

## Supporting Information

### **Yb(OTf)<sub>3</sub> catalysed regioselective synthesis of unusual di- and tri- substituted 3,4-dihydrothiochromeno[3,2-e][1,3]thiazin-5(2H)-one derivatives through a pseudo four-component hetero-Diels-Alder Reaction**

Karuna Mahato,<sup>a</sup> Prasanta Ray Bagdi<sup>a</sup> and Abu T. Khan<sup>\*a,b</sup>

<sup>a</sup>*Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati 781 039, India*

Tel.: +91 361 2582305; Fax: +91 361 2582349

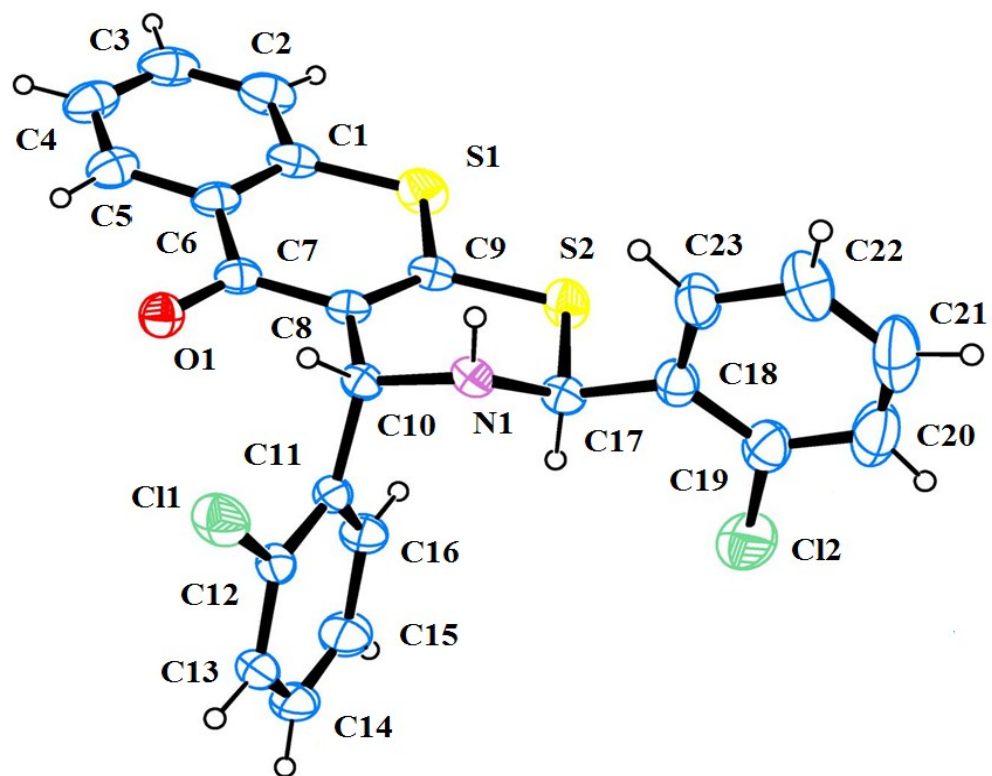
<sup>b</sup>*Present address: Vice-Chancellor, Aliah University, IIA/27, New Town, Near Eco-Space, Kolkata-700 156, India*

E-mail: atk@iitg.ernet.in (A.T. Khan)

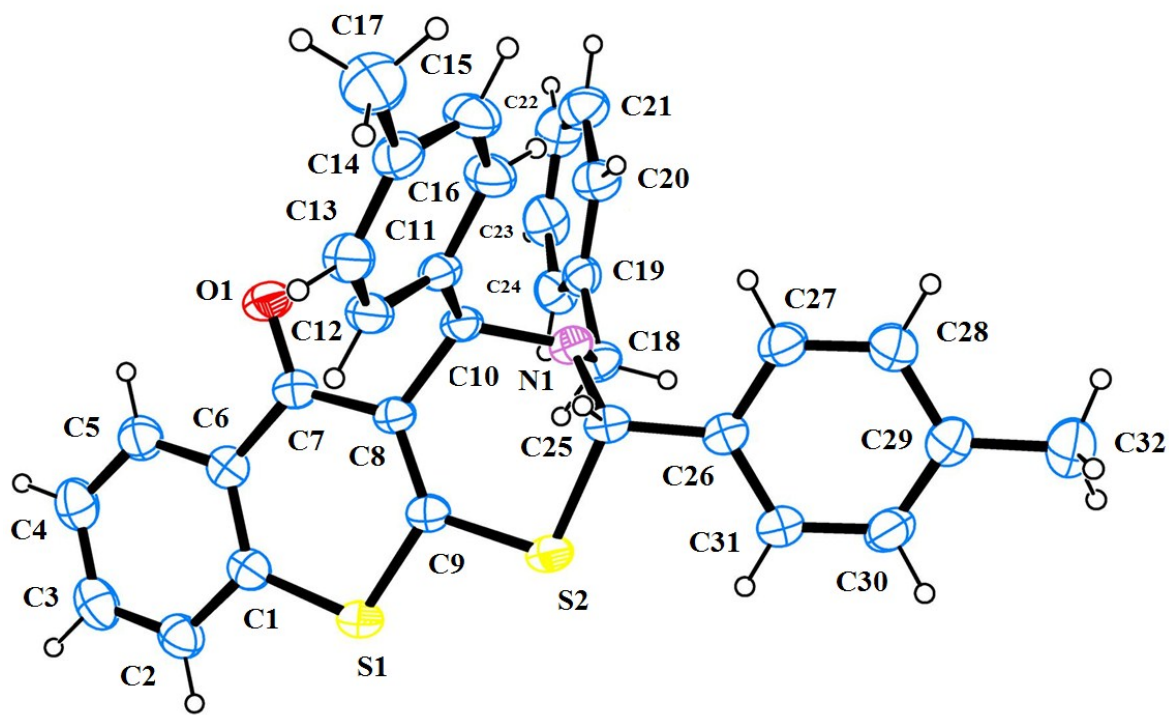
Title page	1
General Experimental Procedure	2
ORTEP diagram of Compound <b>4f</b> and <b>6b</b>	3-4
Crystal Data and Structure Refinement for Compound <b>4f</b> and <b>6b</b>	5
Copies of <sup>1</sup> H NMR, <sup>13</sup> C NMR and HRMS spectra of all Compounds	6-84

## I. General Information and Methods

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on 400 MHz, 600 MHz and 100 MHz, 150 MHz spectrometer TMS as internal reference; chemical shifts ( $\delta$  scale) are reported in parts per million (ppm).  $^1\text{H}$  NMR Spectra are reported in the order: multiplicity, coupling constant ( $J$  value) in hertz (Hz) and no of protons; signals were characterized as s (singlet), d (doublet), t (triplet), m (multiplet) and bs (broad). IR spectra were recorded in KBr. HRMS spectra were recorded using ESI (TOF) mode. The X-ray crystal structures were determined with a diffractometer. Complete crystallographic data of **4f** (CCDC no. 1029813) and **6b** (CCDC no. 1029814) for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-1223-336033, e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk) or via: [www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk)).



**Figure 1.** 30% probability of ORTEP ellipsoids of 4f

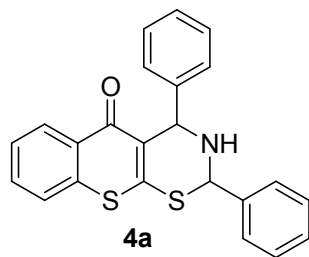


**Figure 2.** 30% probability of ORTEP ellipsoids of **6b**

**Table 1** Crystal Data and Structure Refinement for Compound **4f** and **6b**

Entry	Identification code	Compound <b>4f</b>	Compound <b>6b</b>
01	Empirical formula	C <sub>23</sub> H <sub>15</sub> Cl <sub>2</sub> N O S <sub>2</sub>	C <sub>32</sub> H <sub>27</sub> N O S <sub>2</sub>
02	Formula weight	456.38	505.67
03	Temperature	296(2) K	296(2) K
04	Wavelength	0.71073	0.71073
05	Radiation type	Mo K $\alpha$	Mo K $\alpha$
06	Radiation source	Fine-focus sealed tube	Fine-focus sealed tube
07	Crystal system	Triclinic	Monoclinic
08	Space group	P-1	P2 <sub>1</sub> /c
09	Cell length	a 10.2935(7) b 10.5264(9) c 10.7561(9)	a 11.6518(3) b 15.2049(4) c 14.9453(4)
10	Cell Angle	$\alpha$ 84.384(7) $\beta$ 66.574(7) $\delta$ 76.989(6)	$\alpha$ 90.00 $\beta$ 101.788(2) $\delta$ 90.00
11	Cell Volume	1041.89(16)	2591.93(12)
12	Density	1.458	1.300
13	Completeness to theta	28.87° / 99.6%	25.03° / 99.6%
14	Absorption correction	multi-scan	multi-scan
15	Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
16	Index ranges	-13 $\leq$ h $\leq$ 13, -14 $\leq$ k $\leq$ 7, -14 $\leq$ l $\leq$ 14	-12 $\leq$ h $\leq$ 12, - 16 $\leq$ k $\leq$ 16, -16 $\leq$ l $\leq$ 16
17	Reflection number	5468	4580
18	Theta range	3.25-28.87	1.79-25.03
19	Cell formula units Z	2	4
20	CCDC no	1029813	1029814

# <sup>1</sup>H NMR spectra the compound: 4a

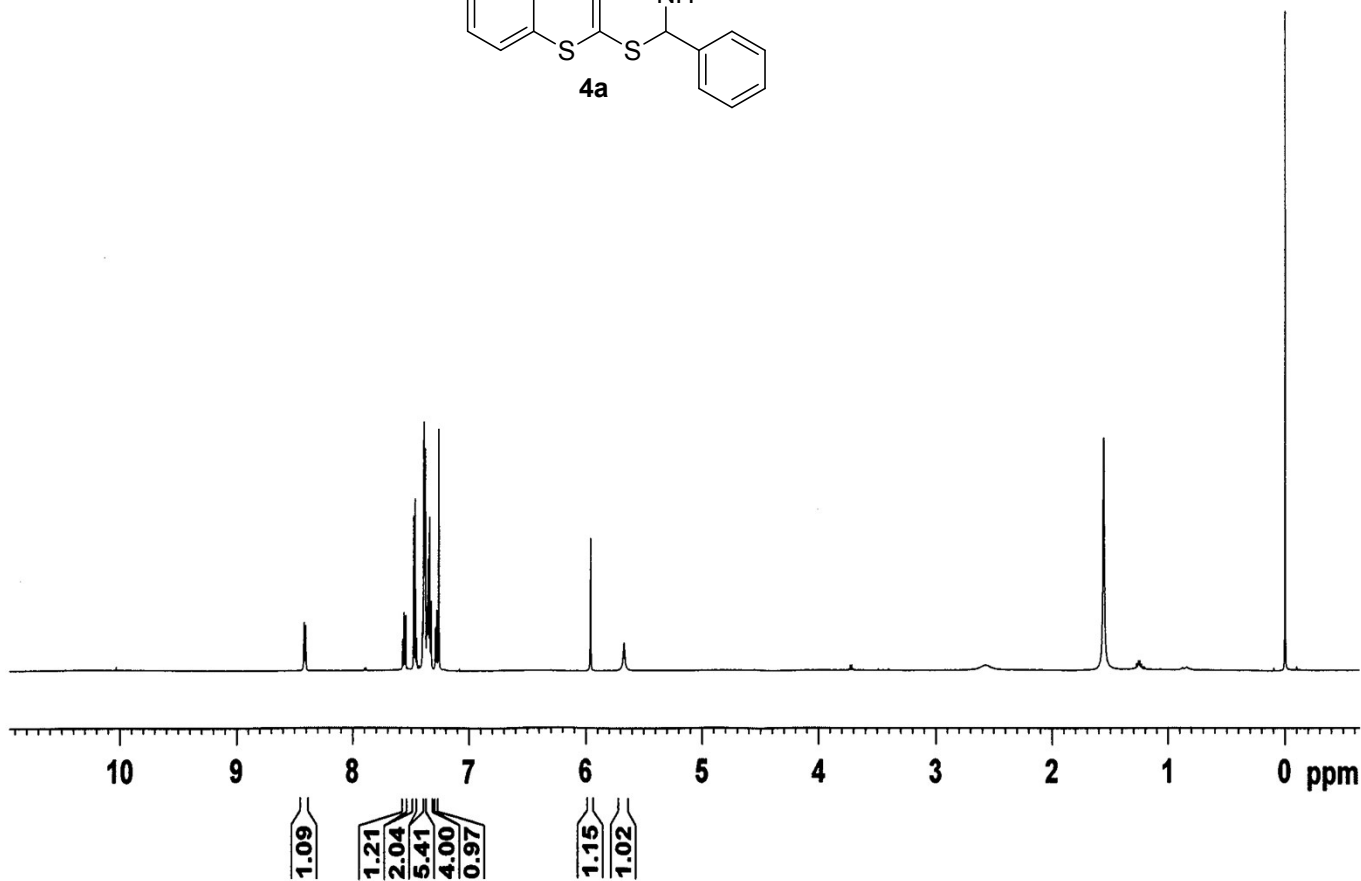


Current Data Parameters  
NAME KM-BEN-2-1H  
EXPNO 1  
PROCNO 1

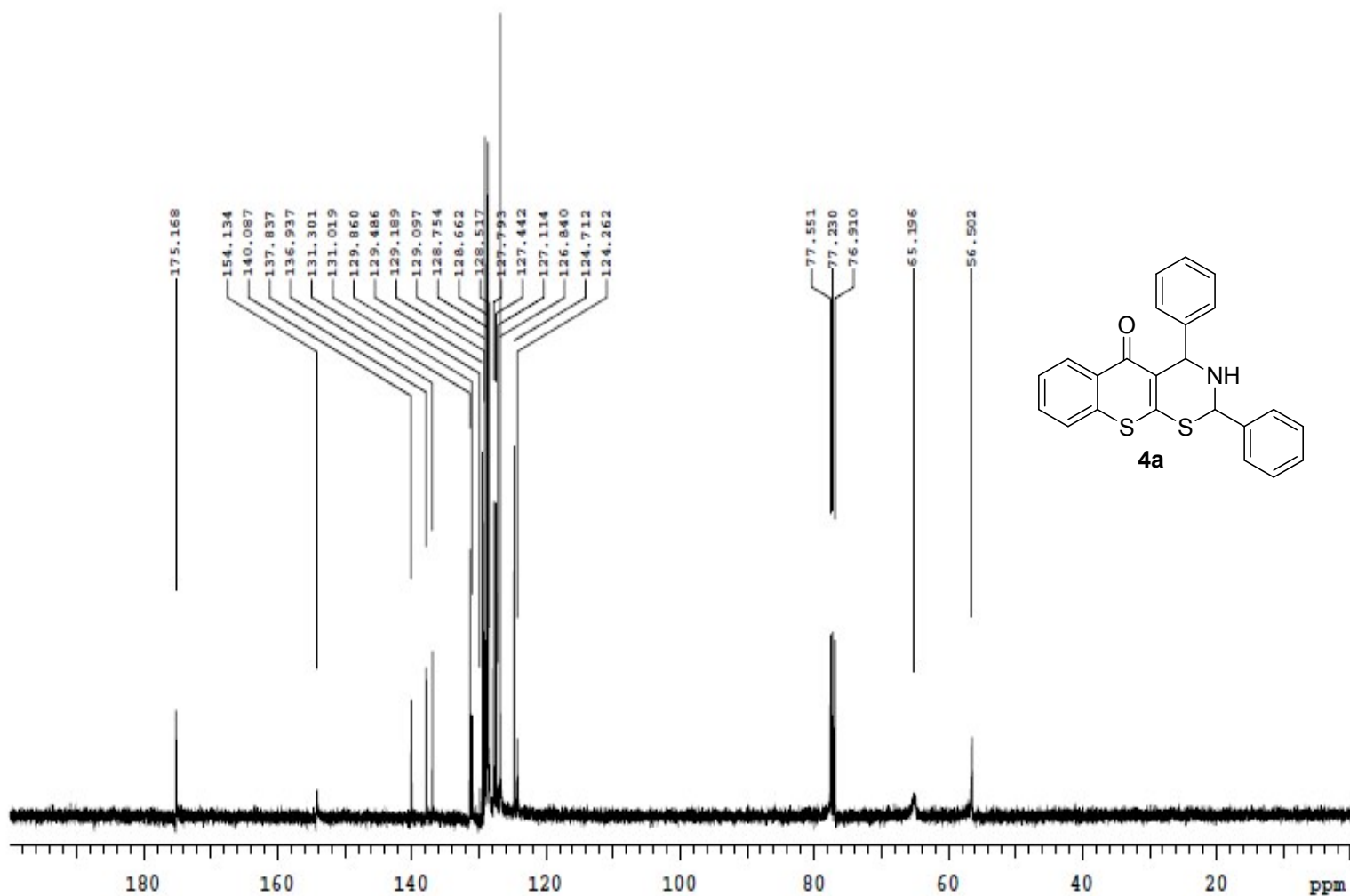
F2 - Acquisition Parameters  
Date\_ 20150226  
Time\_ 11.59  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 113  
DW 41.600 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
SF01 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700137 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



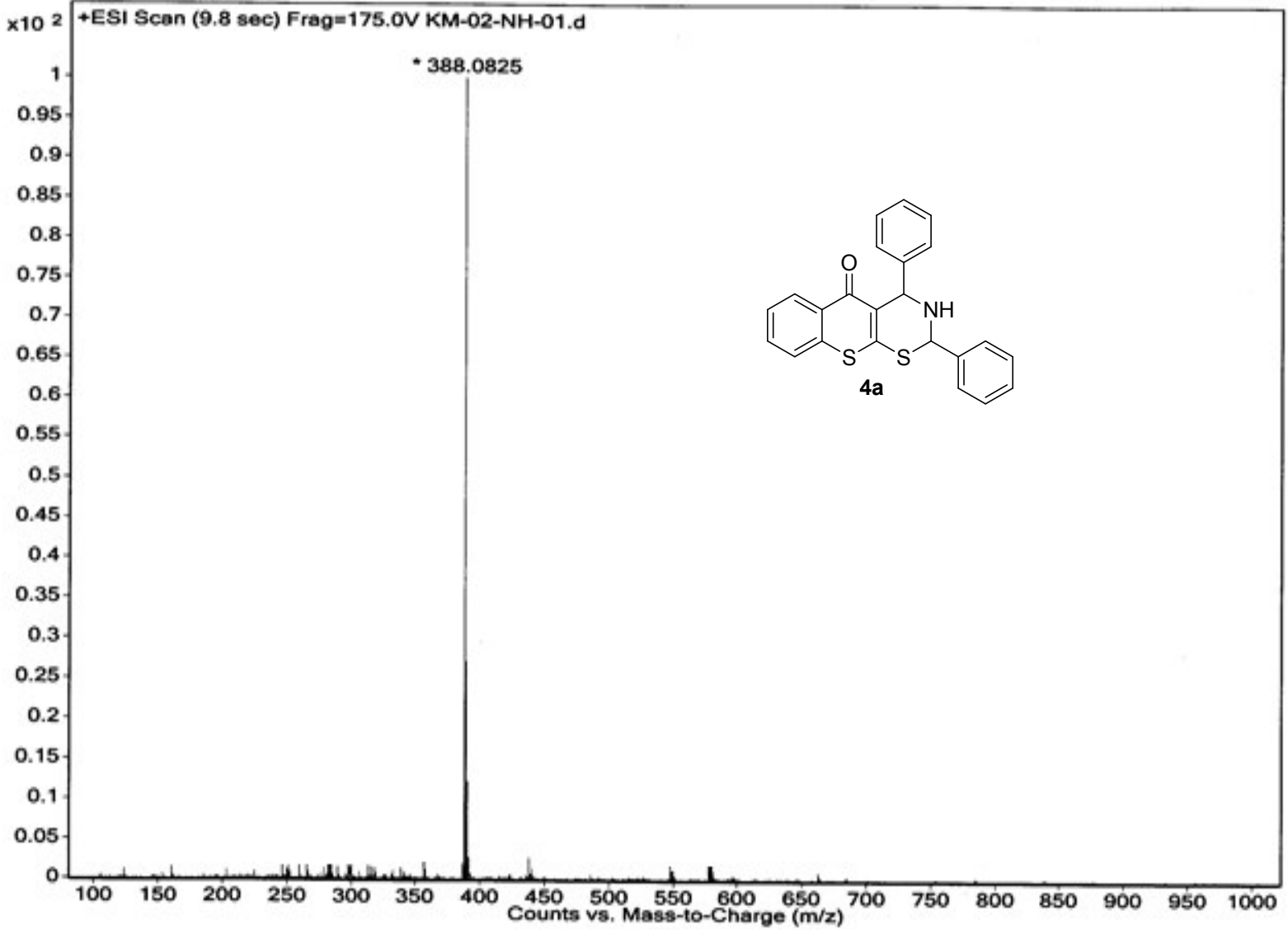
# <sup>13</sup>CNMR spectra of compound: 4a



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 610 repetitions	<b>OBSERVE</b> C13, 100.5425947 <b>DECOUPLE</b> H1, 399.8540270 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 23 minutes	<b>EM-02-NH-1-13C</b> Solvent: D2O Temp. 25.0 C / 298.1 K Operator: chem File: EM-02-NH-1-13C Mercury-400 "IITG-NMR"
---	--	--	---

# HRMS spectra of compound: 4a

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time





# <sup>1</sup>H NMR spectra the compound: 4b

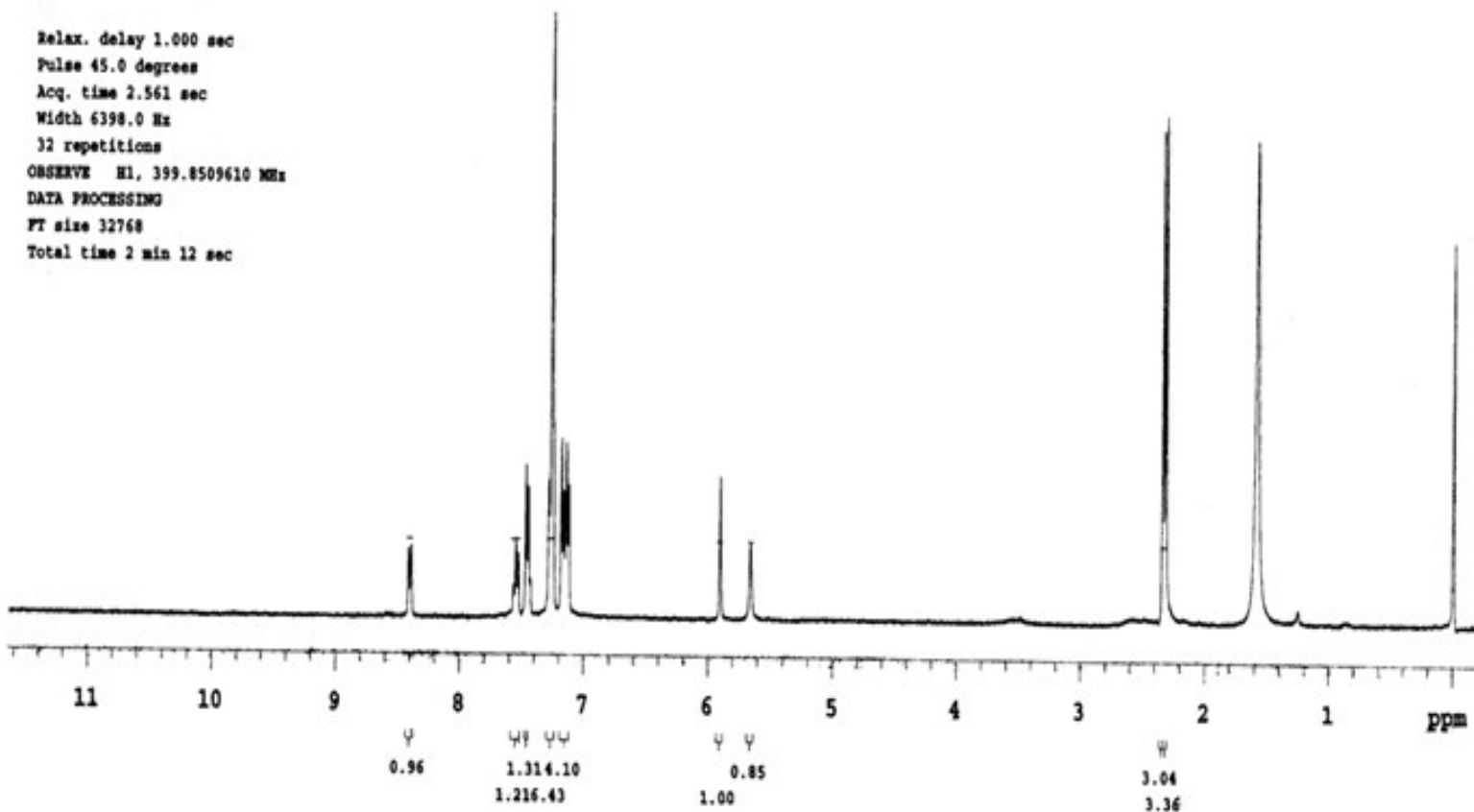
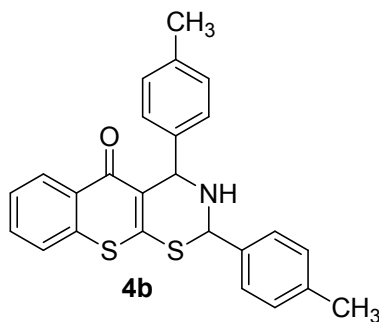
Sample Name:  
EM-02-NH-05-1H  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: EM-02-NH-05-1H

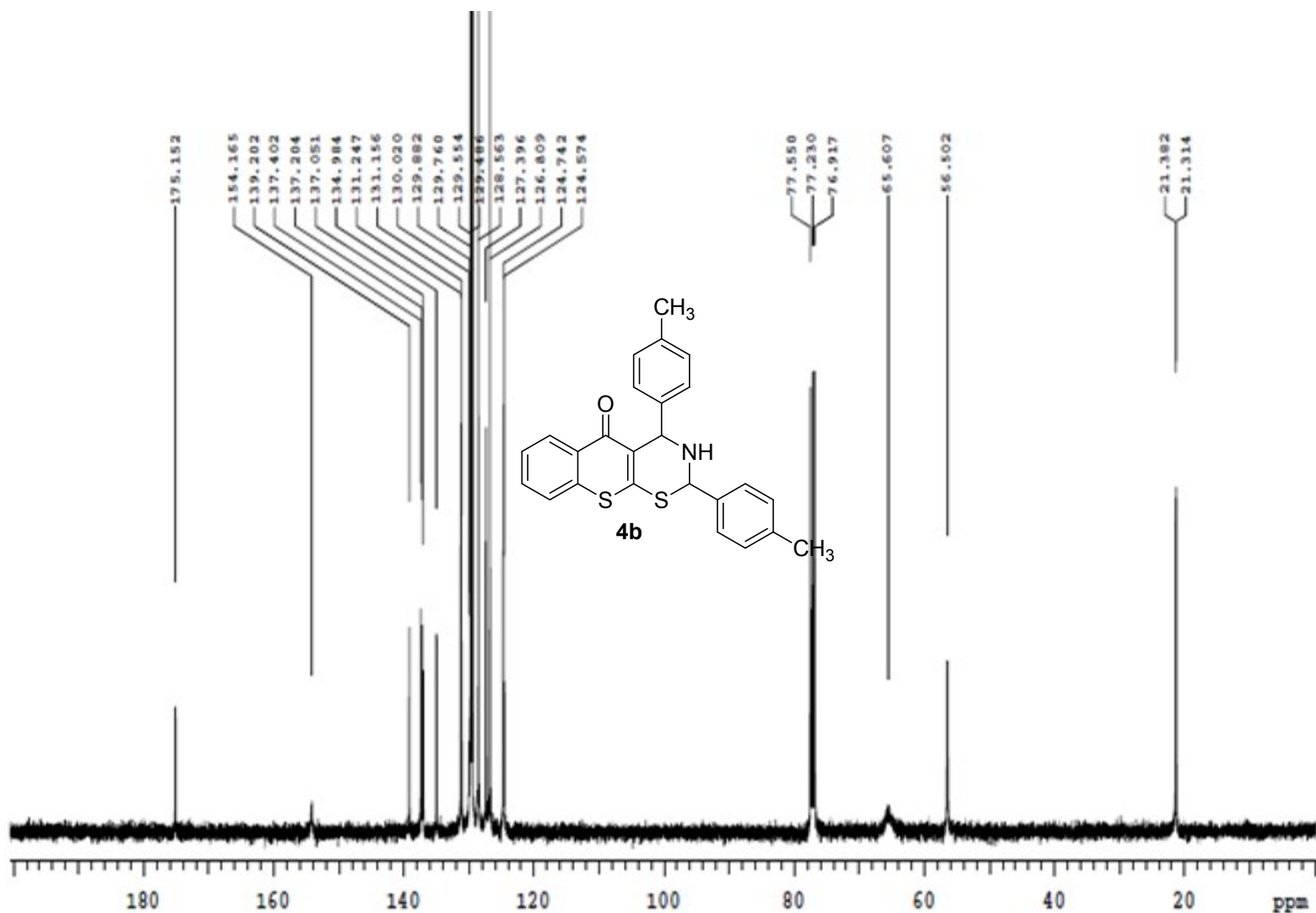
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Mar 4 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509610 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



### <sup>13</sup>CNMR spectra of compound: 4b



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
3752 repetitions

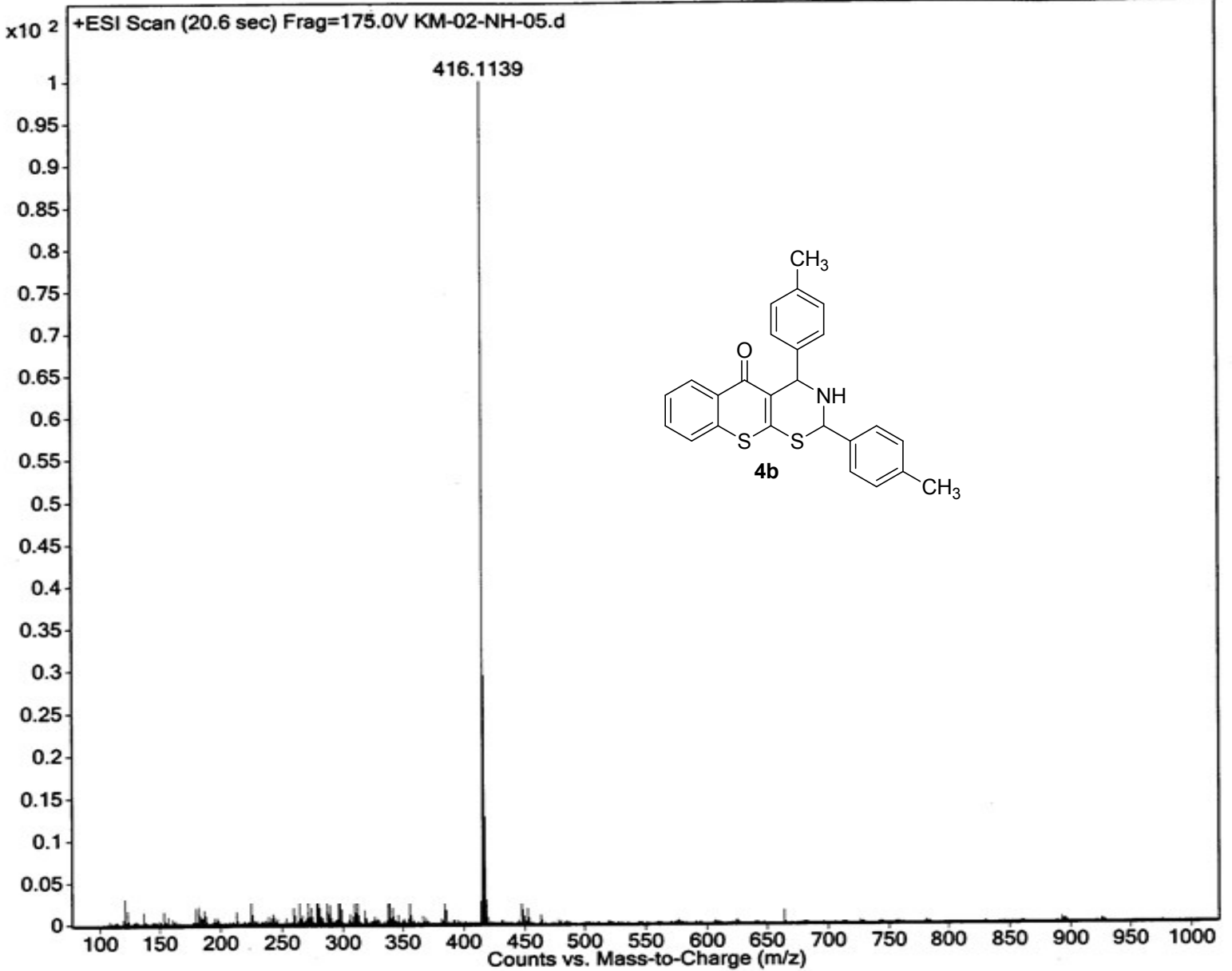
OBSERVE C13, 100.5425870  
DECOUPLE H1, 399.8529994  
Power 42 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 2.4 hours

KM-02-NH-05-13C  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: KM-02-NH-05-13C  
Mercury-400 \*IITG-NMR\*

# HRMS spectra of compound: 4b

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra the compound: 4c

Sample Name:

KM-02-NH-02

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/home/chem/data/study

Sample directory:

PICHYDRA-ZN-tit-4-01

Fidfile: KM-02-NH-02

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 7 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

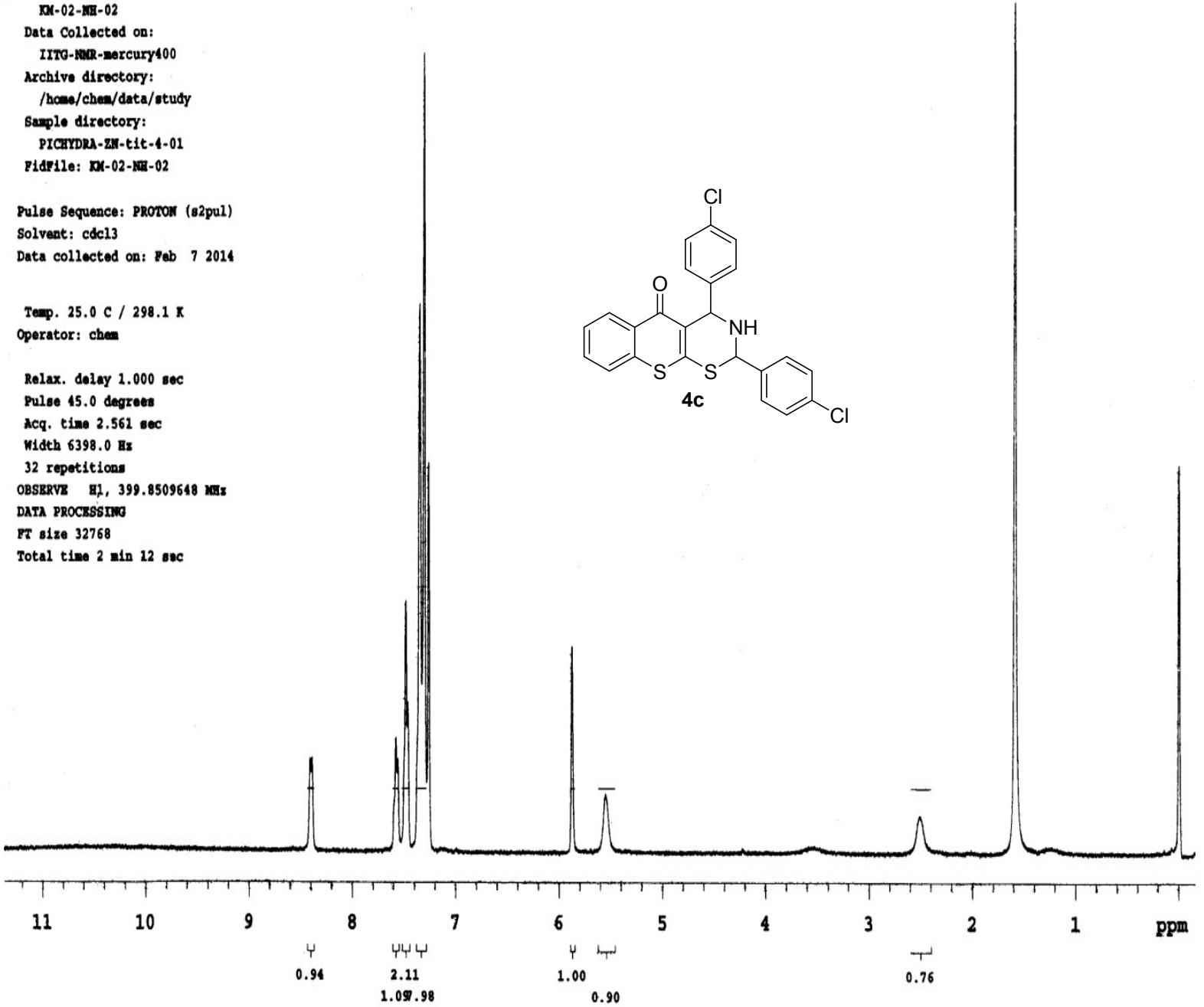
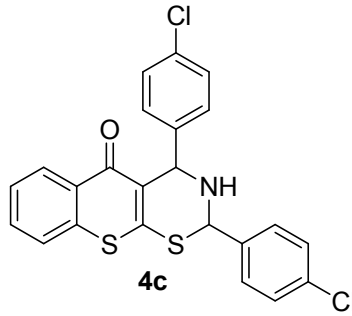
32 repetitions

OBSERVE H1, 399.8509648 MHz

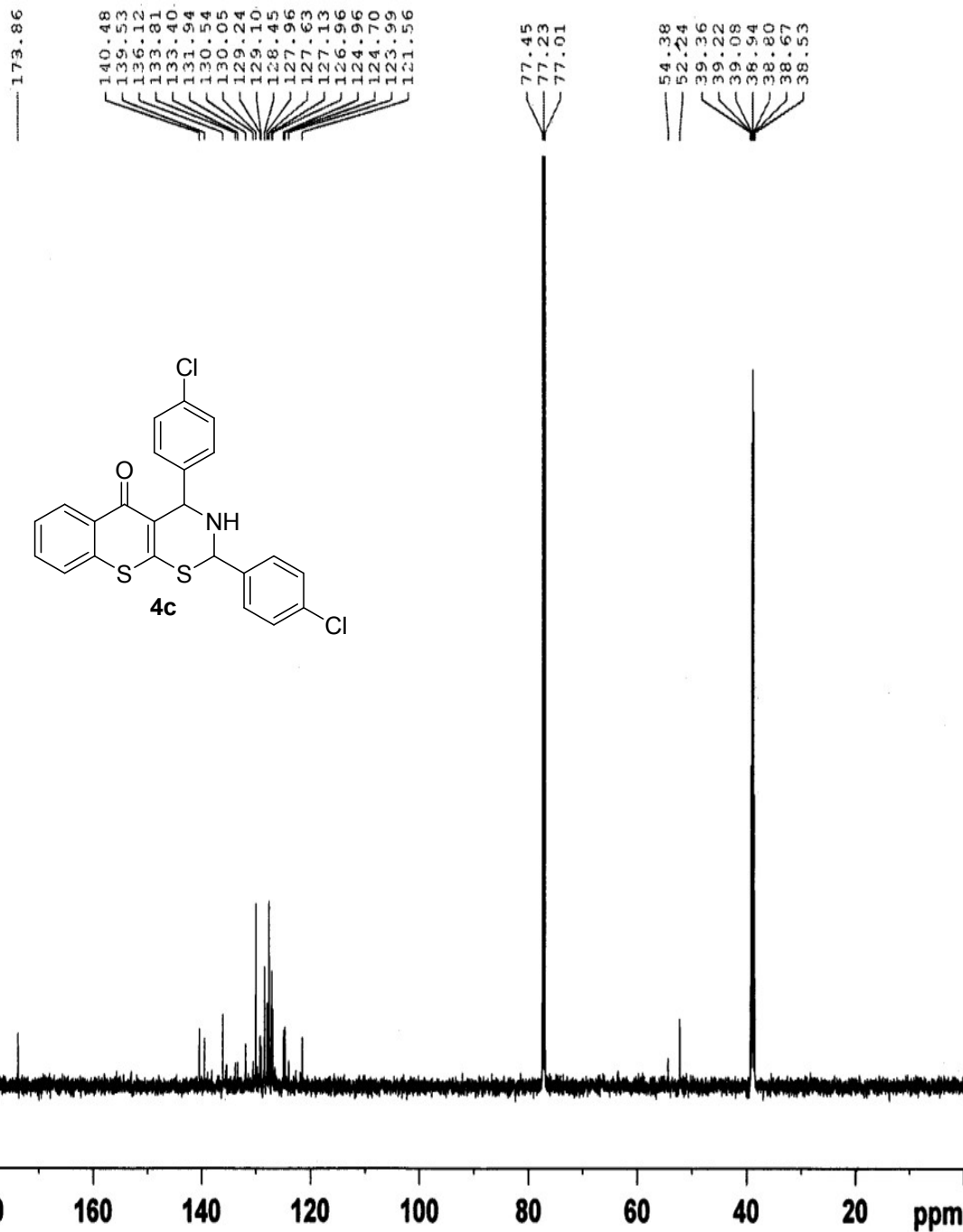
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



