Supporting Information

$Yb(OTf)_3$ 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

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l. General Information and Methods

^{1}H and ^{13}C NMR spectra were recorded on 400 MHz, 600 MHz and 100 MHz, 150 MHz spectrometer TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). ^{1}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 or via: www.ccdc.cam.ac.uk).

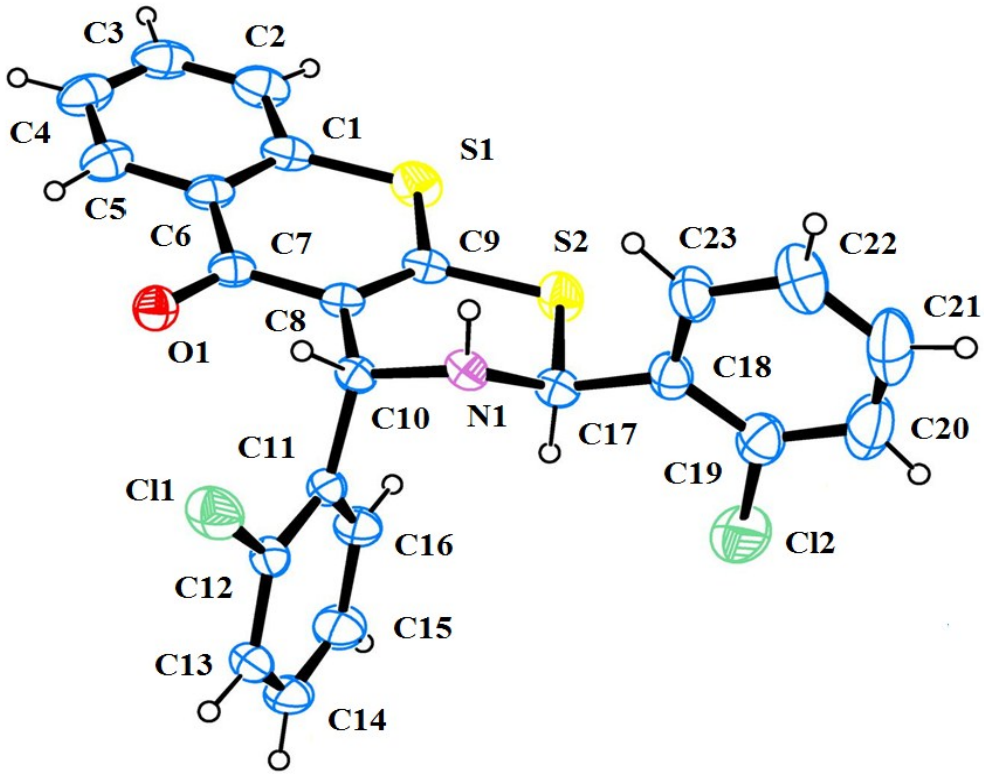


Figure 1. 30% probability of ORTEP ellipsoids of **4f**

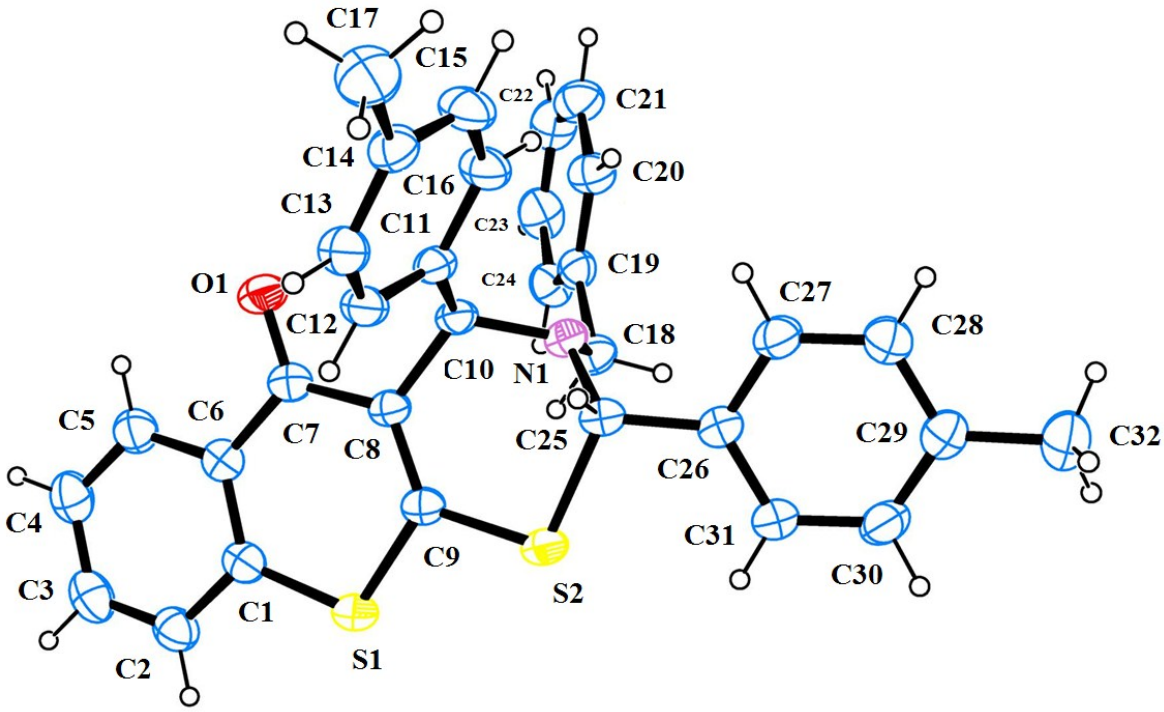
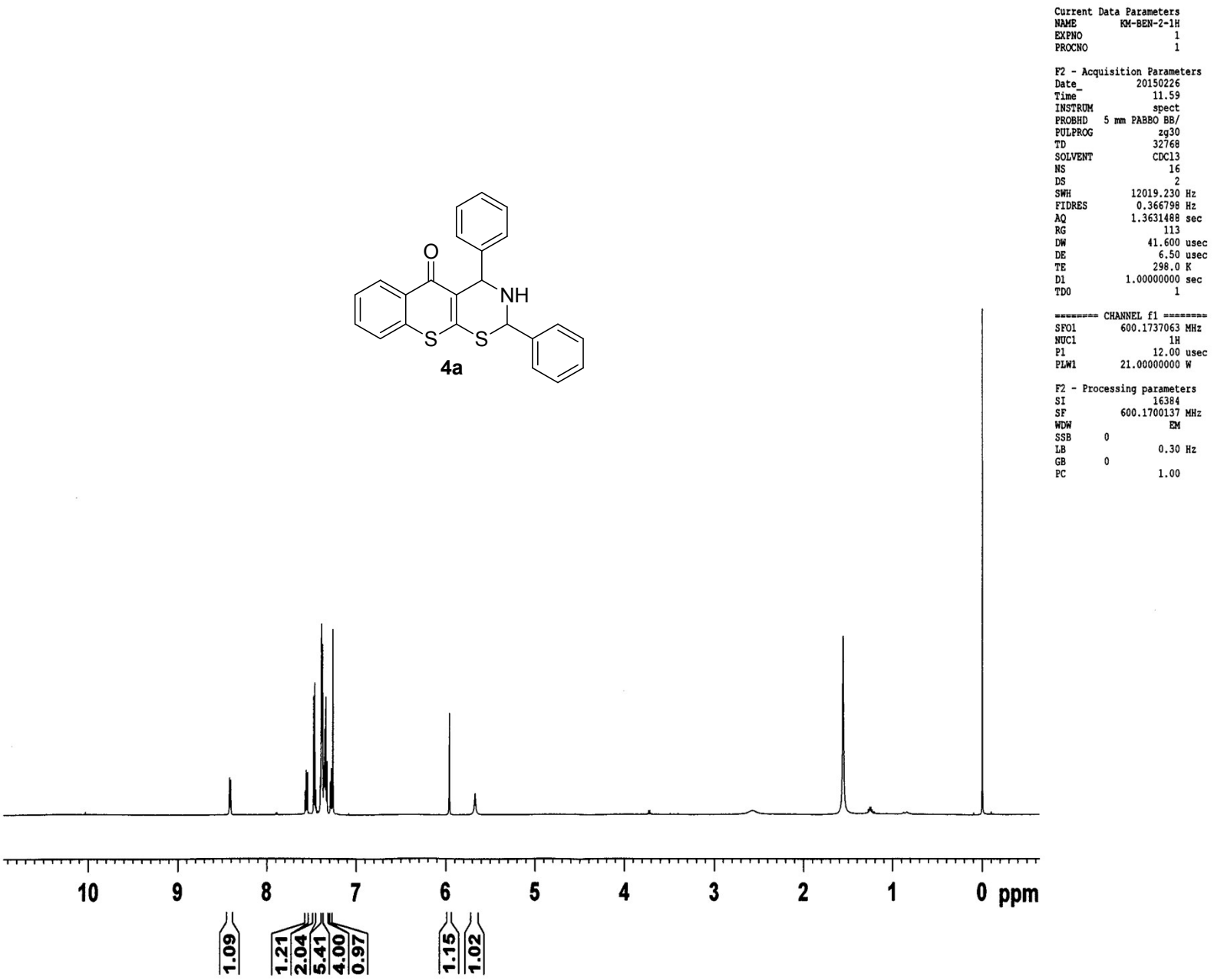


Figure 2. 30% probability of ORTEP ellipsoids of **6b**

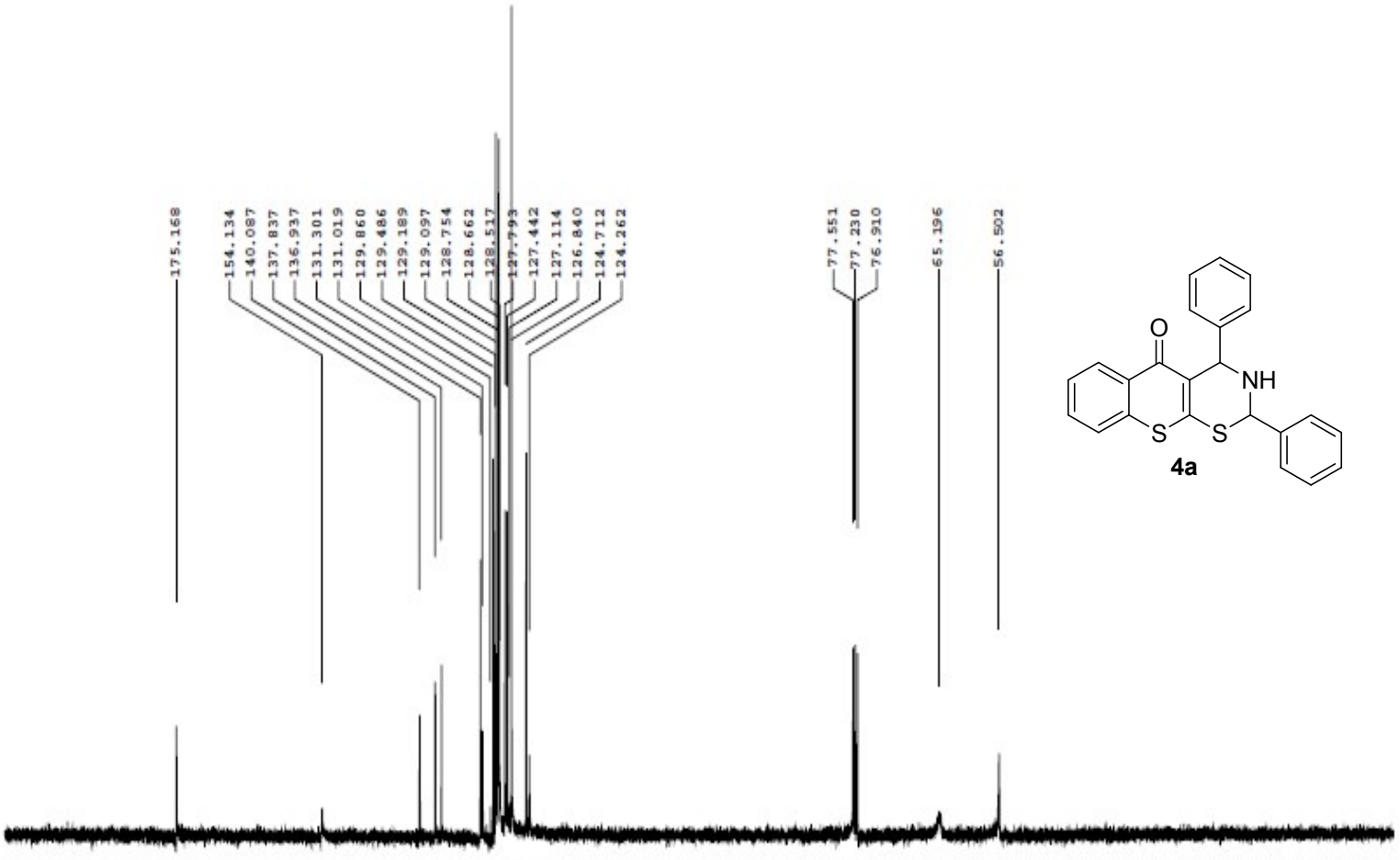
Table 1 Crystal Data and Structure Refinement for Compound **4f** and **6b**

Entry	Identification code	Compound **4f**	Compound **6b**
01	Empirical formula	C23 H15 Cl2 N O S2	C32 H27 N O S2
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\a	Mo K\a
06	Radiation source	Fine-focus sealed tube	Fine-focus sealed tube
07	Crystal system	Triclinic	Monoclinic
08	Space group	P-1	P21/c
09	Cell length	a 10.2935(7) b10.5264(9) c 10.7561(9)	a 11.6518(3) b 15.2049(4) c 14.9453(4)
10	Cell Angle	α 84.384(7) β 66.574(7) δ 76.989(6)	α 90.00 β 101.788(2) δ 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 F2	Full-matrix least-squares on F2
16	Index ranges	-13<=h<=13, -14<=k<=7, -14<=l<=14	-12<=h<=12, -16<=k<=16, -16<=l<=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

[1]HNMR spectra the compound: 4a



^{13}CNMR spectra of compound: 4a



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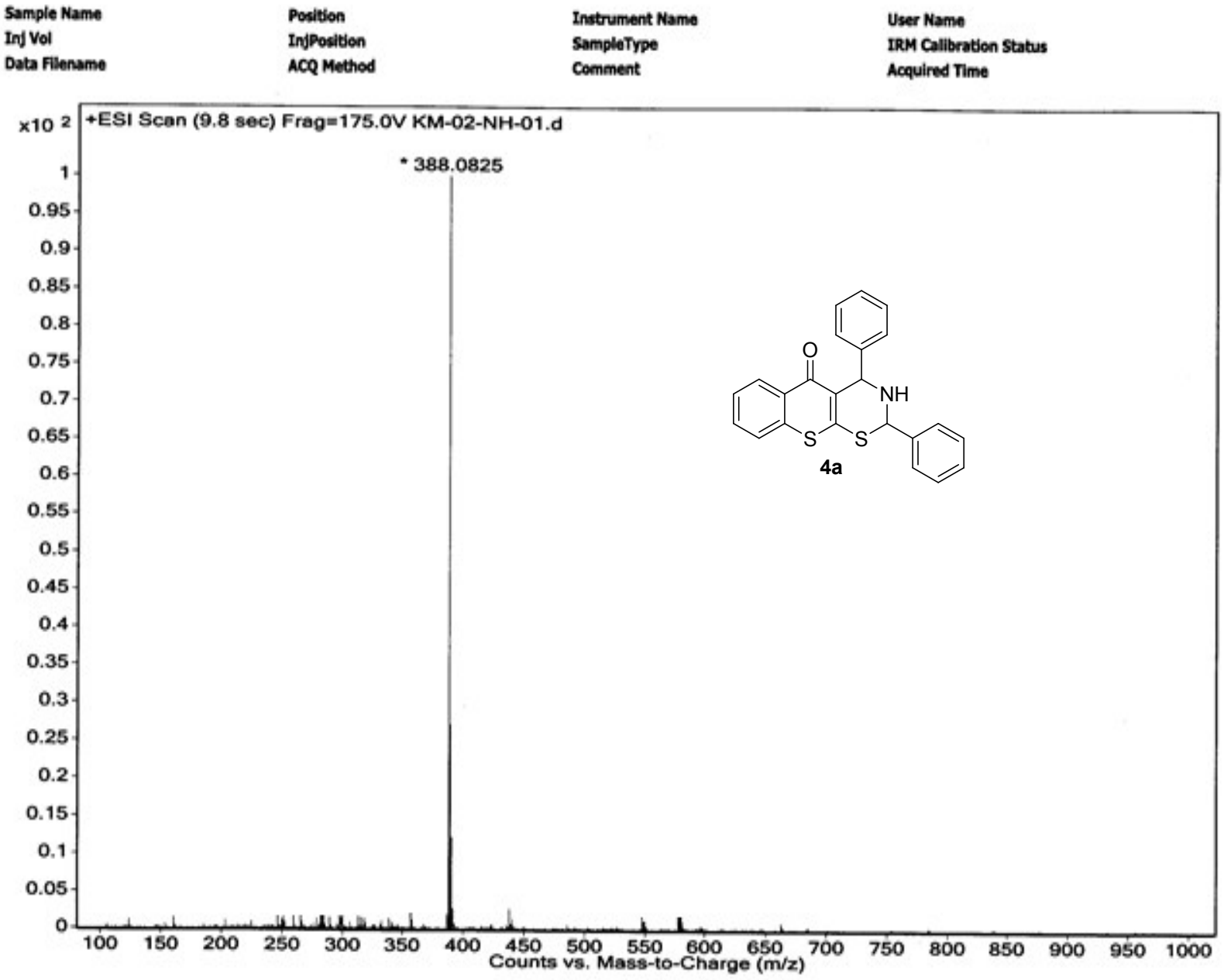
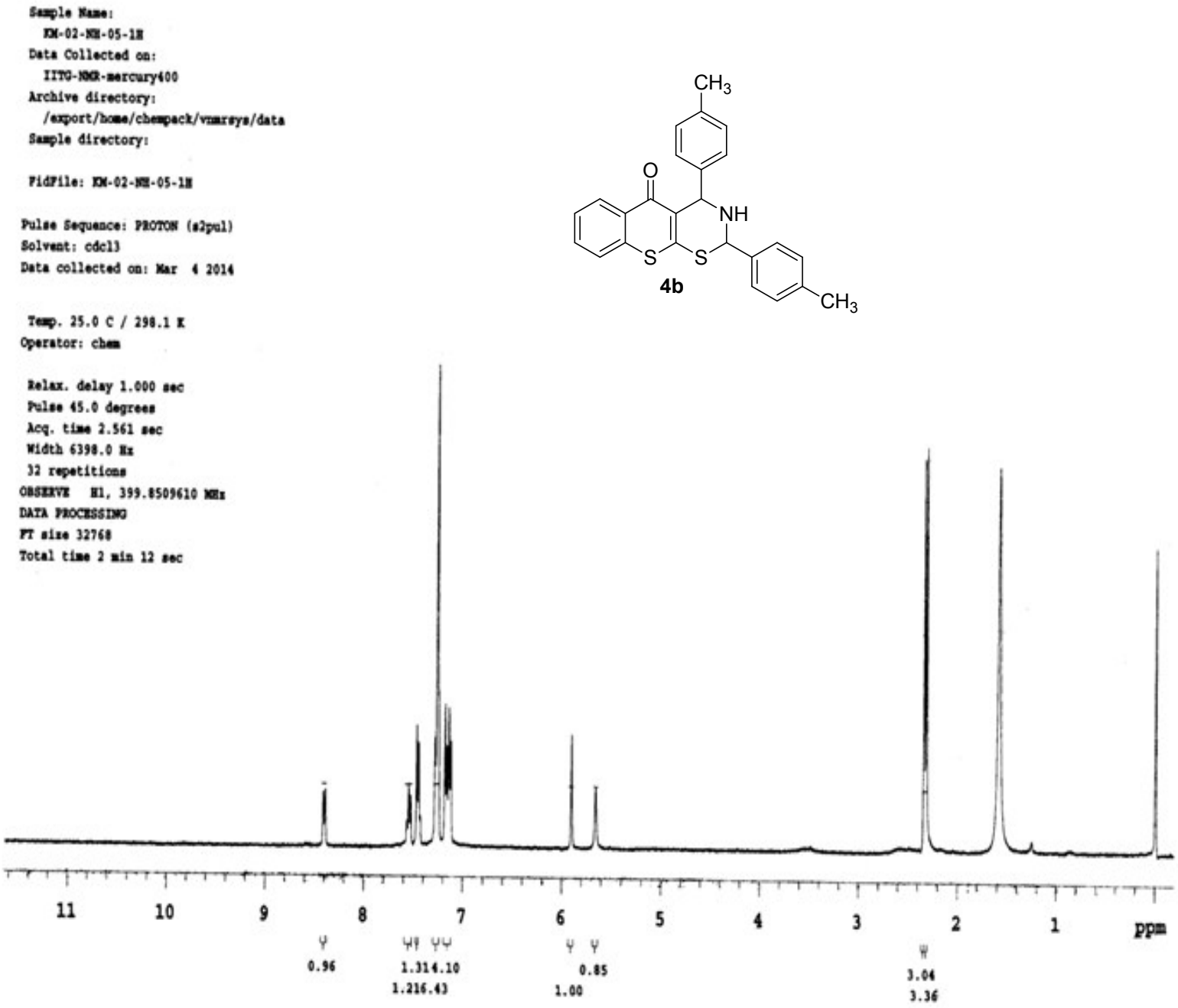
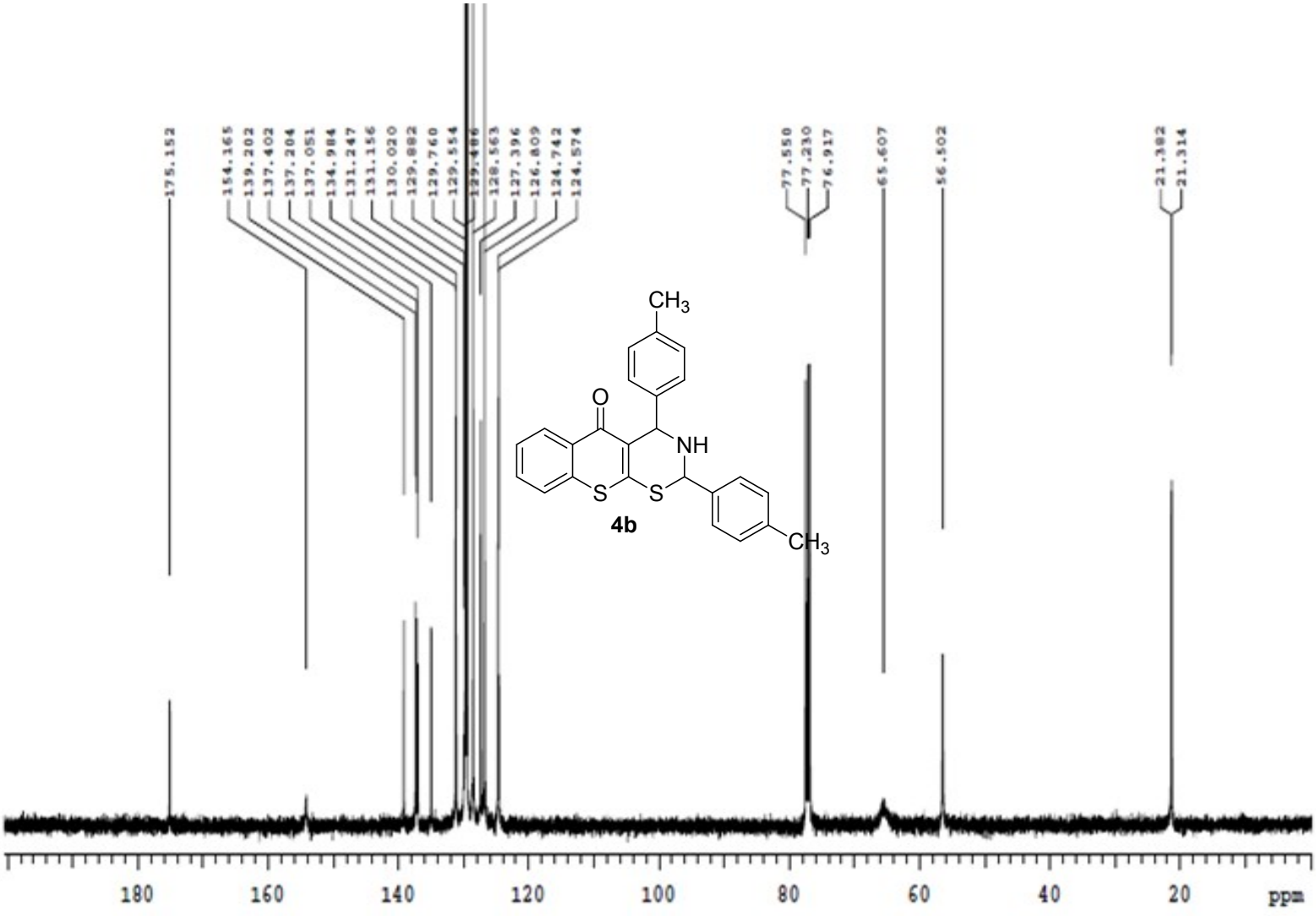
HRMS spectra of compound: 4a



[1]HNMR spectra the compound: 4b



^{13}CNMR spectra of compound: 4b



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HRMS spectra of compound: 4b

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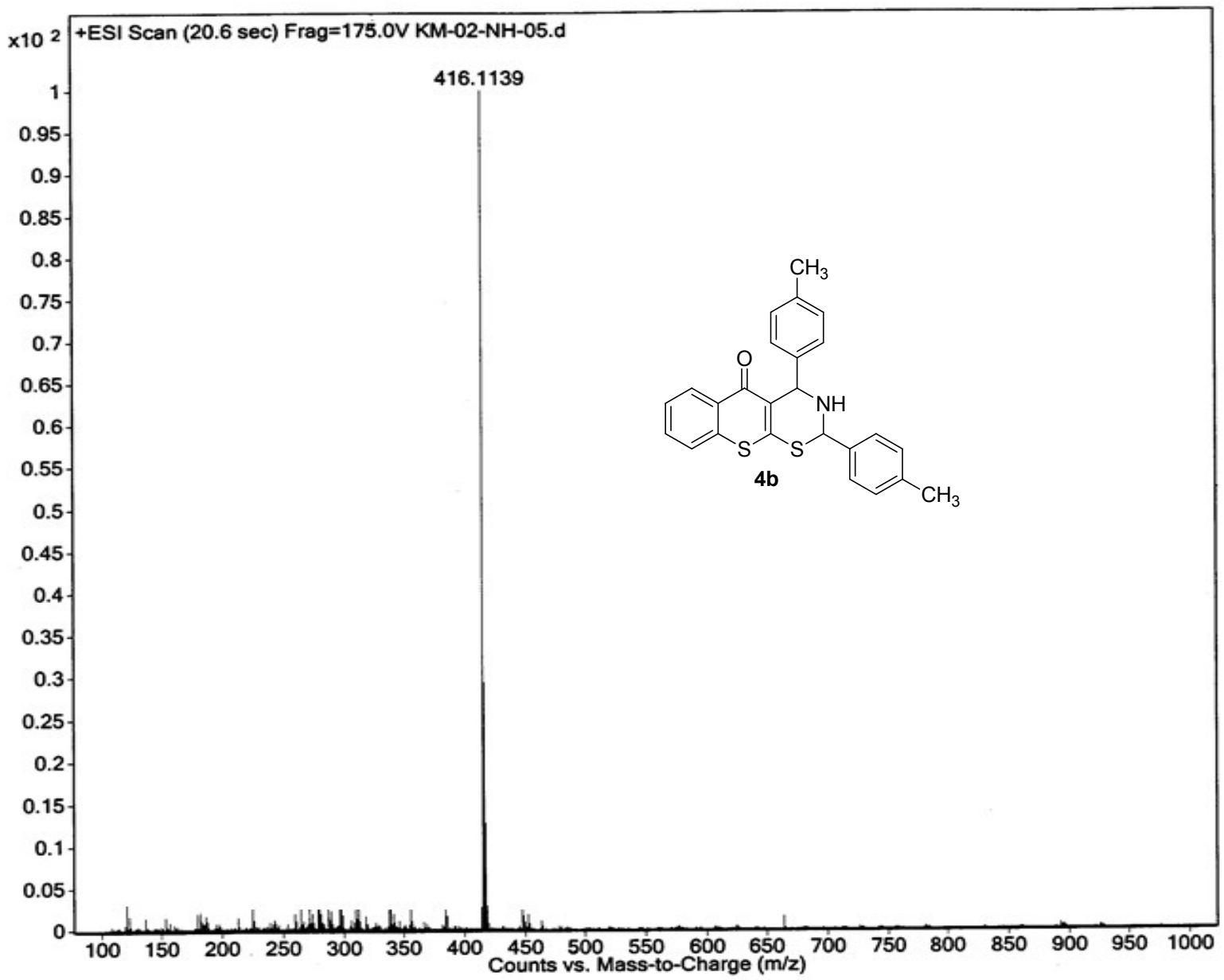
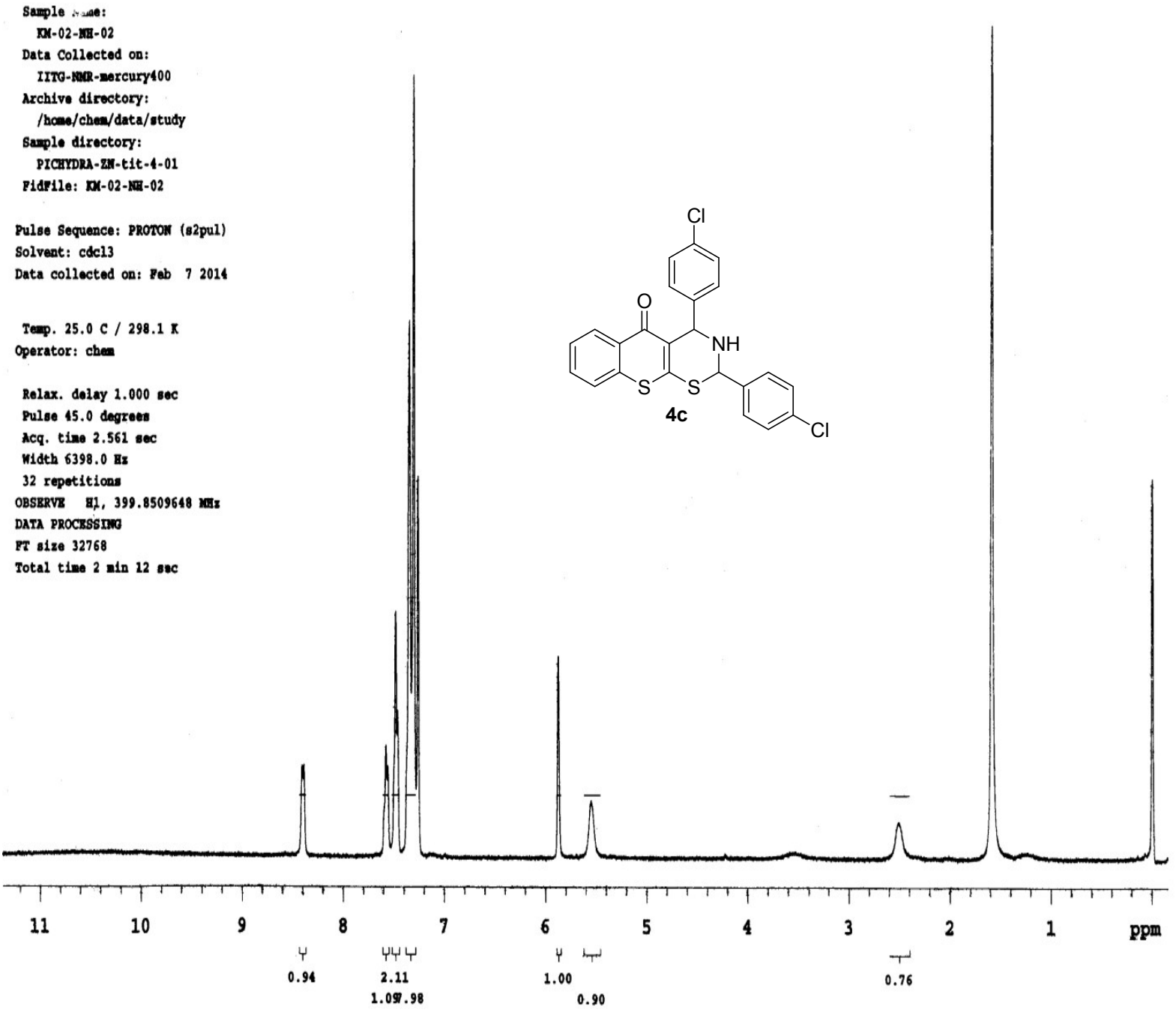
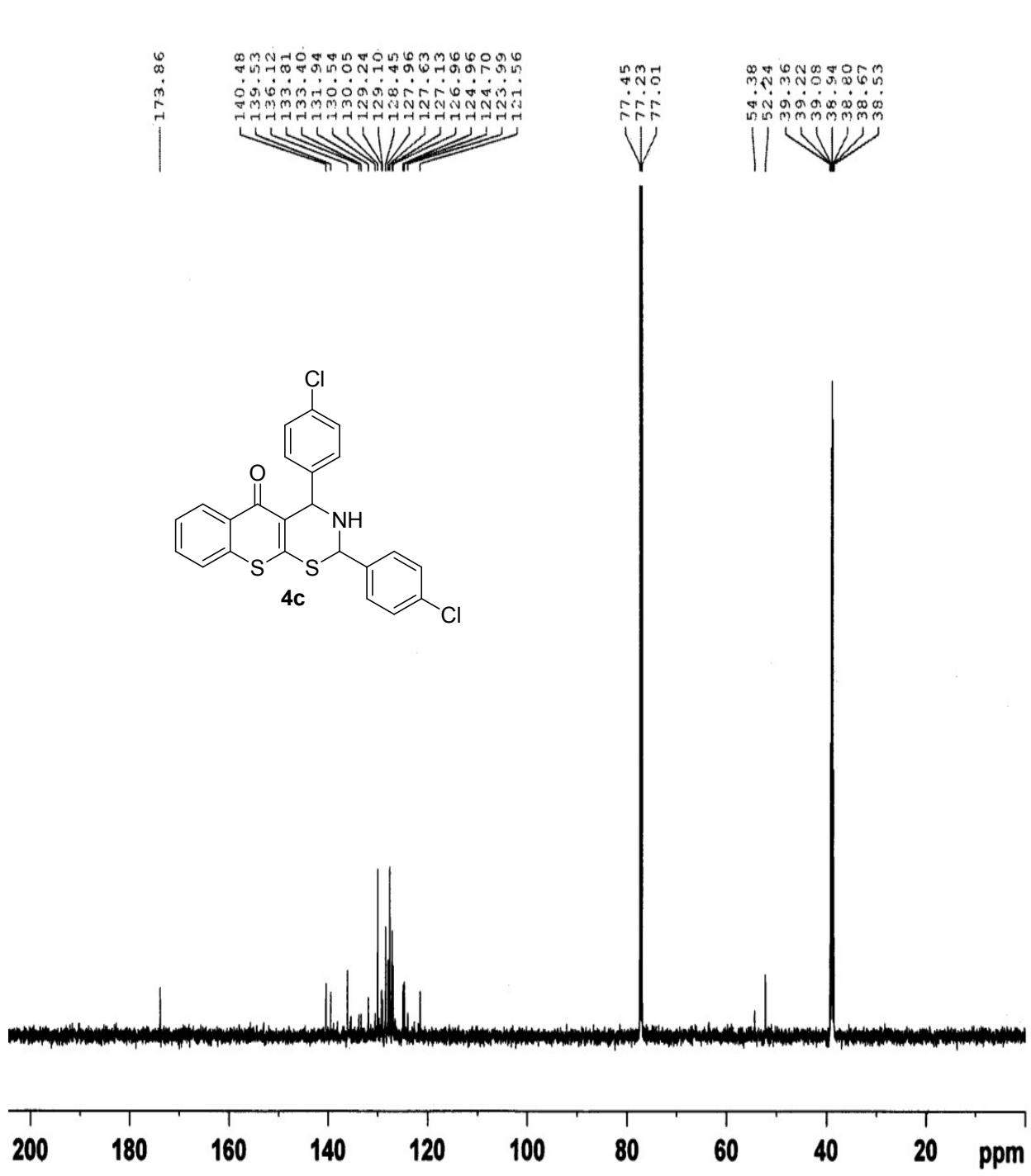
Data Filename	ACQ Method	Comment	Acquired Time



[1]HNMR spectra the compound: 4c



^{13}CNMR spectra of compound: 4c



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PROCNO                   1

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PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                     235
DS                       2
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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
TD0                      1

======== CHANNEL f1 ========
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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
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WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
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HRMS spectra of compound: 4c

