

I-GS-072-2

Sample Name:

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

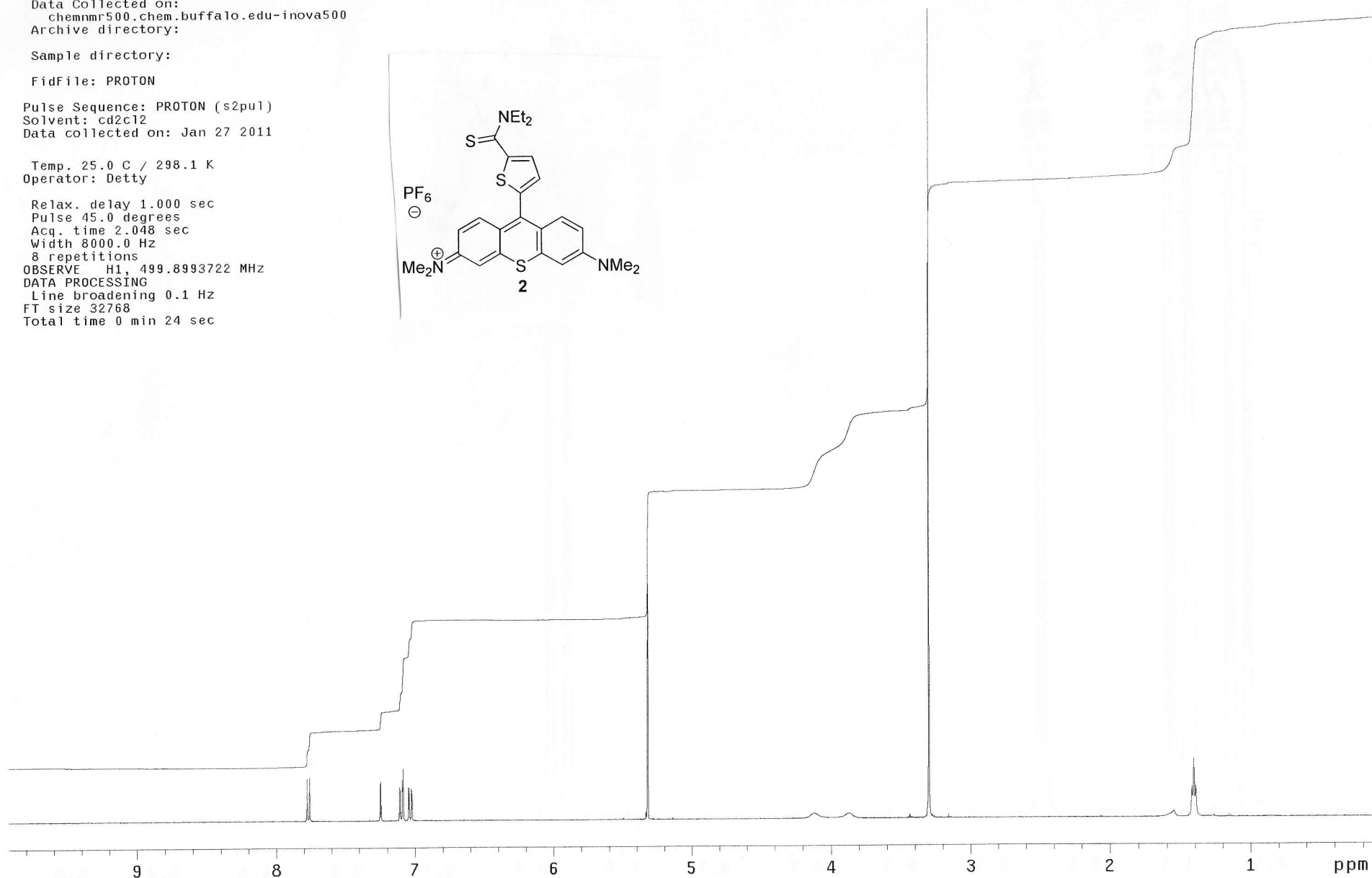
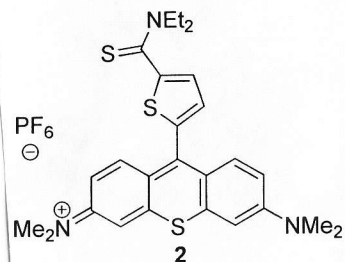
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2c12
Data collected on: Jan 27 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

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



I-GS-072-13C

Sample Name:

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

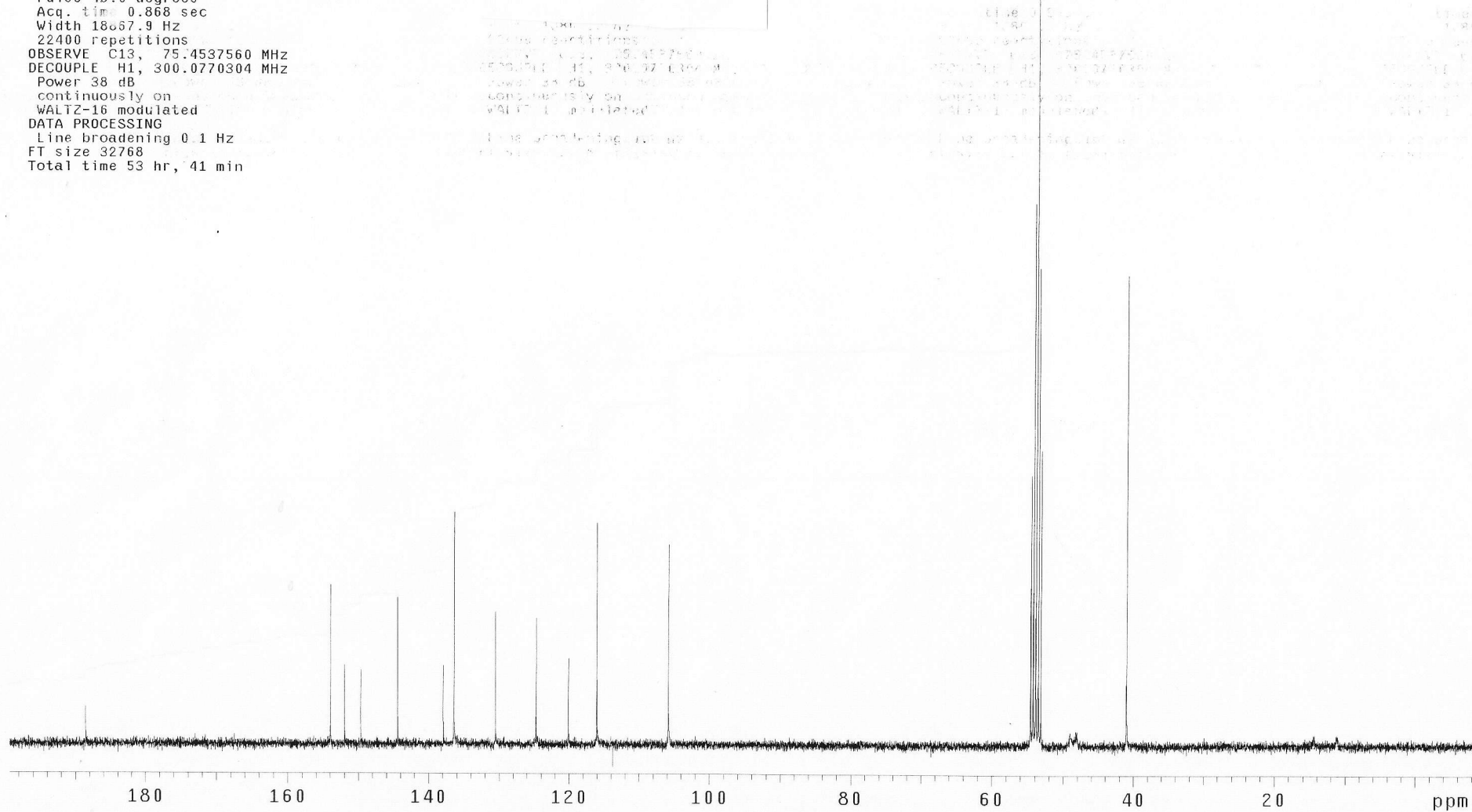
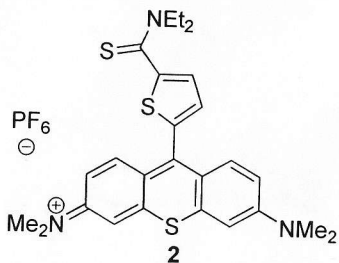
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: cd3cn
Data collected on: Apr 19 2011

Temp. 23.0 C / 296.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18667.9 Hz
22400 repetitions
OBSERVE C13, 75.4537560 MHz
DECOUPLE H1, 300.0770304 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 53 hr, 41 min



Data File C:\HPCHEM\1\DATA\DETTY1\DETTY002.D

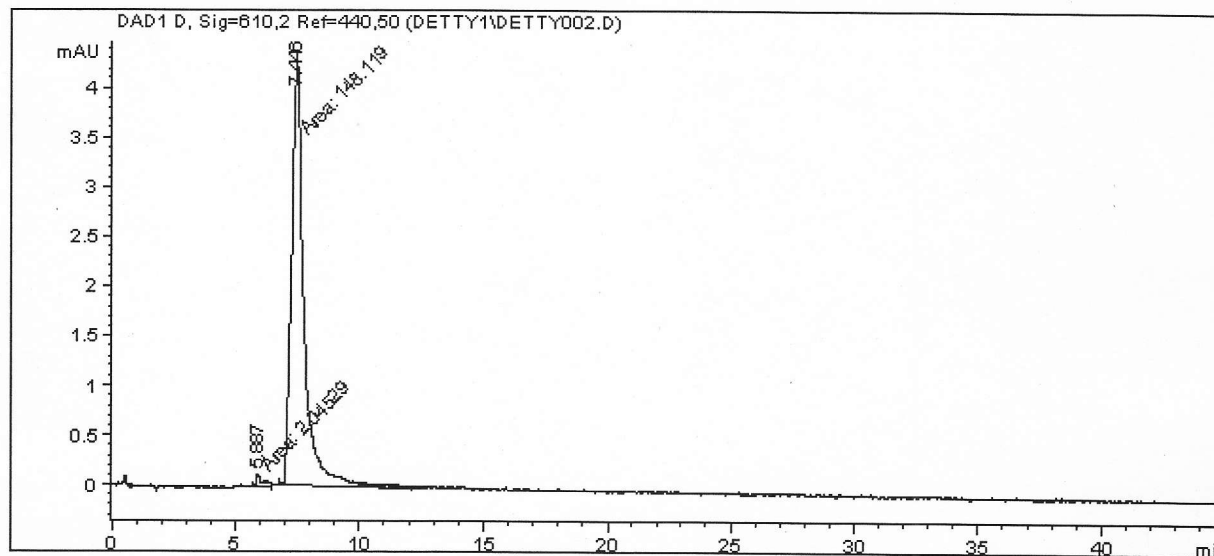
Sample Name: 072

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=====
Injection Date : 6/27/2011 7:49:41 PM      Seq. Line : 2
Sample Name    : 072                        Location  : Vial 2
Acq. Operator  : JCV                        Inj      : 1
                                           Inj Volume: 3 µl

Acq. Method   : C:\HPCHEM\1\METHODS\CODY\DET610NM.M
Last changed  : 6/27/2011 6:57:46 PM by JCV
Analysis Method : C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed  : 6/28/2011 6:13:32 PM by JCV
                (modified after loading)
=====

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                          Area Percent Report
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Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

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Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.887	MM	0.2865	2.04529	1.18997e-1	1.3620
2	7.446	MM	0.5798	148.11896	4.25782	98.6380

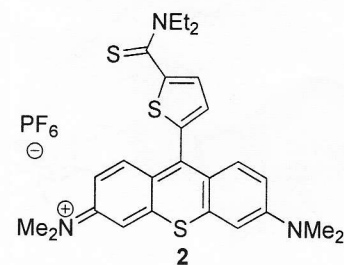
```
Totals :                      150.16424    4.37682
```

Results obtained with enhanced integrator!

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*** End of Report ***
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I-GS-093

Sample Name:

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

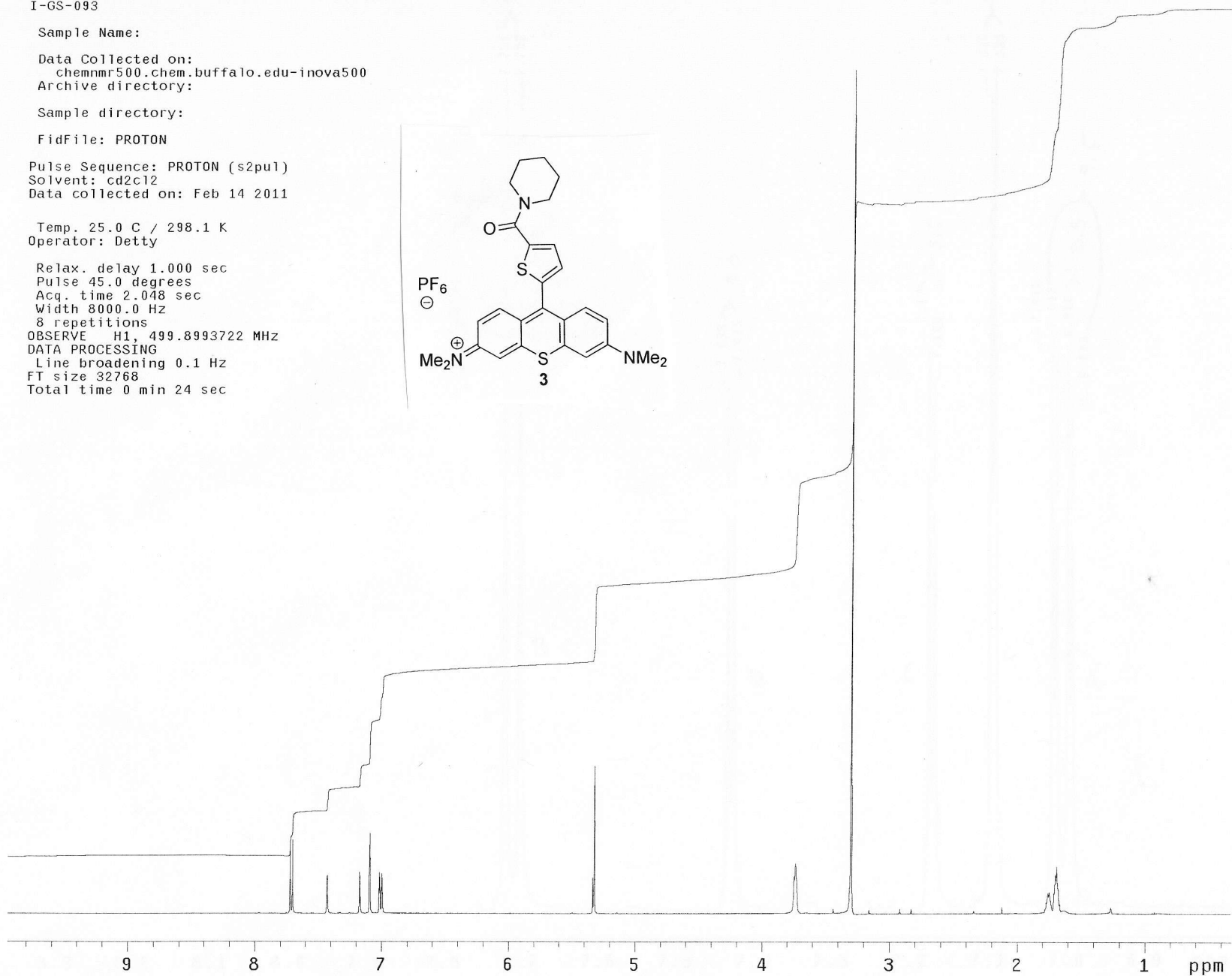
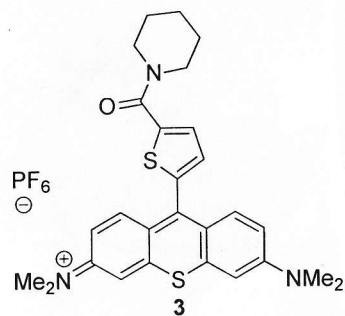
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2c12
Data collected on: Feb 14 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

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



I-GS-093-13C

Sample Name:

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

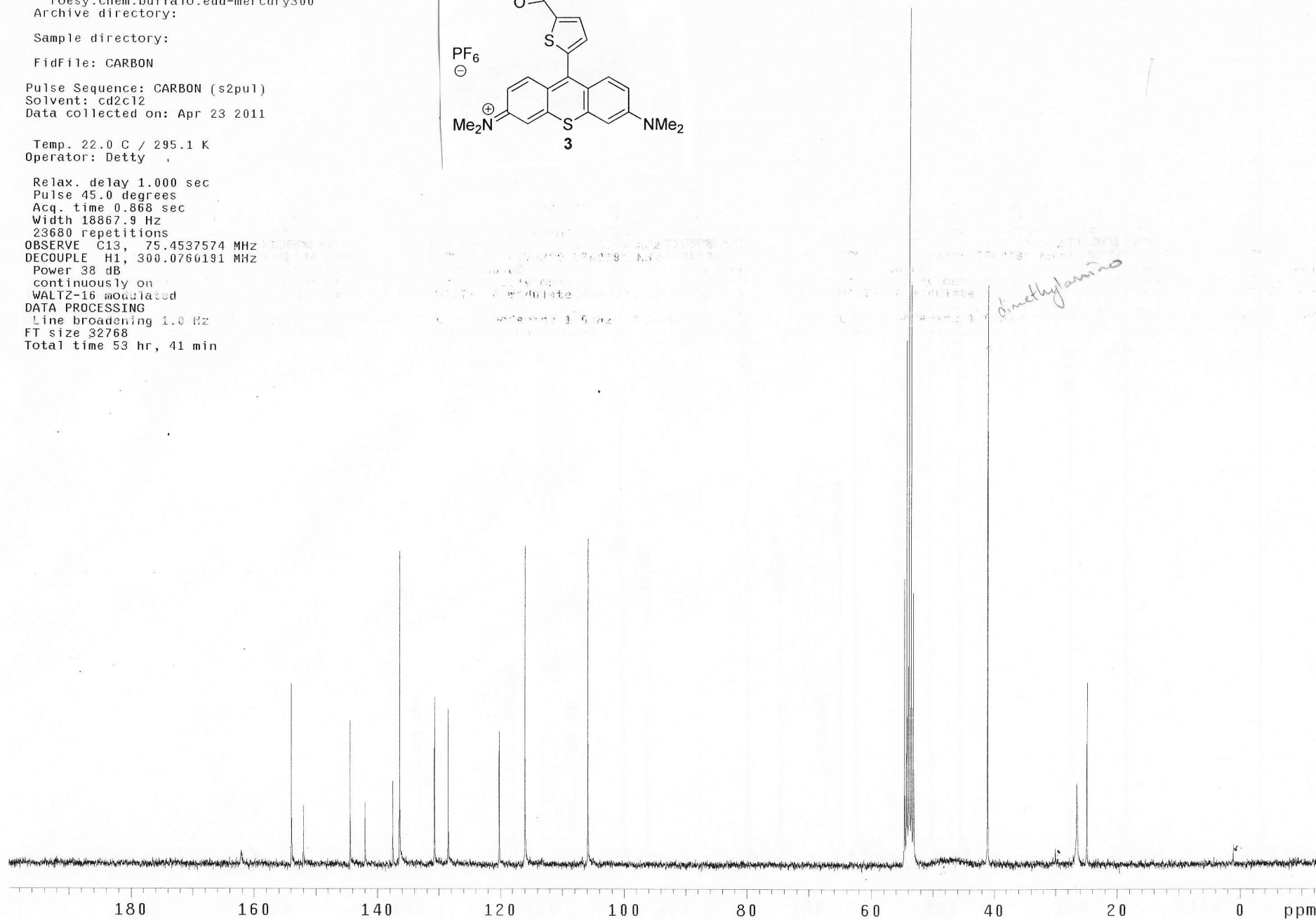
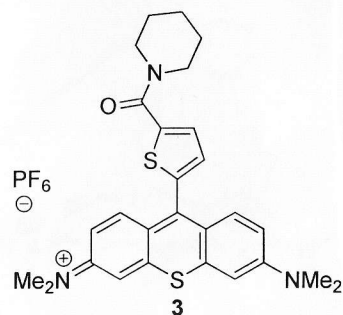
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cd2c12
Data collected on: Apr 23 2011

Temp. 22.0 C / 295.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
23680 repetitions
OBSERVE C13, 75.4537574 MHz
DECOUPLE H1, 300.0760191 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 53 hr, 41 min



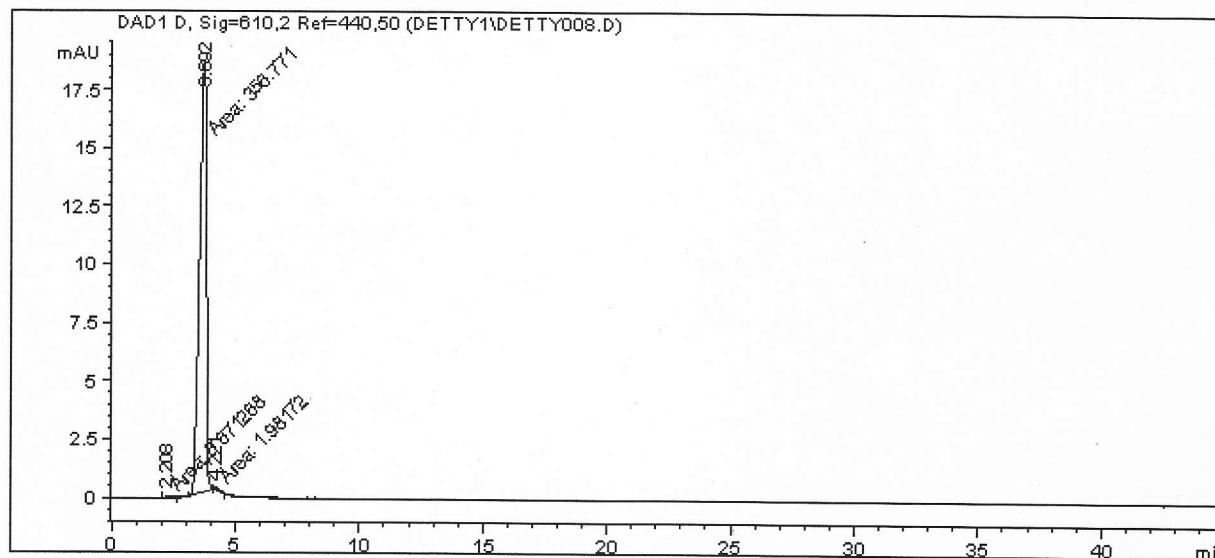
Data File C:\HPCHEM\1\DATA\DETTY1\DETTY008.D

Sample Name: 093

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=====
Injection Date : 6/28/2011 12:27:14 AM      Seq. Line : 8
Sample Name    : 093                          Location  : Vial 8
Acq. Operator  : JCV                           Inj      : 1
                                           Inj Volume: 3 µl
Acq. Method    : C:\HPCHEM\1\METHODS\CODY\DET610NM.M
Last changed   : 6/27/2011 6:57:46 PM by JCV
Analysis Method: C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed   : 6/28/2011 6:26:29 PM by JCV
                (modified after loading)
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                          Area Percent Report
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Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.208	MM	0.1229	6.71268e-1	9.10290e-2	0.1868
2	3.692	MM	0.3236	356.77057	18.37569	99.2619
3	4.221	MM	0.2492	1.98172	1.32532e-1	0.5514

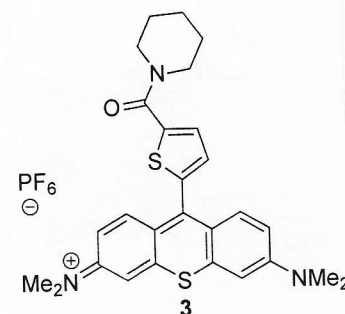
```
Totals :                      359.42355   18.59925
```

Results obtained with enhanced integrator!

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*** End of Report ***

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I-GS-087

Sample Name:

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

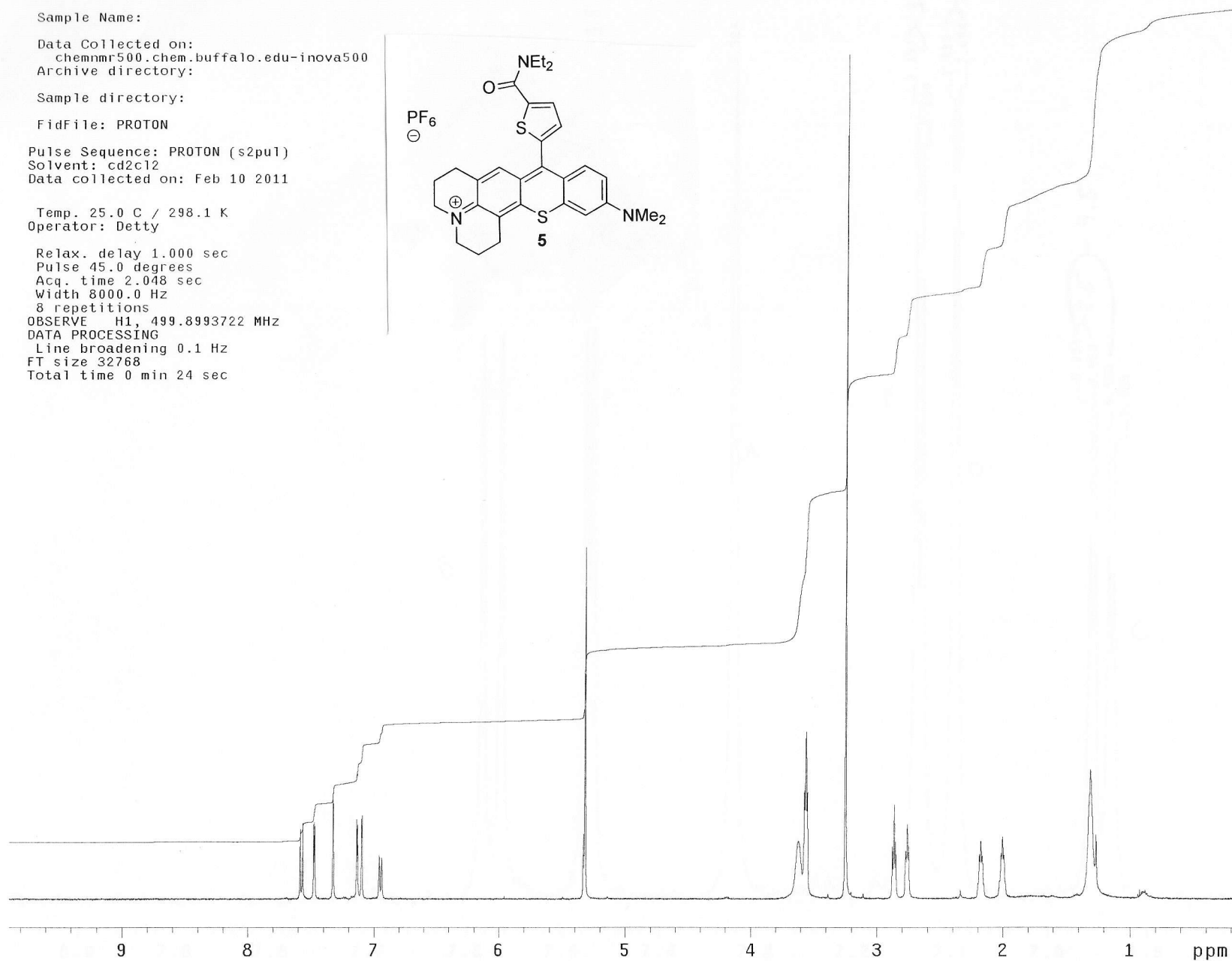
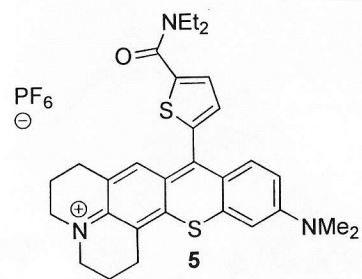
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd2cl2
Data collected on: Feb 10 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

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



I-GS-087-13C

Sample Name:

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

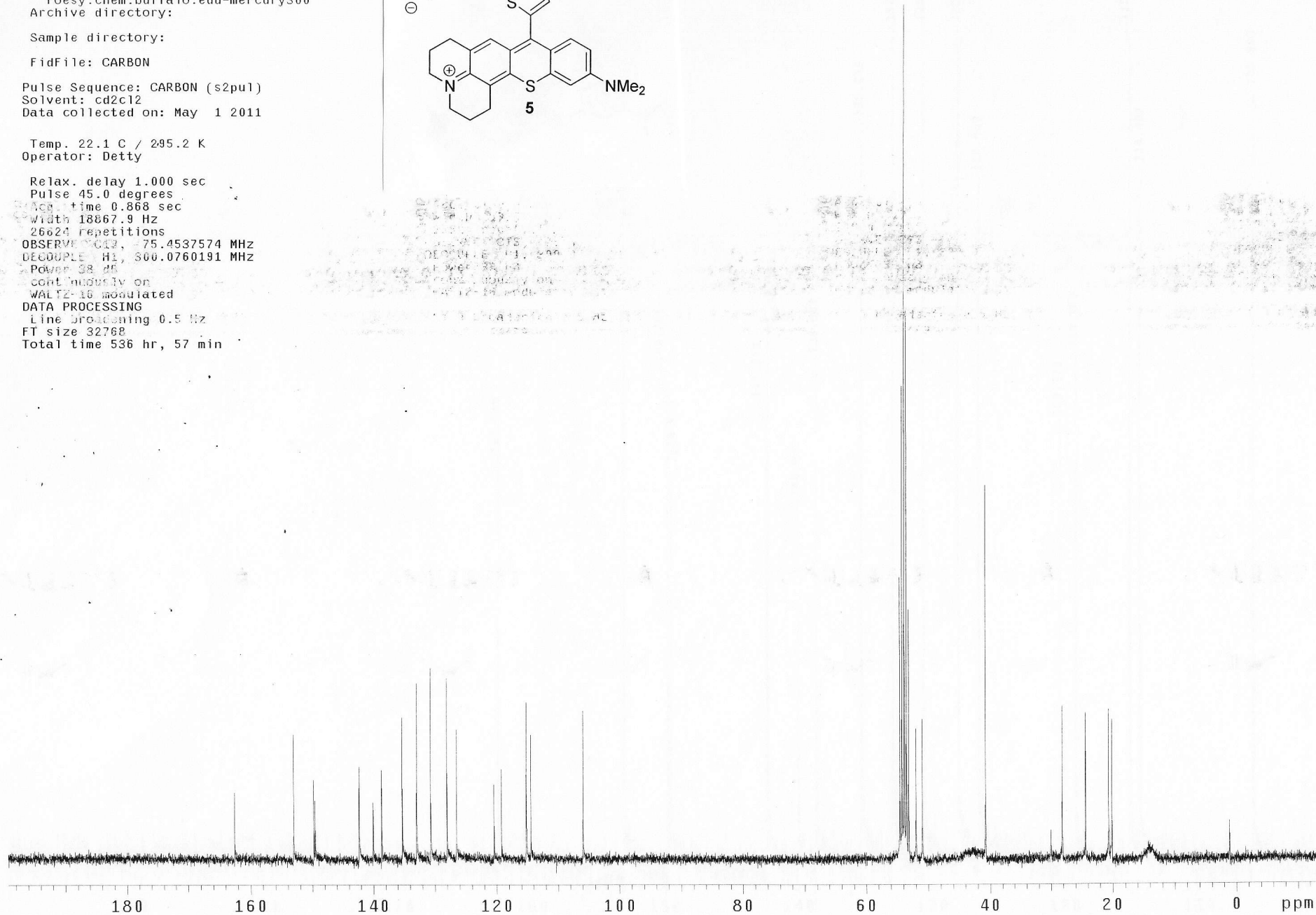
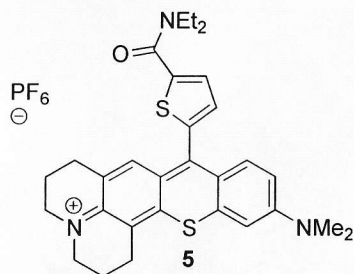
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cd2c12
Data collected on: May 1 2011

Temp. 22.1 C / 295.2 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
26624 repetitions
OBSERVE C13, 75.4537574 MHz
DECOUPLE H1, 500.0760191 MHz
Power 38 dB
cont. moduly on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 536 hr, 57 min



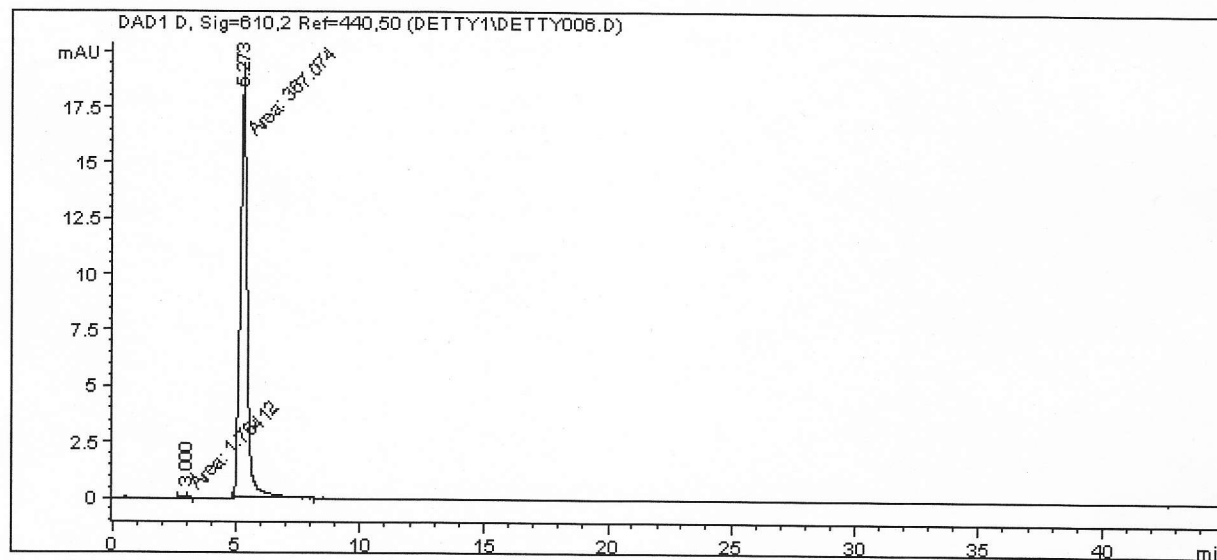
Data File C:\HPCHEM\1\DATA\DETTY1\DETTY006.D

Sample Name: 087

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=====
Injection Date   : 6/27/2011 10:54:44 PM      Seq. Line :    6
Sample Name     : 087                          Location  : Vial 6
Acq. Operator   : JCV                          Inj       :    1
                                                Inj Volume: 3 µl
Acq. Method    : C:\HPCHEM\1\METHODS\CODY\DET610NM.M
Last changed   : 6/27/2011 6:57:46 PM by JCV
Analysis Method: C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed   : 6/28/2011 6:21:42 PM by JCV
                (modified after loading)
=====

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                          Area Percent Report
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Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.000	MM	0.1614	1.76412	1.82134e-1	0.4783
2	5.273	MM	0.3156	367.07419	19.38569	99.5217

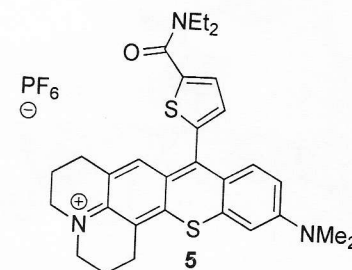
```
Totals :                      368.83831  19.56782
```

Results obtained with enhanced integrator!