<sup>13</sup>CNMR spectra of compound: 4c



Current Data Parameters  
NAME KM-02-NH-4CL-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140826  
Time\_ 9.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 235  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 298.9 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

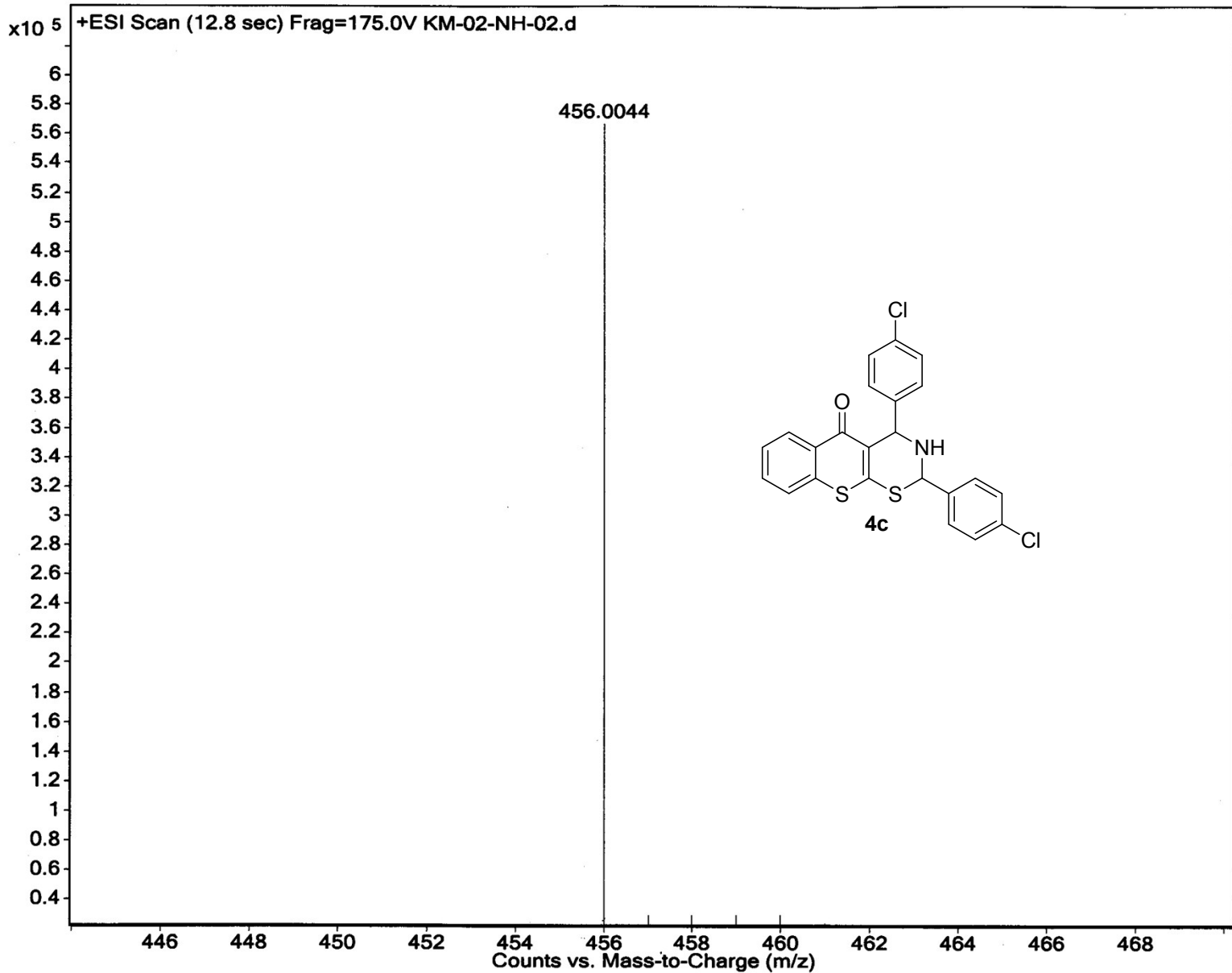
----- CHANNEL f1 -----  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

----- CHANNEL f2 -----  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9137350 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

# HRMS spectra of compound: 4c

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>HNMR spectra the compound: 4d

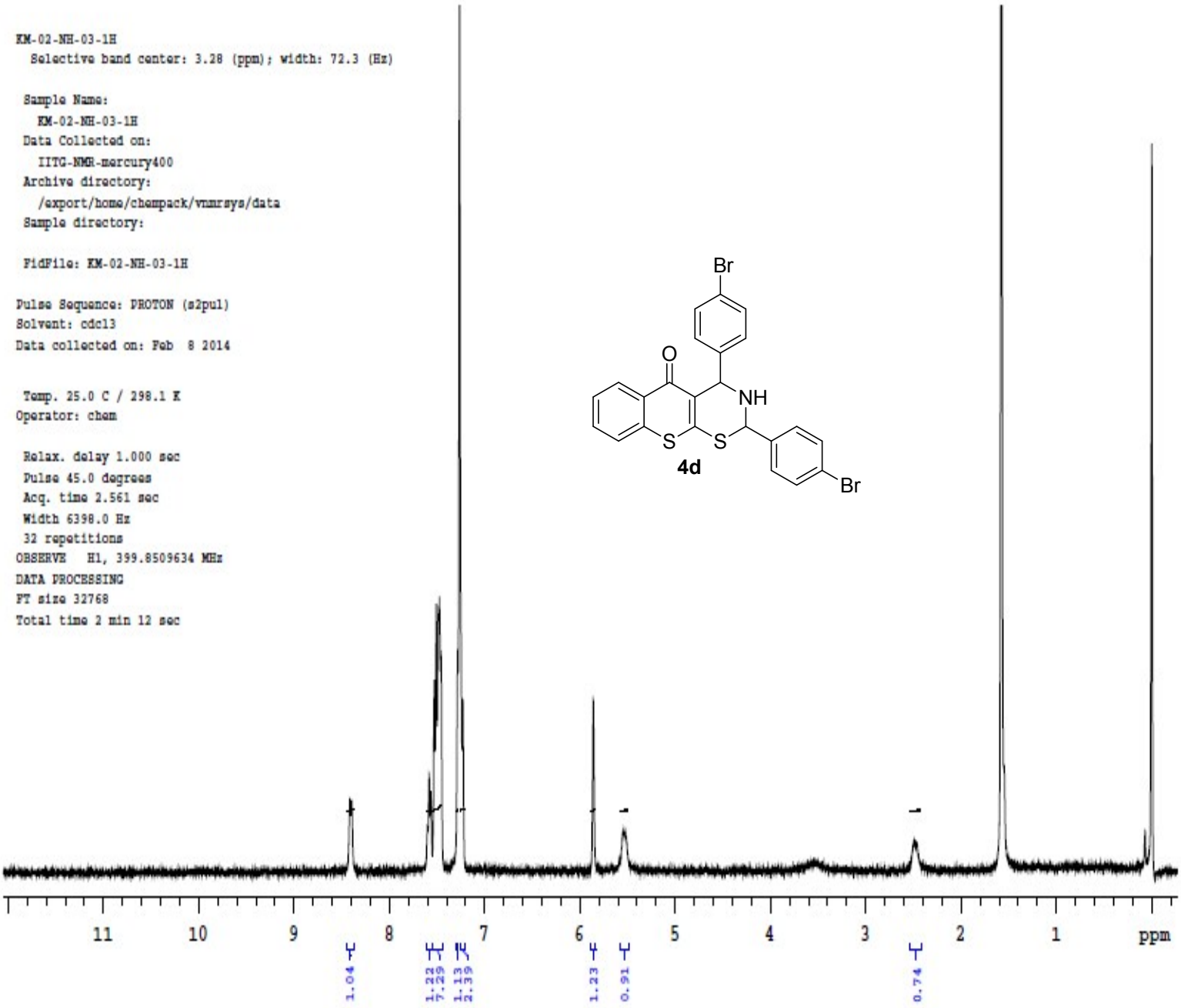
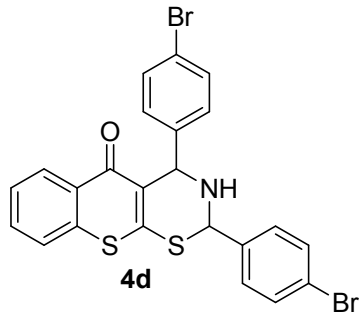
EM-02-NH-03-1H  
Selective band center: 3.28 (ppm); width: 72.3 (Hz)

Sample Name:  
EM-02-NH-03-1H  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

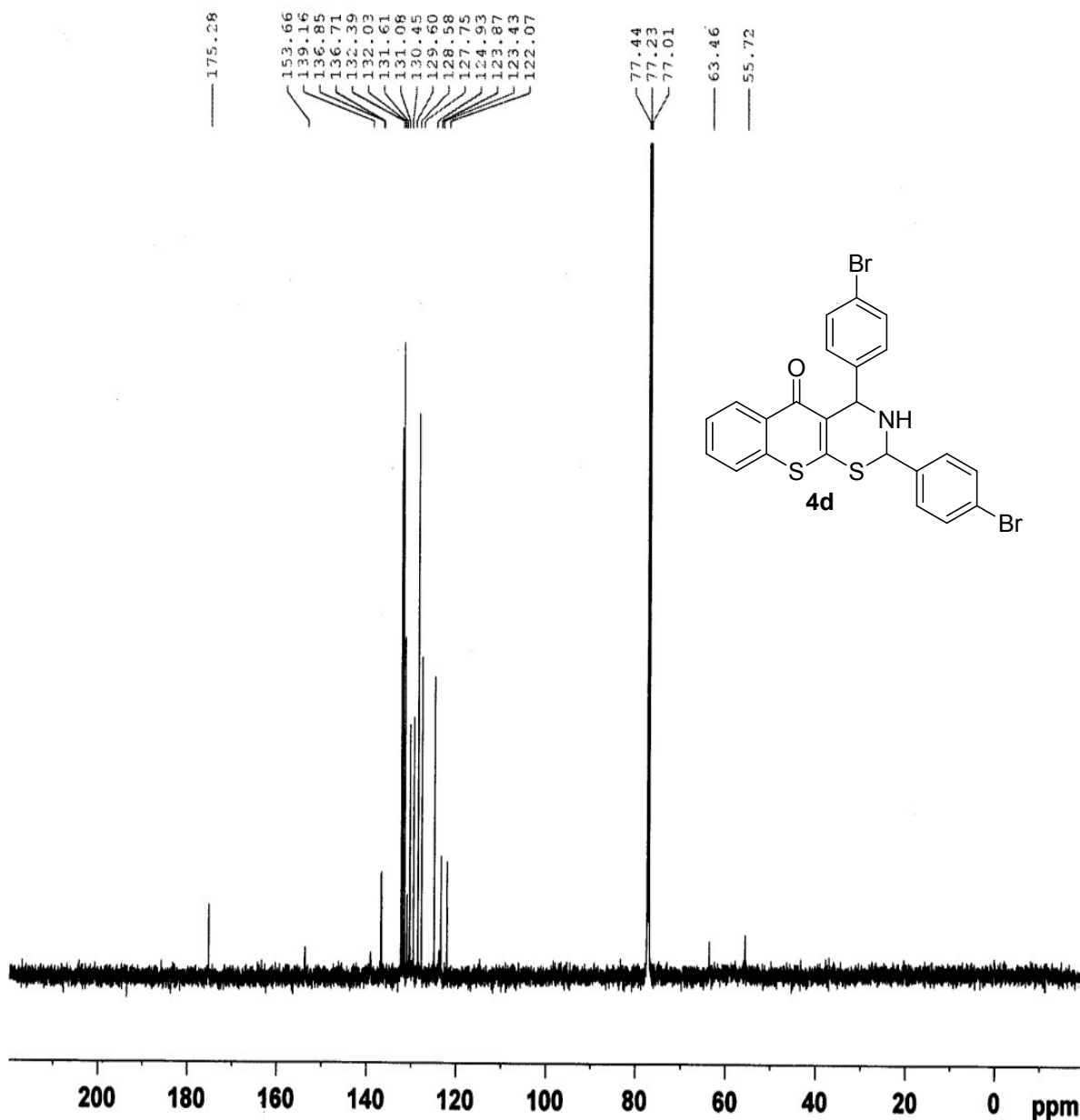
FidFile: EM-02-NH-03-1H  
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Feb 8 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509634 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



<sup>13</sup>CNMR spectra of compound: 4d



Current Data Parameters  
 NAME KM-02-NH-03-13C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20140901  
 Time 10.11  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 1251  
 DS 2  
 SWH 36057.691 Hz  
 FIDRES 1.100393 Hz  
 AQ 0.4543829 sec  
 RG 65.24  
 DW 13.867 usec  
 DE 6.50 usec  
 TE 302.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 150.9279571 MHz  
 NUC1 13C  
 P1 10.50 usec  
 PLW1 95.00000000 W

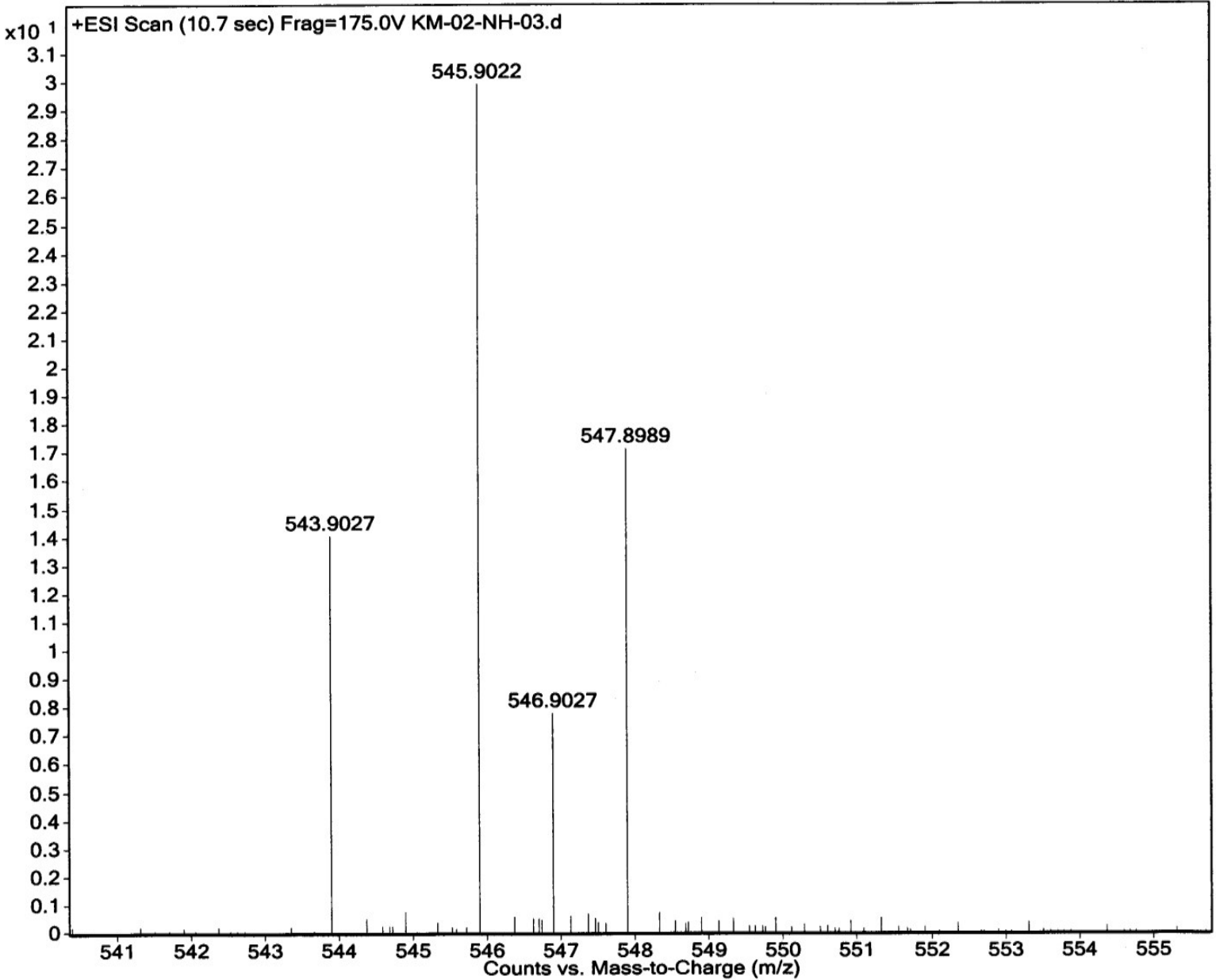
==== CHANNEL f2 =====  
 SFO2 600.1724007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 70.00 usec  
 PLW2 21.00000000 W  
 PLW12 0.61714000 W  
 PLW13 0.30239999 W

F2 - Processing parameters  
 SI 16384  
 SF 150.9128347 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

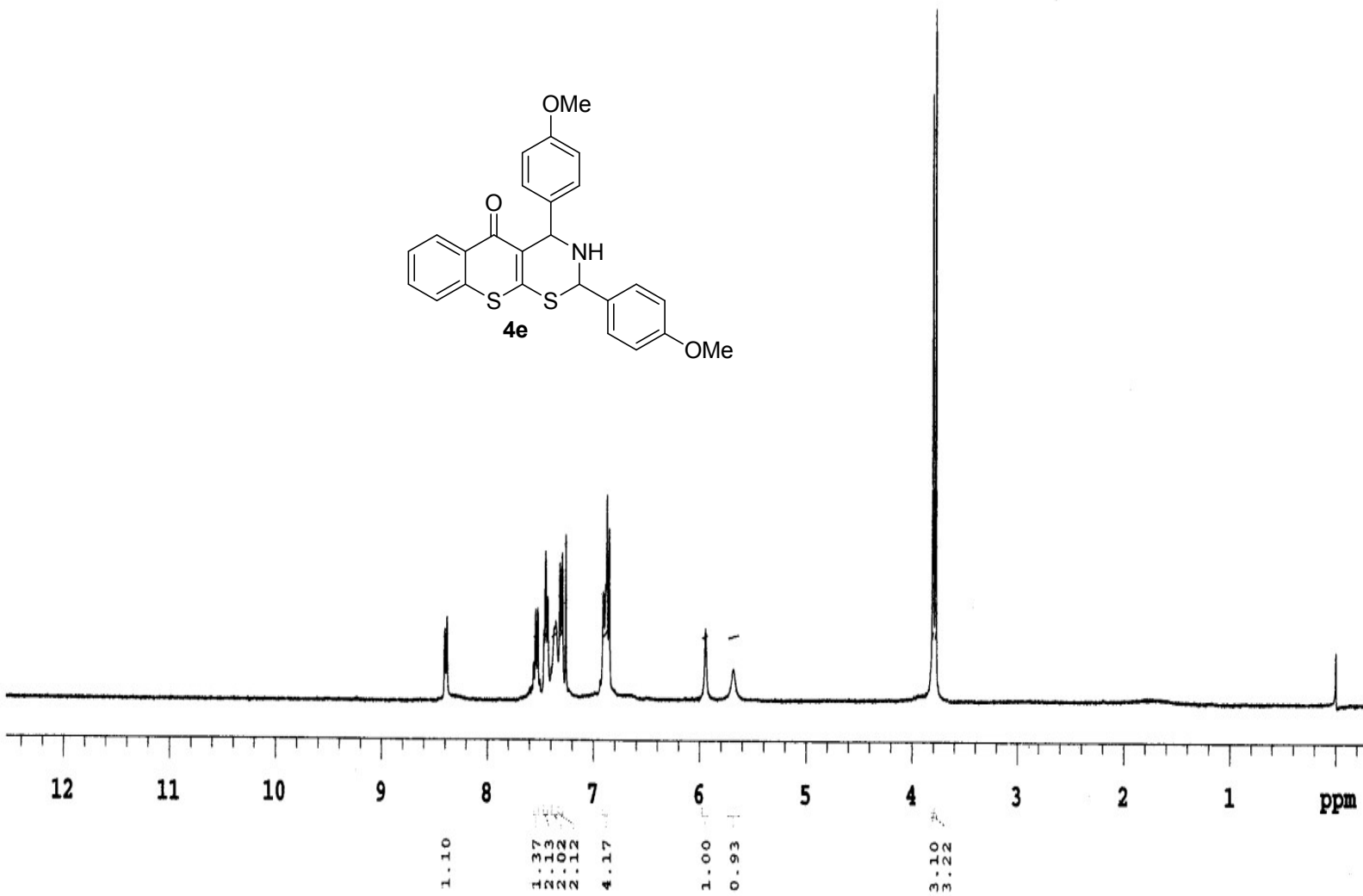
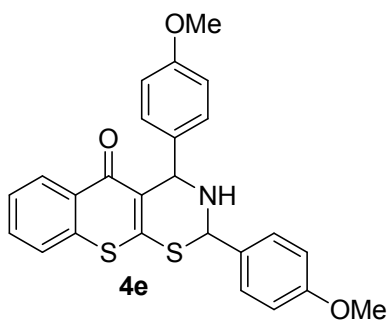


HRMS spectra of compound: 4d

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR spectra the compound: 4e



PULSE SEQUENCE DATA PROCESSING OBSERVED F1, 399.8509613

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

32 repetitions

DATA PROCESSING

FT size 32768

Total time 1 minutes

EXP:03-NMR-06

Solvent: cdcl3

Temp. 25.0 C / 298.1 K

Operator: chem

Mercury-400 "IITG-NMR"

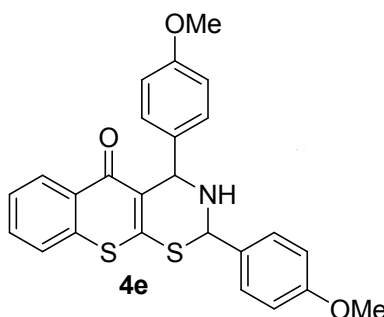
<sup>13</sup>CNMR spectra of compound: 4e



175.03  
 160.43  
 159.25  
 137.19  
 132.31  
 131.90  
 131.26  
 131.16  
 130.82  
 129.89  
 129.79  
 129.53  
 129.36  
 128.40  
 128.12  
 127.41  
 125.57  
 124.74  
 124.68  
 114.52  
 114.22

77.43  
 77.23  
 77.01

56.57  
 55.57  
 55.44



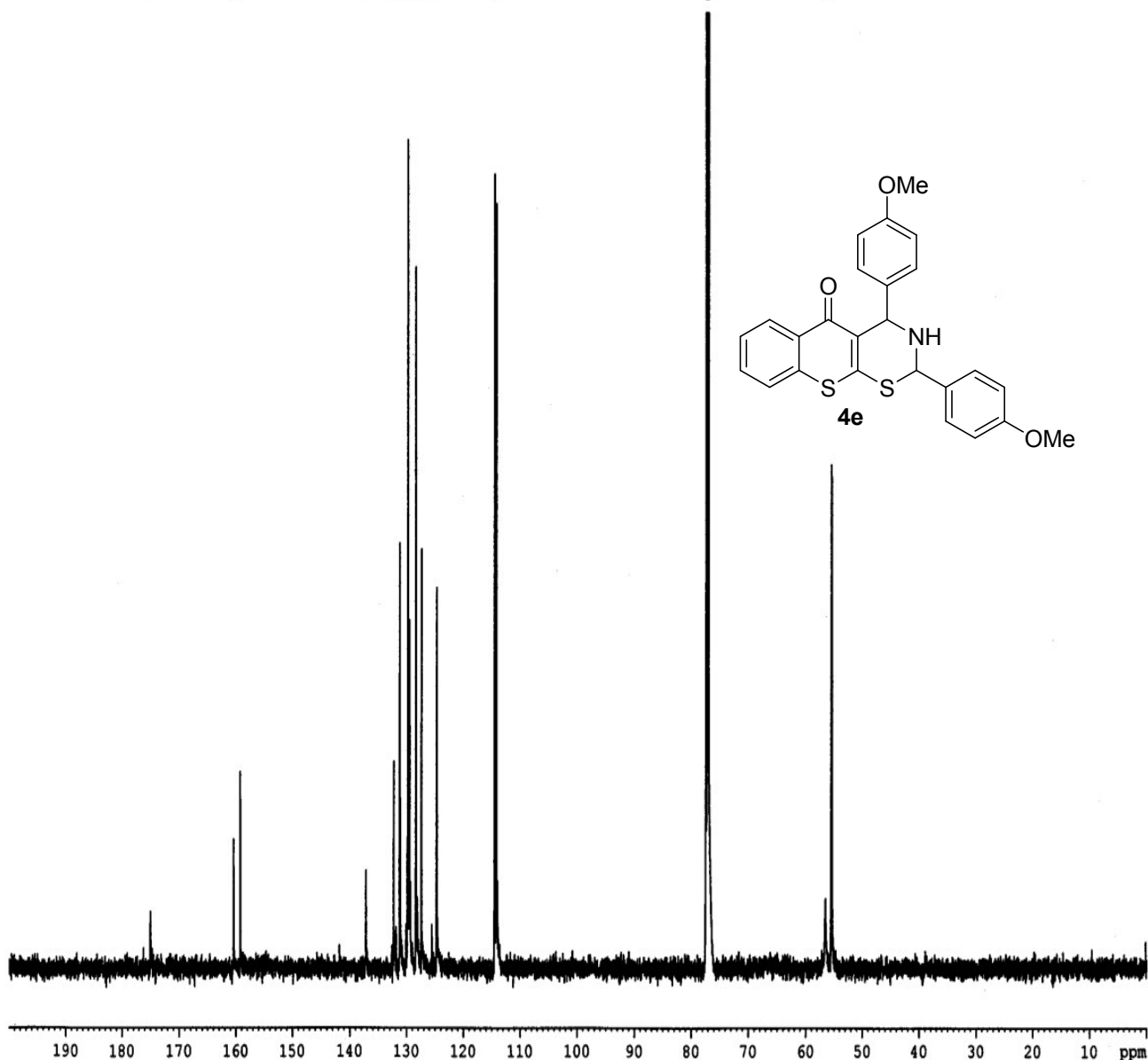
Current Data Parameters  
 NAME KM\_02NH\_06\_13C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20140325  
 Time 9.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 889  
 DS 2  
 SWH 36057.691 Hz  
 FIDRES 1.100393 Hz  
 AQ 0.4543829 sec  
 RG 65.24  
 DW 13.867 usec  
 DE 6.50 usec  
 TE 301.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 SFO1 150.9279571 MHz  
 NUC1 13C  
 P1 10.50 usec  
 PLW1 95.00000000 W

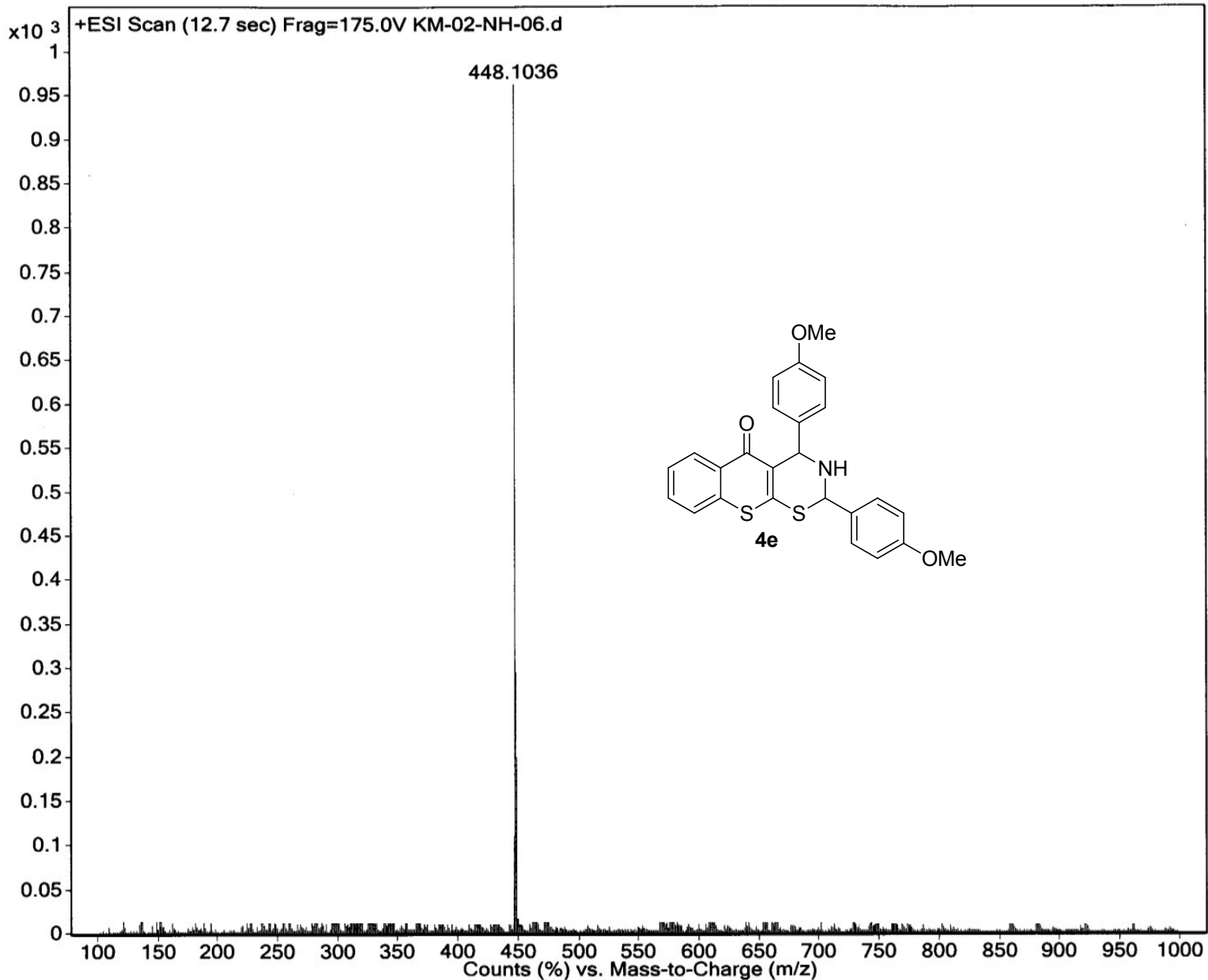
===== CHANNEL f2 =====  
 SFO2 600.1724007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 70.00 usec  
 PLW2 21.00000000 W  
 PLW12 0.61714000 W  
 PLW13 0.30239999 W

F2 - Processing parameters  
 SI 16384  
 SF 150.9128396 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

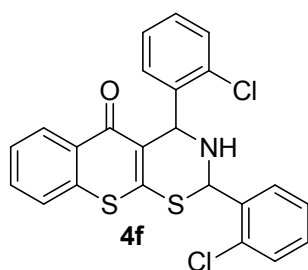


# HRMS spectra of compound: 4e

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR spectra the compound: 4f

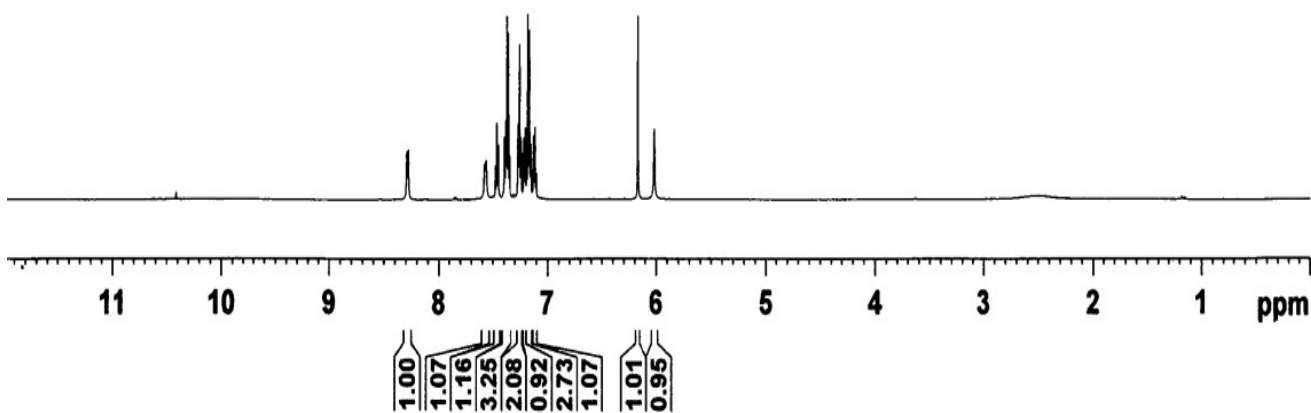


Current Data Parameters  
NAME KM-02-21\_1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131023  
Time 9.43  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 80.22  
DW 41.600 usec  
DE 6.50 usec  
TE 300.1 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PIW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700631 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>CNMR spectra of compound: 4f



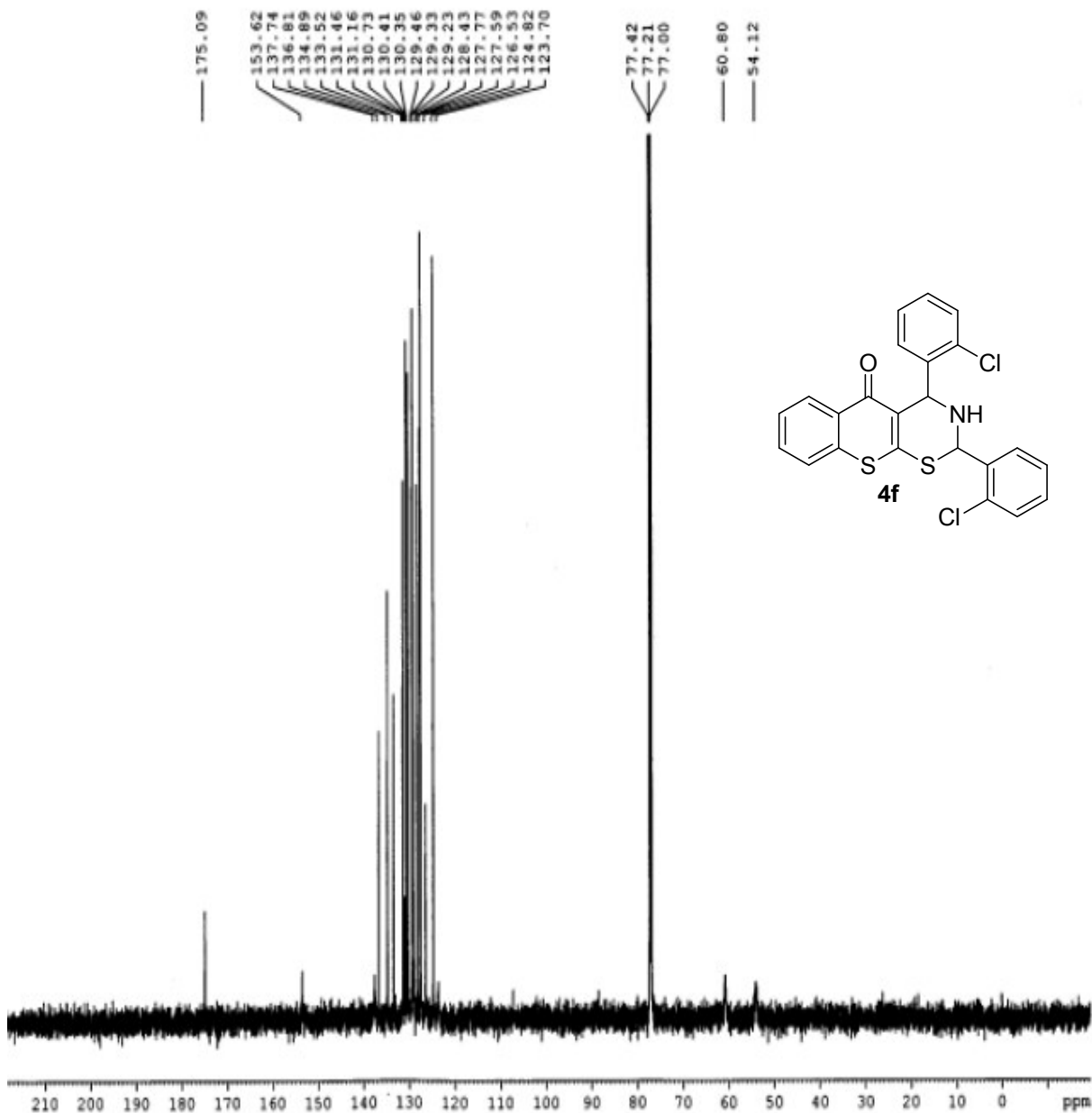
Current Data Parameters  
 NAME KM-2-Cl-13C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150225  
 Time\_ 9.41  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 413  
 DS 2  
 SWH 36057.691 Hz  
 FIDRES 1.100393 Hz  
 AQ 0.4543829 sec  
 RG 65.24  
 DW 13.867 usec  
 DE 6.50 usec  
 TE 298.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 SFO1 150.9279571 MHz  
 NUC1 13C  
 P1 10.50 usec  
 PLW1 95.00000000 W

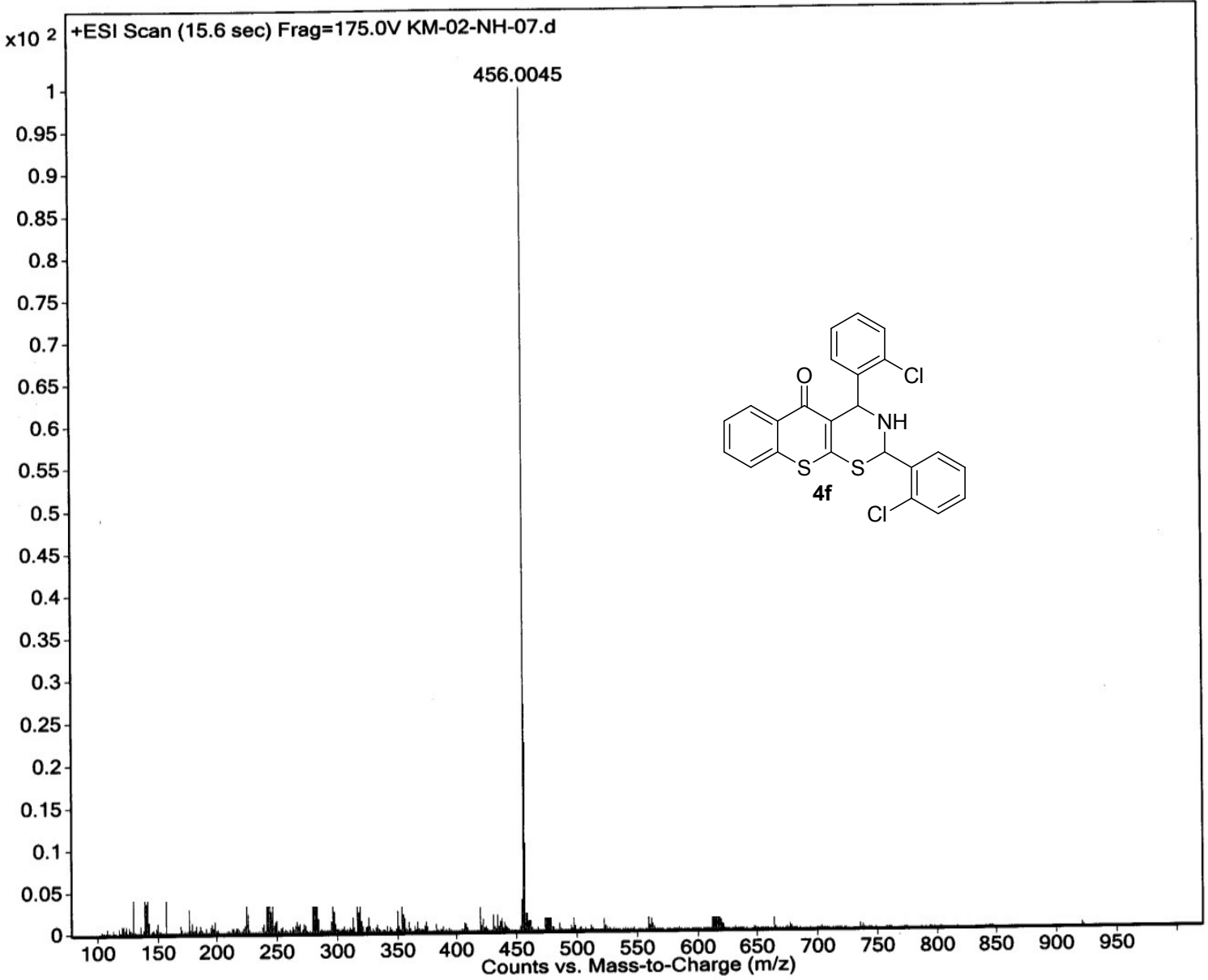
----- CHANNEL f2 -----  
 SFO2 600.1724007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 70.00 usec  
 PLW2 21.00000000 W  
 PLW12 0.61714000 W  
 PLW13 0.30239999 W

