

Supporting Information

Oxidative cross coupling reaction mediated by I_2/H_2O_2 : A novel approach for construction of fused thiazole containing coumarin derivatives.

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Experimental General

Melting points were determined on a Büchi melting point apparatus. IR spectra were recorded on Perkin-Elmer 281 IR spectrophotometer. ^1H NMR spectra were recorded on Bruker 600 MHz and Varian 400 MHz spectrometer with TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). ^1H 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 dd (doublet of double). HRMS spectra were recorded using WATERS MS system, Q-TOF premier and data analyzed using Mass Lynx 4.1. The X-ray crystal structures were determined with a Siemen P-4 diffractometer. Complete crystallographic data of **2a** (CCDC 1013314) 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).

Crystallographic Description: Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated $\text{MoK}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) at 298 K. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. The structure was solved by direct methods implemented in SHELX-97 program and refined by full-matrix least-squares methods on F^2 . All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. Compound **2a** empirical formula $\text{C}_{16}\text{H}_9\text{NO}_2\text{S}$, pale yellow crystal, formula wt 301.29, Monoclinic, $P -1$, $a = 8.2110(2) \text{ \AA}$, $b = 8.9277(2) \text{ \AA}$, $c = 9.0926(2) \text{ \AA}$, $V = 652.53(3) \text{ \AA}^3$, $Z = 2$, $F(000) = 288.0$, $\text{GOF}(S) = 1.049$. Final indices $R_{\text{obs}} = 0.0330$, $wR_{\text{obs}} = 0.0887$ with $I > 2\sigma(I)$; $R_{\text{all}} = 0.0361$, $wR_{\text{all}} = 0.0913$ for all data.