Sample Name	**Position**	**Instrument Name**	**User Name**
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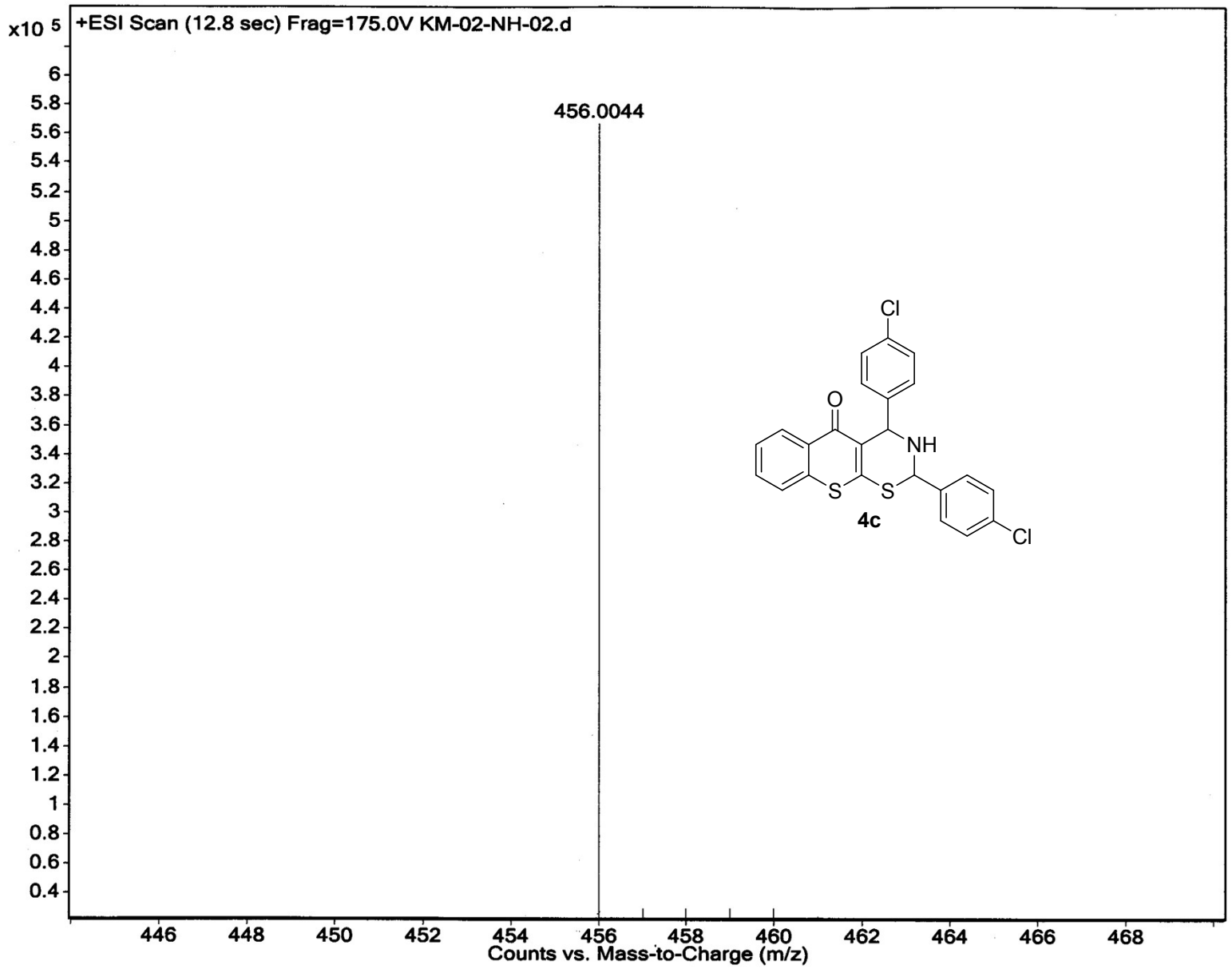
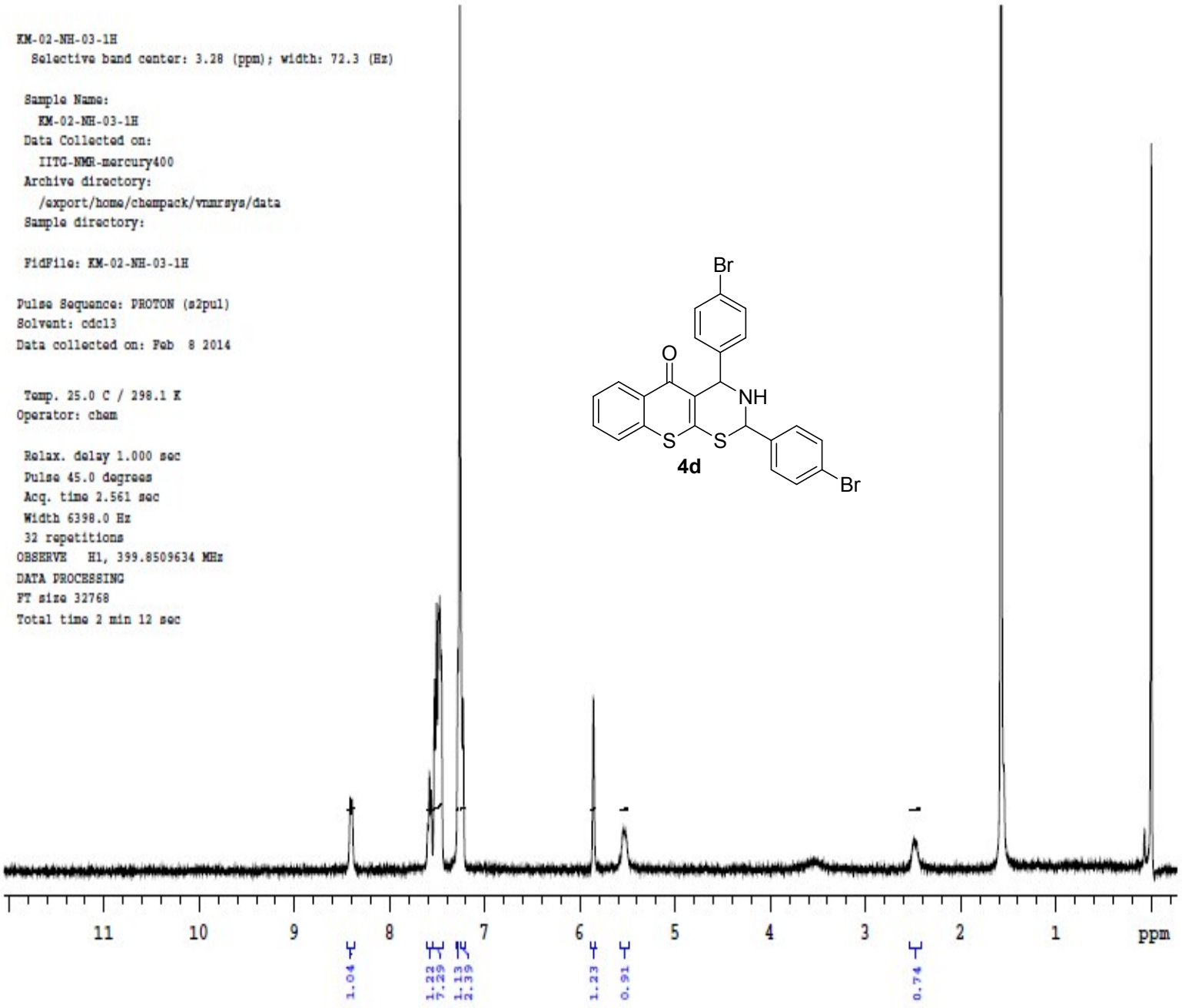
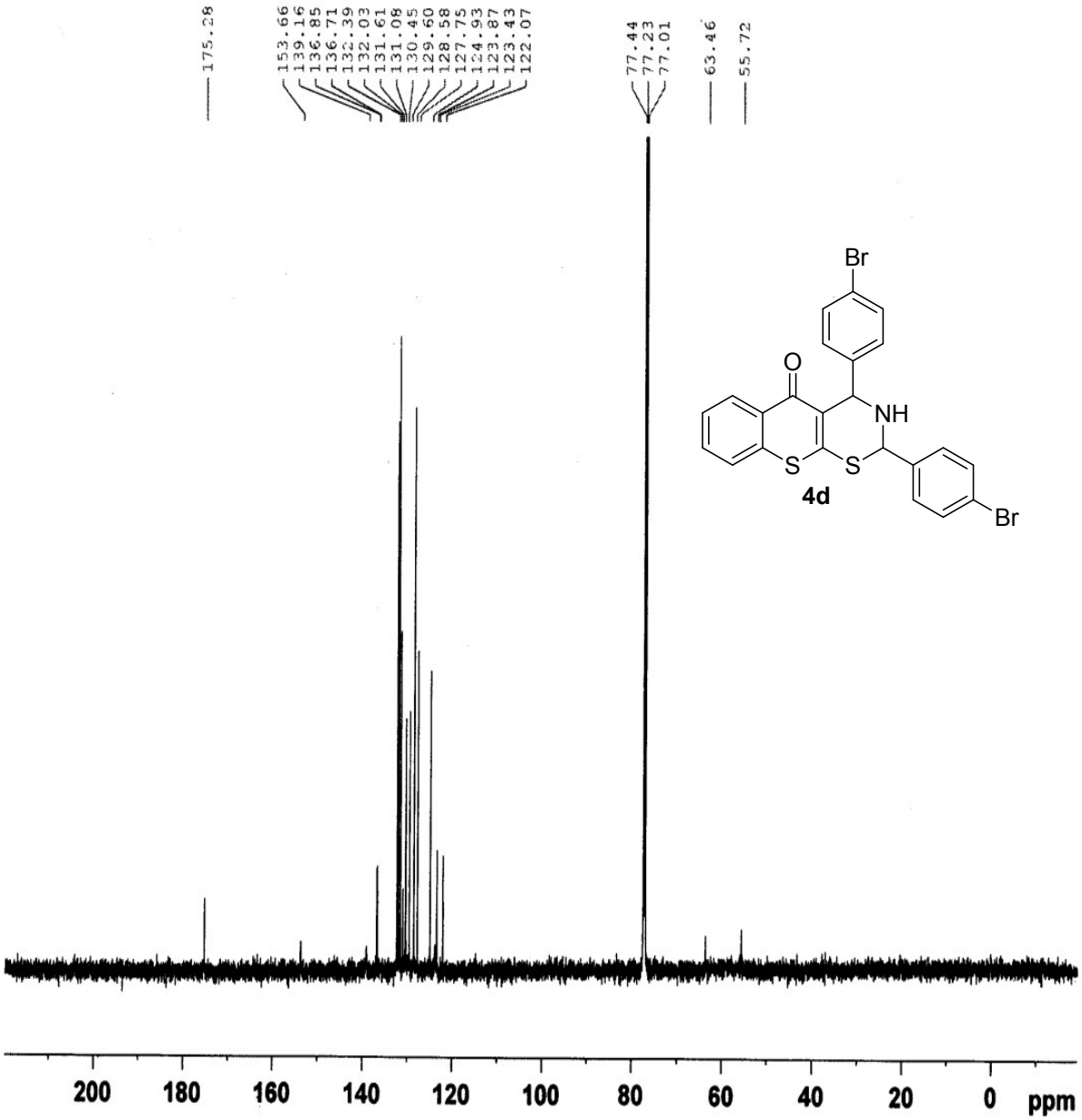
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 4d



^{13}CNMR spectra of compound: 4d



4d

BRUKER

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PROCNO                  1

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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 ========
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NUC1                13C
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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
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LB                 1.00 Hz
GB        0
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HRMS spectra of compound: 4d

Sample Name	**Position**	**Instrument Name**	**User Name**
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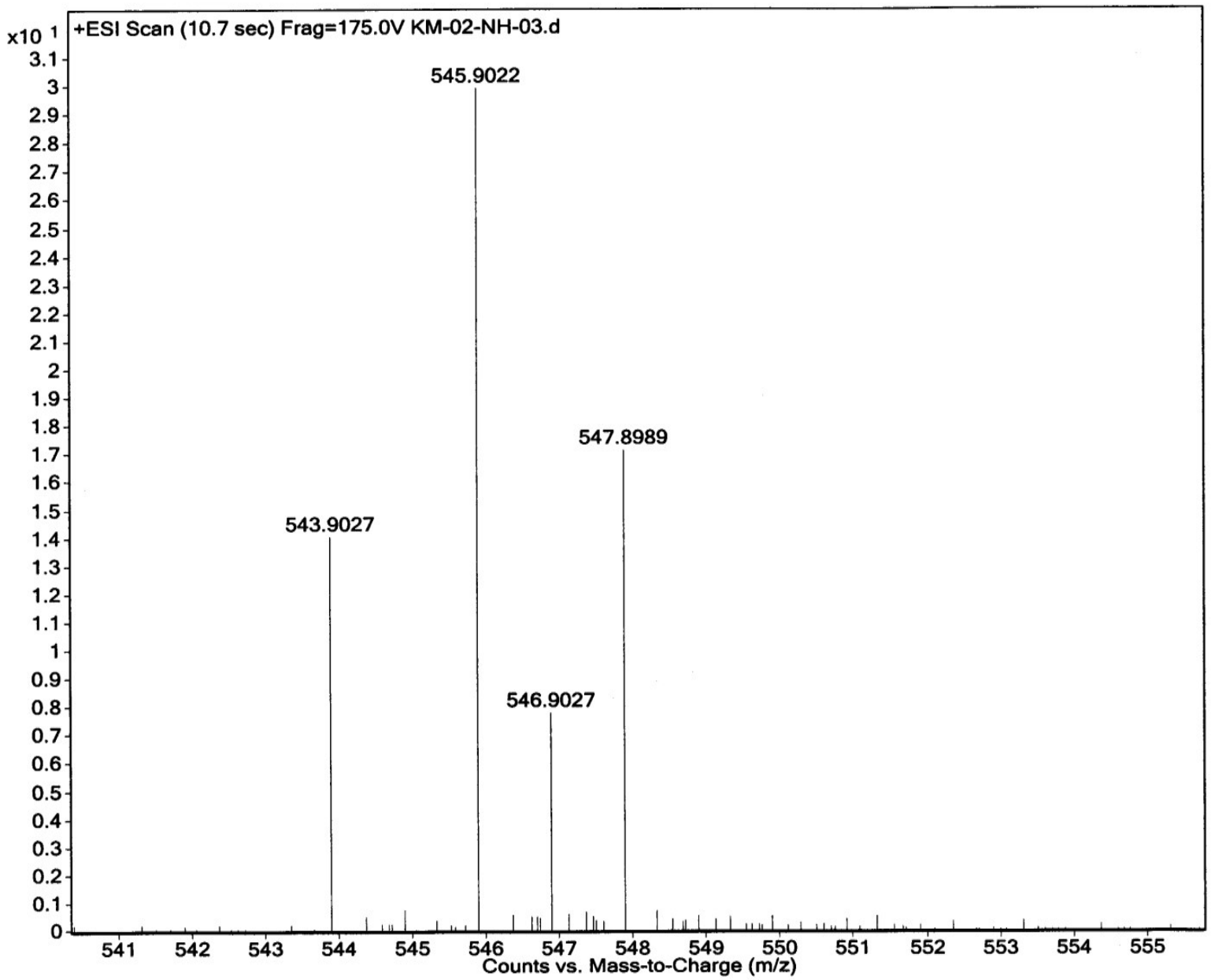
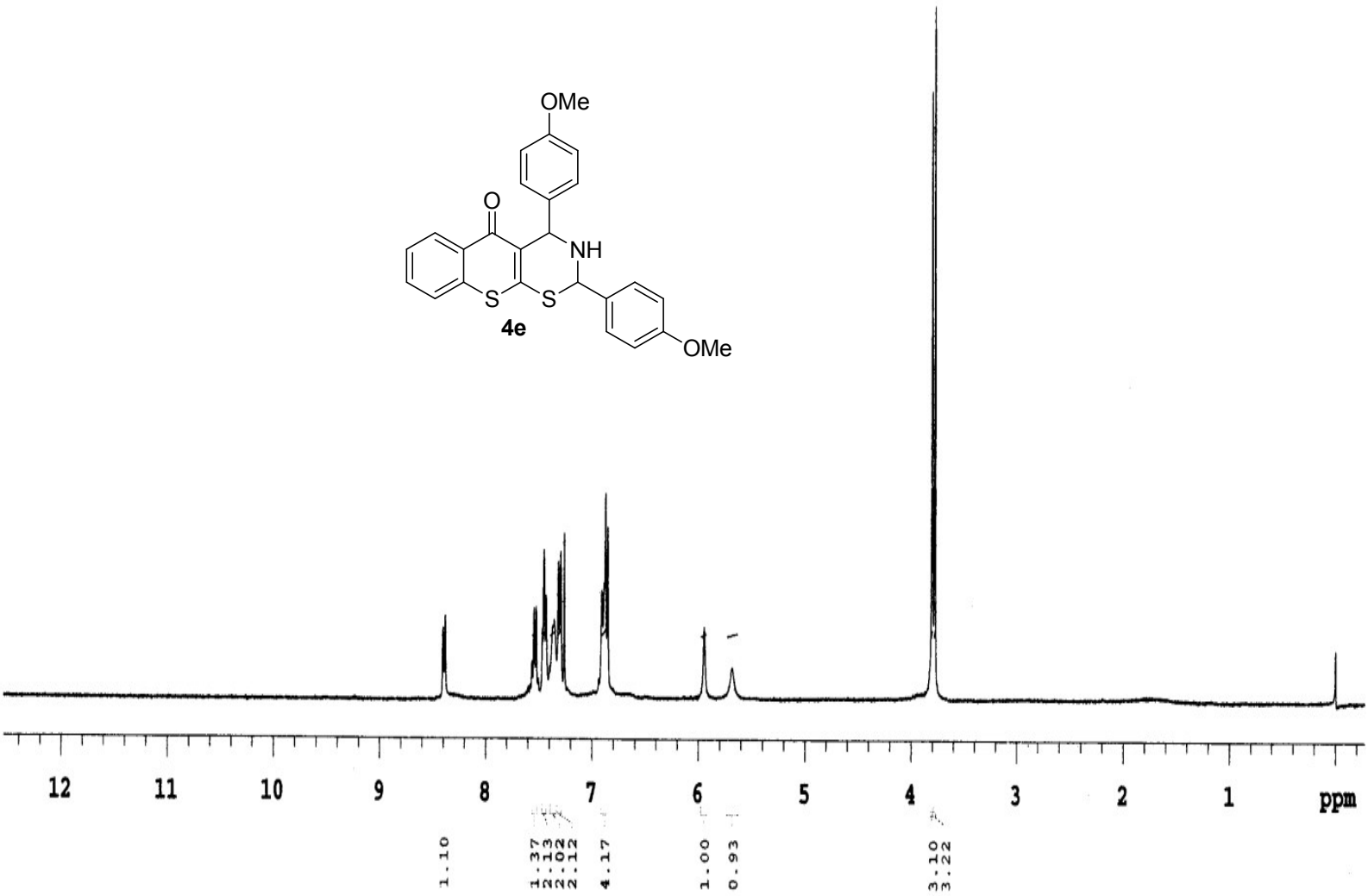


[1]HNMR spectra the compound: 4e



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32 repetitions

DATA PROCESSING
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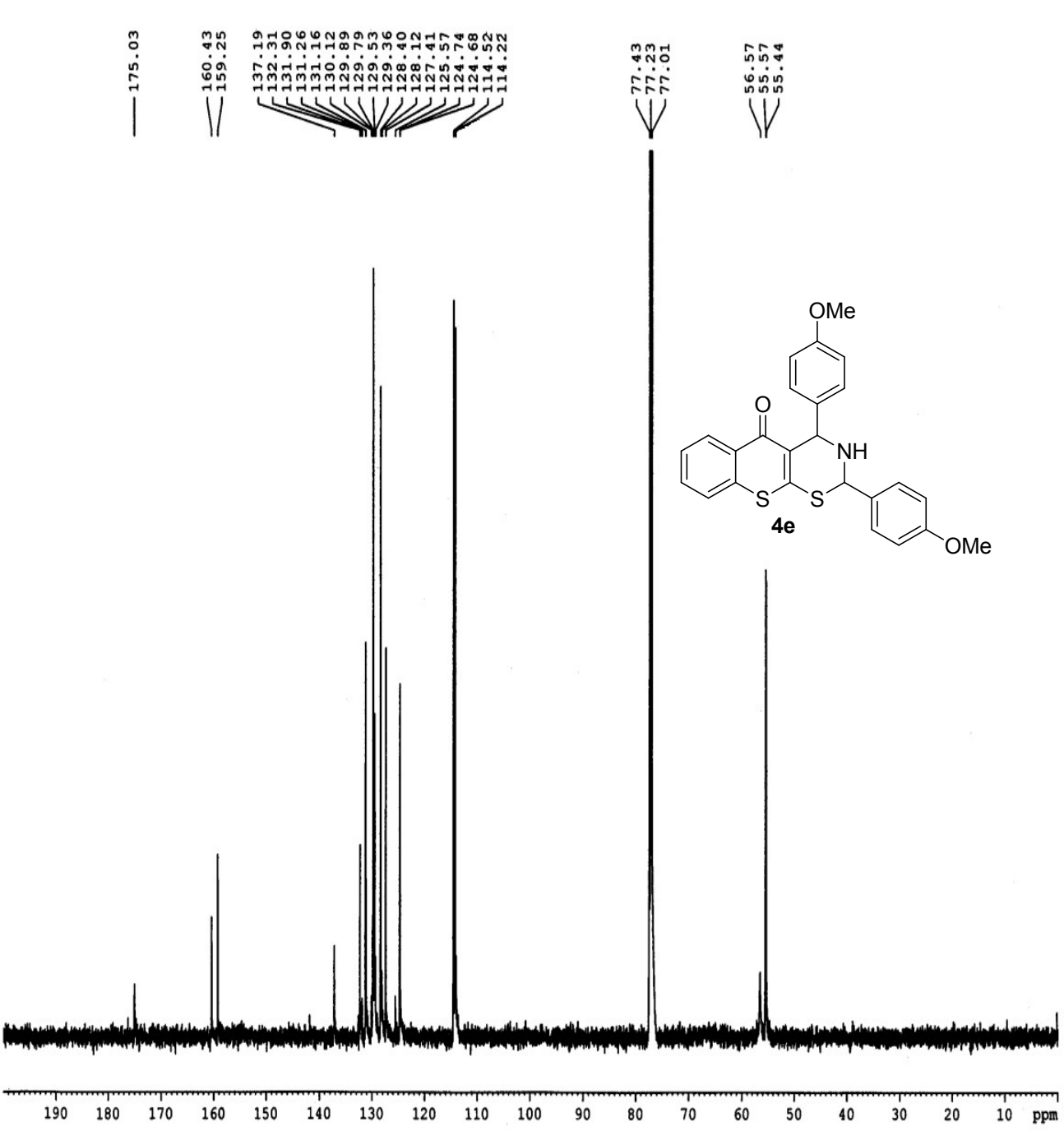
Total time 1 minutes

[illegible]-06

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

^{13}CNMR spectra of compound: 4e



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PULPROG zgpg30
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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 ========
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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
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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**
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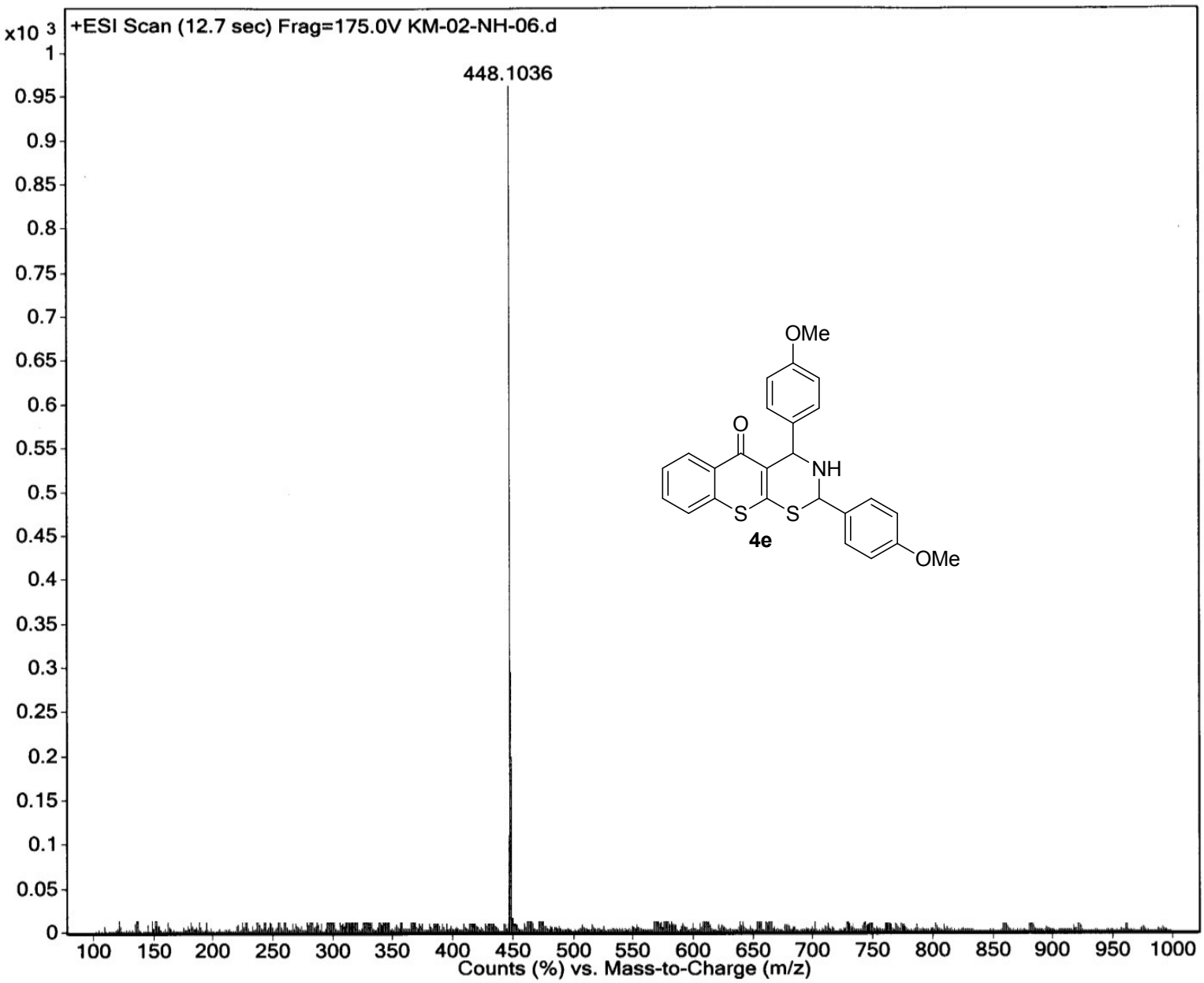
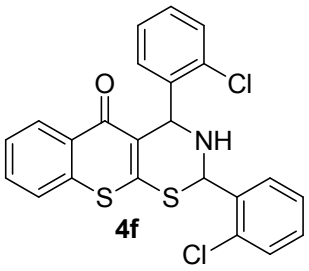


[1]HNMR spectra the compound: 4f



4f

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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

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NUC1                 1H
P1                12.00 usec
PLW1         21.00000000 W

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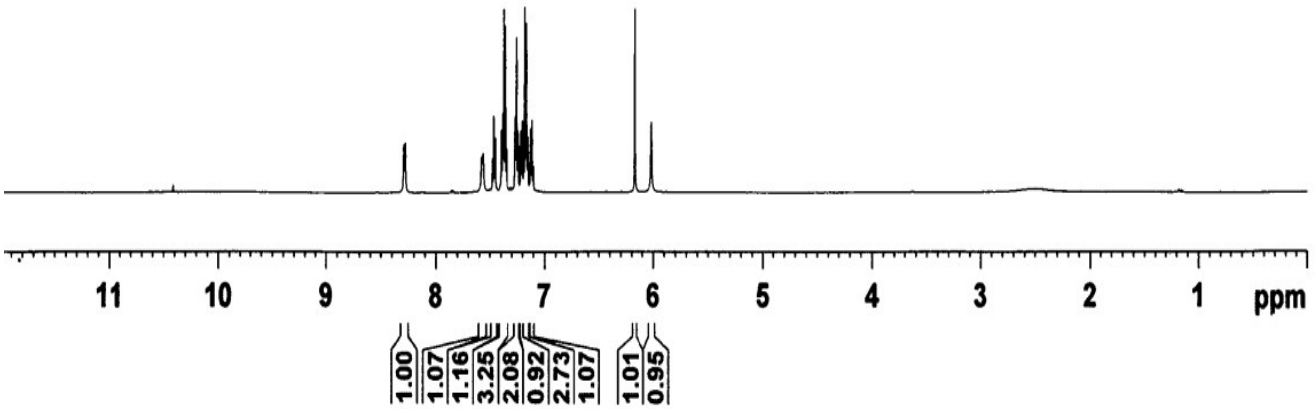
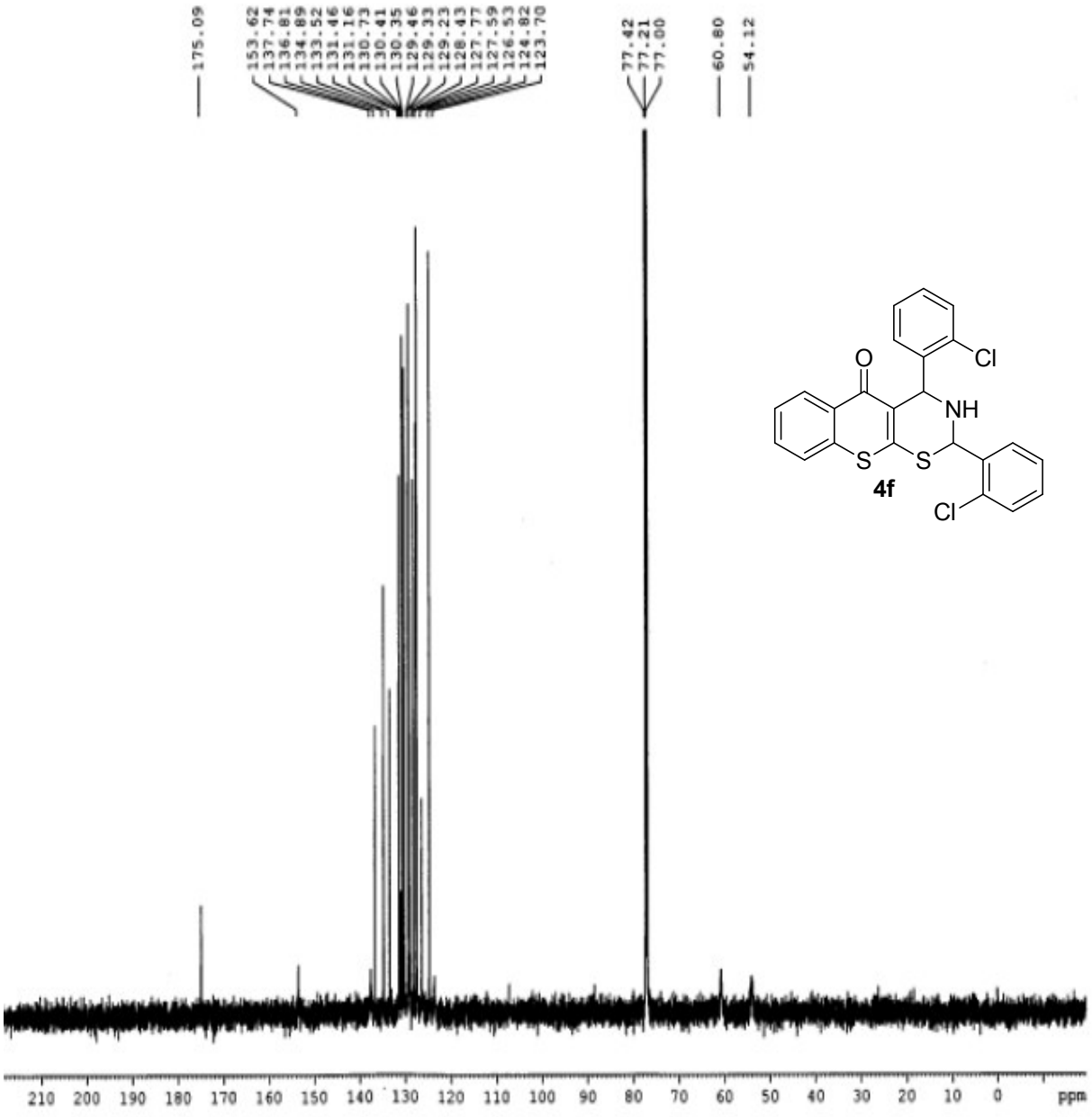


^{13}CNMR spectra of compound: 4f



4f

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Current Data Parameters
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PROCNO 1

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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
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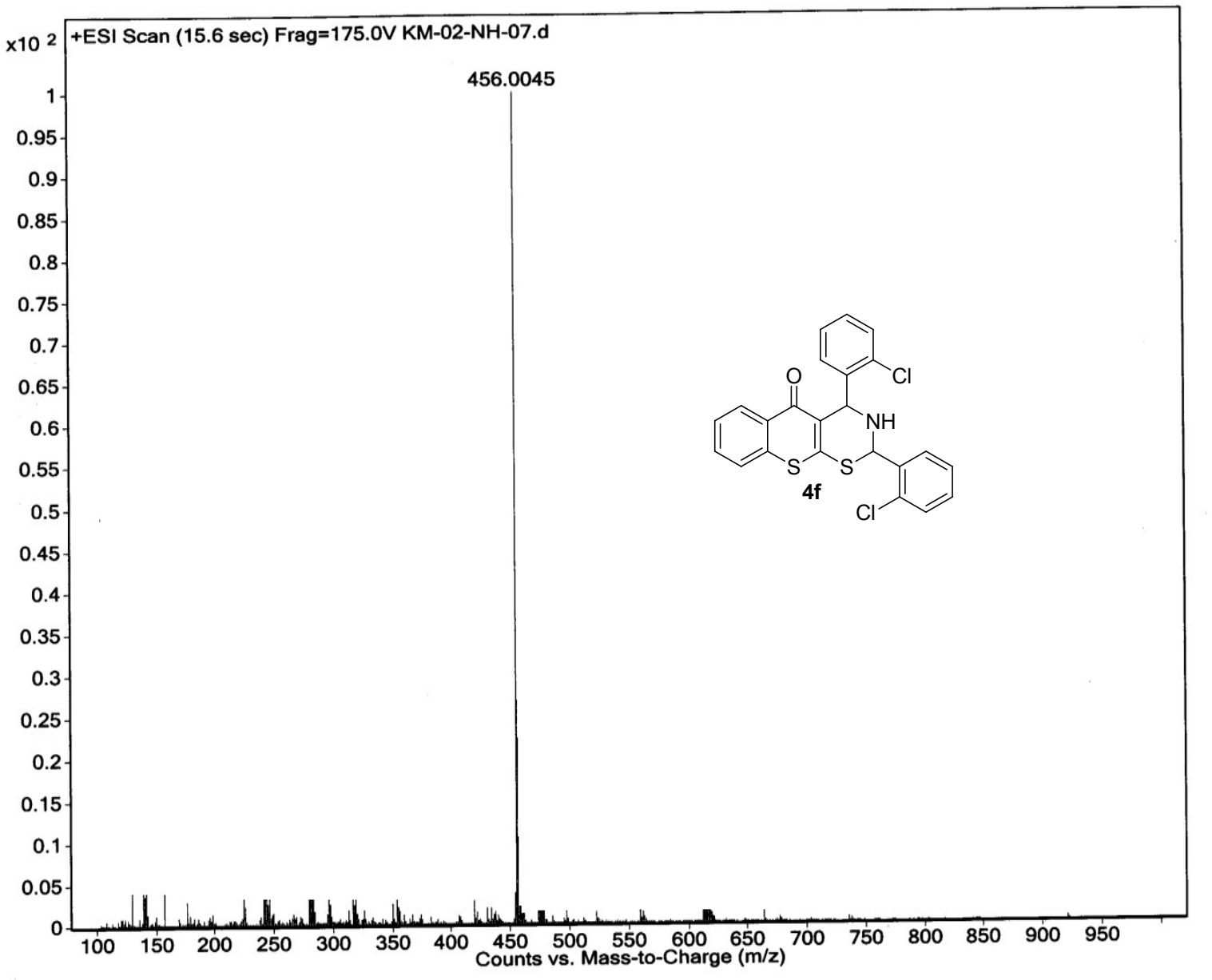
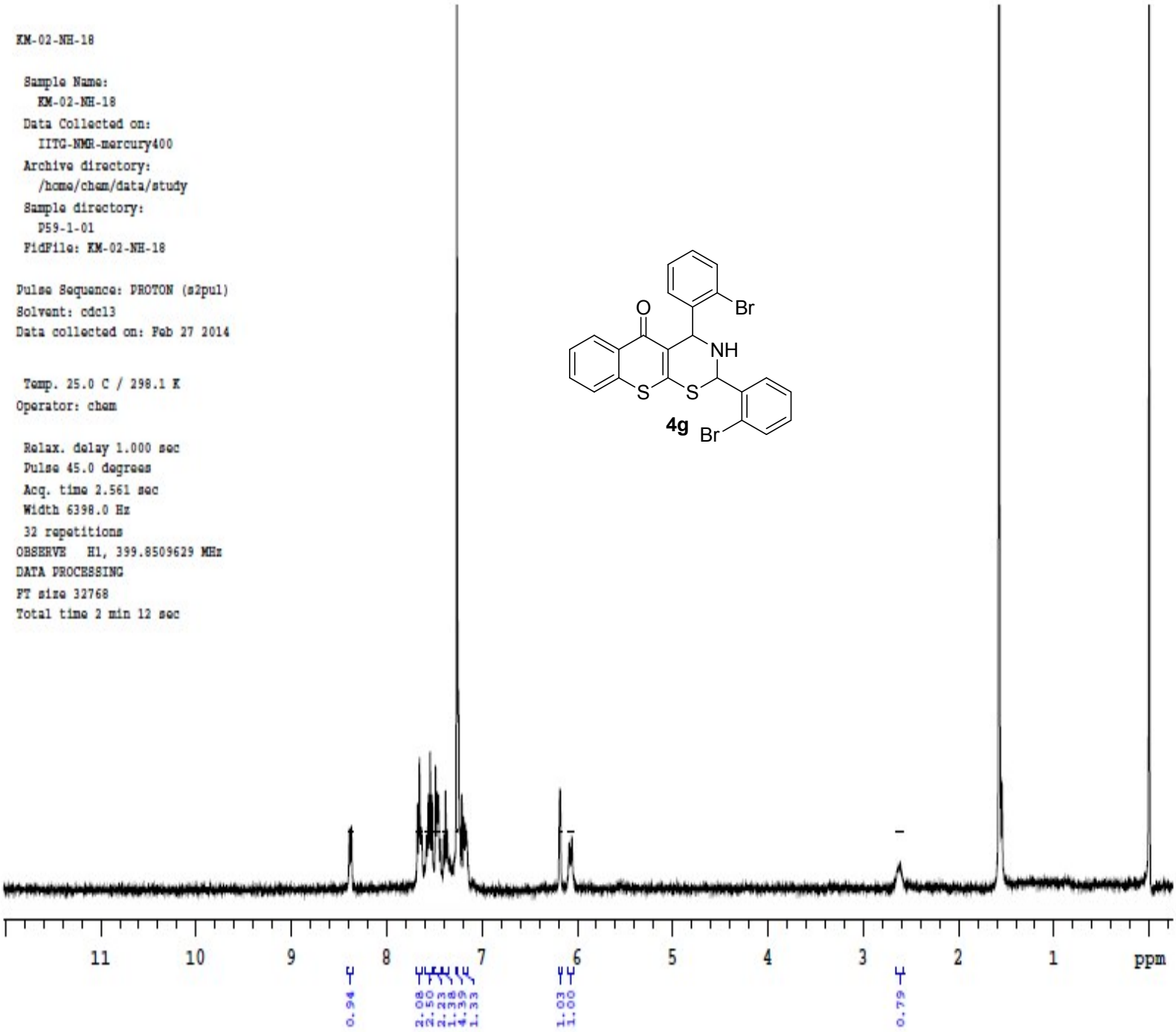
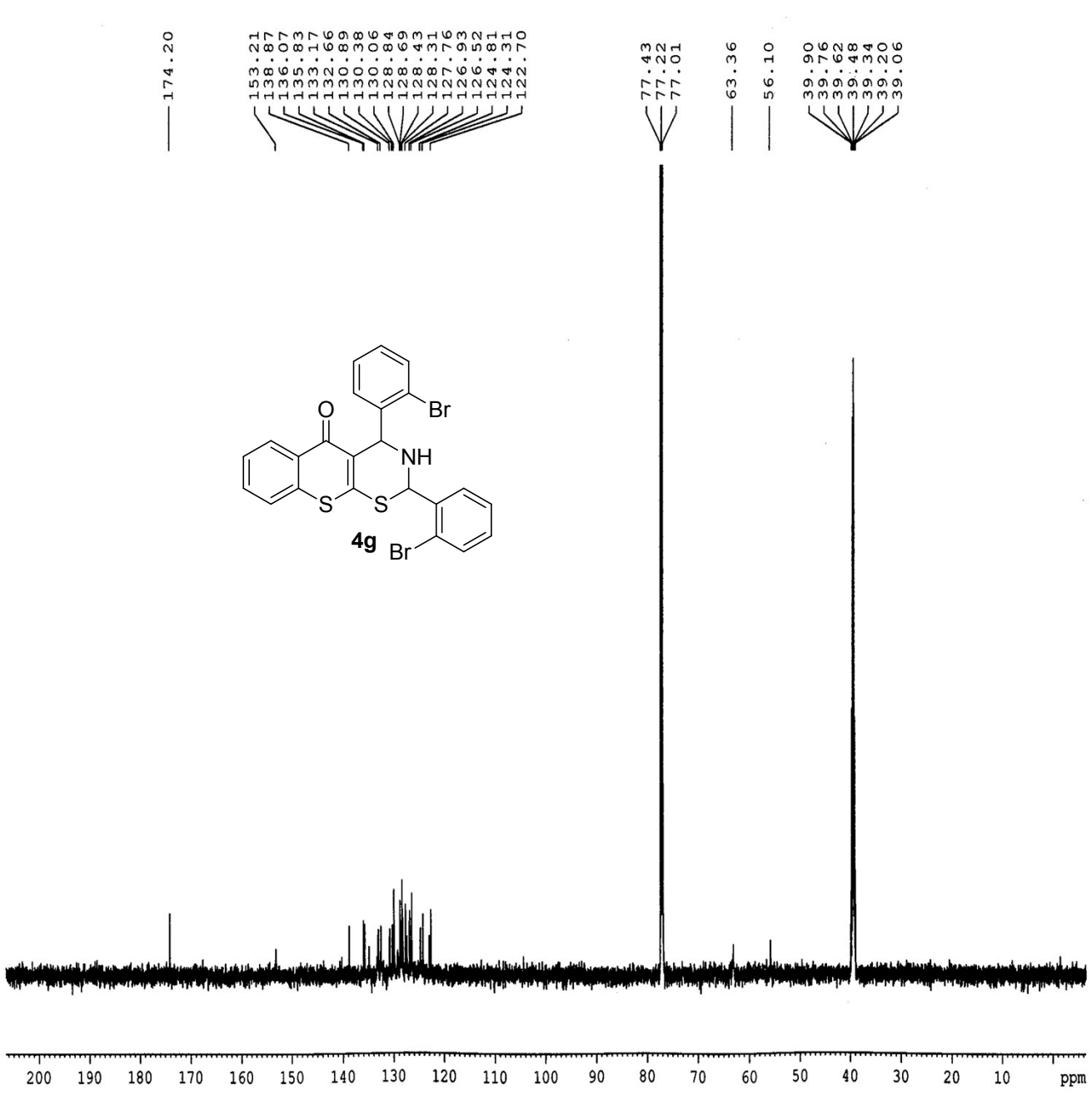


