

Stereoselective Synthesis of Morpholines Via Copper-Promoted Oxyamination of Alkenes

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Supporting Information II: NMR Spectra of New Compounds

fs-V-28proton

Sample Name:

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

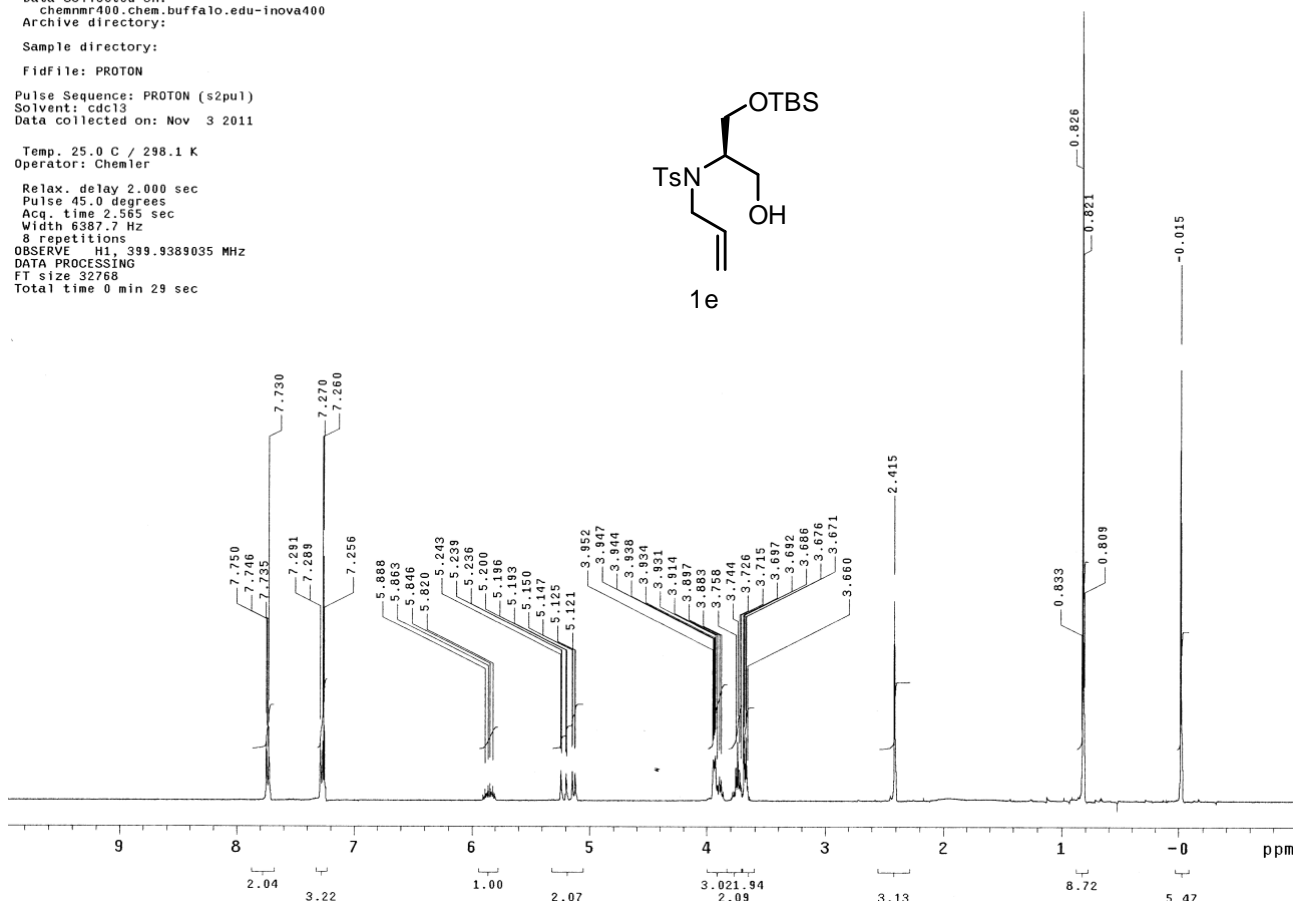
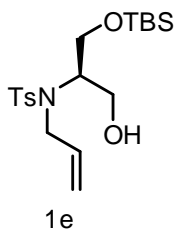
Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 3 2011

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.585 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9389035 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 29 sec



fs-V-28-carbon

Sample Name:

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

Sample directory:

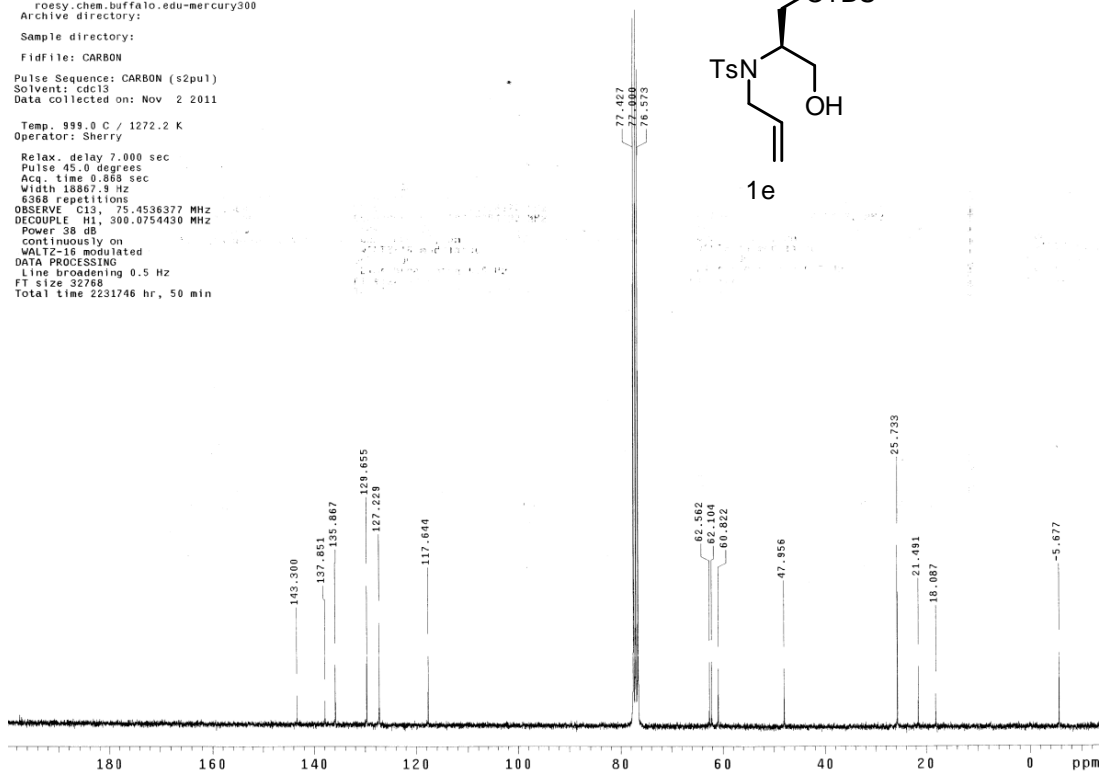
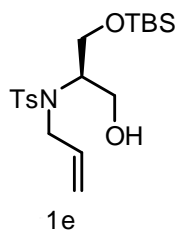
Fidfile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 2 2011

Temp. 99.9 C / 1272.2 K
Operator: Sherry

Relax. delay 7.000 sec
Pulse 45.0 degrees
Acq. time 0.869 sec
Width 18867.3 Hz

6368 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 2231746 hr, 50 min



fs-III-288-proton

Sample Name:

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

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)

Solvent: cdcl3

Data collected on: Oct 12 2011

Operator: Sherry

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8000.0 Hz

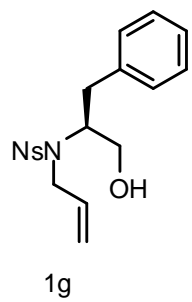
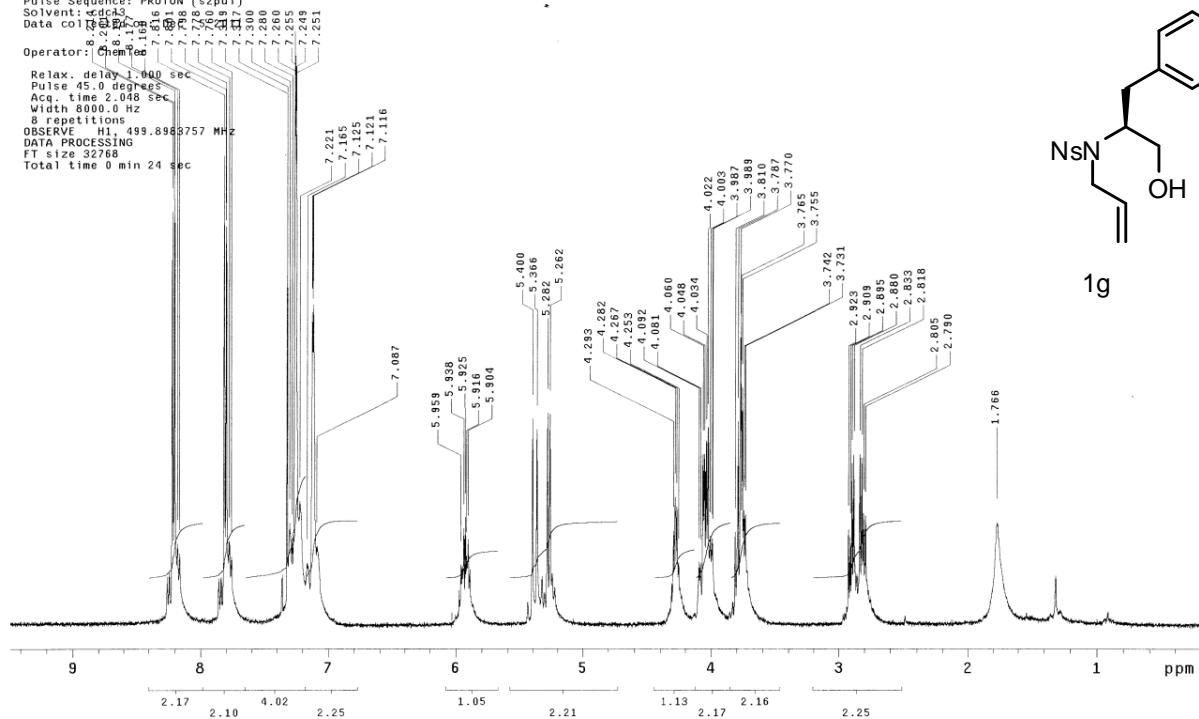
8 repetitions

OBSERVE H1, 499.8983757 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 24 sec



fs-III-288

Sample Name:

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

Archive directory:

Sample directory:

FidFile: fs-III-288-carbon

Pulse Sequence: CARBON (s2pu1)

Solvent: cdcl3

Data collected on: Oct 12 2011

Temp. 25.0 C / 298.1 K

Operator: Sherry

Relax. delay 6.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

7488 repetitions

OBSERVE C13, 75.4536366 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

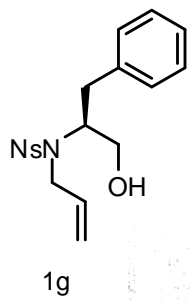
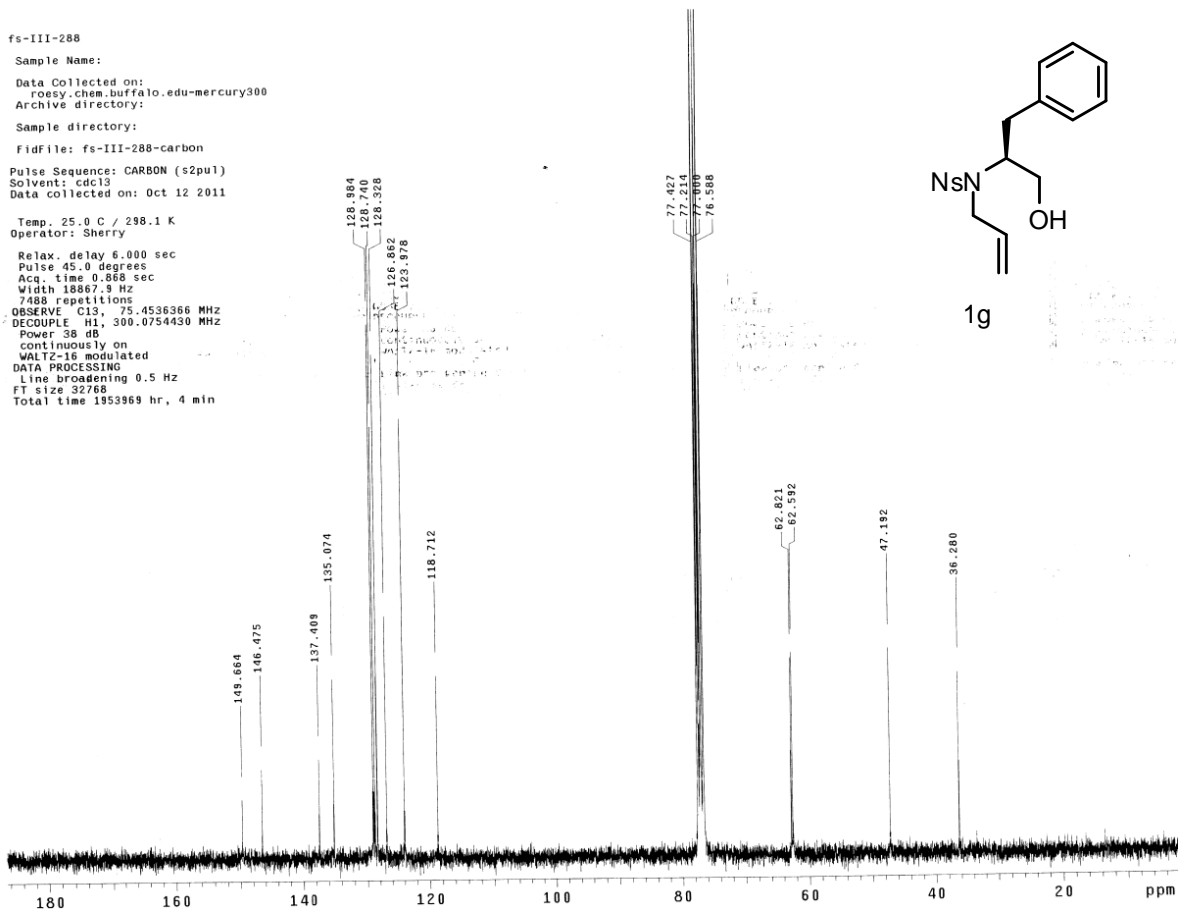
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 1953969 hr, 4 min

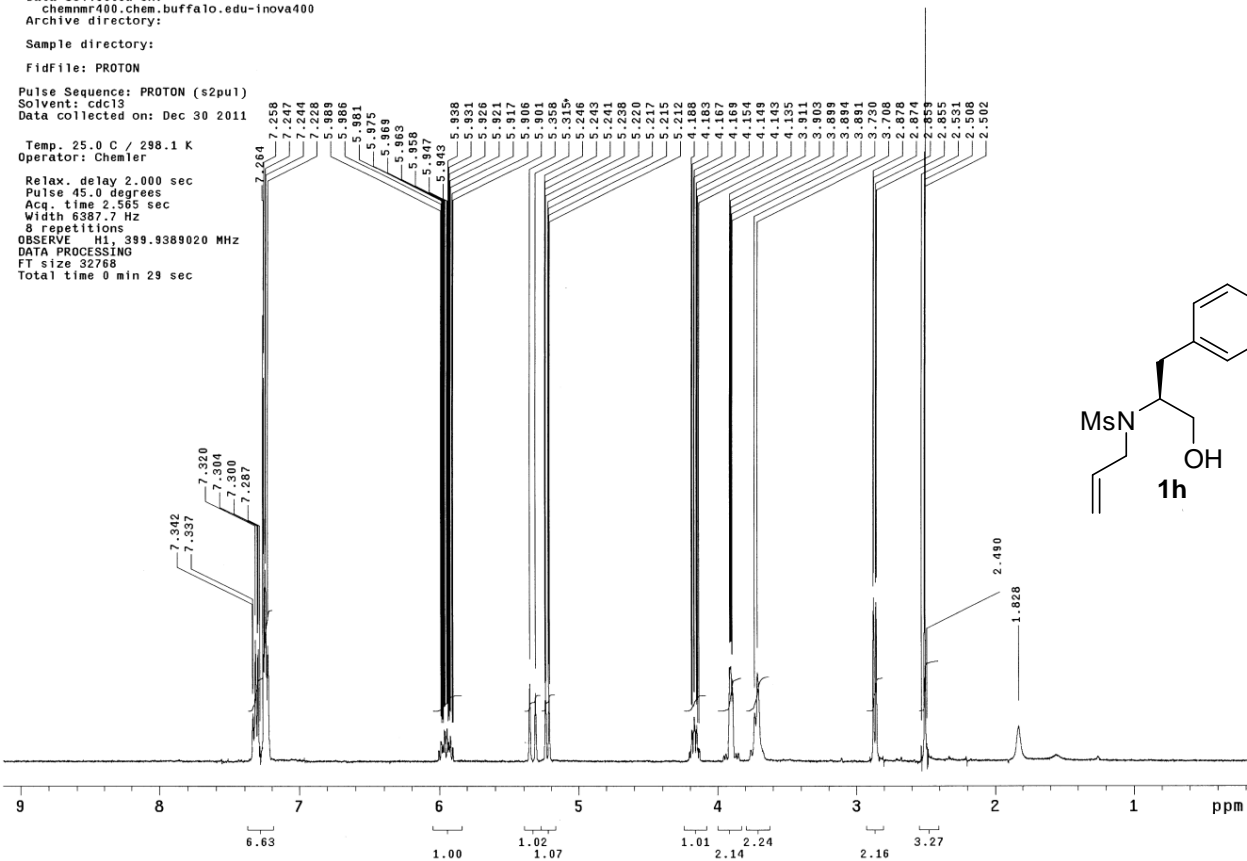


fs-V-46-proton

Sample Name:
Data Collected on:
chemnmr400.chem.buffalo.edu-inova400
Archive directory:
Sample directory:
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Dec 30 2011

Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.9389020 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 29 sec



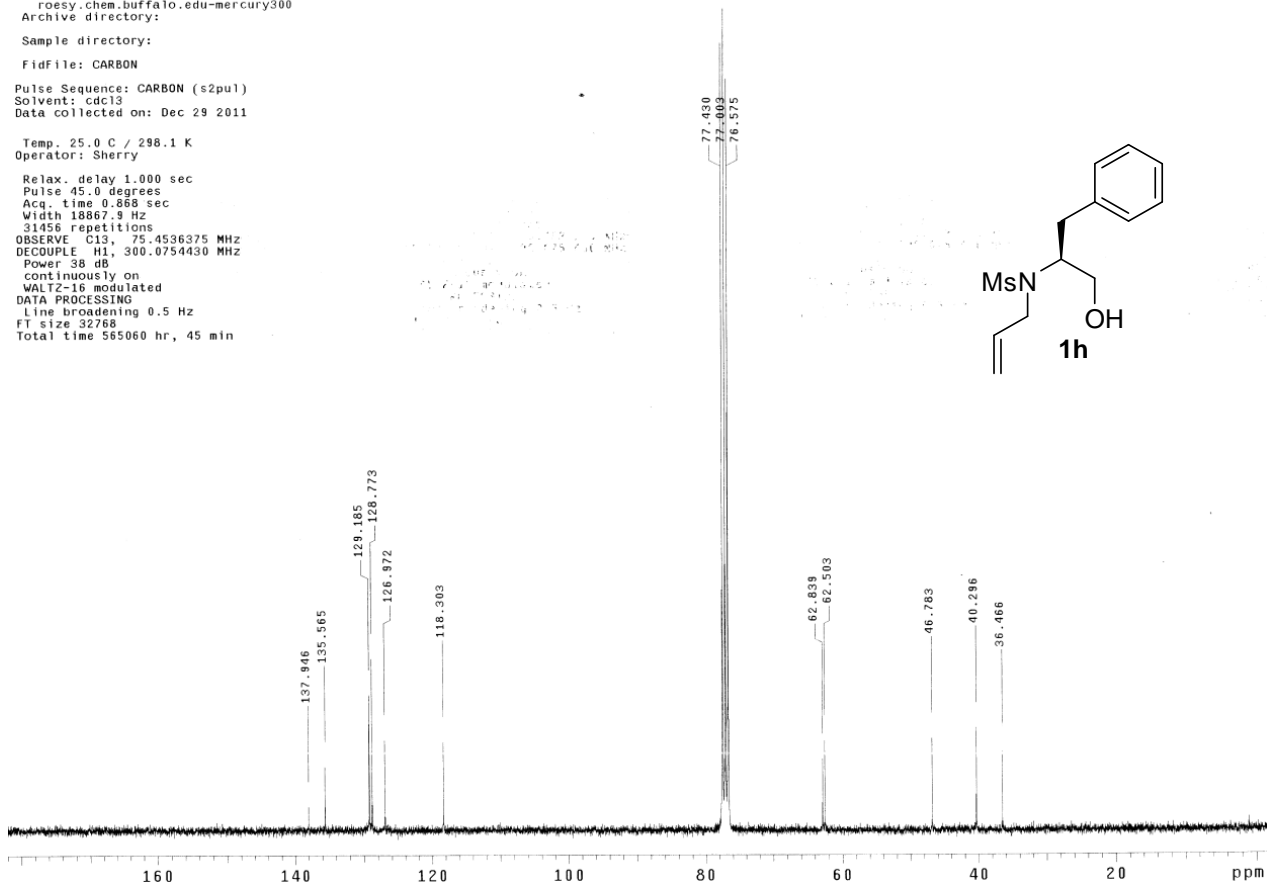
fs-V-46proton

Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Dec 29 2011

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
31456 repetitions
OBSERVE C13, 75.4536375 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 565060 hr, 45 min



fs-II-12hNMRredo

Sample Name:

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

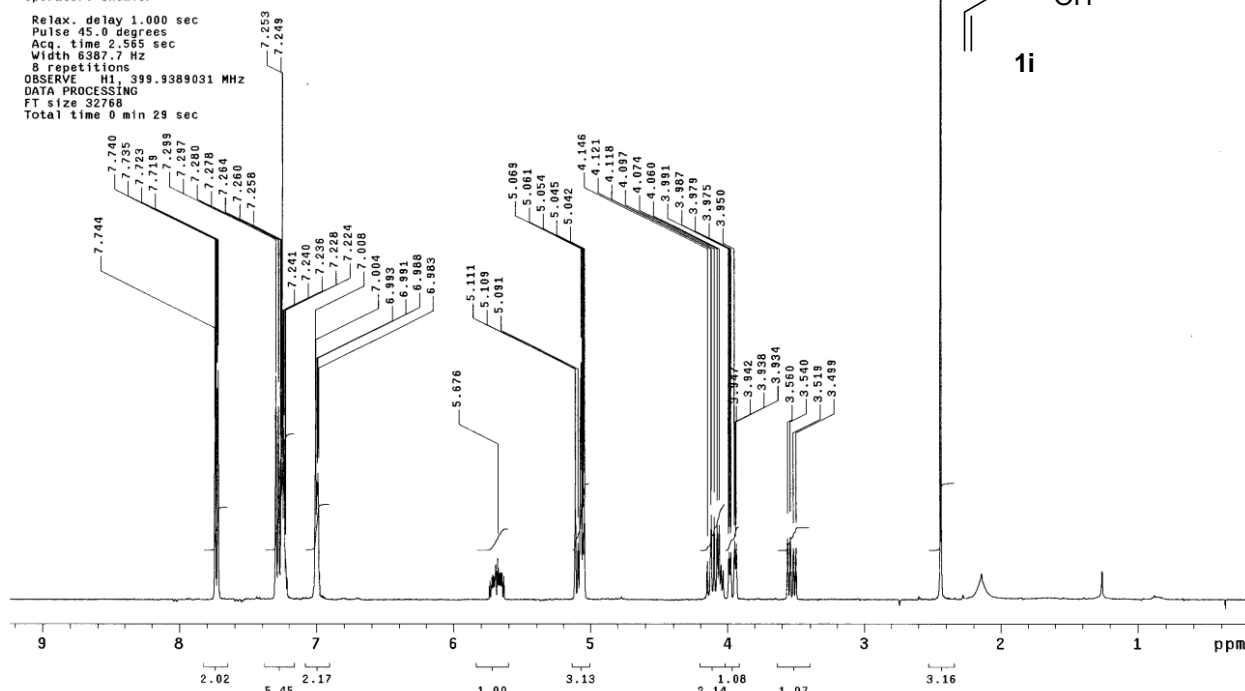
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: May 1 2012

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
3 repetitions
OBSERVE H1, 399.9389031 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 29 sec



fs-iv-266carbon2

Sample Name:

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

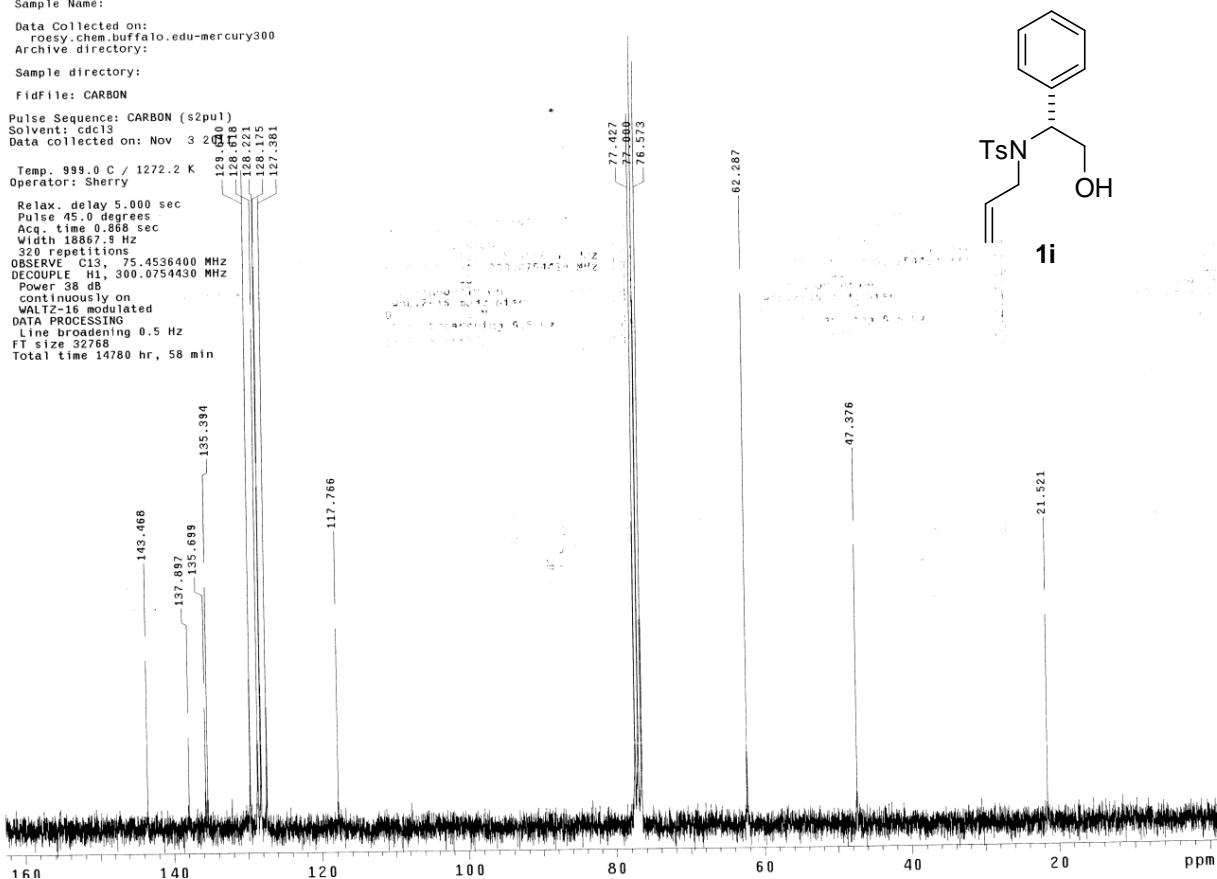
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Nov 3 2012

Temp. 99.0 C / 1272.2 K
Operator: Sherry

Relax. delay 5.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
320 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 14780 hr, 58 min



fs-IV-239-proton

Sample Name:

Data Collected on: chemmr400.chem.buffalo.edu-inova400
Archive directory:

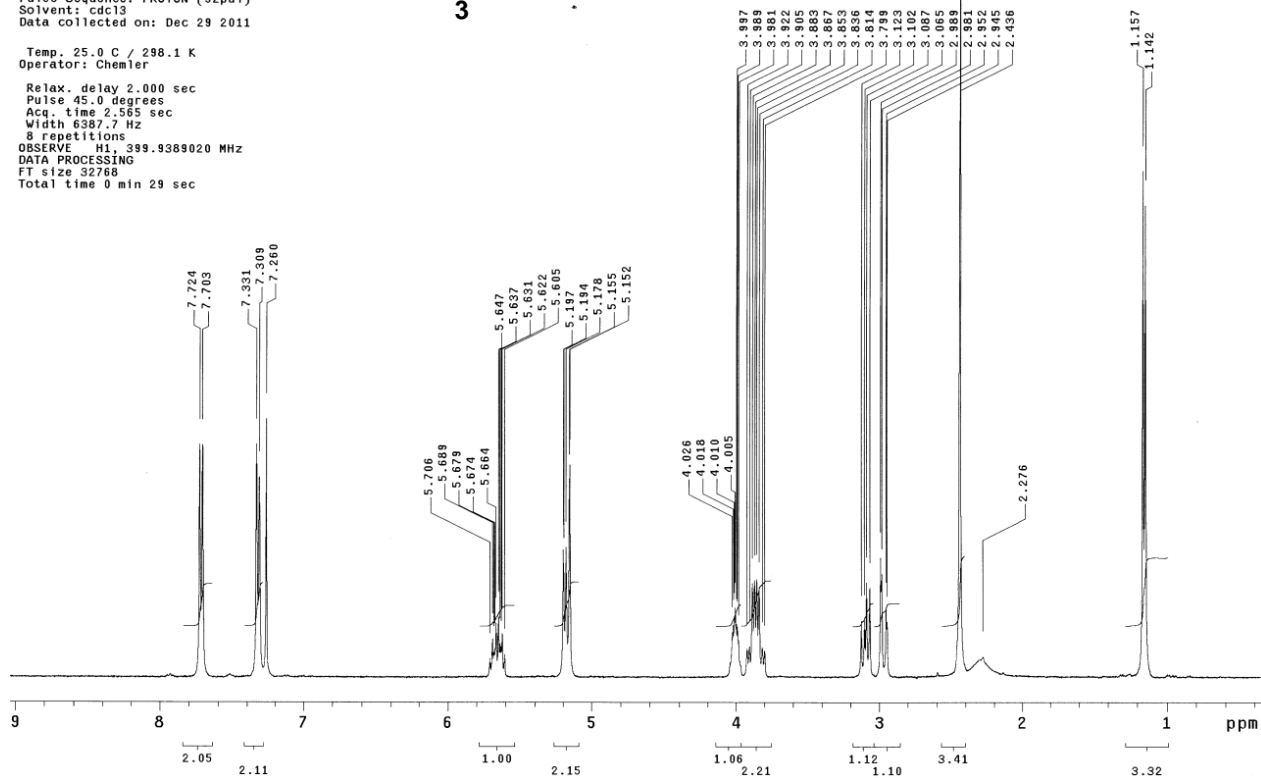
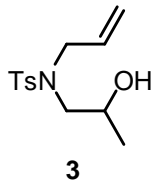
Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Dec 29 2011

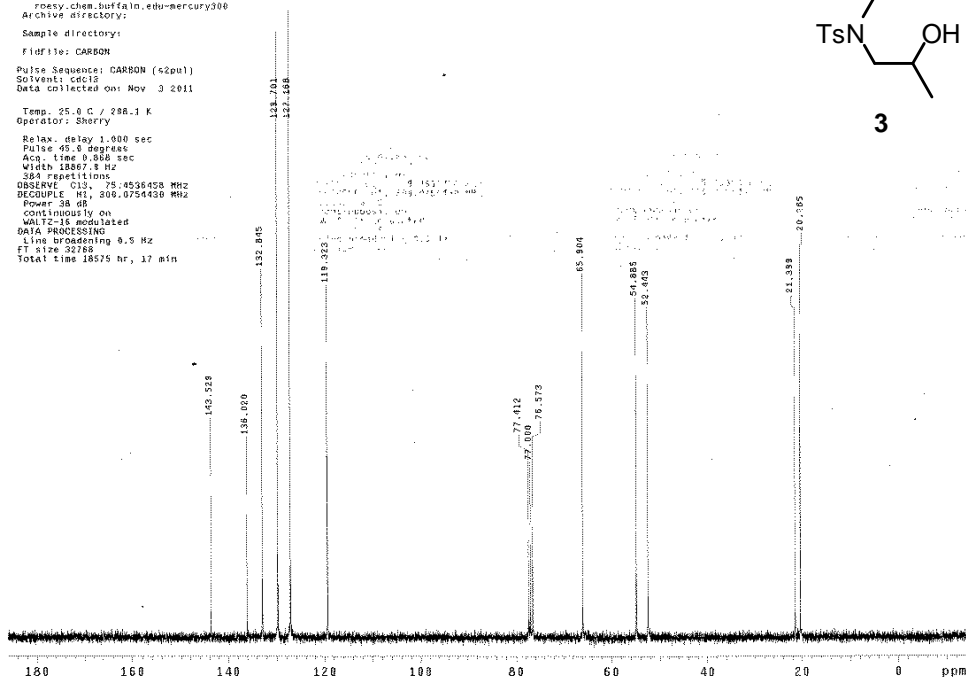
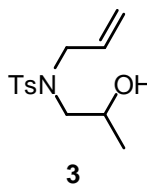
Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.565 sec
Width 6387.7 Hz
8 repetitions
OBSERVE H1, 399.938020 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 29 sec



fs-IV-239-carbon
Sample Name:
Data Collected on: roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
Fidfile: CARBON
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 3 2011

Temp. 25.0 C / 298.1 K
Operator: Sherry
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.958 sec
Width 18867.8 Hz
384 repetitions
OBSERVE C13, 75.4538428 MHz
DECOUPLE H1, 399.9754428 MHz
Power 38 dB
continuous ly on
WALTZ-16 modulated
DATA PROCESSING
Sine broadening 0.5 Hz
FT size 32768
Total time 18576 hr, 17 min



fs-III-207-hp1c

Sample Name:

Data Collected on:
chemmp908.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pu1)

Solvent: cdcl3

Data collected on: Jul 14 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.868 sec

Width 8000.0 Hz

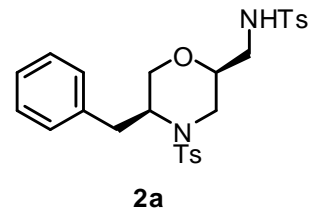
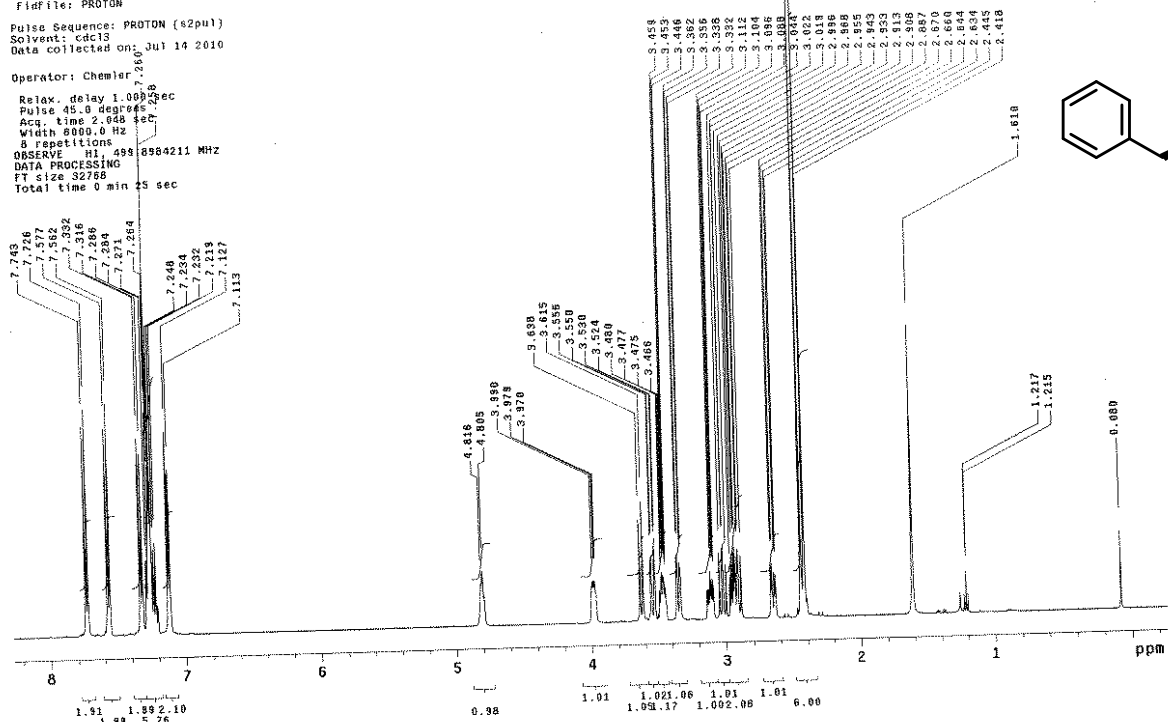
0 repetitions

OBSERVE H1 498.8984211 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 25 sec



fs-III-207-carbon

Sample Name:

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

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cdcl3

Data collected on: Jul 16 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 13867.9 Hz

25046 repetitions

OBSERVE C13, 75.4536375 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

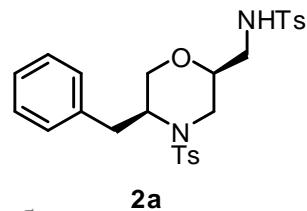
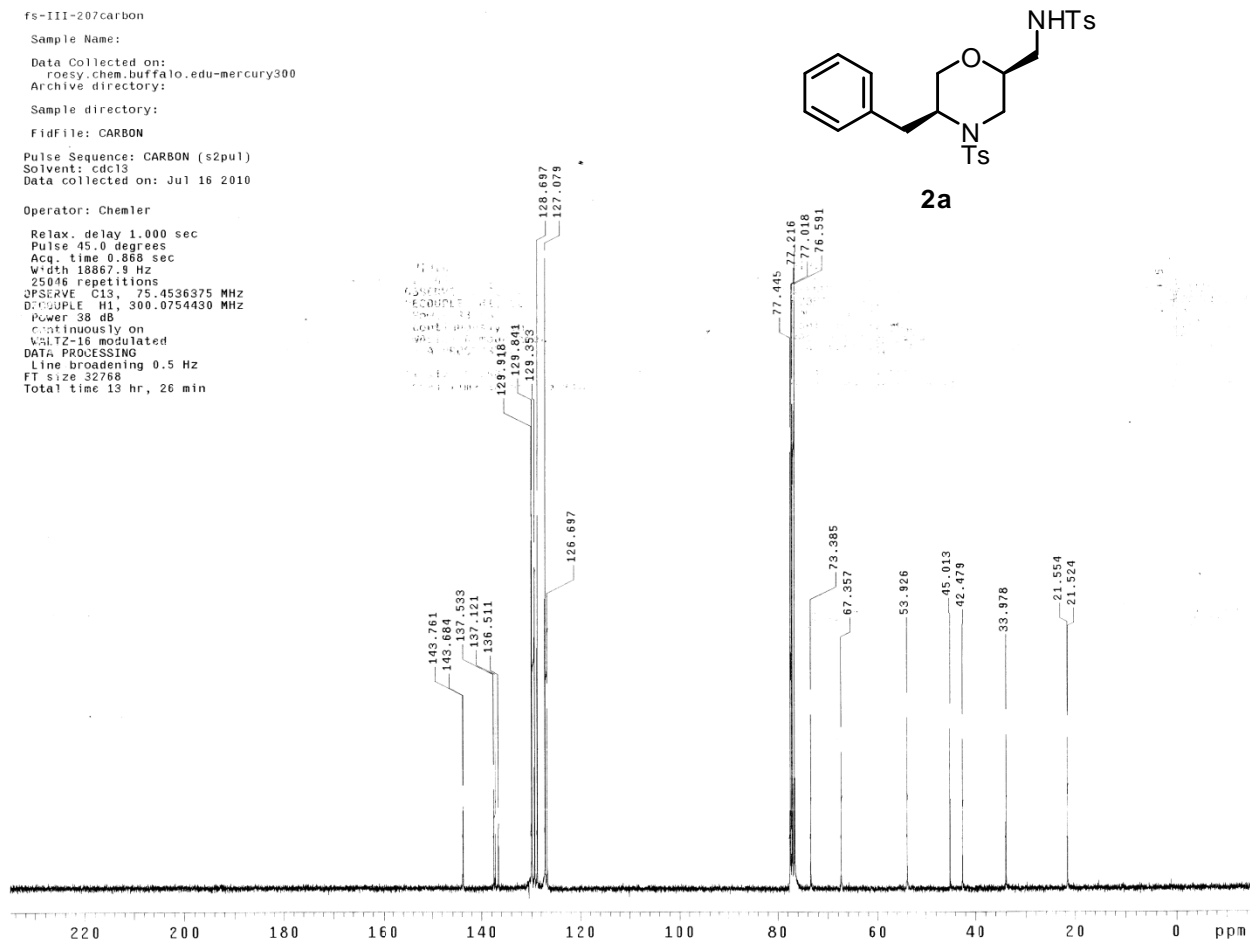
WALTZ-16 modulated

DATA PROCESSING

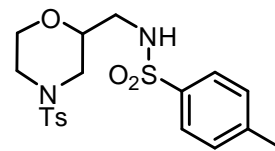
Line broadening 0.5 Hz

FT size 32768

Total time 13 hr, 26 min

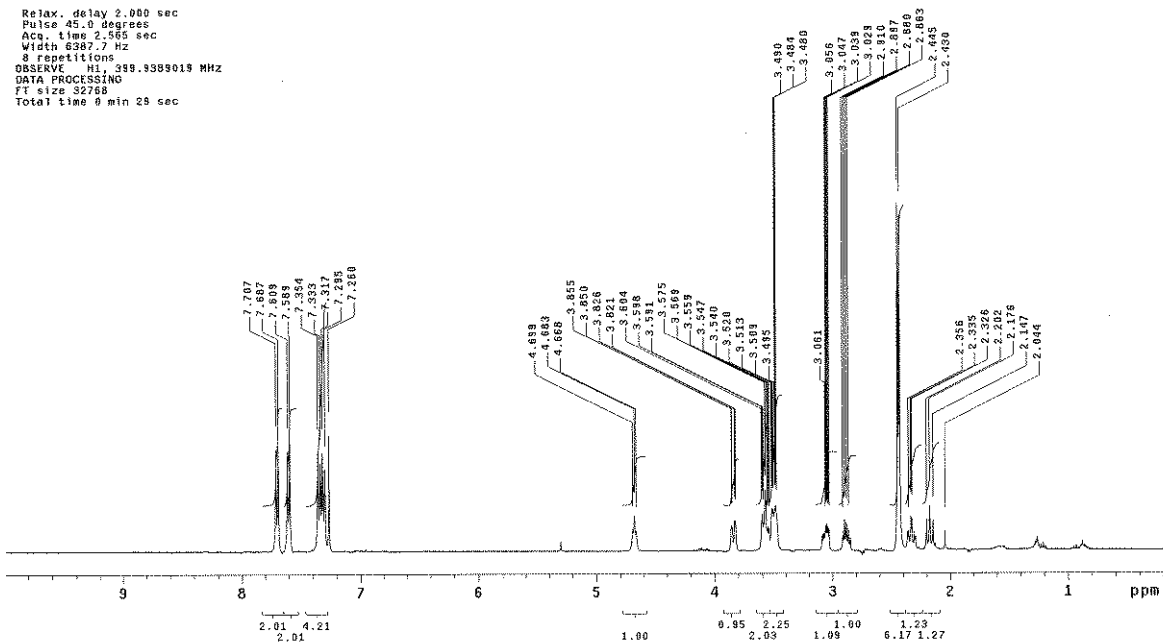


fs-III-234-proton
 Sample Name:
 Data Collected on:
 chemnar480.chem.buffalo.edu-inova480
 Archive directory:
 Sample directory:
 Fidfile: fs-III-234-proton
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jan 14 2012



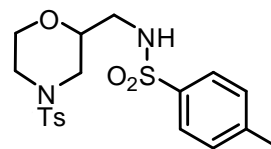
2b

Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 2.505 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 399.9389015 MHZ
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec

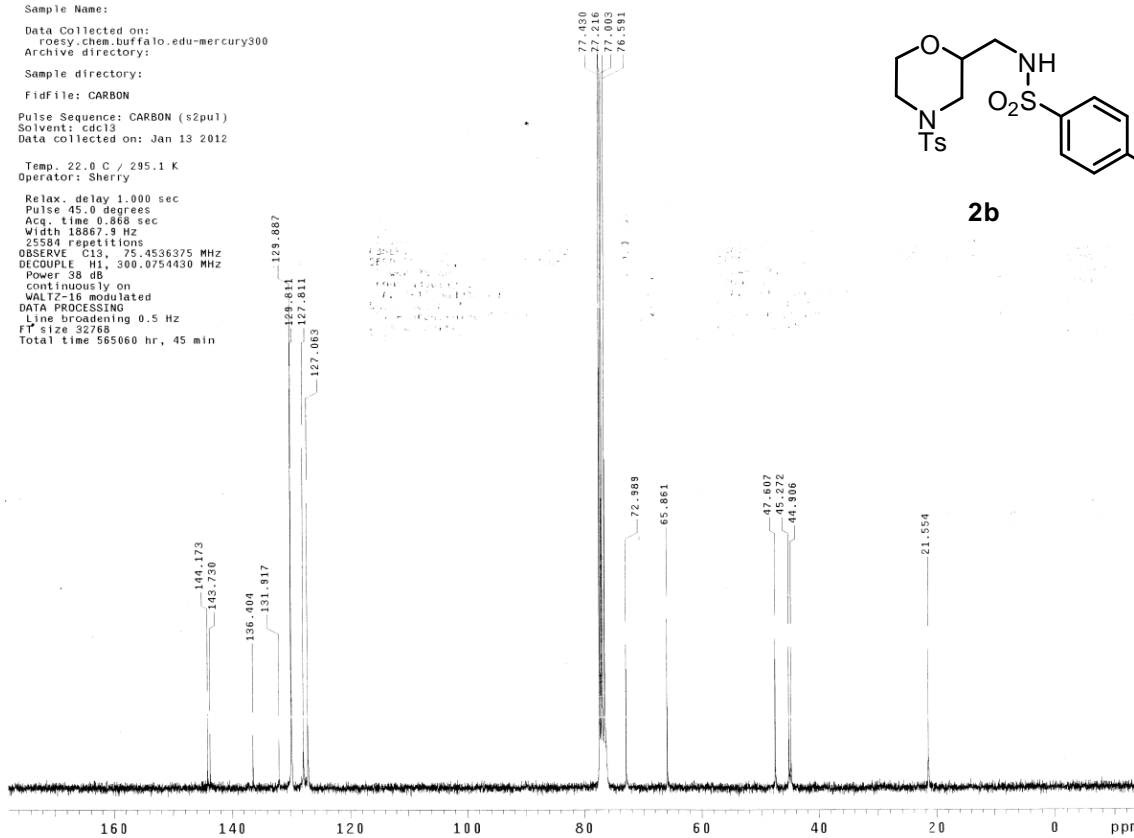


fs-III-234-carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: CARBON
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jan 13 2012

Temp. 22.0 C / 295.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 25584 repetitions
 OBSERVE C13, 75.4536375 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 565060 hr, 45 min

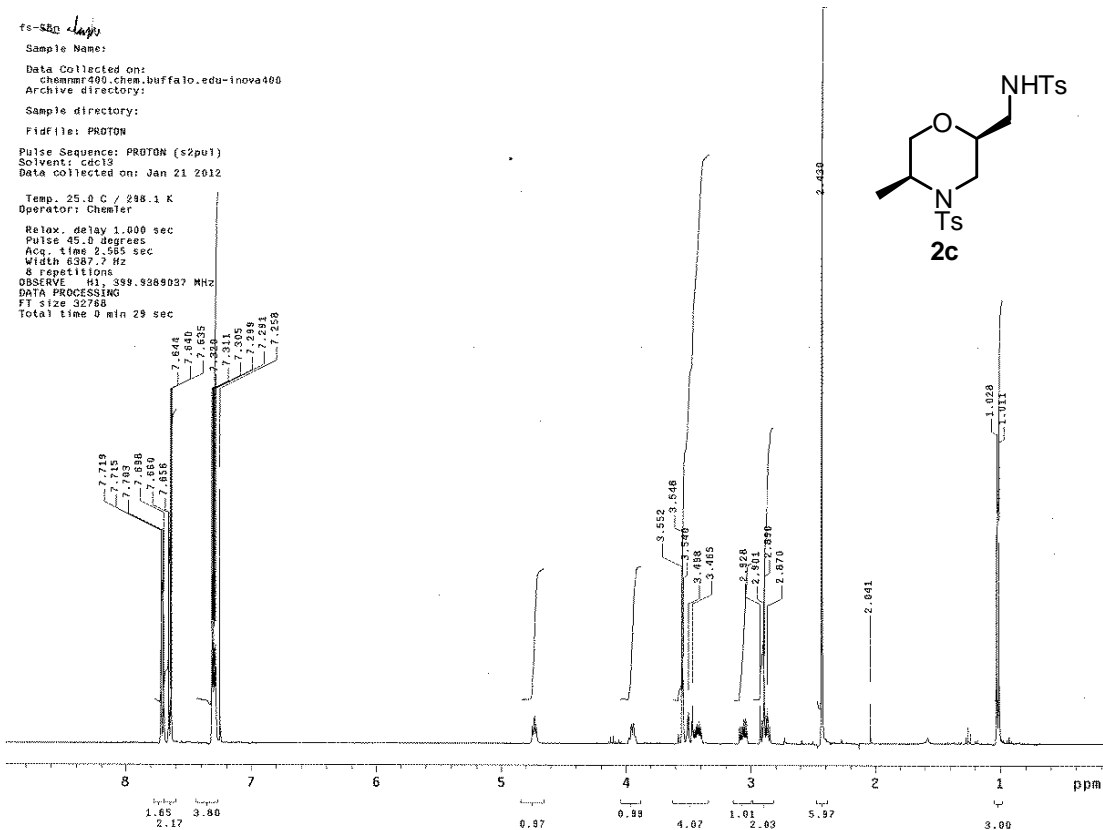


2b



fs-SBQ *shery*
 Sample Name:
 Data Collected on:
 chemmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jan 21 2012

