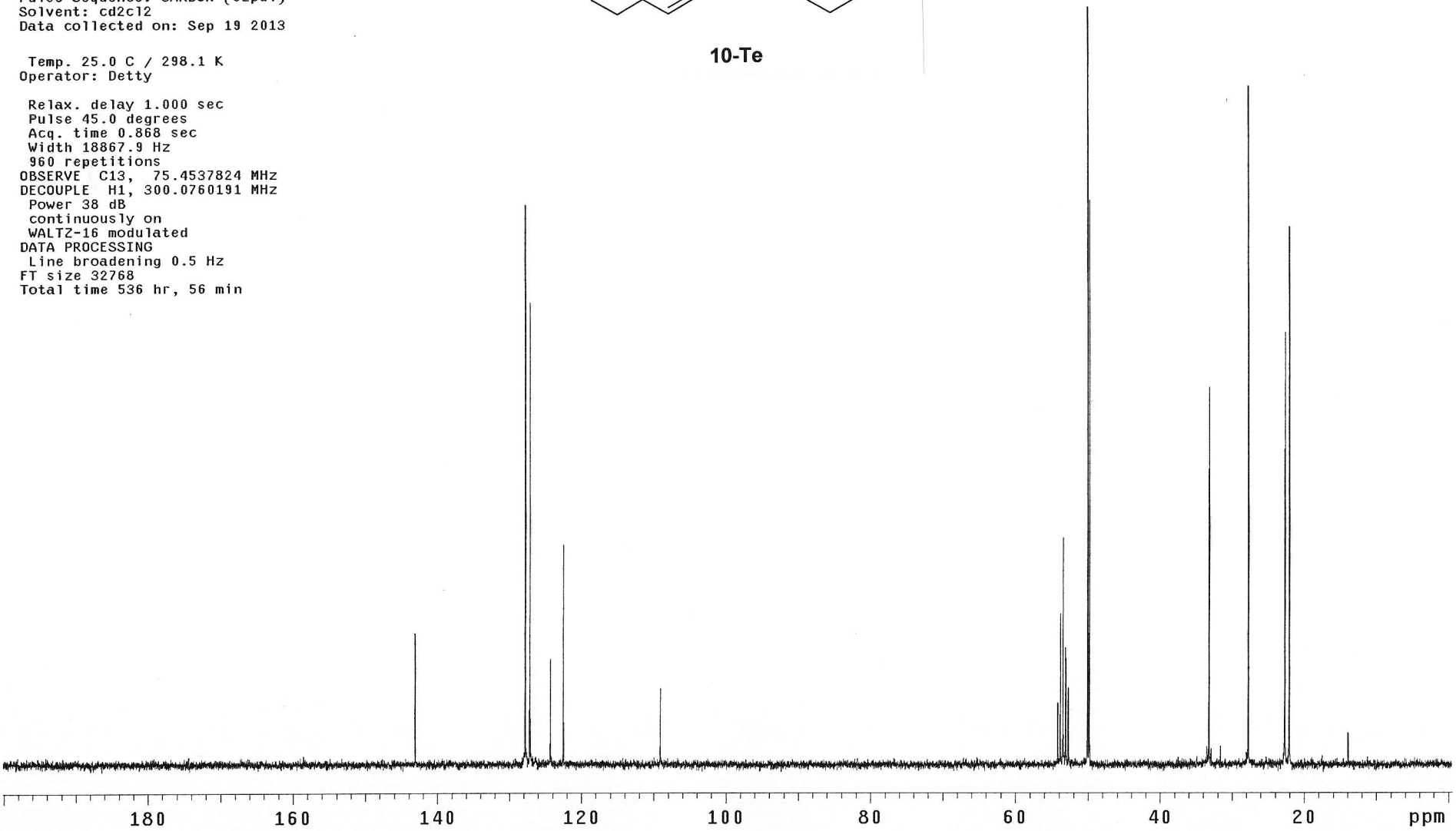
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 19 2013

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
960 repetitions
OBSERVE C13, 75.4537824 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



10-Te



2-bdc-134-topspot

Sample Name:

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

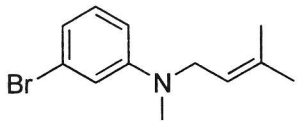
Sample directory:

FidFile: 2-bdc-134-topspot

Pulse Sequence: s2pul
Solvent: cdcl3
Data collected on: Feb 17 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984093 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 15 sec



11

2-bdc-134-13C-2

Sample Name:

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

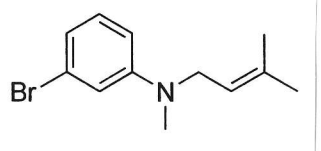
Sample directory:

FidFile: 2-bdc-134-13C-2

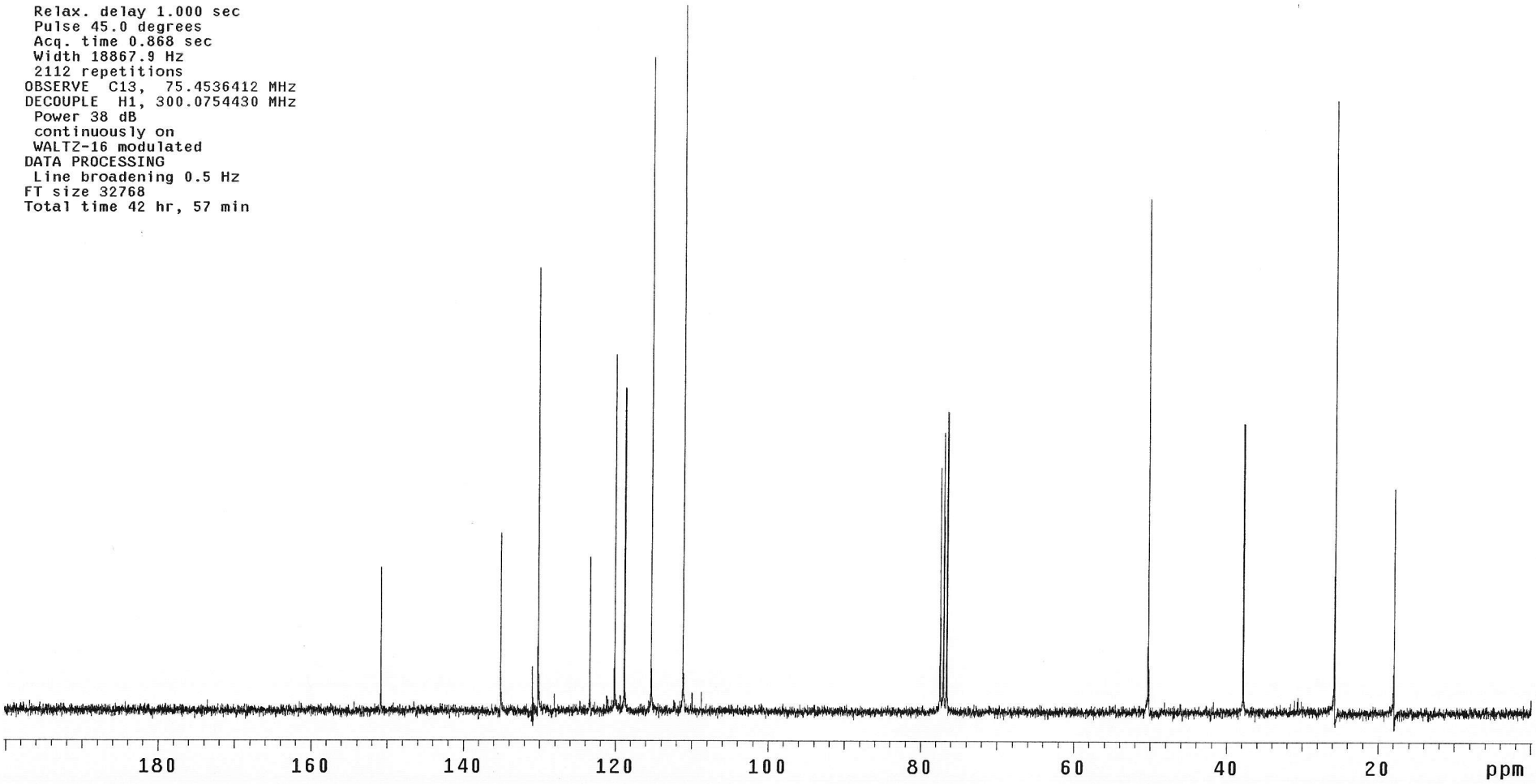
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Feb 21 2011

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
2112 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



11



1-jeh-037

Sample Name:
I-MB-027
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

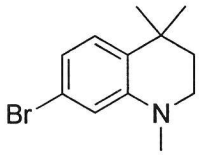
Sample directory:

FidFile: 1-jeh-037

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Feb 1 2011

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



12

1-jeh-037-13C

Sample Name:

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

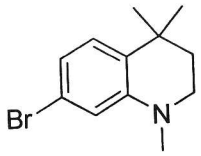
Sample directory:

FidFile: 1-jeh-037-13c

Pulse Sequence: CARBON (s2pul)
Solvent: D2O
Data collected on: Dec 7 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
4544 repetitions
OBSERVE C13, 75.4536405 MHz
DECOUPLE H1, 300.0762142 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



12

II-GS-251-pure

Sample Name:

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

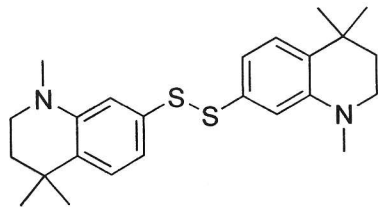
Sample directory:

FidFile: II-GS-251-pure

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 8 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, 499.8984102 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



13-S

II-GS-251-13C

Sample Name:

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

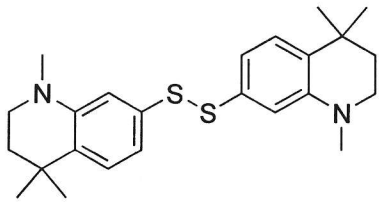
Sample directory:

FidFile: II-GS-251-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 8 2013

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, 75.4536527 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



13-S

II-GS-166/169-column-spot2

Sample Name:

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

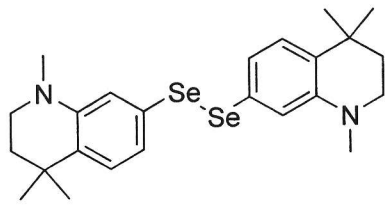
Sample directory:

FidFile: II-GS-166_169-column-spot2

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 26 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, 499.8984107 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



13-Se

II-GS-168-13C

Sample Name:

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

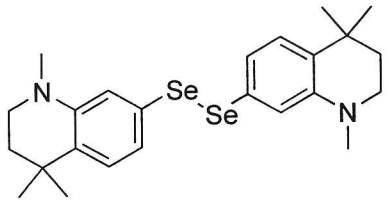
Sample directory:

FidFile: II-GS-168-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 28 2013

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
192 repetitions
OBSERVE C13, 75.4536838 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



13-Se

II-GS-232-solid

Sample Name:

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

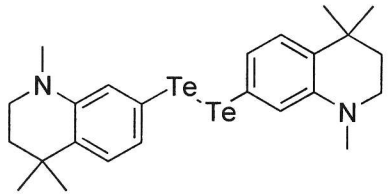
Sample directory:

FidFile: II-GS-232-solid

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 4 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984263 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