[1]HNMR spectra the compound: 4g



^{13}CNMR spectra of compound: 4g



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PROCNO                 1

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PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
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           2.00000000 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          150.9136604 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
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[1]HNMR spectra the compound: 4g

Sample Name	KM-02-NH-18	**Position**	-1	**Instrument Name**	Instrument 1	**User Name**	
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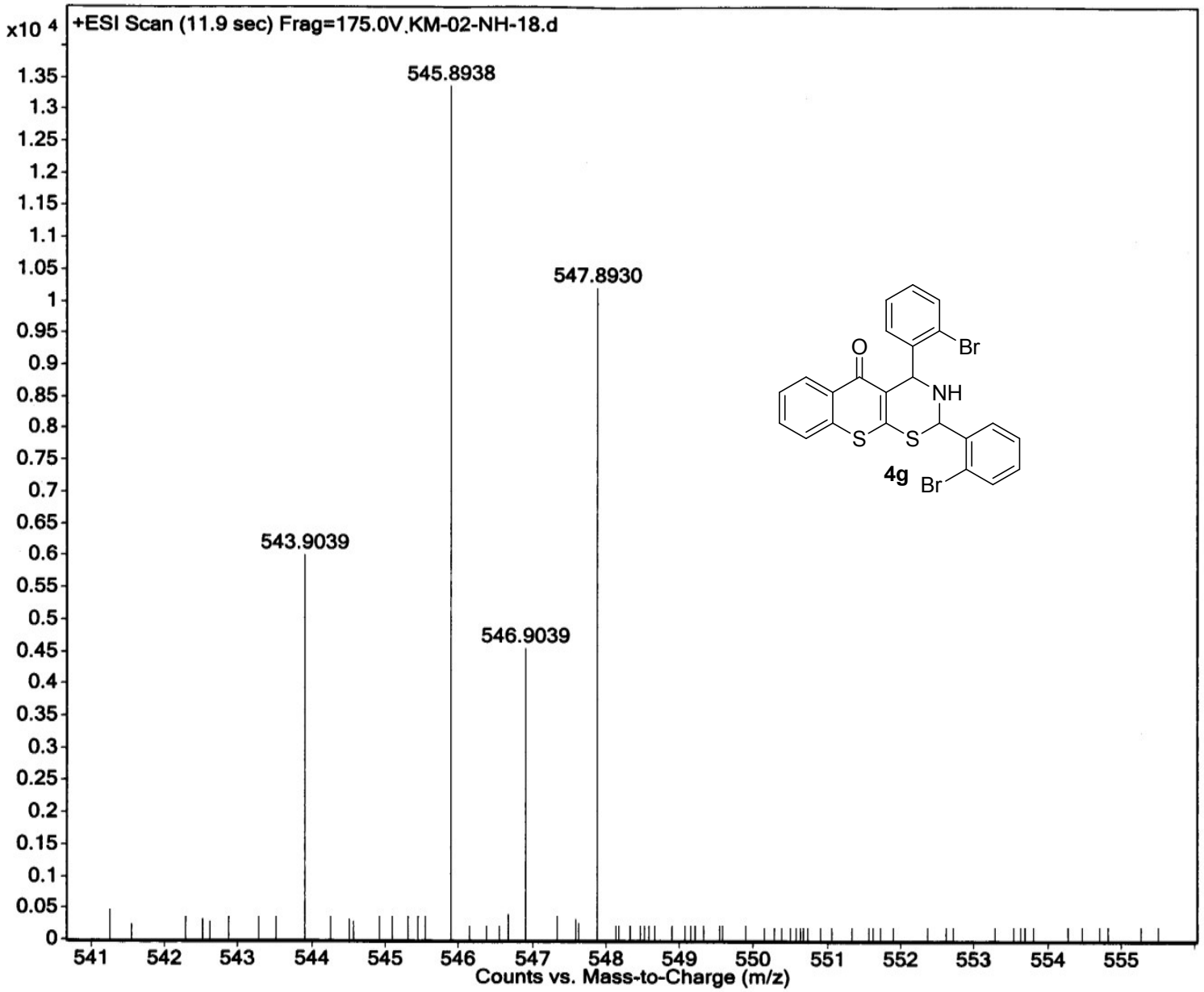
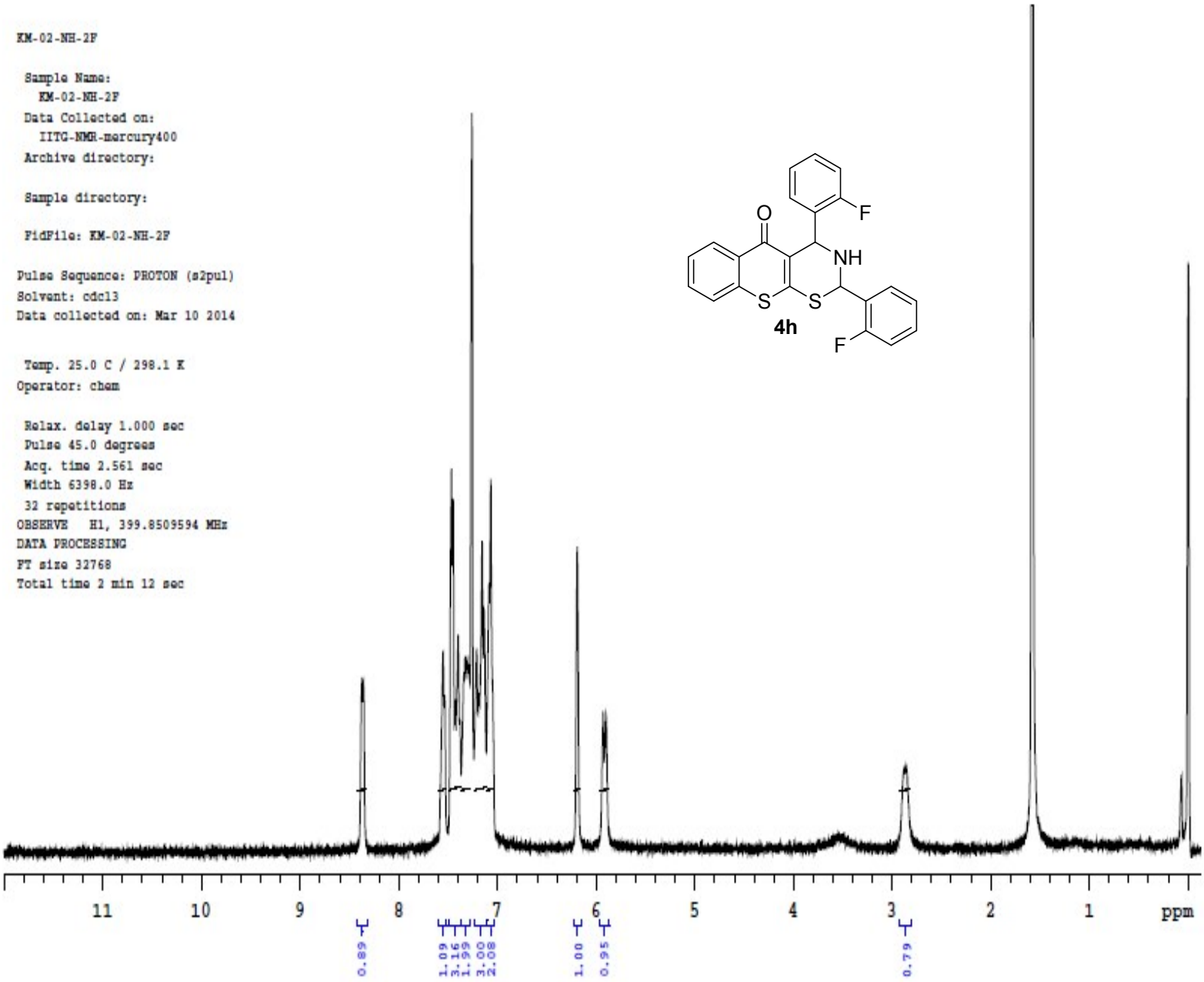
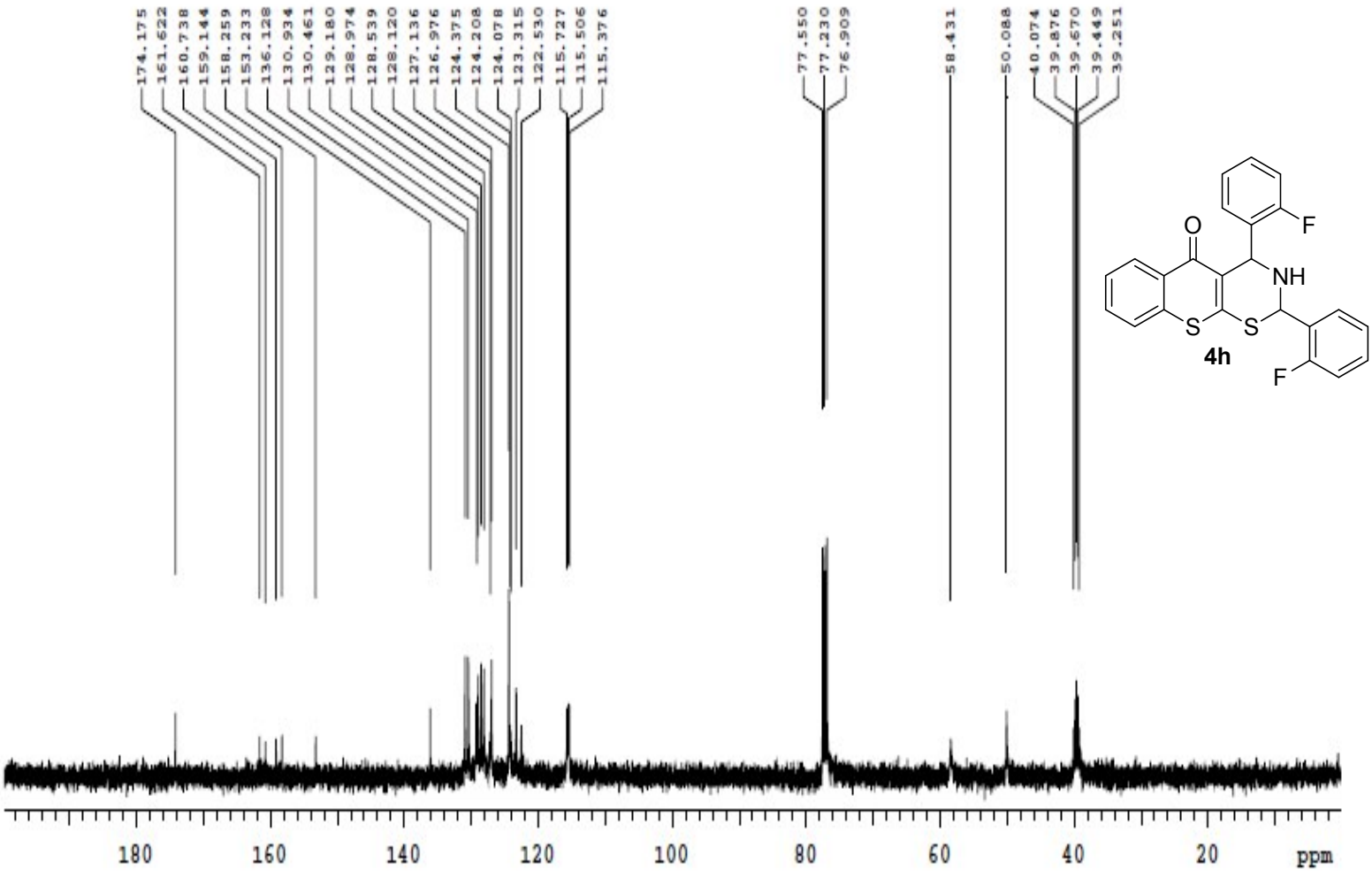


[1]HNMR spectra the compound: 4h



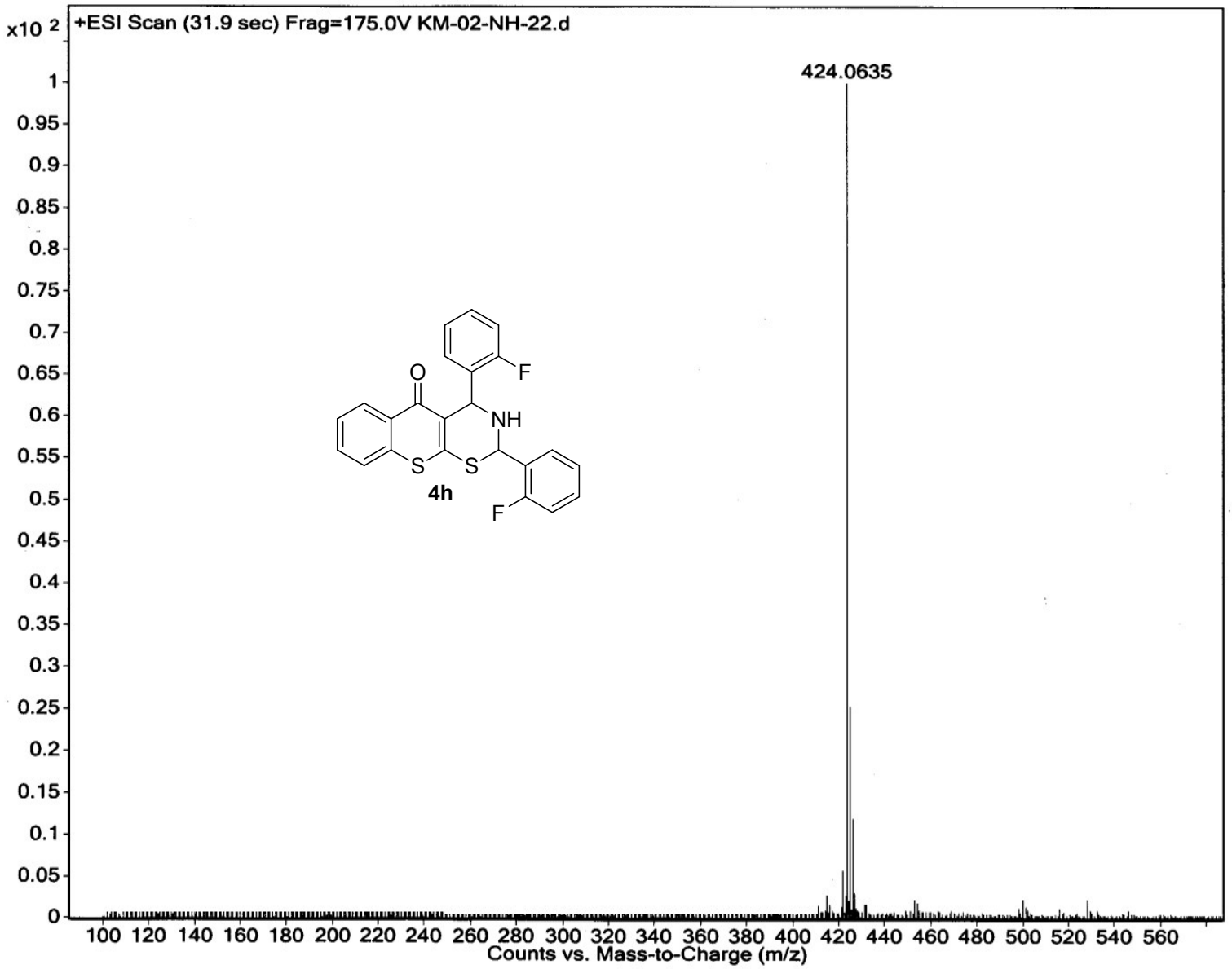
^{13}CNMR spectra of compound: 4h



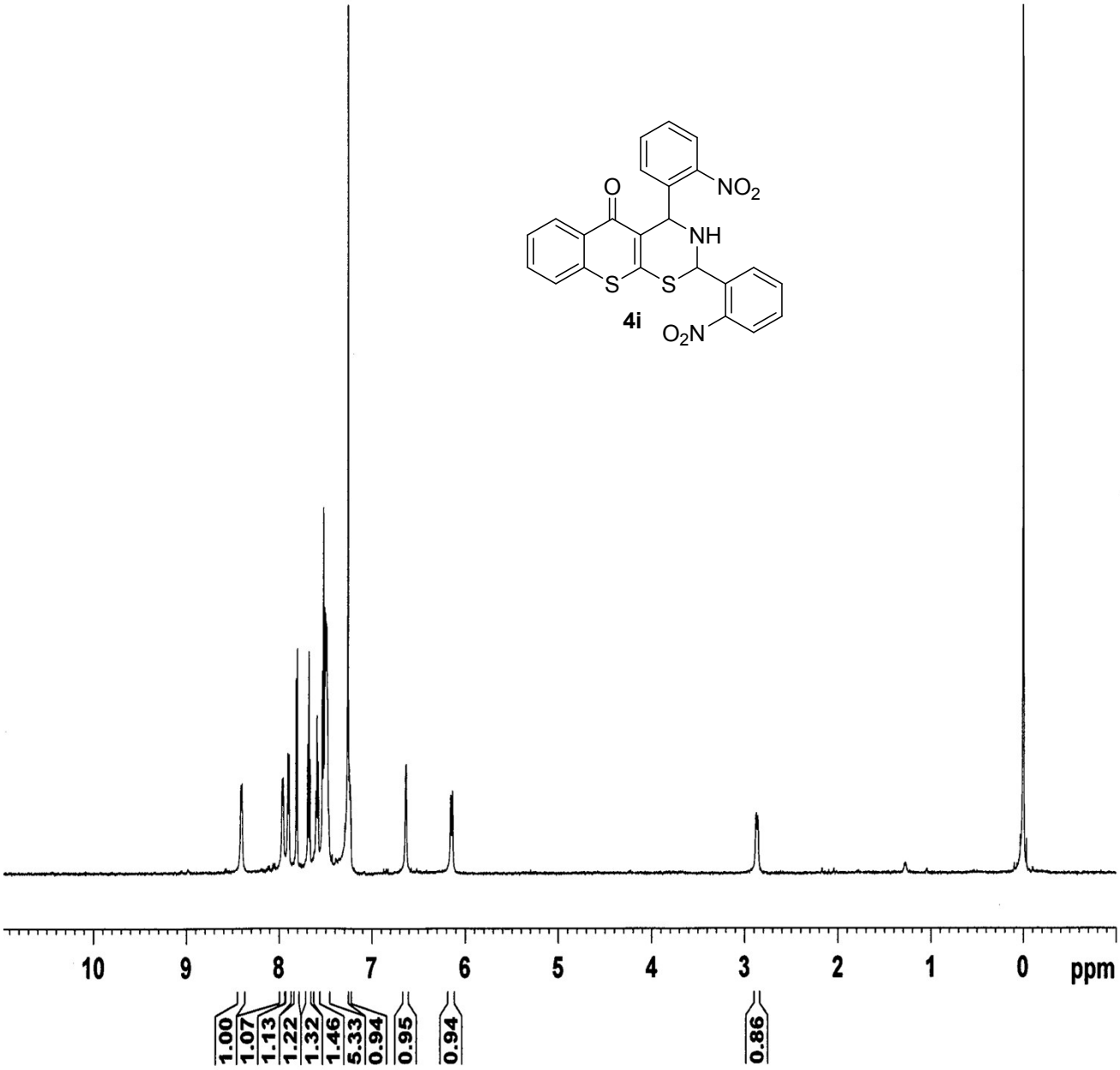
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1610 repetitions	OBSERVE C13, 100.5431207 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 61 minutes		KM-02-NH-2F-13C Solvent: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



[1]HNMR spectra the compound: 4i

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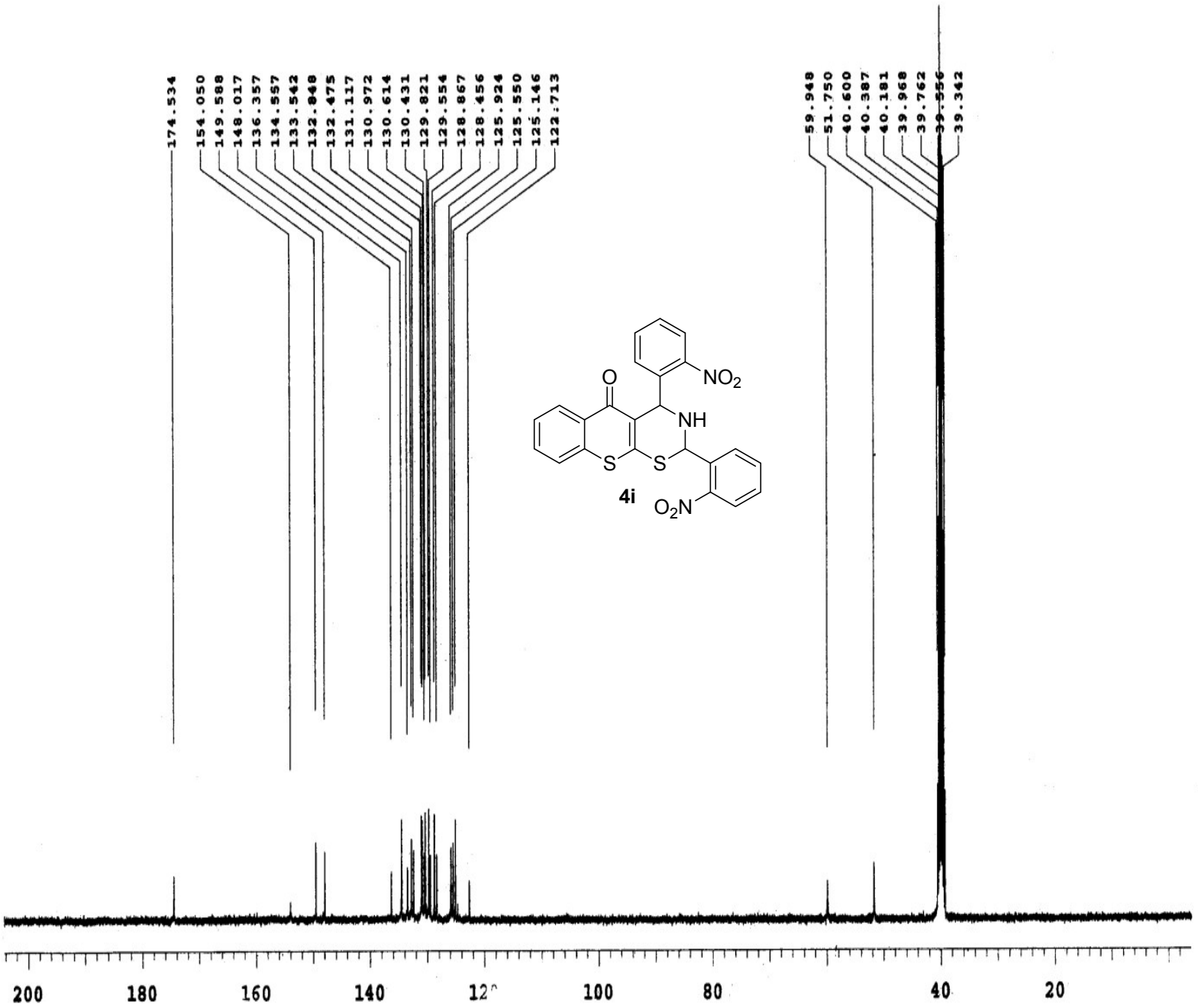
Current Data Parameters
NAME      KM_02_NH_11_1H
EXPNO                  1
PROCNO                 1

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
TD0                    1

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

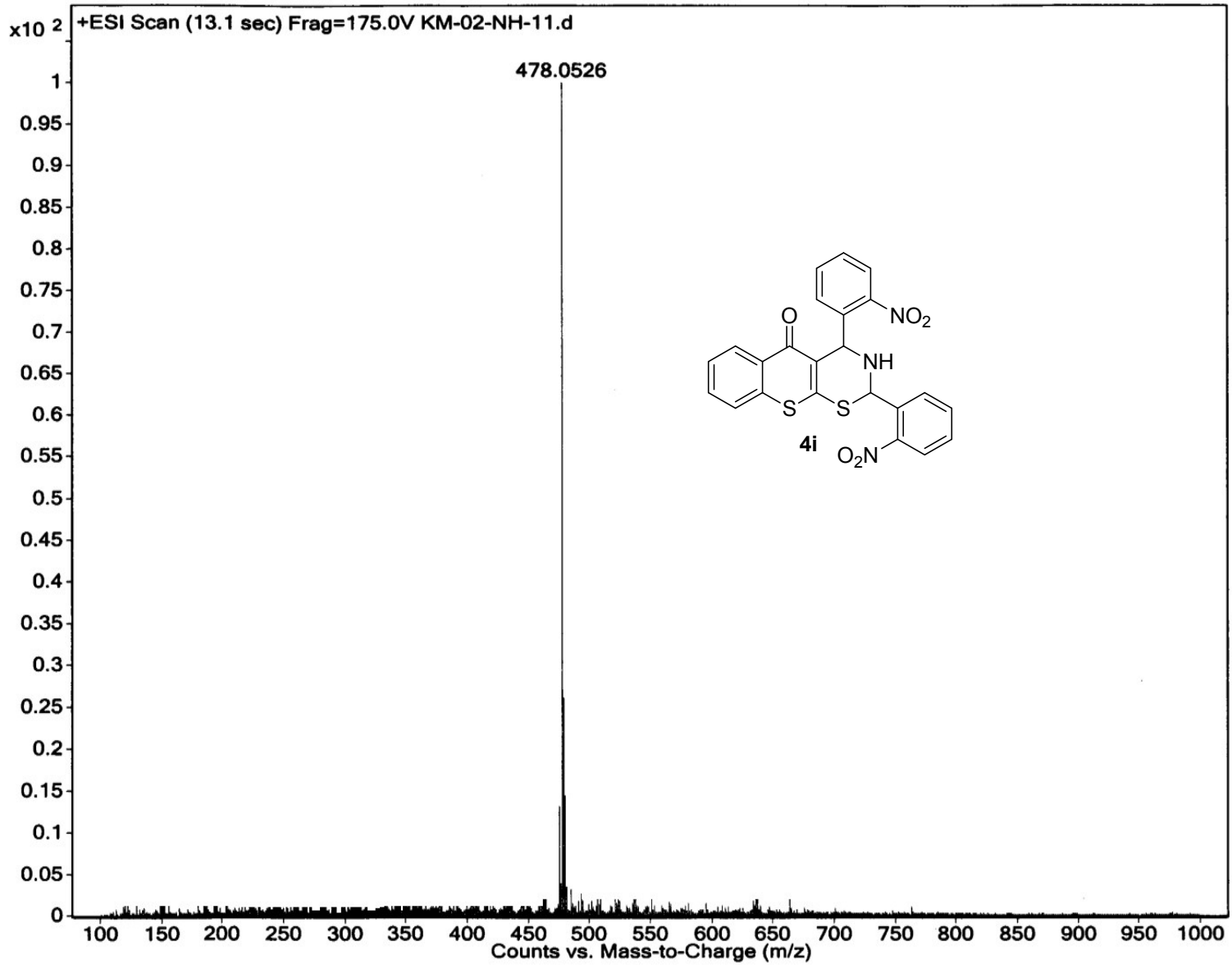
F2 - Processing parameters
SI                16384
SF           600.1700148 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}CNMR spectra of compound: 4i



