

Diastereo- and Enantioselective Copper-Catalyzed Intramolecular Carboamination of Alkenes for the Synthesis of Hexahydro-1*H*-Benz[*f*]indoles

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Supporting Information 2: ¹H NMR and ¹³C NMR of substrates and products

20100629dibenzyl lactone

Sample Name:

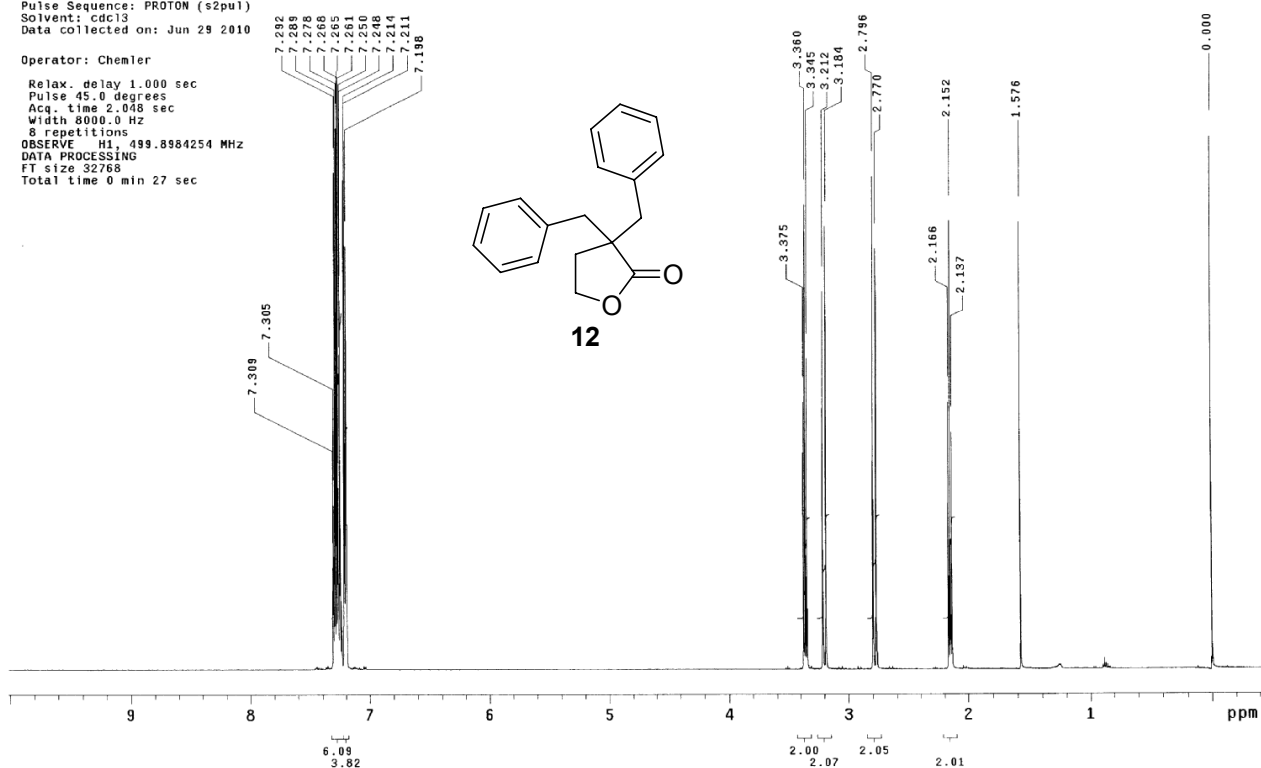
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Jun 29 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984254 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 27 sec

20100629dibenzyl lactoneC13

Sample Name:

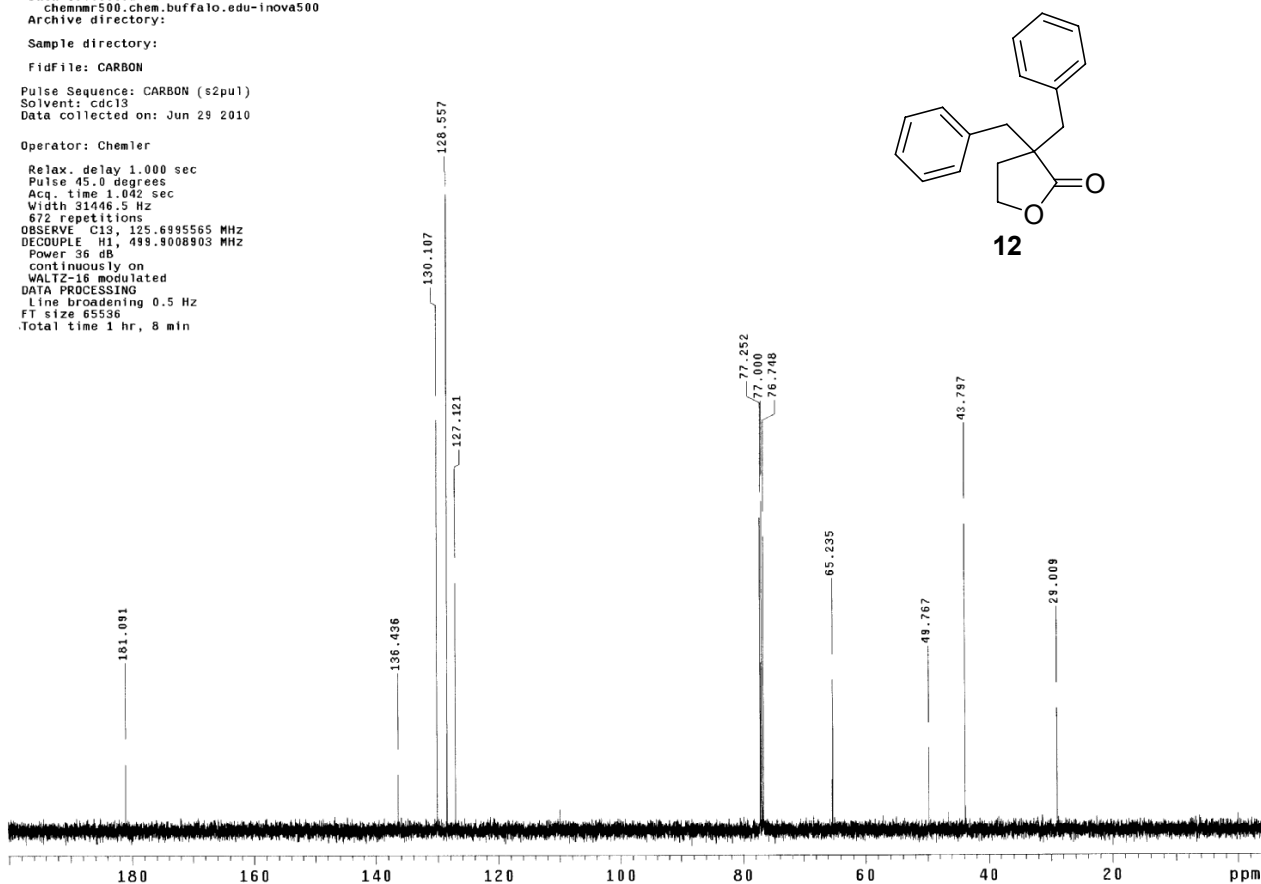
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Jun 29 2010

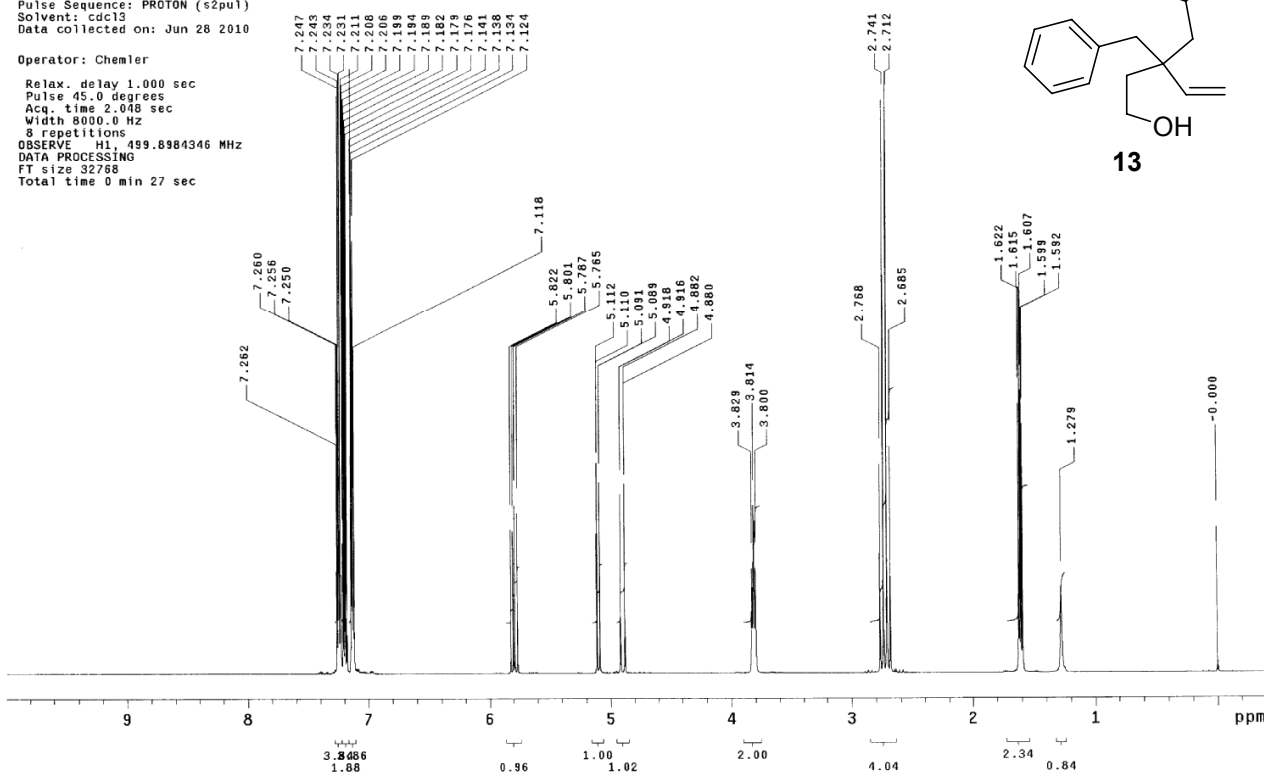
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
672 repetitions
OBSERVE C13, 125.6995565 MHz
DECOUPLE H1, 499.8008903 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 1 hr, 8 min

20100628dibenzylalcohol

Sample Name:
 Data Collected on:
 chemmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jun 28 2010

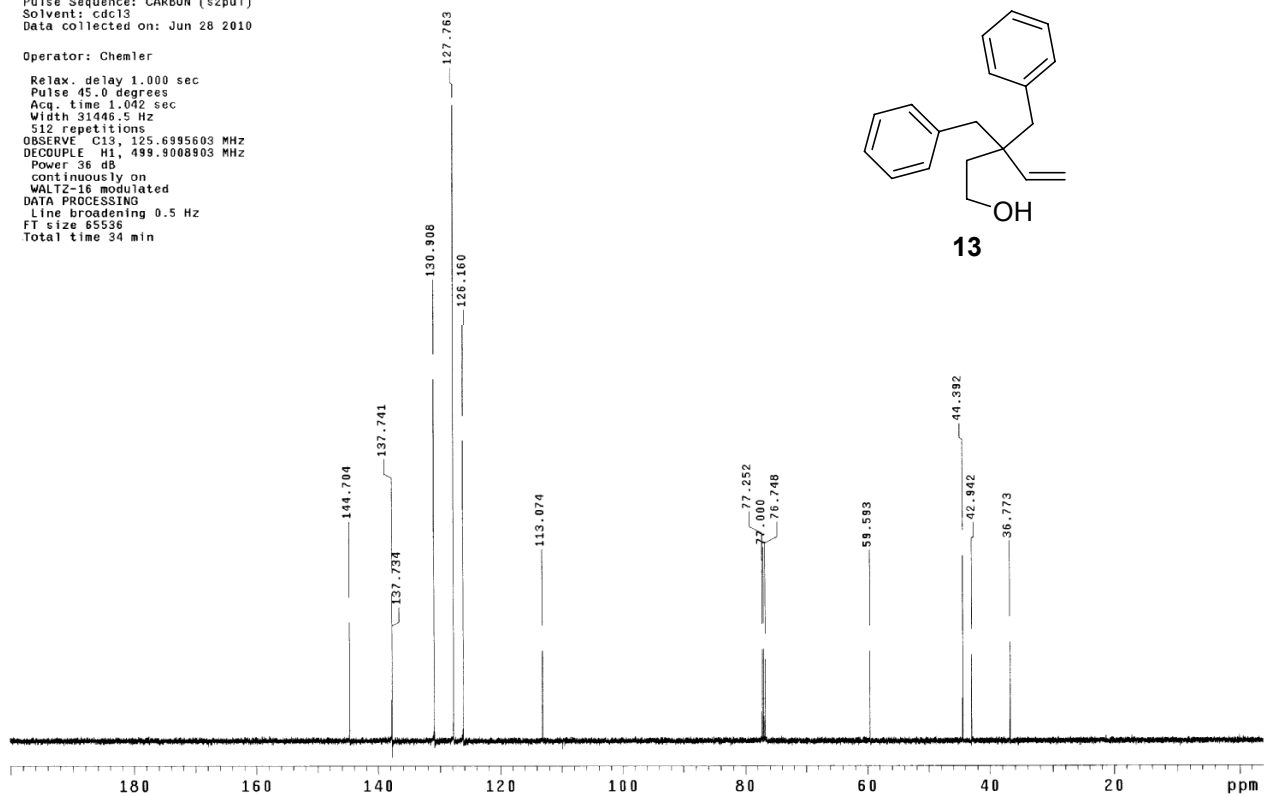
Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.6984346 MHz
 DATA PROCESSING
 FT size 32788
 Total time 0 min 27 sec



20100628dibenzylalcohol1C13

Sample Name:
 Data Collected on:
 chemmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 Fidfile: CARBON
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jun 28 2010

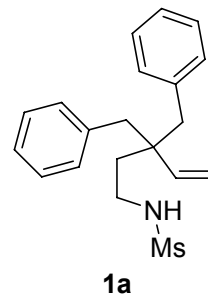
Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.042 sec
 Width 31446.5 Hz
 512 repetitions
 OBSERVE C13, 125.6995603 MHz
 DECOUPLE H1, 499.9008903 MHz
 Power 36 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 65536
 Total time 34 min



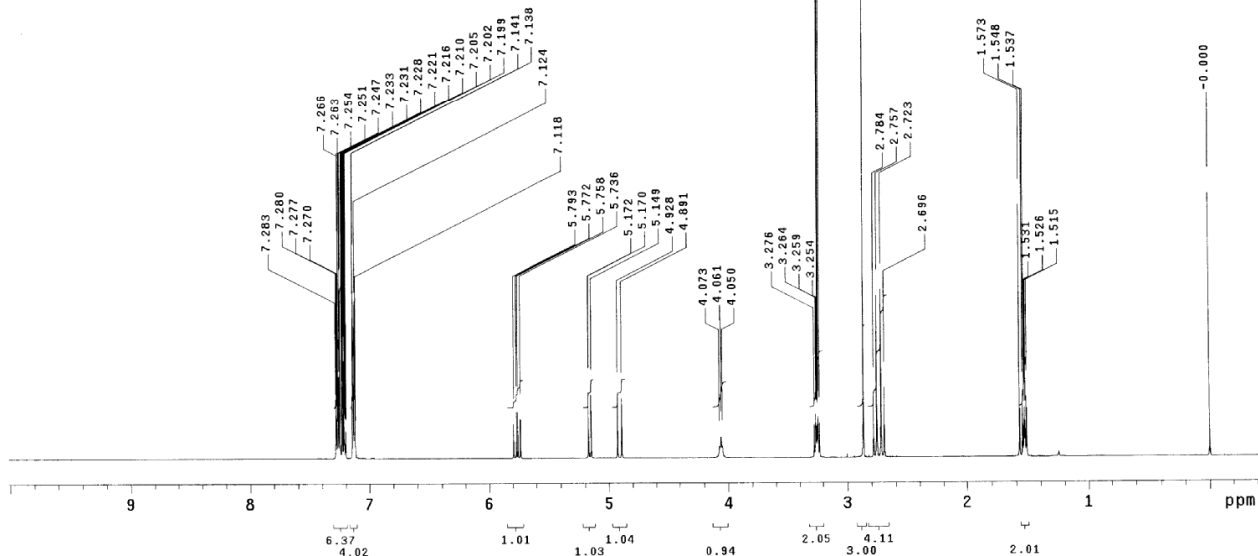
20100628Msdibenzylsubstrate

Sample Name:
 Data Collected on:
 chemnmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdc13
 Data collected on: Jun 28 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.8964256 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 27 sec



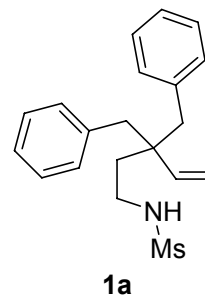
1a



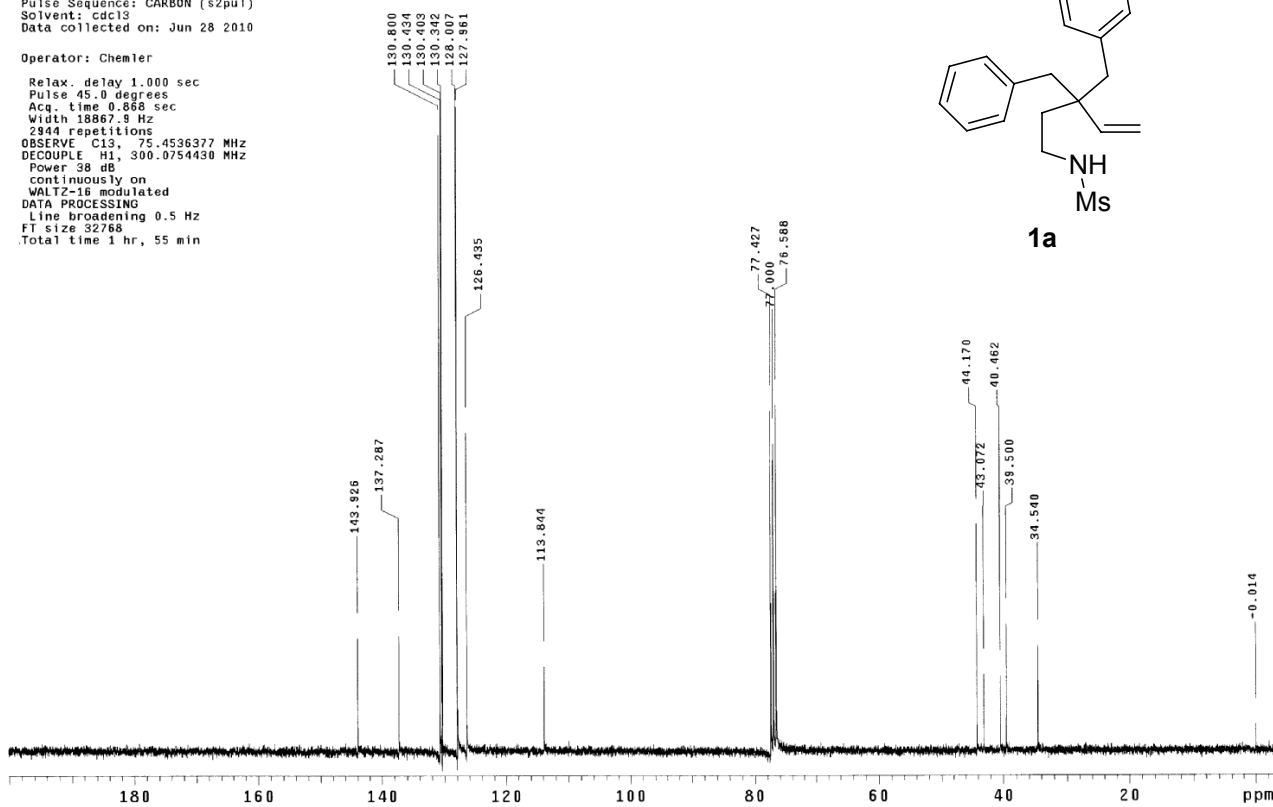
20100628MsdibenzylsubstrateC13

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: Jun 28 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.3 Hz
 2844 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 1 hr, 55 min



1a



20100708SESDibenzylsubstrate

Sample Name:

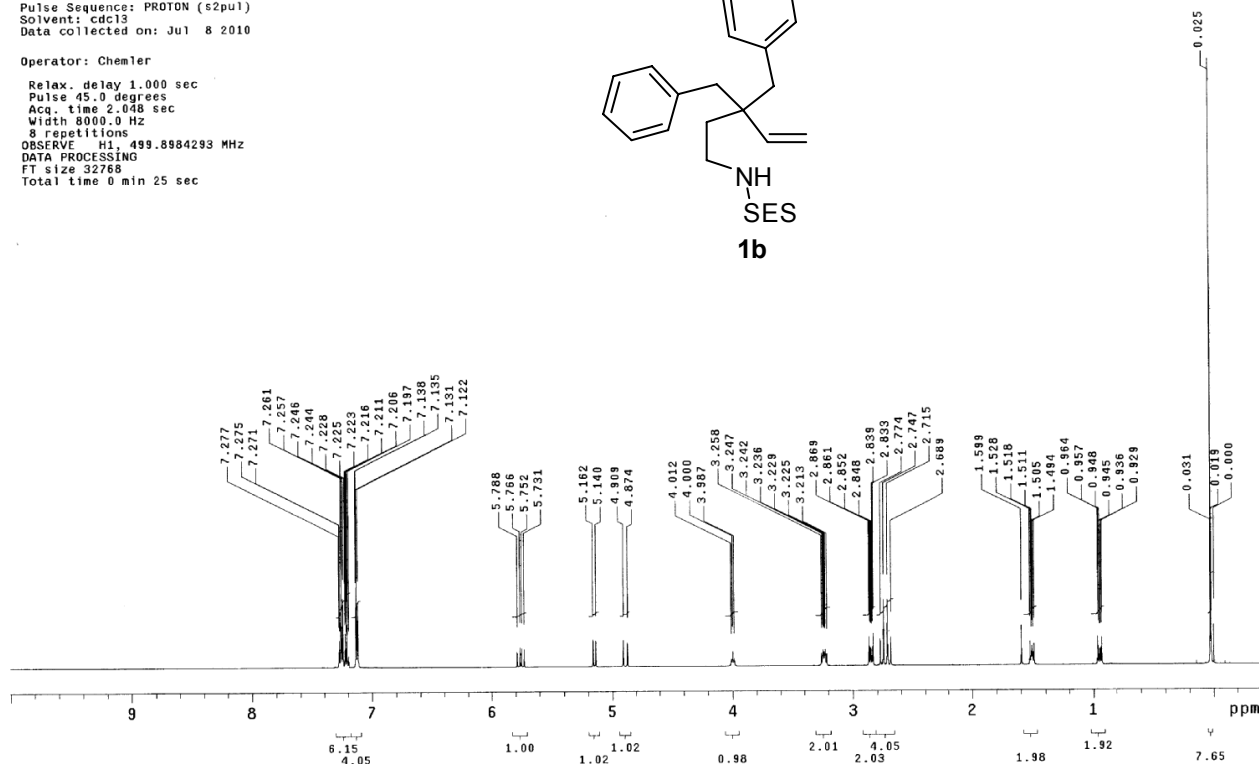
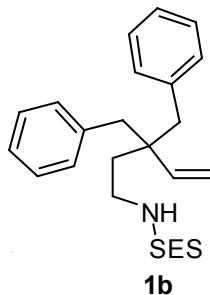
Data Collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Jul 8 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984293 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100708SESDibenzylsubstrateC13

Sample Name:

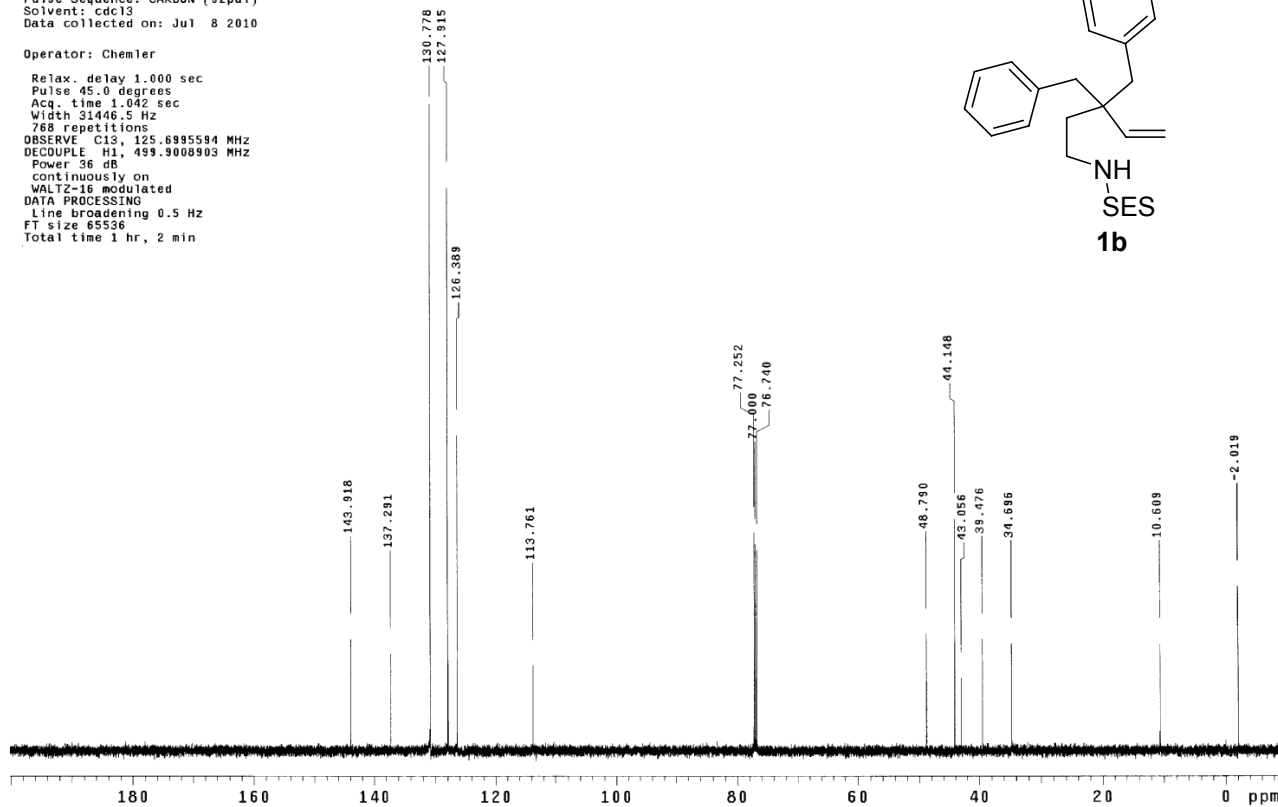
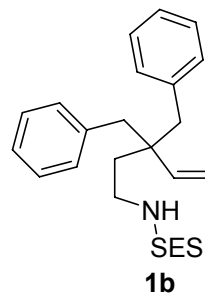
Data Collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Jul 8 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
768 repetitions
OBSERVE C13, 125.6985584 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 1 hr, 2 min

20100630Bsubstrate

Sample Name:

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

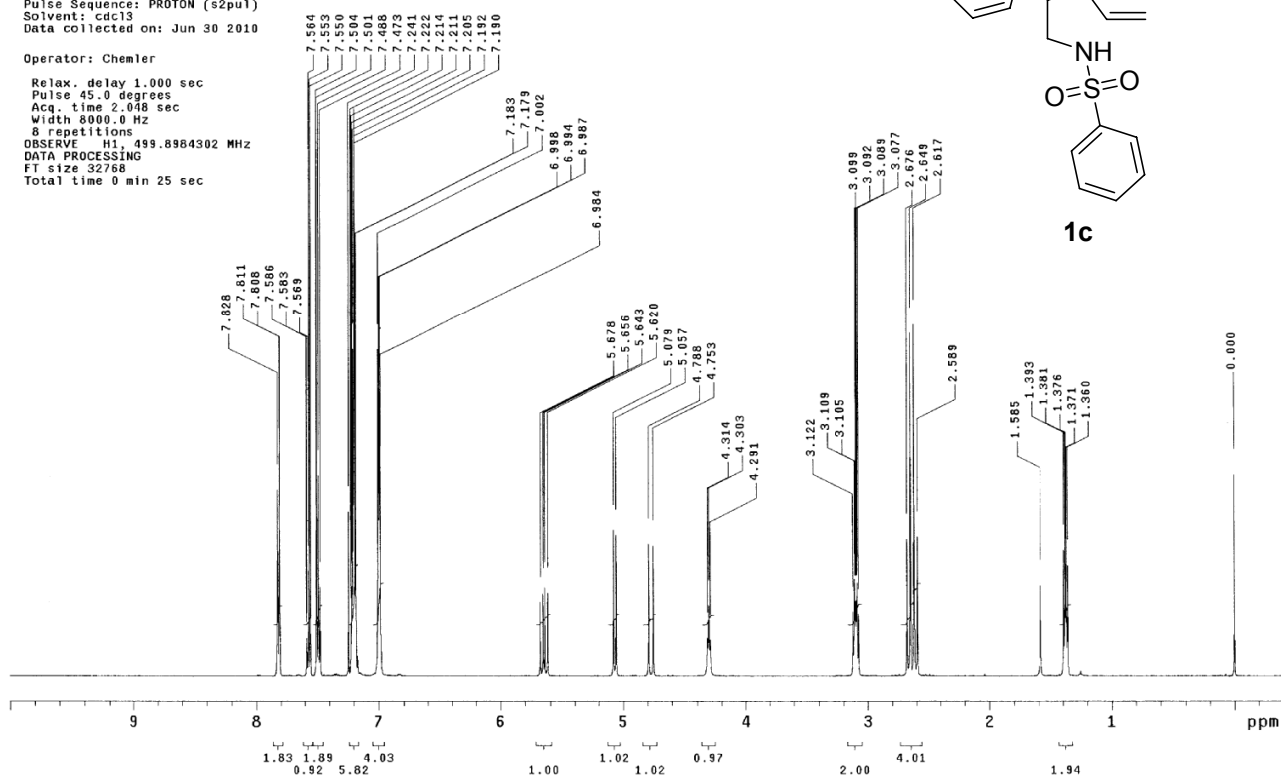
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Jun 30 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984302 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100628dibenzylalcohol1C13

Sample Name:

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

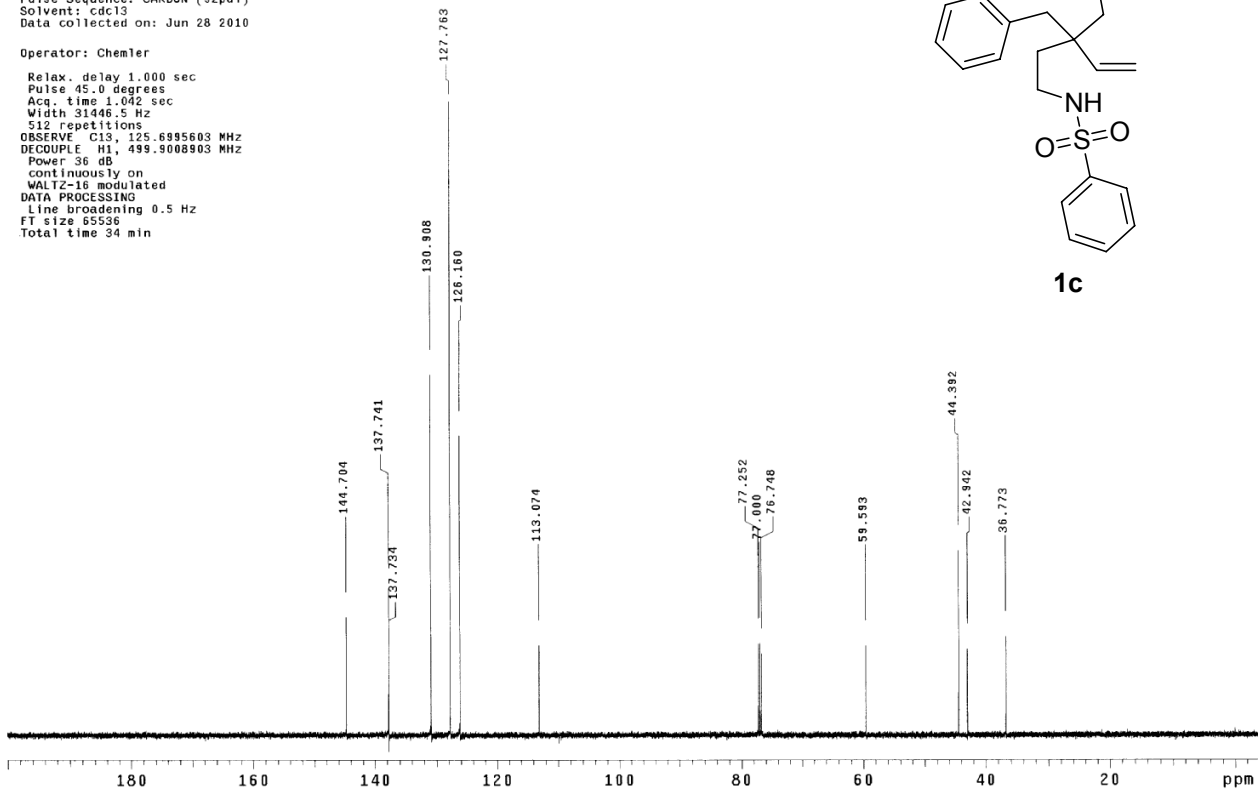
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Jun 28 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
512 repetitions
OBSERVE C13, 125.6985603 MHz
DECOUPLE H1, 499.9086903 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 34 min

20090921dibenzylsubstrate

Sample Name:

Archive directory:

Sample directory:

FidFile: H1

Pulse Sequence: s2pu1

Solvent: CDCl3

Data collected on: Sep 21 2009

Operator: Chemler

Mercury-300B8 "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec

Pulse 39.7 degrees

Acq. time 1.891 sec

Width 10000.0 Hz

16 repetitions

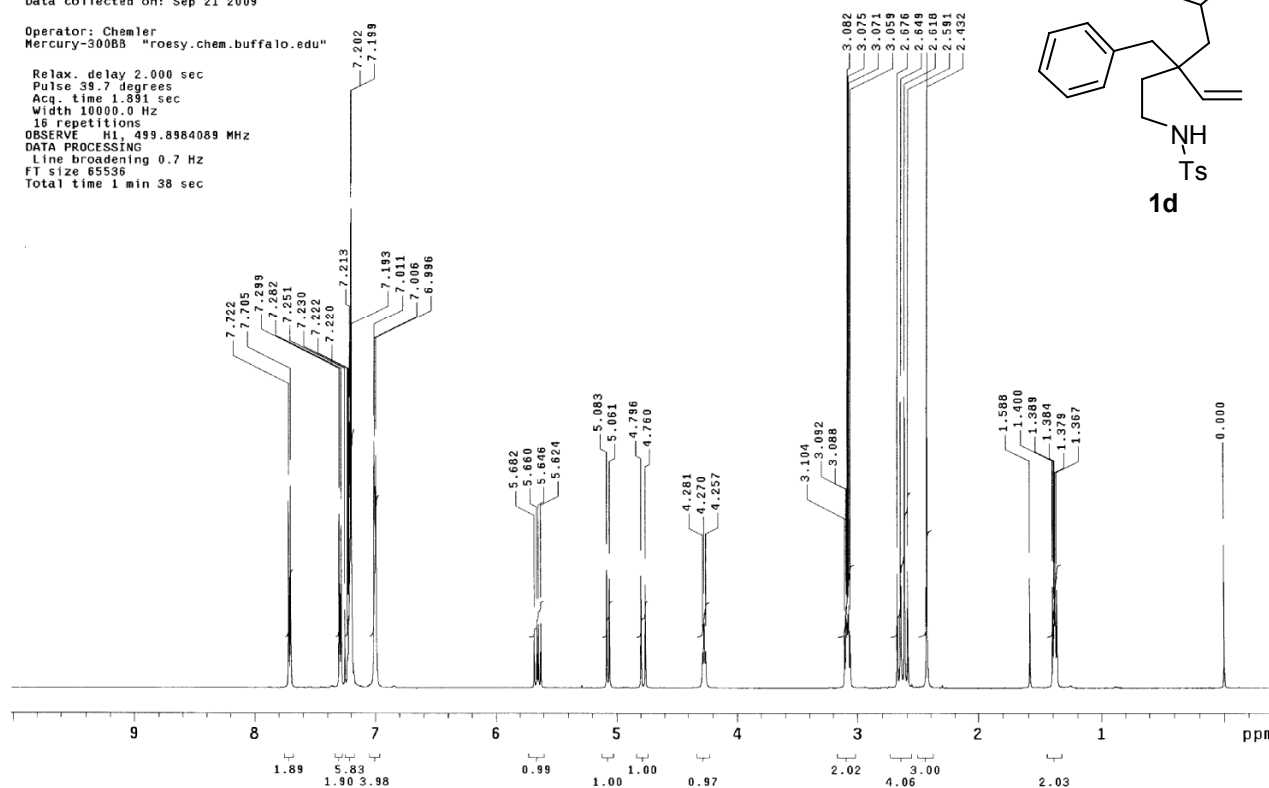
OBSERVE H1, 499.8984089 MHz

DATA PROCESSING

Line broadening 0.7 Hz

FT size 65536

Total time 1 min 38 sec



20100629dibenzylsubstrateC13

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 29 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 15867.9 Hz

2048 repetitions

OBSERVE C13, 75.4536400 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

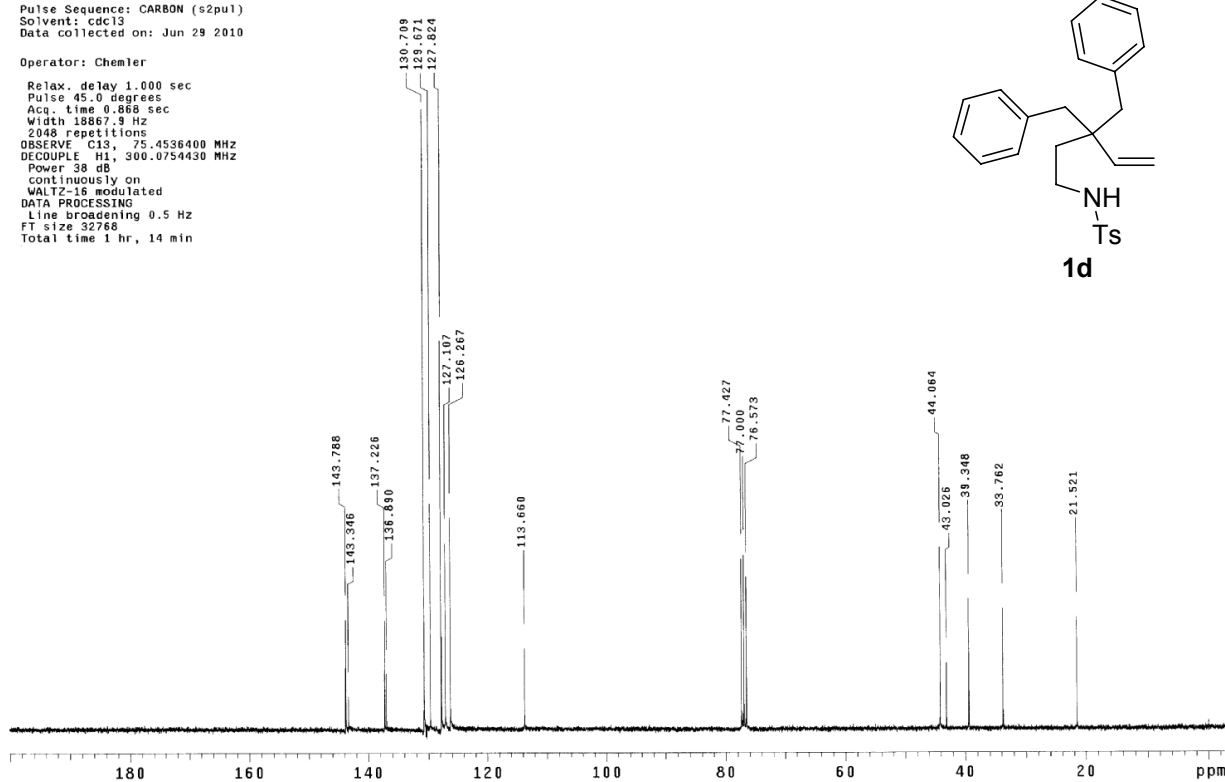
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 1 hr, 14 min



20100630PMBSDibenzylsubstrate

Sample Name:

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

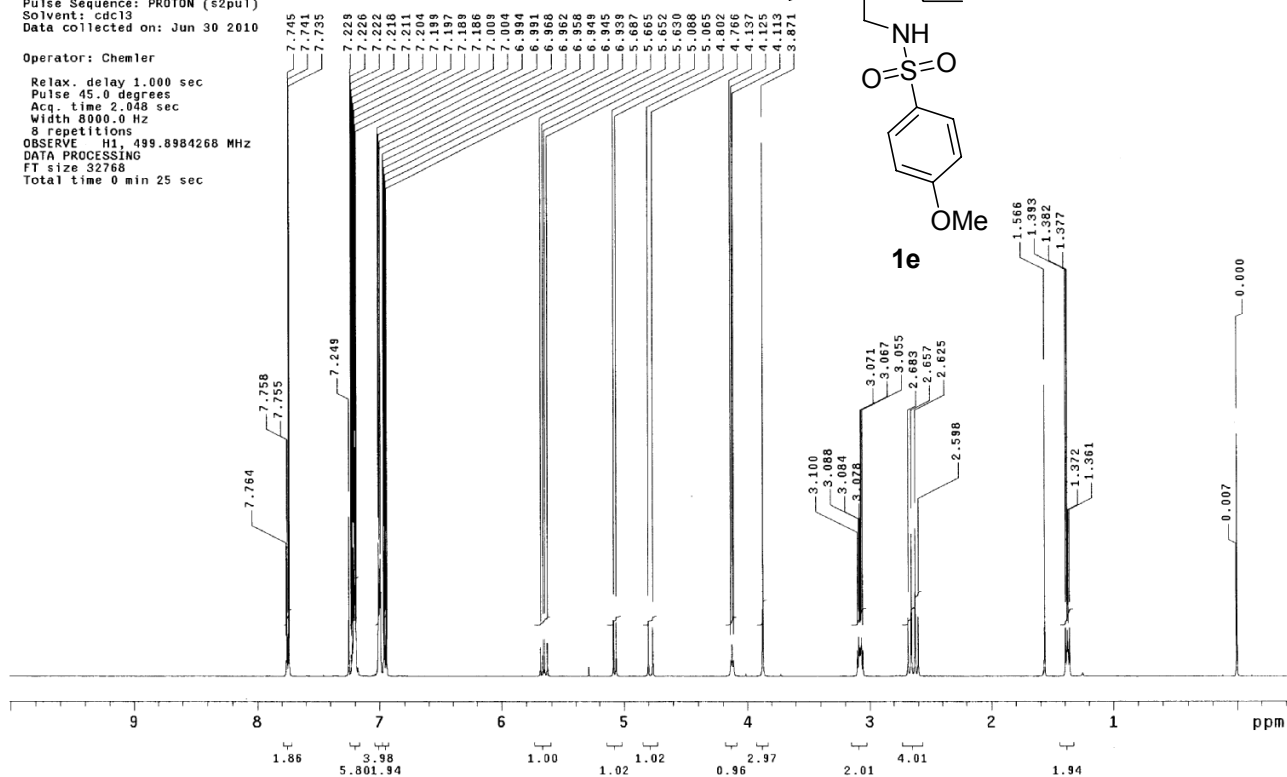
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Jun 30 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984268 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100630PMBSDibenzylsubstrateC13

Sample Name:

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

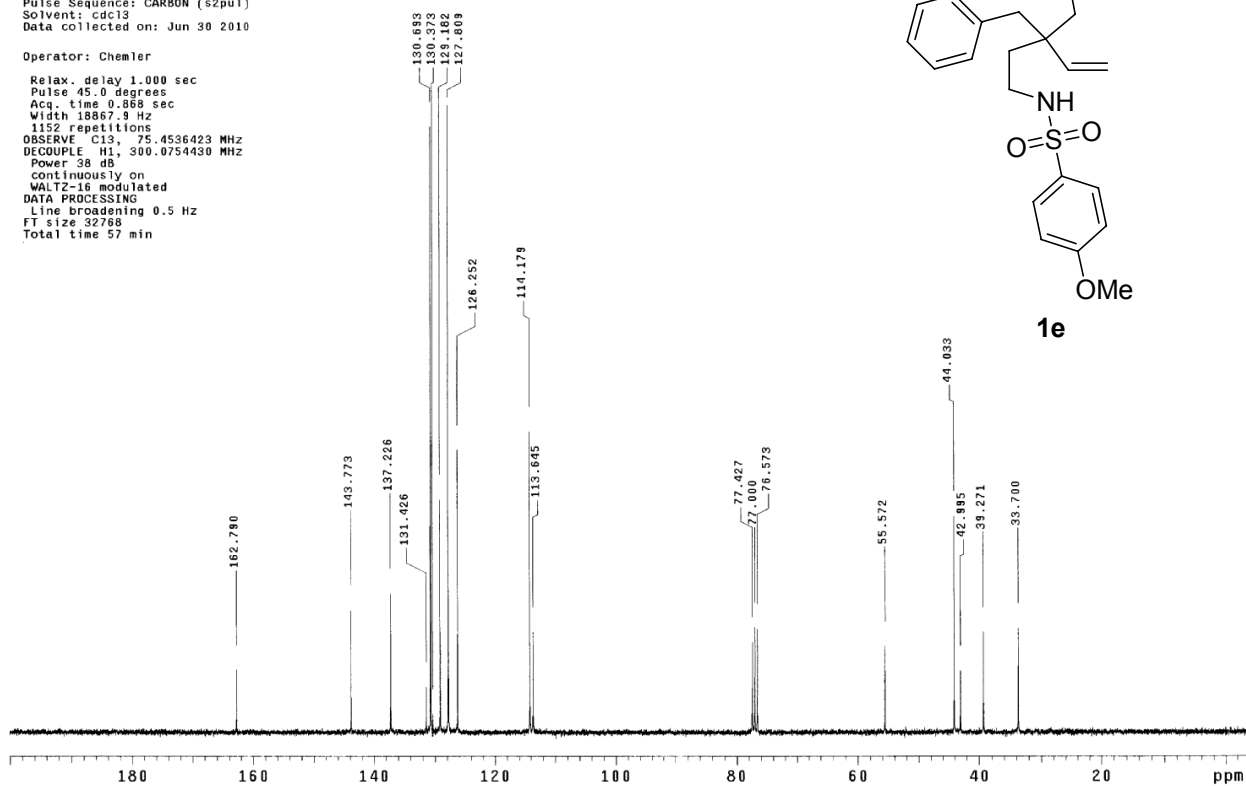
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Jun 30 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 19867.8 Hz
1152 repetitions
OBSERVE C13, 75.4536423 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 57 min

20100702Nsdibenzylsubstrate

Sample Name:

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

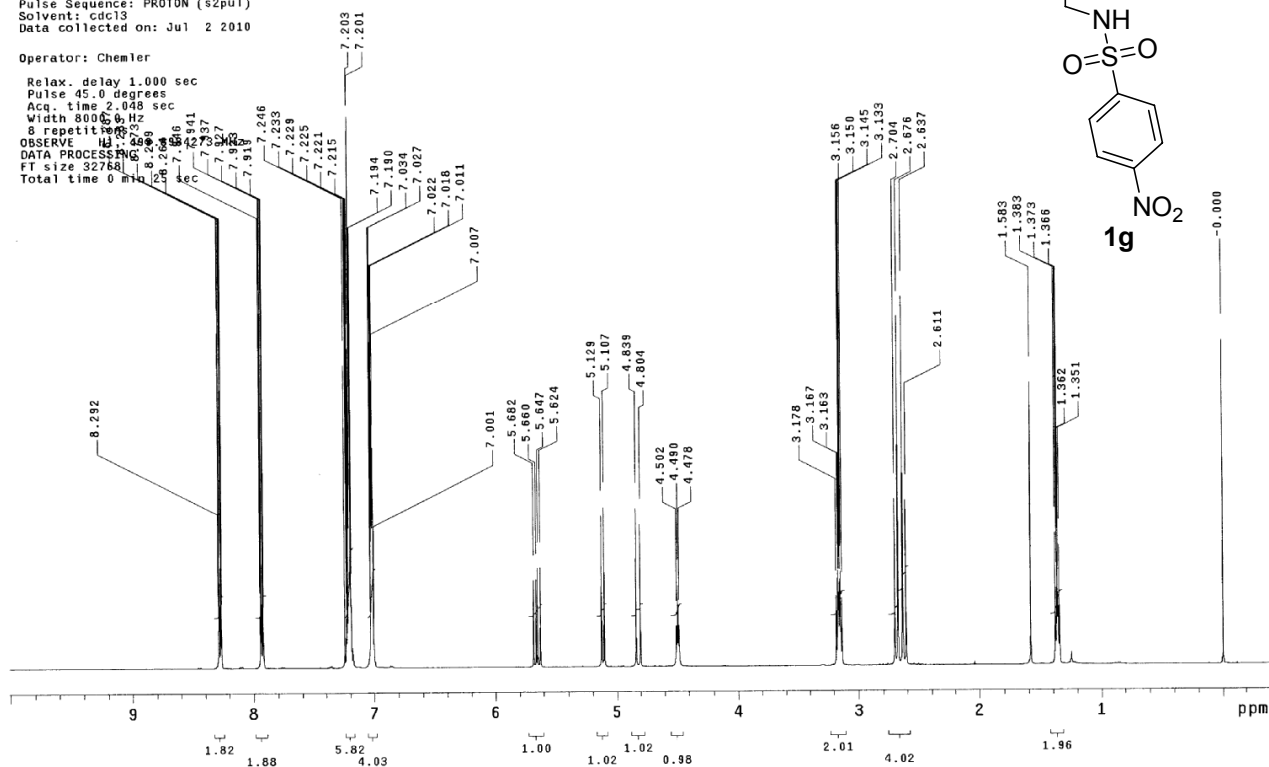
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2010

Operator: Chemier

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
S repetitions 5
OBSERVE H1 250.136 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 23

20100702NsdibenzylsubstrateC13

Sample Name:

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

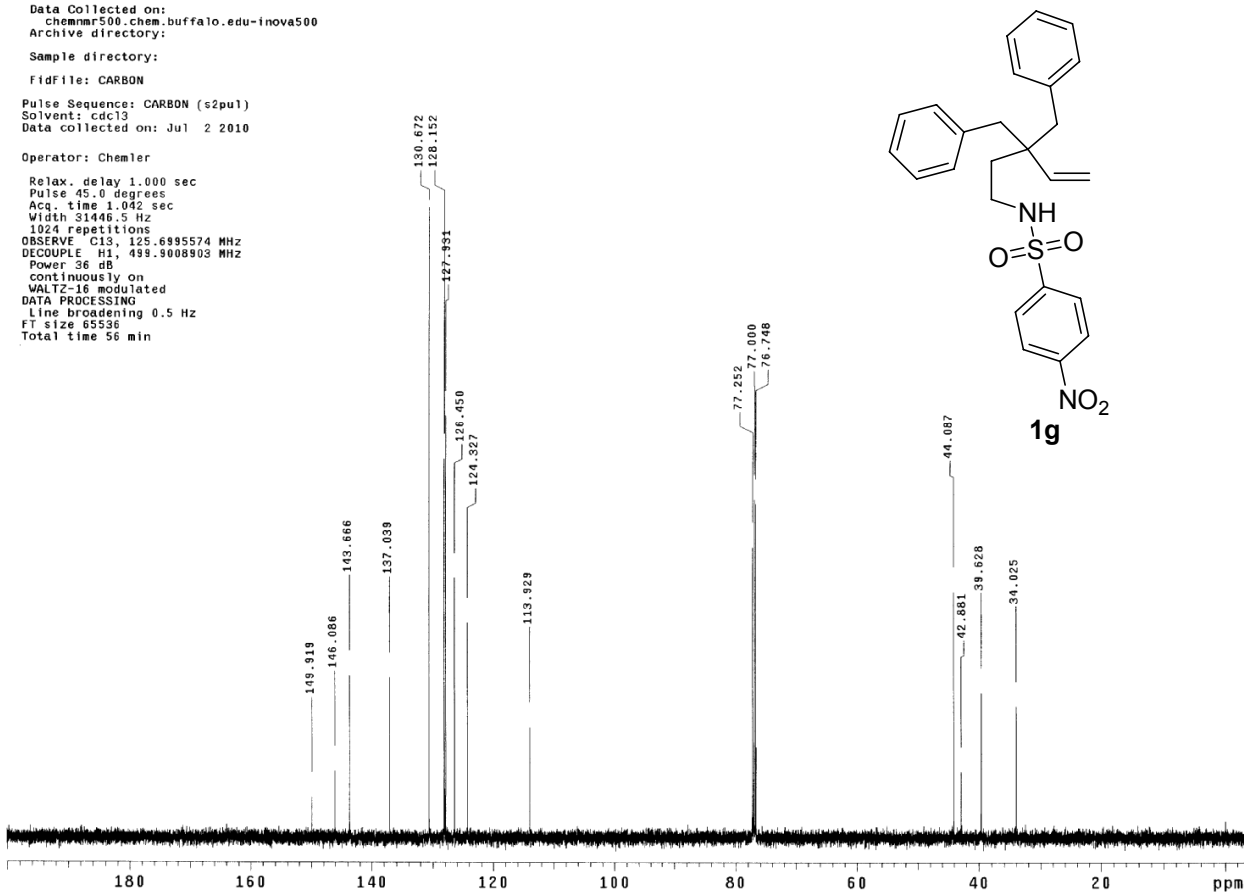
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 2 2010