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*** End of Report ***
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I-GS-085-1

Sample Name:
I-MB-029top
Data Collected on:
chemnmr500.chem.buffalo.edu-inovc
Archive directory:

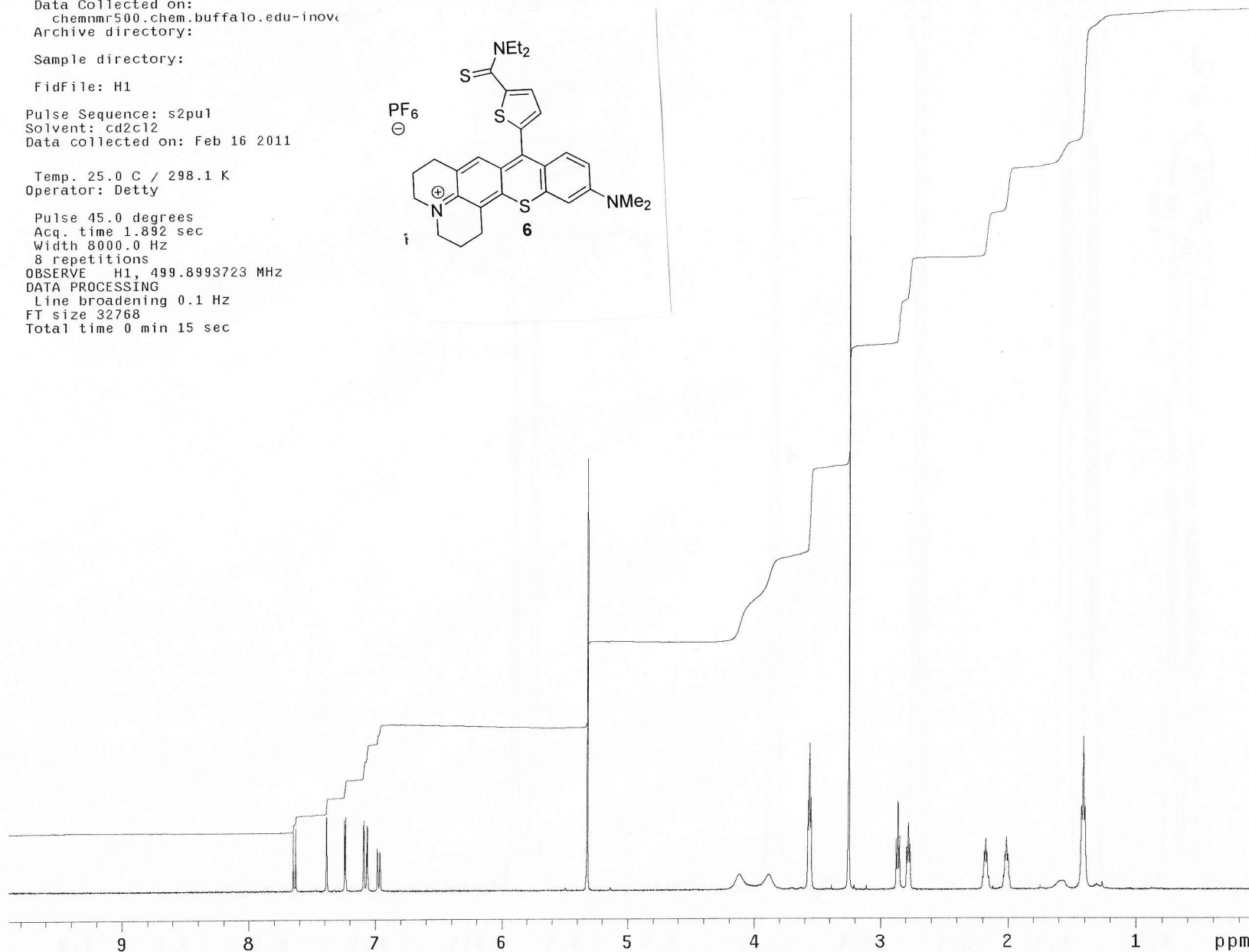
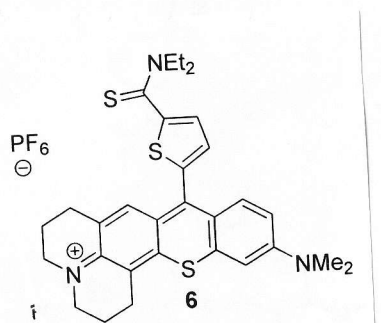
Sample directory:

FidFile: H1

Pulse Sequence: s2pu1
Solvent: cd2c12
Data collected on: Feb 16 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

Pulse 45.0 degrees
Acq. time 1.892 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993723 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 15 sec



I-GS-085-13C

Sample Name:

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

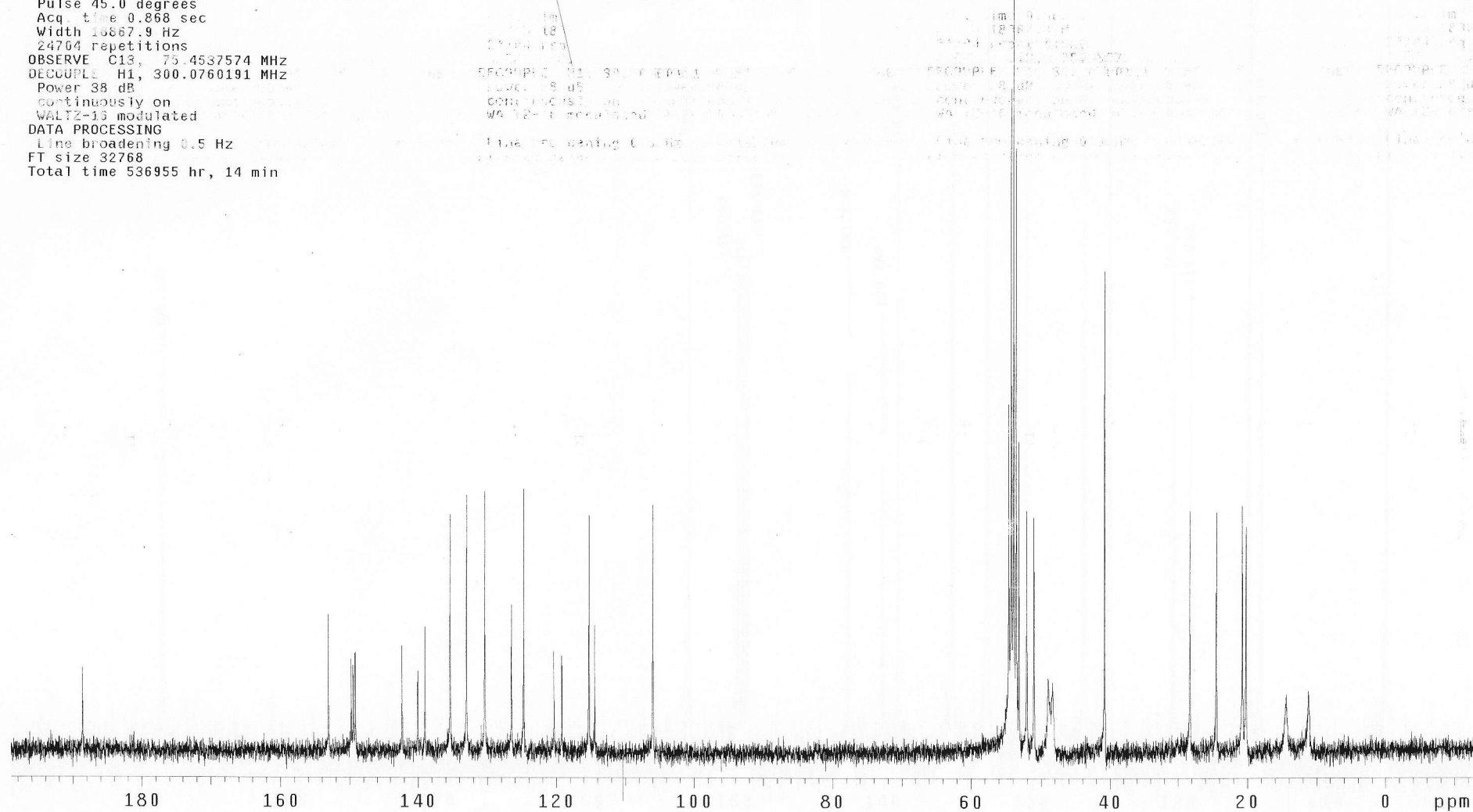
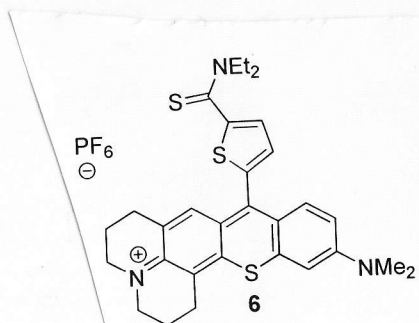
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cd2c12
Data collected on: Apr 24 2011

Temp. 21.6 C / 294.8 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 16567.9 Hz
24704 repetitions
OBSERVE C13, 75.4537574 MHz
DECUPLE H1, 300.0760191 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 536955 hr, 14 min



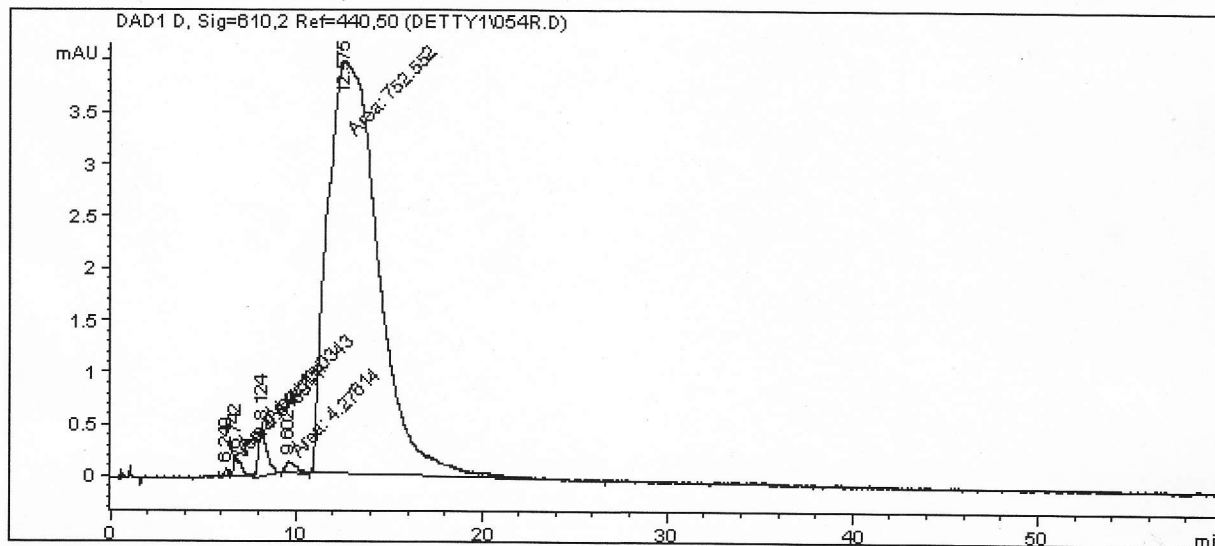
Data File C:\HPCHEM\1\DATA\DETTY1\054R.D

Sample Name: 054R

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=====
Injection Date   : 6/28/2011 4:58:55 PM
Sample Name     : 054R
Accr. Operator  : JCV
Location       : Vial 1
Inj Volume     : 3 µl
Acq. Method    : C:\HPCHEM\1\METHODS\CODY\DET054.M
Last changed   : 6/28/2011 4:55:44 PM by JCV
                (modified after loading)
Analysis Method : C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed   : 6/28/2011 6:10:56 PM by JCV
                (modified after loading)
=====

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=====
Area Percent Report
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Sorted By      : Signal
Multiplier    : 1.0000
Dilution      : 1.0000
Sample Amount  : 5.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.249	MM	0.1896	8.46911e-1	7.44468e-2	0.1089
2	6.742	MM	0.4287	4.94734	1.92330e-1	0.6362
3	8.124	MM	0.5260	15.03427	4.76363e-1	1.9333
4	9.602	MM	0.6507	4.27614	1.09531e-1	0.5499
5	12.575	MM	3.1715	752.55219	3.95473	96.7718

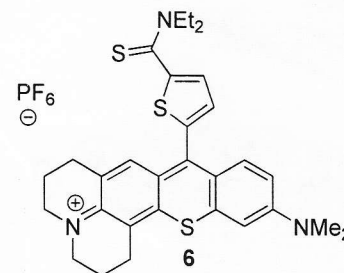
```
Totals :                777.65684    4.80740
```

Results obtained with enhanced integrator!