F2 - Processing parameters  
 SI 16384  
 SF 150.9128423 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



# HRMS spectra of compound: 4f

Sample Name	KM-02-NH-07	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	KM-02-NH-07.d	ACQ Method		Comment		Acquired Time	5/13/2014 3:24:26 PM



# <sup>1</sup>HNMR spectra the compound: 4g

KM-02-NH-18

Sample Name:

KM-02-NH-18

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/home/chem/data/study

Sample directory:

P59-1-01

FidFile: KM-02-NH-18

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 27 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

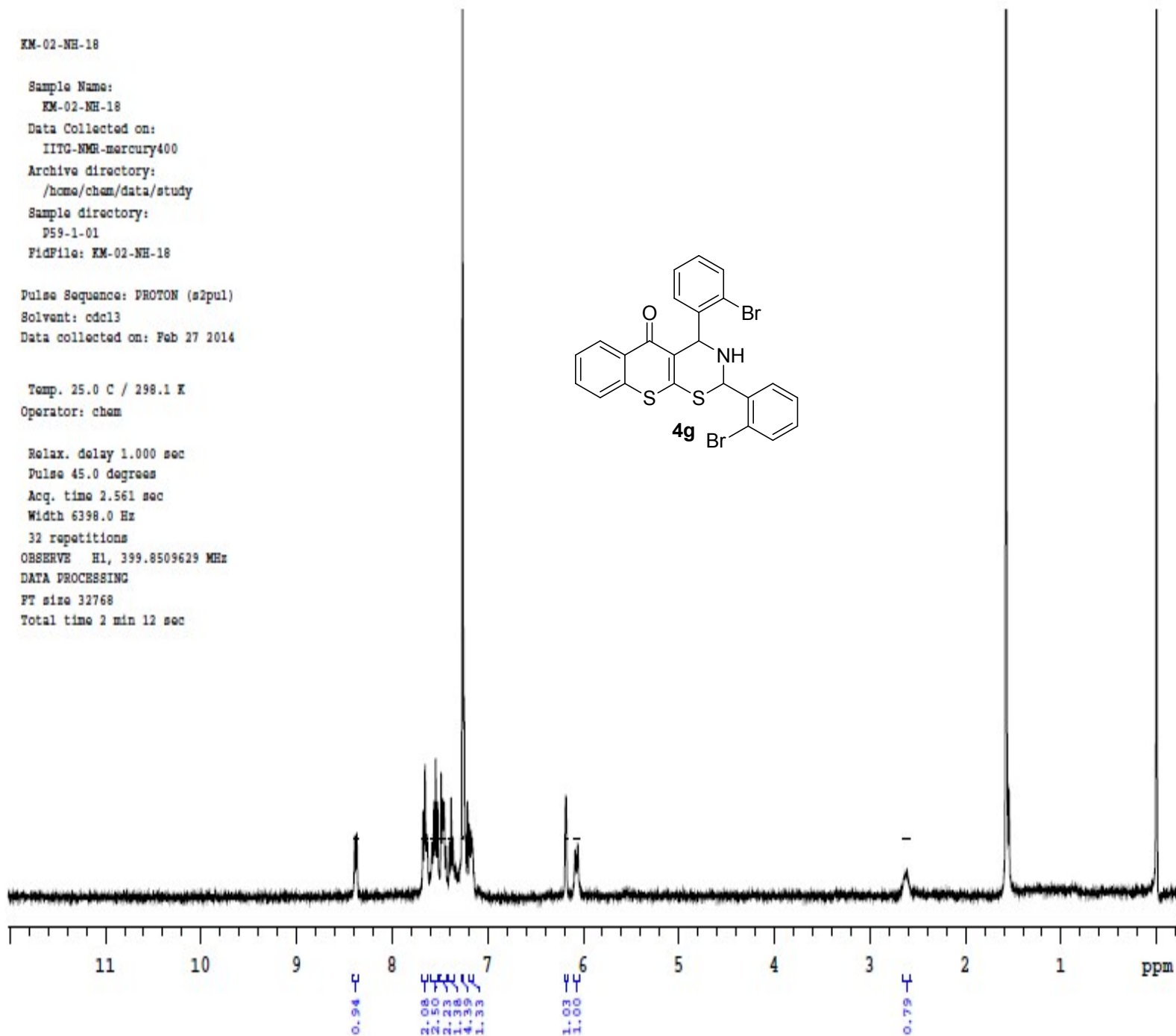
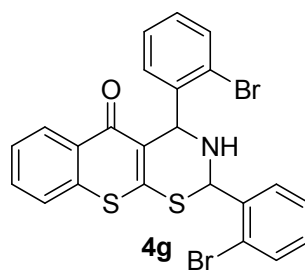
32 repetitions

OBSERVE H1, 399.8509629 MHz

DATA PROCESSING

FT size 32768

Total time 2 min 12 sec





<sup>13</sup>CNMR spectra of compound: 4g



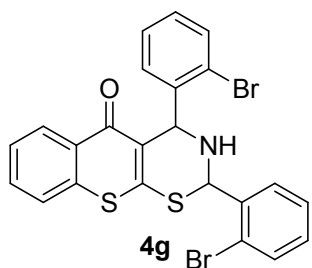
174.20

153.21  
138.87  
136.07  
135.83  
133.17  
132.66  
130.89  
130.38  
130.06  
128.84  
128.69  
128.43  
128.31  
127.76  
126.93  
126.52  
124.81  
124.31  
122.70

77.43  
77.22  
77.01

63.36  
56.10

39.90  
39.76  
39.62  
39.48  
39.34  
39.20  
39.06



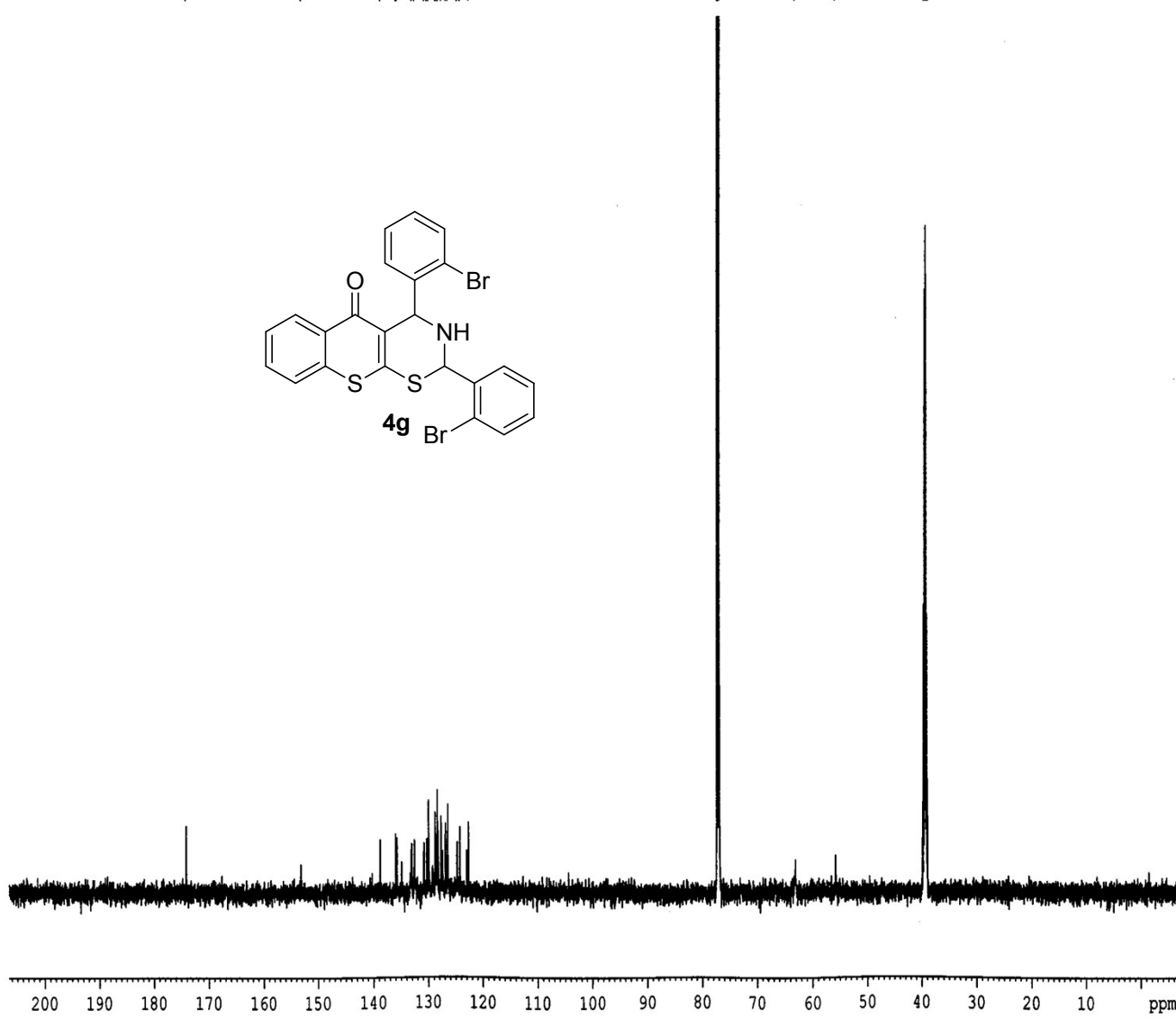
Current Data Parameters  
NAME KM-02-NH2Br-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150210  
Time 12.35  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDC13  
NS 434  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 297.9 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

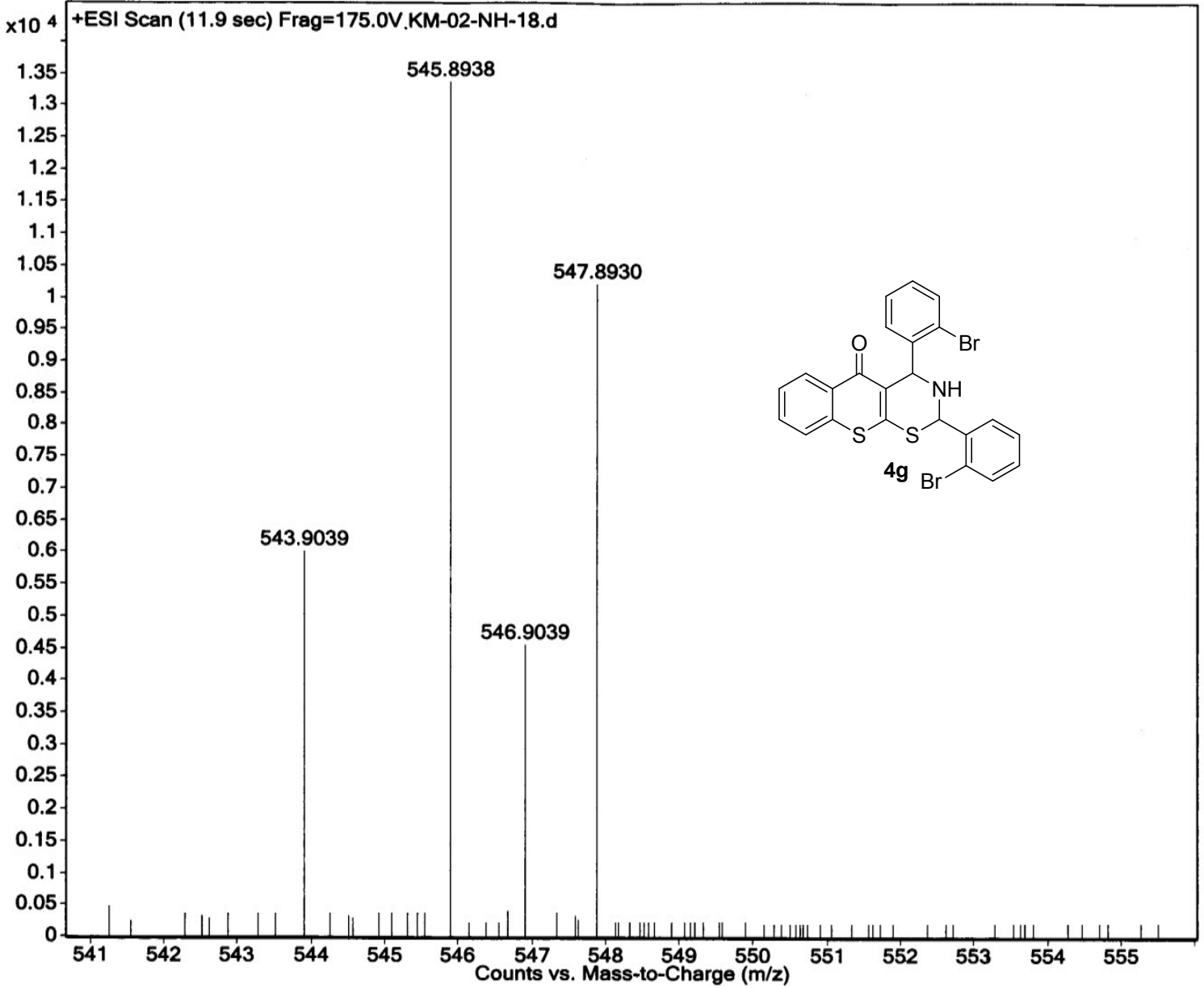
==== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9136604 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



<sup>1</sup>HNMR spectra the compound: 4g

Sample Name	KM-02-NH-18	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	KM-02-NH-18.d	ACQ Method		Comment		Acquired Time	10/14/2014 11:08:35 AM



# <sup>1</sup>H NMR spectra the compound: 4h

KM-02-NH-2F

Sample Name:  
KM-02-NH-2F

Data Collected on:  
IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: KM-02-NH-2F

Pulse Sequence: PROTON (s2pul)

Solvent: cdc13

Data collected on: Mar 10 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

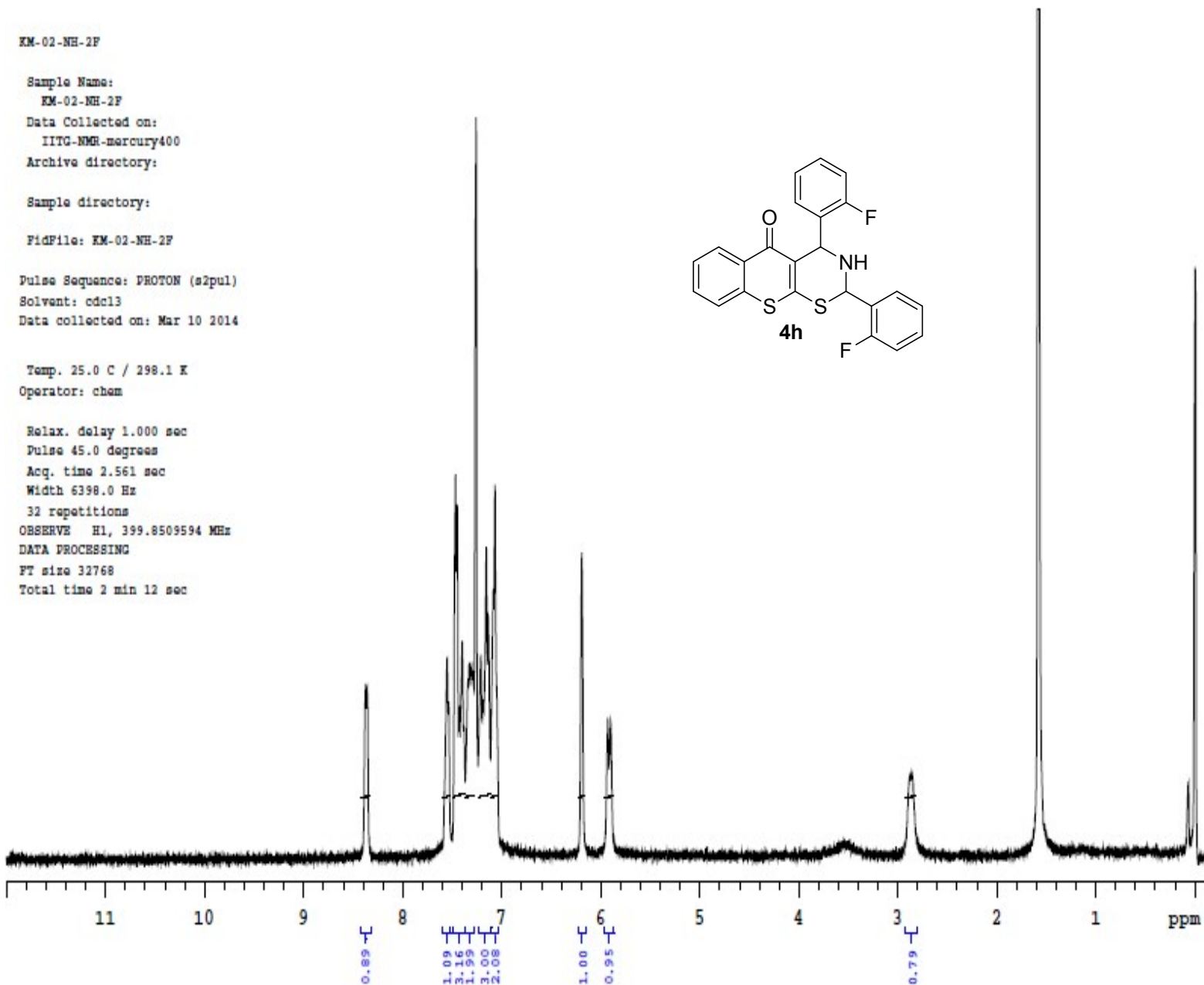
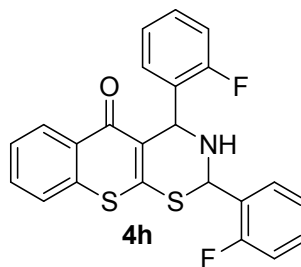
32 repetitions

OBSERVE H1, 399.8509594 MHz

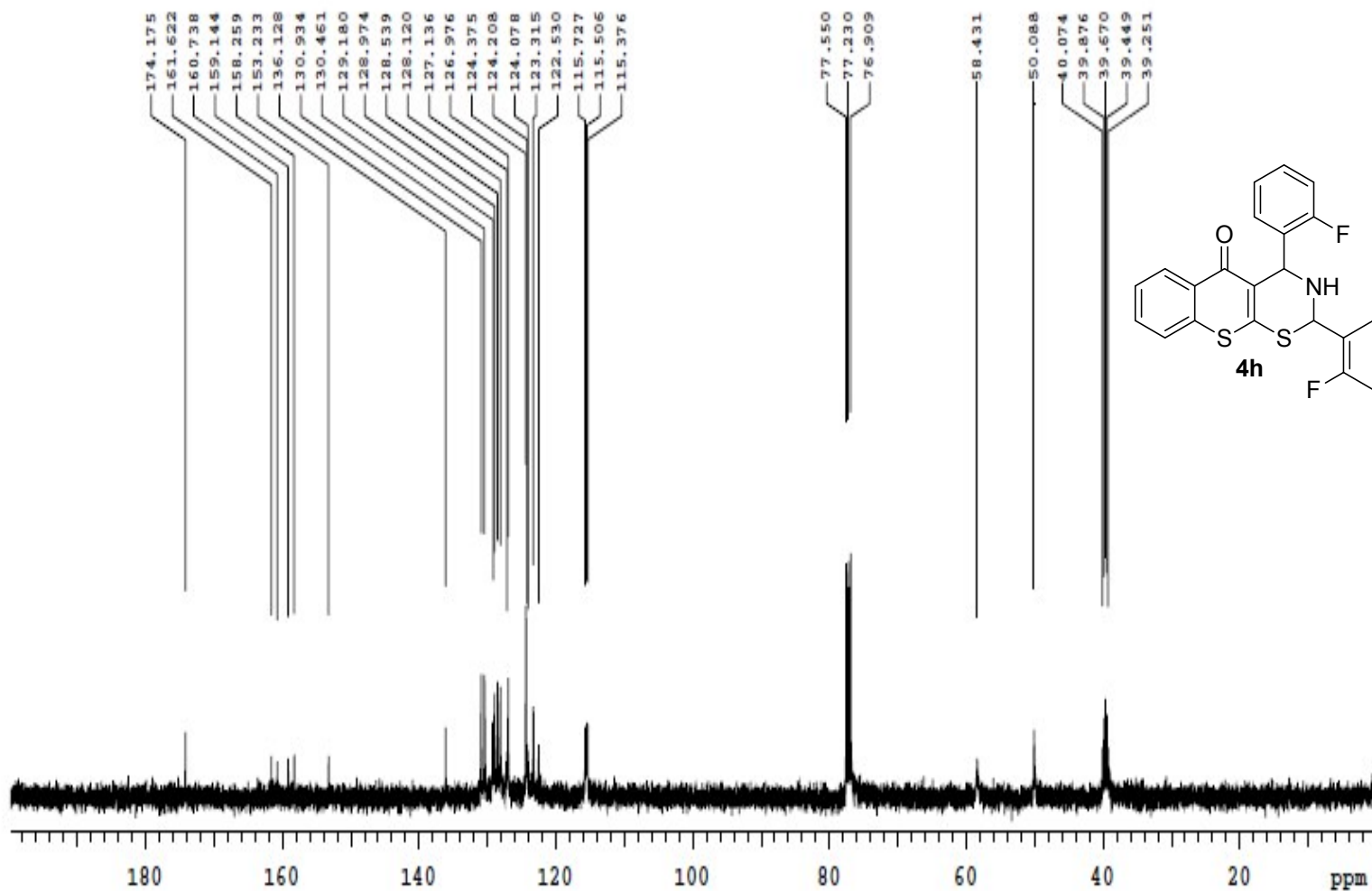
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



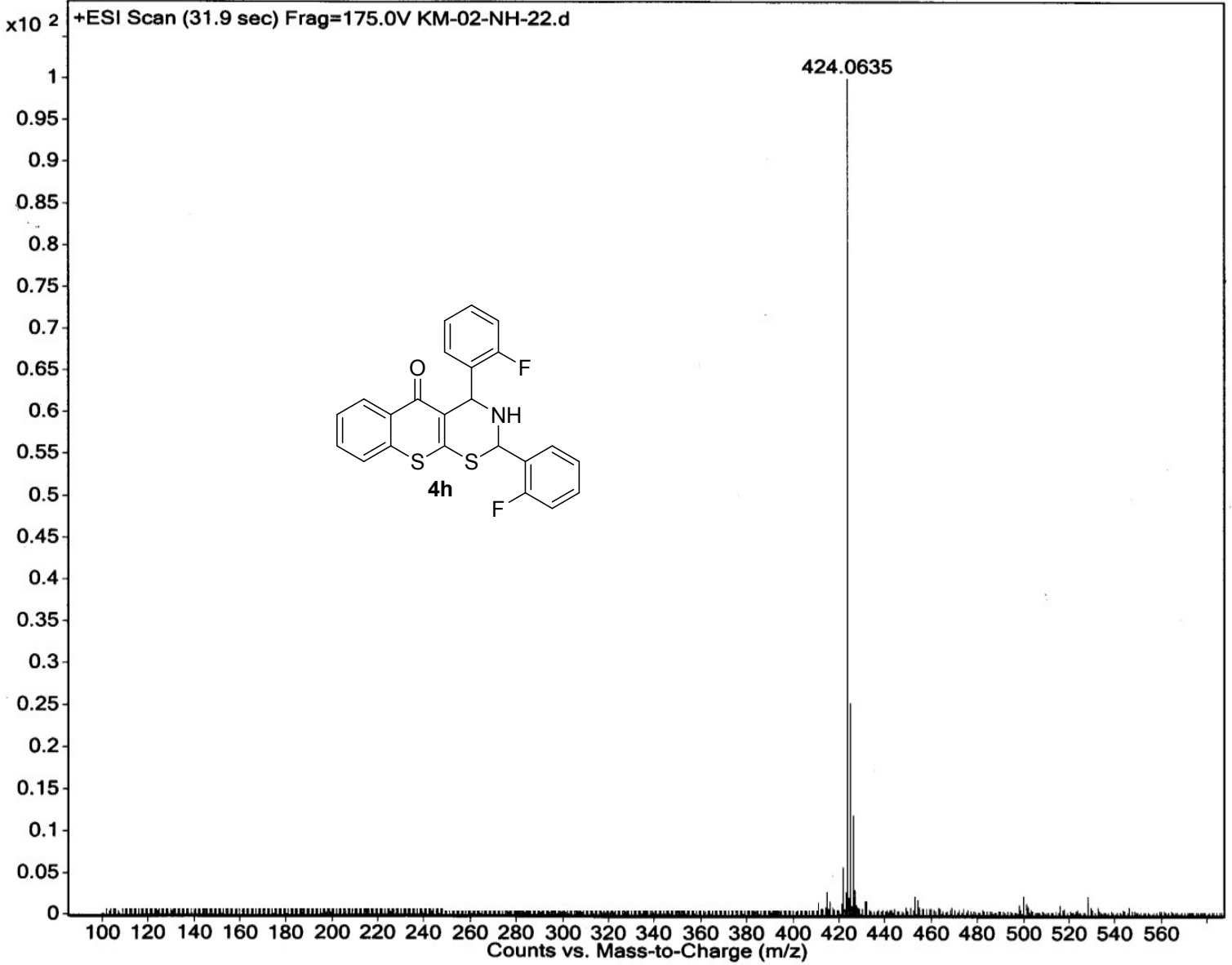
### <sup>13</sup>CNMR spectra of compound: 4h



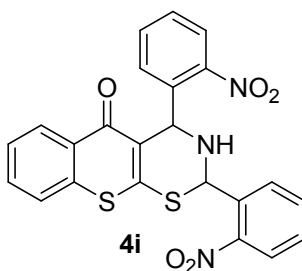
<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1610 repetitions	<b>OBSERVE</b> C13, 100.5431207 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 61 minutes	<b>EM-02-NH-2F-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: EM-02-NH-2F-13C Mercury-400 "IITG-NMR"
--	--	--	---

# HRMS spectra of compound: 4h

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>HNMR spectra the compound: 4i

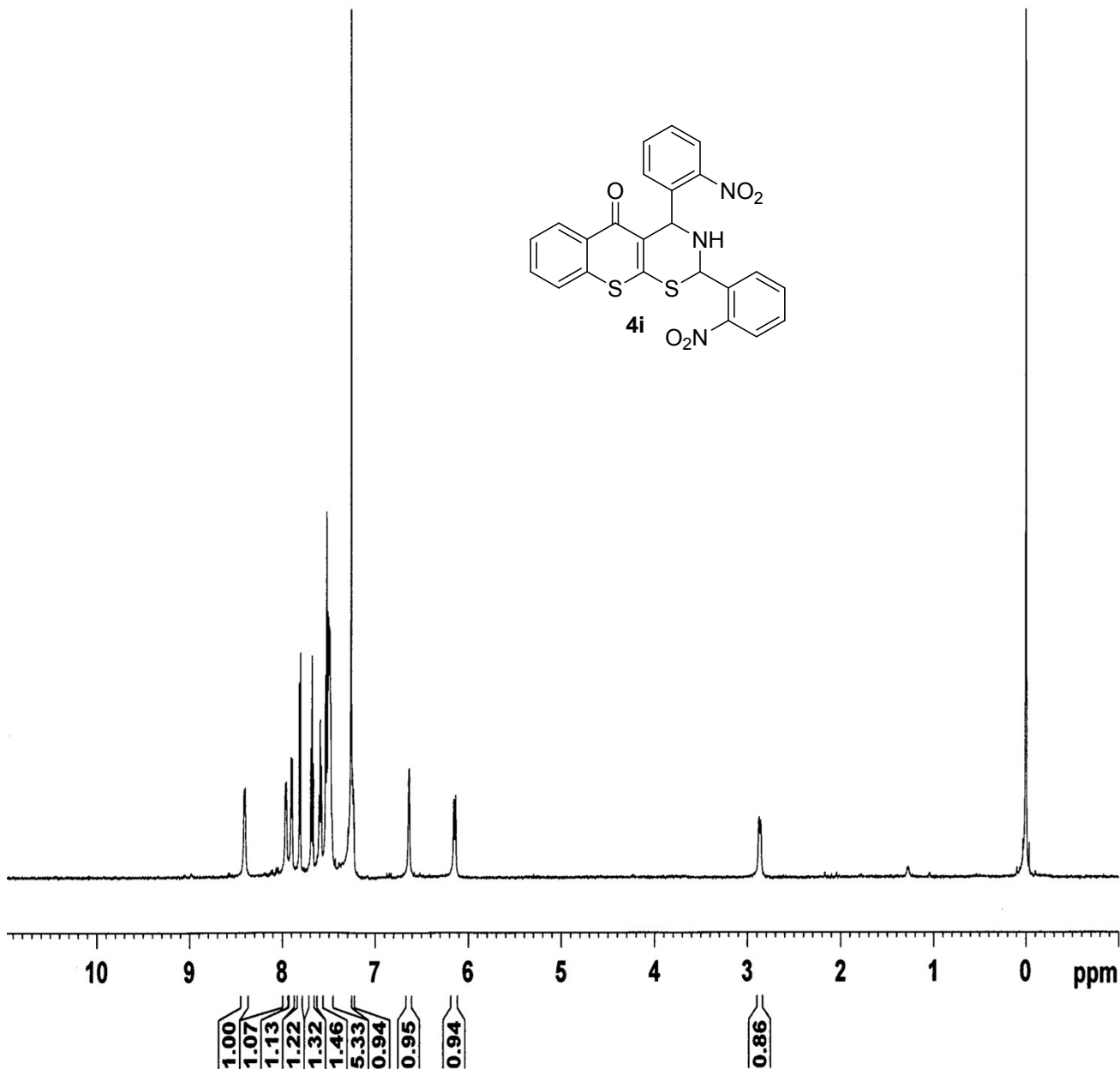


Current Data Parameters  
NAME KM\_02\_NH\_11\_1H  
EXPNO 1  
PROCNO 1

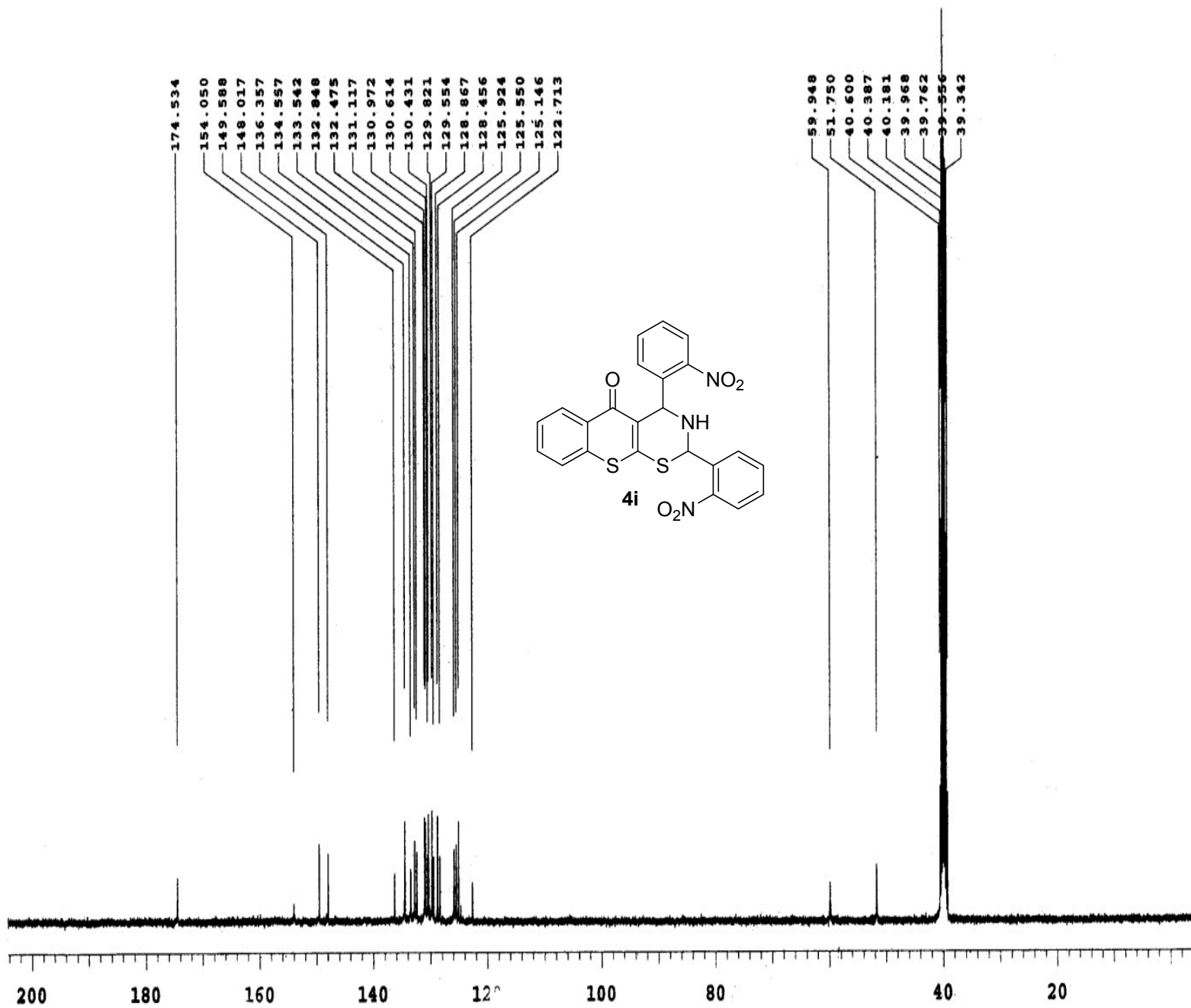
F2 - Acquisition Parameters  
Date 20140219  
Time 9.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 143.33  
DW 41.600 usec  
DE 6.50 usec  
TE 300.2 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700148 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

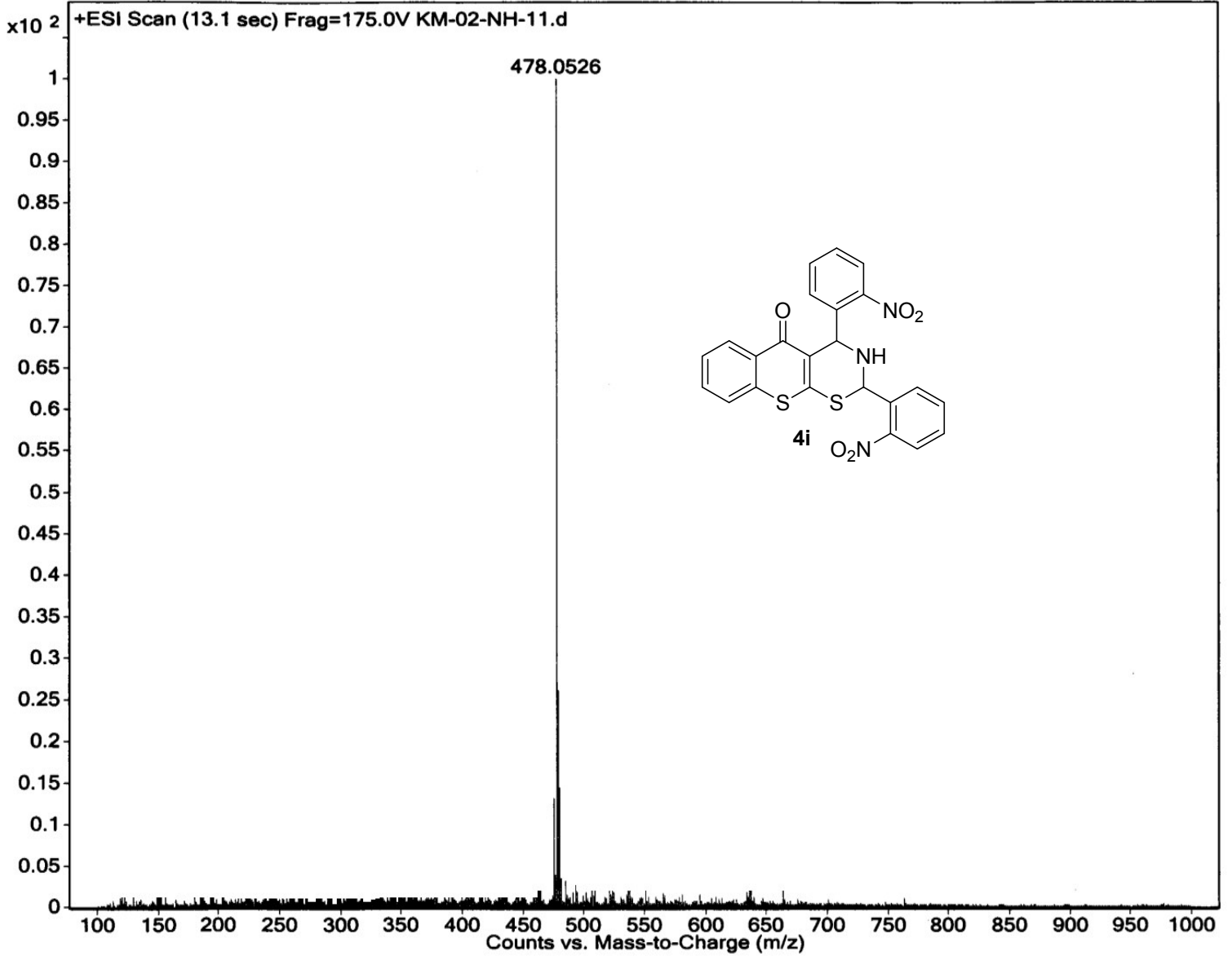


<sup>13</sup>CNMR spectra of compound: 4i



# HRMS spectra of compound: 4i

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time





# <sup>1</sup>H NMR spectra the compound: 4j

EM-02-NH-CN

Sample Name:

EM-02-NH-CN

Data Collected on:

IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: EM-02-NH-CN

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 11 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

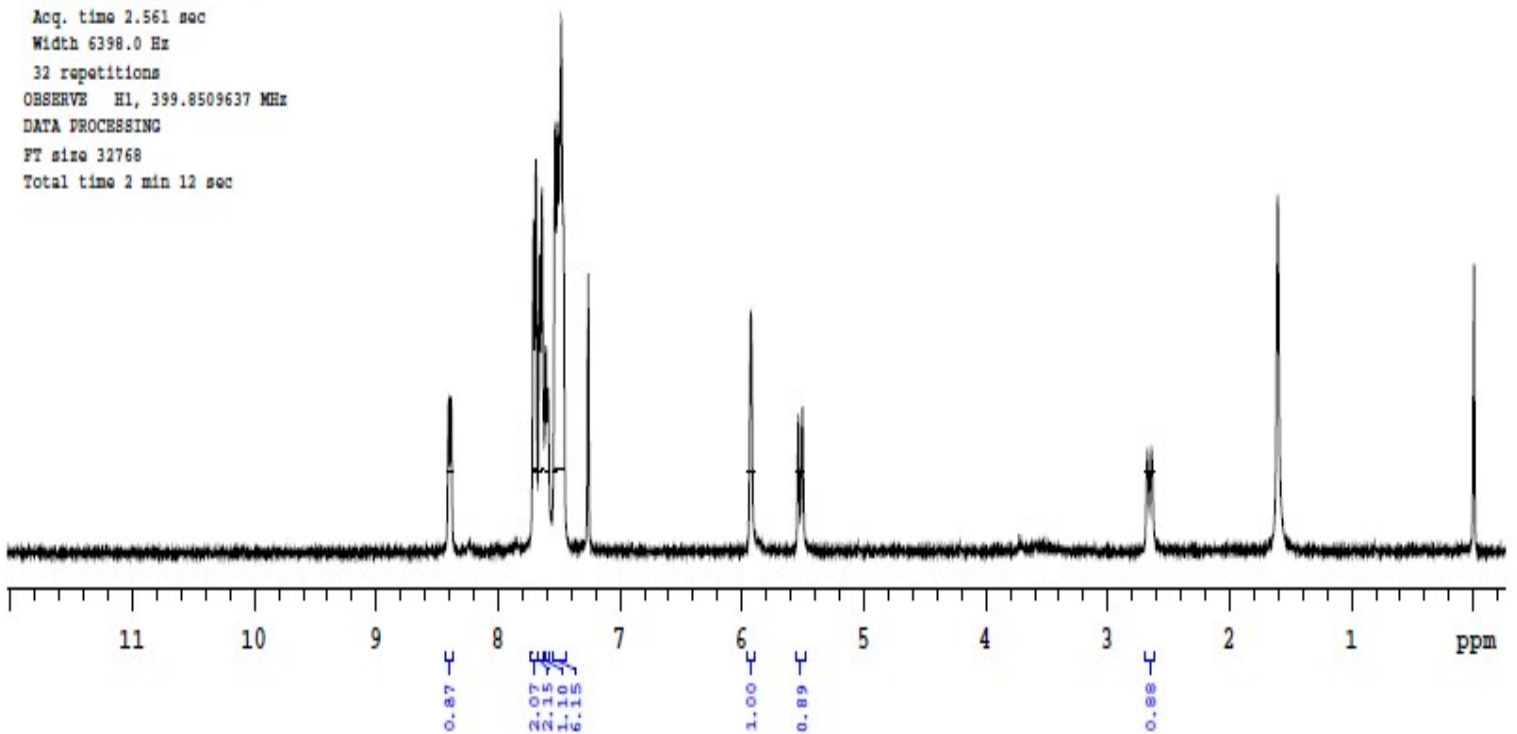
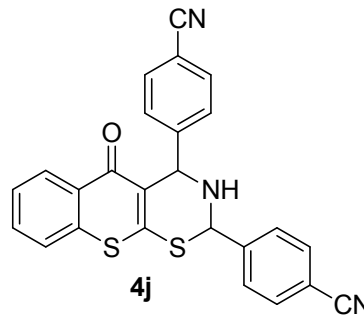
32 repetitions