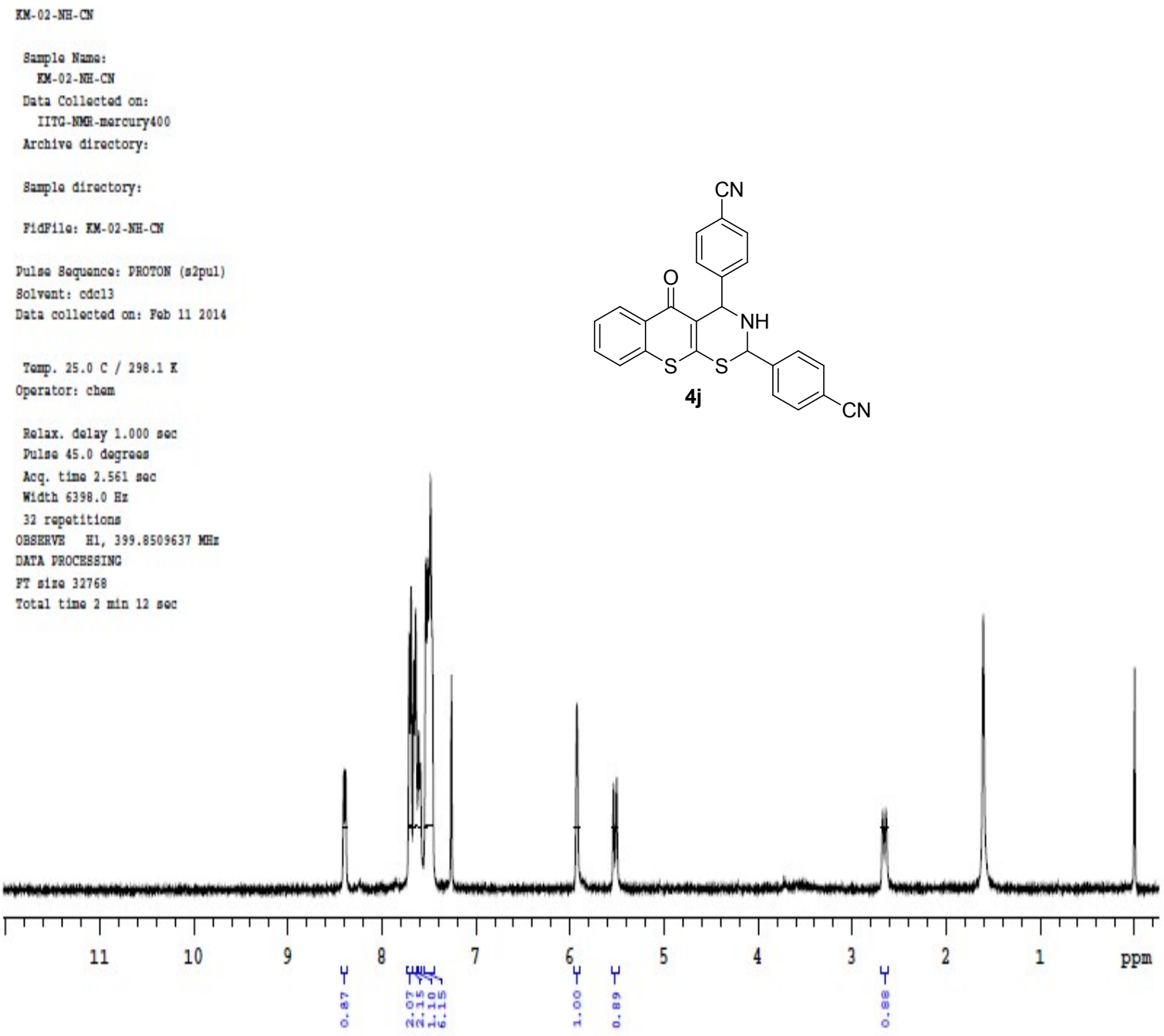
HRMS spectra of compound: 4i

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

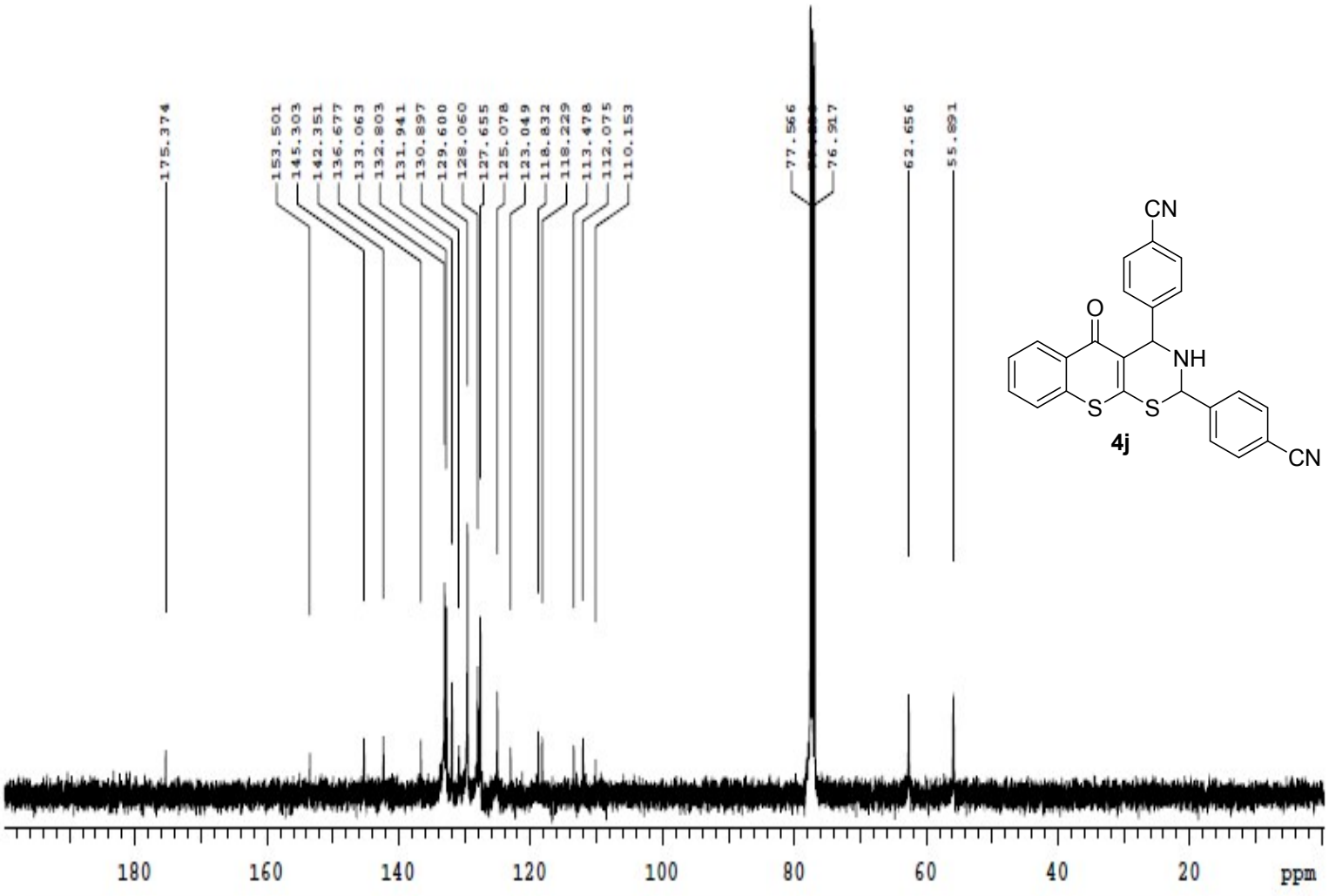


4i

[1]HNMR spectra the compound: 4j



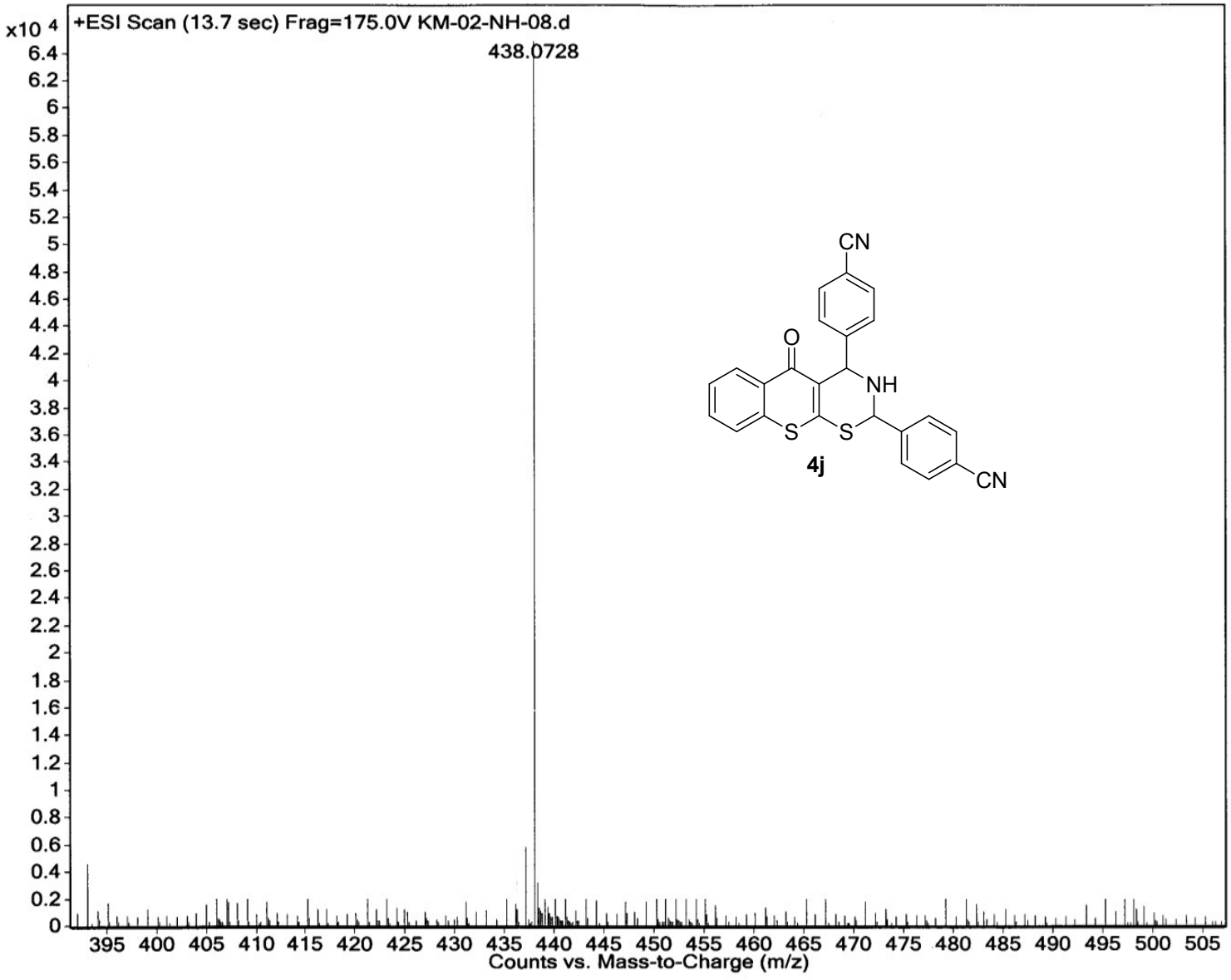
^{13}CNMR spectra of compound: 4j



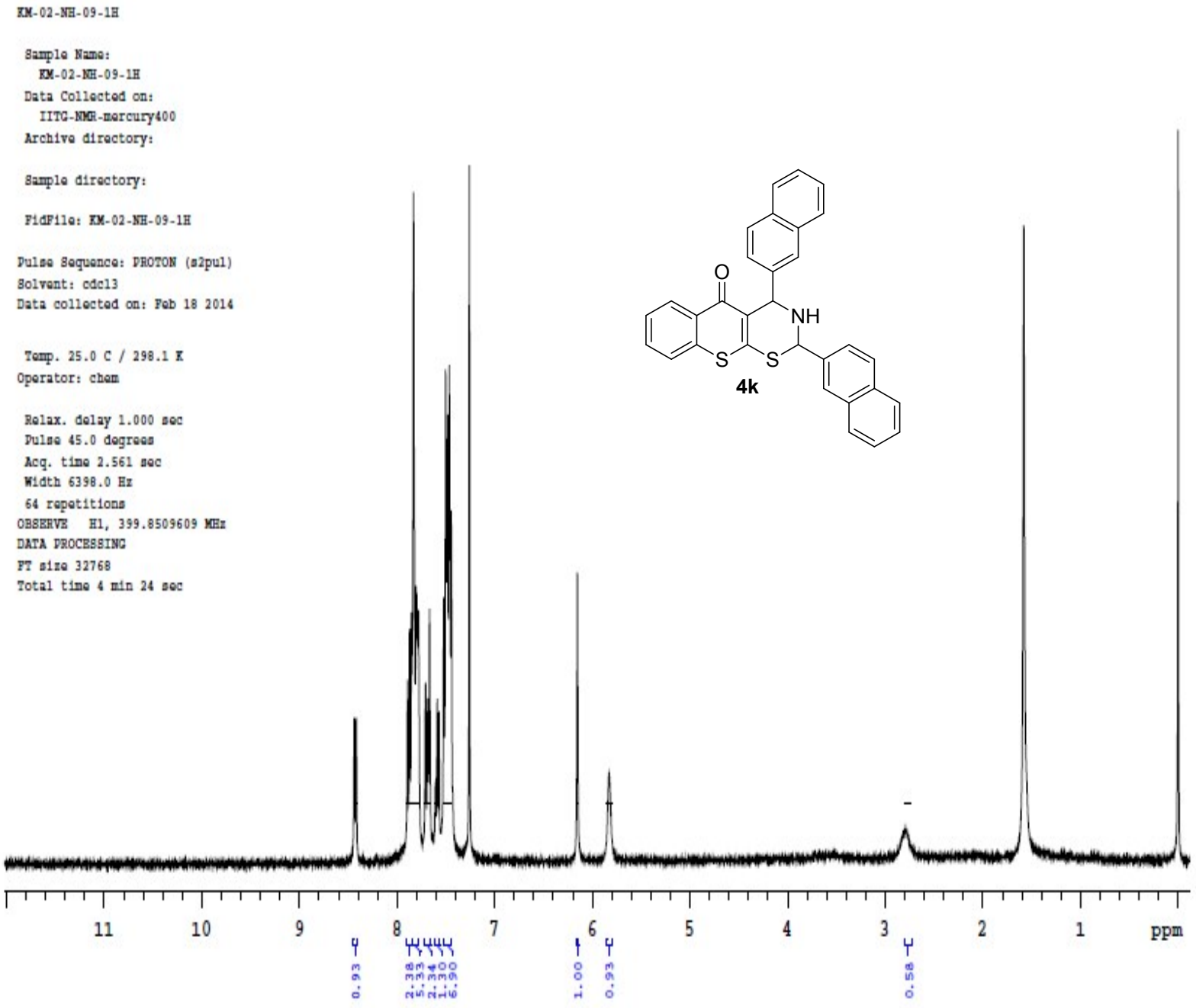
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 12170 repetitions	OBSERVE C13, 100.5425893 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 7.8 hours		KM-NH-RR-13C Solvent: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

HRMS spectra of compound: 4j

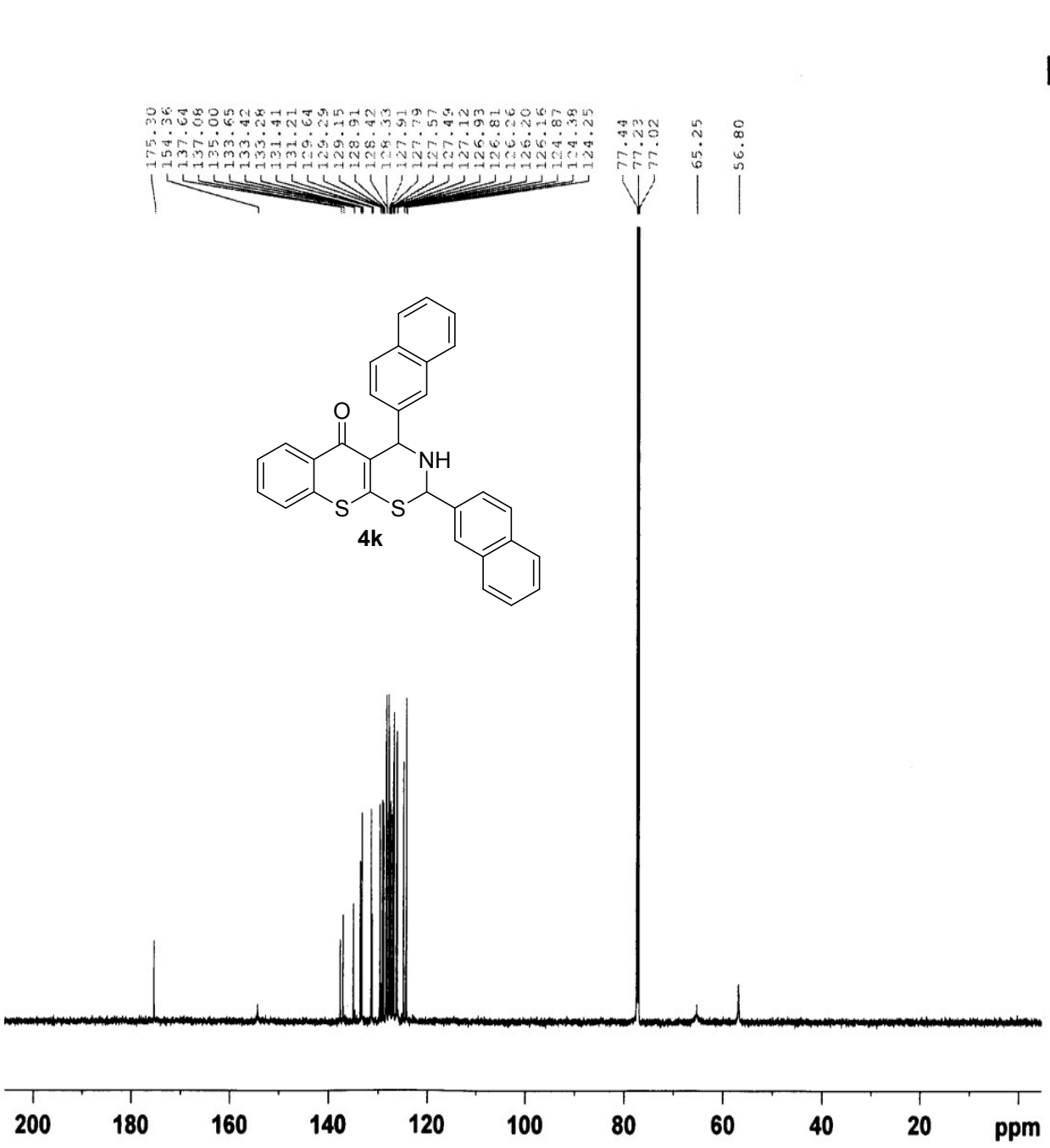
Sample Name	KM-02-NH-08	**Position**	-1	**Instrument Name**	Instrument 1	**User Name**	
Inj Vol	-10	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	KM-02-NH-08.d	**ACQ Method**		**Comment**		**Acquired Time**	10/14/2014 11:06:59 AM



[1]HNMR spectra the compound: 4k



^{13}CNMR spectra of compound: 4k



BRUKER

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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

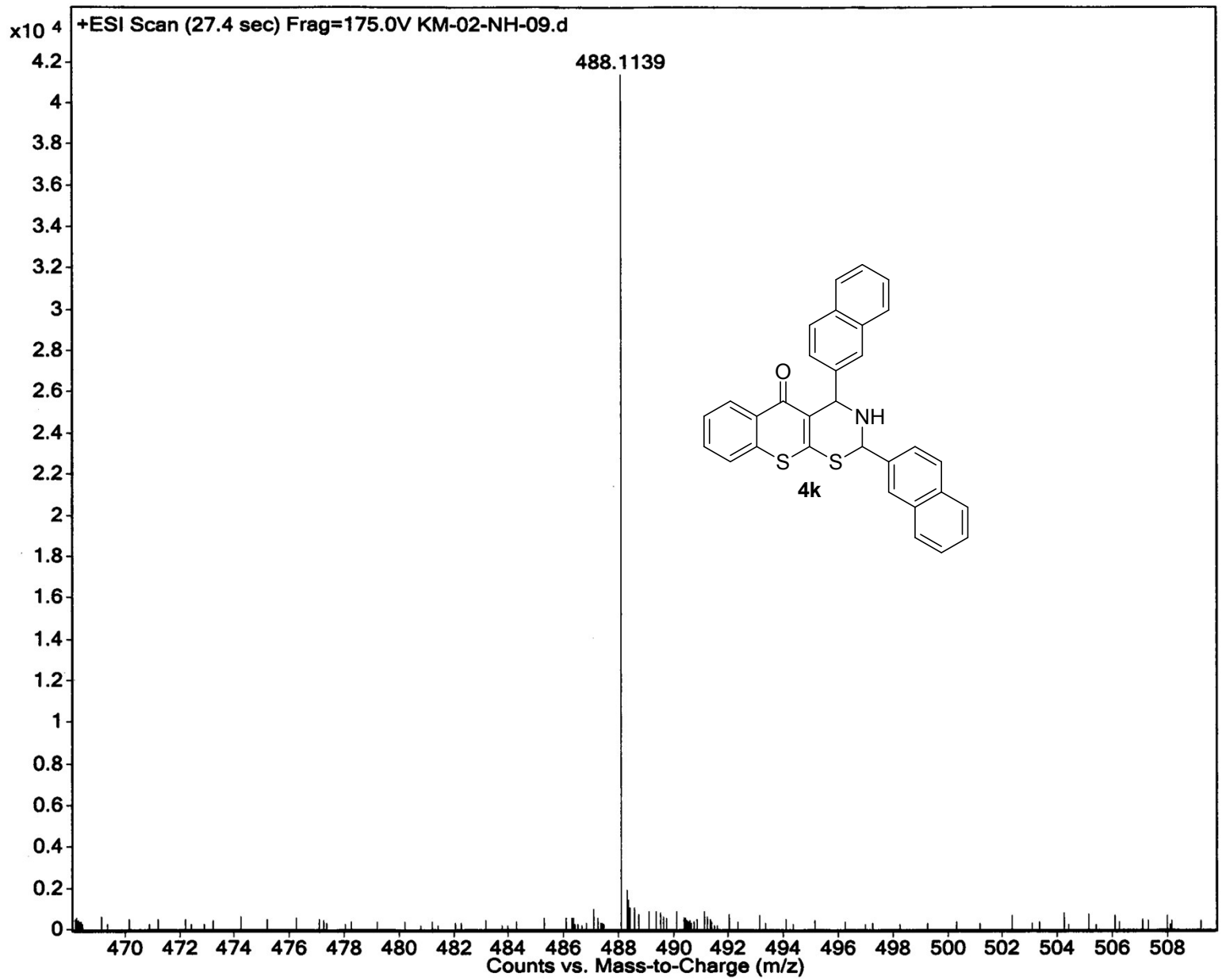
======== CHANNEL f1 ========
SFO1          150.9279571 MHz
NUC1                    13C
P1                   10.50 usec
PLW1          95.00000000 W

======== 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

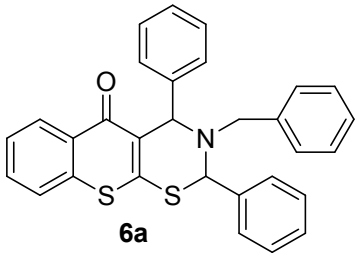
F2 - Processing parameters
SI                   16384
SF            150.9128414 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

HRMS spectra of compound: 4k

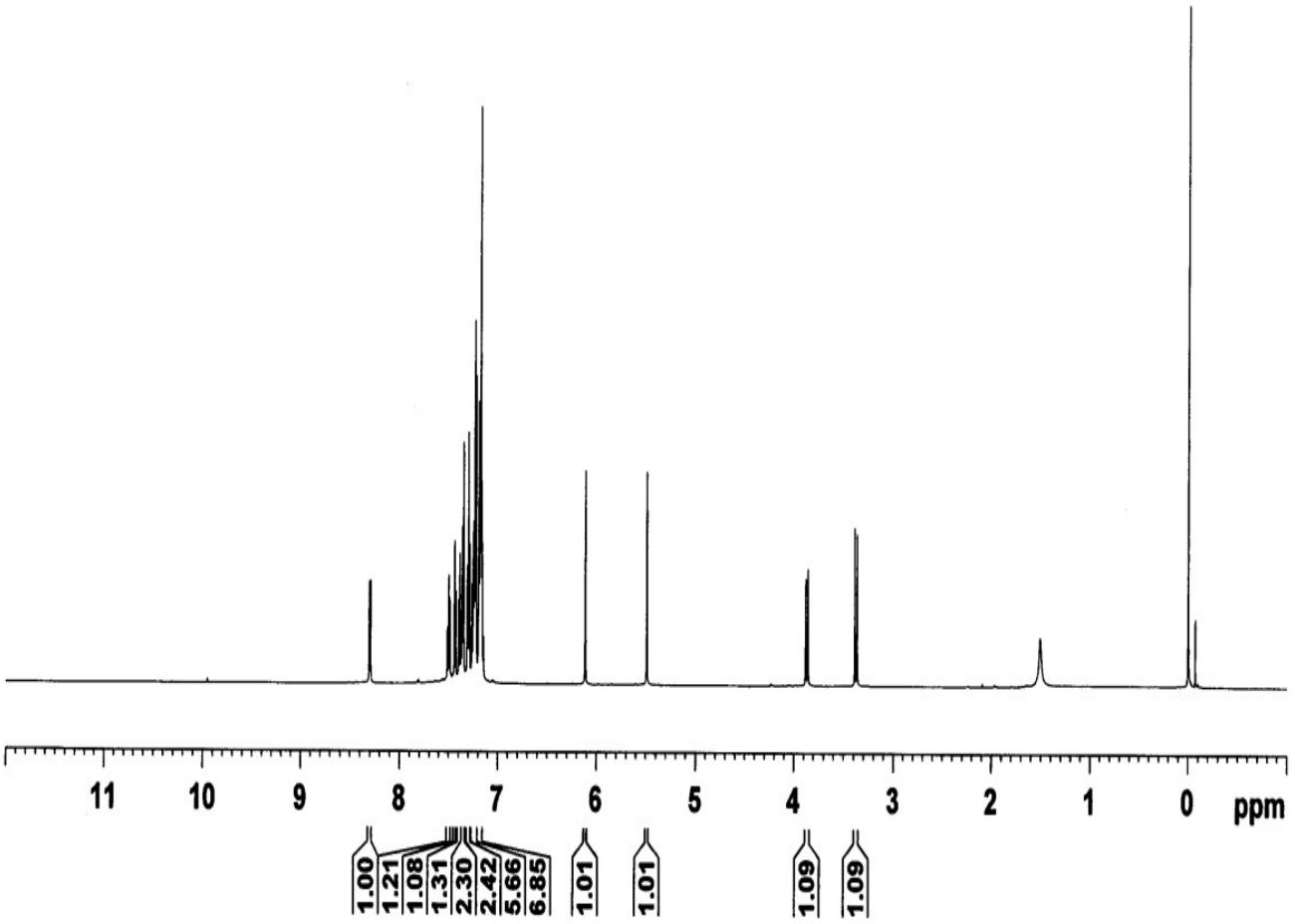
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 6a



6a

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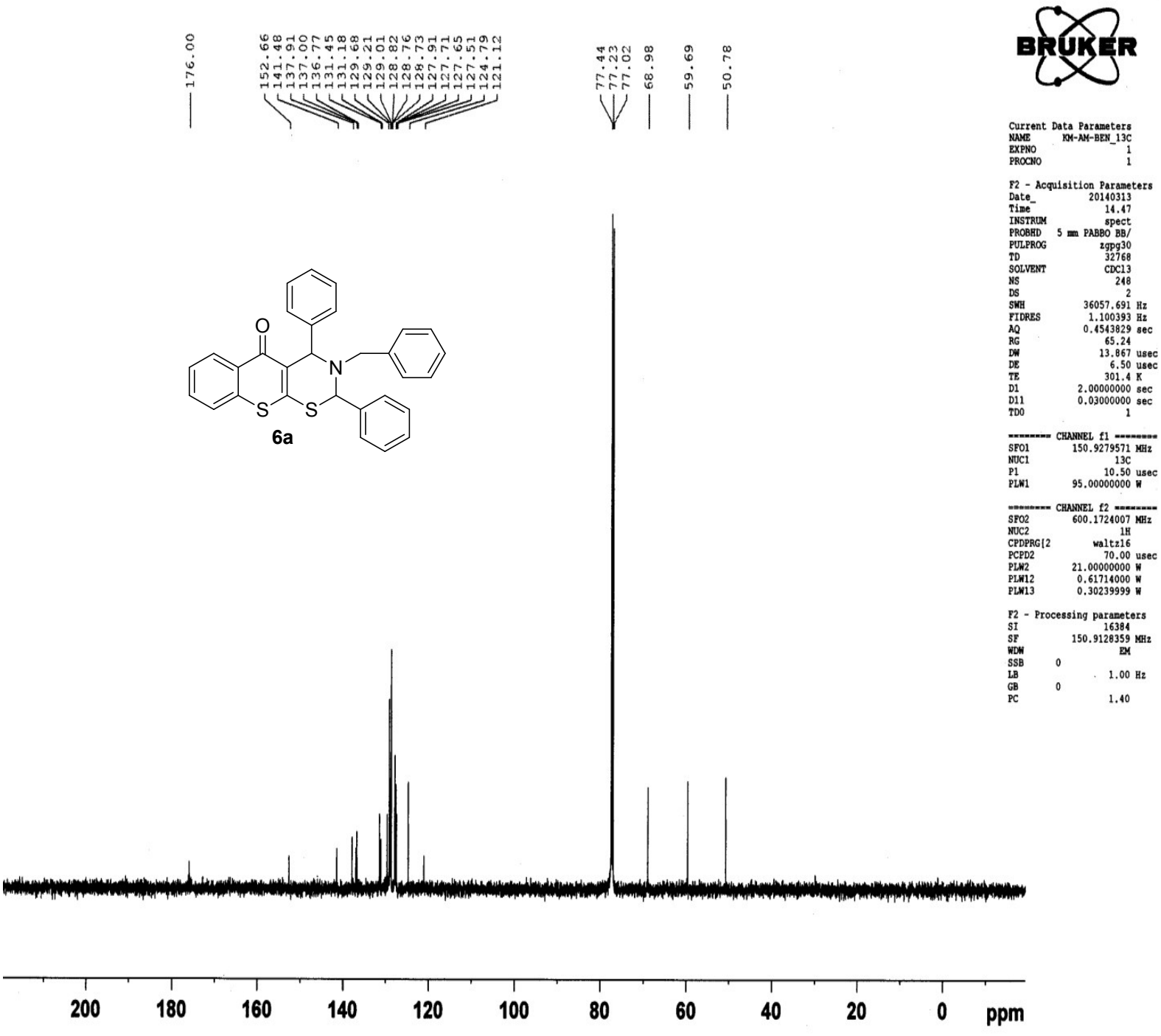
Current Data Parameters
NAME      KM_AM_BEN_ 1H
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20140314
Time              13.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDC13
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           1.00000000 sec
TD0                   1

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

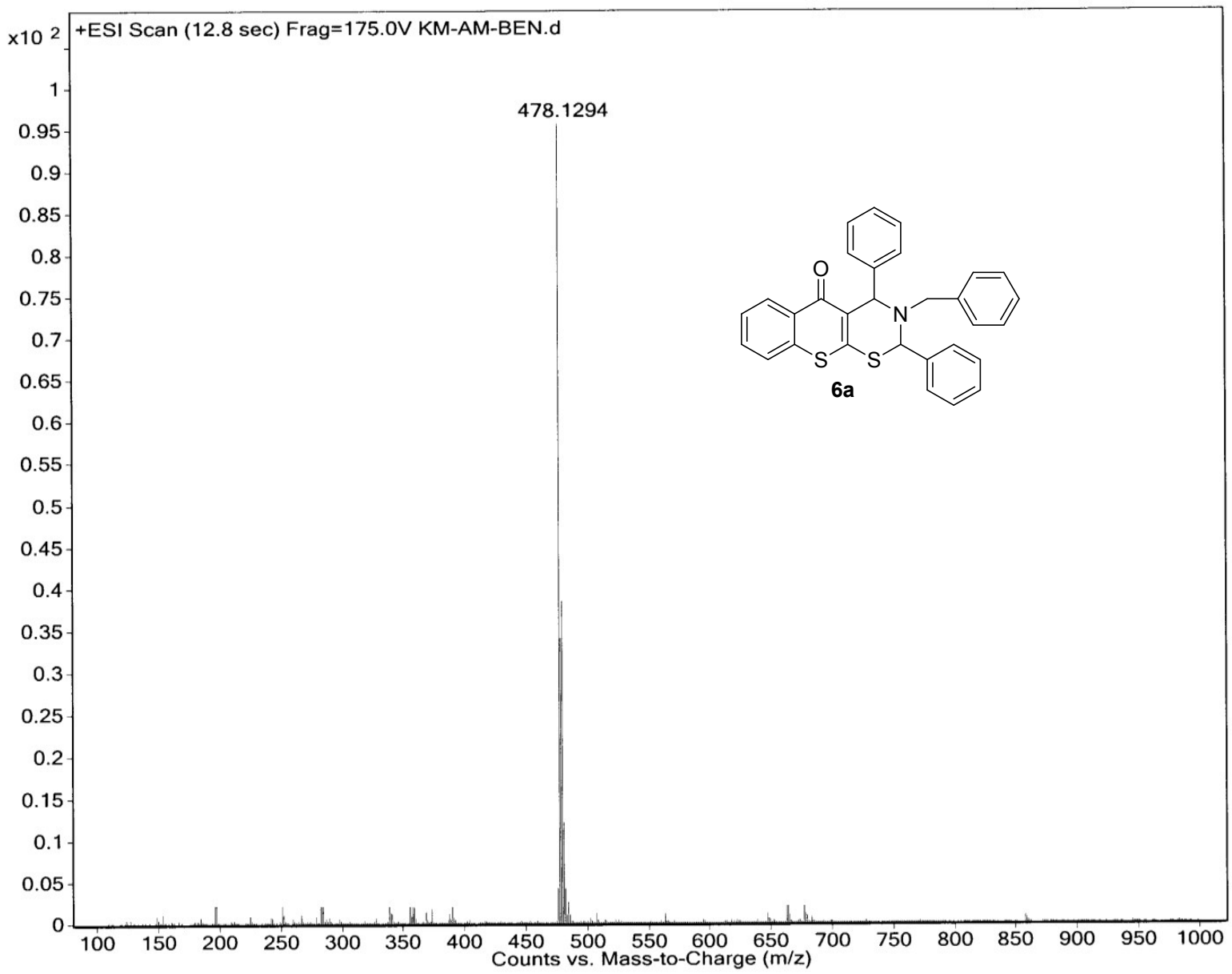
F2 - Processing parameters
SI                16384
SF           600.1700644 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}CNMR spectra of compound: 6a