Operator: Chemier

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
1024 repetitions
OBSERVE C13 125.6985574 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 56 min

20091030difluorobenzylbutyrolactone

Sample Name:

Archive directory:

Sample directory:

FidFile: H1

Pulse Sequence: s2pu1

Solvent: CDC13

Data collected on: Oct 30 2009

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec

Pulse 39.7 degrees

Acq. time 1.891 sec

Width 10000.0 Hz

16 repetitions

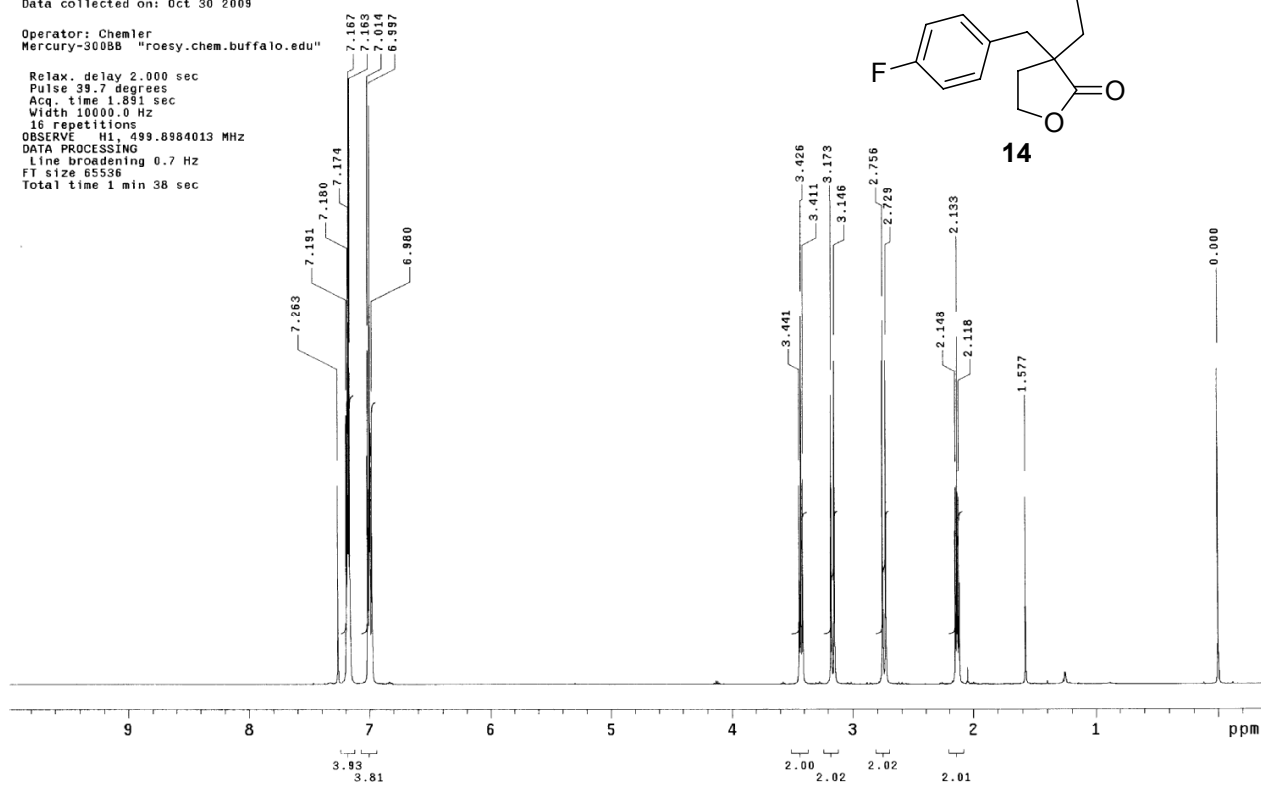
OBSERVE H1; 499.8984013 MHz

DATA PROCESSING

Line broadening 0.7 Hz

FT size 65536

Total time 1 min 38 sec



20091031difluorobenzylbutyrolactoneC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)

Solvent: CDC13

Data collected on: Oct 31 2009

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

748 repetitions

OBSERVE C13; 75.4536599 MHz

DECOUPLE H1; 300.0754431 MHz

Power 1023 dB

continuously on

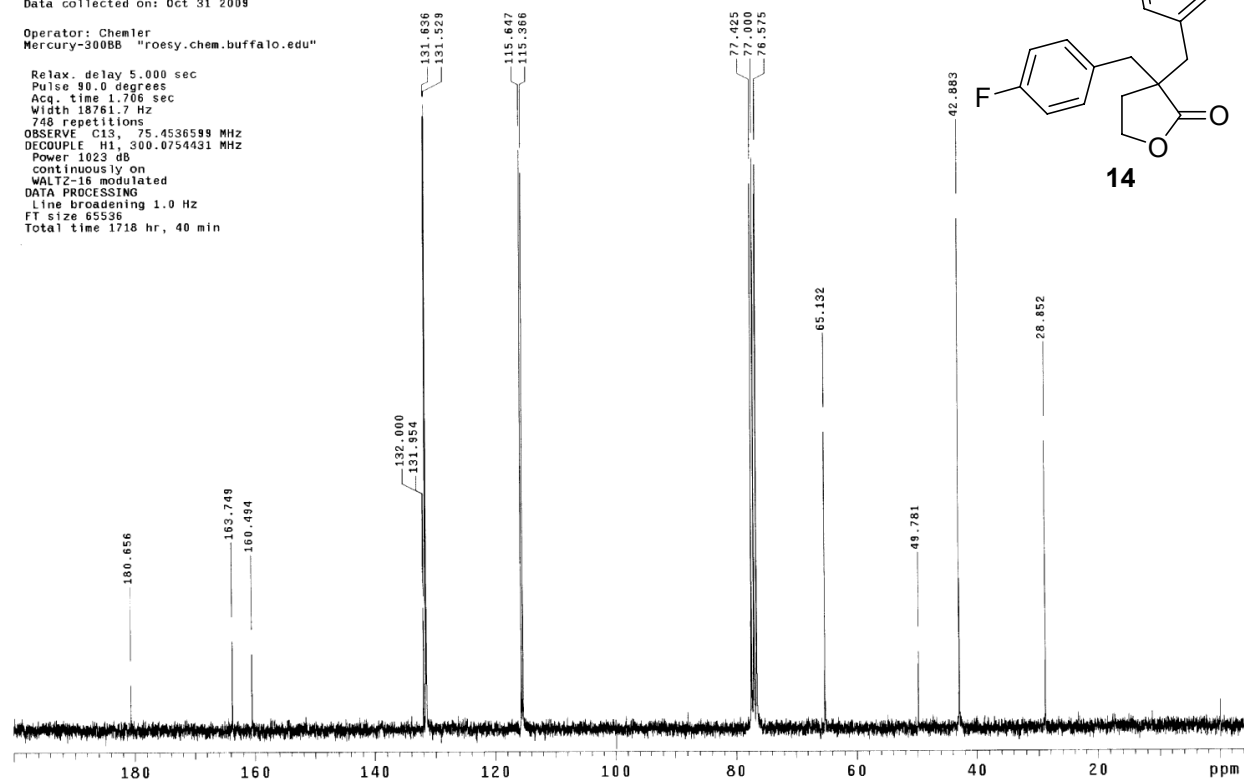
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1718 hr, 40 min



20100705difluorobenzylalcoholalkene

Sample Name:

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

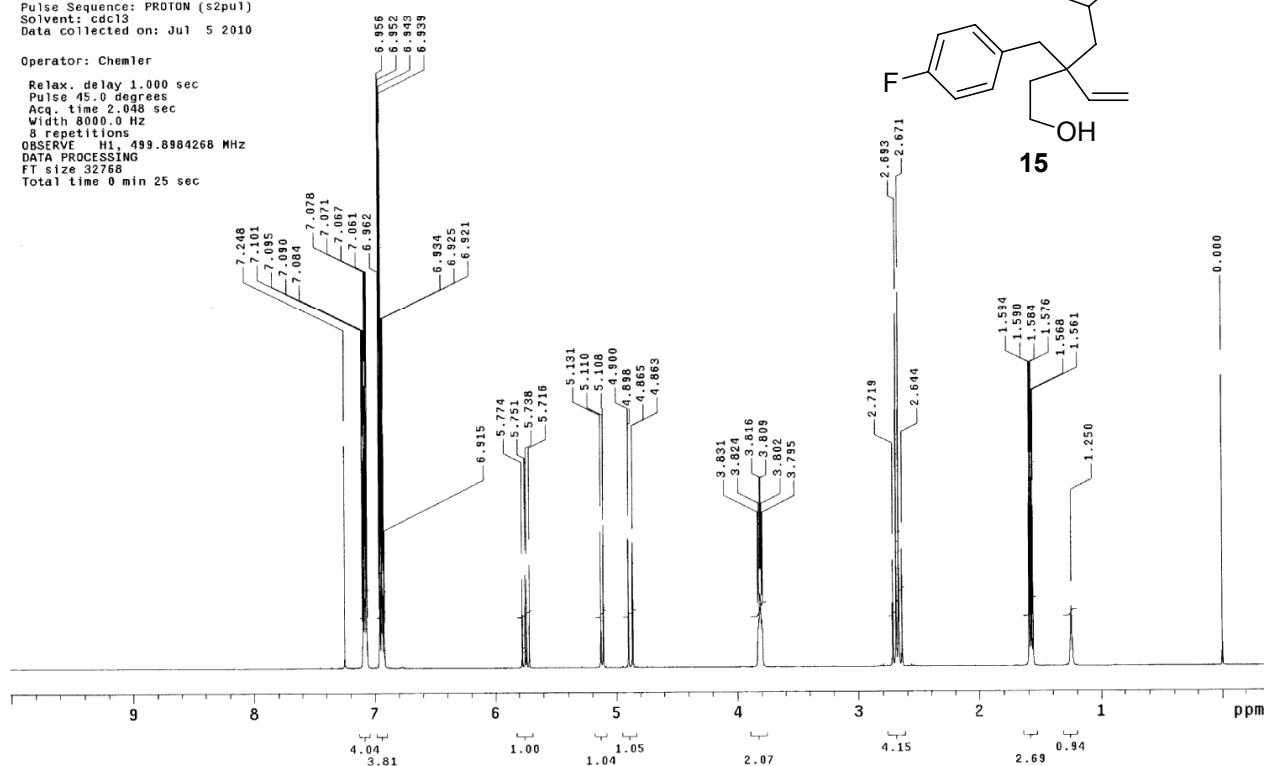
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Jul 5 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984268 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

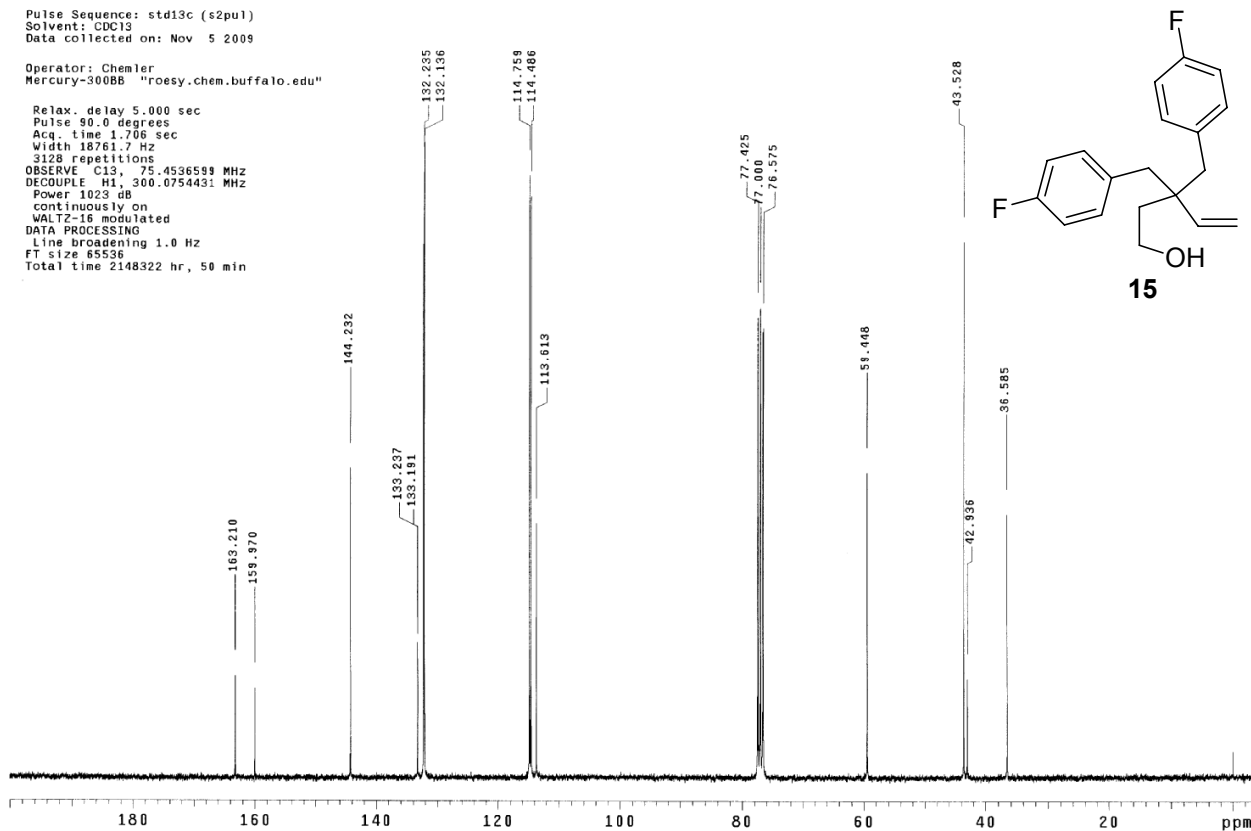
20091105difluorobenzylalcoholC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)
Solvent: CDCl3
Data collected on: Nov 5 2009Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 5.000 sec
Pulse 90.0 degrees
Acq. time 1.706 sec
Width 18761.7 Hz
3128 repetitions
OBSERVE C13, 75.4536599 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2148322 hr, 50 min

20100702difluorosubstrate

Sample Name:

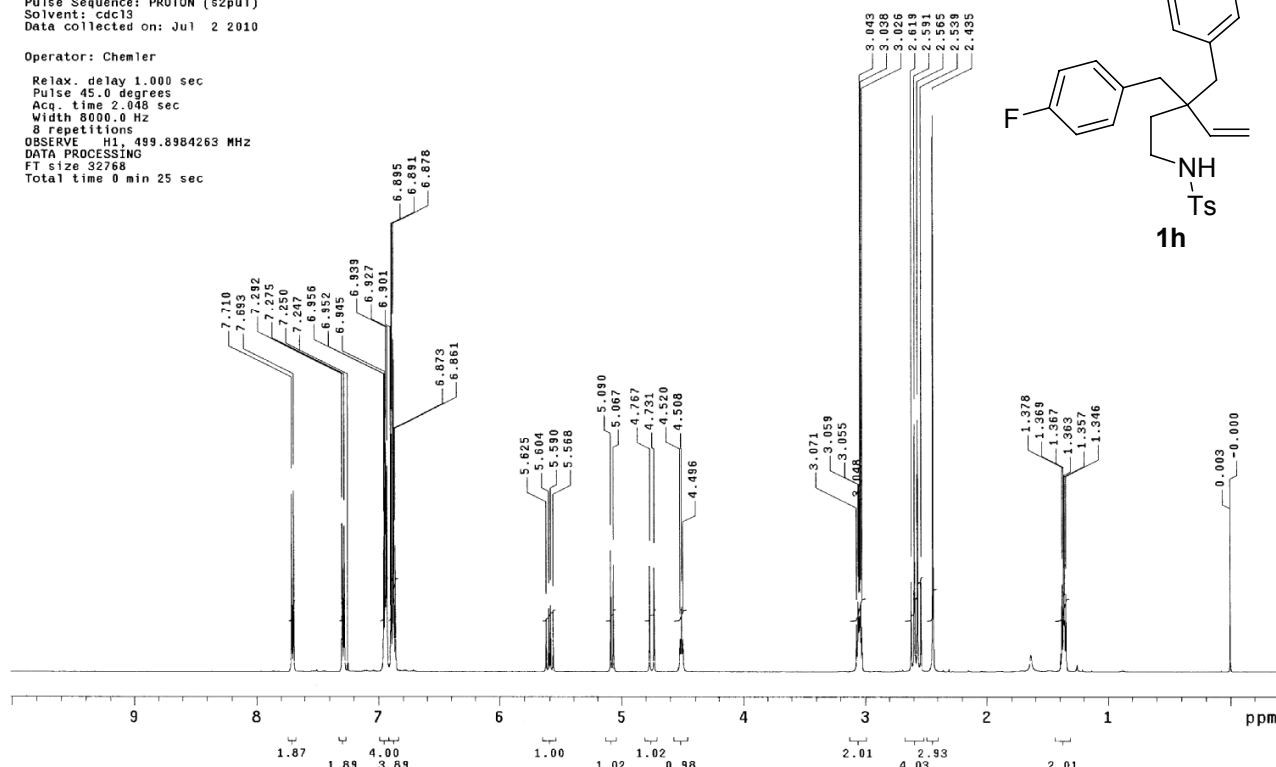
Data Collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Jul 2 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 5000.0 Hz
8 repetitions
OBSERVE H1, 499.8984263 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100702difluorosubstrateC13

Sample Name:

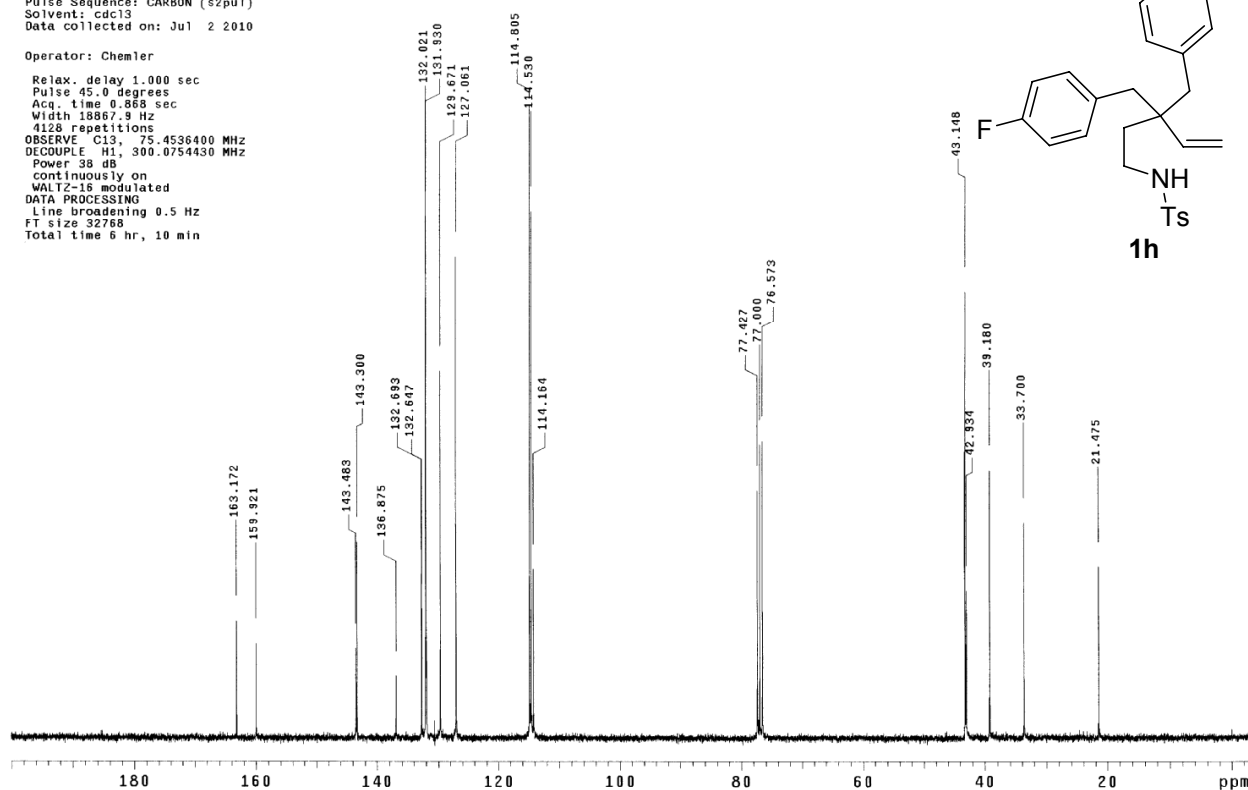
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Jul 2 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4128 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 6 hr, 10 min

20100610diomethylactone

Sample Name:

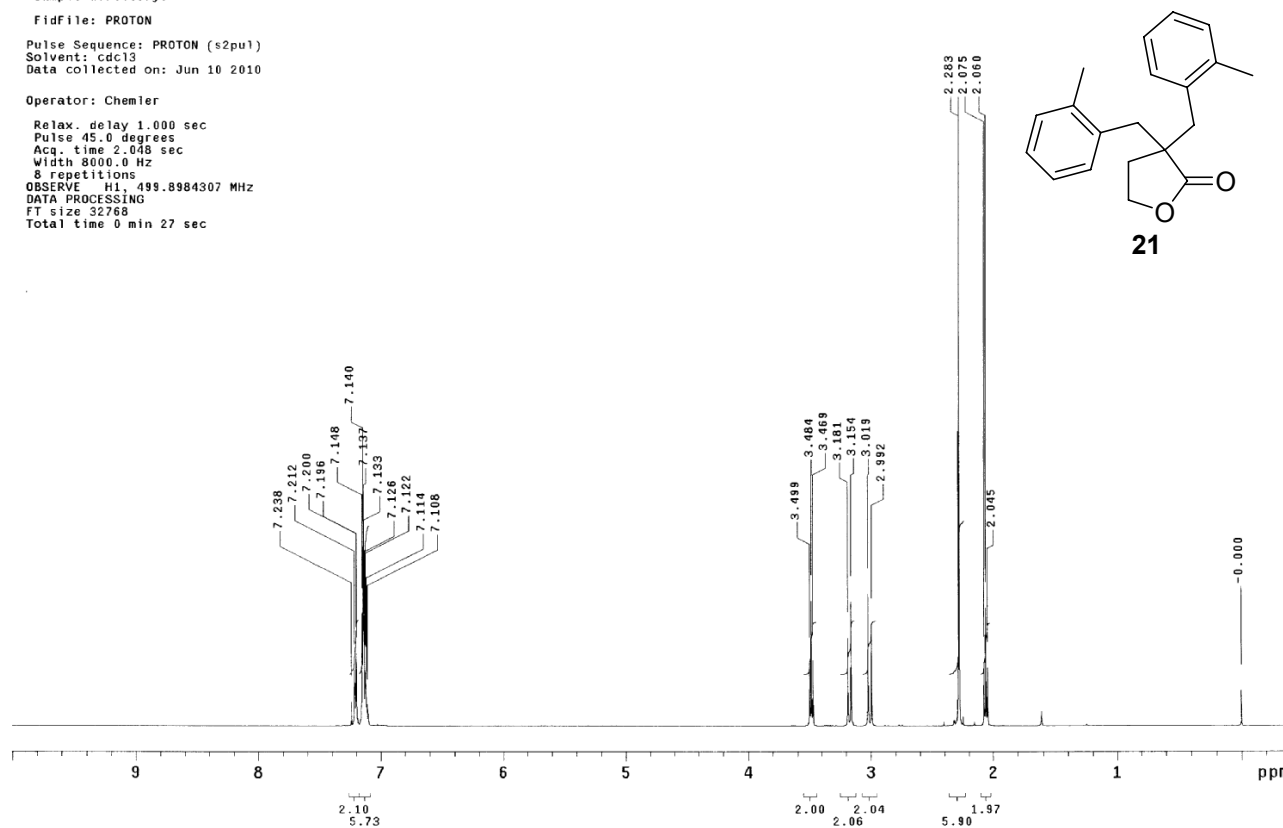
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Jun 10 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984307 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 27 sec

20100610diomethylactoneC13

Sample Name:

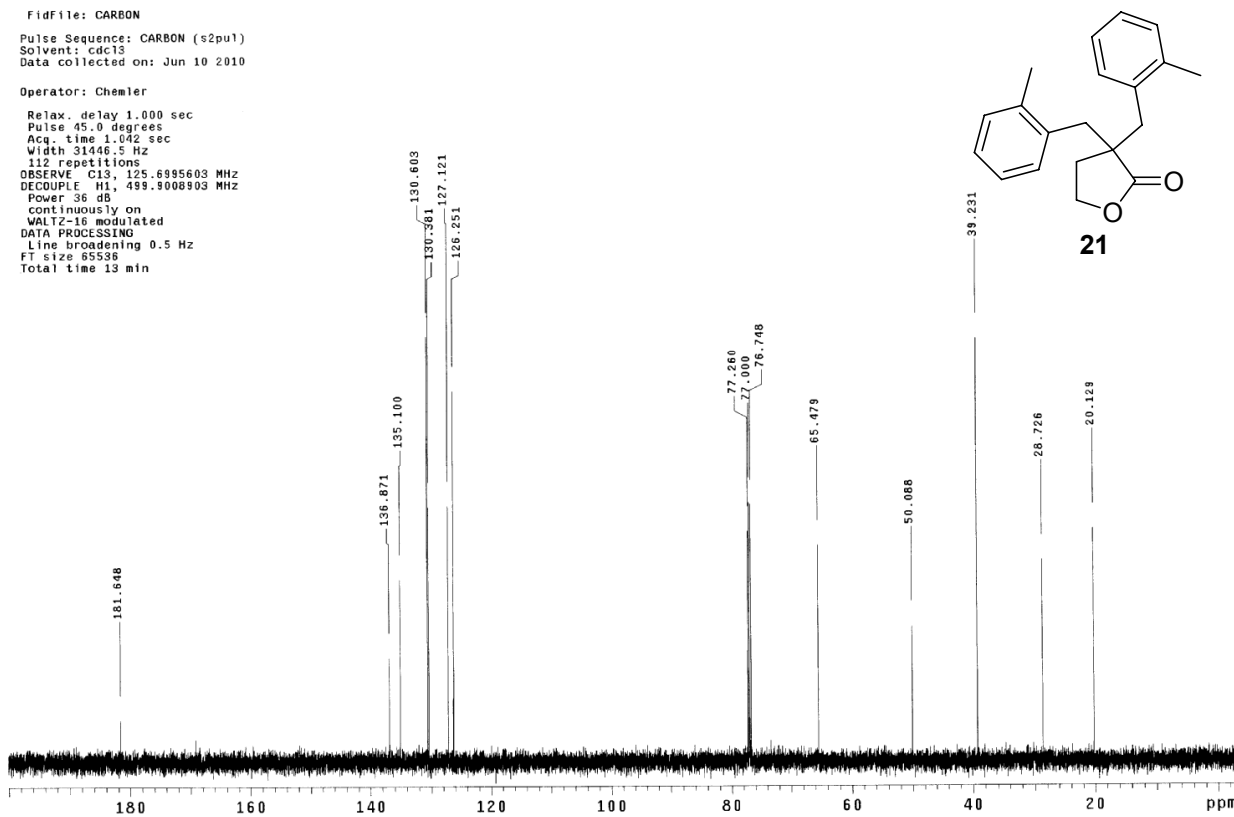
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Jun 10 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
112 repetitions
OBSERVE C13, 125.6995603 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 13 min

20091104dimethylalkenealcohol

Sample Name:

Archive directory:

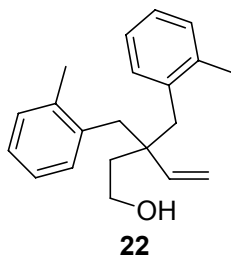
Sample directory:

Fidfile: H1

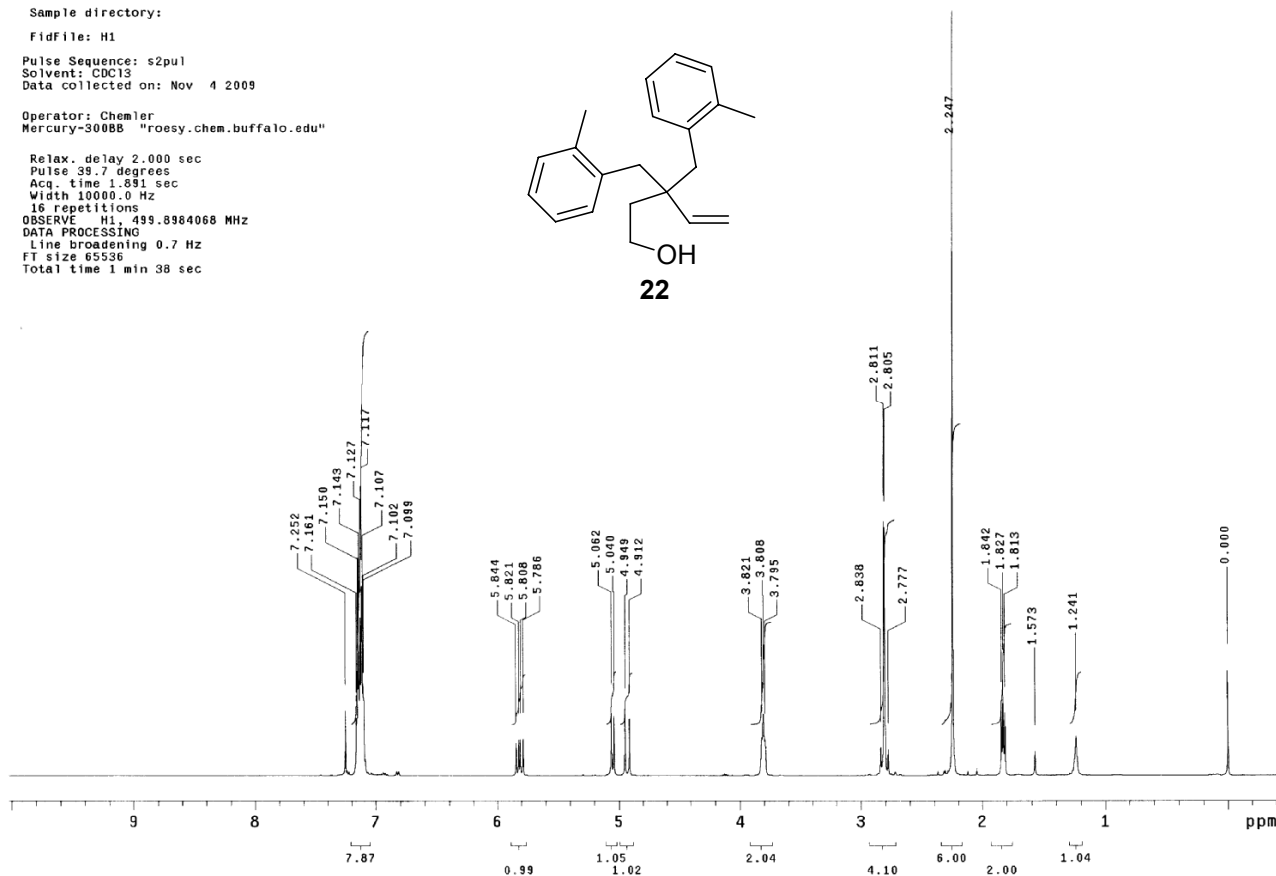
Pulse Sequence: s2pul

Solvent: CDCl3

Data collected on: Nov 4 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 2.000 sec
Pulse 39.7 degrees
Acq. time 1.891 sec
Width 10000.0 Hz
16 repetitions
OBSERVE H1, 499.8984068 MHz
DATA PROCESSING
Line broadening 0.7 Hz
FT size 65536
Total time 1 min 38 sec

22



20091106dimethylalkenealcohol1C13

Sample Name:

Archive directory:

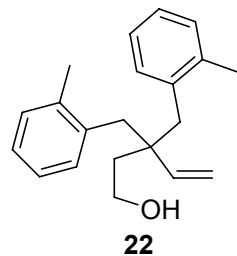
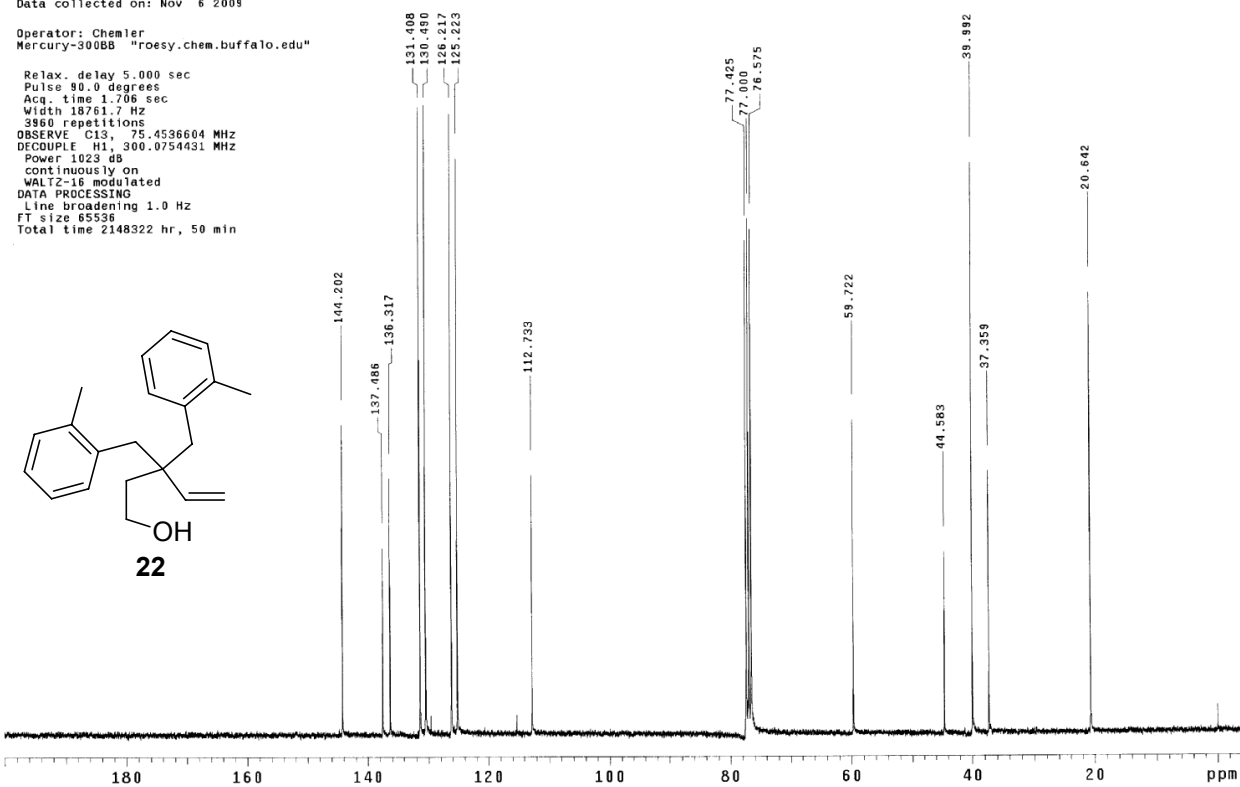
Sample directory:

Fidfile: std13c

Pulse Sequence: std13c (s2pul)

Solvent: CDCl3

Data collected on: Nov 6 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 5.000 sec
Pulse 90.0 degrees
Acq. time 1.706 sec
Width 18761.7 Hz
3860 repetitions
OBSERVE C13, 75.4536604 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2148322 hr, 50 min

22

20091212diomethylsubstrate5

Sample Name:

Archive directory:

Sample directory:

Fidfile: H1

Pulse Sequence: s2pu1

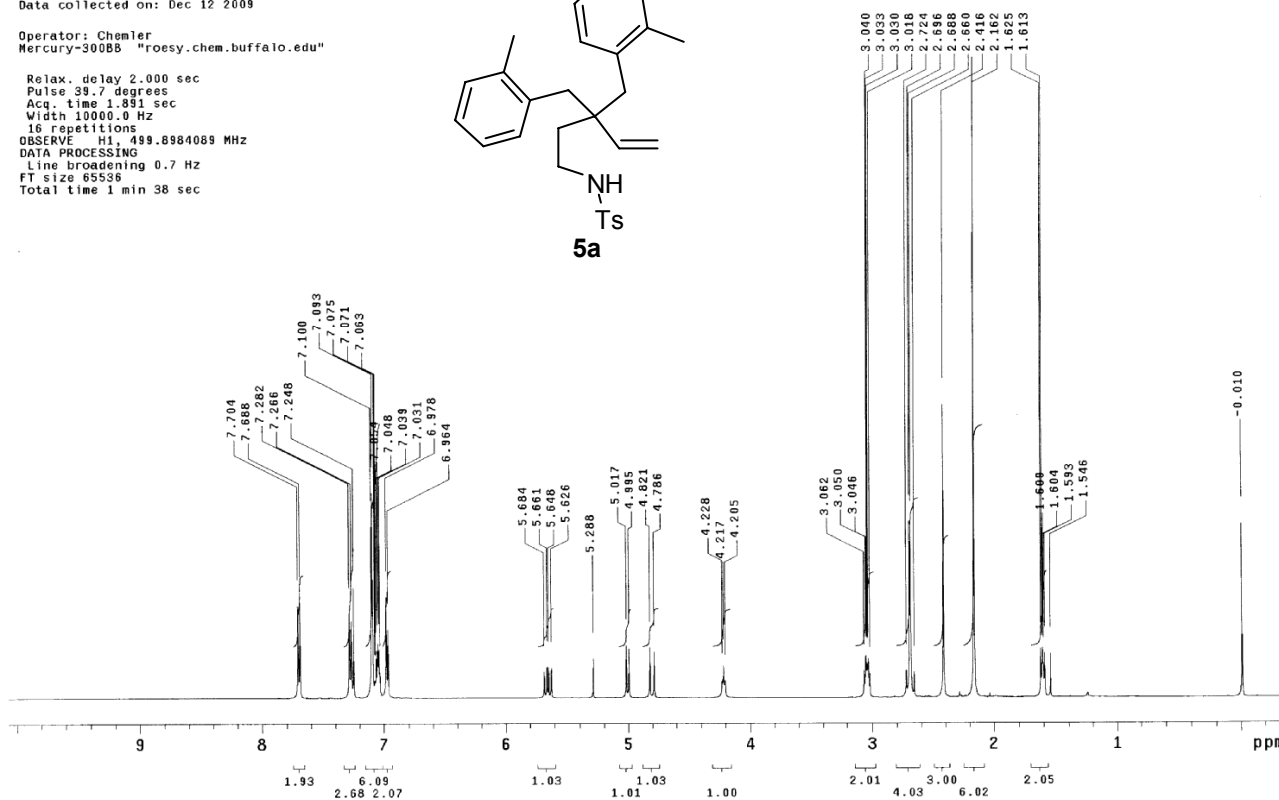
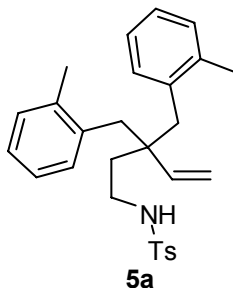
Solvent: CDCl3

Data collected on: Dec 12 2009

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.881 sec
 Width 10000.0 Hz
 16 repetitions
 OBSERVE H1 499.8984089 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min 38 sec



20091216diomethylsubstrateC13

Sample Name:

Archive directory:

Sample directory:

Fidfile: std13c

Pulse Sequence: std13c (s2pu1)

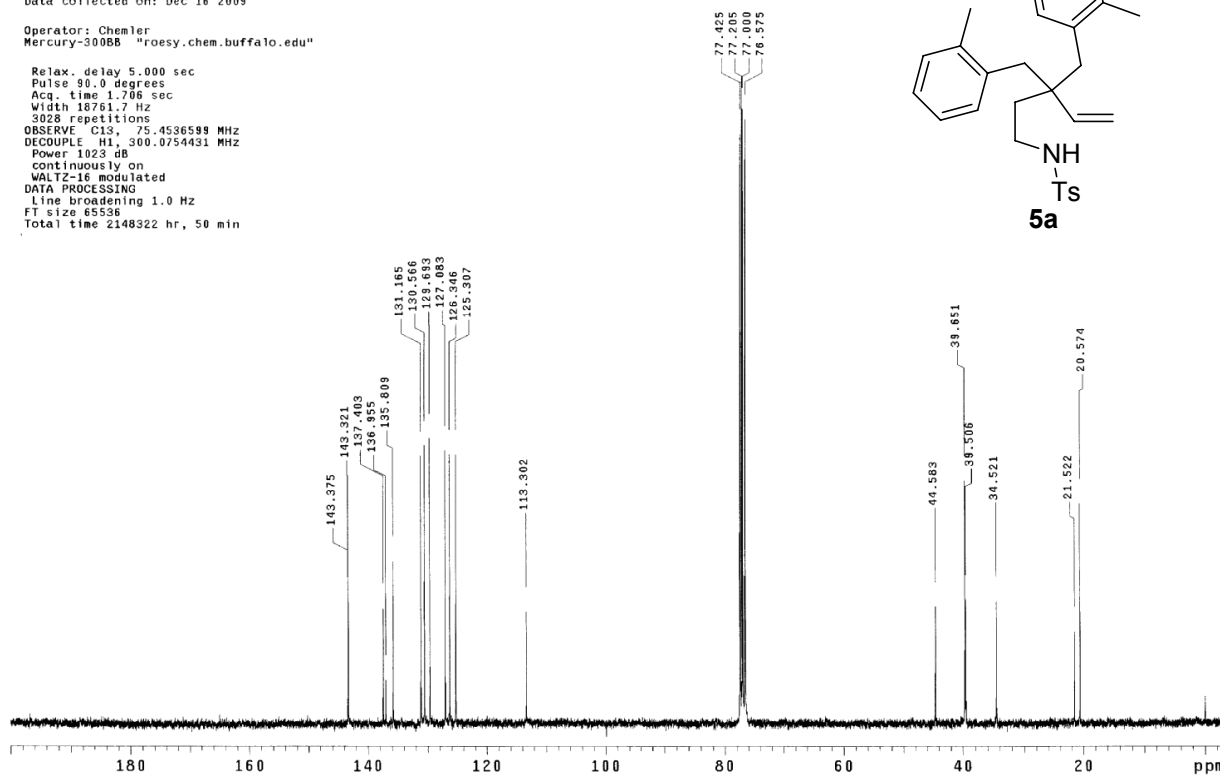
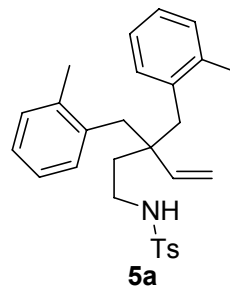
Solvent: CDCl3

Data collected on: Dec 16 2009

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec
 Pulse 30.0 degrees
 Acq. time 1.706 sec
 Width 18761.7 Hz
 3028 repetitions
 OBSERVE C13 75.4536599 MHz
 DECOUPLE H1 300.0754431 MHz
 Power 1023 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 2148322 hr, 50 min



20091012ditrifluoromethylbenzylbutyrolactone

Sample Name:

Archive directory:

Sample directory:

FidFile: std1h

Pulse Sequence: std1h (s2pul)

Solvent: CDCl3

Data collected on: Oct 12 2009

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 1.000 sec

Pulse 47.9 degrees

Acq. time 1.800 sec

Width 6000.6 Hz

16 repetitions

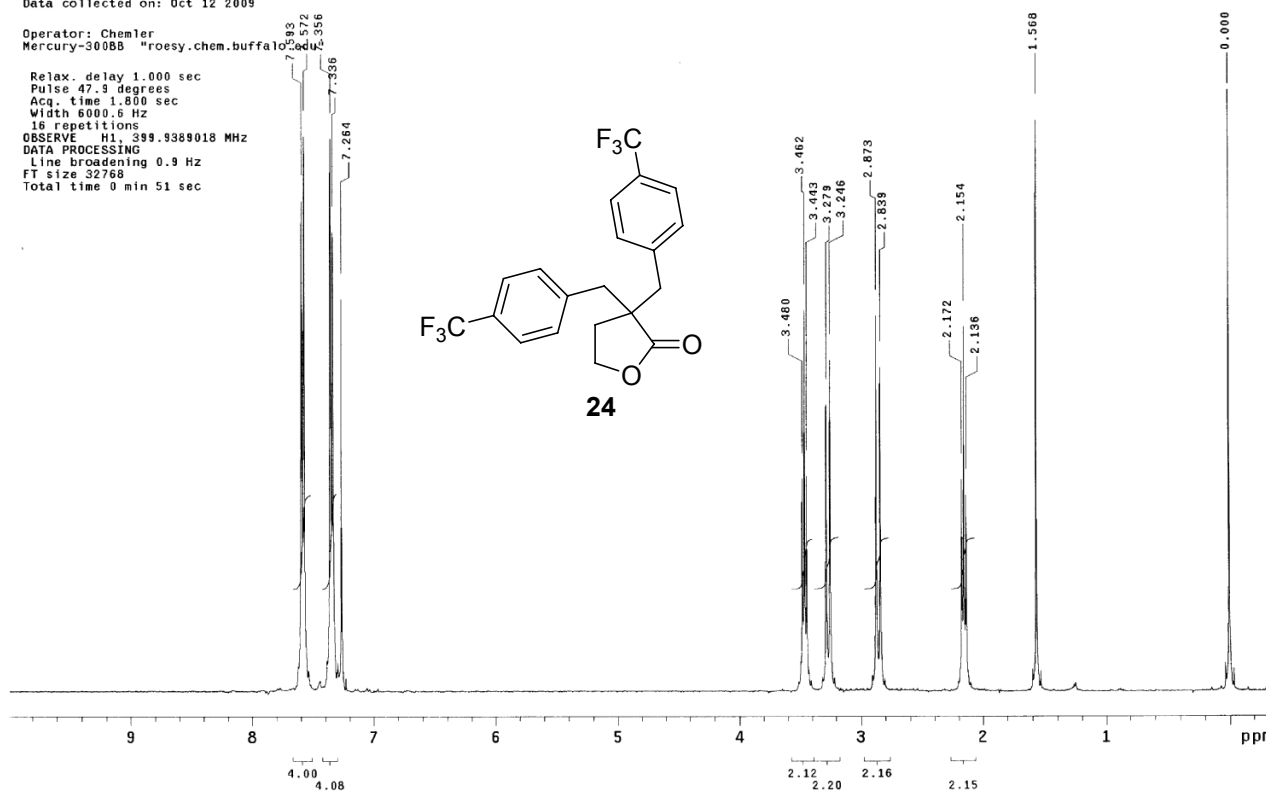
OBSERVE H1, 399.9389018 MHz

DATA PROCESSING

Line broadening 0.9 Hz

FT size 32768

Total time 0 min 51 sec



20091016ditrifluoromethylbenzylbutyrolactoneC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pul)

Solvent: CDCl3

Data collected on: Oct 16 2009

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

5838 repetitions

OBSERVE C13, 75.4536593 MHz

DECOUPLE H1, 300.0754431 MHz

Power 1023 db

continuously on

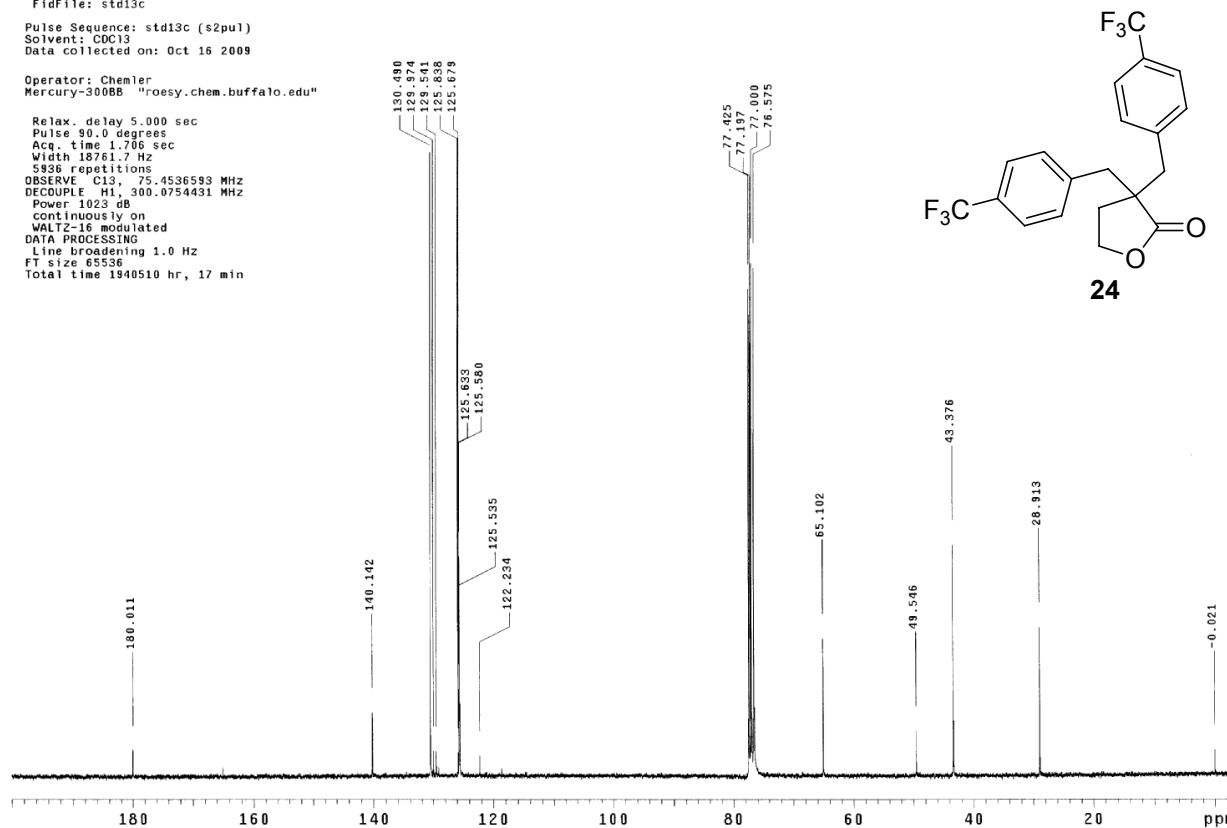
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1940510 hr, 17 min



20091018ditrifluoromethylbenzylalkenealcohol12

Sample Name:

Archive directory:

Sample directory:

FidFile: H1

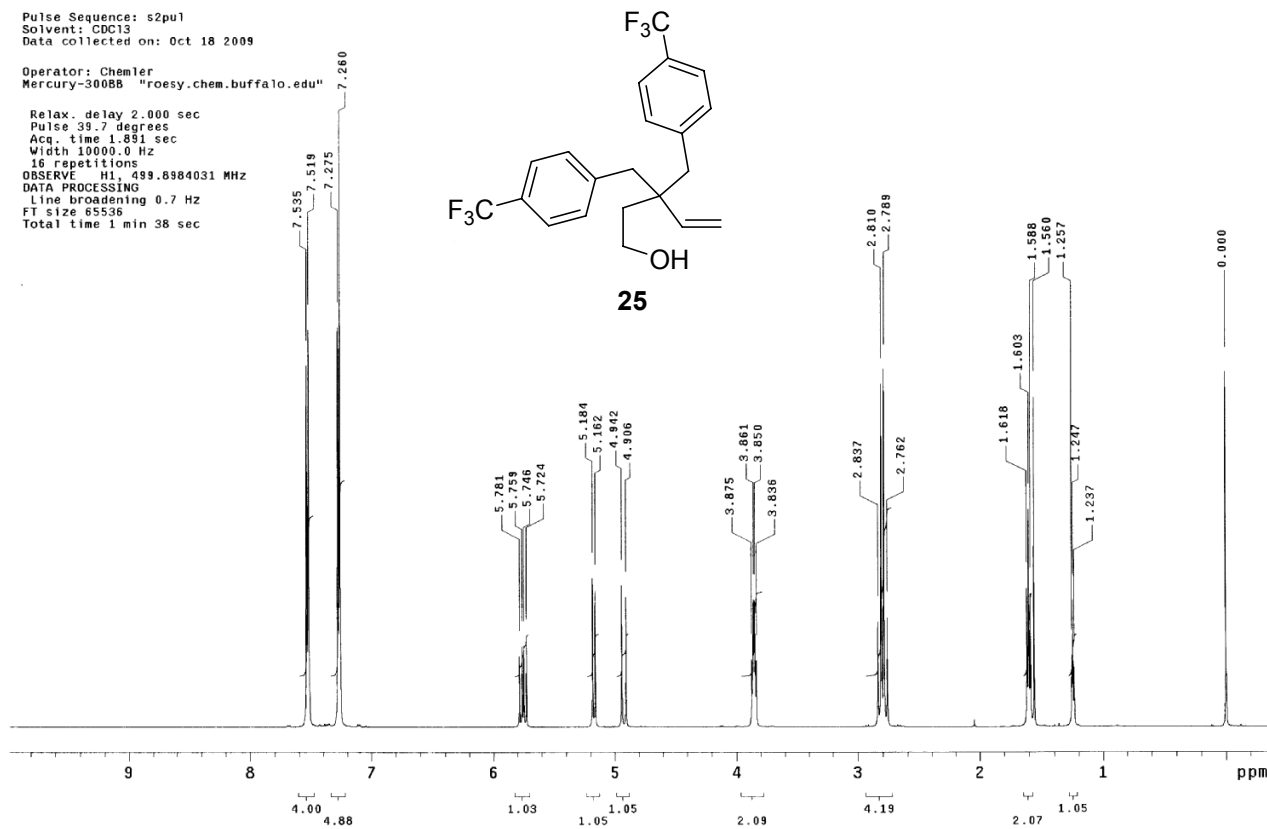
Pulse Sequence: s2pu1

Solvent: CDCl3

Data collected on: Oct 18 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec
Pulse 39.7 degrees
Acq. time 1.891 sec
Width 10000.0 Hz
16 repetitions
OBSERVE H1, 499.8984031 MHz
DATA PROCESSING
Line broadening 0.7 Hz
FT size 65536
Total time 1 min 38 sec



20091018ditrifluoromethylbenzylalkenealcohol13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

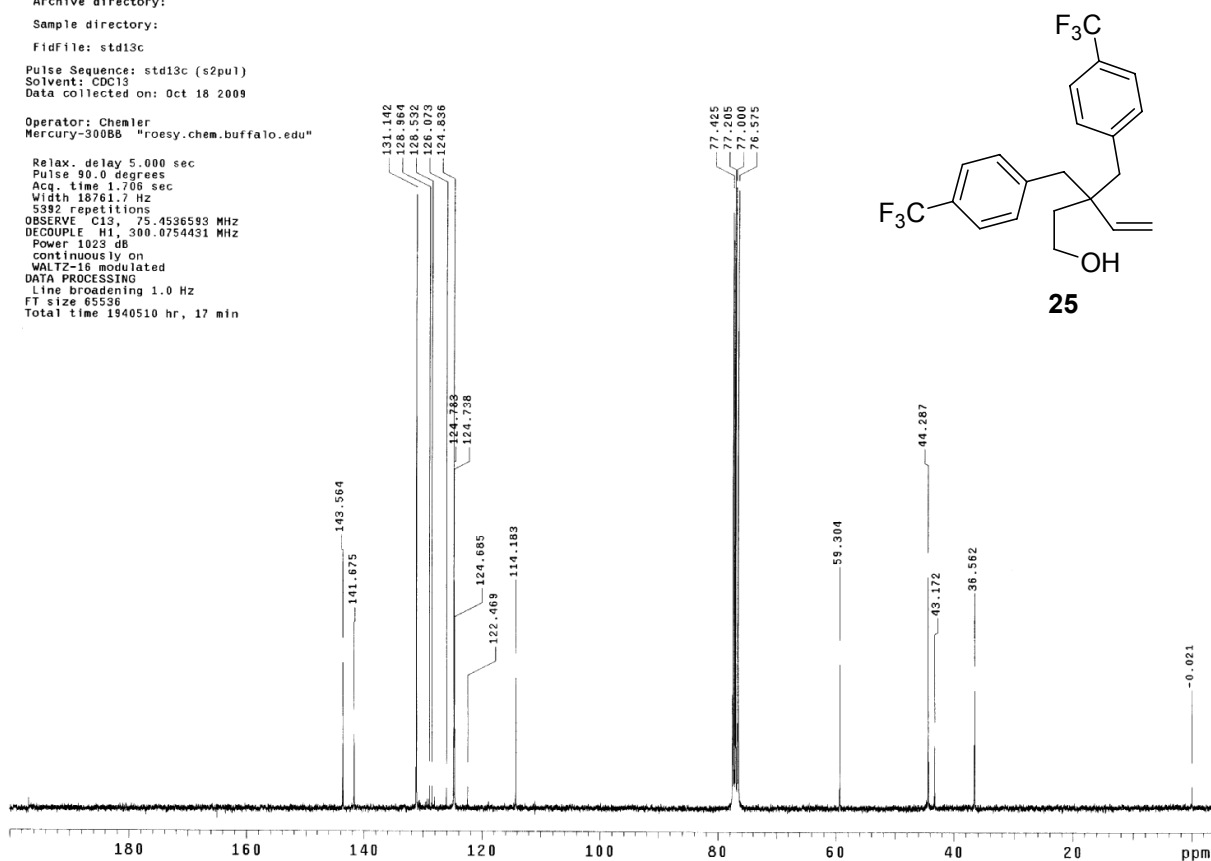
Pulse Sequence: std13c (s2pu1)

Solvent: CDCl3

Data collected on: Oct 18 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec
Pulse 90.0 degrees
Acq. time 1.706 sec
Width 18761.7 Hz
5392 repetitions
OBSERVE C13, 75.4536593 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 1940510 hr, 17 min



20091119dtrifluoromethylsubstrate

Sample Name:

Archive directory:

Sample directory:

FidFile: H1

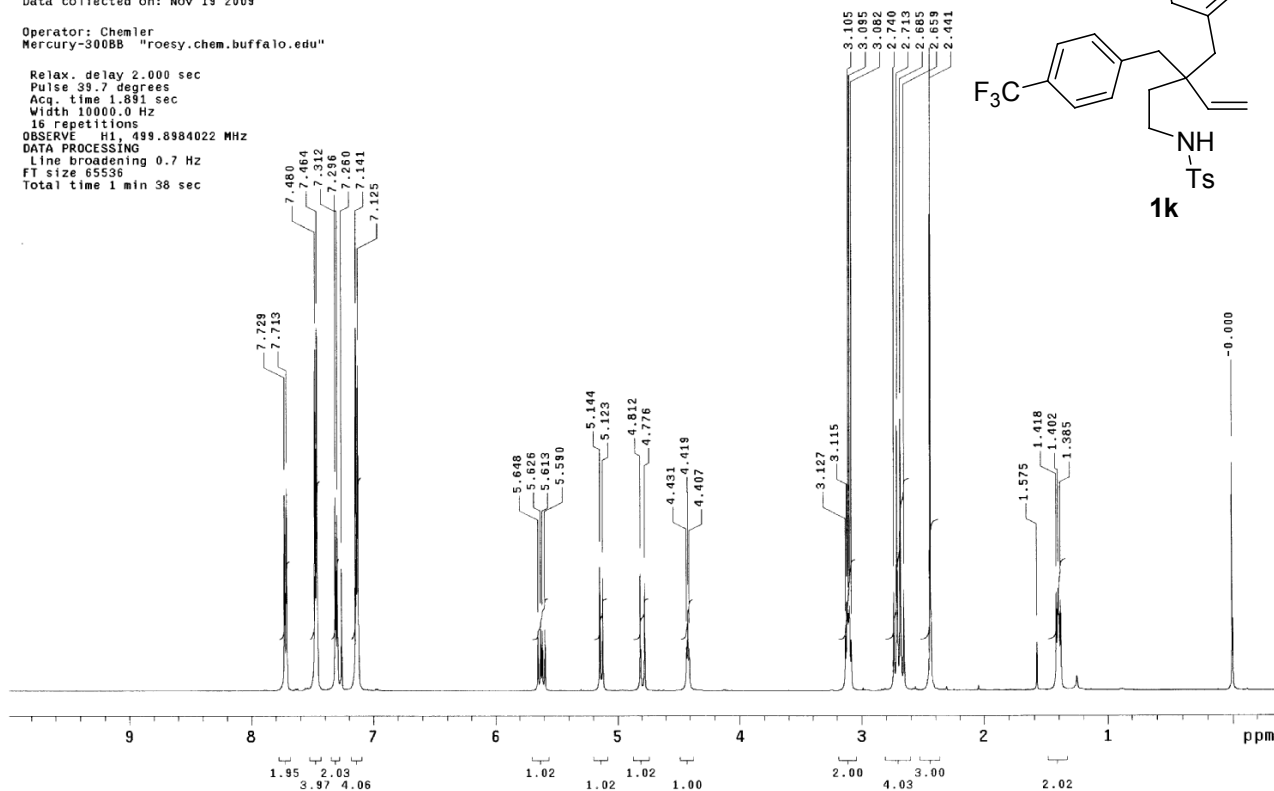
Pulse Sequence: s2pul

Solvent: CDCl3

Data collected on: Nov 19 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.891 sec
 Width 10000.0 Hz
 16 repetitions
 OBSERVE H1, 499.8984022 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min 38 sec



20091130dtrifluoromethylsubstrateC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

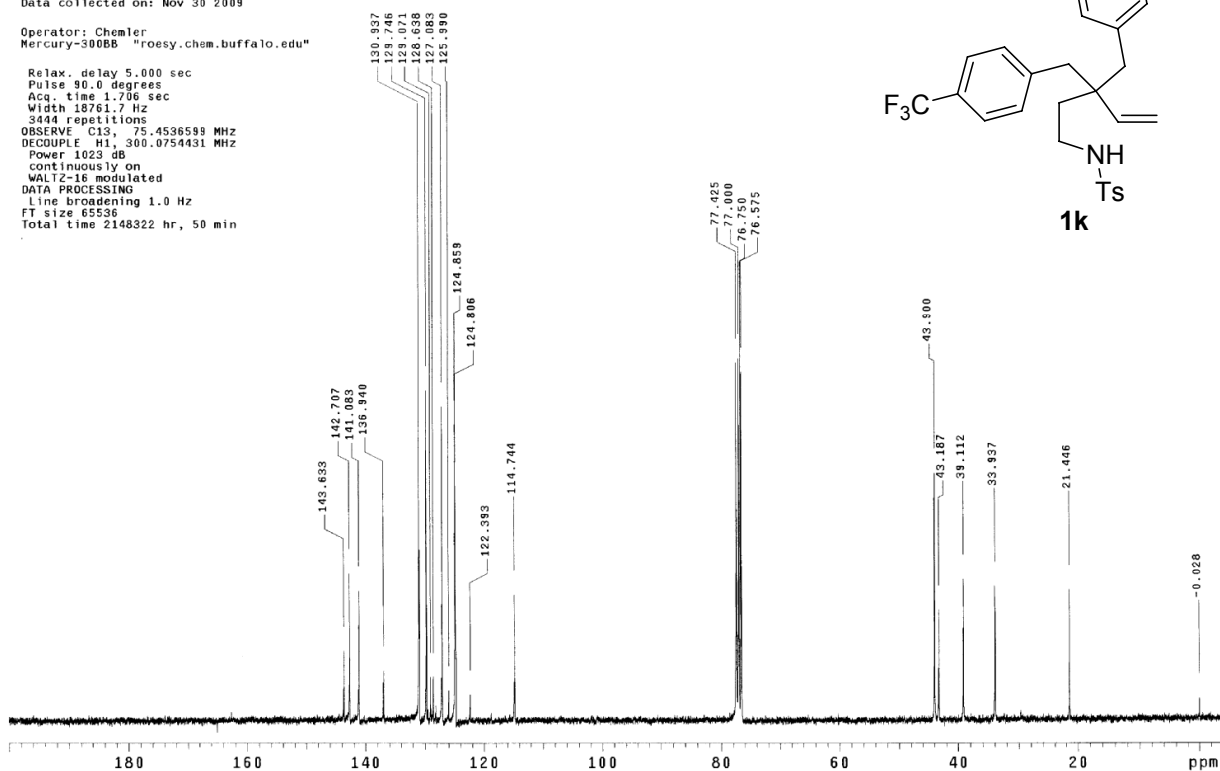
Pulse Sequence: std13c (s2pul)

Solvent: CDCl3

Data collected on: Nov 30 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec
 Pulse 90.0 degrees
 Acq. time 1.706 sec
 Width 18761.7 Hz
 3444 repetitions
 OBSERVE C13, 75.4536599 MHz
 DECOUPLE H1, 300.0754431 MHz
 Power 1023 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 2148322 hr, 50 min



20090929Tsbutyrolactam

Sample Name:

Archive directory:

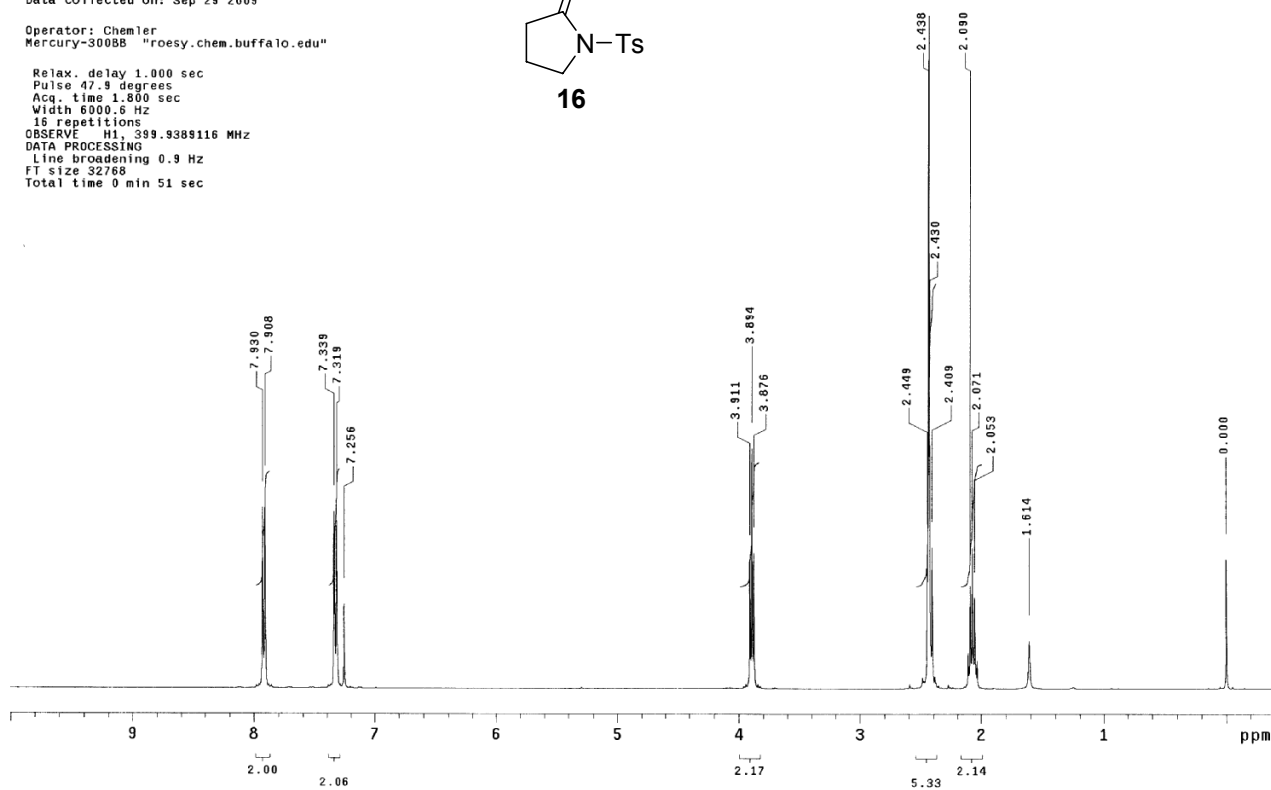
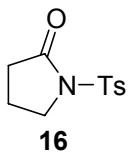
Sample directory:

FidFile: std1h

Pulse Sequence: std1h (s2pu1)

Solvent: CDCl3

Data collected on: Sep 29 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 1.000 sec
Pulse 47.9 degrees
Acq. time 1.800 sec
Width 6000.6 Hz
16 repetitions
OBSERVE H1, 399.9389116 MHz
DATA PROCESSING
Line broadening 0.9 Hz
FT size 32768
Total time 0 min 51 sec

20091022TsbutyrolactamC13

Sample Name:

Archive directory:

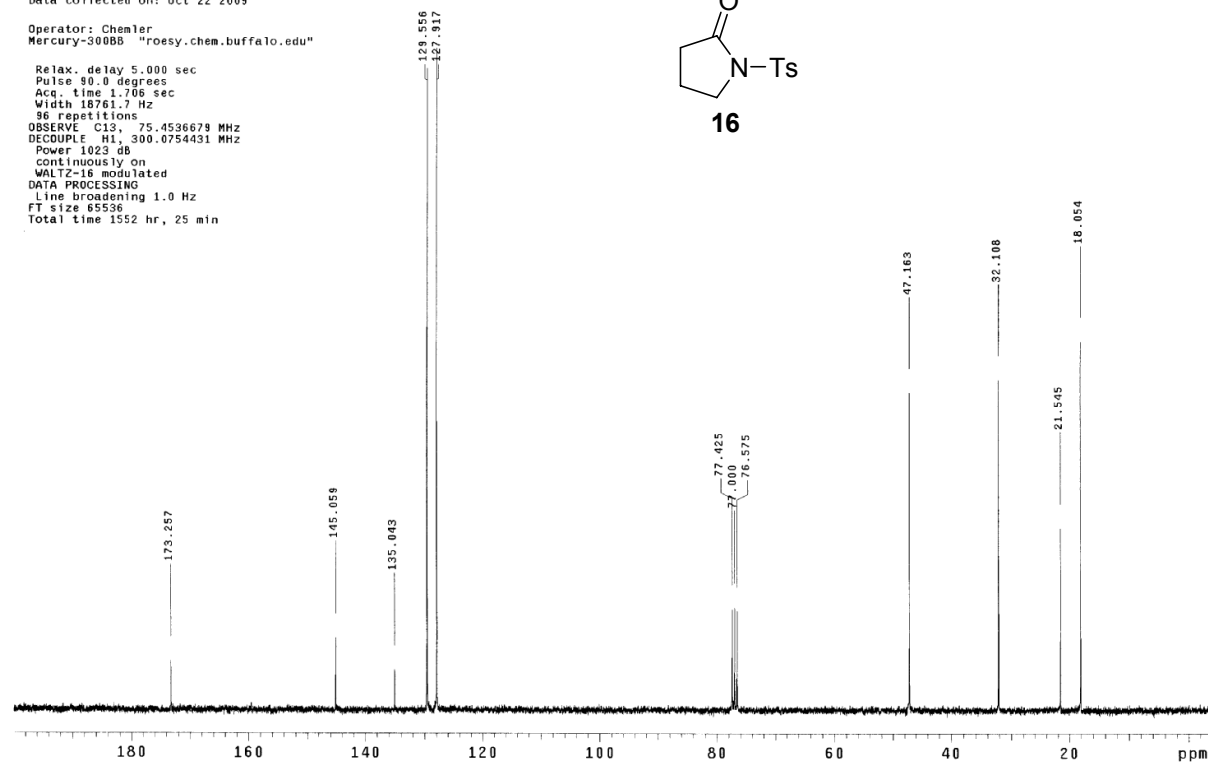
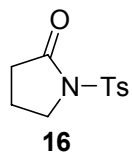
Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)

Solvent: CDCl3

Data collected on: Oct 22 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 5.000 sec
Pulse 80.0 degrees
Acq. time 1.706 sec
Width 18761.7 Hz
36 repetitions
OBSERVE C13, 75.4536679 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 db
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 85536
Total time 1552 hr, 25 min

20100201d3methoxyllactam

Sample Name:

Archive directory:

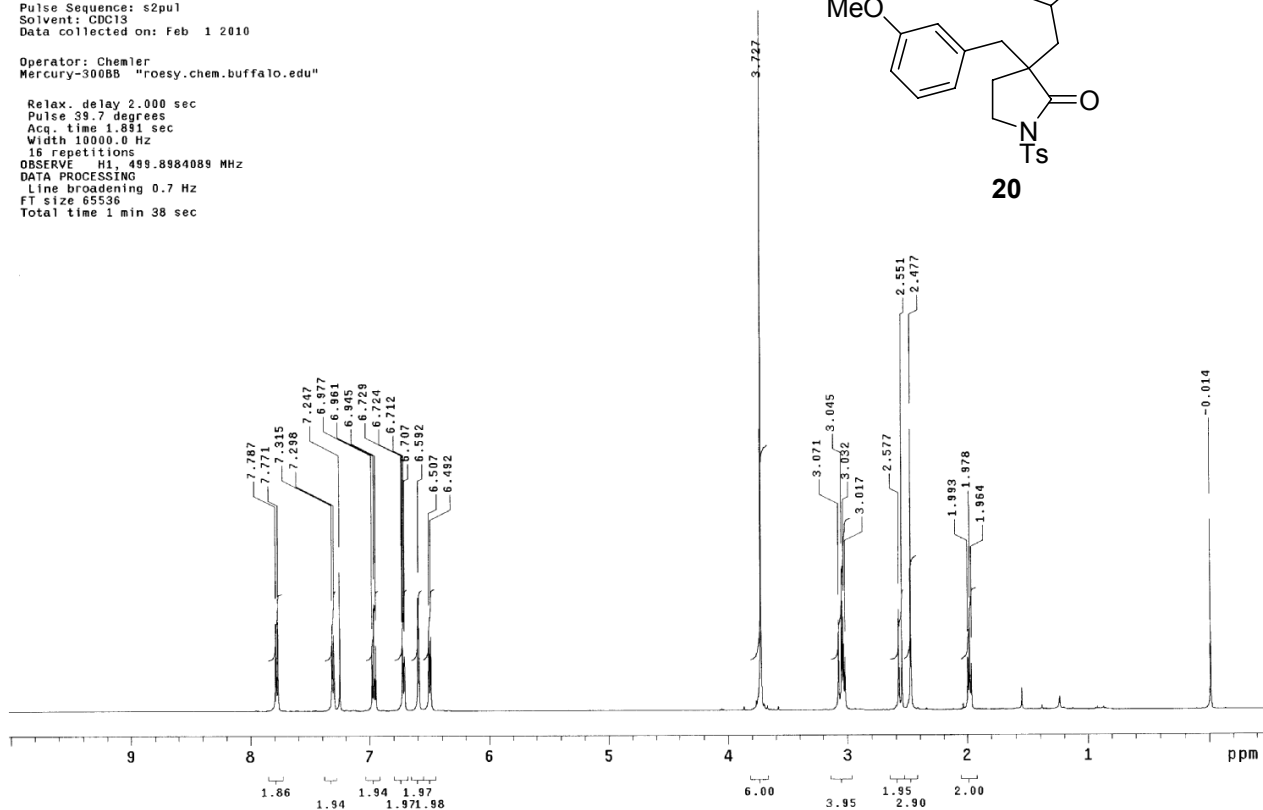
Sample directory:

FidFile: H1

Pulse Sequence: s2pul

Solvent: CDCl3

Data collected on: Feb 1 2010

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 2.000 sec
Pulse 39.7 degrees
Acq. time 1.891 sec
Width 10000.0 Hz
15 repetitions
OBSERVE H1, 499.8984089 MHz
DATA PROCESSING
Line broadening 0.7 Hz
FT size 65536
Total time 1 min 38 sec

20100201d3methoxyllactamC13

Sample Name:

Archive directory:

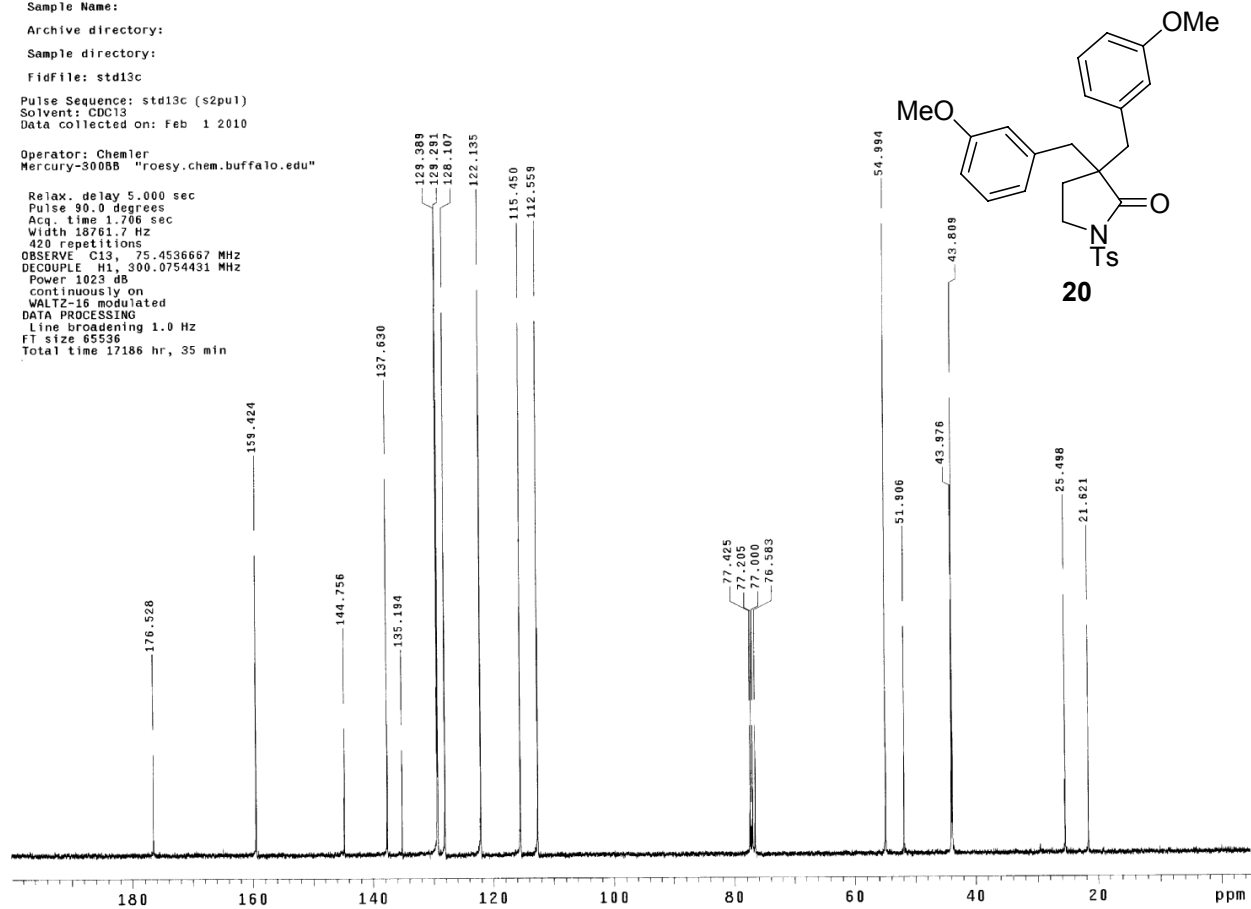
Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pul)

Solvent: CDCl3

Data collected on: Feb 1 2010

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 5.000 sec
Pulse 90.0 degrees
Acq. time 1.706 sec
Width 18781.7 Hz
420 repetitions
OBSERVE C13, 75.4536667 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 17186 hr, 35 min

20100224di3methoxy1substrate

Sample Name:

Archive directory:

Sample directory:

FidFile: H1

Pulse Sequence: s2pu1

Solvent: CDCl3

Data collected on: Feb 24 2010

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec

Pulse 39.7 degrees

Acq. time 1.891 sec

Width 10000.0 Hz

16 repetitions

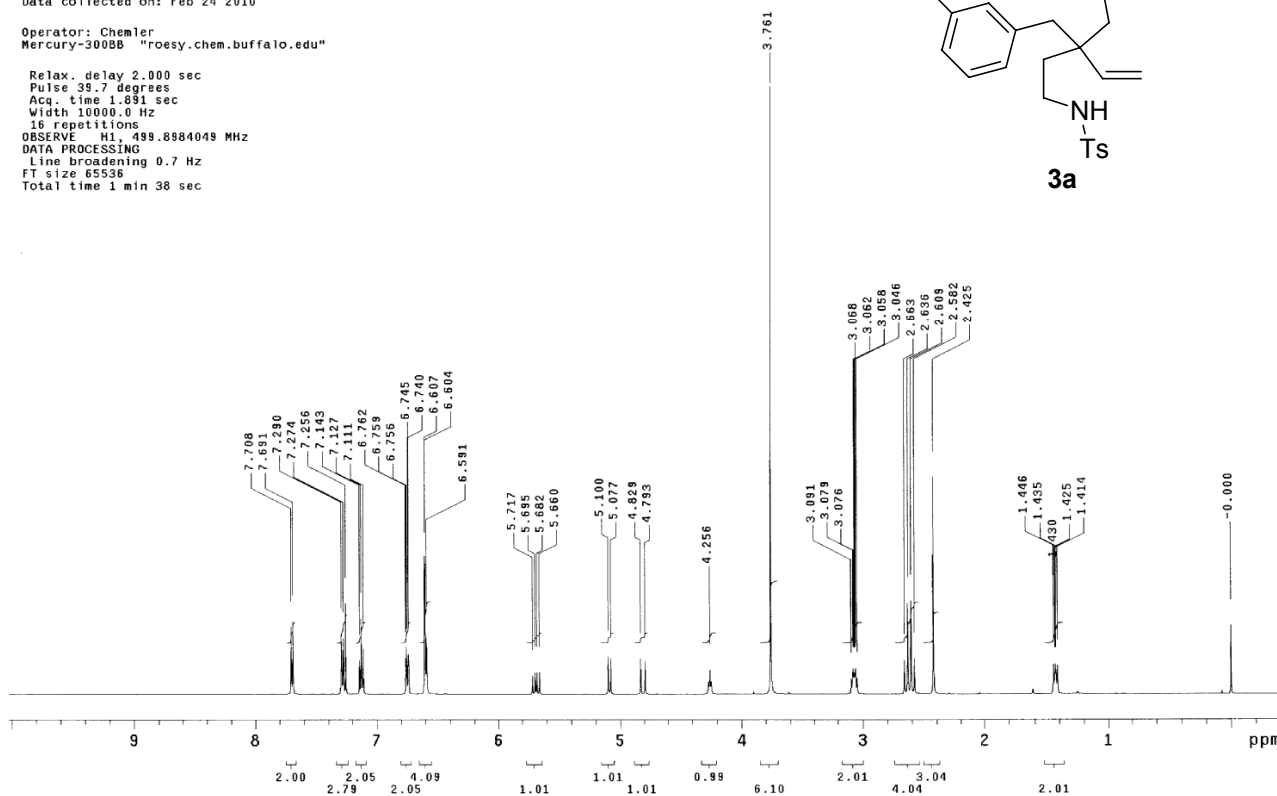
OBSERVE H1, 499.8984049 MHz

DATA PROCESSING

Line broadening 0.7 Hz

FT size 65536

Total time 1 min 38 sec



20100224di3methoxy1substrateC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)

Solvent: CDCl3

Data collected on: Feb 24 2010

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

3272 repetitions

OBSERVE C13, 75.4536627 MHz

DECOUPLE H1, 300.0754431 MHz

Power 1023 dB

continuously on

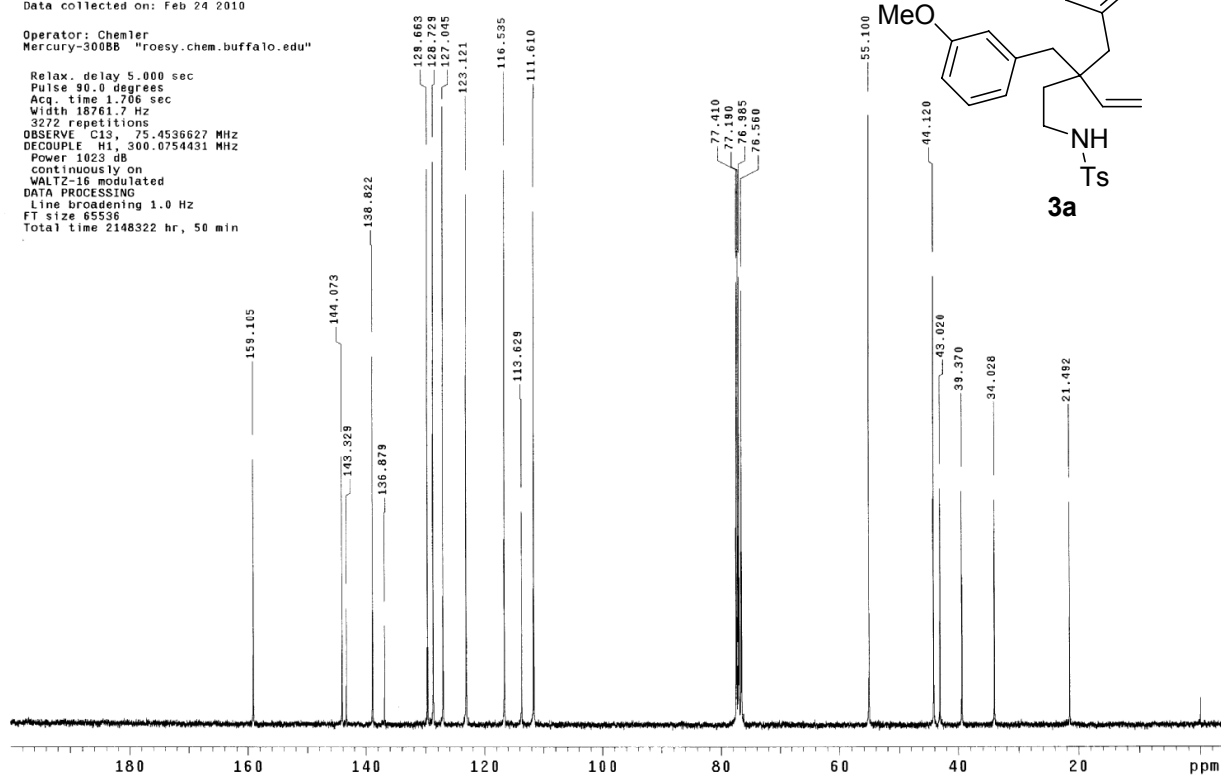
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2148322 hr, 50 min



20100726dithiomethylactamb

Sample Name:

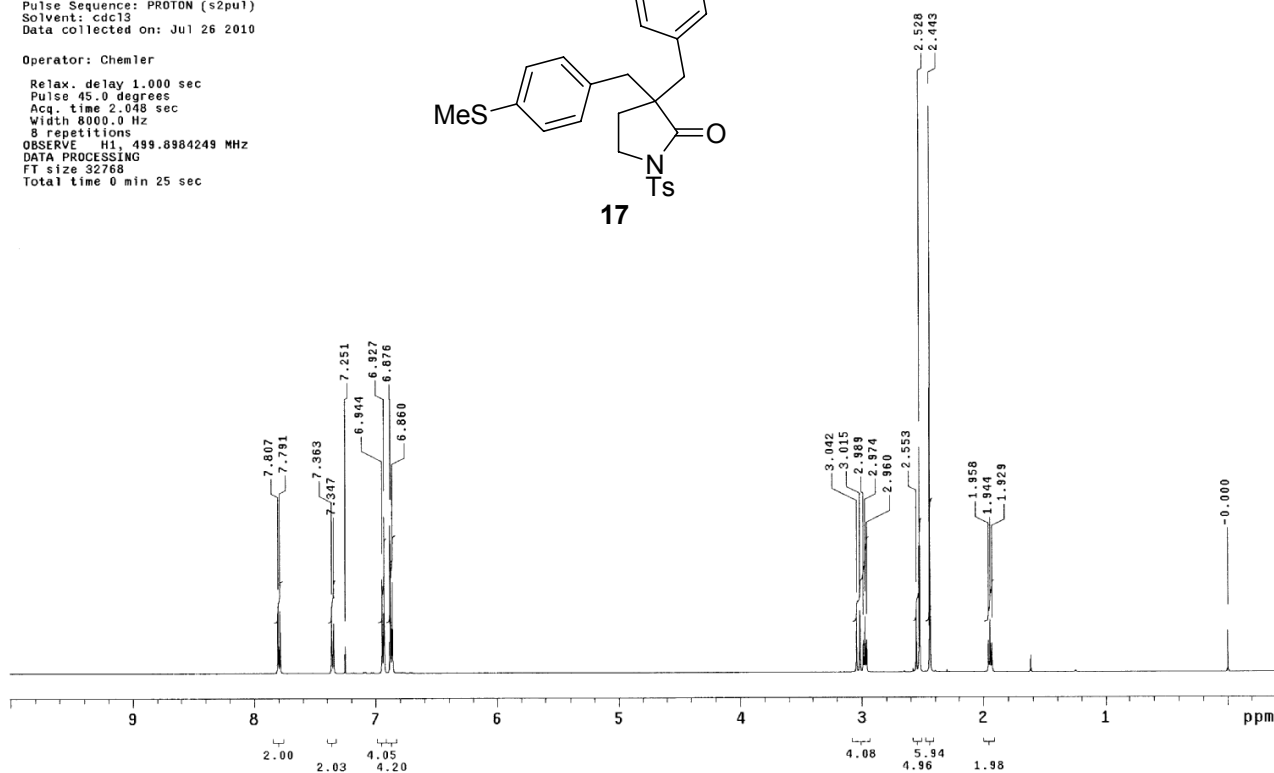
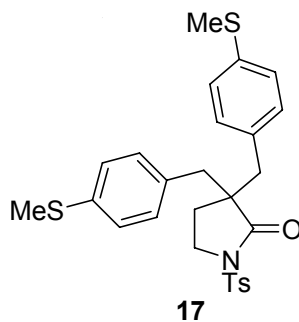
Data Collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Jul 26 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984249 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100727dithiomethylactamC13B

Sample Name:

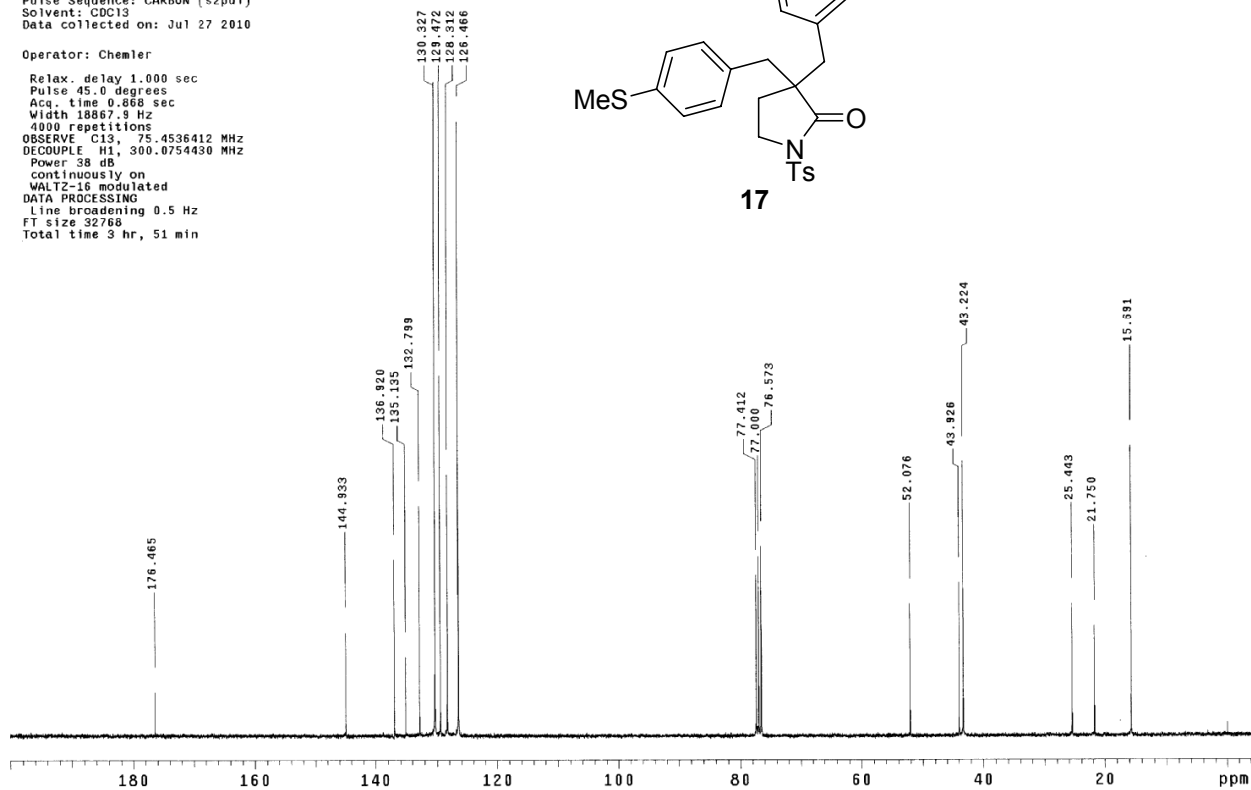
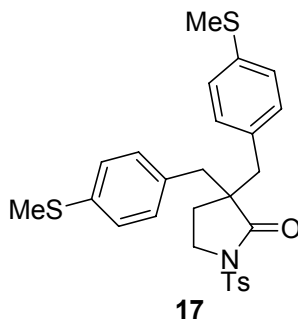
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: CDC13
Data collected on: Jul 27 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
4000 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 3 hr, 51 min

20100817dithiomethylsubstrate

Sample Name:

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

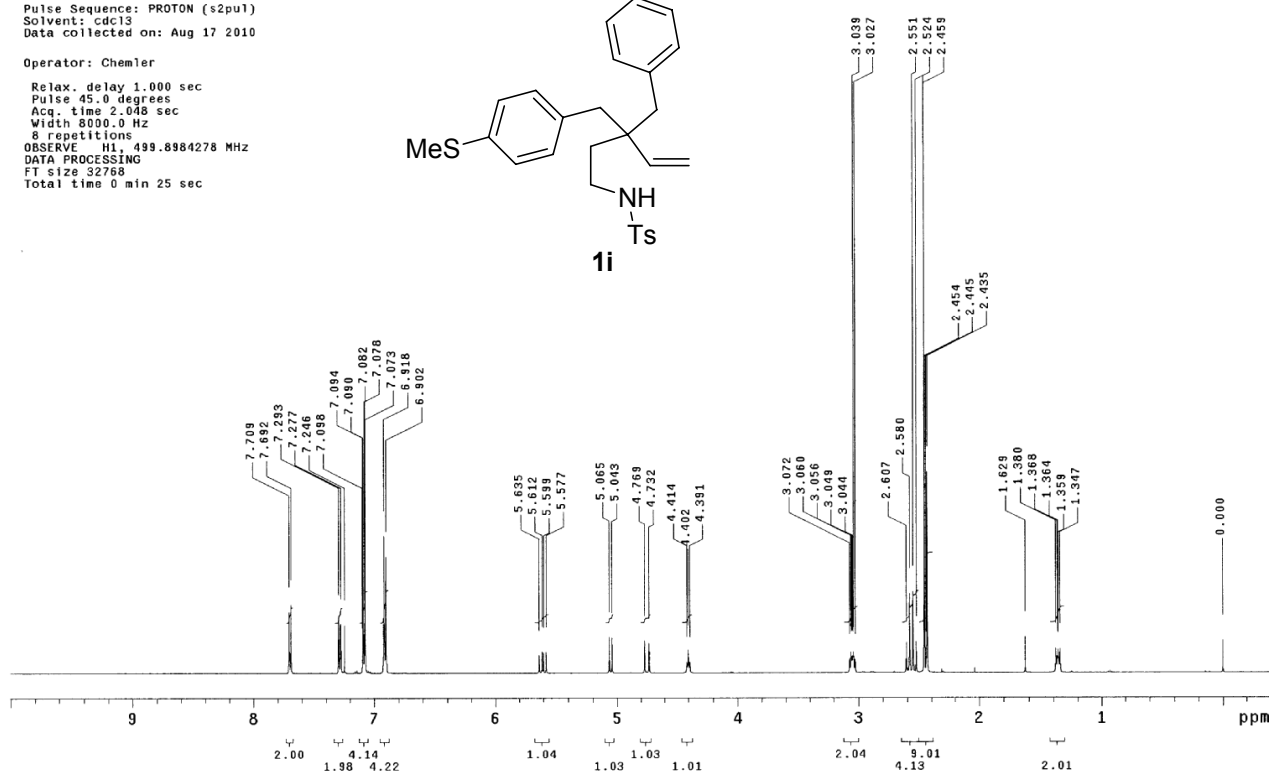
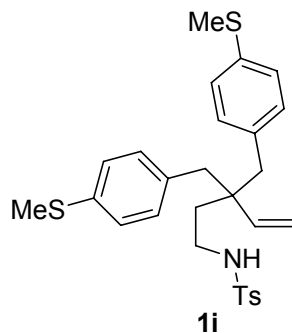
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Aug 17 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984278 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100817dithiomethylsubstrateC13

Sample Name:

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

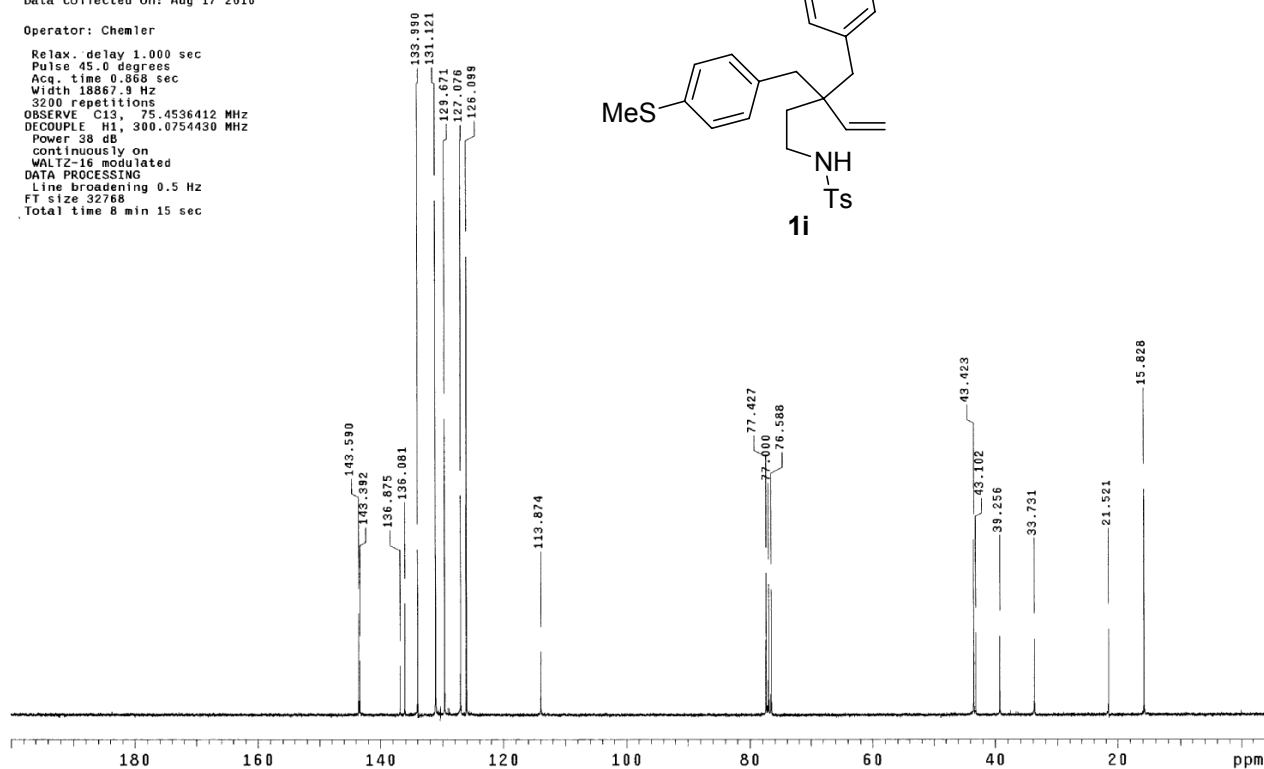
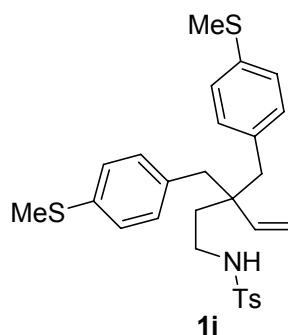
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Aug 17 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3200 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 8 min 15 sec

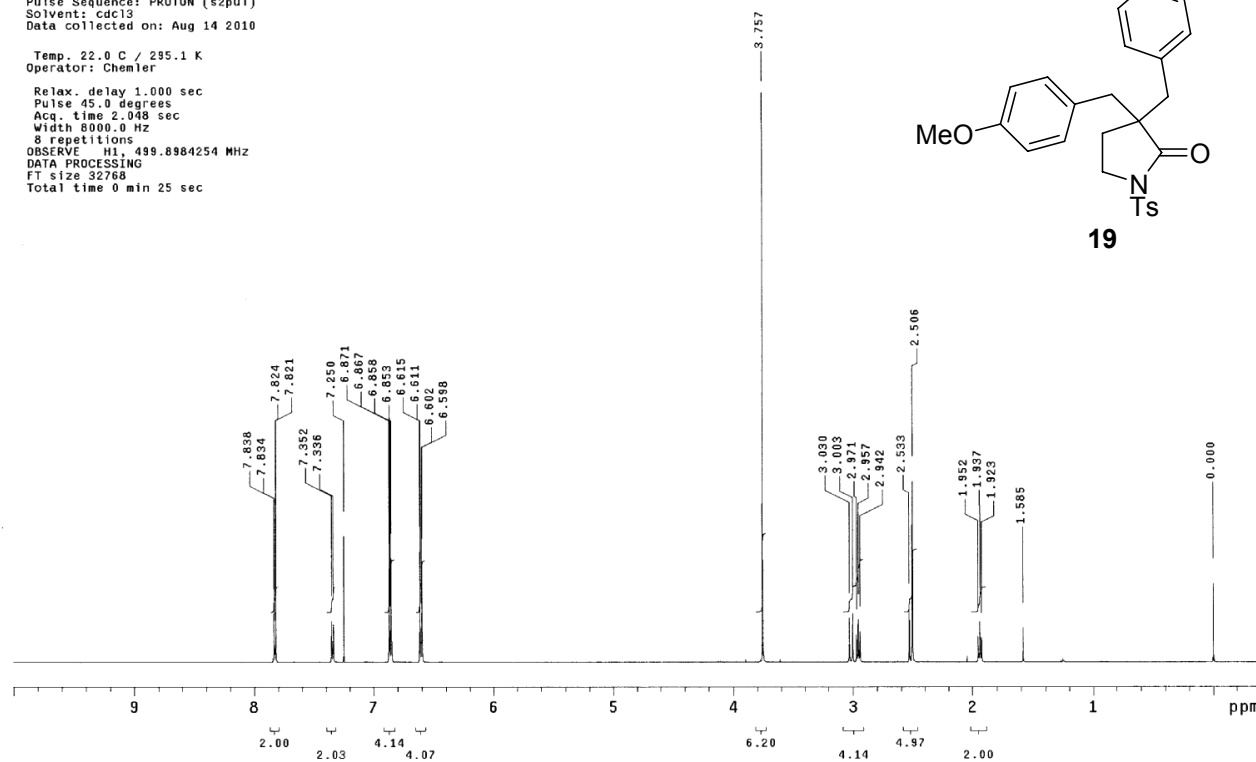
20100814dimethoxyllactam

Sample Name:

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

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: Aug 14 2010Temp. 22.0 C / 295.1 K
Operator: ChemlerRelax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.948 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984254 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100816dimethoxyllactamC13

Sample Name:

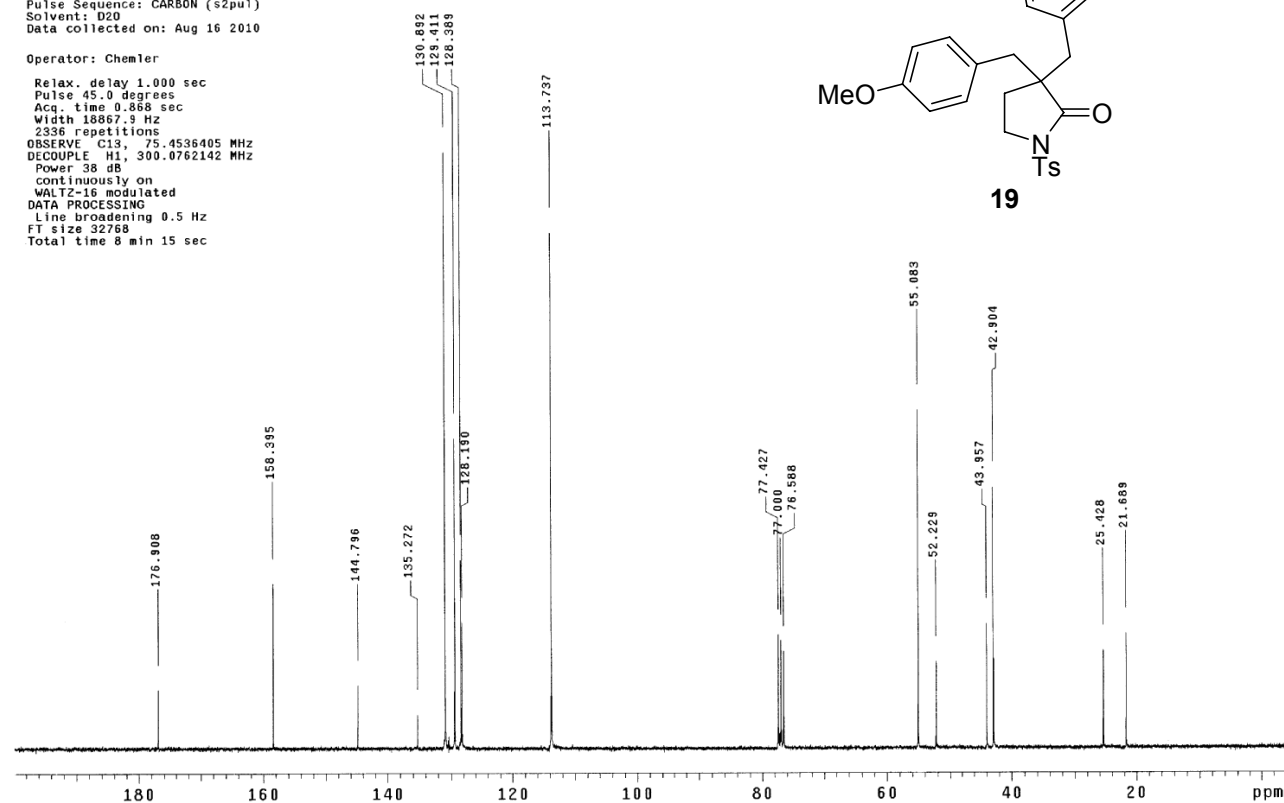
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: D2O
Data collected on: Aug 16 2010

Operator: Chemler

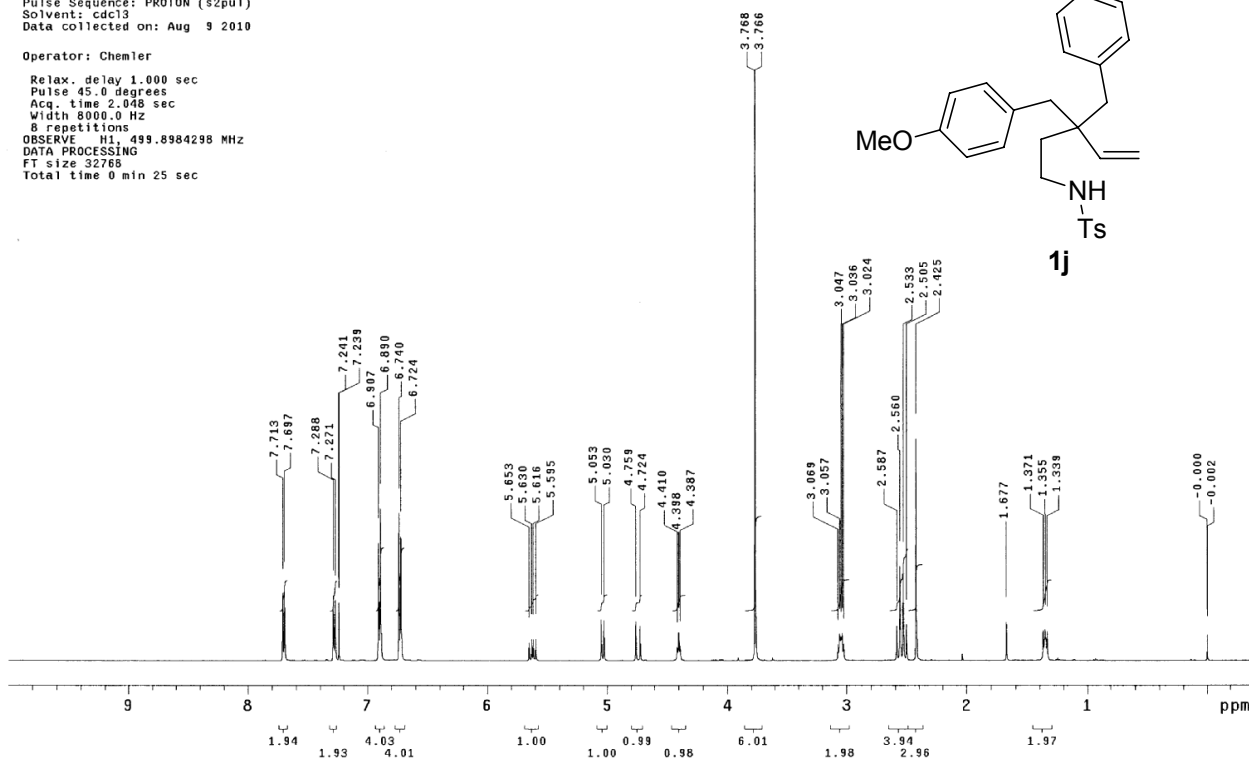
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2336 repetitions
OBSERVE C13, 75.4536405 MHz
DECOUPLE H1, 300.0762142 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 8 min 15 sec

20100809dimethoxysubstrate

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: Aug 9 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.848 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.8984298 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 25 sec

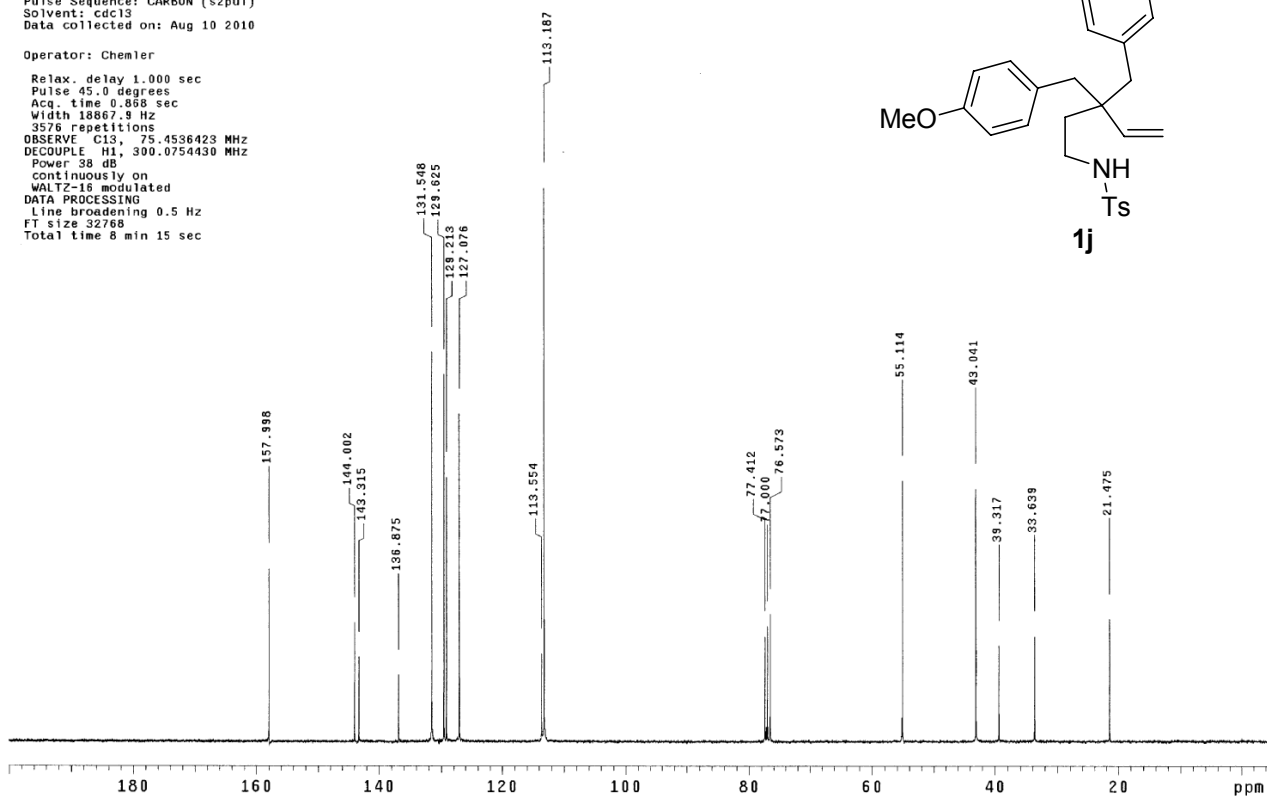


20100810dimethoxysubstrateC13

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: Aug 10 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 3576 repetitions
 OBSERVE C13, 75.4536423 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 8 min 15 sec



20091123diomethoxybutyrolactam

Sample Name:

Archive directory:

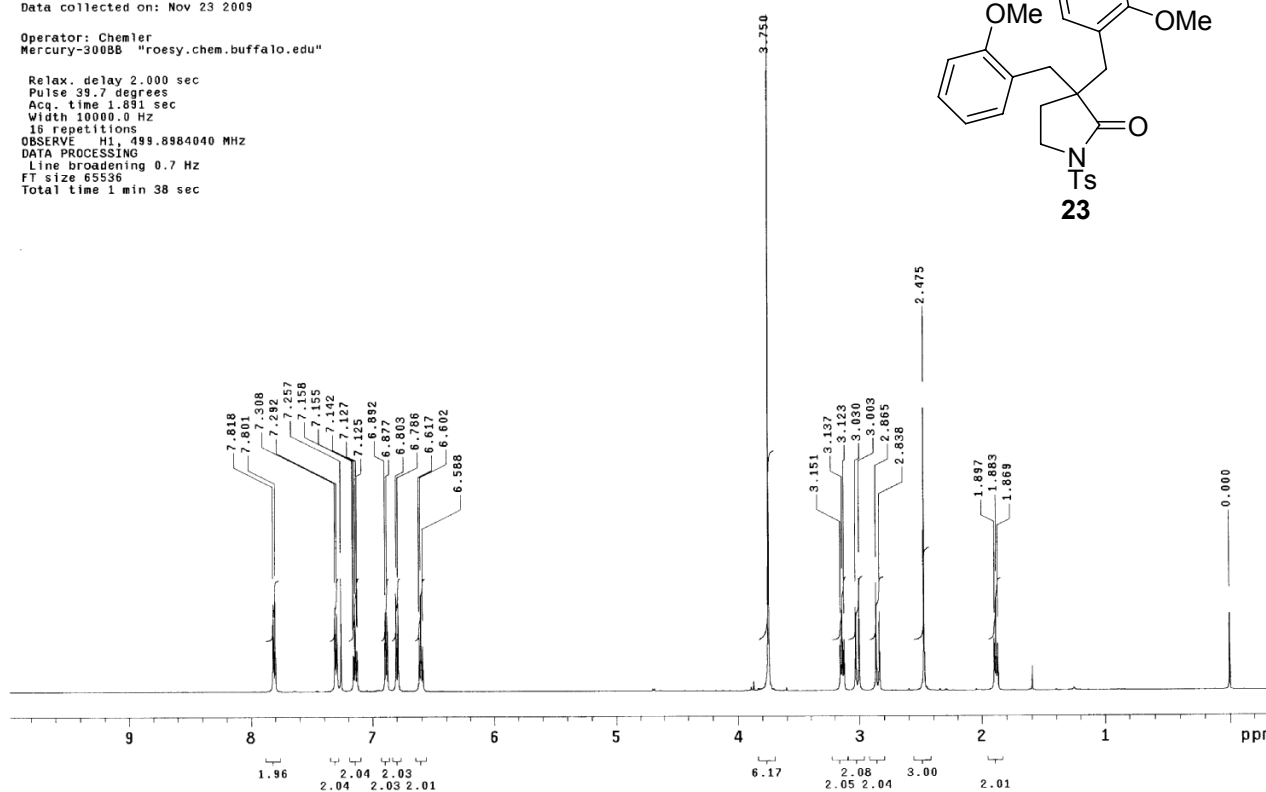
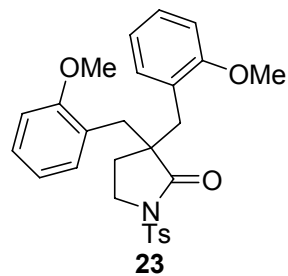
Sample directory:

FidFile: H1

Pulse Sequence: s2pu1

Solvent: CDCl3

Data collected on: Nov 23 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 2.000 sec
Pulse 39.7 degrees
Acq. time 1.891 sec
Width 10000.0 Hz
16 repetitions
OBSERVE H1, 499.8984040 MHz
DATA PROCESSING
Line broadening 0.7 Hz
FT size 65536
Total time 1 min 38 sec

20091123diomethoxybutyrolactamC13

Sample Name:

Archive directory:

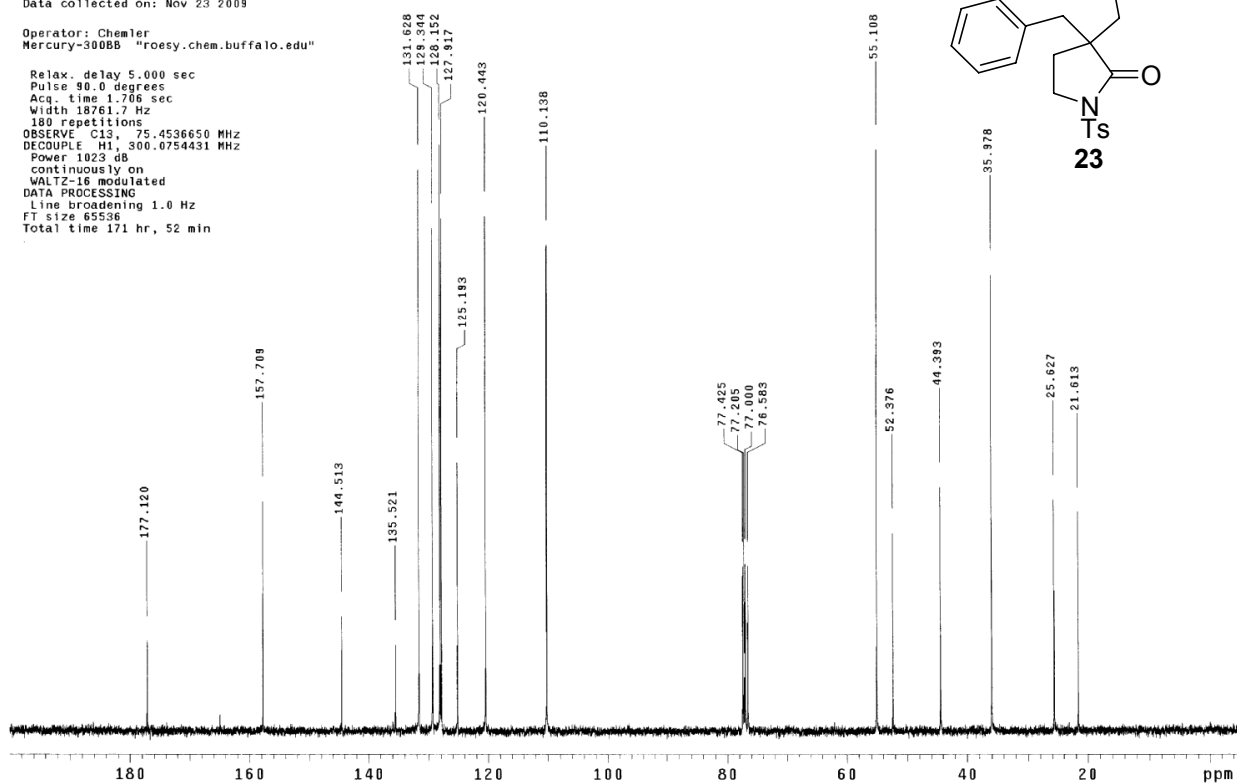
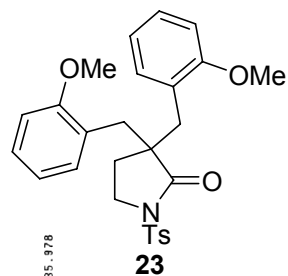
Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)

Solvent: CDCl3

Data collected on: Nov 23 2009

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 5.000 sec
Pulse 90.0 degrees
Acq. time 1.706 sec
Width 18761.7 Hz
180 repetitions
OBSERVE C13, 75.4536650 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 171 hr, 52 min

20100624diomethoxylsubstrate

Sample Name:

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

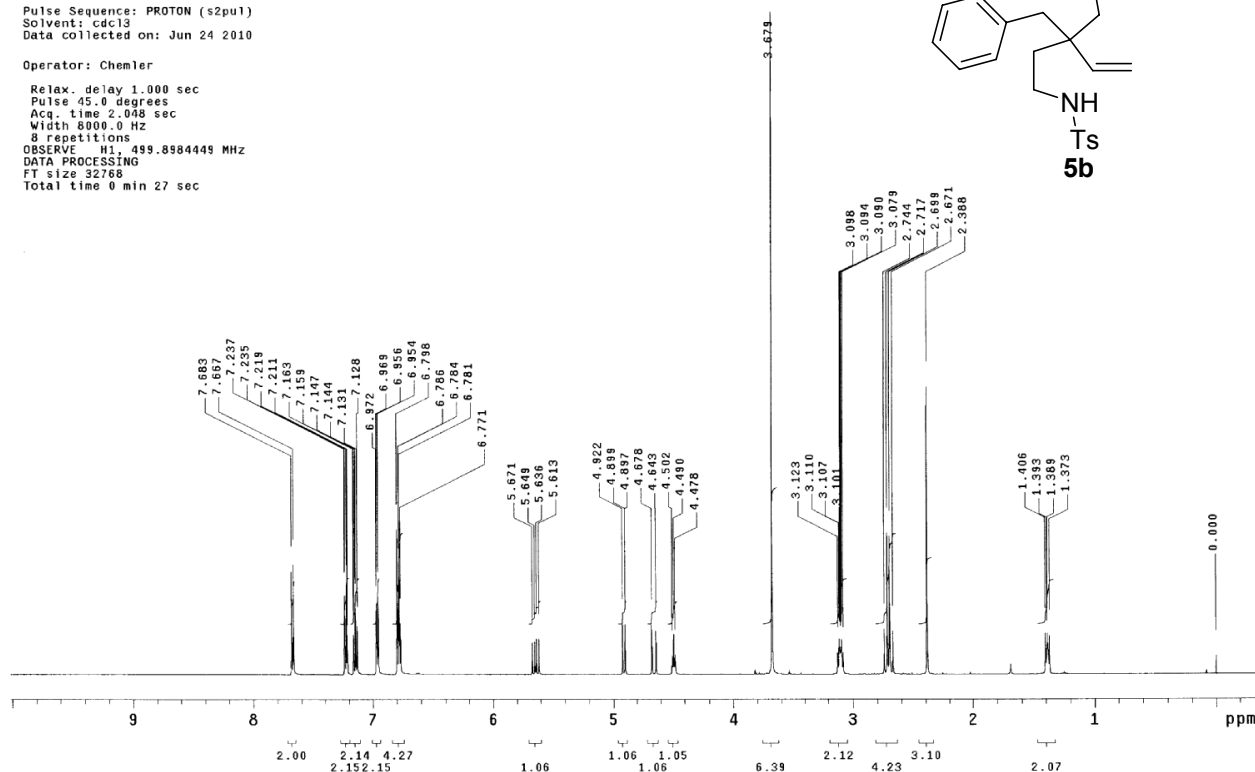
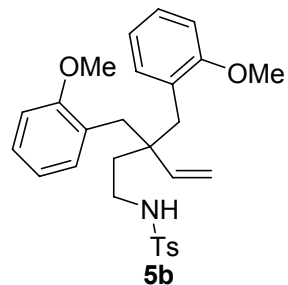
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Jun 24 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984449 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 27 sec

20100624diomethoxylsubstrateC13

Sample Name:

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

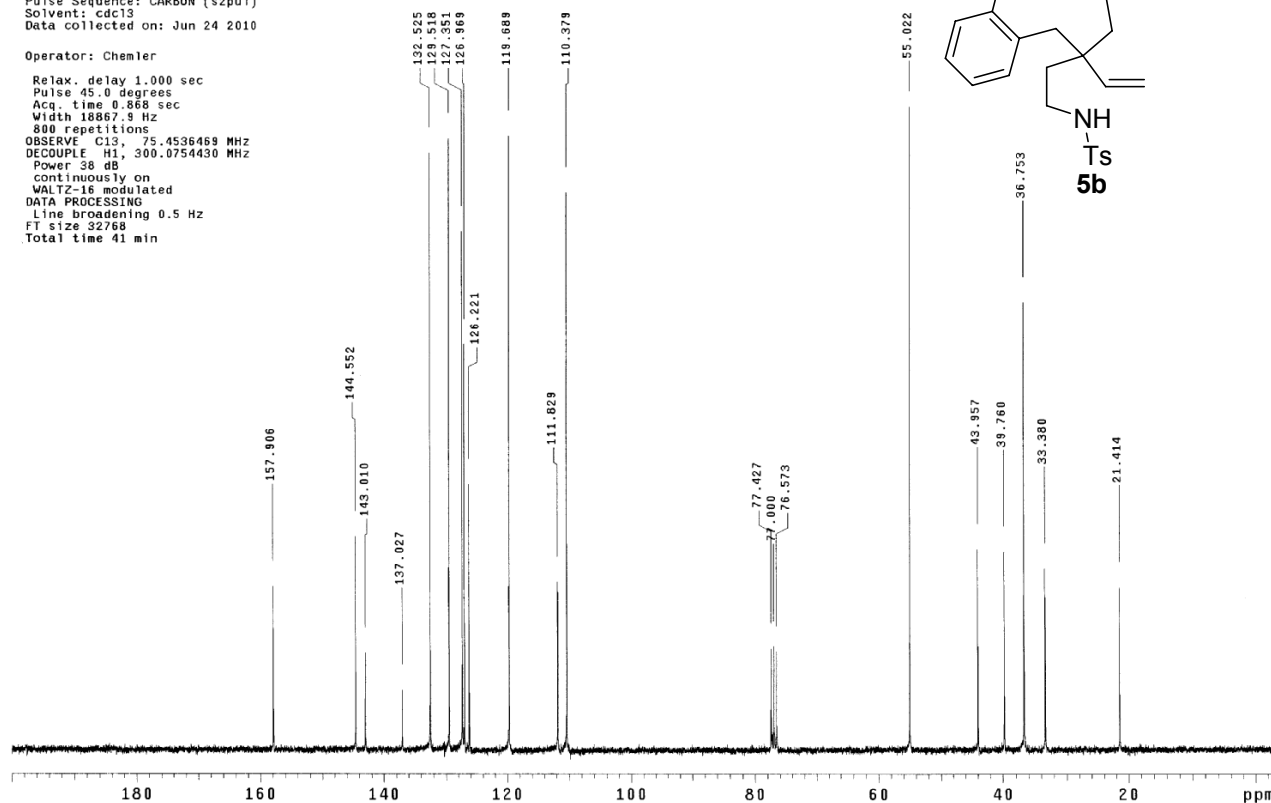
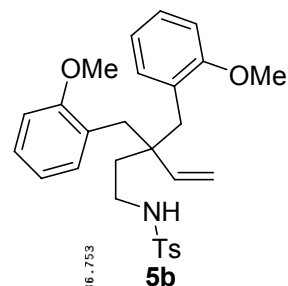
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Jun 24 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
800 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 41 min

20100802omethoxylactone1

Sample Name:

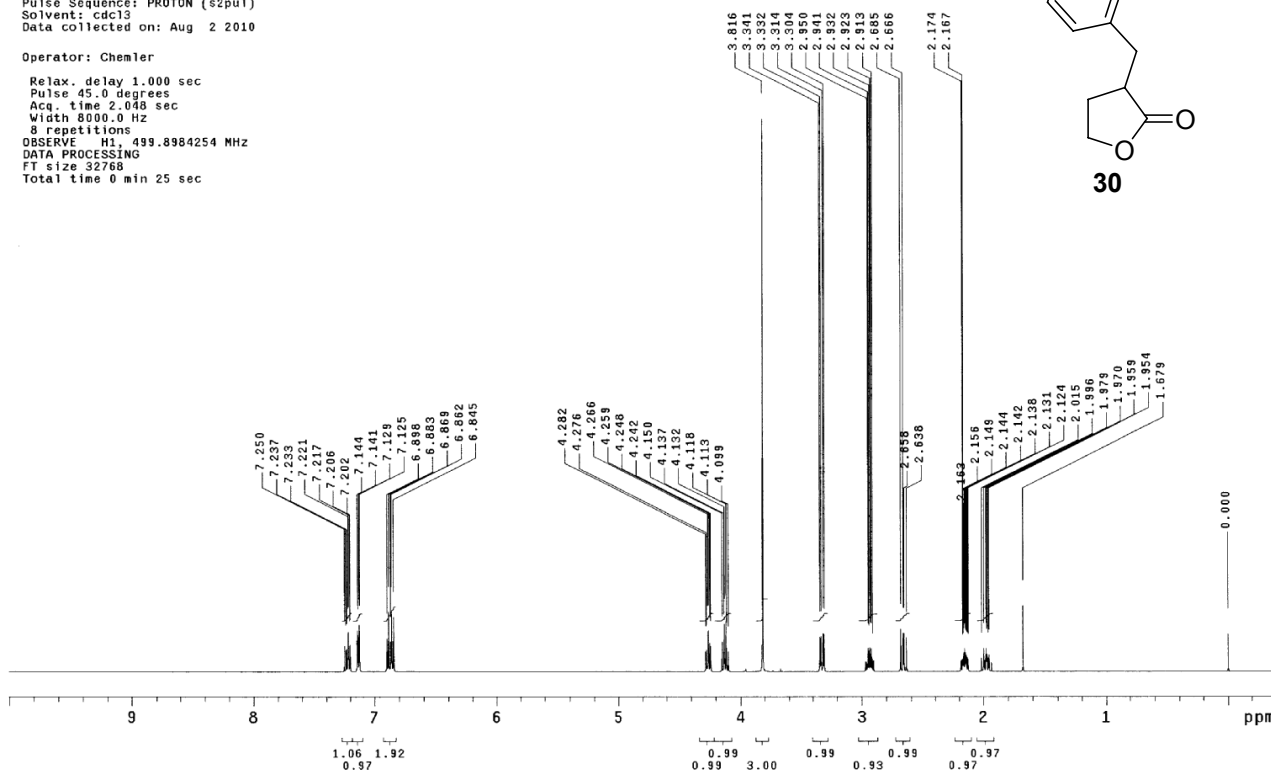
Data Collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Aug 2 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984254 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100802omethoxylactoneC13

Sample Name:

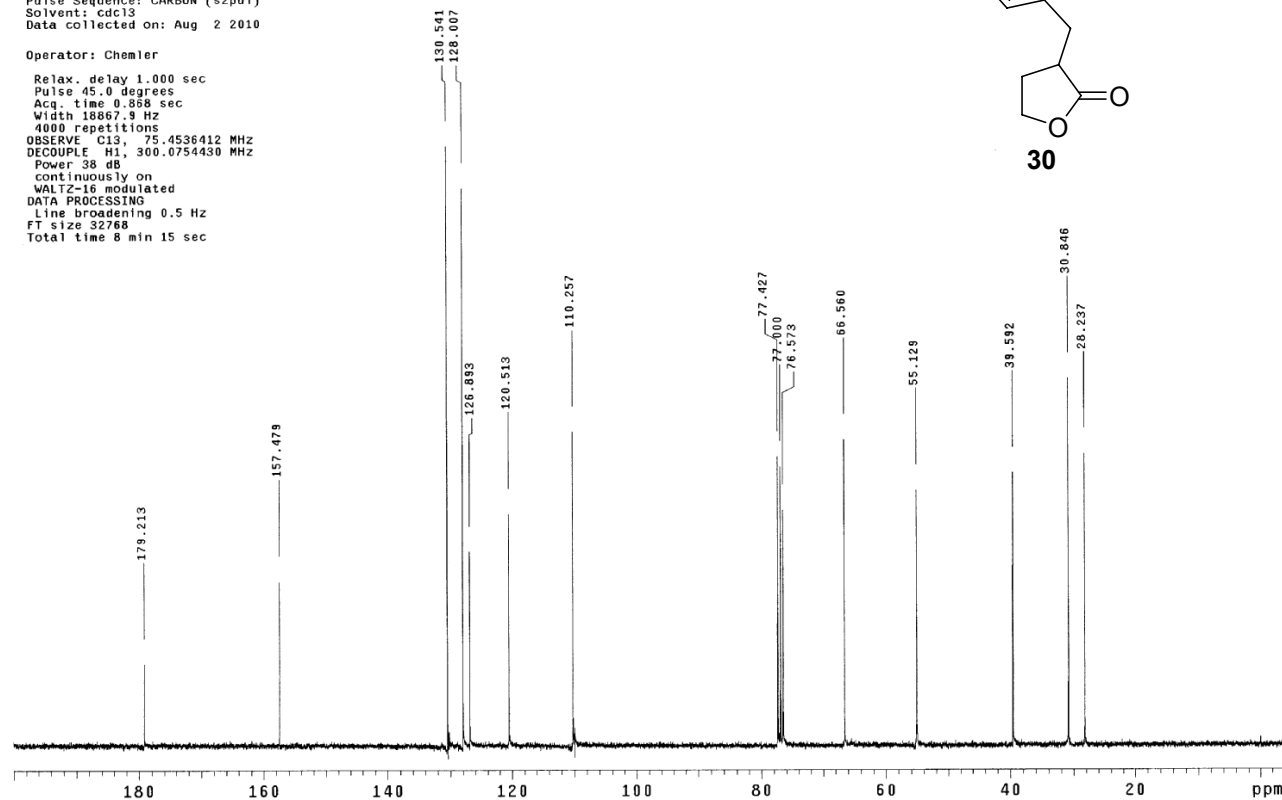
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Aug 2 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.858 sec
Width 18867.9 Hz
4000 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 8 min 15 sec

20100805omethoxyla1coho1

Sample Name:

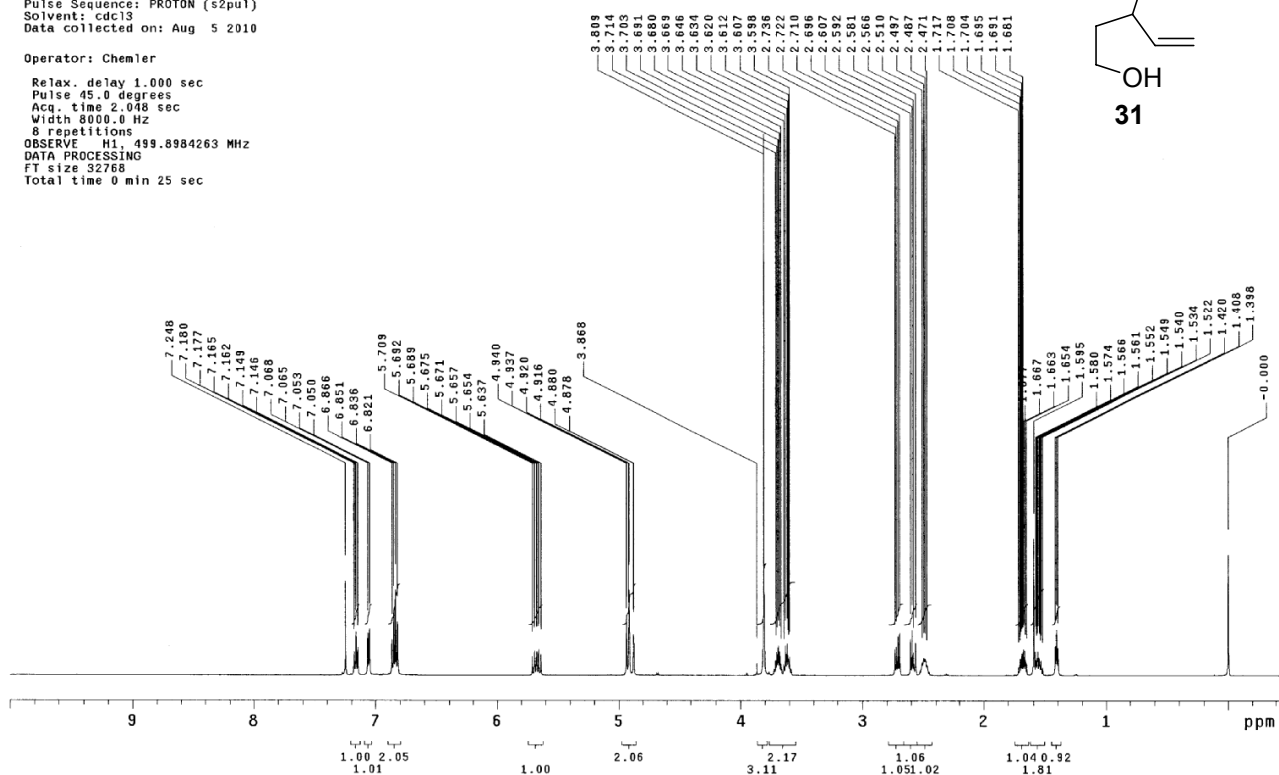
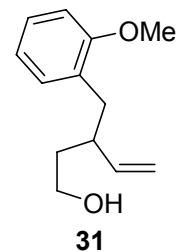
Data Collected on:
chemmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Aug 5 2010

Operator: Chemler

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
FT size 32768
Total time 0 min 25 sec

20100805omethoxyla1coho1C13

Sample Name:

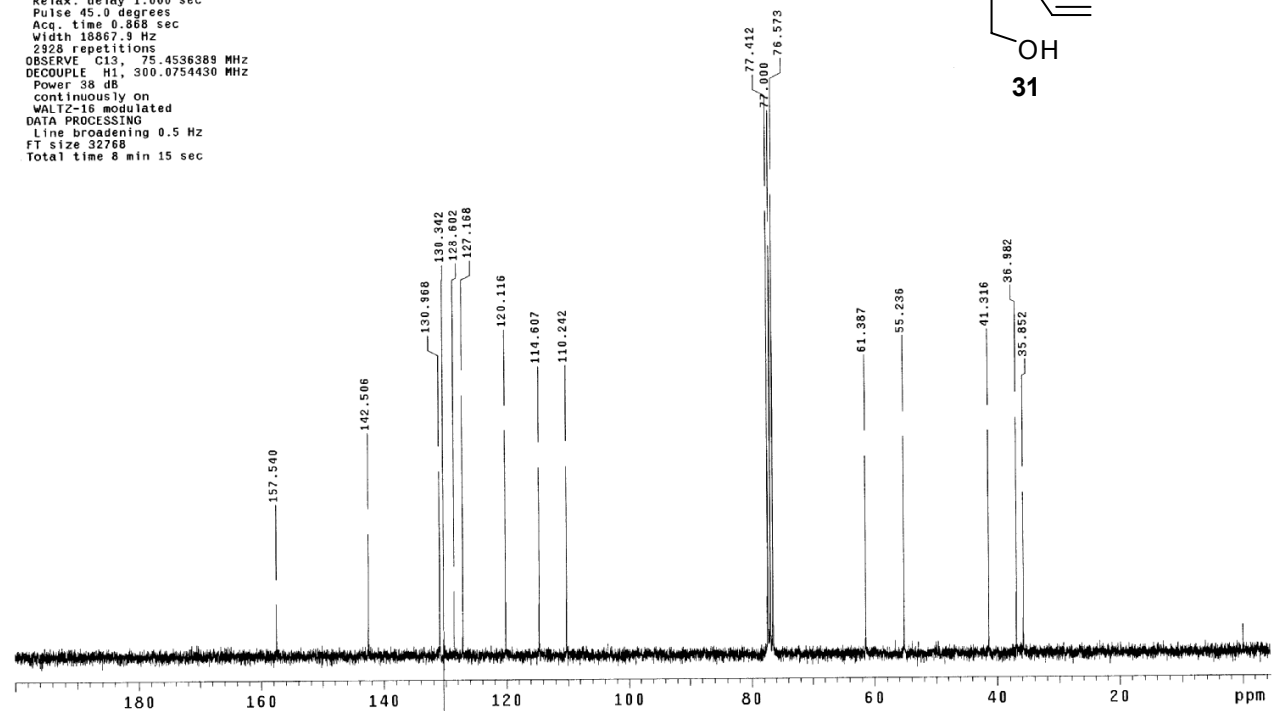
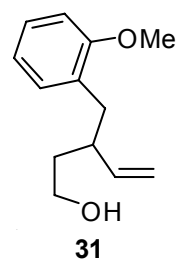
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Aug 5 2010

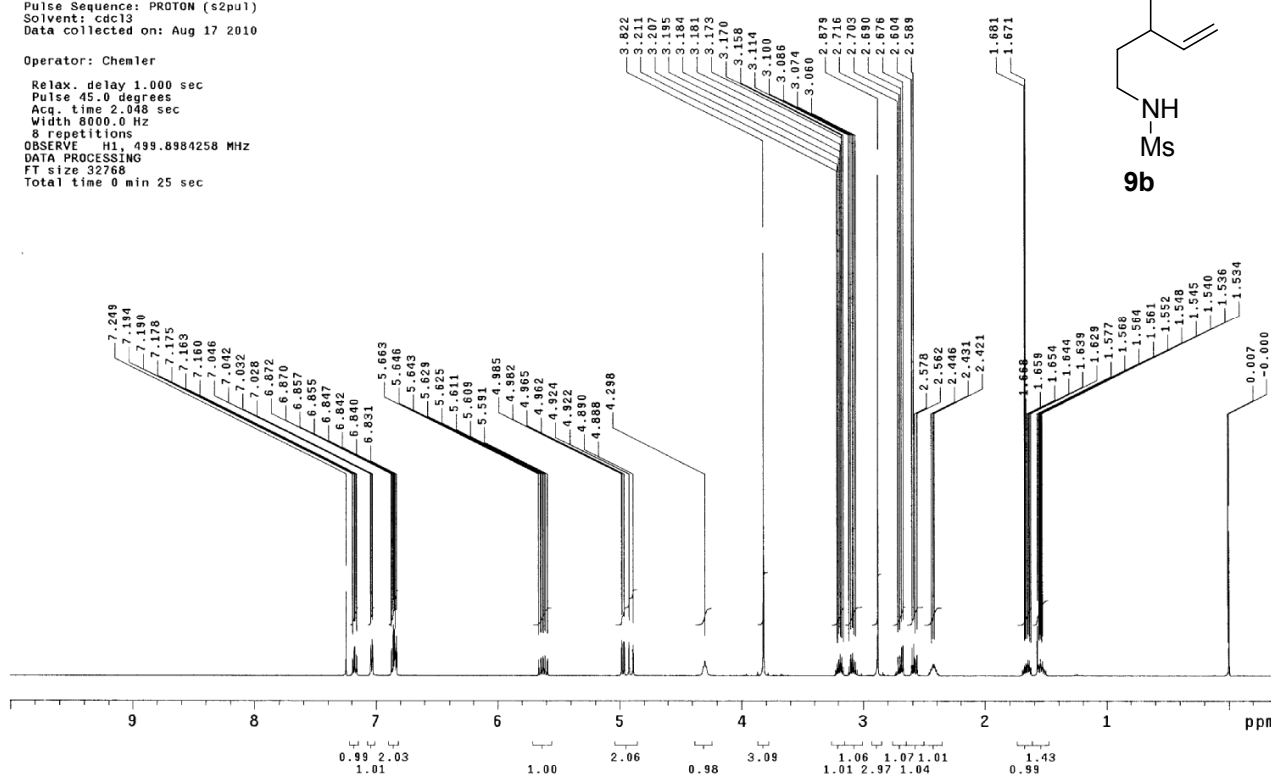
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2328 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 8 min 15 sec

20100817omethoxylsubstrate

Sample Name:
 Data Collected on:
 chemmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Aug 17 2010

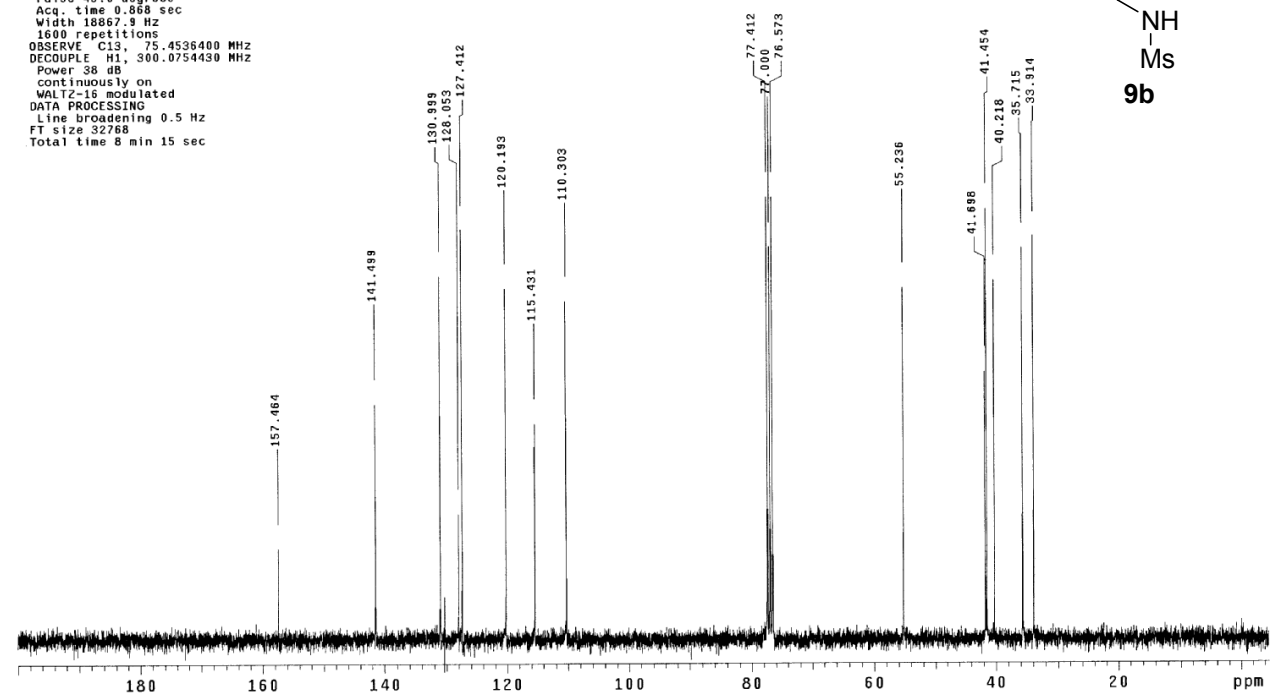
Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.8984258 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 25 sec



20100817omethoxylsubstrateC13

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: Aug 17 2010

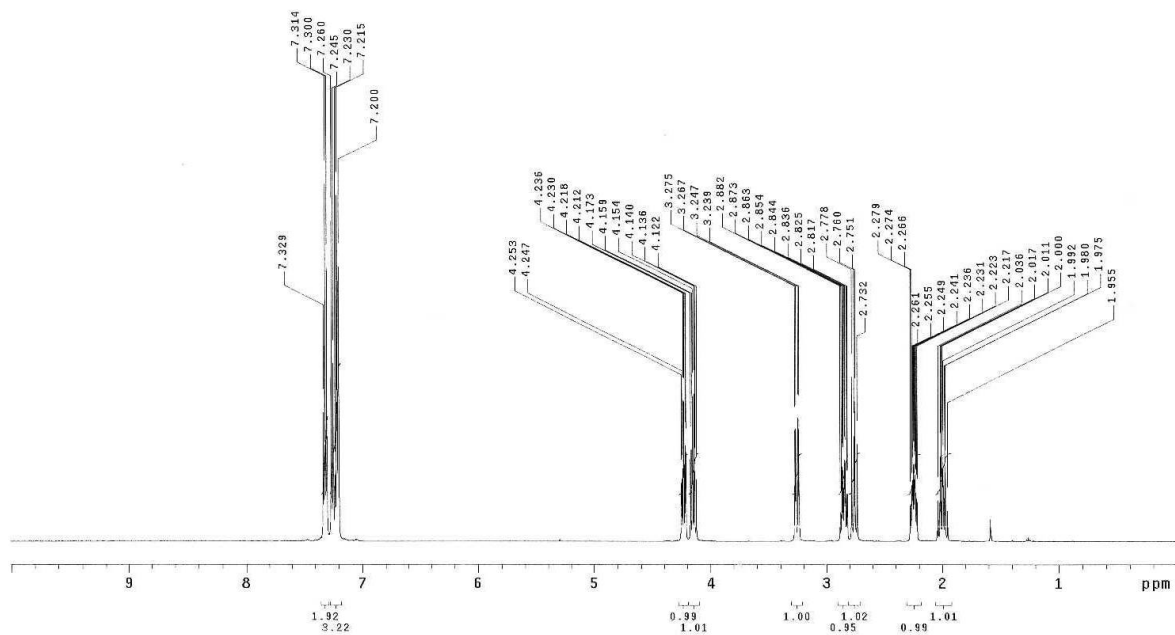
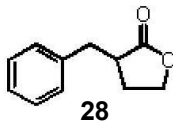
Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 1600 repetitions
 OBSERVE C13, 75.4536400 MHz
 DECOUPLE H1, 300.0754430 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 8 min 15 sec



T-215-P

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 INOVA-500 "tocsy.chem.buffalo.edu"

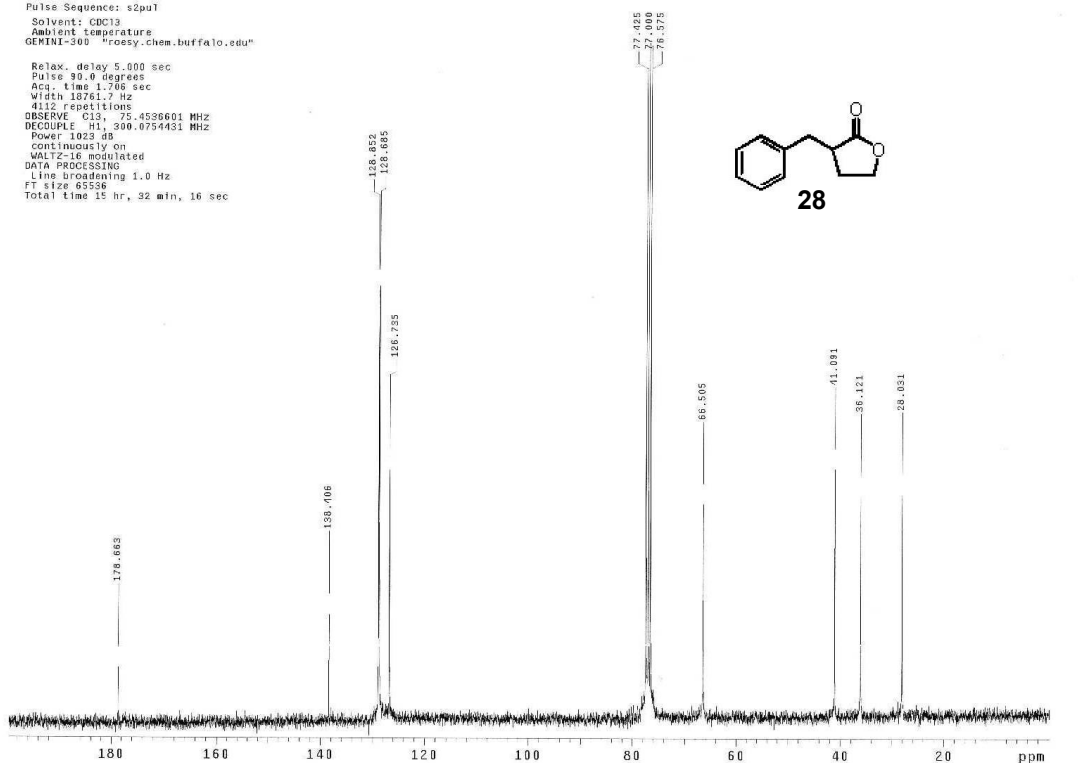
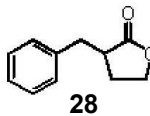
Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.891 sec
 Width 10000.9 Hz
 16 repetitions
 OBSERVE H1, 499.8564024 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min, 18 sec



T-215-P-CMNR

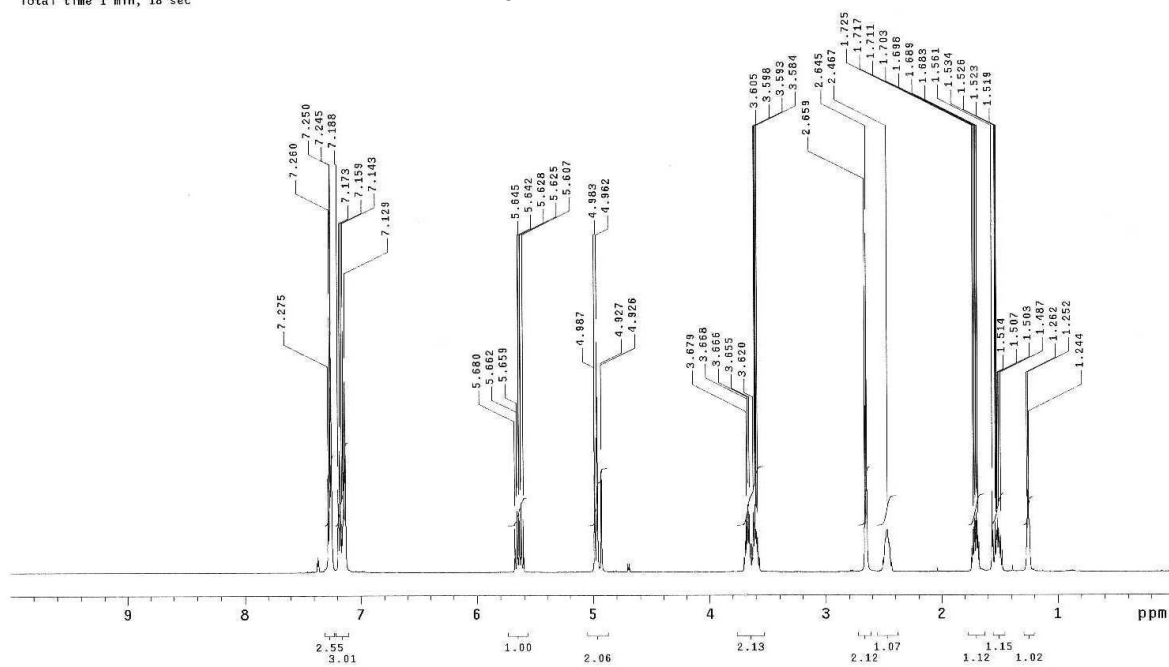
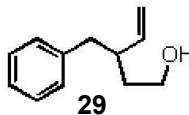
Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 GEMINI-500 "tocsy.chem.buffalo.edu"

Relax. delay 5.000 sec
 Pulse 90.0 degrees
 Acq. time 1.706 sec
 Width 18761.7 Hz
 412 repetitions
 OBSERVE C13, 75.4536601 MHz
 DECOUPLE H1, 300.0754431 MHz
 Power 1023 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 15 hr, 32 min, 16 sec