OBSERVE H1, 399.8509637 MHz

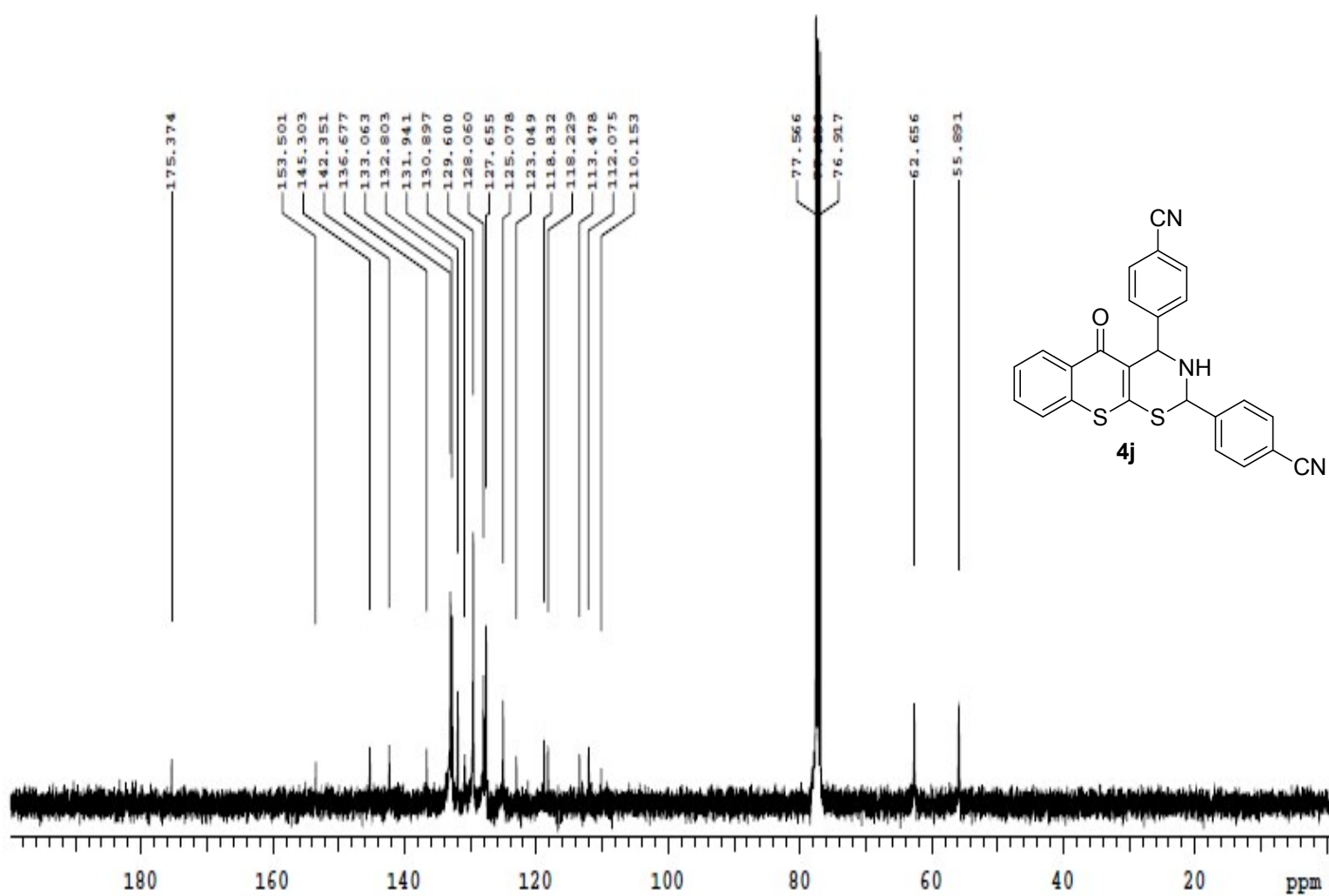
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



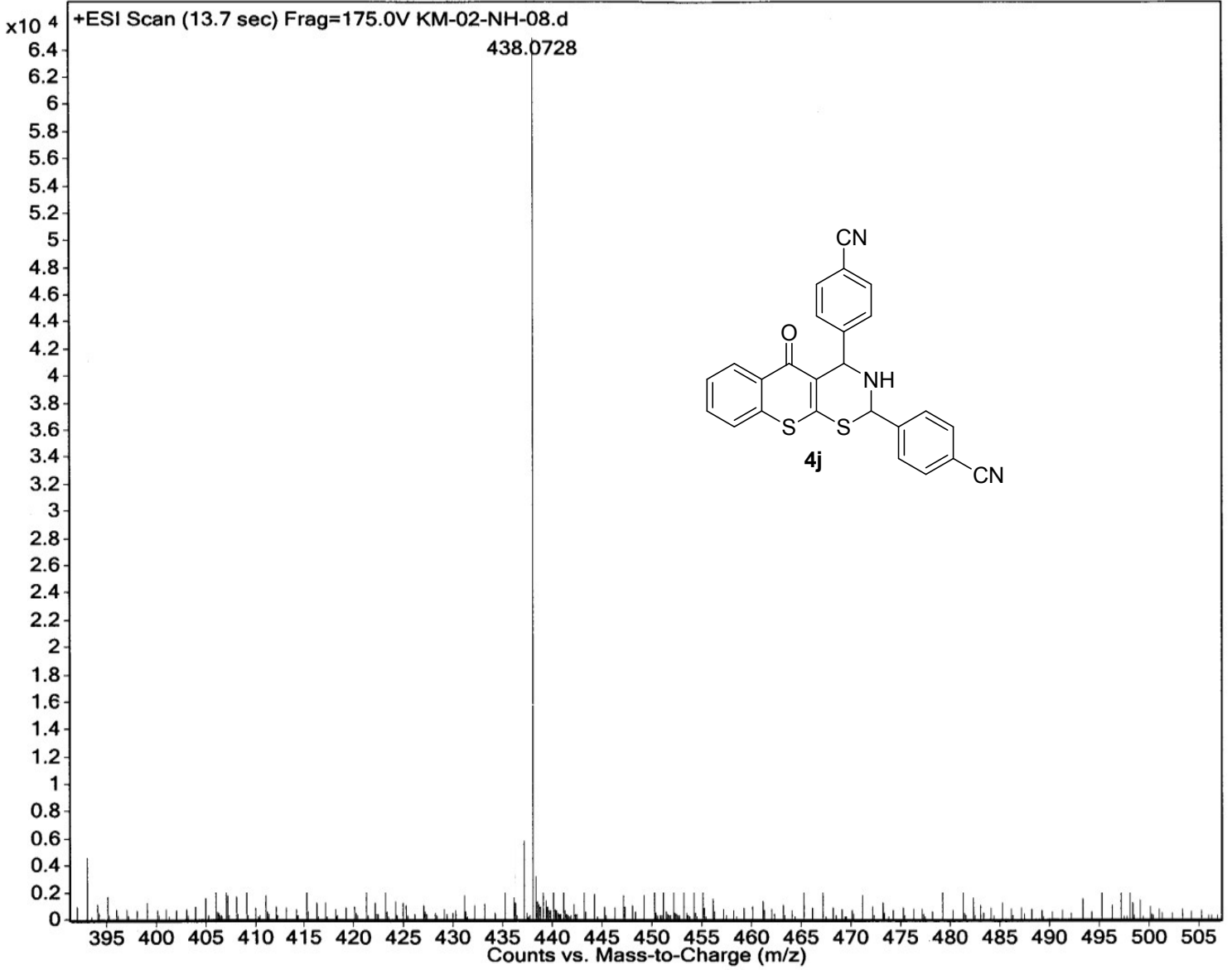
### <sup>13</sup>CNMR spectra of compound: 4j



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 12170 repetitions	<b>OBSERVE</b> C13, 100.5425893 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 7.8 hours	<b>EM-NH-RR-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: EM-NH-RR-13C Mercury-400 "IITG-NMR"
---	--	---	---

# HRMS spectra of compound: 4j

<b>Sample Name</b>	KM-02-NH-08	<b>Position</b>	-1	<b>Instrument Name</b>	Instrument 1	<b>User Name</b>	
<b>Inj Vol</b>	-10	<b>InjPosition</b>		<b>SampleType</b>	Sample	<b>IRM Calibration Status</b>	Success
<b>Data Filename</b>	KM-02-NH-08.d	<b>ACQ Method</b>		<b>Comment</b>		<b>Acquired Time</b>	10/14/2014 11:06:59 AM



# <sup>1</sup>H NMR spectra the compound: 4k

KM-02-NH-09-1H

Sample Name:

KM-02-NH-09-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: KM-02-NH-09-1H

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 18 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

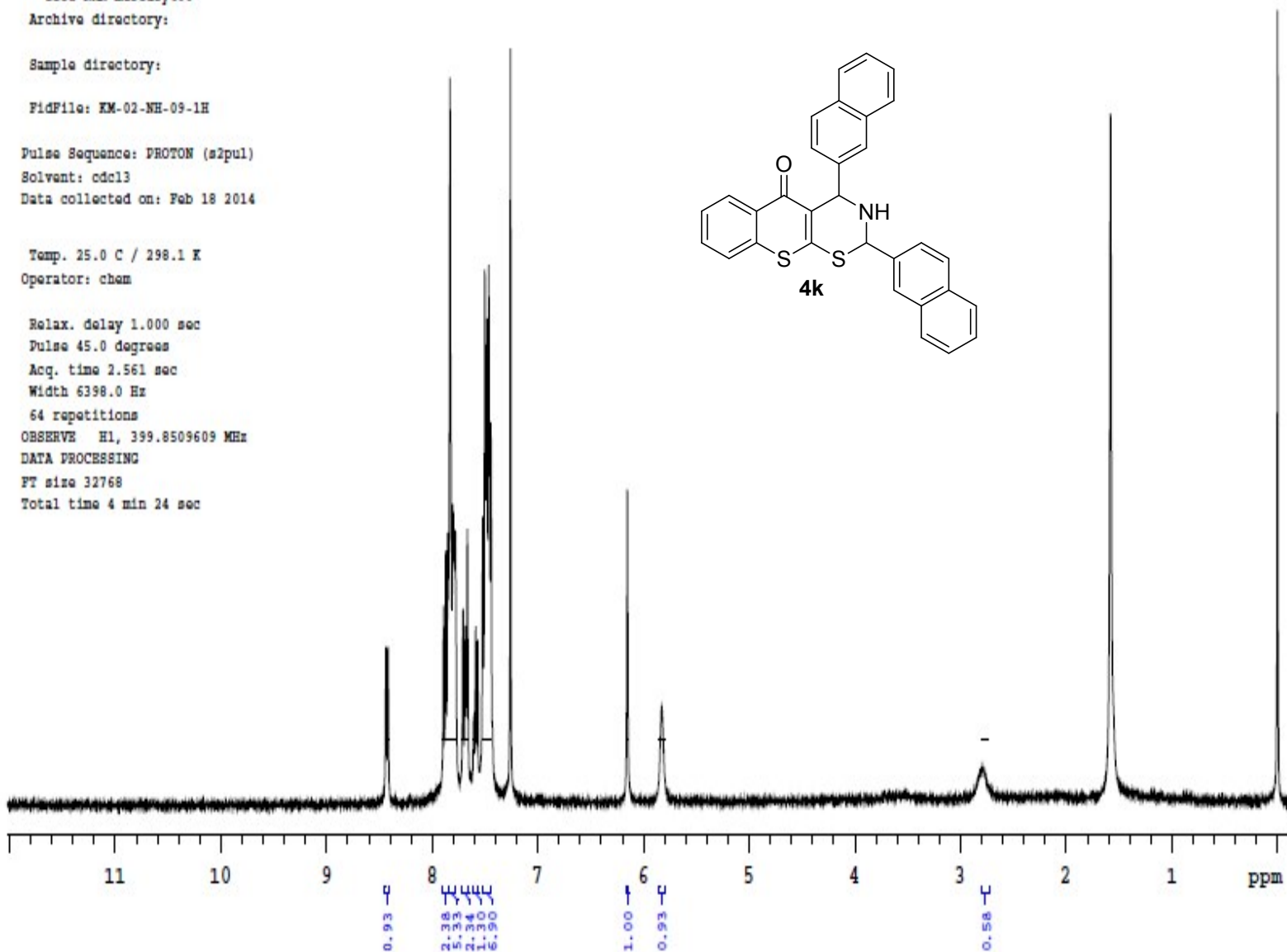
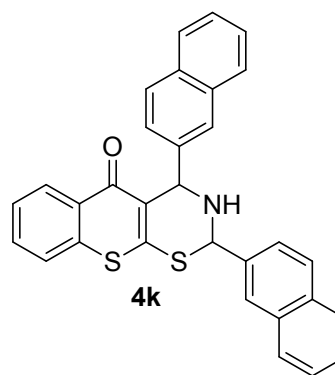
64 repetitions

OBSERVE H1, 399.8509609 MHz

DATA PROCESSING

FT size 32768

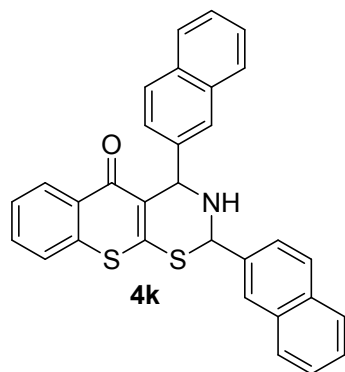
Total time 4 min 24 sec



<sup>13</sup>CNMR spectra of compound: 4k



175.30  
154.26  
137.64  
137.08  
135.00  
133.65  
133.42  
133.28  
131.41  
131.21  
129.64  
129.29  
129.15  
128.91  
128.42  
128.33  
127.91  
127.79  
127.57  
127.49  
127.12  
126.93  
126.81  
126.26  
126.20  
126.16  
124.87  
124.38  
124.25



77.44  
77.23  
77.02  
65.25  
56.80

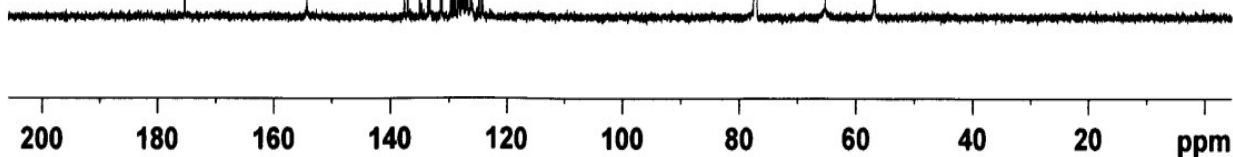
Current Data Parameters  
NAME KM-02-NH-09a-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140217  
Time 12.50  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 939  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 300.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

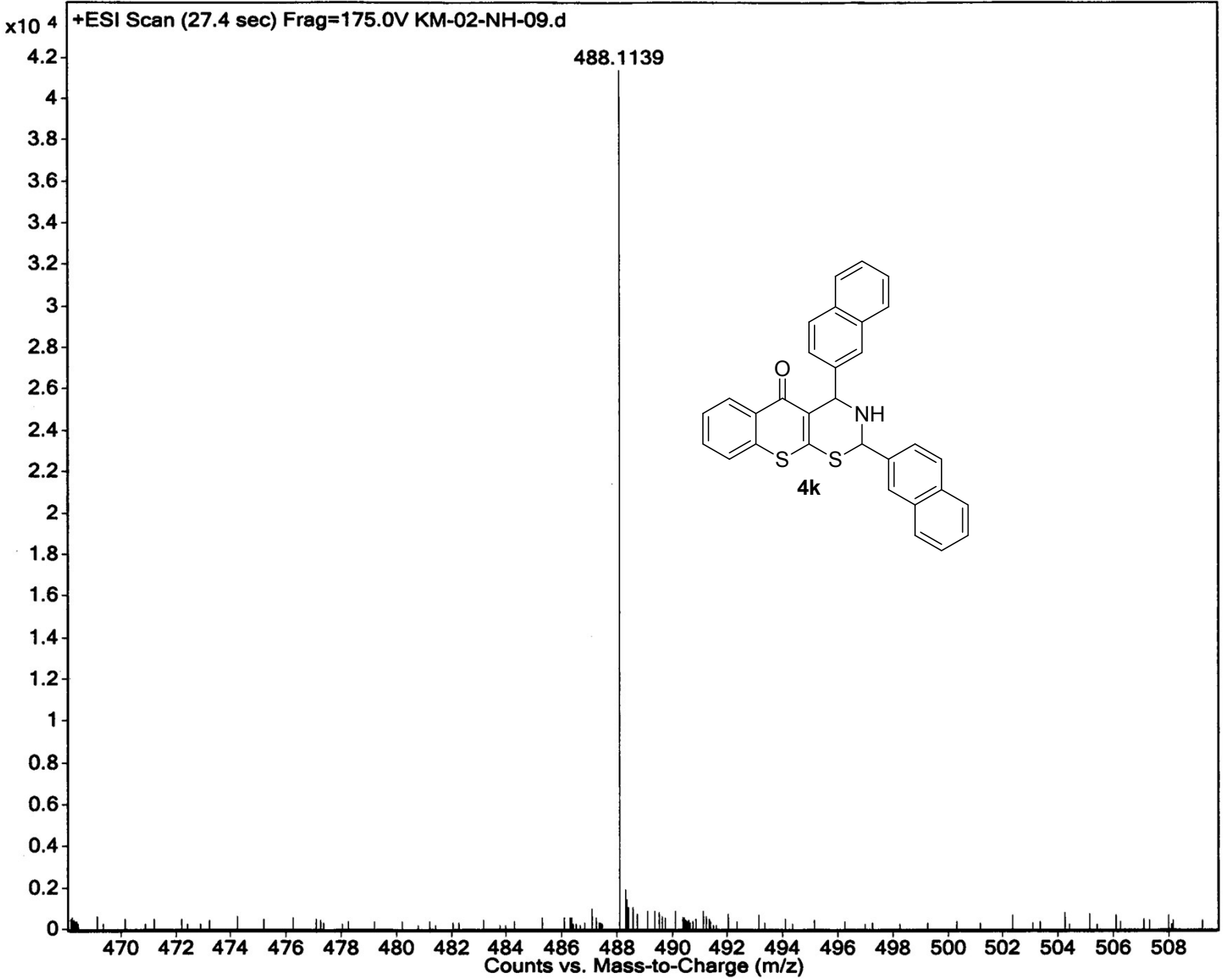
==== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128414 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

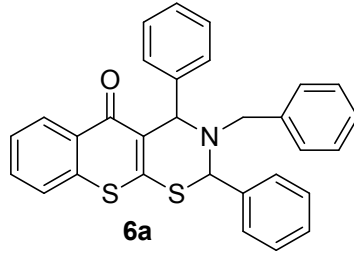


HRMS spectra of compound: 4k

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra the compound: 6a

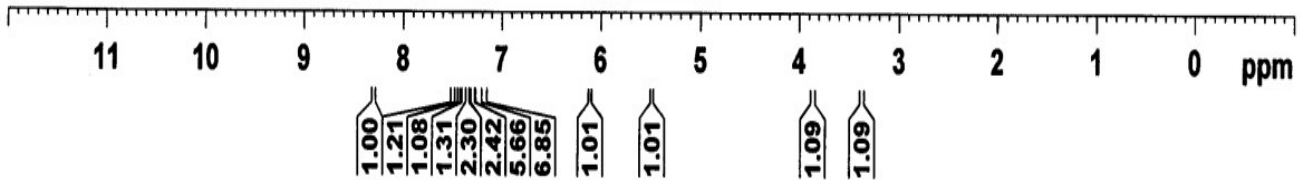
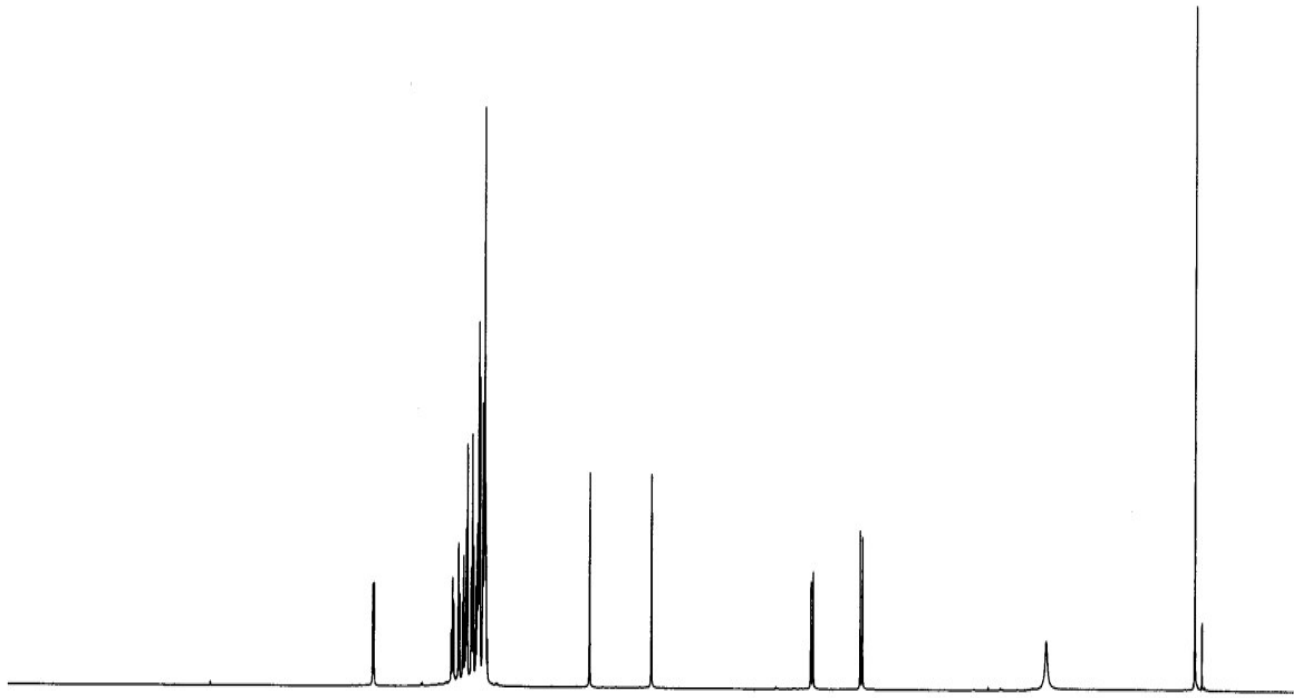


Current Data Parameters  
NAME KM\_AM\_BEN\_1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140314  
Time\_ 13.42  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 80.22  
DW 41.600 usec  
DE 6.50 usec  
TE 300.8 K  
D1 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700644 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

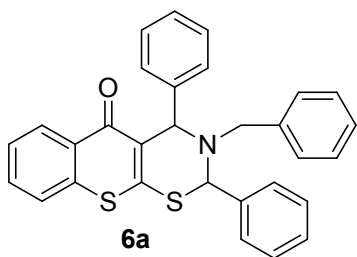


<sup>13</sup>CNMR spectra of compound: 6a



176.00  
 152.66  
 141.48  
 137.91  
 137.00  
 136.77  
 131.45  
 131.18  
 129.68  
 129.21  
 129.01  
 128.82  
 128.76  
 128.73  
 127.91  
 127.71  
 127.65  
 127.51  
 124.79  
 121.12

77.44  
 77.23  
 77.02  
 68.98  
 59.69  
 50.78



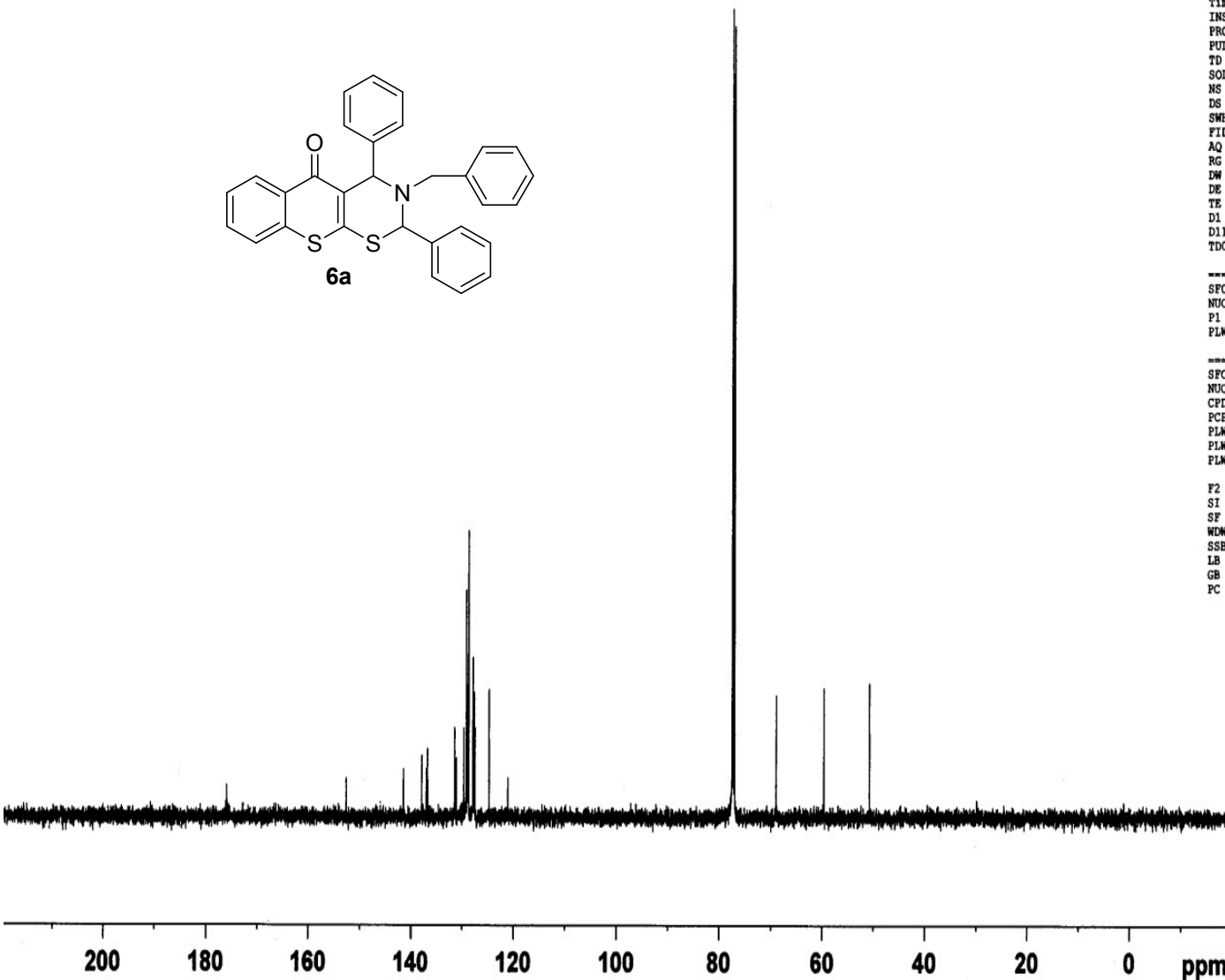
Current Data Parameters  
 NAME KM-AM-BEN\_13C  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20140313  
 Time 14.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 248  
 DS 2  
 SWH 36057.691 Hz  
 FIDRES 1.100393 Hz  
 AQ 0.4543829 sec  
 RG 65.24  
 DW 13.867 usec  
 DE 6.50 usec  
 TE 301.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 150.9279571 MHz  
 NUC1 13C  
 P1 10.50 usec  
 PLW1 95.00000000 W

===== CHANNEL f2 =====  
 SFO2 600.1724007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 70.00 usec  
 PLW2 21.00000000 W  
 PLW12 0.61714000 W  
 PLW13 0.30239999 W

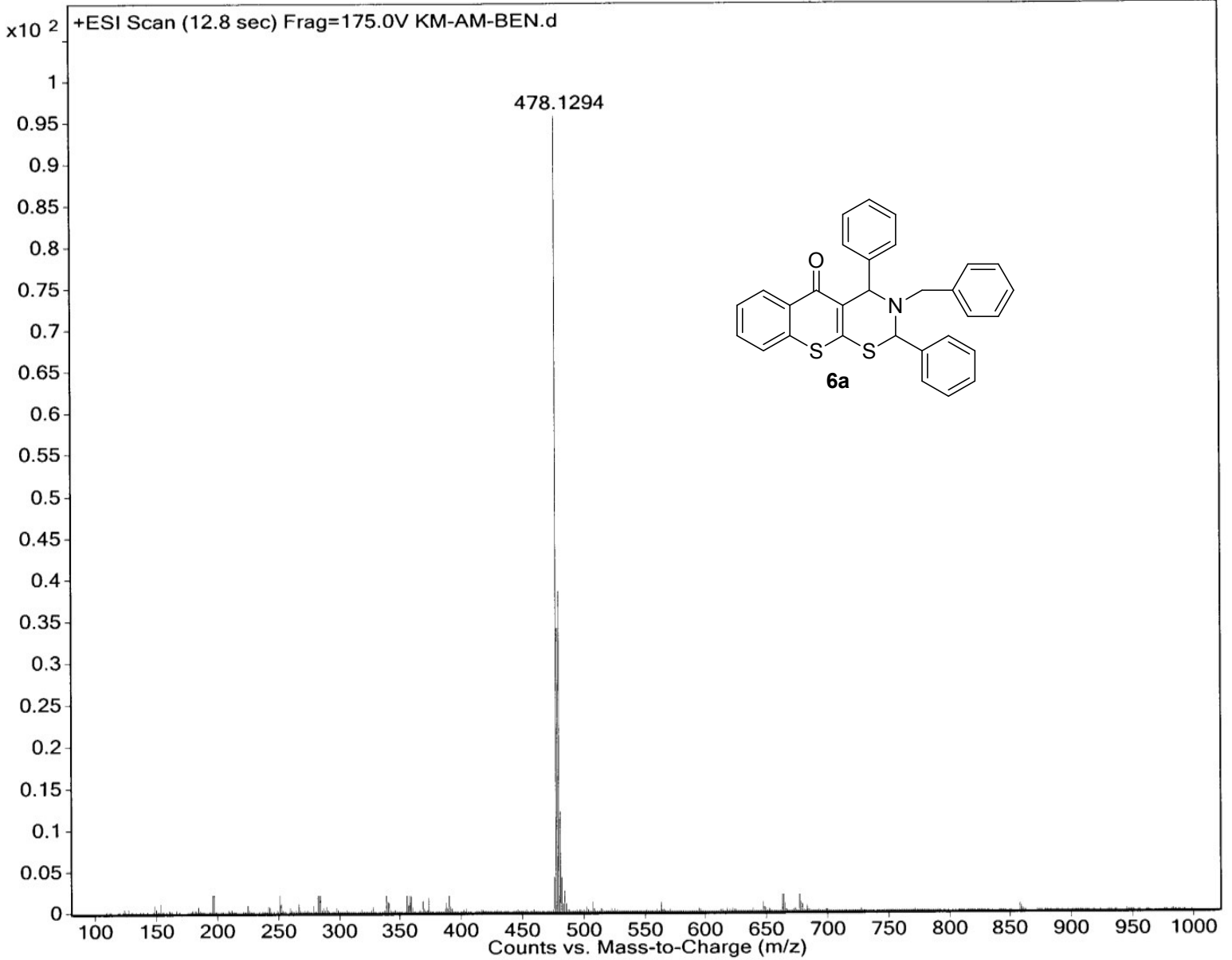
F2 - Processing parameters  
 SI 16384  
 SF 150.9128359 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



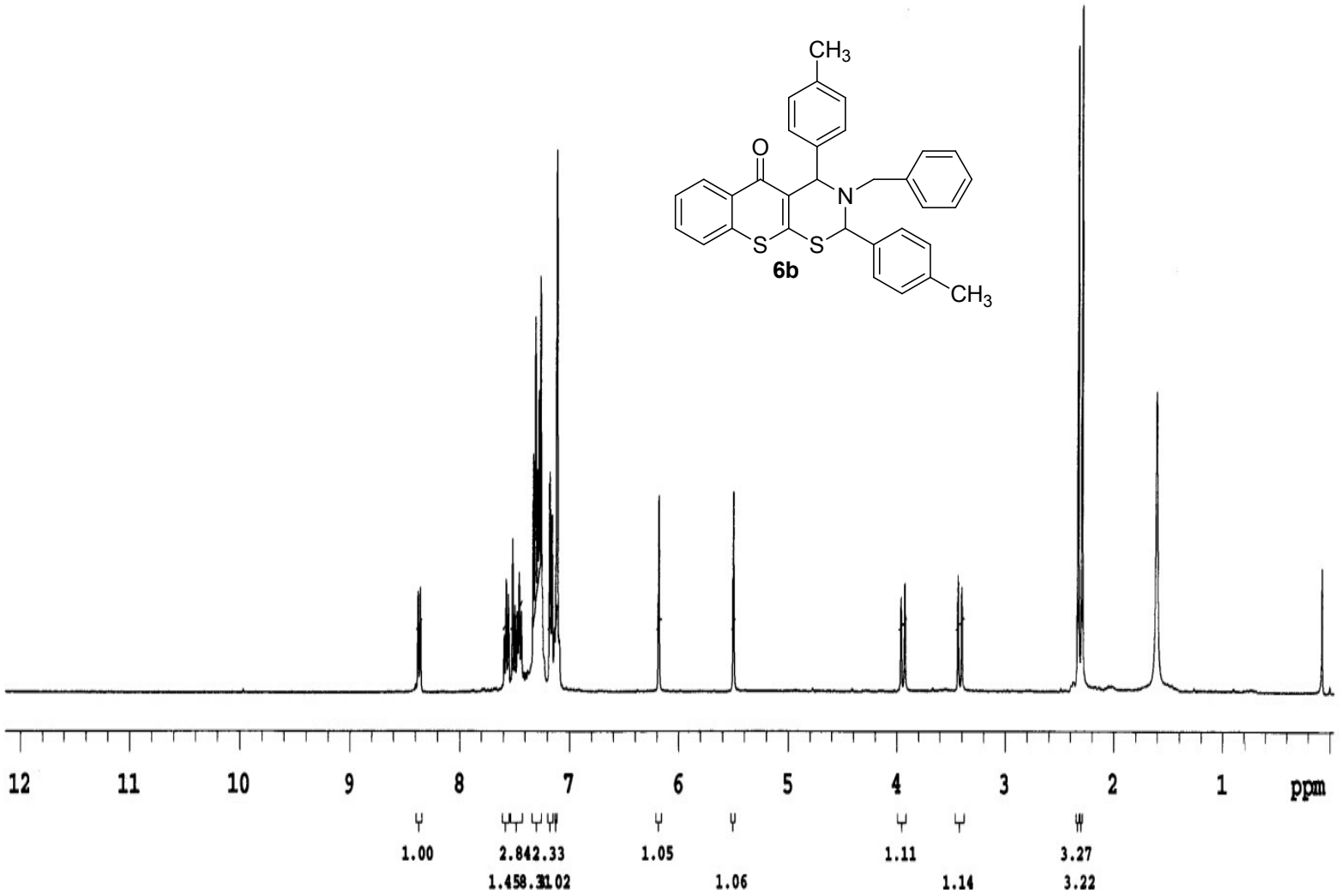


# HRMS spectra of compound: 6a

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

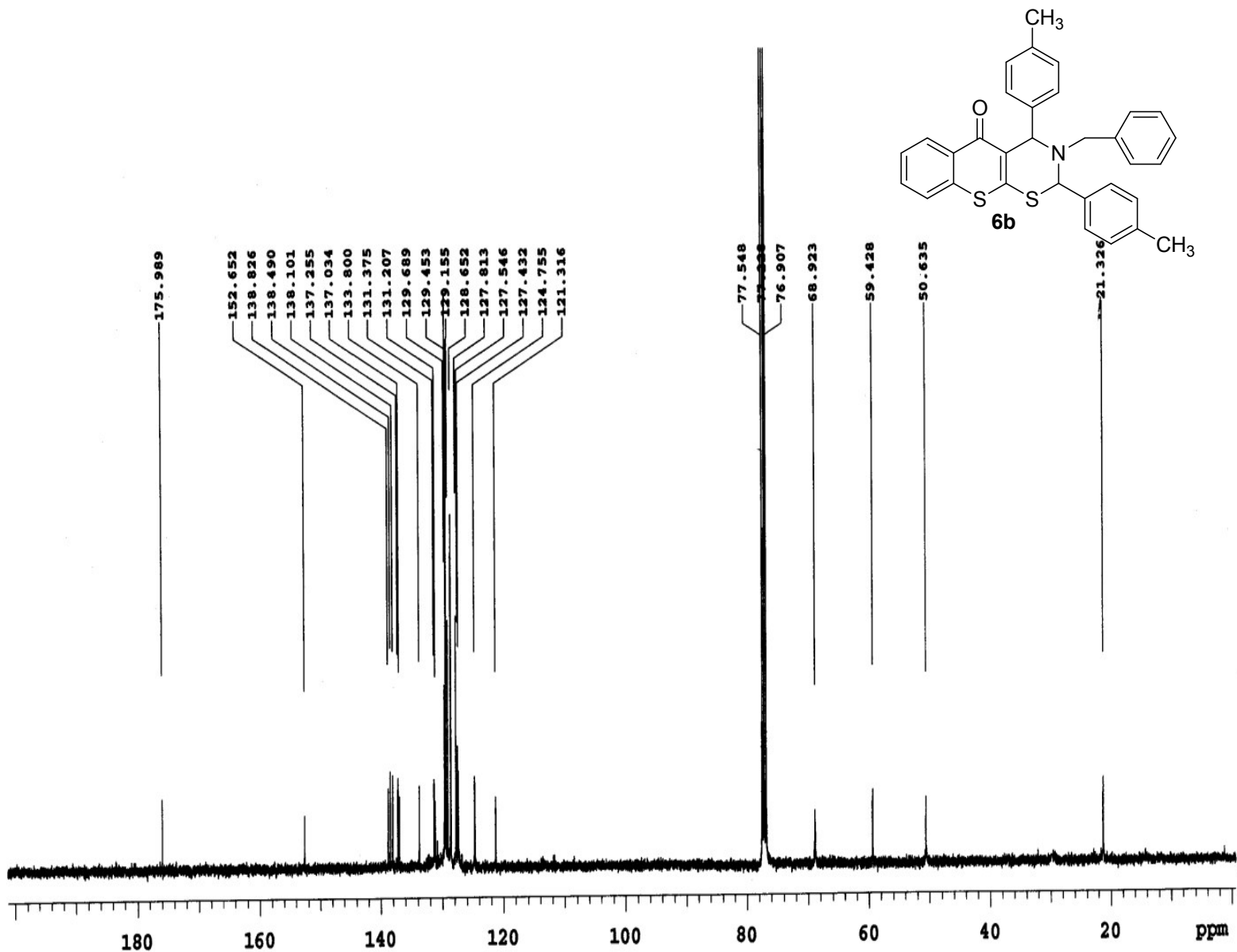


<sup>1</sup>HNMR spectra the compound: 6b



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	<b>OBSERVE</b> H1, 399.8509634	<b>DATA PROCESSING</b> FT size 32768 Total time 1 minutes	<b>KM-4Me-02-1H</b>  Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: KM-4Me-02-1H Mercury-400 *IITG-NMR*
---	--------------------------------	---	---

<sup>13</sup>CNMR spectra of compound: 6b



**PULSE SEQUENCE**  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.304 sec  
 Width 25125.6 Hz  
 12530 repetitions