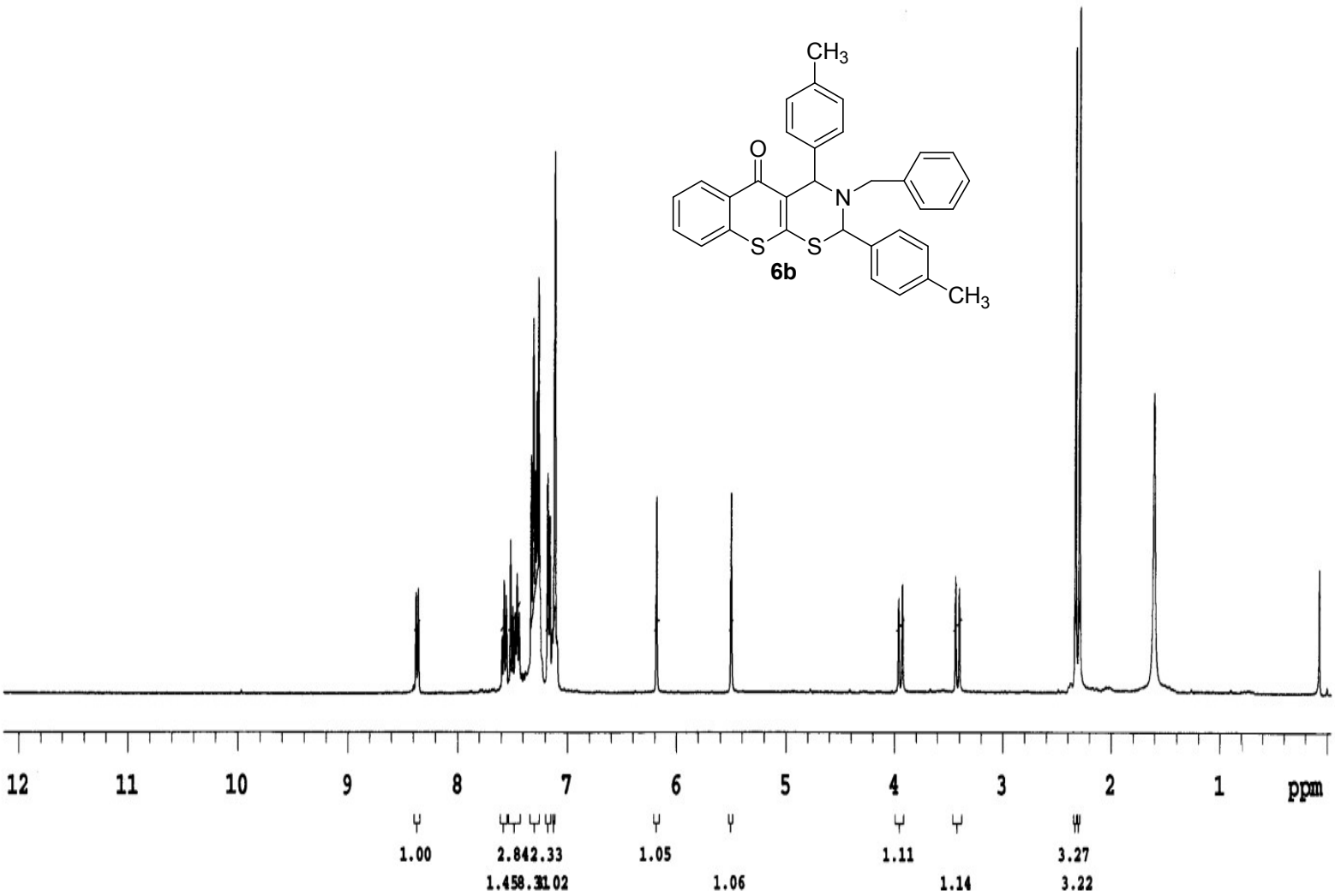


HRMS spectra of compound: 6a

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

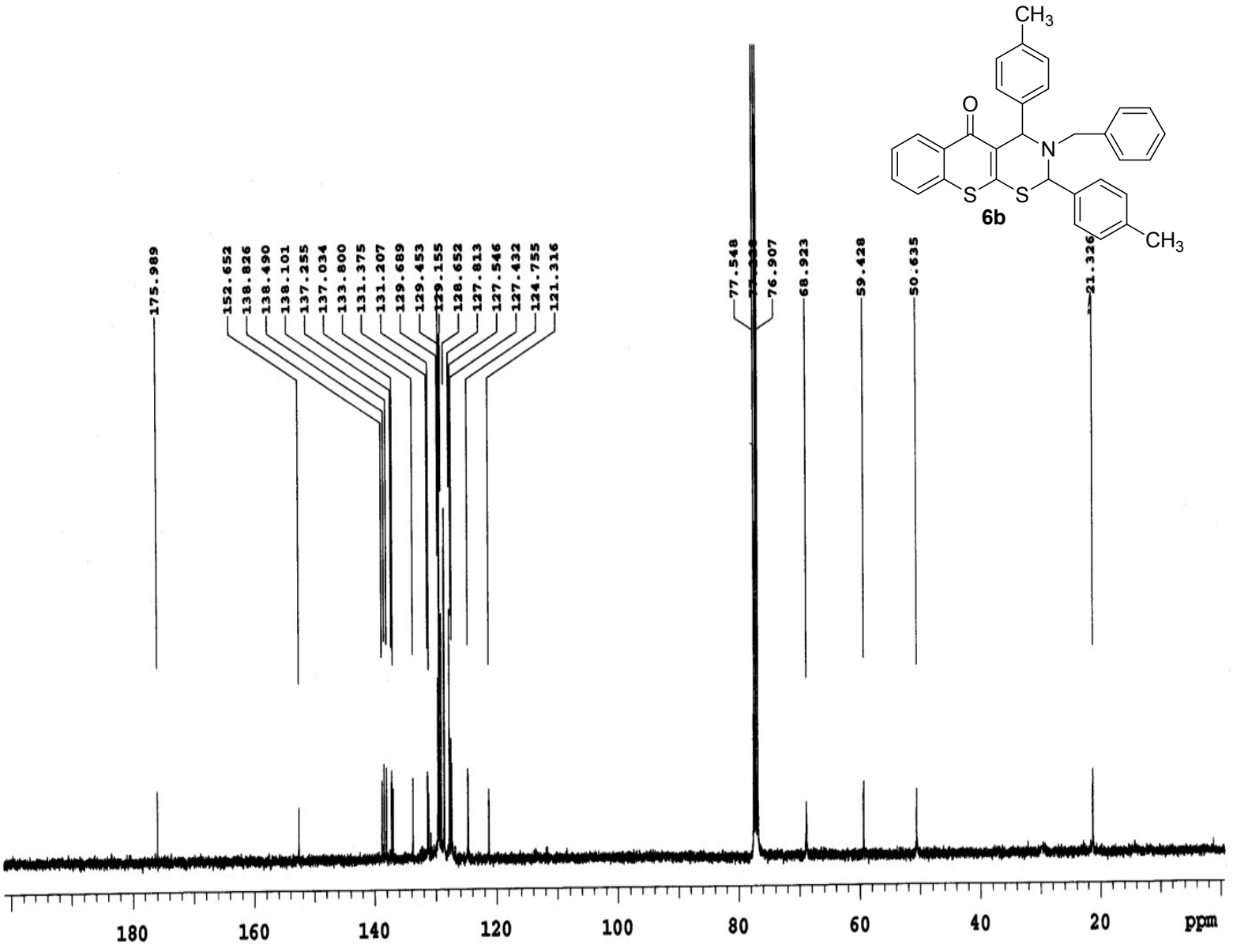


[1]HNMR spectra the compound: 6b



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

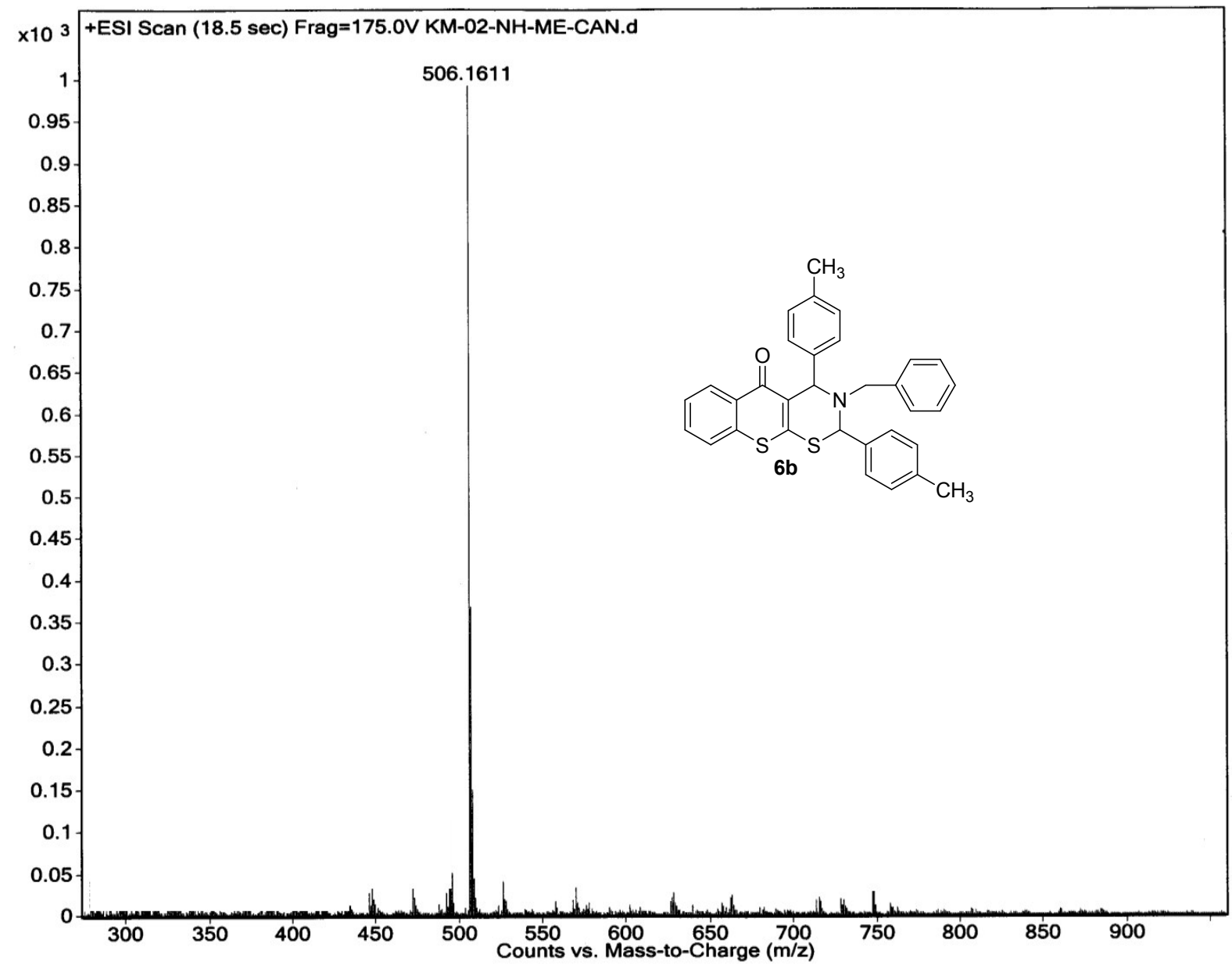
^{13}CNMR spectra of compound: 6b



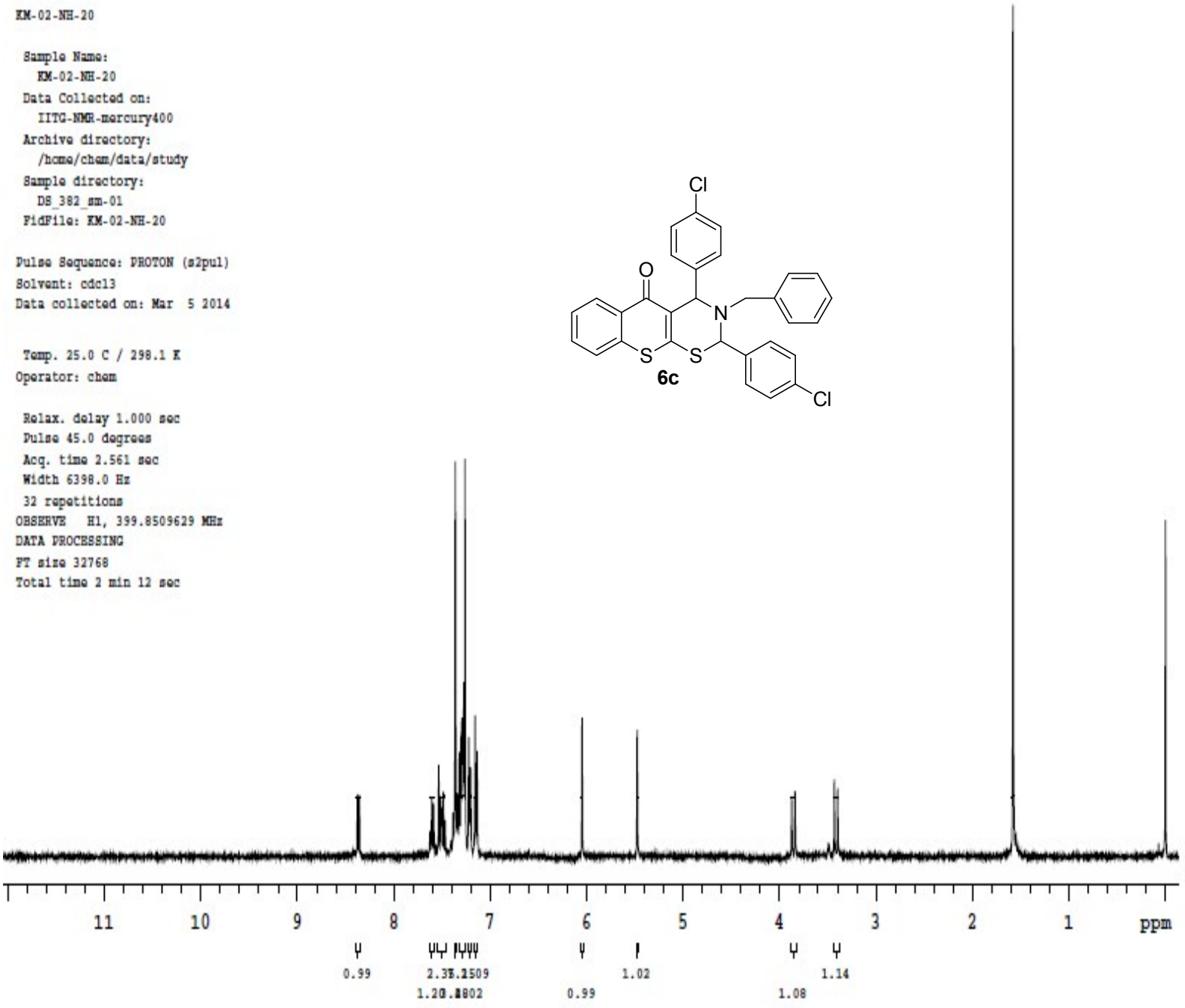
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 12530 repetitions	OBSERVE C13, 100.5425819 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 8.0 hours		KM-4Me-02-13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"

HRMS spectra of compound: 6b

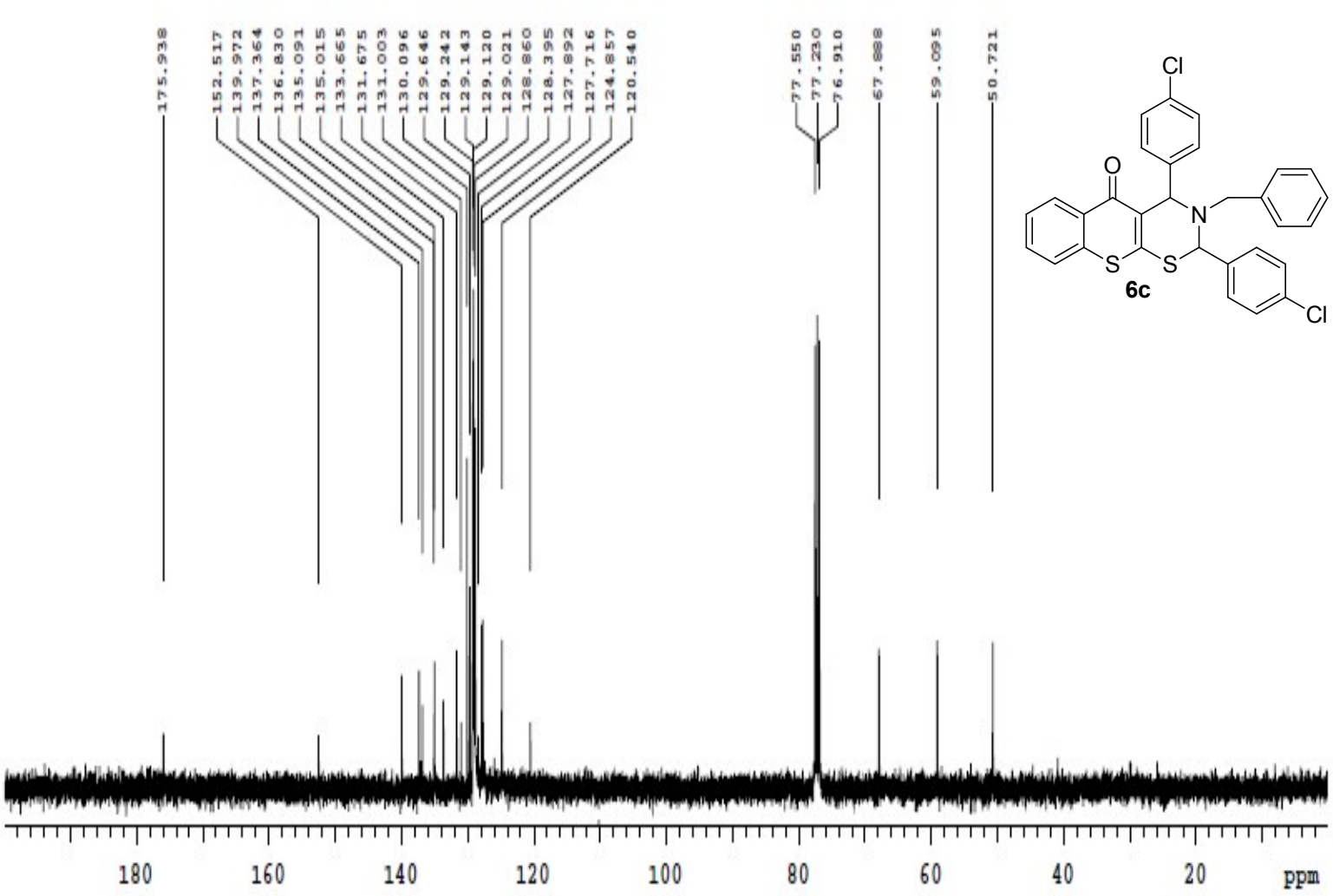
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 6c



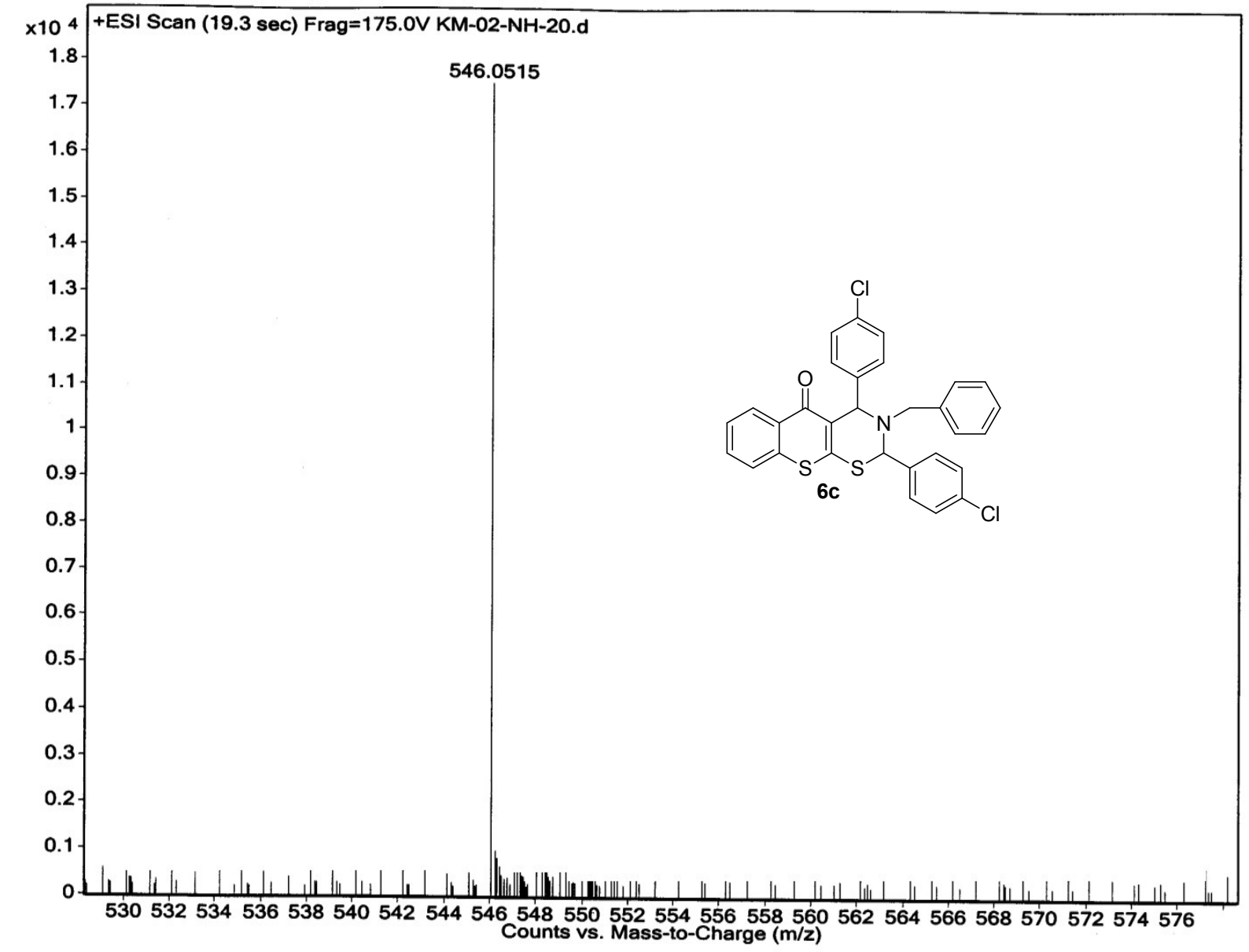
^{13}CNMR spectra of compound: 6c



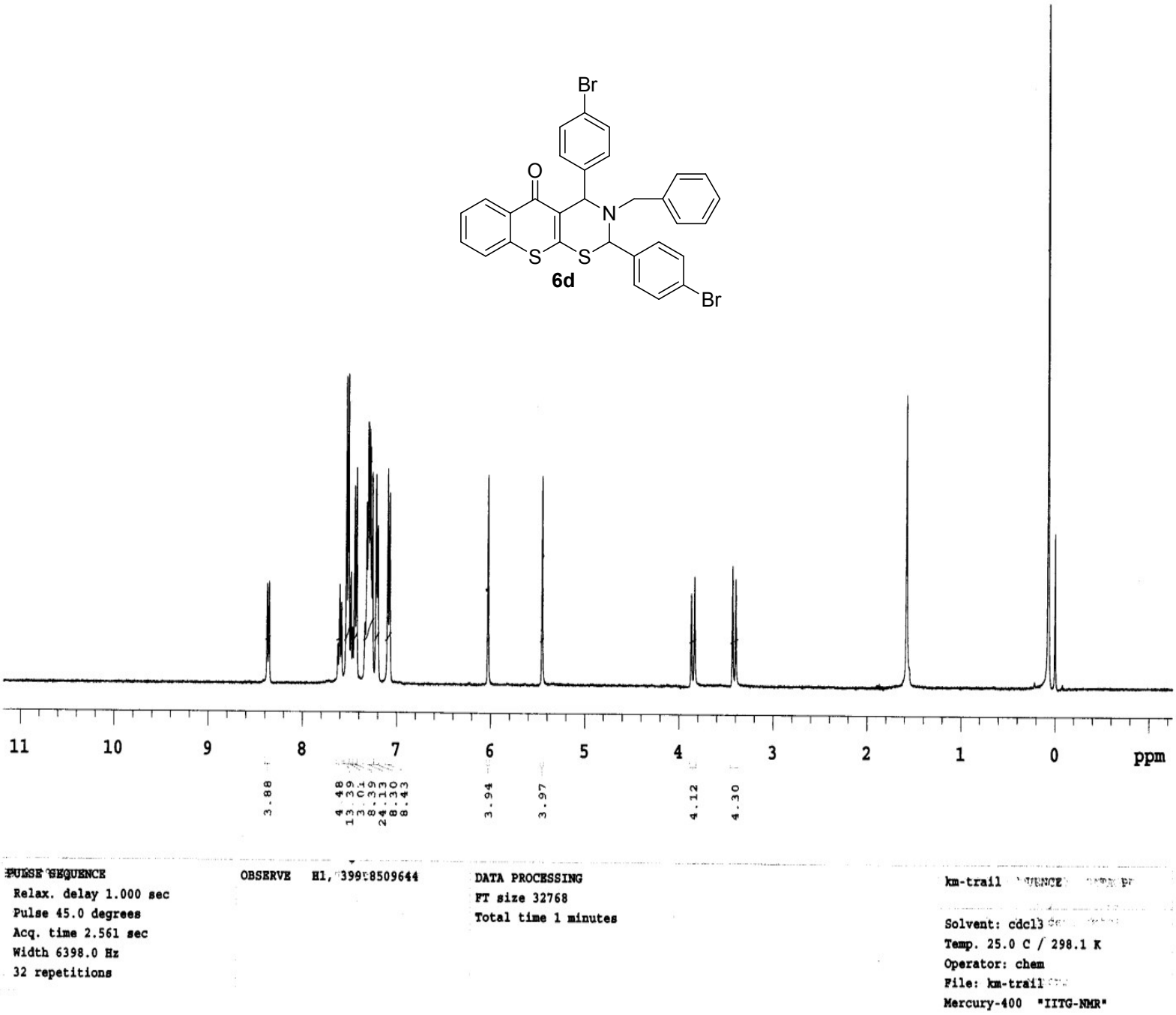
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 840 repetitions	OBSERVE C13, 100.5425840 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 32 minutes		KM-02-NH-20-13C Solvent: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

HRMS spectra of compound: 6c

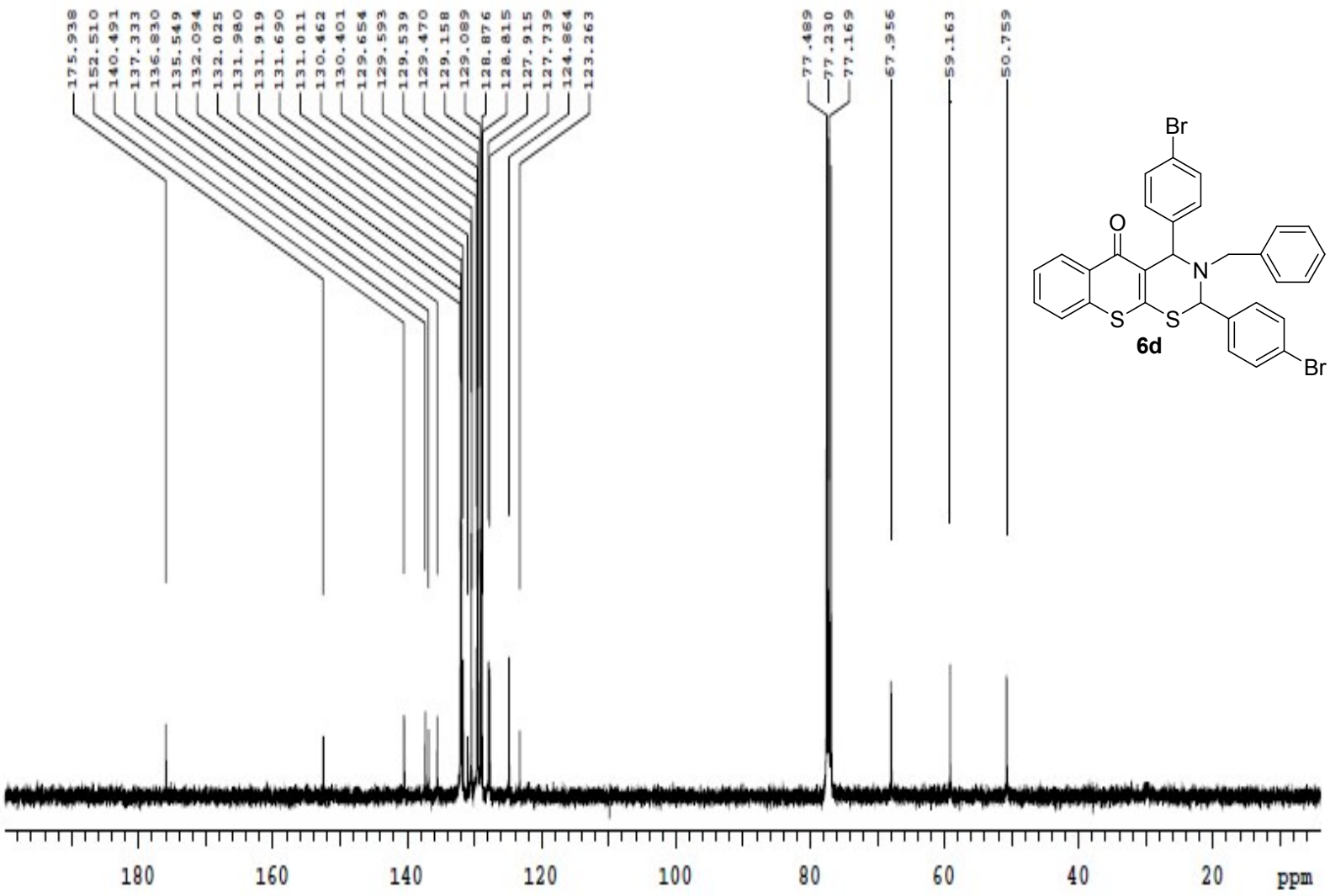
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



[1]HNMR spectra the compound: 6d



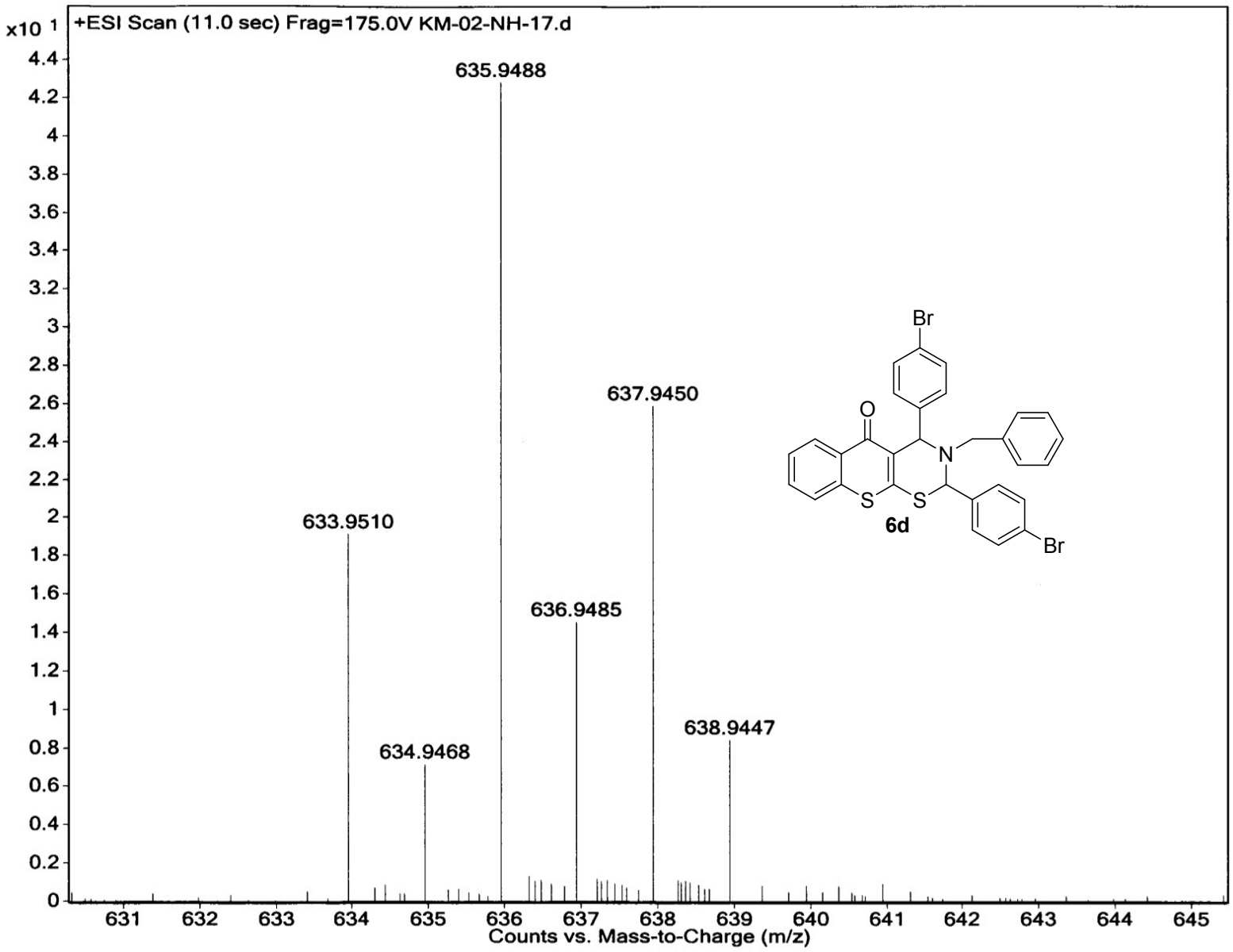
^{13}CNMR spectra of compound: 6d



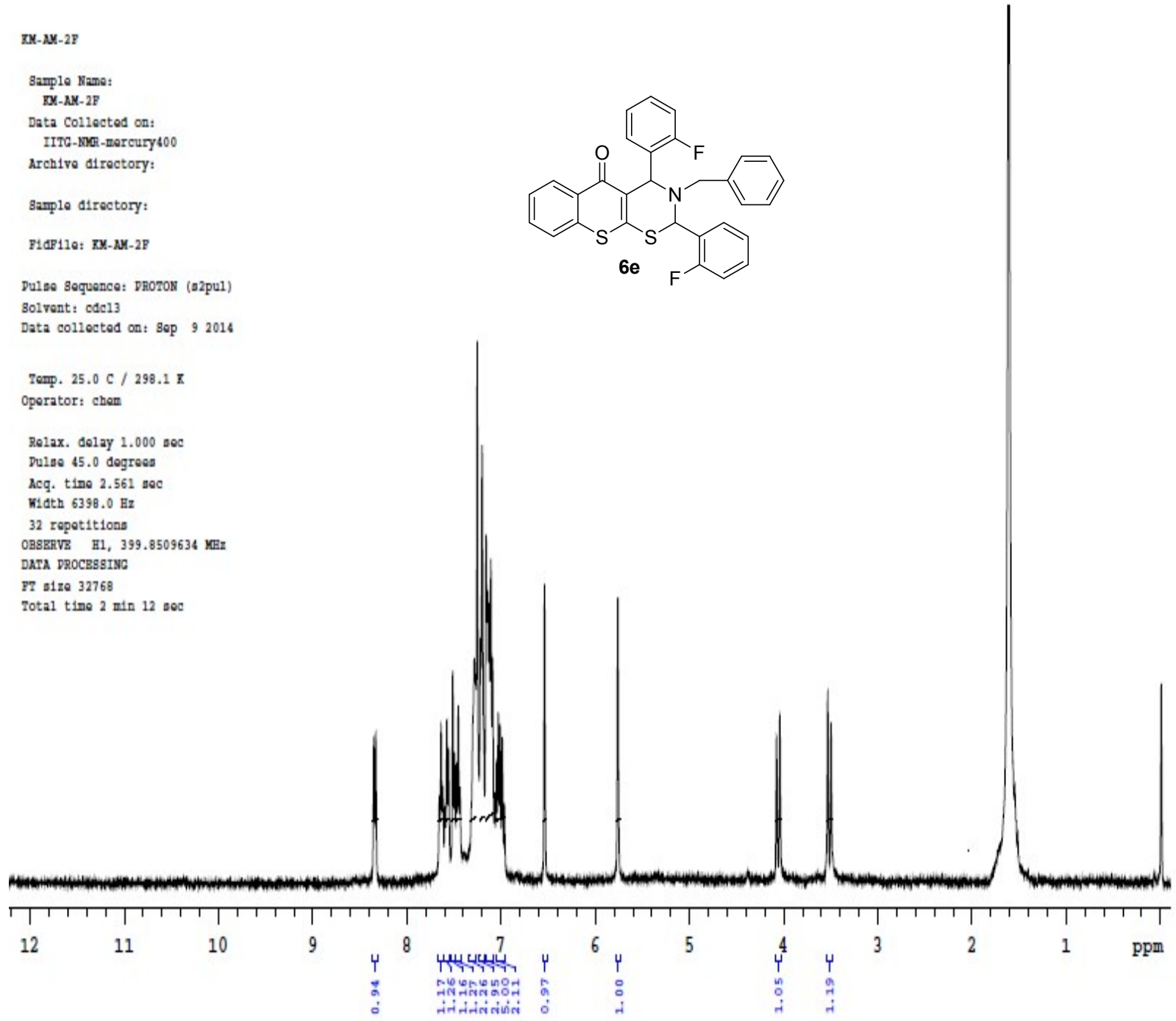
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 9050 repetitions	OBSERVE C13, 100.5426154 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 5.8 hours		KM-AM-1-13C Solvent: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

HRMS spectra of compound: 6d

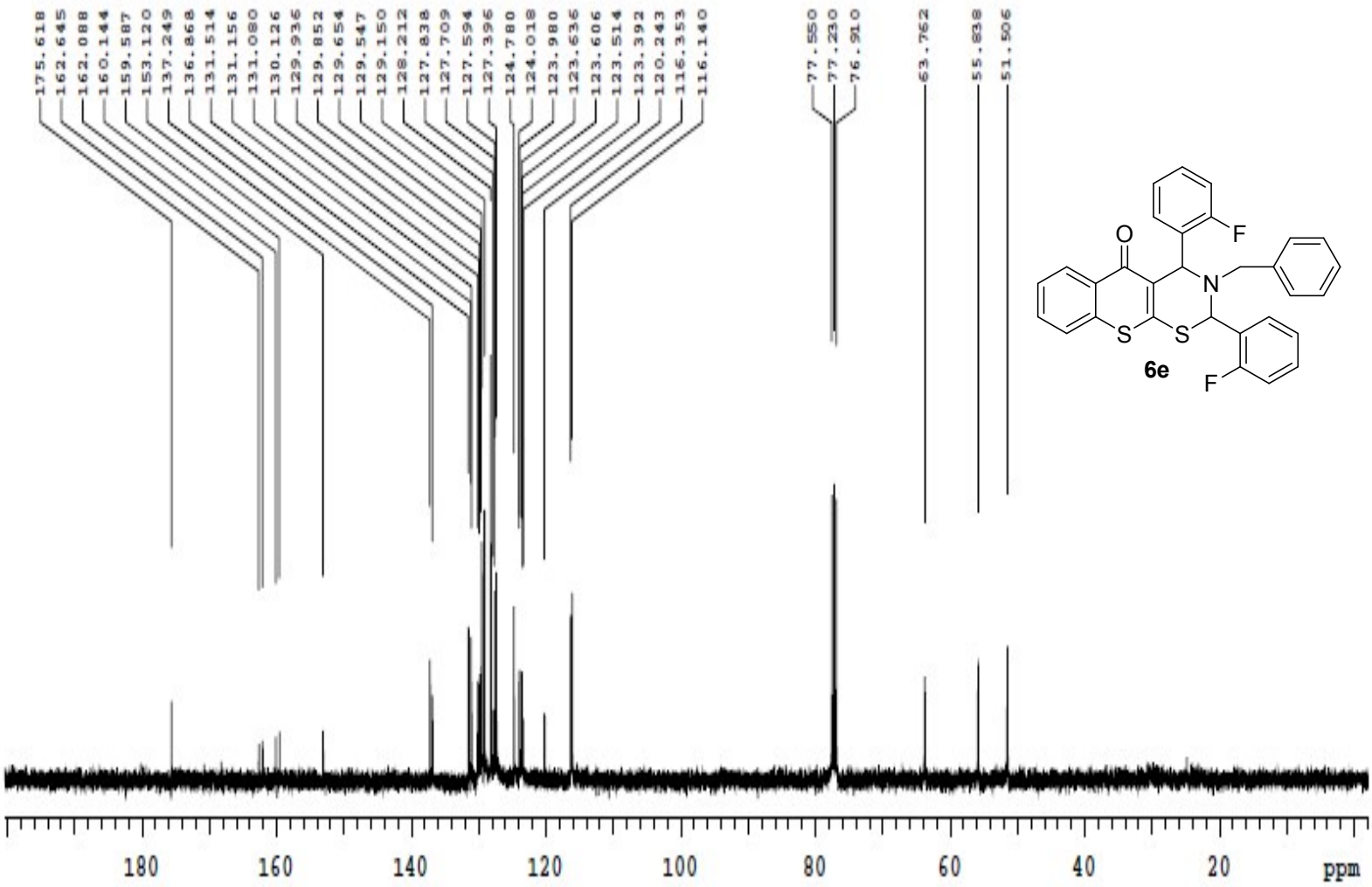
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 6e



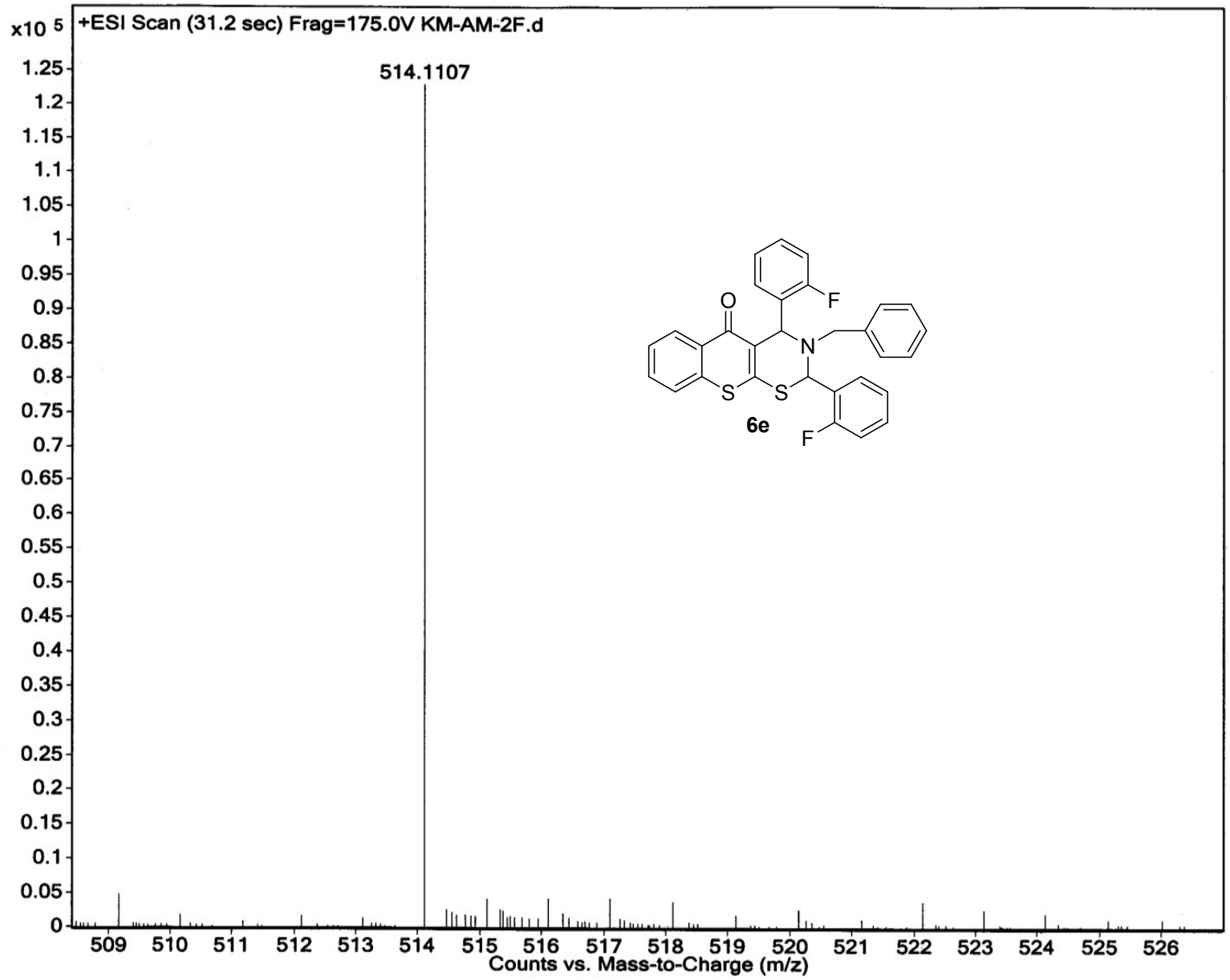
^{13}CNMR spectra of compound: 6e



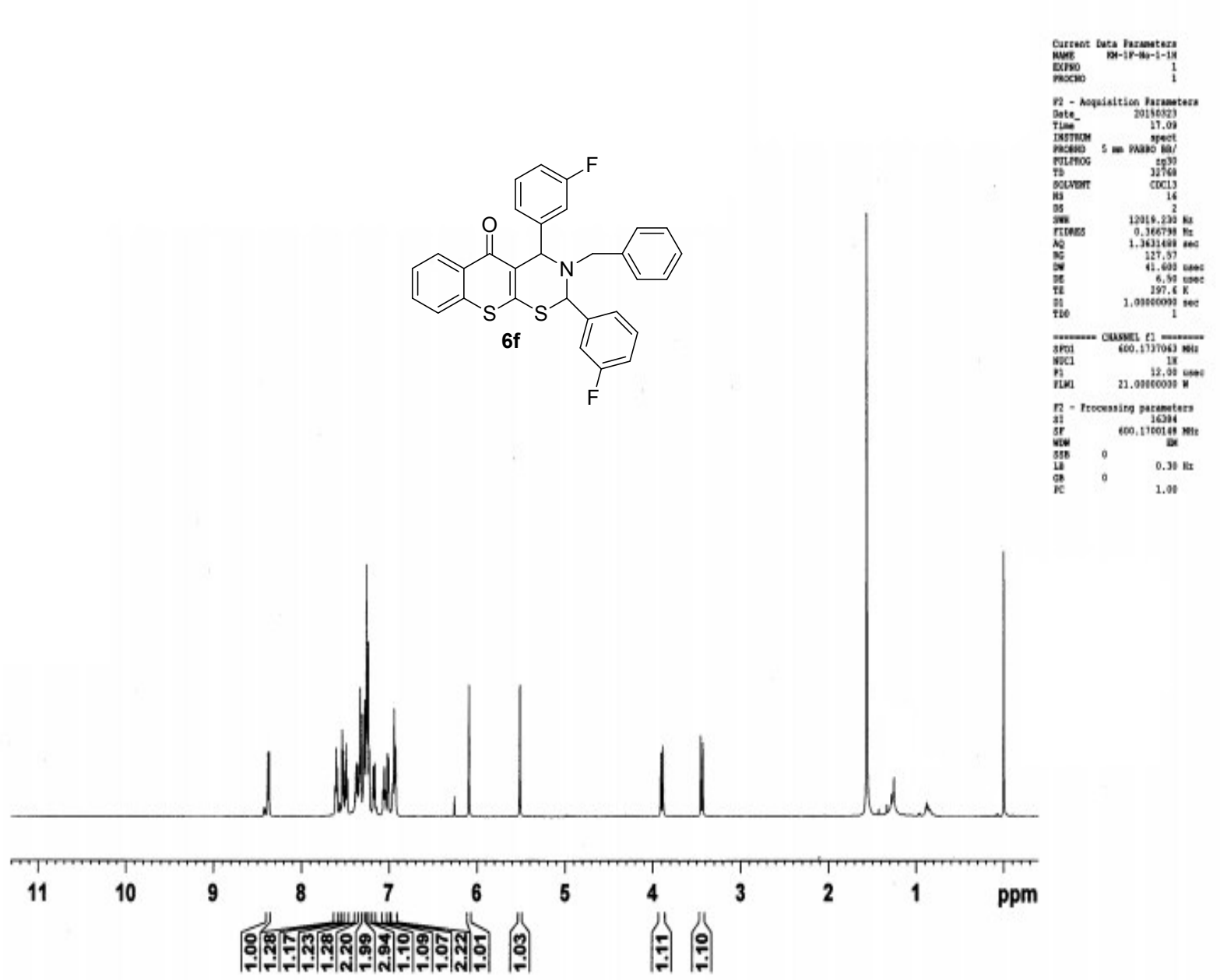
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 640 repetitions	OBSERVE C13, 100.5425863 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 24 minutes		KM-AM-2F-13C Solvent: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

