

Copper-Catalyzed Alkene Diamination: Synthesis of Chiral 2-Aminomethyl Indolines and Pyrrolidines

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The State University of New York, Buffalo, NY 14260, schemler@buffalo.edu

Supporting Information II

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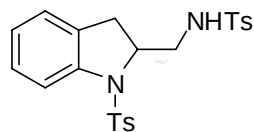
NMR Spectra	S-2
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NMR Spectra

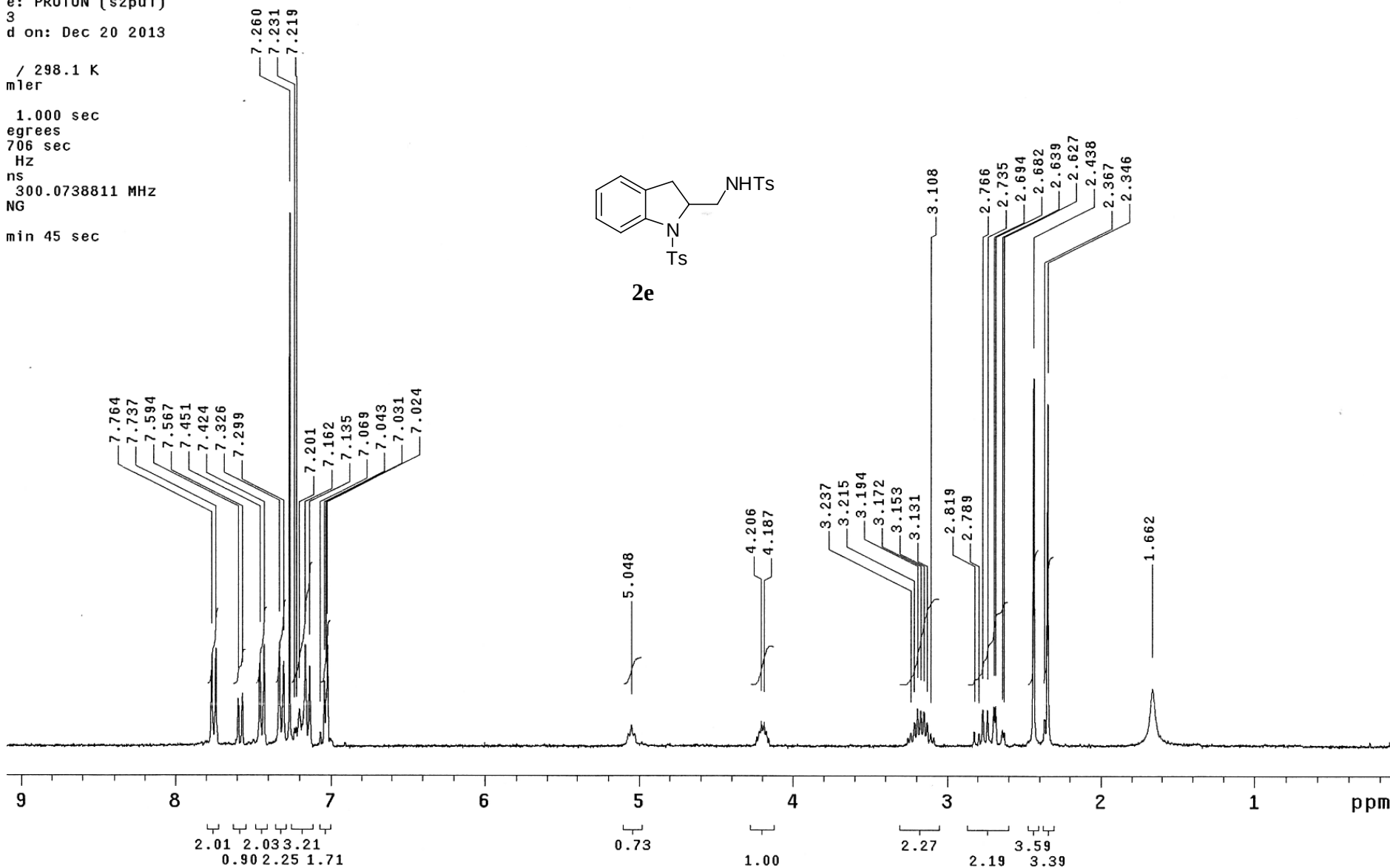
e: PROTON (s2pu1)
3
d on: Dec 20 2013

/ 298.1 K
mler

1.000 sec
egrees
706 sec
Hz
ns
300.0738811 MHz
NG
min 45 sec



2e



blt1-rxn196pg205pure2prep2

Sample Name:

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

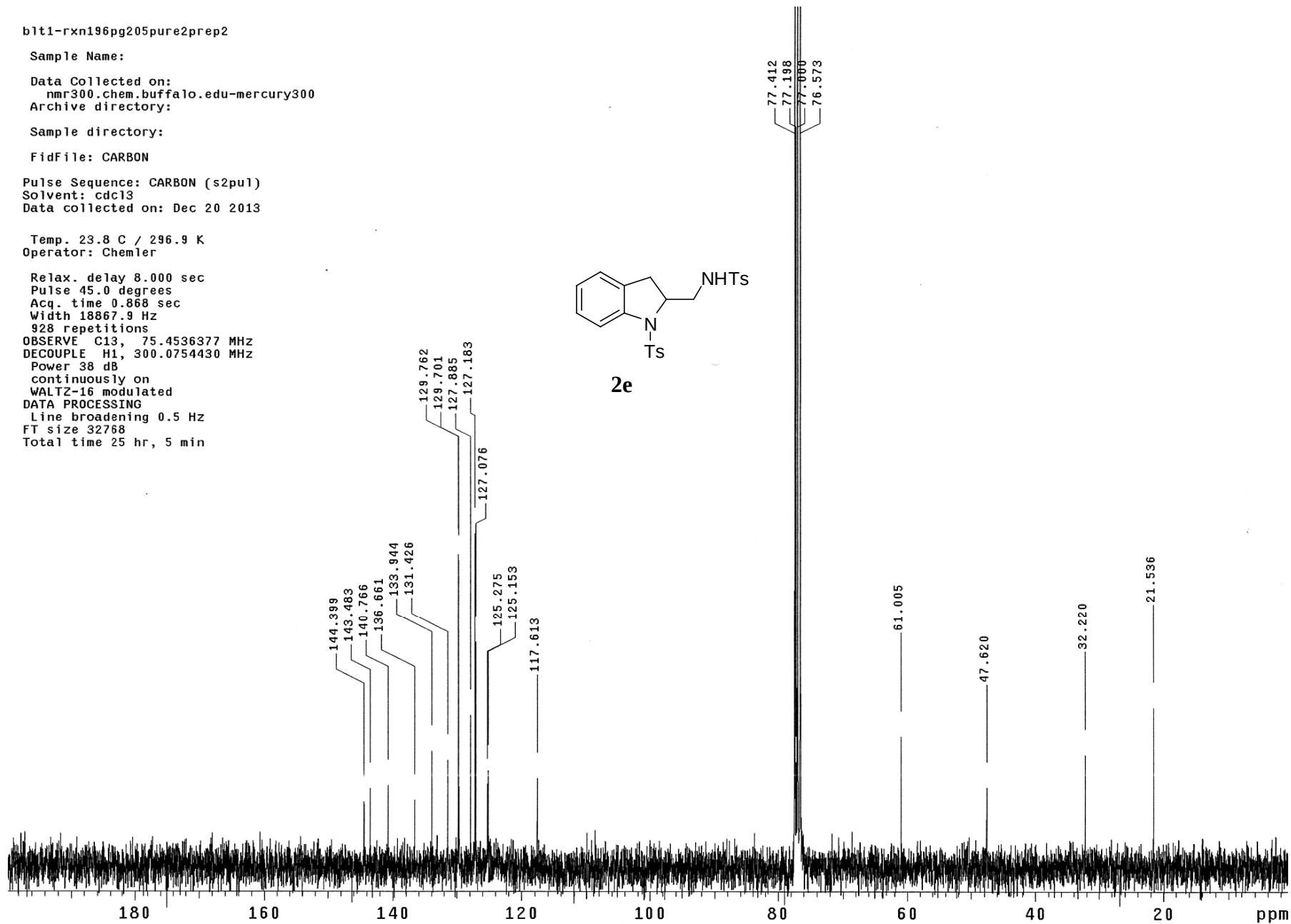
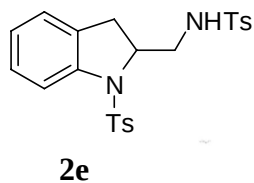
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Dec 20 2013

Temp. 23.8 C / 296.9 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
928 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 25 hr, 5 min



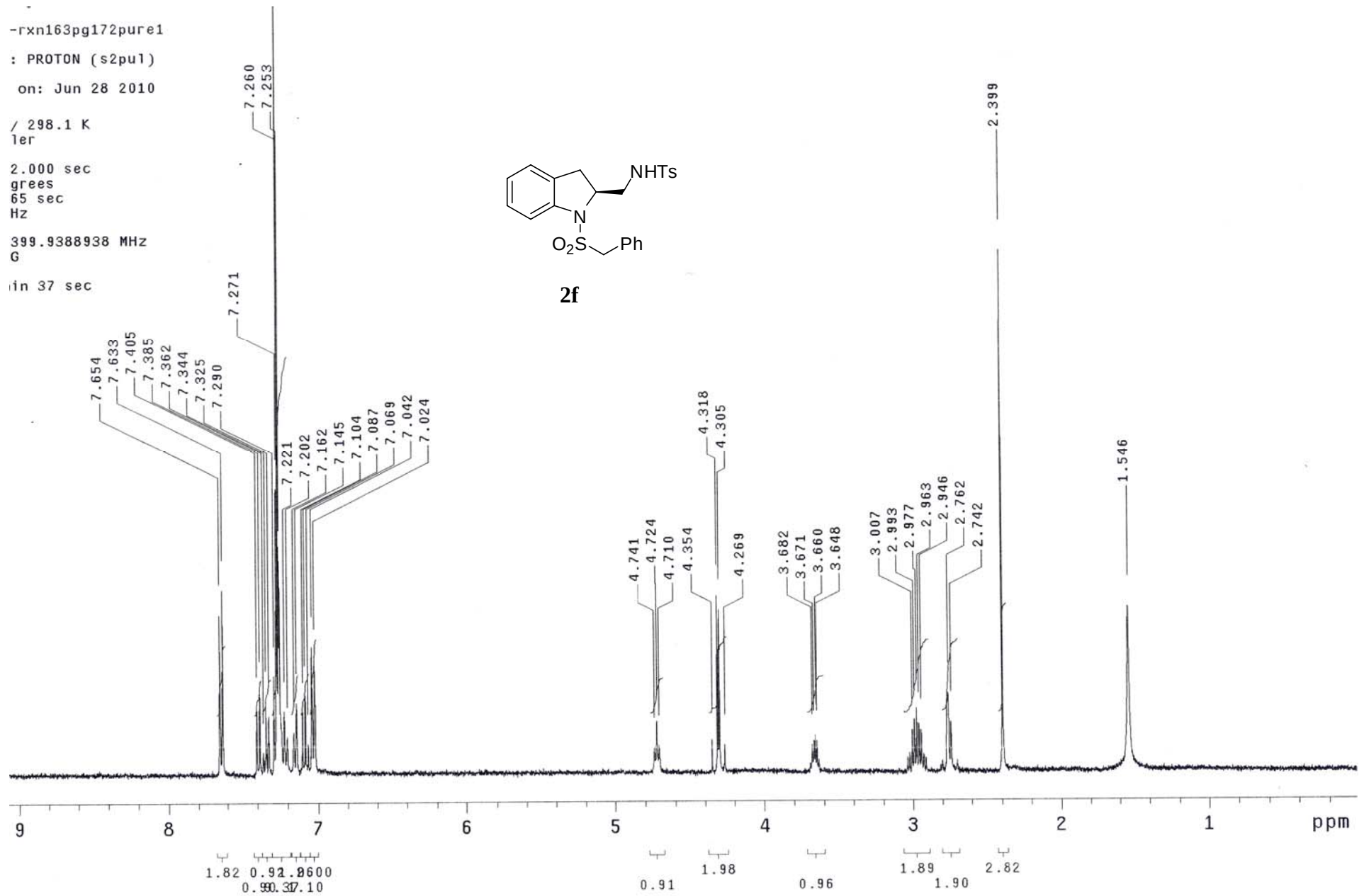
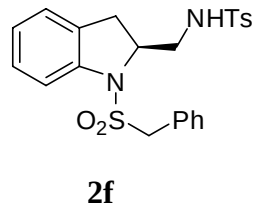
-rxn163pg172pure1

: PROTON (s2pu1)

on: Jun 28 2010

/ 298.1 K
1er2.000 sec
grees
65 sec
Hz399.9388938 MHz
G

in 37 sec



blt3-rxn165pg185CNMR

Sample Name:

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

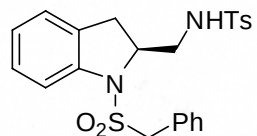
Sample directory:

FidFile: CARBON

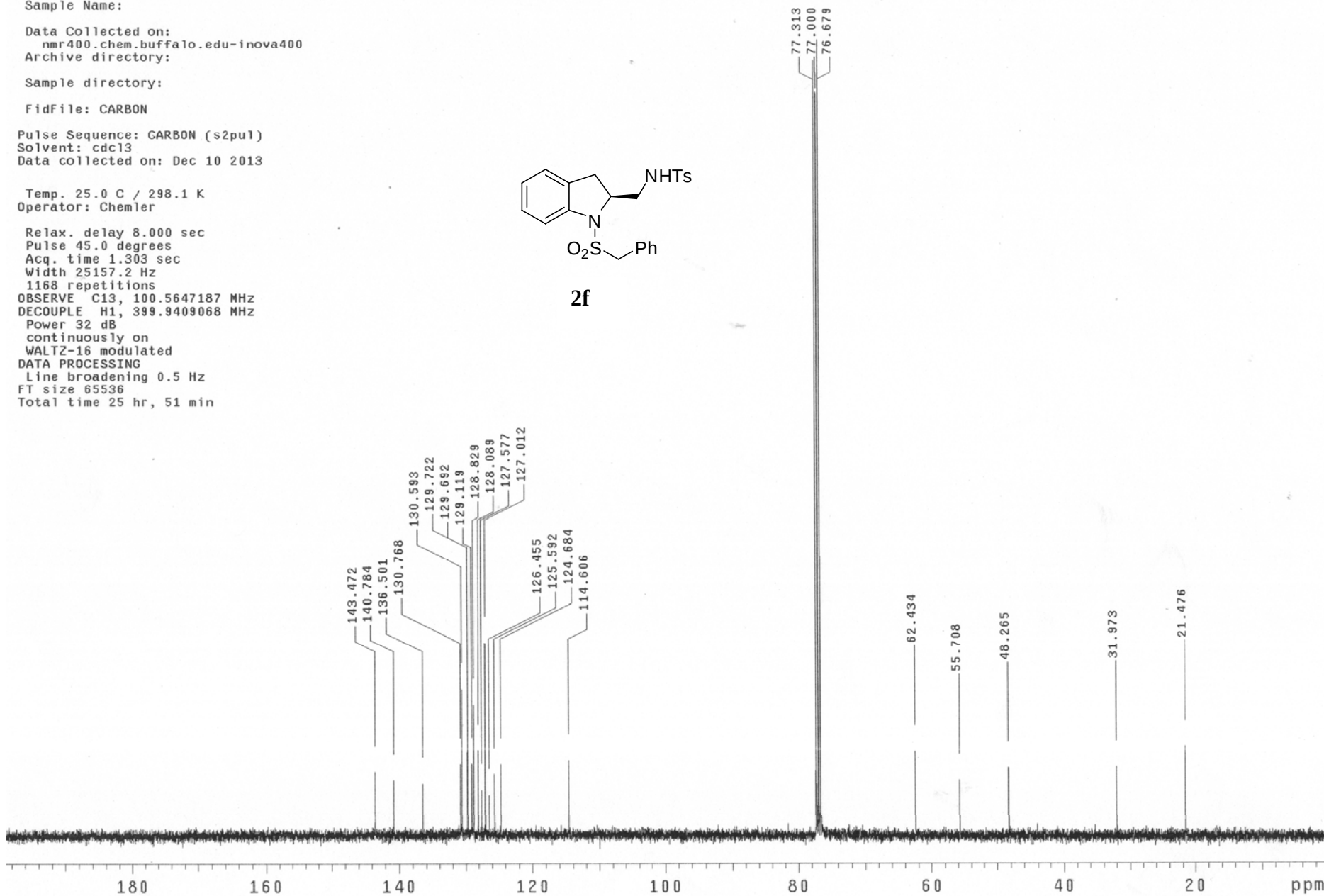
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Dec 10 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
1168 repetitions
OBSERVE C13, 100.5647187 MHz
DECOUPLE H1, 399.9409068 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 25 hr, 51 min



2f



: PROTON (s2pul)

on: Jul 18 2013

/ 298.1 K
ry

1.000 sec

grees

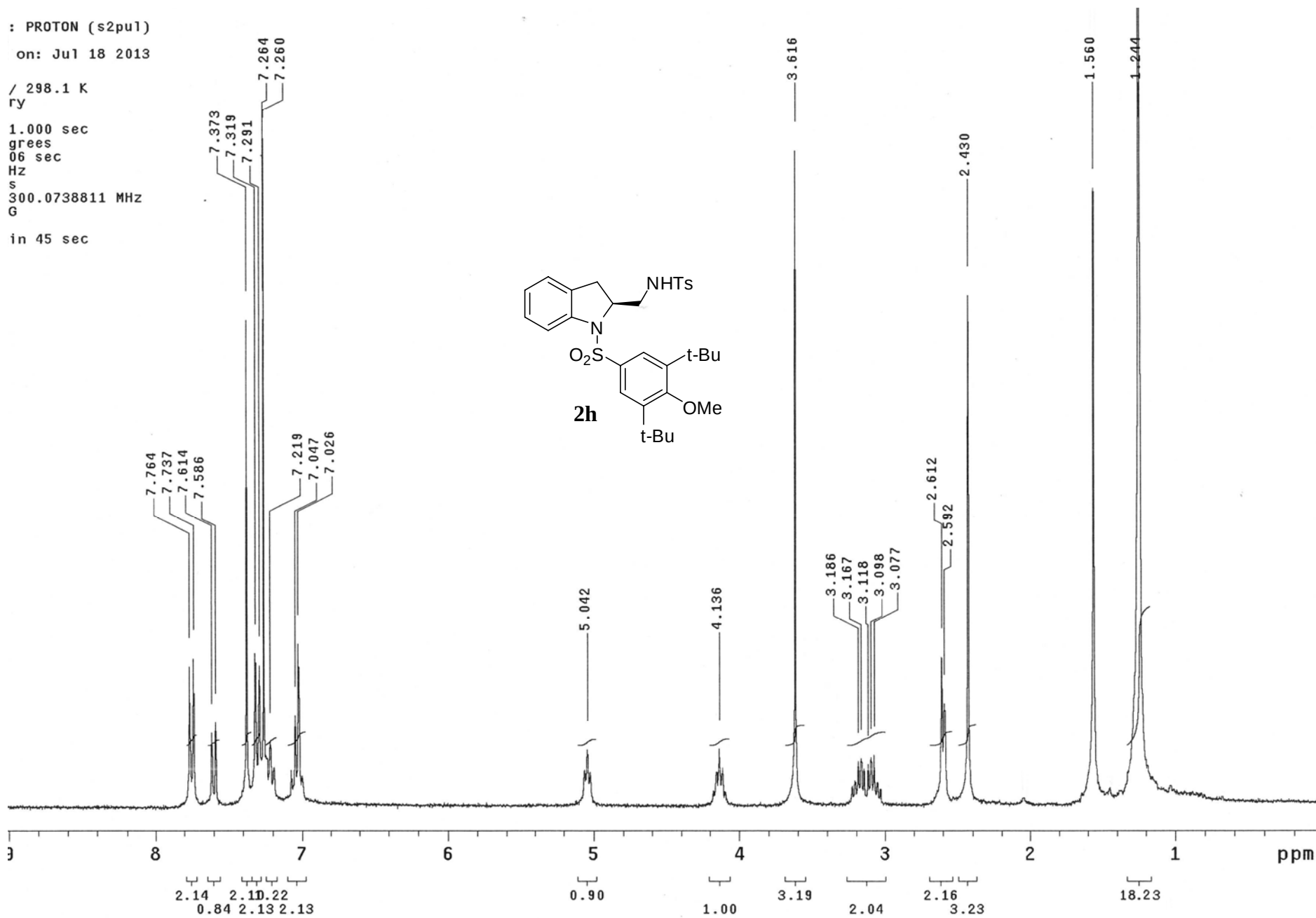
06 sec

Hz

300.0738811 MHz

G

in 45 sec



blt3-rxn700pg120prep2carbon

Sample Name:

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

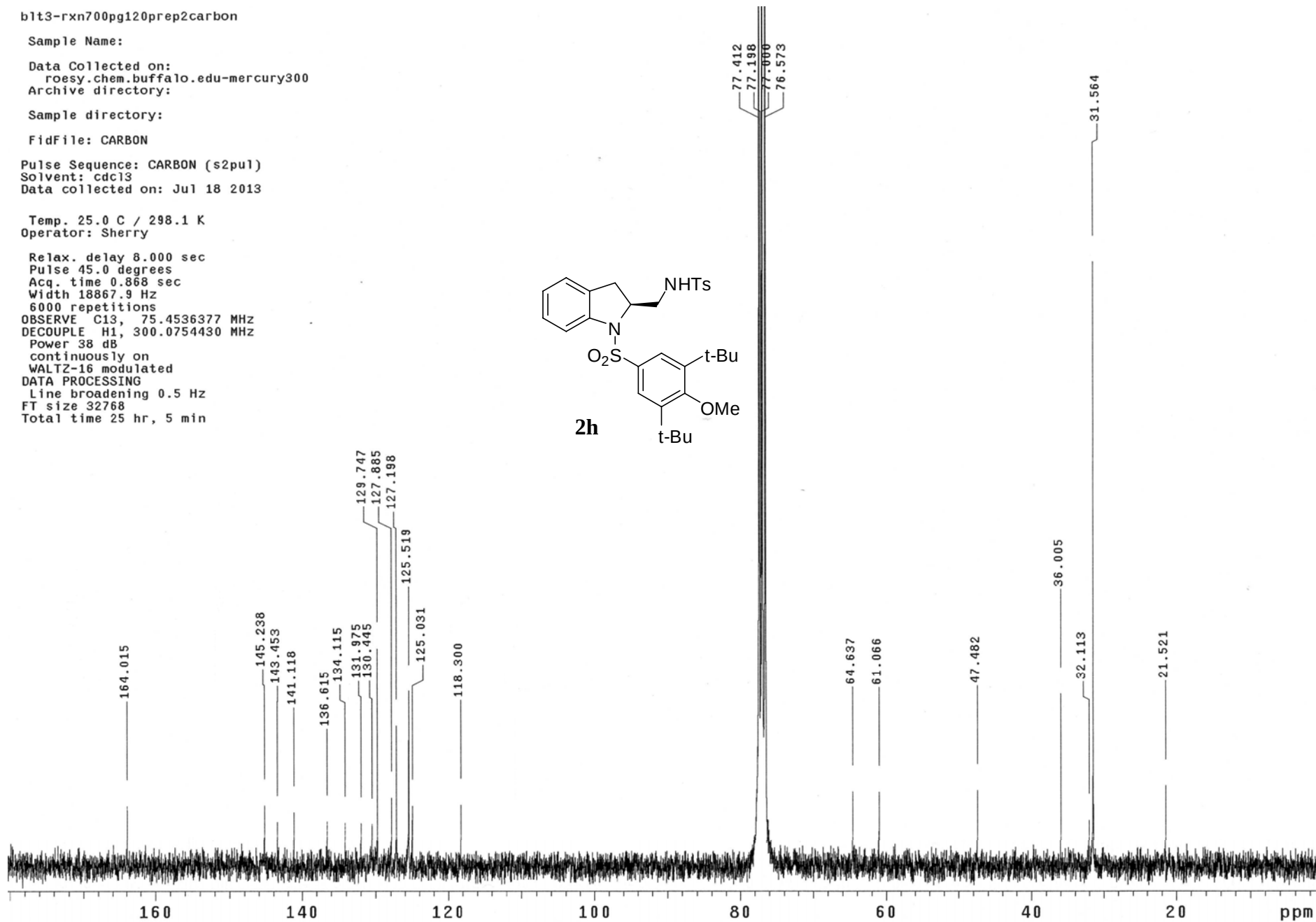
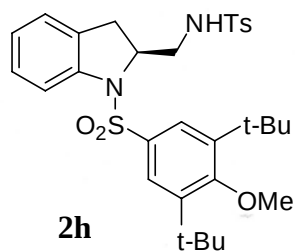
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Jul 18 2013

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6000 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 25 hr, 5 min



ed on:
l.chem.buffalo.edu-inova400
ctory:

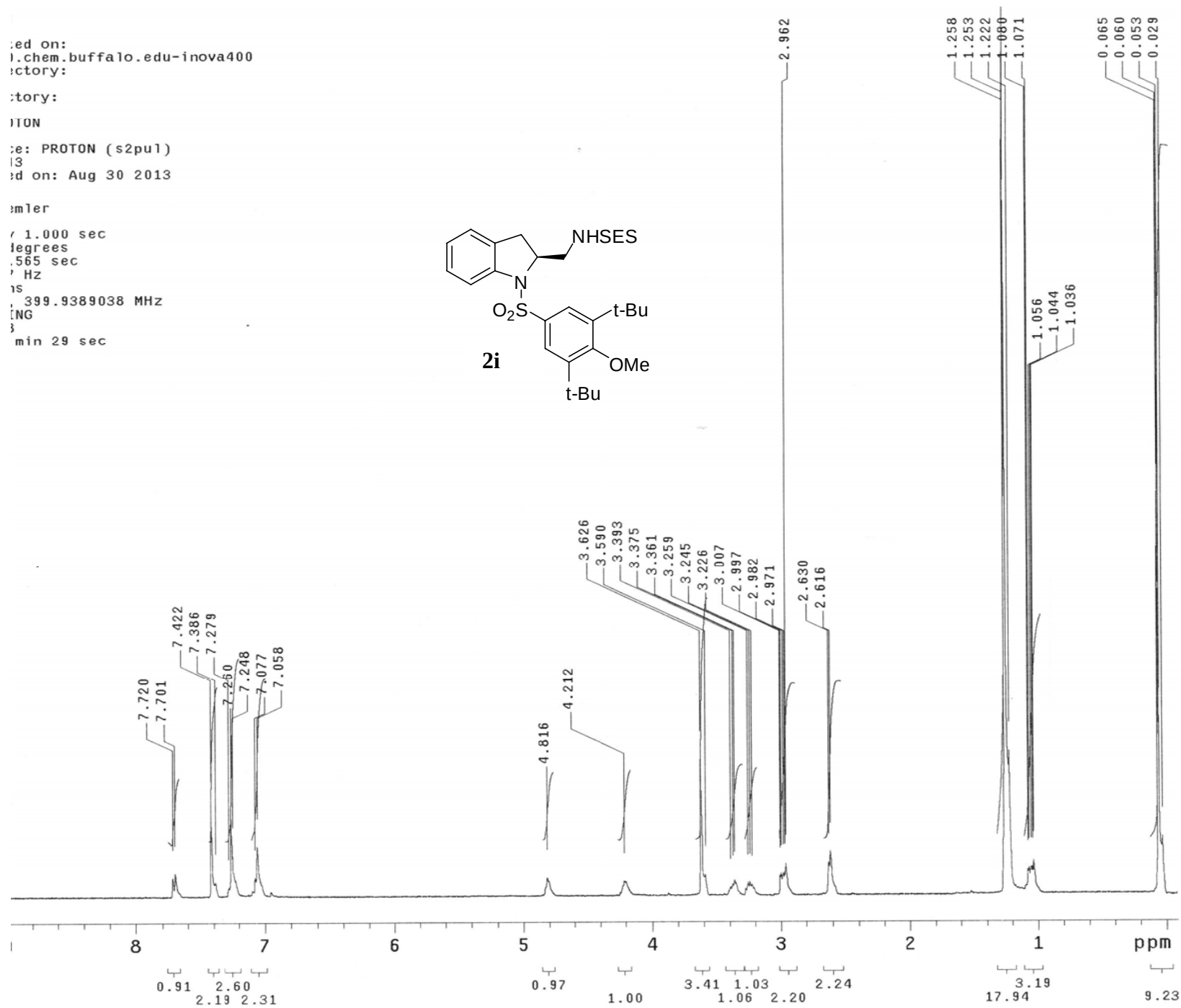
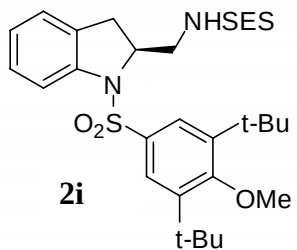
ctory:

ITON

re: PROTON (s2pu1)
13
ed on: Aug 30 2013

mler

/ 1.000 sec
egrees
.565 sec
' HZ
is
.399.9389038 MHz
[NG
} min 29 sec



blt3-rxn749pg169pure1prep1carbon

Sample Name:

Data Collected on:

roesy.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: CARBON

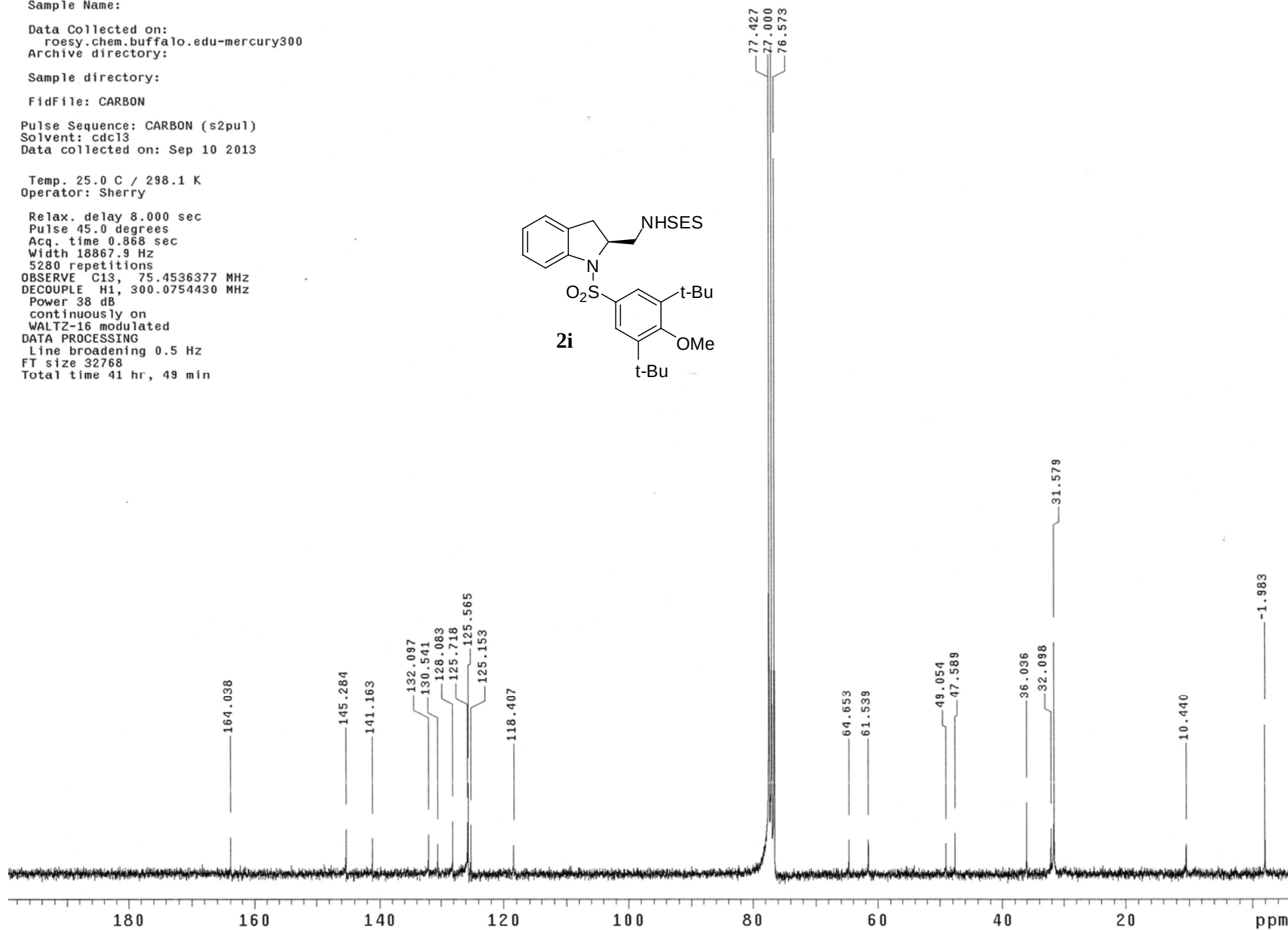
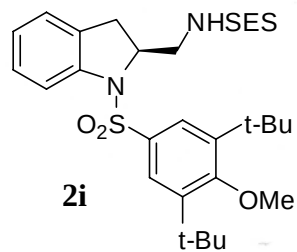
Pulse Sequence: CARBON (s2pu1)

Solvent: cdc13

Data collected on: Sep 10 2013

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
5280 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 41 hr, 49 min



sted on:
m.buffalo.edu-mercury300
ectory:

actory:

OTON

ice: PROTON (s2pu1)
:13
ed on: Sep 4 2013

C / 298.1 K
erry

y 1.000 sec

degrees

1.706 sec

.1 Hz

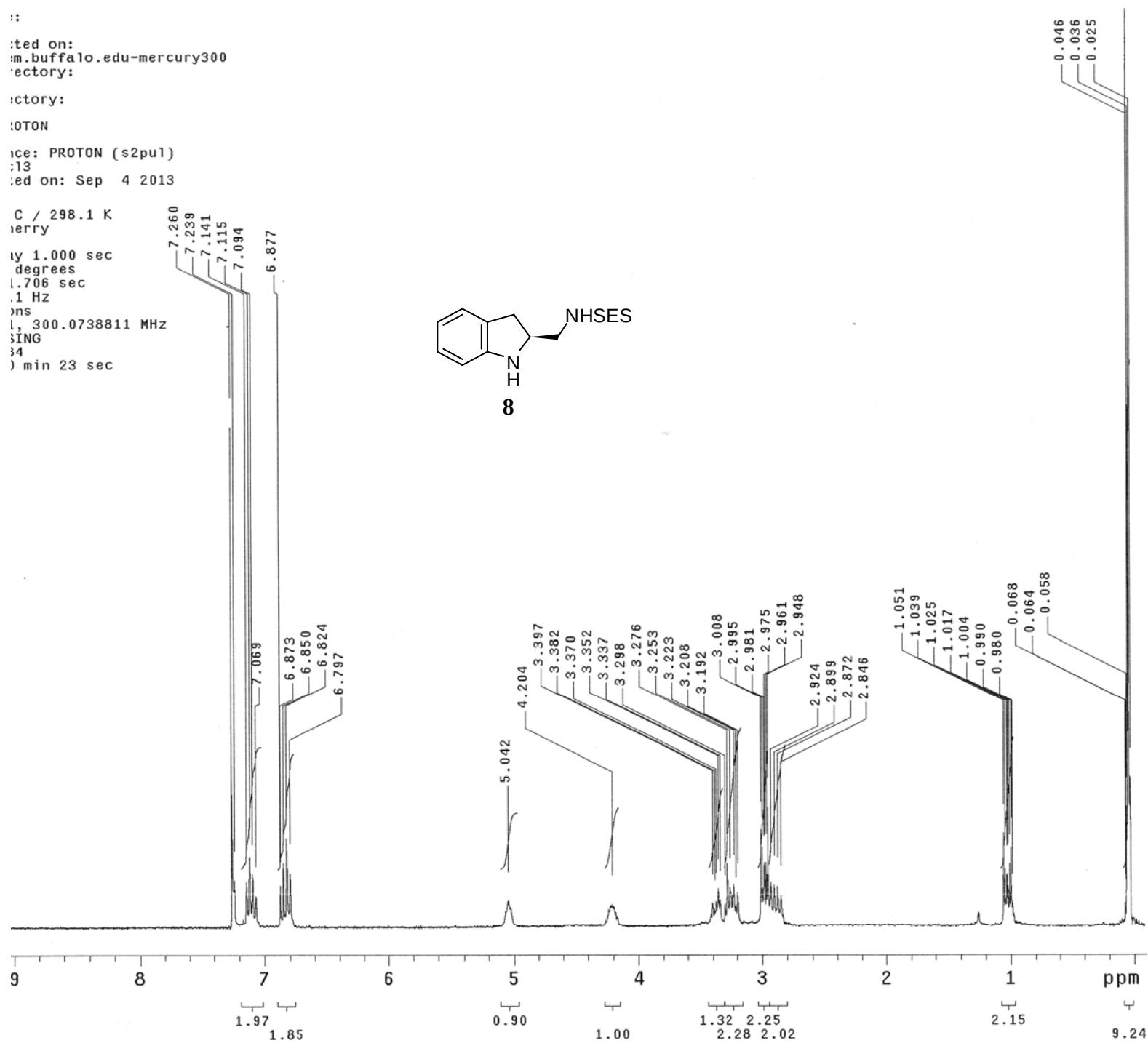
ns

L, 300.0738811 MHz

ING

34

) min 23 sec



blt3-rxn744pg164carbon

Sample Name:

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

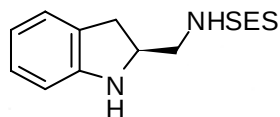
Sample directory:

FidFile: CARBON

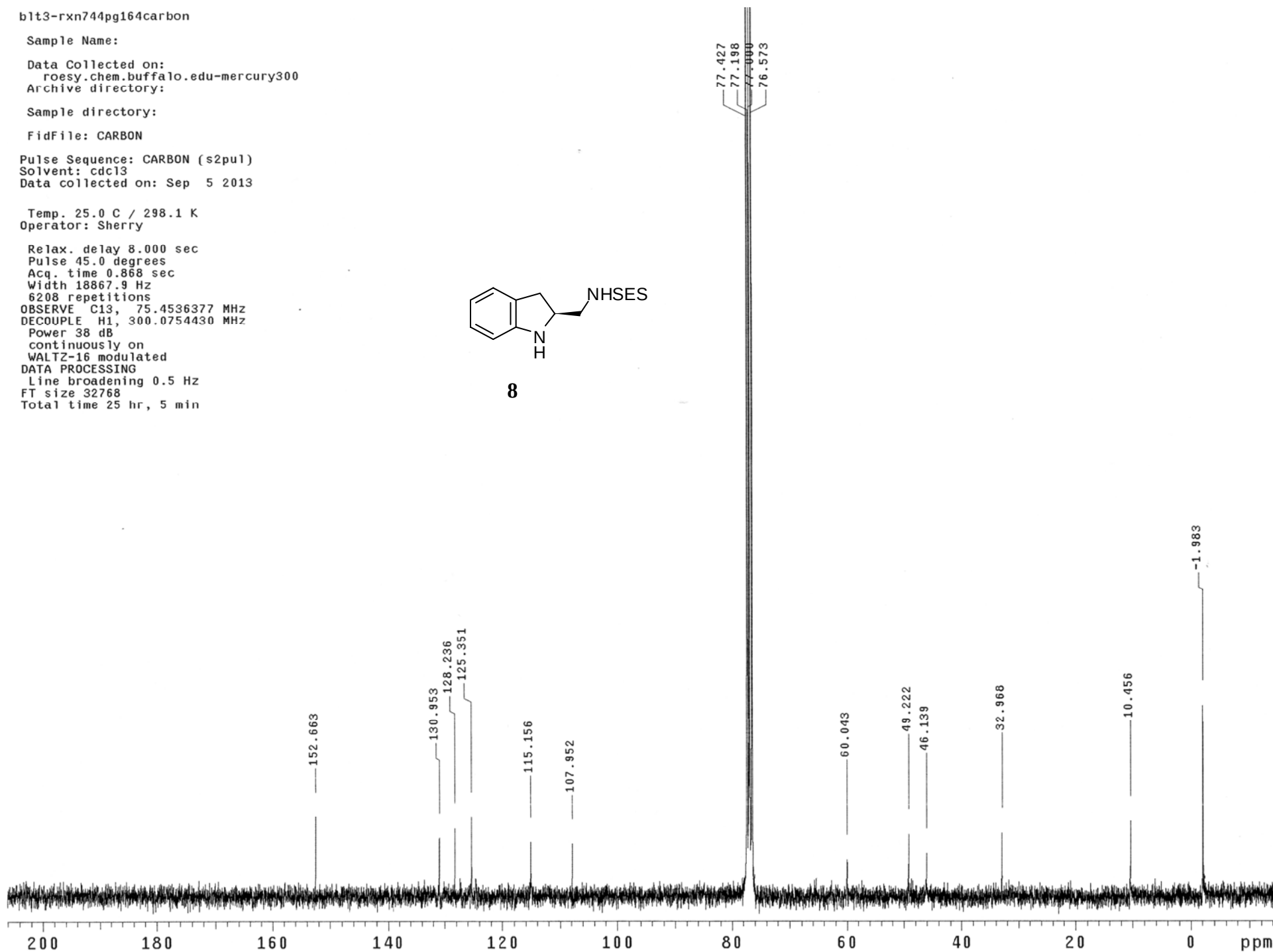
Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Sep 5 2013

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6208 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 25 hr, 5 min



8



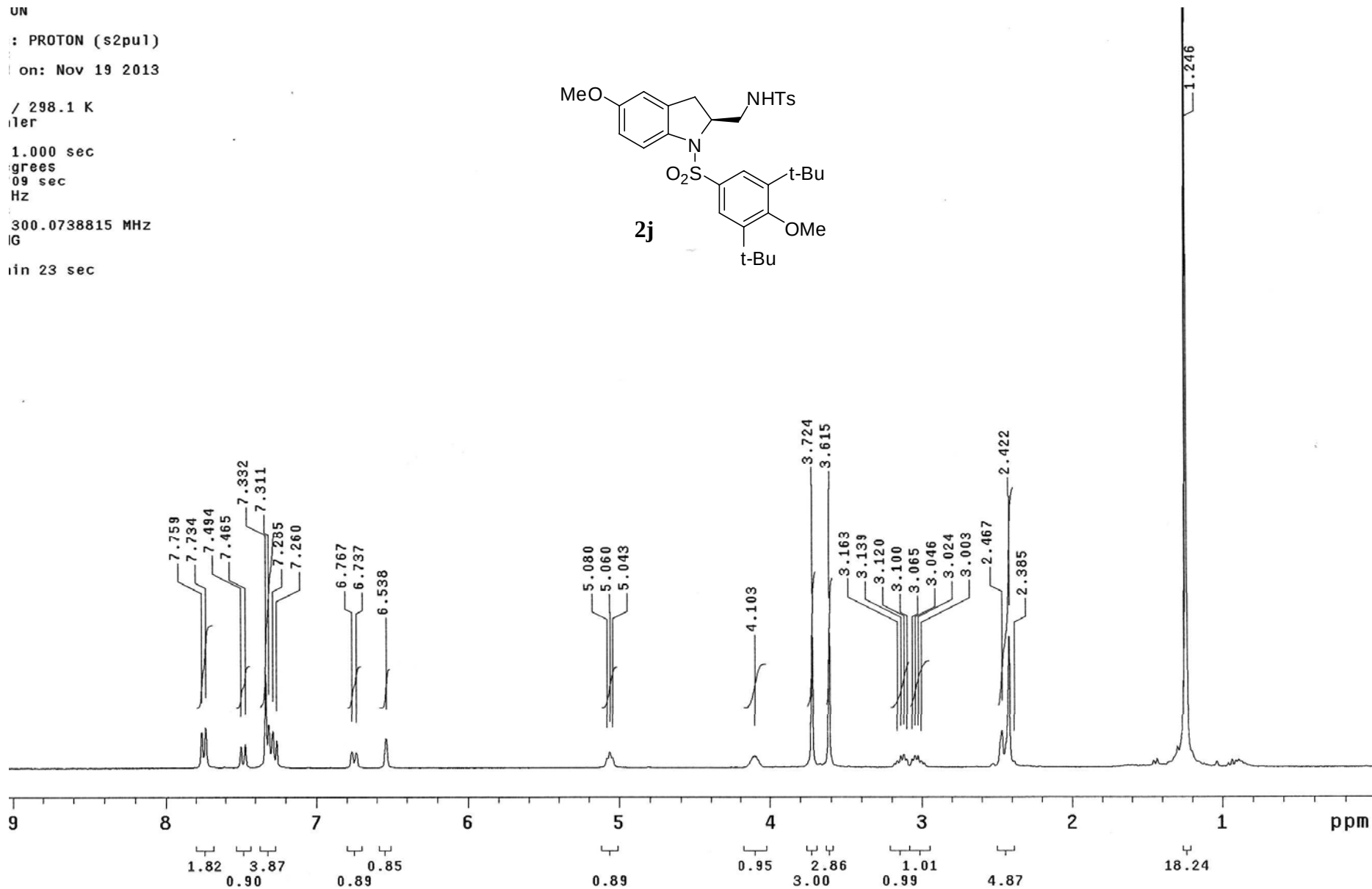
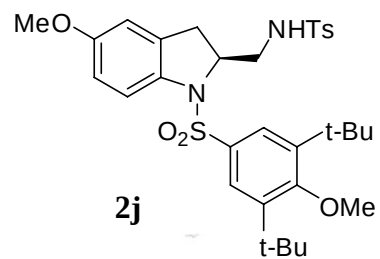
UN

: PROTON (s2pul)

on: Nov 19 2013

/ 298.1 K
r1.000 sec
grees
09 sec
Hz300.0738815 MHz
IG

in 23 sec



blt3-rxn767pg187pure1carbon

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cdcl3

Data collected on: Nov 19 2013

Temp. 23.8 C / 296.9 K

Operator: Chemler

Relax. delay 8.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

560 repetitions

OBSERVE C13, 75.4536389 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

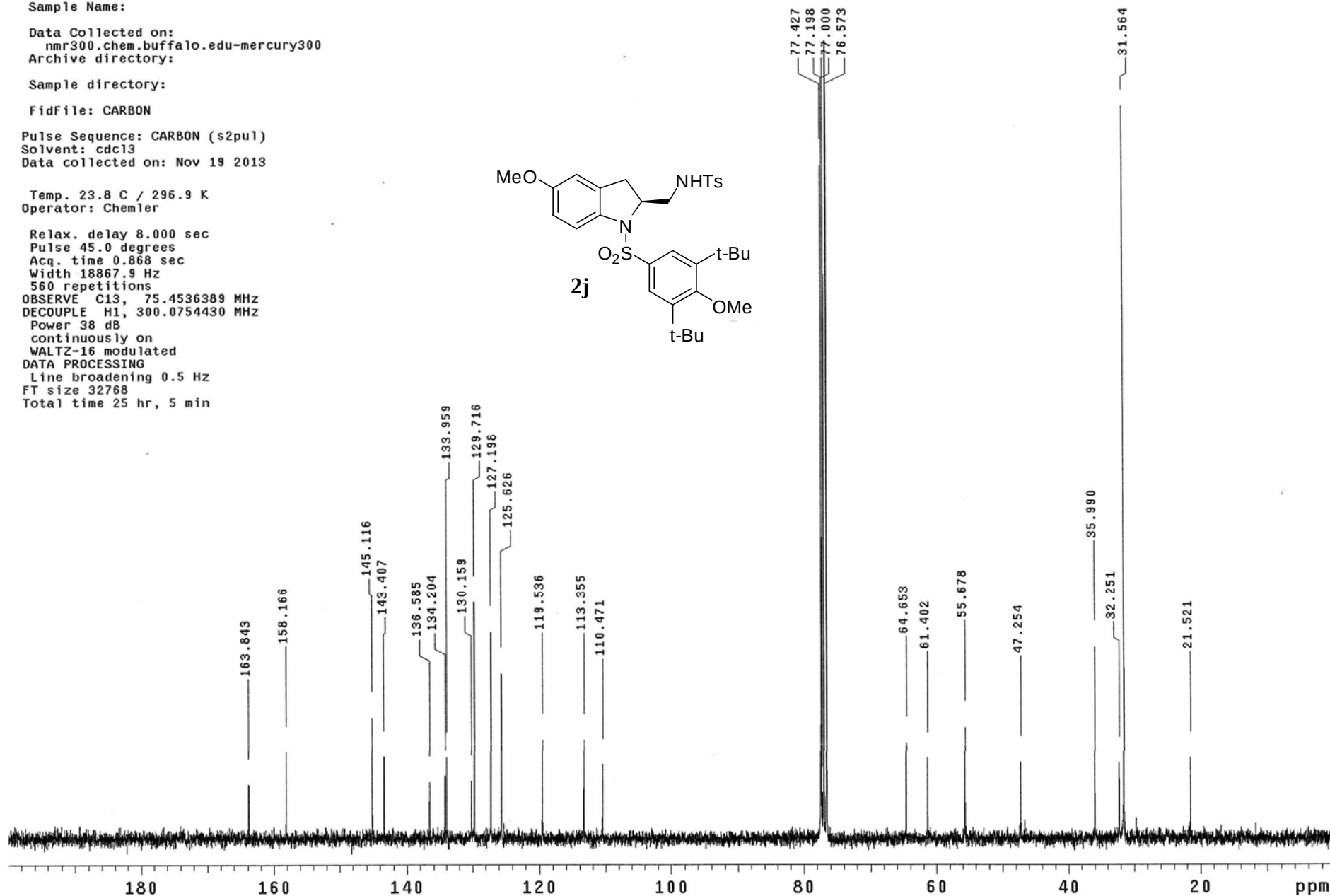
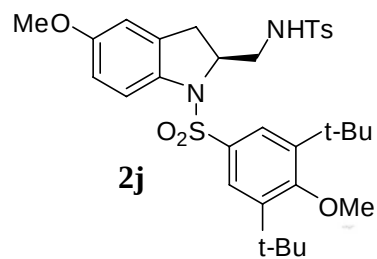
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 25 hr, 5 min



File Name:

a Collected on:
mr300.chem.buffalo.edu/mercury300
hive directory:

File directory:

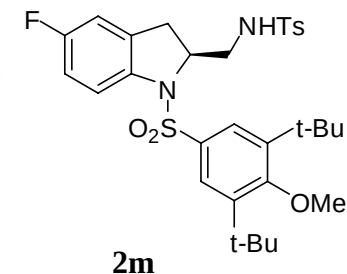
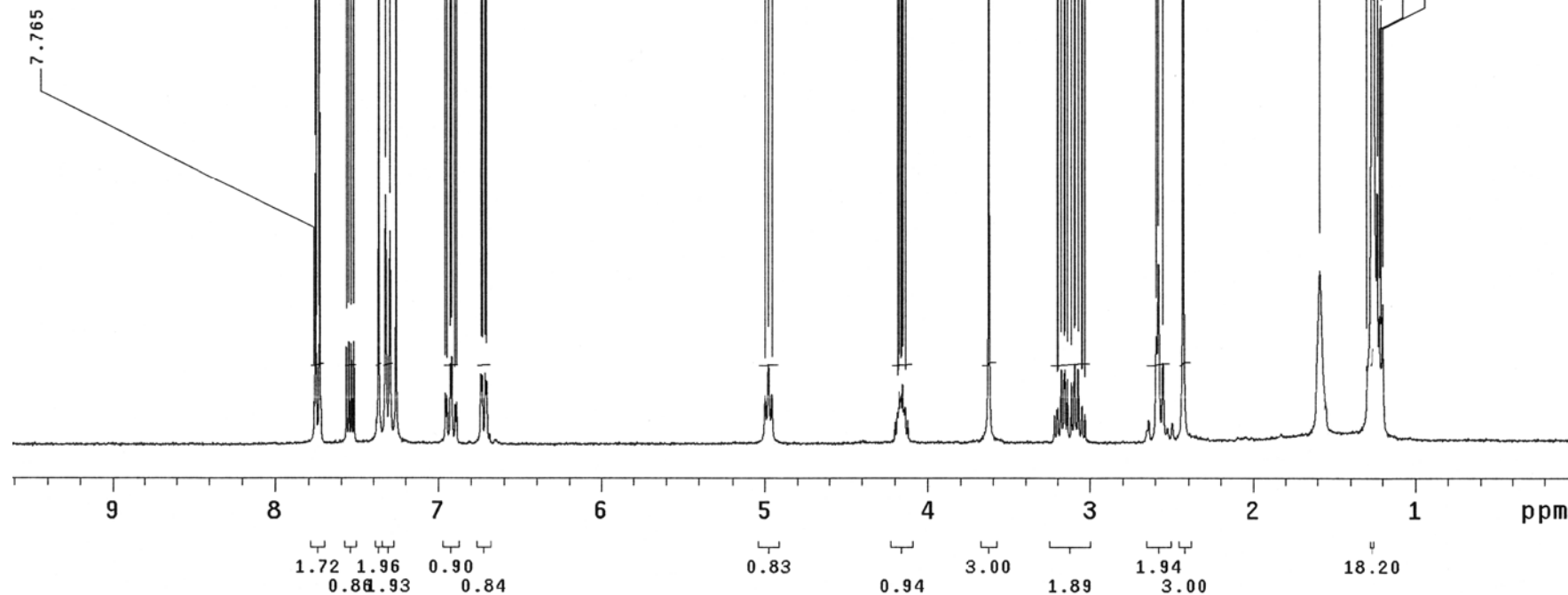
File: PROTON

e Sequence: PROTON (s2pul)
ent: cdcl3
collected on: Dec 5 2013

p. 25.0 C / 298.1 K
ator: Chemler

ax. delay 1.000 sec
se 45.0 degrees
. time 1.709 sec
th 4793.9 Hz
repetitions
RVE H1, 300.0738815 MHz

PROCESSING
ize 16384
1 t 7.765



blt3-rxn780pg200pure1carbon

Sample Name:

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

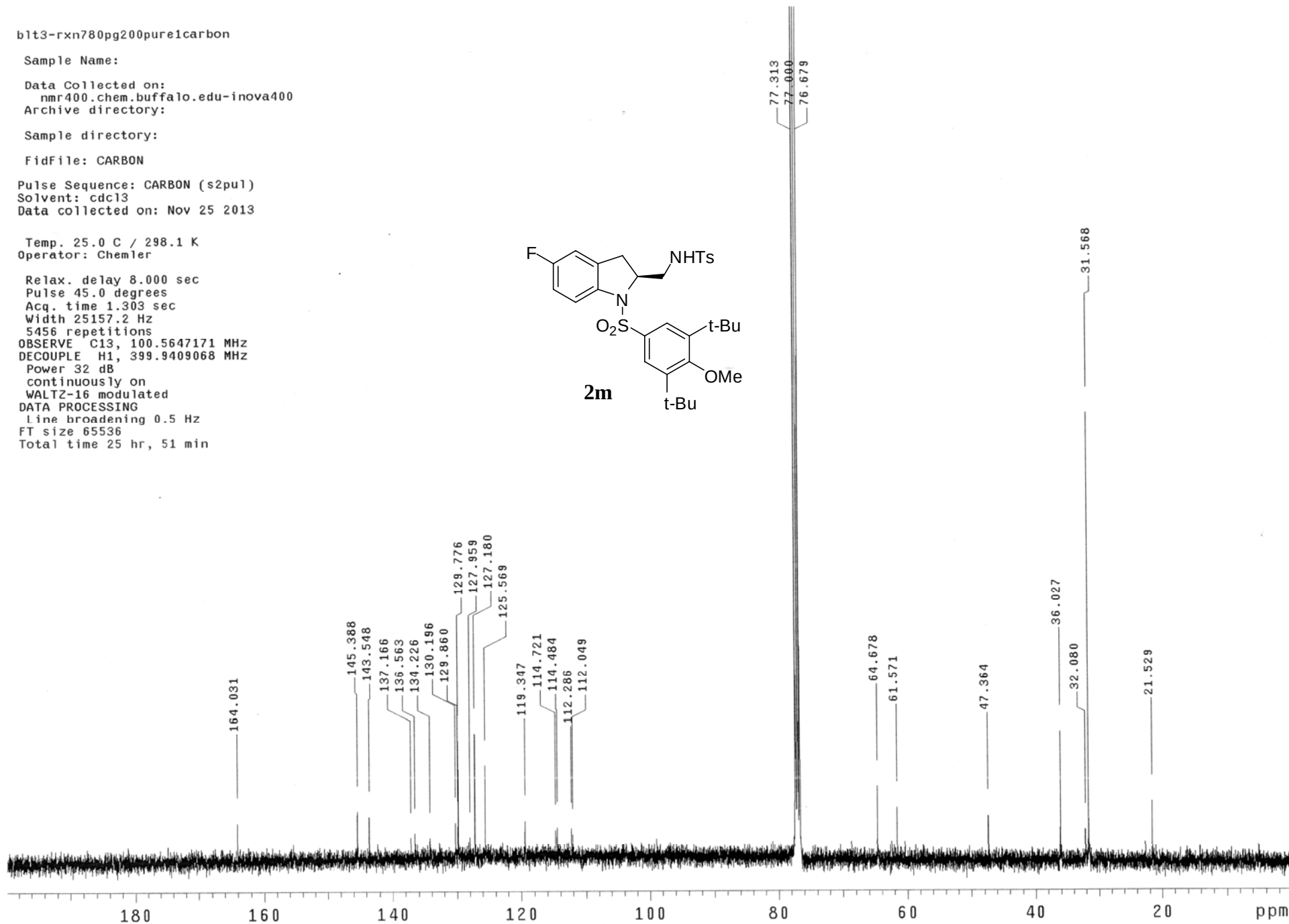
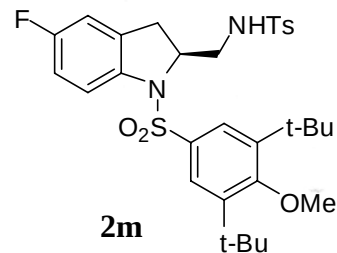
Sample directory:

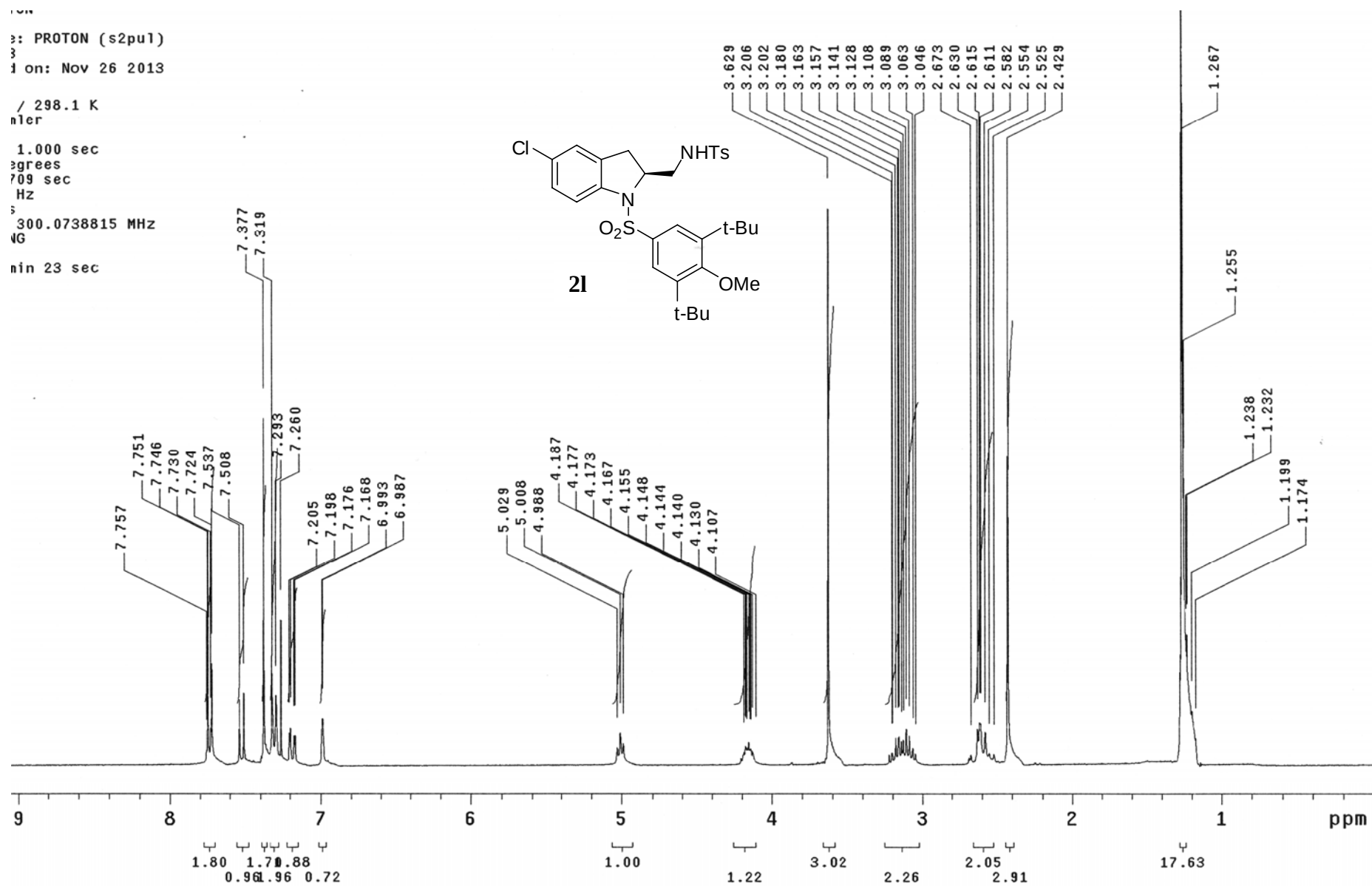
FidFile: CARBON

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

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
5456 repetitions
OBSERVE C13, 100.5647171 MHz
DECOUPLE H1, 399.9409068 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 25 hr, 51 min





b1t3-rxn788pg208pure1prep1carbon

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on: Nov 26 2013

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 8.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

608 repetitions

OBSERVE C13, 75.4536377 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

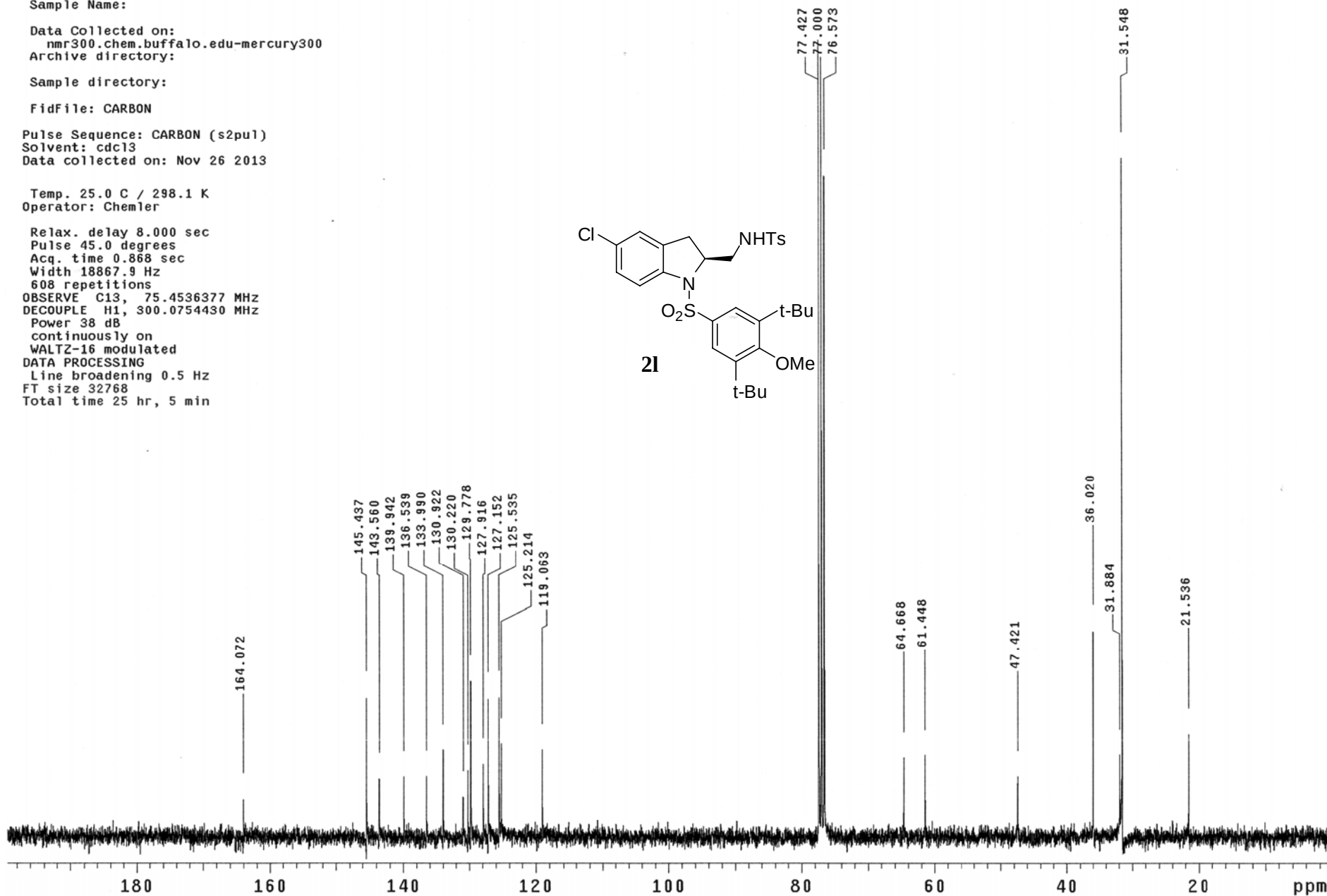
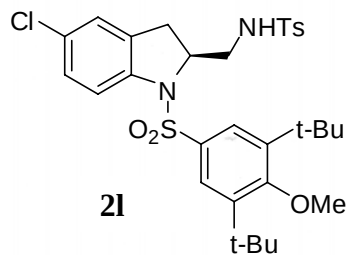
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 25 hr, 5 min



Dry:

ON

: PROTON (s2pu1)

on: Dec 2 2013

/ 298.1 K

iter

1.000 sec

degrees

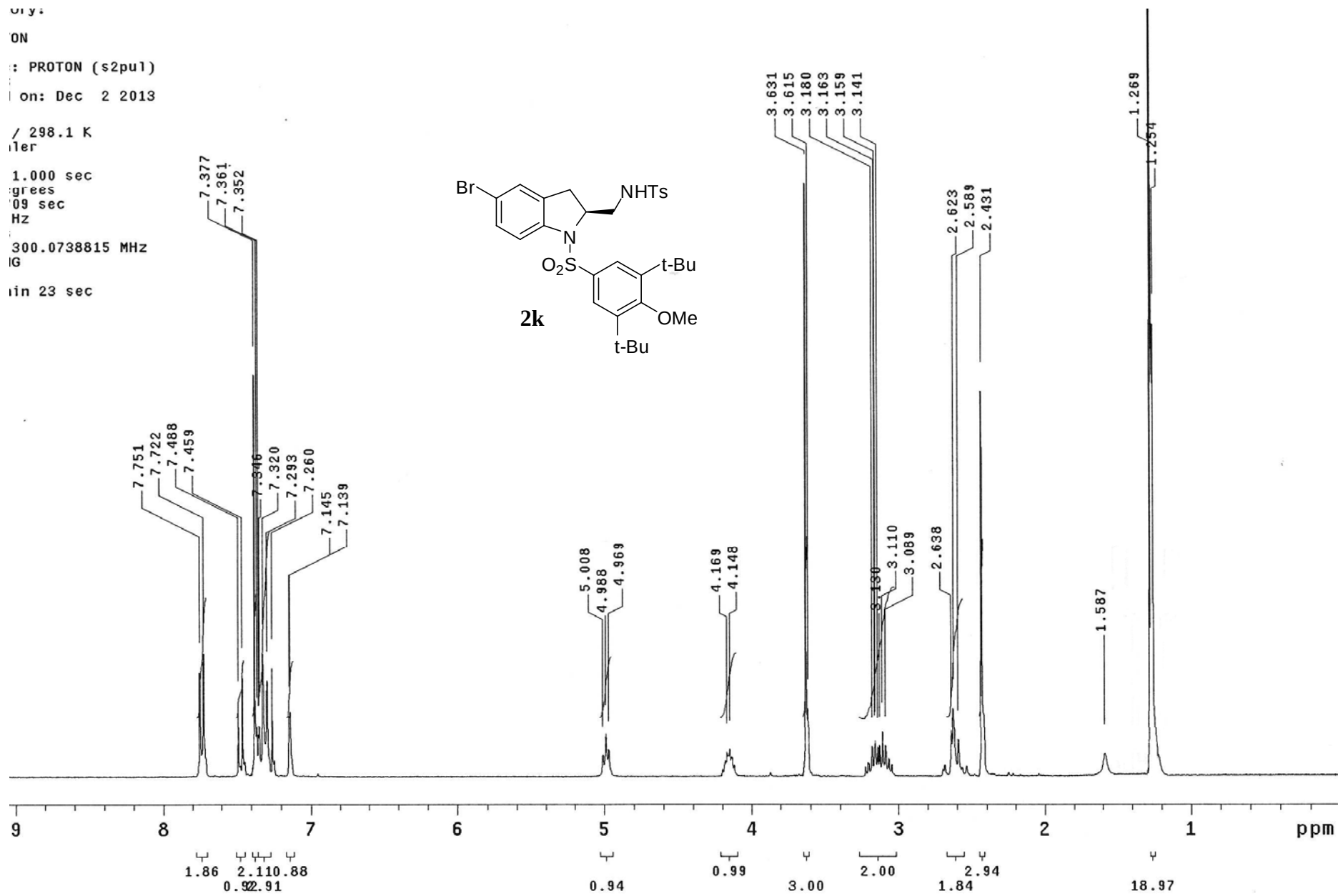
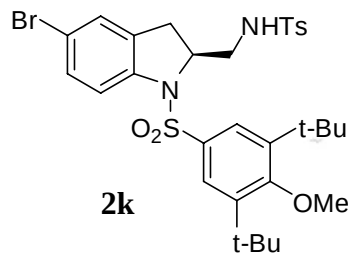
09 sec

Hz

300.0738815 MHz

IG

in 23 sec



blt3-rxn768pg188pure1prep1carbon

Sample Name:

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

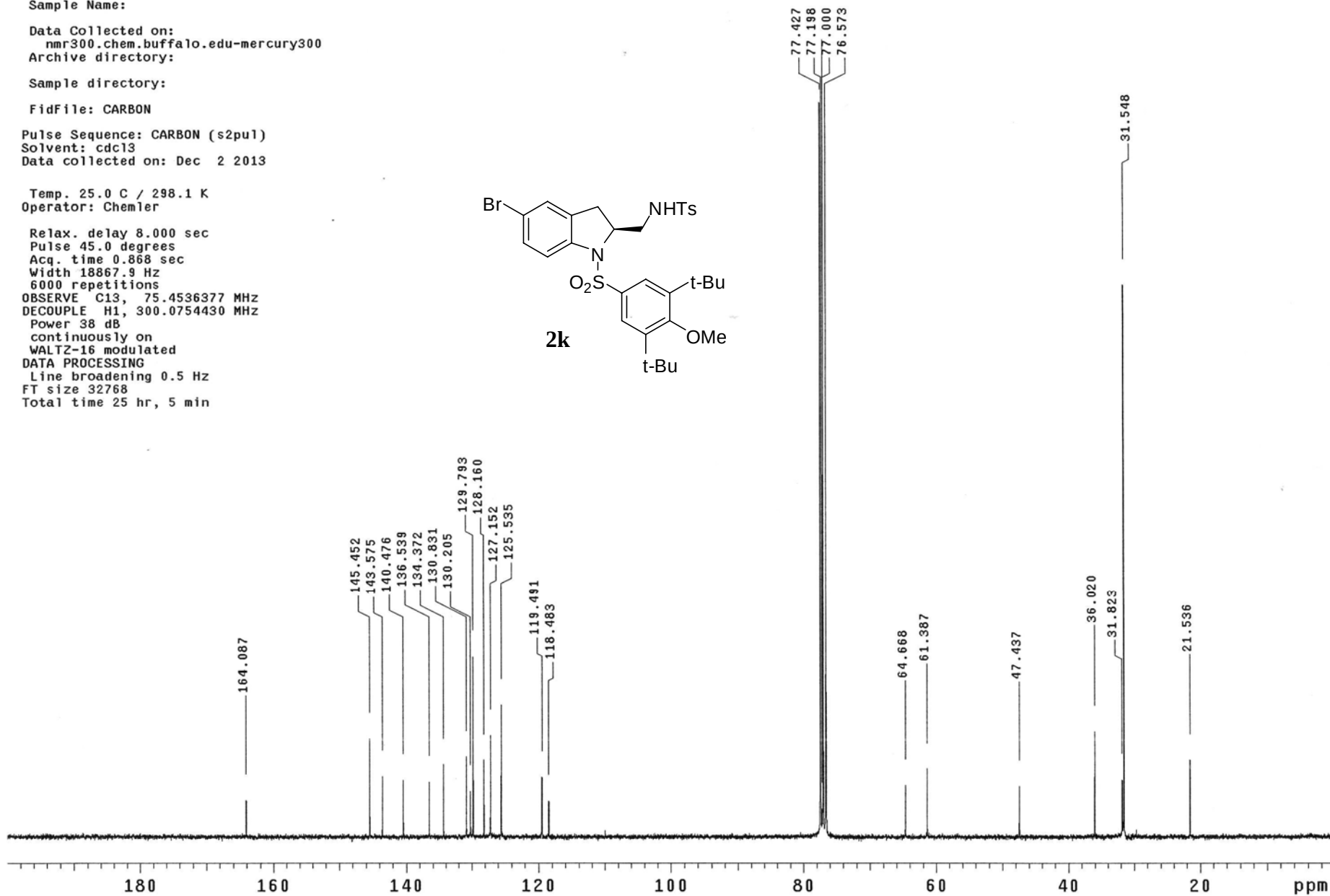
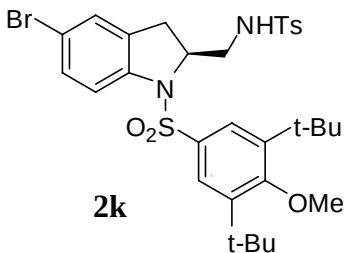
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Dec 2 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6000 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 25 hr, 5 min



ed on:
n.buffalo.edu-mercury300
ctory:

tory:

TON

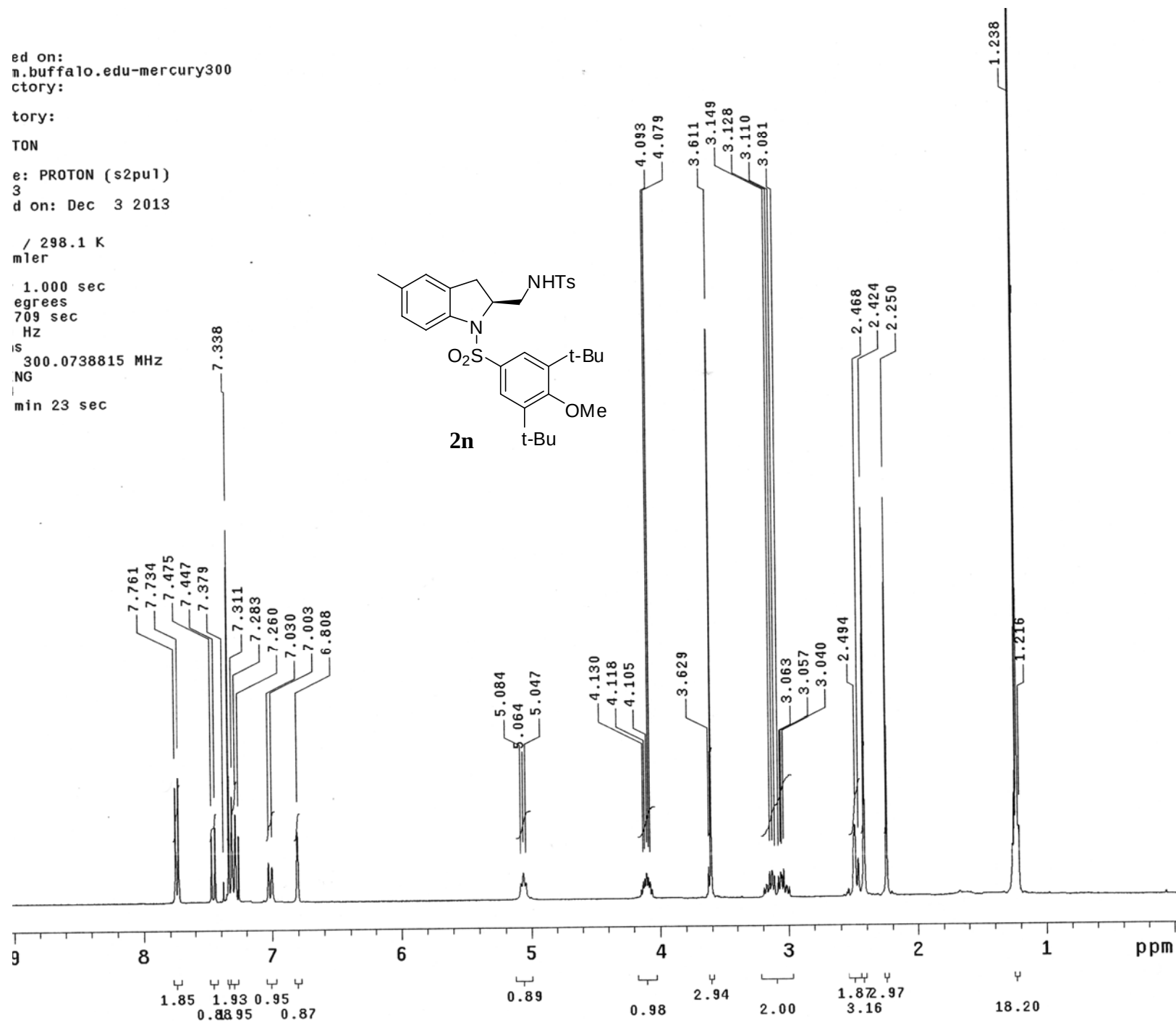
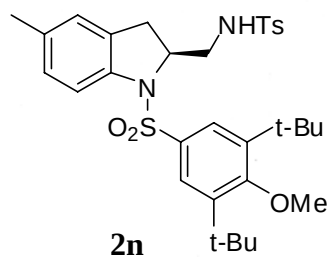
e: PROTON (s2pu1)
3
d on: Dec 3 2013

/ 298.1 K
mler

1.000 sec
egrees
709 sec
Hz

is
300.0738815 MHz
NG

min 23 sec



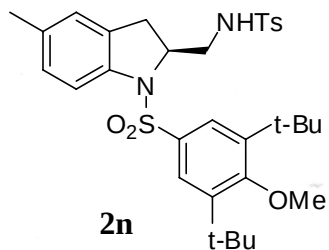
blt3-rxn789pg209pure1prep1

Sample Name:

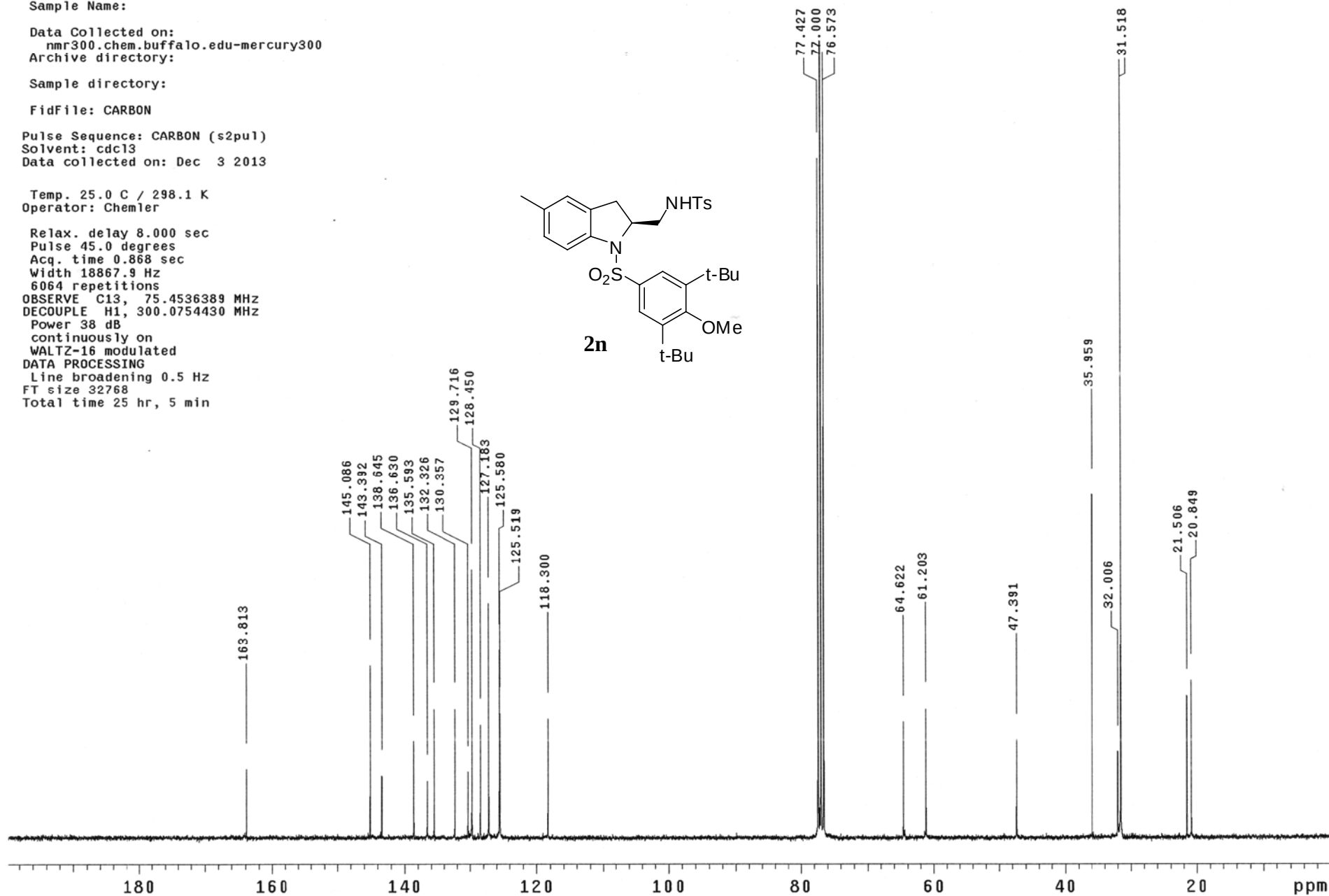
Data Collected on:
nmr300.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Dec 3 2013Temp. 25.0 C / 298.1 K
Operator: ChemlerRelax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6064 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 25 hr, 5 min

2n



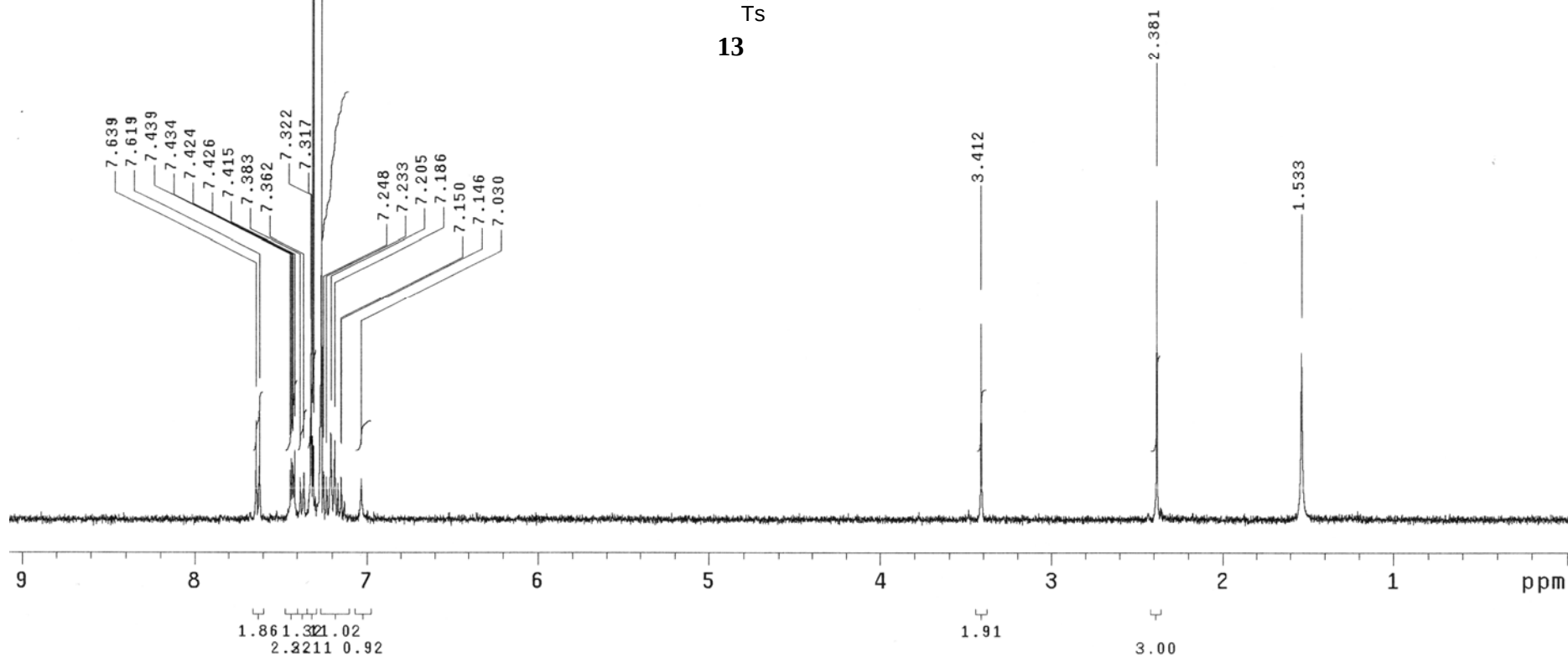
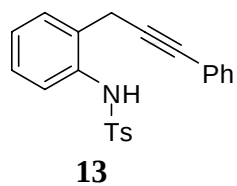
1: PROTON (s2pu1)
1 on: Aug 1 2013

/ 298.1 K
1.000 sec

degrees
65 sec

Hz
399.9389027 MHz
IG

in 29 sec



blt3-rxn718pg138pure1carbon

Sample Name:

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

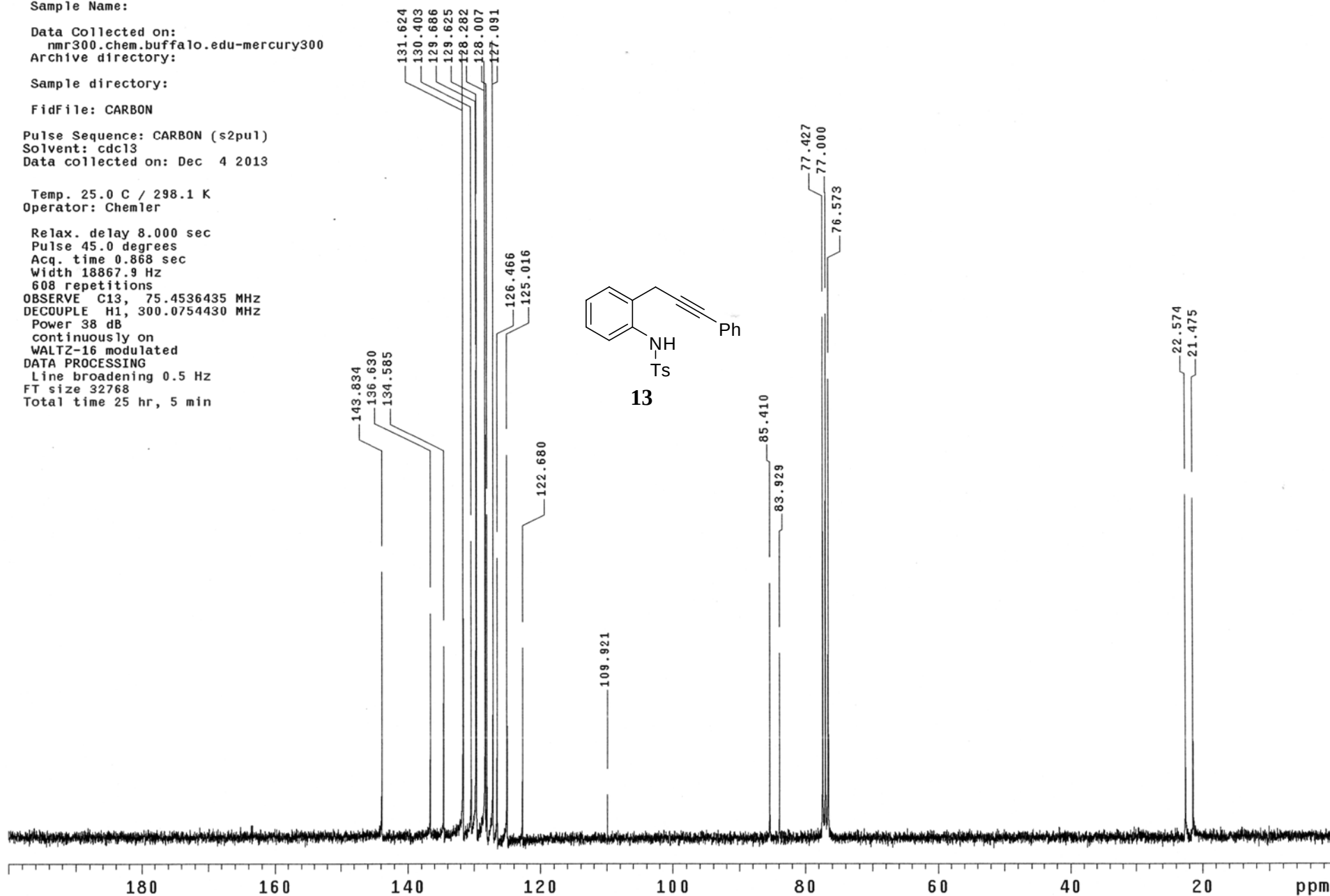
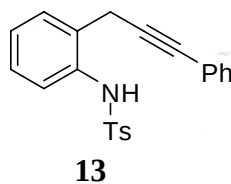
Sample directory:

FidFile: CARBON

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

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
608 repetitions
OBSERVE C13, 75.4536435 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 25 hr, 5 min



PROTON (s2pu1)

n: Jun 12 2012

r

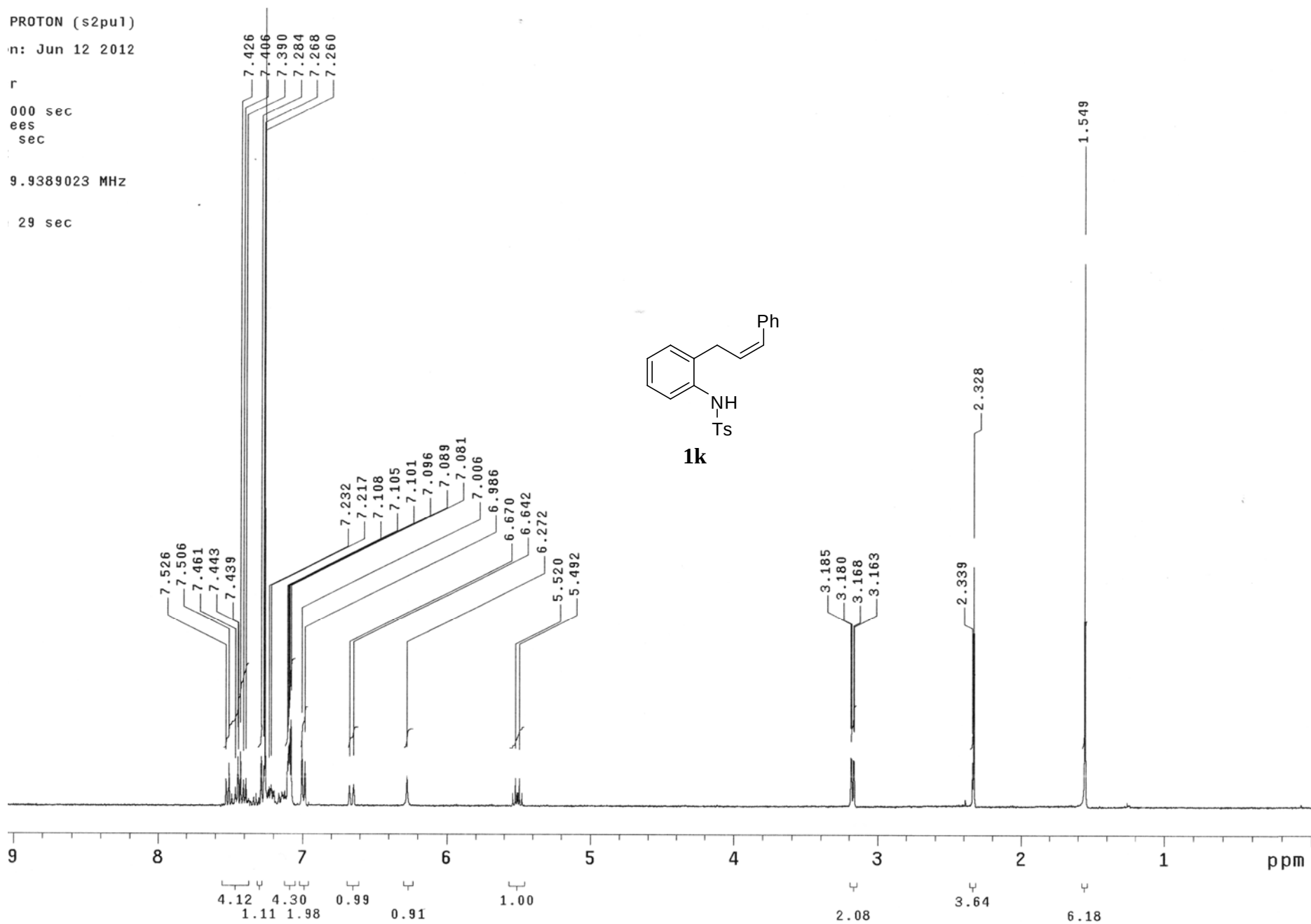
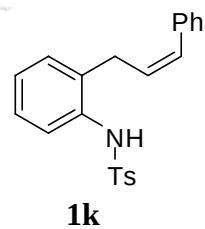
000 sec

ees

sec

9.9389023 MHz

29 sec



blt3-rxn721pg141carbon

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 19 2013

Temp. 25.0 C / 298.1 K

Operator: Sherry

Relax. delay 8.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

5936 repetitions

OBSERVE C13, 75.4536377 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

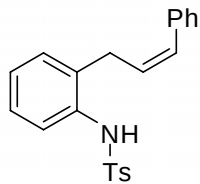
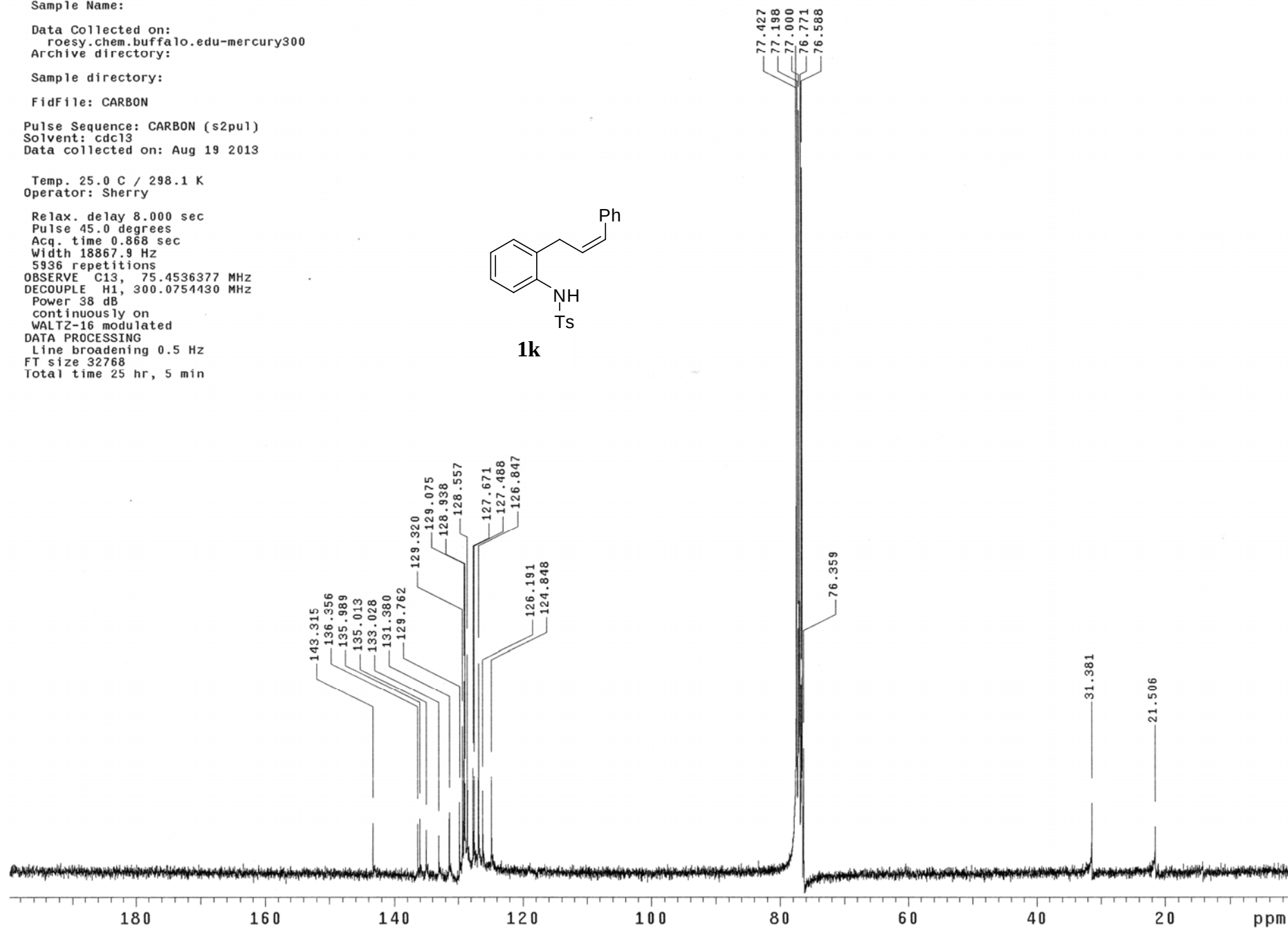
WALTZ-16 modulated

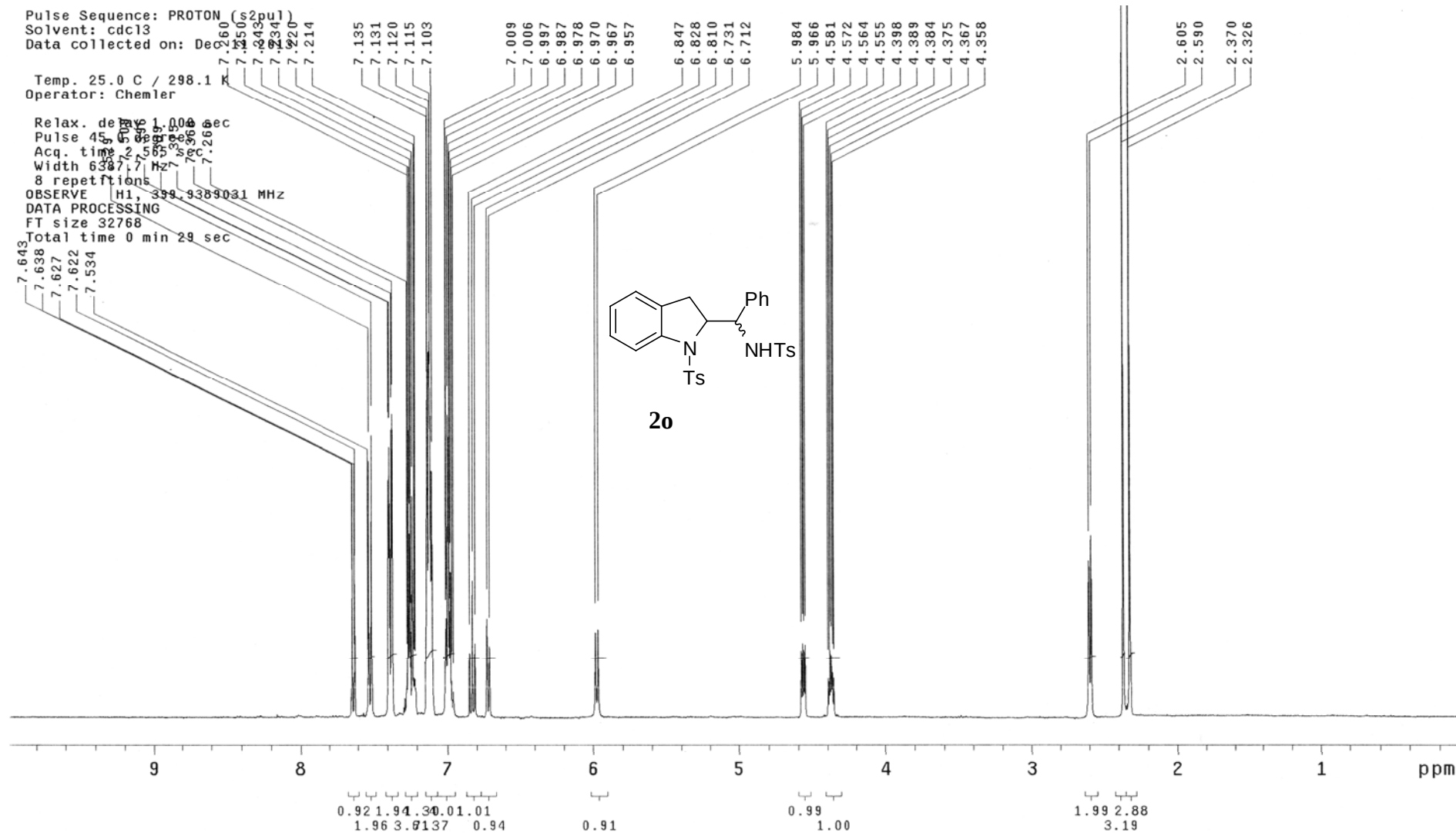
DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 25 hr, 5 min

**1k**



blt3-rxn709pg129pure1prep2major

Sample Name:

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

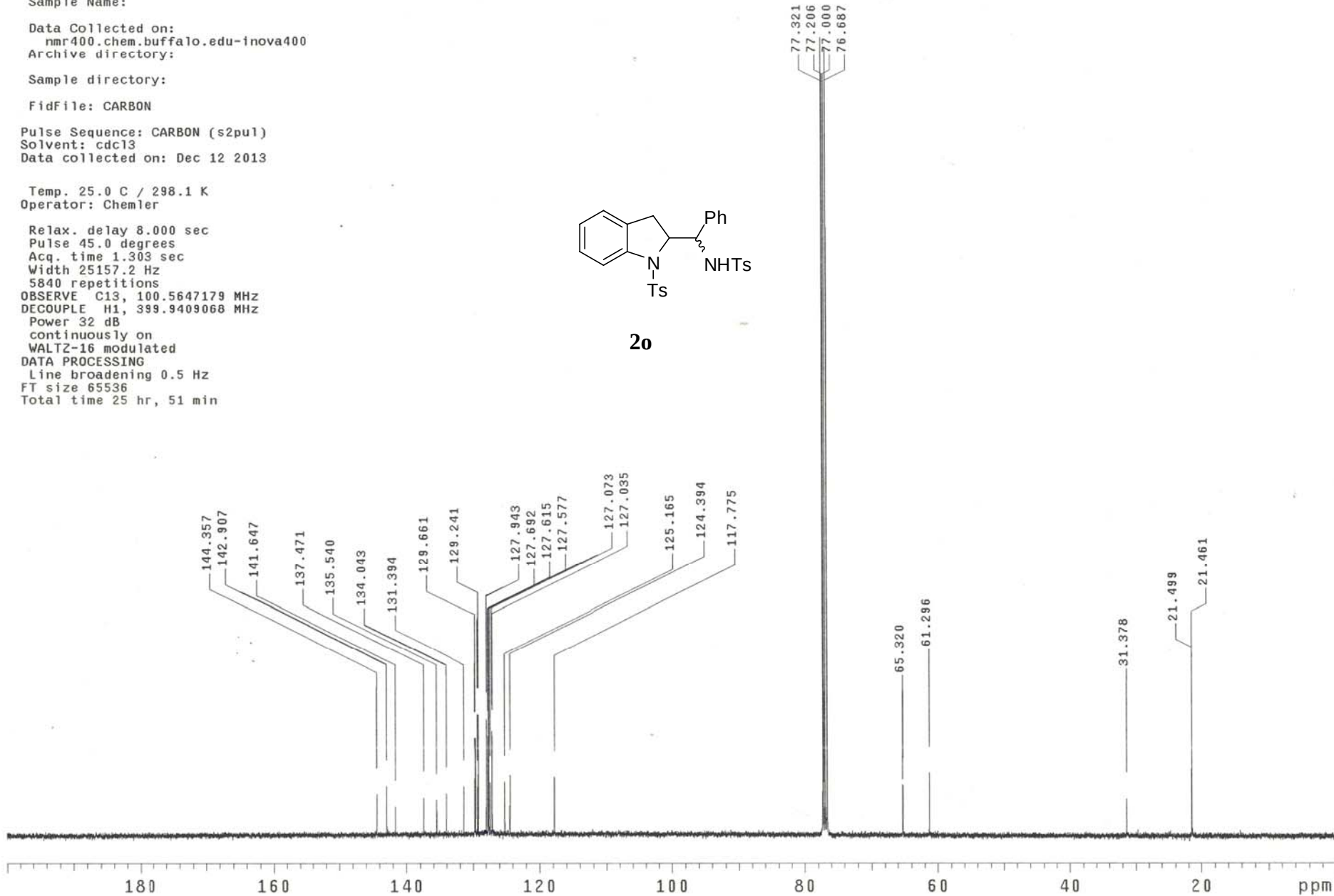
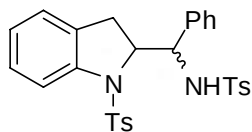
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 12 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
5840 repetitions
OBSERVE C13, 100.5647179 MHz
DECOUPLE H1, 399.9409068 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 25 hr, 51 min



b1t3-rxn709pg129pure1prep1

Sample Name:

Data Collected on:

nmr400.chem.buffalo.edu-inova400-7

Archive directory:

```

Archive directory:
/export/home/chempack/vnmr/sys/data

```

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)

Solvent: cdcl_3

Data collected on: Dec 11 2013

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 1.000 sec

Relax. delay 1.000
Pulse 45.0 degrees

Pulse 45.0 degrees
Acq. time 2.565 sec

Width 6387.7 Hz

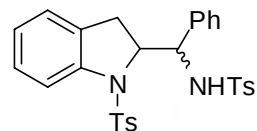
8 repetitions

OBSERVE H1, 399.9389022 MHz

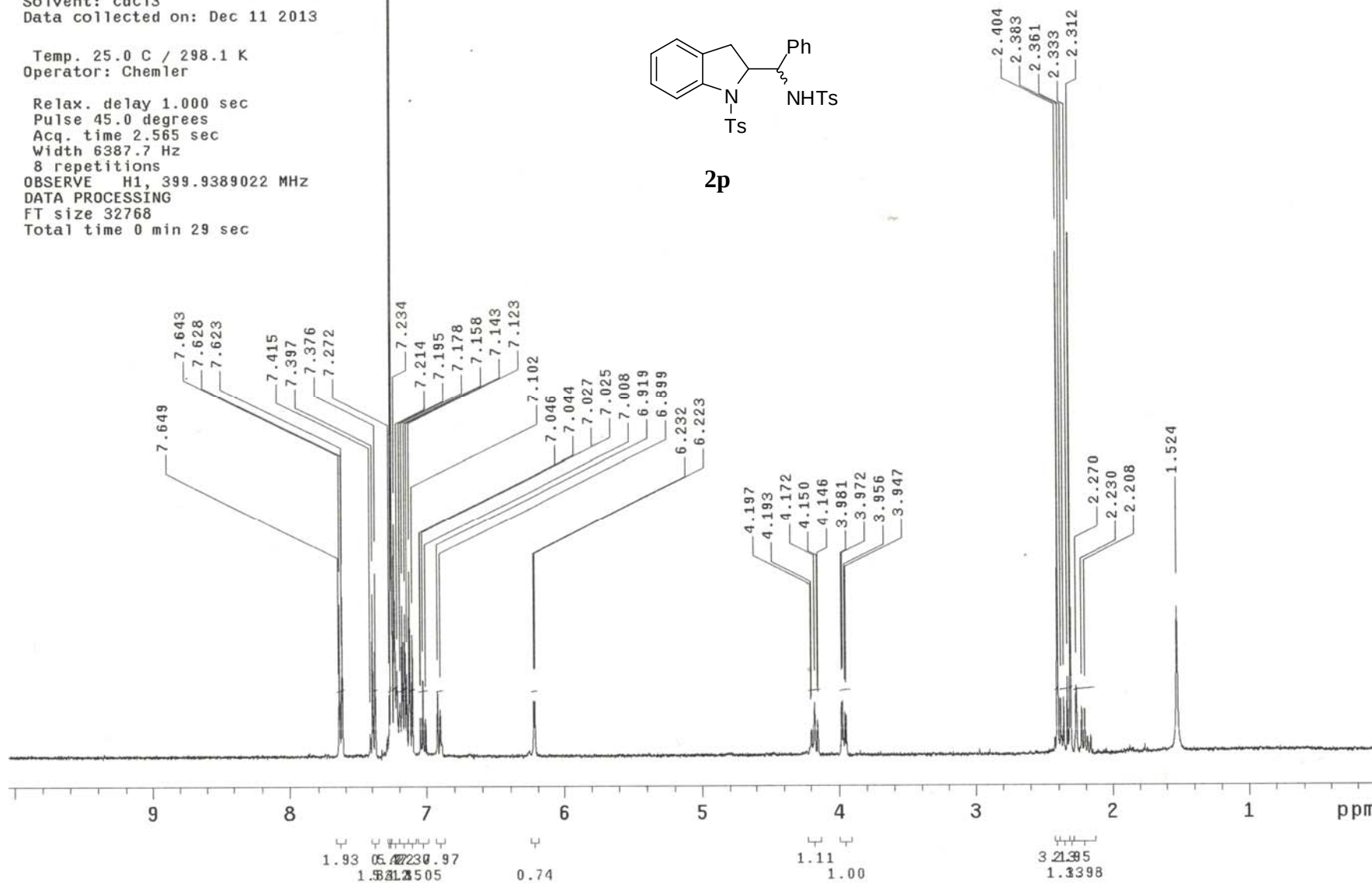
DATA PROCESSING

```
DATA PROCESSING
FT size 32768
```

Total time 0 min 29 sec



2p



blt3-rxn709pg129pure1prep1

Sample Name:

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

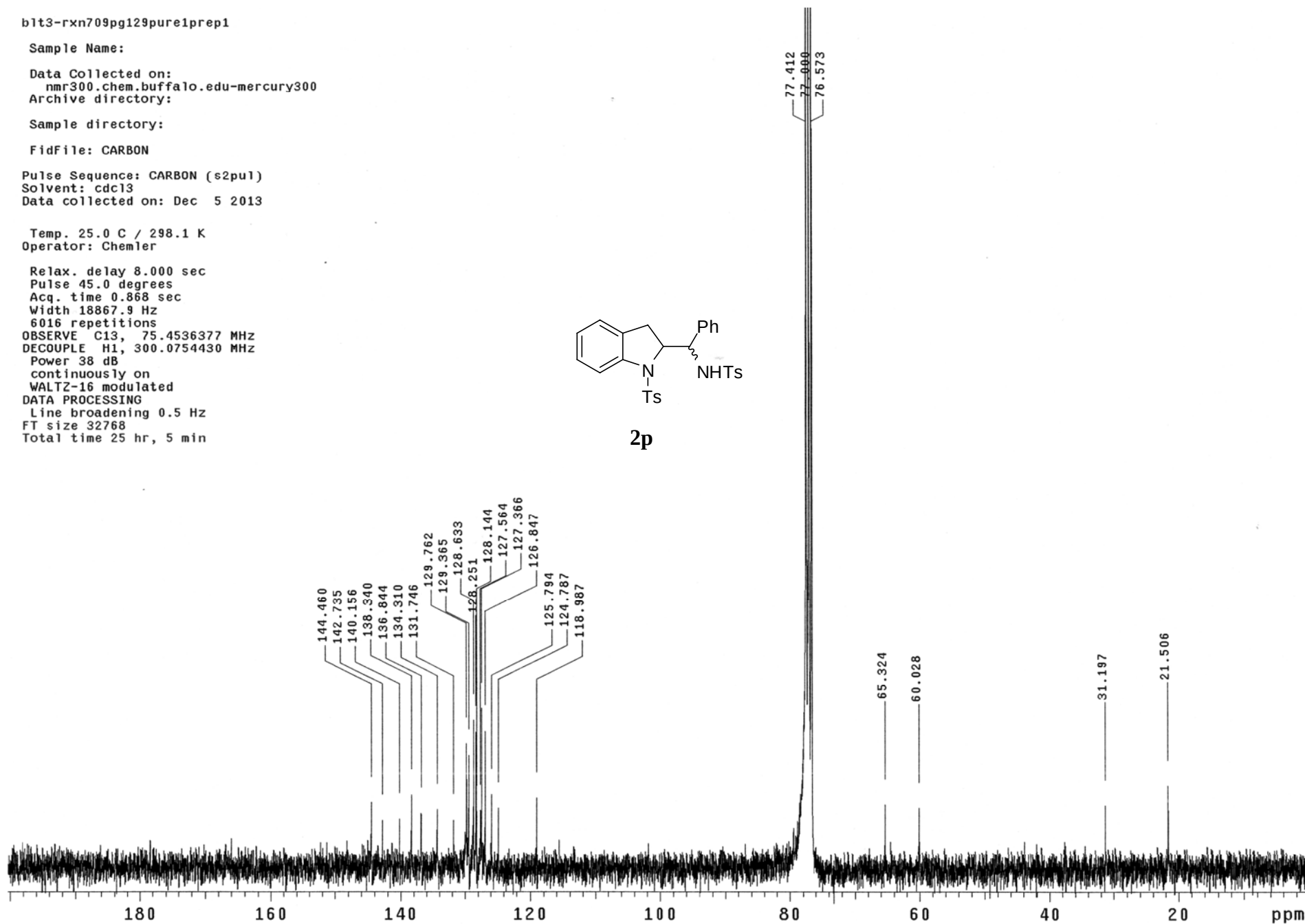
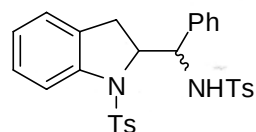
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 5 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6016 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 25 hr, 5 min



: PROTON (s2pu1)

on: Jun 11 2013

/ 298.1 K

ler

1.000 sec

grees

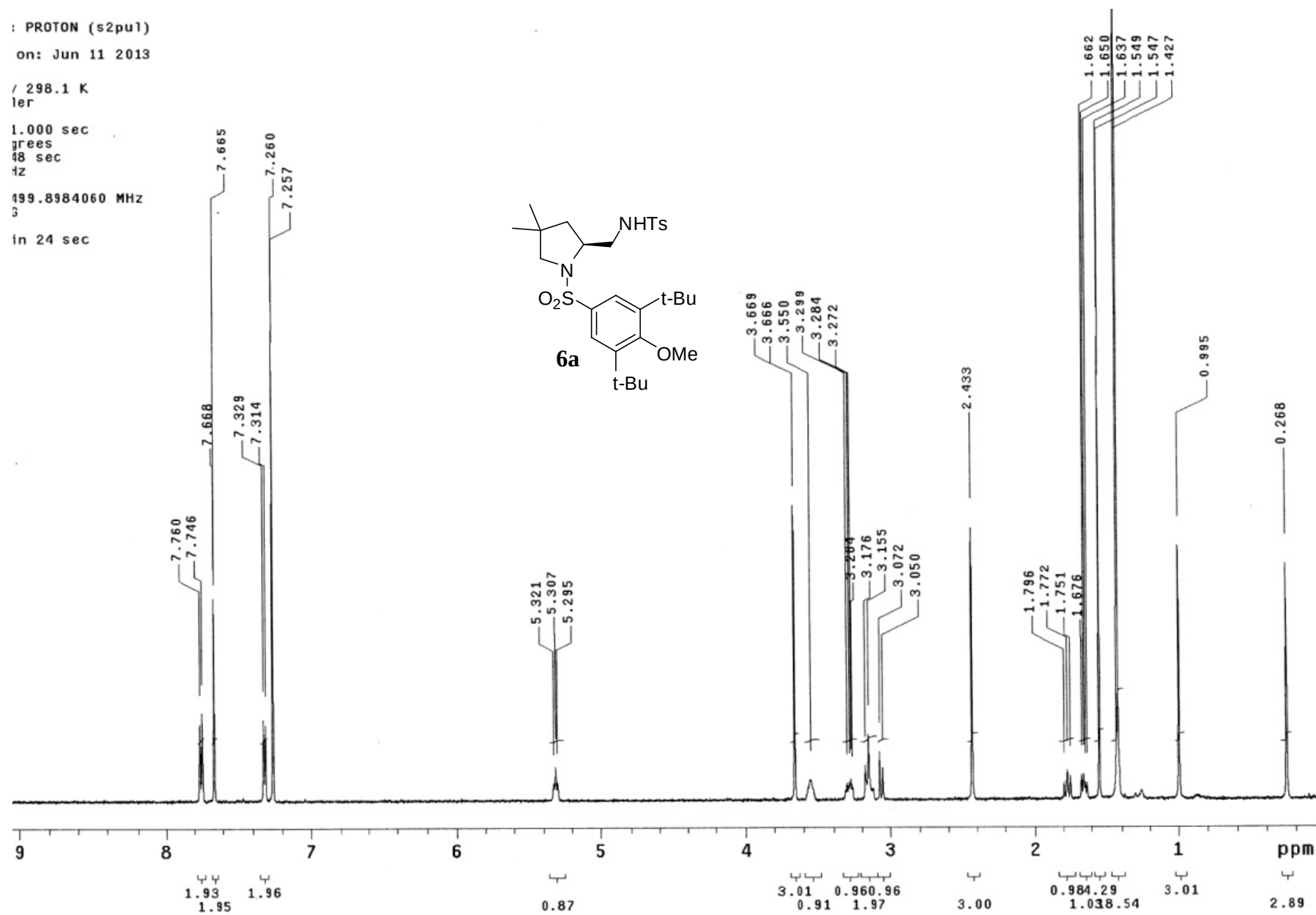
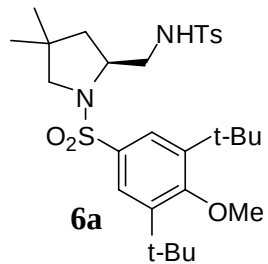
48 sec

Hz

499.8984060 MHz

3

in 24 sec



blt3-rxn781pg201pure1prep1

Sample Name:

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

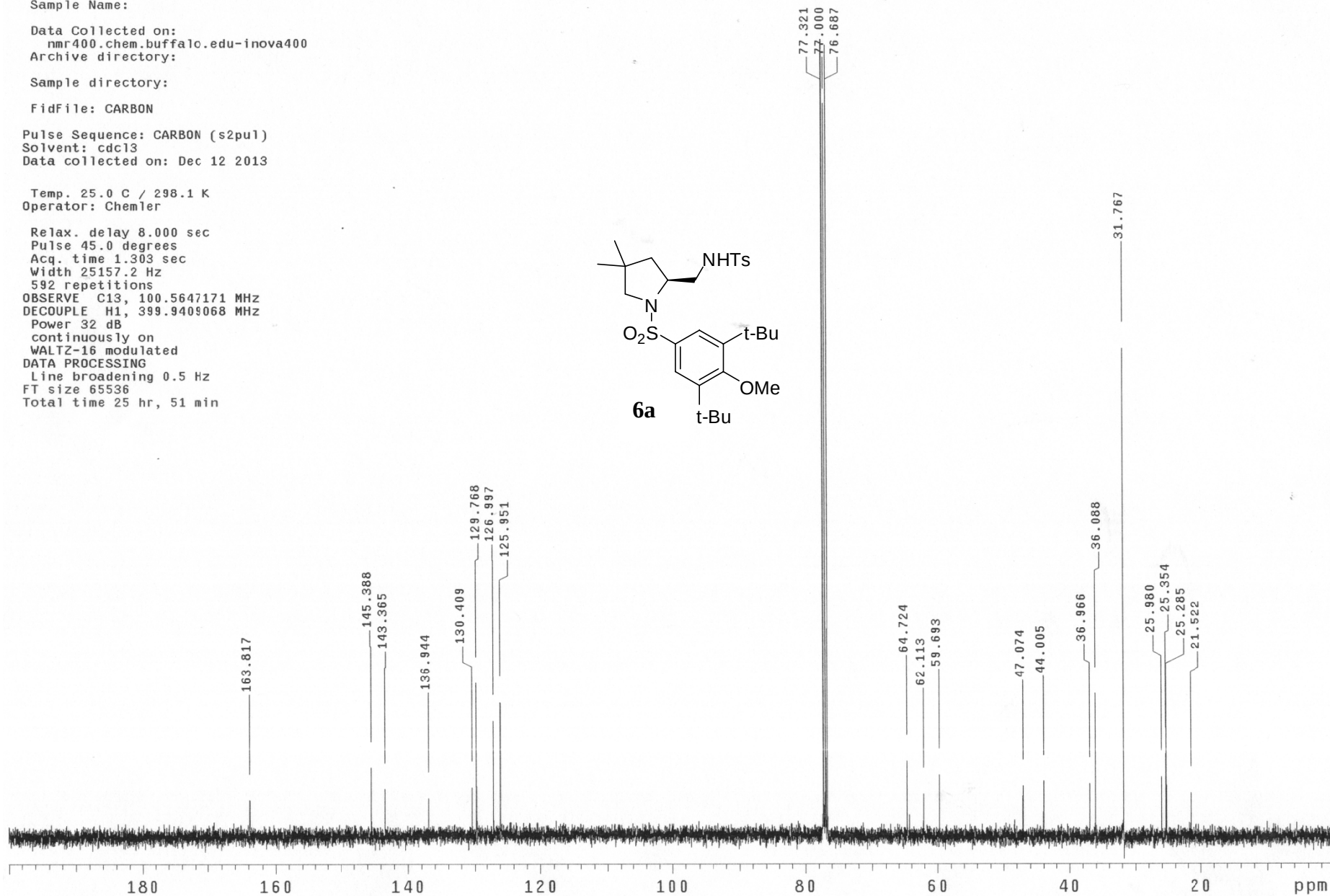
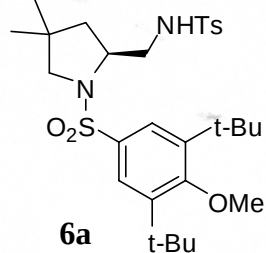
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 12 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
592 repetitions
OBSERVE C13, 100.5647171 MHz
DECOUPLE H1, 399.9409068 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 25 hr, 51 min



: PROTON (s2pul)

on: Jul 8 2013

ler

1.000 sec

grees

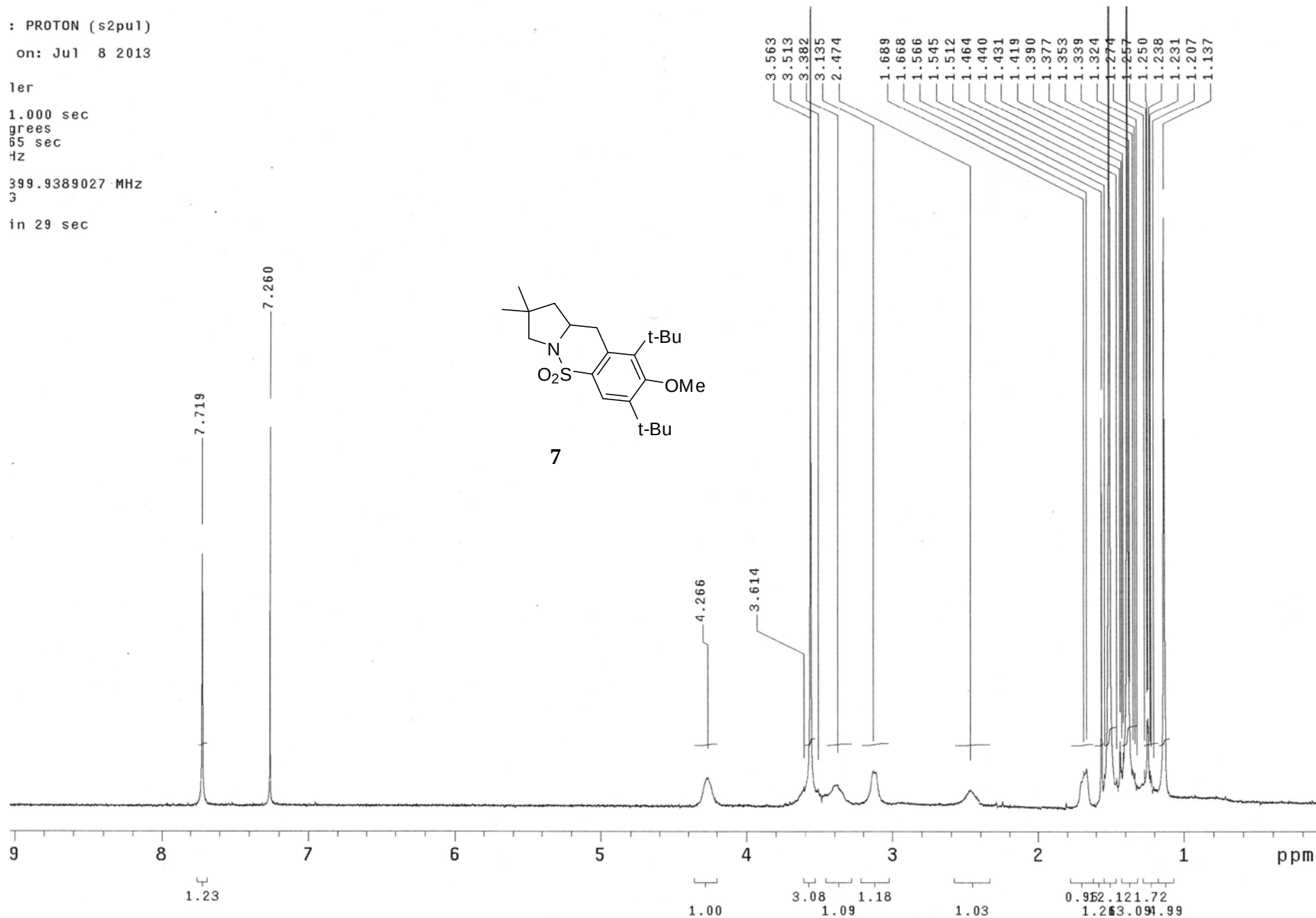
65 sec

Hz

399.9389027 MHz

3

in 29 sec



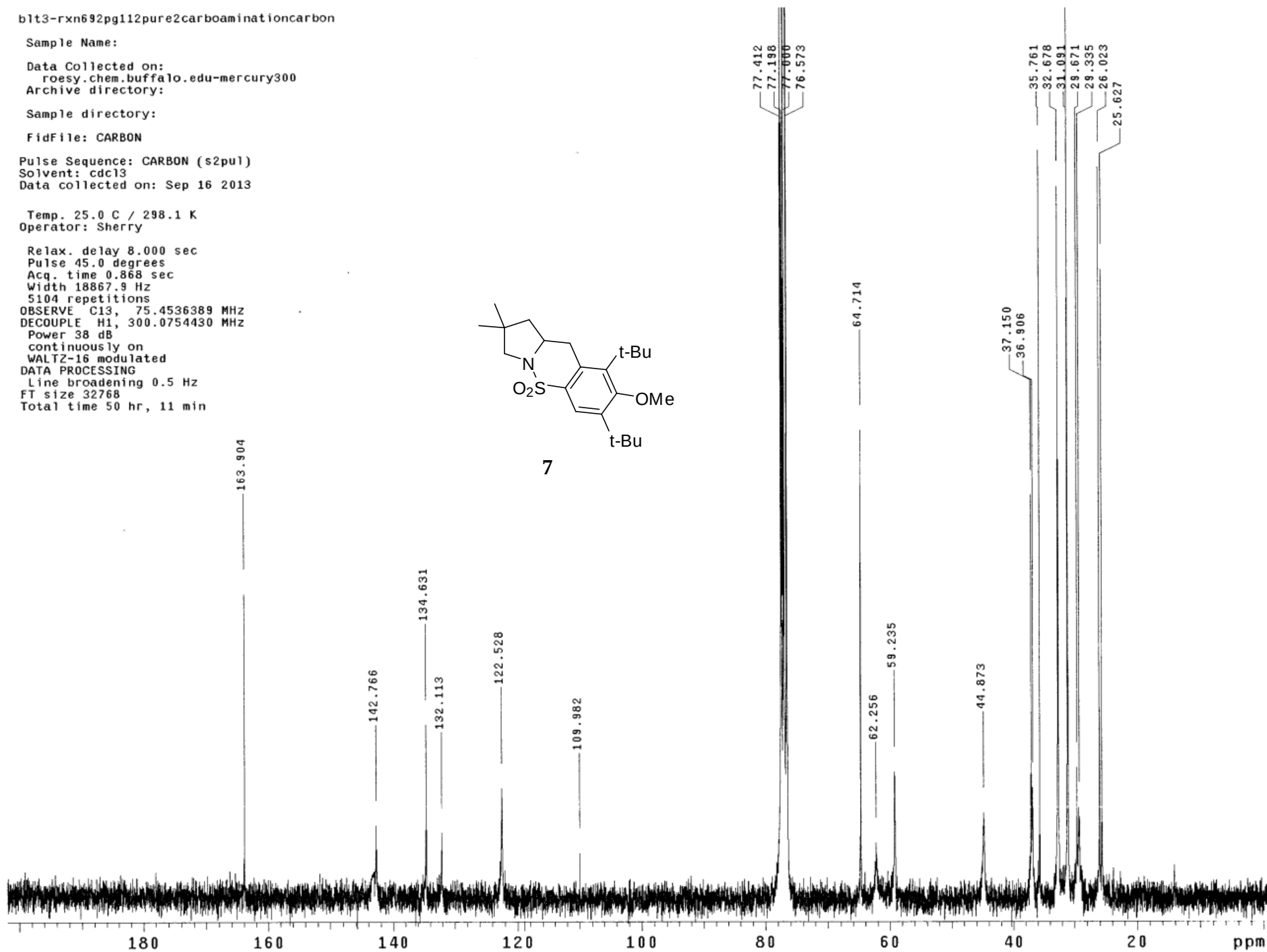
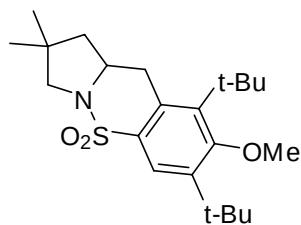
blt3-rxn692pg112pure2carboaminationcarbon

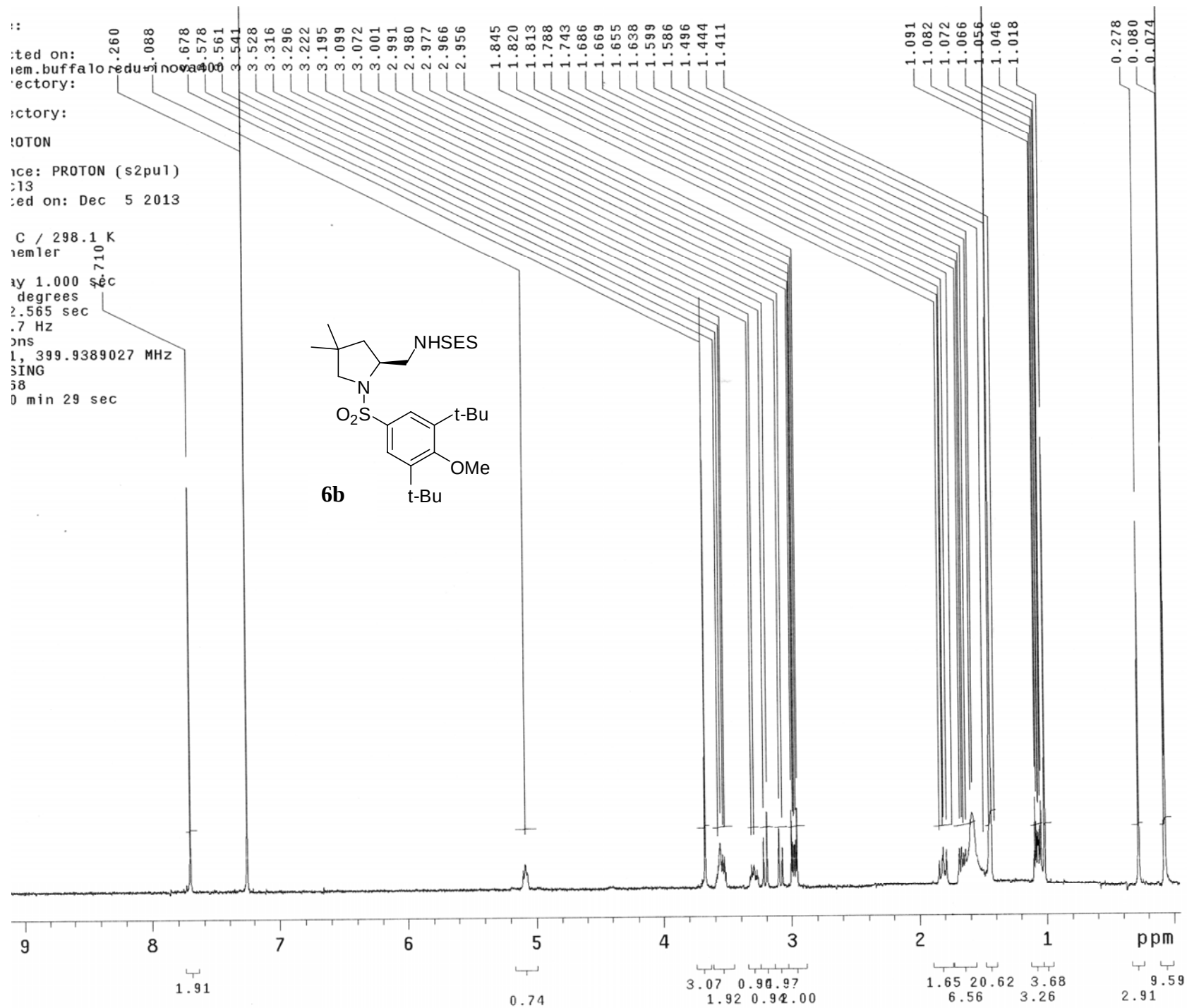
Sample Name:

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

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Sep 16 2013Temp. 25.0 C / 298.1 K
Operator: SherryRelax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
5104 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 50 hr, 11 min



blt3-rxn705pg125pure1prep1

Sample Name:

Data Collected on:

nmr400.chem.buffalo.edu-inova400

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Dec 5 2013

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 8.000 sec

Pulse 45.0 degrees

Acq. time 1.303 sec

Width 25157.2 Hz

5680 repetitions

OBSERVE C13, 100.5647182 MHz

DECOUPLE H1, 399.9409068 MHz

Power 32 dB

continuously on

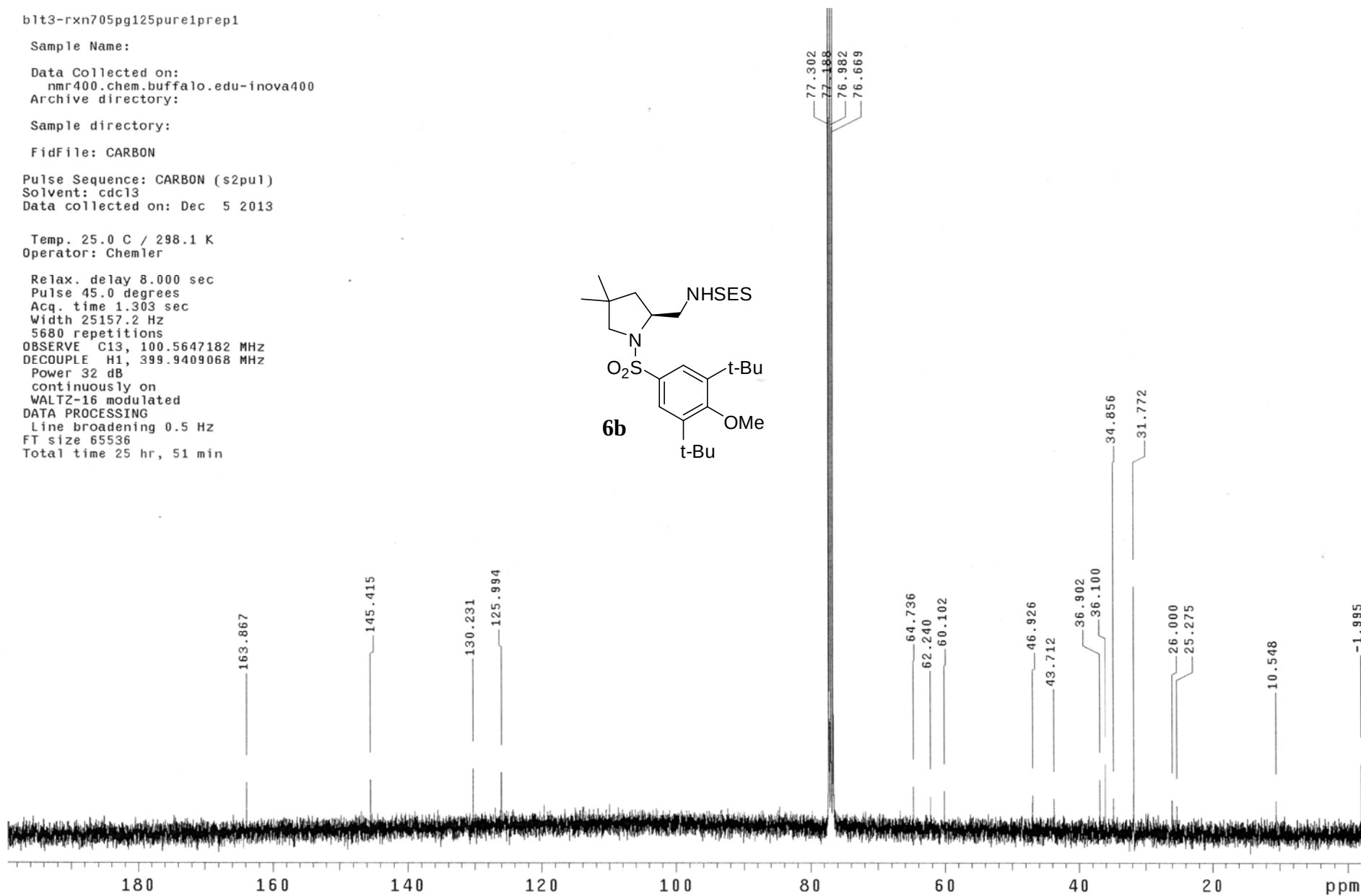
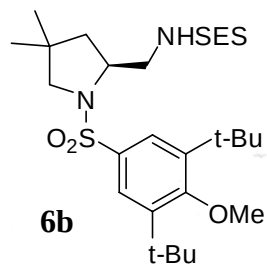
WALTZ-16 modulated

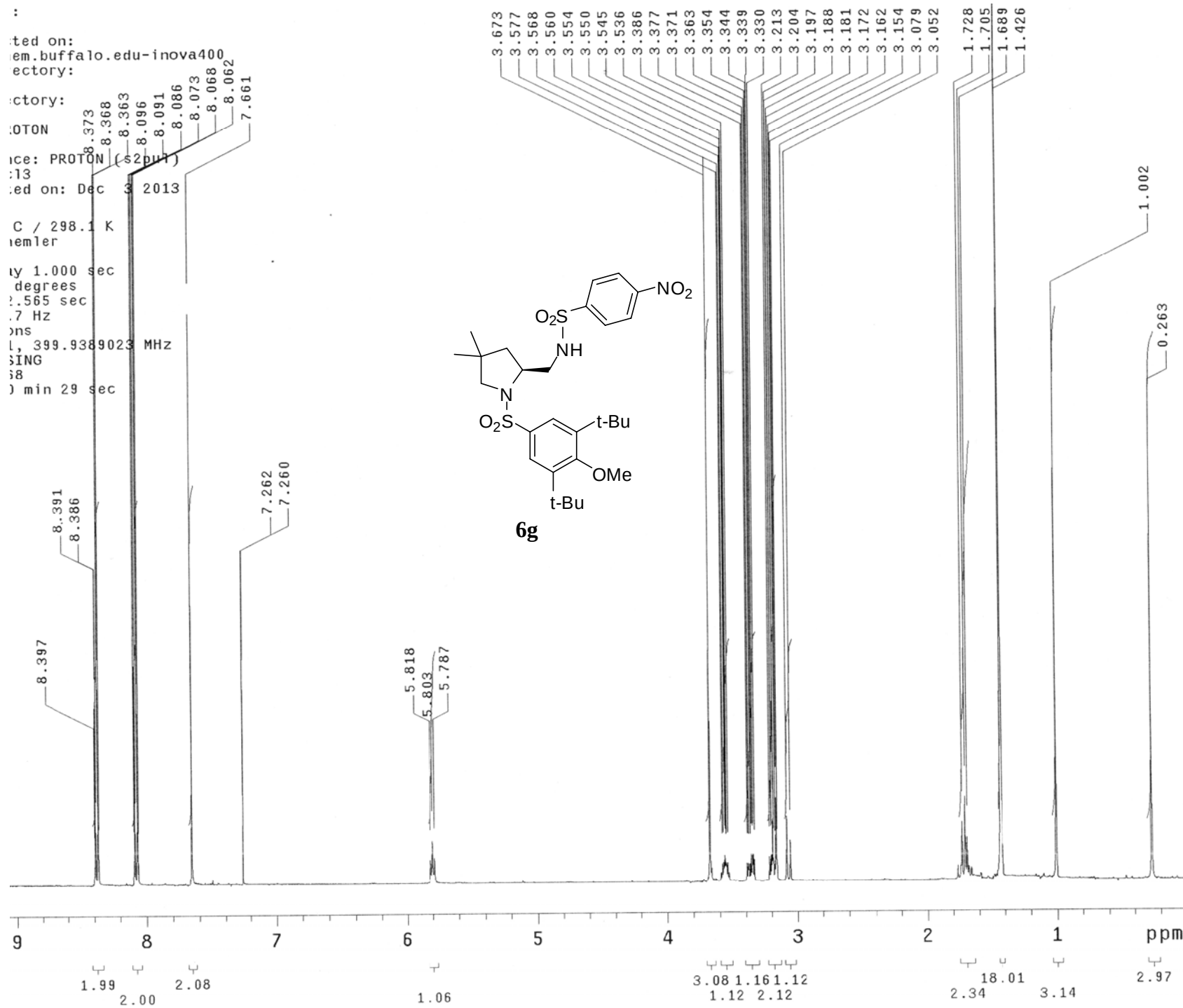
DATA PROCESSING

Line broadening 0.5 Hz

FT size 65536

Total time 25 hr, 51 min





blt3-rxn708pg118pureprep2carbon

Sample Name:

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

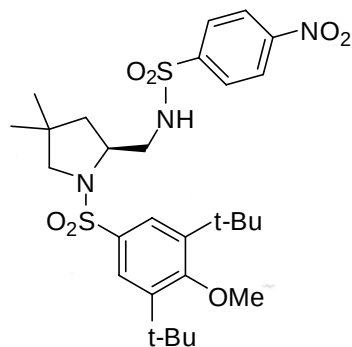
Sample directory:

FidFile: CARBON

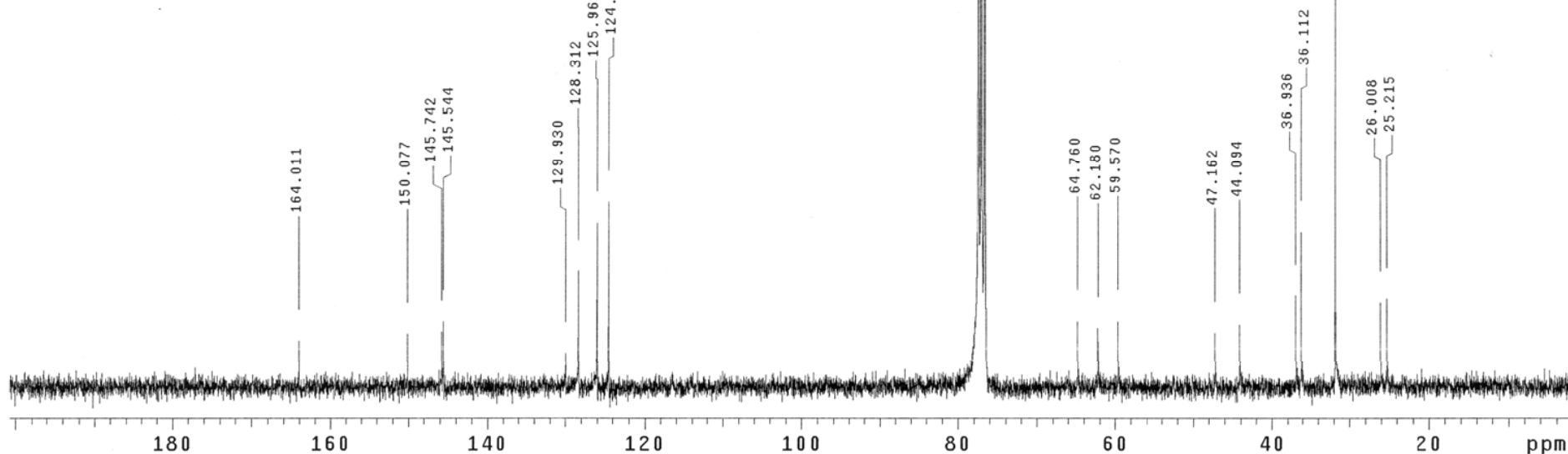
Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Sep 17 2013

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6160 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 25 hr, 5 min



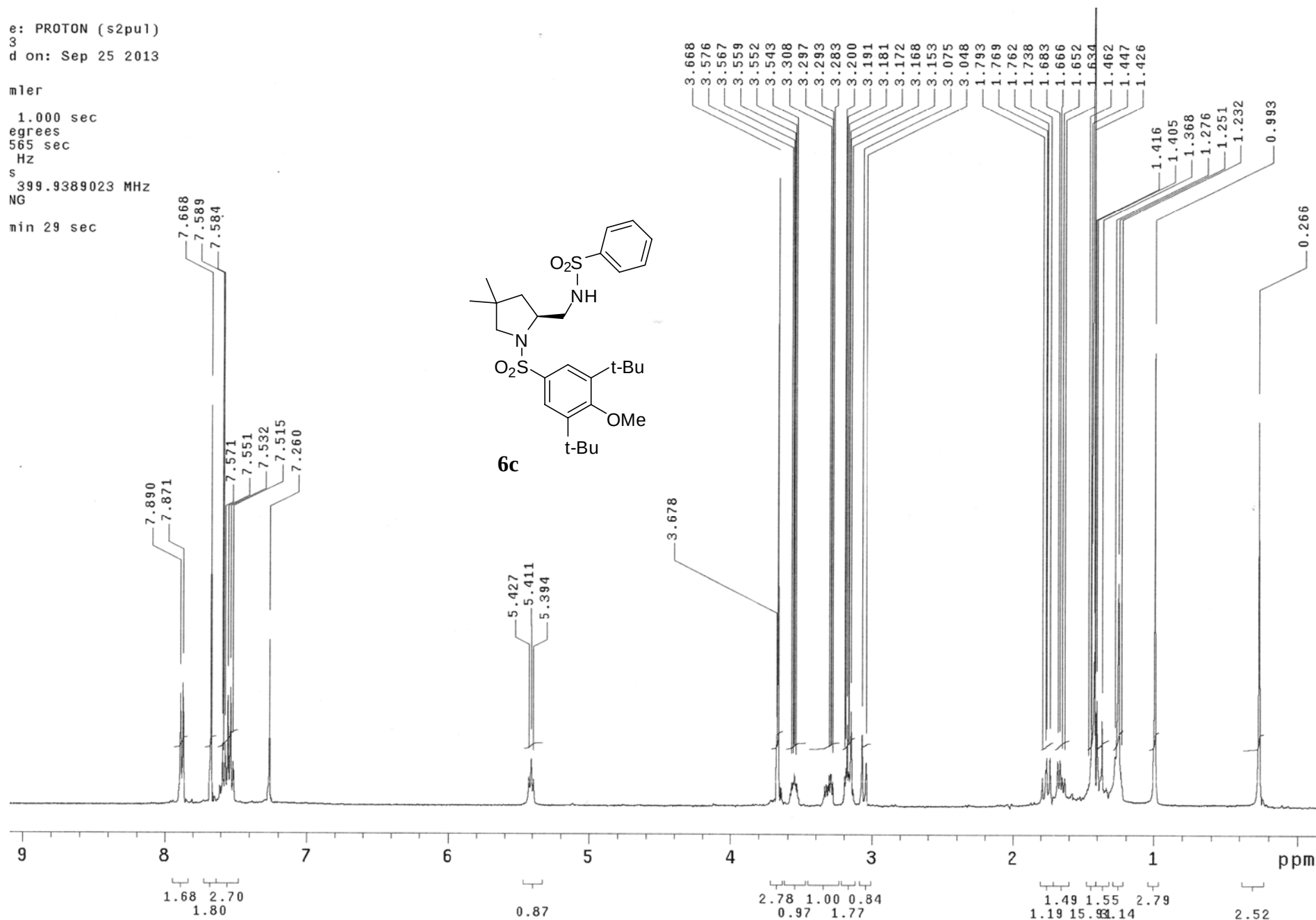
6g



e: PROTON (s2pu1)
3
d on: Sep 25 2013

mler

1.000 sec
egrees
565 sec
Hz
s
399.9389023 MHz
NG
min 29 sec



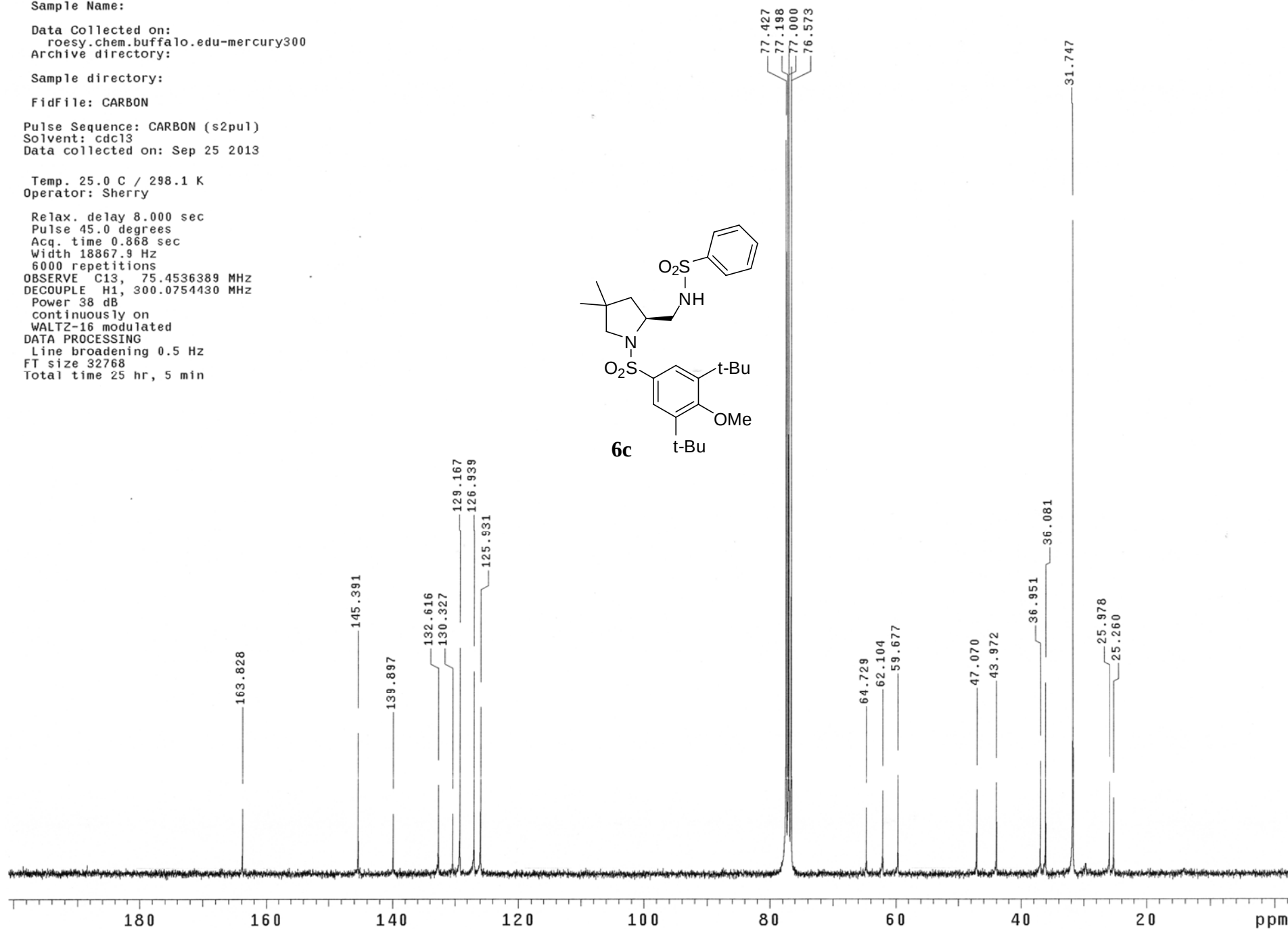
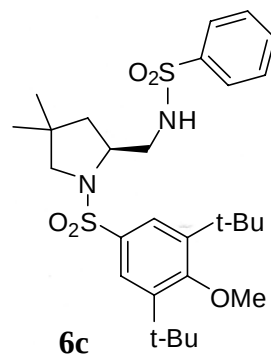
blt3-rxn728pg148pure1carbon

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: Sep 25 2013Temp. 25.0 C / 298.1 K
Operator: SherryRelax. delay 8.000 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 25 hr, 5 min

3:

cted on:
em.buffalo.edu-mercury300
ectory:

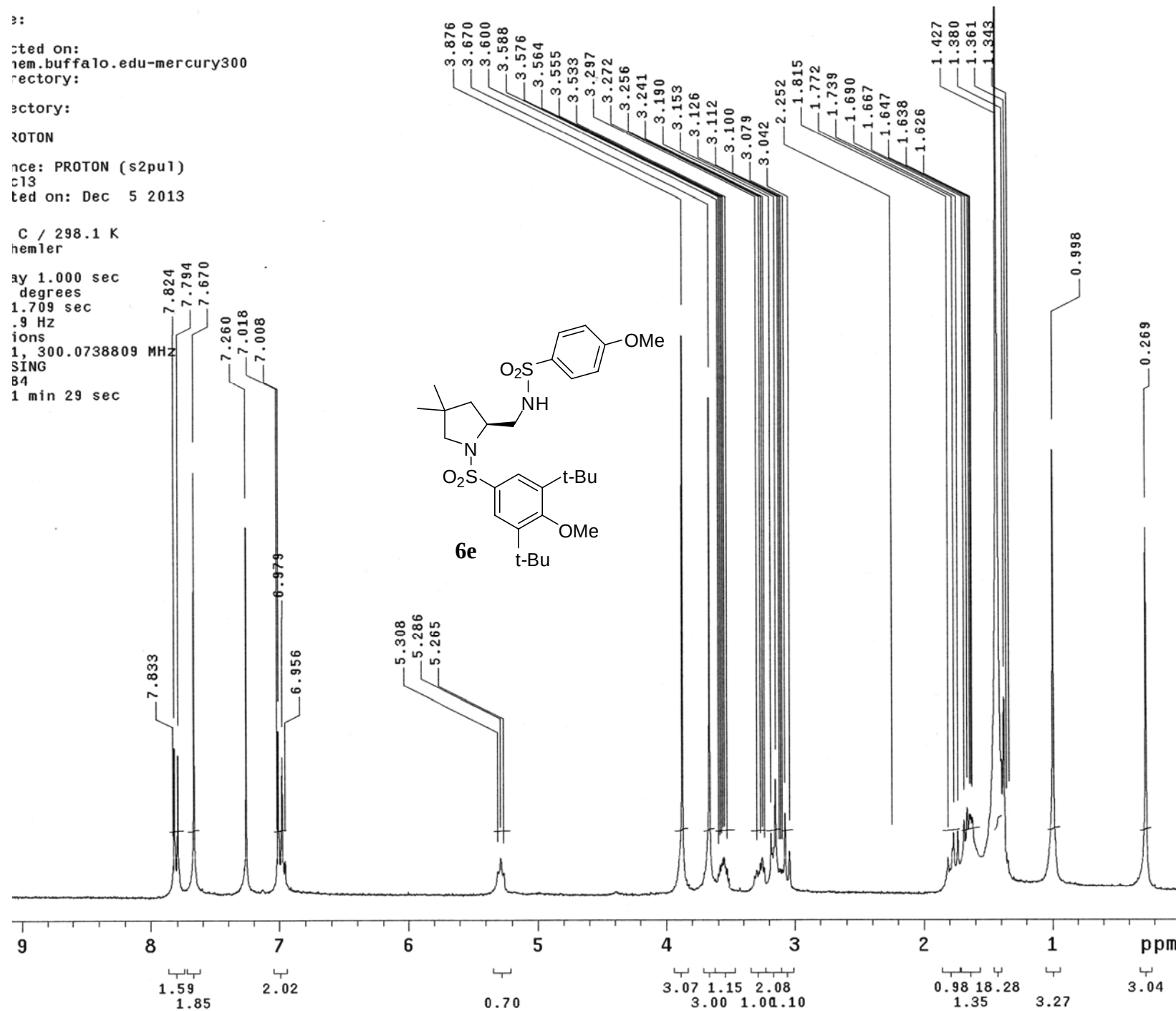
actory:

ROTON

nce: PROTON (s2pu1)
c13
ted on: Dec 5 2013

C / 298.1 K
hemler

ay 1.000 sec
degrees
1.709 sec
.9 Hz
ions
1,300.0738809 MHz
SING
B4
1 min 29 sec



b1t3-rxn737pg157pure1prep1

Sample Name:

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

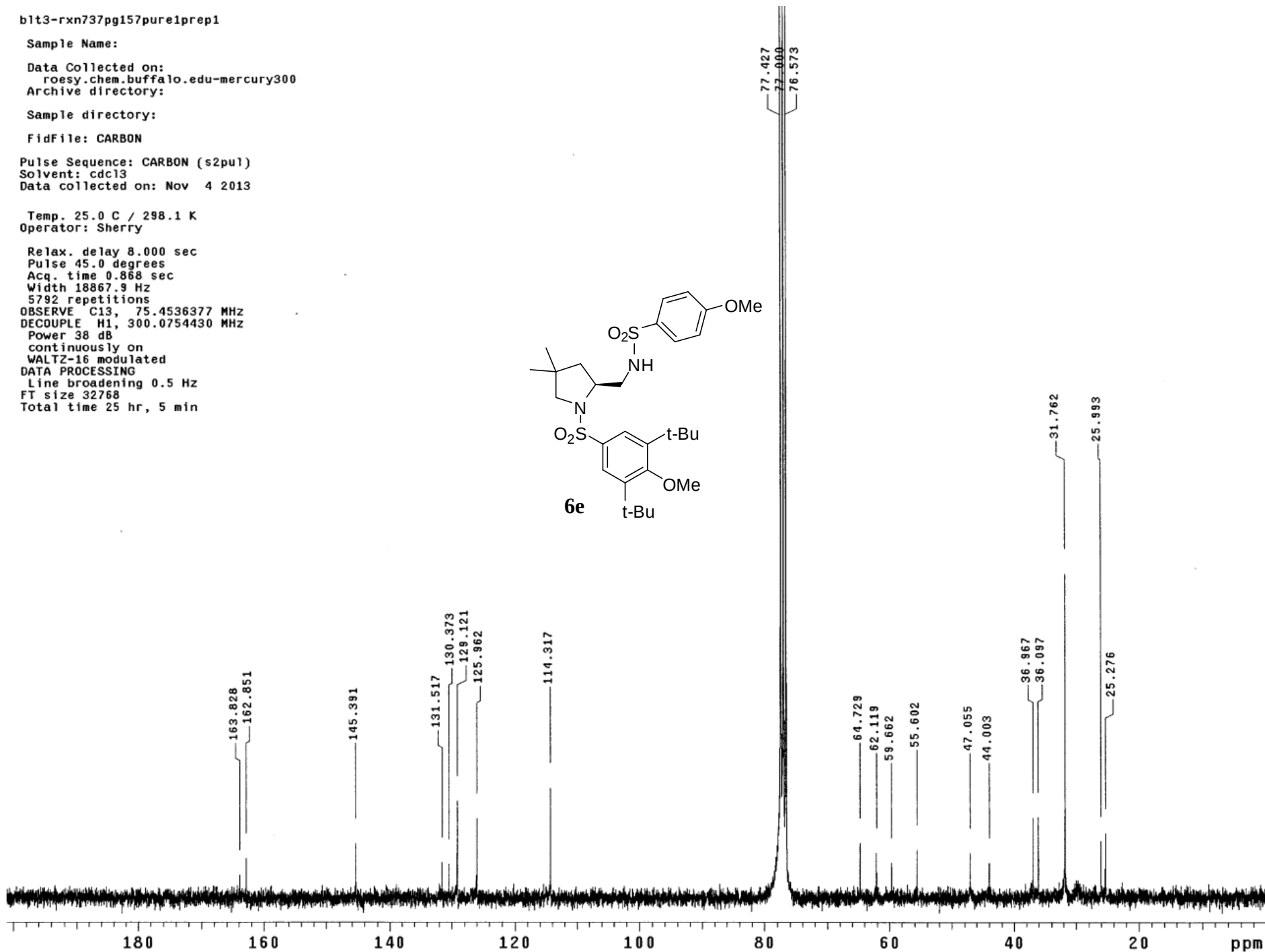
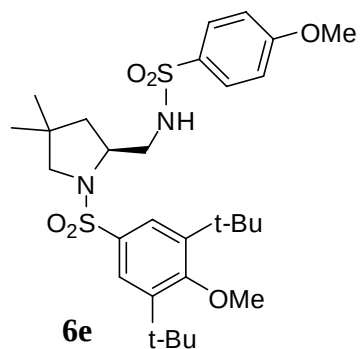
Sample directory:

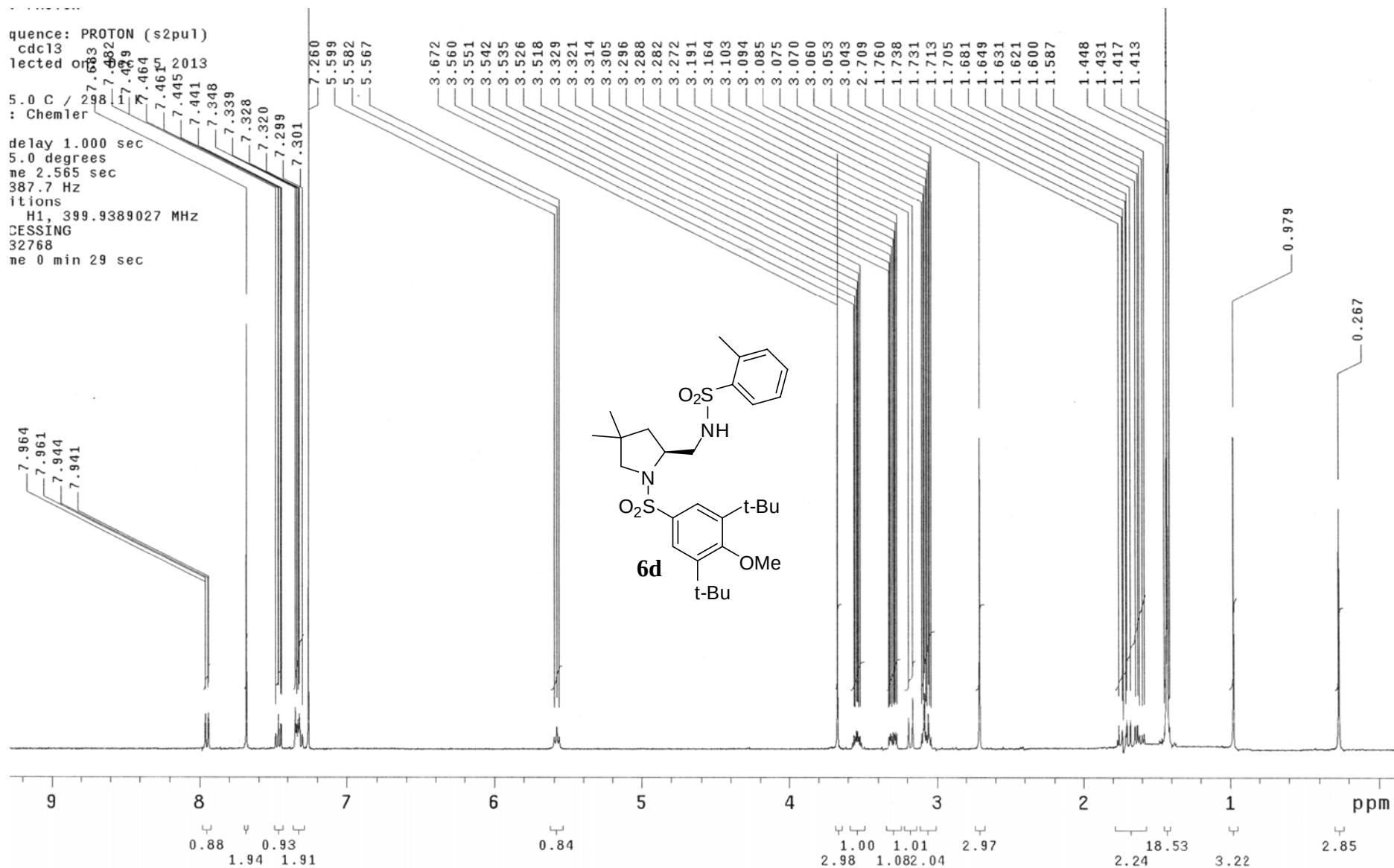
FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Nov 4 2013

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
5792 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 25 hr, 5 min





blt3-rxn719pg139pure1carbon

Sample Name:

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

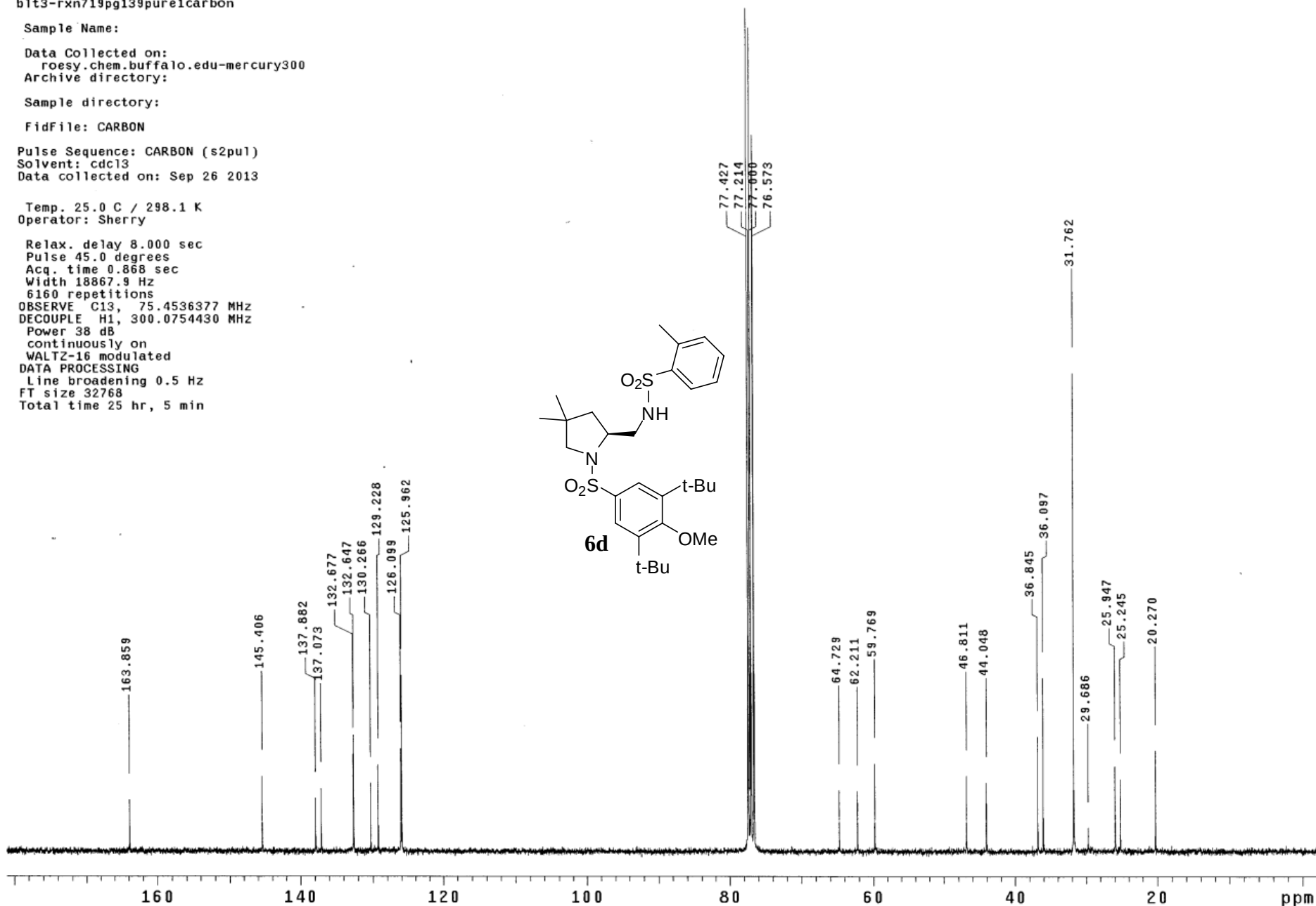
Sample directory:

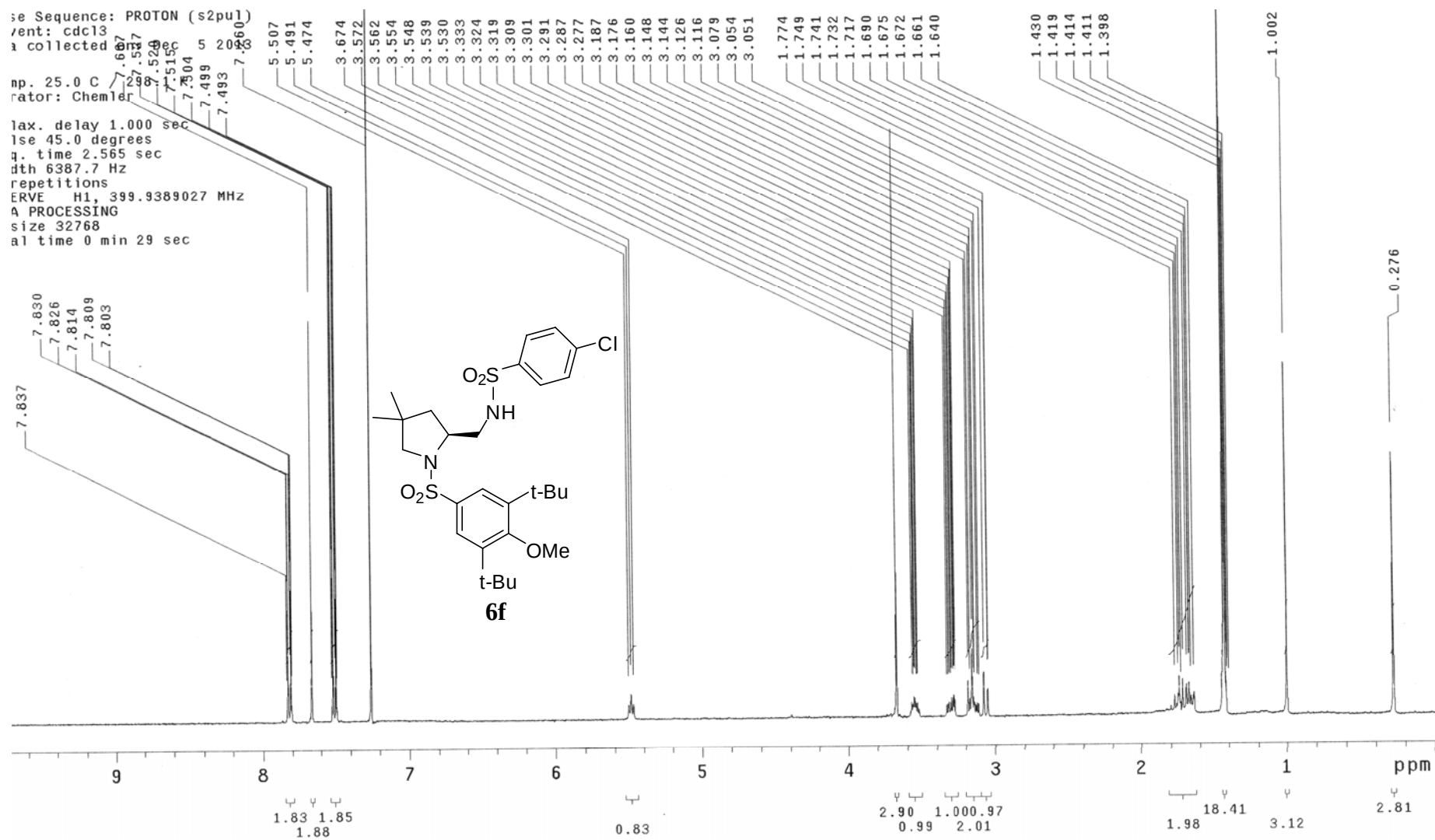
FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Sep 26 2013

Temp. 25.0 C / 298.1 K
Operator: SherryRelax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6160 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 25 hr, 5 min



b1t3-rxn738pg158pure1prep1carbon

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

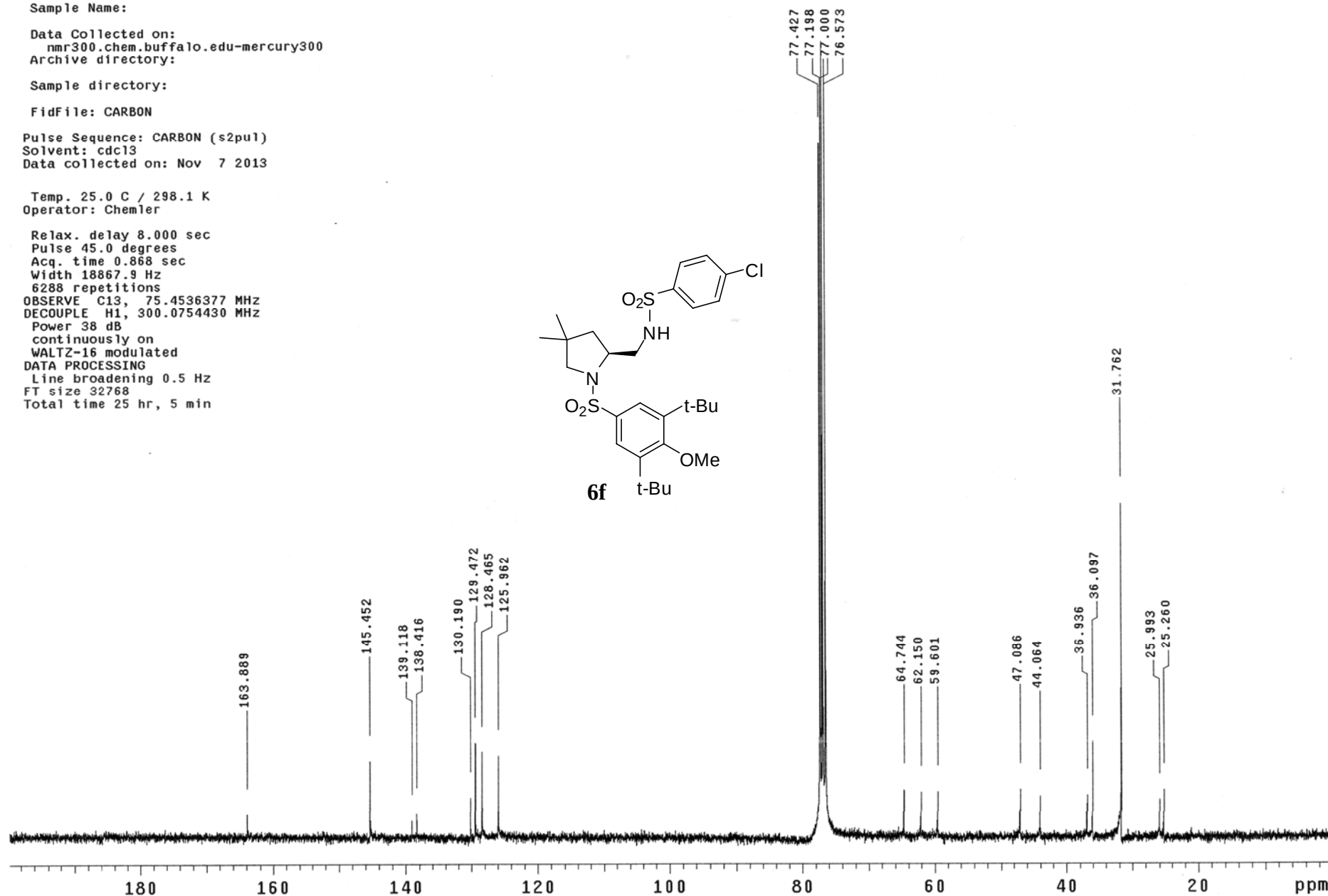
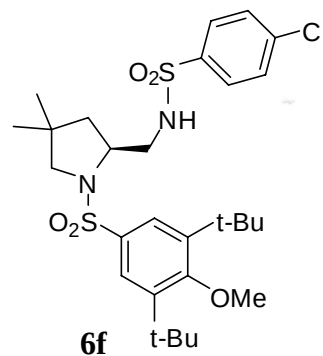
Pulse Sequence: CARBON (s2pu1)