13-Te

II-GS-232-13C

Sample Name:

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

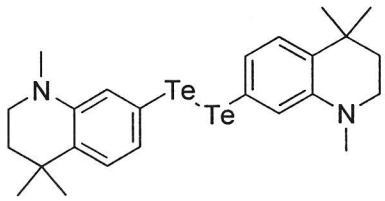
Sample directory:

FidFile: II-GS-232-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 4 2013

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, 75.4536642 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 5369 hr, 21 min



13-Te

II-MK-119

Sample Name:

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

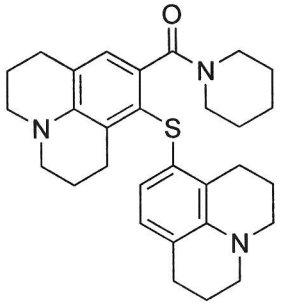
Sample directory:

FidFile: II-MK-119

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 7 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, 499.8993761 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



15-S

STANDARD CARBON PARAMETERS

Sample Name: II -MK-119 carbon

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

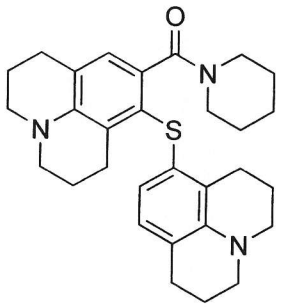
Sample directory:

FidFile: II-MK-119carbon

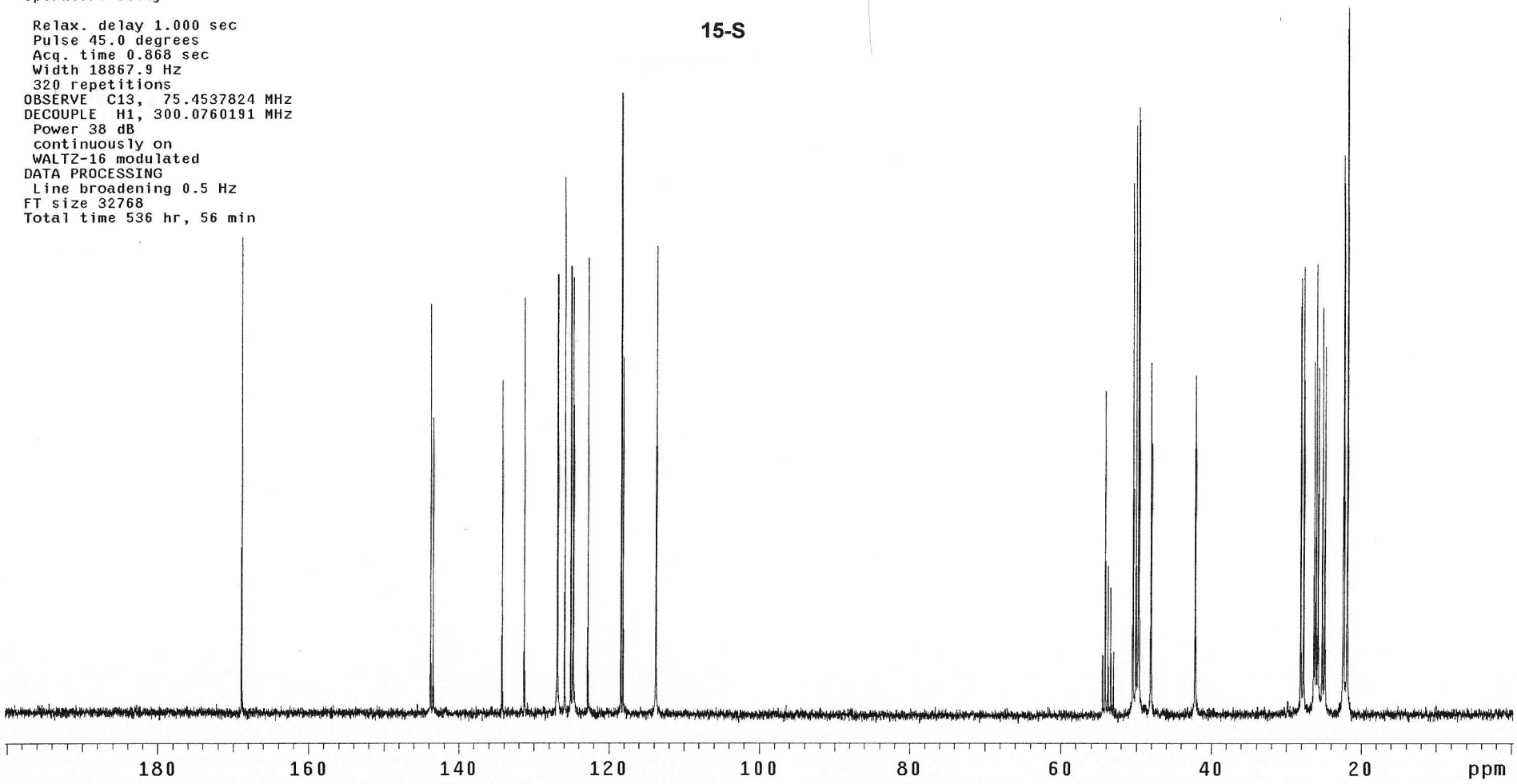
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Aug 7 2013

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
320 repetitions
OBSERVE C13, 75.4537824 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



15-S



II-MK-092

Sample Name:

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

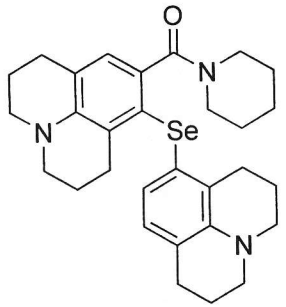
Sample directory:

FidFile: II-MK-092

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: May 9 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, 499.8993780 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