HRMS spectra of compound: 6e

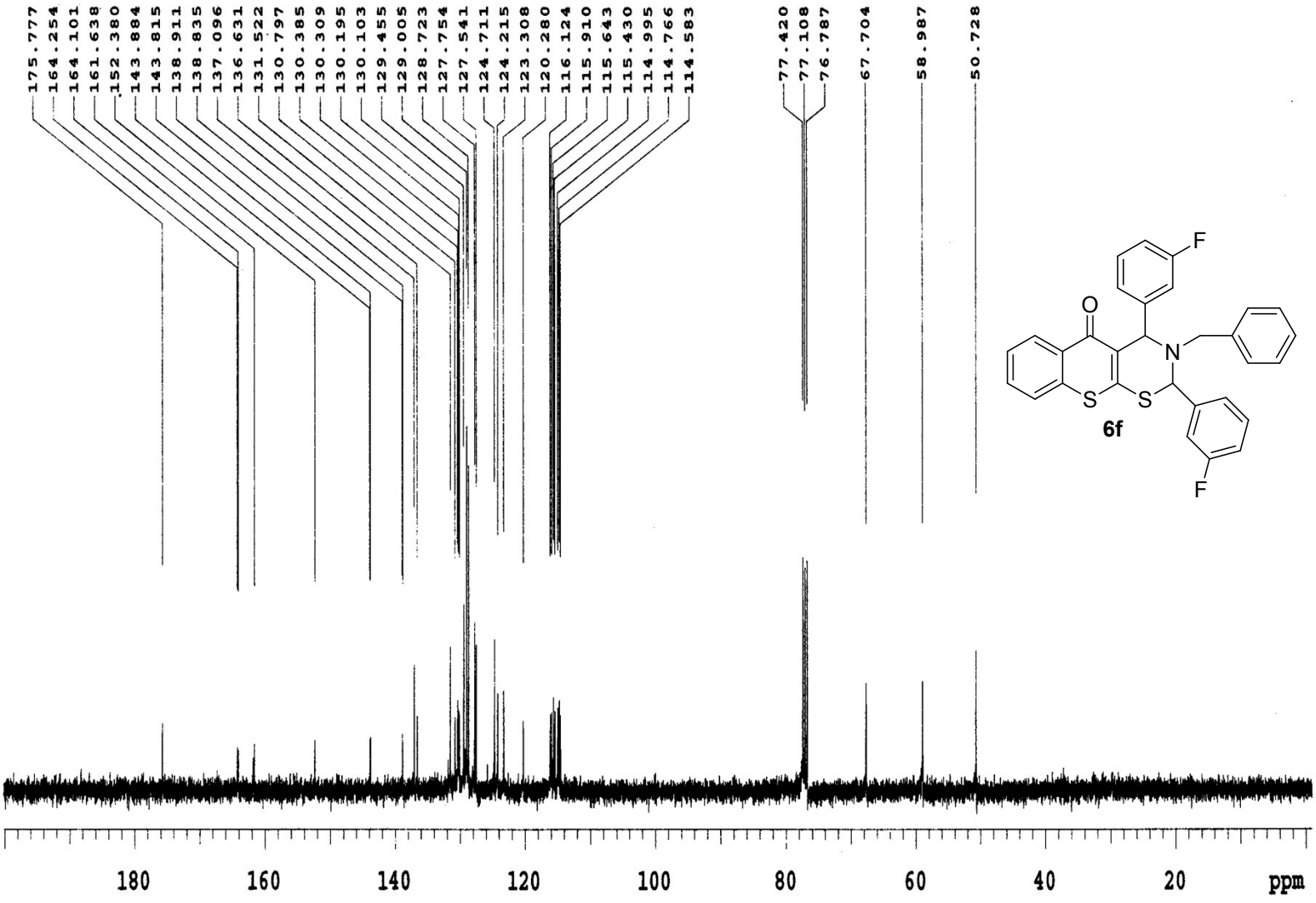
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 6f



^{13}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, 100.5426047
DECOUPLE H1, 399.8529994
Power 42 dB
continuously on
WALTZ-16 modulated

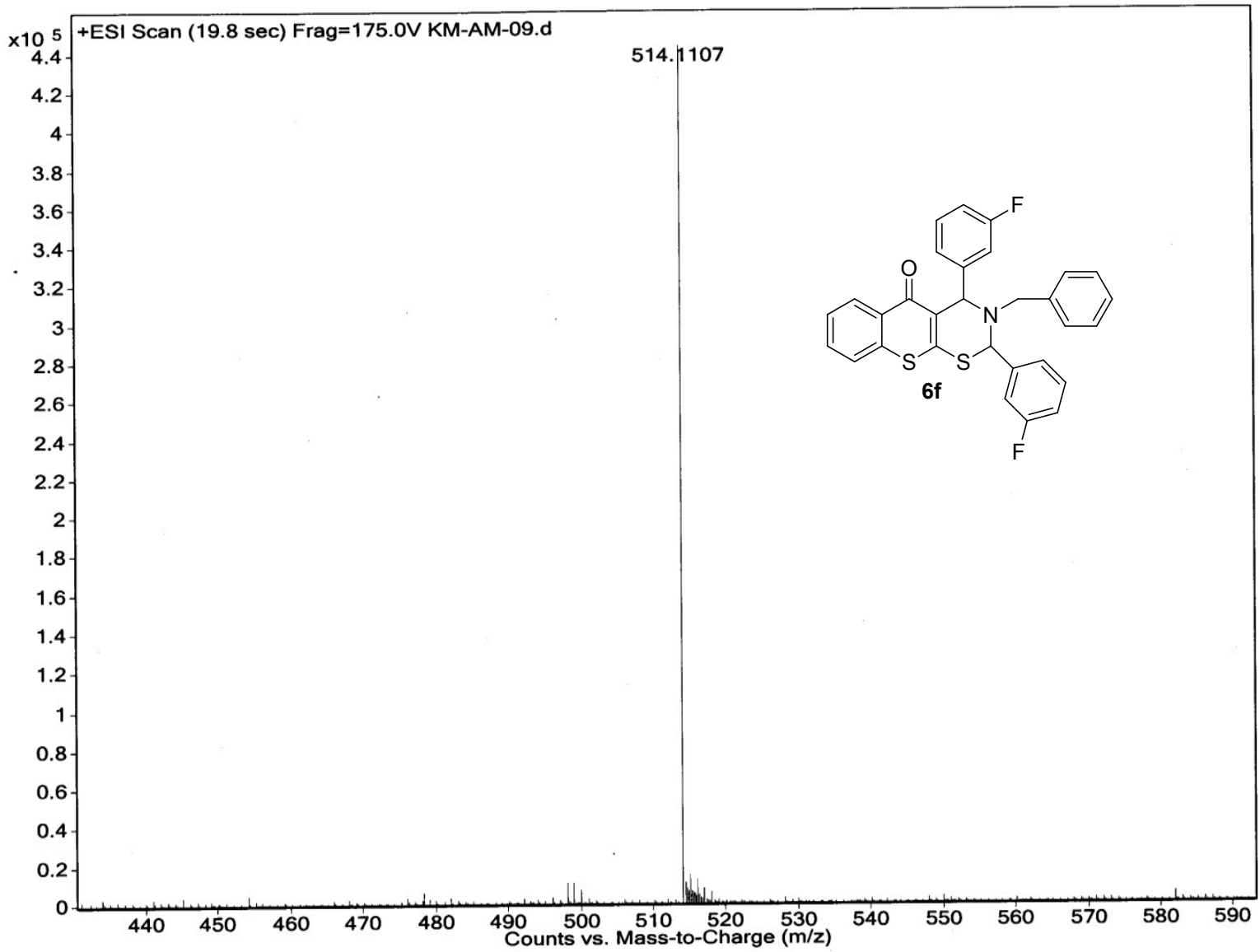
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 4 minutes

KM-AM-05-13C

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

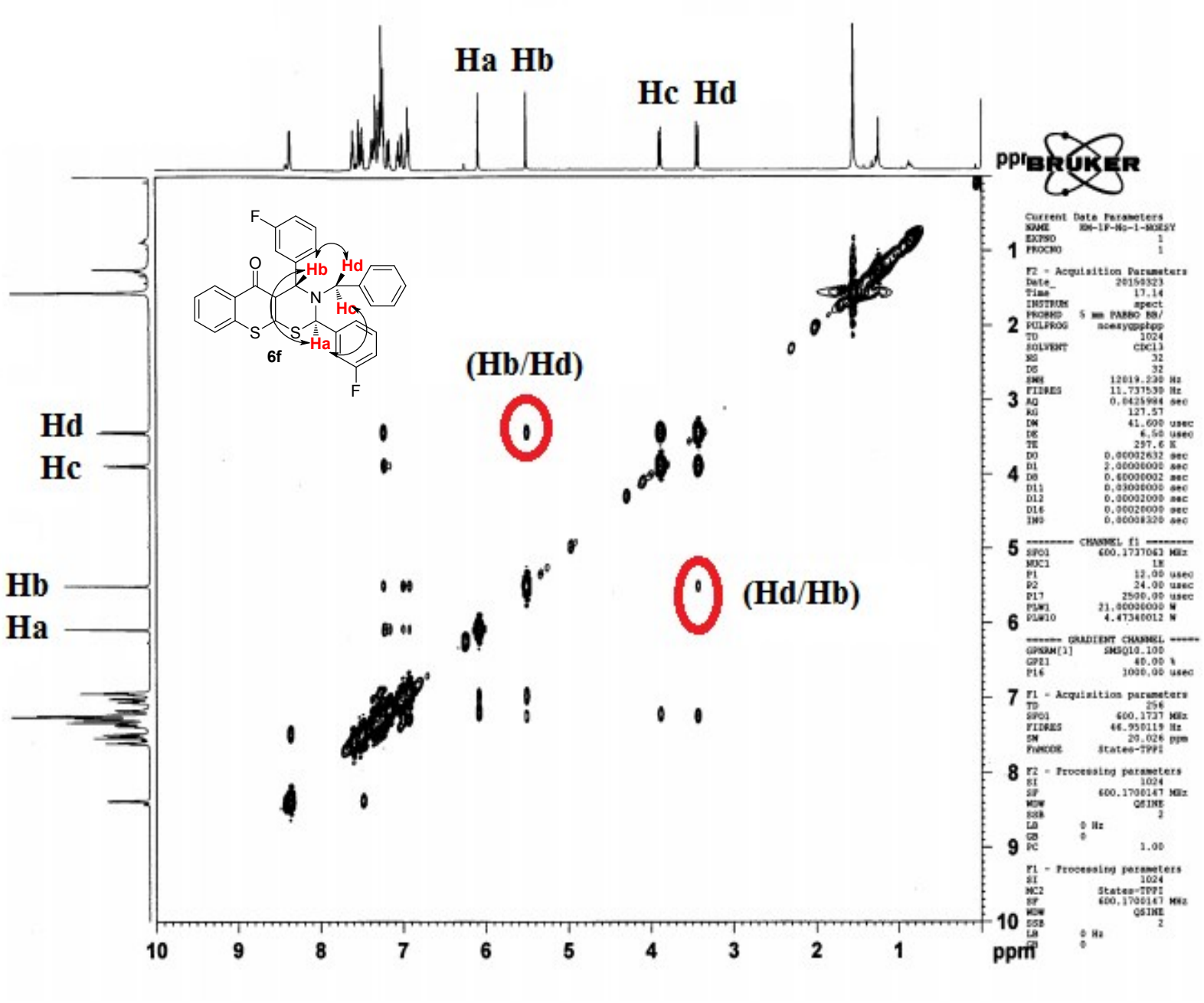
HRMS spectra of compound: 6f

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

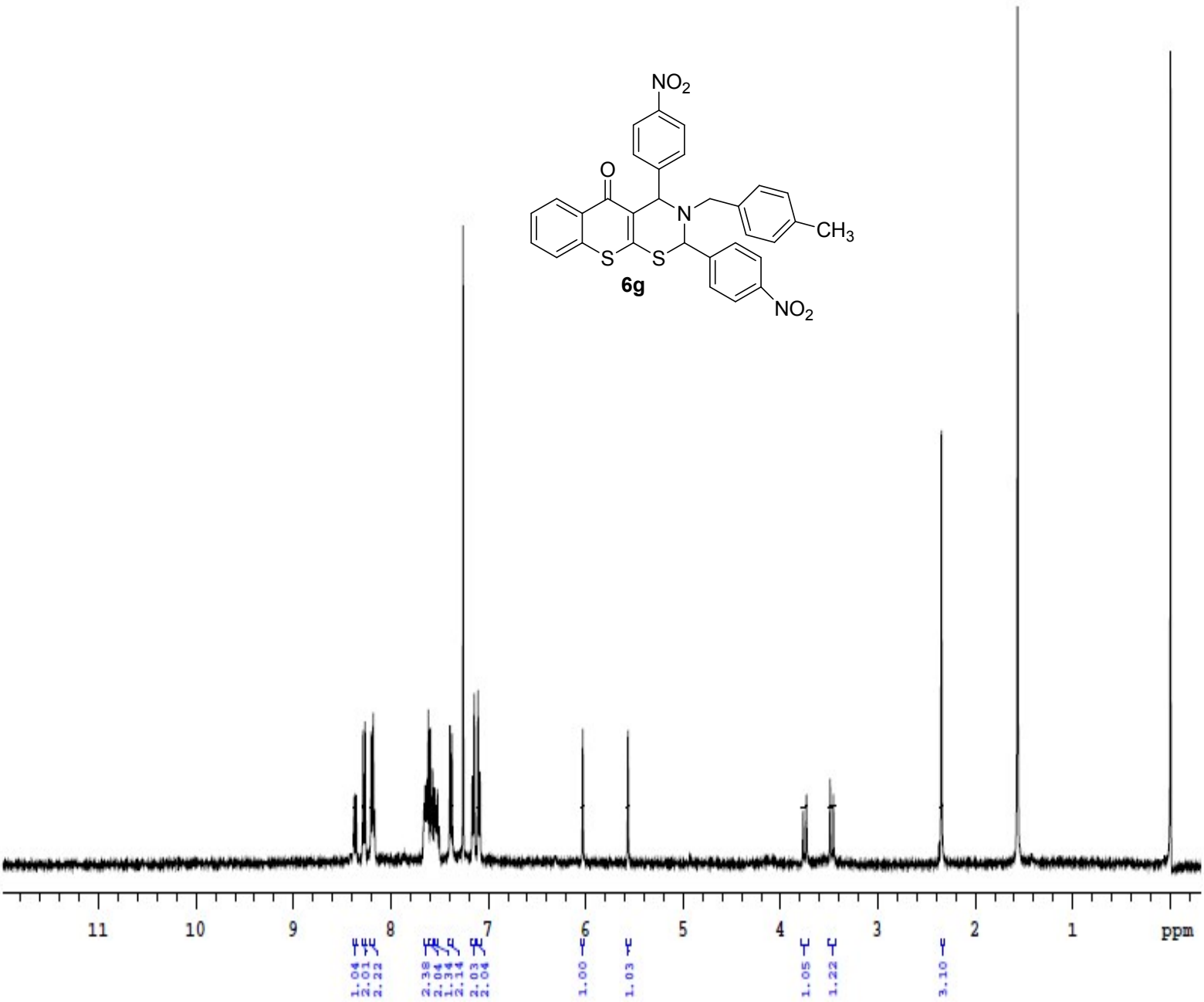


6f

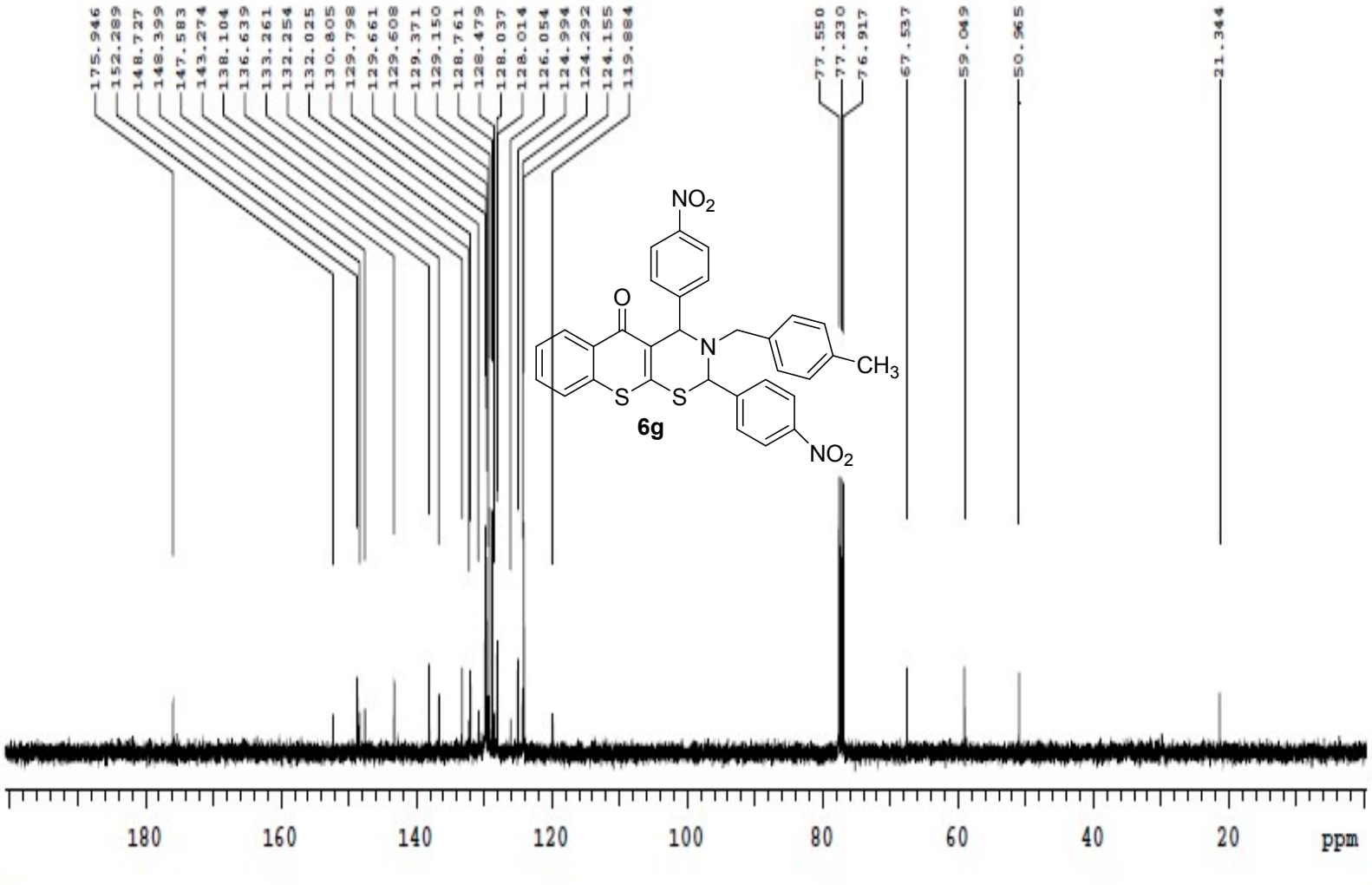
NOEs spectra of compound: 6f



[1]HNMR spectra the compound: 6g



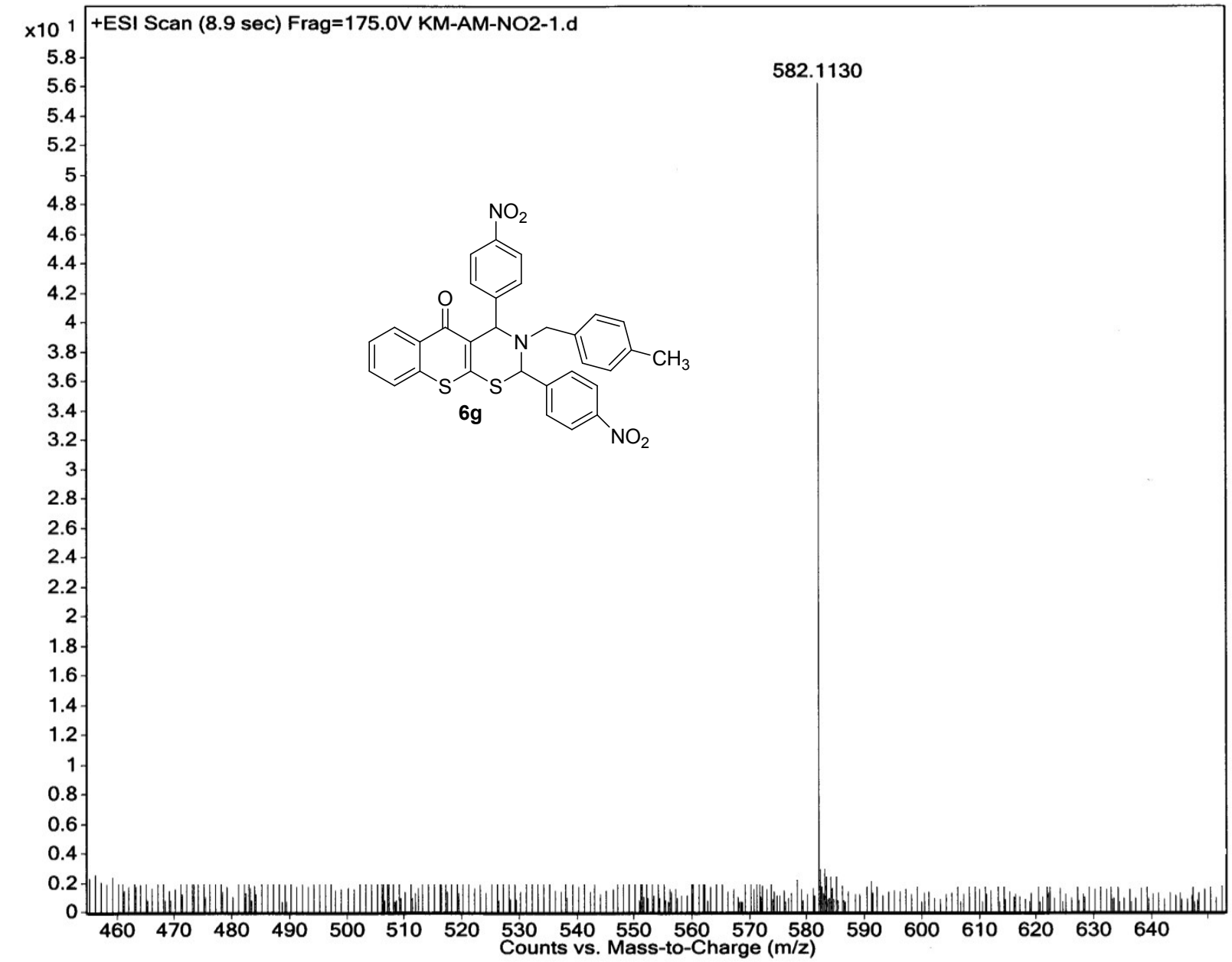
^{13}CNMR spectra of compound: 6g



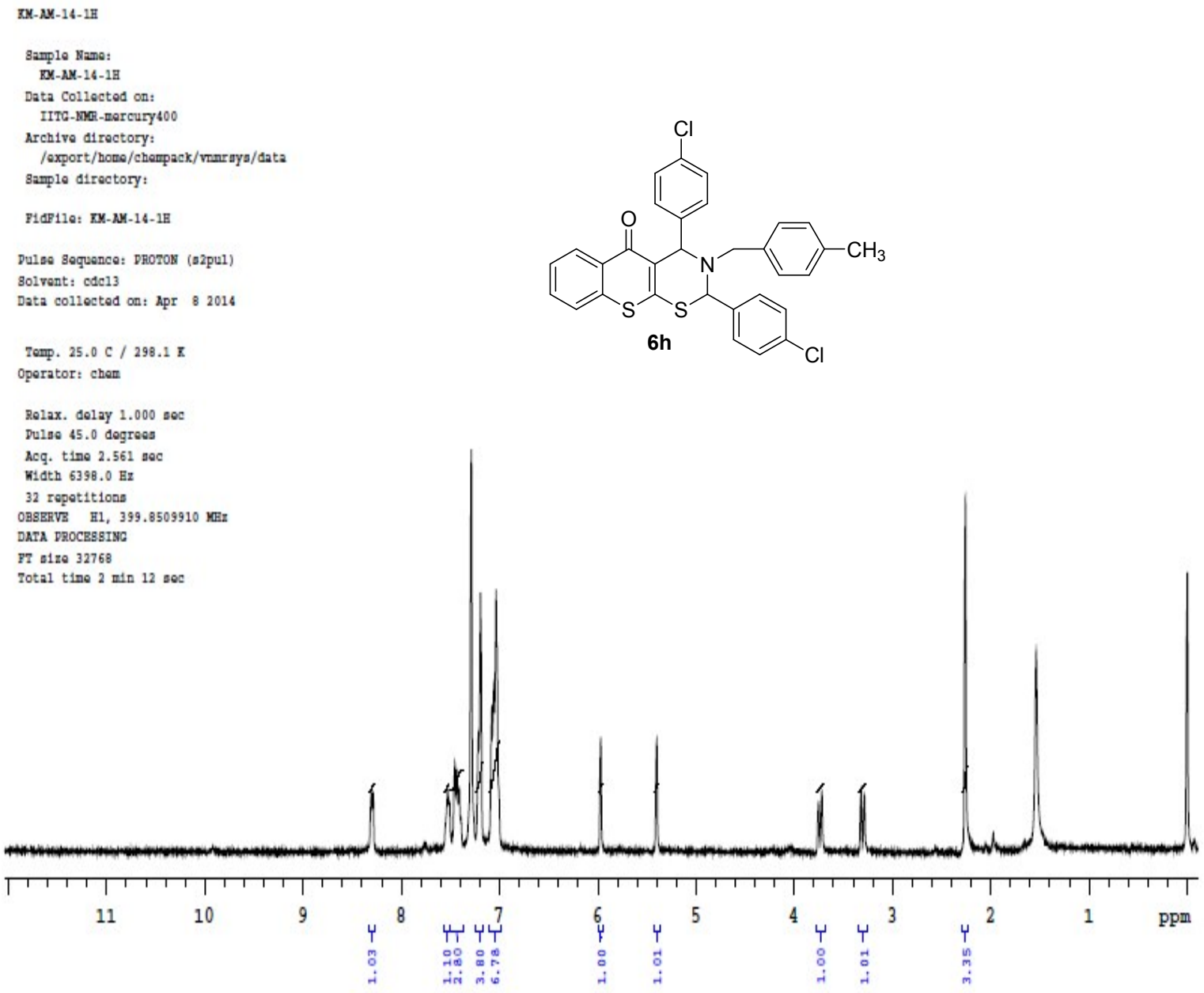
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 300 repetitions	OBSERVE C13, 100.5425855 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 11 minutes		KM-AM-NO2-13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: KM-AM-NO2-13C Mercury-400 "IITG-NMR"

HRMS spectra of compound: 6g

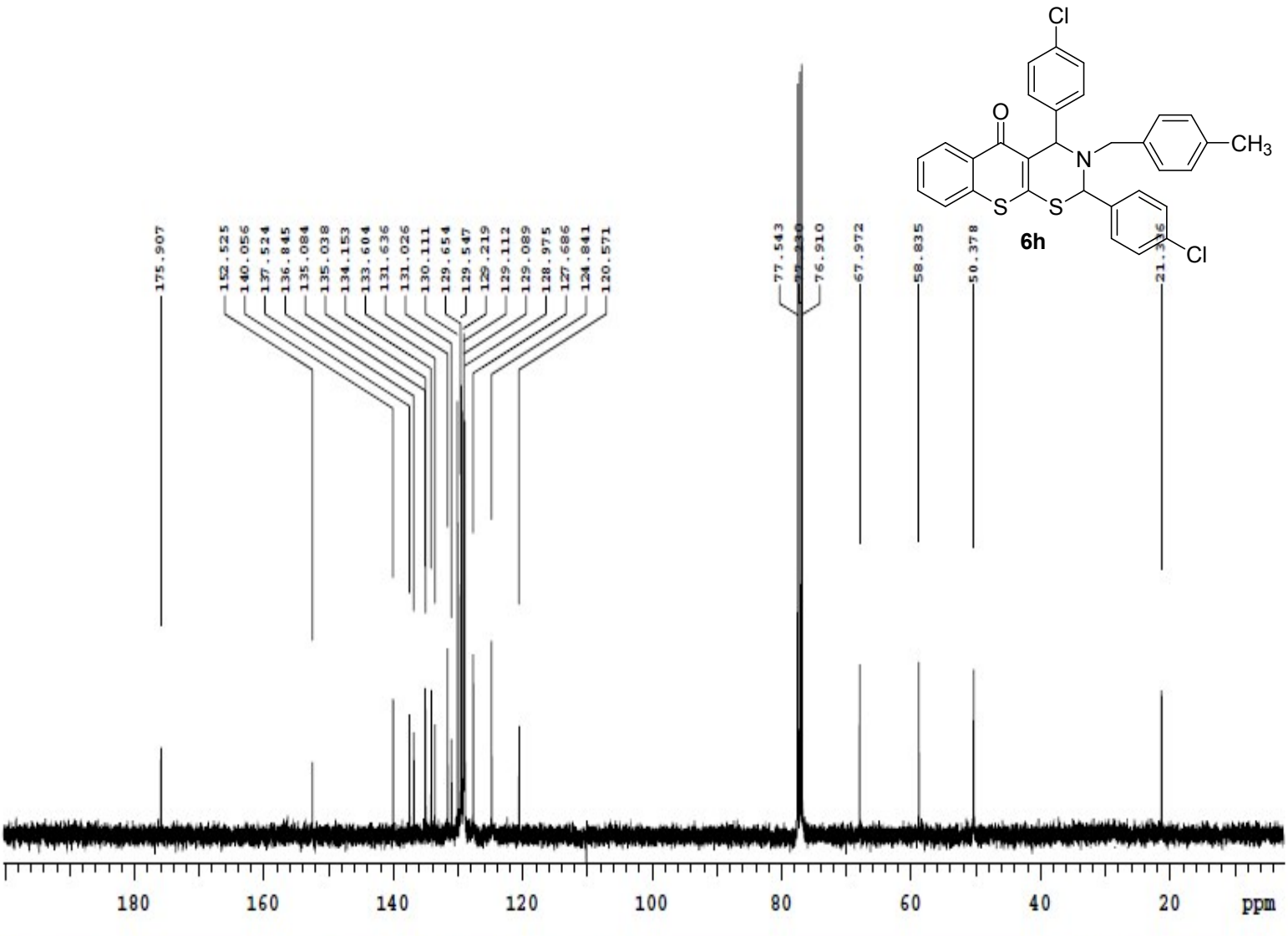
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 6h



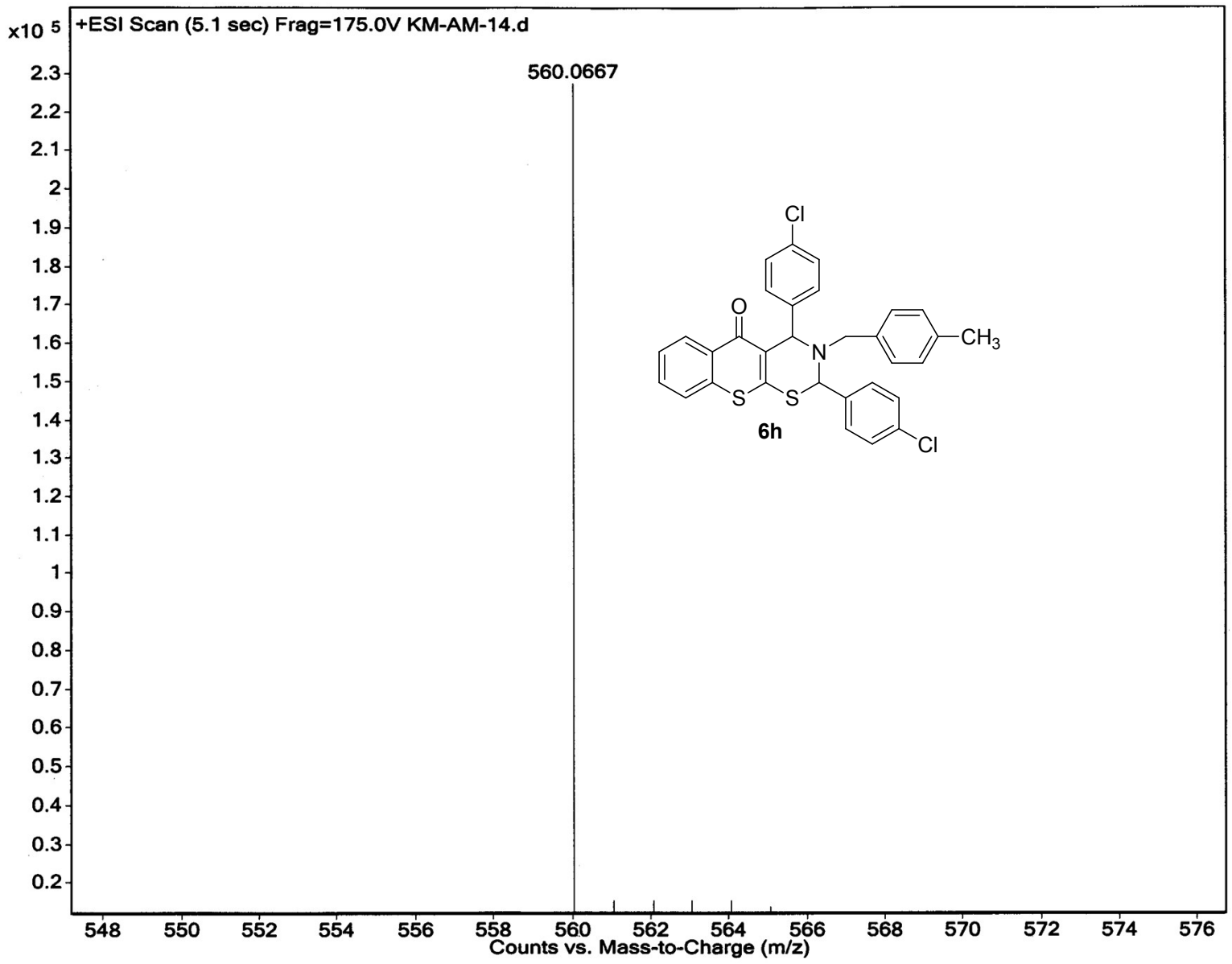
^{13}CNMR spectra of compound: 6h



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

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**



^{1}HNMR spectra the compound: 6i

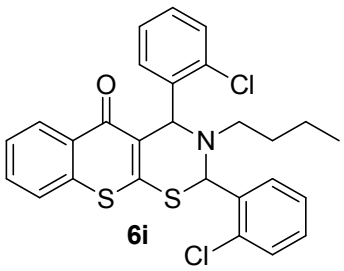
km-bam-h

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

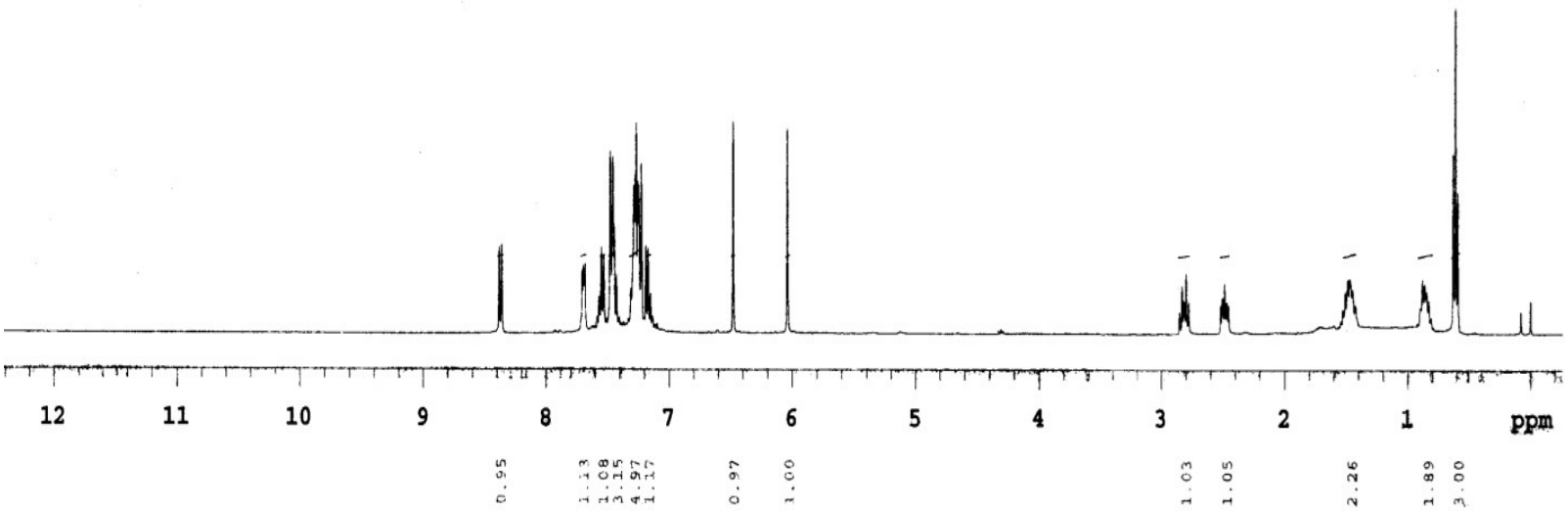
Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Apr 12 2014