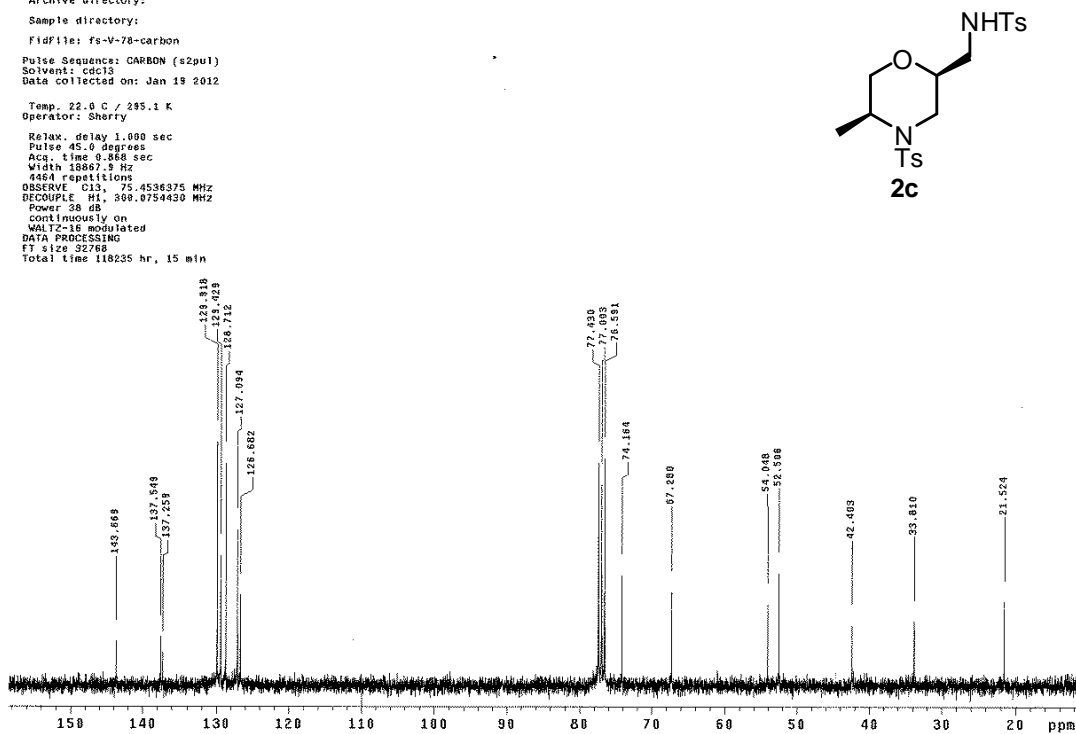
Temp. 25.0 C / 298.1 K
 Operator: Chemter
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.565 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 399.9389037 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



STANDARD PROTON PARAMETERS

Sample Name:
 Data Collected on:
 rosey.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: fs-v-78-carbon
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jan 19 2012

Temp. 22.0 C / 295.1 K
 Operator: Shery
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 4464 repetitions
 OBSERVE C13, 75.4536375 MHz
 DECOUPLE H1, 399.0754450 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 FT size 32768
 Total time 118235 hr, 15 min



fs-1p-pro-carbon

Sample Name:

Data Collected on:
chemm400.chem.buffalo.edu-inova400

Archive directory:

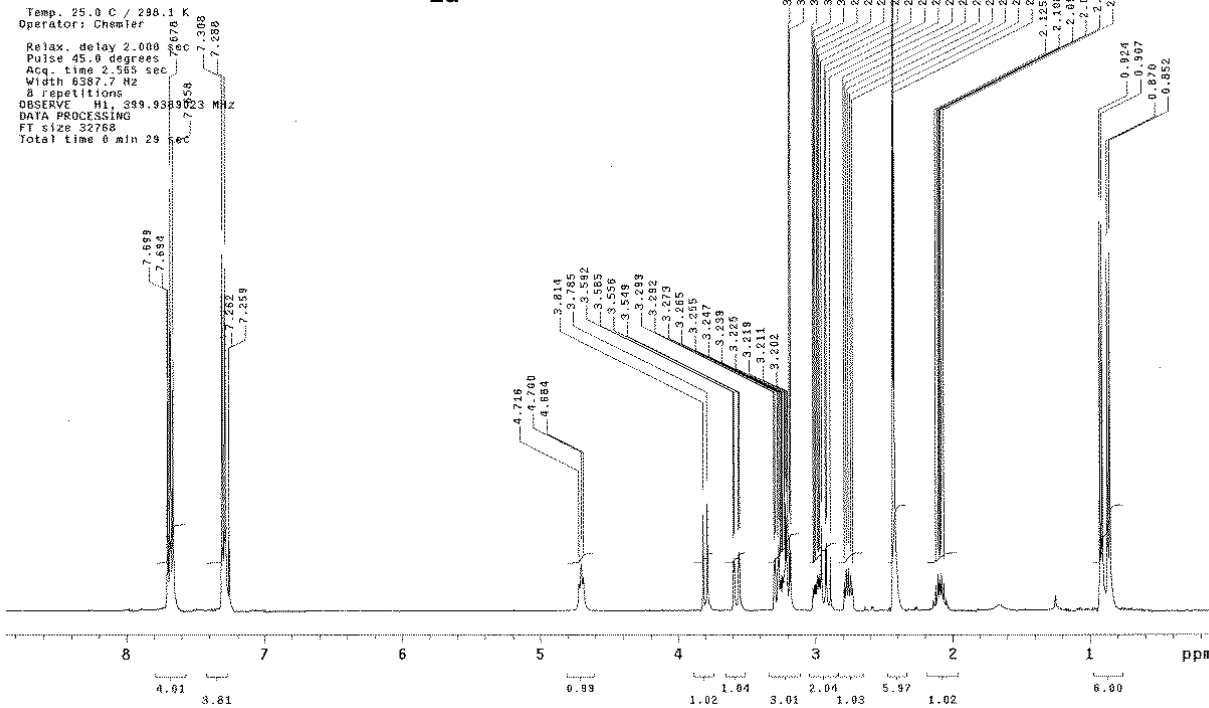
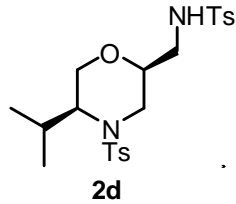
Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pu1)

Solvent: cdc13

Data collected on: Jan 17 2012



fs-111-1p-13c-trs-1-carbon

Sample Name:

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

Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cdc13

Data collected on: Aug 3 2010

Operator: Chemler

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18667.5 Hz

5616 repetitions

OBSERVE C13, 75.4536375 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

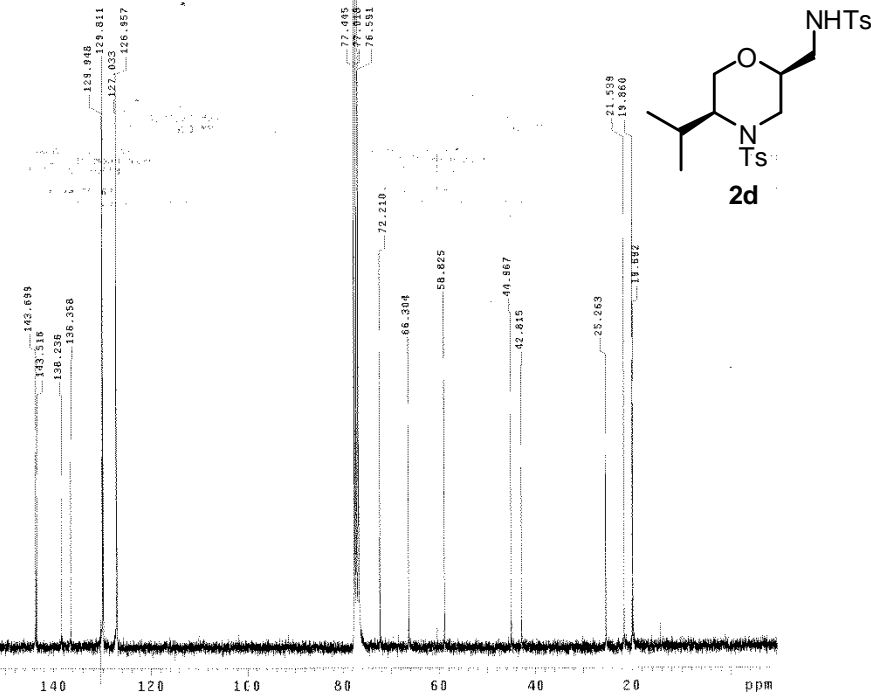
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 92768

Total time 23 hr, 30 min



fs-II-12f-NMRreda

Sample Name:

Data Collected on:
chemnar400.chem.buffalo.edu-inova400

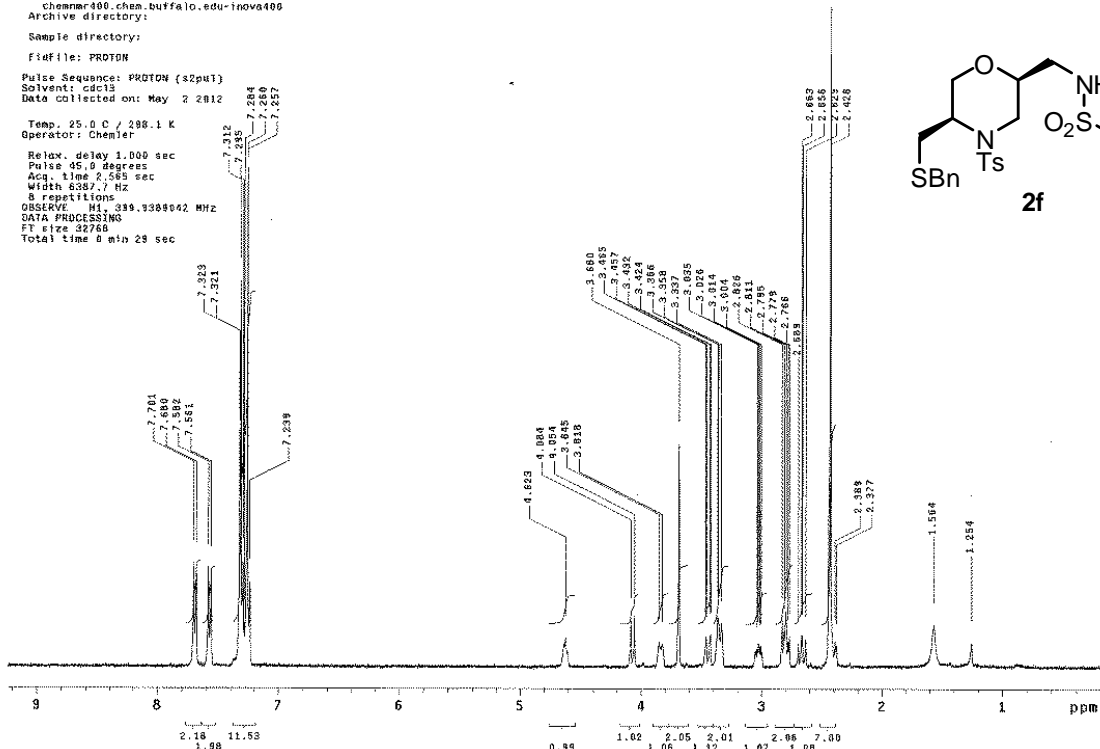
Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: May 2 2012

Temp. 25.0 C / 298.1 K
Operator: Chemler
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.585 sec
Width 6387.7 Hz
6 repetitions
OBSERVE H1, 399.9388042 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 28 sec



STANDARD CARBON PARAMETERS

Sample Name:

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

Archive directory:

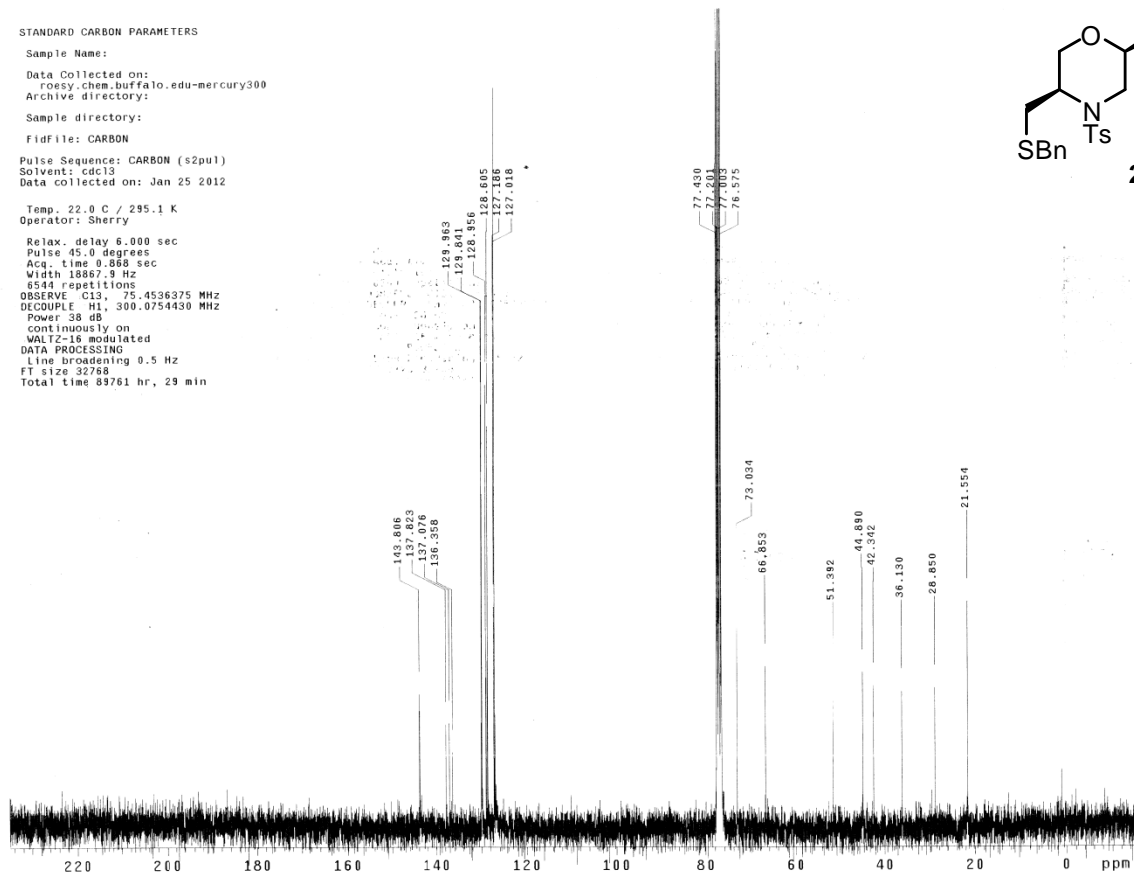
Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Jan 25 2012

Temp. 22.0 C / 295.1 K
Operator: Sherry

Relax. delay 6.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6544 repetitions
OBSERVE C13, 75.4536375 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 89761 hr, 29 min



fs-V-77

Sample Name:

Data Collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:

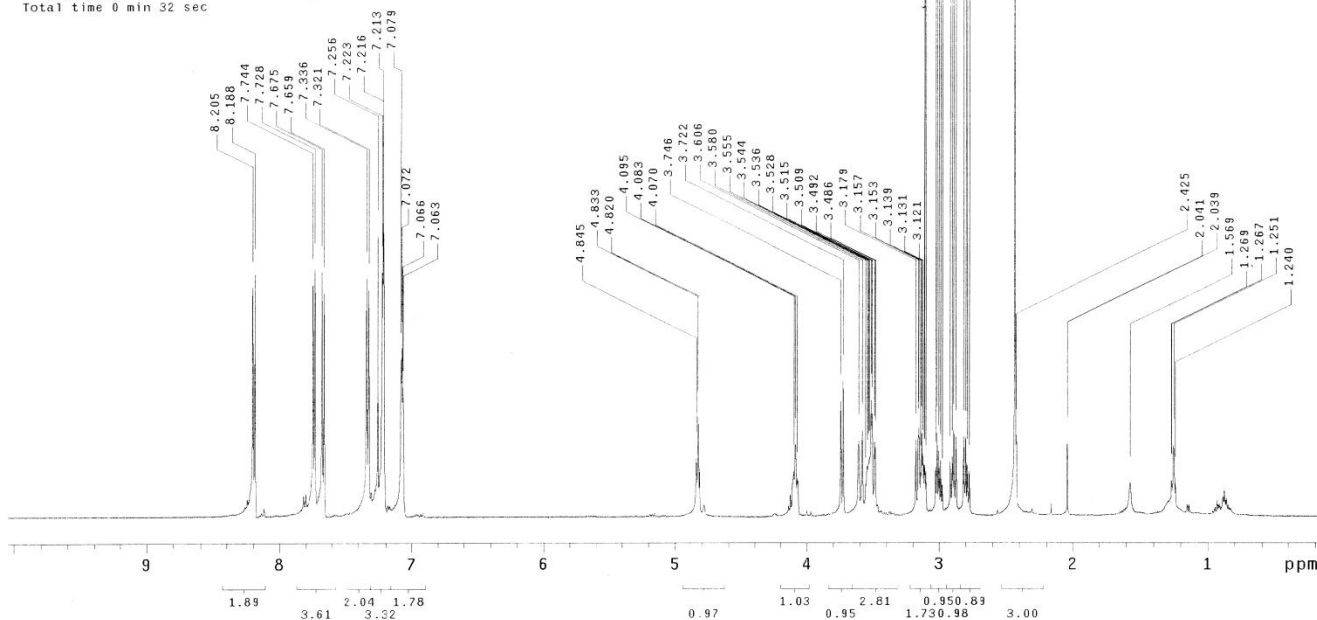
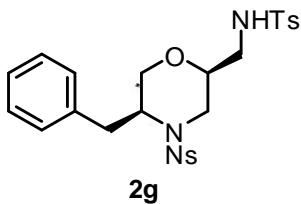
Sample directory:

Fidfile: PROTON

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

Operator: Chemler

Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1 499.8984089 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 32 sec



fs-IV-236-carbon

Sample Name:

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

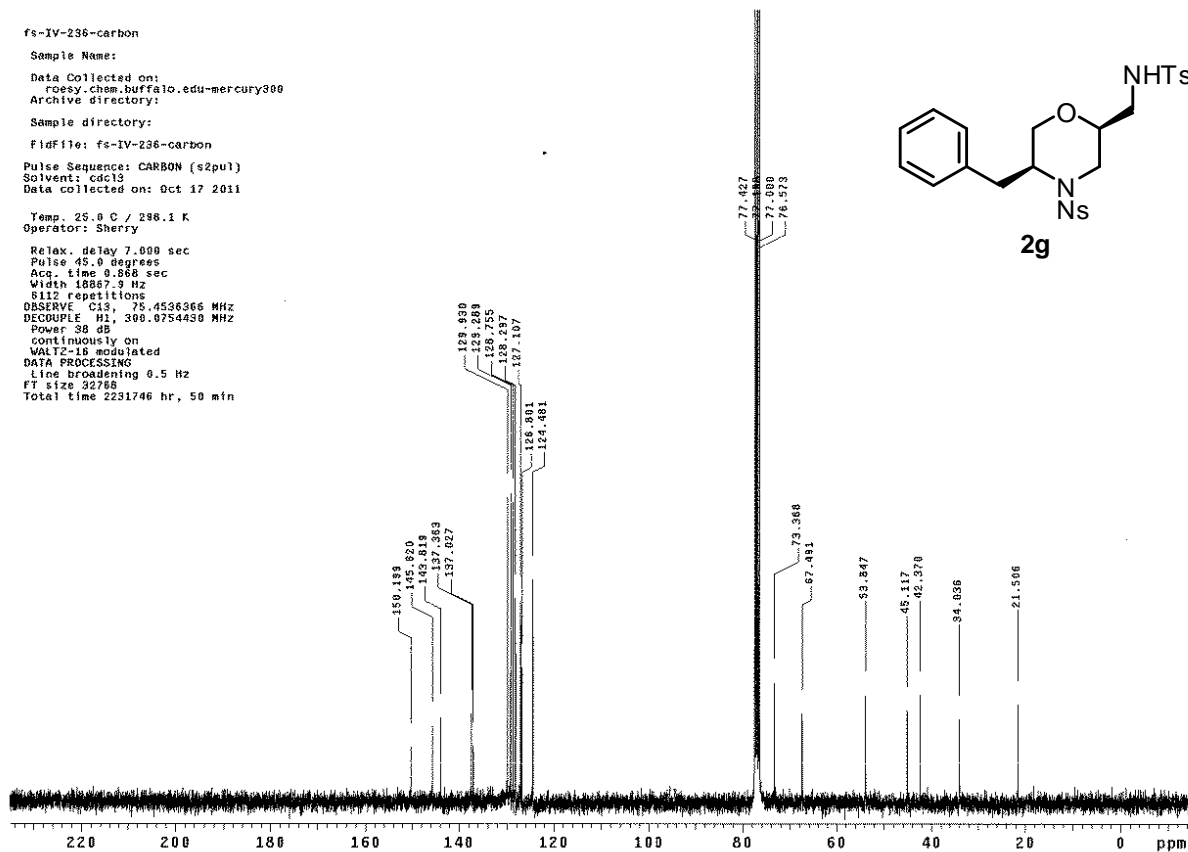
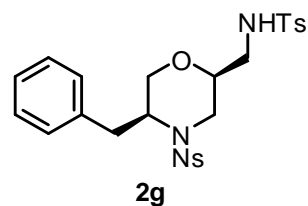
Sample directory:

Fidfile: fs-IV-236-carbon

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Oct 17 2011

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 7.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
812 repetitions
OBSERVE C13 76.4536366 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 2231746 hr, 50 min



fs-IV-236-proton

Sample Name:

Data Collected on:
Chemmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)

Solvent: cdcl3

Data Collected on: Oct 18 2011

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.565 sec

Width 6387.7 Hz

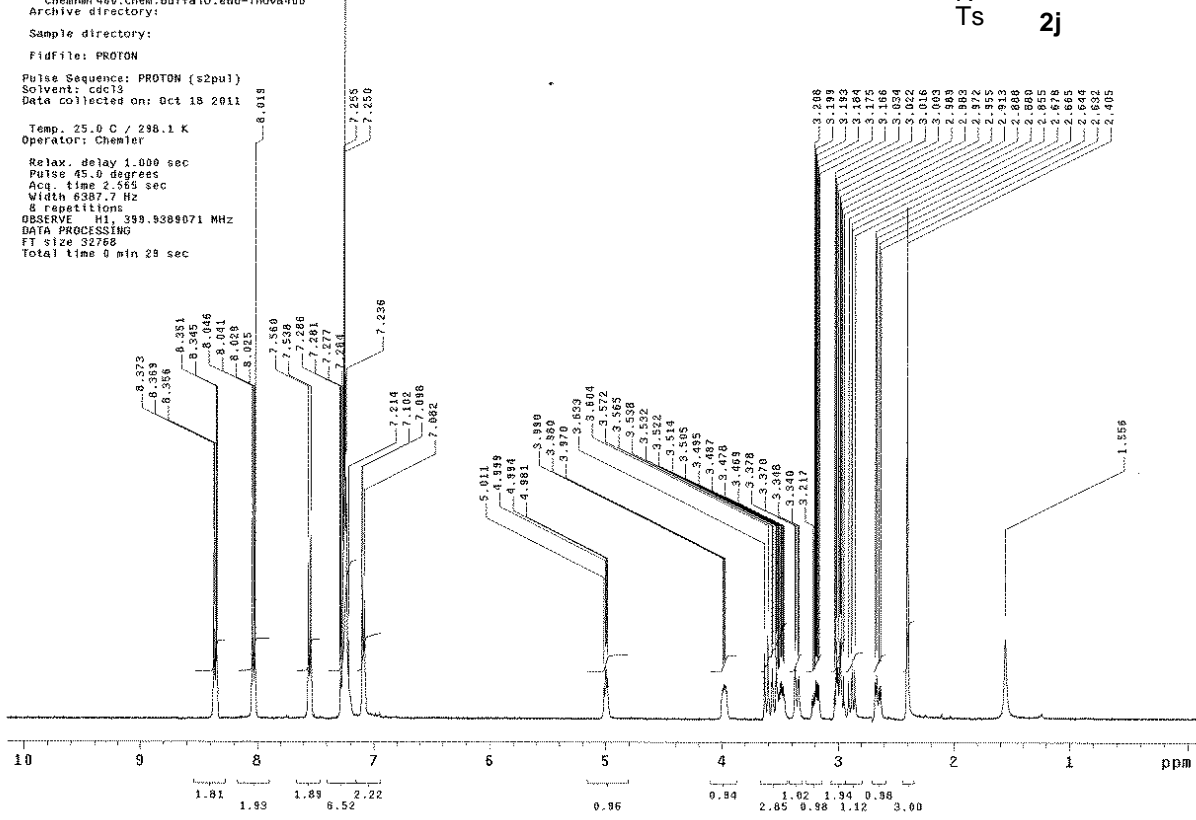
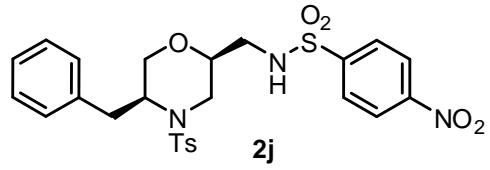
8 repetitions

OBSERVE H1, 399.9389071 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 28 sec



fs-IV-236-carbon

Sample Name:

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

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cdcl3

Data collected on: Oct 17 2011

Temp. 26.6 C / 299.8 K

Operator: Sherry

Relax. delay 7.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.8 Hz

6112 repetitions

OBSERVE C13, 75.4536366 MHz

DECUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

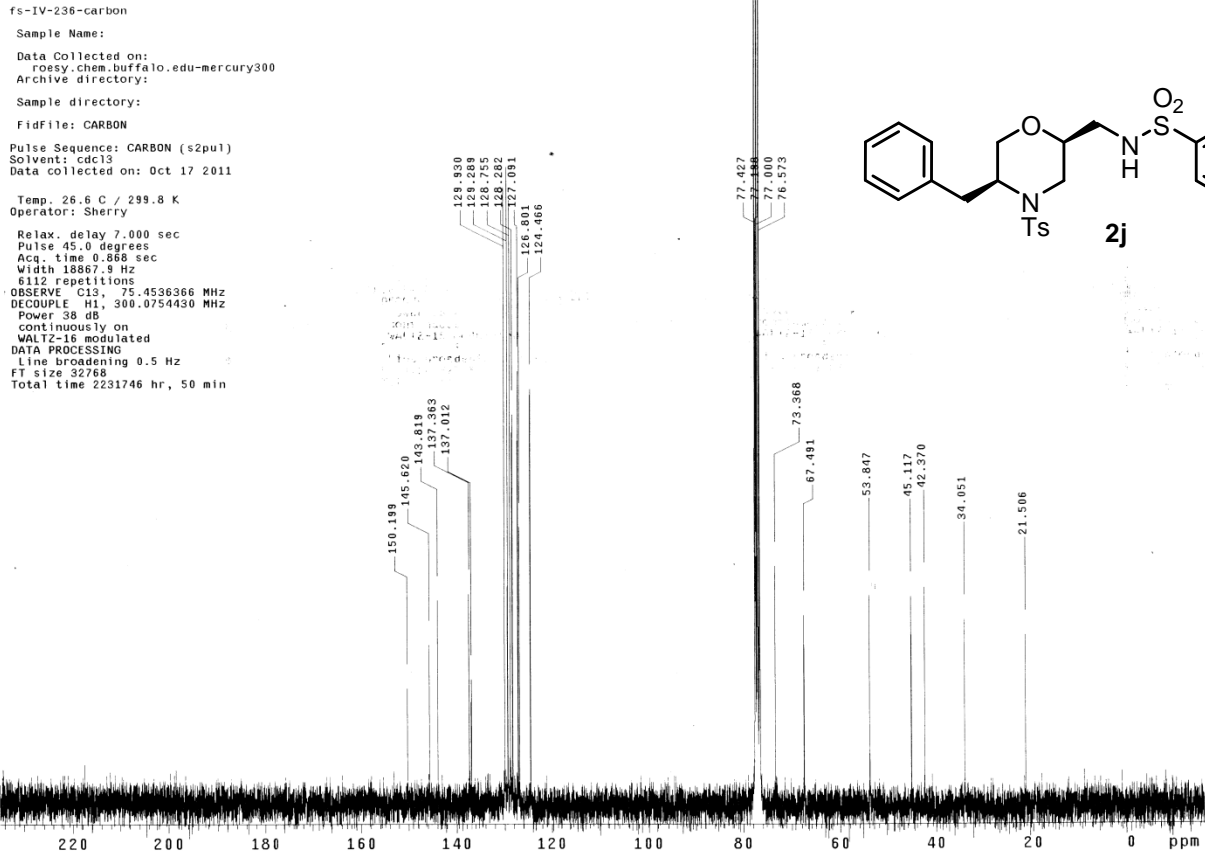
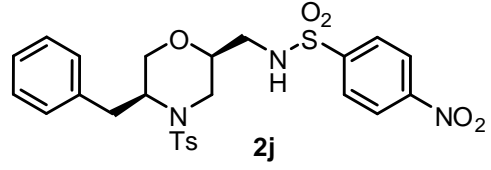
WALTZ-16 modulated

DATA PROCESSING

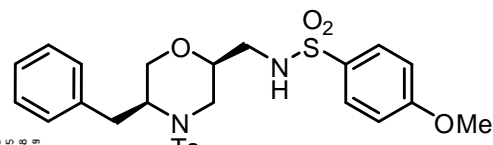
Line broadening 0.5 Hz

FT size 32768

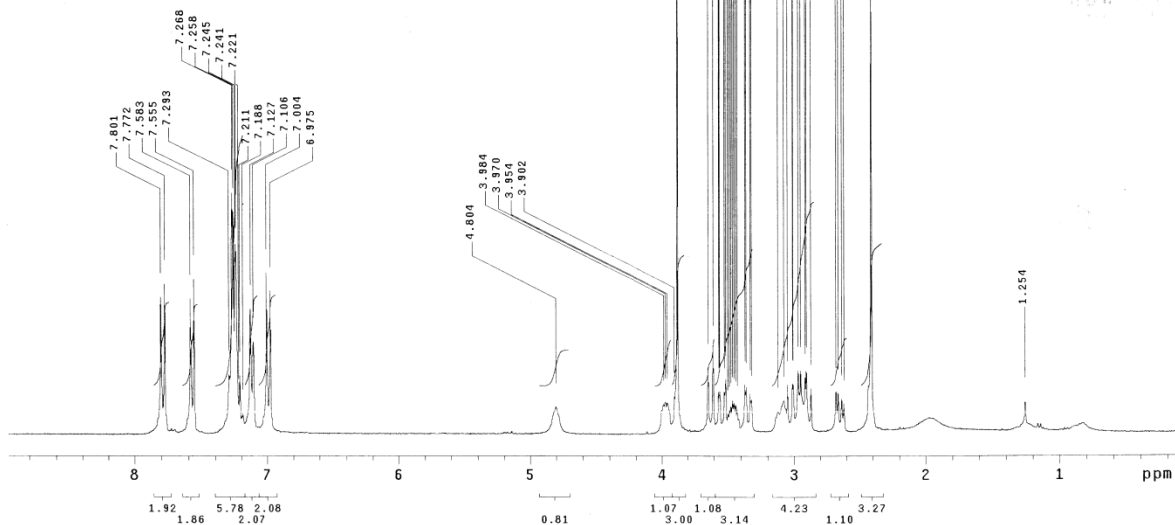
Total time 2291746 hr, 50 min



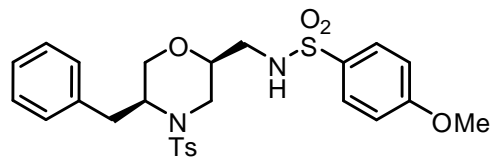
fs-IV-240-proton
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Oct 12 2011
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.706 sec
 Width 4803.1 Hz
 8 repetitions
 OBSERVE H1, 300.0738816 MHZ
 DATA PROCESSING
 FT size 16384
 Total time 0 min 23 sec



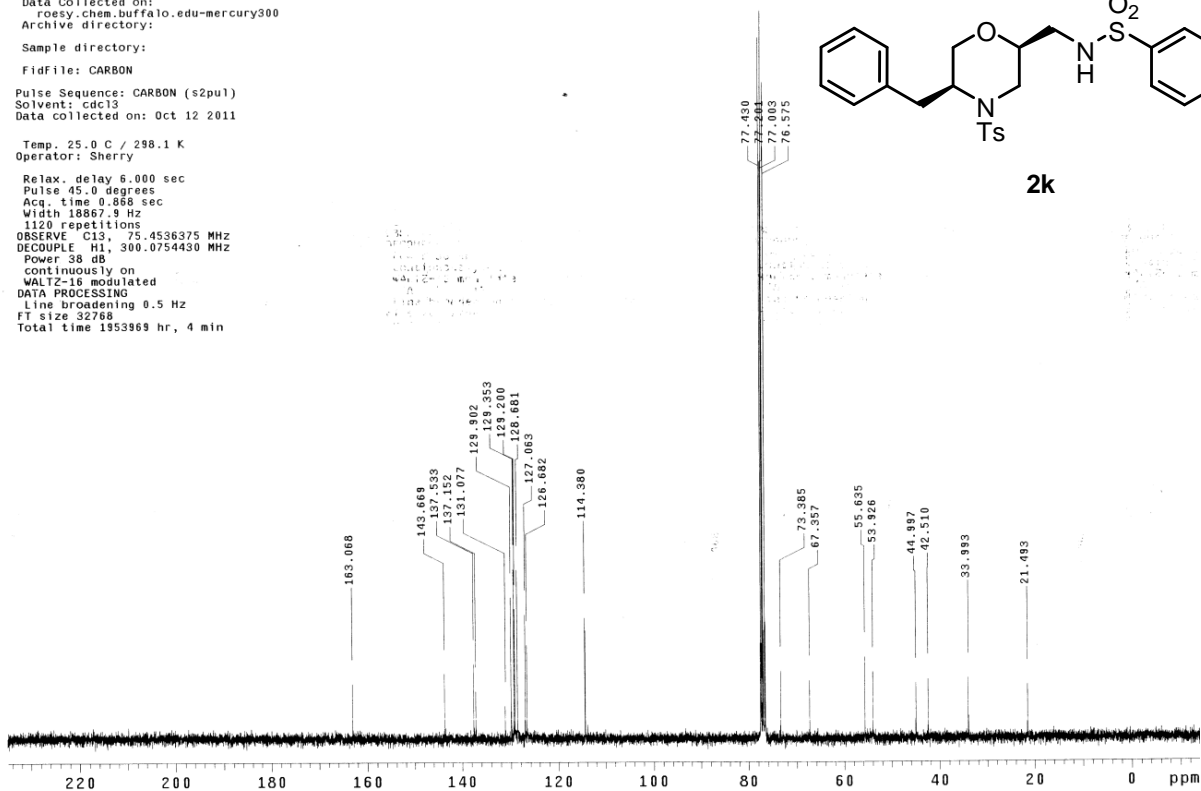
2k



fs-IV-240-carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: CARBON
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Oct 12 2011
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 6.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 1120 repetitions
 OBSERVE C13, 75.4536375 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 1953969 hr, 4 min



2k



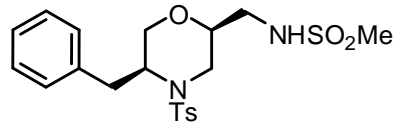
fs-v-mscap-major-1

Sample Name:
DC-13Rf_2
Data Collected on:
chemm300.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
FidFile: PRDTON

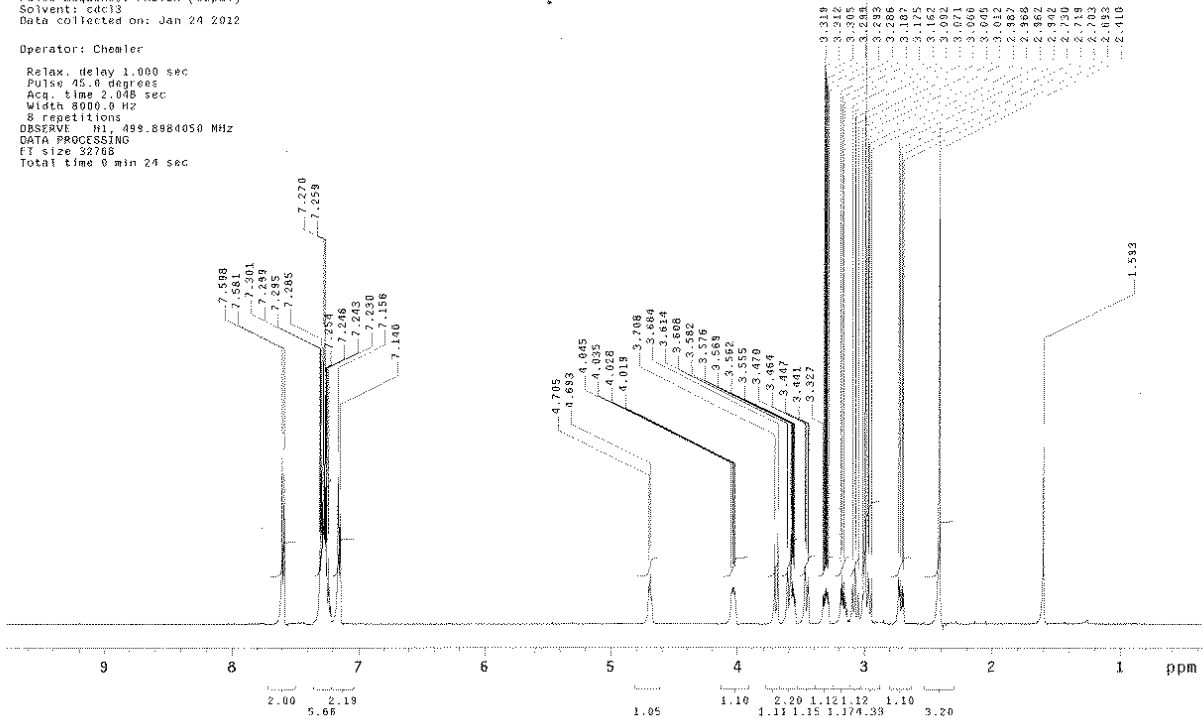
Pulse Sequence: PRDTON (s2pul)
Solvent: cdcl3
Data collected on: Jan 24 2012

Operator: Chewler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE N1, 499.8984050 MHz
DATA PROCESSING
F1 size 32768
Total time 0 min 24 sec



cis-21



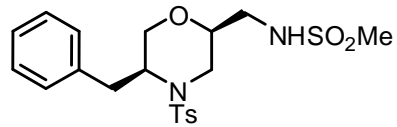
fs-v-83major-carbon

Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
FidFile: CARBON

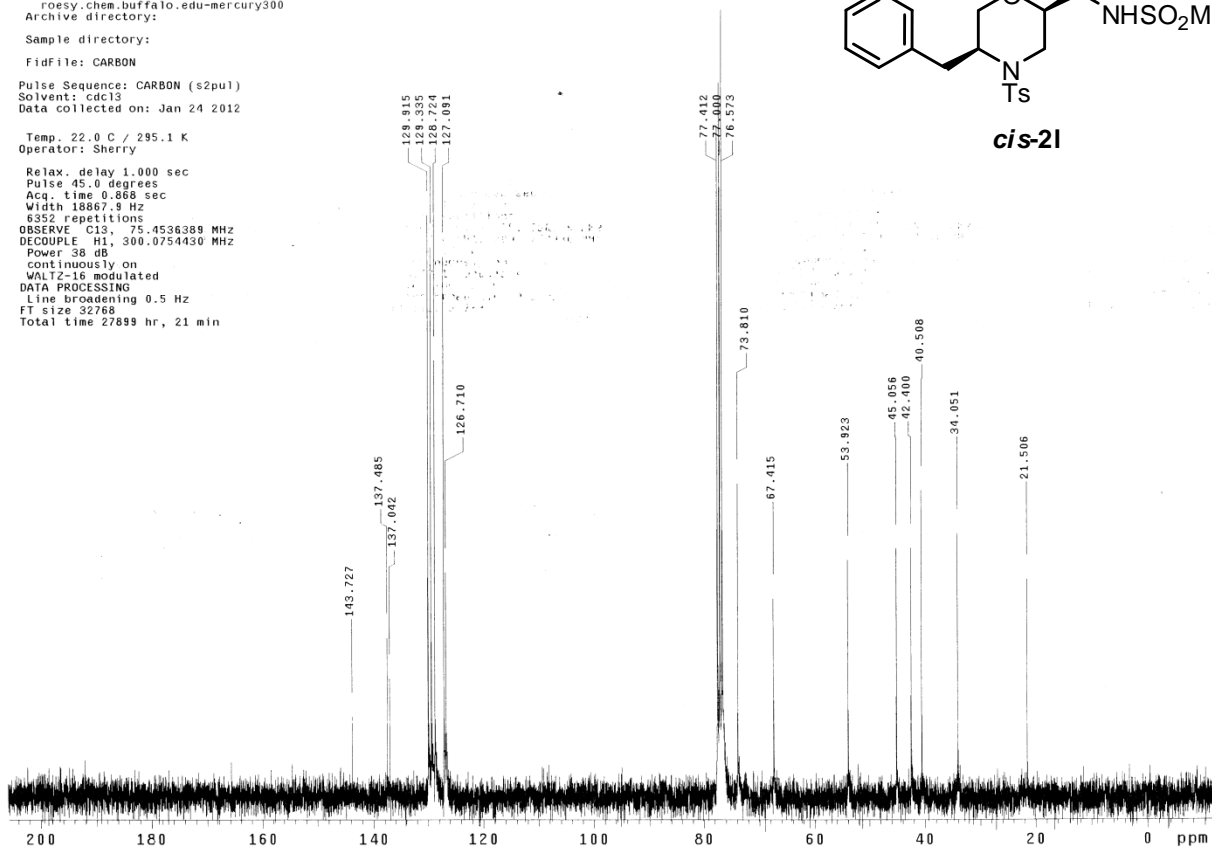
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jan 24 2012

Temp. 22.0 C / 295.1 K
Operator: Sherry

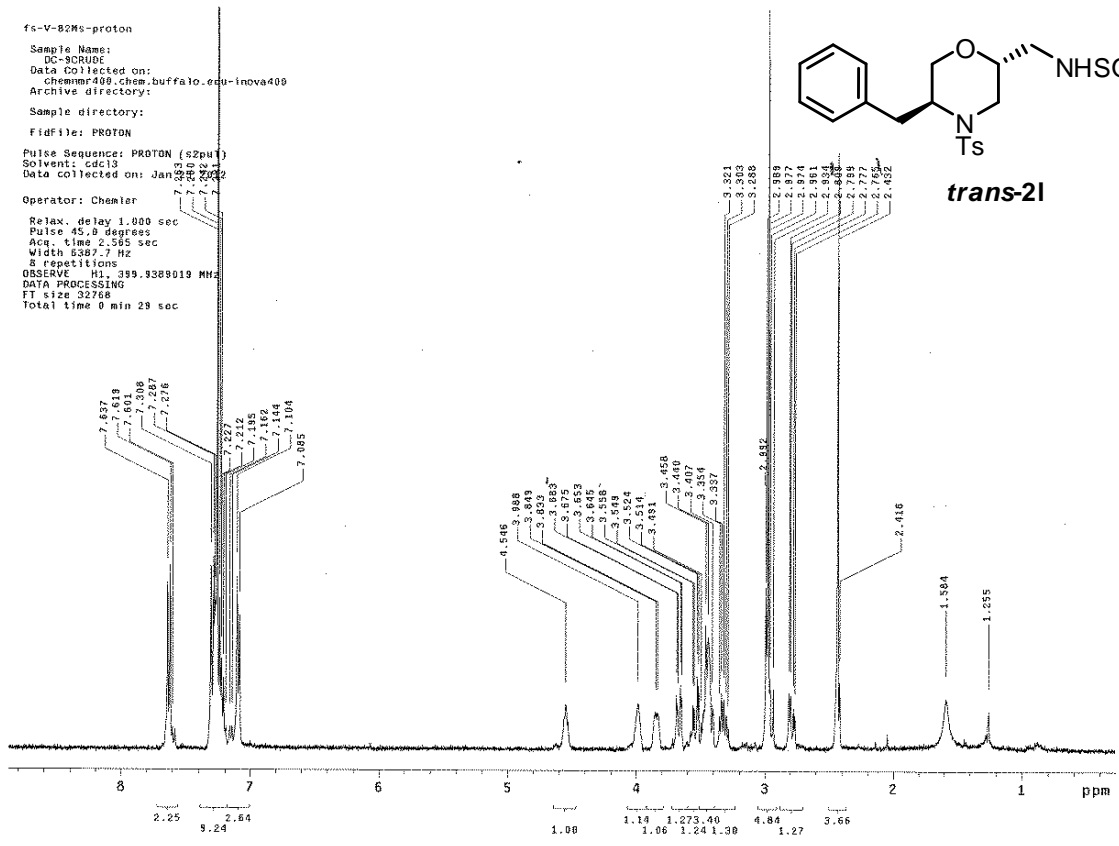
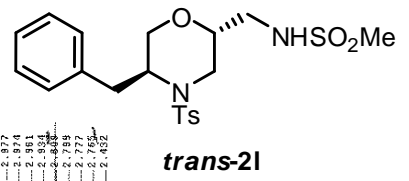
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6352 repetitions
OBSERVE C13, 75.4536389 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
F1 size 32768
Total time 27899 hr, 21 min



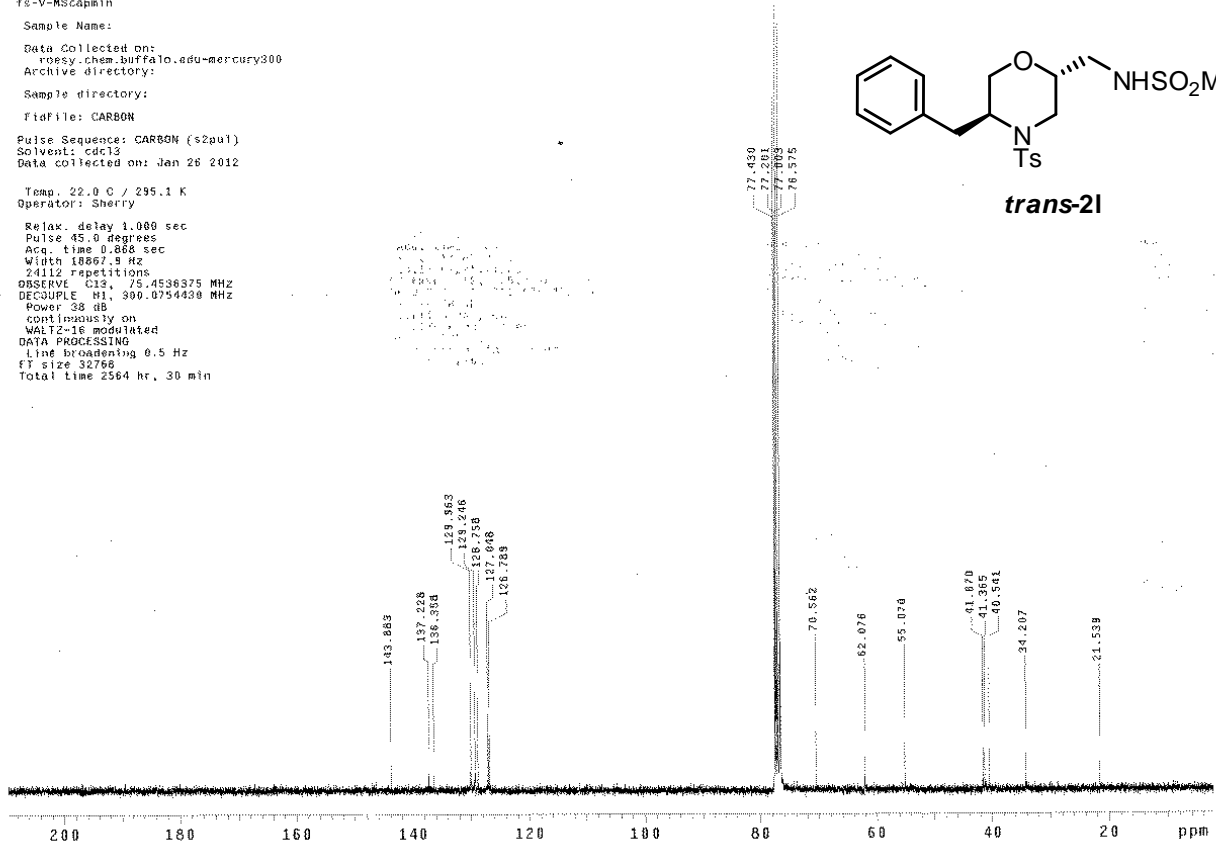
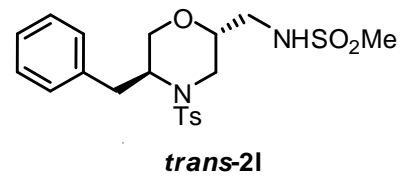
cis-21



fs-V-82Ms-proton
 Sample Name: DC-9CRUDE
 Data Collected on: chemmr408.chem.buffalo.edu-inova409
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdc13
 Data collected on: Jan 26 2012
 Operator: Chemier
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.395 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1, 359.9389019 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



fs-V-MScapin
 Sample Name:
 Data Collected on: roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdc13
 Data collected on: Jan 26 2012
 Temp. 22.0 C / 295.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.3 Hz
 24112 repetitions
 OBSERVE C13, 75.4536375 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 2564 hr, 30 min



fs-IV-SES-prton2

Sample Name:

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

Sample directory:

Fidfile: PROTON

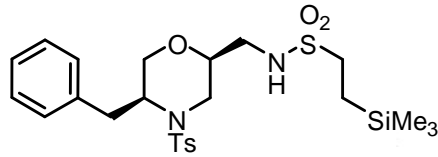
Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

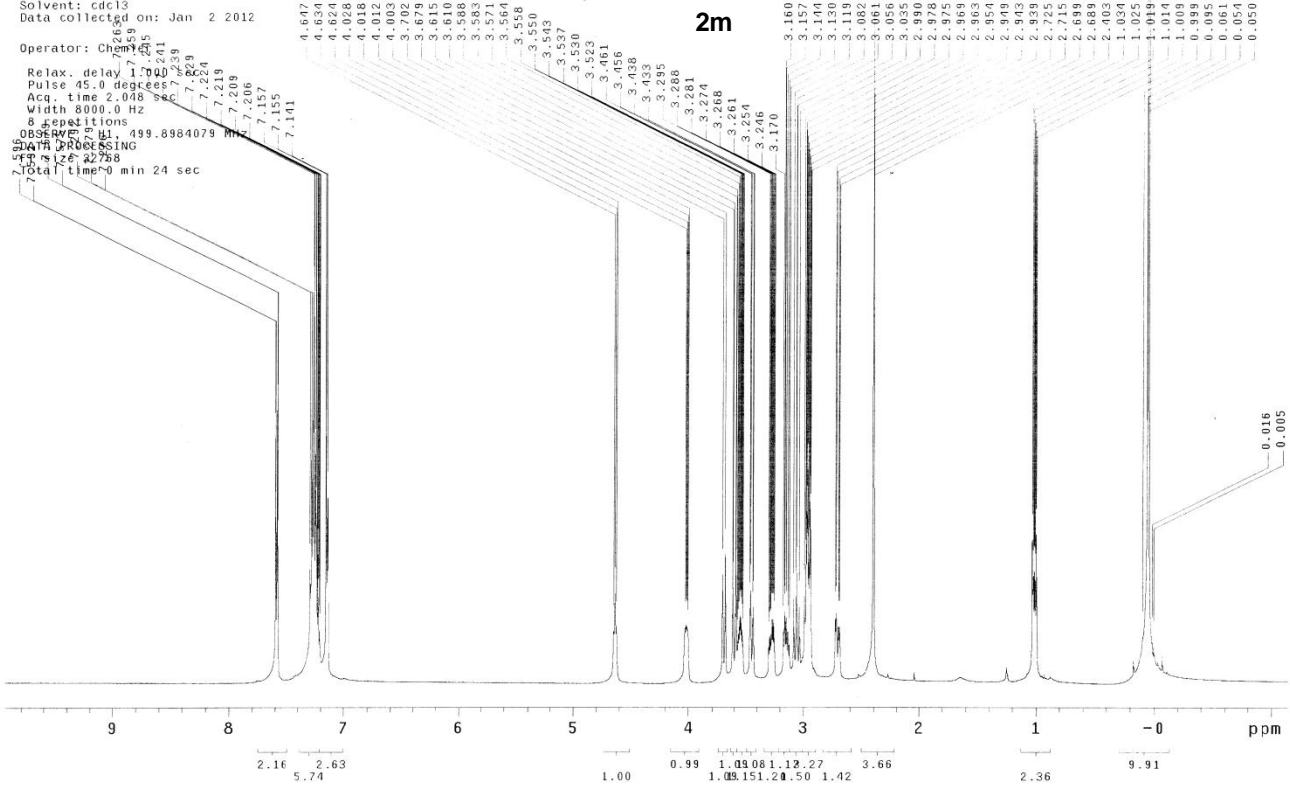
Data collected on: Jan 2 2012

Operator: Chemler

Relax. delay 1.700 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE F1: 499.8984079 MHz
DATA PROCESSING
FT size 22758
Total time 0 min 24 sec