15-Se

II-MK-092carbon

Sample Name:

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

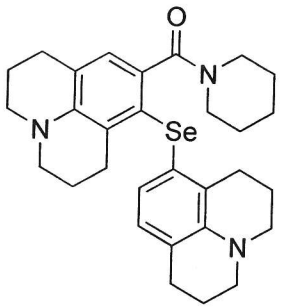
Sample directory:

FidFile: II-MK-092carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: May 9 2013

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
320 repetitions
OBSERVE C13, 75.4537824 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



15-Se

II-MK-101

Sample Name:

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

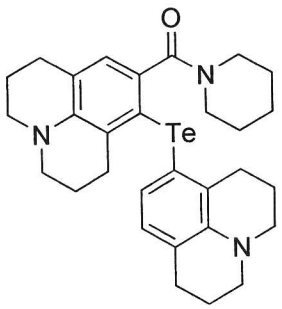
Sample directory:

FidFile: II-MK-101

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 4 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993775 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



15-Te

II-MK-101carbon

Sample Name:

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

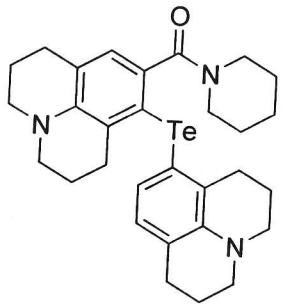
Sample directory:

FidFile: II-MK-101carbon

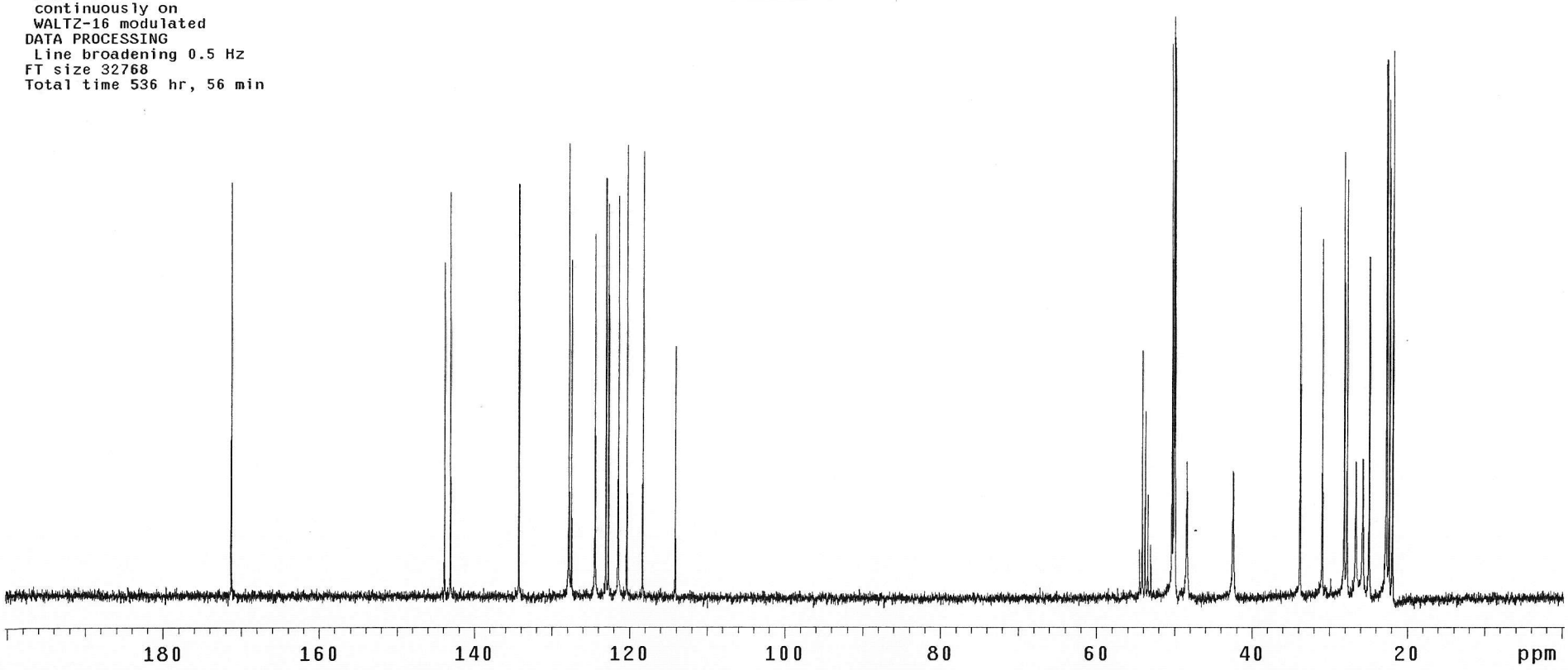
Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jun 4 2013

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
320 repetitions
OBSERVE C13, 75.4537824 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



15-Te



II-GS-265-vacuum

Sample Name:

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

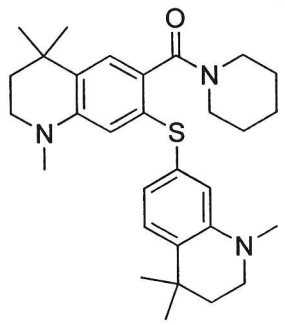
Sample directory:

FidFile: II-GS-265-vacuum

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 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, 499.8984039 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



17-S

II-GS-265-13C

Sample Name:

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

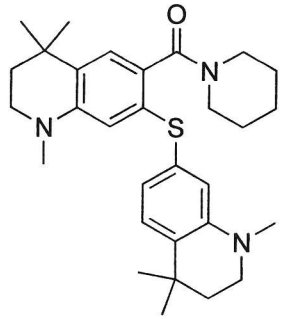
Sample directory:

FidFile: II-GS-265-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 14 2013

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
448 repetitions
OBSERVE C13, 75.4536780 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



17-S

II-GS-174-spot2

Sample Name:

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

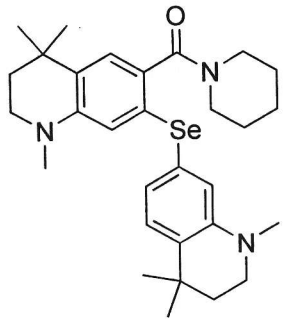
Sample directory:

FidFile: II-GS-174-spot2

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 2 2013

Temp. 19.0 C / 292.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.820 sec
Width 9000.9 Hz
8 repetitions
OBSERVE H1, 499.8983264 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 23 sec



17-Se

II-GS-174-spot2-13C

Sample Name:

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

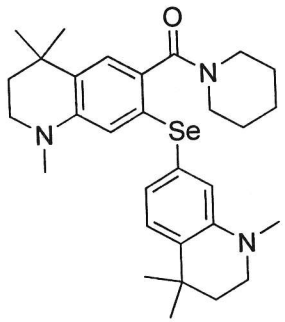
Sample directory:

FidFile: II-GS-174-spot2-13C

Pulse Sequence: CARBON (s2pul)
Solvent: D2O
Data collected on: Feb 2 2013

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
1408 repetitions
OBSERVE C13, 75.4536762 MHz
DECOUPLE H1, 300.0762142 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



17-Se

II-GS-244-spot3

Sample Name:

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

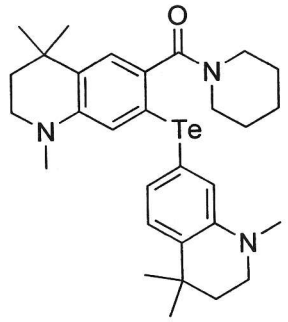
Sample directory:

FidFile: II-GS-244-spot3

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 6 2013

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



17-Te

II-GS-244-13C

Sample Name:

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

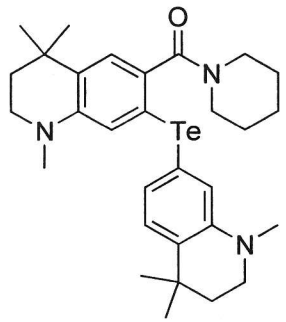
Sample directory:

FidFile: II-GS-244-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jun 6 2013

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
640 repetitions
OBSERVE C13, 75.4536746 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 5369 hr, 21 min



17-Te

II-GS-273-spot4

Sample Name:

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

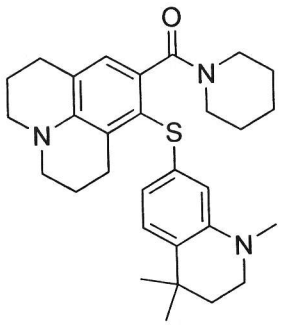
Sample directory:

FidFile: II-GS-274-spot4

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 26 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, 499.8984005 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



18-S

II-GS-273-13C

Sample Name:

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

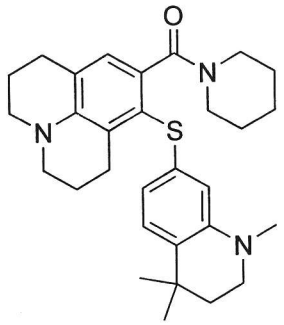
Sample directory:

FidFile: II-GS-273-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 6 2013

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
30720 repetitions
OBSERVE C13, 75.4537597 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 5369 hr, 21 min



18-S

II-GS-200-spot2-dry2

Sample Name:

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

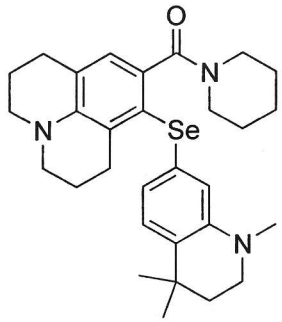
Sample directory:

FidFile: II-GS-200-spot2-dry2

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984000 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



18-Se

II-GS-200-13C

Sample Name:

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

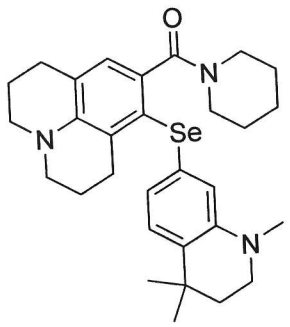
Sample directory:

FidFile: II-GS-200-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 16 2013

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
832 repetitions
OBSERVE C13, 75.4536469 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 53 hr, 41 min



18-Se

II-GS-280

Sample Name:

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

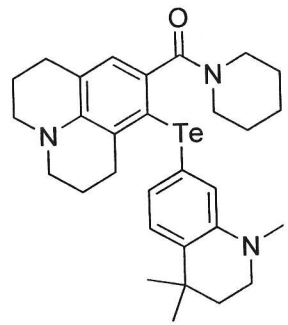
Sample directory:

FidFile: II-GS-280

Pulse Sequence: PRESAT
Solvent: cdcl3
Data collected on: Aug 6 2013

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, 499.8984000 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 41 sec



18-Te

II-GS-280-13C

Sample Name:

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

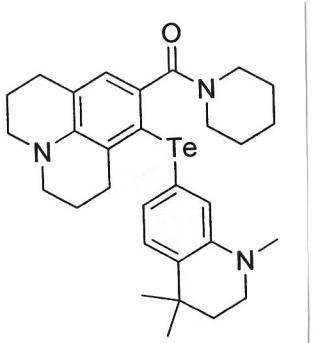
Sample directory:

FidFile: II-GS-280-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 6 2013

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
320 repetitions
OBSERVE C13, 75.4536573 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 53 hr, 41 min