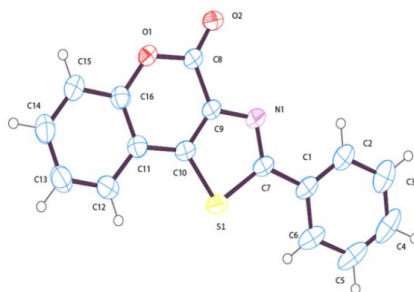
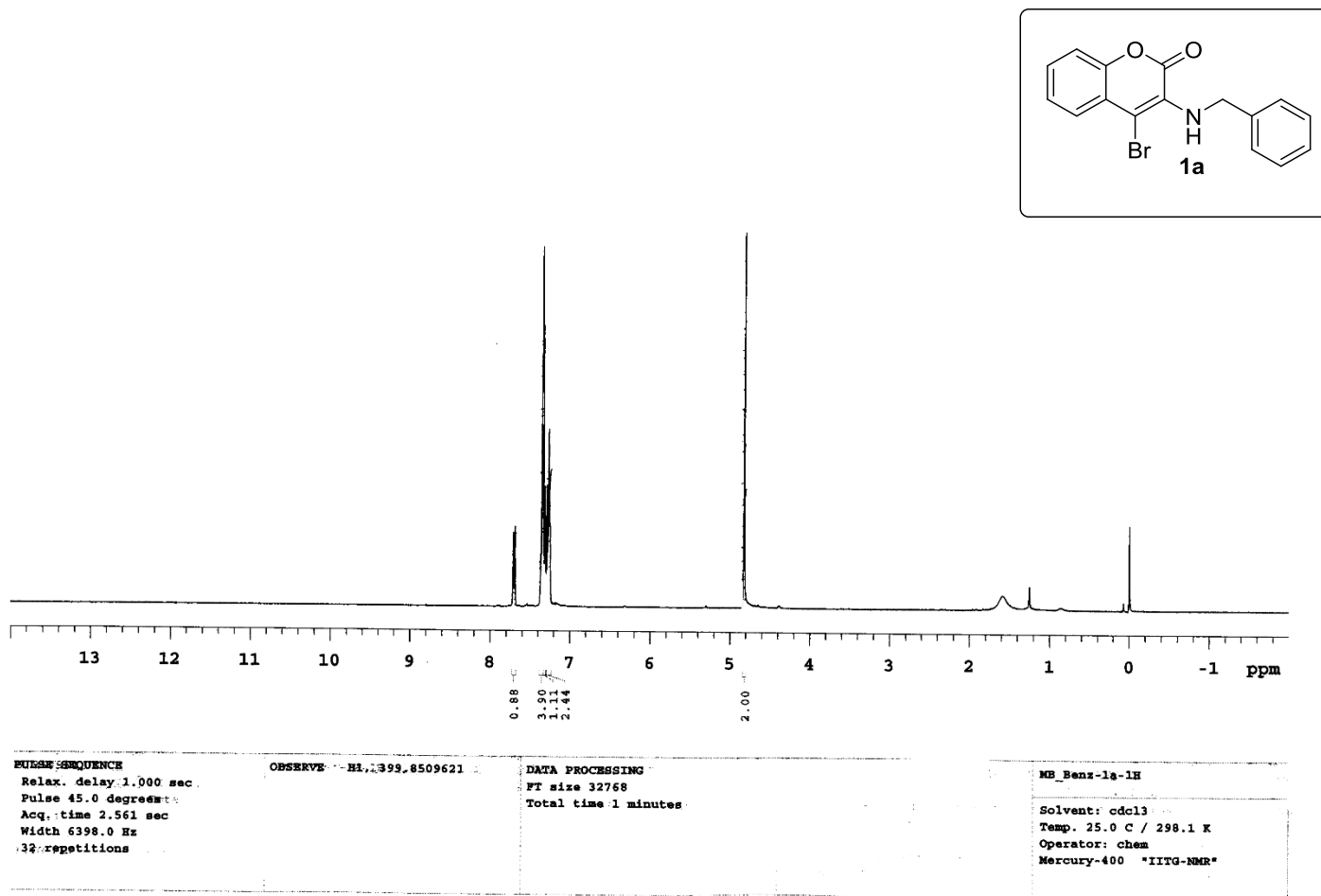