2m



fs-IV-222-carbon

Sample Name:

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

Sample directory:

Fidfile: fs-IV-222-carbon

Pulse Sequence: CARBON (s2pul)

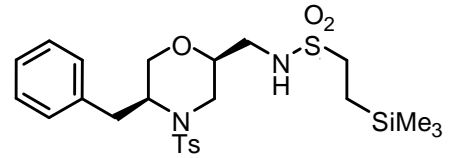
Solvent: cdcl3

Data collected on: Aug 1 2011

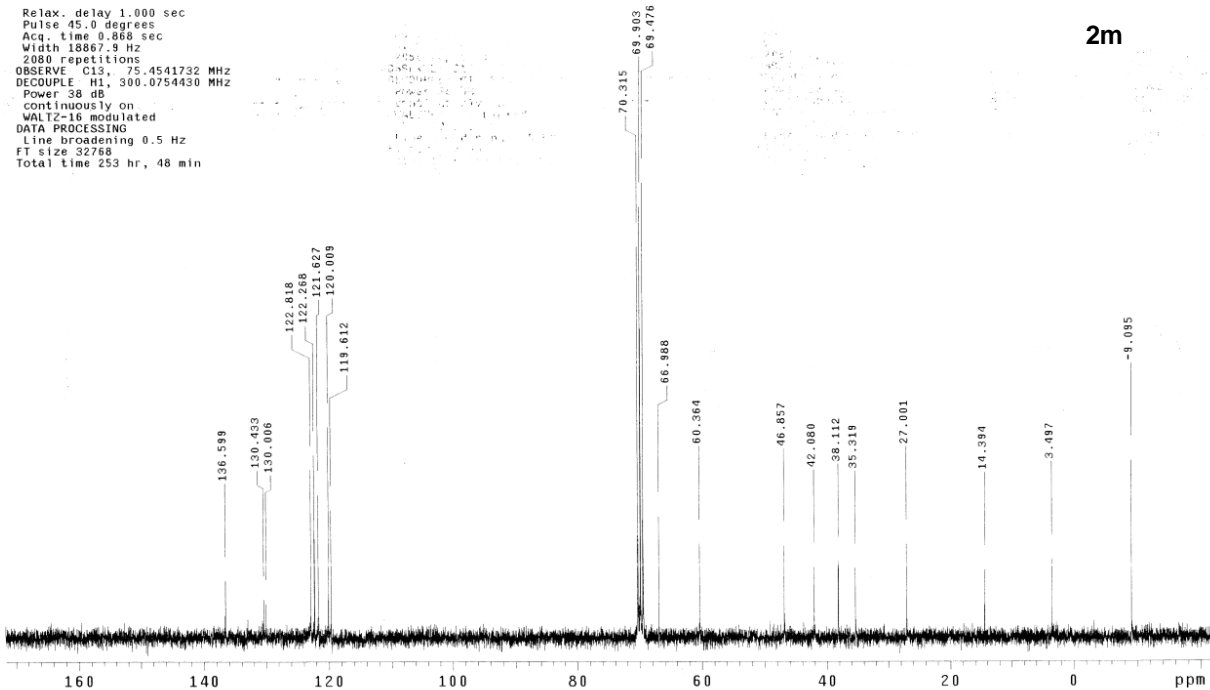
Temp. 22.0 C / 295.1 K

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2080 repetitions
OBSERVE C13, 75.4541732 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 253 hr, 48 min



2m



fs-V-Bzcapmajor-prton

Sample Name:
DC34crude
Data collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:

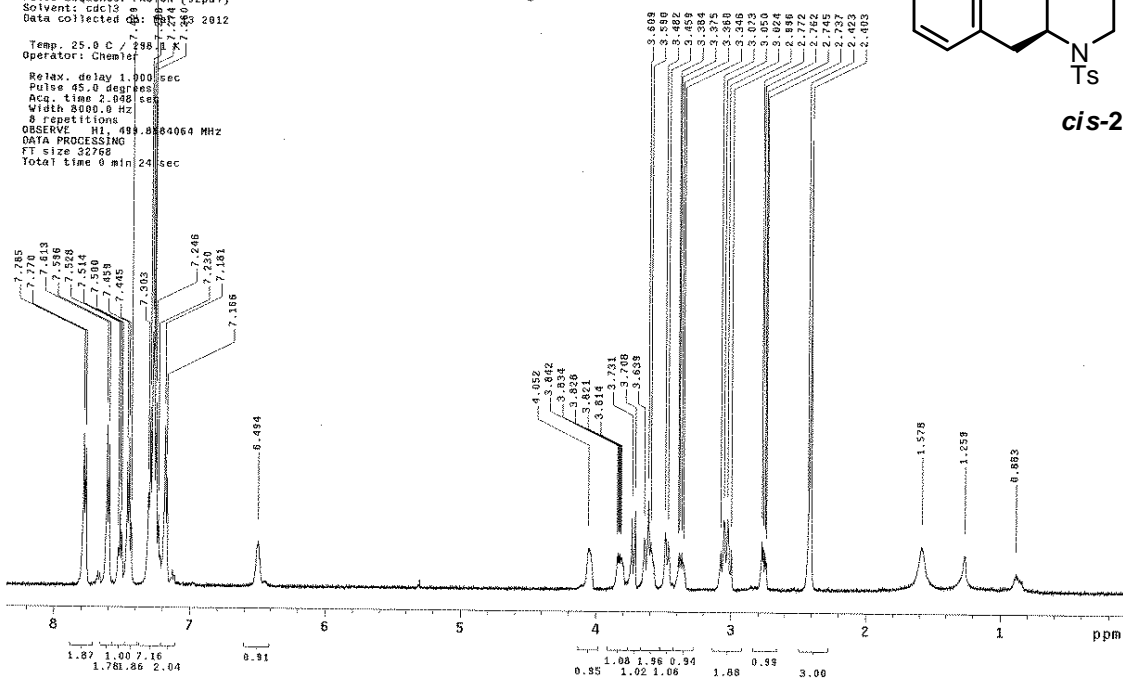
FidFile: PROTDN

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 18 2012

Temp: 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.008 sec
Width 3000.0 Hz
8 repetitions
OBSERVE H1, 499.8364064 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 24 sec



fs-IV-152-carbon

Sample Name:
Data collected on:
rossy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

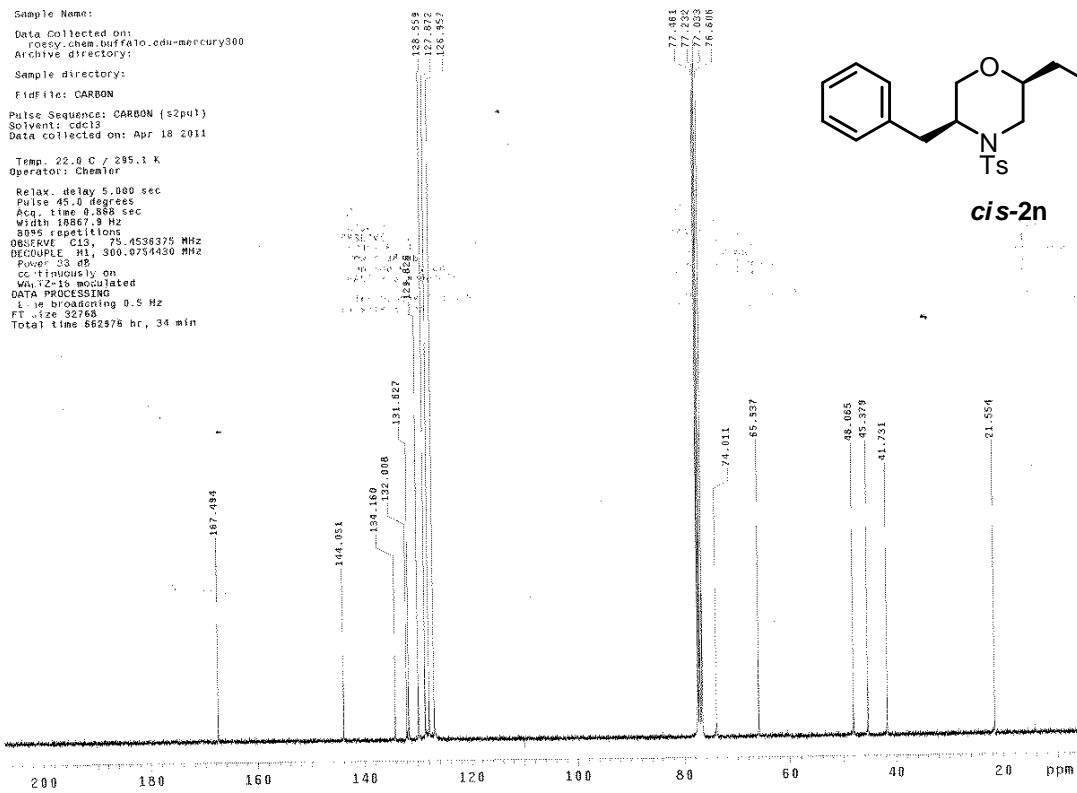
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 18 2011

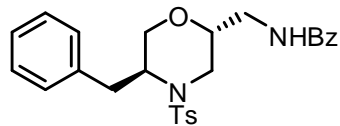
Temp: 22.0 C / 295.1 K

Operator: Chemler

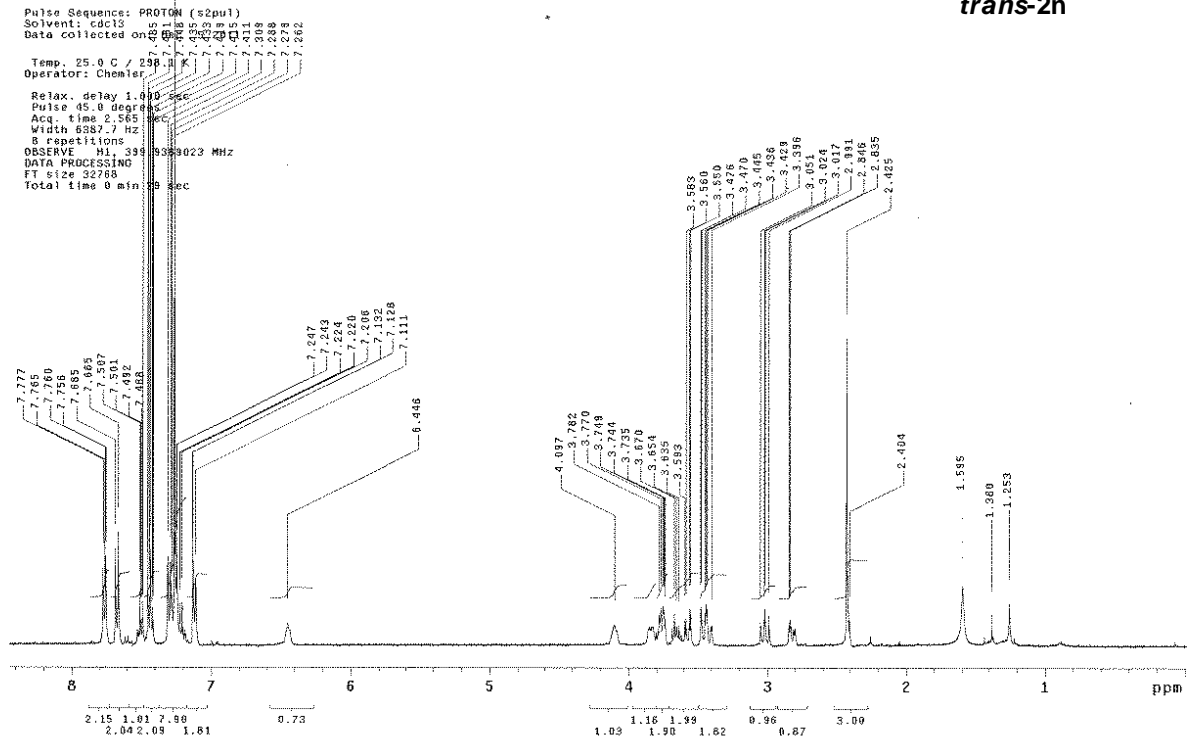
Relax. delay 5.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.3 Hz
3095 repetitions
OBSERVE C13, 75.4536375 MHz
REQUIRE H1, 300.0254450 MHz
Power 33 dB
cc: 1100000
Waltz-16 modulated
DATA PROCESSING
1.0 Hz broadening 0.5 Hz
FT size 32768
Total time 562578 hr, 34 min



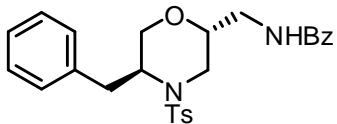
fs-IV-142-min
 Sample Name:
 Data Collected on:
 chemmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: 7/26/11
 Temp. 25.0 C / 298.1 K
 Operator: Chemist
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.565 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE M1, 398.9023 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 39 sec



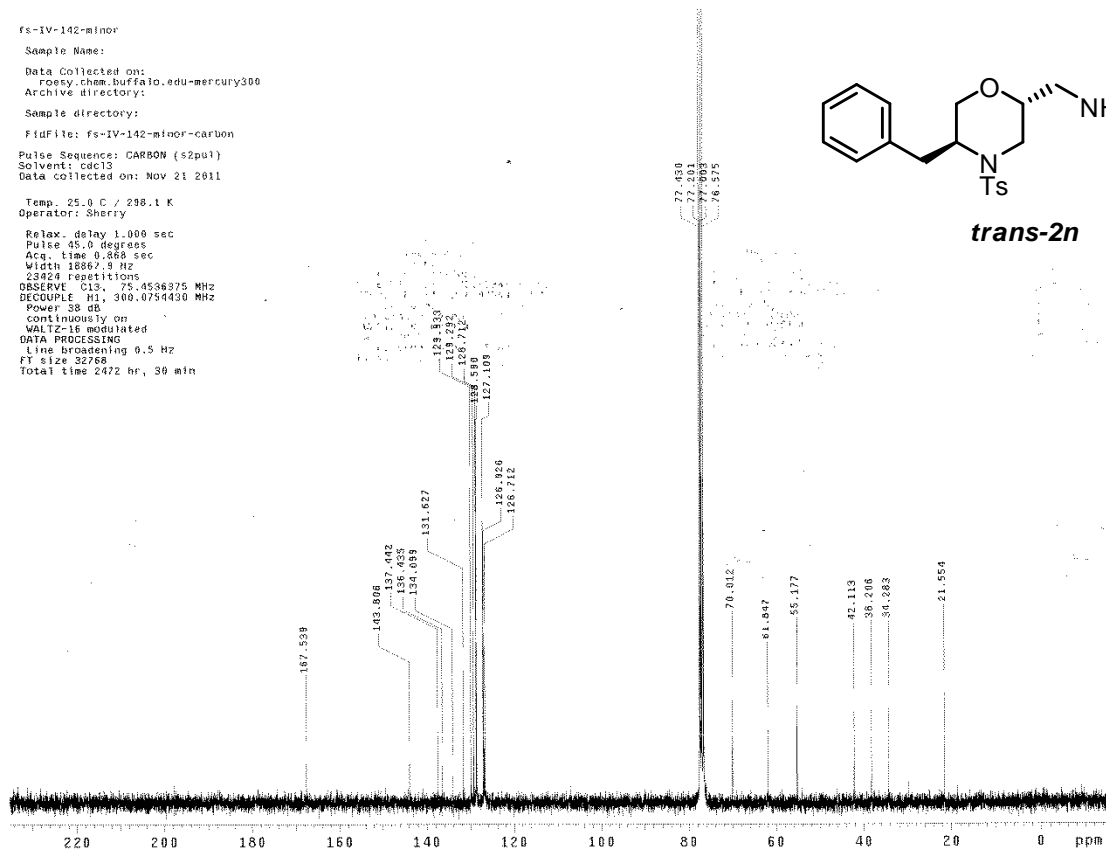
trans-2n



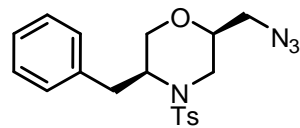
fs-IV-142-minor
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: fs-IV-142-minor-carbon
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Nov 21 2011
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.888 sec
 Width 16867.9 Hz
 23024 repetitions
 OBSERVE C13, 75.4536375 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 2472 hr, 39 min



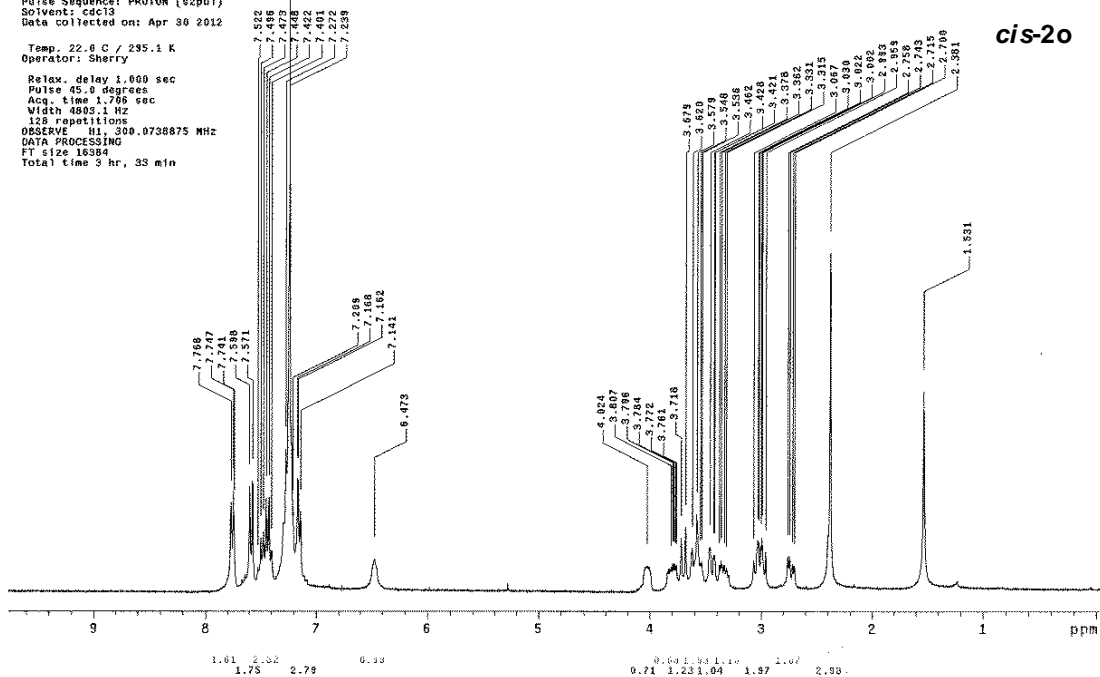
trans-2n



fs-cis-II-27dNMR
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Apr 30 2012
 Temp: 22.6 C / 295.1 K
 Operator: Sherry
 Relax. delay 1.600 sec
 Pulse 45.0 degrees
 Acq. time 1.706 sec
 Width 4803.1 Hz
 128 repetitions
 OBSERVE H1, 300.0738875 MHz
 DATA PROCESSING
 FT size 16384
 Total time 3 hr, 33 min

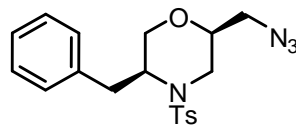


cis-20



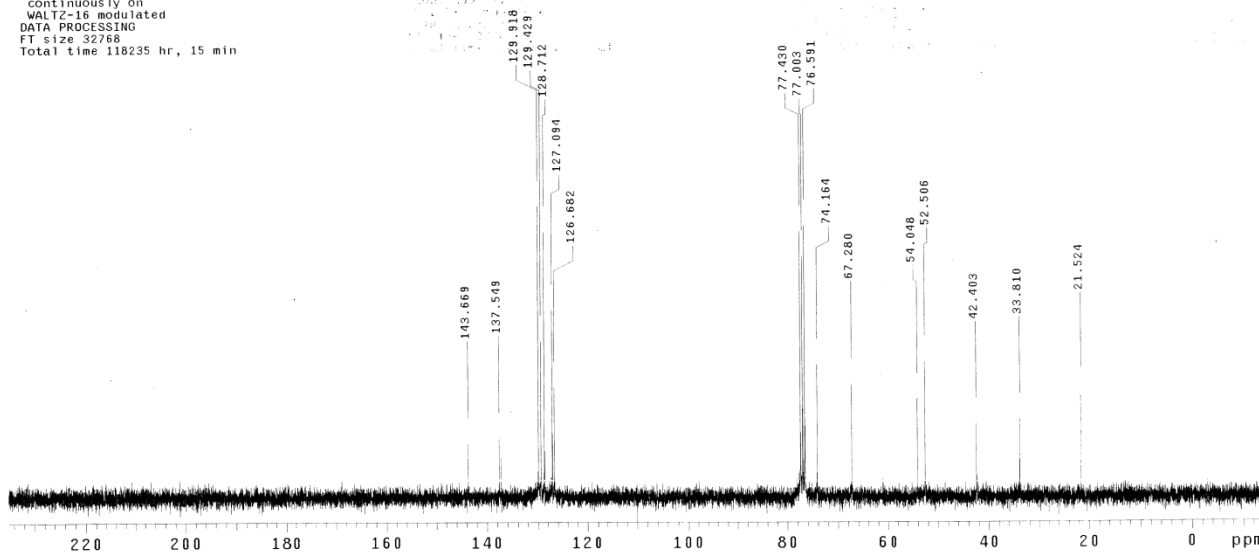
STANDARD PROTON PARAMETERS

Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: fs-V-78-carbon
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jan 19 2012



cis-20

Temp: 22.0 C / 295.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 4464 repetitions
 OBSERVE C13, 75.4536375 MHz
 DECOUPLE H1, 300.0754430 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 FT size 32768
 Total time 118235 hr, 15 min



fs-V-N3-minor

Sample Name:

Date Collected on:
chemmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3

Data collected on: Feb 21 2012

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.585 sec

Width 6387.7 Hz

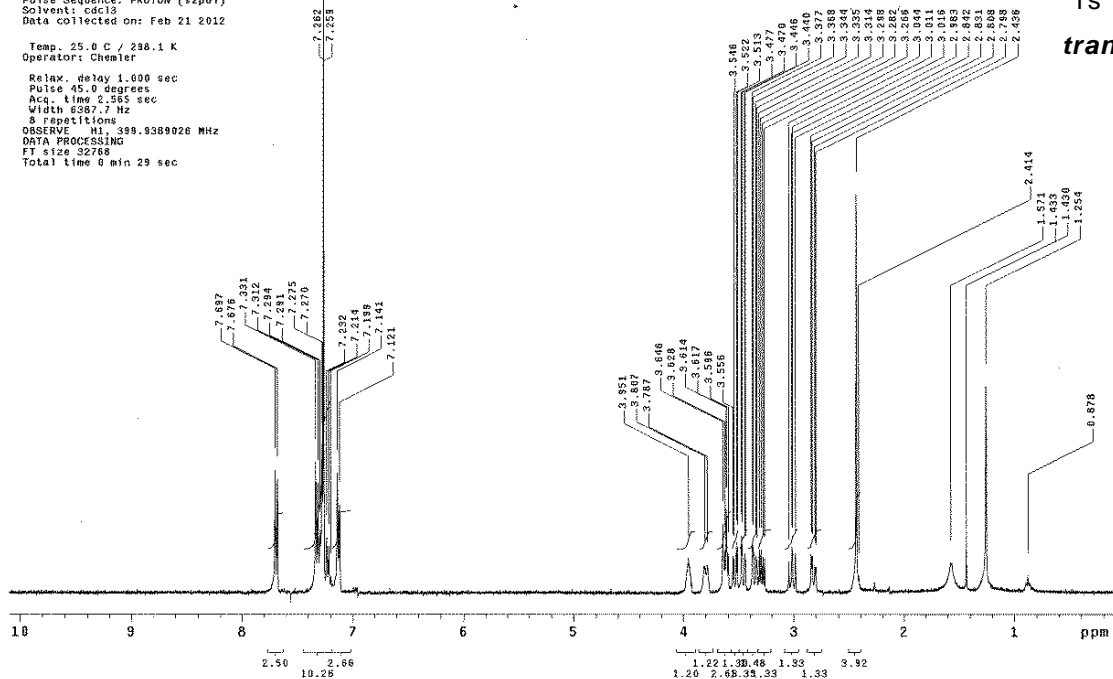
8 Repetitions

OBSERVE H1, 399.9389026 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 29 sec



fs-V-53-carbon-min

Sample Name:

Date Collected on:
roesy.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cdcl3