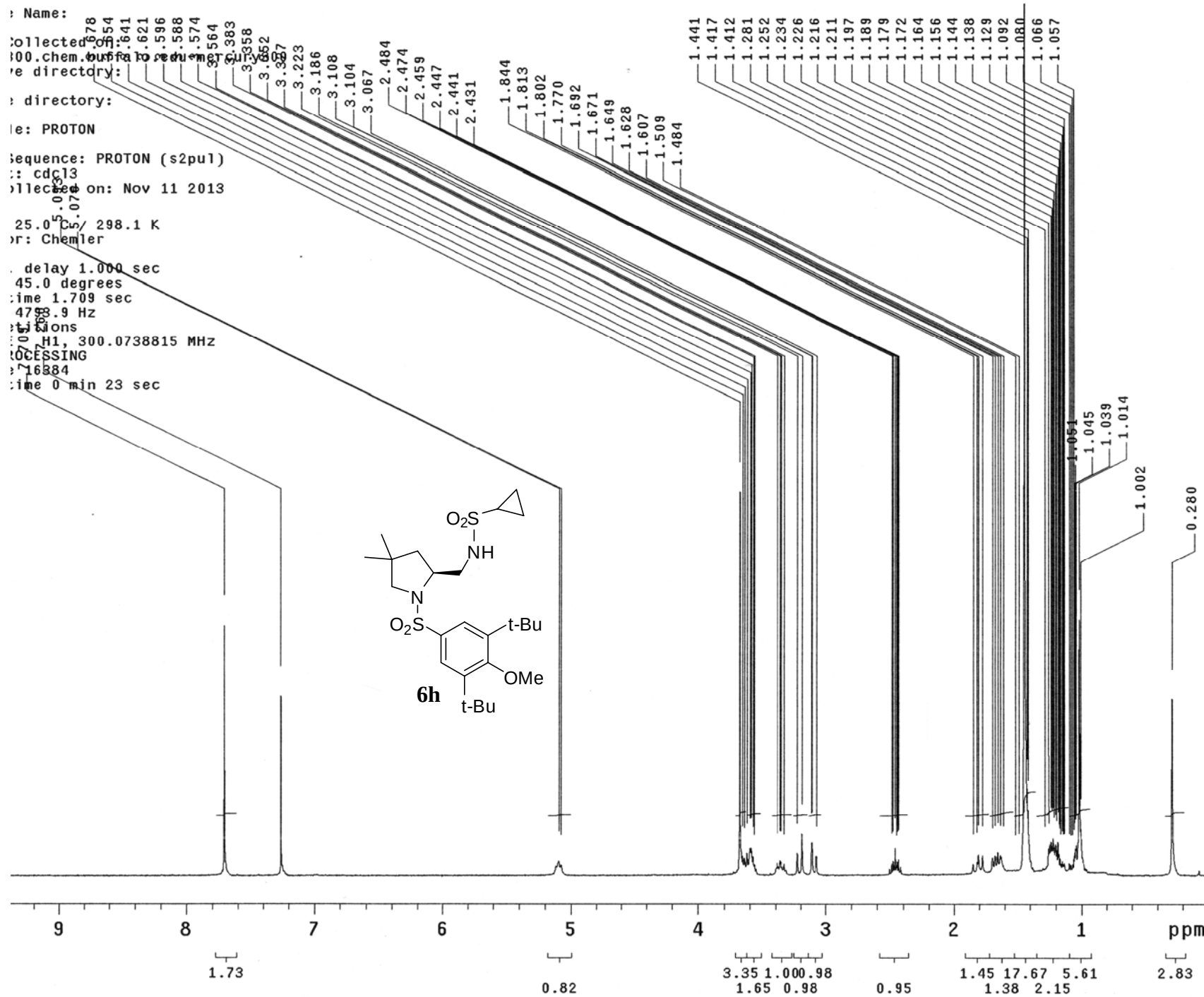
Solvent: cdcl3

Data collected on: Nov 7 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6288 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 25 hr, 5 min





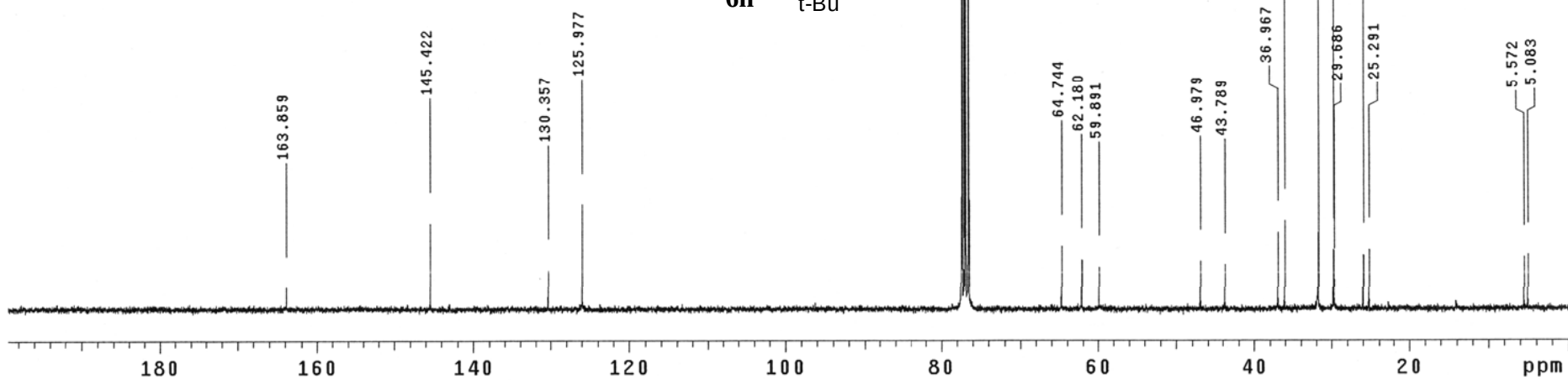
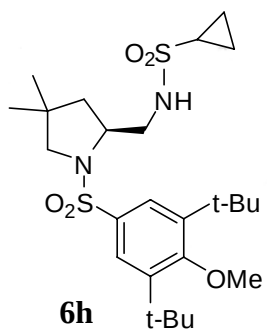
blt3-rxn777pg197pure1carbon

Sample Name:

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

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdcl3
Data collected on: Nov 11 2013Temp. 23.8 C / 296.9 K
Operator: ChemlerRelax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6128 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 25 hr, 5 min

ie:

ected on:
hem.buffalo.edu-mercury300
rectory:

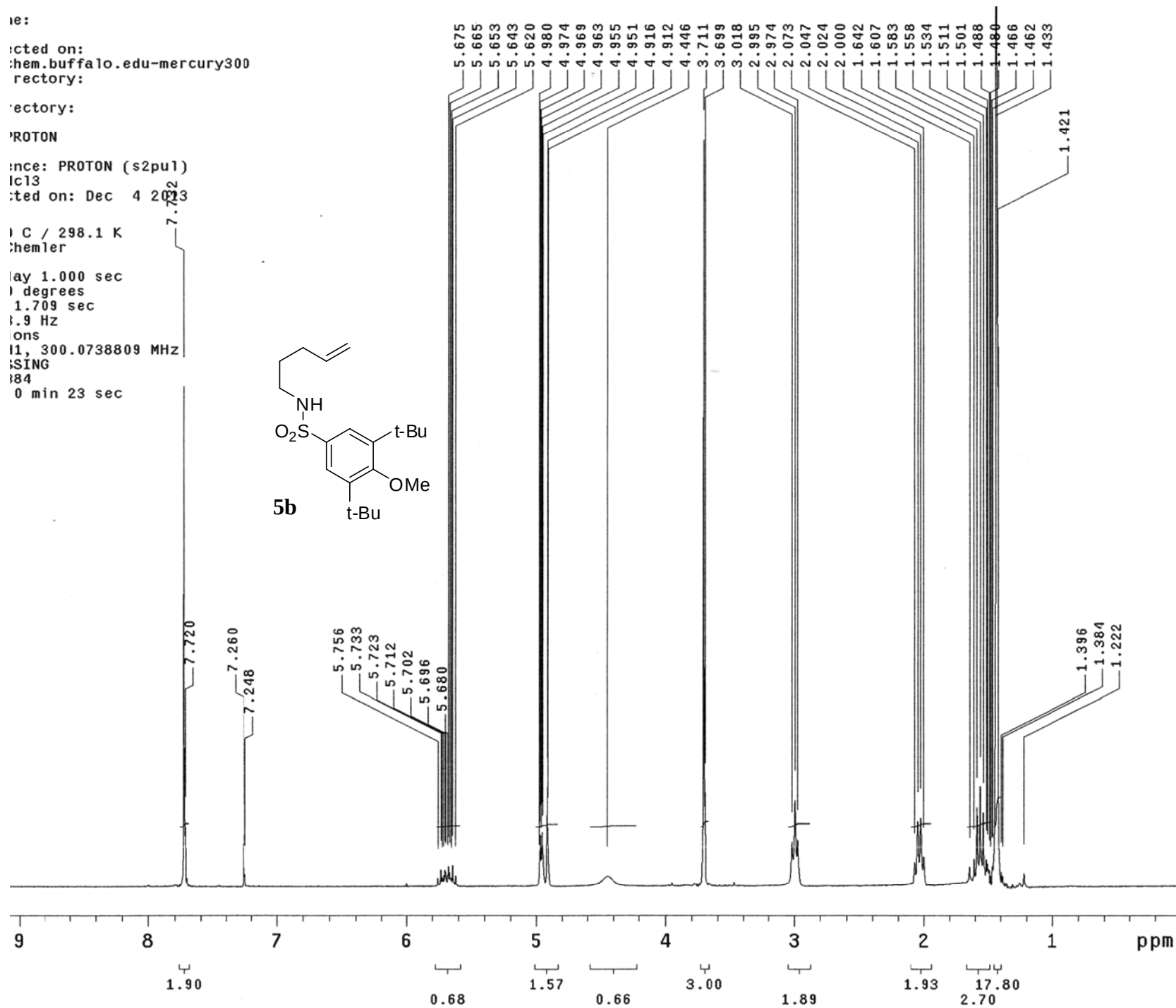
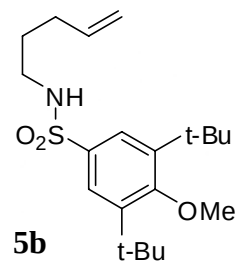
rectory:

PROTON

nce: PROTON (s2pu1)
lc13
ted on: Dec 4 2013

1 C / 298.1 K
hemler

lay 1.000 sec
degrees
1.709 sec
9 Hz
ons
11, 300.0738809 MHz
SING
84
0 min 23 sec



blt3-unsubstituted

Sample Name:

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

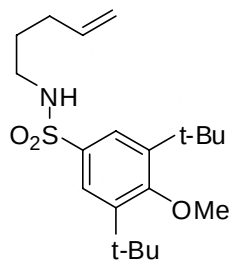
Sample directory:

FidFile: CARBON

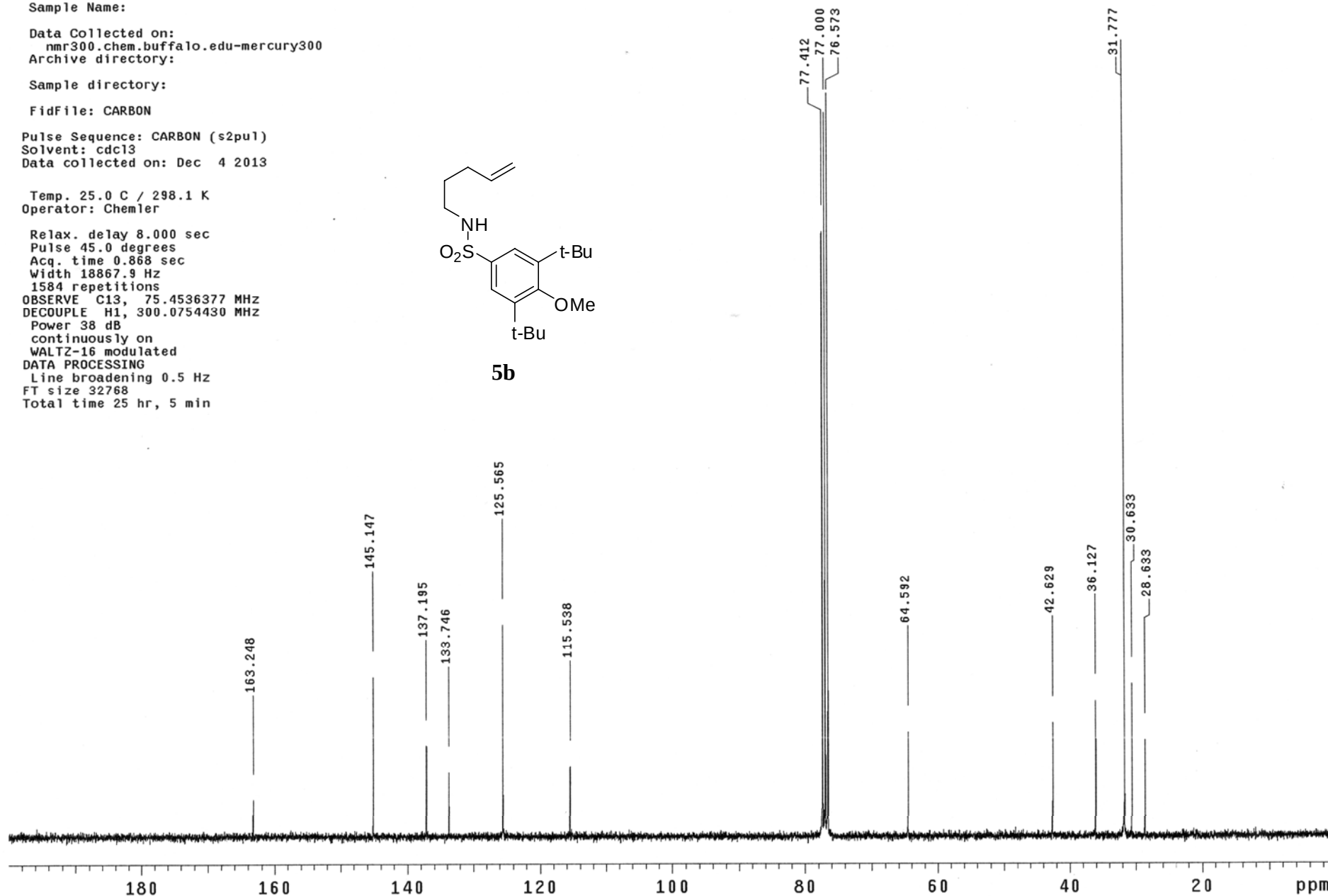
Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 4 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
1584 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 25 hr, 5 min



5b



rxn387pg102pure1

PROTON (s2pu1)

on: Feb 13 2012

298.1 K
er

1.000 sec

rees

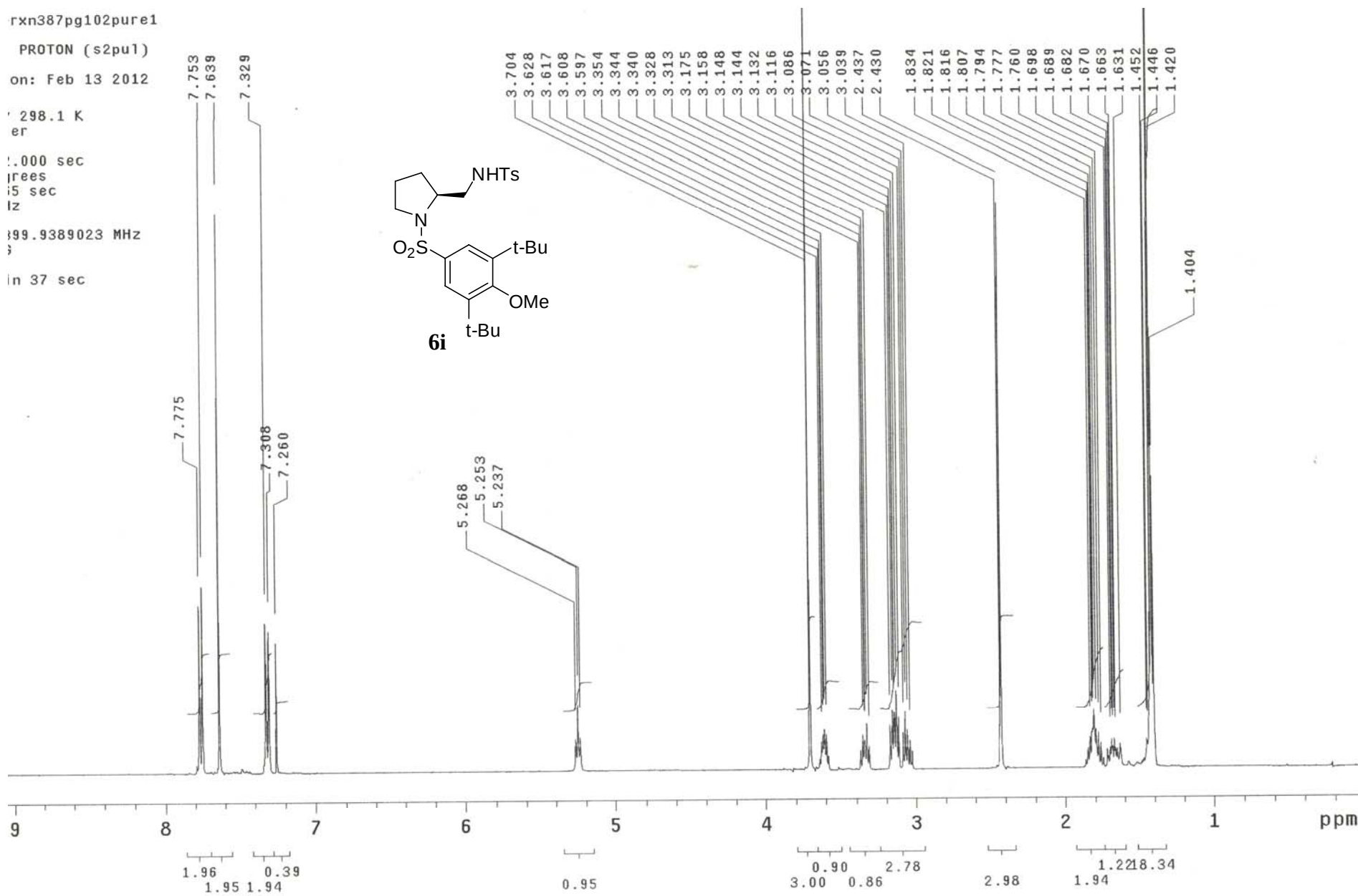
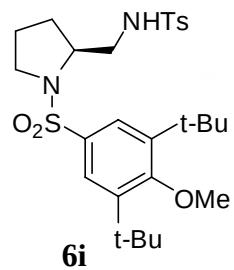
5 sec

12

399.9389023 MHz

3

in 37 sec



blt3-rxn695pg115prep2carbon

Sample Name:

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

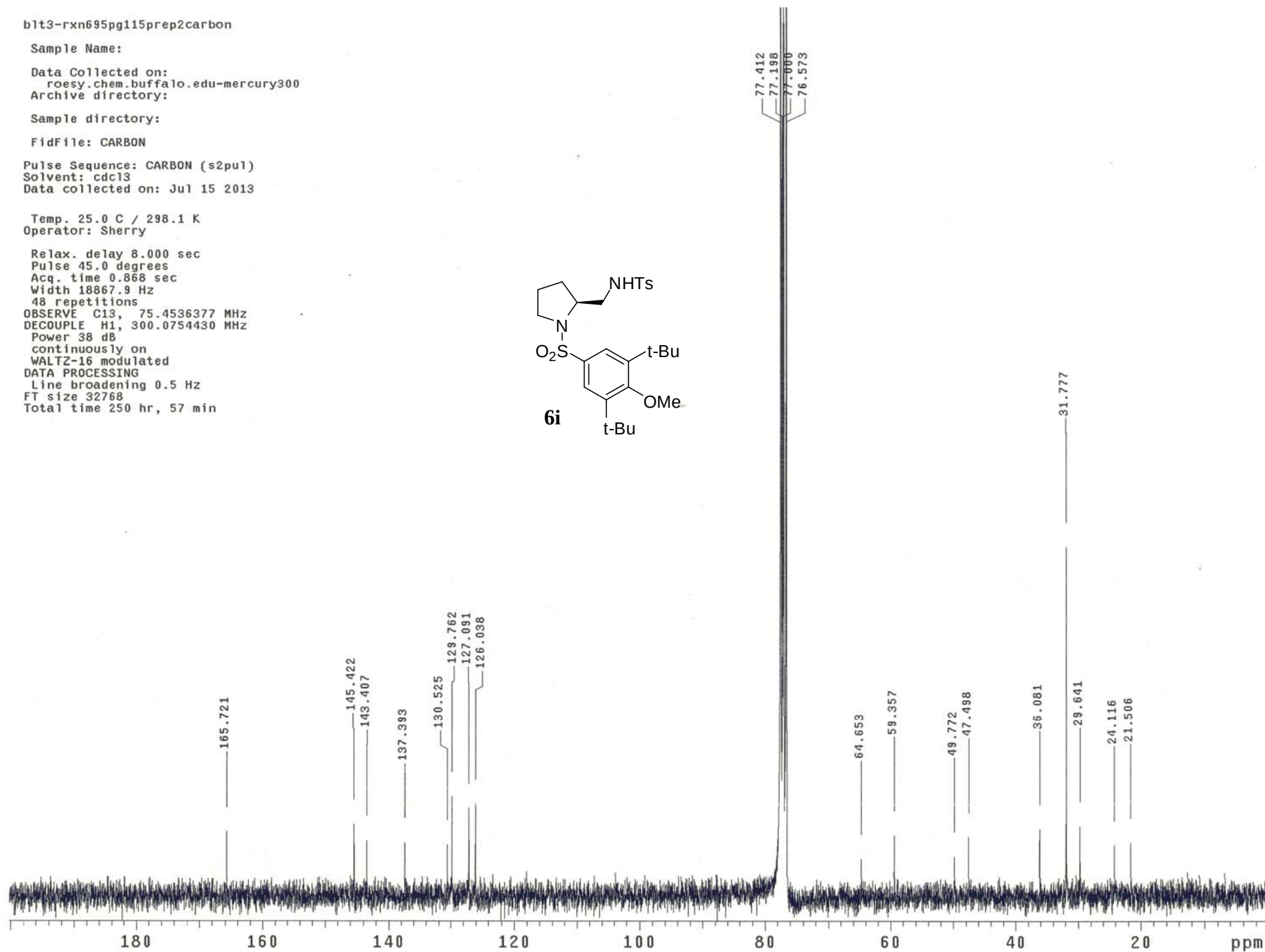
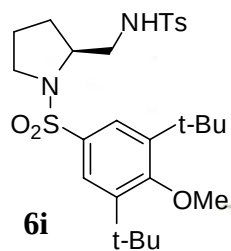
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Jul 15 2013

Temp. 25.0 C / 298.1 K
Operator: Sherry

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
48 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 250 hr, 57 min



::

ted on:
em.buffalo.edu-mercury300
ectory:

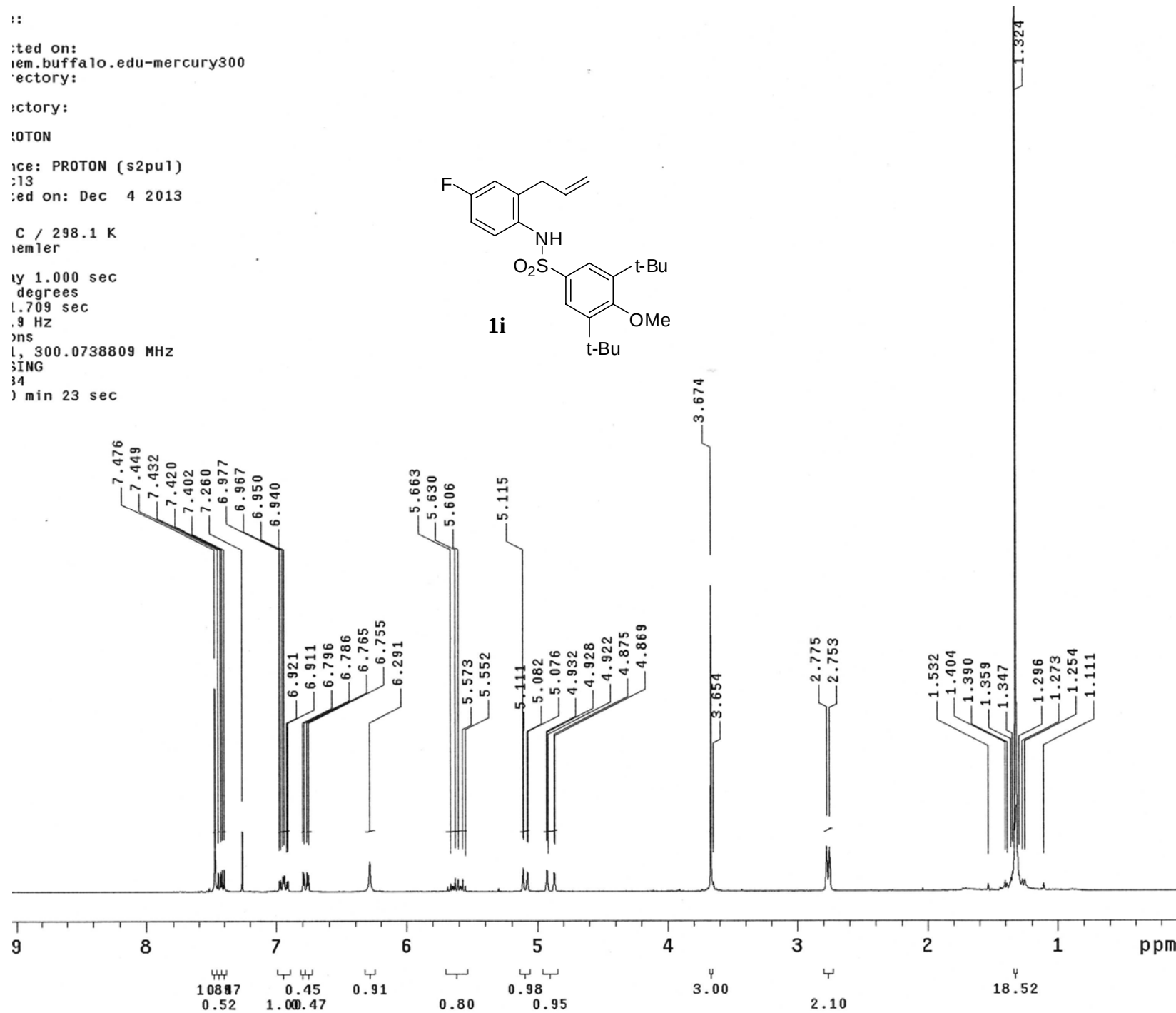
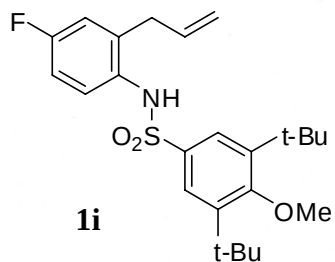
ctory:

OTON

ice: PROTON (s2pu1)
:13
ed on: Dec 4 2013

C / 298.1 K
emler

y 1.000 sec
degrees
1.709 sec
.9 Hz
ns
l, 300.0738809 MHz
SING
4
min 23 sec



blt3-rxn769pg189pure1

Sample Name:

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

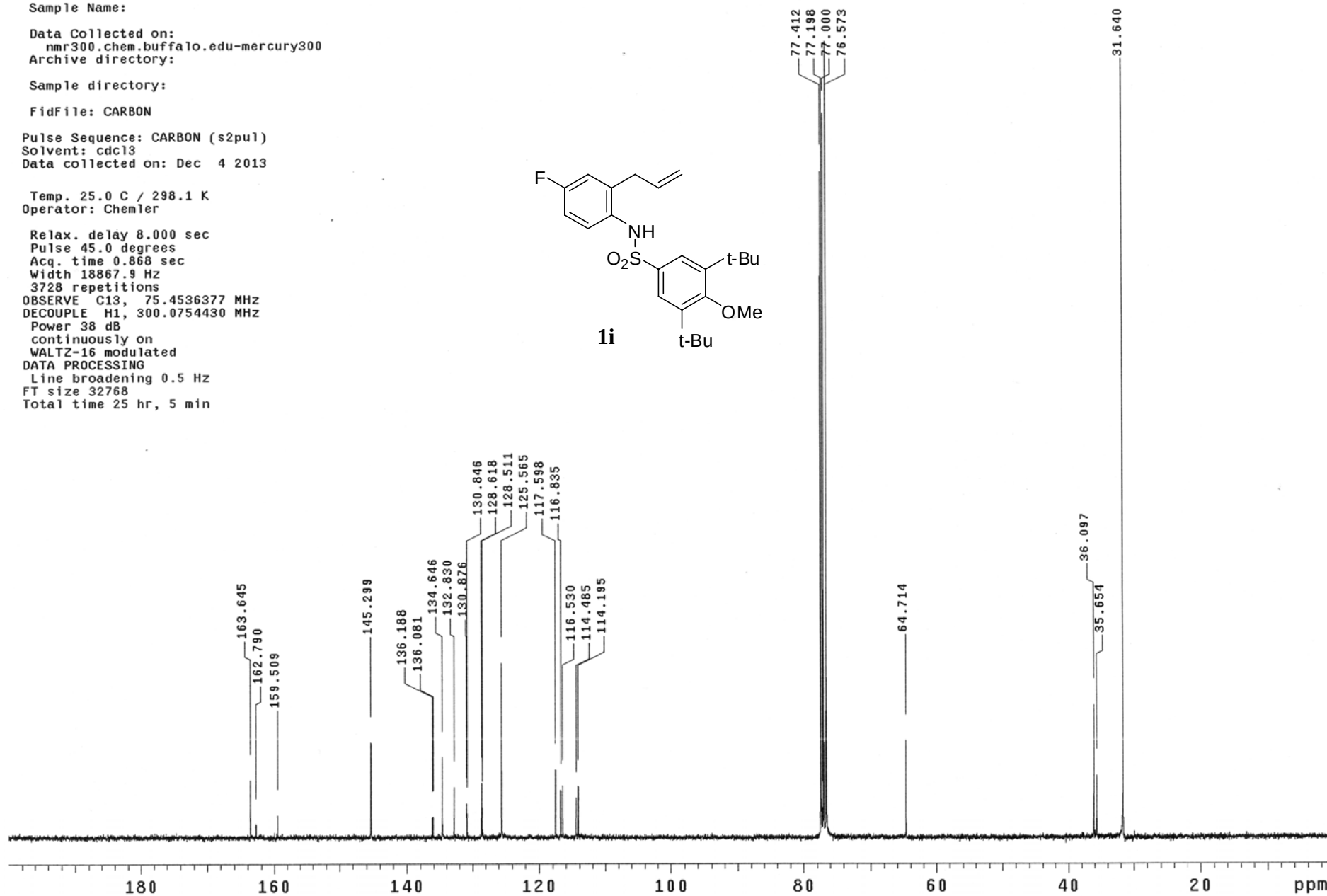
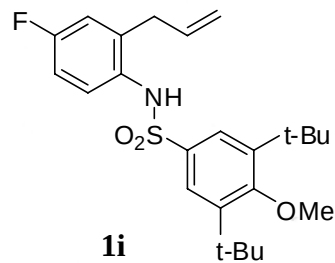
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 4 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3728 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 25 hr, 5 min



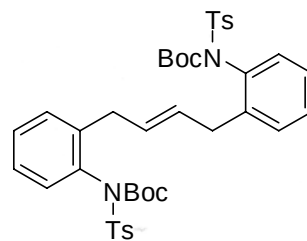
3
e: PROTON (s2pul)
d on: Nov 7 2013

/ 298.1 K
nler

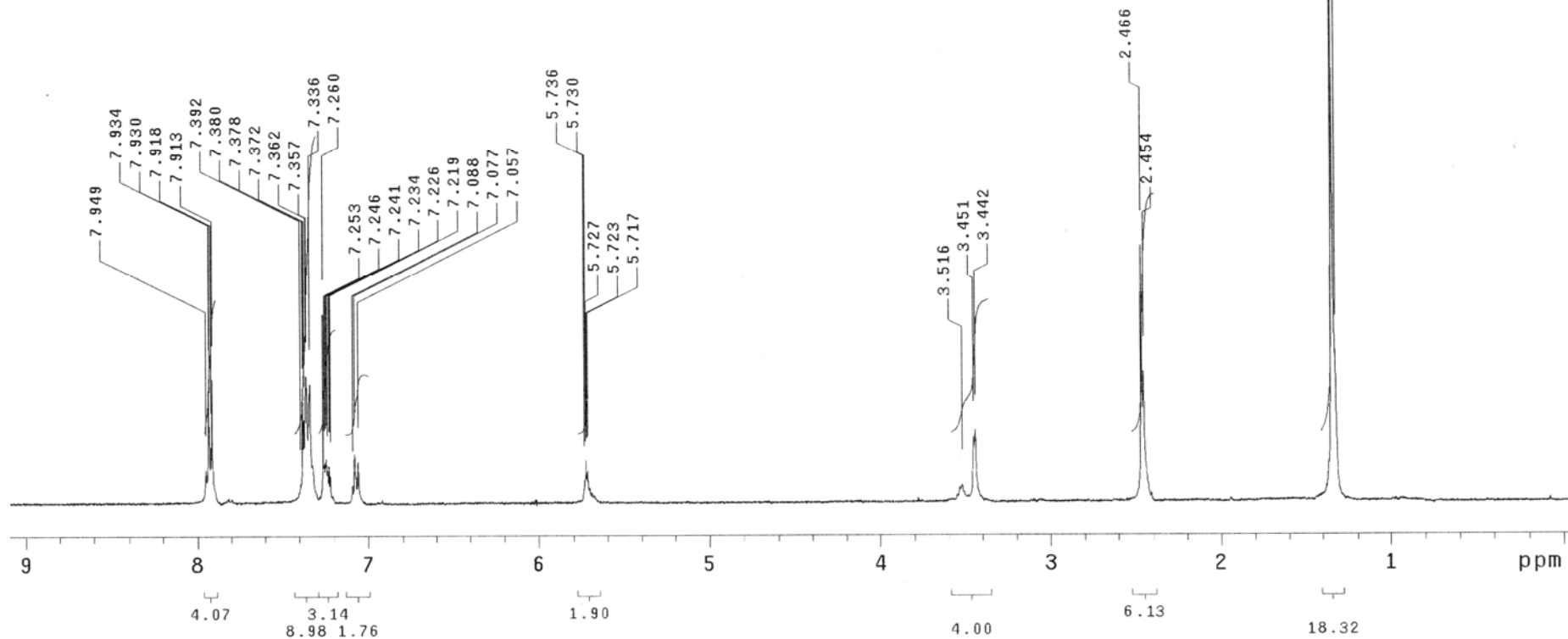
egrees
565 sec
Hz

S
399.9389026 MHz
NG

min 21 sec



15



blt3-rxn784pg204pure3carbon

Sample Name:

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

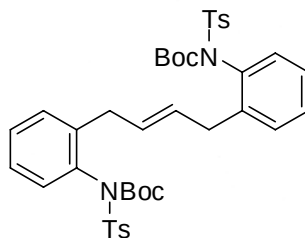
Sample directory:

FidFile: CARBON

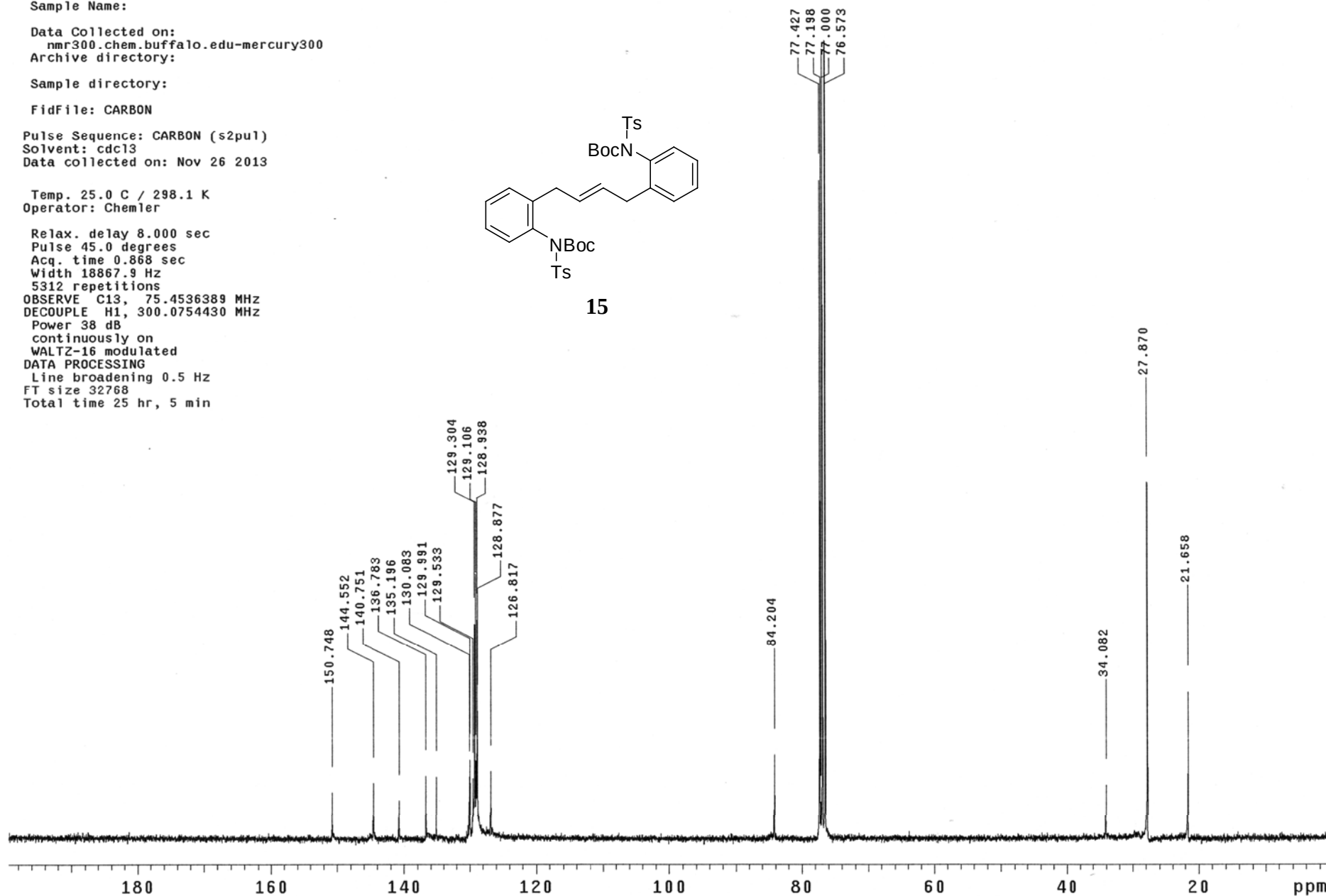
Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Nov 26 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
5312 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 25 hr, 5 min



15



ctory:

OTON

ice: PROTON (s2pu1)

13

ed on: Nov 13 2013

C / 298.1 K

emler

y 1.000 sec

degrees

.709 sec

9 Hz

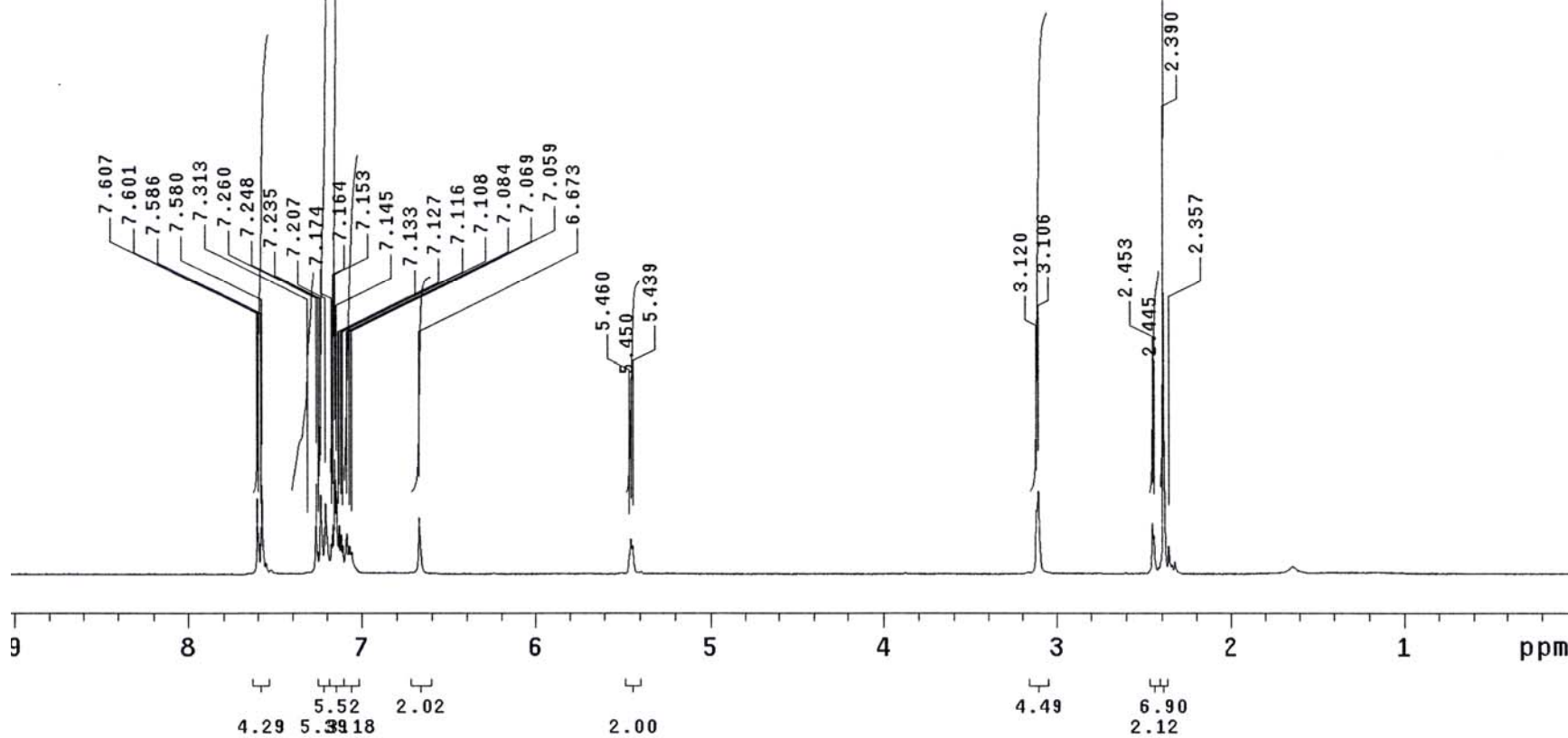
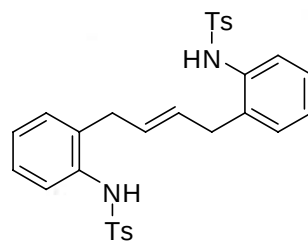
ns

, 300.0738809 MHz

ING

4

min 23 sec



blt3-rxn791pg211pure1

Sample Name:

Data Collected on:

nmr300.chem.buffalo.edu-mercury300

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)

Solvent: cdc13

Data collected on: Dec 9 2013

Temp. 25.0 C / 298.1 K

Operator: Chemler

Relax. delay 8.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

5472 repetitions

OBSERVE C13, 75.4536377 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuously on

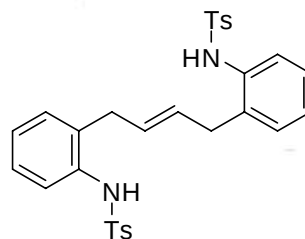
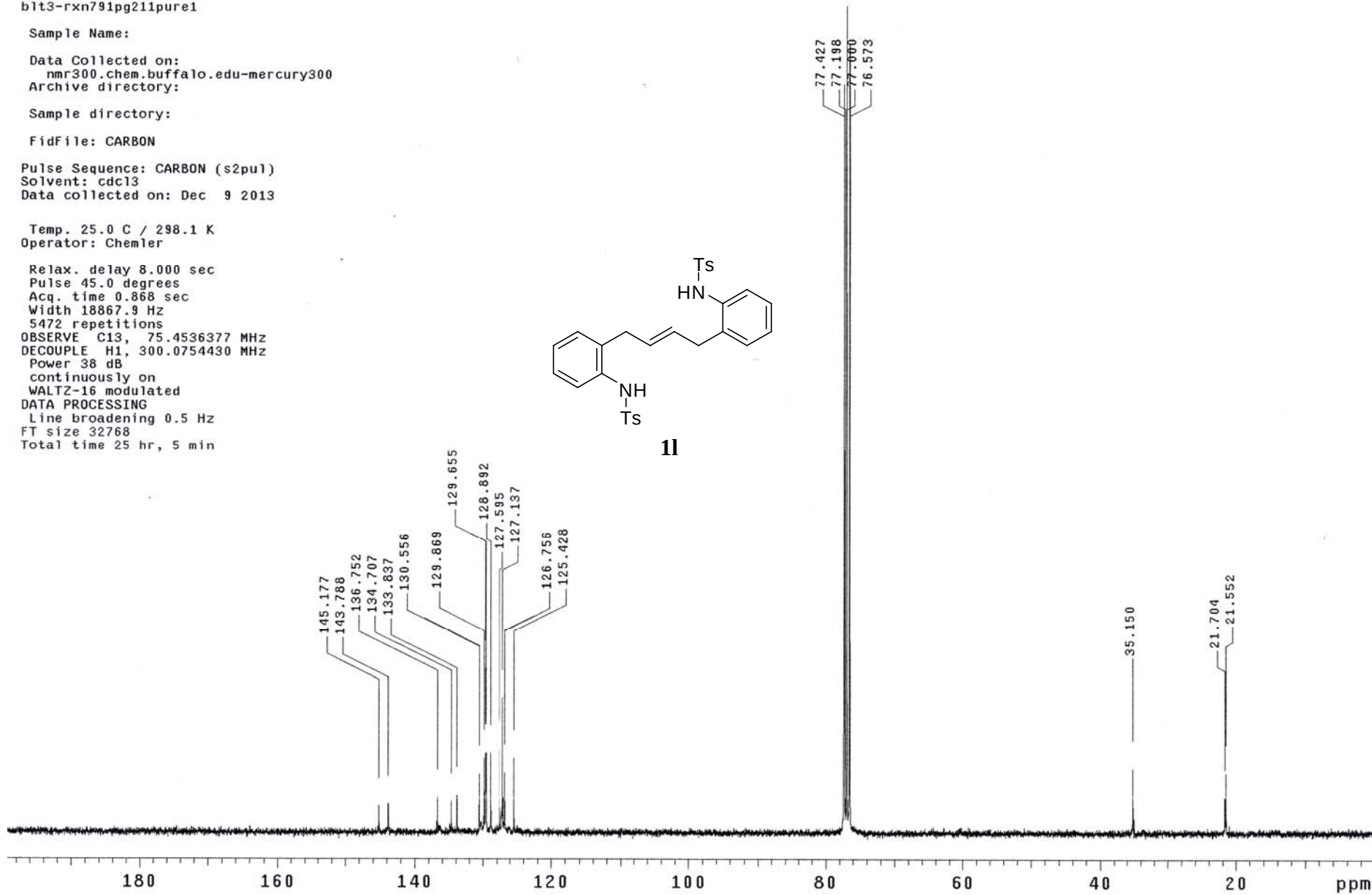
WALTZ-16 modulated

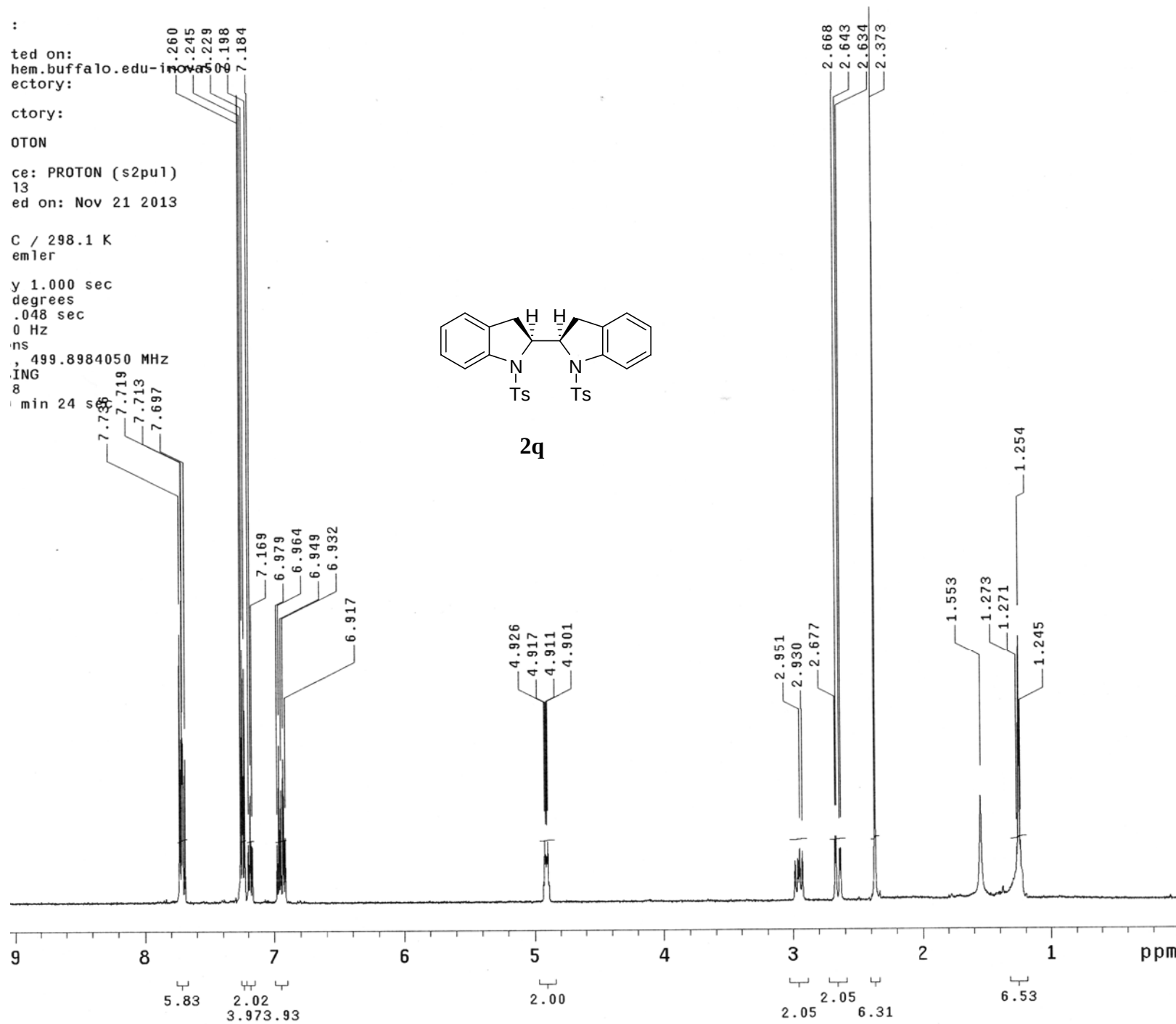
DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 25 hr, 5 min

**11**



blt3-rxn782pg202pure1

Sample Name:

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

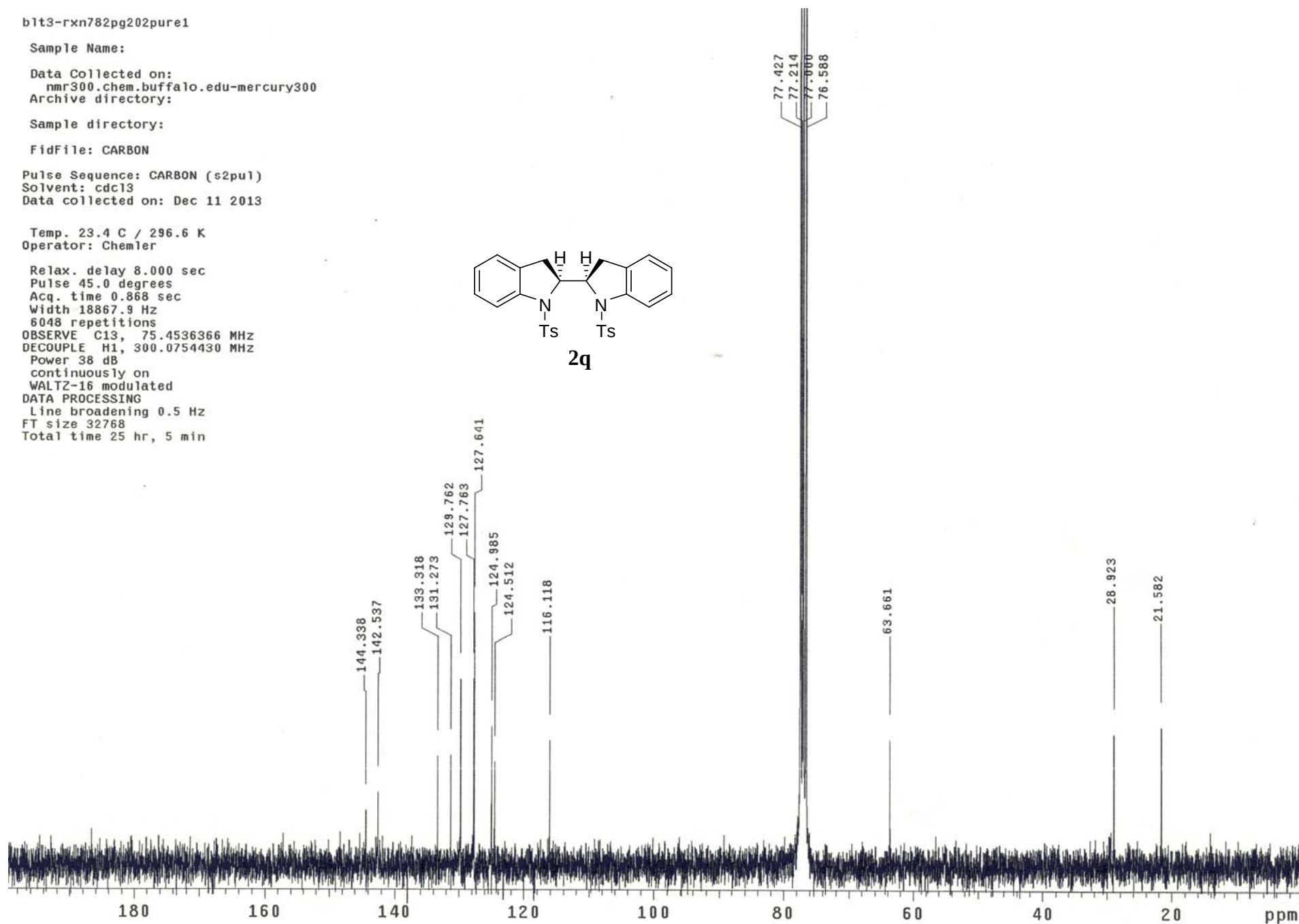
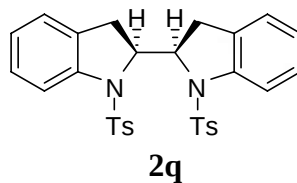
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 11 2013

Temp. 23.4 C / 296.6 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
6048 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 25 hr, 5 min



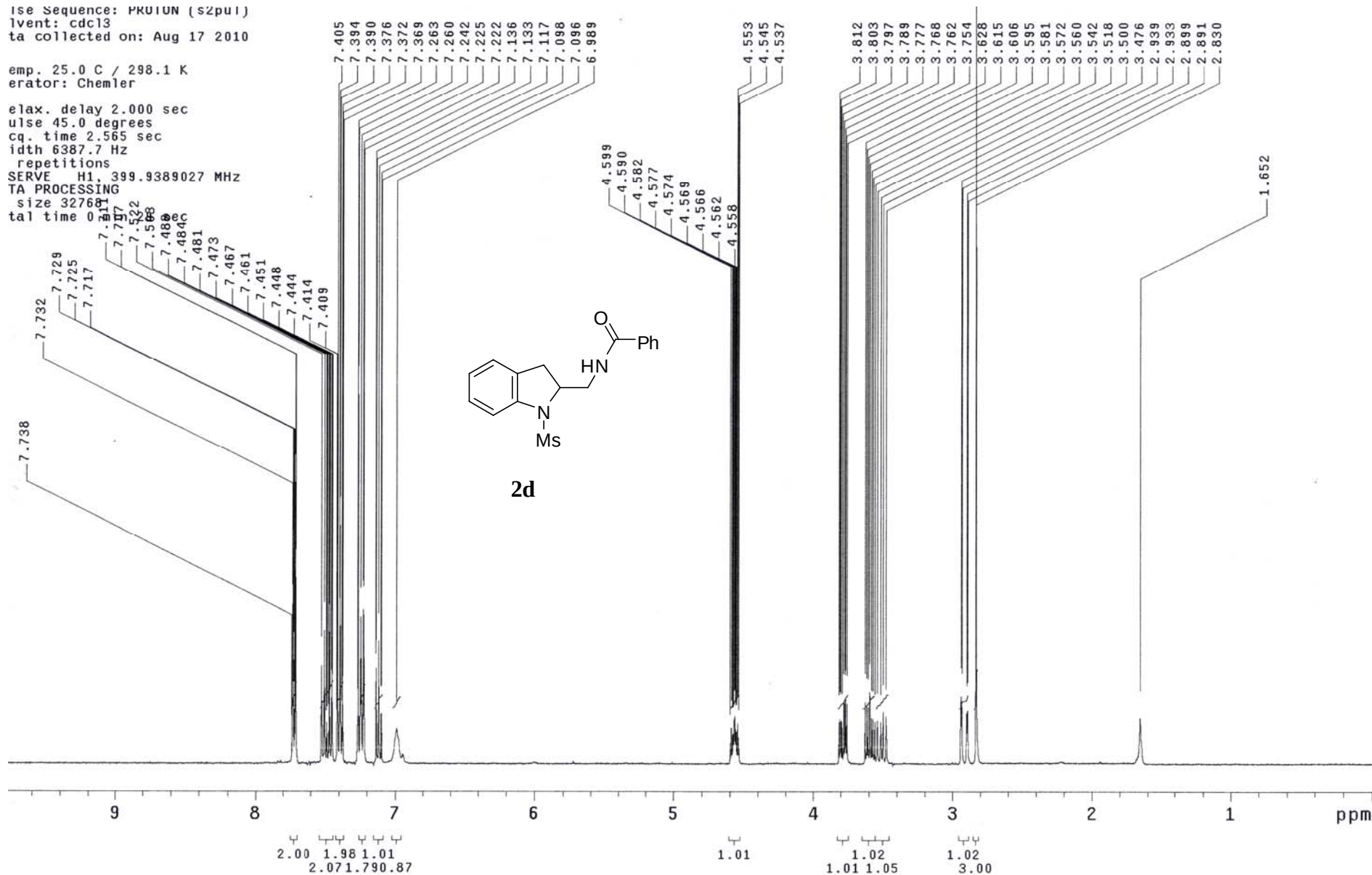
use Sequence: PRUION (s2pul)
lvent: cdcl3
ta collected on: Aug 17 2010

emp. 25.0 C / 298.1 K
erator: Chemler

elax. delay 2.000 sec
ulse 45.0 degrees
cq. time 2.565 sec
idth 6387.7 Hz
repetitions

SERVE H1, 399.9389027 MHz
TA PROCESSING

size 32768
tal time 0.61



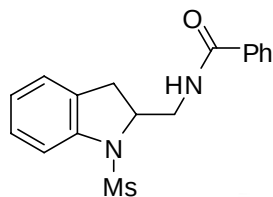
blt1-rxn191pg200CNMR

Sample Name:

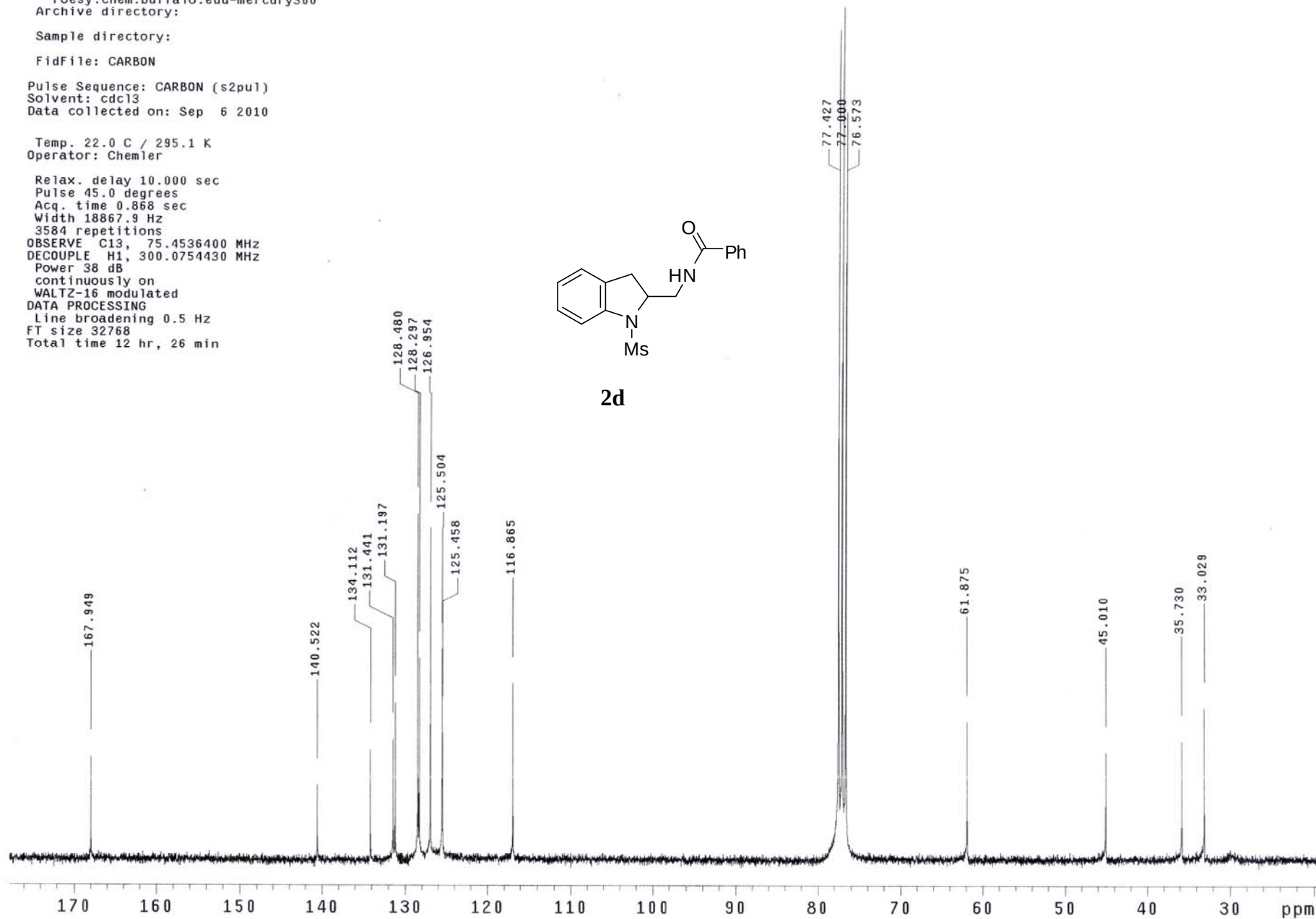
Data Collected on:
roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Sep 6 2010Temp. 22.0 C / 295.1 K
Operator: ChemlerRelax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
3584 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 12 hr, 26 min

2d



Sample Name:

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

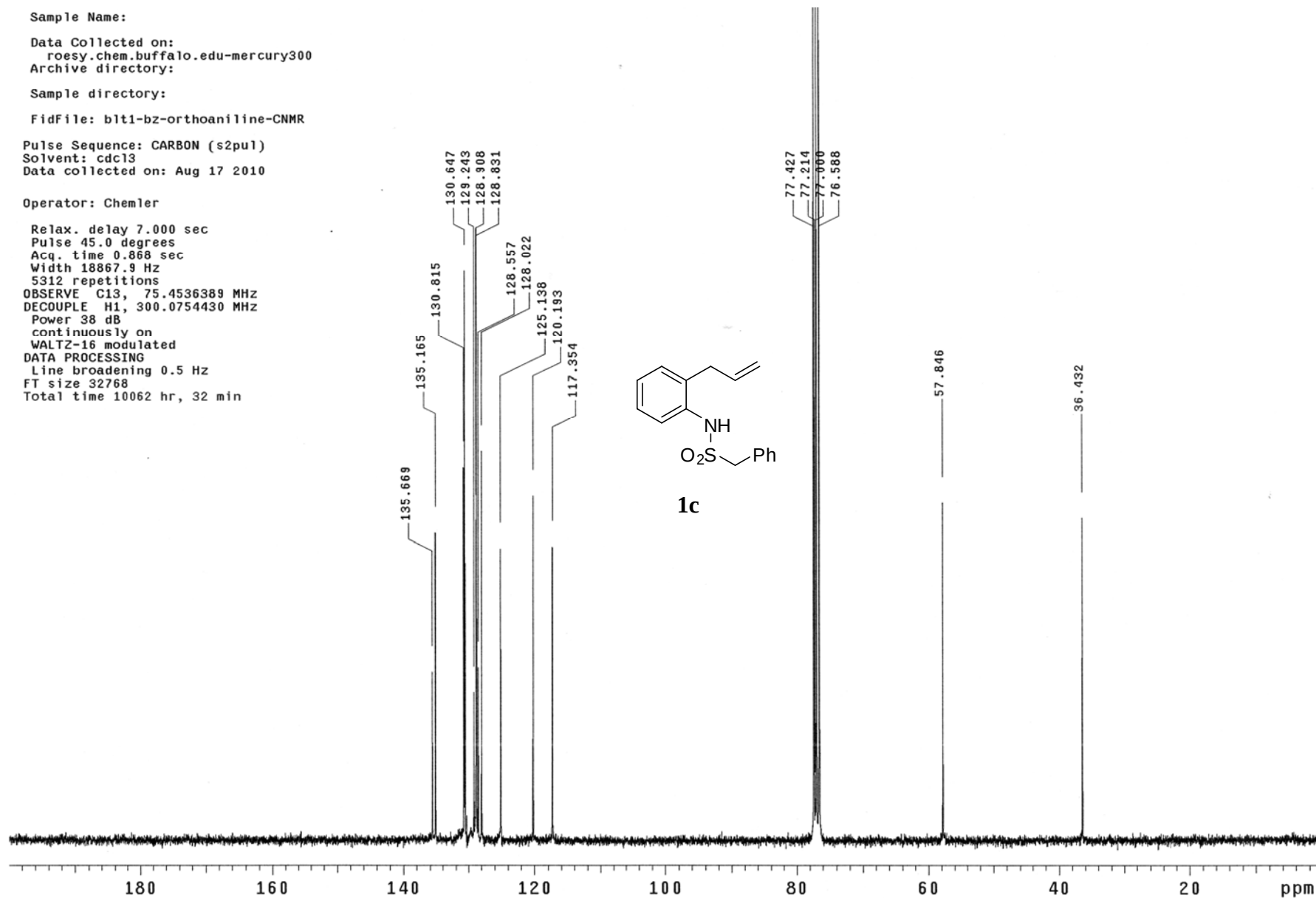
Sample directory:

FidFile: blt1-bz-orthoaniline-CNMR

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

Operator: Chemler

Relax. delay 7.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
5312 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 10062 hr, 32 min

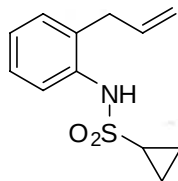
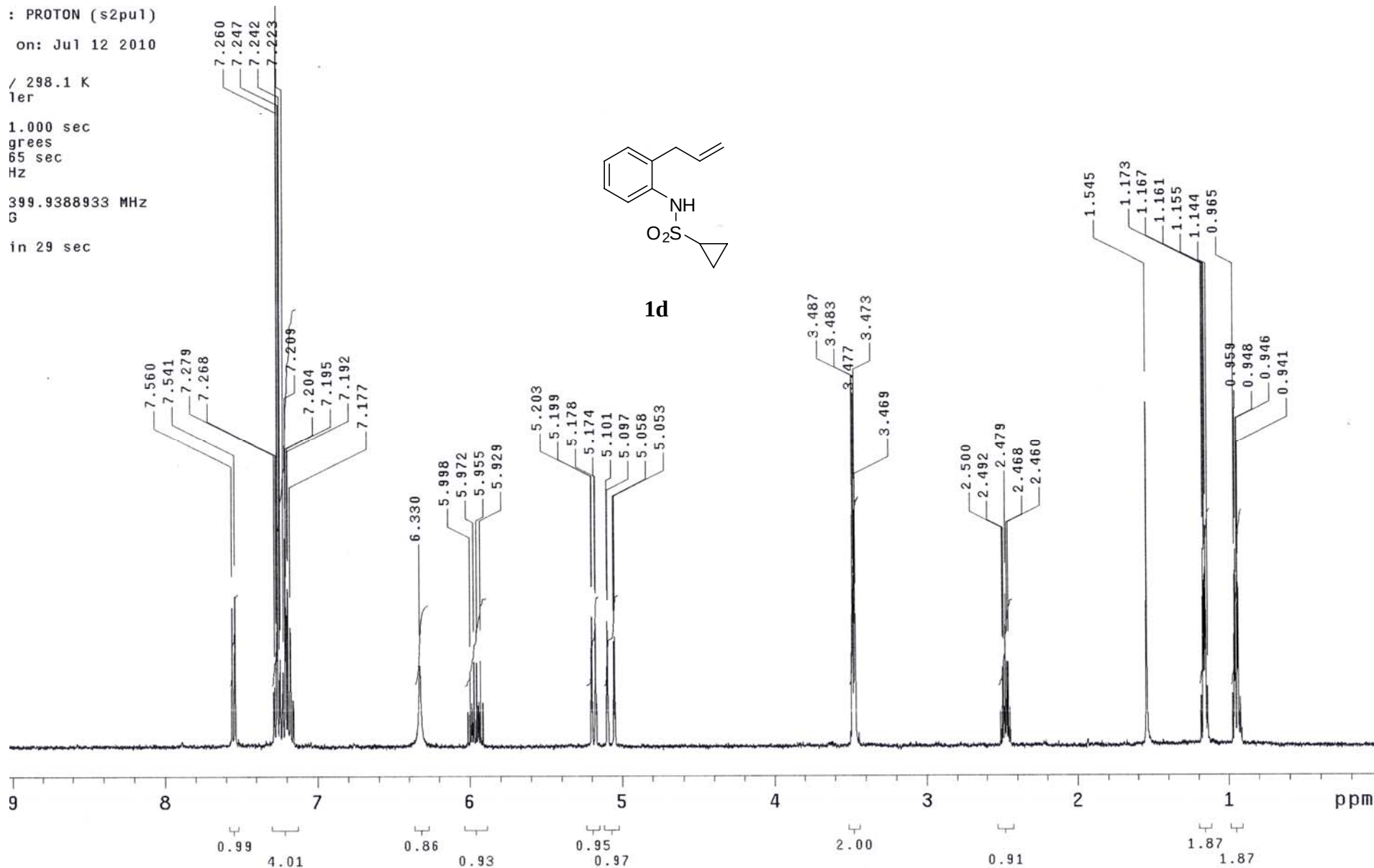