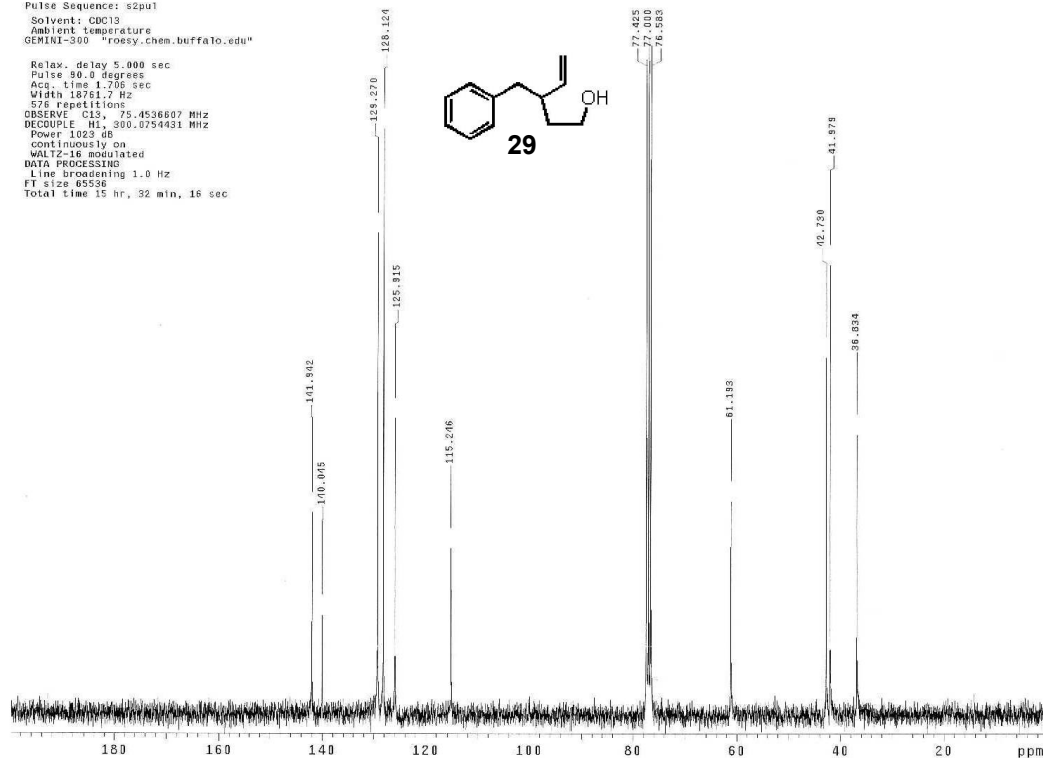
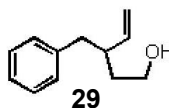
T-233-P2
 Pulse Sequence: s2pu1
 Solvent: CDC13
 Ambient temperature
 INOVA-500 "tocsy.chem.buffalo.edu"

Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.891 sec
 Width 10000.0 Hz
 16 repetitions
 OBSERVE H1, 499.8984103 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min, 18 sec



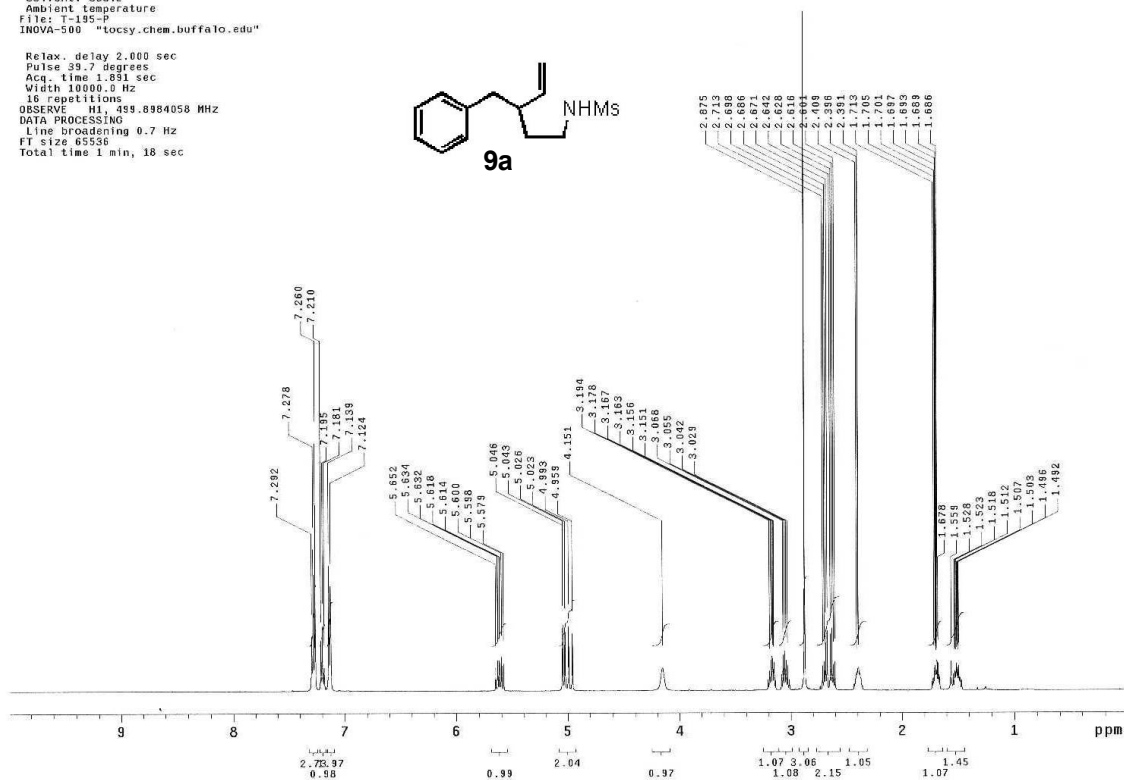
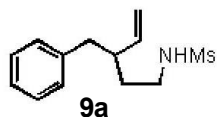
T-233-P2-CMRR
 Pulse Sequence: s2pu1
 Solvent: CDC13
 Ambient temperature
 GEMINI-300 "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec
 Pulse 90.0 degrees
 Acq. time 1.708 sec
 Width 18751.7 Hz
 576 repetitions
 OBSERVE C13, 75.4536607 MHz
 DECOUPLE H1, 300.0754431 MHz
 Power 1023 dB
 Continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 15 hr, 32 min, 16 sec



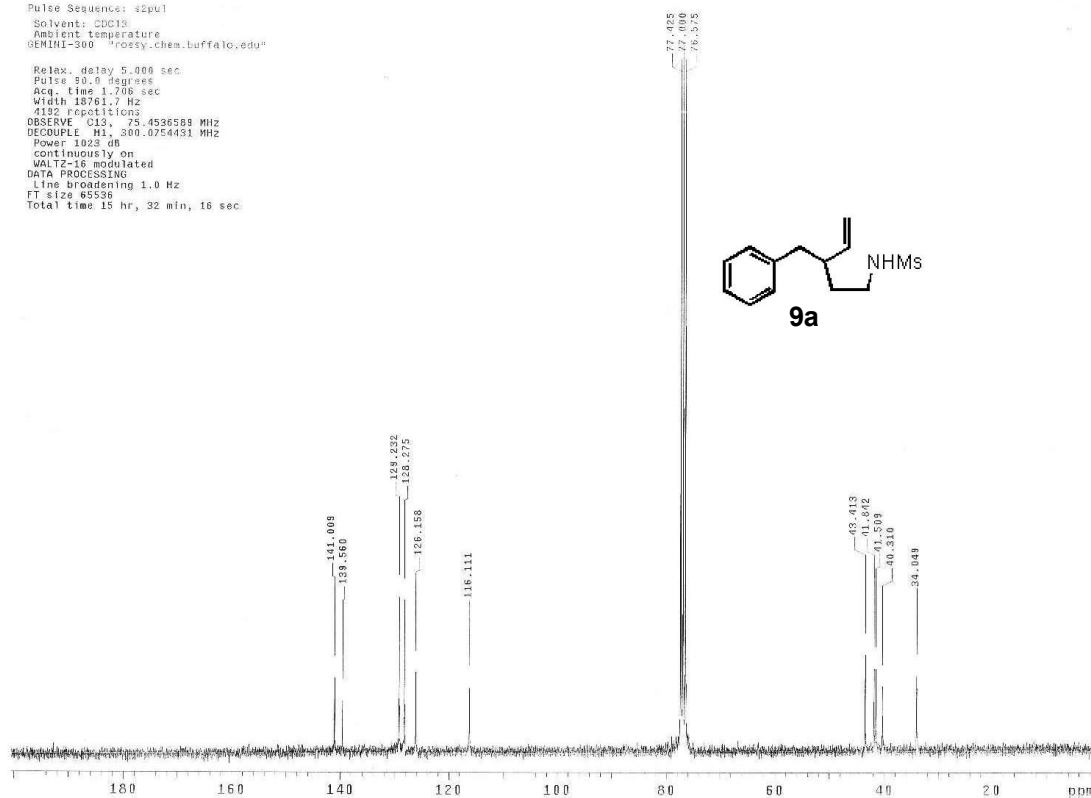
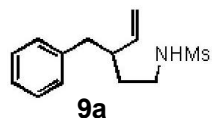
T-195-P
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 File: T-195-P
 INOVA-500 "tocsy.chem.buffalo.edu"

Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.891 sec
 Width 10000.0 Hz
 16 repetitions
 OBSERVE H1, 499.8984058 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min, 18 sec



T-195-P-CHIR
 Pulse Sequence: s2pul
 Solvent: CDCl3
 Ambient temperature
 GENIINI-300 "rossy.chem.buffalo.edu"

Relax. delay 5.000 sec
 Pulse 30.0 degrees
 Acq. time 1.708 sec
 Width 13761.7 Hz
 4192 repetitions
 OBSERVE C13, 75.4536588 MHz
 DECOUPLE H1, 300.0754451 MHz
 Power 1023 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 85536
 Total time 15 hr, 32 min, 16 sec



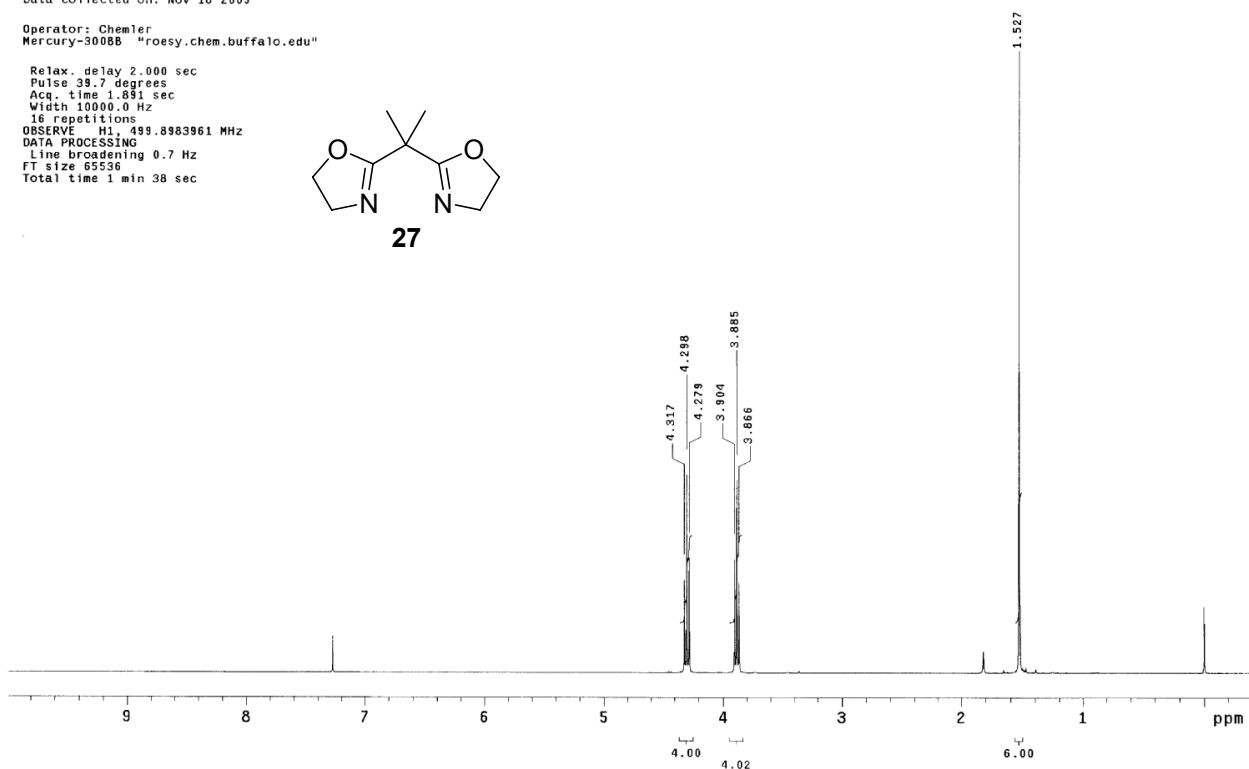
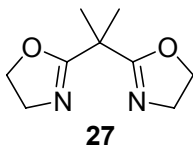
2009111811gand

Sample Name:
 Archive directory:
 Sample directory:
 FidFile: H1

Pulse Sequence: s2pul
 Solvent: CDCl3
 Data collected on: Nov 18 2009

Operator: Chemler
 Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.891 sec
 Width 10000.0 Hz
 18 repetitions
 OBSERVE H1, 499.8983961 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min 38 sec



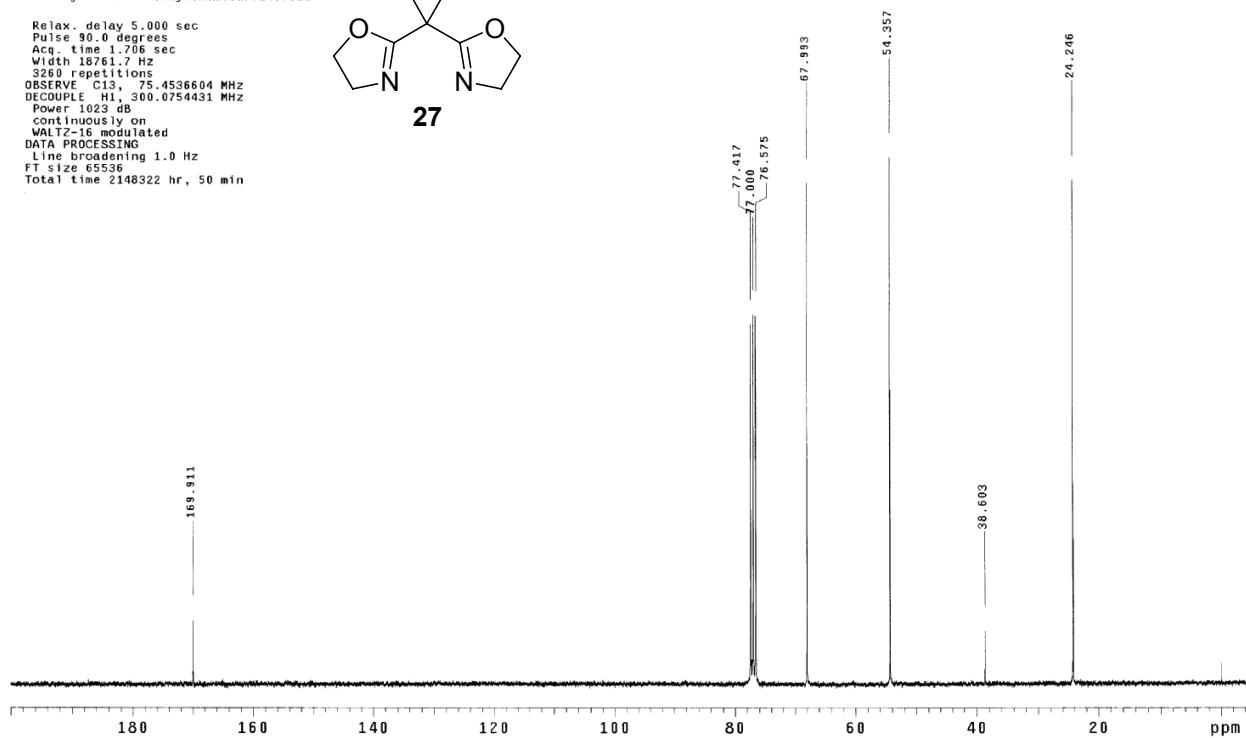
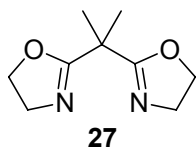
2009111911gandC13

Sample Name:
 Archive directory:
 Sample directory:
 FidFile: std13c

Pulse Sequence: std13c (s2pul)
 Solvent: CDCl3
 Data collected on: Nov 19 2009

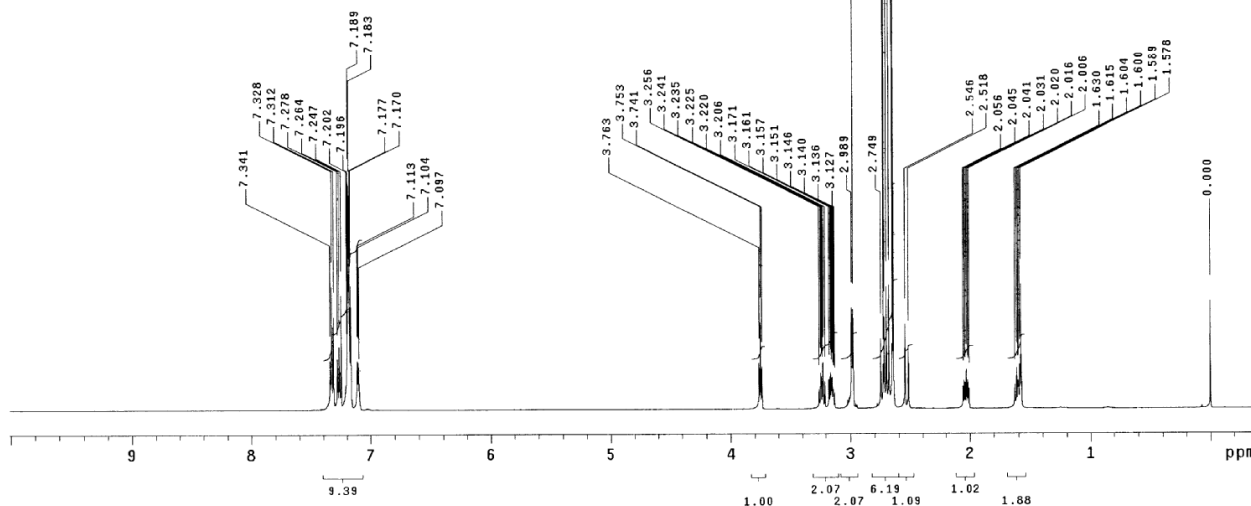
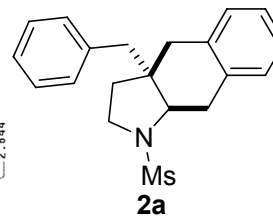
Operator: Chemler
 Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec
 Pulse 90.0 degrees
 Acq. time 1.706 sec
 Width 18761.7 Hz
 3260 repetitions
 OBSERVE C13, 75.4536604 MHz
 DECOUPLE H1, 300.0754431 MHz
 Power 1023 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 2148322 hr, 50 min



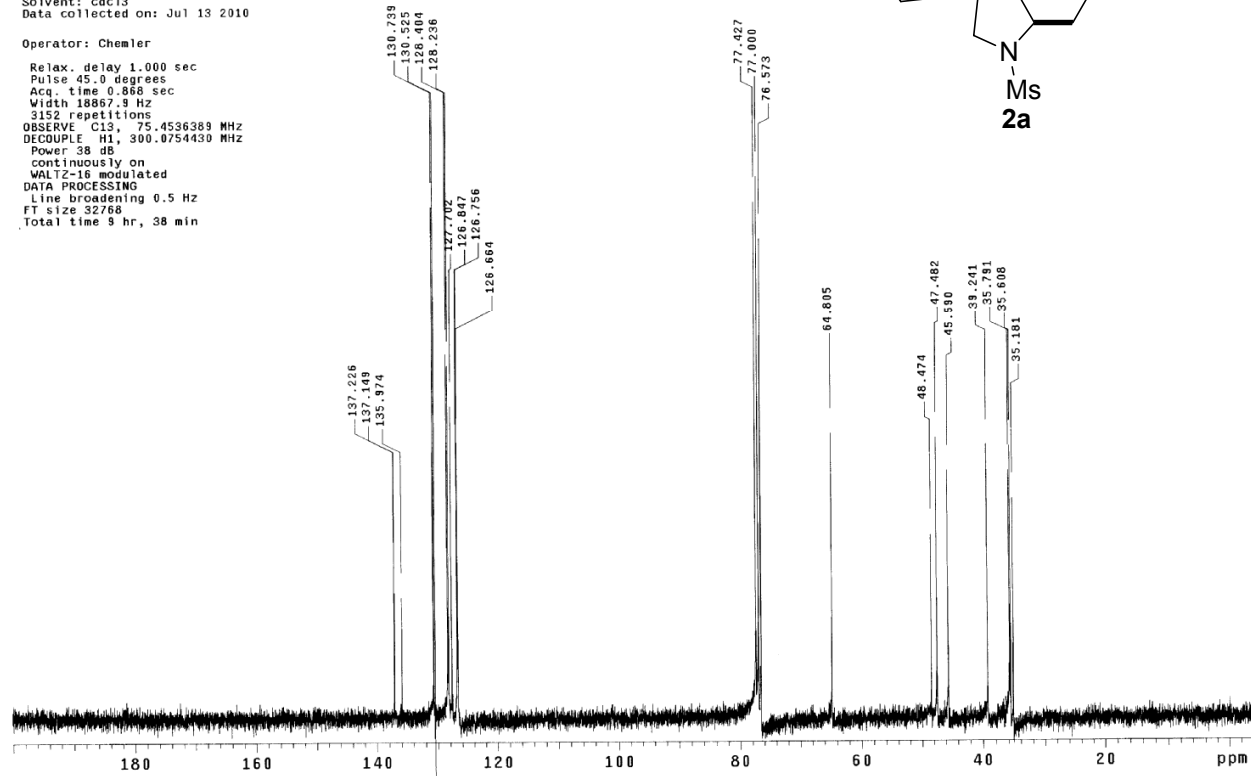
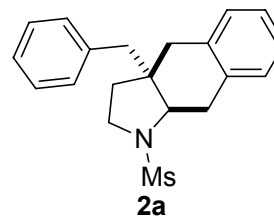
20100713Msdibenzylproduct
 Sample Name:
 Data Collected on:
 chemmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 Fidfile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdc13
 Data collected on: Jul 13 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.8984268 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 25 sec



20100713MsdibenzylproductC13
 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: Jul 13 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 3152 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 9 hr, 38 min



20100713SESDibenzylproduct

Sample Name:

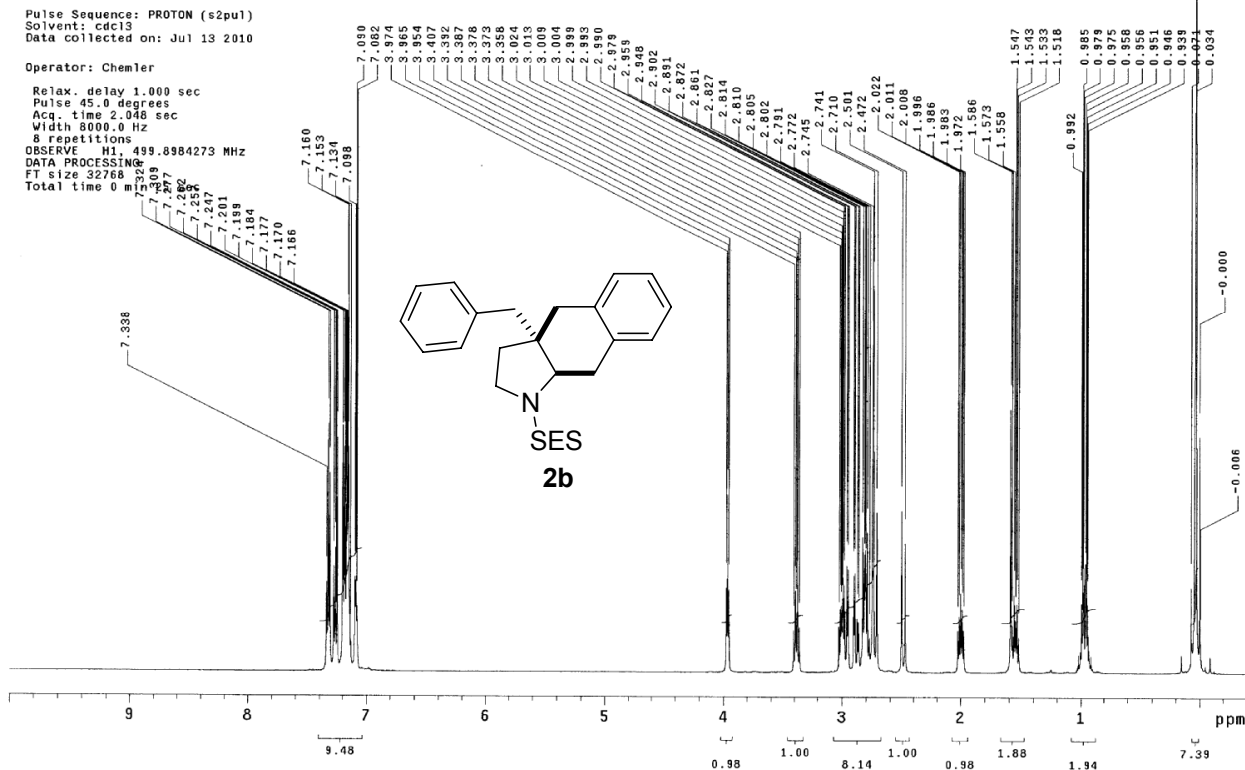
Data Collected on:
Chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdCl3
Data collected on: Jul 13 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984273 MHz
DATA PROCESSING
FT size 32768
Total time 0 m

20100713SESDibenzylproductC13

Sample Name:

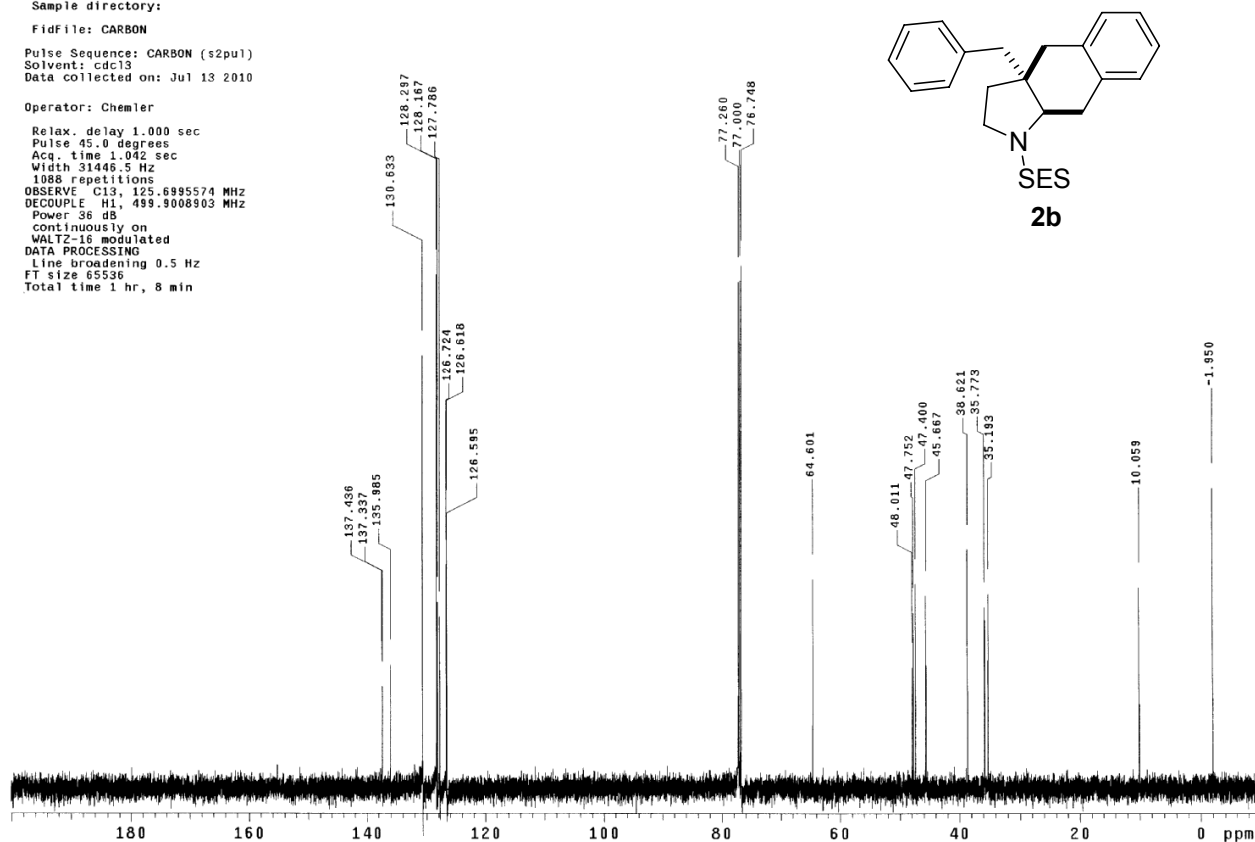
Data Collected on:
Chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdCl3
Data collected on: Jul 13 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
1888 repetitions
OBSERVE C13, 125.6995574 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 1 hr, 8 min

20100714BSsubstrate

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: Jul 14 2010

Operator: Chemler

Relax. delay 7.000 sec

Pulse 45.0 degrees

Acq. time 7.048 sec

Width 8000.0 Hz

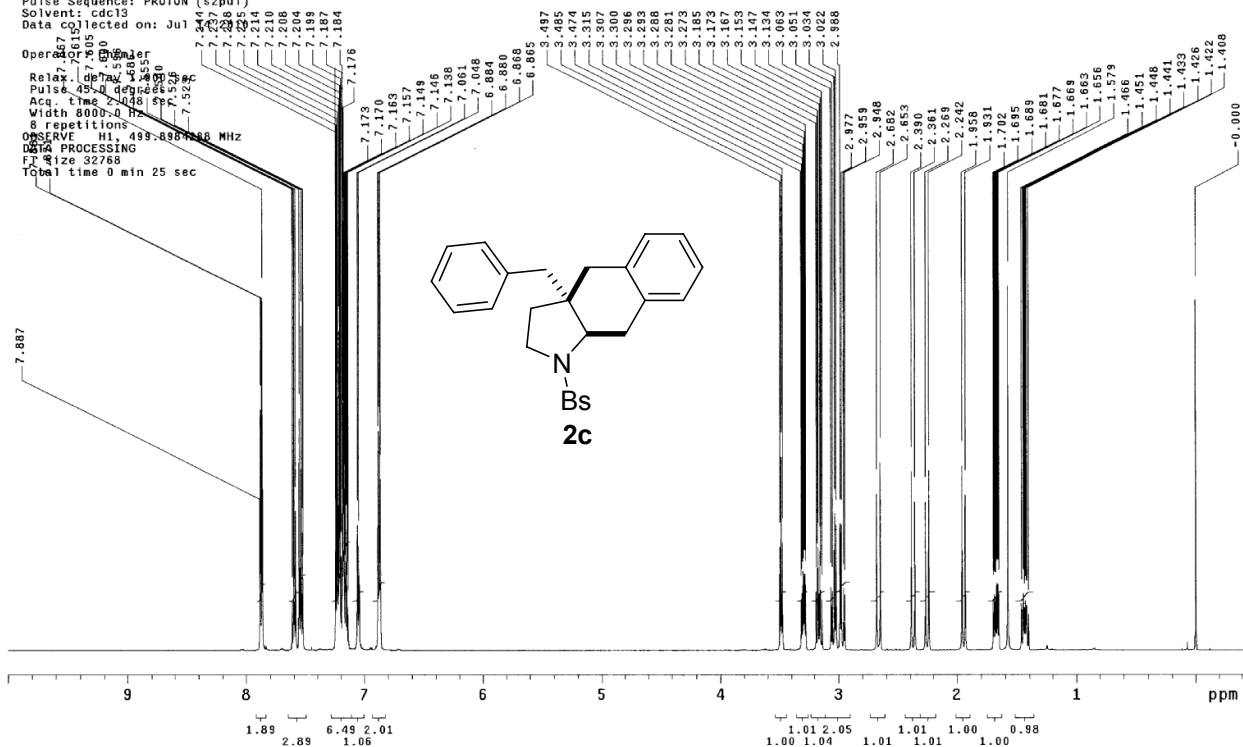
8 repetitions

OBSERVE H1 499.8357488 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 25 sec



20100714BSsubstrateC13

Sample Name:

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

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Jul 14 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 1.042 sec

Width 31446.5 Hz

1200 repetitions

OBSERVE C13, 125.6895574 MHz

DECOUPLE H1, 499.8008903 MHz

Power 36 dB

continuously on

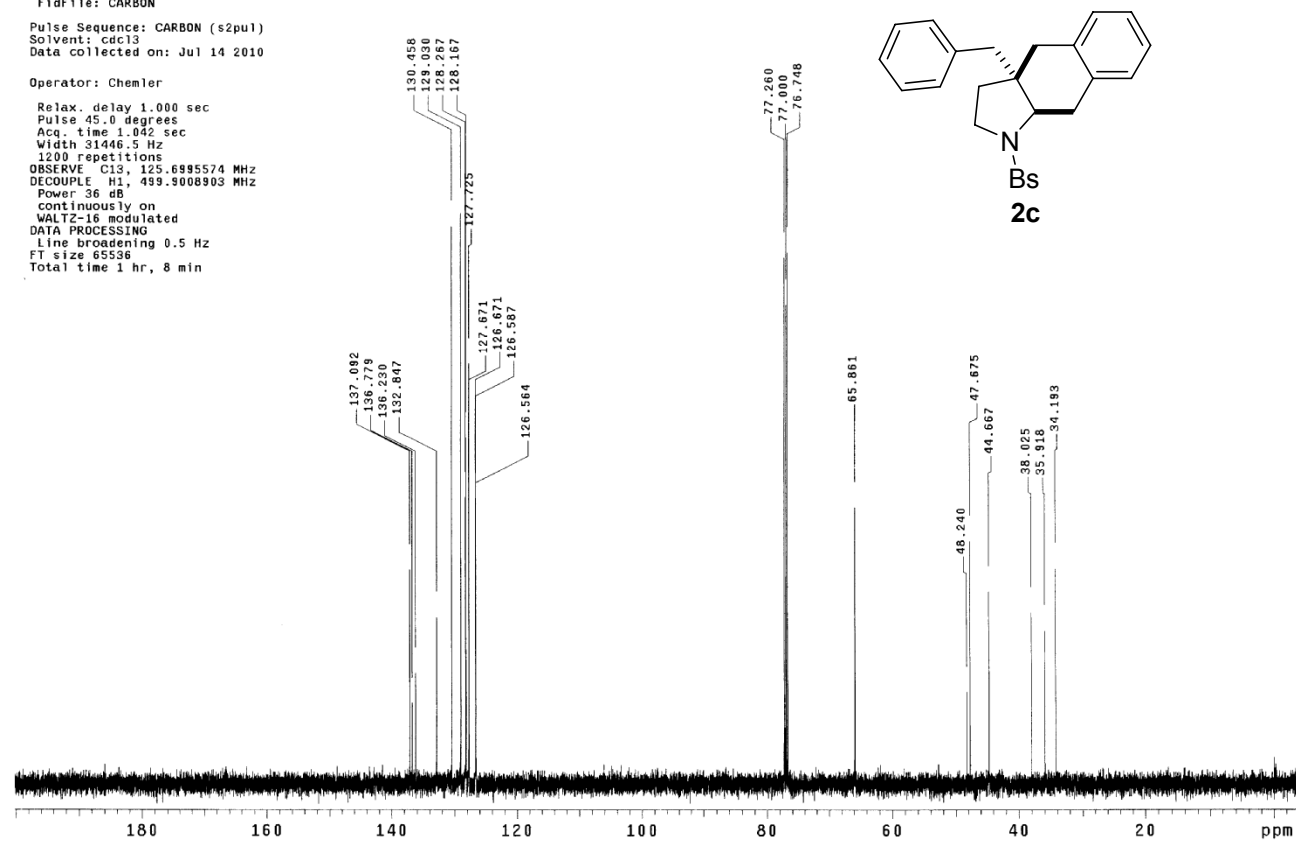
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 1 hr, 8 min



20100719dibenzylproduct

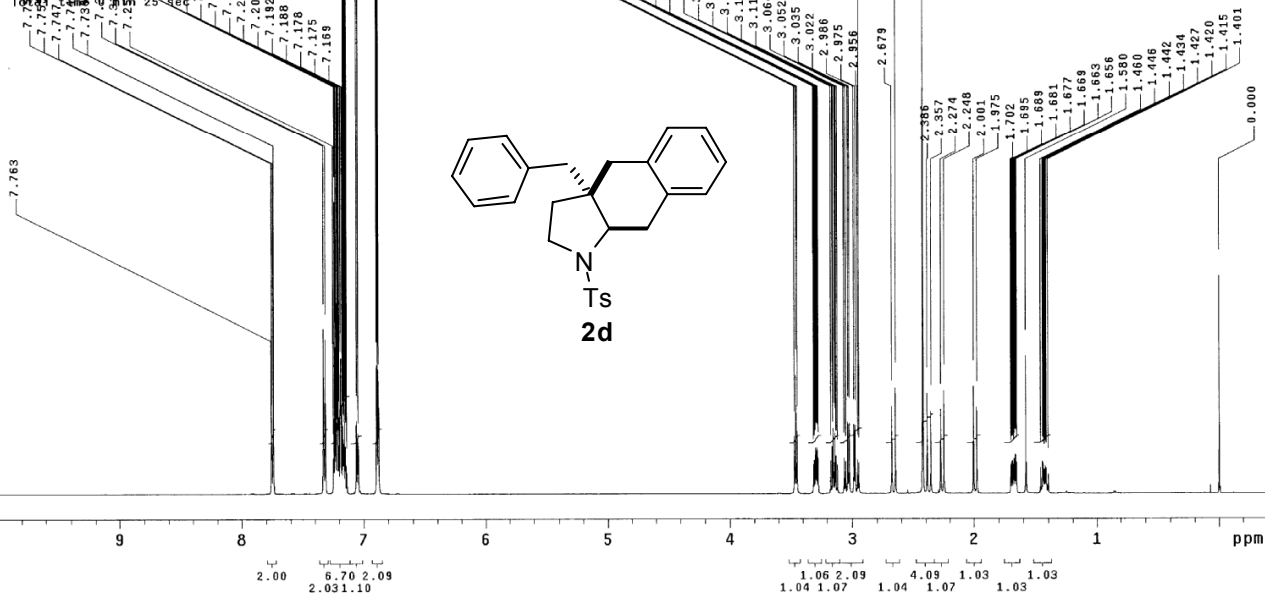
Sample Name:
Data Collected on:
chemmrs500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
Fidfile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: Jul 19 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.832834 MHz

DATA PROCESSING
FT size 32736
Total time 9.376 min



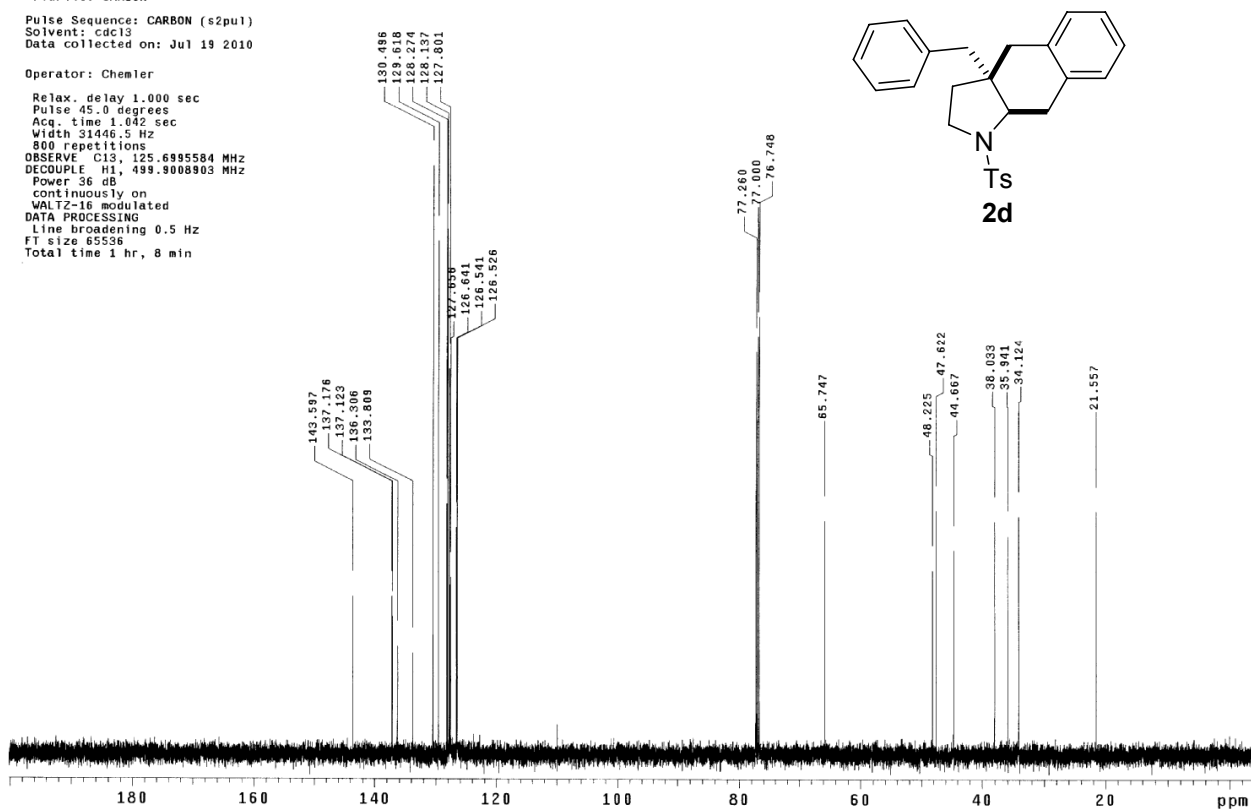
20100719dibenzylproductC13

Sample Name:
Data Collected on:
chemmrs500.chem.buffalo.edu-inova500
Archive directory:
Sample directory:
Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Jul 19 2010

Operator: Chemler

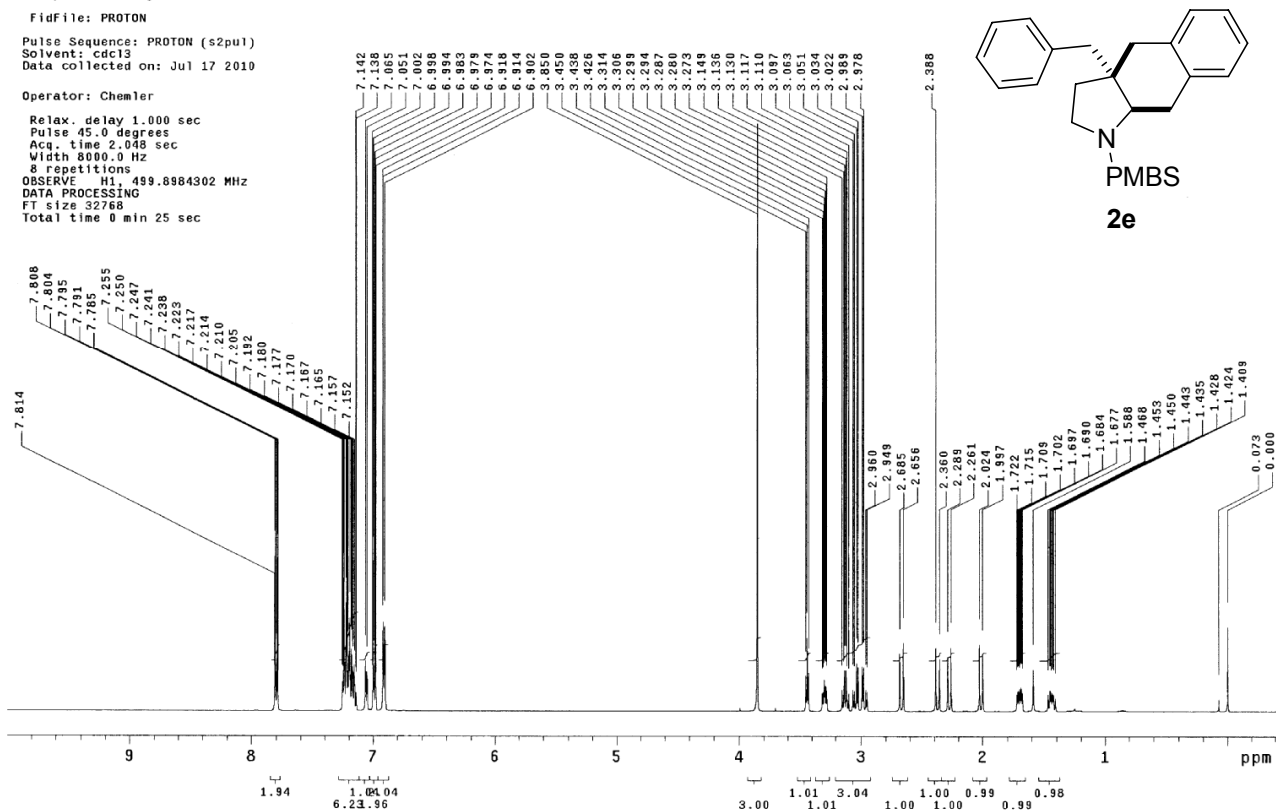
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
800 repetitions
OBSERVE C13, 125.6995584 MHz
DECOUPLE H1, 499.9008903 MHz
Power 36 dB
CONTINUOUSLY ON
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 6558
Total time 1 hr, 8 min



20100717PMBSdibenzylproduct

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: Jul 17 2010

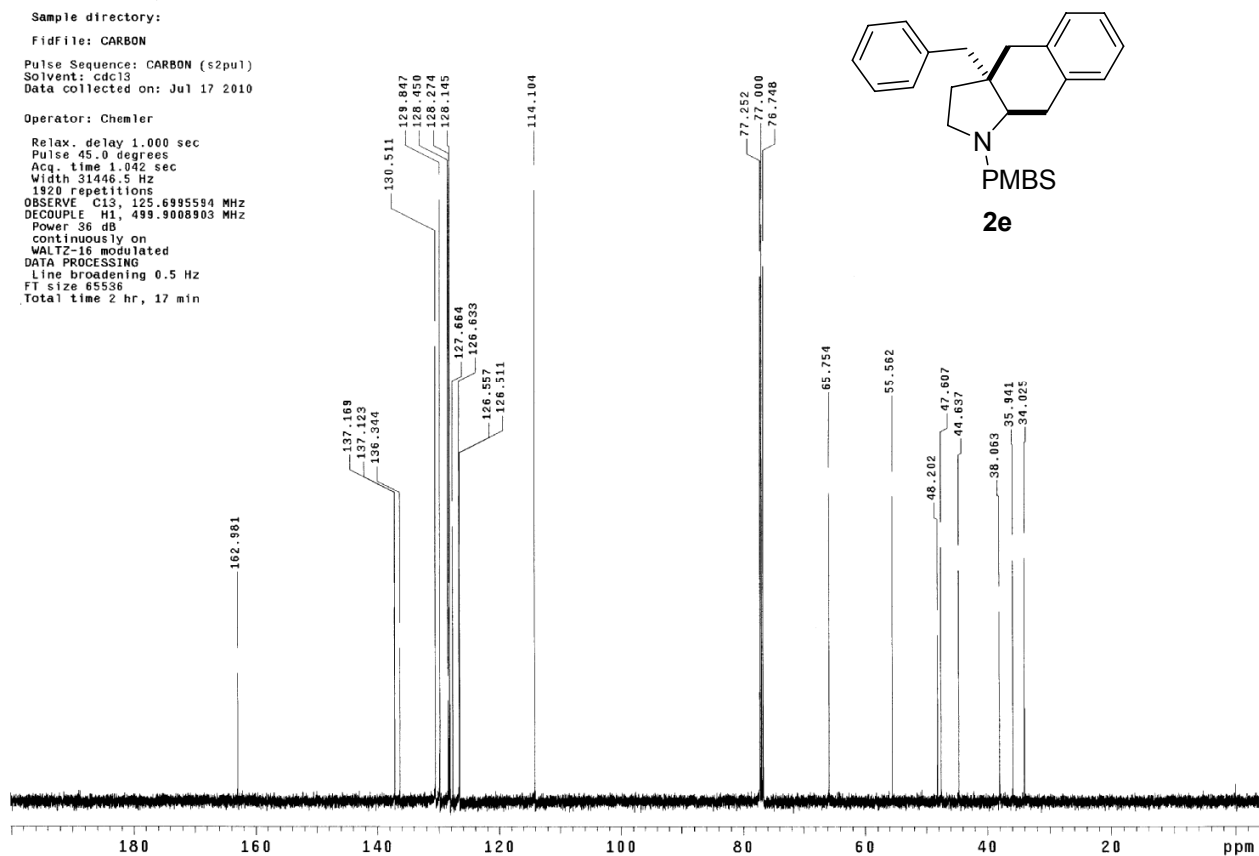
Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.8984302 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 25 sec



20100717PMBSdibenzylproductC13

Sample Name:
 Data Collected on:
 chemnmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pul)
 Solvent: cdcl3
 Data collected on: Jul 17 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.042 sec
 Width 31446.5 Hz
 1920 repetitions
 OBSERVE C13, 125.6995554 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 2 hr, 17 min



20100711PCBSproduct

Sample Name:

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

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Jul 11 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 deg

Acq. time 2.048 sec

Width 8000.0 Hz

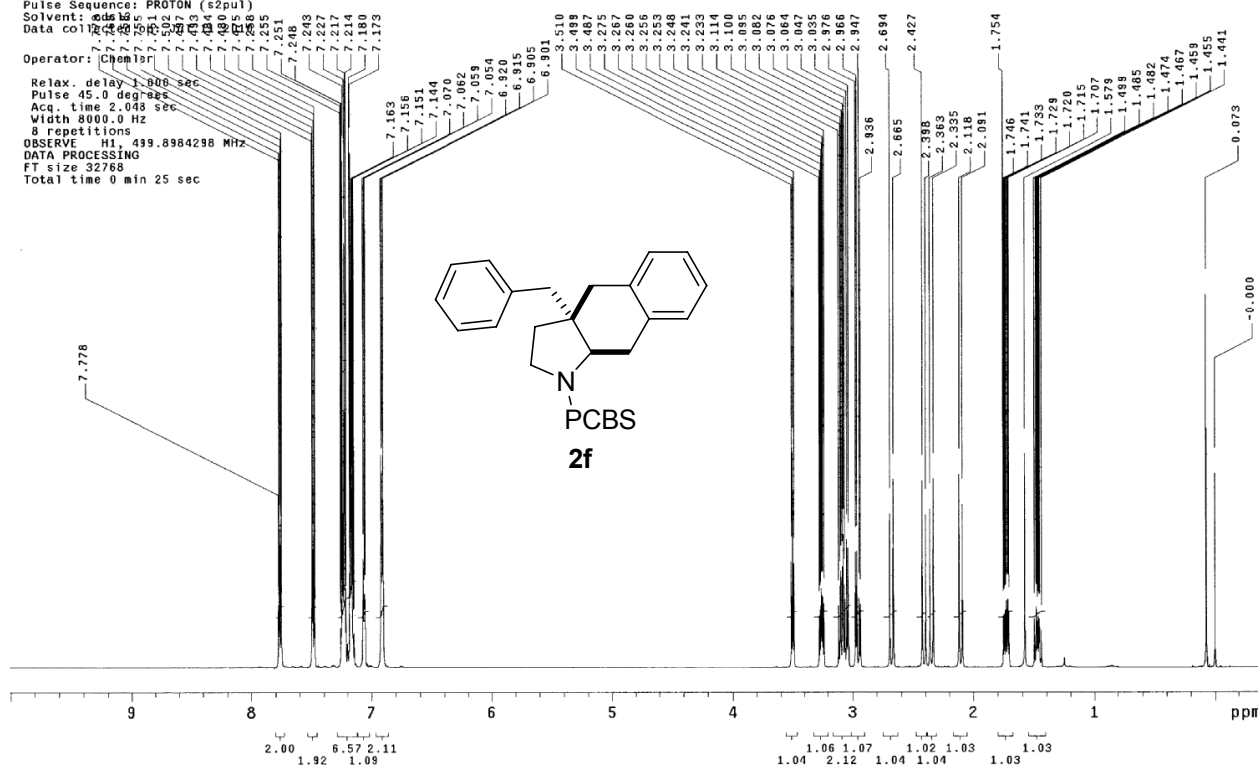
8 repetitions

OBSERVE H1, 499.8984298 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 25 sec