**OBSERVE** C13, 100.5425819  
**DECOUPLE** H1, 399.8529994  
 Power 42 dB  
 continuously on  
 WALTZ-16 modulated

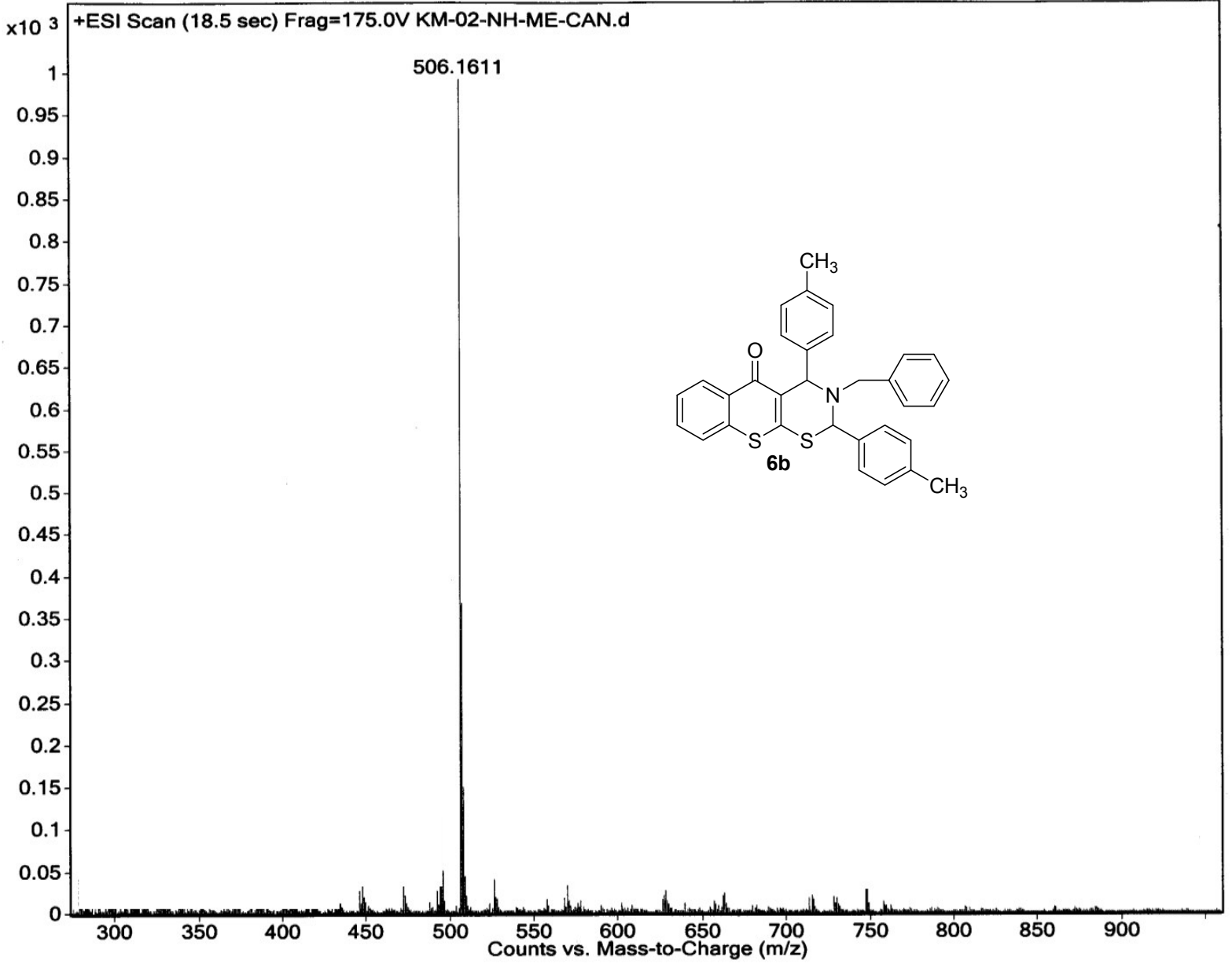
**DATA PROCESSING**  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 8.0 hours

KM-4Me-02-13C

Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 "IITG-NMR"

HRMS spectra of compound: 6b

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra the compound: 6c

KM-02-NH-20

Sample Name:

KM-02-NH-20

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/home/chem/data/study

Sample directory:

DB\_382\_sm-01

Fidfile: KM-02-NH-20

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 5 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

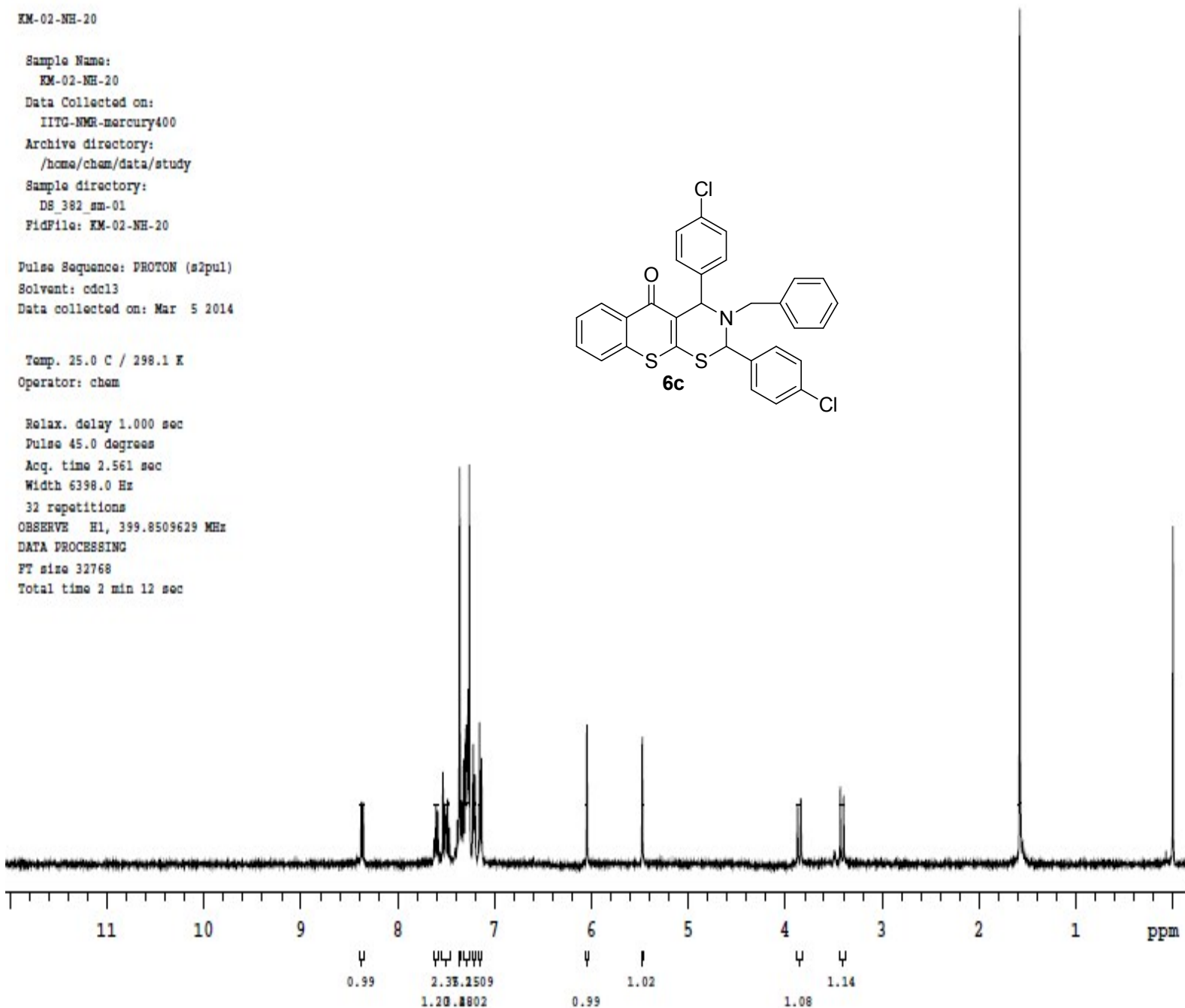
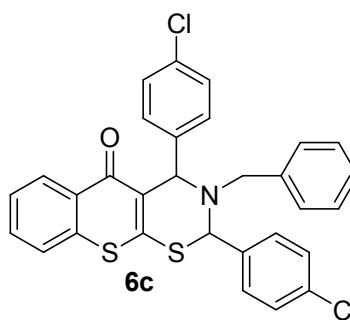
32 repetitions

OBSERVE H1, 399.8509629 MHz

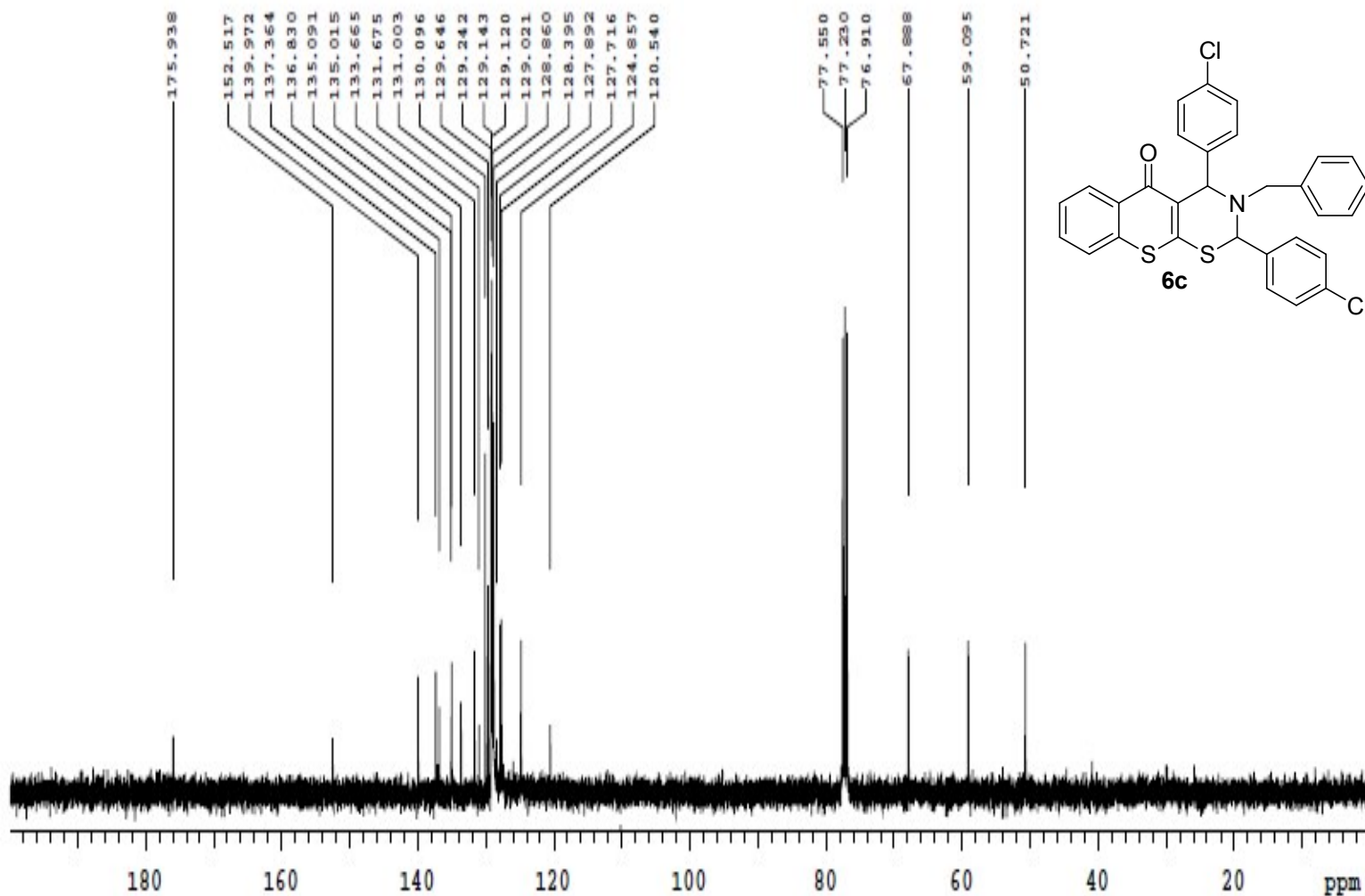
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



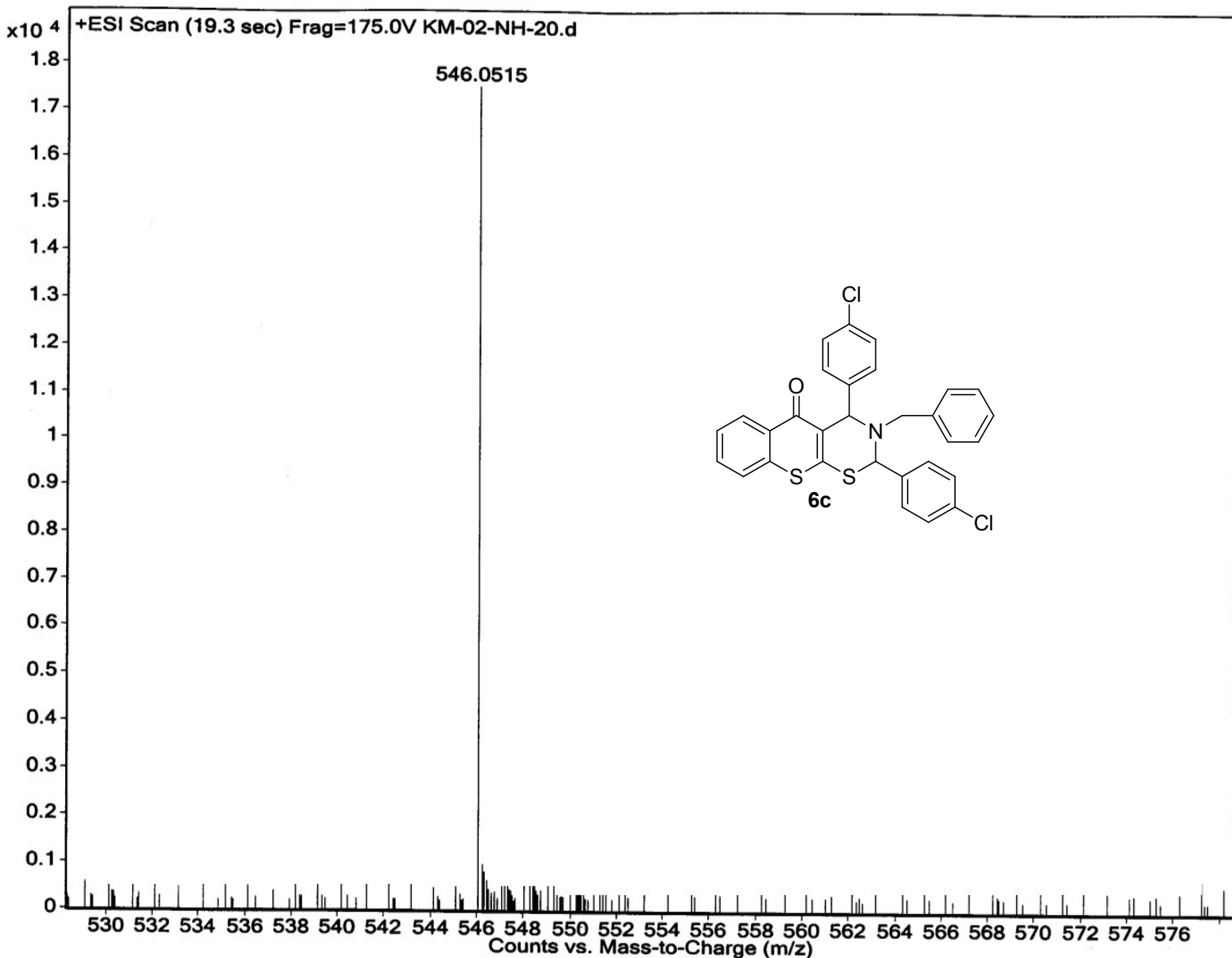
<sup>13</sup>CNMR spectra of compound: 6c



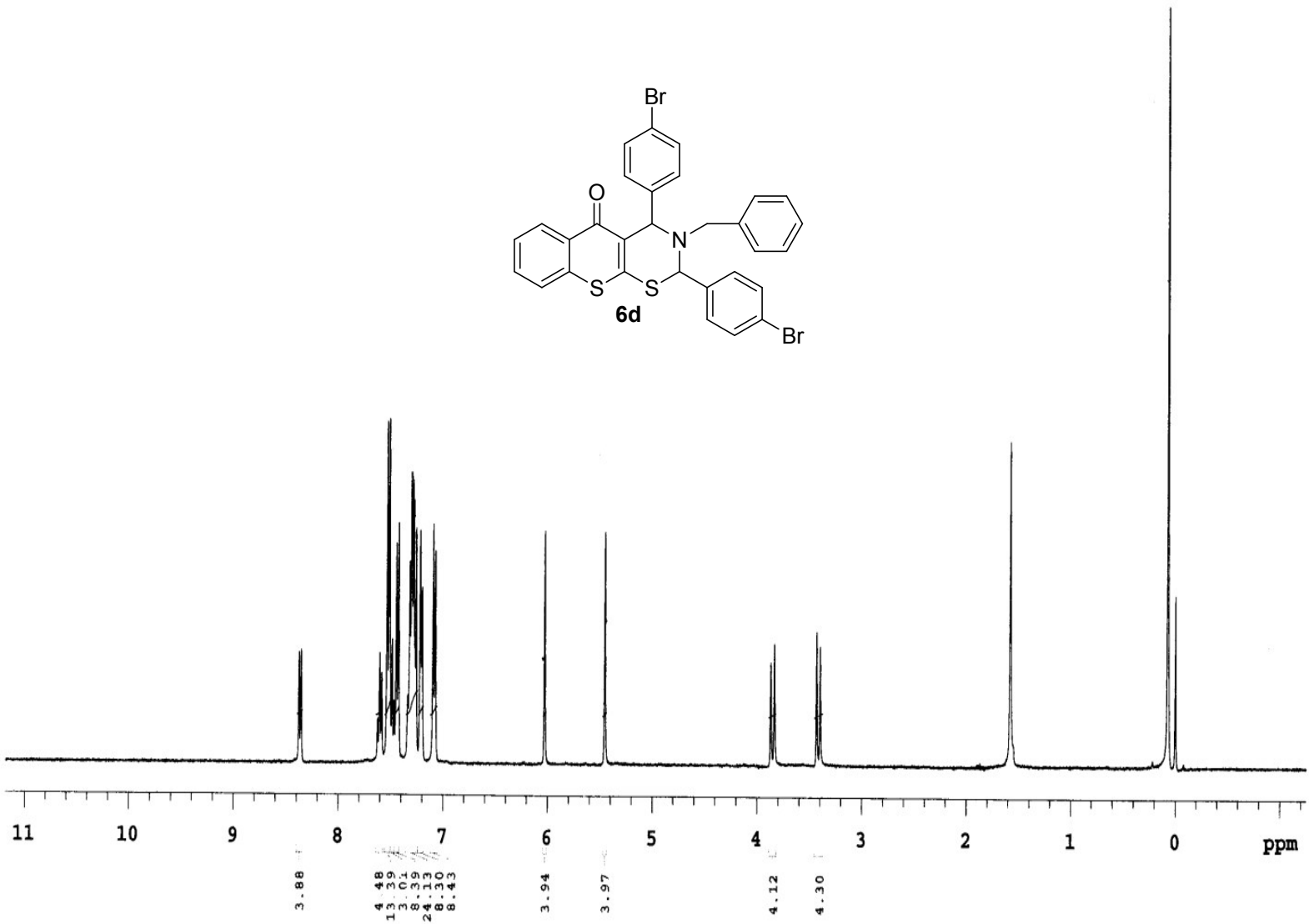
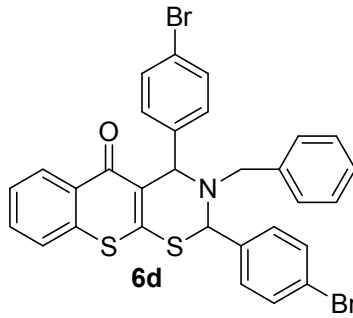
<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 840 repetitions	<b>OBSERVE</b> C13, 100.5425840 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 32 minutes	<b>EM-02-NH-20-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: EM-02-NH-20-13C Mercury-400 "IITG-NMR"
---	--	--	---

# HRMS spectra of compound: 6c

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>H NMR spectra the compound: 6d



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions

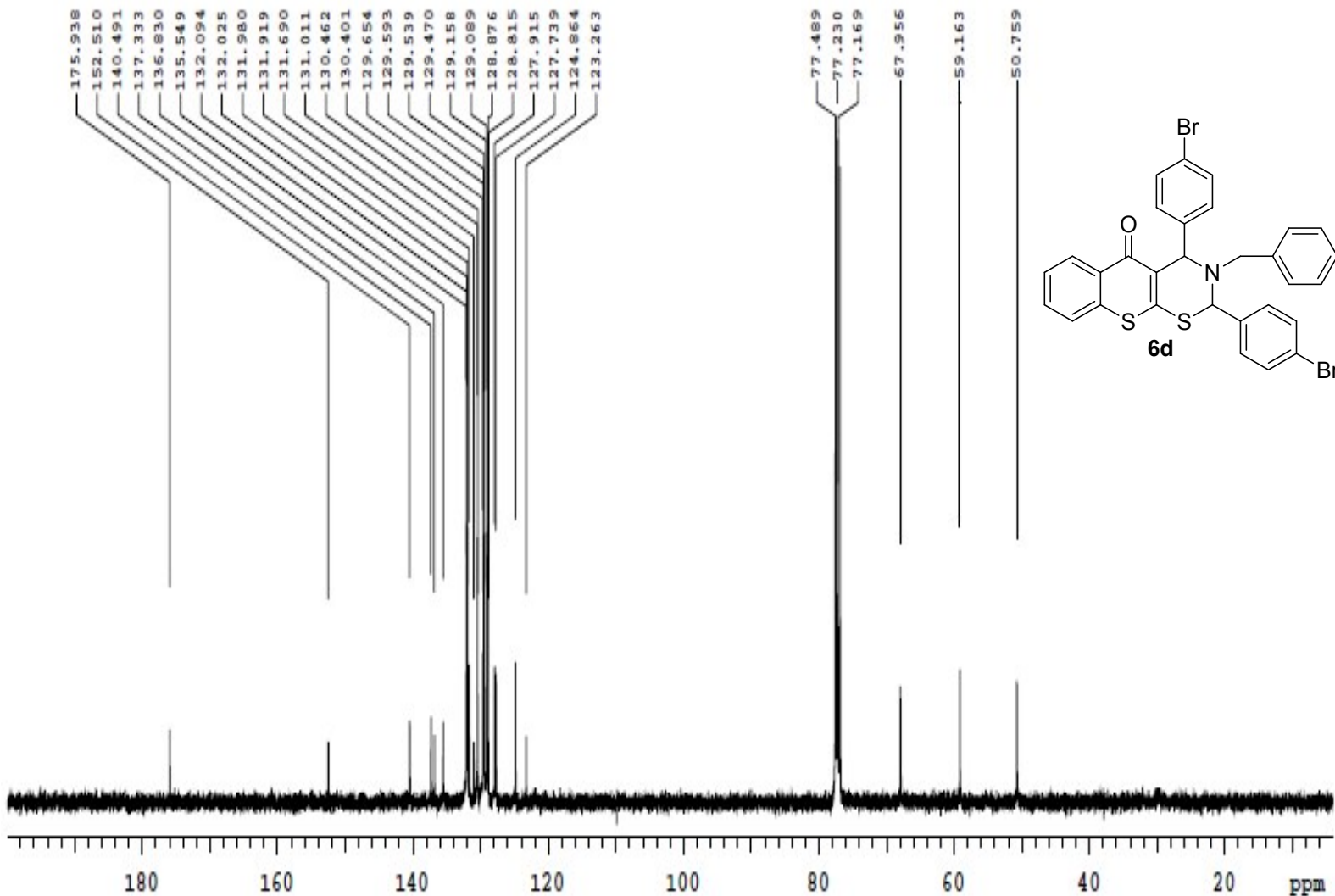
OBSERVE H1, 39908509644

DATA PROCESSING  
FT size 32768  
Total time 1 minutes

km-trail SOURCE: DATA PF  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: km-trail  
Mercury-400 "IITG-NMR"



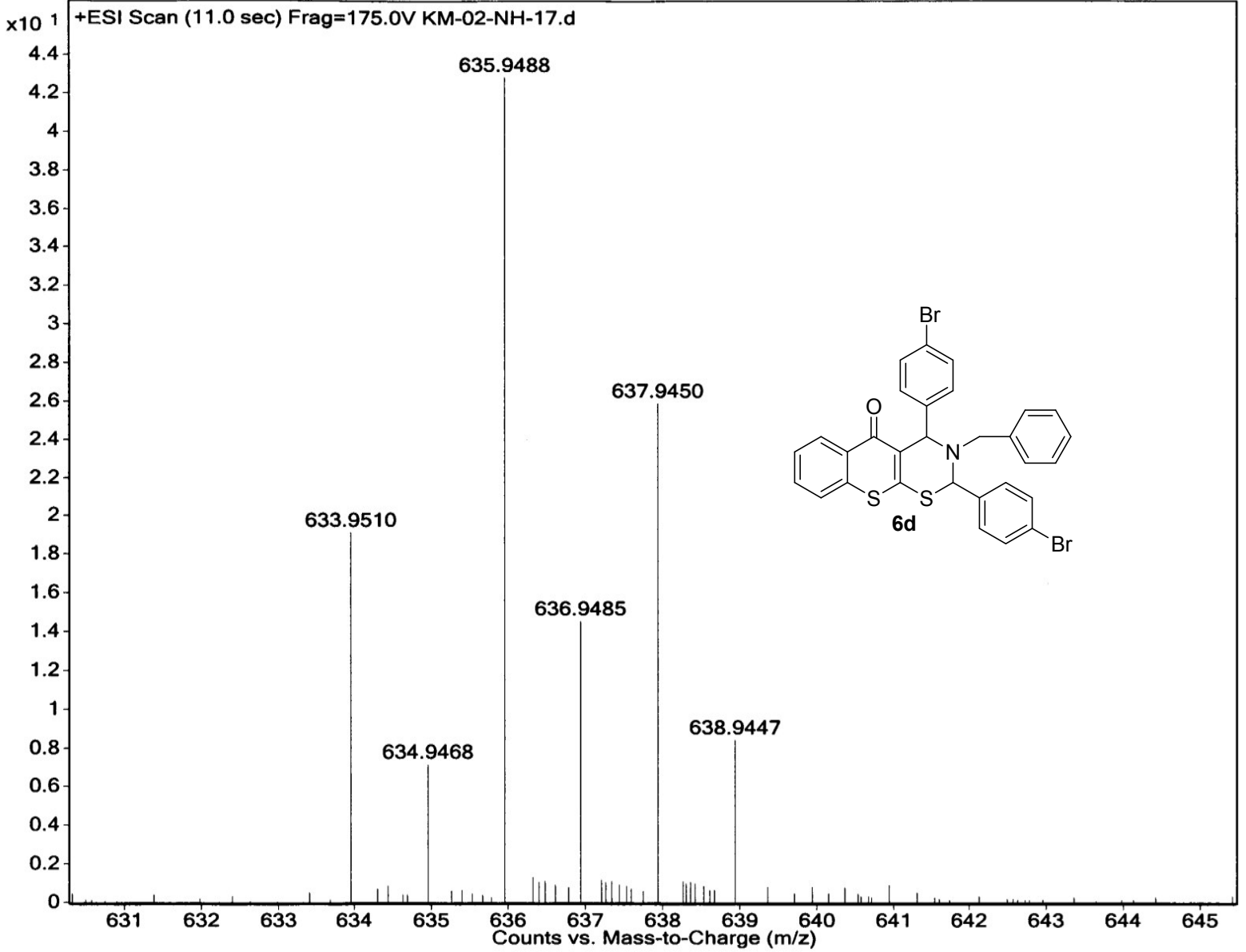
### <sup>13</sup>CNMR spectra of compound: 6d



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 9050 repetitions	<b>OBSERVE</b> C13, 100.5426154 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 5.8 hours	<b>KM-AM-1-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: KM-AM-1-13C Mercury-400 "IITG-NMR"
--	--	---	---

# HRMS spectra of compound: 6d

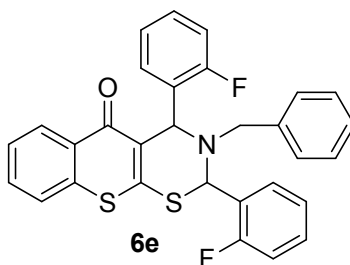
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra the compound: 6e

KM-AM-2F

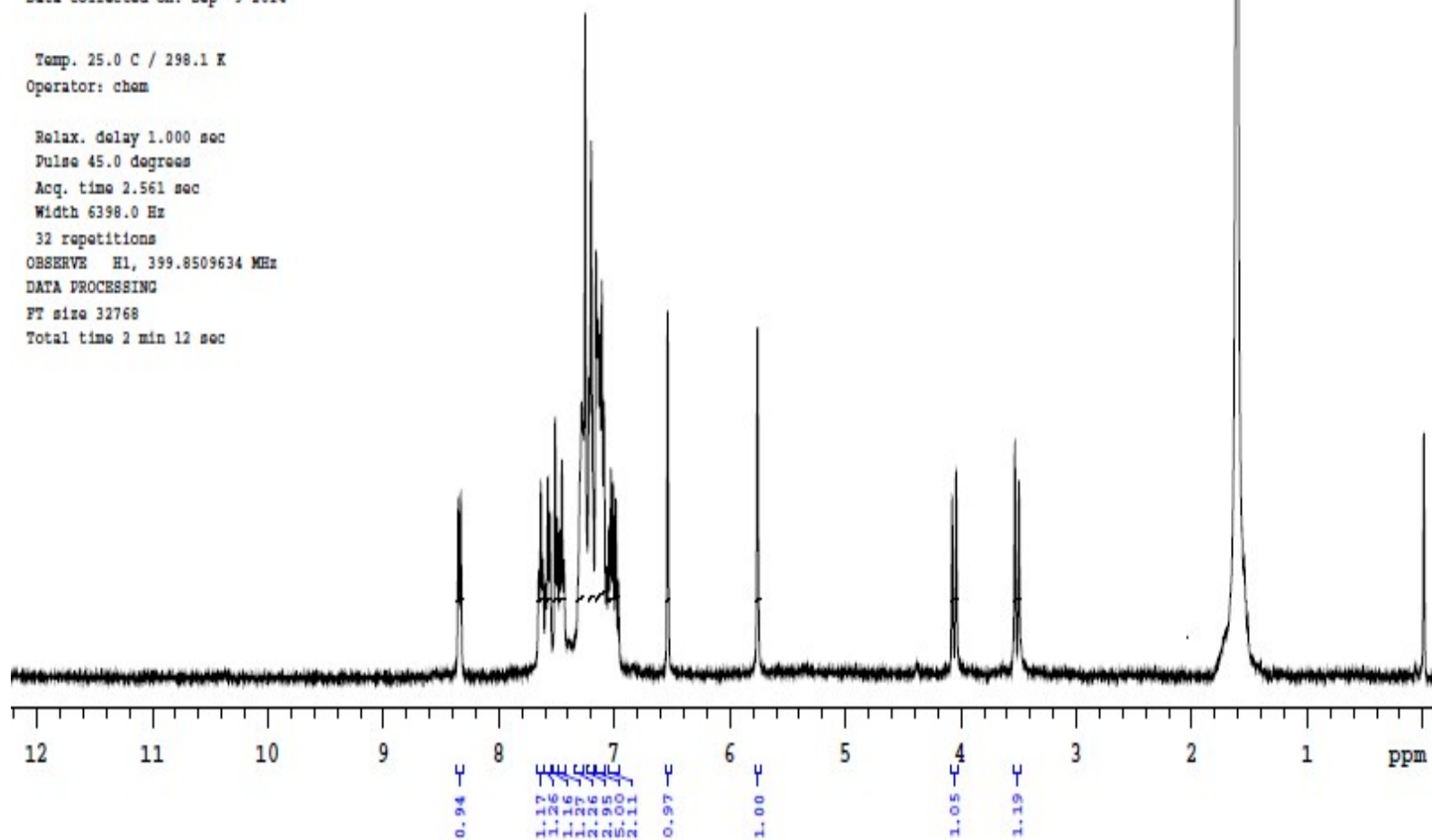
Sample Name:  
KM-AM-2F  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
Sample directory:  
FidFile: KM-AM-2F



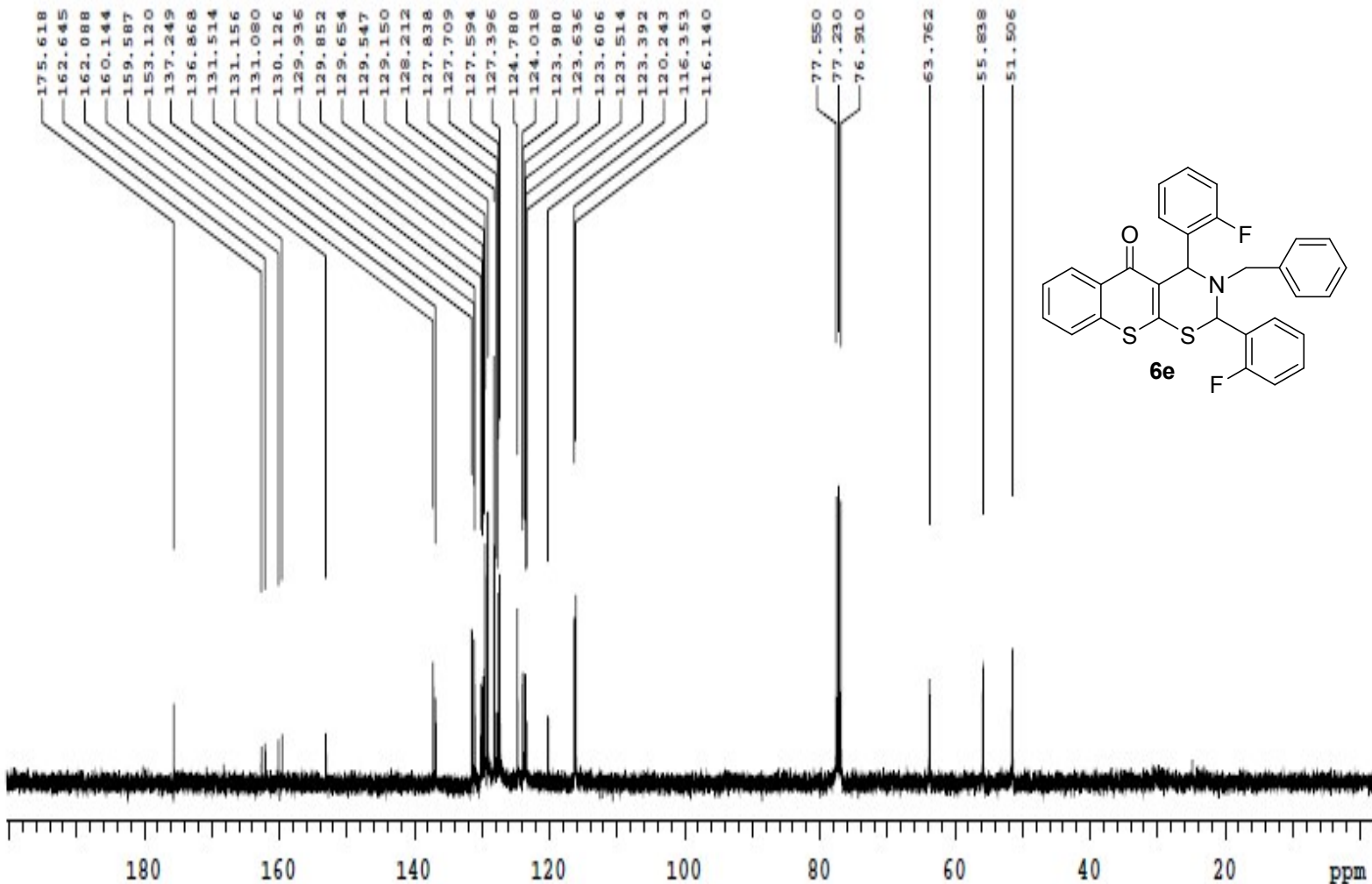
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Sep 9 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509634 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



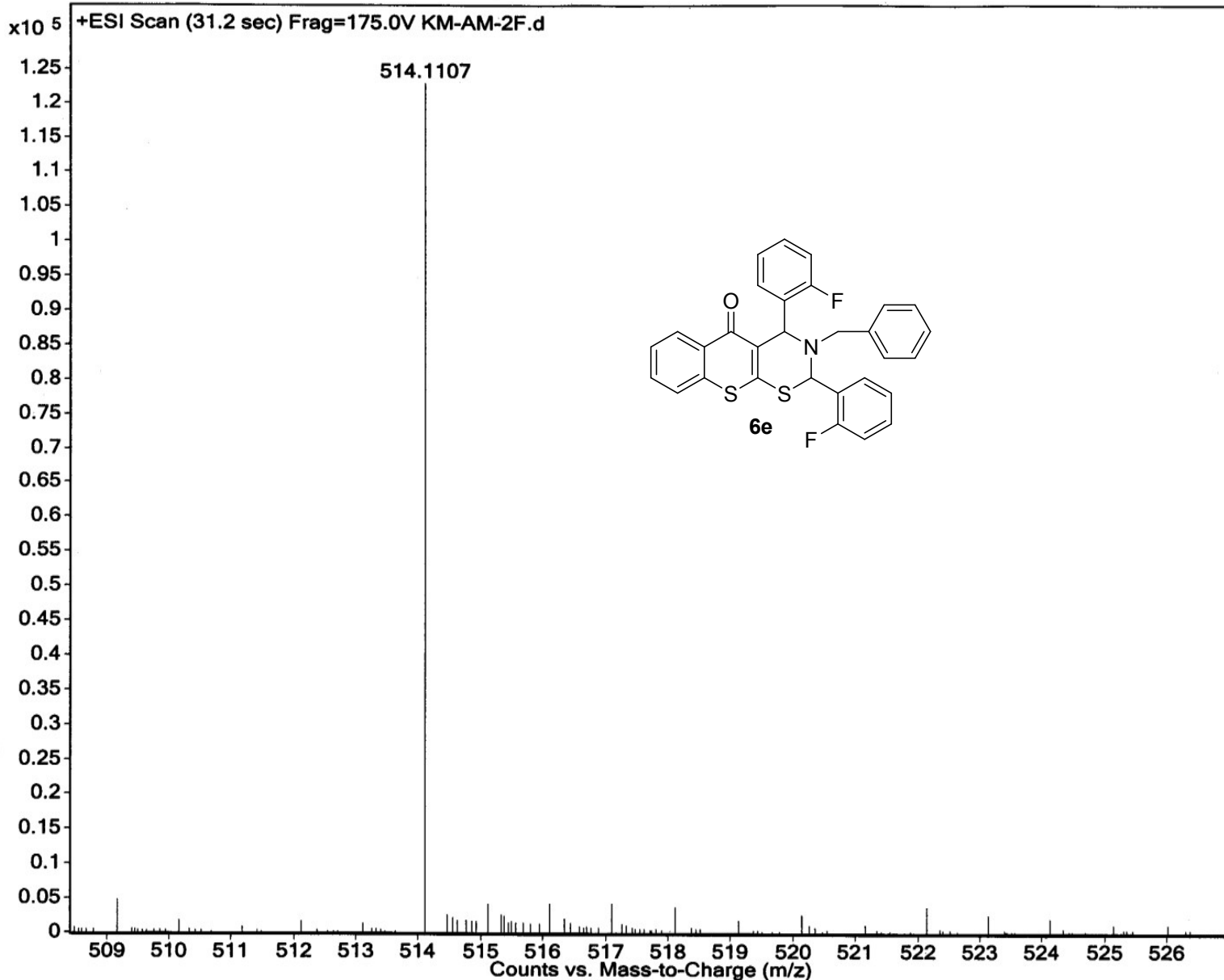
<sup>13</sup>CNMR spectra of compound: 6e