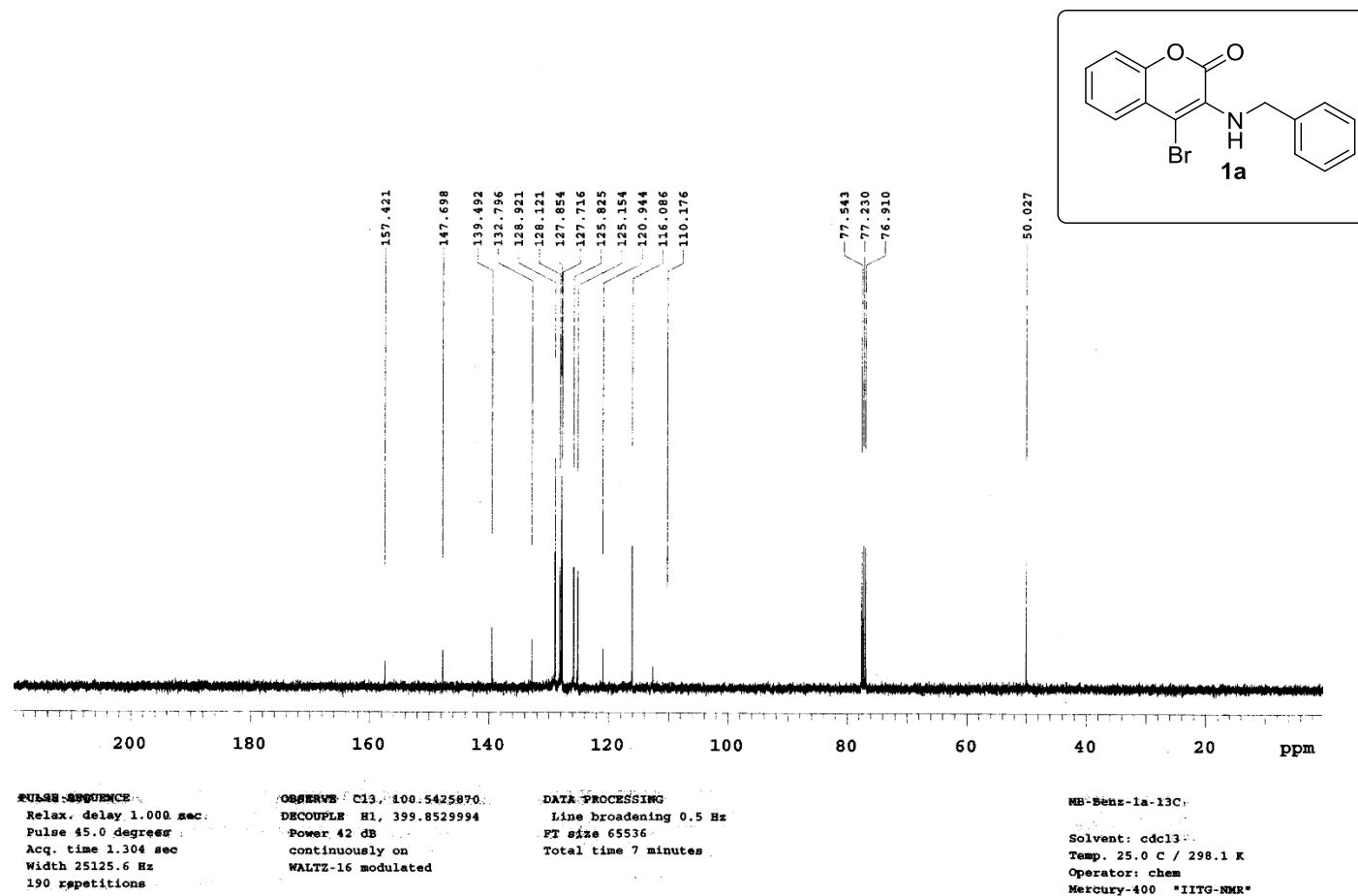