20100711PCBSproductC13

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: Jul 11 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

11728 repetitions

OBSERVE C13, 75.4536400 MHz

DECUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

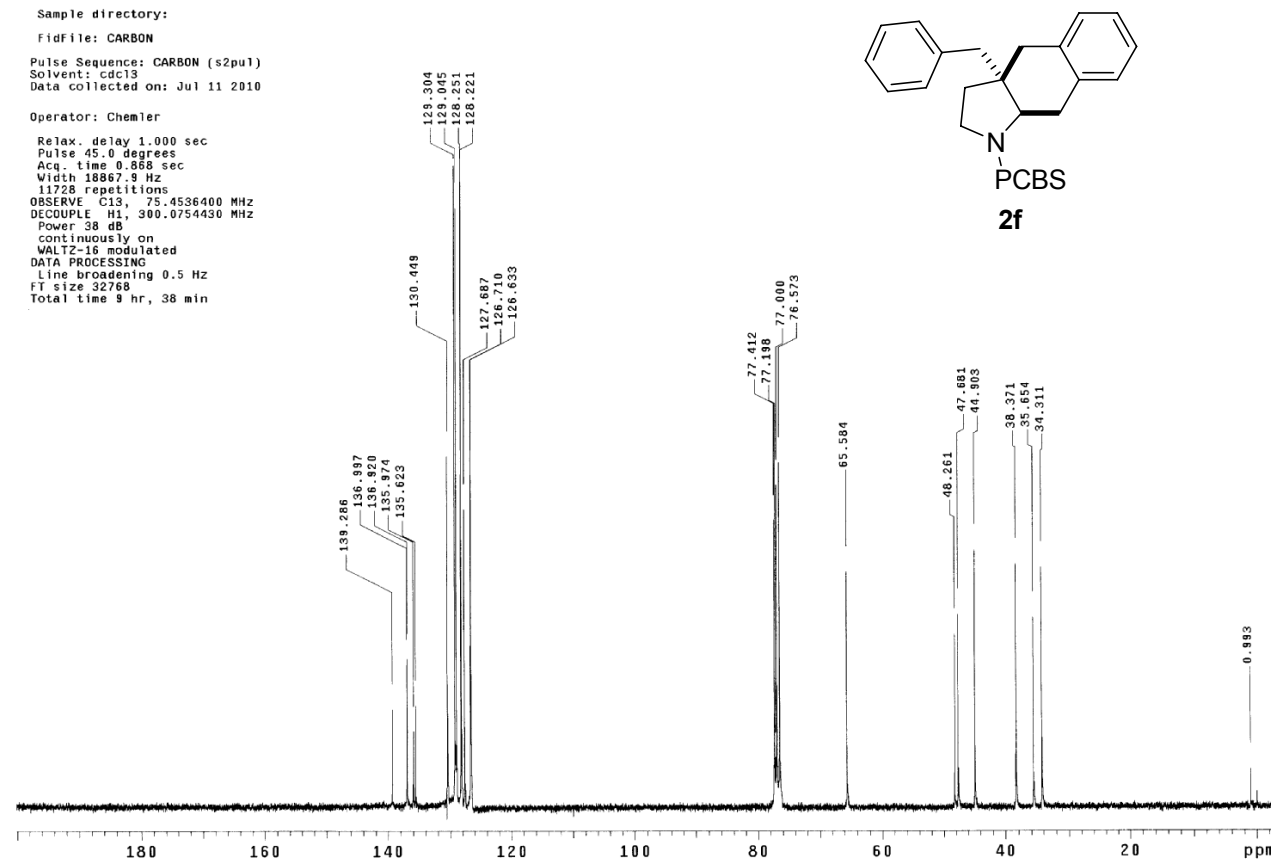
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 9 hr, 38 min



20100814Nsproduct

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: Aug 16 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.048 sec

Width 8000.0 Hz

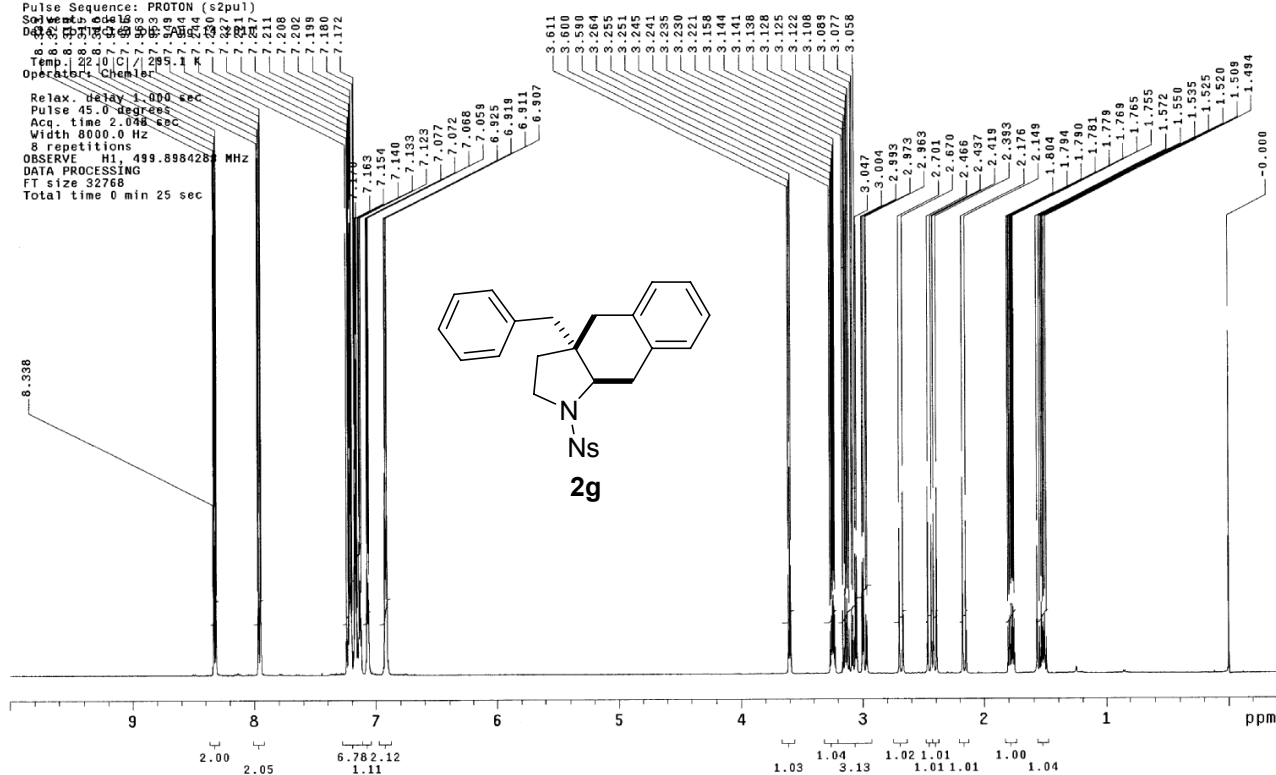
8 repetitions

OBSERVE H1, 499.8984280 MHz

DATA PROCESSING

FT size 32768

Total time 0 min 25 sec



20100816NsproductC13

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: Aug 16 2010

Operator: Chemler

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

4688 repetitions

OBSERVE C13, 75.4536400 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

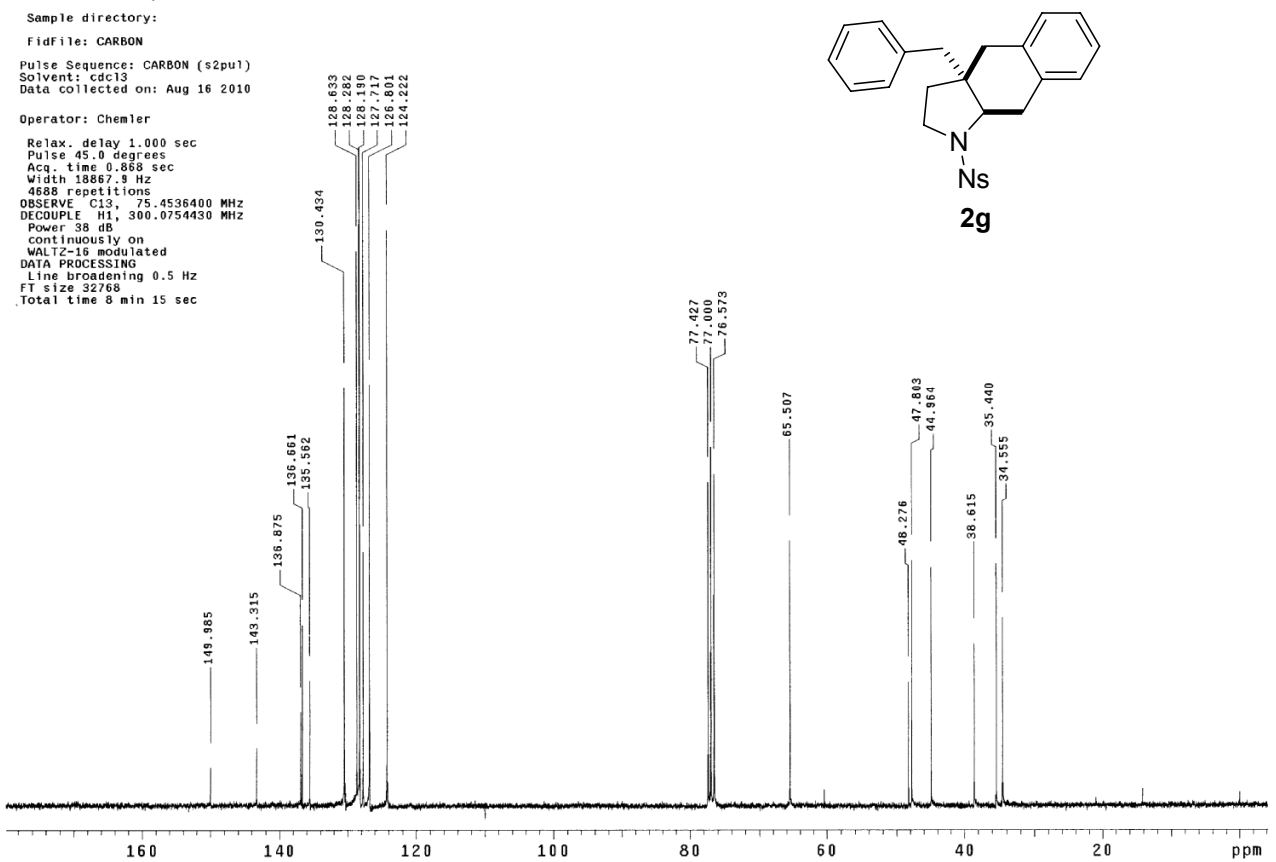
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 8 min 15 sec



20100711difluorobenzylproduct

Sample Name:

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

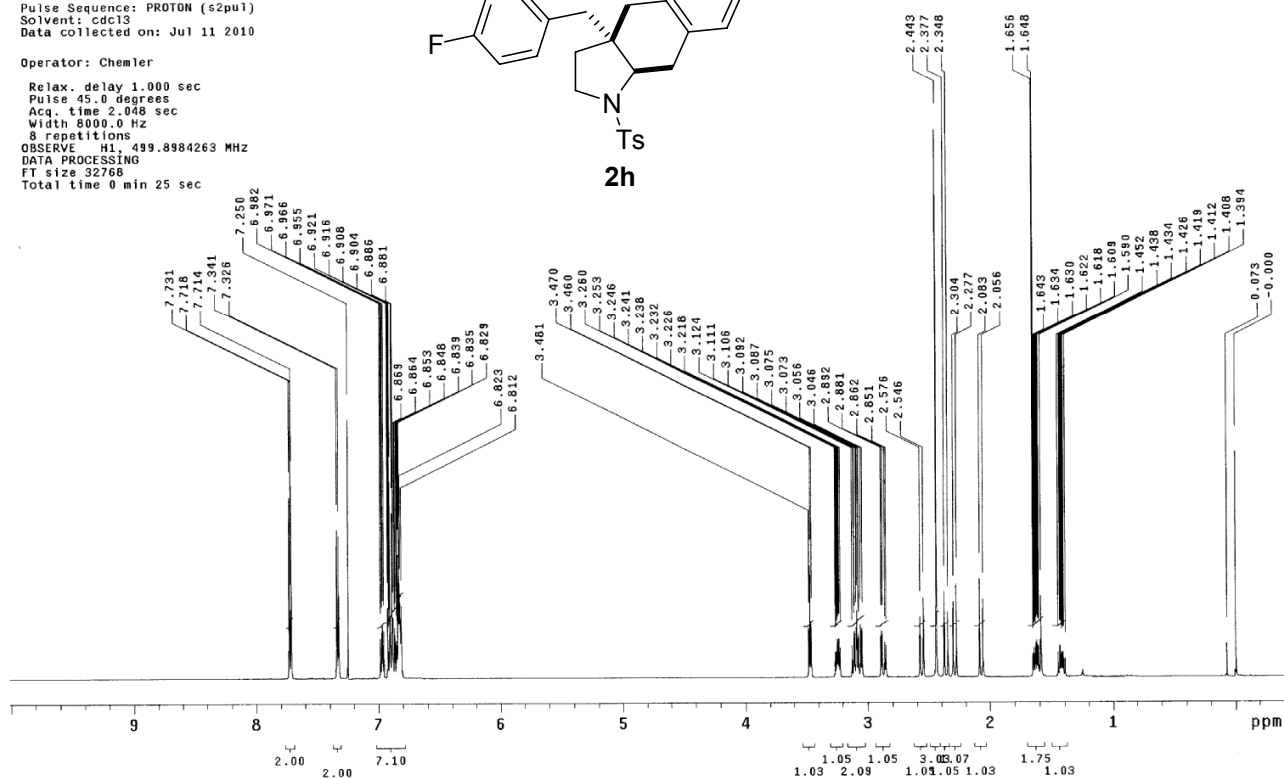
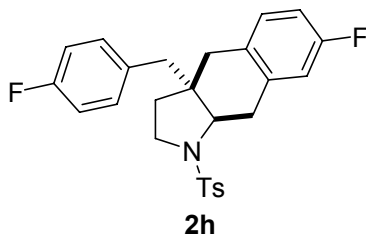
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: Jul 11 2010

Operator: Chemler

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
FT size 32768
Total time 0 min 25 sec

20100711difluorobenzylproductC13

Sample Name:

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

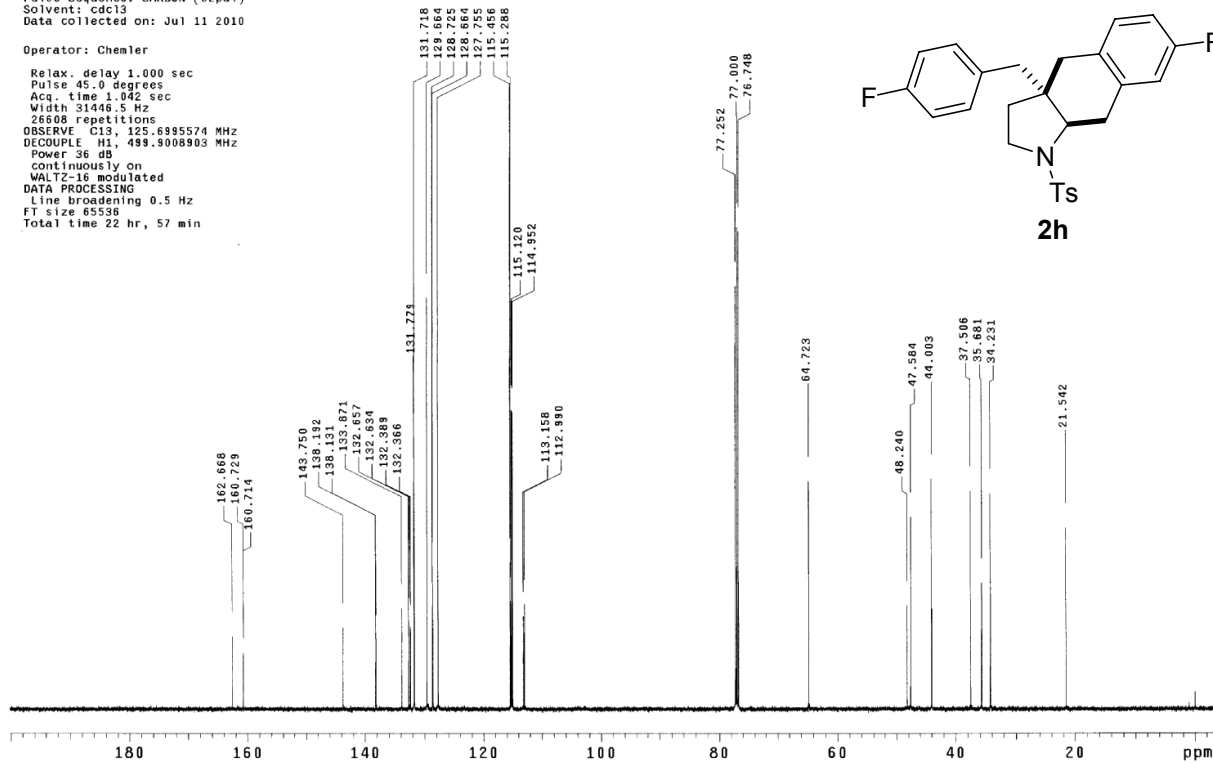
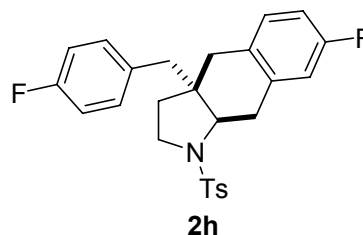
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Jul 11 2010

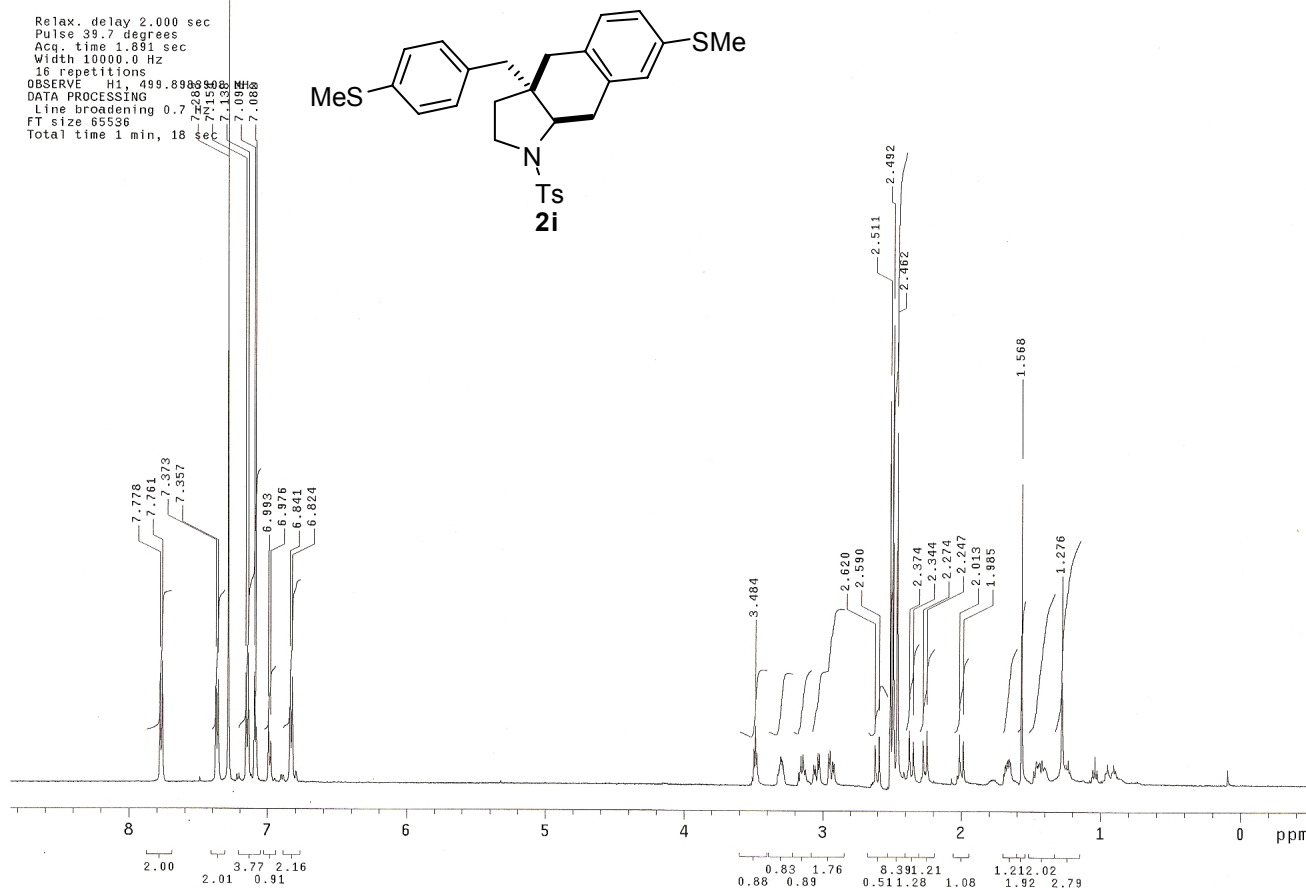
Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31448.5 Hz
26508 repetitions
OBSERVE C13, 125.6985574 MHz
DECOUPLE H1, 499.9008903 MHz
Power 56 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 22 hr, 57 min

STANDARD PROTON PARAMETERS

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 INOVA-500 "tocsy.chem.buffalo.edu"

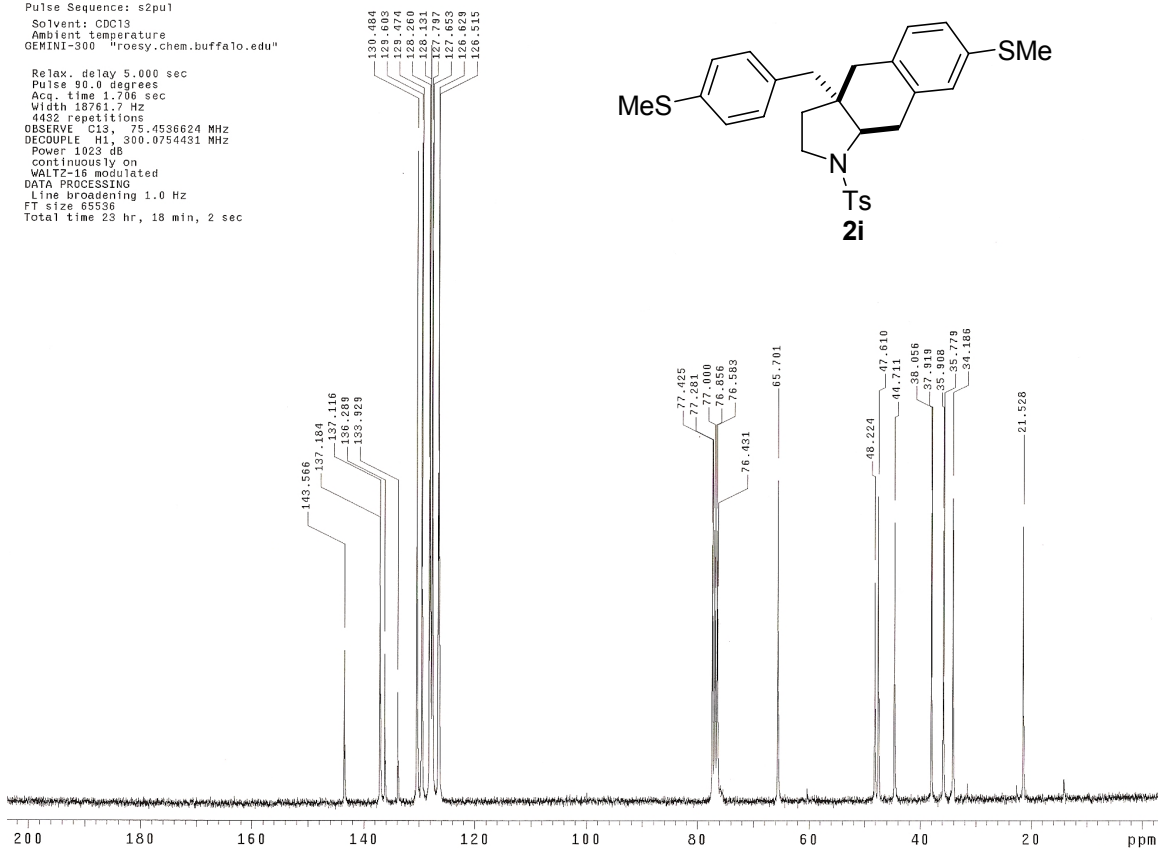
Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.891 sec
 Width 10000.0 Hz
 16 repetitions
 OBSERVE H1, 499.899990 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min, 18 sec



Imran-040209

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 GEMINI-300 "rossy.chem.buffalo.edu"

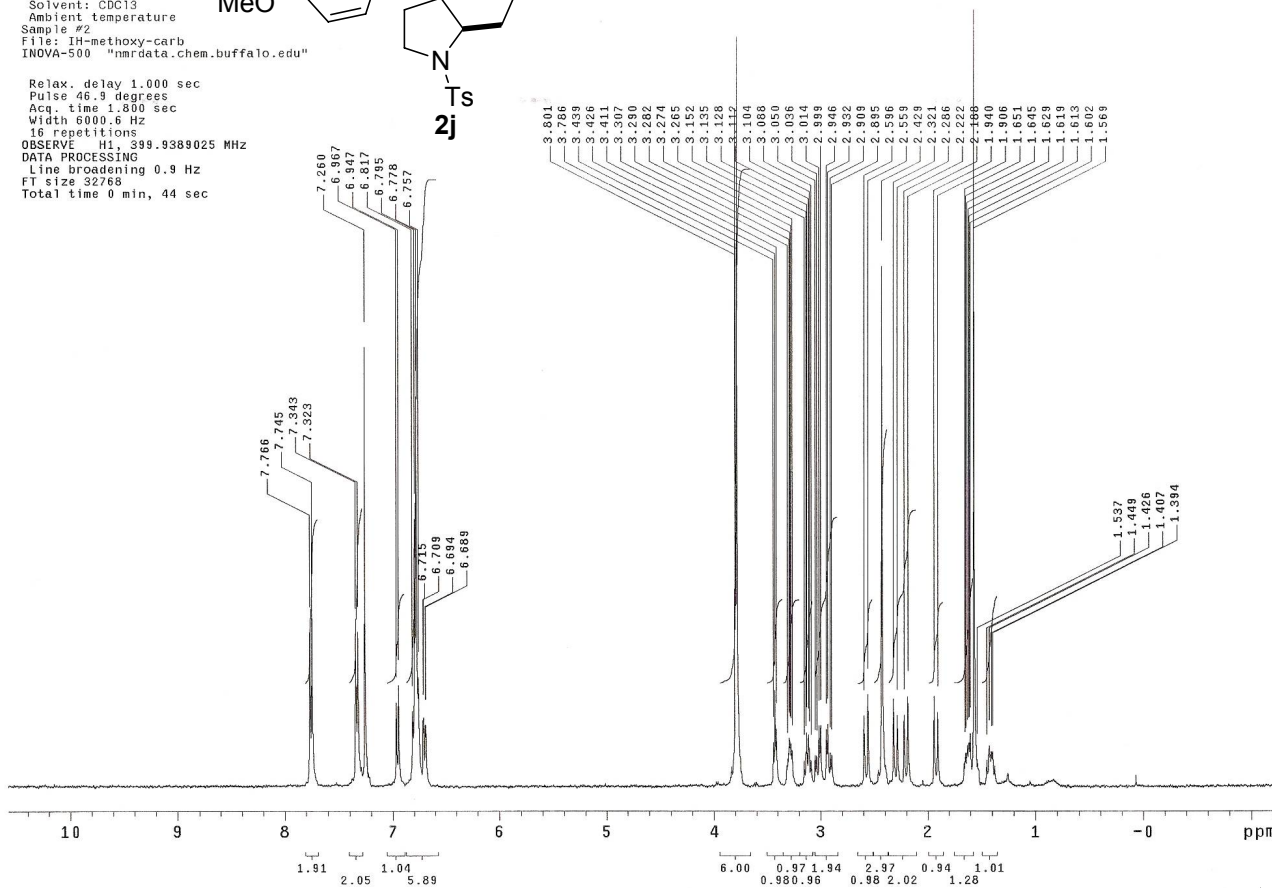
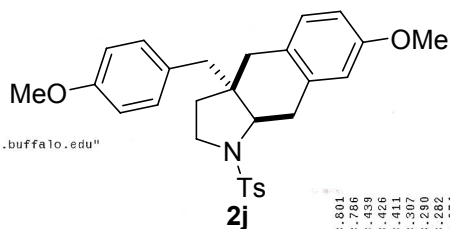
Relax. delay 5.000 sec
 Pulse 90.0 degrees
 Acq. time 1.796 sec
 Width 18761.7 Hz
 4432 repetitions
 OBSERVE C13, 75.4536624 MHz
 DECOUPLE H1, 300.0754431 MHz
 Power 1023 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 23 hr, 18 min, 2 sec



STANDARD 1H OBSERVE

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 Sample #2
 File: 1H-methoxy-carb
 INOVA-500 "nmrdata.chem.buffalo.edu"

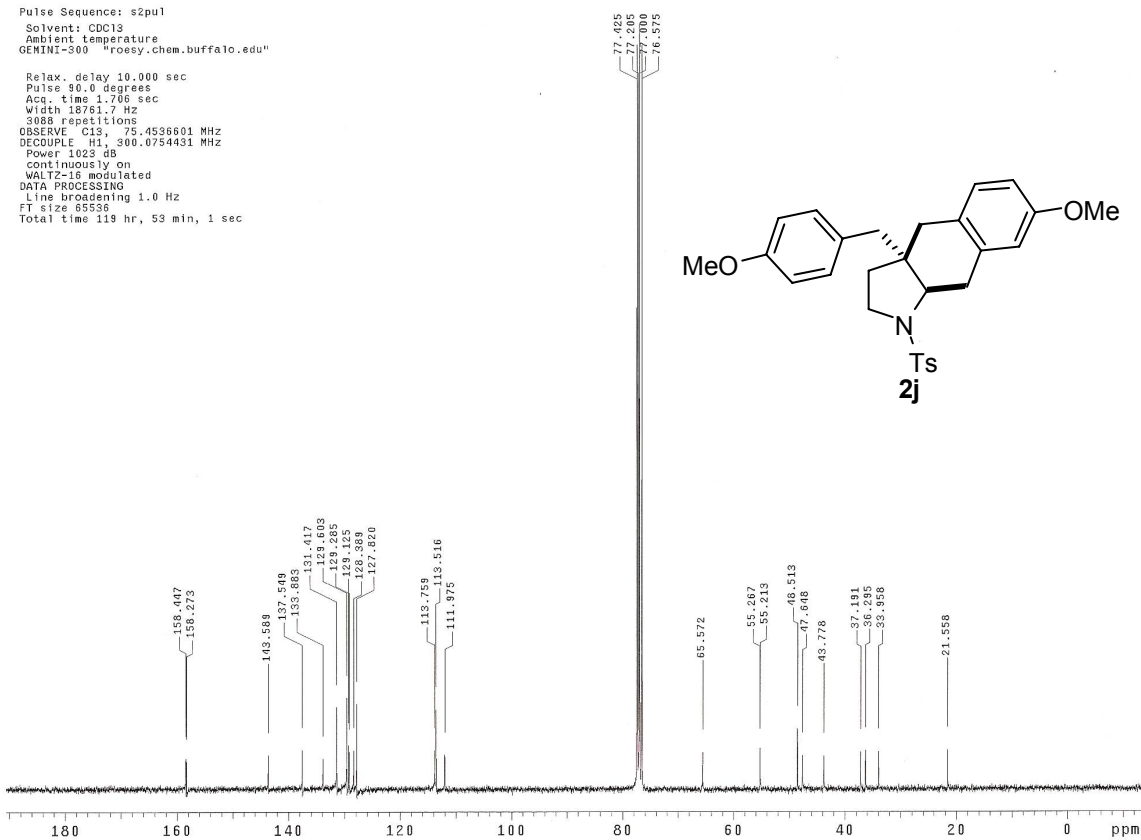
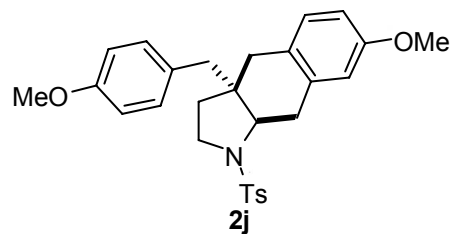
Relax. delay 1.000 sec
 Pulse 46.9 degrees
 Acq. time 1.800 sec
 Width 6000.6 Hz
 16 repetitions
 OBSERVE H1, 399.9389025 MHz
 DATA PROCESSING
 Line broadening 0.9 Hz
 FT size 32768
 Total time 0 min, 44 sec



1H-p-methoxy-carb-prod

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 GENIINI-300 "roesy.chem.buffalo.edu"

Relax. delay 10.000 sec
 Pulse 90.0 degrees
 Acq. time 1.706 sec
 Width 18761.7 Hz
 3088 repetitions
 OBSERVE C13, 75.4536601 MHz
 DECOUPLE H1, 300.6754431 MHz
 Power 1023 db
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 119 hr, 53 min, 1 sec



20100708di3methoxy1paraproduct

Sample Name:

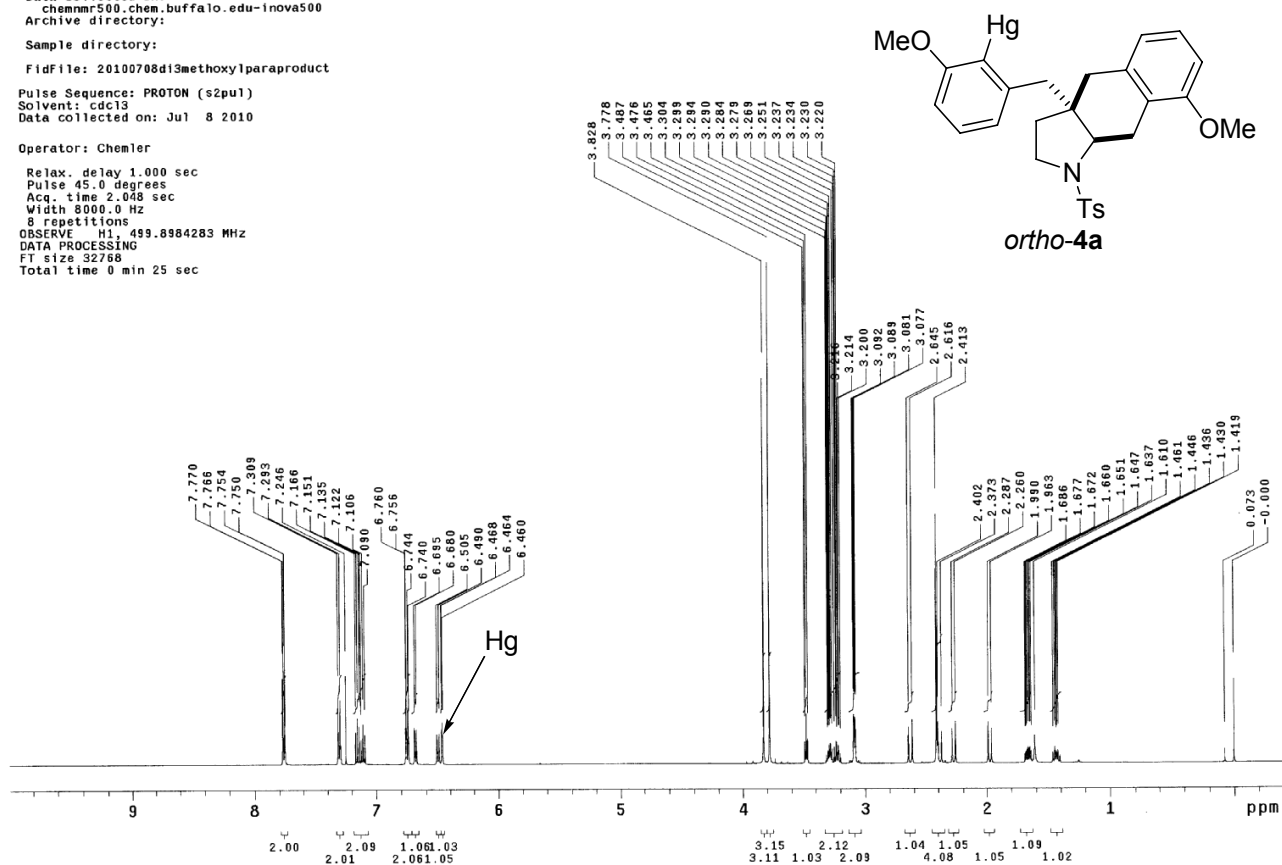
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

Fidfile: 20100708di3methoxy1paraproduct

Pulse Sequence: PROTON (s2pul)
Solvent: cdc13
Data collected on: Jul 8 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984283 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100617di3methoxy1orthoproductC13

Sample Name:

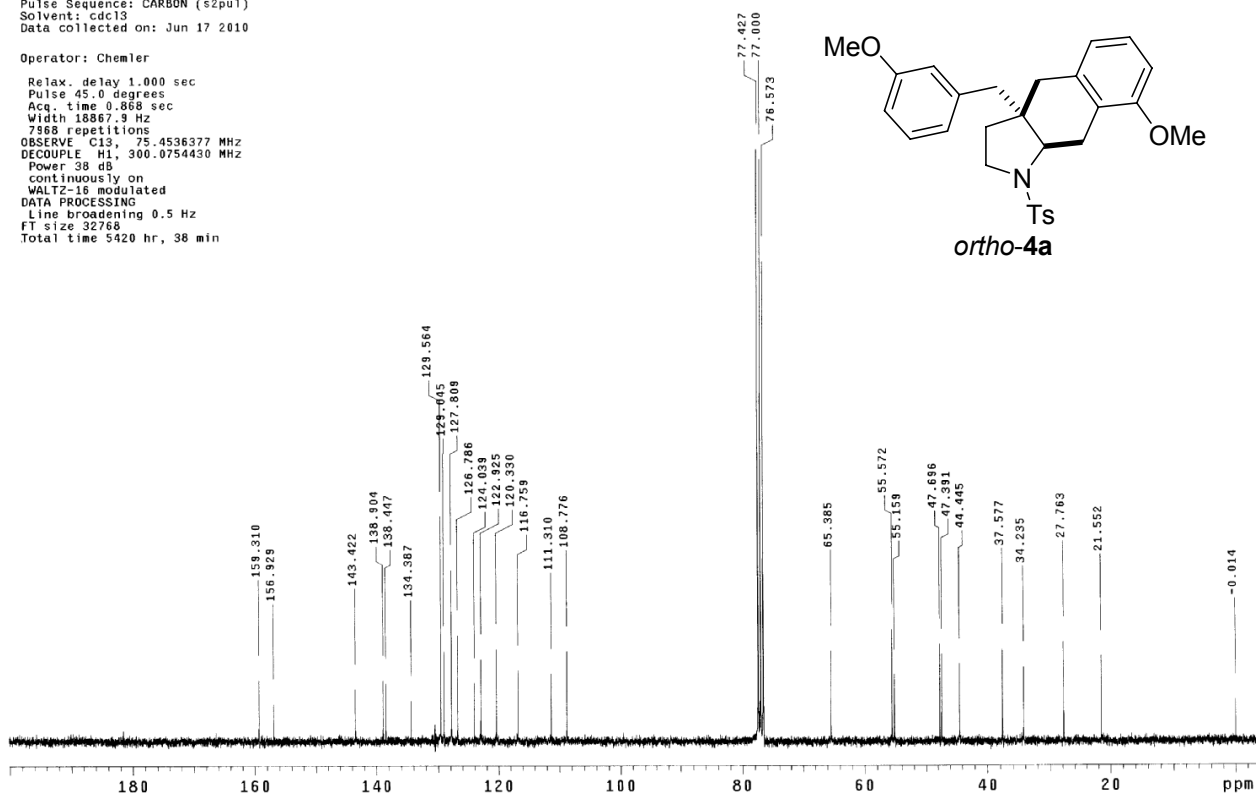
Data Collected on:
Roesy.Chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Jun 17 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
788 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 5420 hr, 38 min

20100701d13methoxylparaproduct

Sample Name:

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

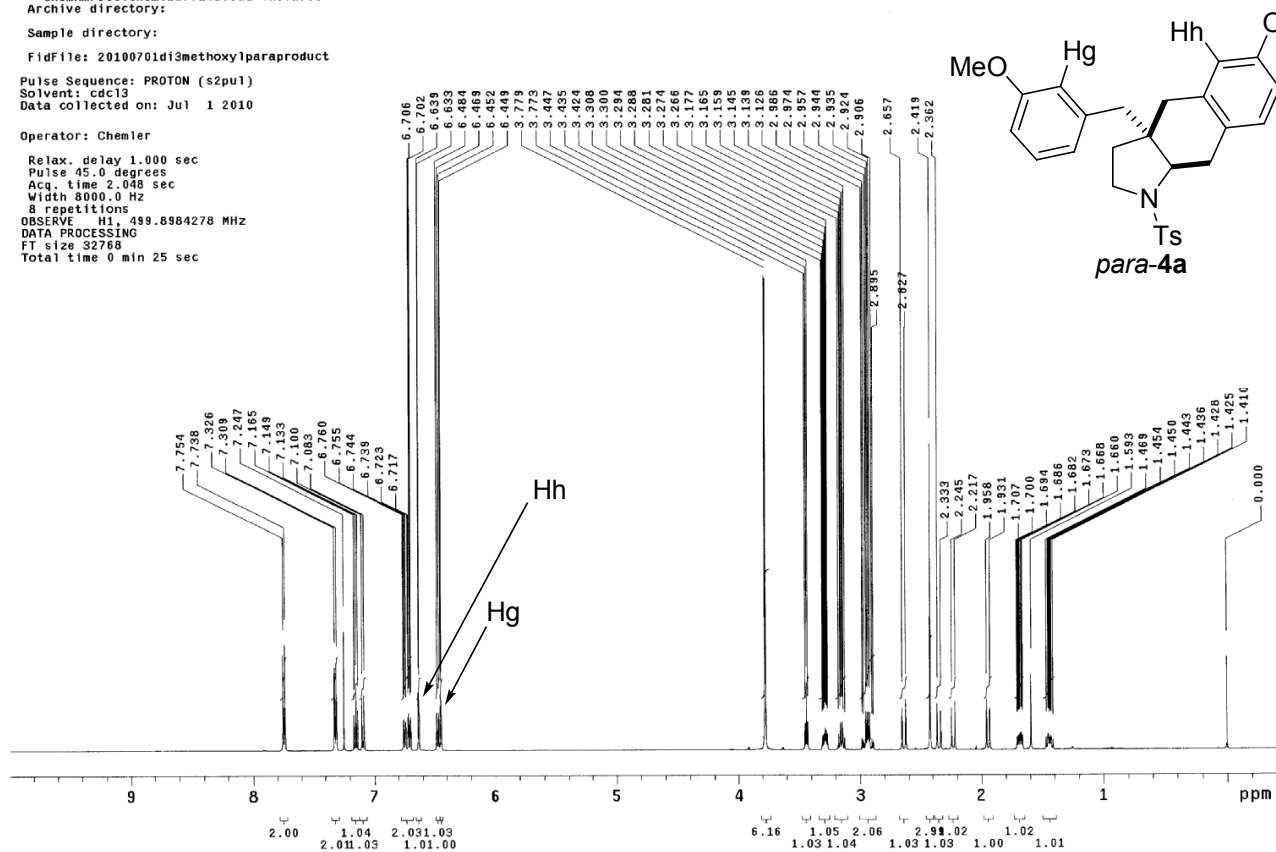
Archive directory:

Sample directory:

FidFile: 20100701d13methoxylparaproduct

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Ju 1 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitionsOBSERVE H1, 499.8984278 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

20100701d13methoxylparaproductC13

Sample Name:

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

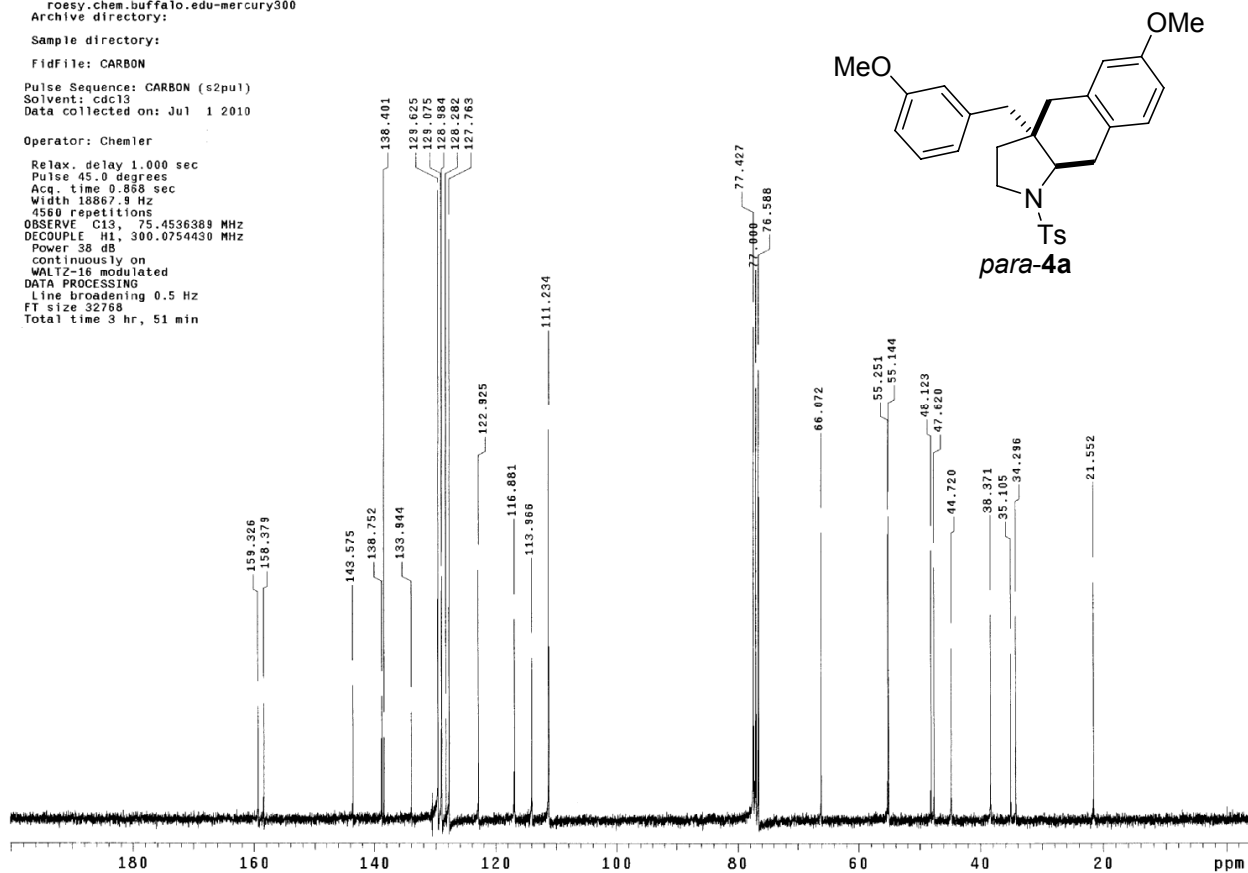
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Ju 1 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.869 sec
Width 18867.9 Hz
4580 repetitionsOBSERVE 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 3 hr, 51 min

20100617d13methoxyortho-productNOESY1D

Sample Name:

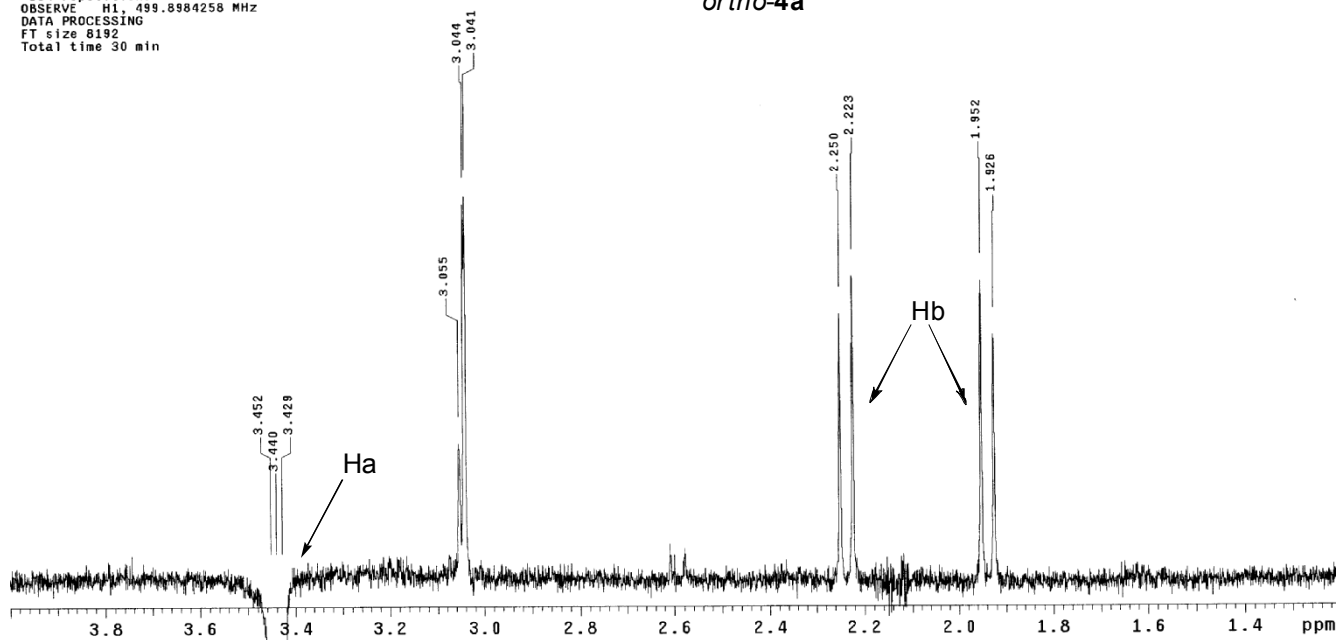
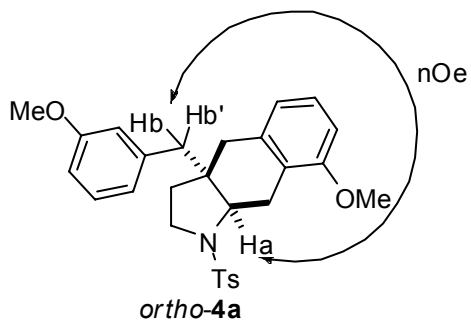
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100617d13methoxyortho-productNOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jun 17 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.925 sec
Width 1400.6 Hz
384 repetitions
OBSERVE H1, 499.8984258 MHz
DATA PROCESSING
FT size 6192
Total time 30 min

20100701d13methoxy1paraproductNOESY1D

Sample Name:

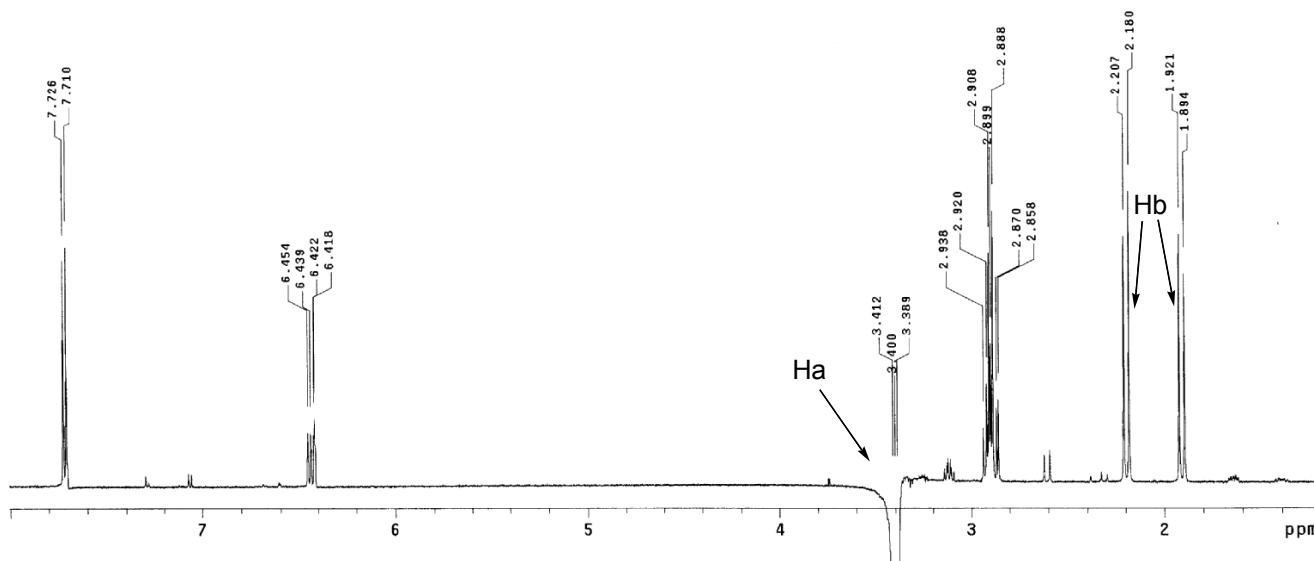
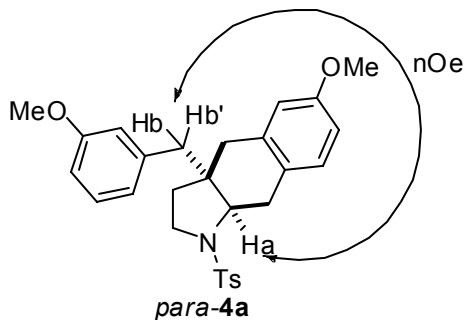
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100701d13methoxy1paraproductNOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jul 1 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.402 sec
Width 3410.1 Hz
10752 repetitions
OBSERVE H1, 499.8984268 MHz
DATA PROCESSING
FT size 16384
Total time 12 hr, 45 min