Temp. 25.0 C / 298.1 K
Operator: chem

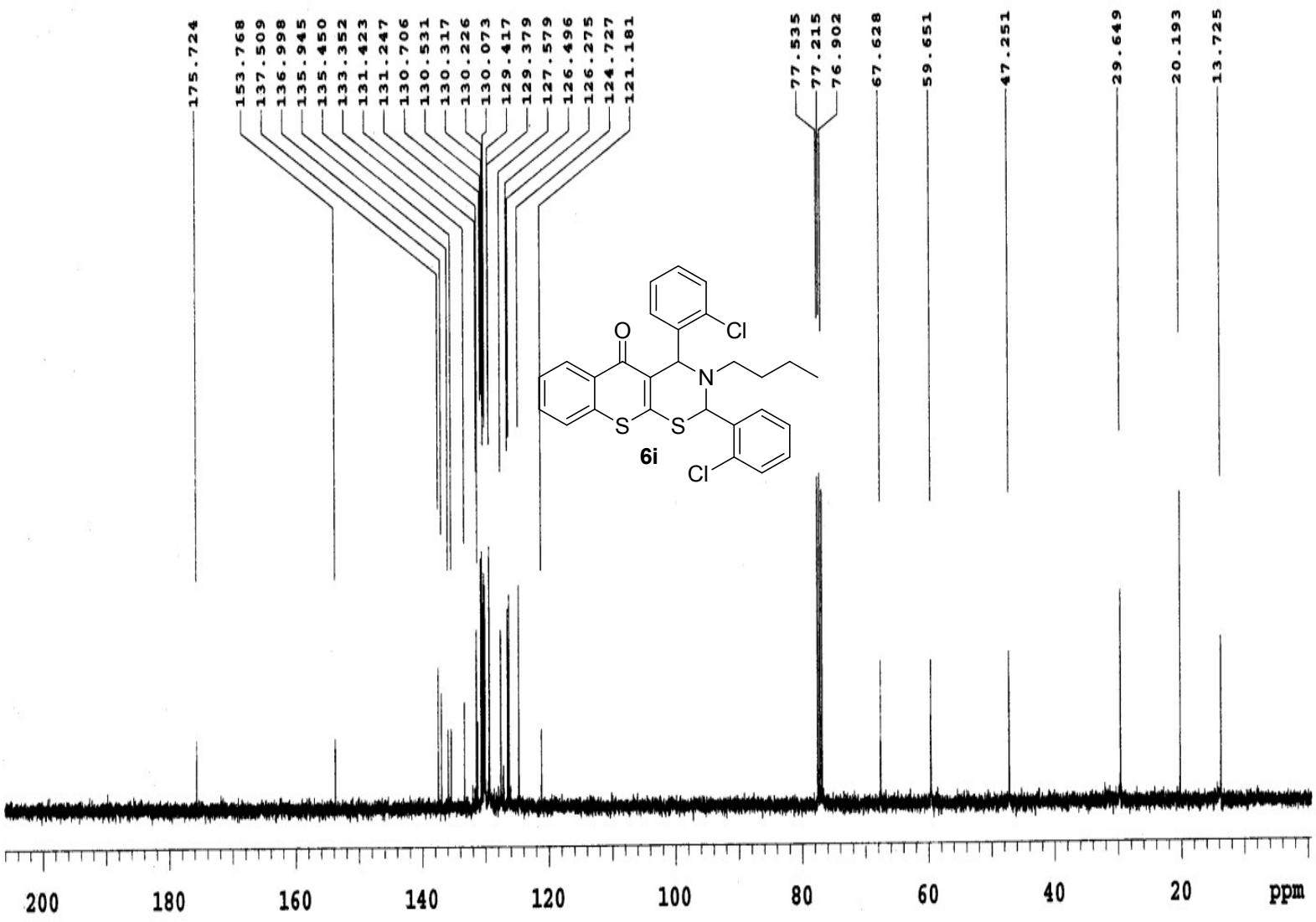
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
32 repetitions
OBSERVE H1, 399.8509652 MHz
DATA PROCESSING
FT size 32768
Total time 2 min 12 sec



6i



^{13}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

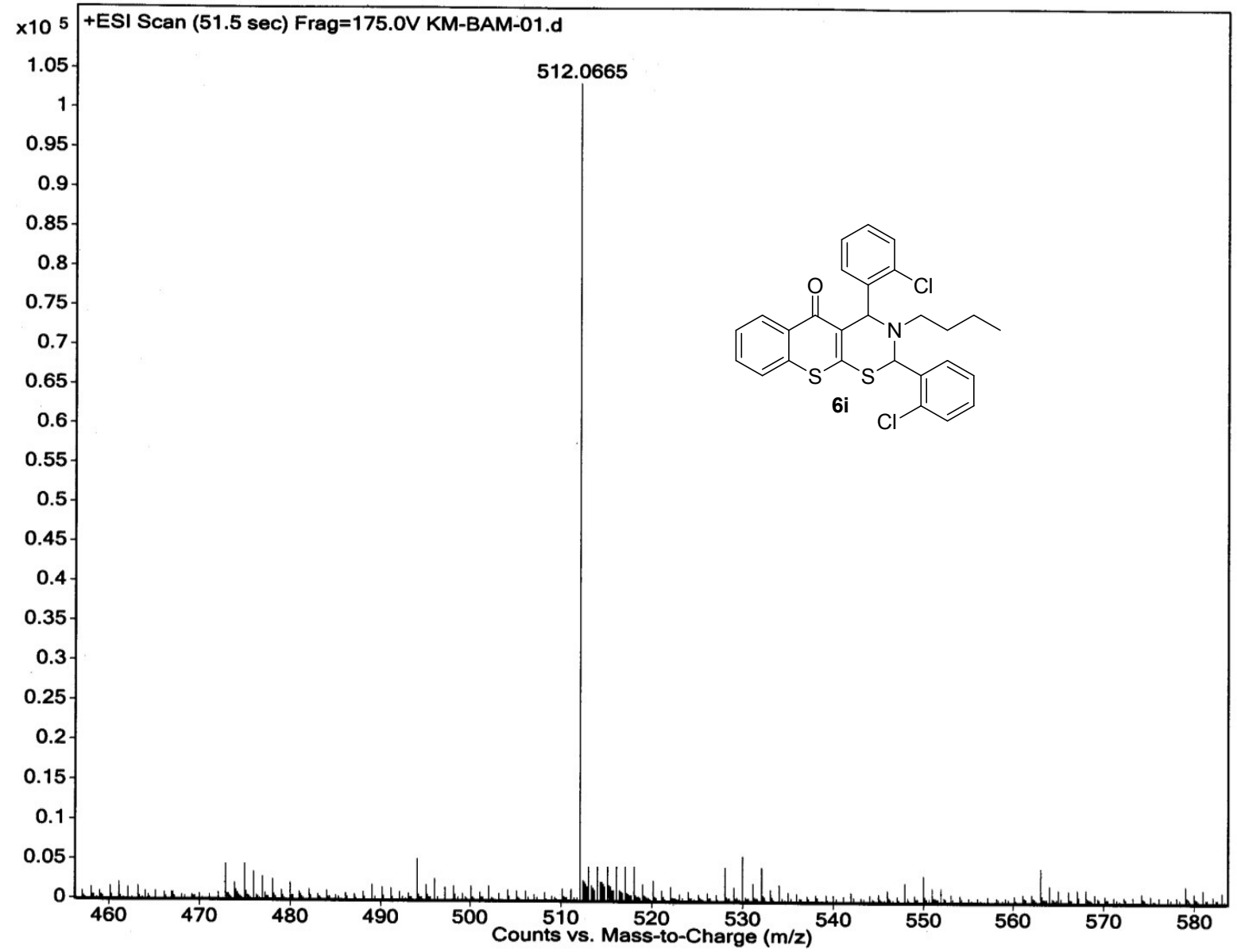
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 19 minutes

Km-BAM-1-13C

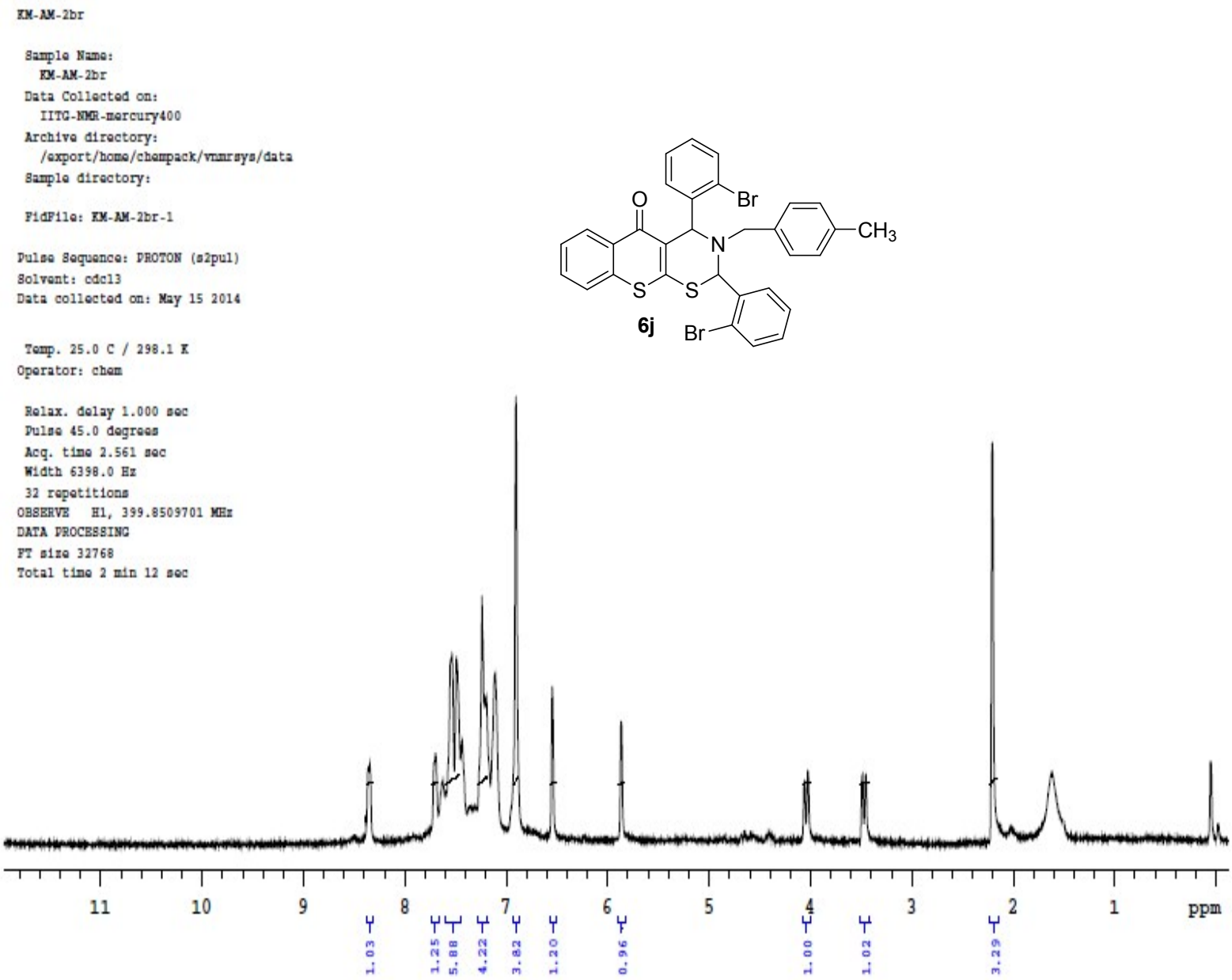
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem
Mercury-400 "IITG-NMR"

HRMS spectra of compound: 6i

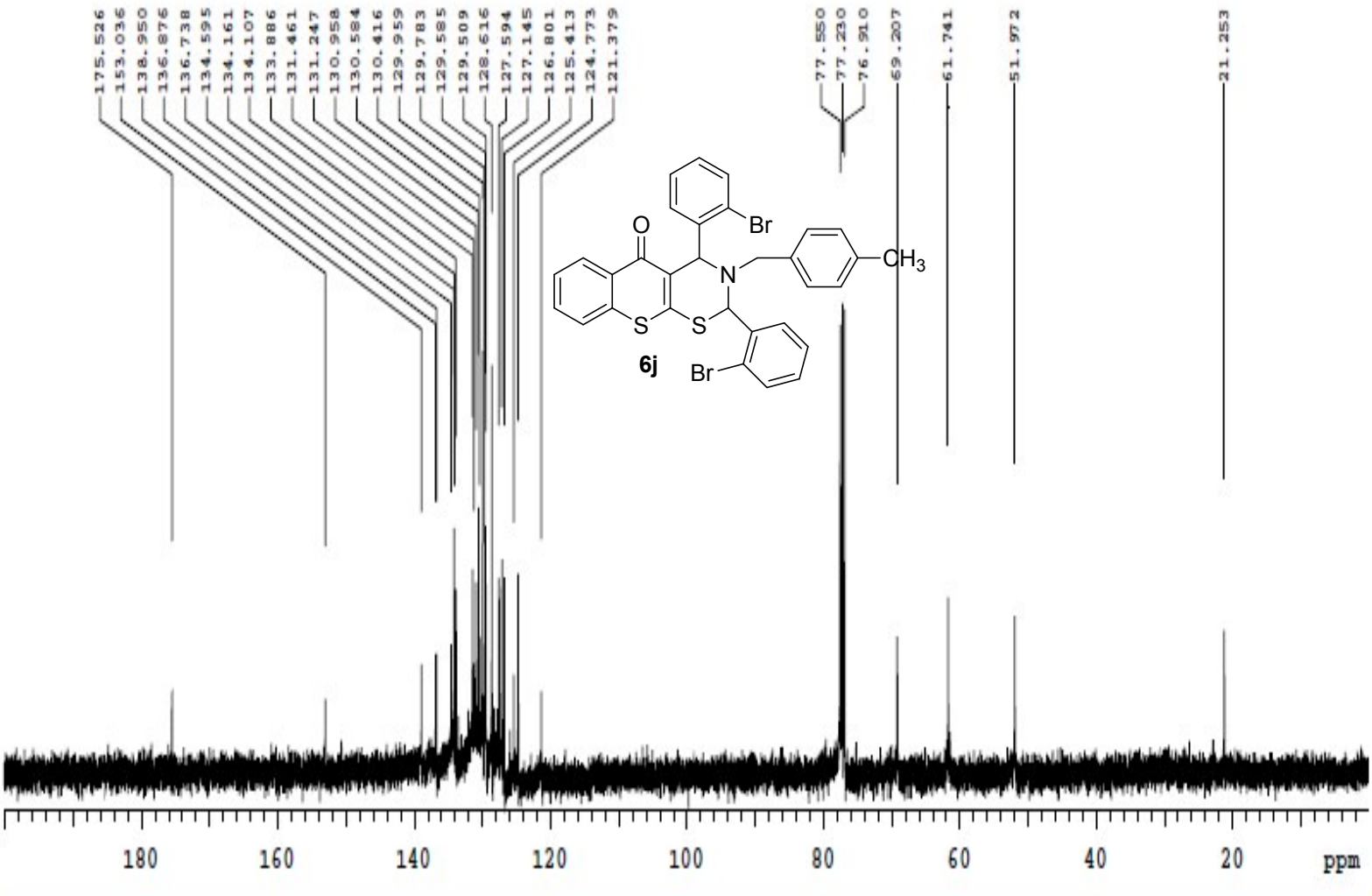
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 6j



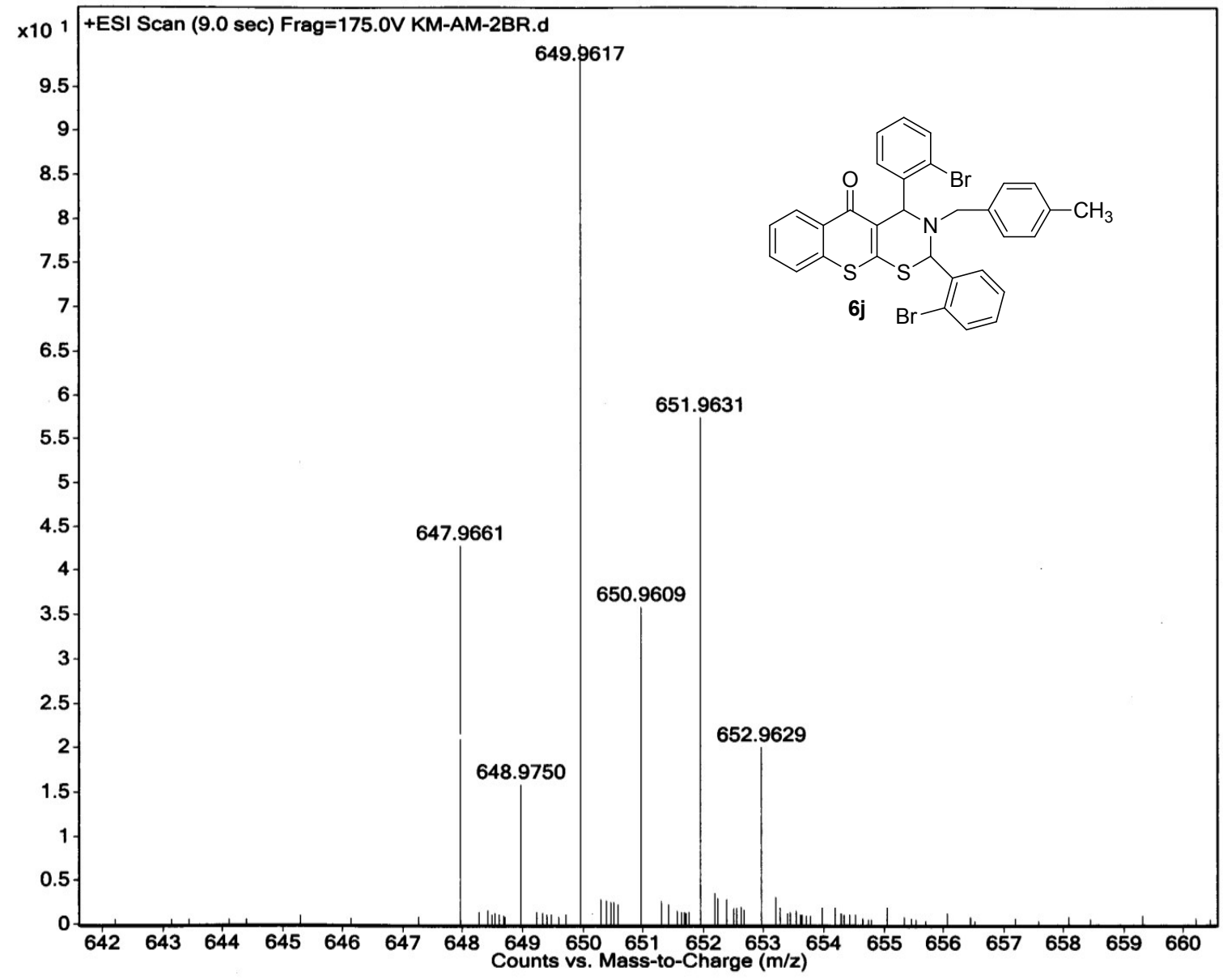
^{13}CNMR spectra of compound: 6j



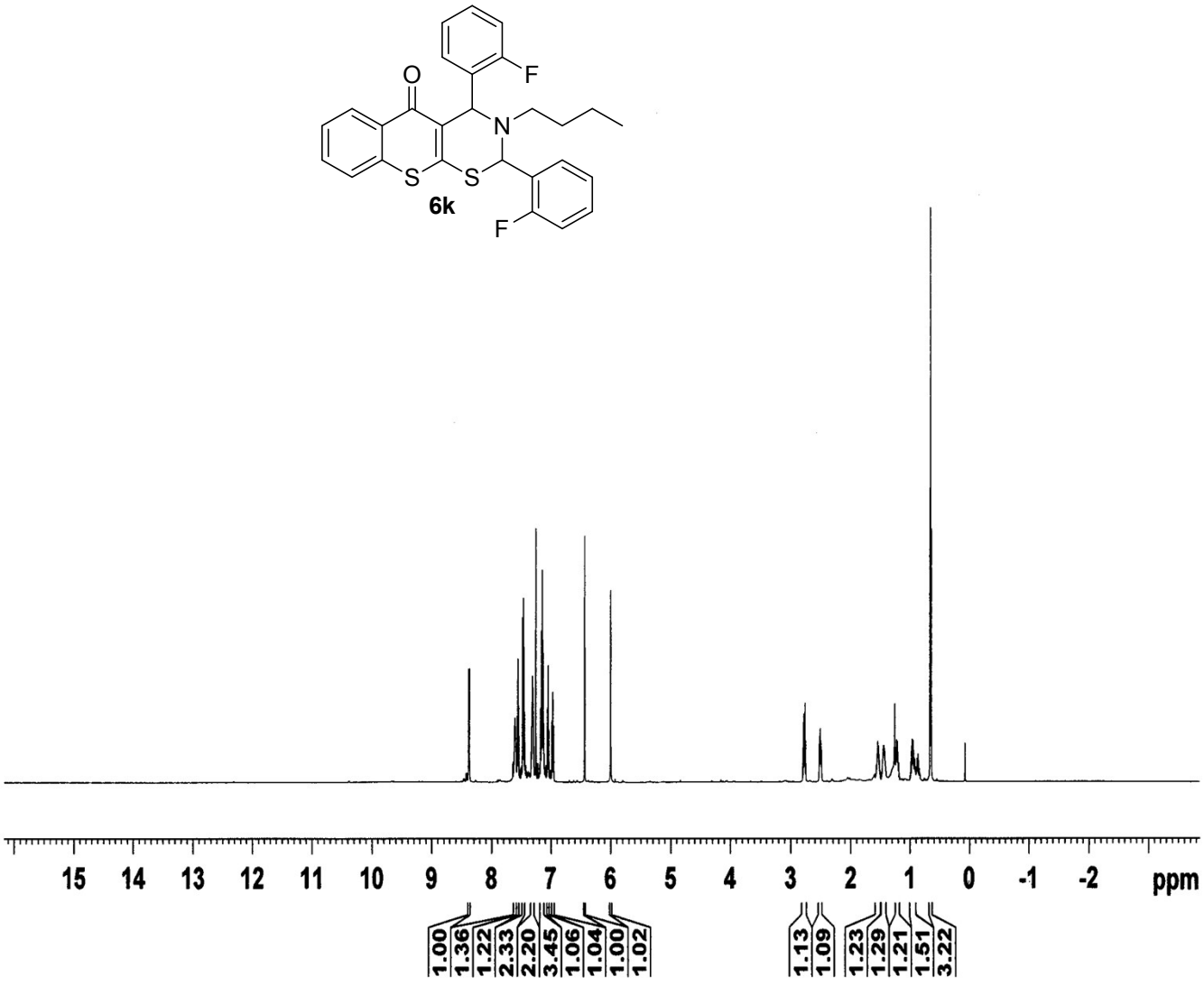
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 950 repetitions	OBSERVE C13, 100.5425732 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 36 minutes		Km-AM-2Br-13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: Km-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**



[1]HNMR spectra the compound: 6k



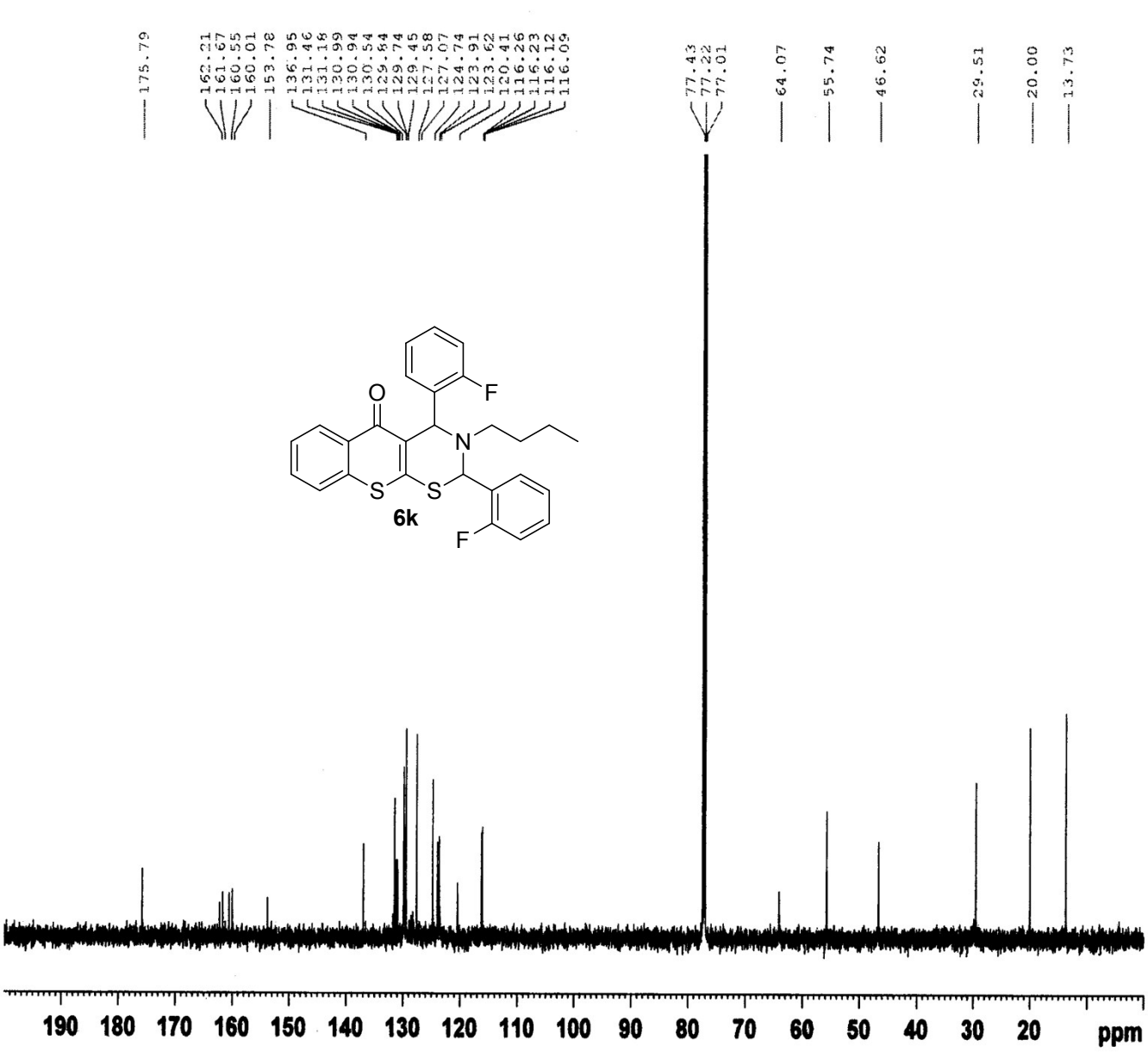

```
Current Data Parameters
NAME        KM-BAM-2F-1H
EXPNO                  1
PROCNO                 1

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
TD0                   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
```

^{13}CNMR spectra of compound: 6k



BRUKER

```
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
TD0                    1

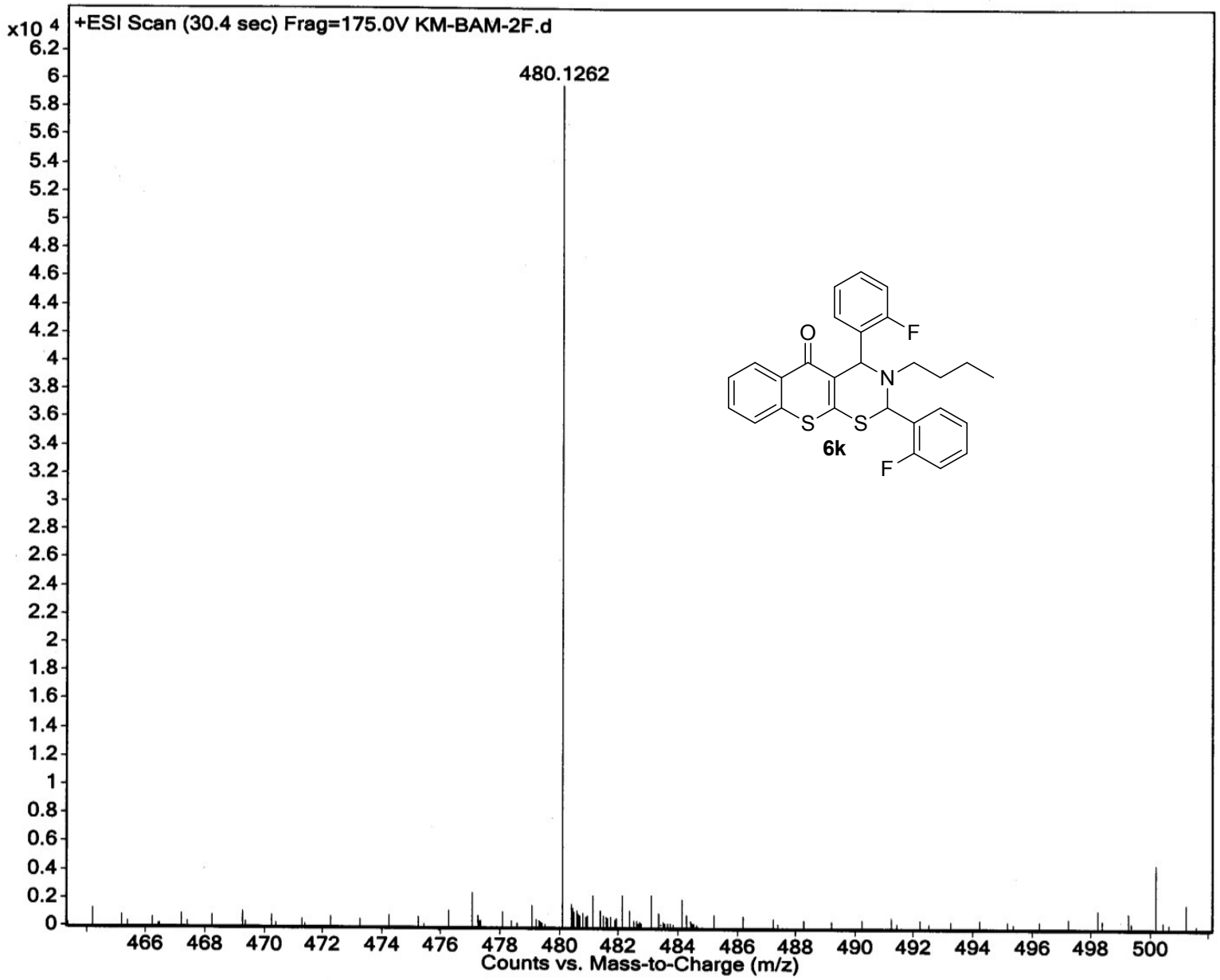
======== CHANNEL f1 ========
SFO1         150.9279571 MHz
NUC1                  13C
P1                 10.50 usec
PLW1         95.00000000 W

======== 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

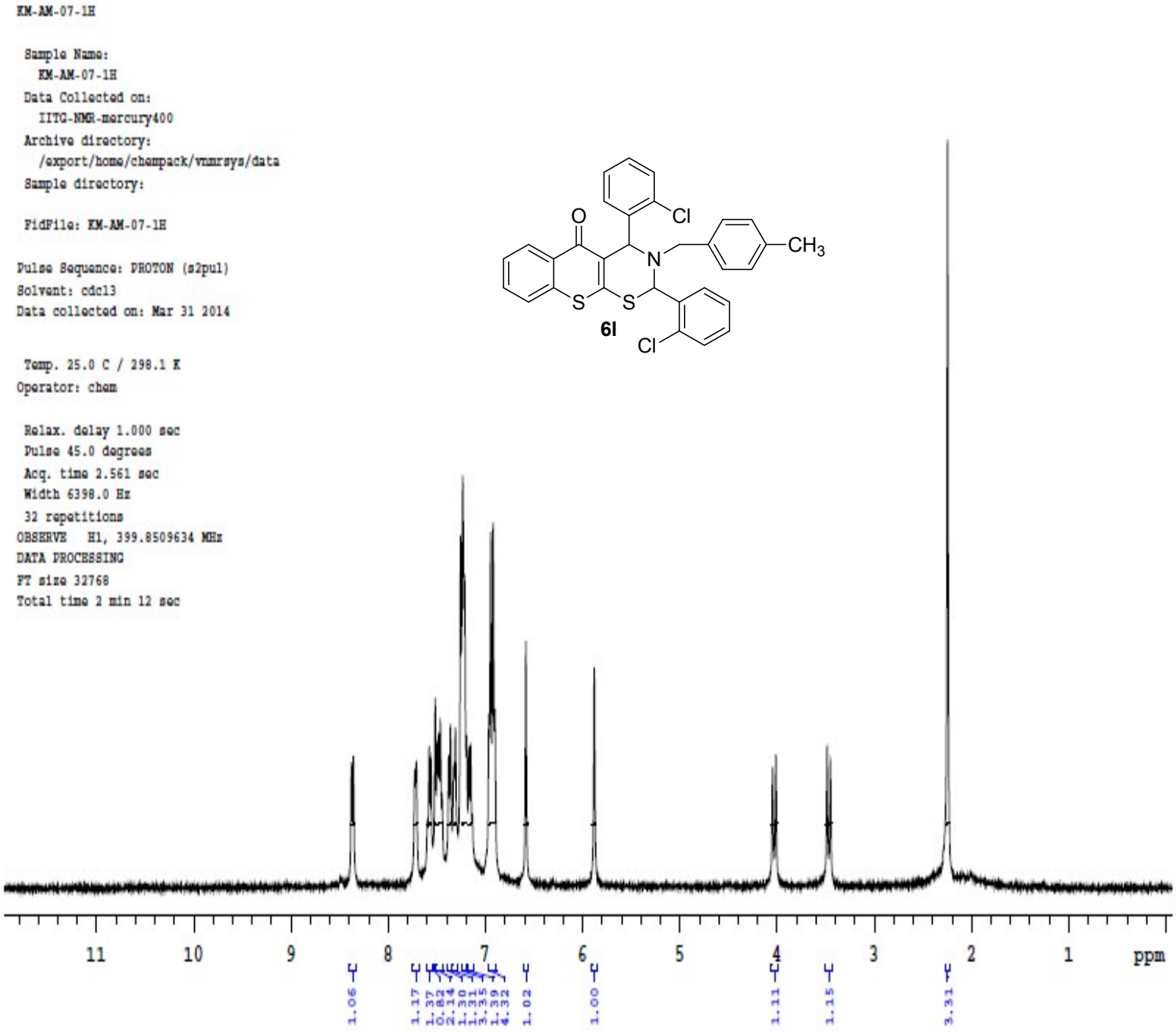
F2 - Processing parameters
SI                 16384
SF           150.9128403 MHz
WDW                   EM
SSB        0
LB                 1.00 Hz
GB         0
PC                 1.40
```