18-Te

1-JH-038

Sample Name:

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

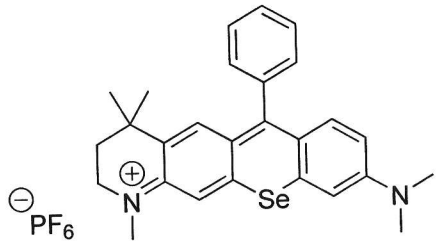
Sample directory:

FidFile: 1-JH-038dry

Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Jul 20 2012

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.9010670 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



20-Se

1-JH-038

Sample Name:

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

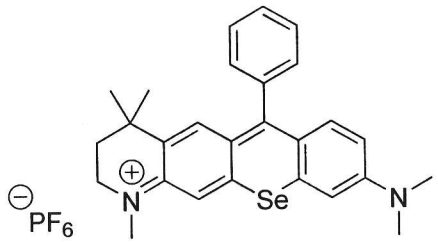
Sample directory:

FidFile: 1-JH-038dry

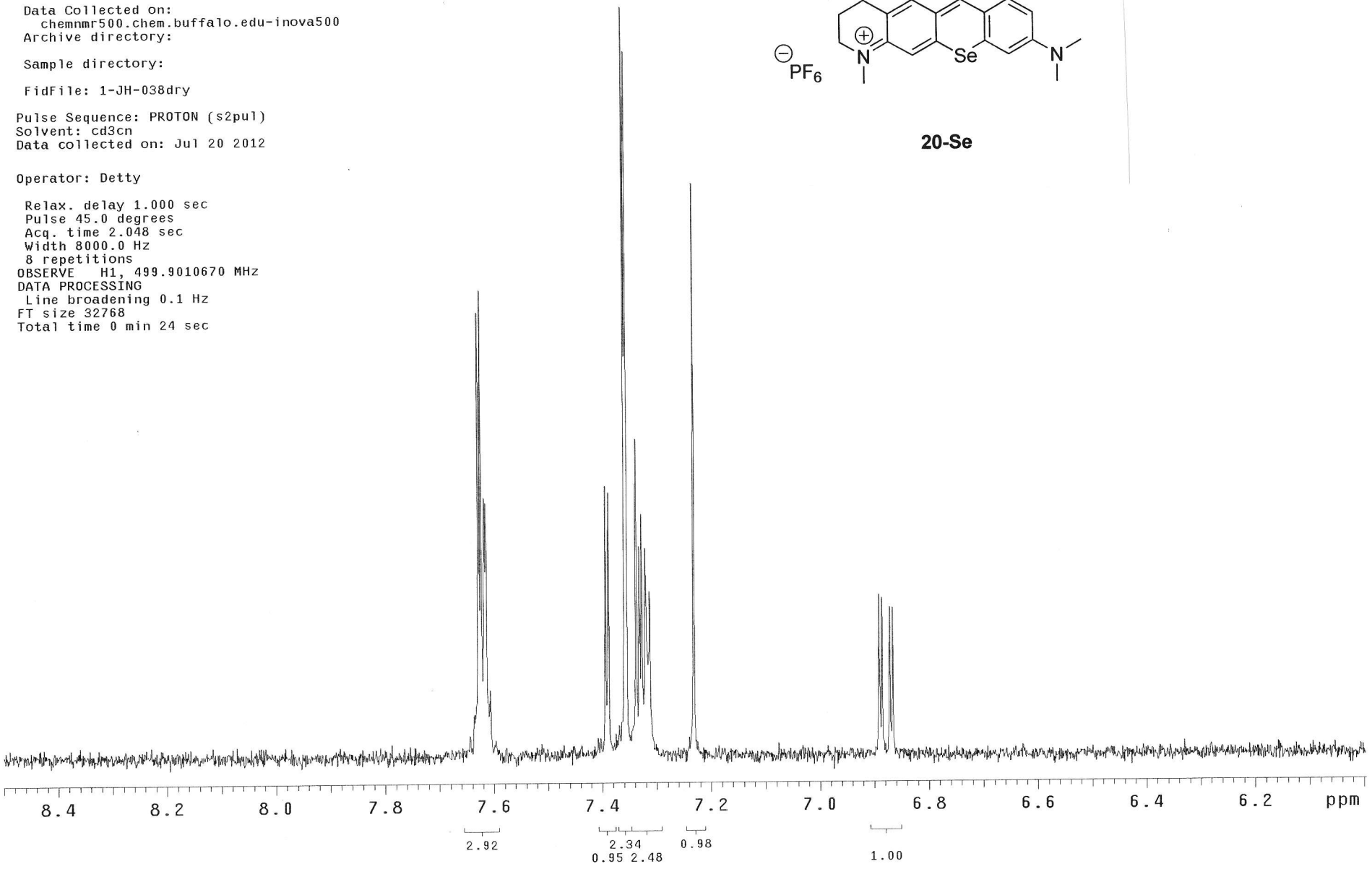
Pulse Sequence: PROTON (s2pul)
Solvent: cd3cn
Data collected on: Jul 20 2012

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.9010670 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



20-Se



1-JH-038

Sample Name:

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

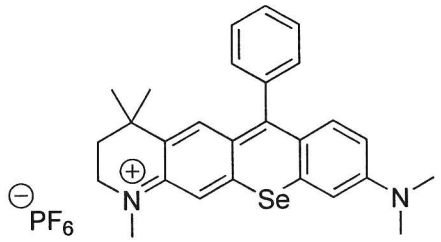
Sample directory:

FidFile: 1-JH-038-C13

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jul 22 2012

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
25344 repetitions
OBSERVE C13, 125.6997487 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 569 hr, 43 min



20-Se

I-JH-029

Sample Name:

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

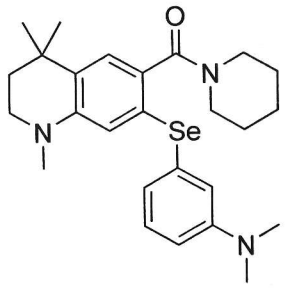
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Feb 10 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, 499.8983787 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



22

I-JH-029carbon

Sample Name:

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

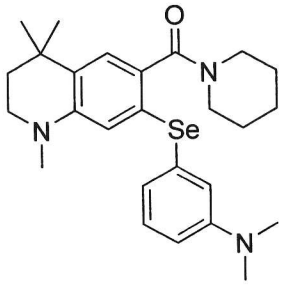
Sample directory:

FidFile: I-JH-029carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 25 2013

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
1024 repetitions
OBSERVE C13, 75.4536631 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



22

II-GS-284-recrystallization

Sample Name:

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

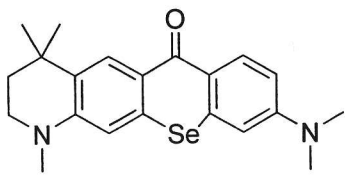
Sample directory:

FidFile: II-GS-284-recrystallization

Pulse Sequence: PRESAT
Solvent: cdcl3
Data collected on: Aug 12 2013

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, 499.8984048 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 41 sec



23

STANDARD CARBON PARAMETERS

Sample Name:

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

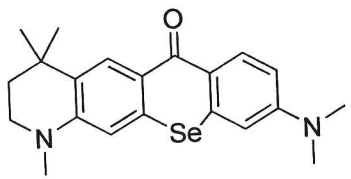
Sample directory:

FidFile: II-GS-284-13C-2

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 14 2013

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3072 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 53 hr, 41 min



23

II-MK-148

Sample Name:

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

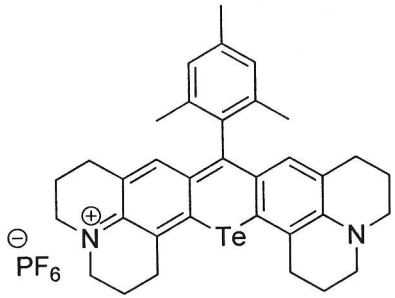
Sample directory:

FidFile: II-MK-148

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
Data collected on: Sep 28 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, 499.8993717 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



27

II-MK-148carbon

Sample Name:

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

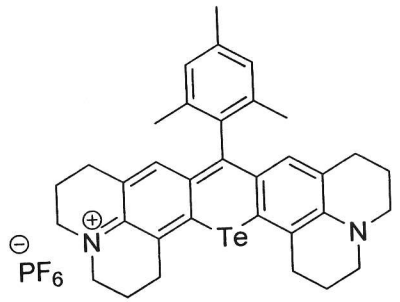
Sample directory:

FidFile: II-MK-148carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
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 0.868 sec
Width 18867.9 Hz
28224 repetitions
OBSERVE C13, 75.4537824 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



27

III-GS-072-hexanes

Sample Name:

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

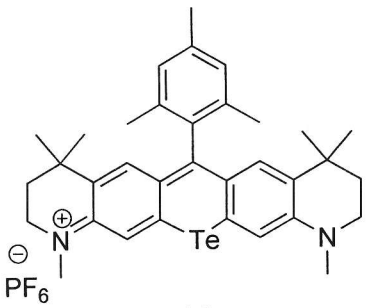
Sample directory:

FidFile: III-GS-072-hexanes

Pulse Sequence: PROTON (s2pul)
Solvent: cd2cl2
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, 499.8993712 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



29

III-GS-072-13C

Sample Name:

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

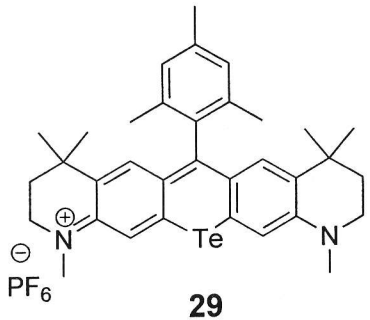
Sample directory:

FidFile: III-GS-072-13C

Pulse Sequence: CARBON (s2pul)
Solvent: cd2cl2
Data collected on: Jan 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
32768 repetitions
OBSERVE C13, 75.4537585 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 53693 hr, 34 min



29

Telluride
II-MK-148MeOH-dTFA

Sample Name:

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

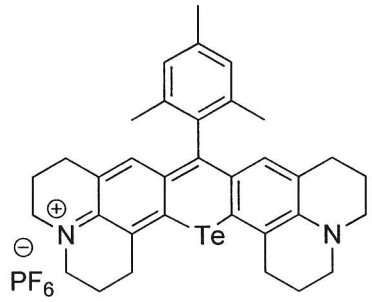
Sample directory:

FidFile: II-MK-148MeOHb-dTFA

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
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 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.9003752 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



27

CF_3CO_2D/CD_3OD

Telluroxide
II-MK-148MeOHb-dTFA-H2O2d

Sample Name:

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

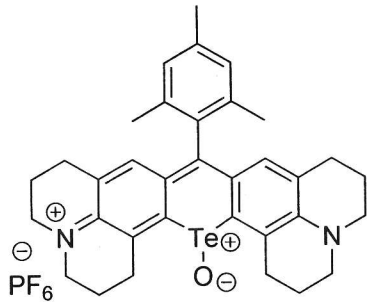
Sample directory:

FidFile: PRESAT

Pulse Sequence: PRESAT
Solvent: cd3od
Data collected on: Feb 17 2014

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, 499.9003708 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 41 sec



28

CF_3CO_2D/CD_3OD

II-MK-148telluroxideCarbon

Sample Name:

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

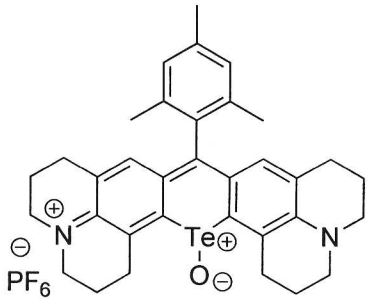
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Feb 18 2014

Temp. 23.5 C / 296.6 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
25088 repetitions
OBSERVE C13, 75.4539064 MHz
DECOUPLE H1, 300.0766253 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



28

CF_3CO_2D/CD_3OD

II-MK-148telluroxideCarbon

Sample Name:

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

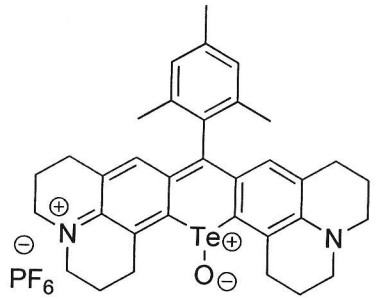
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd3od
Data collected on: Feb 18 2014

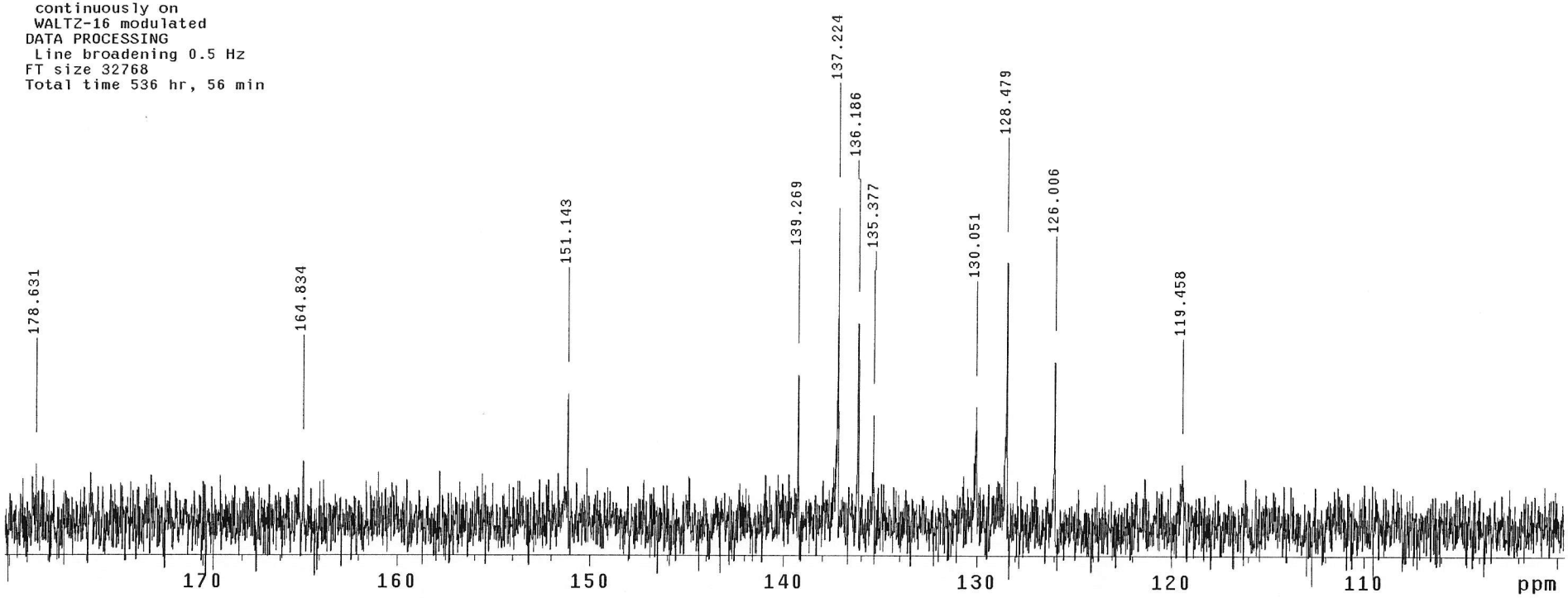
Temp. 23.6 C / 296.8 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
25152 repetitions
OBSERVE C13, 75.4539064 MHz
DECOUPLE H1, 300.0766253 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



28

CF_3CO_2D/CD_3OD



III-GS-072-MeOH and CF3CO2D

Sample Name:

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

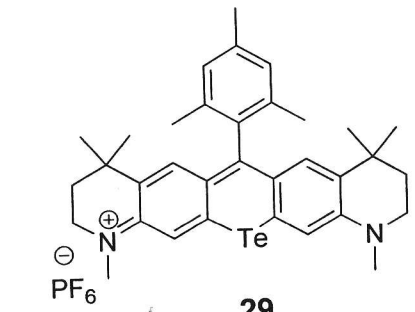
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd3od
Data collected on: Feb 18 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, 499.9003716 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



CF3CO2D/CD3OD

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III-GS-072-MeOH-H2O2 and CF3CO2D

Sample Name:

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

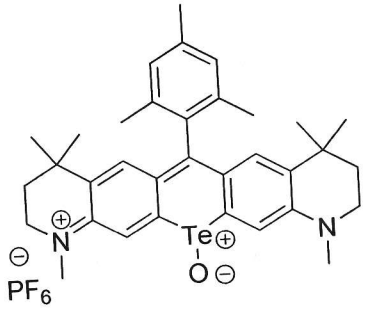
Sample directory:

FidFile: PRESAT

Pulse Sequence: PRESAT
Solvent: cd3od
Data collected on: Feb 18 2014

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, 499.9003711 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 41 sec



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CF_3CO_2D/CD_3OD