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*** End of Report ***

```



I-GS-075

Sample Name:

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

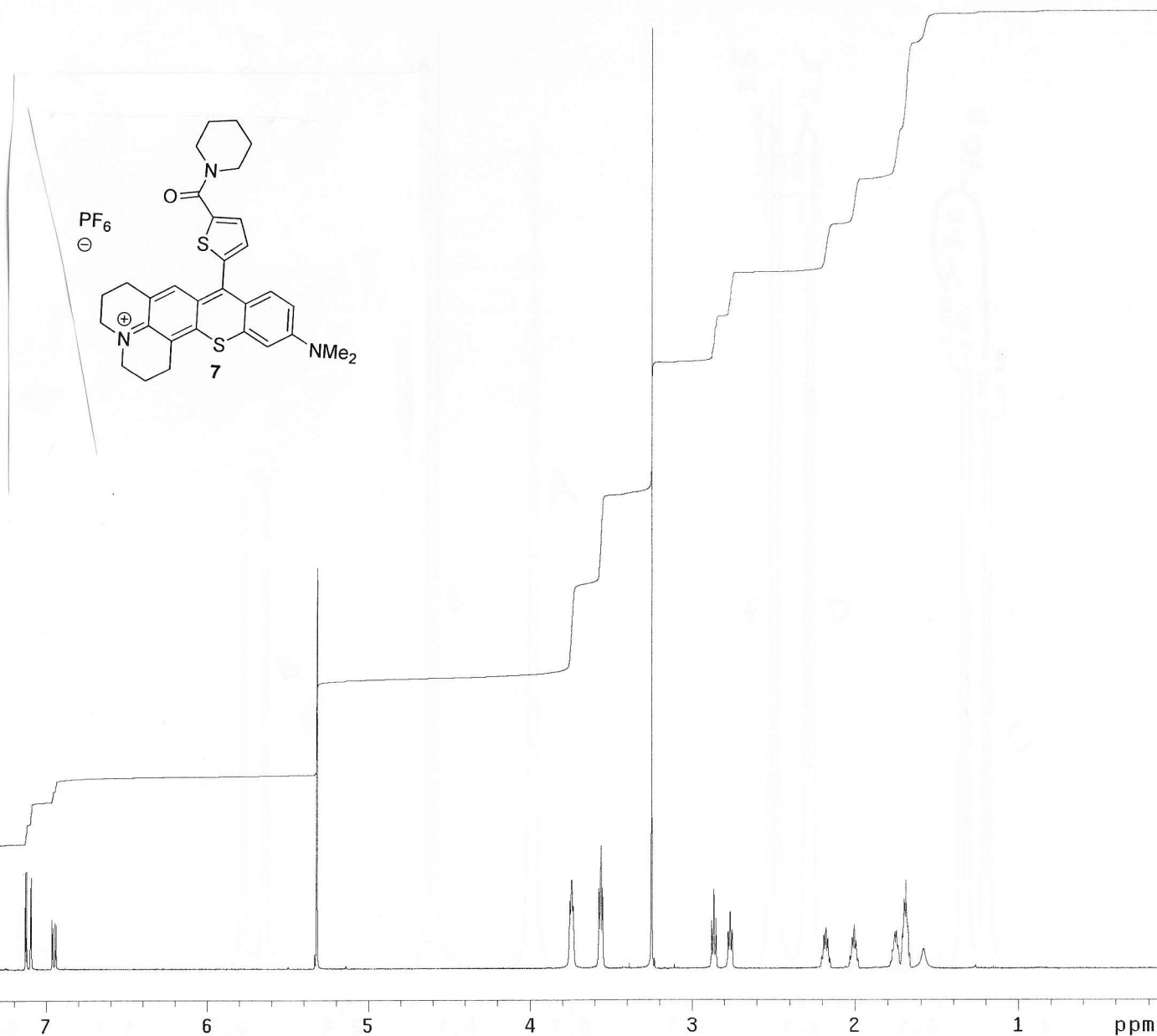
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2c12
Data collected on: Jan 27 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

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



I-GS-075

Sample Name:

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

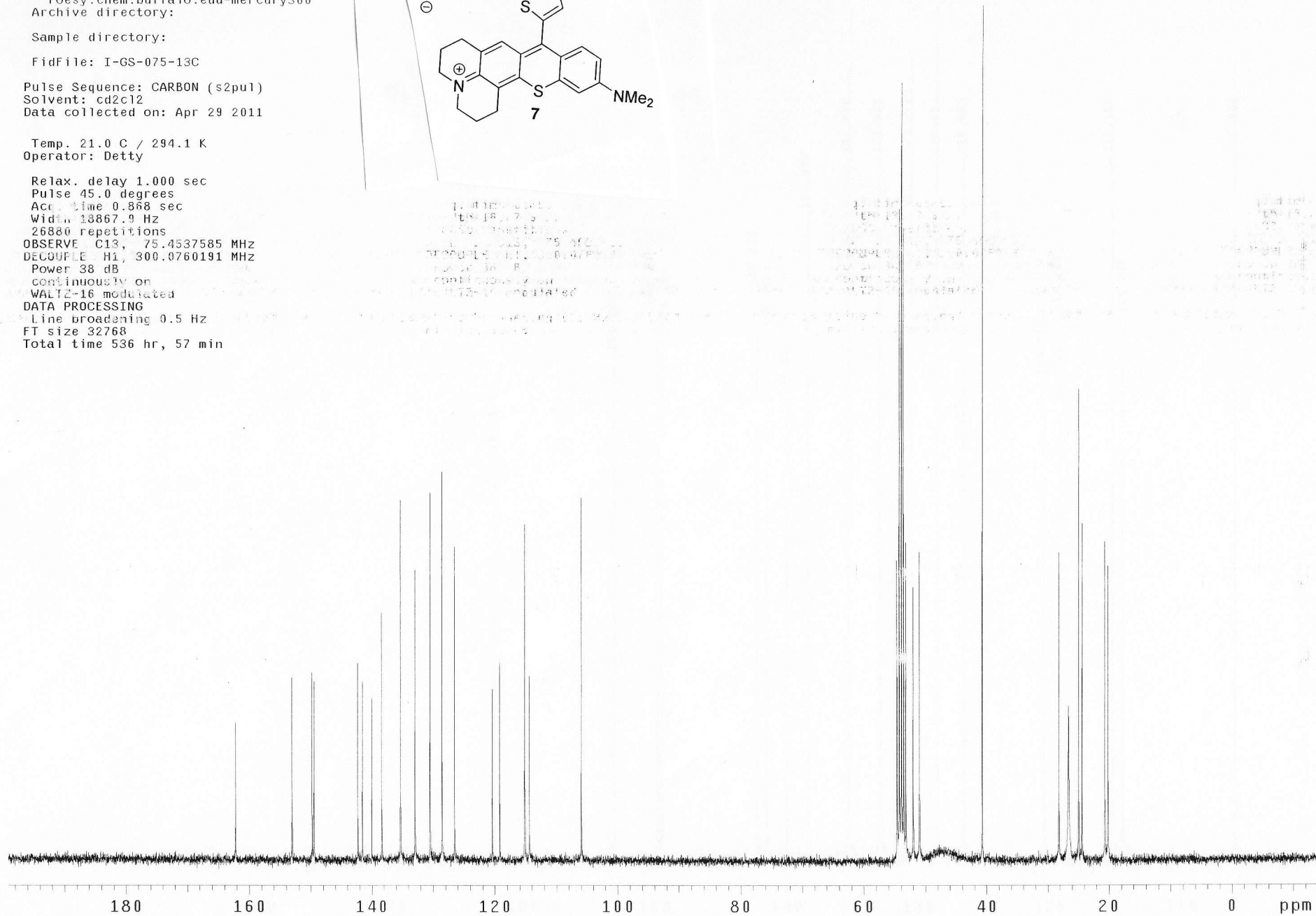
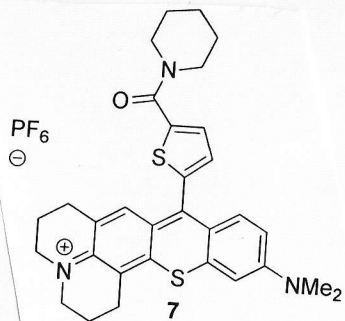
Sample directory:

FidFile: I-GS-075-13C

Pulse Sequence: CARBON (s2pu1)
Solvent: cd2c12
Data collected on: Apr 29 2011

Temp. 21.0 C / 294.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 13867.9 Hz
26880 repetitions
OBSERVE C13, 75.4537585 MHz
DECOUPLE H1, 300.0760191 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 536 hr, 57 min



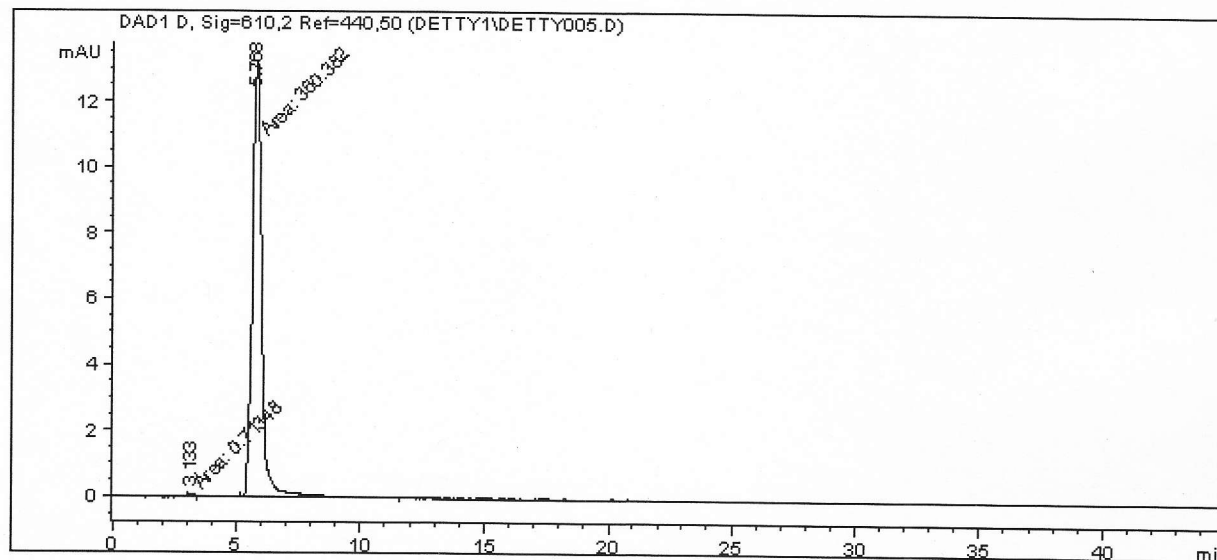
Data File C:\HPCHEM\1\DATA\DETTY1\DETTY005.D

Sample Name: 075

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=====
Injection Date   : 6/27/2011 10:08:31 PM      Seq. Line :    5
Sample Name     : 075                          Location  : Vial 5
Acq. Operator   : JCV                          Inj      :    1
                                                Inj Volume: 3 µl
Acq. Method     : C:\HPCHEM\1\METHODS\CODY\DET610MM.M
Last changed    : 6/27/2011 6:57:46 PM by JCV
Analysis Method : C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed    : 6/28/2011 6:20:22 PM by JCV
                  (modified after loading)
=====

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=====
                          Area Percent Report
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Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.133	MM	0.1641	7.13480e-1	7.24673e-2	0.1976
2	5.768	MM	0.4576	360.38196	13.12644	99.8024

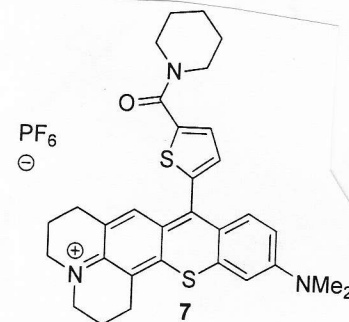
```
Totals :                      361.09544  13.19891
```

Results obtained with enhanced integrator!

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*** End of Report ***
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```



Instrument 1 6/28/2011 6:21:41 PM JCV

Page 1 of 1

1-A0-238-2

Sample Name:

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

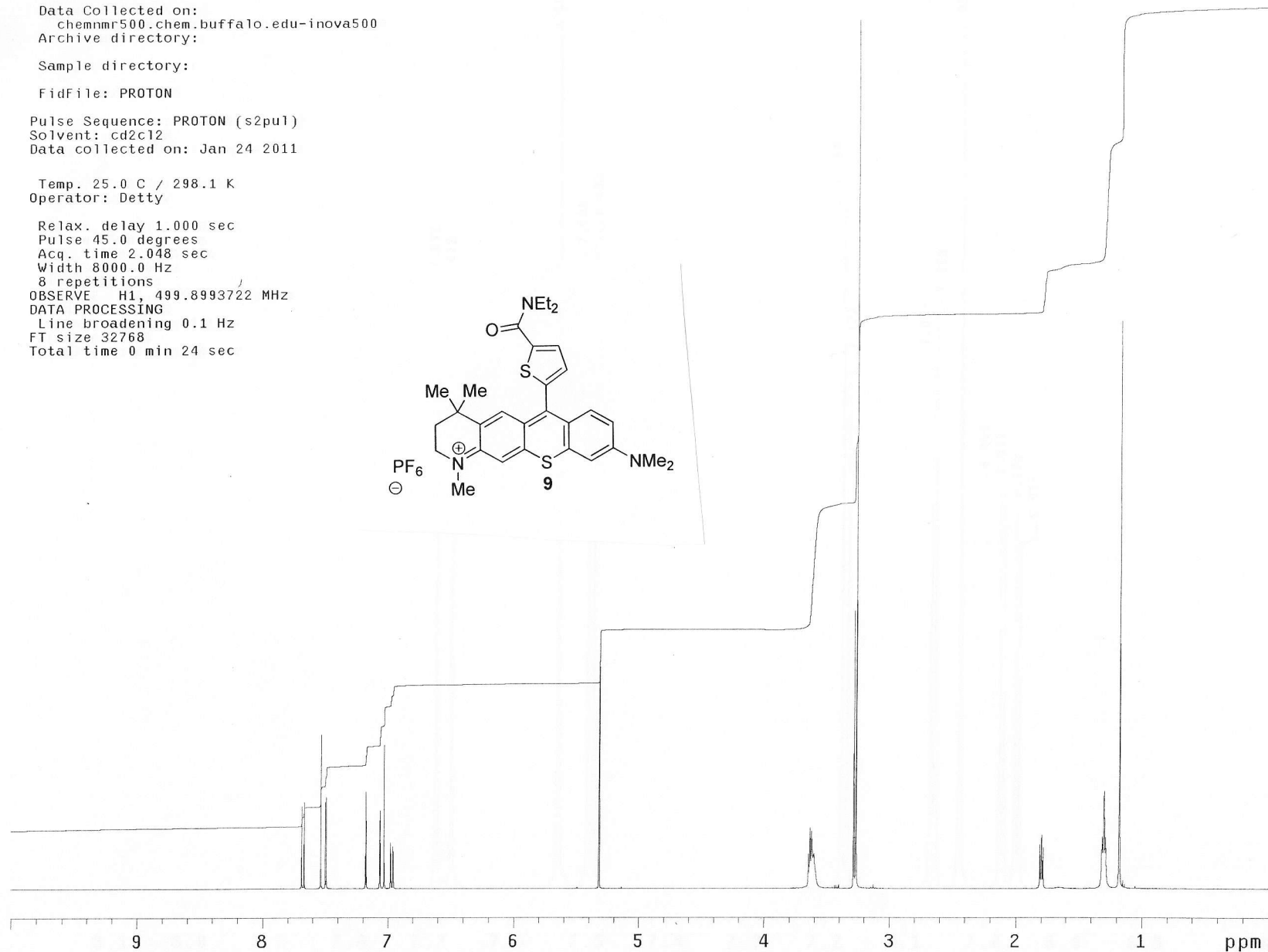
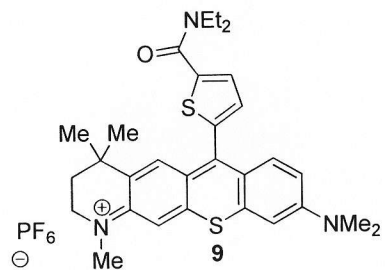
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: cd2c12
Data collected on: Jan 24 2011

Temp. 25.0 C / 298.1 K
Operator: Detty

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



1-A0-238-13C-2

Sample Name:

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

Archive directory:

Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)

Solvent: cd2c12

Data collected on: Jan 24 2011

Temp. 21.0 C / 294.1 K

Operator: Detty

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 0.868 sec

Width 18867.9 Hz

4608 repetitions

OBSERVE C13, 75.4537528 MHz

DECOUPLE H1, 300.0760191 MHz

Power 38 dB

continuously on

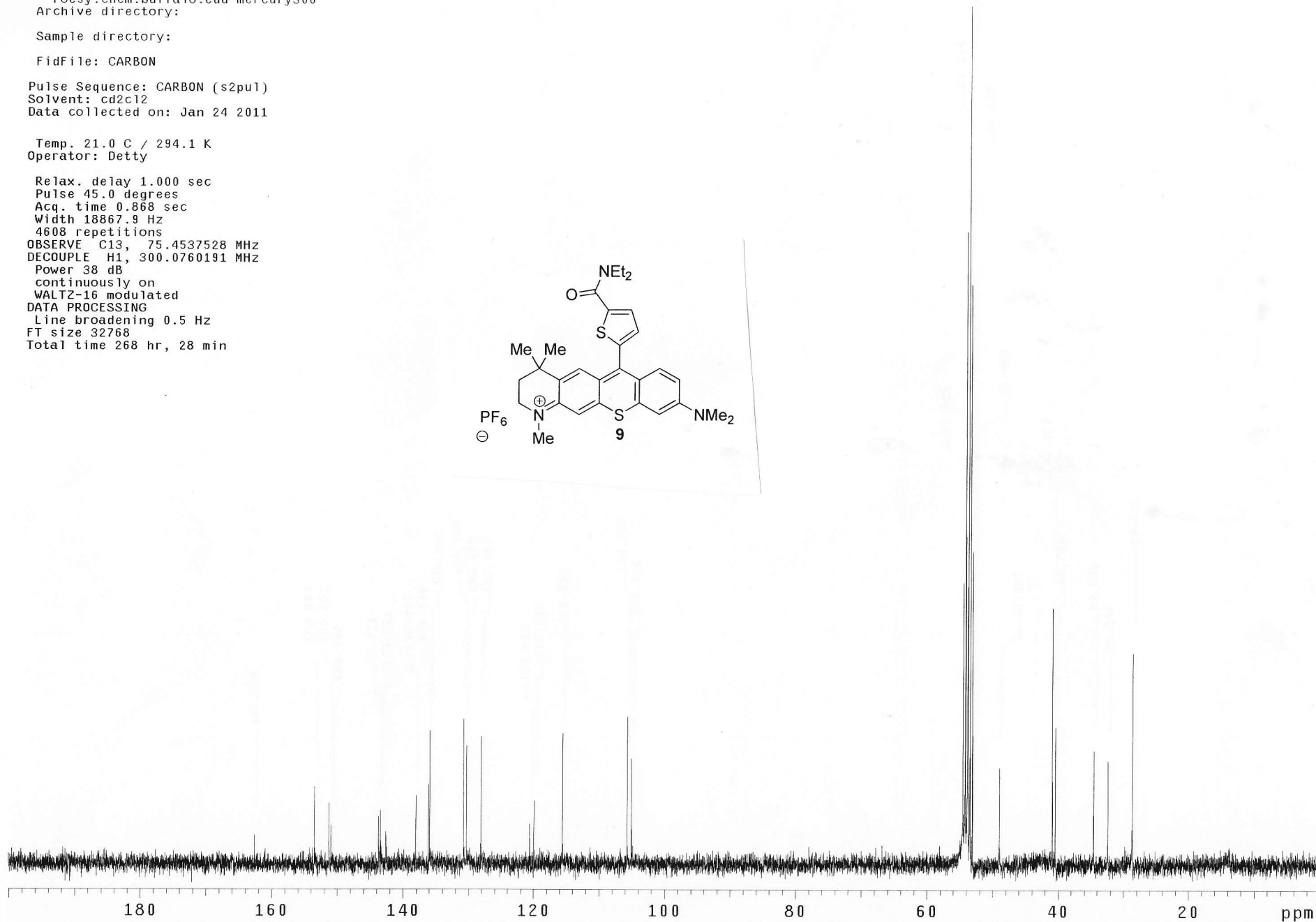
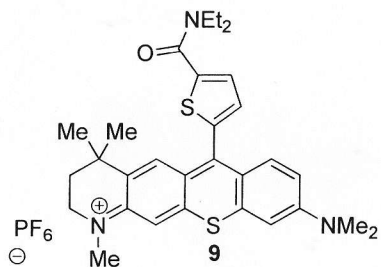
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.5 Hz

FT size 32768

Total time 268 hr, 28 min



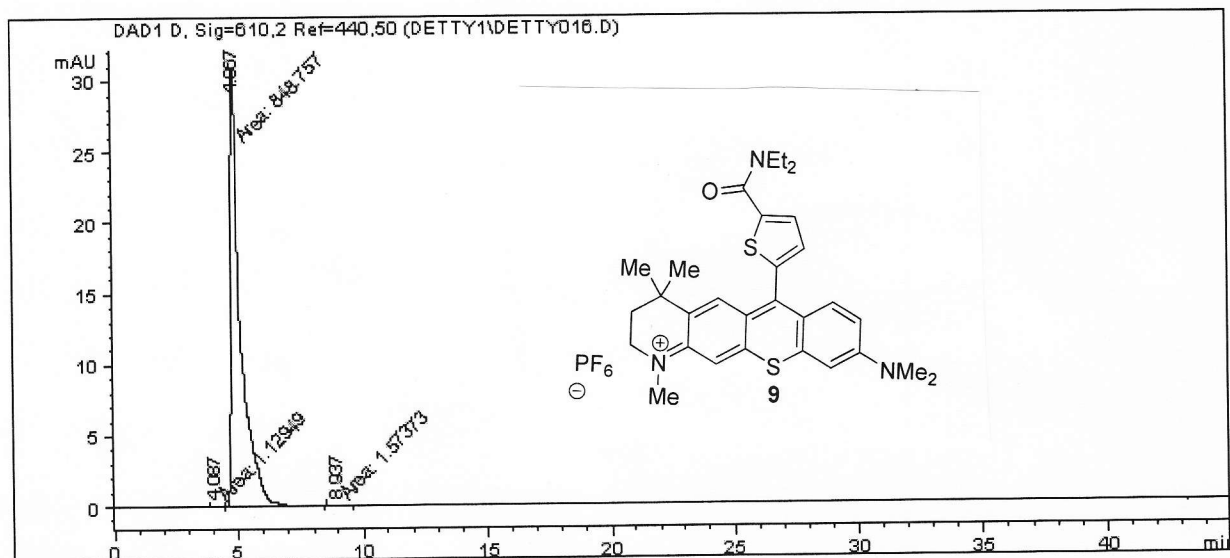
Data File C:\HPCHEM\1\DATA\DETTY1\DETTY016.D

Sample Name: 238

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=====
Injection Date : 6/28/2011 6:37:52 AM      Seq. Line : 16
Sample Name    : 238                        Location  : Vial 16
Acq. Operator  : JCV                        Inj      : 1
                                           Inj Volume: 3 µl
Acq. Method    : C:\HPCHEM\1\METHODS\CODY\DET610NM.M
Last changed   : 6/27/2011 6:57:46 PM by JCV
Analysis Method : C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed   : 6/28/2011 6:34:14 PM by JCV
                (modified after loading)
=====

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=====
                          Area Percent Report
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Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs

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Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.087	MM	0.3064	1.12949	6.14385e-2	0.1327
2	4.867	MM	0.4601	848.75684	30.74488	99.6825
3	8.937	MM	0.5441	1.57373	4.82028e-2	0.1848