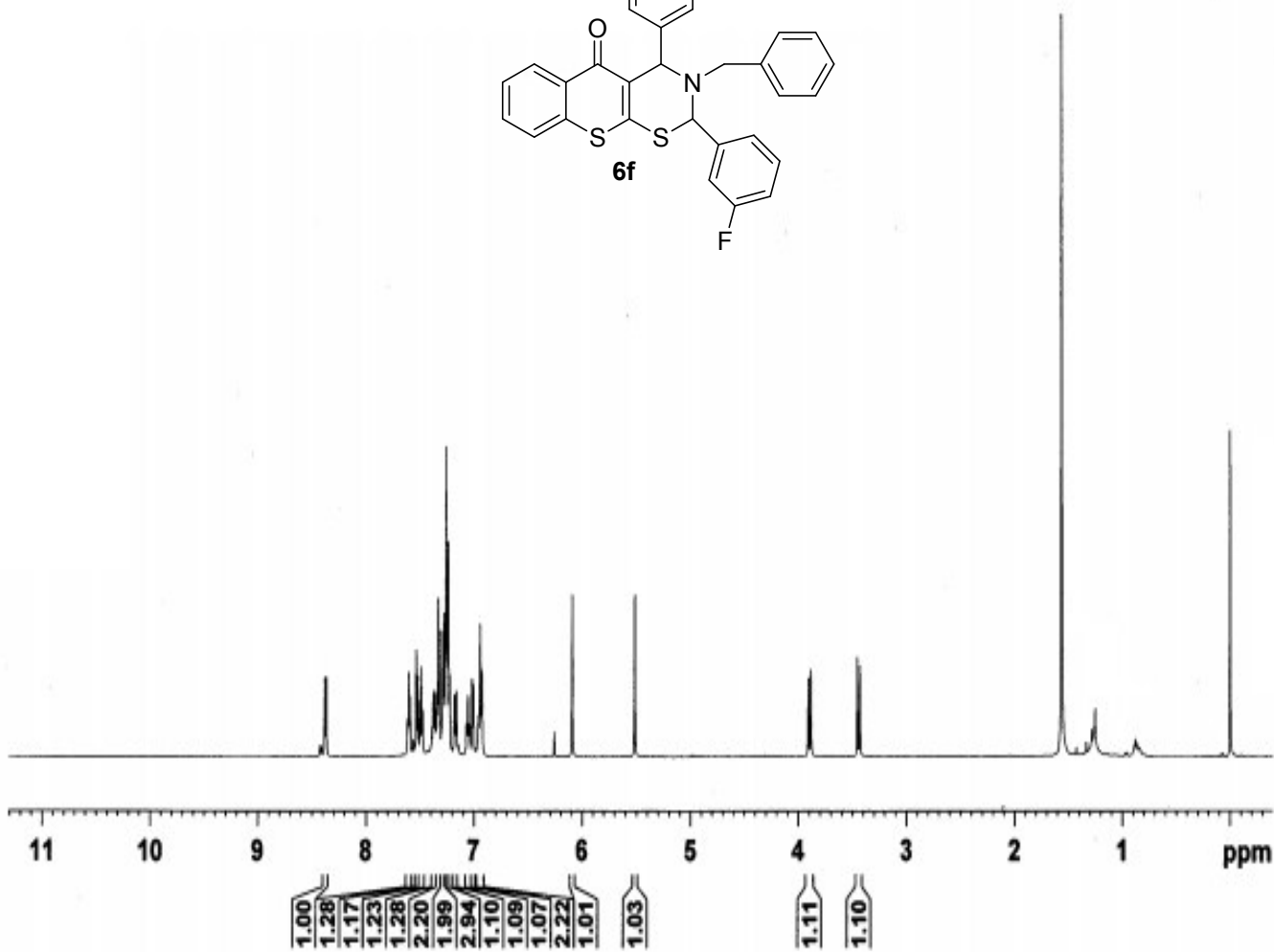
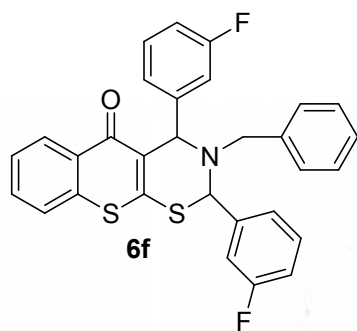
<p><b>PULSE SEQUENCE</b>                  Relax. delay 1.000 sec                  Pulse 45.0 degrees                  Acq. time 1.304 sec                  Width 25125.6 Hz                  640 repetitions</p>	<p><b>OBSERVE</b> C13, 100.5425863                  DECOUPLE H1, 399.8529994                  Power 42 dB                  continuously on                  WALTZ-16 modulated</p>	<p><b>DATA PROCESSING</b>                  Line broadening 0.5 Hz                  FT size 65536                  Total time 24 minutes</p>	<p><b>EM-AM-2F-13C</b>                  Solvent: cdcl3                  Temp. 25.0 C / 298.1 K                  Operator: chem                  File: EM-AM-2F-13C                  Mercury-400 "IITG-NMR"</p>
--	--	---	--

# HRMS spectra of compound: 6e

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



<sup>1</sup>HNMR spectra the compound: 6f



```

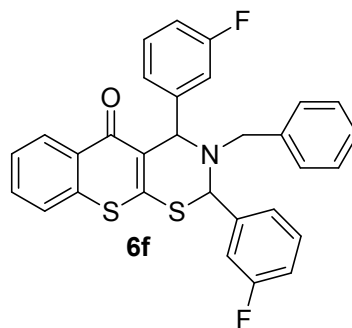
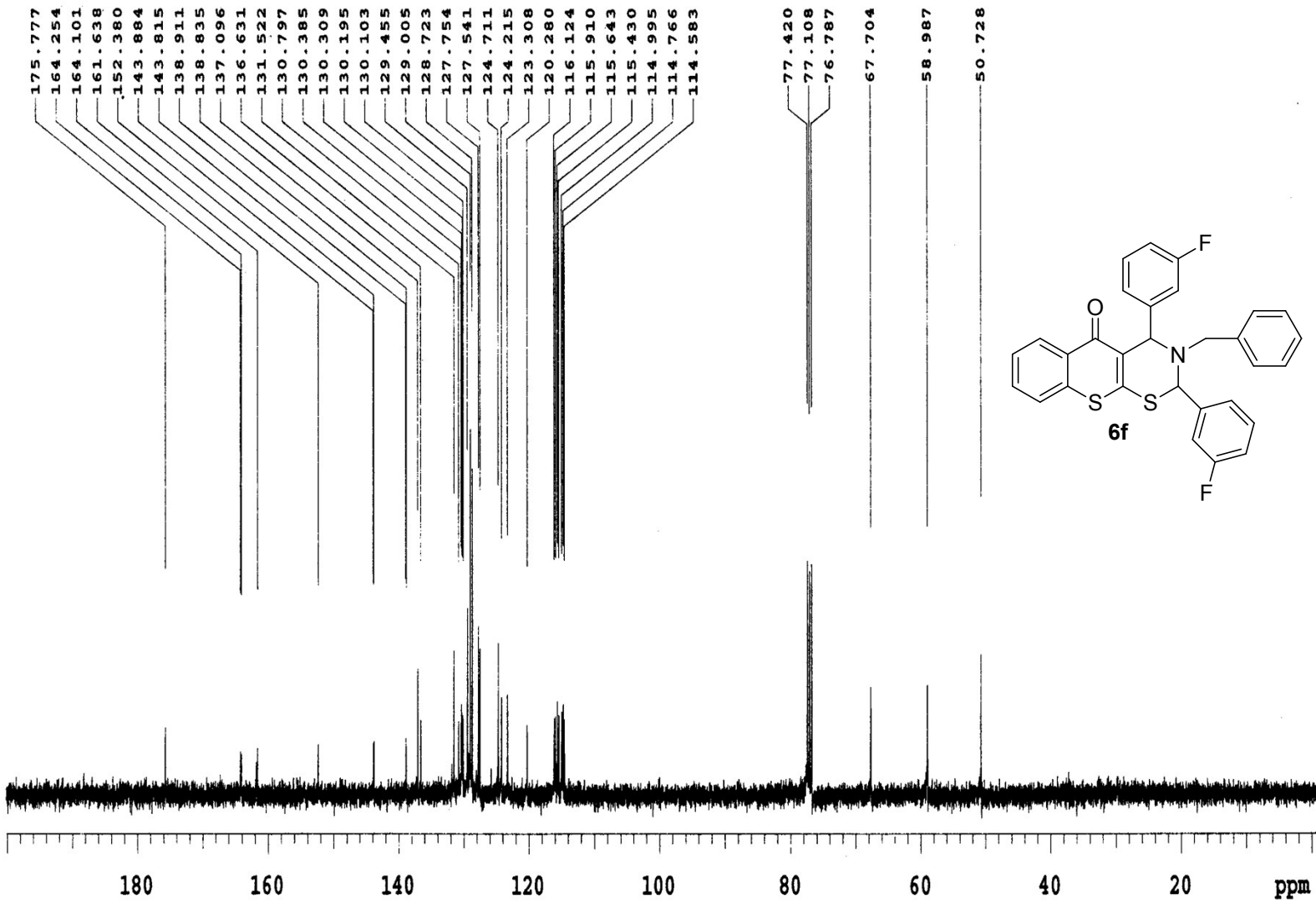
Current Data Parameters
NAME      FM-1P-No-1-1H
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    2016023
Time     17.09
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       2
SWH      12019.230 Hz
FIDRES   0.366798 Hz
AQ       1.3431488 sec
RG       327.57
DW       41.600 usec
DE       6.50 usec
TE       297.6 K
SI       1.00000000 sec
TSD     1

===== CHANNEL f1 =====
SFO1    400.137043 MHz
NUC1     1H
P1      12.00 usec
PL1     21.00000000 W

F2 - Processing parameters
SI      16384
SF      400.137043 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
    
```

<sup>13</sup>CNMR spectra of compound: 6f



**PULSE SEQUENCE**  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.304 sec  
 Width 25125.6 Hz  
 120 repetitions

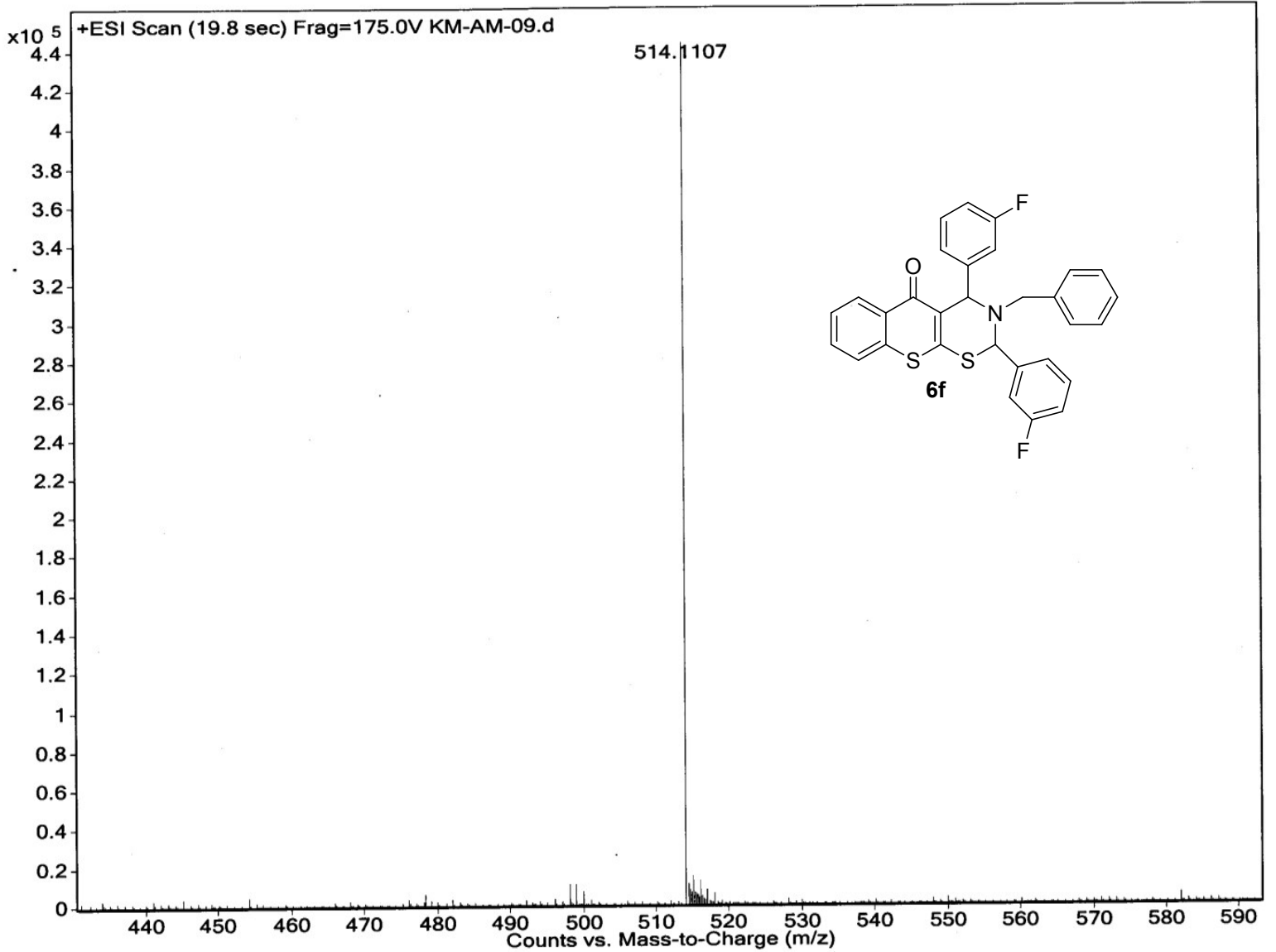
**OBSERVE** C13, 210055426047  
**DECOUPLE** H1, 399.8529994  
 Power 42 dB  
 continuously on  
**WALTZ-16** modulated

**DATA PROCESSING**  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 4 minutes

**NAME** 6f  
**Solvent**: cdcl3  
**Temp.** 25.0 C / 298.1 K  
**Operator**: chem  
**Mercury-400** "1H-NMR"

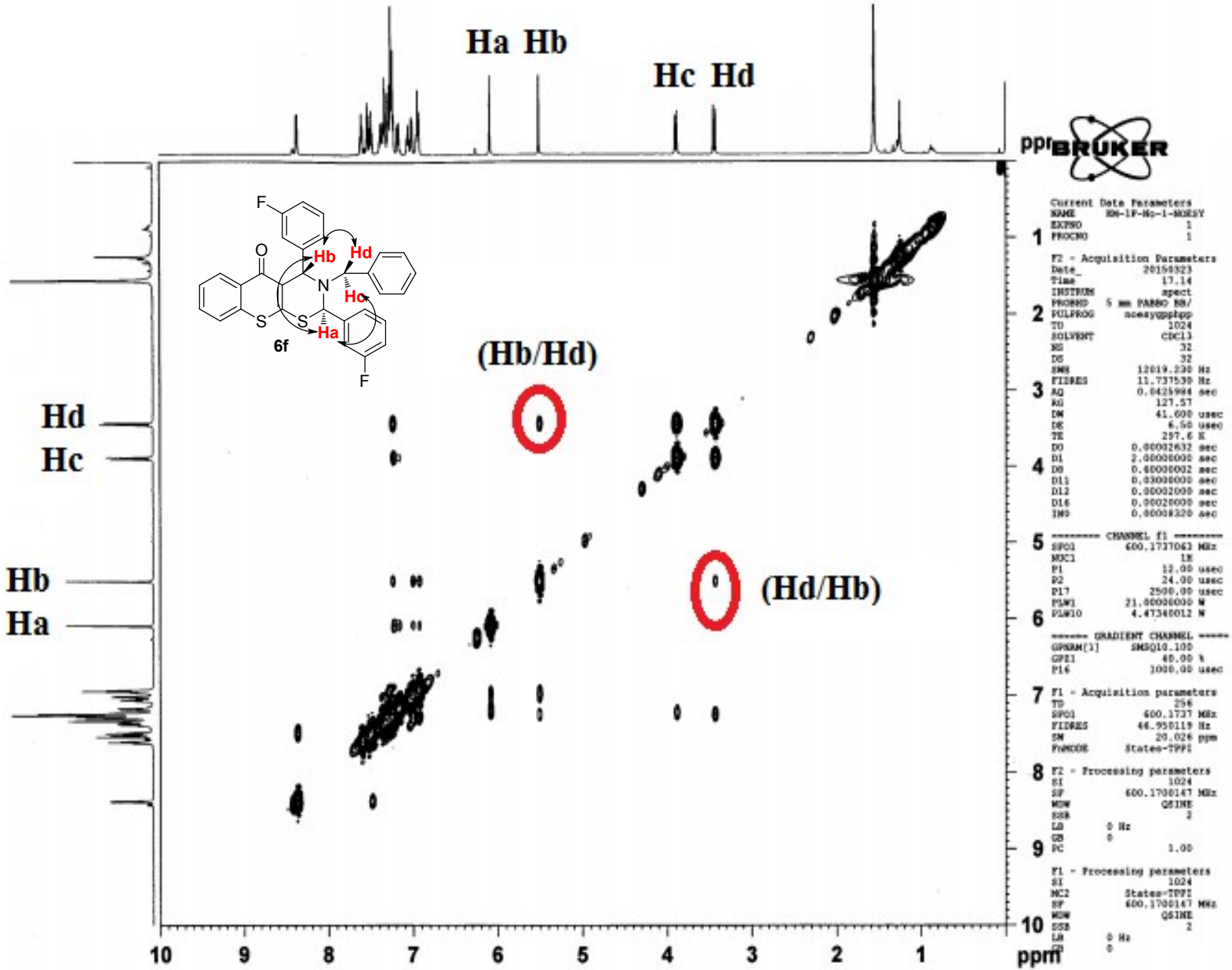
# HRMS spectra of compound: 6f

Sample Name	KM-AM-09	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	KM-AM-09.d	ACQ Method		Comment		Acquired Time	9/10/2014 12:02:42 PM

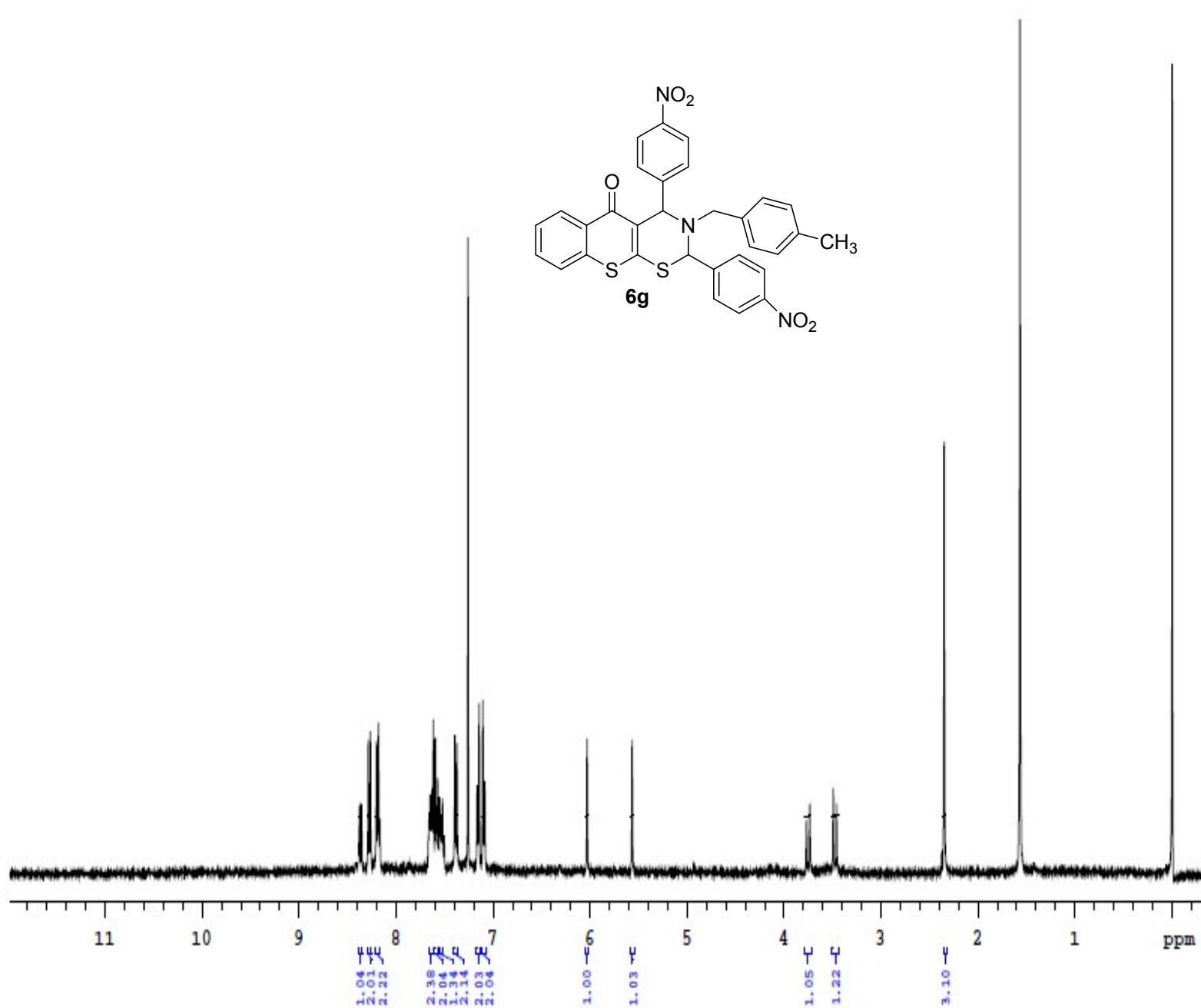




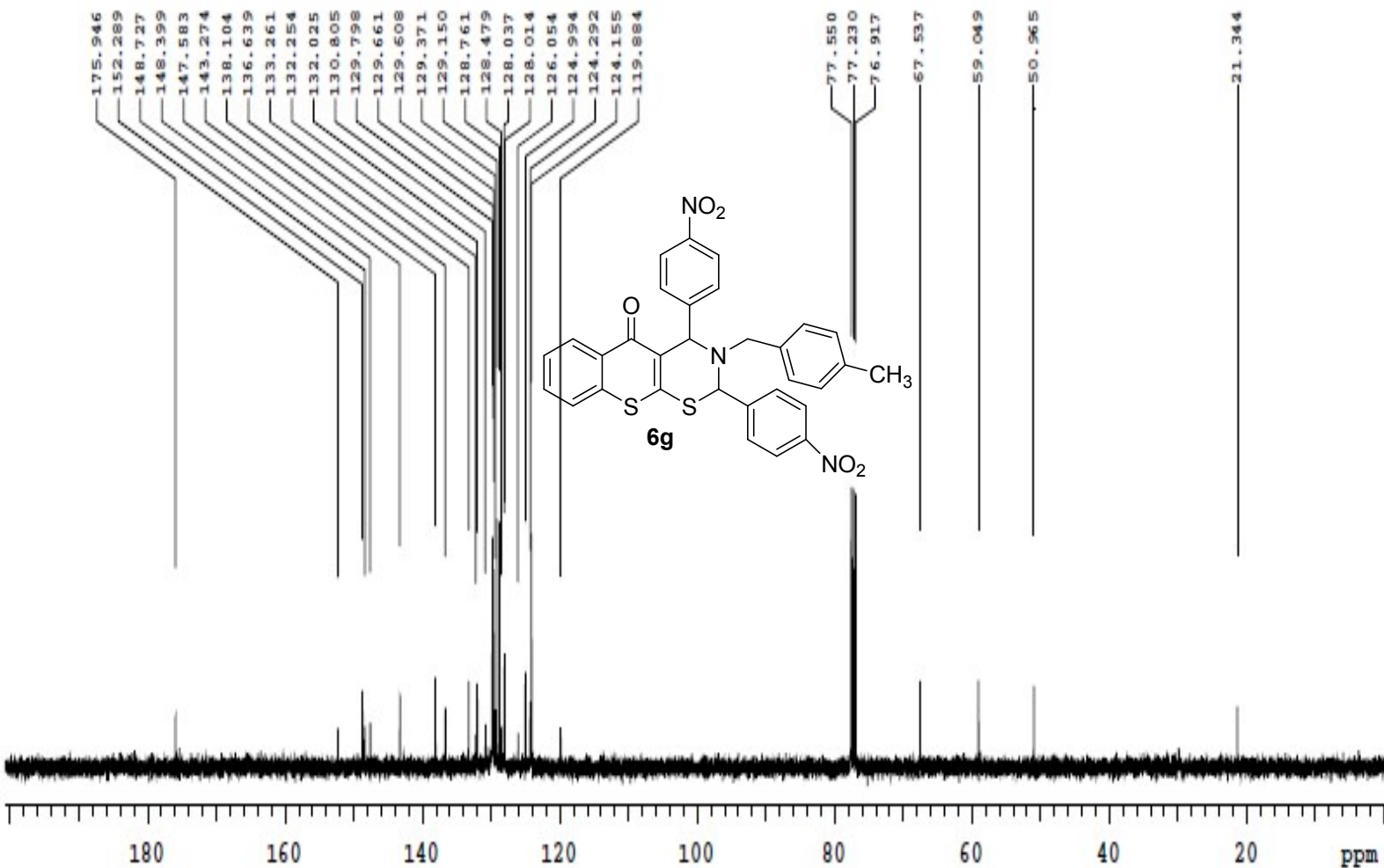
NOEs spectra of compound: 6f



<sup>1</sup>HNMR spectra the compound: 6g



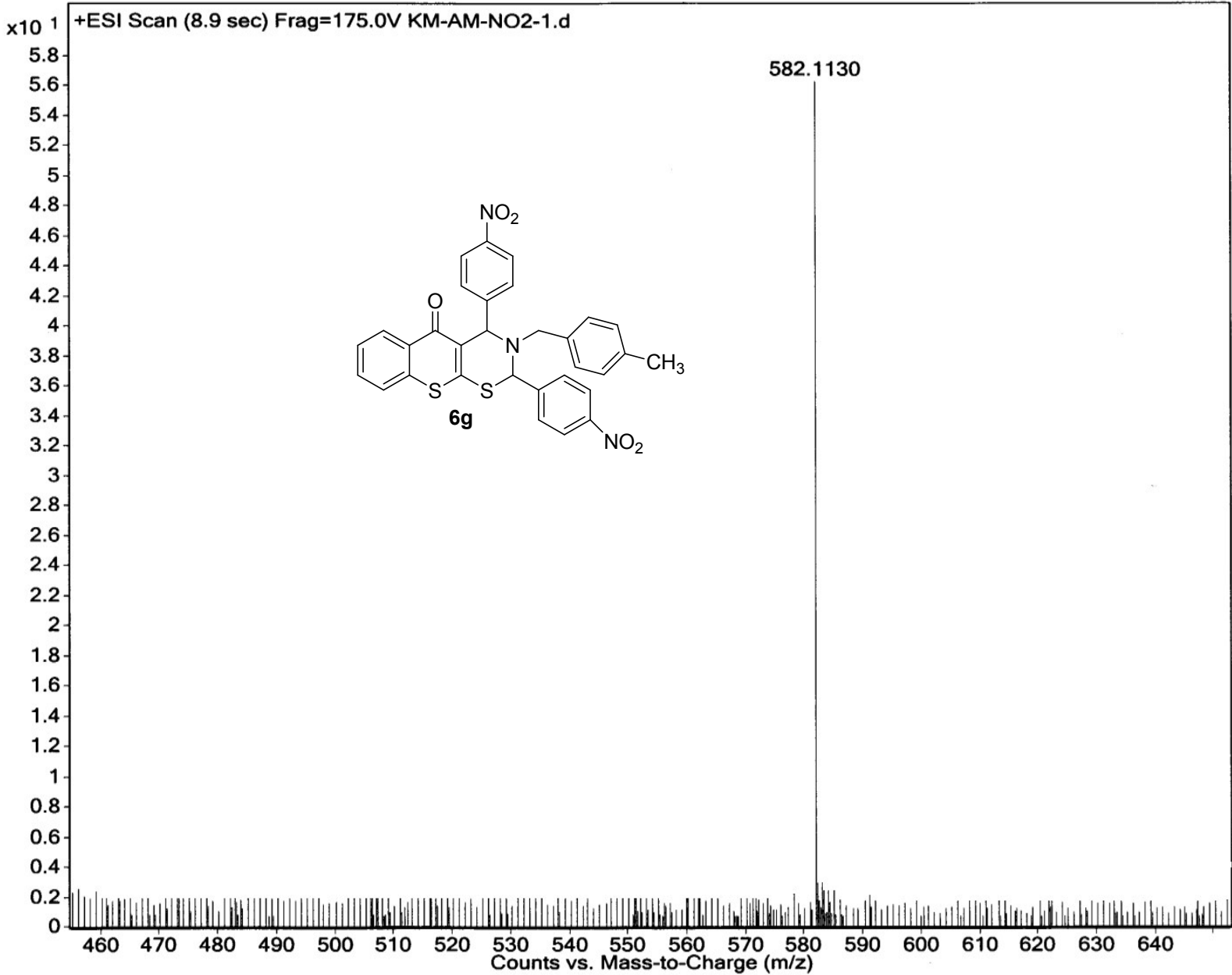
<sup>13</sup>CNMR spectra of compound: 6g



<p><b>PULSE SEQUENCE</b>                  Relax. delay 1.000 sec                  Pulse 45.0 degrees                  Acq. time 1.304 sec                  Width 25125.6 Hz                  300 repetitions</p>	<p><b>OBSERVE</b> C13, 100.5425855  <b>DECOUPLE</b> H1, 399.8529994                  Power 42 dB                  continuously on                  WALTZ-16 modulated</p>	<p><b>DATA PROCESSING</b>                  Line broadening 0.5 Hz                  FT size 65536                  Total time 11 minutes</p>	<p><b>EM-AM-N02-13C</b>                  Solvent: cdcl3                  Temp. 25.0 C / 298.1 K                  Operator: chem                  File: EM-AM-N02-13C                  Mercury-400 "IITG-NMR"</p>
--	---	---	--

# HRMS spectra of compound: 6g

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra the compound: 6h

KM-AM-14-1H

Sample Name:

KM-AM-14-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

FidFile: KM-AM-14-1H

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Apr 8 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

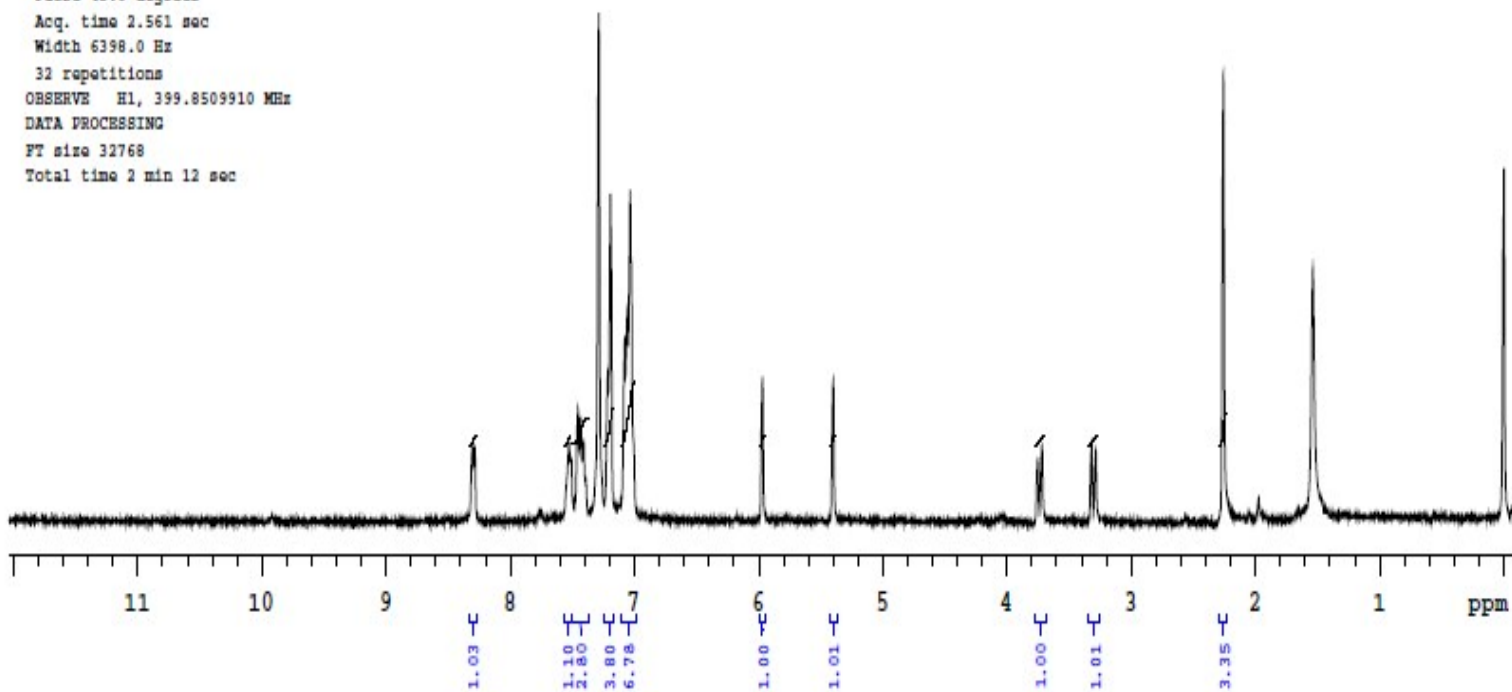
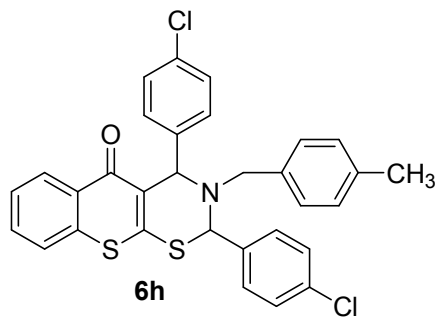
32 repetitions

OBSERVE H1, 399.8509910 MHz

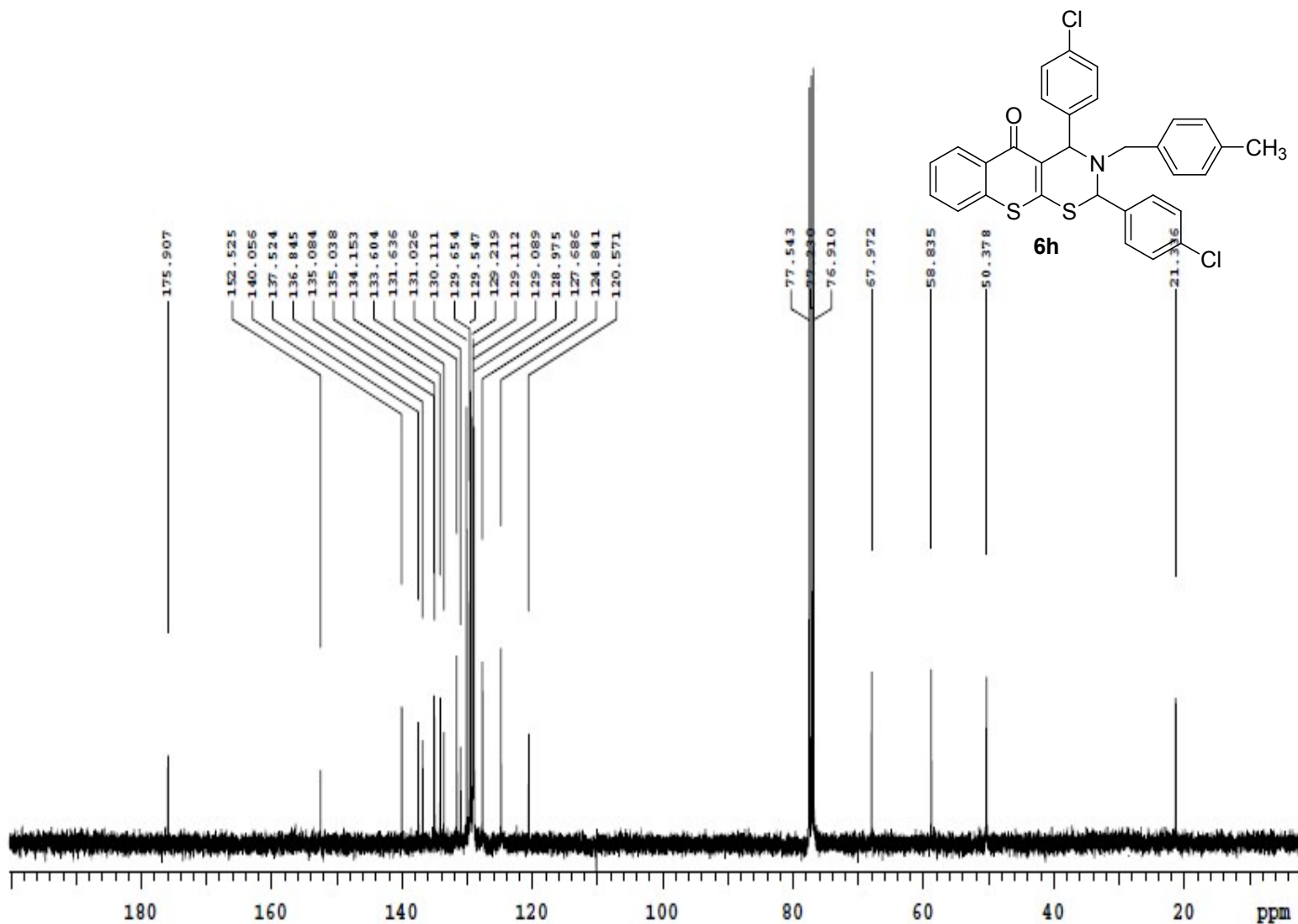
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



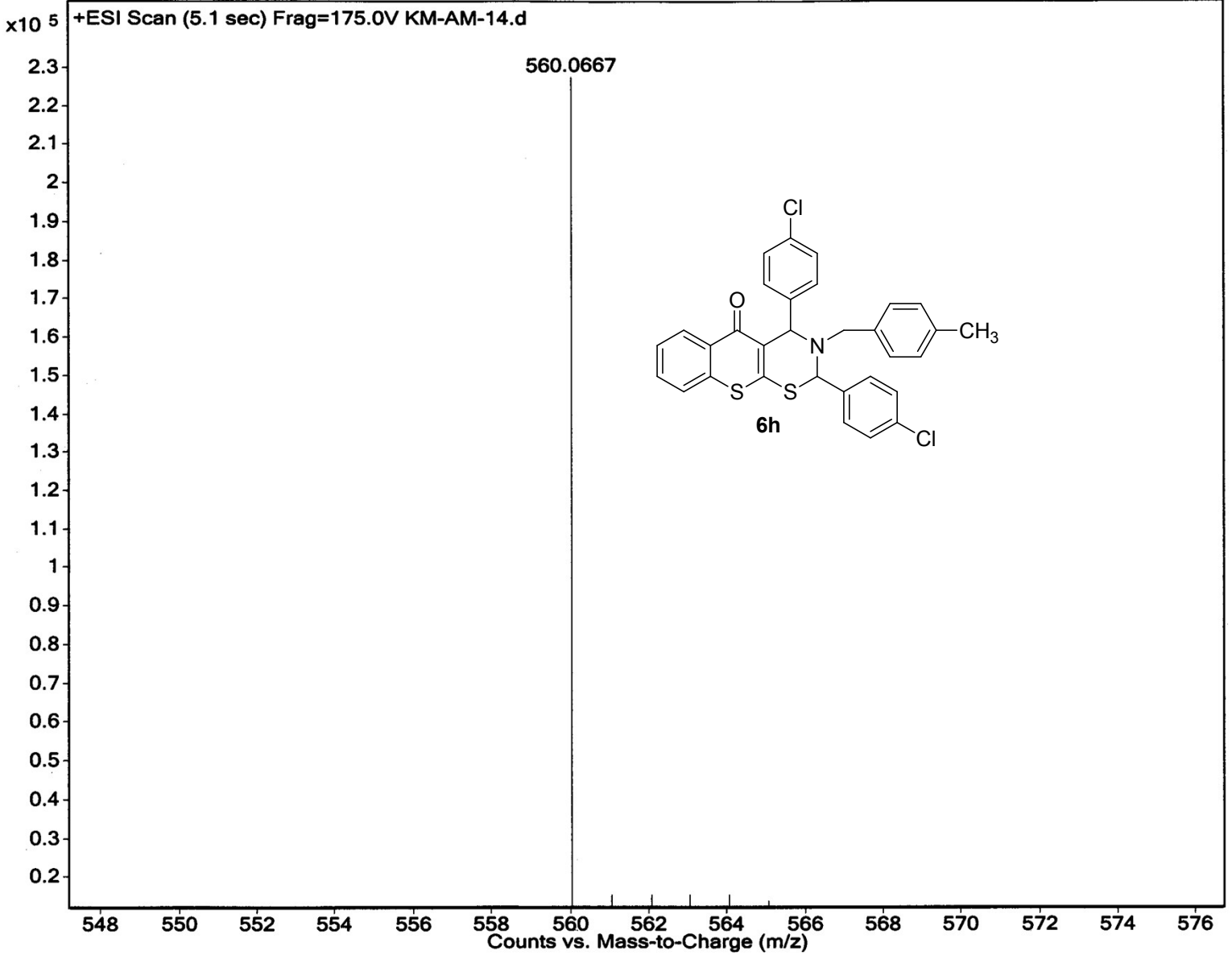
<sup>13</sup>CNMR spectra of compound: 6h