: PROTON (s2pu1)

on: Jul 12 2010

/ 298.1 K
1er1.000 sec
grees
65 sec
Hz399.9388933 MHz
G

in 29 sec

**1d**

roesy.chem.buffalo.edu-mercury300
Archive directory:

Sample directory:

FidFile: ass

Pulse Sequence: CARBON (s2pul)

Solvent: cdcl3

Data collected on Apr 27 2010

Operator: Chemler

Relax. delay 10.000

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

4096 repetitions

OBSERVE C13, 75.4536375 MHz

DECOUPLE H1, 300.0754430 MHz

Power 38 dB

continuous on

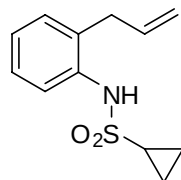
WALTZ-16 modulated

DATA PROCESSING

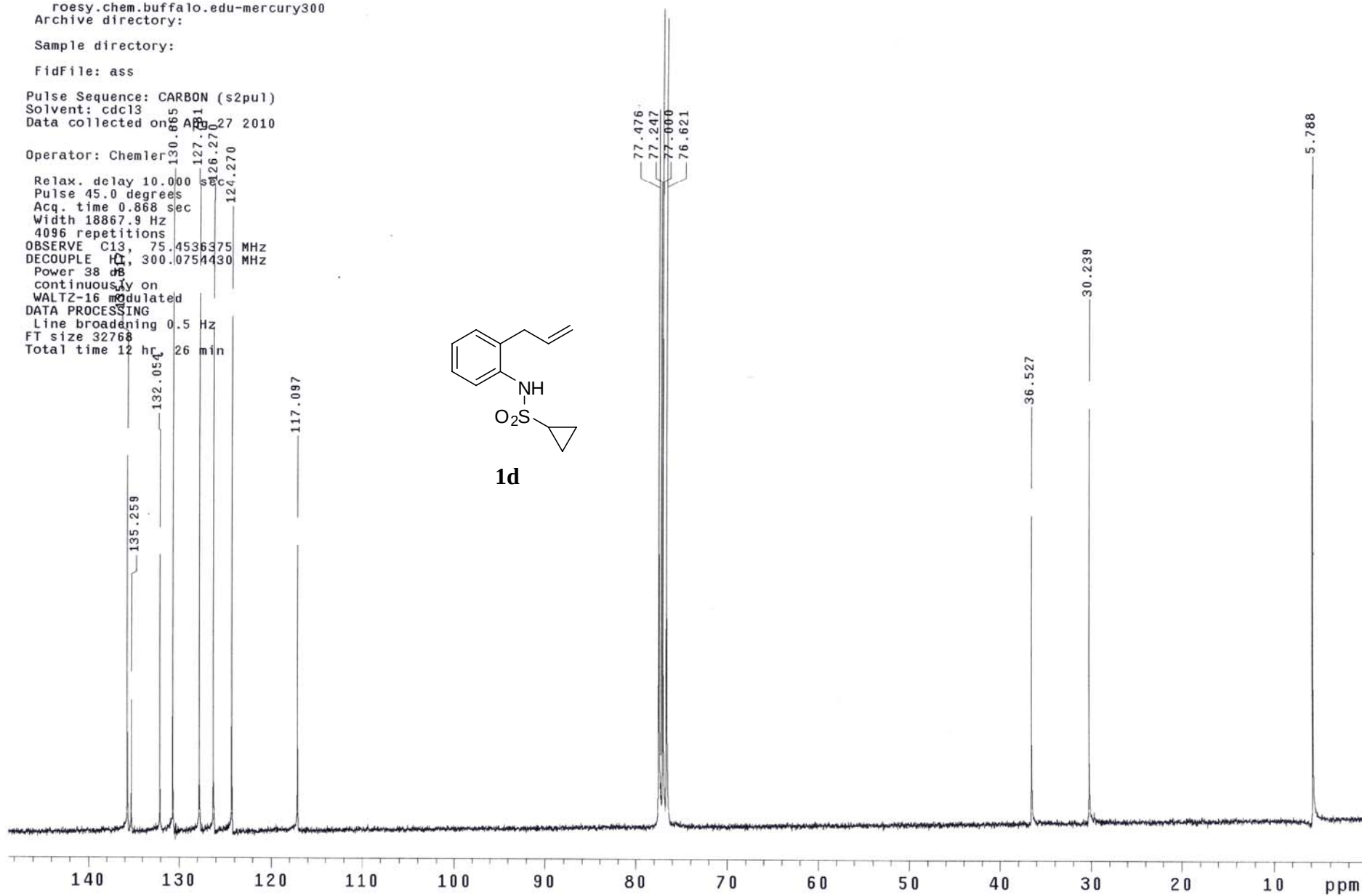
Line broadening 0.5 Hz

FT size 32768

Total time 12 hr 26 min



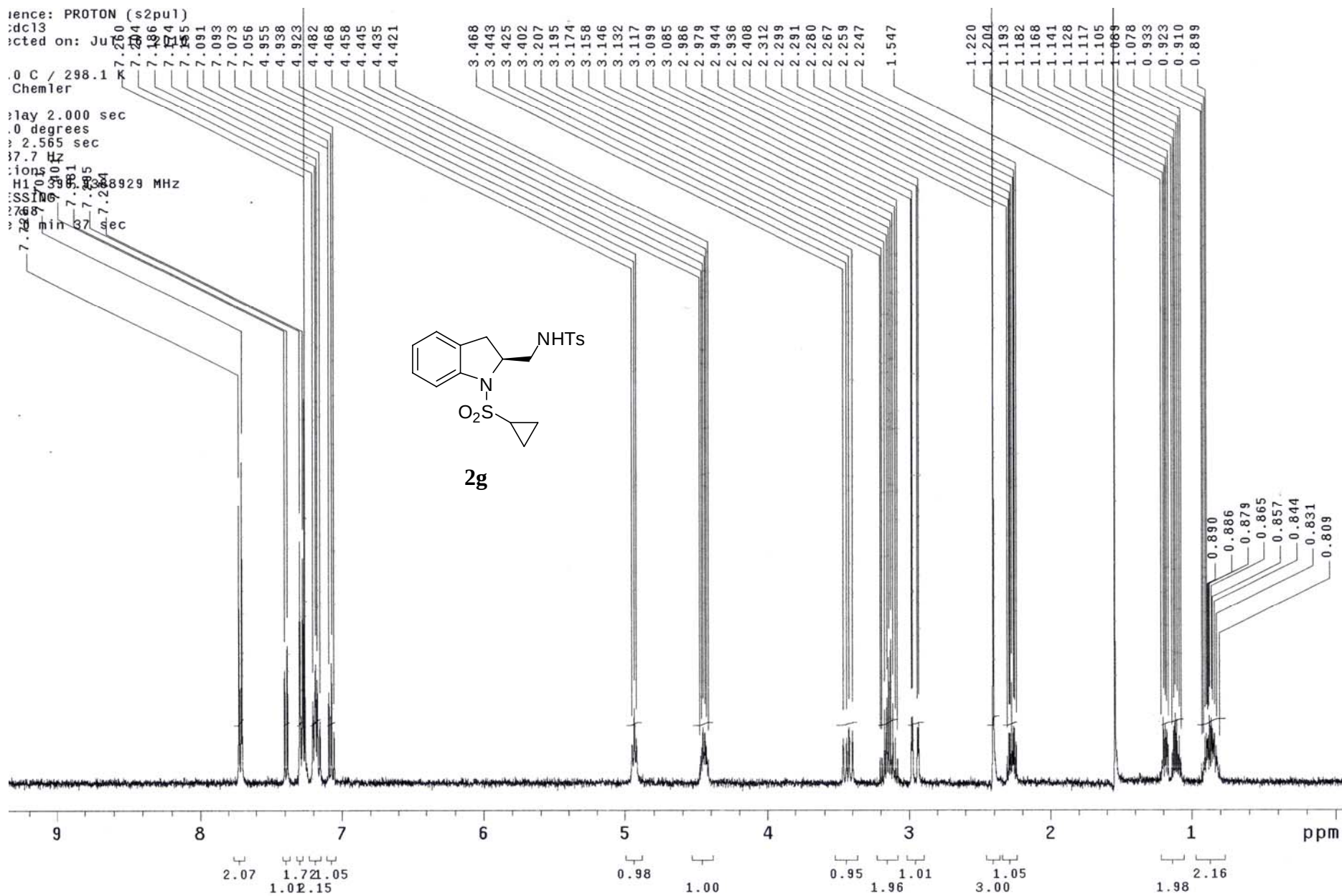
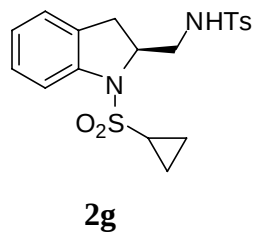
1d



```

play 2.000 sec
0 degrees
2.565 sec
37.7 Hz
ions
H1 0.3951
SSING 7.738929 MHZ
2768 7.738929
2 min 37 sec

```



b1t1-rxn172pg181CNMR

Sample Name:

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

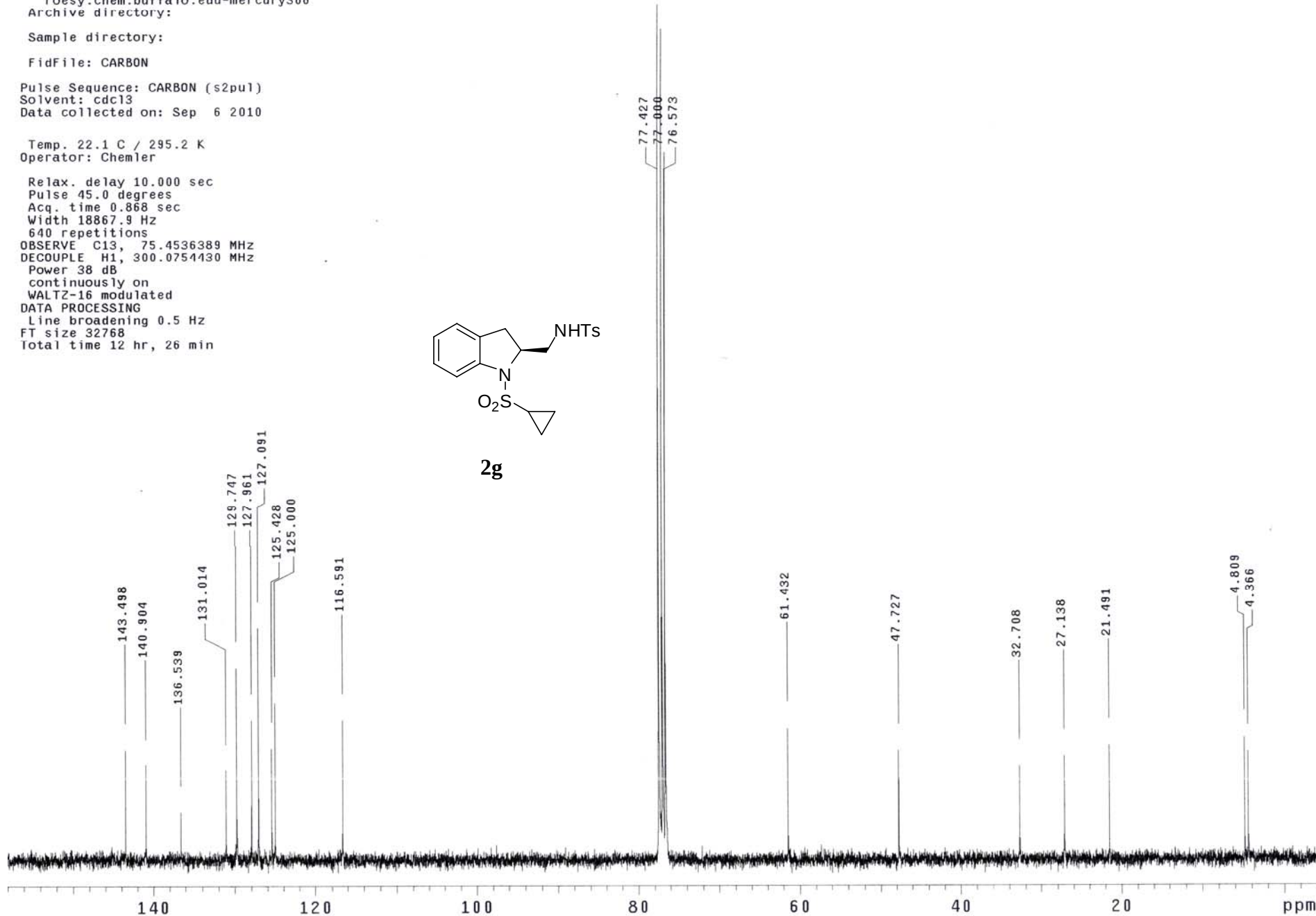
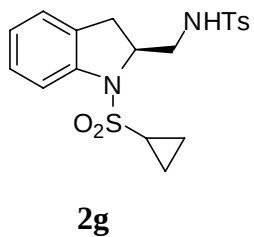
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Sep 6 2010

Temp. 22.1 C / 295.2 K
Operator: Chemler

Relax. delay 10.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
640 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 12 hr, 26 min

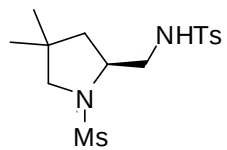
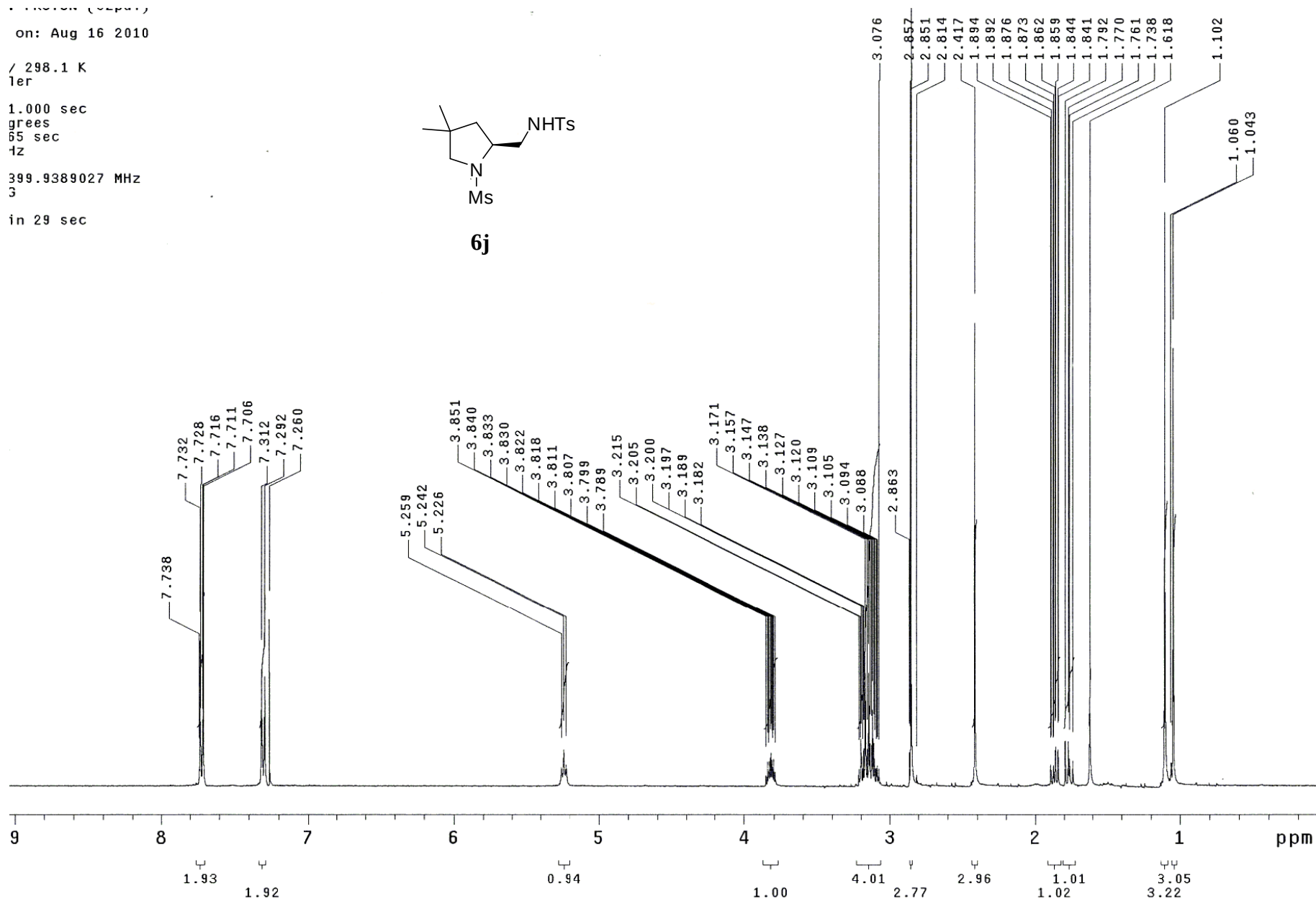


1H NMR (CDCl3)

Date: Aug 16 2010

/ 298.1 K
1er1.000 sec
grees
65 sec
42399.9389027 MHz
3

in 29 sec

**6j**

blt1-rxn185pg194prepcarbon

Sample Name:

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

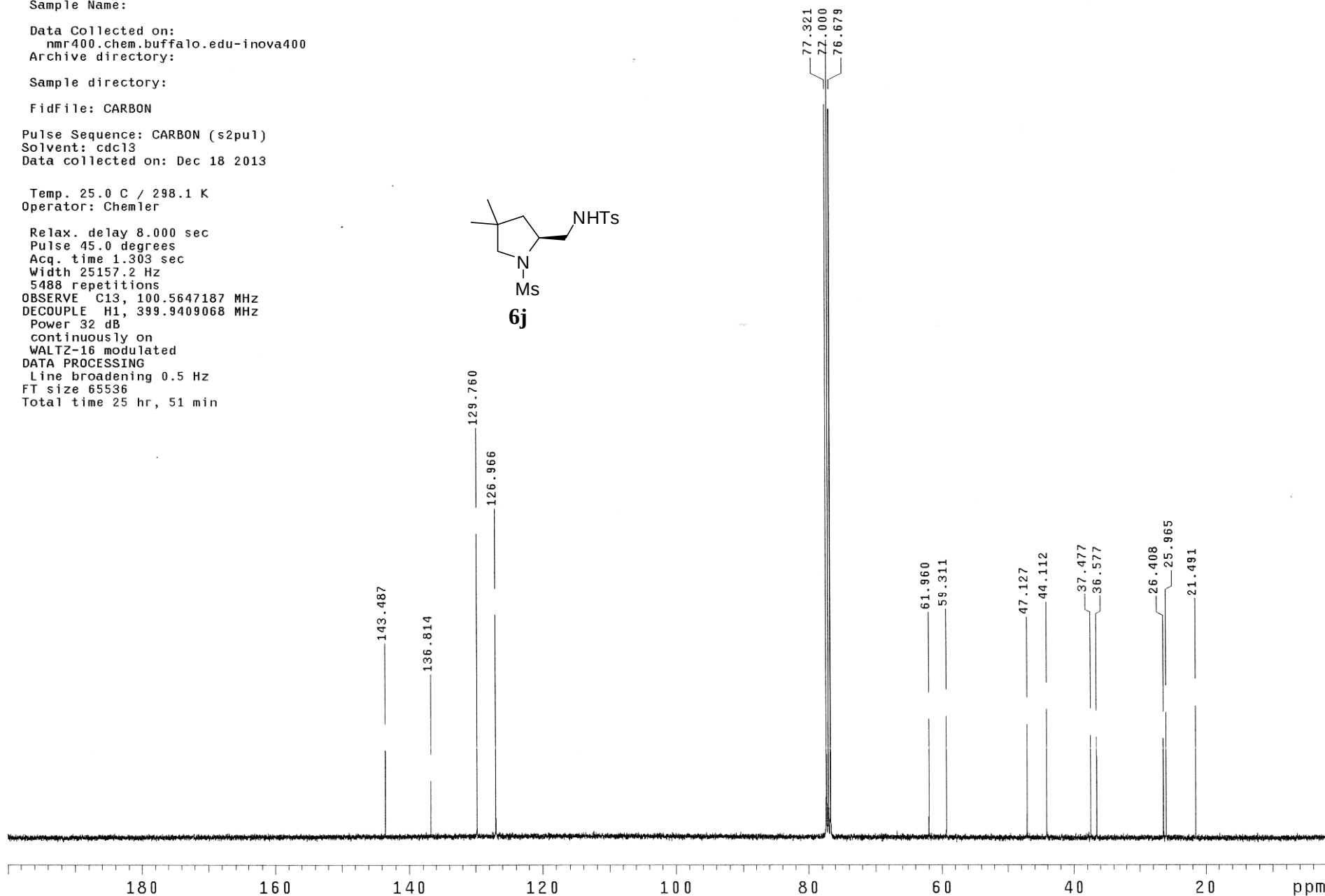
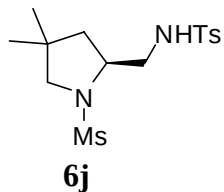
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 18 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
5488 repetitions
OBSERVE C13, 100.5647187 MHz
DECOUPLE H1, 399.9409068 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 25 hr, 51 min



ed on:
.chem.buffalo.edu-inova400
ctory:

tory:

TON

e: PROTON (s2pul)

3

d on: Dec 20 2012

/ 298.1 K
mler

1.000 sec

egrees

565 sec

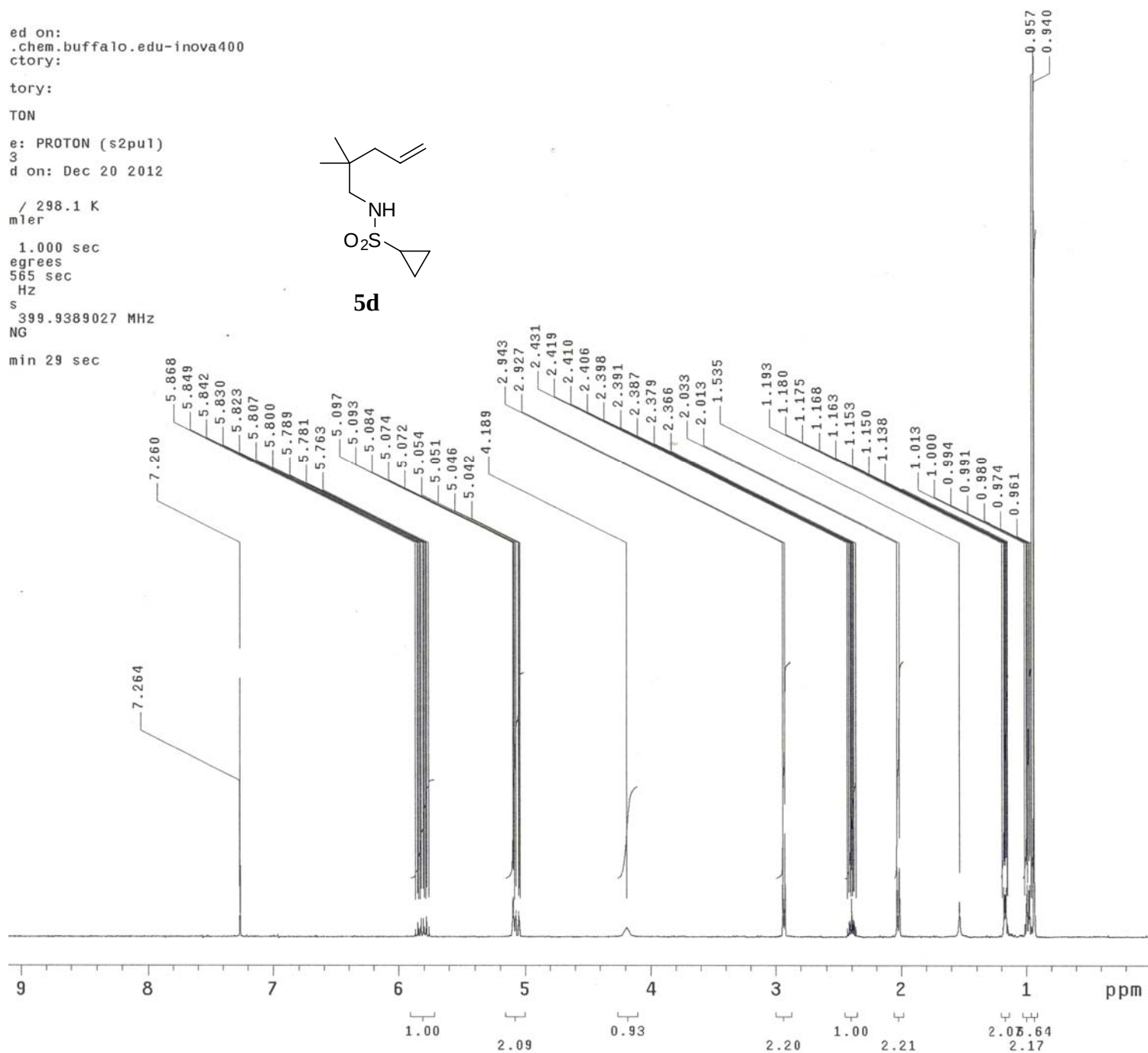
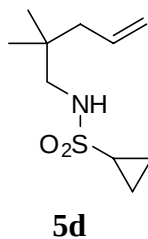
Hz

s

399.9389027 MHz

NG

min 29 sec



blt2-rxn568pg283pure1

Sample Name:

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

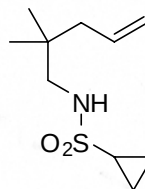
Sample directory:

FidFile: CARBON

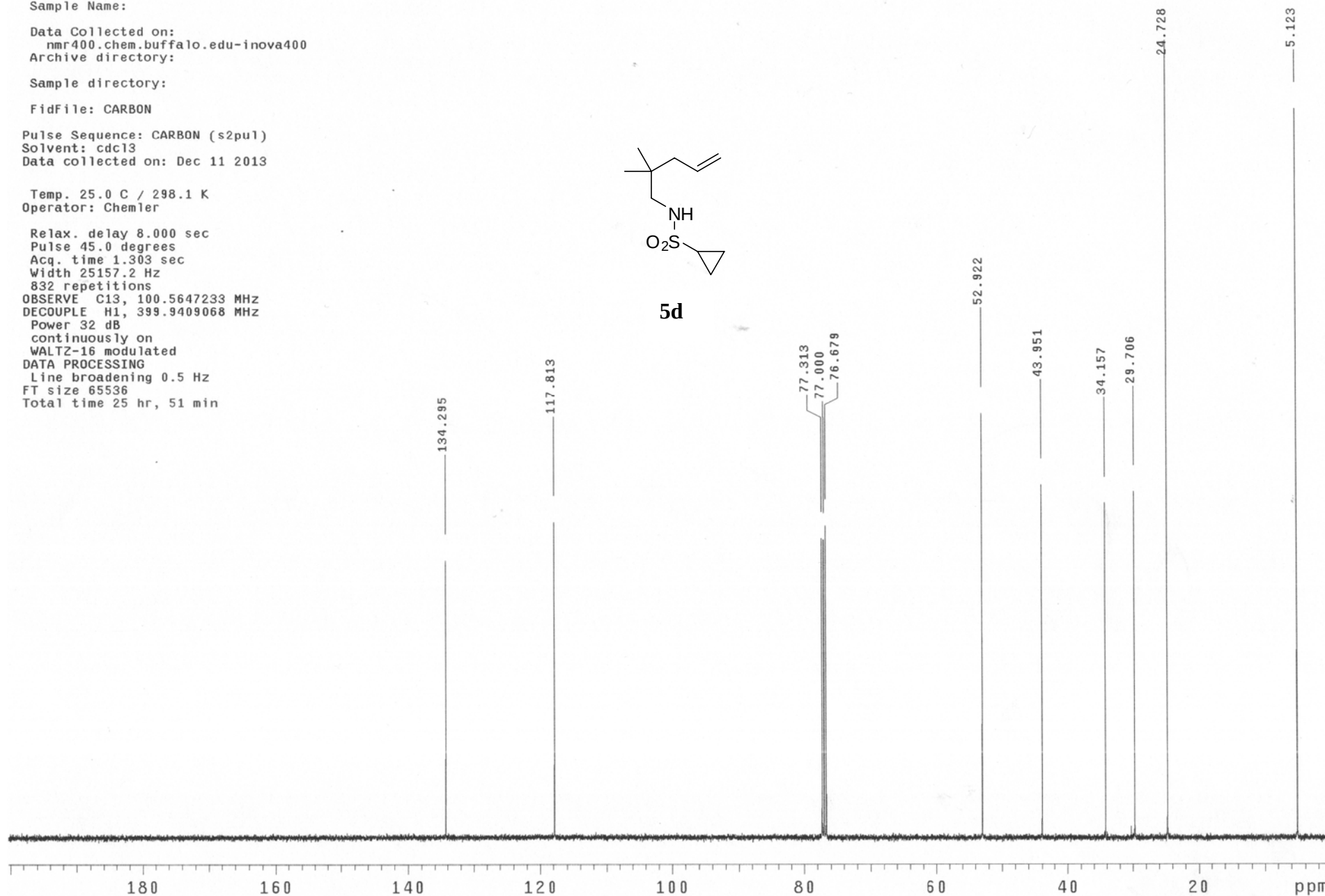
Pulse Sequence: CARBON (s2pul)
Solvent: cdc13
Data collected on: Dec 11 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

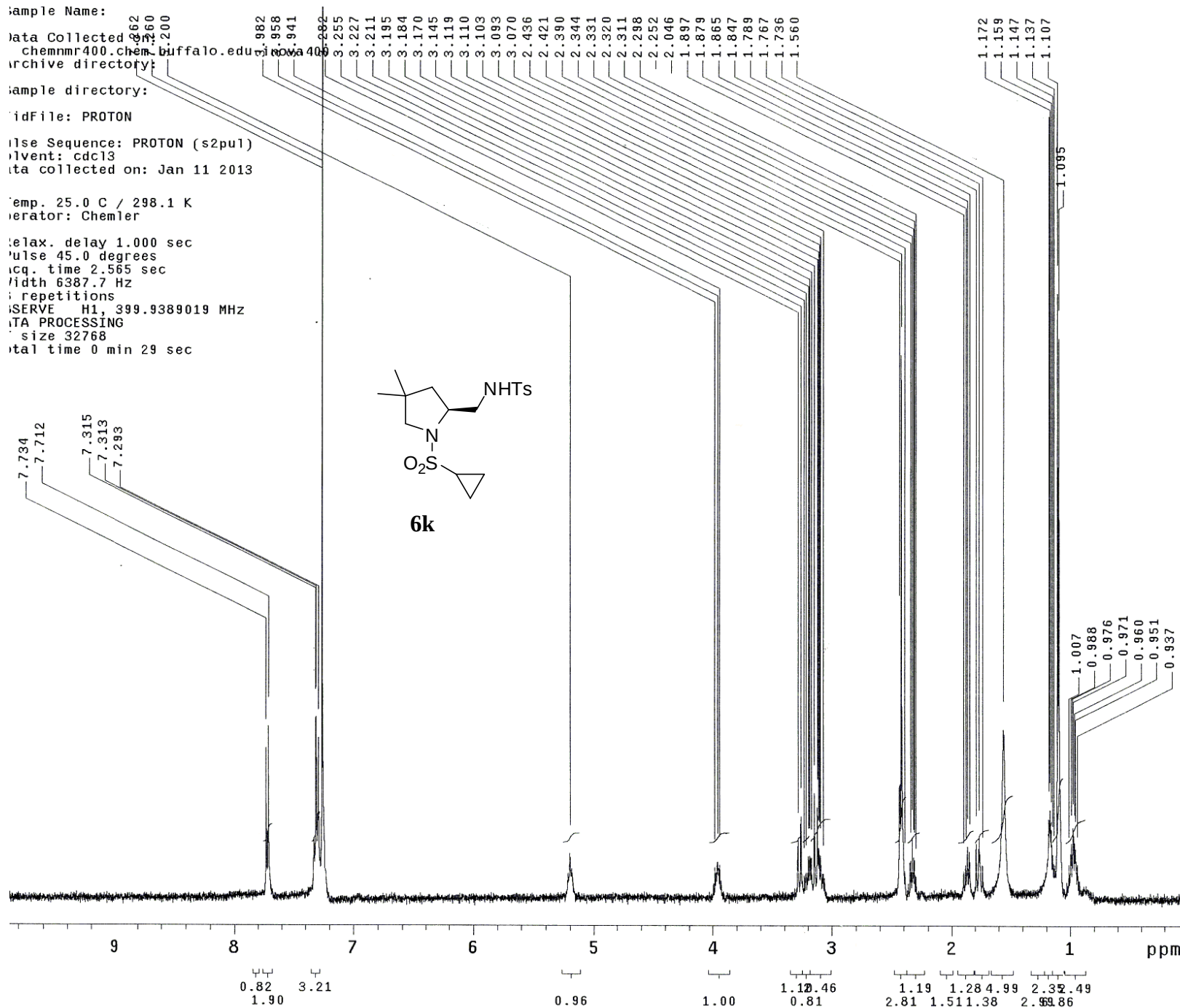
Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
832 repetitions
OBSERVE C13, 100.5647233 MHz
DECOUPLE H1, 399.9409068 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 25 hr, 51 min



5d



Sample Name:
 Data Collected: 11/11/2013
 chemnmr400.chem.buffalo.edu/nova400
 Archive directory:
 Sample directory:
 File: PROTON
 Pulse Sequence: PROTON (s2pu1)
 Solvent: cdc13
 Data collected on: Jan 11 2013
 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
 Repetitions
 ASERVE H1, 399.9389019 MHz
 DATA PROCESSING
 Size 32768
 Total time 0 min 29 sec



blt2-rxn570pg185prepcarbon

Sample Name:

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

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cdc13
Data collected on: Dec 10 2013

Temp. 25.0 C / 298.1 K
Operator: Chemler

Relax. delay 8.000 sec
Pulse 45.0 degrees
Acq. time 1.303 sec
Width 25157.2 Hz
4400 repetitions
OBSERVE C13, 100.5647187 MHz
DECOUPLE H1, 399.9409068 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 25 hr, 51 min