```
Totals :                      851.46006    30.85453
```

Results obtained with enhanced integrator!

```

=====
*** End of Report ***
=====

```

Instrument 1 6/28/2011 6:36:21 PM JCV

Page 1 of 1

1-A0-237-7

Sample Name:

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

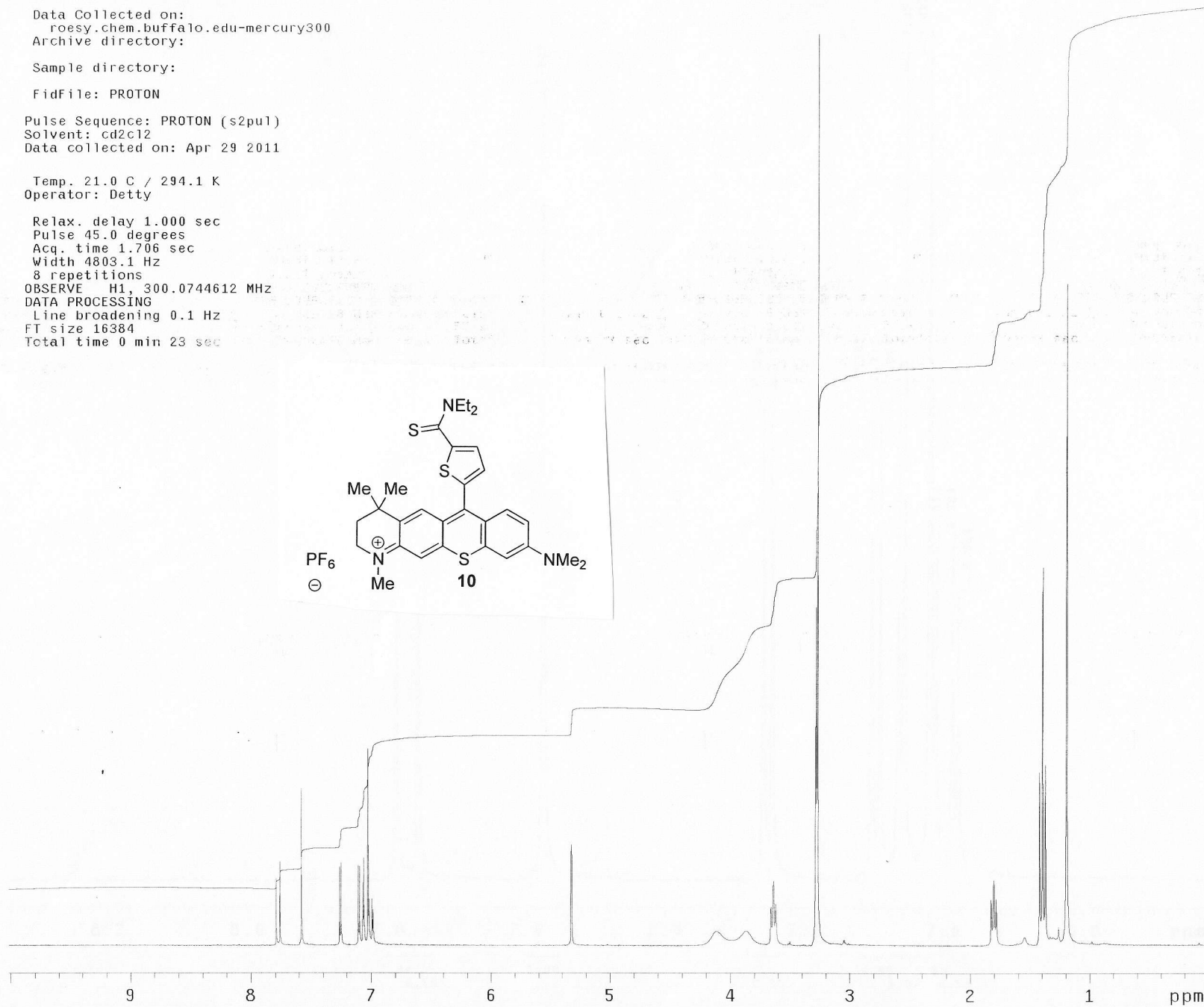
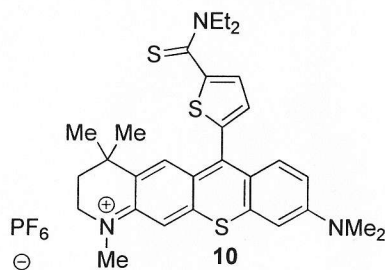
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd2c12
Data collected on: Apr 29 2011

Temp. 21.0 C / 294.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.706 sec
Width 4803.1 Hz
8 repetitions
OBSERVE H1, 300.0744612 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 16384
Total time 0 min 23 sec



STANDARD CARBON PARAMETERS

Sample Name: 1-A0-237-13 C

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

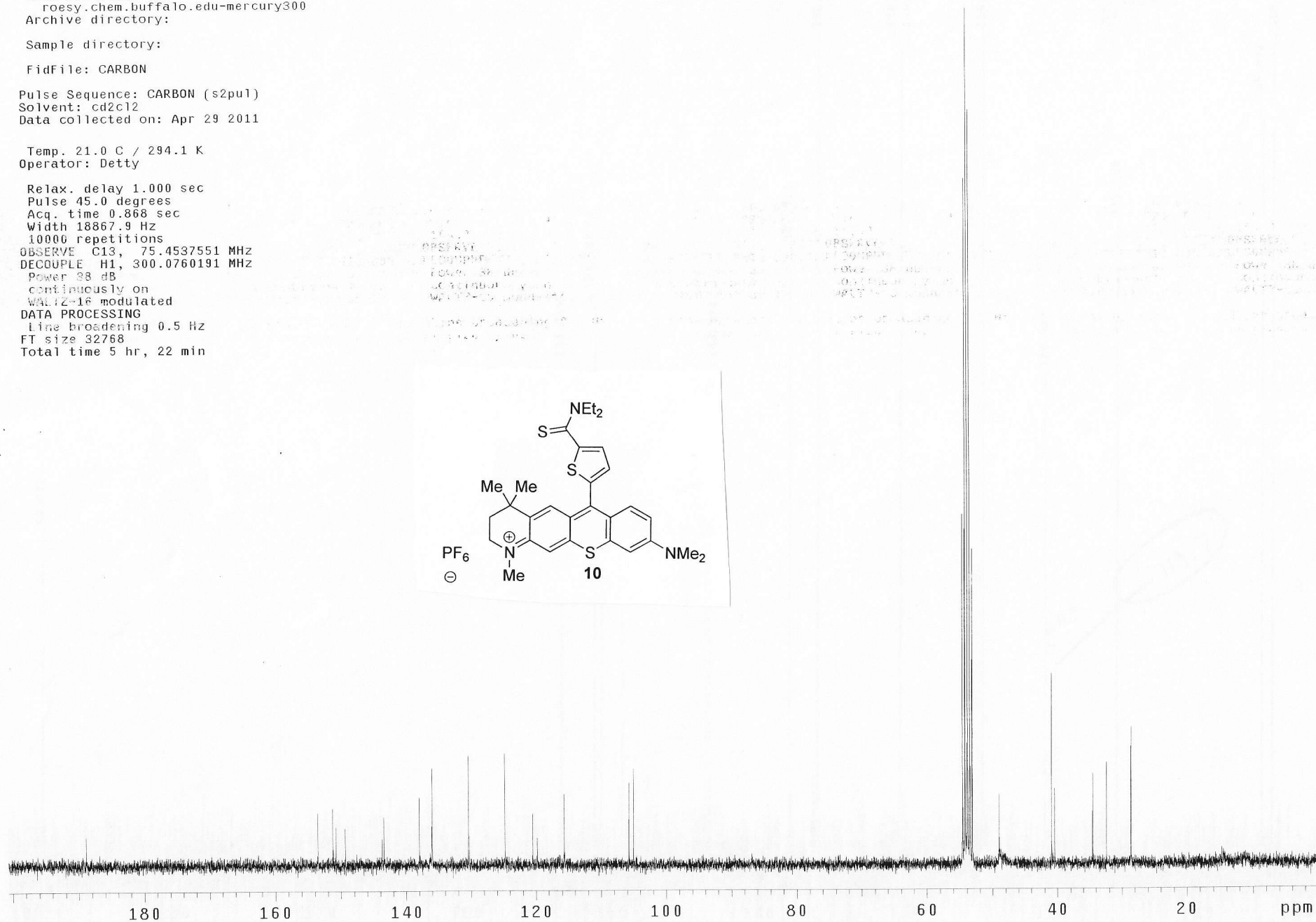
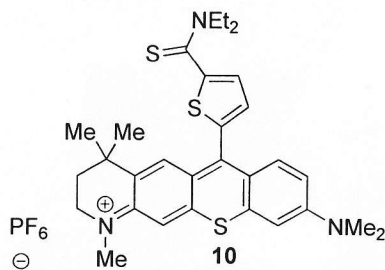
Sample directory:

FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cd2cl2
Data collected on: Apr 29 2011

Temp. 21.0 C / 294.1 K
Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
10000 repetitions
OBSERVE C13, 75.4537551 MHz
DECOUPLE H1, 300.0760191 MHz
Power 28 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 5 hr, 22 min



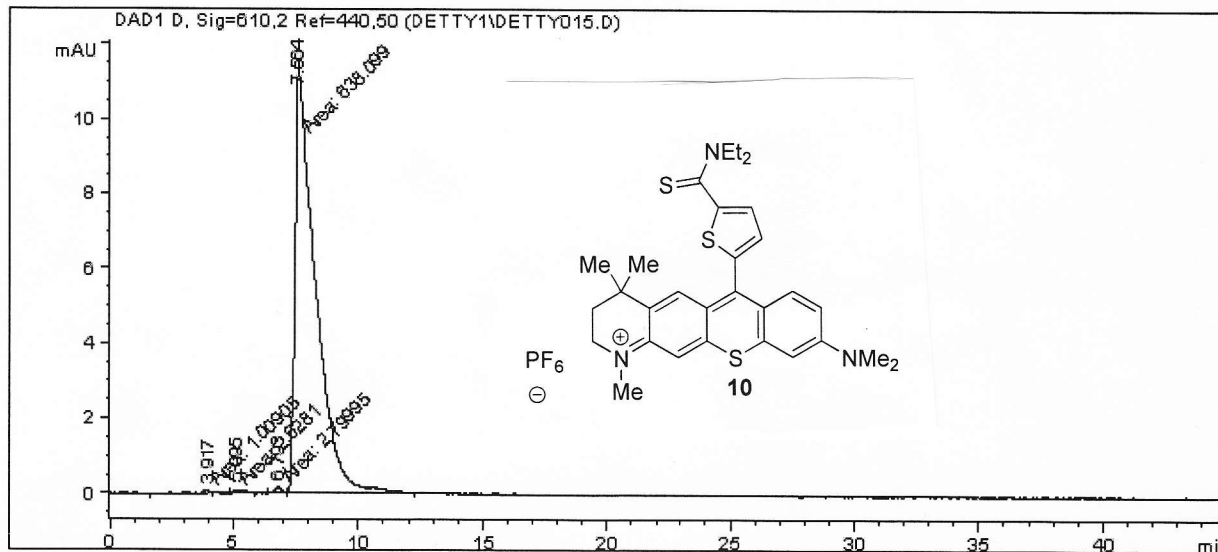
Data File C:\HPCHEM\1\DATA\DETTY1\DETTY015.D

Sample Name: 237

```

=====
Injection Date : 6/28/2011 5:51:37 AM      Seq. Line : 15
Sample Name    : 237                        Location  : Vial 15
Acq. Operator  : JCV                       Inj      : 1
                                                Inj Volume: 3 µl
Acq. Method   : C:\HPCHEM\1\METHODS\CODY\DET610NM.M
Last changed  : 6/27/2011 6:57:46 PM by JCV
Analysis Method : C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed  : 6/28/2011 6:32:54 PM by JCV
                (modified after loading)
=====

```



```

=====
                          Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier    :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.917	MM	0.2112	1.00905	7.96317e-2	0.1566
2	5.095	MM	0.4687	2.62810	9.34609e-2	0.4077
3	6.793	MM	0.2965	2.79995	1.57371e-1	0.4344
4	7.564	MM	0.9230	638.09924	11.52272	99.0013

```
Totals :                644.53634  11.85318
```

Results obtained with enhanced integrator!

```

=====
*** End of Report ***

```

Instrument 1 6/28/2011 6:34:14 PM JCV

Page 1 of 1

1-A0-280-3

Sample Name:

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

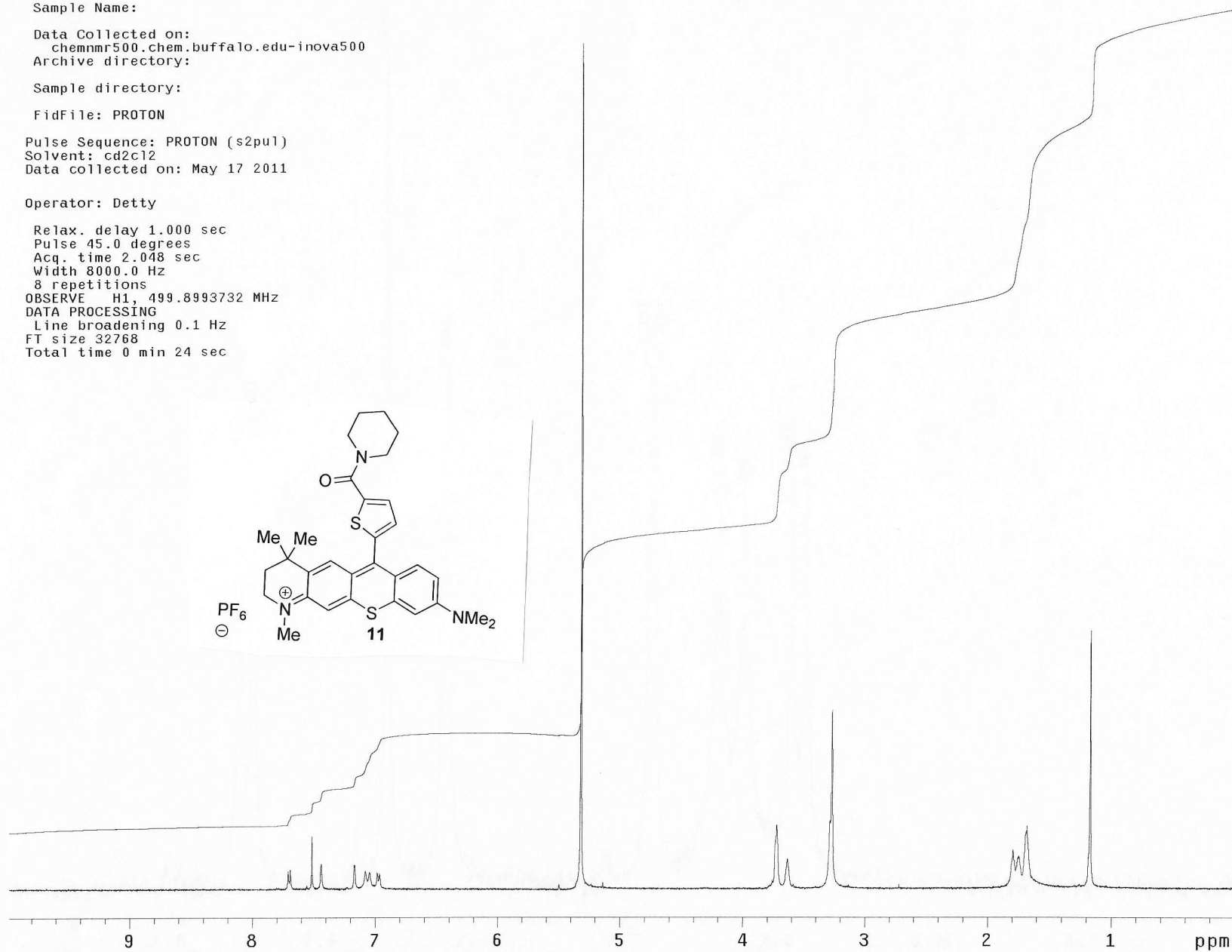
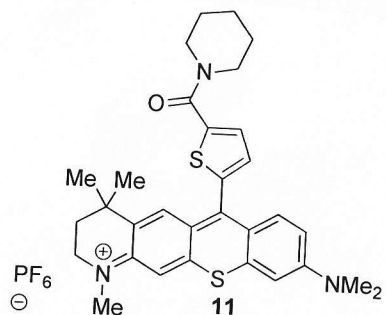
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd2c12
Data collected on: May 17 2011