<p>PULSE SEQUENCE</p> <p>Relax. delay 1.000 sec</p> <p>Pulse 45.0 degrees</p> <p>Acq. time 1.304 sec</p> <p>Width 25125.6 Hz</p> <p>1590 repetitions</p>	<p>OBSERVE C13, 100.5425840</p> <p>DECOUPLE H1, 399.8529994</p> <p>Power 42 dB</p> <p>continuously on</p> <p>WALTZ-16 modulated</p>	<p>DATA PROCESSING</p> <p>Line broadening 0.5 Hz</p> <p>FT size 65536</p> <p>Total time 61 minutes</p>	<p>EM-AM-14-13C</p> <p>Solvent: cdcl3</p> <p>Temp. 25.0 c / 298.1 K</p> <p>Operator: chem</p> <p>File: EM-AM-14-13C</p> <p>Mercury-400 *IITC-NMR*</p>
--	---	--	---

# HRMS spectra of compound: 6h

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

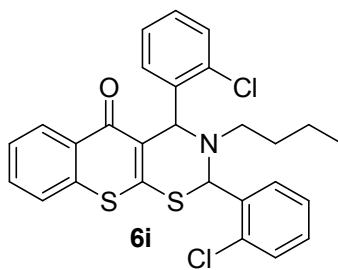


# <sup>1</sup>H NMR spectra the compound: 6i

km-bam-h

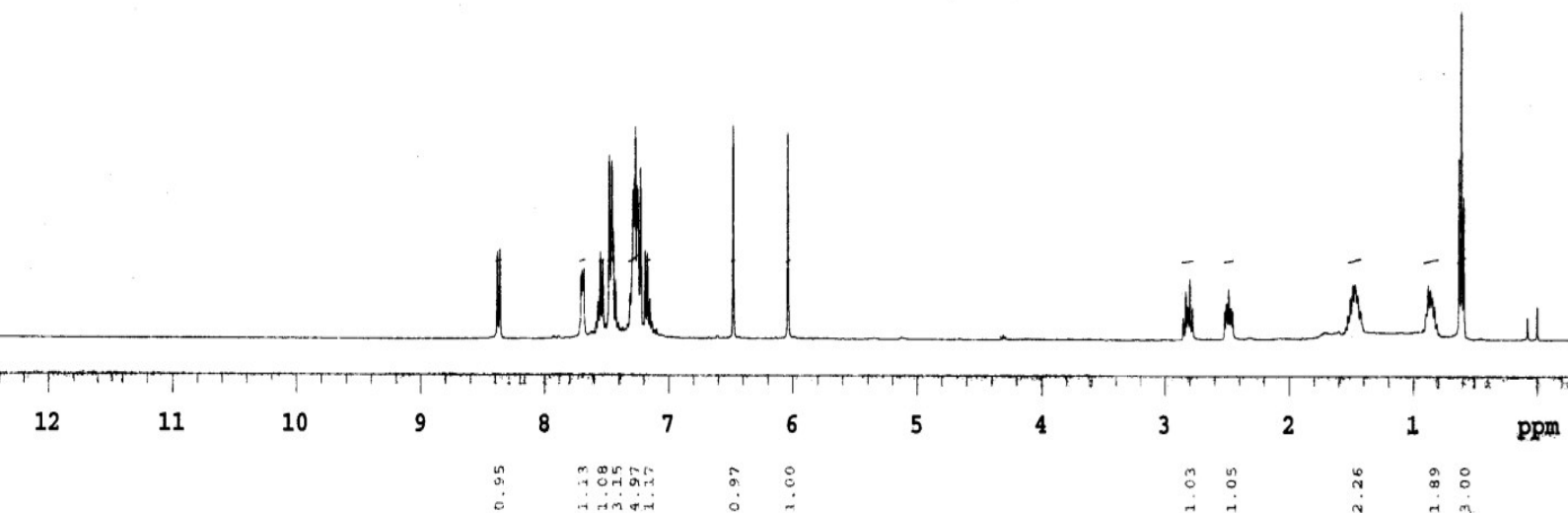
Sample Name:  
km-bam-h1  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
/home/chem/data/study  
Sample directory:  
test-proton-01  
FidFile: PROTON

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 12 2014



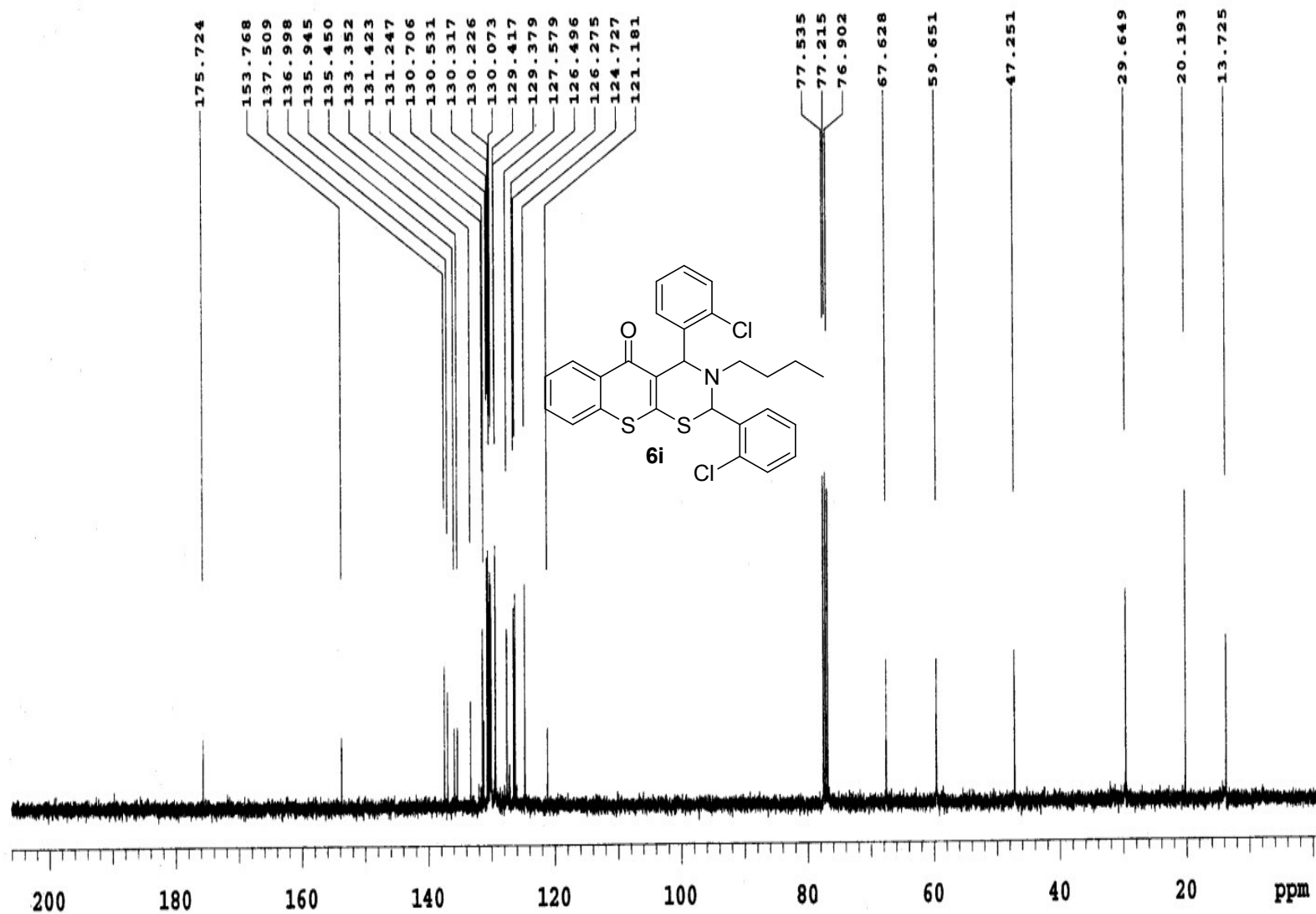
Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509652 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec





<sup>13</sup>CNMR spectra of compound: 6i



PULSE SEQUENCE  
 Relax. delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.304 sec  
 Width 25125.6 Hz  
 500 repetitions

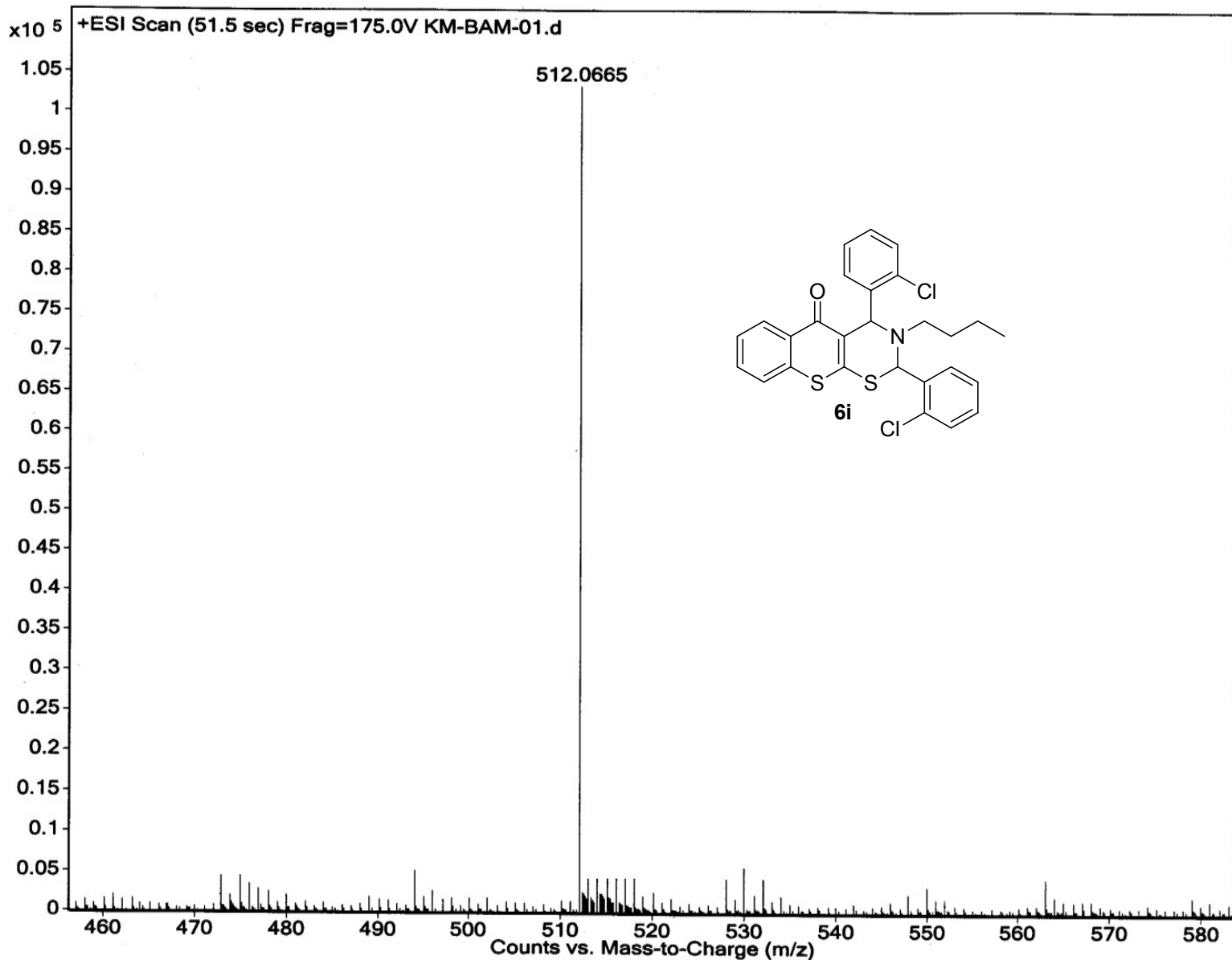
OBSERVE: C13, 100.5425870  
 DECOUPLE H1, 399.8529994  
 Power: 42 dB  
 continuously on  
 WALTZ-16 modulated

DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 19 minutes

Kn-BAM-1-13C  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 "IITG-NMR"

# HRMS spectra of compound: 6i

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>HNMR spectra the compound: 6j

KM-AM-2br

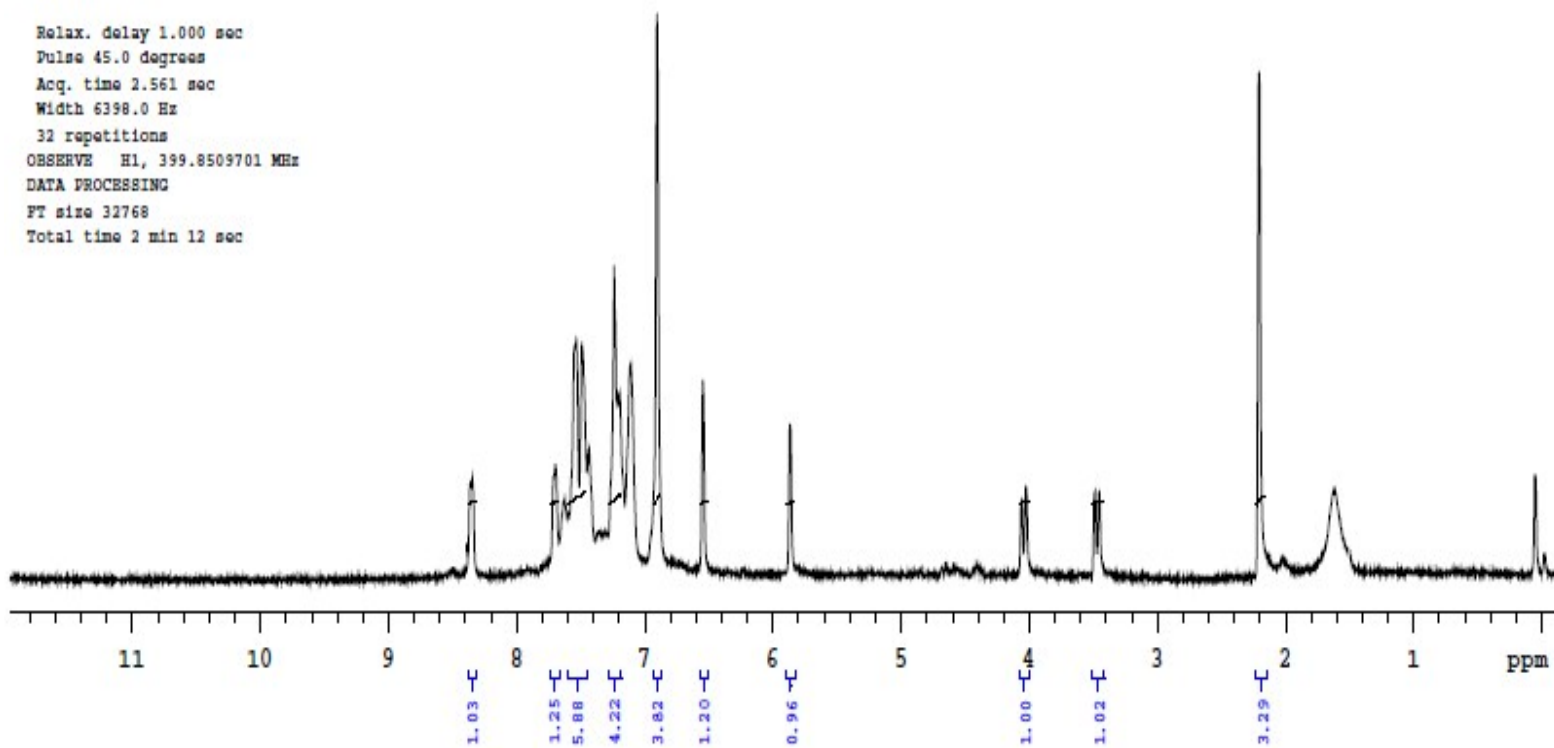
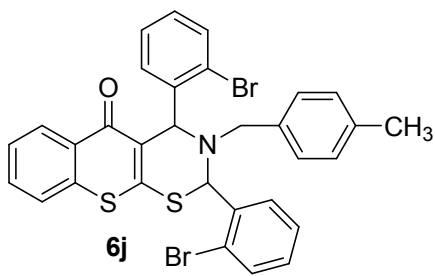
Sample Name:  
KM-AM-2br  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
/export/home/chempack/vnmrsys/data  
Sample directory:

FidFile: KM-AM-2br-1

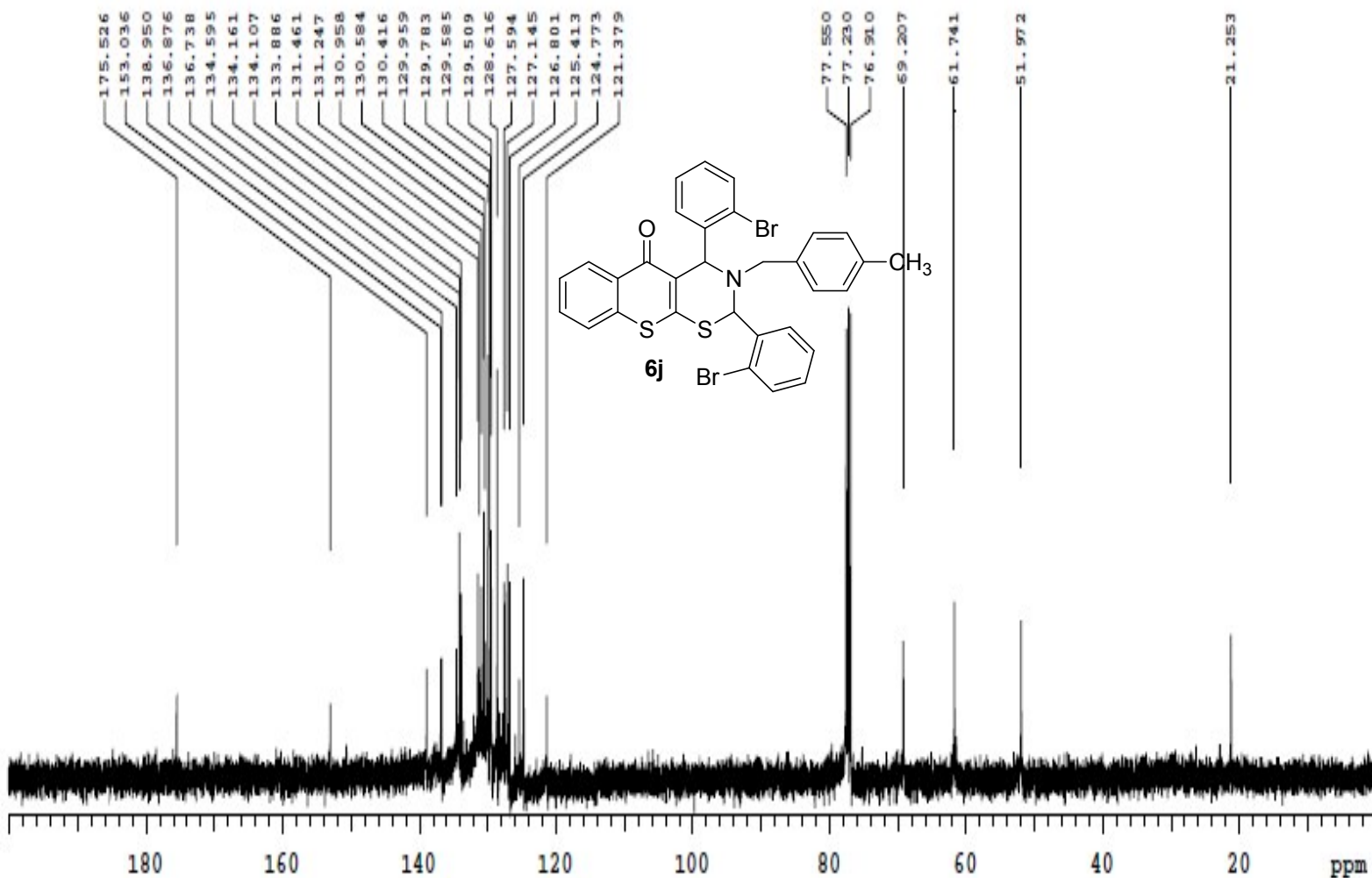
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: May 15 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509701 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



### <sup>13</sup>CNMR spectra of compound: 6j



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
950 repetitions

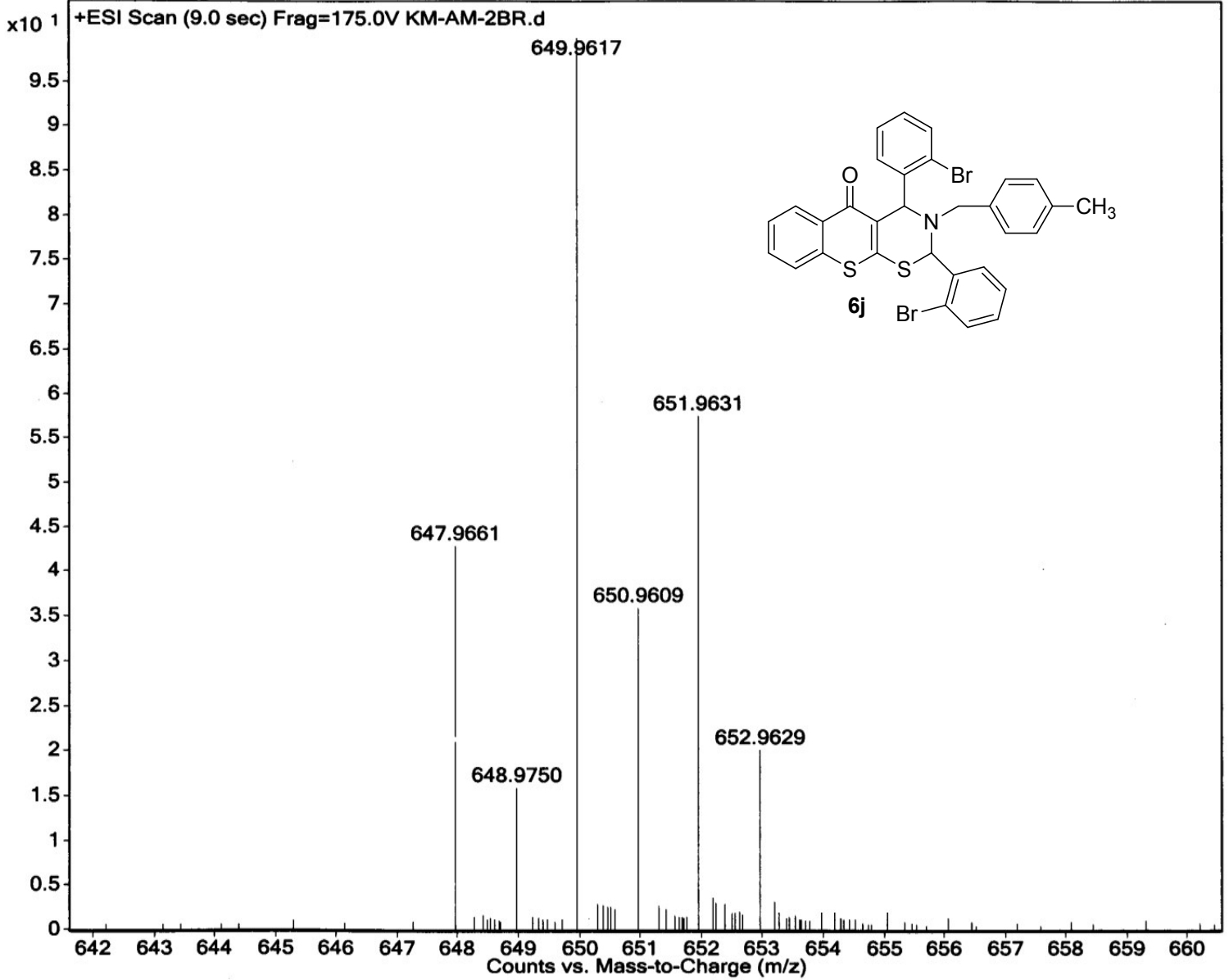
OBSERVE C13, 100.5425732  
DECOUPLE H1, 399.8529994  
Power 42 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 36 minutes

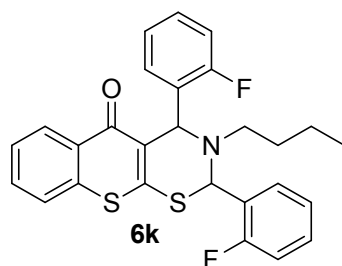
Ex-AM-2Br-13C  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: Ex-AM-2Br-13C  
Mercury-400 "IITG-NMR"

# HRMS spectra of compound: 6j

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra the compound: 6k

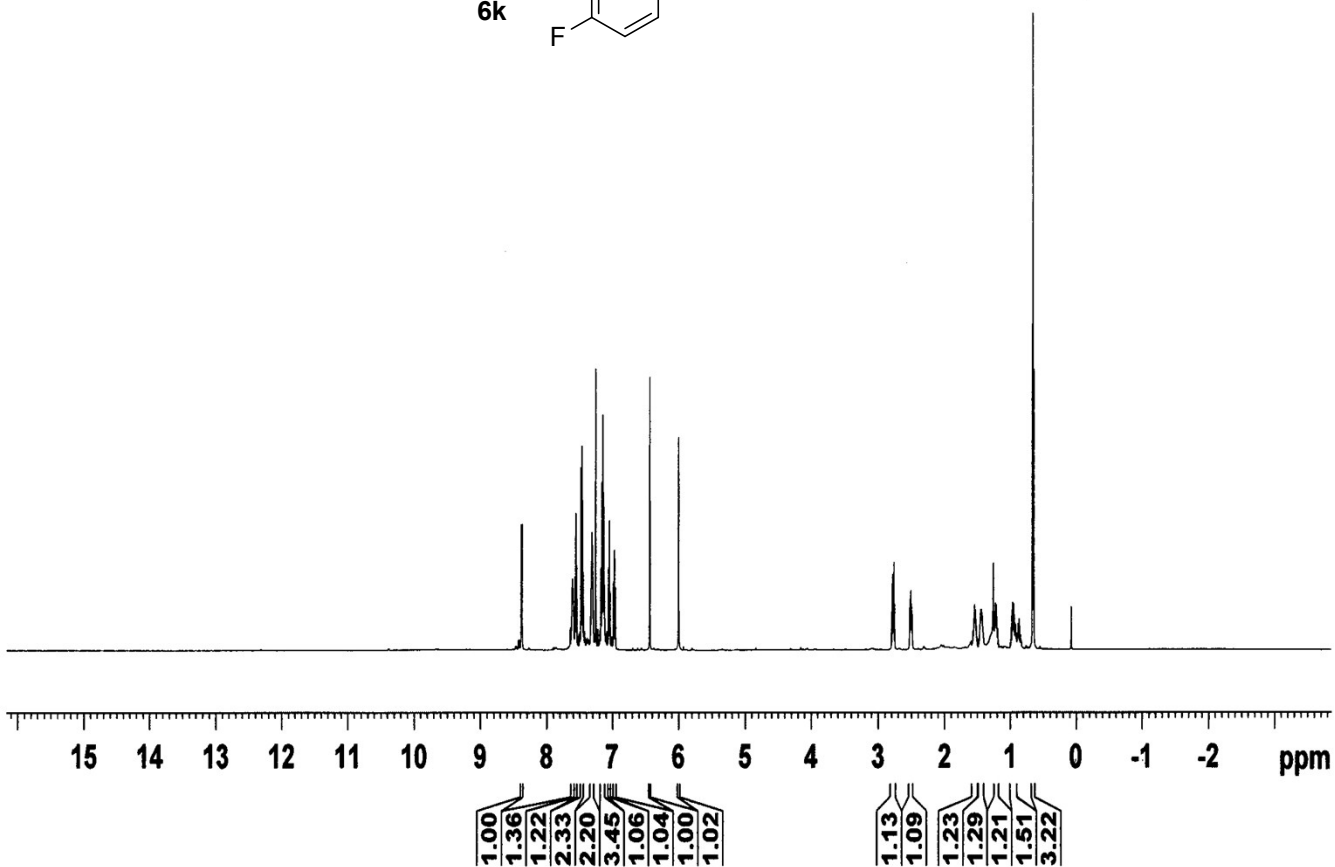


Current Data Parameters  
NAME RM-BAM-2F-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150210  
Time 10.19  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 65.24  
DW 41.600 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700137 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

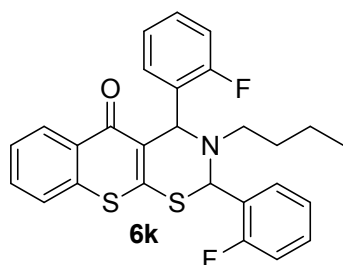


<sup>13</sup>CNMR spectra of compound: 6k



175.79  
162.21  
161.67  
160.55  
160.01  
153.78  
136.95  
131.46  
131.18  
130.99  
130.94  
130.54  
129.84  
129.74  
129.45  
127.58  
127.07  
124.74  
123.91  
123.62  
120.41  
116.26  
116.23  
116.12  
116.09

77.43  
77.22  
77.01  
64.07  
55.74  
46.62  
29.51  
20.00  
13.73



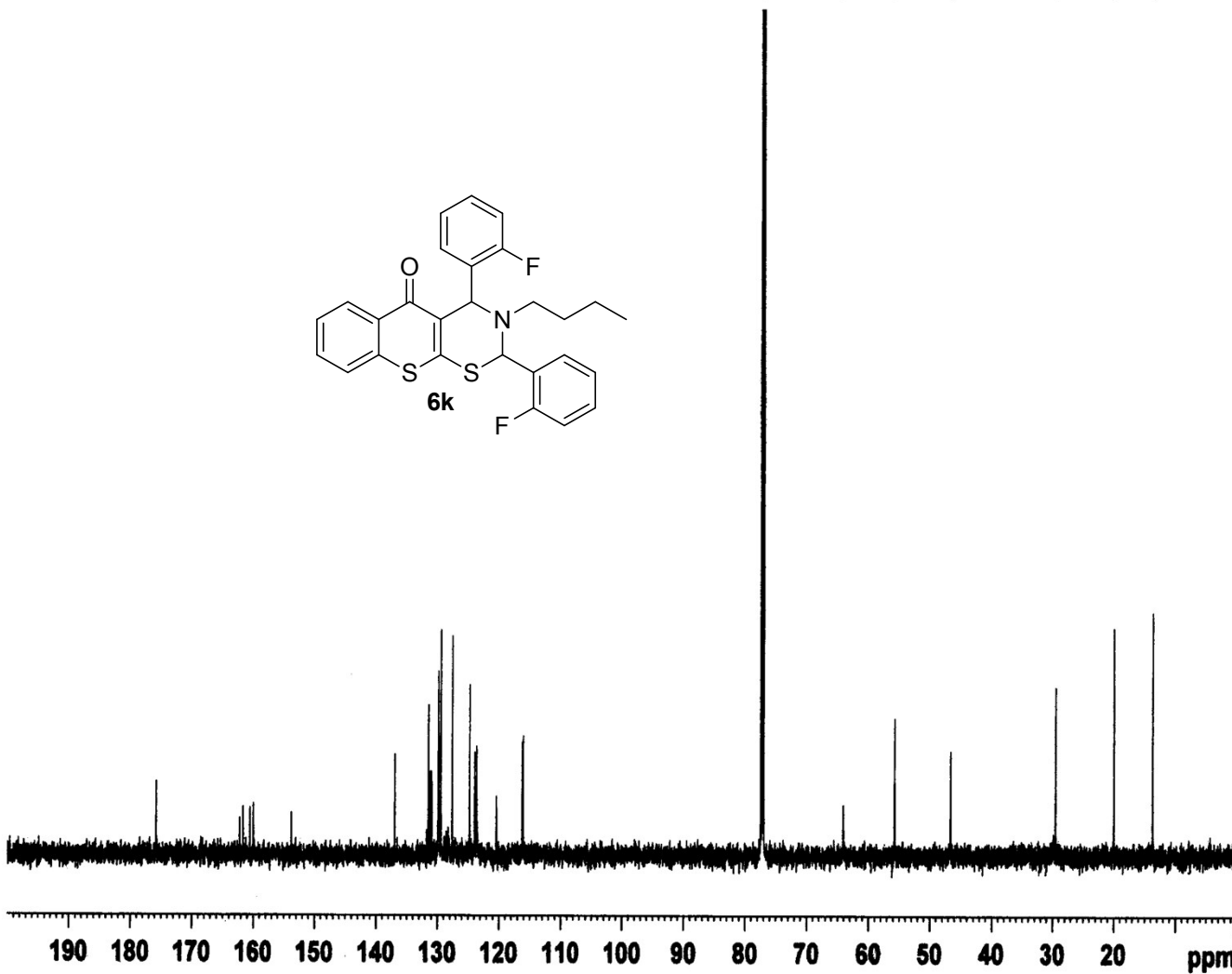
Current Data Parameters  
NAME KM-BAM-2F-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150210  
Time 10.23  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 84  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

----- CHANNEL f1 -----  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

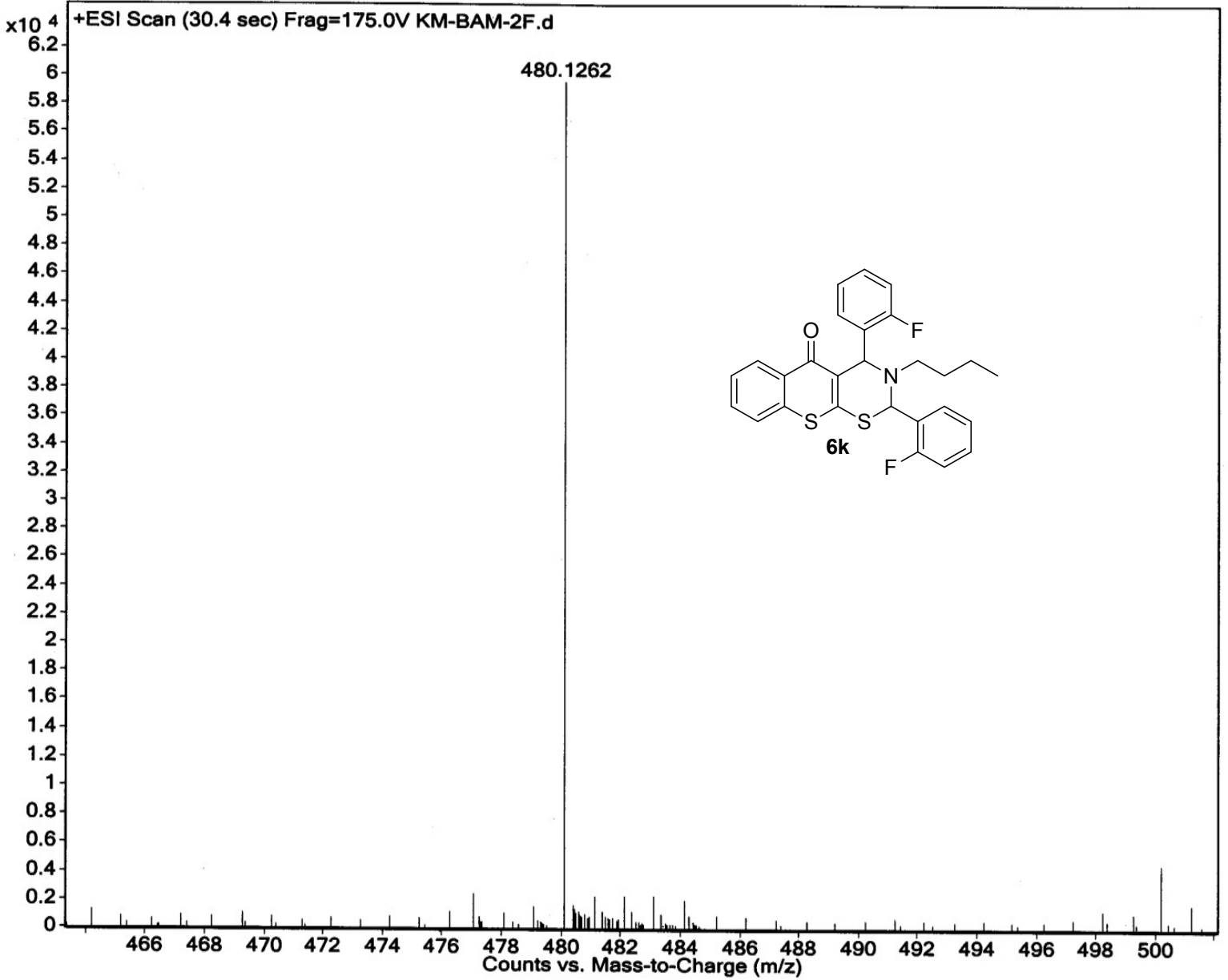
----- CHANNEL f2 -----  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] walzr16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128403 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



# HRMS spectra of compound: 6k

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time





# <sup>1</sup>HNMR spectra the compound: 6l

EM-AM-07-1H

Sample Name:

EM-AM-07-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

FidFile: EM-AM-07-1H

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 31 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

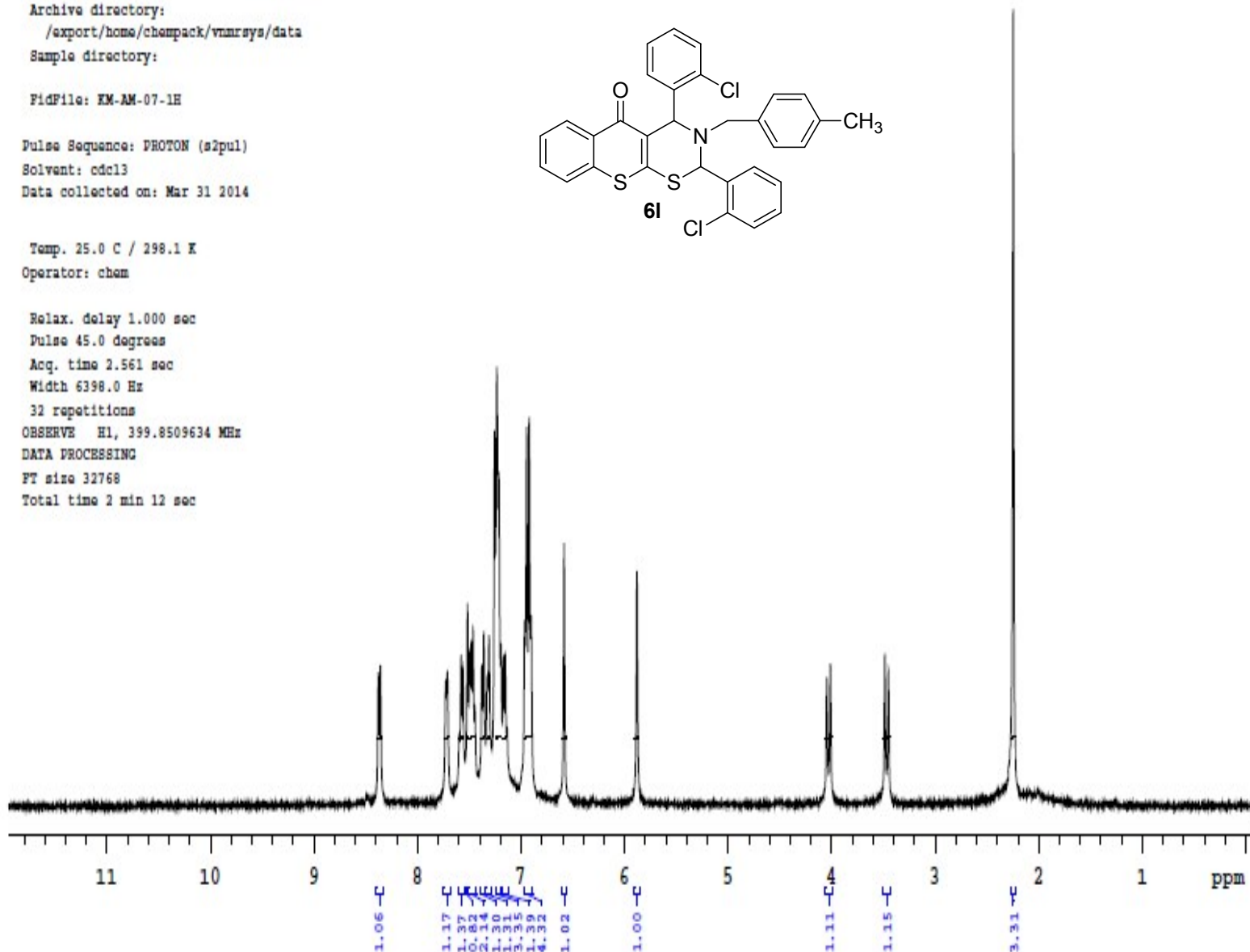
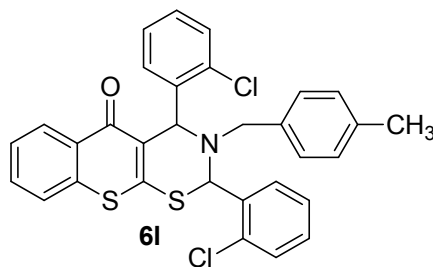
32 repetitions