20100620diomethylcisproduct

Sample Name:

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

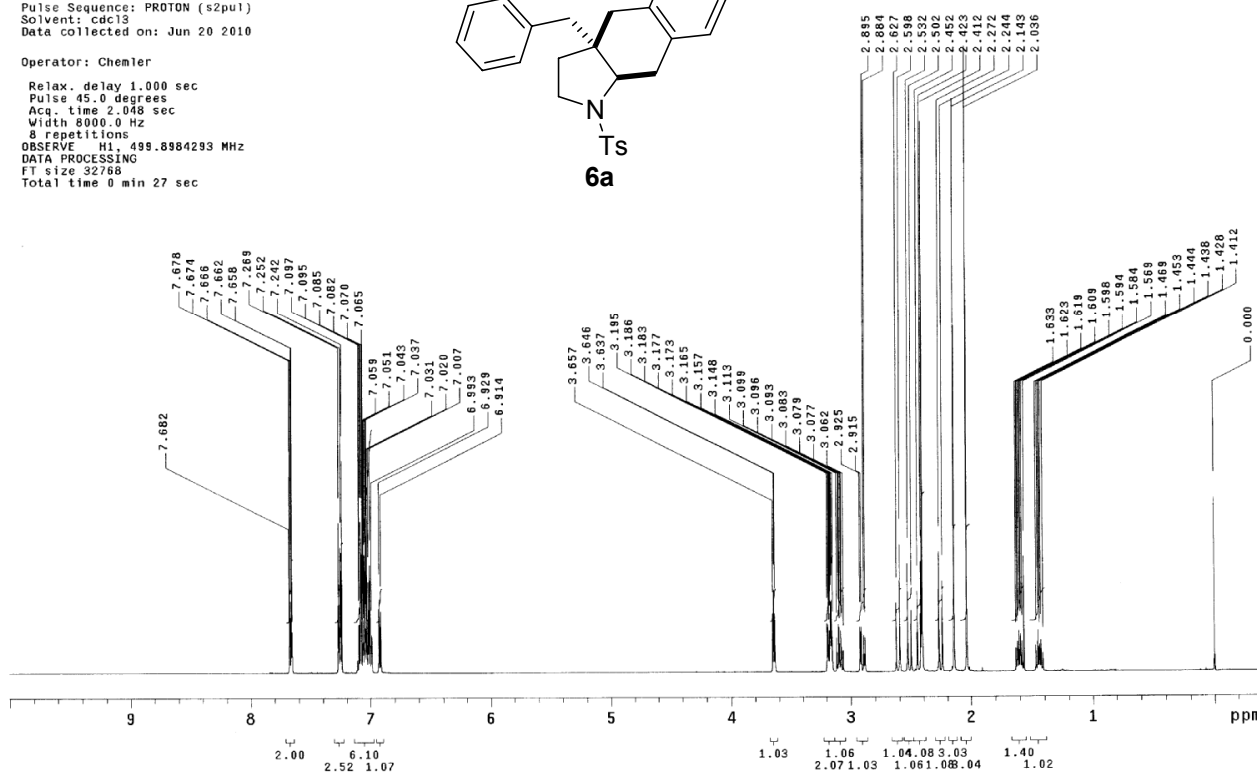
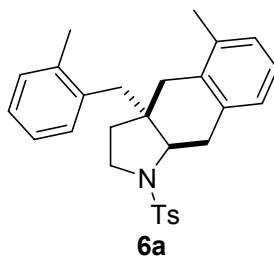
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Jun 20 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984293 MHz
DATA PROCESSING
FT size 32788
Total time 0 min 27 sec

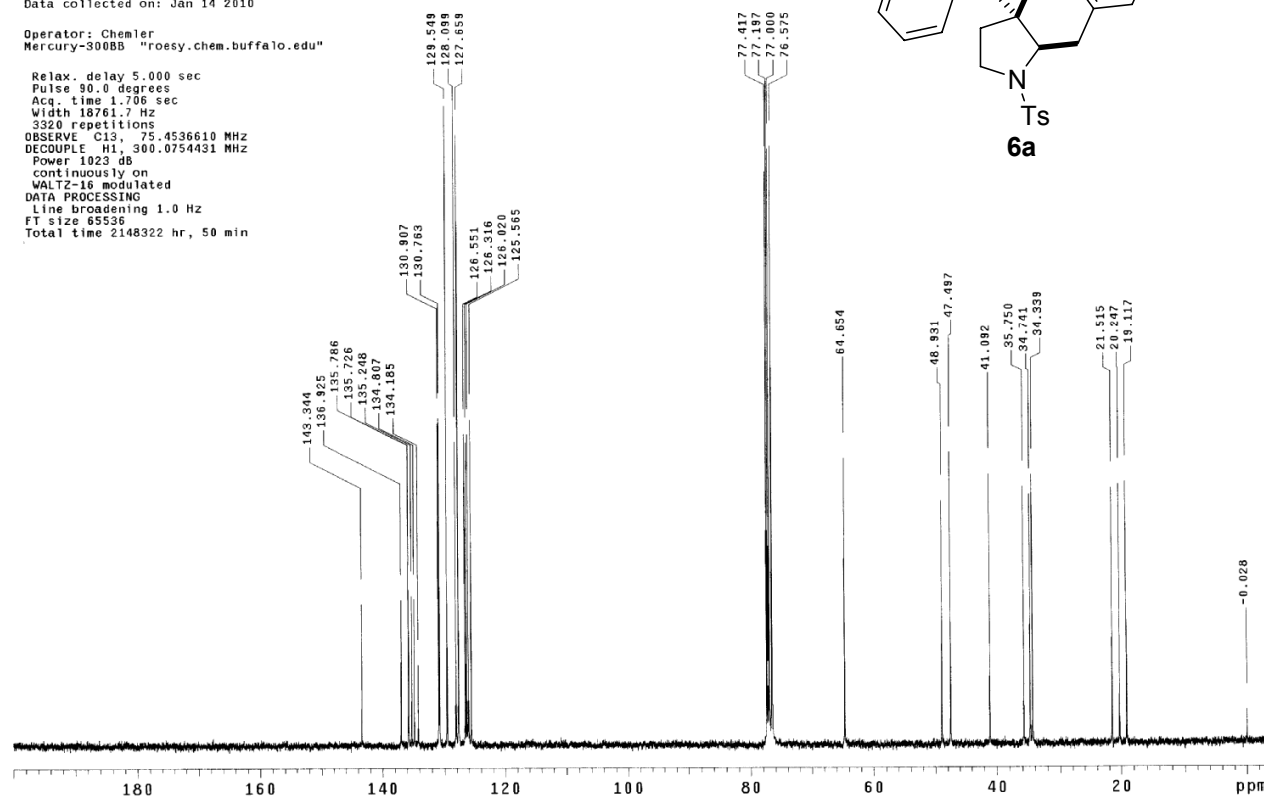
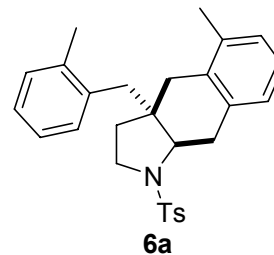
20100114diomethylmajorproductC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)
Solvent: CDC13
Data collected on: Jan 14 2010Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 5.000 sec
Pulse 90.0 degrees
Acq. time 1.708 sec
Width 18761.7 Hz
3320 repetitions
OBSERVE C13, 75.4536610 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2148322 hr, 50 min

20100215diomethylminorproduct

Sample Name:

Archive directory:

Sample directory:

FidFile: H1

Pulse Sequence: s2pu1

Solvent: CDC13

Data collected on: Feb 15 2010

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec

Pulse 39.7 degrees

Acq. time 1.931 sec

Width 10000.0 Hz

16 repetitions

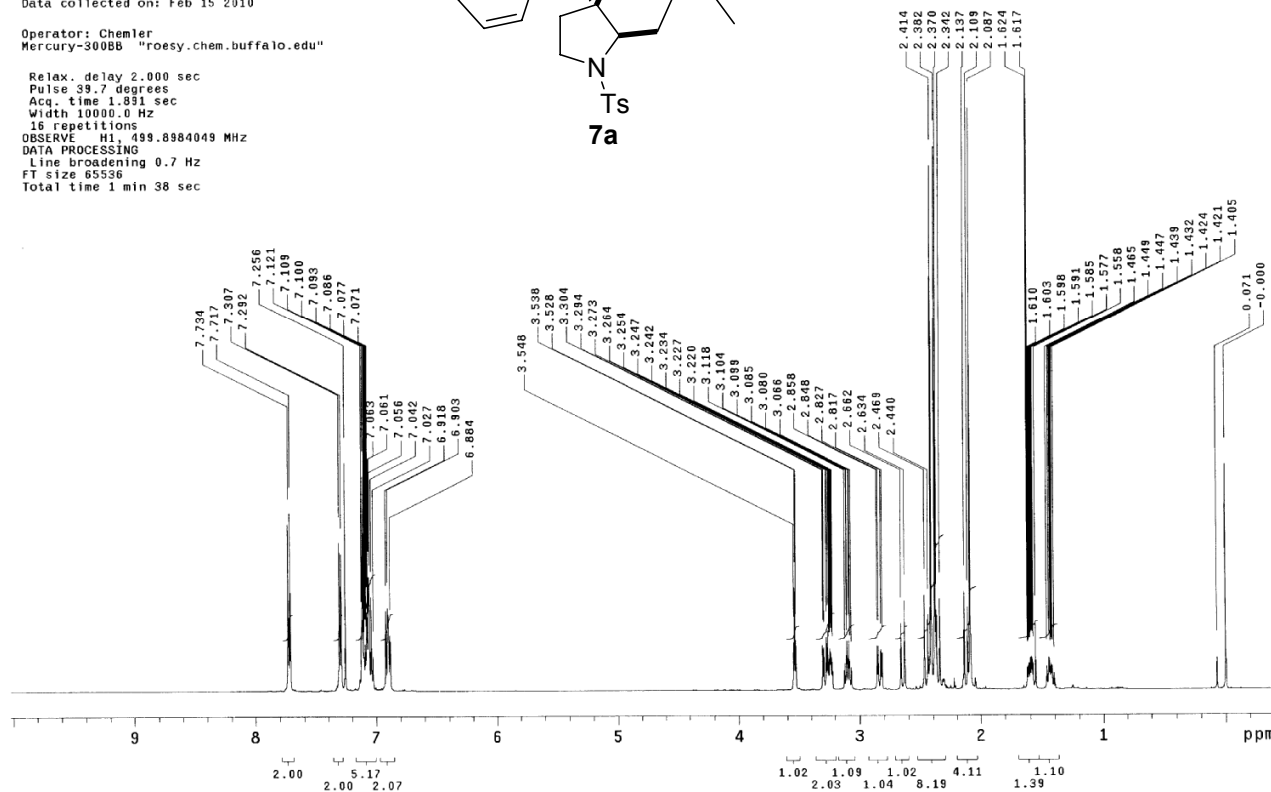
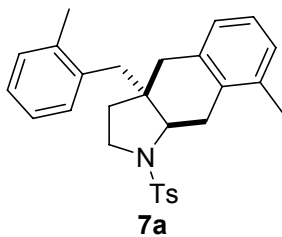
OBSERVE H1, 499.8984049 MHz

DATA PROCESSING

Line broadening 0.7 Hz

FT size 65536

Total time 1 min 38 sec



20100215diomethylminorproductC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)

Solvent: CDC13

Data collected on: Feb 15 2010

Operator: Chemler

Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

2800 repetitions

OBSERVE C13, 75.4536604 MHz

DECOUPLE H1, 300.0754431 MHz

Power 1023 dB

continuously on

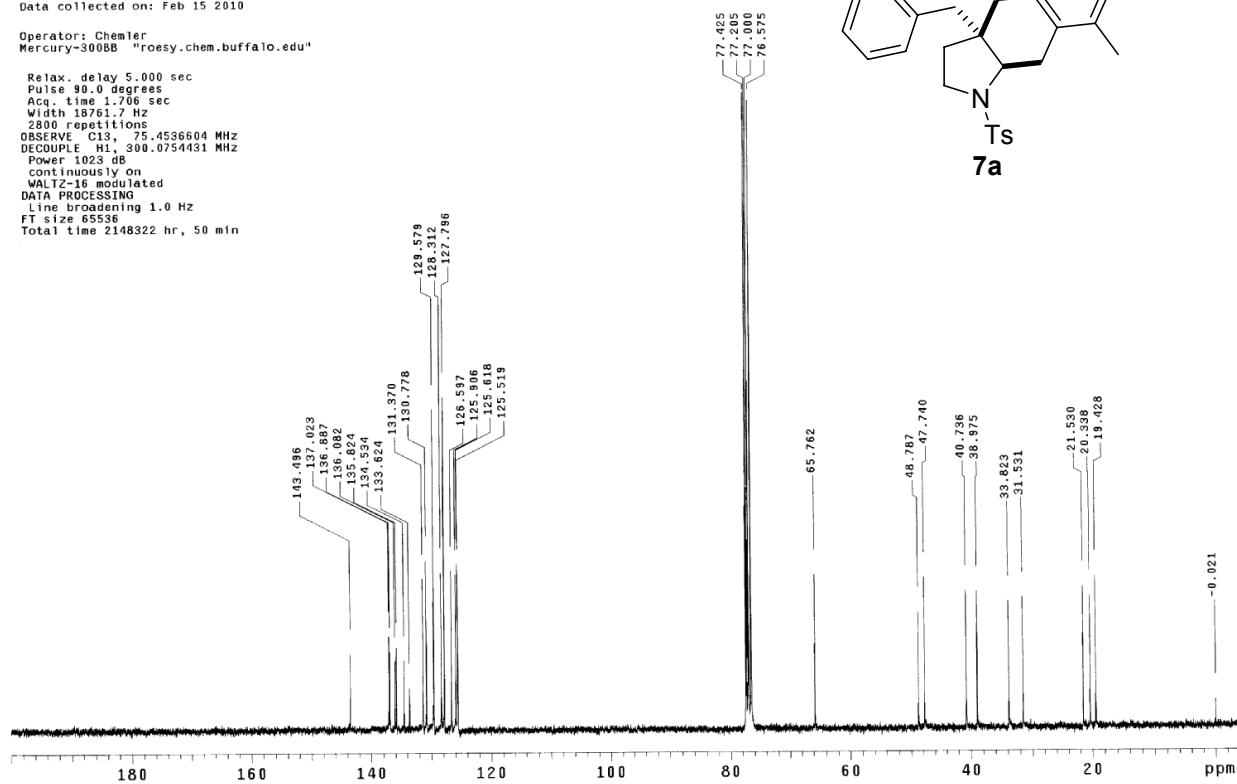
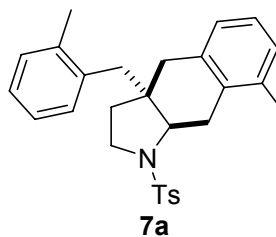
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 2148322 hr, 50 min



20100620diomethylcisproductcosyNOESY1D

Sample Name:

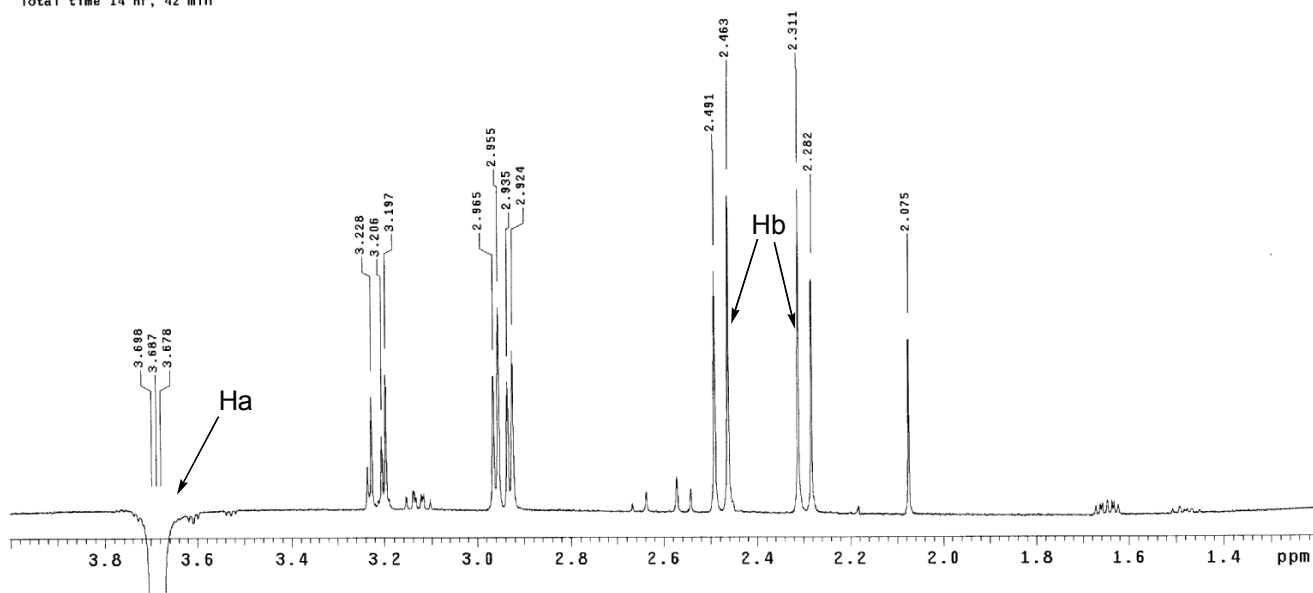
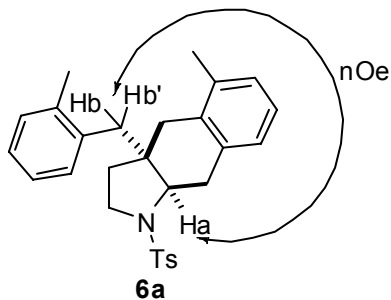
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100620diomethylcisproductcosyNOESY1D

Pulse Sequence: NOESY1D
Solvent: cdc13
Data collected on: Jun 20 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.928 sec
Width 1398.9 Hz
11200 repetitions
OBSERVE H1, 499.8983908 MHz
DATA PROCESSING
FT size 8192
Total time 14 hr, 42 min

20100621diomethyltransproductNOESY1D

Sample Name:

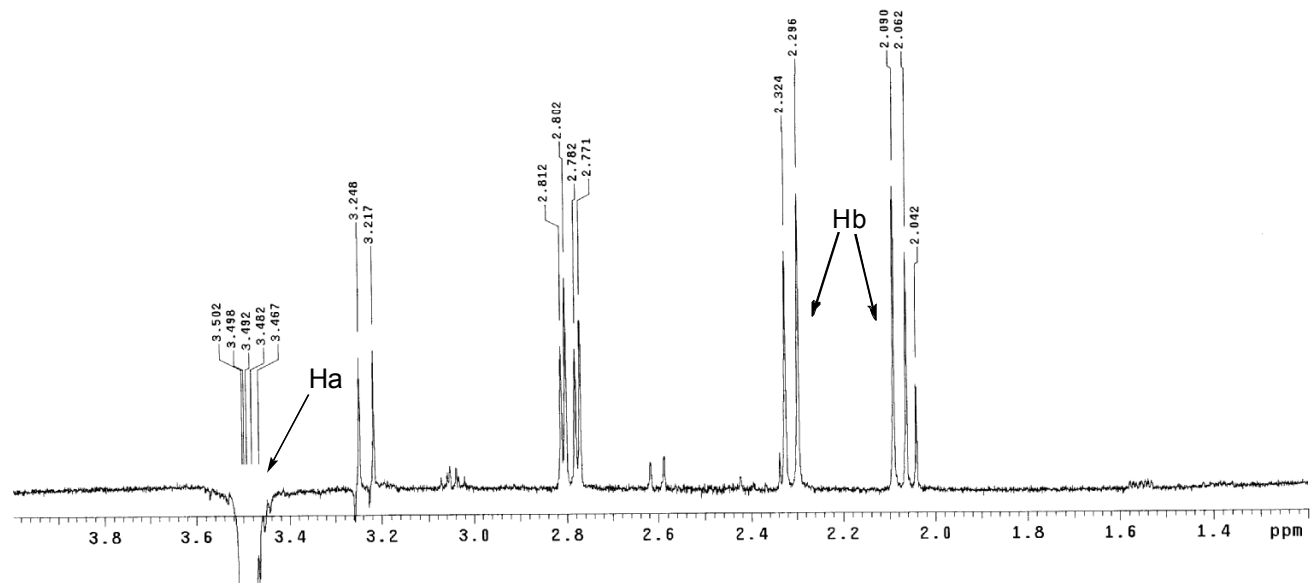
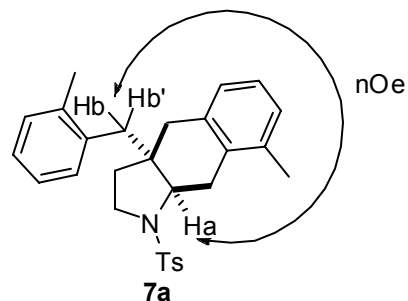
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100621diomethyltransproductNOESY1D

Pulse Sequence: NOESY1D
Solvent: cdc13
Data collected on: Jun 21 2010

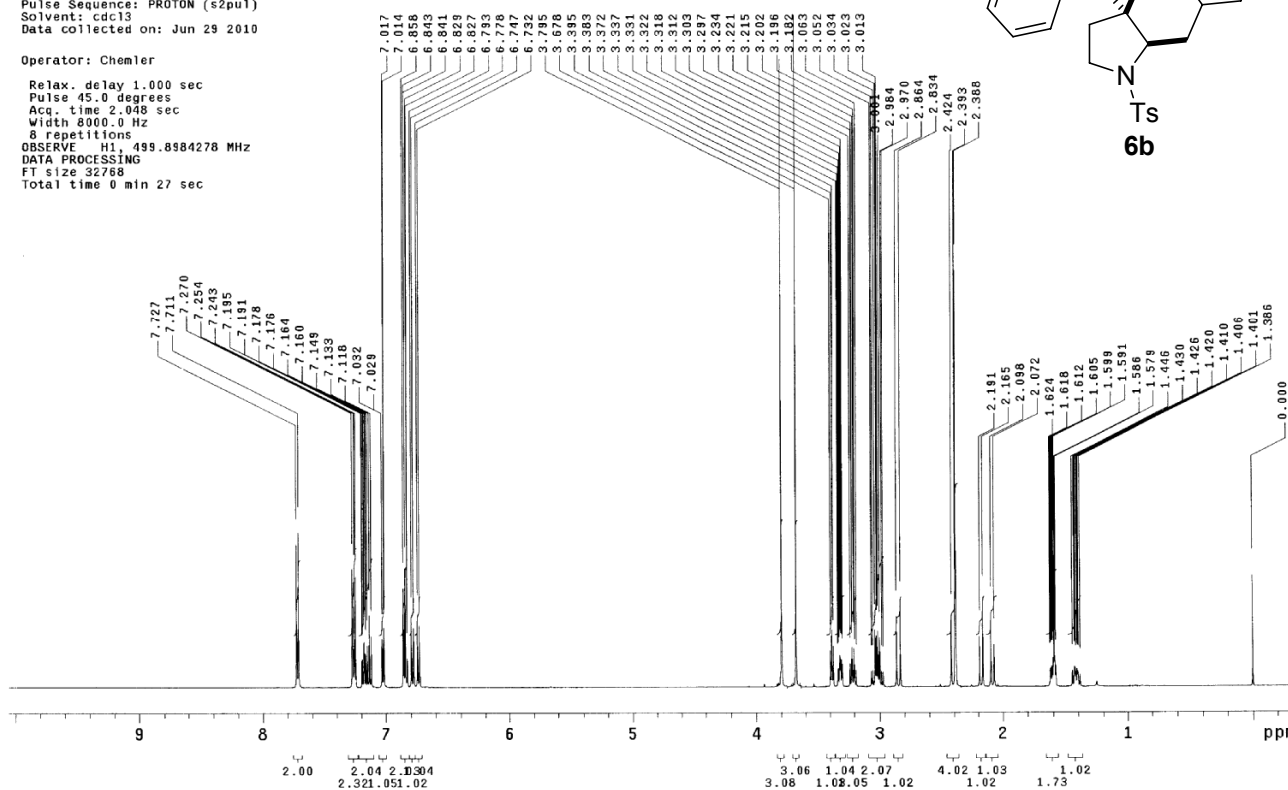
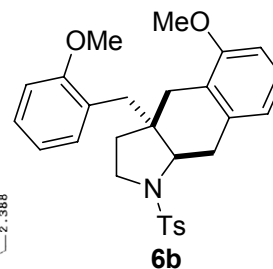
Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.928 sec
Width 1398.9 Hz
9600 repetitions
OBSERVE H1, 499.8984259 MHz
DATA PROCESSING
FT size 8192
Total time 12 hr, 41 min

20100628diomethoxyImajorproduct

Sample Name:
 Data Collected on:
 chemmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 FidFile: PROTON

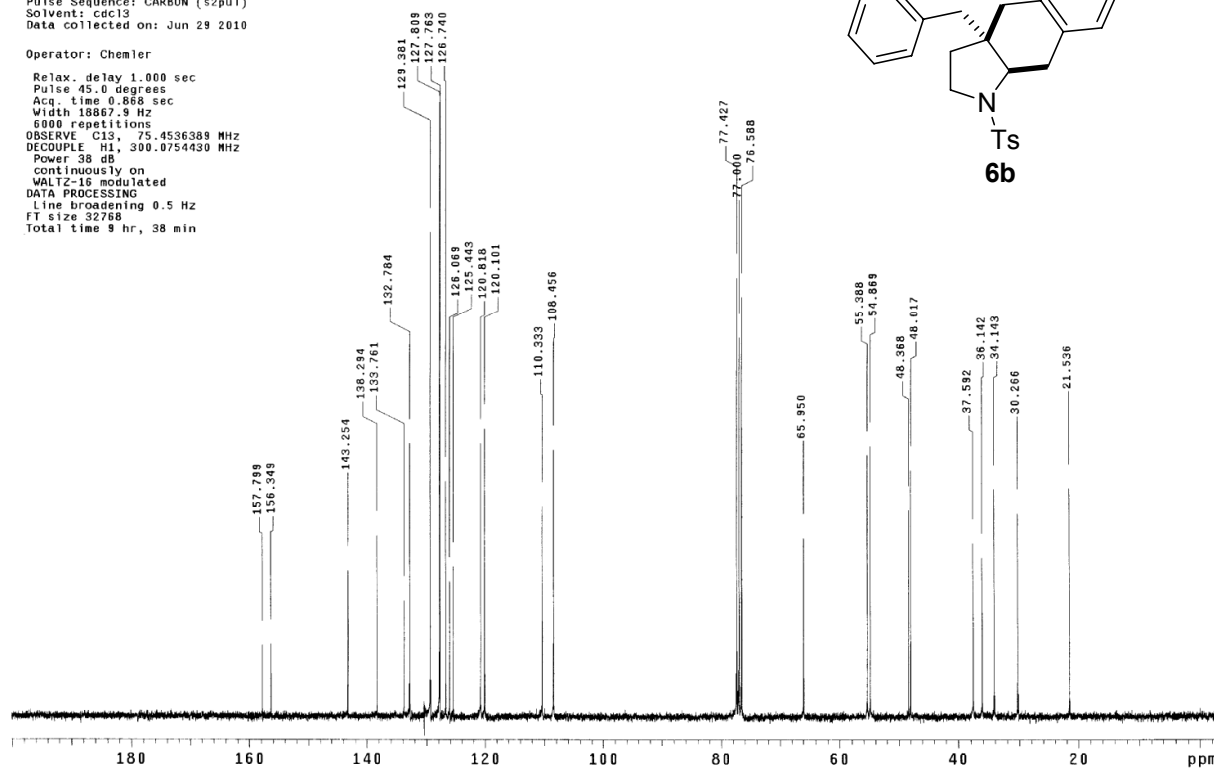
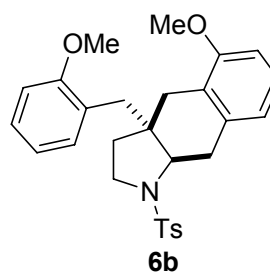
Pulse Sequence: PROTON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jun 29 2010
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1 499.8584278 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 27 sec



20100629diomethoxyImajorproductC13

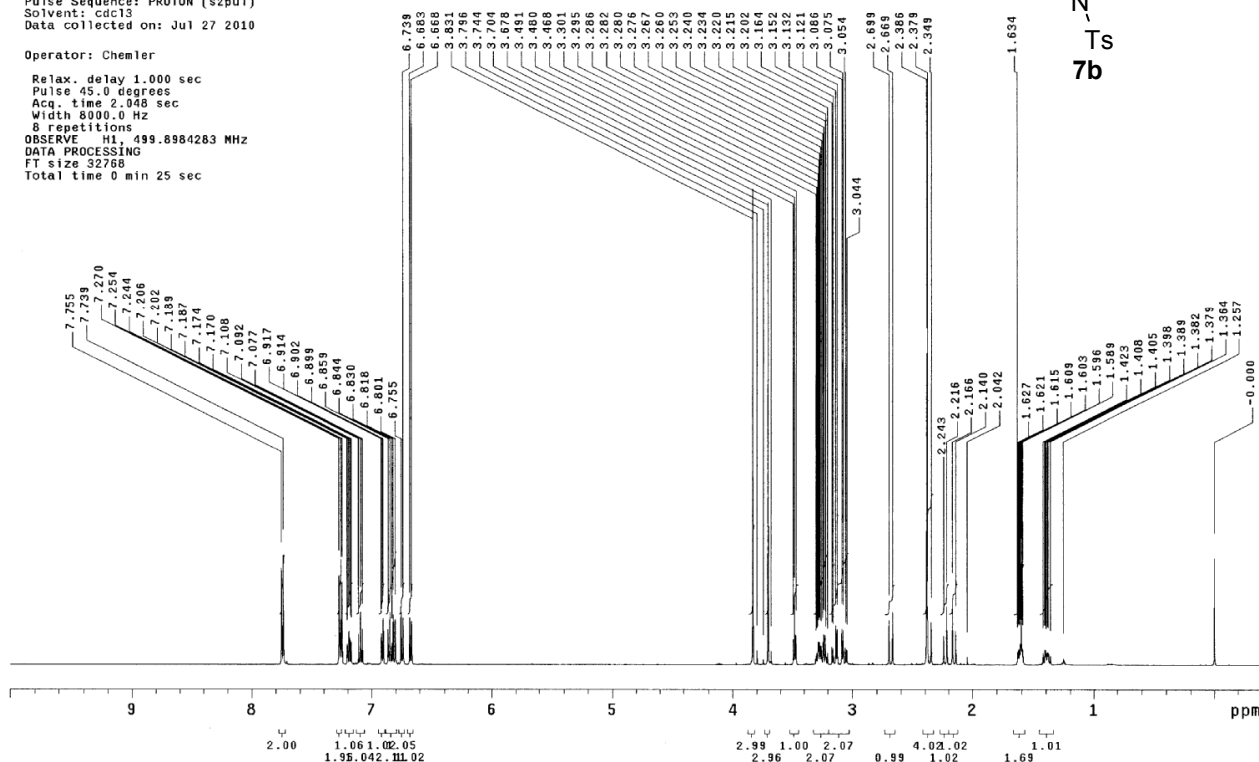
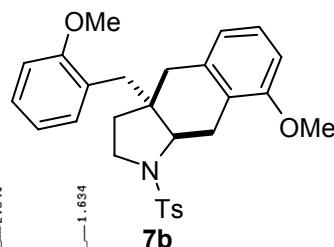
Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
 Solvent: cdcl3
 Data collected on: Jun 29 2010
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 6000 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 9 hr, 38 min



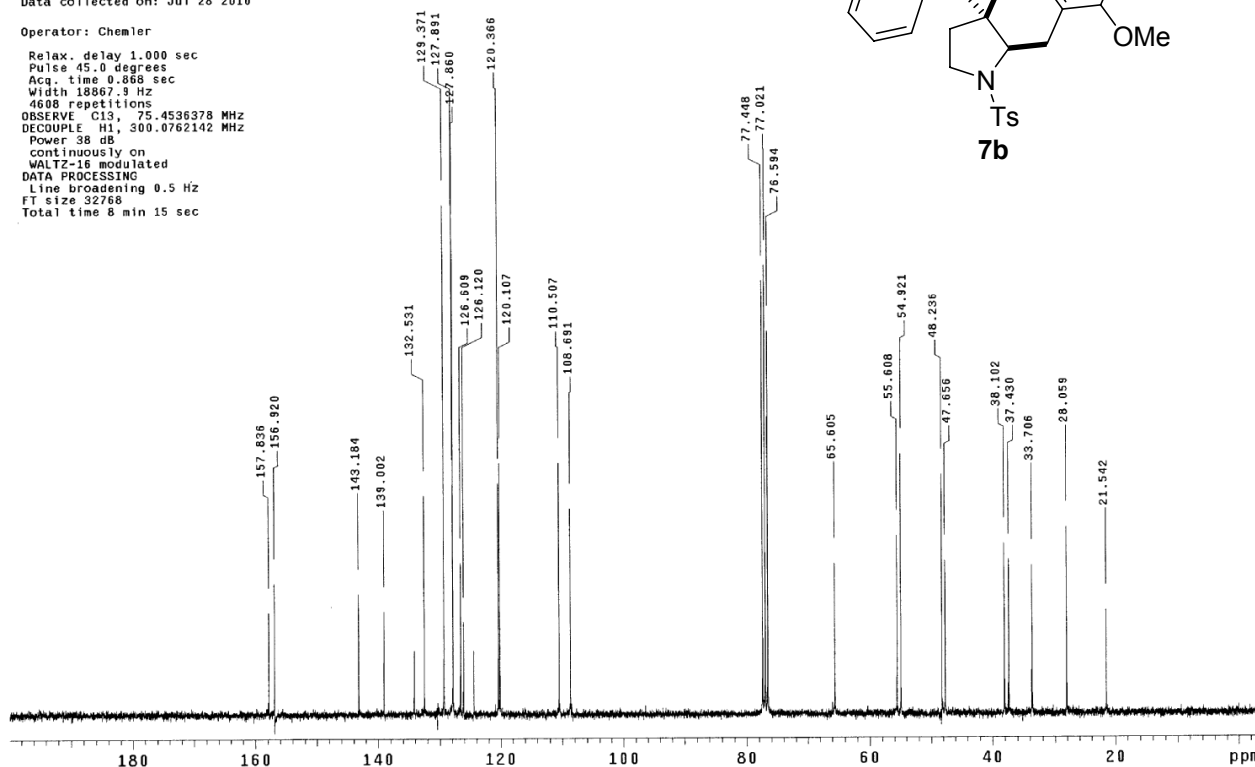
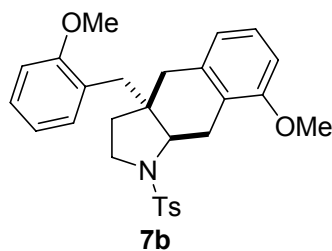
20100727diomethoxyiminorproduct
 Sample Name:
 Data Collected on:
 chemmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pul)
 Solvent: cdc13
 Data collected on: Jul 27 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE H1, 499.8984283 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 25 sec



20100728diomethoxyiminorproductC13
 Sample Name:
 Data Collected on:
 roesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pul)
 Solvent: D2O
 Data collected on: Jul 28 2010

Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18867.9 Hz
 4600 repetitions
 OBSERVE C13, 75.4536378 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 8 min 15 sec



20100630diomethoxylmajorproductNOESY1Db

Sample Name:

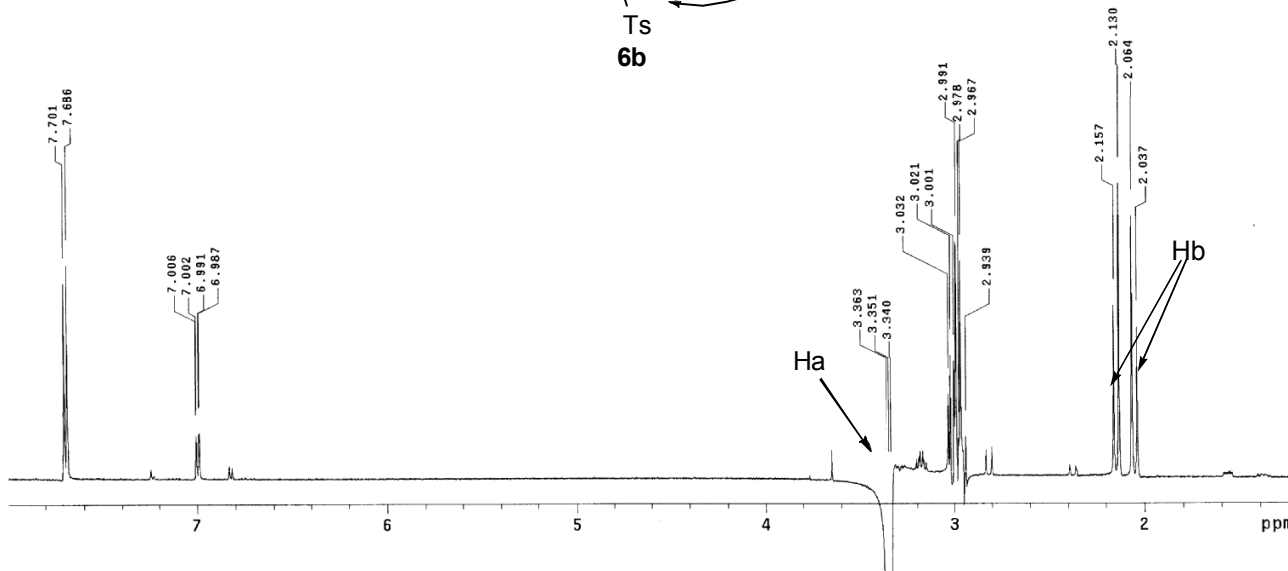
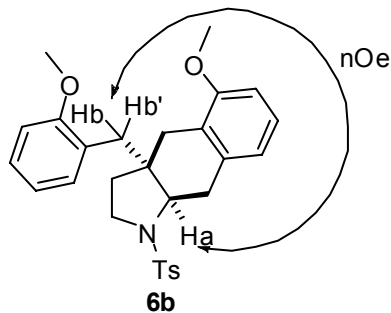
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100630diomethoxylmajorproductNOESY1Db

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jun 30 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.409 sec
Width 3400.2 Hz
10240 repetitions
OBSERVE H1, 499.8984298 MHz
DATA PROCESSING
FT size 16384
Total time 12 hr, 3 min

20100628diomethoxylmajorproductNOESY1D

Sample Name:

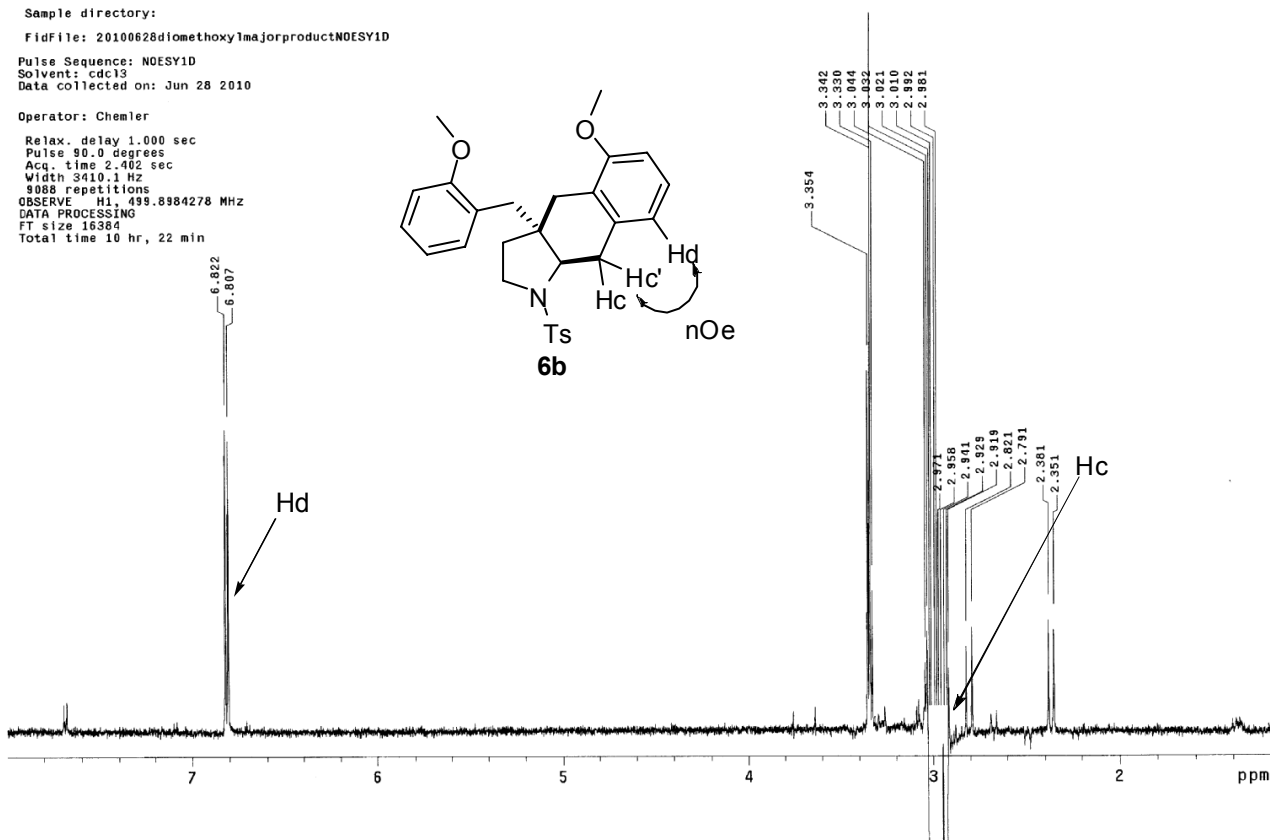
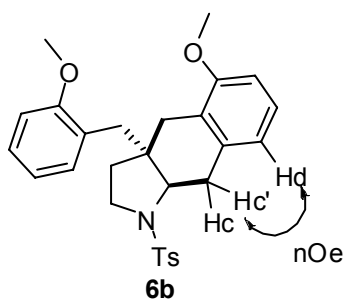
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100628diomethoxylmajorproductNOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jun 28 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.402 sec
Width 3410.1 Hz
9098 repetitions
OBSERVE H1, 499.8984278 MHz
DATA PROCESSING
FT size 16384
Total time 10 hr, 22 min

20100703diomethoxylminorproductNOESY1D

Sample Name:

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

Sample directory:

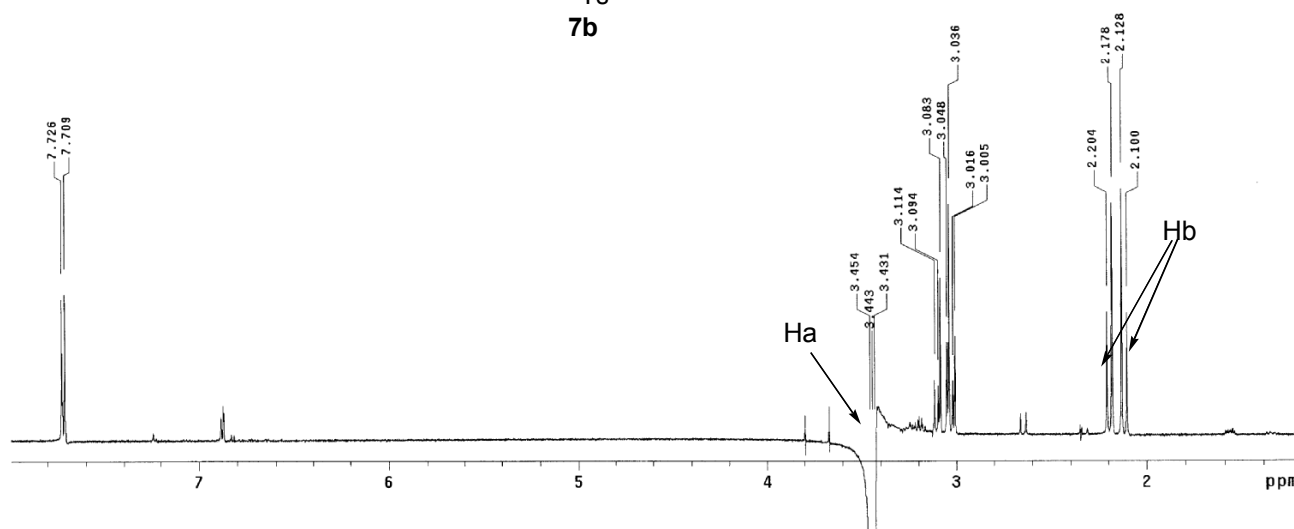
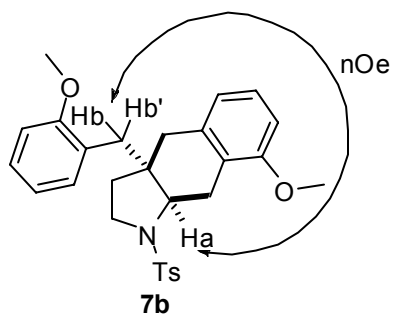
FidFile: 20100703diomethoxylminorproductNOESY1D

Pulse Sequence: NOESY1D

Solvent: cdcl3

Data collected on: Jul 3 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.409 sec
Width 3400.2 Hz
11776 repetitions
OBSERVE H1, 499.8984273 MHz
DATA PROCESSING
FT size 16384
Total time 14 hr, 18 min

20100703diomethoxylminorproductNOESY1Db

Sample Name:

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

Sample directory:

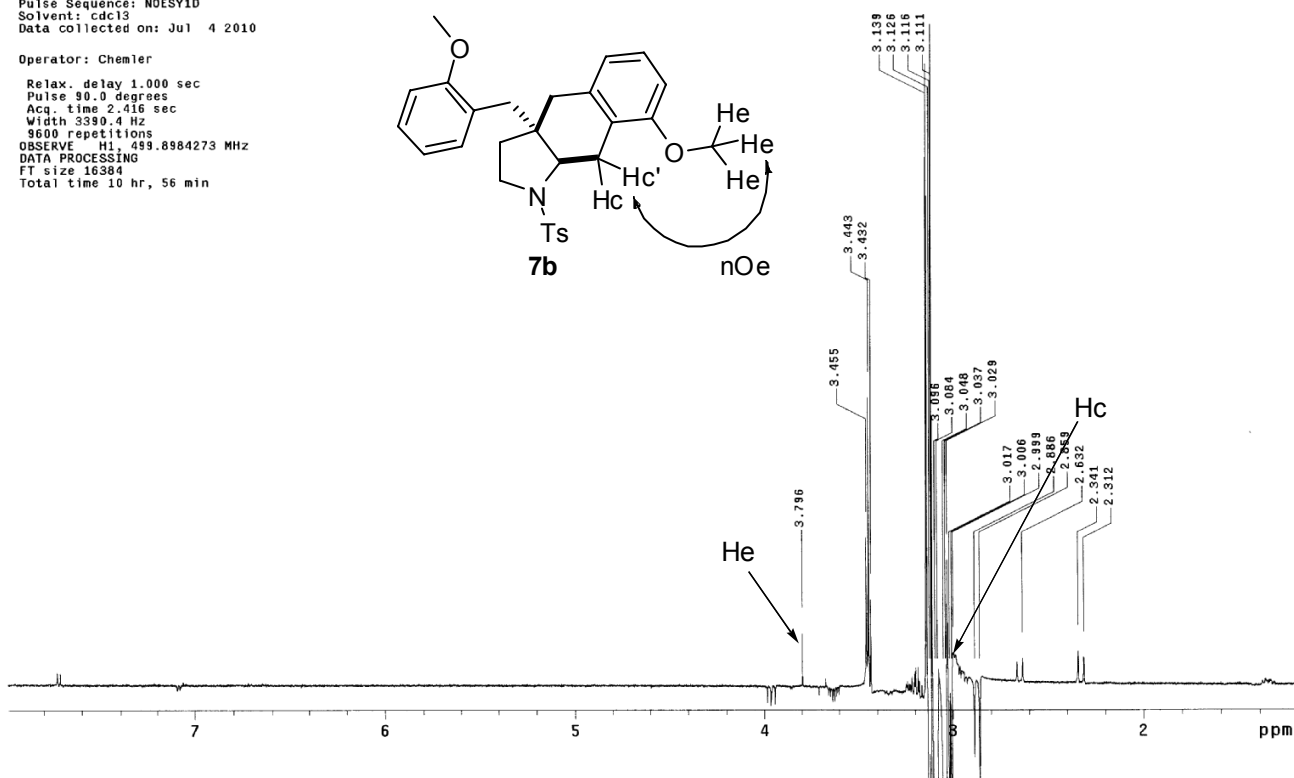
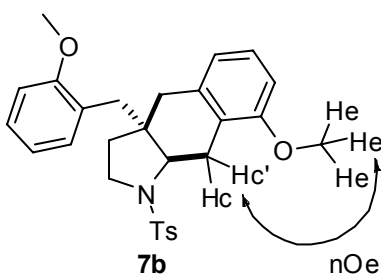
FidFile: 20100703diomethoxylminorproductNOESY1Db

Pulse Sequence: NOESY1D

Solvent: cdcl3

Data collected on: Jul 4 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.416 sec
Width 3390.4 Hz
9600 repetitions
OBSERVE H1, 499.8984273 MHz
DATA PROCESSING
FT size 16384
Total time 10 hr, 56 min

20100704ditrifluoromethylmajorproduct

Sample Name:

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

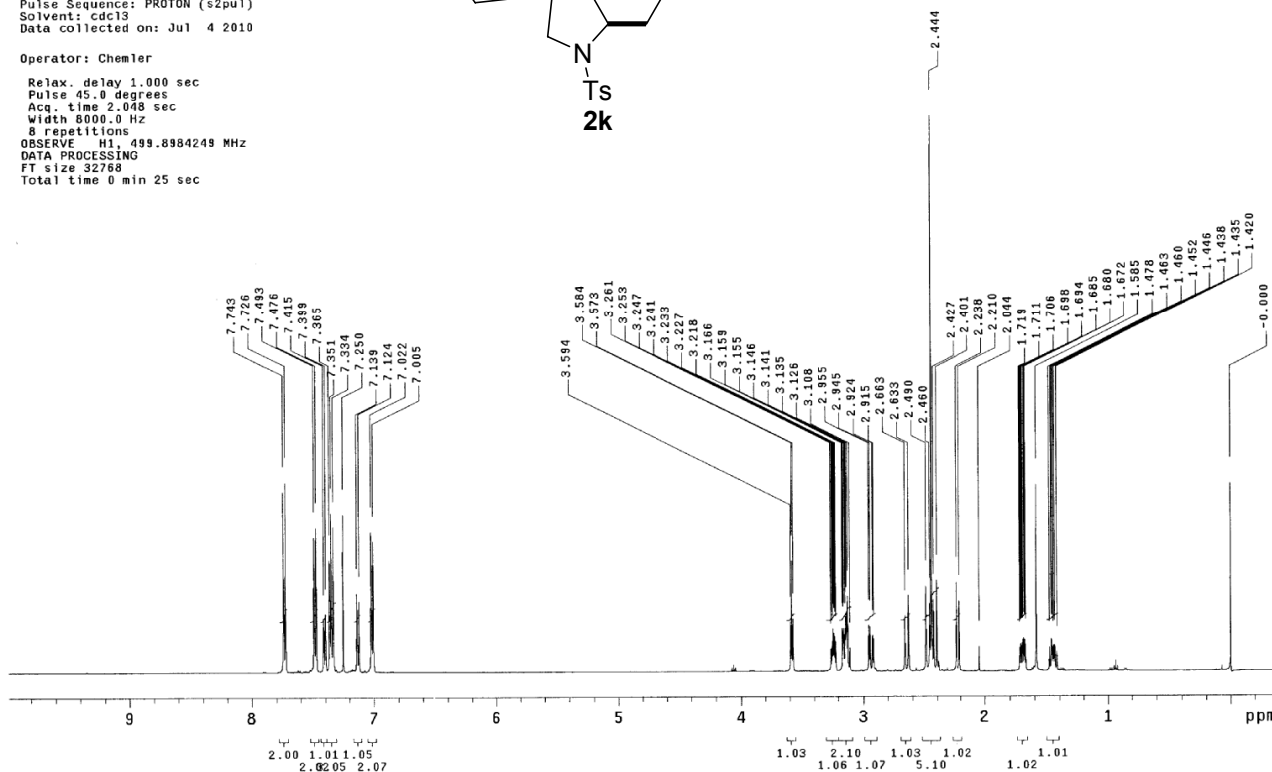
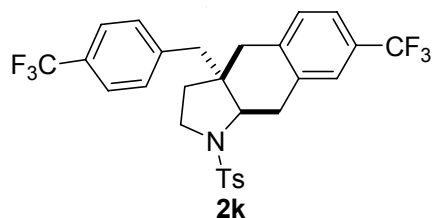
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdcl3
Data collected on: Jul 4 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984248 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

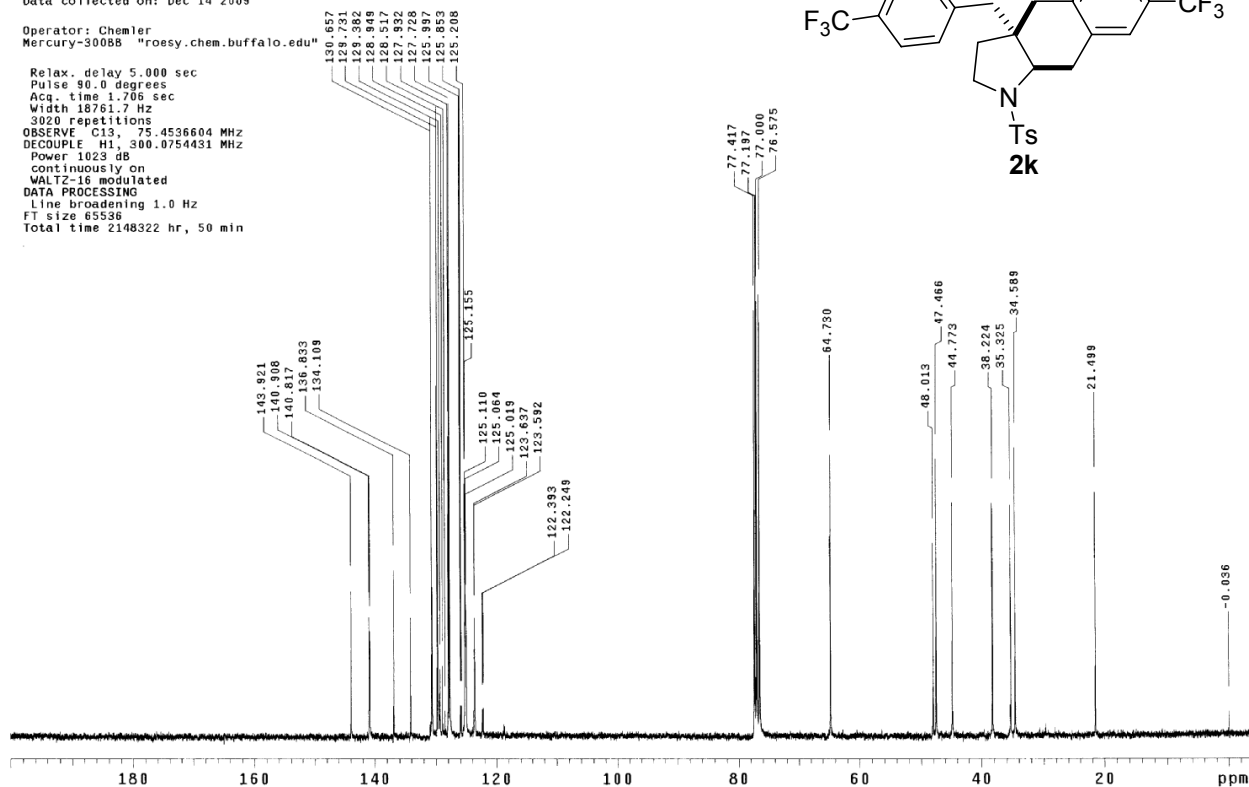
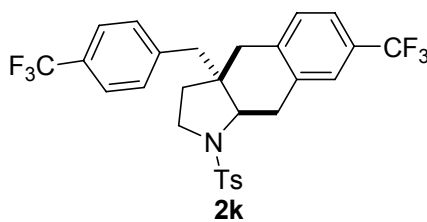
20091214ditrifluoromethylmajorproductC13

Sample Name:

Archive directory:

Sample directory:

FidFile: std13c

Pulse Sequence: std13c (s2pu1)
Solvent: CDC13
Data collected on: Dec 14 2009Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"Relax. delay 5.000 sec
Pulse 90.0 degrees
Acq. time 1.708 sec
Width 18761.7 Hz
3020 repetitions
OBSERVE C13, 75.4536604 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 2148322 hr, 50 min

20100705dinitrifluoromethylaminorproduct

Sample Name:

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

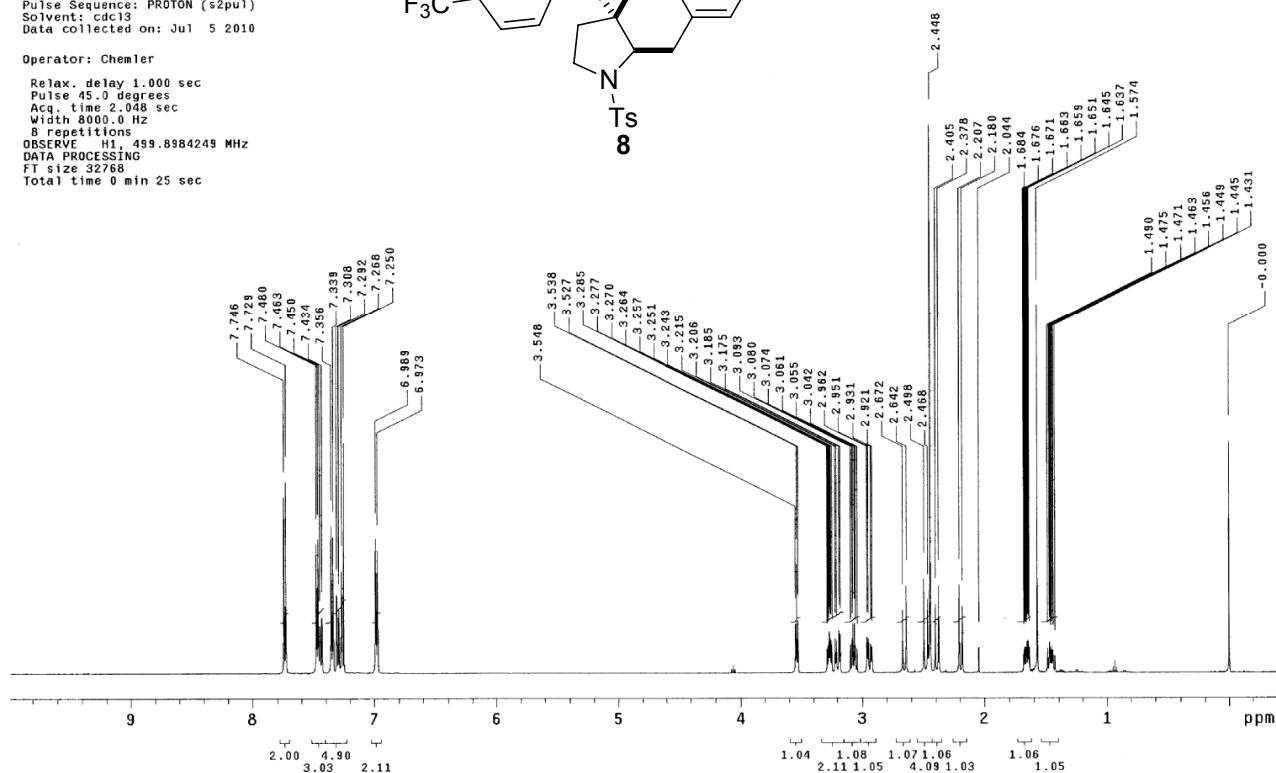
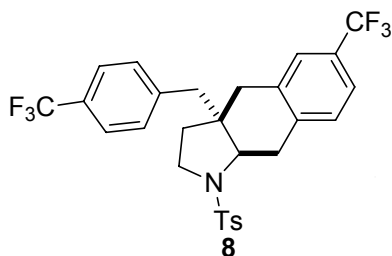
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cdc13
Data collected on: Jul 5 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984249 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 25 sec

2010dinitrifluoromethylaminorproductC13

Sample Name:

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

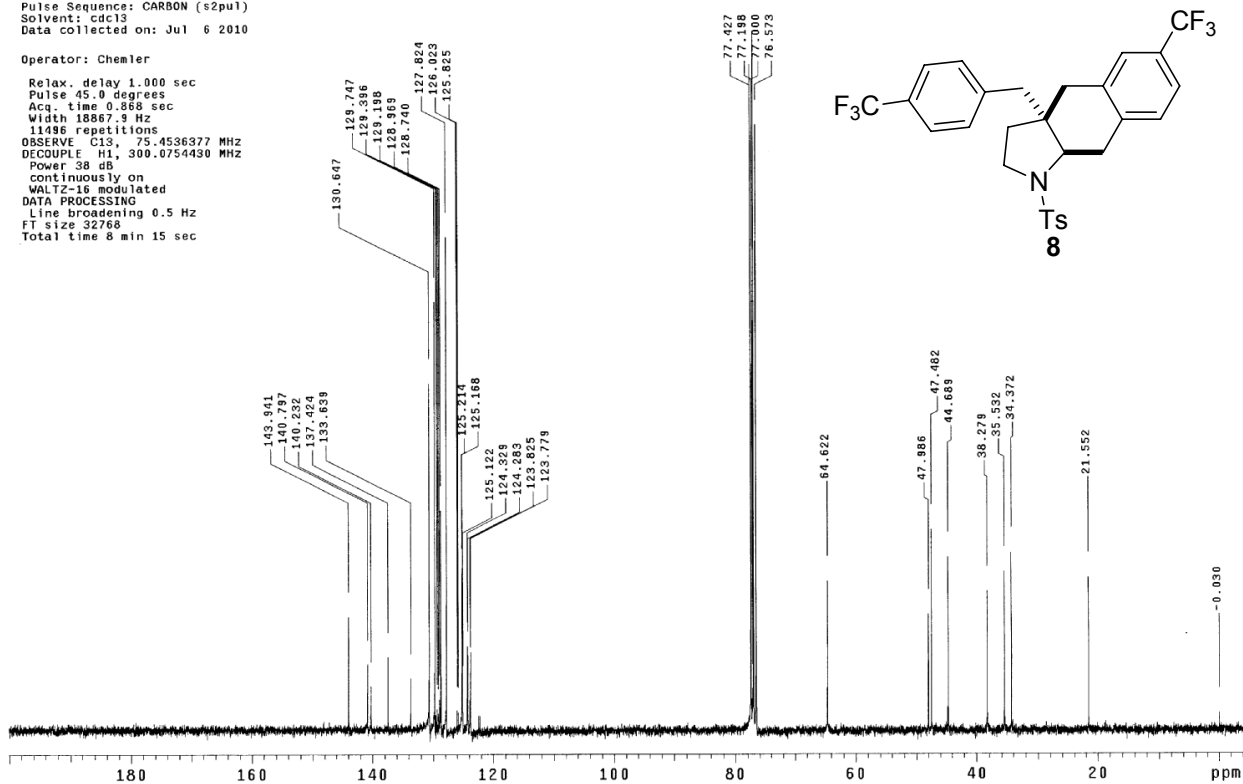
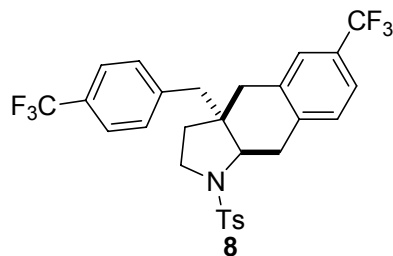
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Jul 6 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.3 Hz
1196 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 8 min 15 sec

20100704dinitrifluoromethylmajorproductNOESY1D

Sample Name:

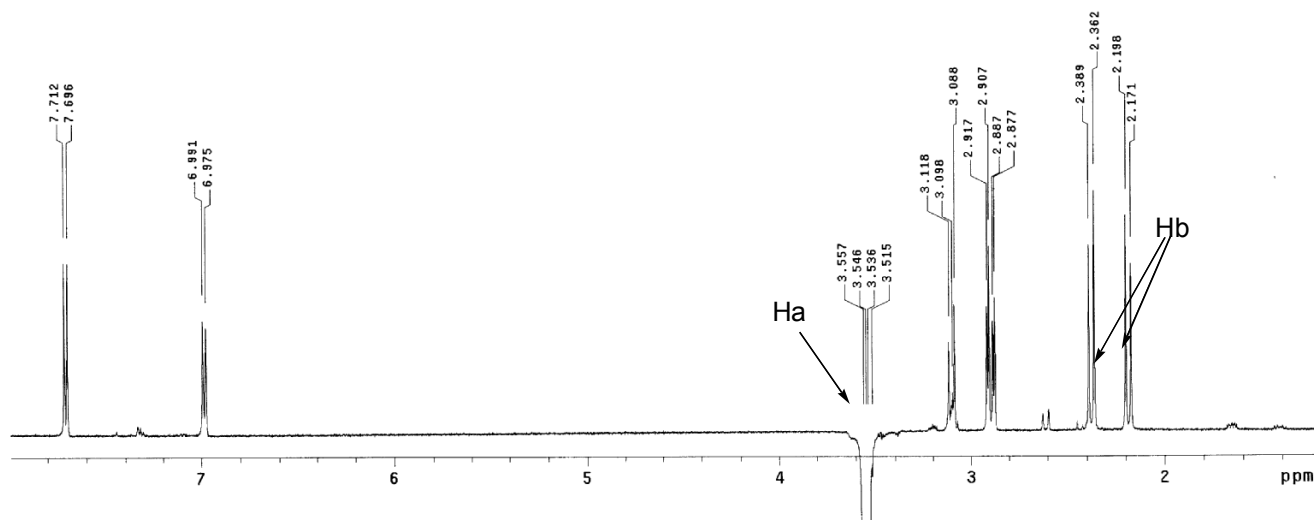
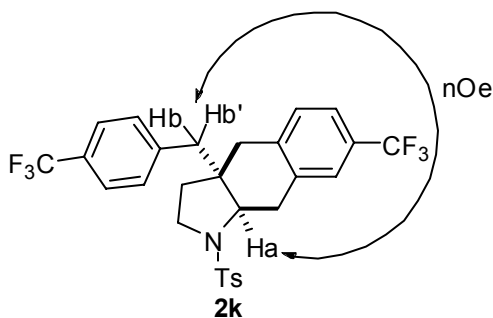
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100704dinitrifluoromethylmajorproductNOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jul 5 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.416 sec
Width 3390.4 Hz
7424 repetitions
OBSERVE H1, 499.8984249 MHz
DATA PROCESSING
FT size 16384
Total time 8 hr, 43 min

20100705dinitrifluoromethylminorproductNOESY1D

Sample Name:

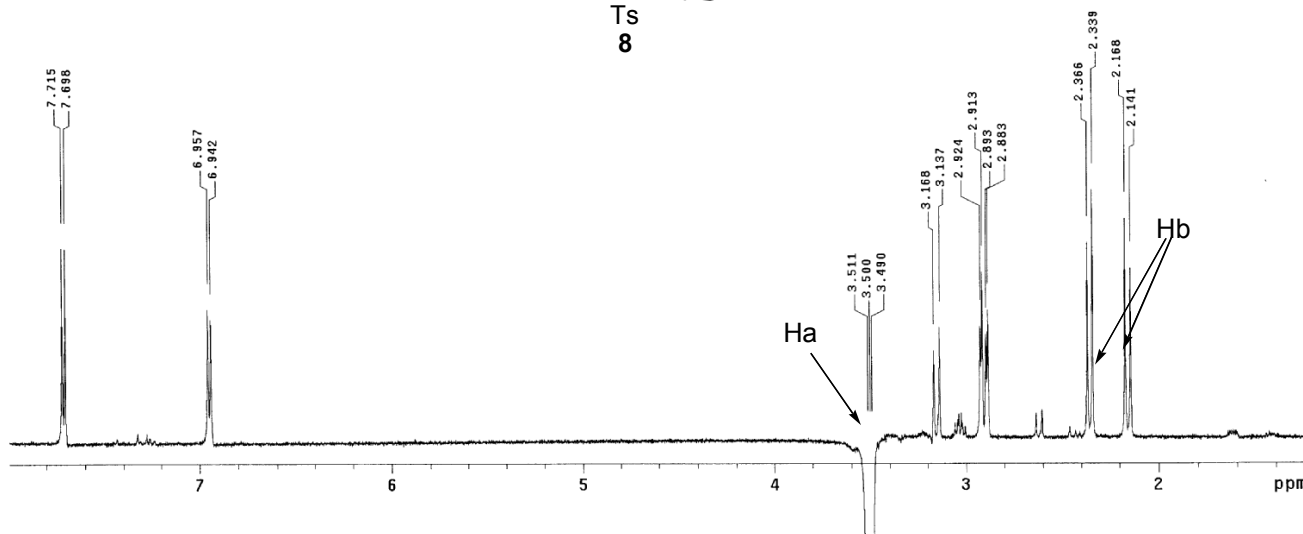
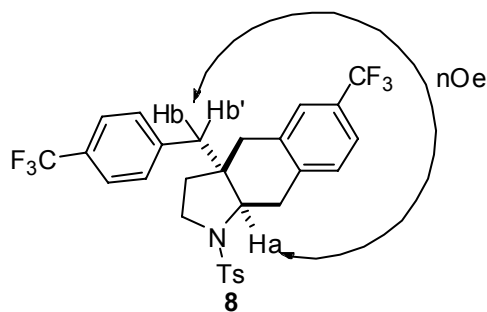
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: 20100705dinitrifluoromethylminorproductNOESY1D

Pulse Sequence: NOESY1D
Solvent: cdcl3
Data collected on: Jul 5 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 2.416 sec
Width 3390.4 Hz
10752 repetitions
OBSERVE H1, 499.8984249 MHz
DATA PROCESSING
FT size 16384
Total time 12 hr, 40 min

20100104benzylcarbonamination

Sample Name:

Archive directory:

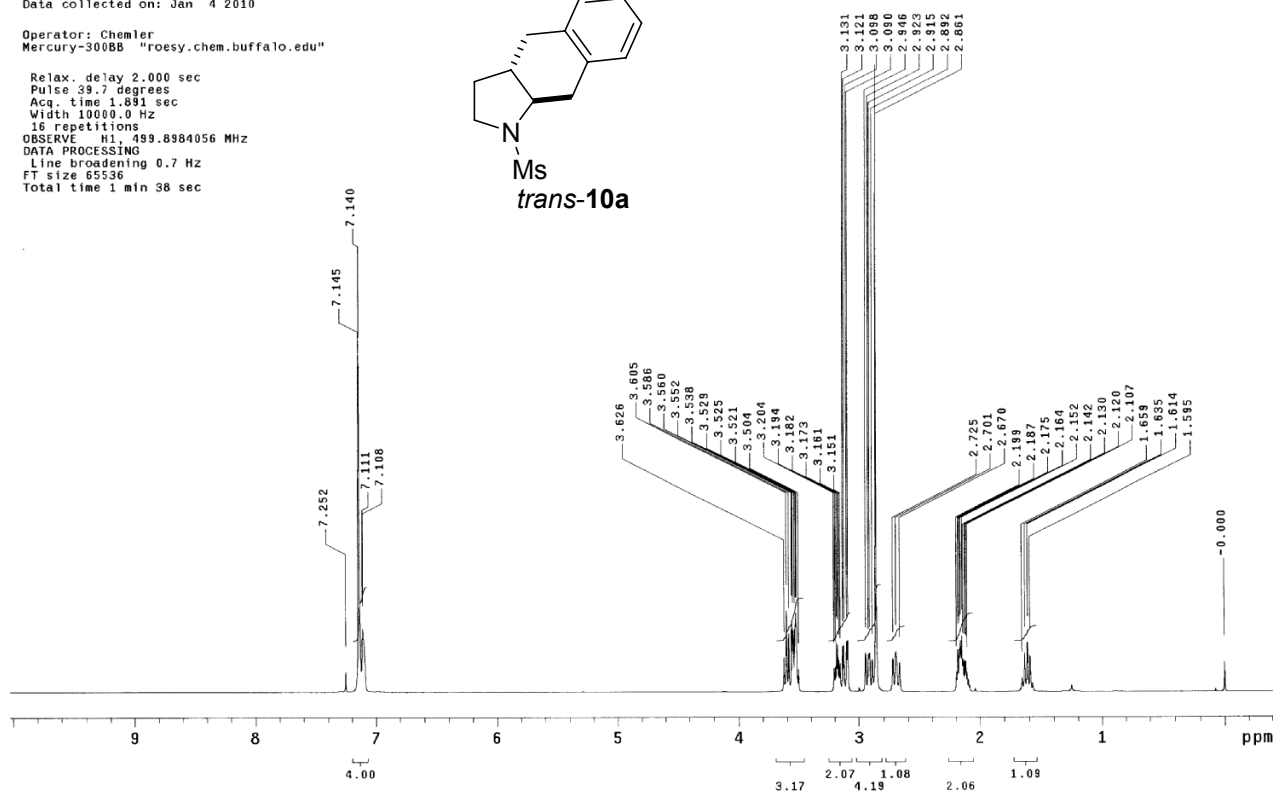
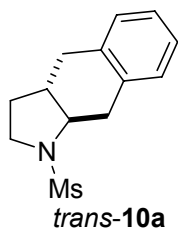
Sample directory:

FidFile: H1

Pulse Sequence: s2pul
 Solvent: CDC13
 Data collected on: Jan 4 2010

Operator: Chemler
 Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec
 Pulse 39.7 degrees
 Acq. time 1.891 sec
 Width 10000.0 Hz
 16 repetitions
 OBSERVE H1, 499.8984056 MHz
 DATA PROCESSING
 Line broadening 0.7 Hz
 FT size 65536
 Total time 1 min 38 sec



20100104benzylcarbonaminationC13

Sample Name:

Archive directory:

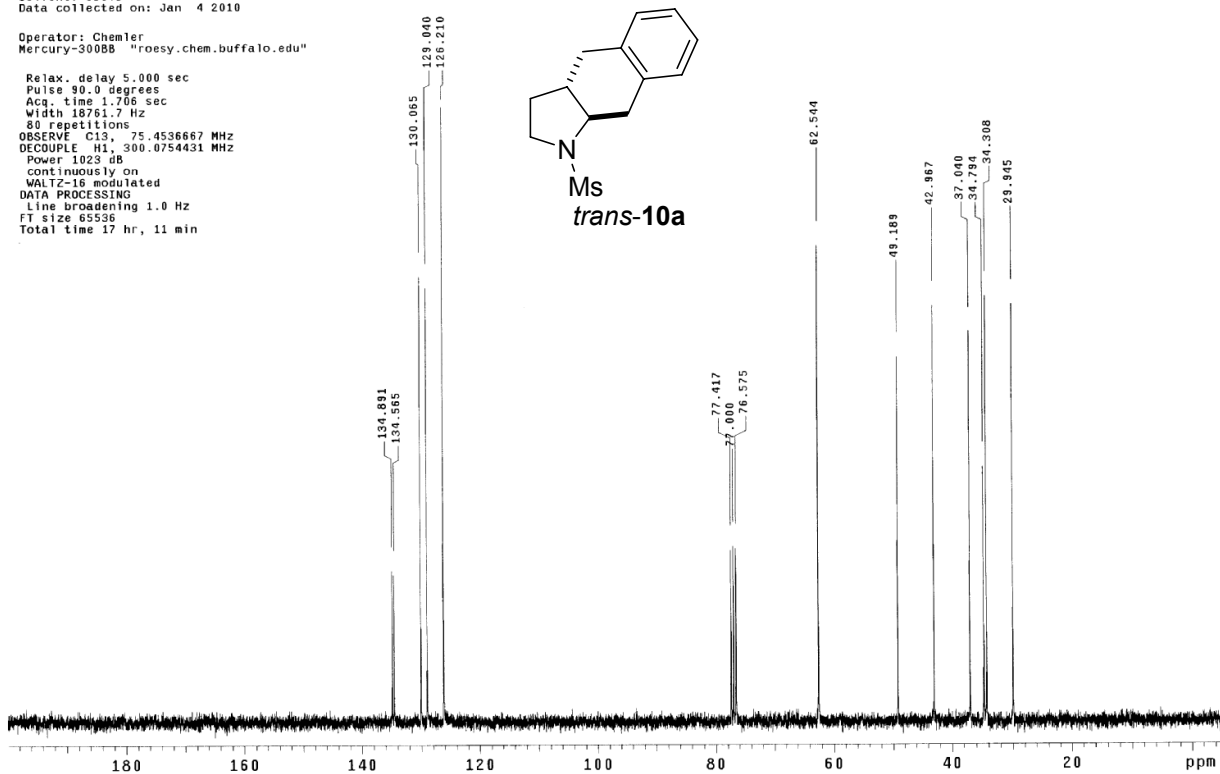
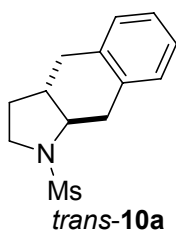
Sample directory:

FidFile: std13c

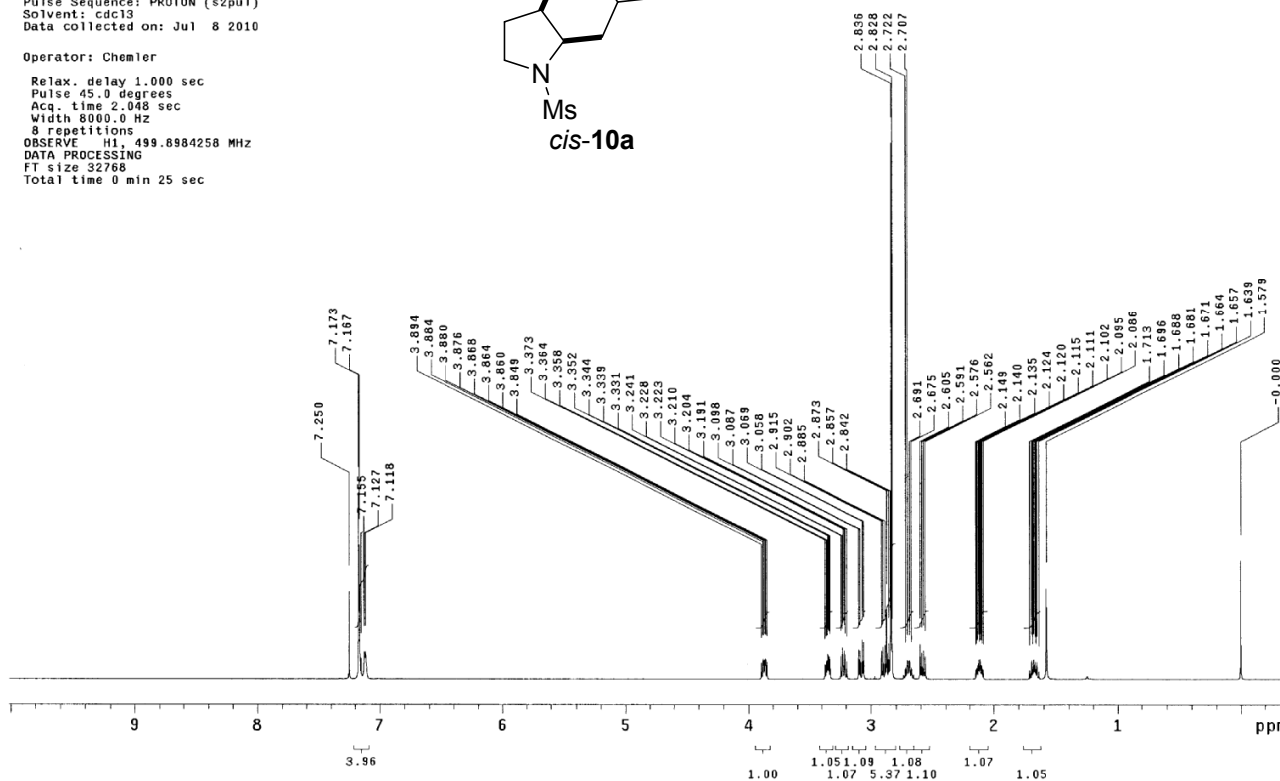
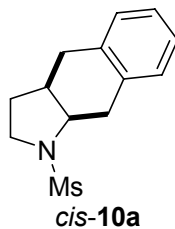
Pulse Sequence: std13c (s2pul)
 Solvent: CDC13
 Data collected on: Jan 4 2010

Operator: Chemler
 Mercury-300BB "roesy.chem.buffalo.edu"

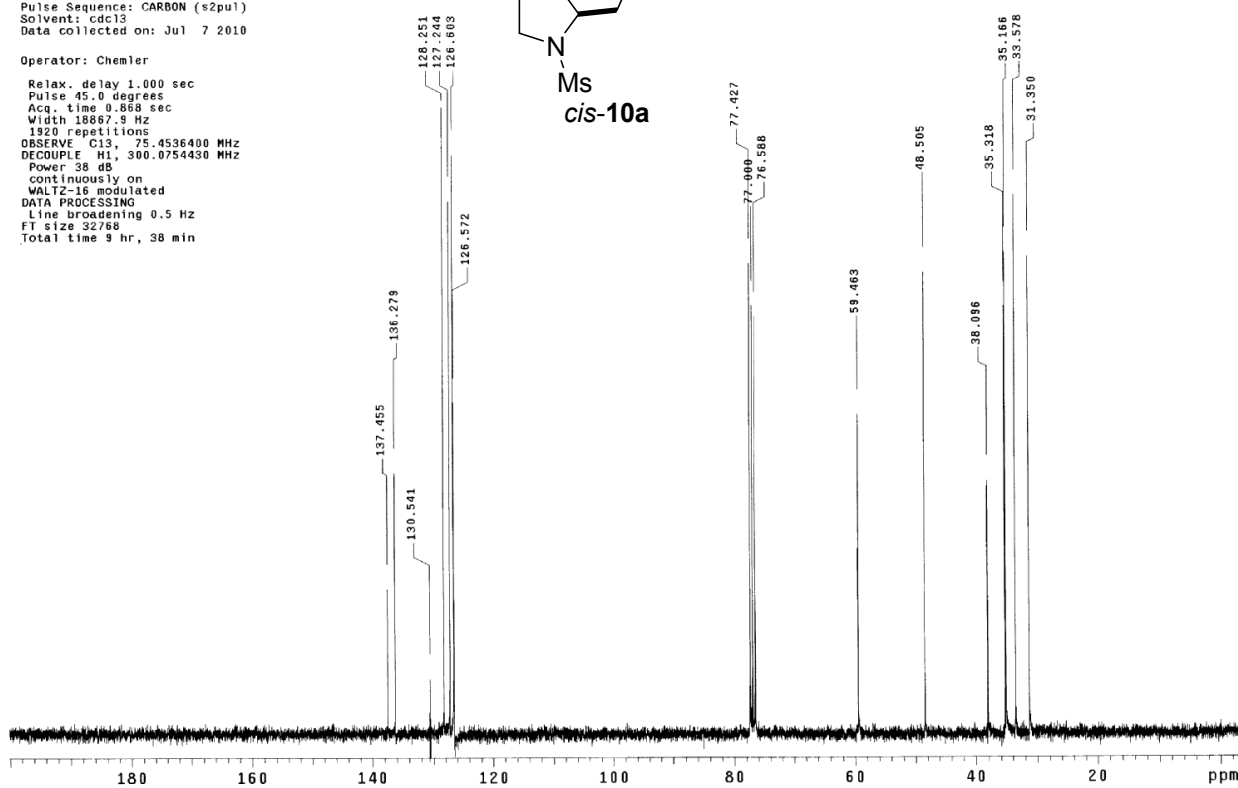
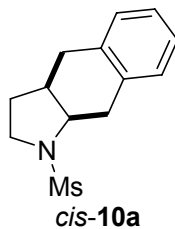
Relax. delay 5.000 sec
 Pulse 90.0 degrees
 Acq. time 1.706 sec
 Width 10761.7 Hz
 80 repetitions
 OBSERVE C13, 75.4536667 MHz
 DECOUPLE H1, 300.0754431 MHz
 Power 1023 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 65536
 Total time 17 hr, 11 min



20100708benzylcisproduct
 Sample Name:
 Data Collected on:
 chemnmr500.chem.buffalo.edu-inova500
 Archive directory:
 Sample directory:
 FidFile: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdc13
 Data collected on: Jul 8 2010
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 2.048 sec
 Width 8000.0 Hz
 8 repetitions
 OBSERVE HI, 499.8984258 MHz
 DATA PROCESSING
 FT size 32768
 Total time 0 min 25 sec



20100707benzylcisproductC13
 Sample Name:
 Data Collected on:
 toesy.chem.buffalo.edu-mercury300
 Archive directory:
 Sample directory:
 FidFile: CARBON
 Pulse Sequence: CARBON (s2pu1)
 Solvent: cdc13
 Data collected on: Jul 7 2010
 Operator: Chemler
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 0.868 sec
 Width 18687.9 Hz
 1920 repetitions
 OBSERVE C13, 75.4536400 MHz
 DECOUPLE HI, 300.0754430 MHz
 Power 38 dB
 continuously on
 WALTZ-16 modulated
 DATA PROCESSING
 Line broadening 0.5 Hz
 FT size 32768
 Total time 9 hr, 38 min



20100609omethoxyltransproduct

Sample Name:

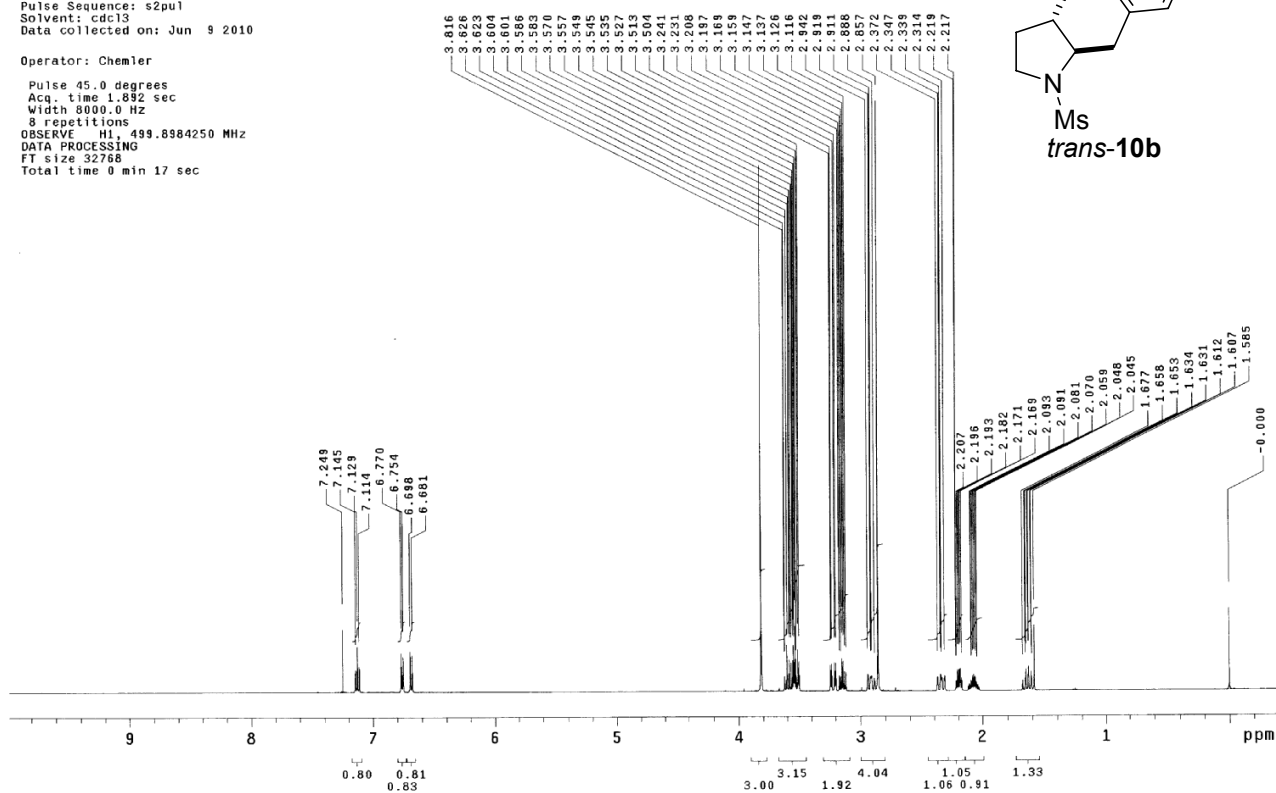
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: H1

Pulse Sequence: s2pu1
Solvent: cdc13
Data collected on: Jun 9 2010

Operator: Chemler

Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8984250 MHz
DATA PROCESSING
FT size 32768
Total time 0 min 17 sec

20100610omethoxyltransproductC13

Sample Name:

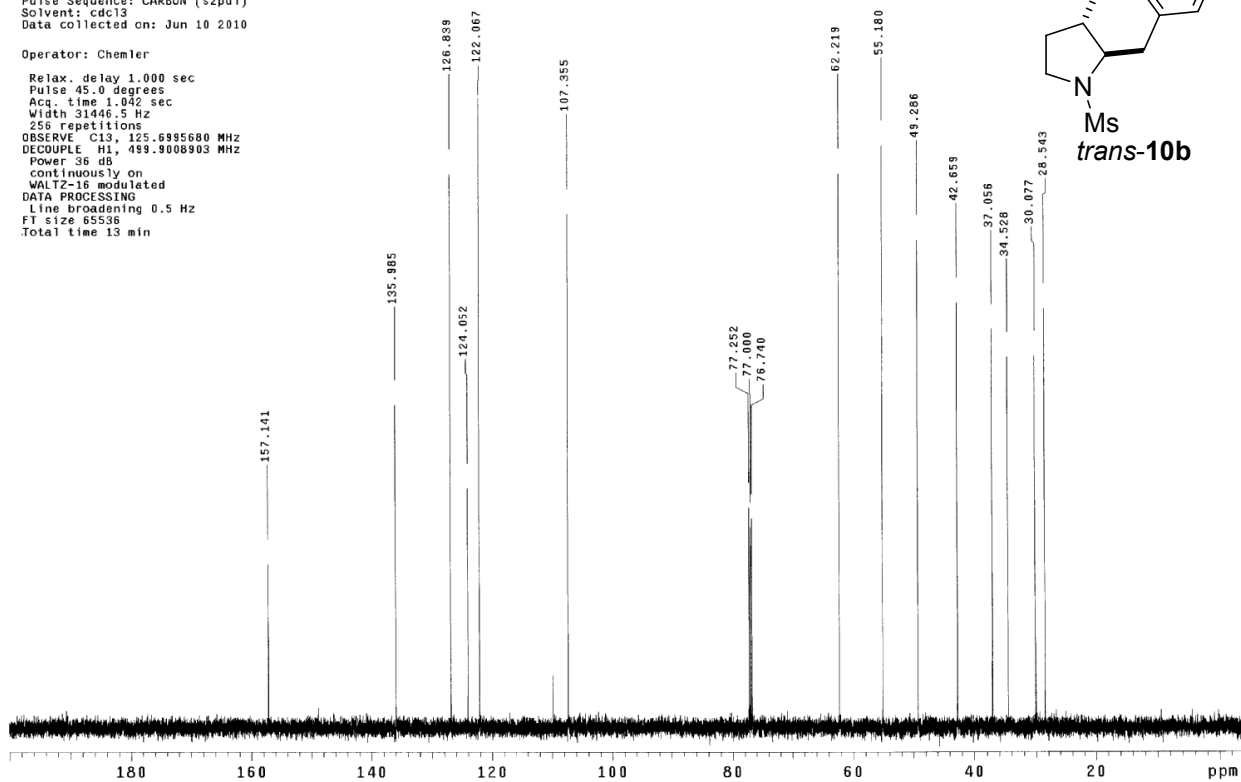
Data Collected on:
chemnmr500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

Fidfile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Jun 10 2010

Operator: Chemler

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.042 sec
Width 31446.5 Hz
256 repetitions
OBSERVE C13, 125.6995680 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 13 min

20100818omethoxylcisproduct

Sample Name:

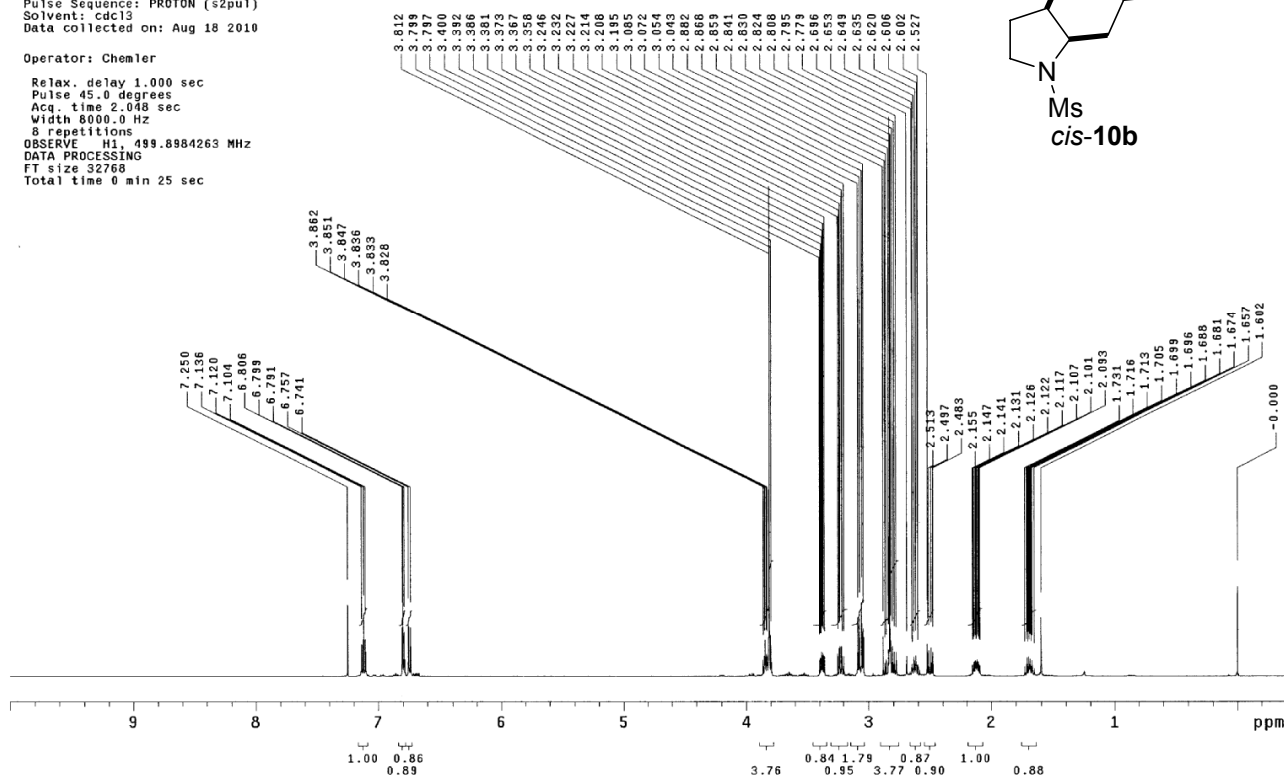
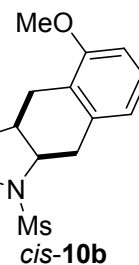
Data Collected on:
chemmrs500.chem.buffalo.edu-inova500
Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Aug 18 2010

Operator: Chemler

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
FT size 32768
Total time 0 min 25 sec

20100818omethoxylcisproductC13

Sample Name:

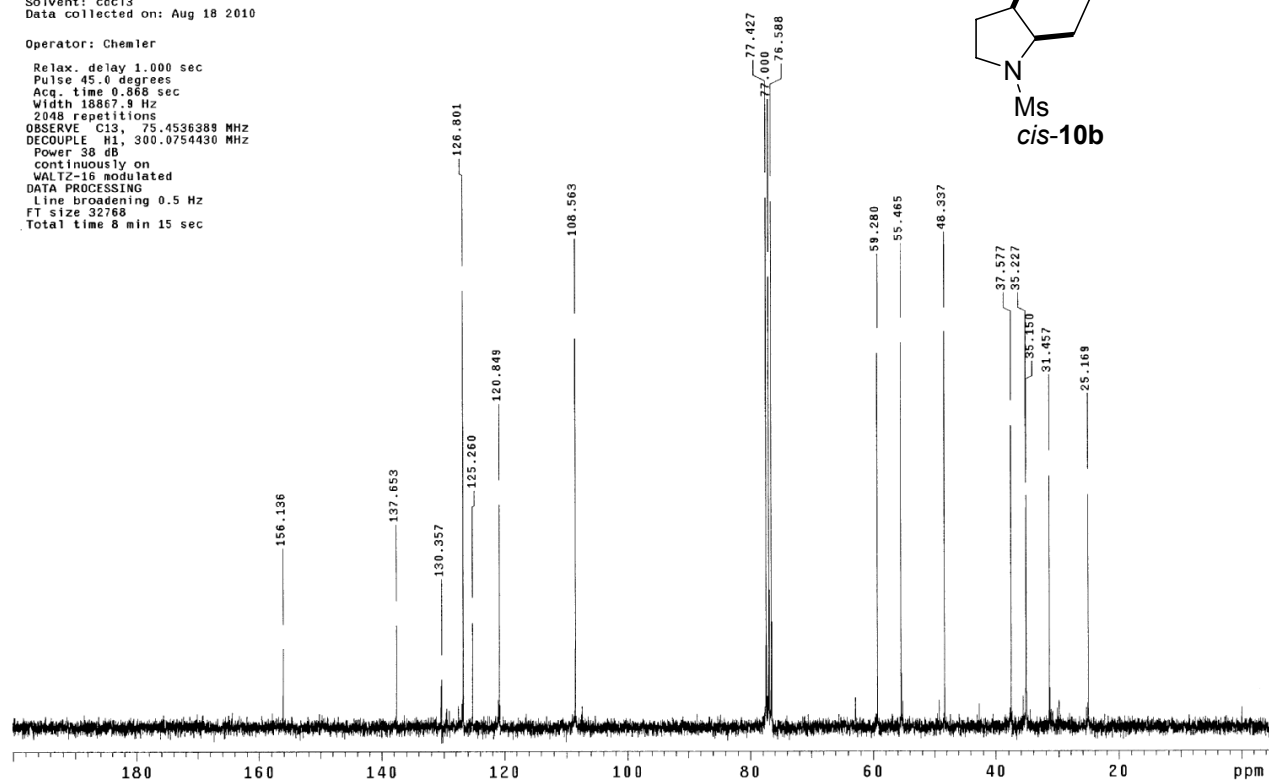
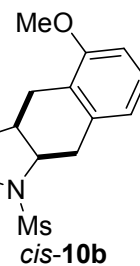
Data Collected on:
rossy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Aug 18 2010

Operator: Chemler

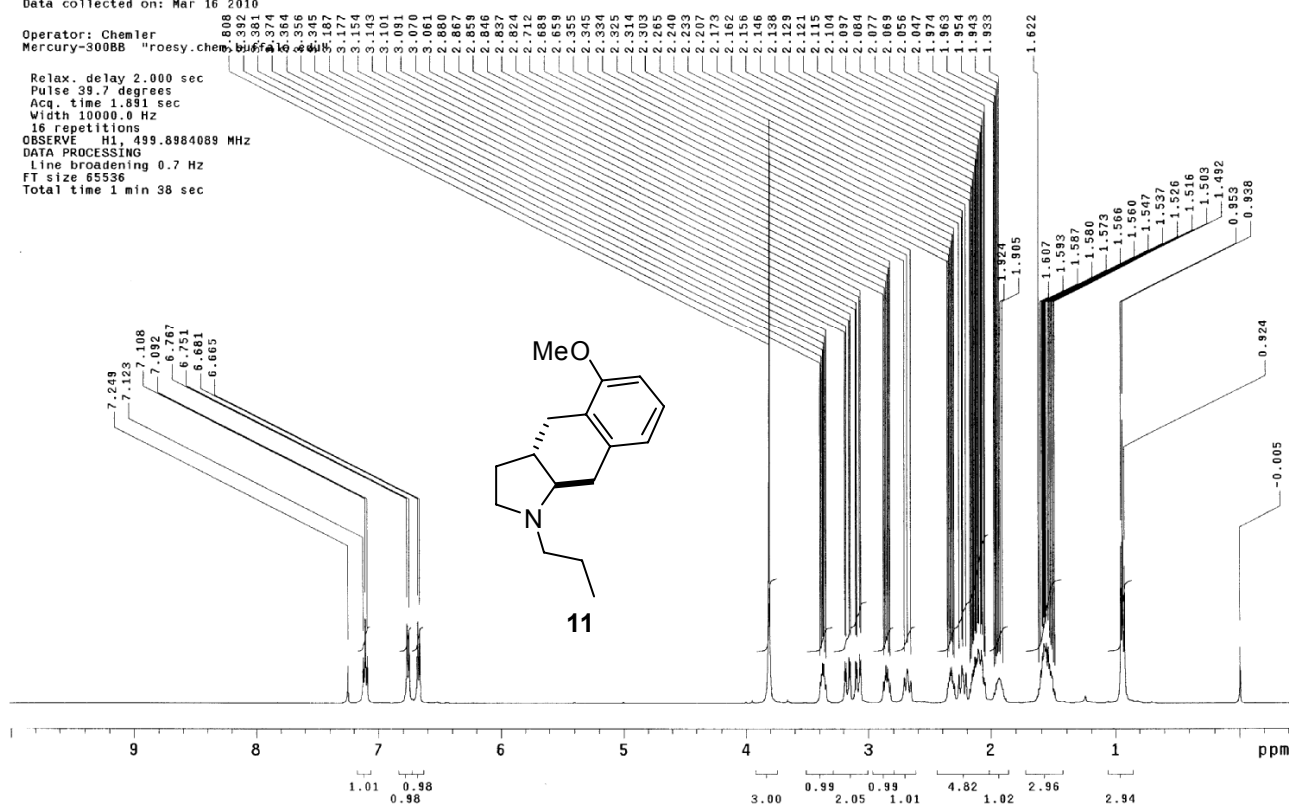
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
2048 repetitions
OBSERVE C13, 75.4536388 MHz
DECOUPLE H1, 300.0754430 MHz
Power 38 dB
continuous ly on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 8 min 15 sec

20100316omethoxypropyl

Sample Name:
Archive directory:
Sample directory:
FidFile: H1

Pulse Sequence: s2pu1
Solvent: CDC13
Data collected on: Mar 16 2010
Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"

Relax. delay 2.000 sec
Pulse 39.7 degrees
Acq. time 1.891 sec
Width 10000.0 Hz
16 repetitions
OBSERVE H1, 499.8984089 MHz
DATA PROCESSING
Line broadening 0.7 Hz
FT size 65536
Total time 1 min 38 sec



20100316omethoxypropylC13

Sample Name:
Archive directory:
Sample directory:
FidFile: std13c

Pulse Sequence: std13c (s2pu1)
Solvent: CDC13
Data collected on: Mar 16 2010

Operator: Chemler
Mercury-300BB "roesy.chem.buffalo.edu"

Pulse 35.5 degrees
Acq. time 1.706 sec
Width 18761.7 Hz
2080 repetitions
OBSERVE C13, 75.4536627 MHz
DECOUPLE H1, 300.0754431 MHz
Power 1023 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 85536
Total time 607 hr, 32 min