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.8993732 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



1-A0-280-13C

Sample Name:

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

Sample directory:

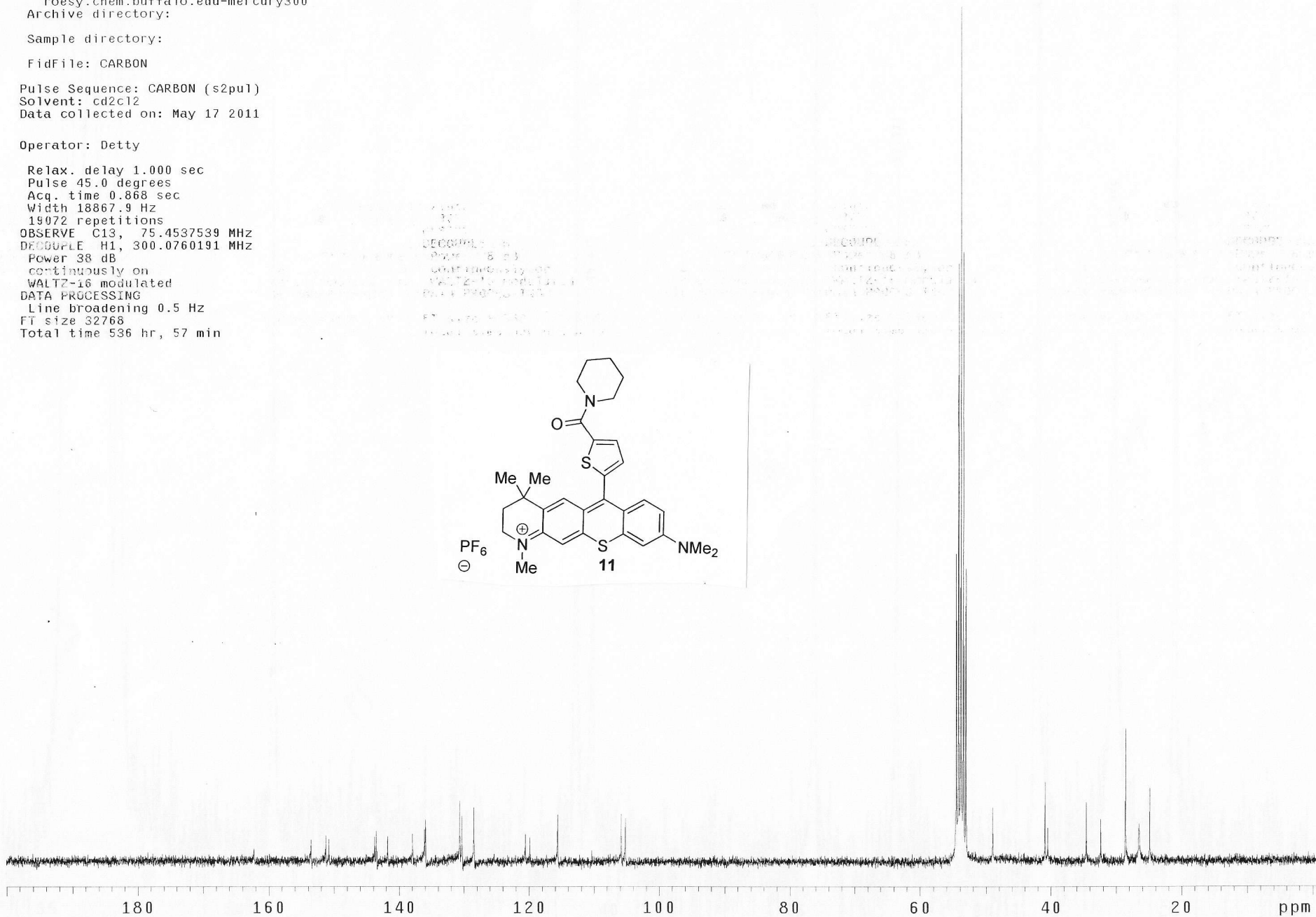
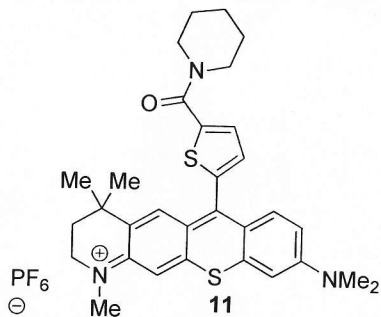
FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)
Solvent: cd2c12
Data collected on: May 17 2011

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 0.868 sec
Width 18867.9 Hz
19072 repetitions
OBSERVE C13, 75.4537539 MHz
DECOUPLE H1, 300.0760191 MHz
Power 38 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 32768
Total time 536 hr, 57 min

13C NMR
75.4537539 MHz
300.0760191 MHz
WALTZ-16
19072
536 hr, 57 min



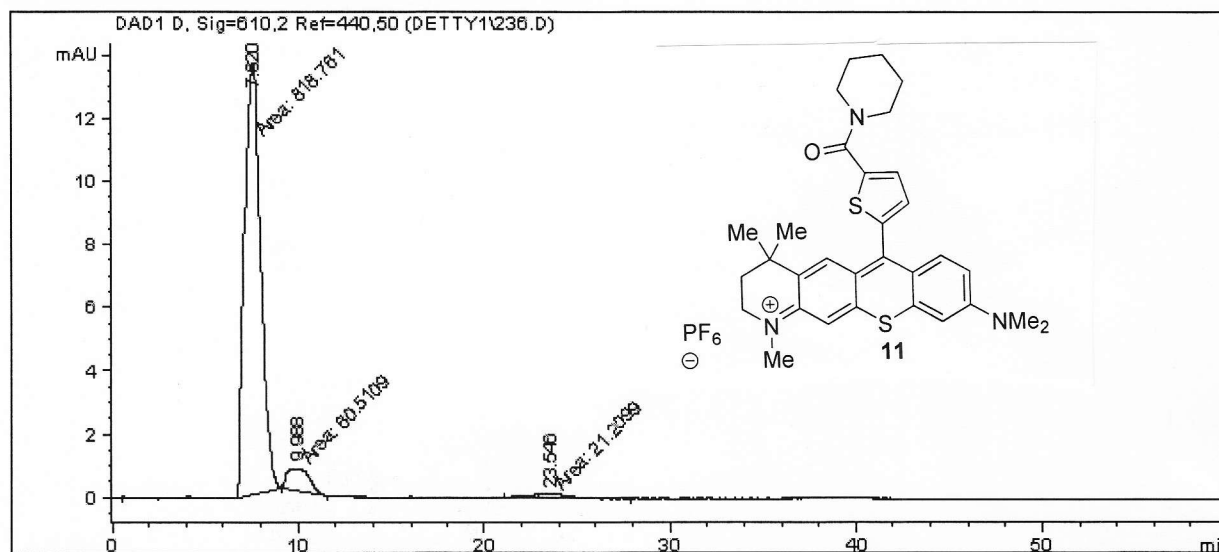
Data File C:\HPCHEM\1\DATA\DETTY1\236.D

Sample Name: 236L1

```

=====
Injection Date   : 7/5/2011 9:51:21 PM
Sample Name     : 236L1
Acq. Operator   : JCV
Location        : Vial 43
Inj Volume     : 3 µl
Acq. Method    : C:\HPCHEM\1\METHODS\CODY\DET610NM.M
Last changed   : 7/5/2011 5:58:53 PM by JCV
Analysis Method: C:\HPCHEM\1\METHODS\CODY\DET717NM.M
Last changed   : 7/5/2011 9:58:58 PM by JCV
                (modified after loading)
=====

```



```

=====
                          Area Percent Report
=====

```

```

Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Sample Amount  :      5.00000 [ng/ul] (not used in calc.)
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.620	MM	1.0041	818.76141	13.59078	90.9248
2	9.988	MM	1.3780	60.51088	7.31891e-1	6.7198
3	23.546	MM	2.9797	21.20992	1.18637e-1	2.3554

```
Totals :                      900.48221  14.44131
```

Results obtained with enhanced integrator!

```

=====
*** End of Report ***

```

1-A0-279-4

Sample Name:

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

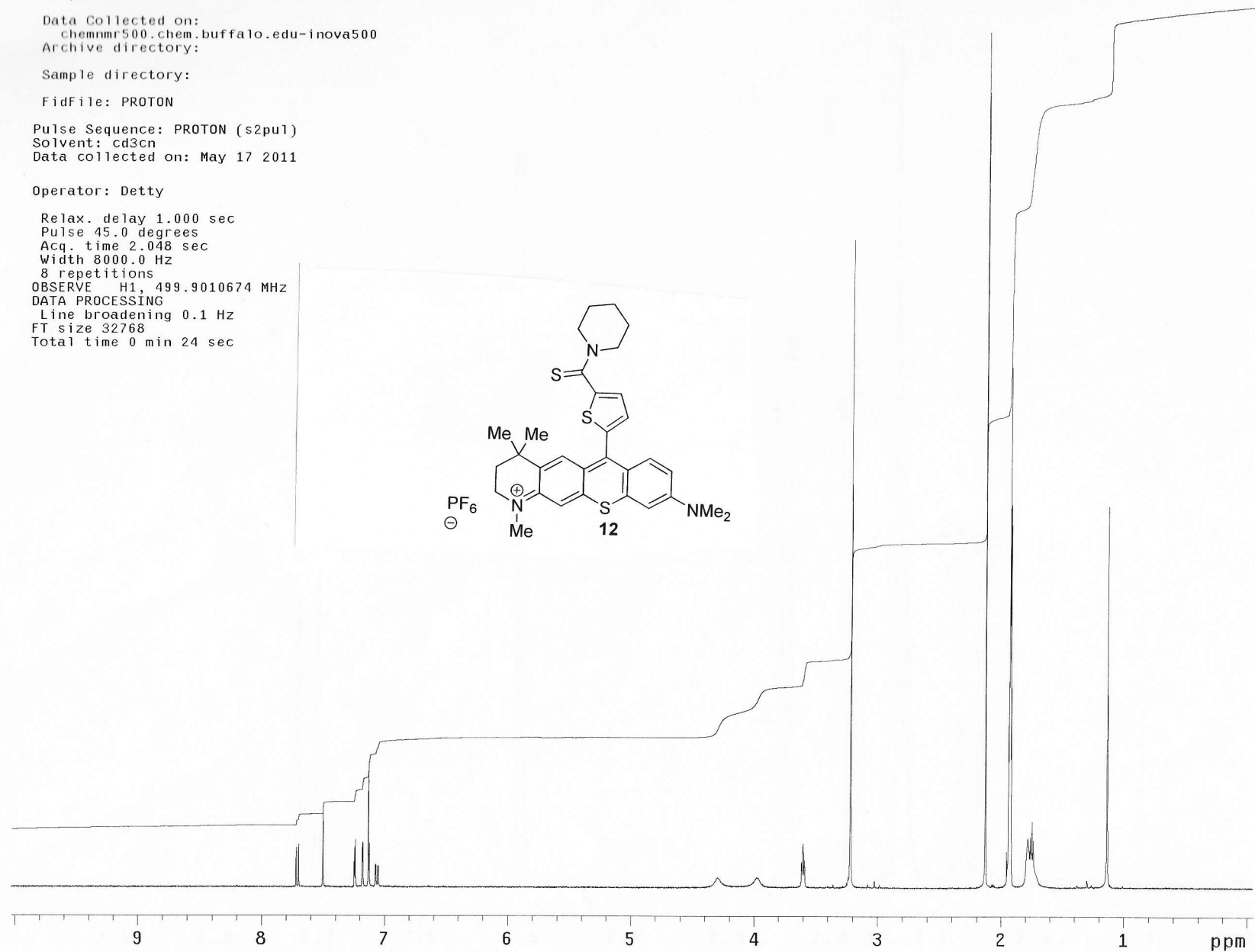
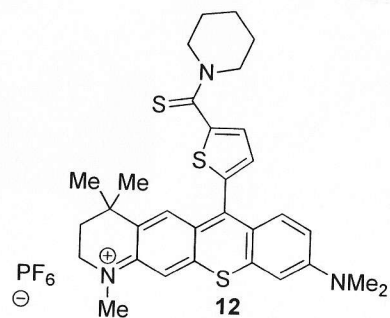
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pu1)
Solvent: cd3cn
Data collected on: May 17 2011

Operator: Detty

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.048 sec
Width 8000.0 Hz
8 repetitions
OBSERVE H1, 499.9010674 MHz
DATA PROCESSING
Line broadening 0.1 Hz
FT size 32768
Total time 0 min 24 sec



1-A0-145

Pulse Sequence: s2pu1

Solvent: cd2c12

Ambient temperature

GEMINI-300 "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

1472 repetitions

OBSERVE C13, 75.4537673 MHz

DECOUPLE H1, 300.0760192 MHz

Power 1023 dB

continuously on

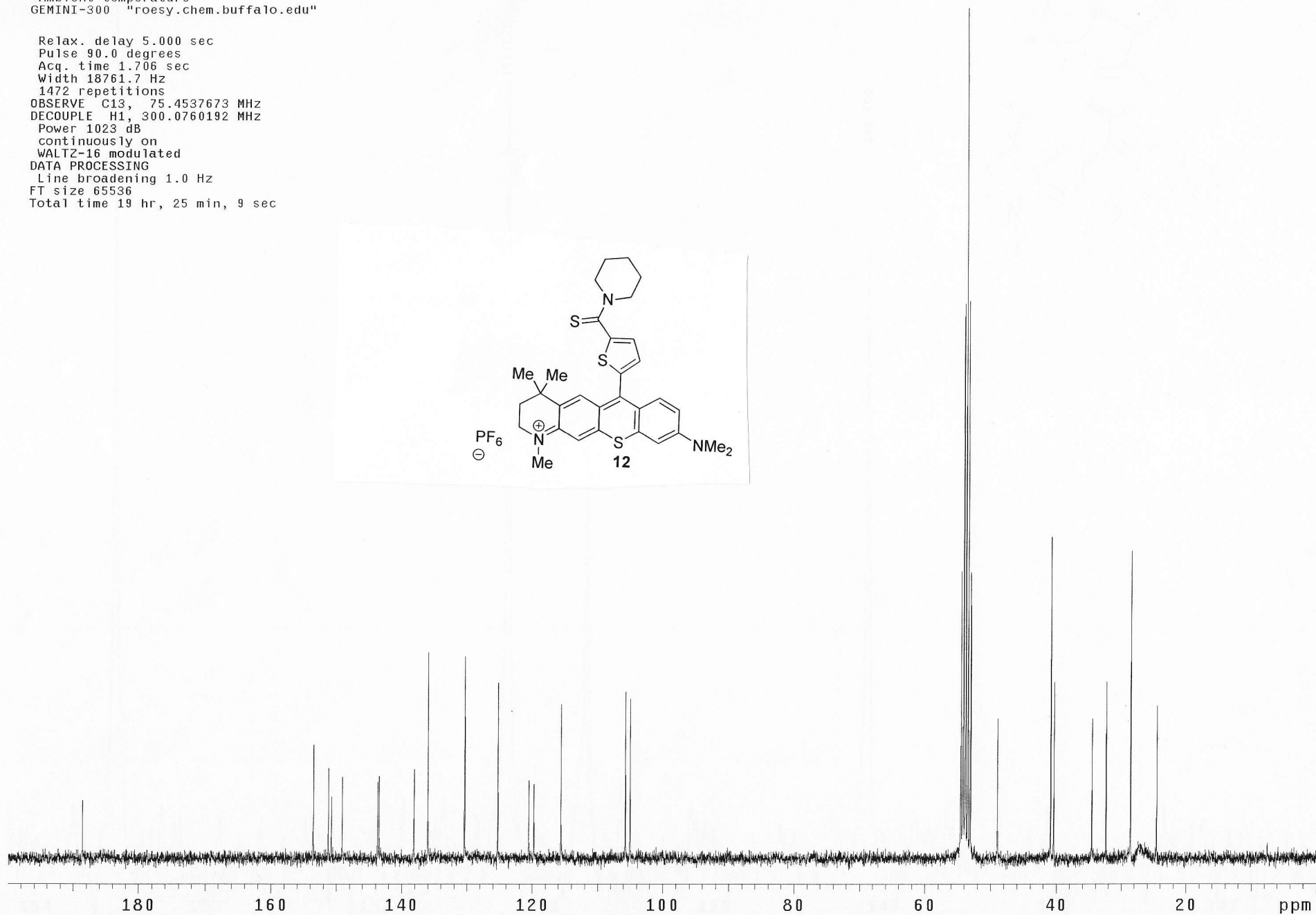
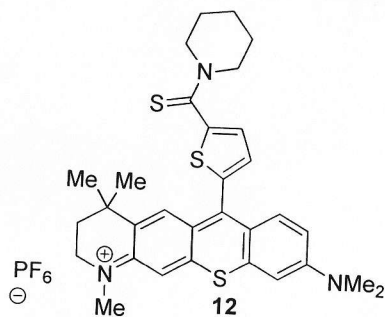
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 19 hr, 25 min, 9 sec



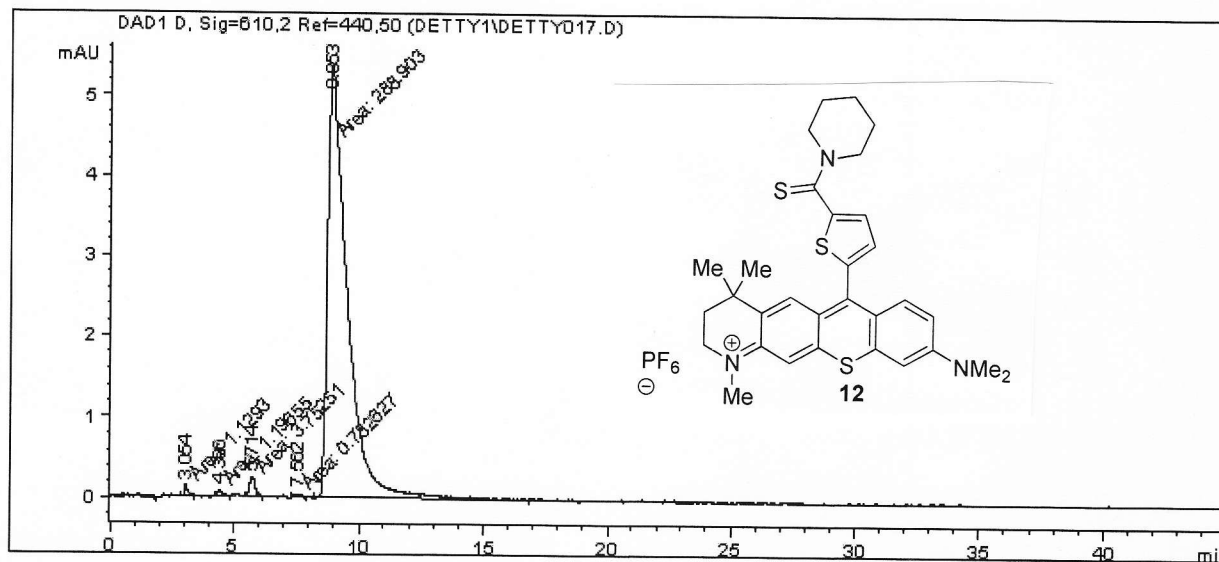
Data File C:\HPCHEM\1\DATA\DETTY1\DETTY017.D

Sample Name: 279