OBSERVE H1, 399.8509634 MHz

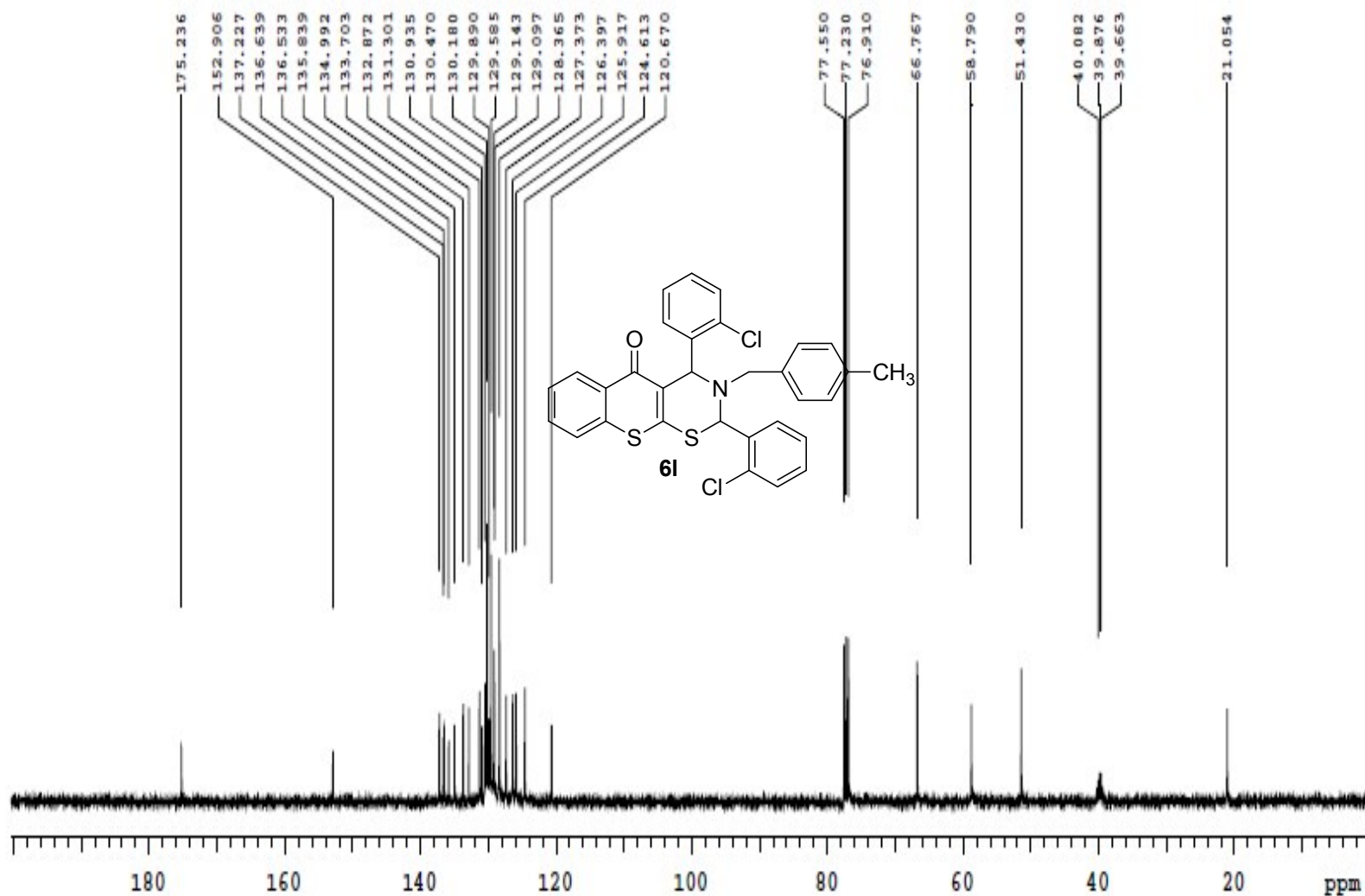
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



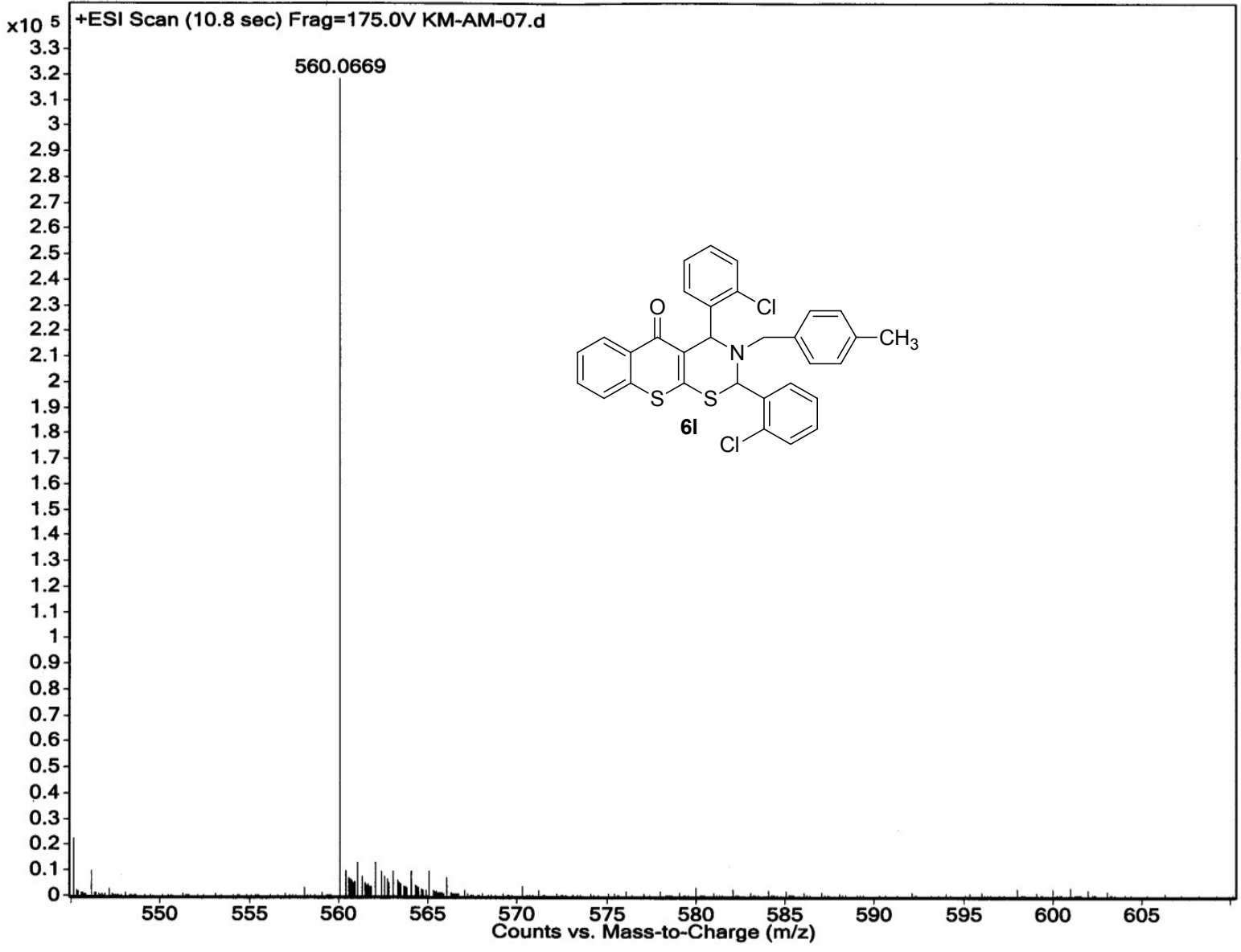
<sup>13</sup>CNMR spectra of compound: 6l



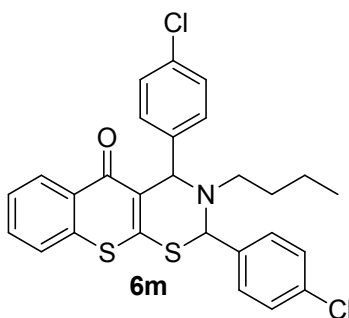
<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1130 repetitions	<b>OBSERVE</b> C13, 100.5425364 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 43 minutes	<b>KM-AM-07-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: KM-AM-07-13C Mercury-400 "IITG-NMR"
--	--	--	---

# HRMS spectra of compound: 6l

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>H NMR spectra compound: 6m

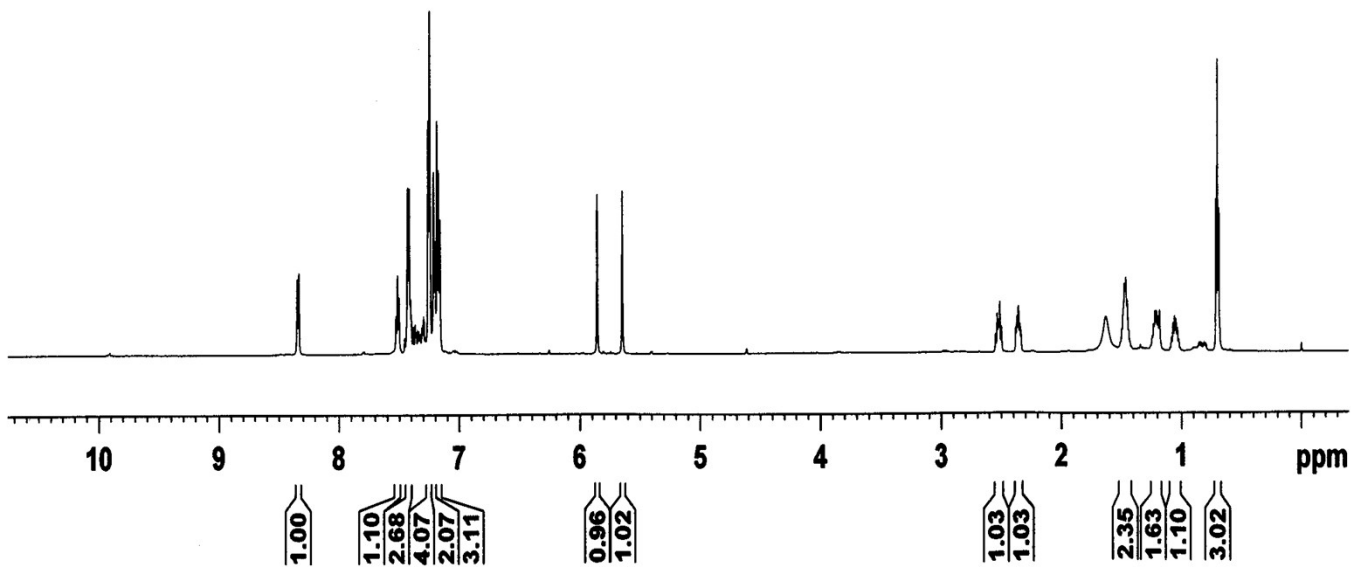


Current Data Parameters  
NAME RM-BAM-4-Cl-1H  
EXPNO 1  
PROCNO 1

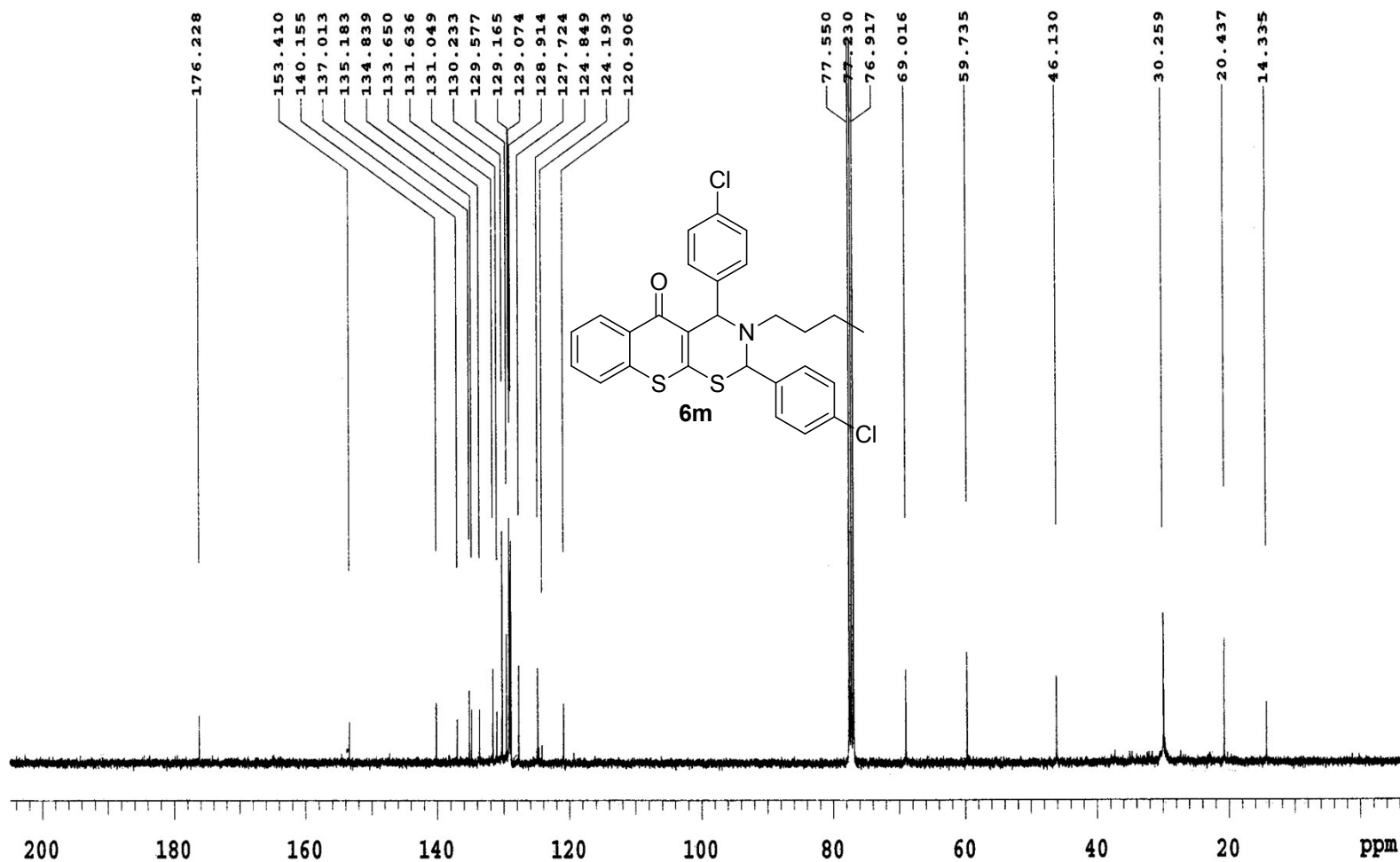
F2 - Acquisition Parameters  
Date 20150223  
Time 12.31  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 113  
DW 41.600 usec  
DE 6.50 usec  
TE 298.5 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

F2 - Processing parameters  
SI 16384  
SF 600.1700579 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>CNMR spectra of compound: 6m



PULSE SEQUENCE  
 Relax delay 1.000 sec  
 Pulse 45.0 degrees  
 Acq. time 1.304 sec  
 Width 25125.6 Hz  
 9300 Repetitions

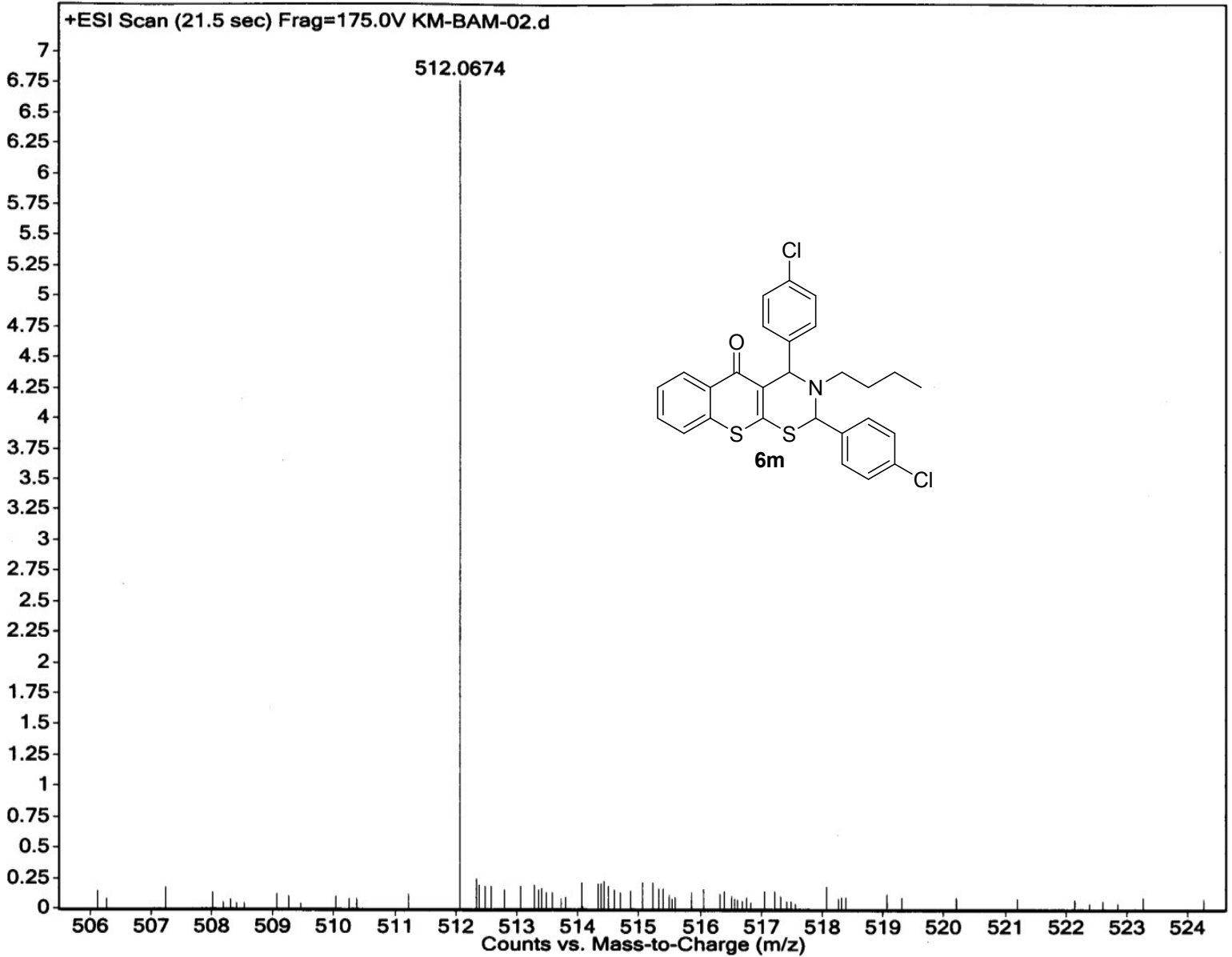
OBSERVE: C13, 100.5425601  
 DECOUPLE: H1, -399.8529994  
 Power 42 dB  
 continuously on  
 WALTZ-16 modulated

DATA PROCESSING  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 6.0 hours

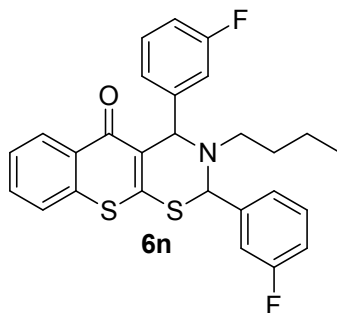
RM-BAM-461-13C  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 "IITG-NMR"

# HRMS spectra of compound: 6m

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



# <sup>1</sup>HNMR spectra the compound: 6n

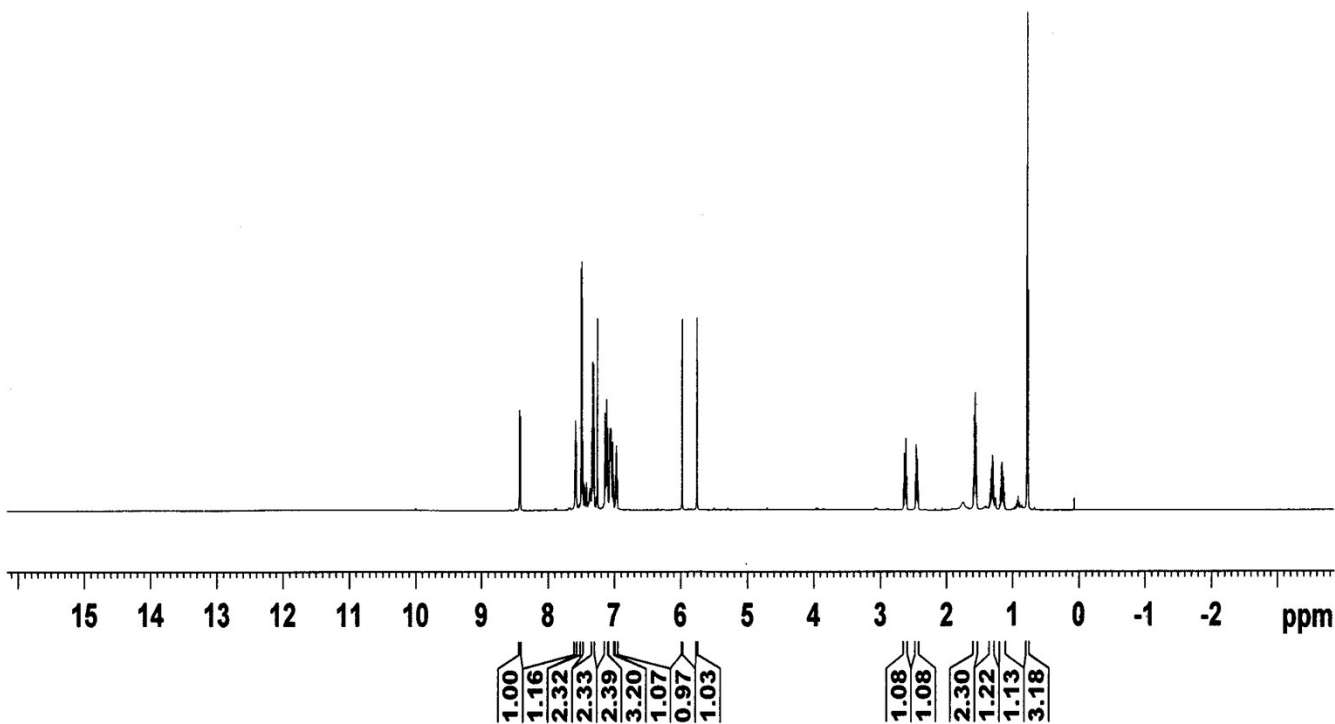


Current Data Parameters  
NAME KM-BAM-3F-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150210  
Time 10.05  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 73.2  
DW 41.600 usec  
DE 6.50 usec  
TE 297.9 K  
D1 1.00000000 sec  
TDO 1

==== CHANNEL f1 =====  
SFO1 600.1737063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.00000000 W

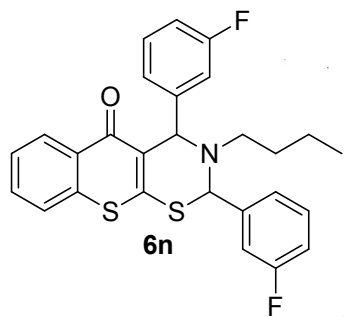
F2 - Processing parameters  
SI 16384  
SF 600.1700137 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>CNMR spectra of compound: 6n



176.23  
164.12  
163.77  
162.49  
162.14  
153.40  
144.20  
139.21  
136.97  
131.63  
131.01  
130.38  
130.29  
129.55  
127.71  
127.53  
127.13  
124.85  
124.48  
123.35  
120.83  
115.90  
115.85  
115.75  
115.04  
114.89  
114.75  
77.44  
77.23  
77.02  
68.96  
59.80  
— 46.25  
— 29.94  
— 20.39  
— 13.94



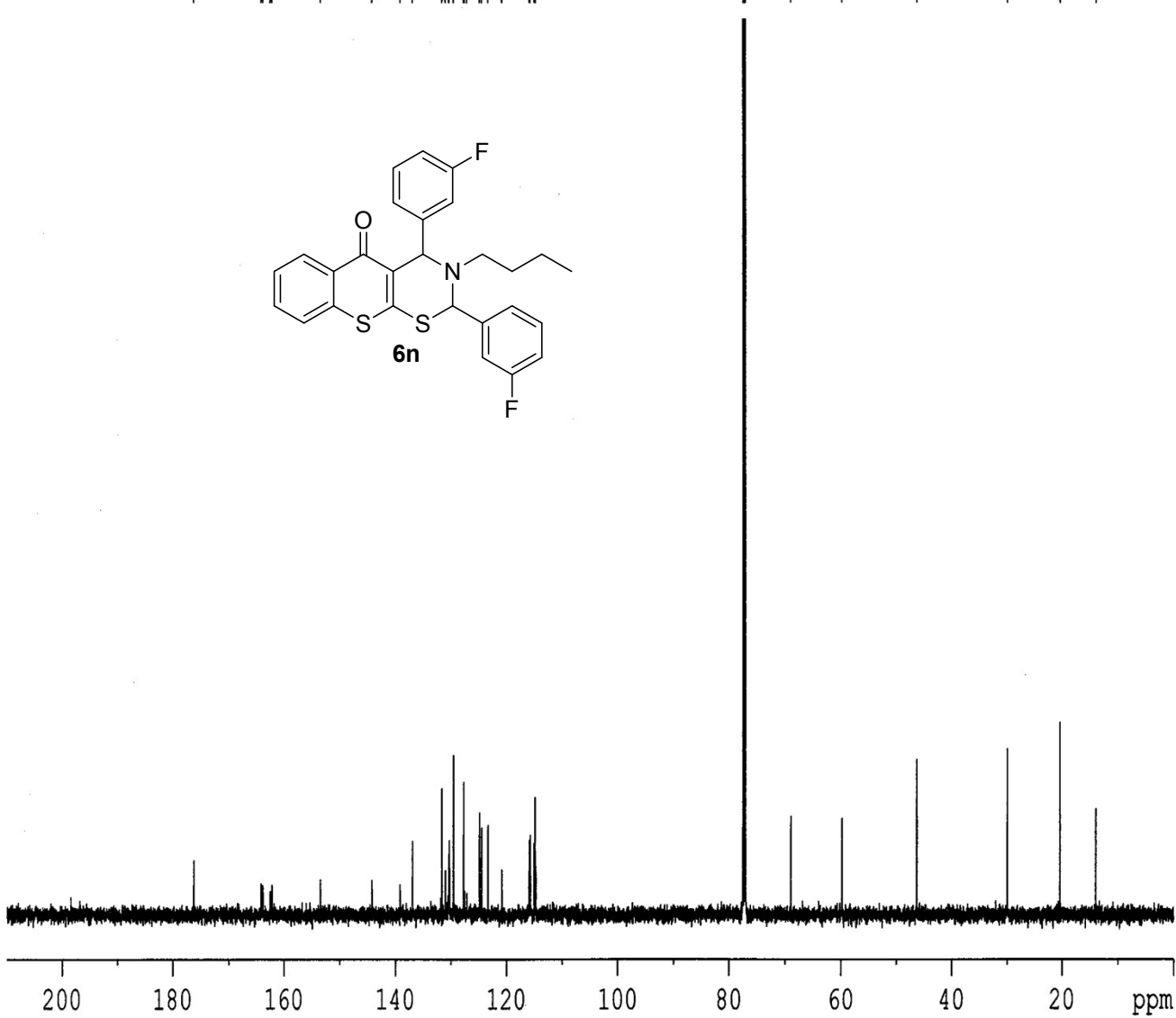
Current Data Parameters  
NAME KM-BAM-3F-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150210  
Time 10.08  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 86  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 127.57  
DW 13.867 usec  
DE 6.50 usec  
TE 298.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

==== CHANNEL f1 =====  
SF01 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

==== CHANNEL f2 =====  
SF02 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLM2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

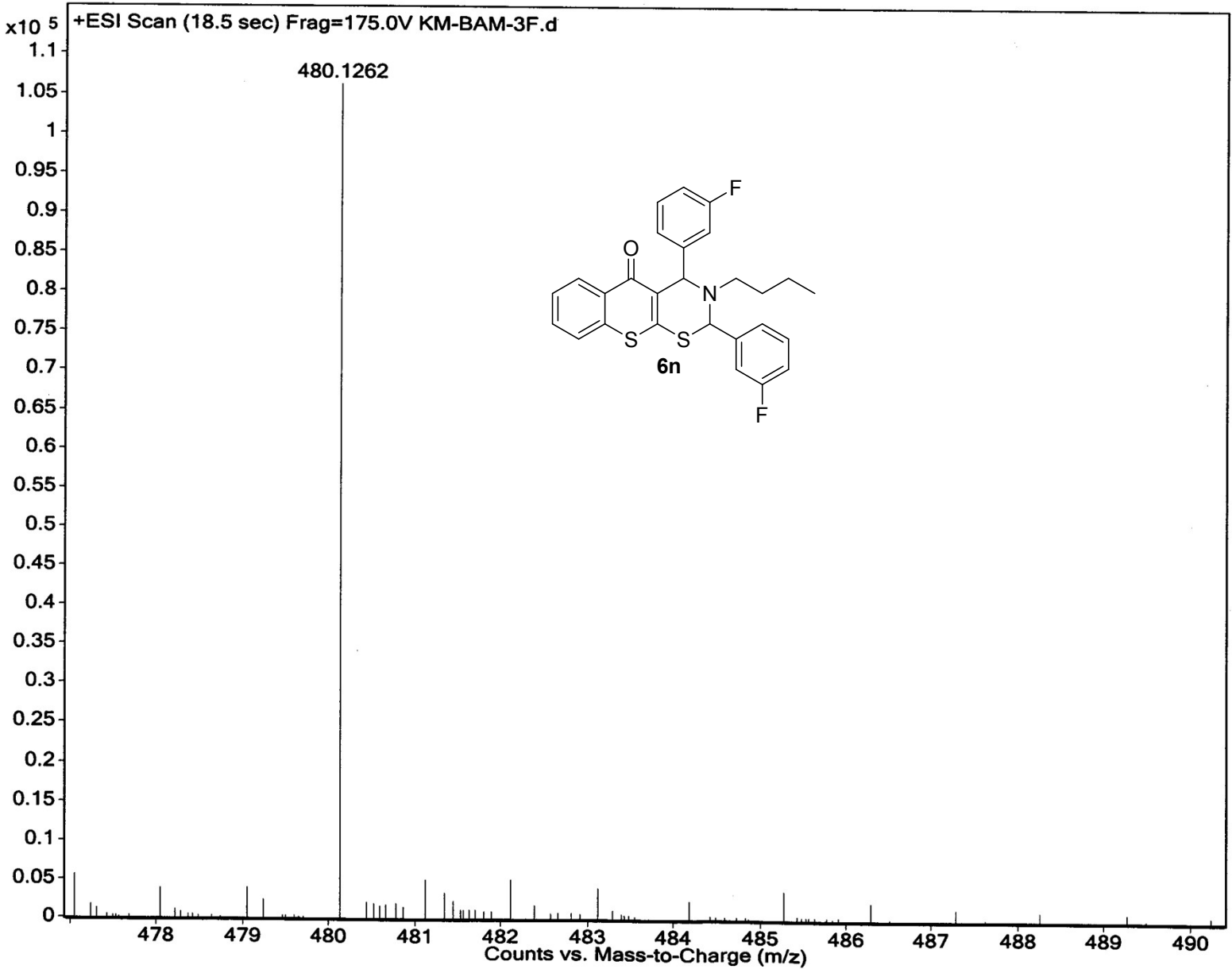
F2 - Processing parameters  
SI 16384  
SF 150.9128382 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





# HRMS spectra of compound: 6n

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



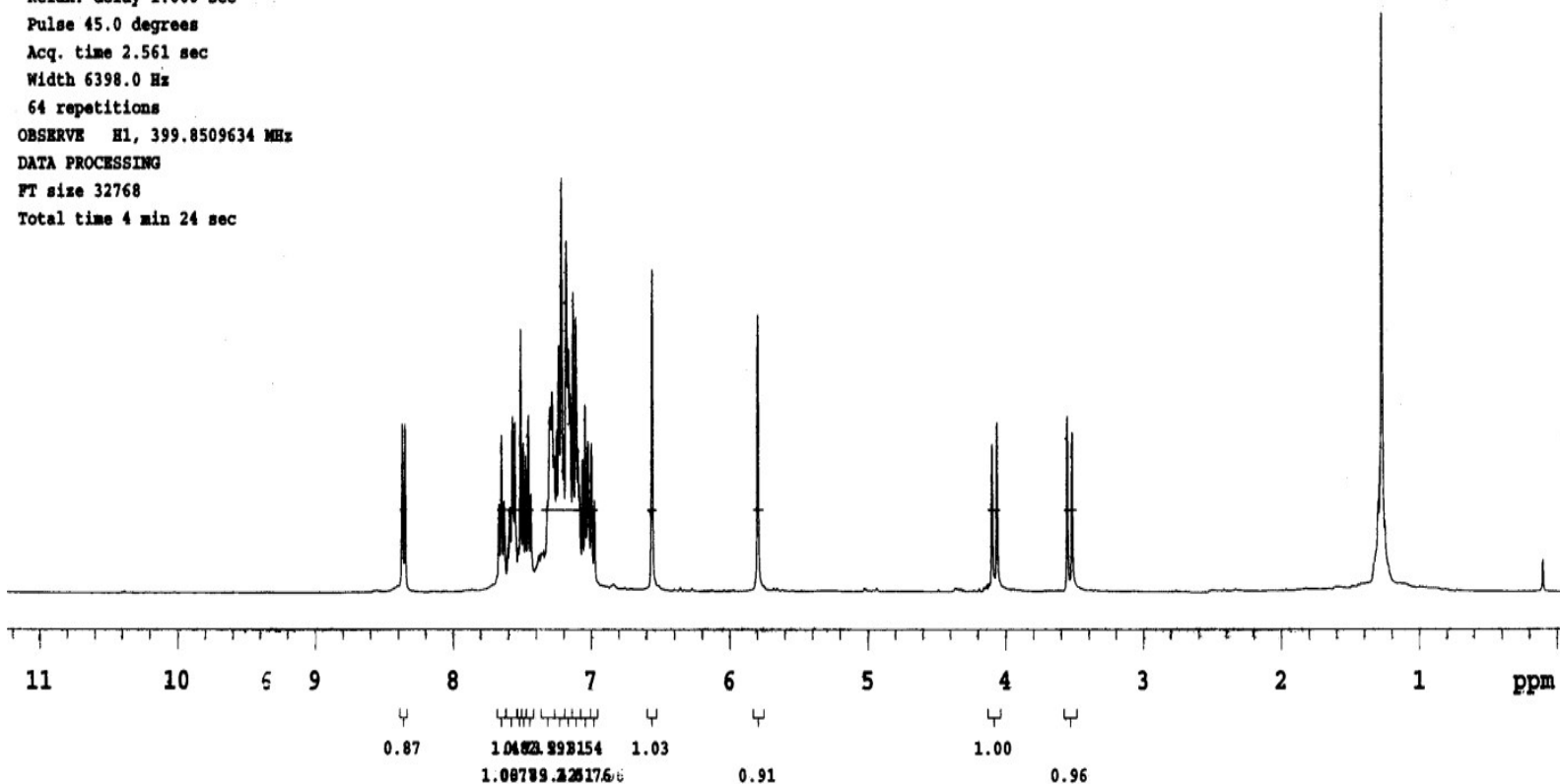
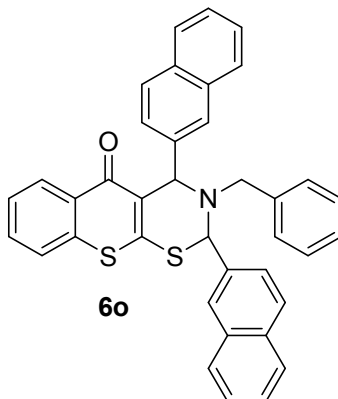
# <sup>1</sup>HNMR spectra the compound: 6o

Sample Name:  
KM-AM-11  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
/home/chem/data/study  
Sample directory:  
PICHYDRA-ZN-tit-4-01  
FidFile: KM-AM-11

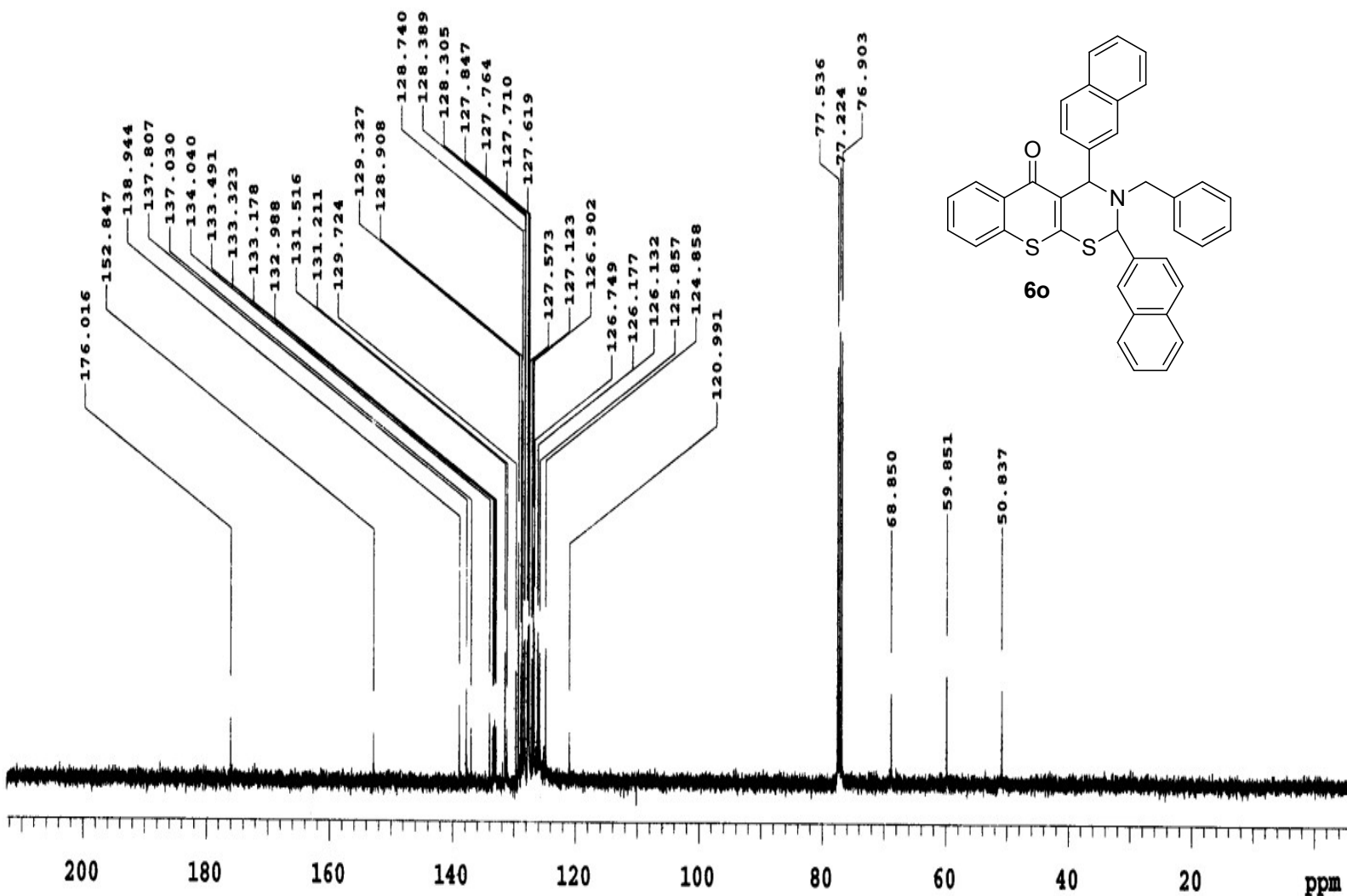
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: Apr 4 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
64 repetitions  
OBSERVE H1, 399.8509634 MHz  
DATA PROCESSING  
FT size 32768  
Total time 4 min 24 sec



<sup>13</sup>CNMR spectra of compound: 60



PULSE SEQUENCE: zgpg30  
 Relax. delay 1.000 sec.  
 Pulse 45.0 degree  
 Acq. time 1.304 sec  
 Width 25125.6 Hz  
 1150 repetitions

OBSERVE: C13, 100.5425892  
 DECOUPLE: H1, 399.8529994  
 Power 42 dB  
 continuously on  
 WALTZ-16 modulated

DATA PROCESSING: zgpg30  
 Line broadening 0.5 Hz  
 FT size 65536  
 Total time 44 minutes

NAME: KM-AM-10-13C  
 Solvent: cdcl3  
 Temp. 25.0 C / 298.1 K  
 Operator: chem  
 Mercury-400 "IITG-NMR"

# HRMS spectra of compound: 6o

Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time