Data collected on: Jan 21 2012

Temp. 22.5 C / 295.6 K

Operator: Sherry

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18367.9 Hz

26496 repetitions

OBSERVE C13, 75.4536366 MHz

DECOUPLE H1, 300.0754430 MHz

Power 39 dB

continuously on

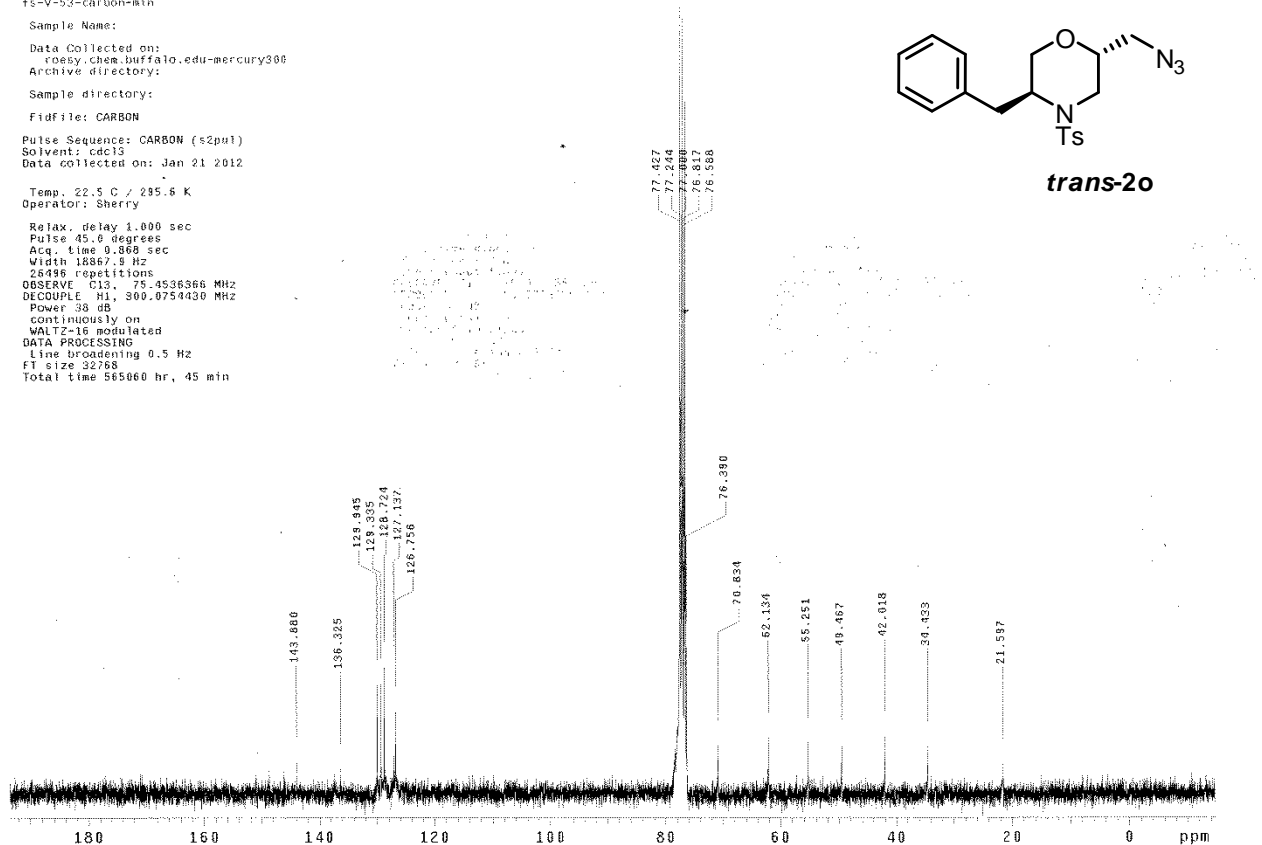
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 565660 hr, 45 min



fs-IV-241-proton

Sample Name:

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

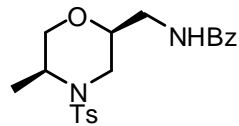
Sample directory:

FidFile: PROTON

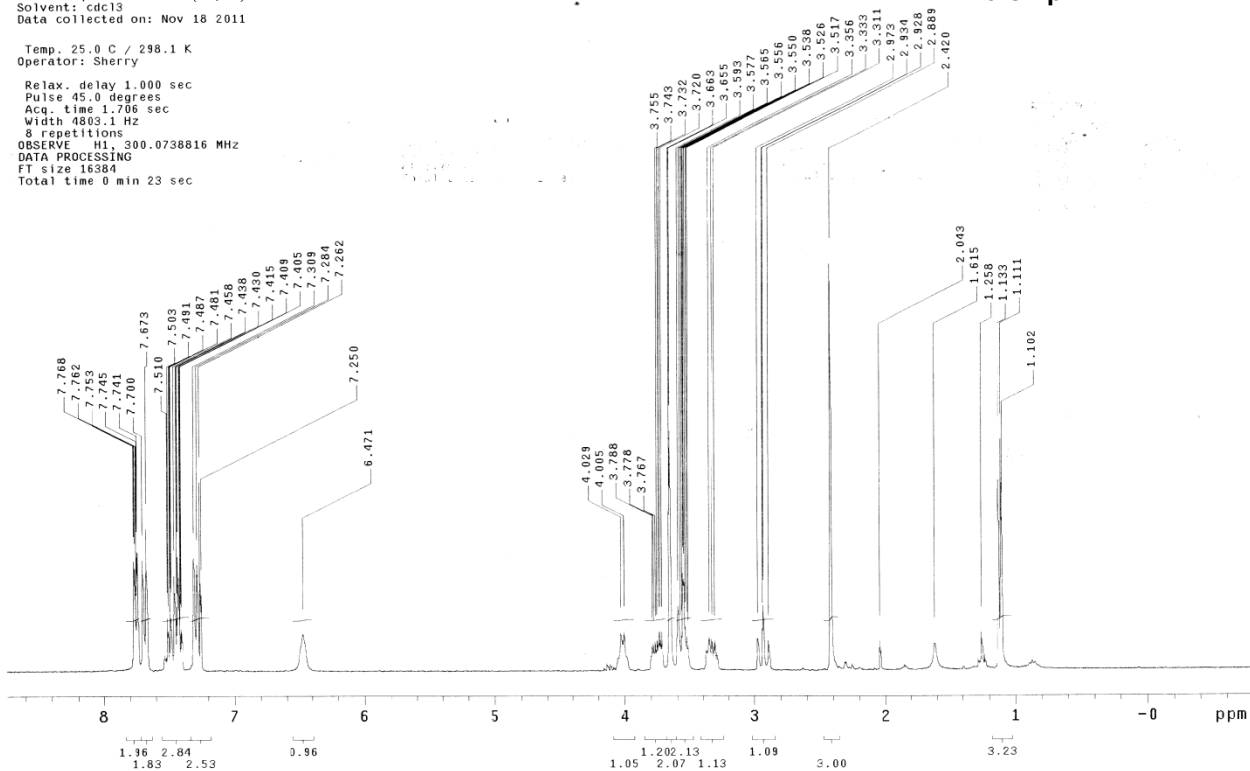
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Nov 18 2011

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.706 sec
Width 4803.1 Hz
8 repetitions
OBSERVE H1, 300.0738816 MHz
DATA PROCESSING
FT size 16384
Total time 0 min 23 sec



cis-2p



STANDARD CARBON PARAMETERS

Sample Name:

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

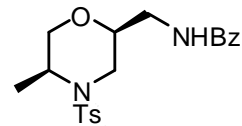
Sample directory:

FidFile: CARBON

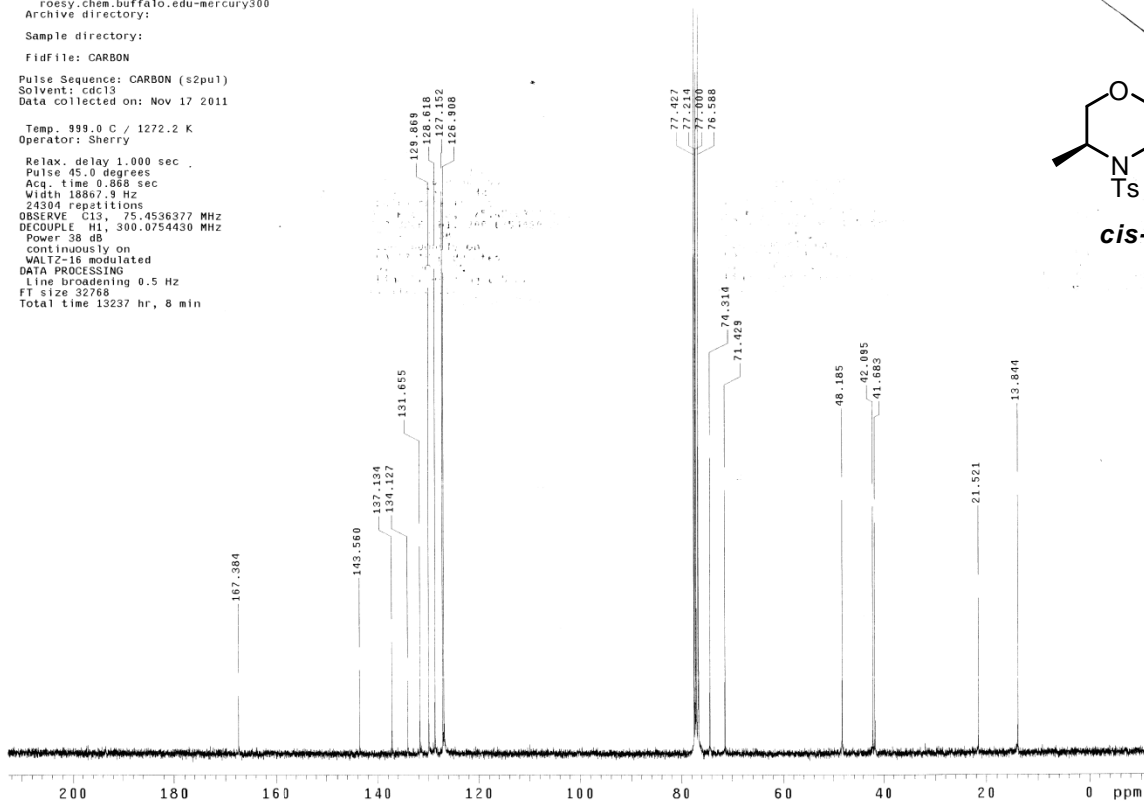
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Nov 17 2011

Temp. 99.0 C / 1272.2 K
Operator: Sherry

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
24304 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 13237 hr, 8 min

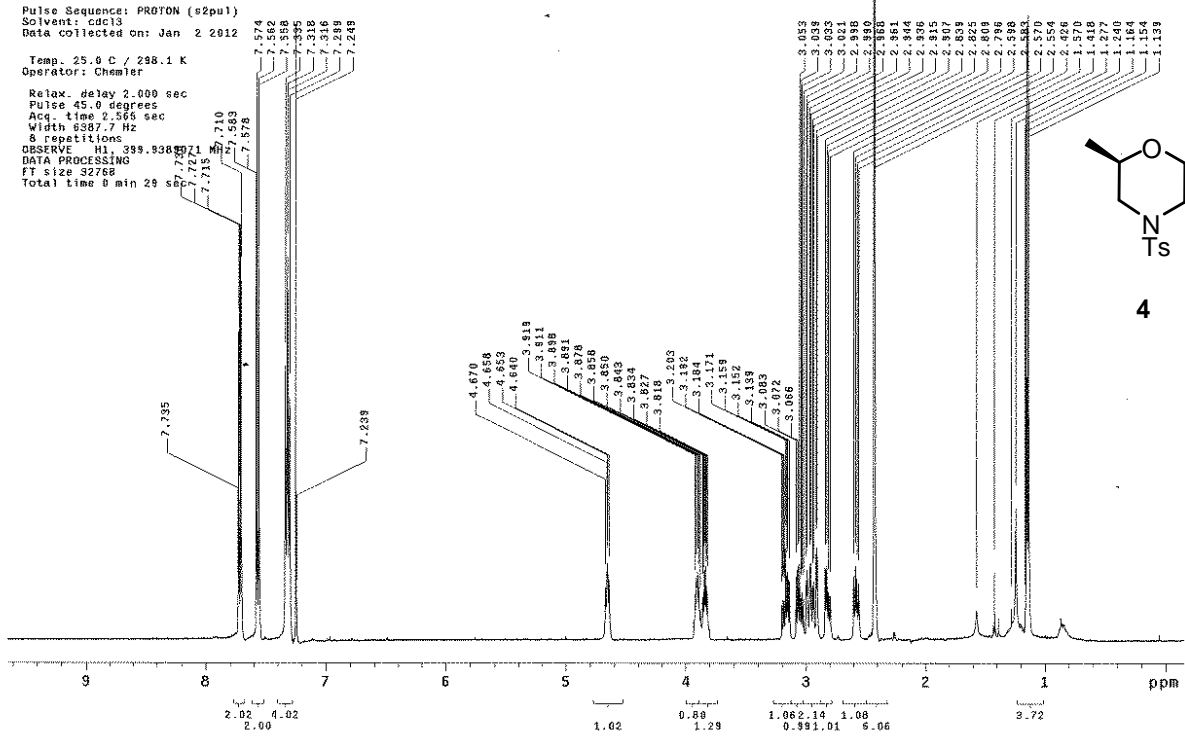


cis-2p

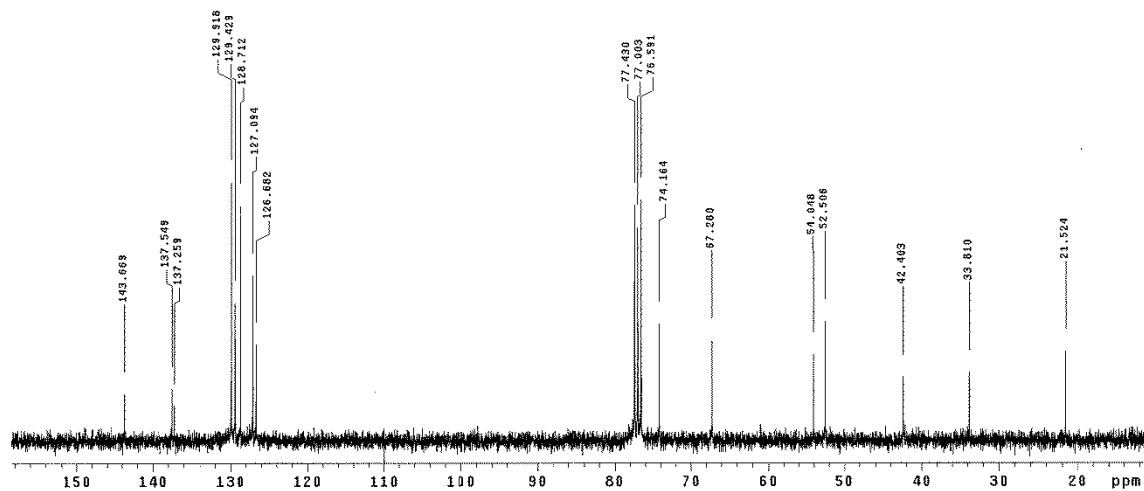


fs-V-56-proton
 Sample Name:
 Data Collected on:
 chemmer400.chem.buffalo.edu-inovq400
 Archive directory:
 Sample directory:
 FidFile: fs-v-56-proton

Pulse Sequence: PROTON (s2pul)
 Solvent: cdcl3
 Data collected on: Jan 2 2012
 Temp. 25.0 C / 298.1 K
 Operator: Chemler
 Relax. delay 2.000 sec
 Pulse 45.0 degrees
 Acq. time 2.556 sec
 Width 6987.7 Hz
 8 repetitions
 OBSERVE H1, 399.9308971
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec

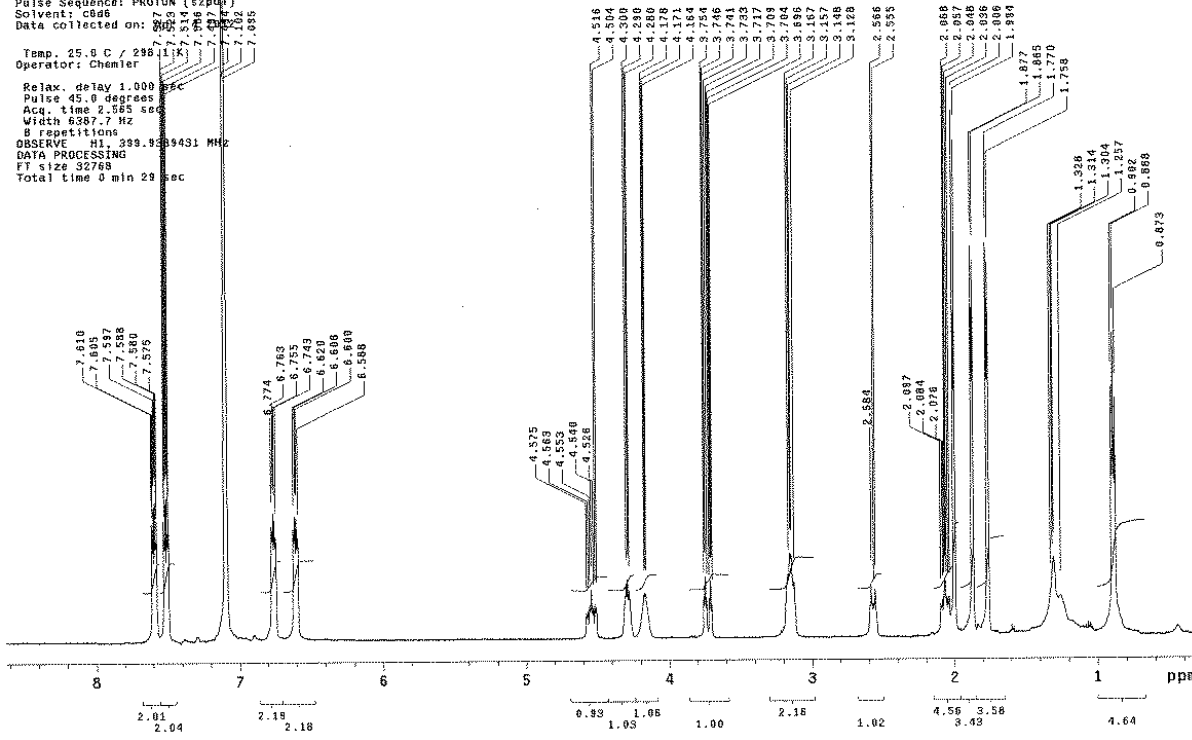
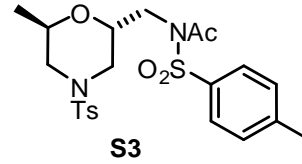


STANDARD PROTON PARAMETERS
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: fs-v-78-carbon
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jan 19 2012
 Temp. 22.0 C / 295.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.866 sec
 Width 18867.8 Hz
 4464 repetitions
 OBSERVE C13, 75.4536375 MHz
 DECOUPLE H1, 306.0754438 MHz
 Power 30 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 FT size 32768
 Total time 118235 hr, 15 min



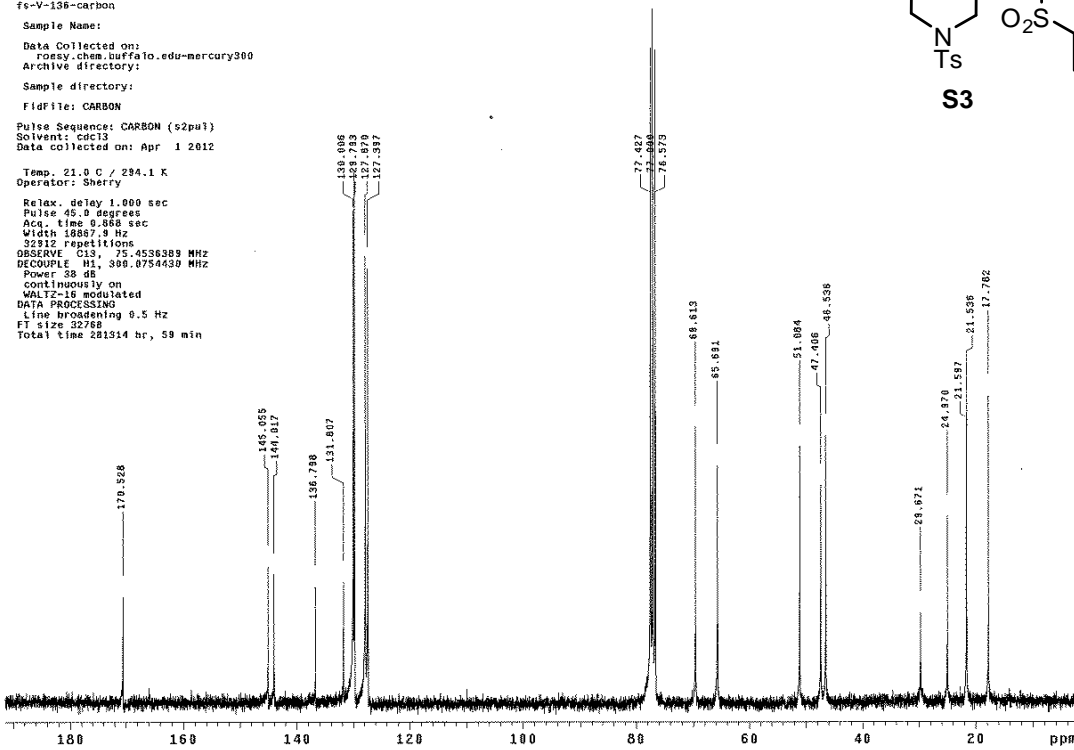
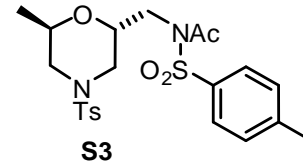
STANDARD PROTON PARAMETERS

Sample Name:
 Data Collected on:
 chemnmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: c8s6
 Data collected on: 2012
 Temp. 25.0 C / 296.15 K
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.565 sec
 Width 6387.7 Hz
 8 repetitions
 OBSERVE H1 399.939431 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 29 sec



13C-V-136-carbon

Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: CARBON
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Apr 1 2012
 Temp. 21.0 C / 294.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.368 sec
 Width 18667.9 Hz
 32912 Repetitions
 OBSERVE C13 TS 4536309 MHz
 DECOUPLE H1 399.0754430 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 281914 hr, 59 min



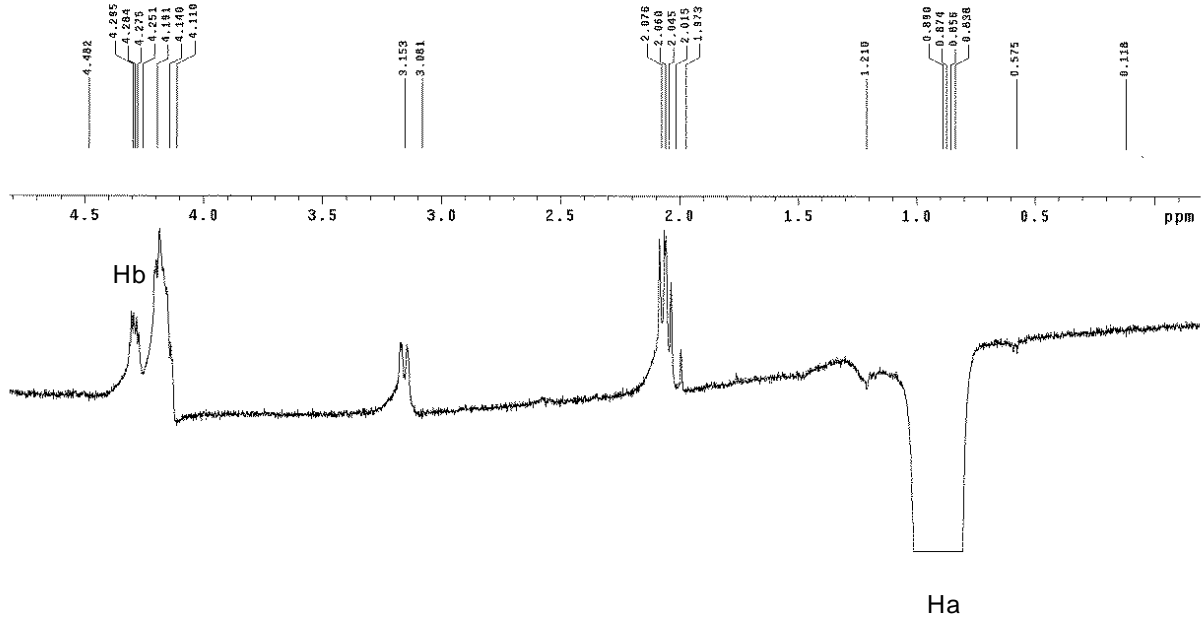
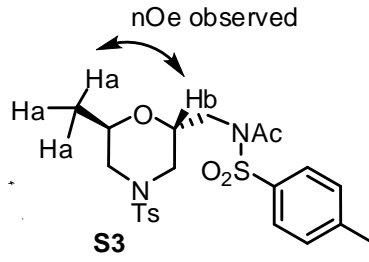
STANDARD PROTON PARAMETERS
 Selective band center: 0.80 (ppm); width: 50.0 (Hz)

Sample Name:
 Data Collected on:
 Chemnmr400.chem.buffalo.edu-inova400
 Archive directory:
 Sample directory:
 Fidfile: NOESY1D

Pulse Sequence: NOESY1D
 Solvent: CDCl3
 Data collected on: Apr 3 2012

Temp. 25.0 C / 298.1 K
 Operator: Chemler

Relax. delay 1.000 sec
 Pulse 90.0 degrees
 Acq. time 2.047 sec
 Width 2000.8 Hz
 3600 repetitions
 OBSERVE H1, 399.9388431 MHz
 DATA PROCESSING
 FT size 8192
 Total time 3 hr, 44 min