```

=====
Injection Date   : 6/28/2011 7:24:06 AM      Seq. Line : 17
Sample Name     : 279                        Location  : Vial 17
Acq. Operator  : JCV                        Inj      : 1
                                           Inj Volume: 3 µl
Acq. Method    : C:\HPCHEM\1\METHODS\CODY\DET610NM.M
Last changed   : 6/27/2011 6:57:46 PM by JCV
Analysis Method: C:\HPCHEM\1\METHODS\CODY\DET238.M
Last changed   : 6/28/2011 6:36:21 PM by JCV
                (modified after loading)
=====

```



```

=====
Area Percent Report
=====

```

```

Sorted By      : Signal
Multiplier    : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs

```

Signal 1: DAD1 D, Sig=610,2 Ref=440,50

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.054	MM	0.1488	1.12930	1.26449e-1	0.3818
2	4.396	MM	0.2429	1.19655	8.21087e-2	0.4046
3	5.714	MM	0.2570	3.75251	2.43331e-1	1.2688
4	7.562	MM	0.3264	7.82627e-1	3.99667e-2	0.2646
5	8.853	MM	0.8969	288.90286	5.36882	97.6802

```
Totals :                295.76385    5.86068
```

Results obtained with enhanced integrator!

```

=====
*** End of Report ***
=====

```


1-A0-059 - recryst

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

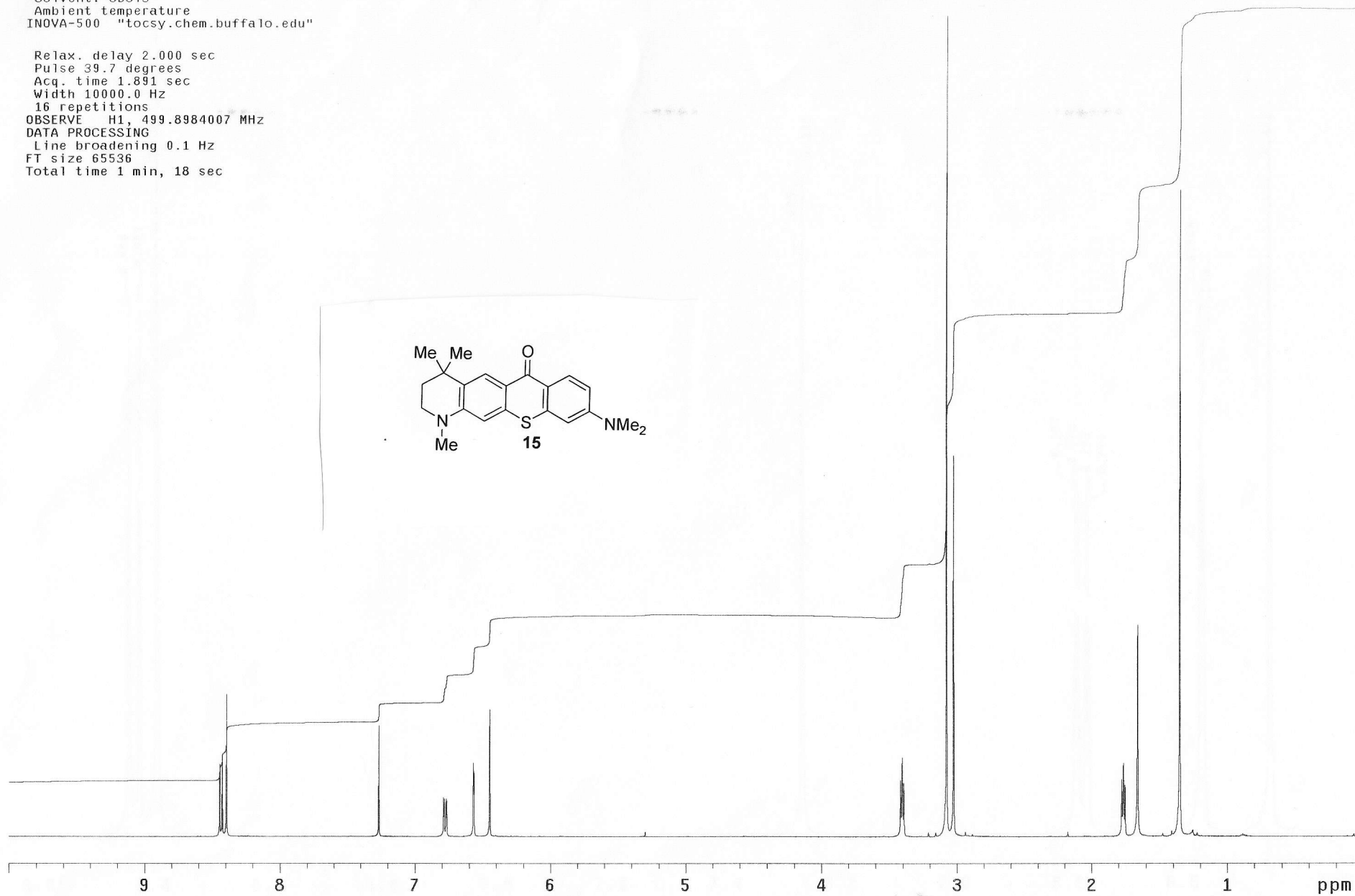
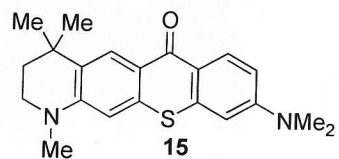
OBSERVE H1, 499.8984007 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 min, 18 sec



1-A0-059-13C

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

GEMINI-300 "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

736 repetitions

OBSERVE C13, 75.4536195 MHz

DECOUPLE H1, 300.0754431 MHz

Power 1023 dB

continuously on

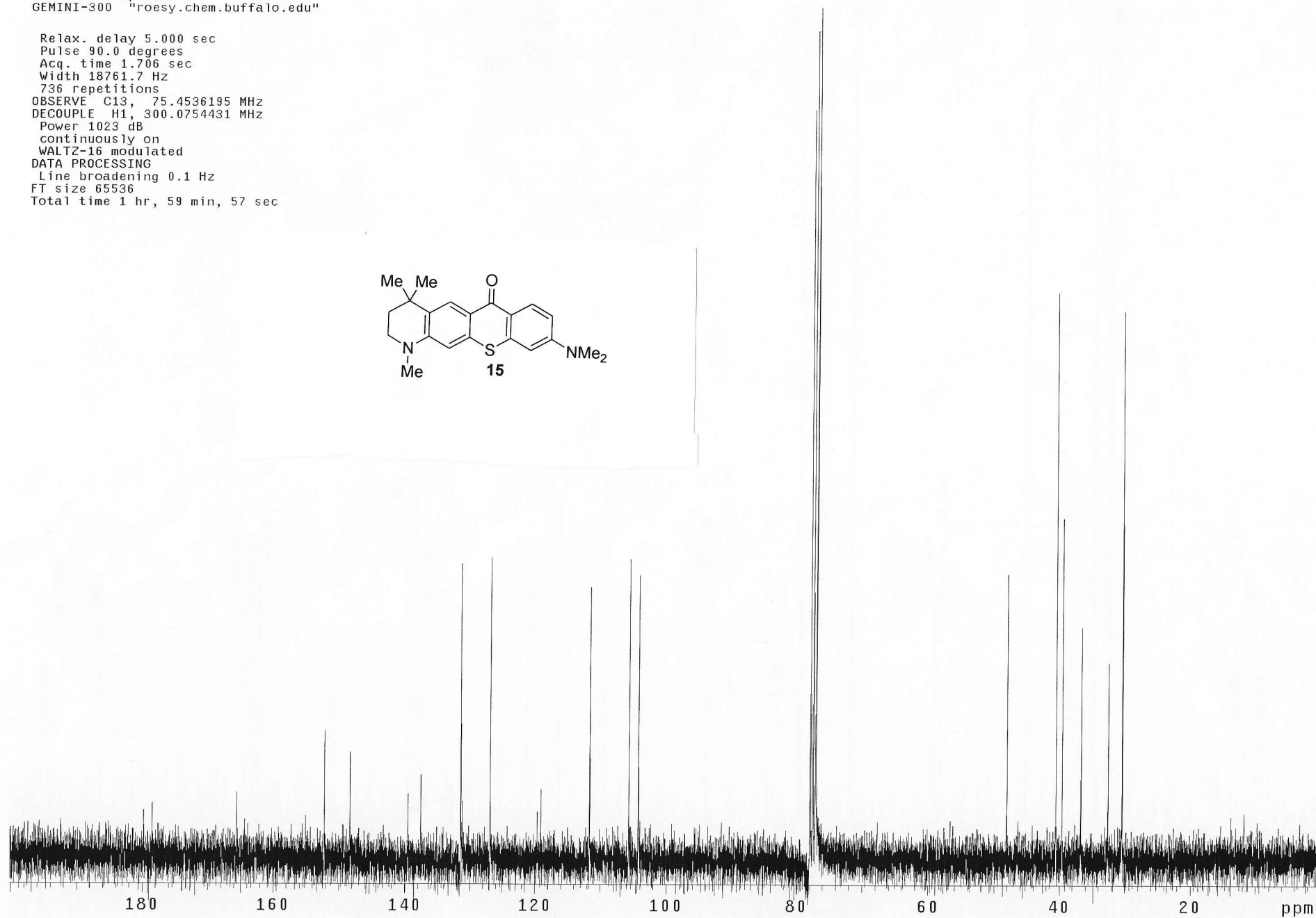
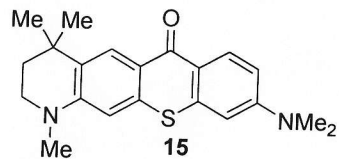
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 hr, 59 min, 57 sec



1-A0-032-b

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

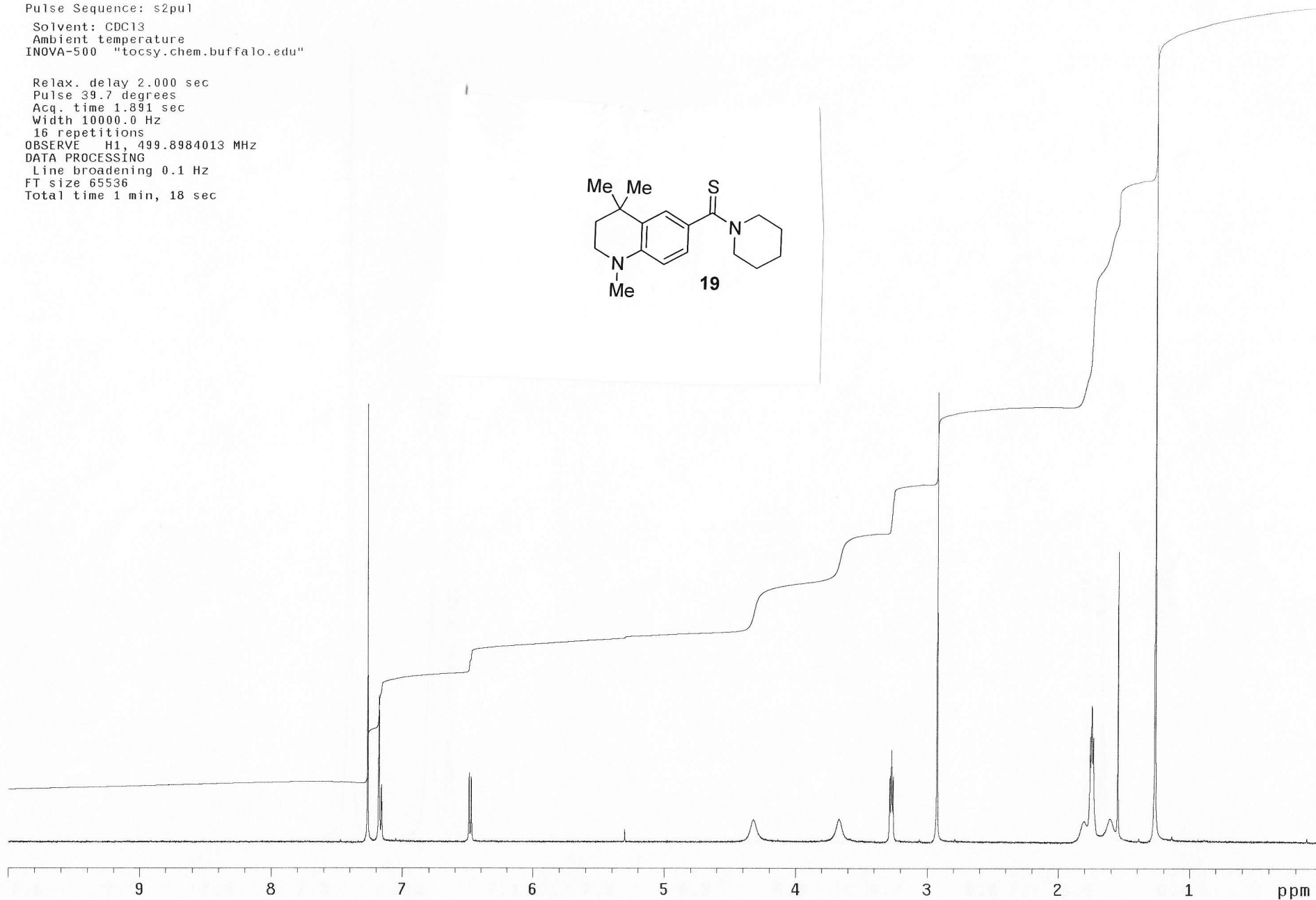
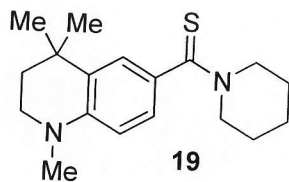
OBSERVE H1, 499.8984013 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 min, 18 sec