HRMS spectra of compound: 6k

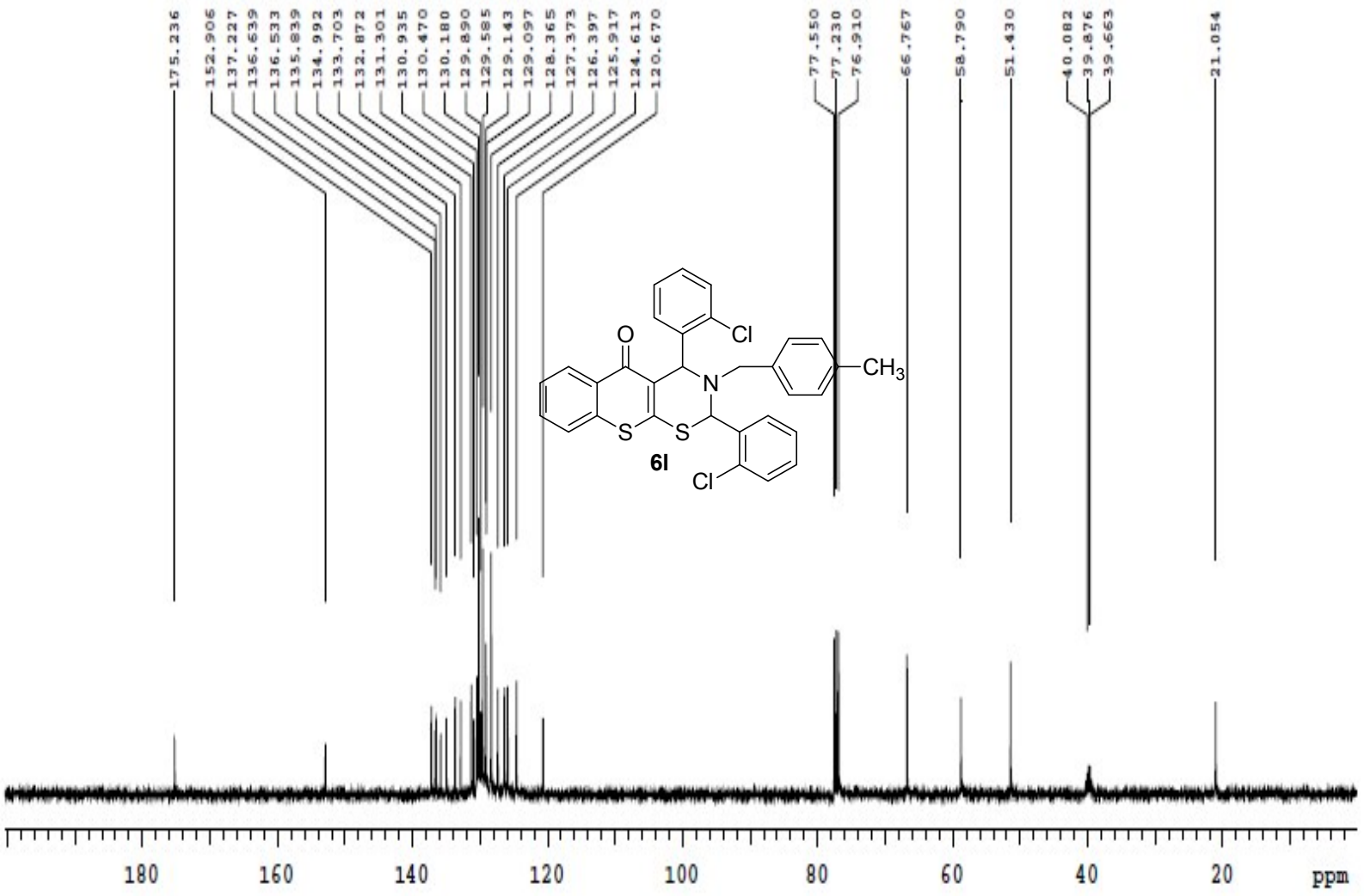
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



[1]HNMR spectra the compound: 6l



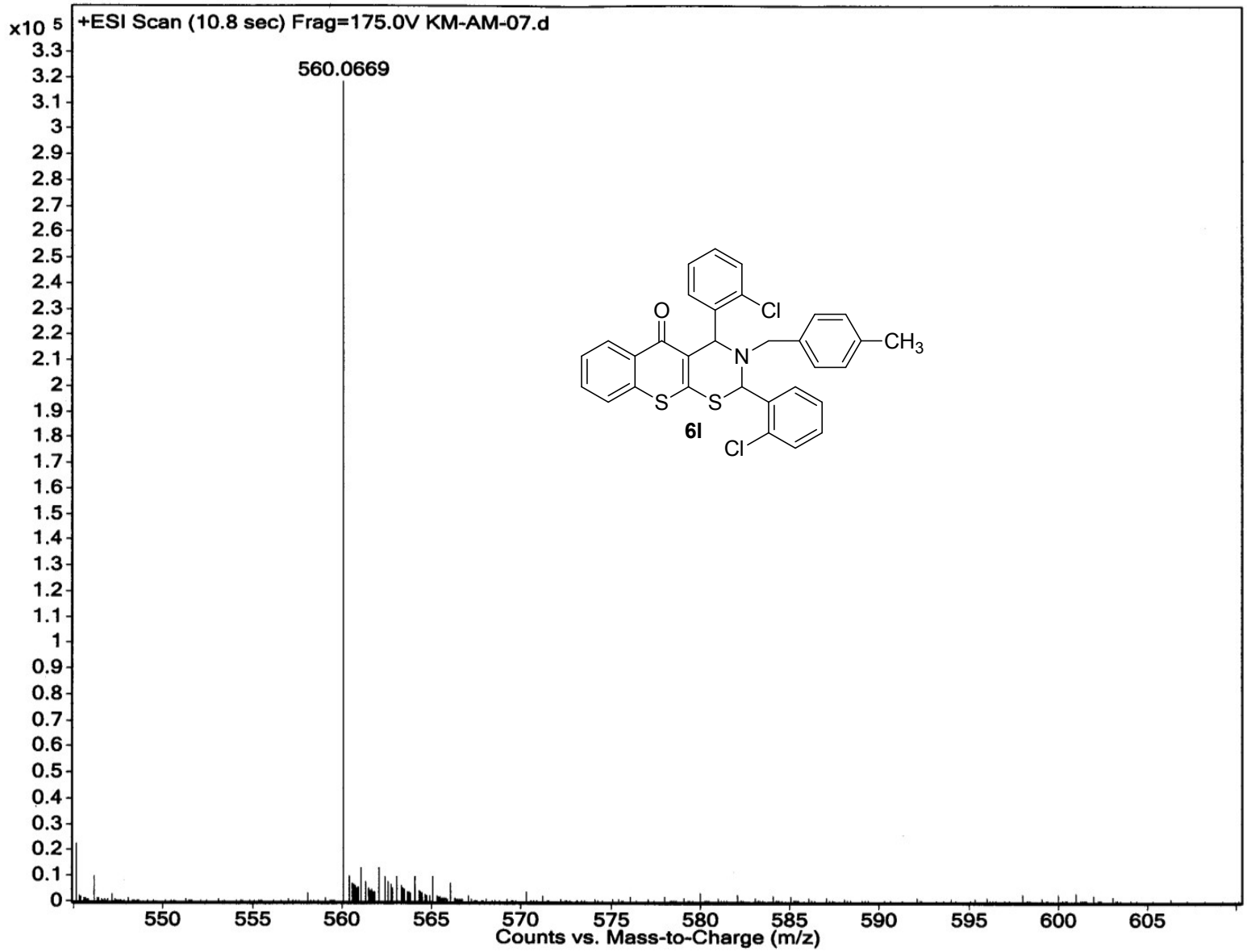
^{13}CNMR spectra of compound: 6l



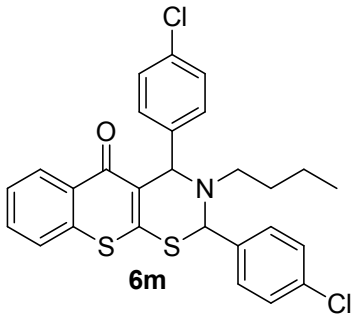
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 1130 repetitions	OBSERVE C13, 100.5425364 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 43 minutes		KM-AM-07-13C Solvent: 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**



[1]HNMR spectra compound: 6m



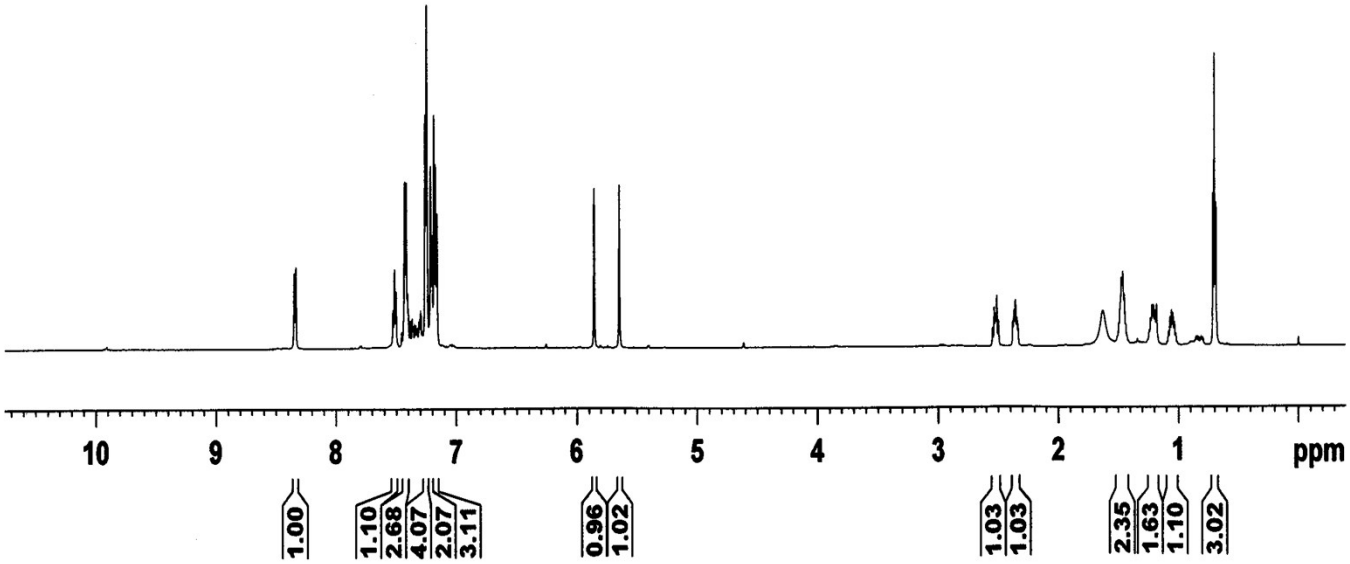
6m

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

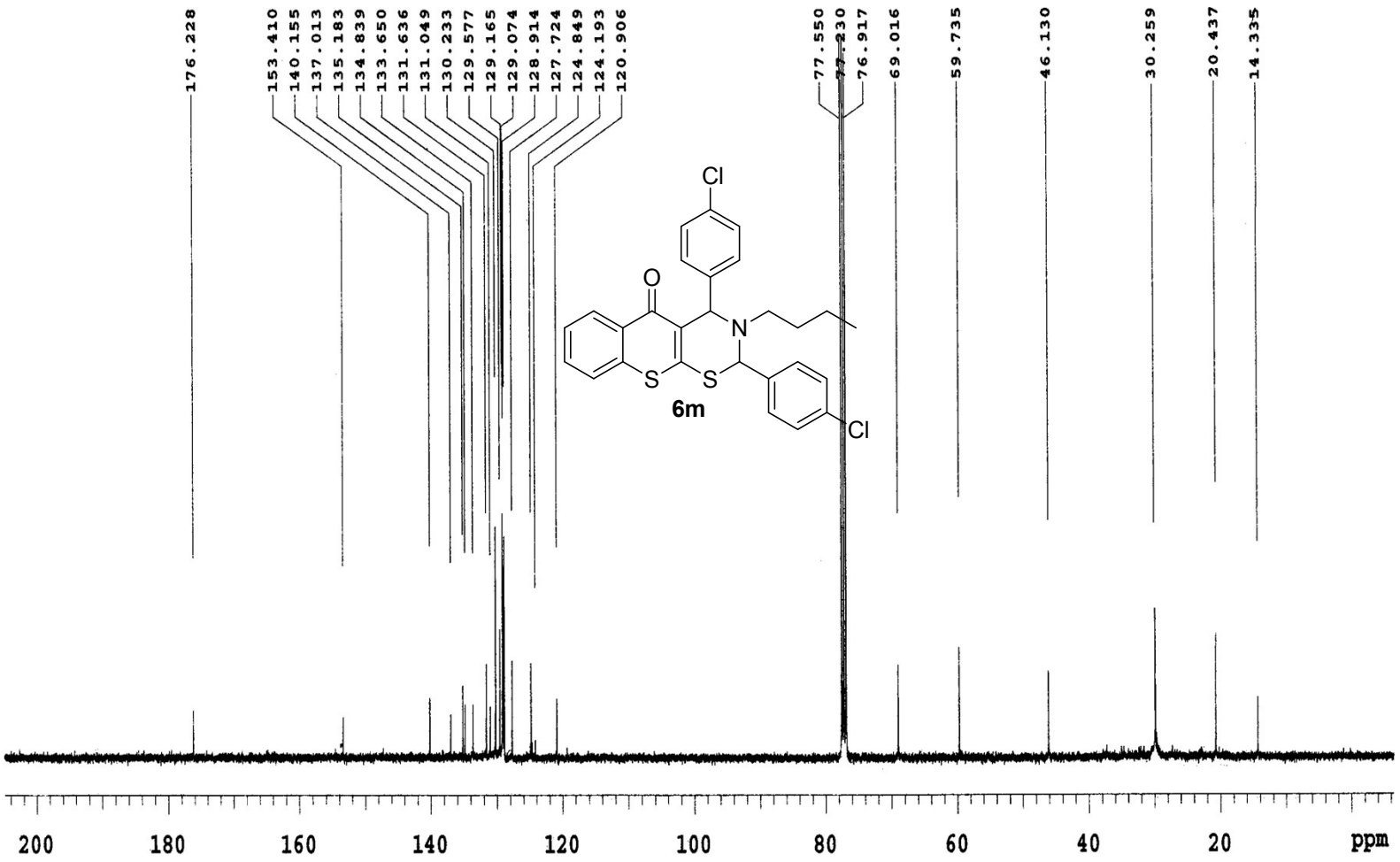
F2 - Acquisition Parameters
Date_           20150223
Time               12.31
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                   113
DW                41.600 usec
DE                 6.50 usec
TE                298.5 K
D1             1.00000000 sec
TD0                    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
```



^{13}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, 100.5425801
DECOUPLE H1, 399.8529994
Power 42 dB
continuously on
WALTZ-16 modulated

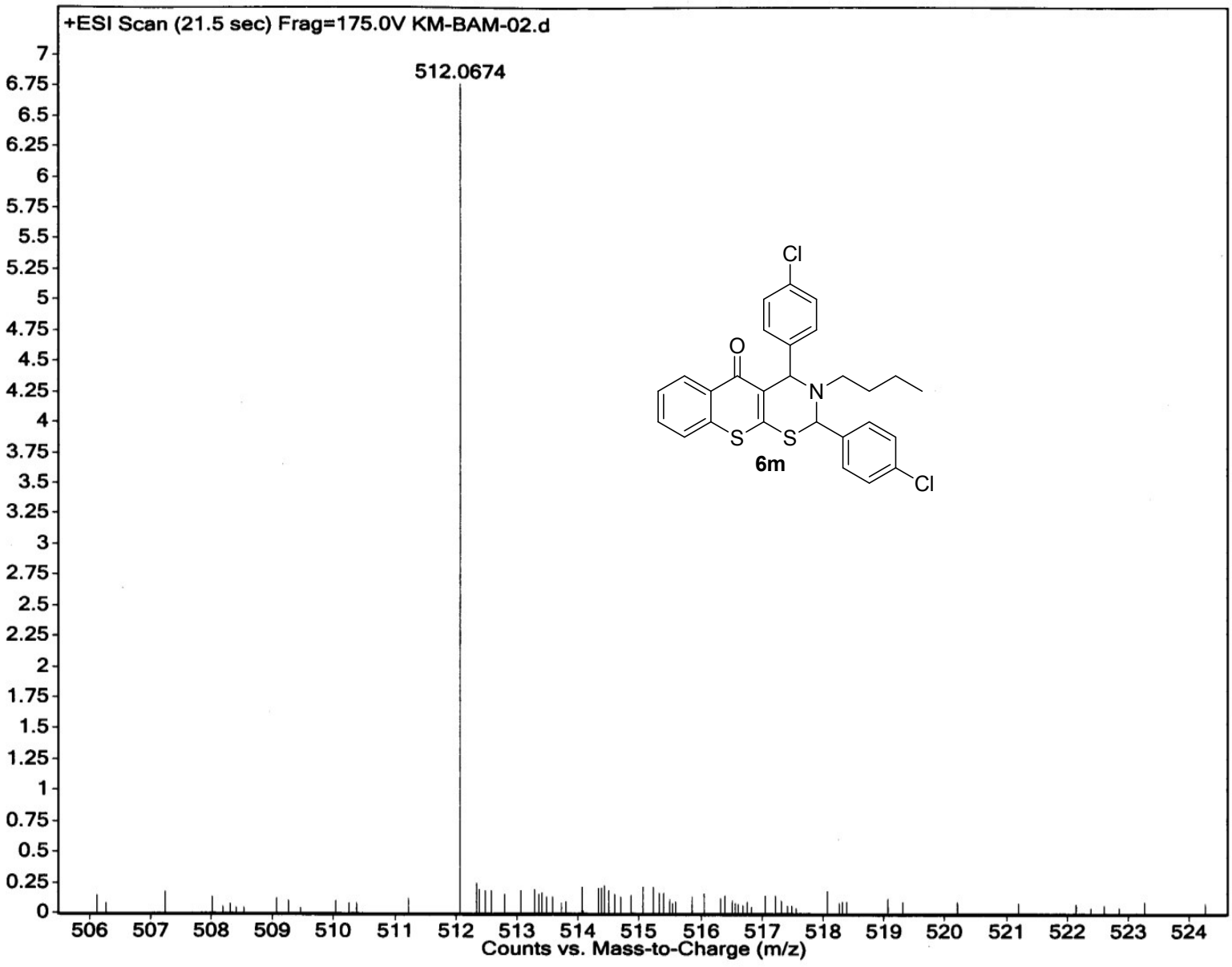
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 6.0 hours

KM-BAM-4Cl-13C

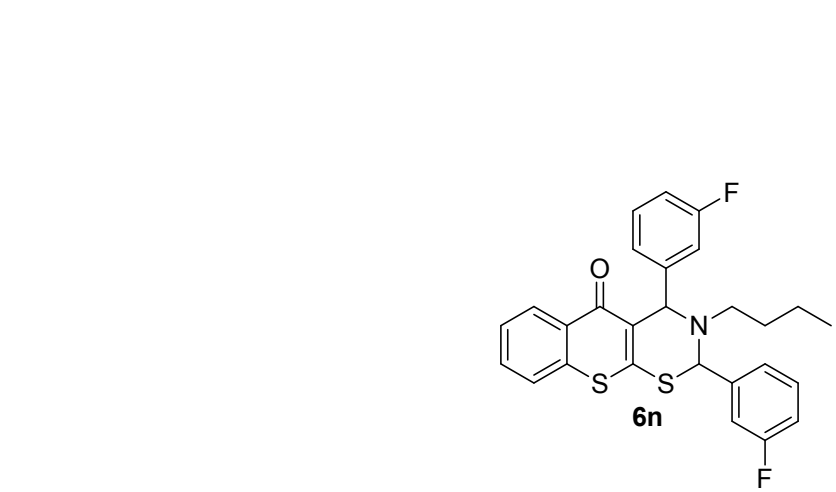
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem
Mercury-400 "IITG-NMR"

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**



[1]HNMR spectra the compound: 6n



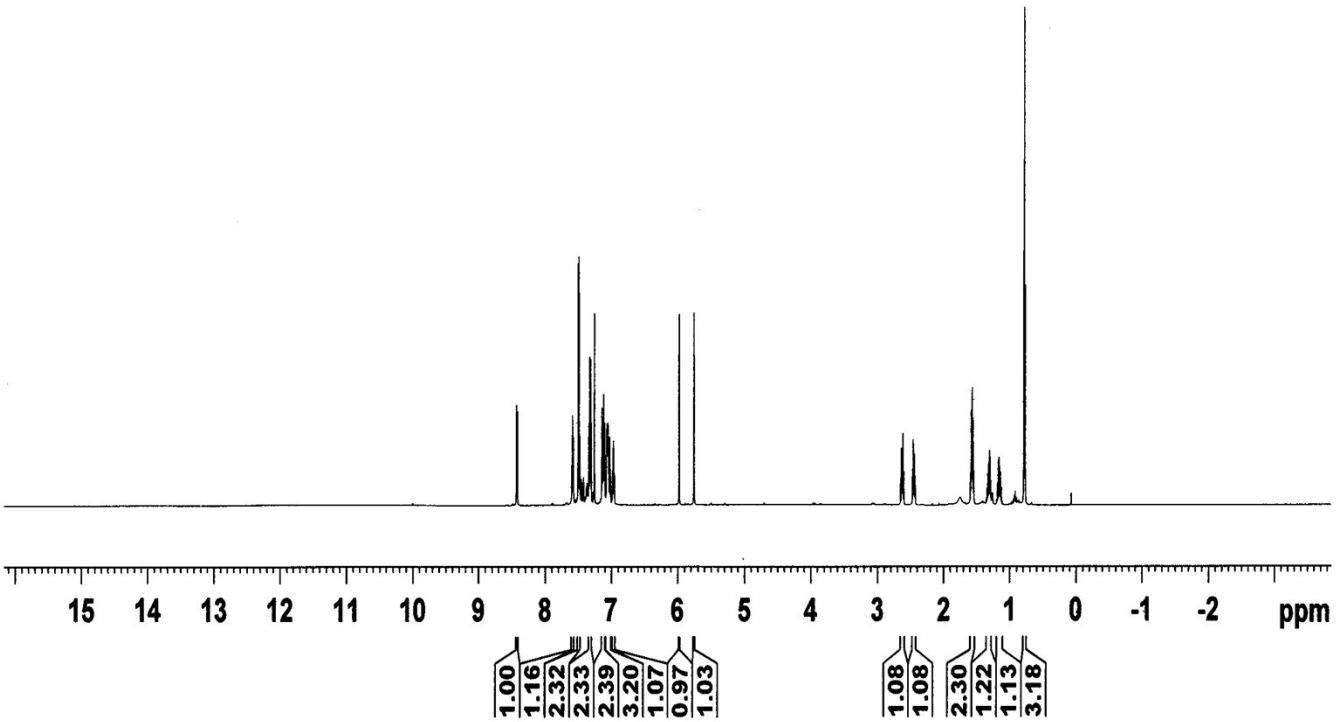
6n

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

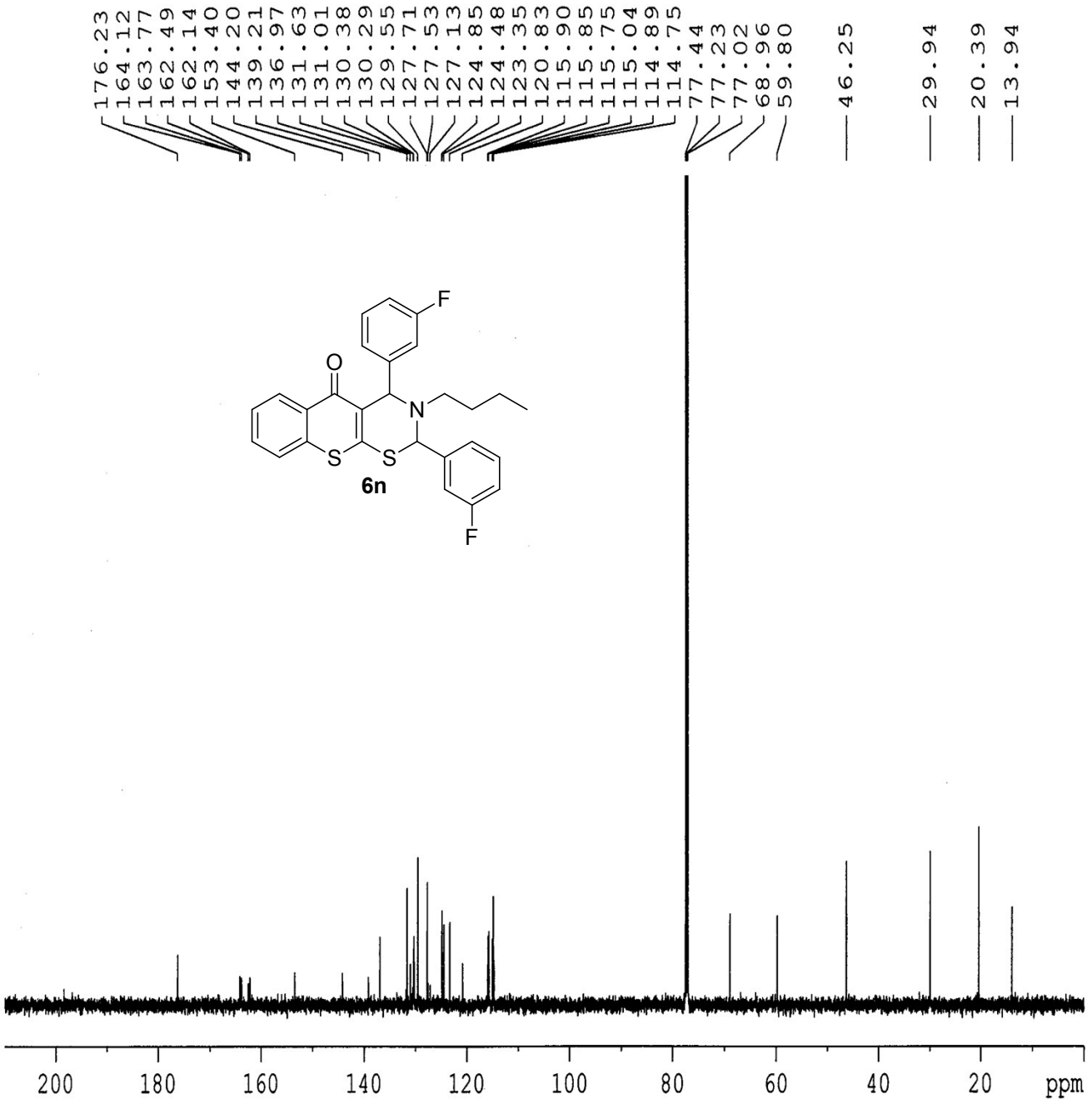
F2 - Acquisition Parameters
Date_           20150210
Time               10.05
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                  73.2
DW                41.600 usec
DE                 6.50 usec
TE                297.9 K
D1            1.00000000 sec
TD0                    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
```



^{13}CNMR spectra of compound: 6n



BRUKER

```
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
TD0                  1

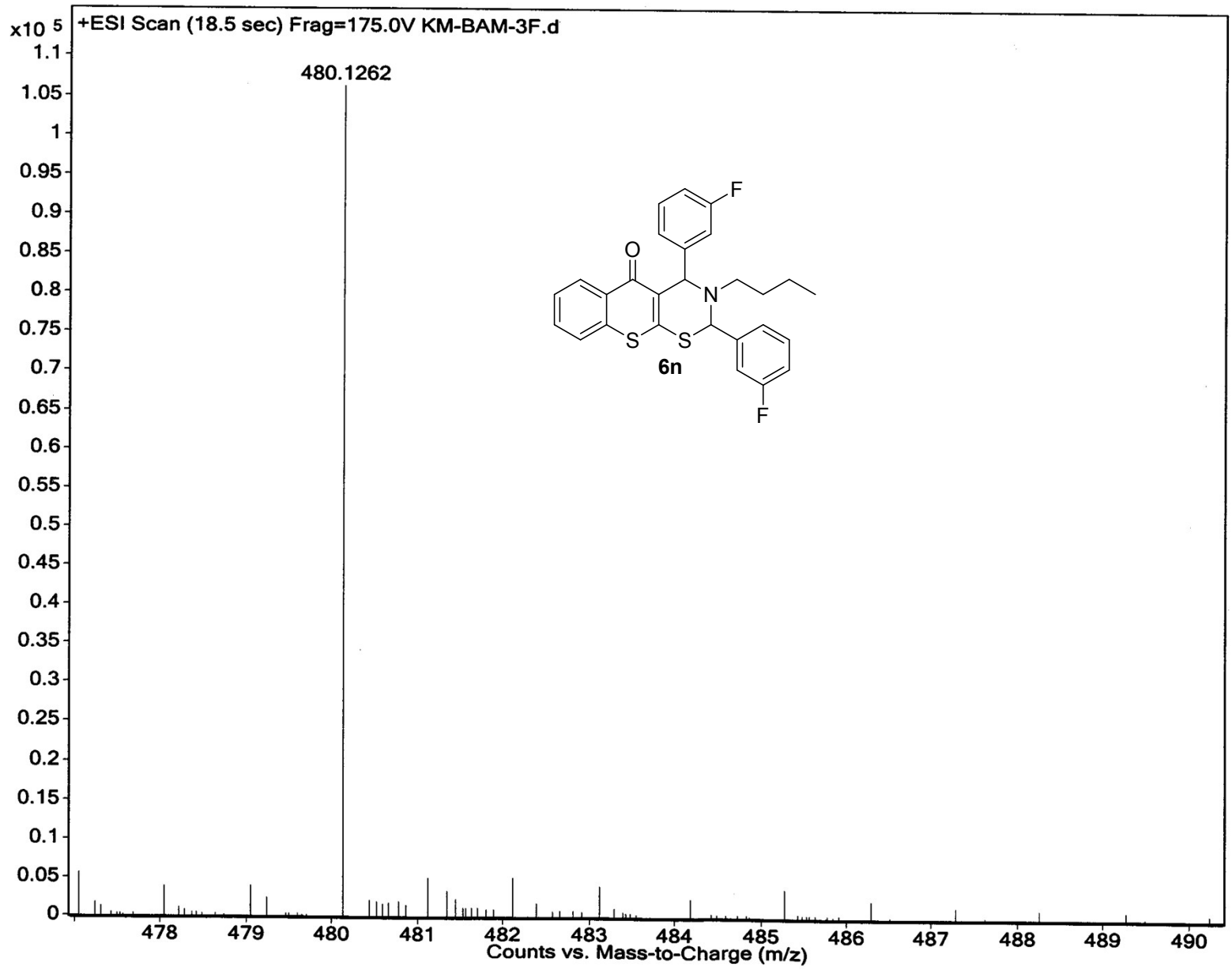
======== CHANNEL f1 ========
SFO1        150.9279571 MHz
NUC1                13C
P1                10.50 usec
PLW1        95.00000000 W

======== 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

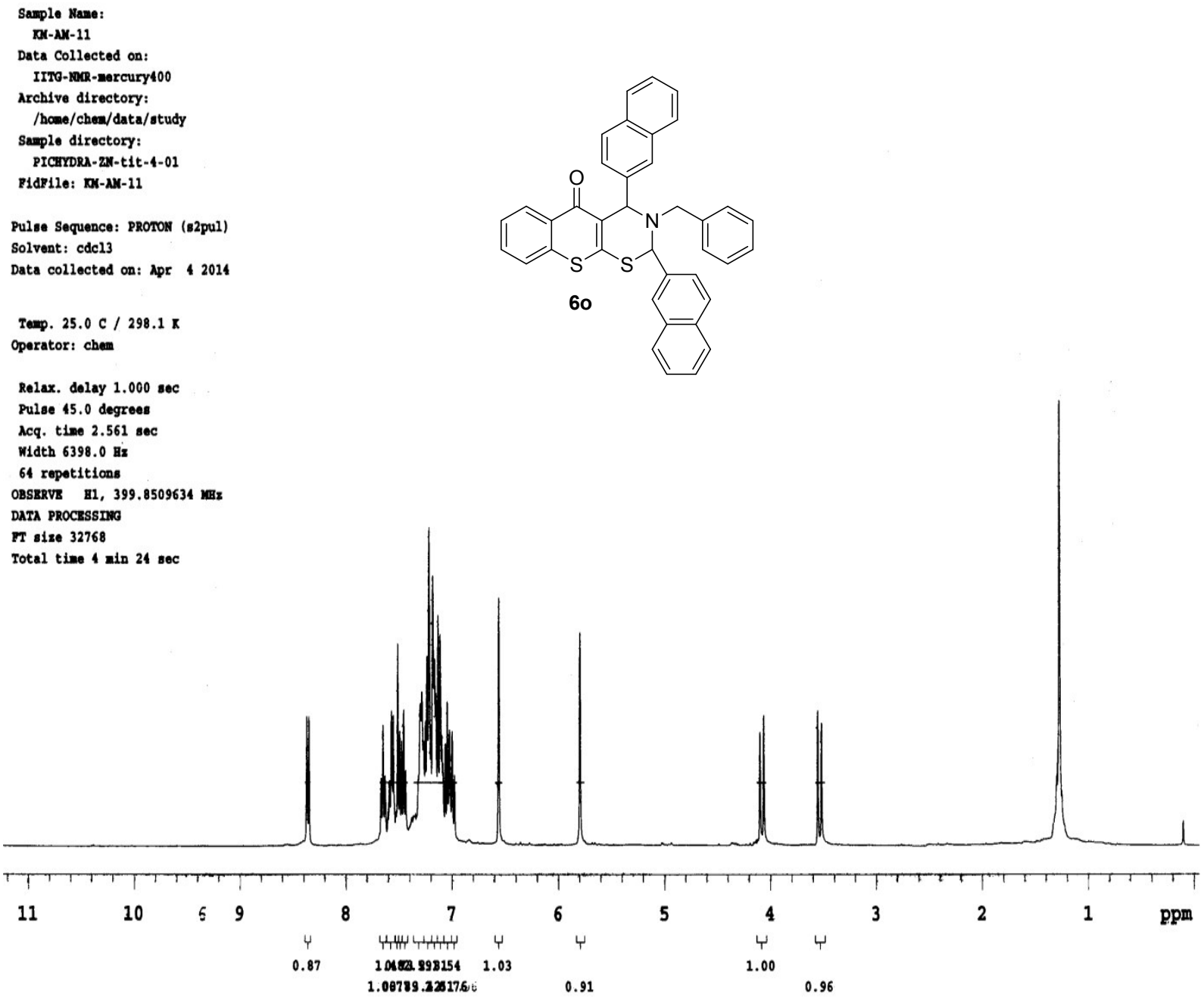
F2 - Processing parameters
SI                 16384
SF          150.9128382 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

HRMS spectra of compound: 6n

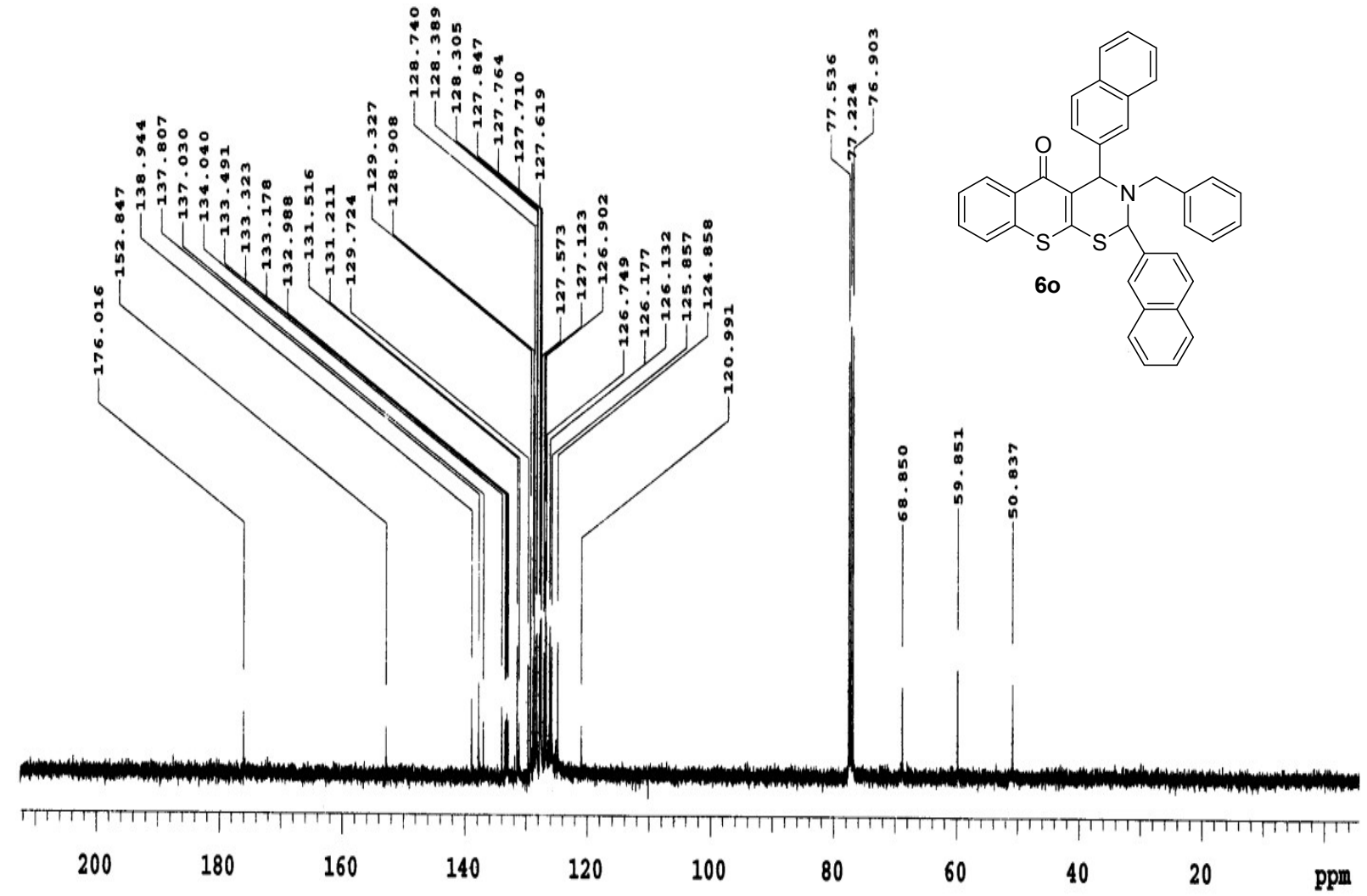
Sample Name	**Position**	**Instrument Name**	**User Name**
Inj Vol	**InjPosition**	**SampleType**	**IRM Calibration Status**
Data Filename	**ACQ Method**	**Comment**	**Acquired Time**



[1]HNMR spectra the compound: 6o



^{13}CNMR spectra of compound: 6o



PULSE SEQUENCE
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
Line broadening 0.5 Hz
FT size 65536
Total time 44 minutes

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