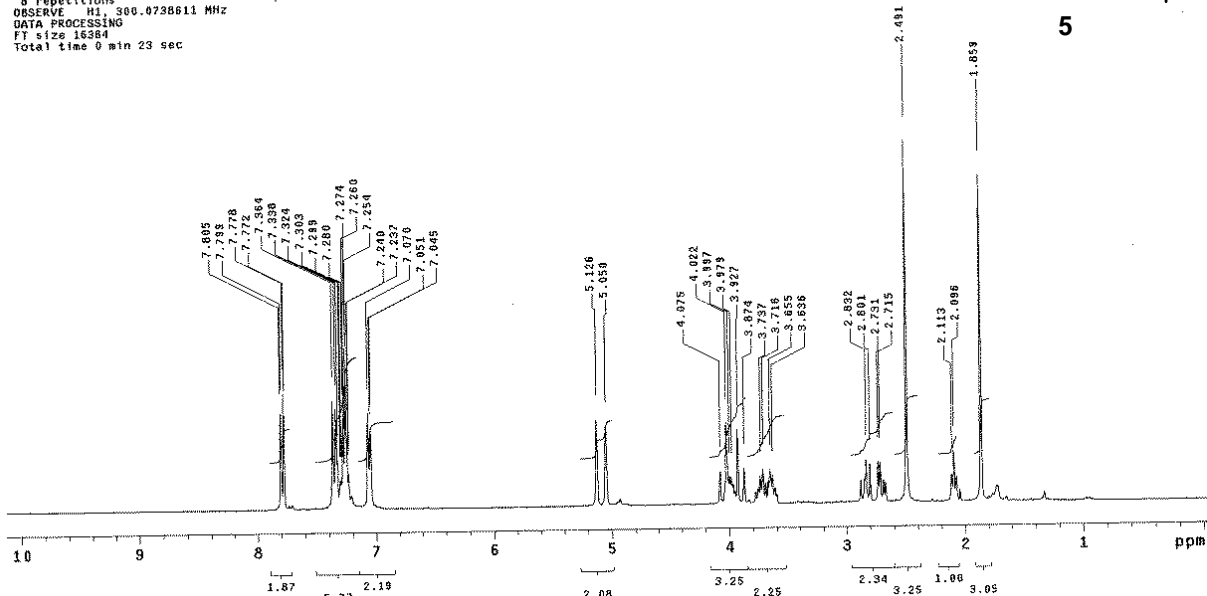
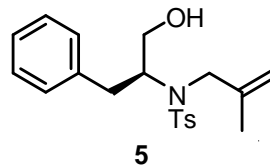
fs-V-168-proton

Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: PROTON

Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jun 8 2012

Temp. 25.0 C / 298.1 K
 Operator: Sherry

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.785 sec
 Width 4803.1 Hz
 8 repetitions
 OBSERVE H1 300.0738611 MHz
 DATA PROCESSING
 FT size 16384
 Total time 0 min 23 sec



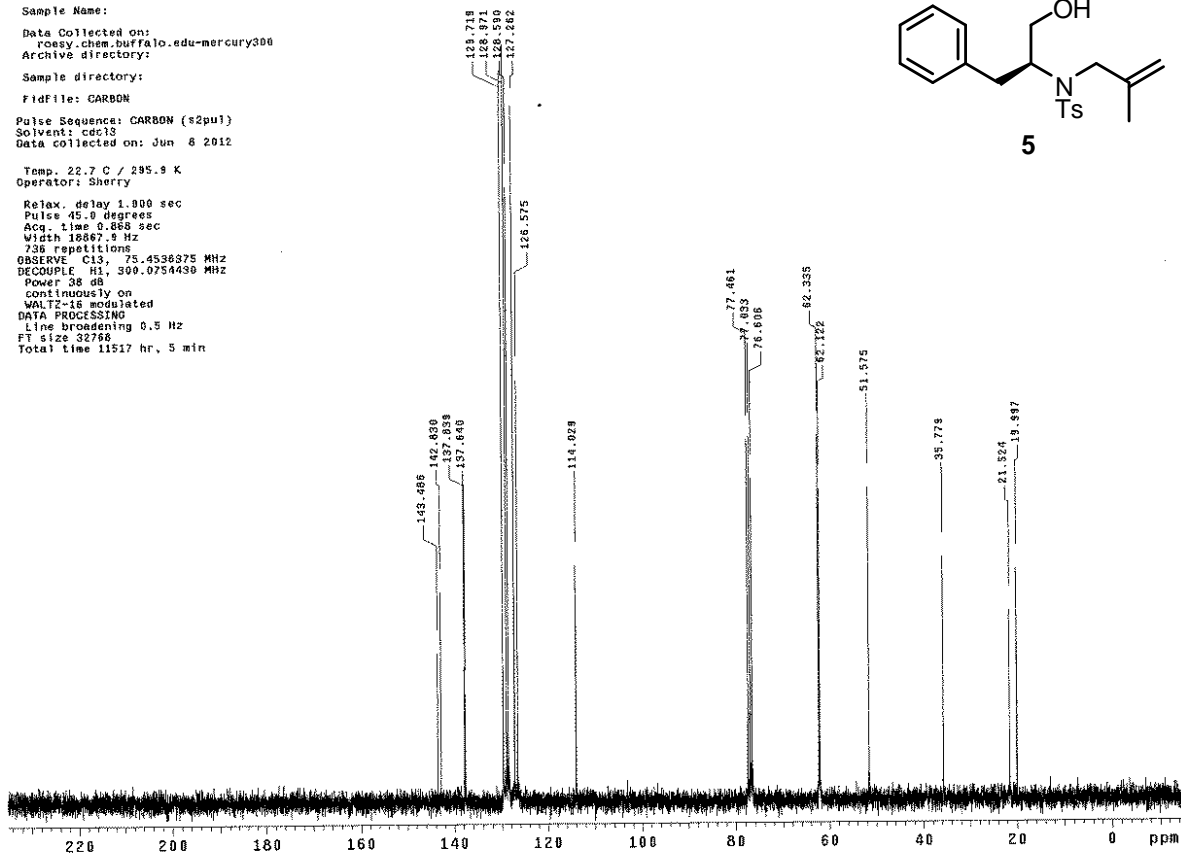
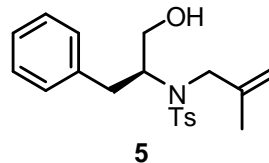
fs-V-168-carbon

Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jun 8 2012

Temp. 22.7 C / 295.9 K
 Operator: Sherry

Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 736 repetitions
 OBSERVE C13 75.4536375 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 11517 hr, 5 min

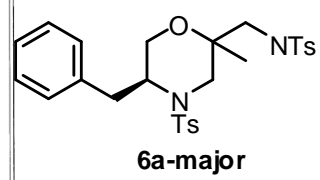
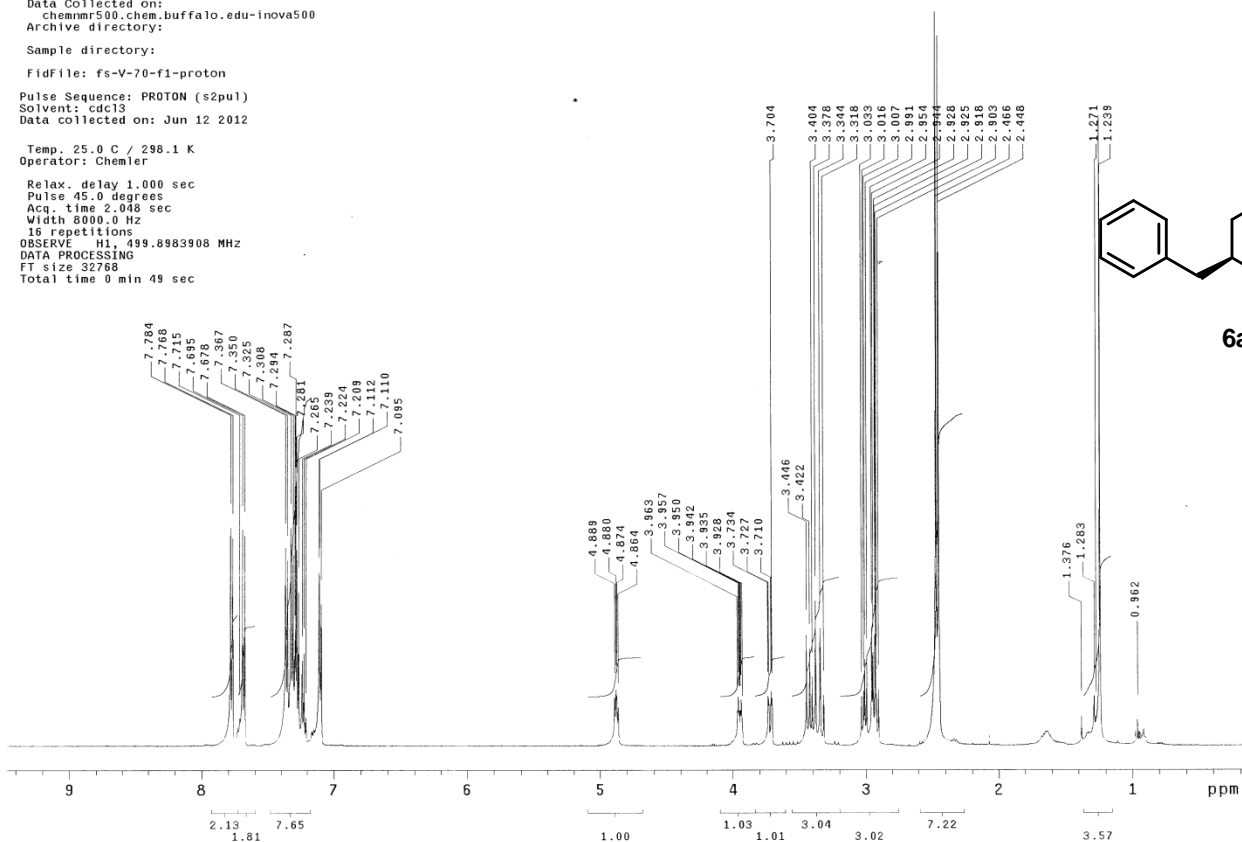


fs-V-70-f1-proton

Sample Name:
DC-99pure
Data Collected on:
chemm500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
Fidfile: fs-V-70-f1-proton
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 12 2012

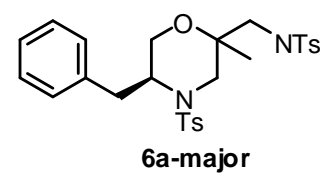
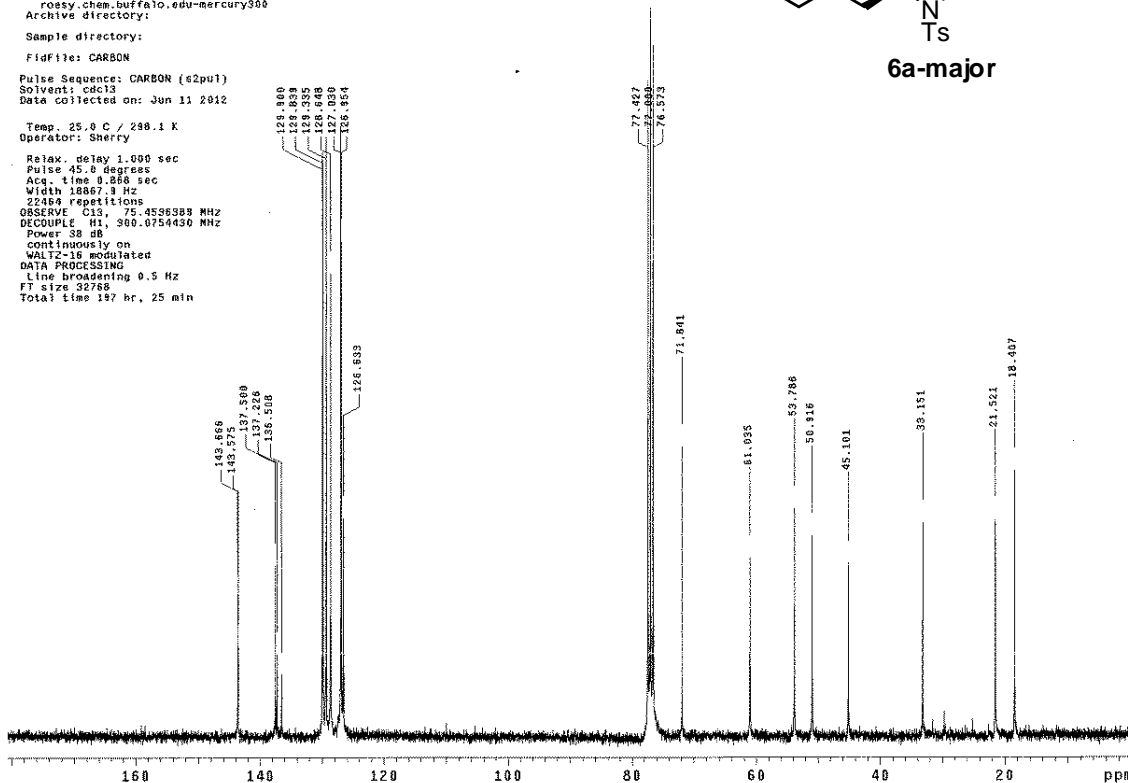
Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
16 repetitions
OBSERVE H1, 499.8983908 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 49 sec

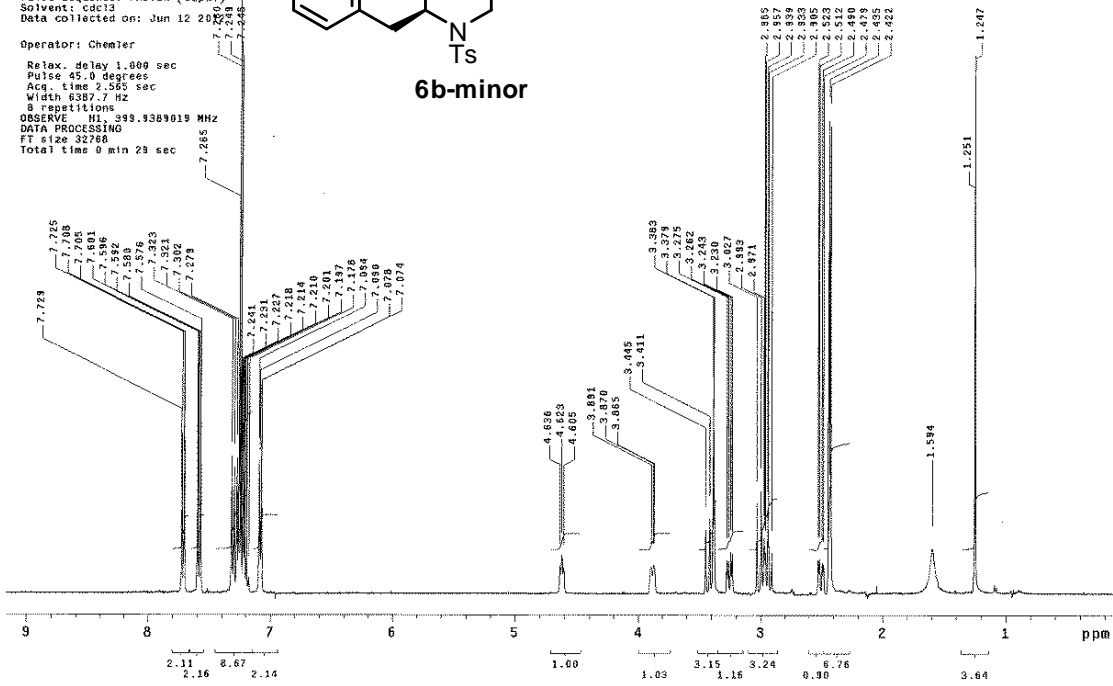
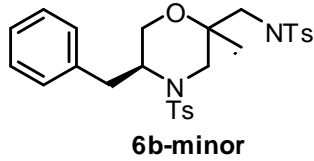


STANDARD CARBON PARAMETERS

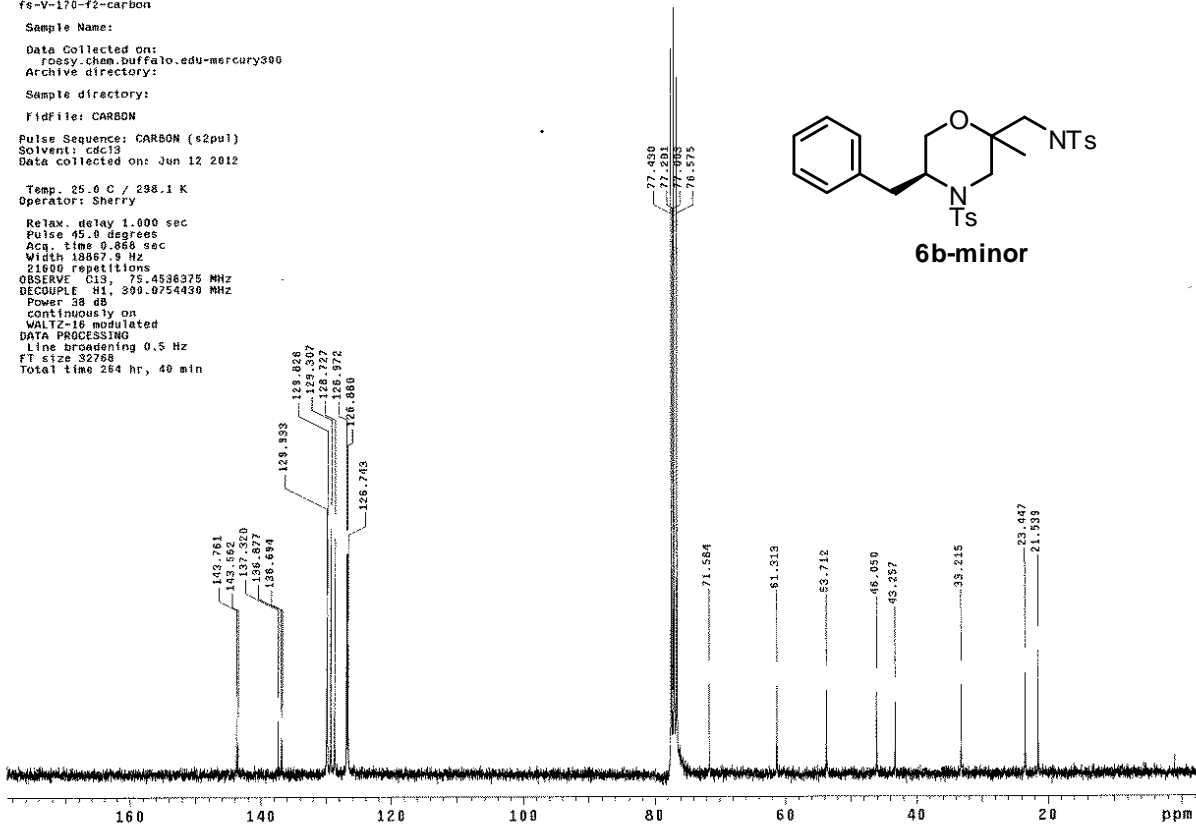
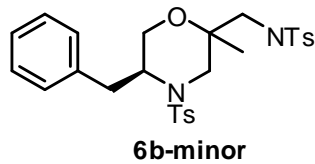
Sample Name:
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:
Sample directory:
Fidfile: CARBON
Pulse Sequence: CARBON (e2pu1)
Solvent: cdcl3
Data collected on: Jun 11 2012
Temp. 25.0 C / 298.1 K
Operator: Sherry
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.008 sec
Width 18867.0 Hz
22464 repetitions
OBSERVE C13, 75.4536388 MHz
DECUPLE H1, 300.6754430 MHz
Power 38 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 197 hr, 25 min



fs-V-70-2proton
 Sample Name:
 Data Collected on:
 chemnar400.chem.buffalo.edu-1mova400
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdc13
 Data collected on: Jun 12 2012
 Operator: Chemler
 Relax. delay 1.800 sec
 Pulse 45.0 degrees
 Acq. time 7.585 sec
 Width 8387.7 Hz
 8 repetitions
 OBSERVE H1 399.9389019 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 23 sec



fs-V-170-f2-carbon
 Sample Name:
 Data Collected on:
 rossy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: CARBON
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdc13
 Data collected on: Jun 12 2012
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18067.5 Hz
 21600 repetitions
 OBSERVE C13 75.4536375 MHz
 DECOUPLE H1 399.0754430 MHz
 Power 38 dB
 CONTINUOUS on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 264 hr, 40 min



fs-ligand-cap-OH-carbon

Sample Name:

Data Collected on:

roesy.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 8 2012

Temp. 25.0 C / 298.1 K

Operator: Sherry

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.705 sec

Width 4893.1 Hz

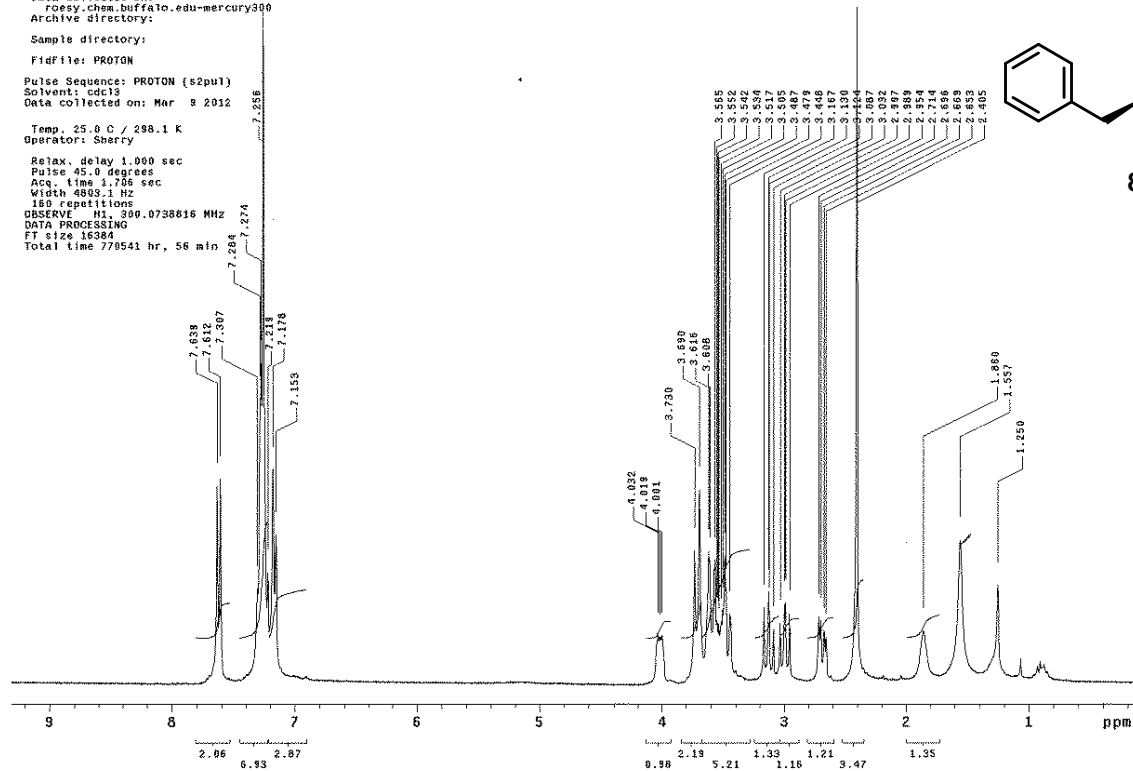
150 repetitions

OBSERVE H1, 300.0738816 MHz

DATA PROCESSING

FT size 18384

Total time 770541 hr, 56 min



fs-ligand-cap-OH-proton

Sample Name:

Data Collected on:

roesy.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Mar 8 2012

Temp. 25.0 C / 298.1 K

Operator: Sherry

Relax. delay 5.000 sec

Pulse 45.0 degrees

Acq. time 0.865 sec

Width 18867.9 Hz

726 repetitions

OBSERVE C13, 75.4536375 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

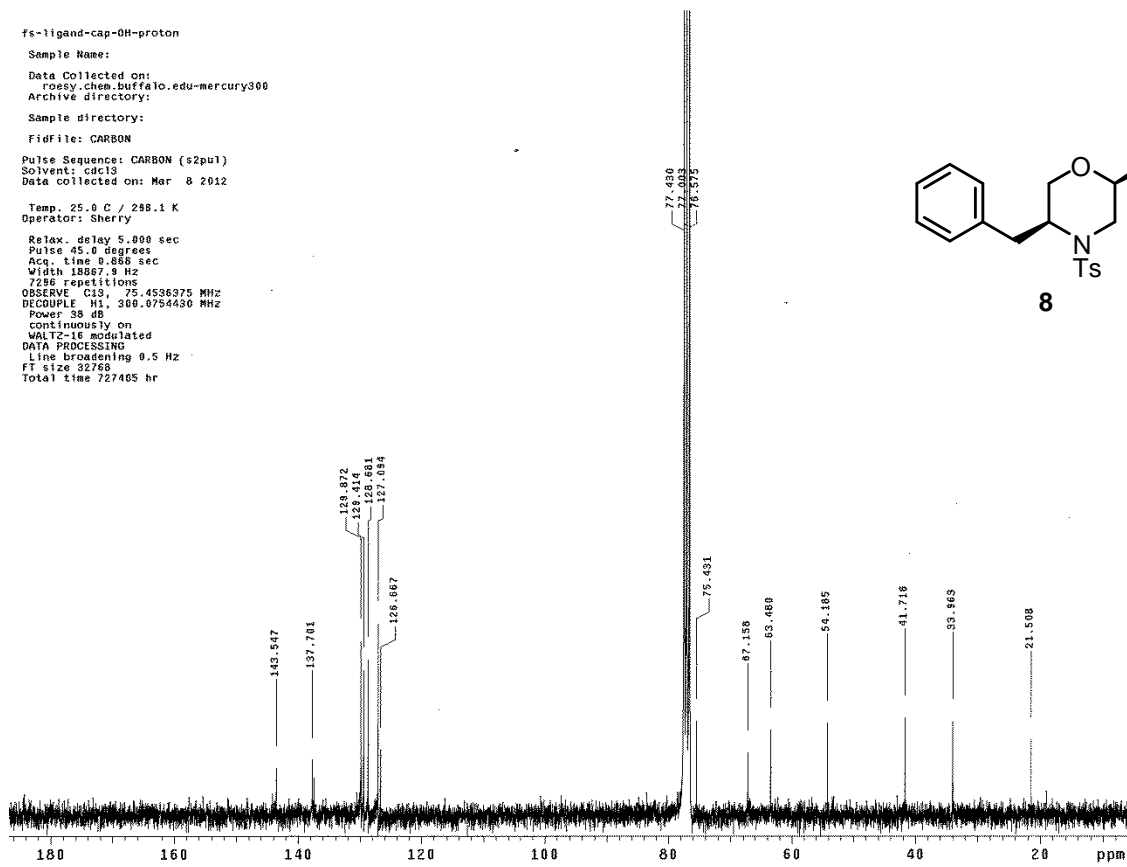
WALTZ-16 modulated

DATA PROCESSING

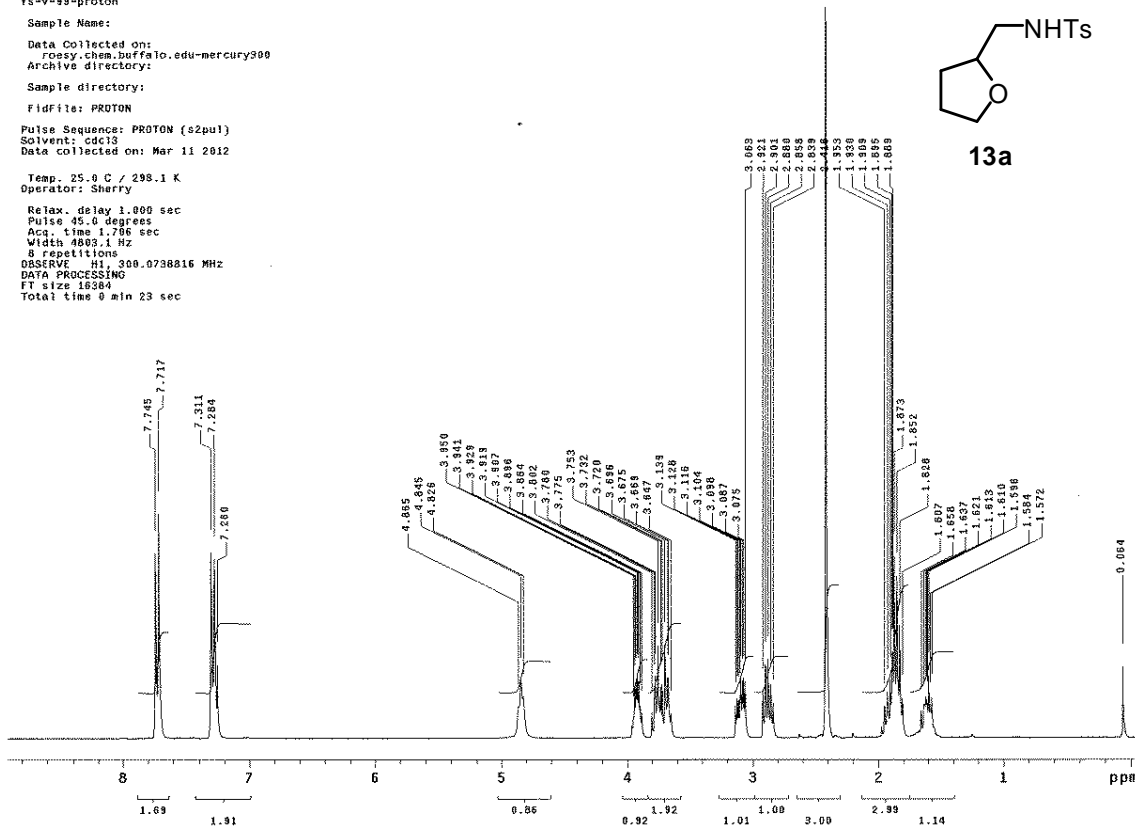
Line broadening 0.5 Hz

FT size 32768

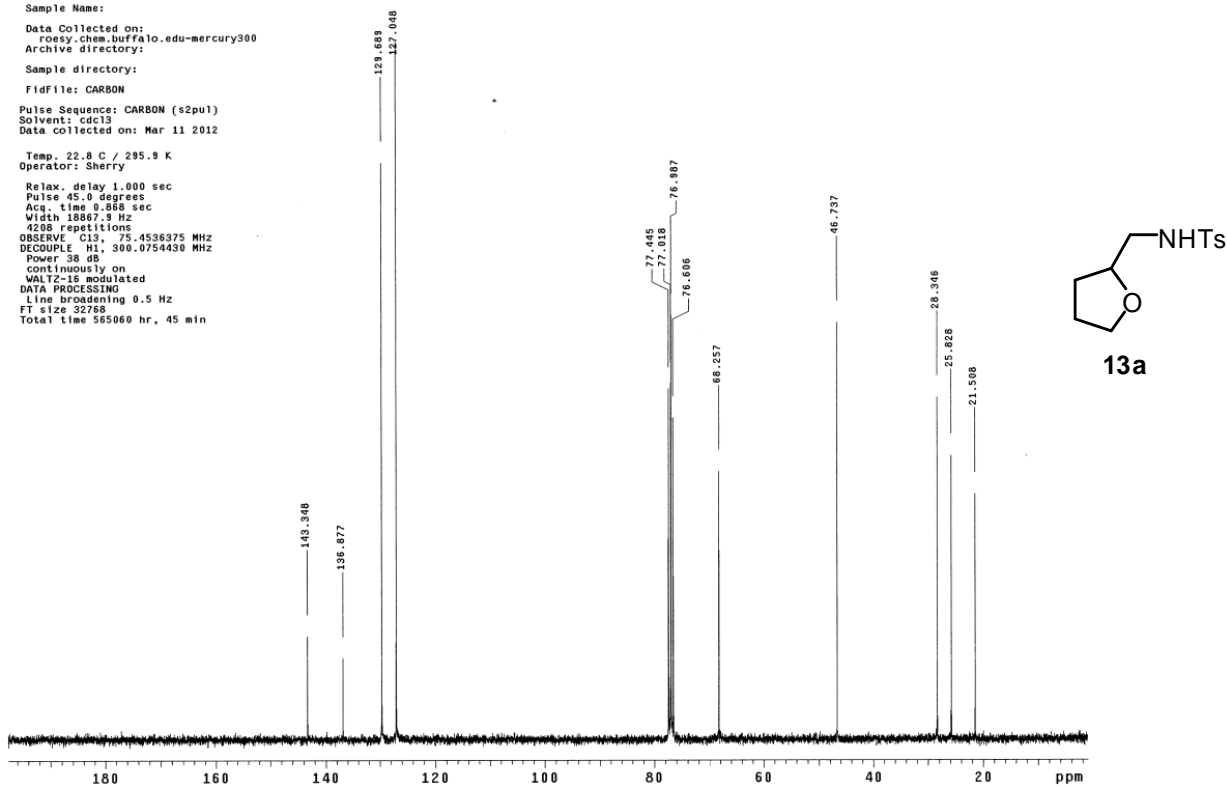
Total time 727405 hr

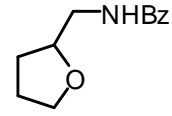


fs-V-99-proton
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Mar 11 2012
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.796 sec
 Width 4603.1 Hz
 8 repetitions
 OBSERVE H1, 300.0738816 MHz
 DATA PROCESSING
 FT size 16384
 Total time 0 min 23 sec



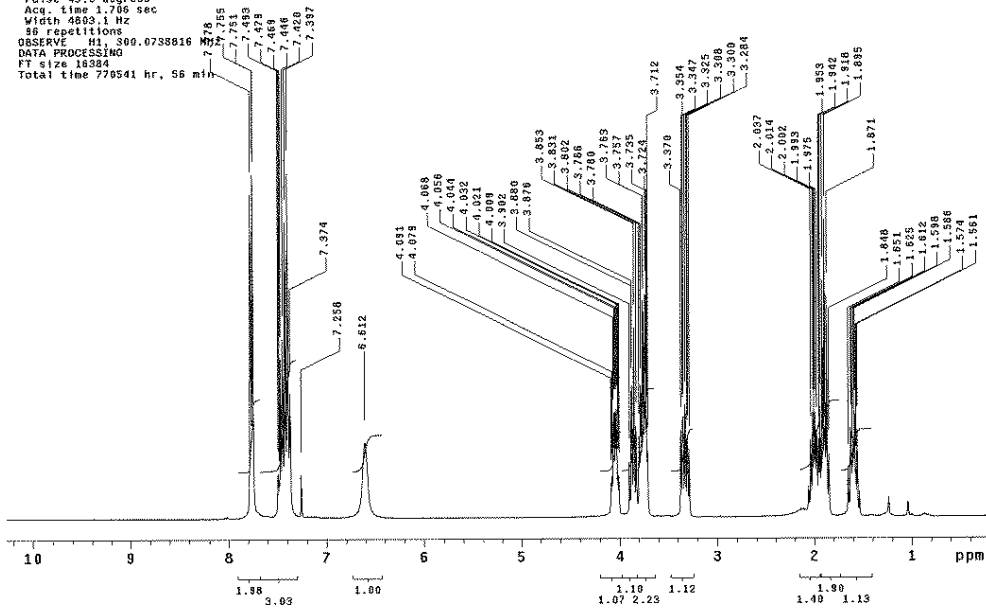
fs-V-99-carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: CARBON
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Mar 11 2012
 Temp. 22.8 C / 295.9 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18697.3 Hz
 4208 repetitions
 OBSERVE C13, 75.4536375 MHz
 DECOUPLE H1, 300.0754450 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 565060 hr, 45 min



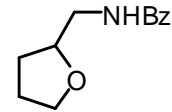


13b

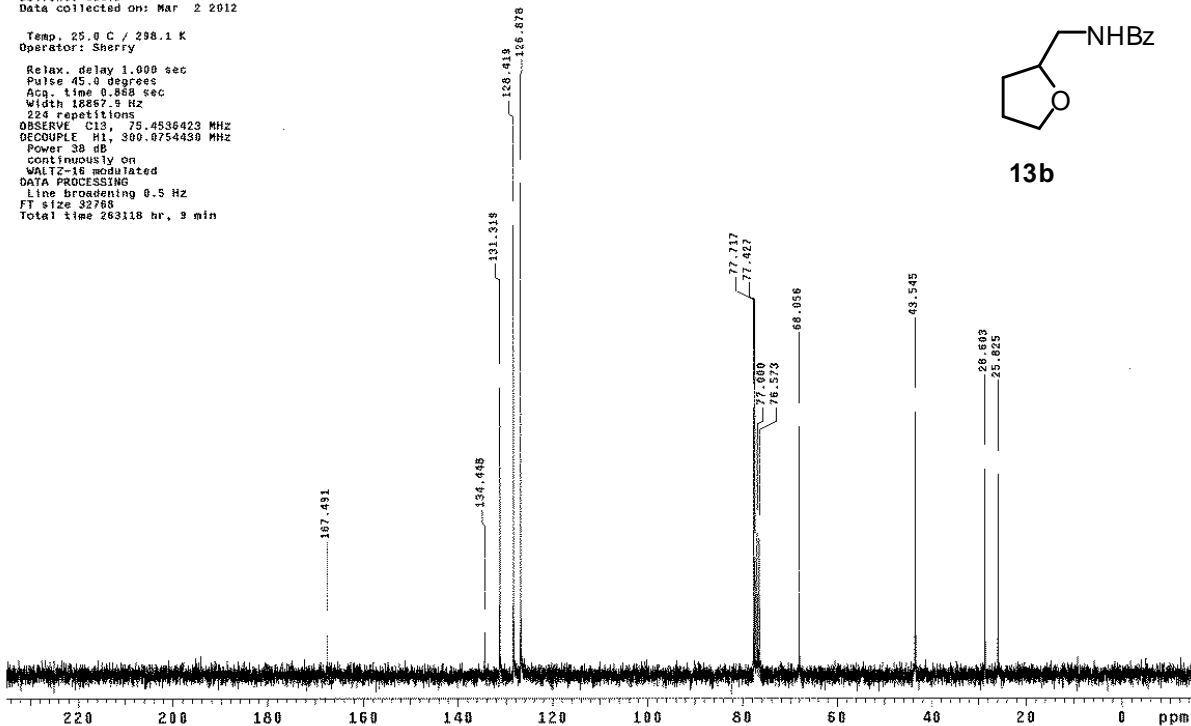
fs-V-110-proton
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Mar 2 2012
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.706 sec
 Width 6603.1 Hz
 56 repetitions
 OBSERVE H1, 300.0738816 MHz
 DATA PROCESSING
 FT size 18384
 Total time 770541 hr, 56 min



fs-V-110-carbon
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 Fidfile: fs-V-110-carbon
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Mar 2 2012
 Temp. 25.0 C / 298.1 K
 Operator: Sherry
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.888 sec
 Width 18867.9 Hz
 224 repetitions
 OBSERVE C13, 75.4536423 MHz
 DECOUPLE H1, 300.0754430 MHz
 Power 30 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 263118 hr, 9 min



13b



fs-V-136-proton

Sample Name:

Data Collected on:
chemmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pu1)

Solvent: cdd6

Data collected on: Apr 5 2012

Temp. 25.0 C / 298.1 K

Operator: Chemlar

Relax. delay 2.000 sec

Pulse 45.0 degrees

Acq. time 2.555 sec

Width 6387.7 Hz

8 repetitions

OBSERVE H1, 399.9389328 MHz

DATA PROCESSING

FT size 32768

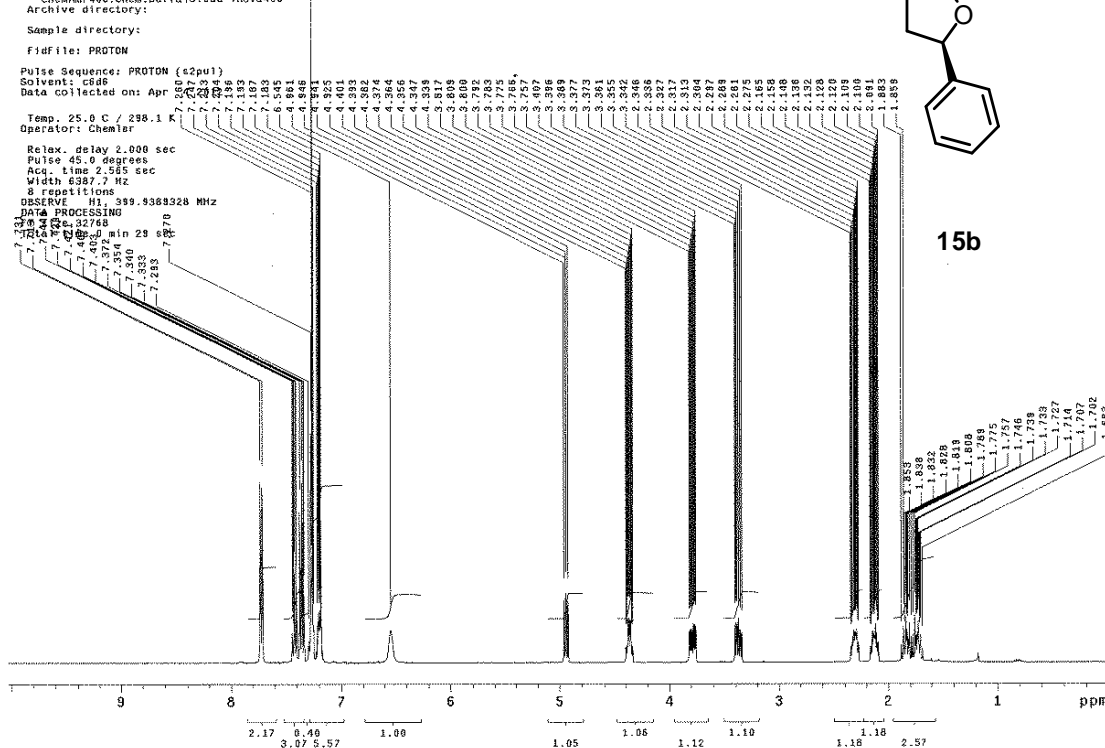
FT resolution 0.082 min 29 6879

FT scan rate 7.40250 min 7.0

FT S/N 1.384

FT F2 1.3333

FT F1 1.283



fs-V-147carbon

Sample Name:

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

Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cdc13

Data collected on: Apr 5 2012

Temp. 22.0 C / 295.1 K

Operator: Sherry

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

2480 repetitions

OBSERVE C13, 75.4596375 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

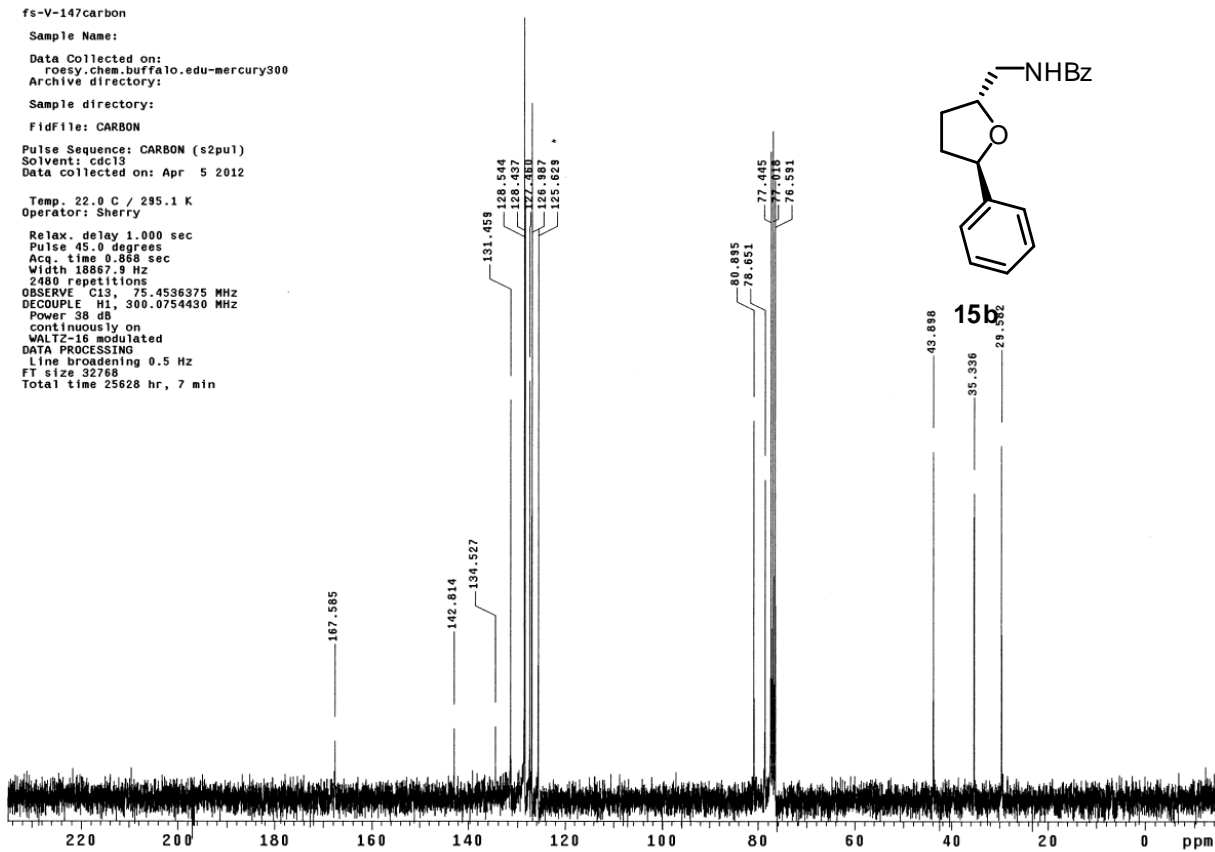
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 25628 hr, 7 min



fs-V-147NDS-1

Sample Name:

Data Collected on:
chemarr408.chem.buffalo.edu~nova408
Archive directory:

Sample directory:

FidFile: NOESY10

Pulse Sequence: NOESY10

Solvent: c6d6

Data collected on: Apr 4 2012

Temp: 25.0 C / 298.1 K

Operator: Chemist

Relax. delay: 1.000 sec

Pulse: 90.0 degrees

Acq. time: 3.032 sec

Width: 2648.7 Hz

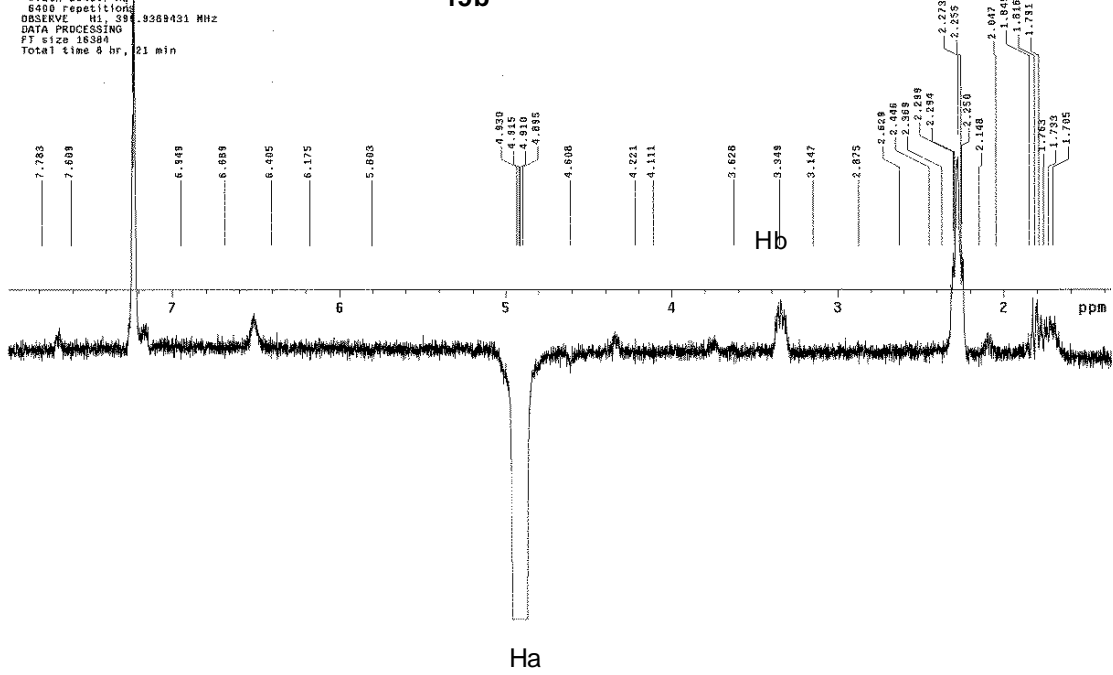
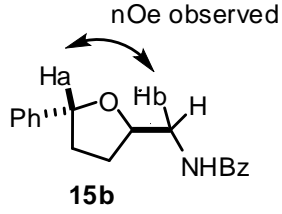
6400 repetitions

DESIKE: 91.3349369431 MHz

DATA PROCESSING

FT size: 16384

Total time: 6 hr, 21 min



fs-V-145-proton

Sample Name:

Data Collected on:
chemarr00.chem.buffalo.edu-inova400

Archive directory:

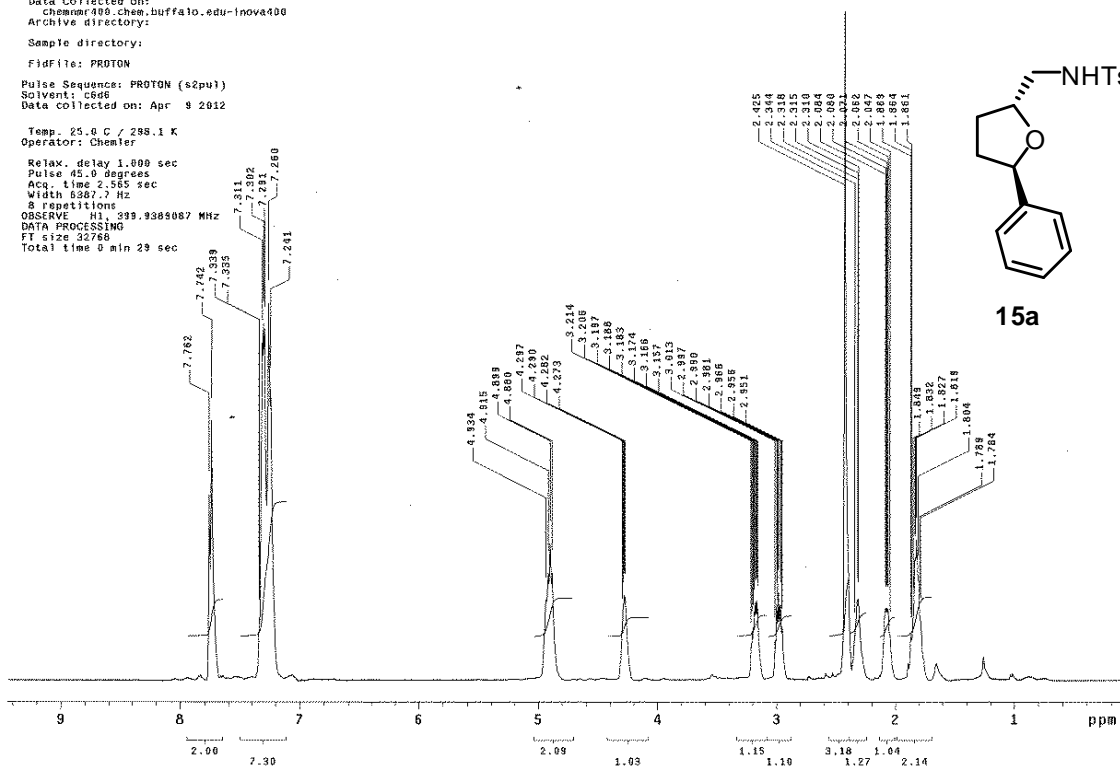
Sample directory:

Fidfile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Apr 9 2012

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.585 sec
Width 6307.7 Hz
8 repetitions
OBSERVE H1, 399.9385087 MHz
DATA PROCESSING
F1 size 32768
Total time 0 min 29 sec



fs-V-145carbon

Sample Name:

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

Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Apr 5 2012

Temp. 22.8 C / 295.9 K
Operator: Sherry

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.888 sec
Width 18867.9 Hz
488 repetitions
OBSERVE C13, 75.4536430 MHz
DECOUPLE H1, 300.0754430 MHz
Power 98 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
F1 size 32768
Total time 187419 hr, 12 min