1-A0-031-carbon-2

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

GEMINI-300 "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

528 repetitions

OBSERVE C13, 75.4536583 MHz

DECOUPLE H1, 300.0754431 MHz

Power 1023 dB

continuously on

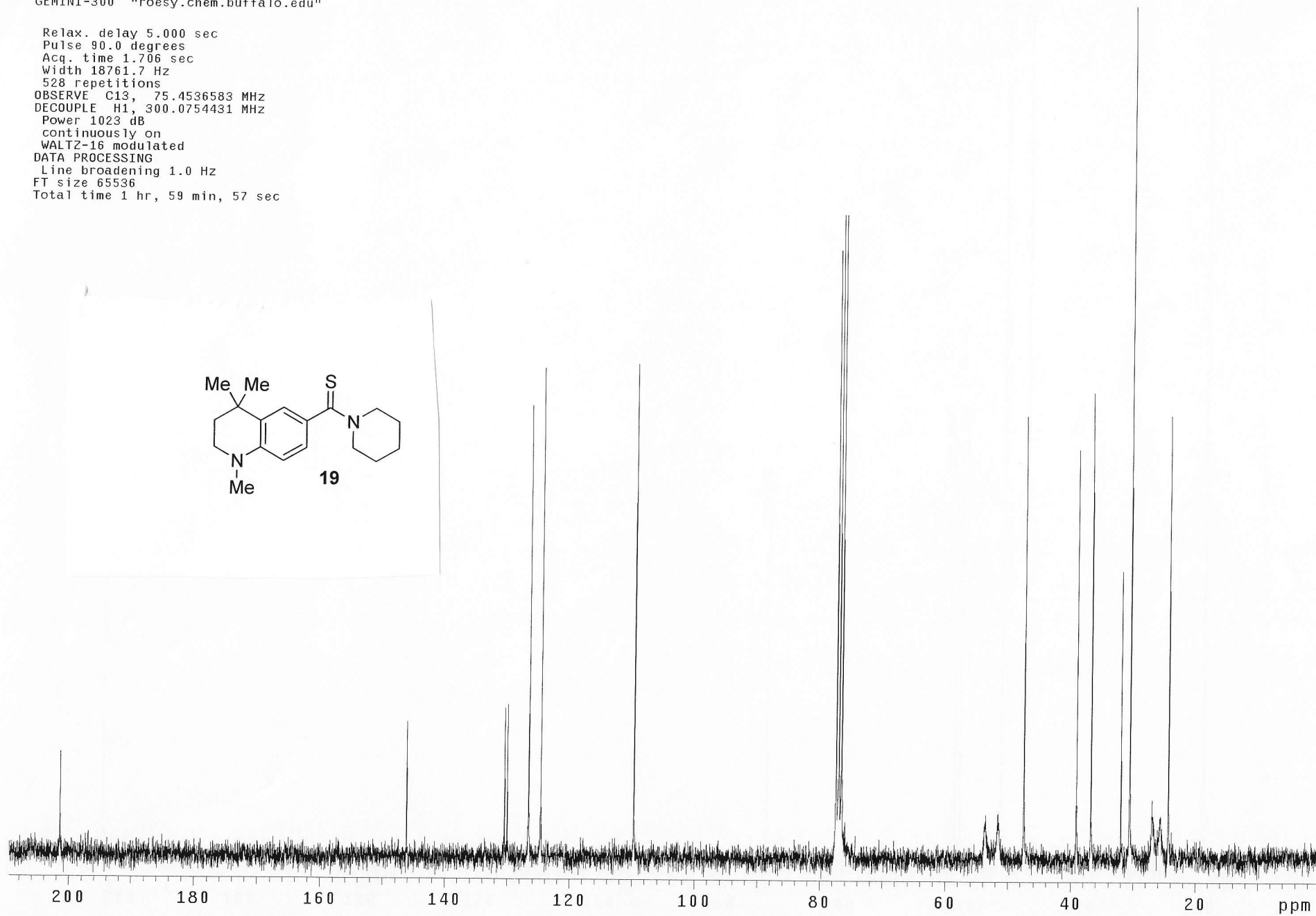
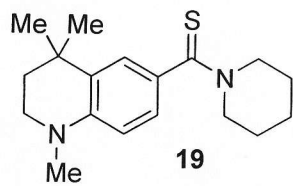
WALTZ-16 modulated

DATA PROCESSING

Line broadening 1.0 Hz

FT size 65536

Total time 1 hr, 59 min, 57 sec



1-A0-049-4

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

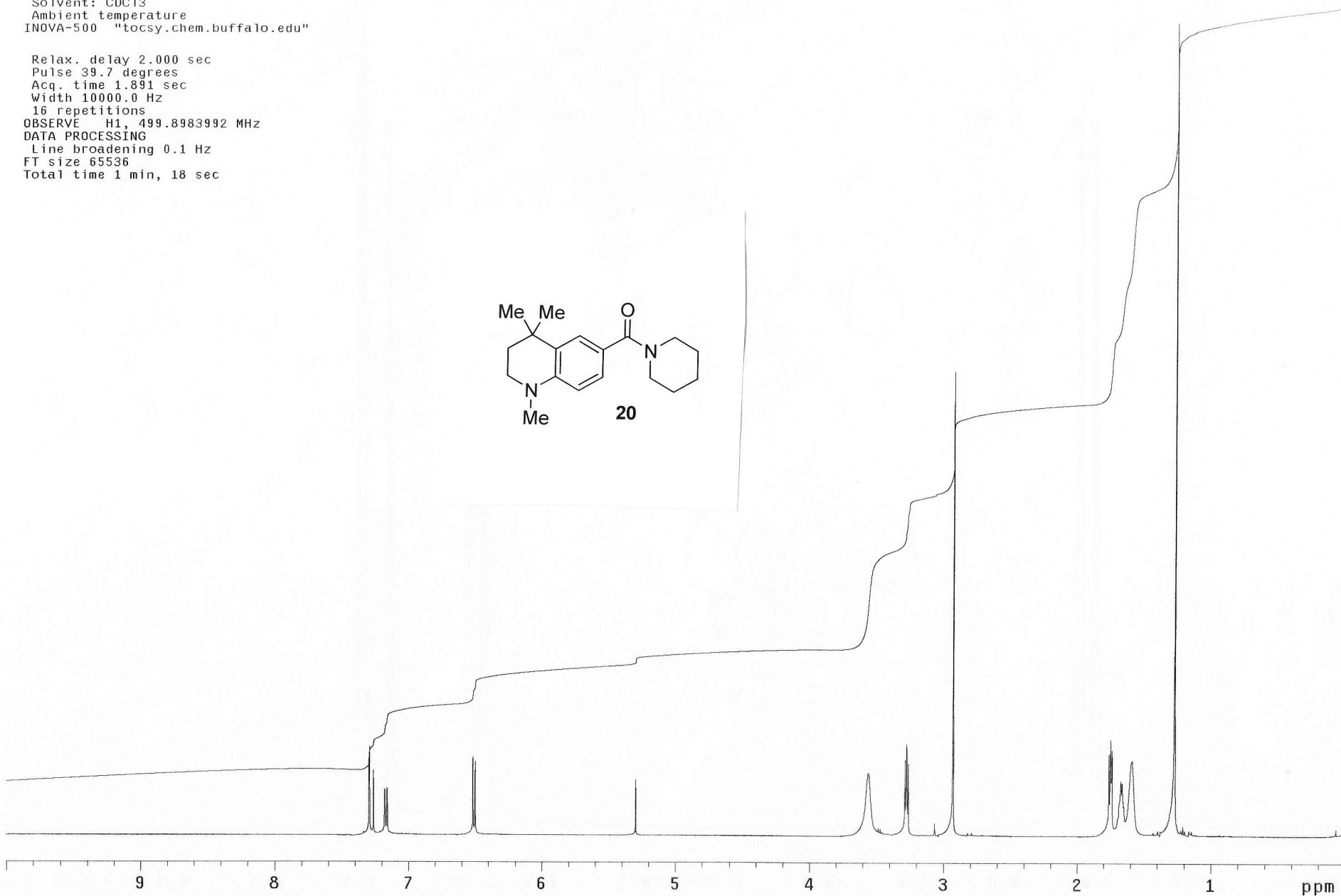
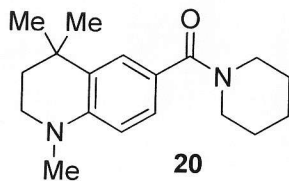
OBSERVE H1, 499.8983992 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 min, 18 sec



1-A0-037-carbon13

Pulse Sequence: s2pu1

Solvent: CDC13

Ambient temperature

GEMINI-300 "roesy.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

672 repetitions

OBSERVE C13, 75.4536195 MHz

DECOUPLE H1, 300.0754431 MHz

Power 1023 dB

continuously on

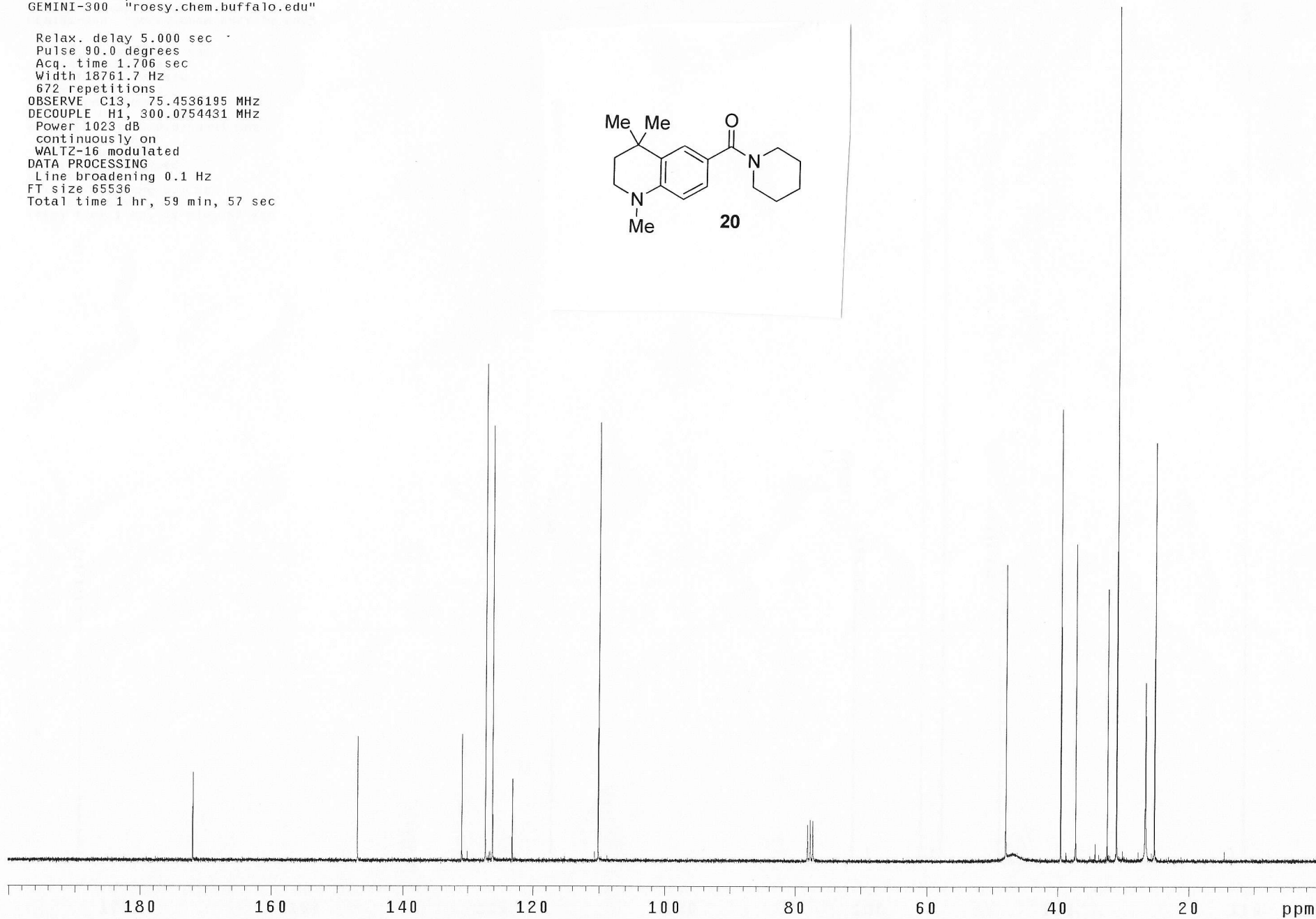
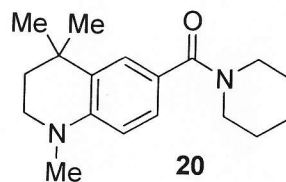
WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 hr, 59 min, 57 sec



1-A0-135-2

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

Sample #2

File: 1-A0-135-2

INOVA-500 "nmrdata.chem.buffalo.edu"

Relax. delay 1.000 sec

Pulse 47.9 degrees

Acq. time 1.800 sec

Width 6000.6 Hz

16 repetitions

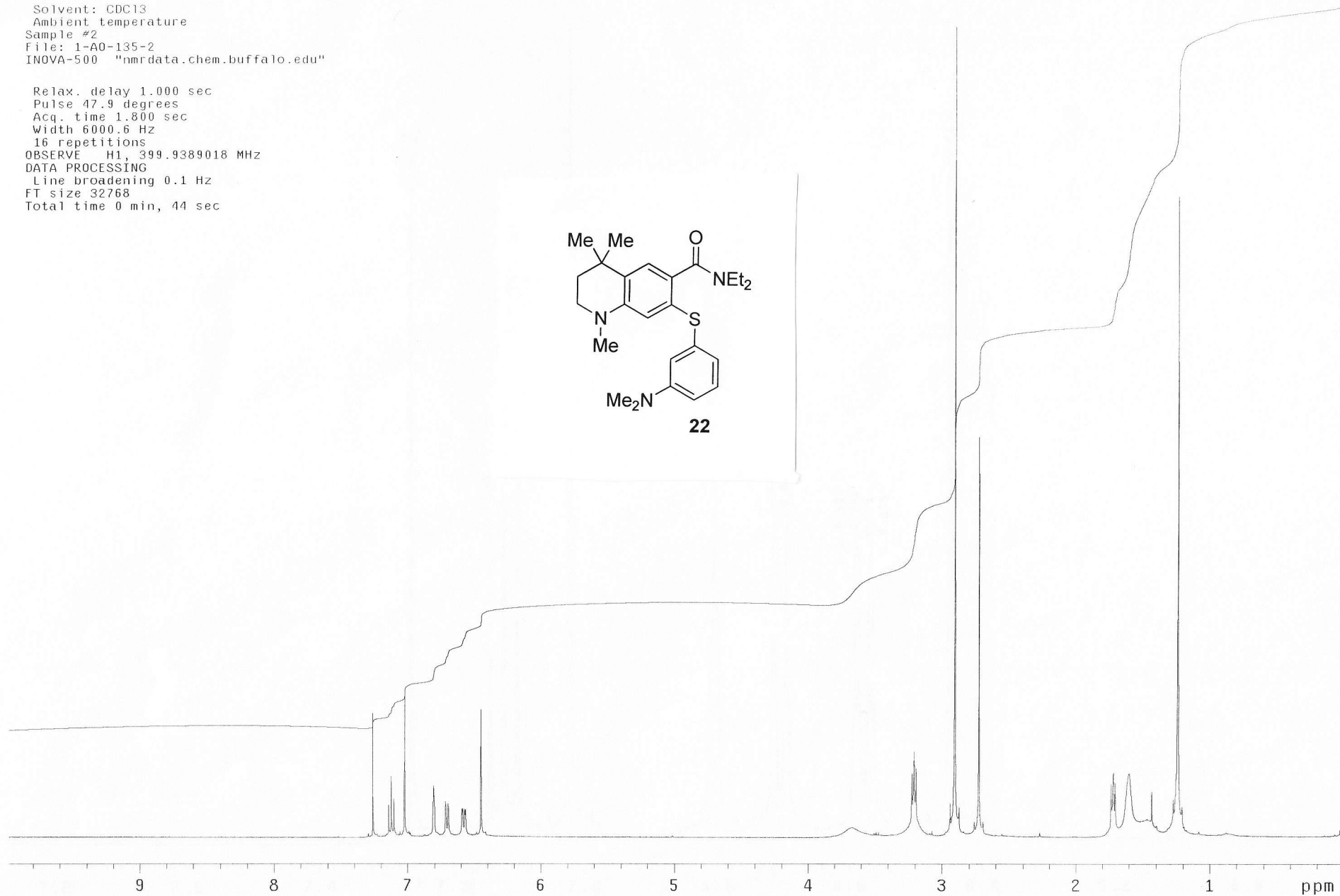
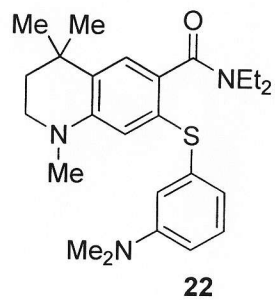
OBSERVE H1, 399.9389018 MHz

DATA PROCESSING

Line broadening 0.1 Hz

FT size 32768

Total time 0 min, 44 sec



1-A0-122-13C

Pulse Sequence: s2pul

Solvent: cd2c12

Ambient temperature

Sample #2

File: 1-A0-122-13C

INOVA-500 "nmrdata.chem.buffalo.edu"

Relax. delay 5.000 sec

Pulse 90.0 degrees

Acq. time 1.706 sec

Width 18761.7 Hz

1024 repetitions

OBSERVE C13, 75.4537682 MHz

DECOUPLE H1, 300.0760192 MHz

Power 1023 dB

continuously on

WALTZ-16 modulated

DATA PROCESSING

Line broadening 0.1 Hz

FT size 65536

Total time 1 hr, 55 min, 2 sec