Figure 1. Single crystal structure of **2a** (CCDC: 1013314)

¹H NMR spectra of **1a**



¹³C NMR spectra of **1a**



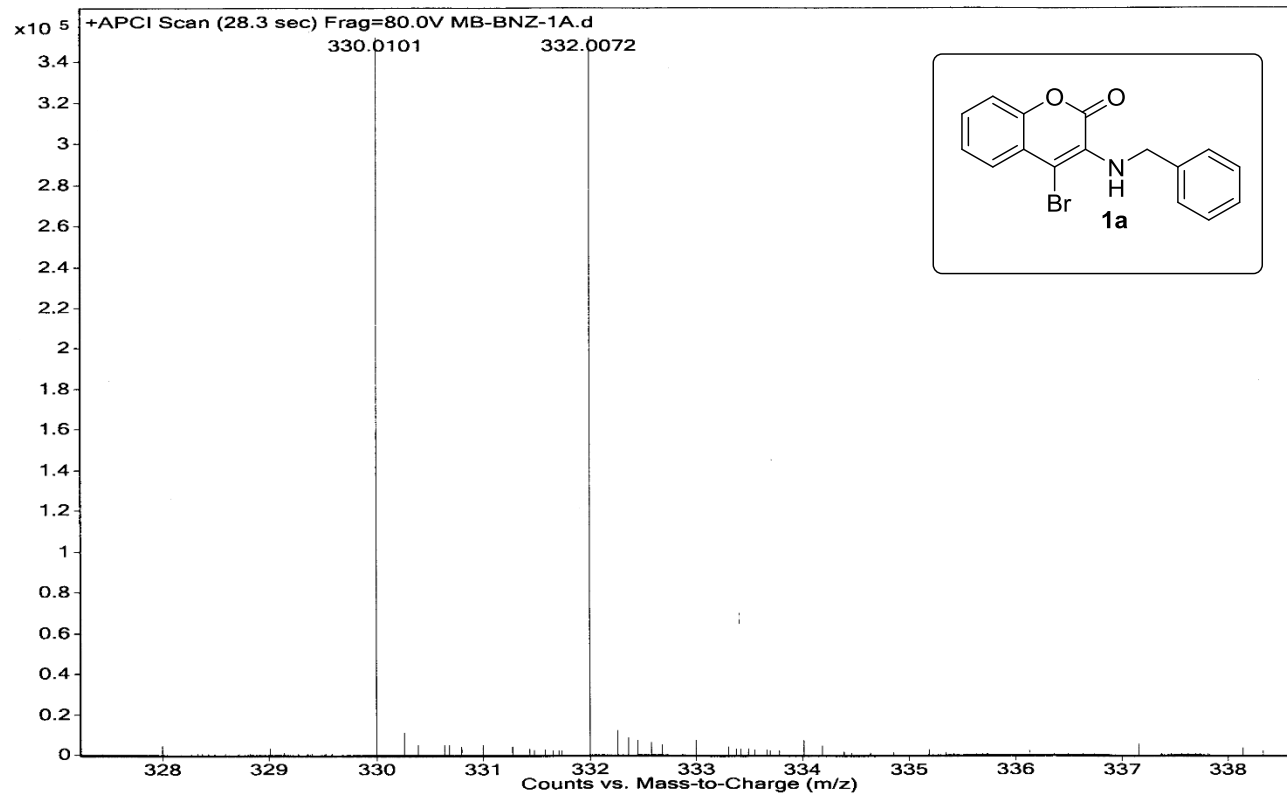
HRMS Spectra of **1a**

Sample Name
Inj Vol
Data Filename

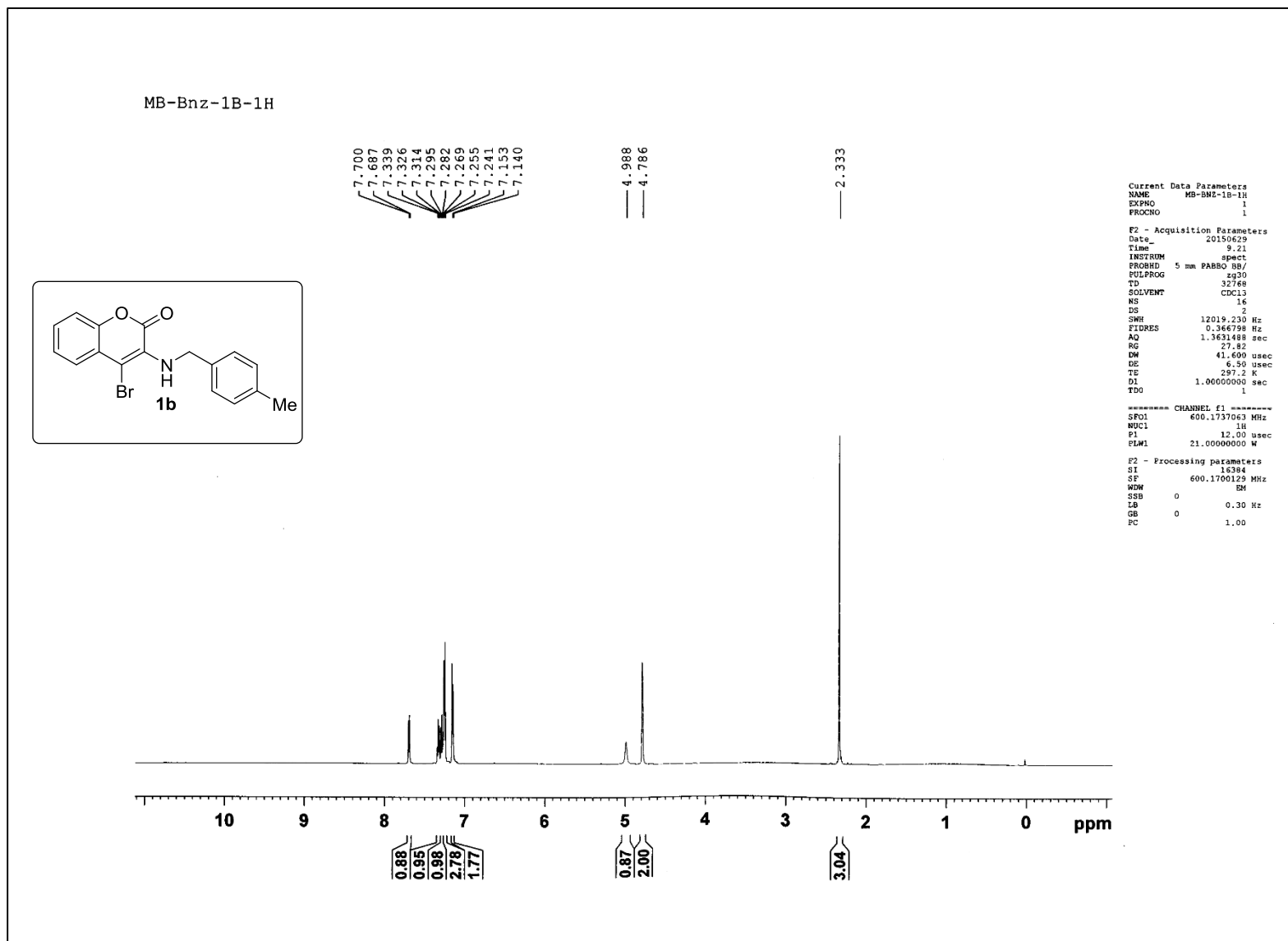
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Instrument Name
SampleType
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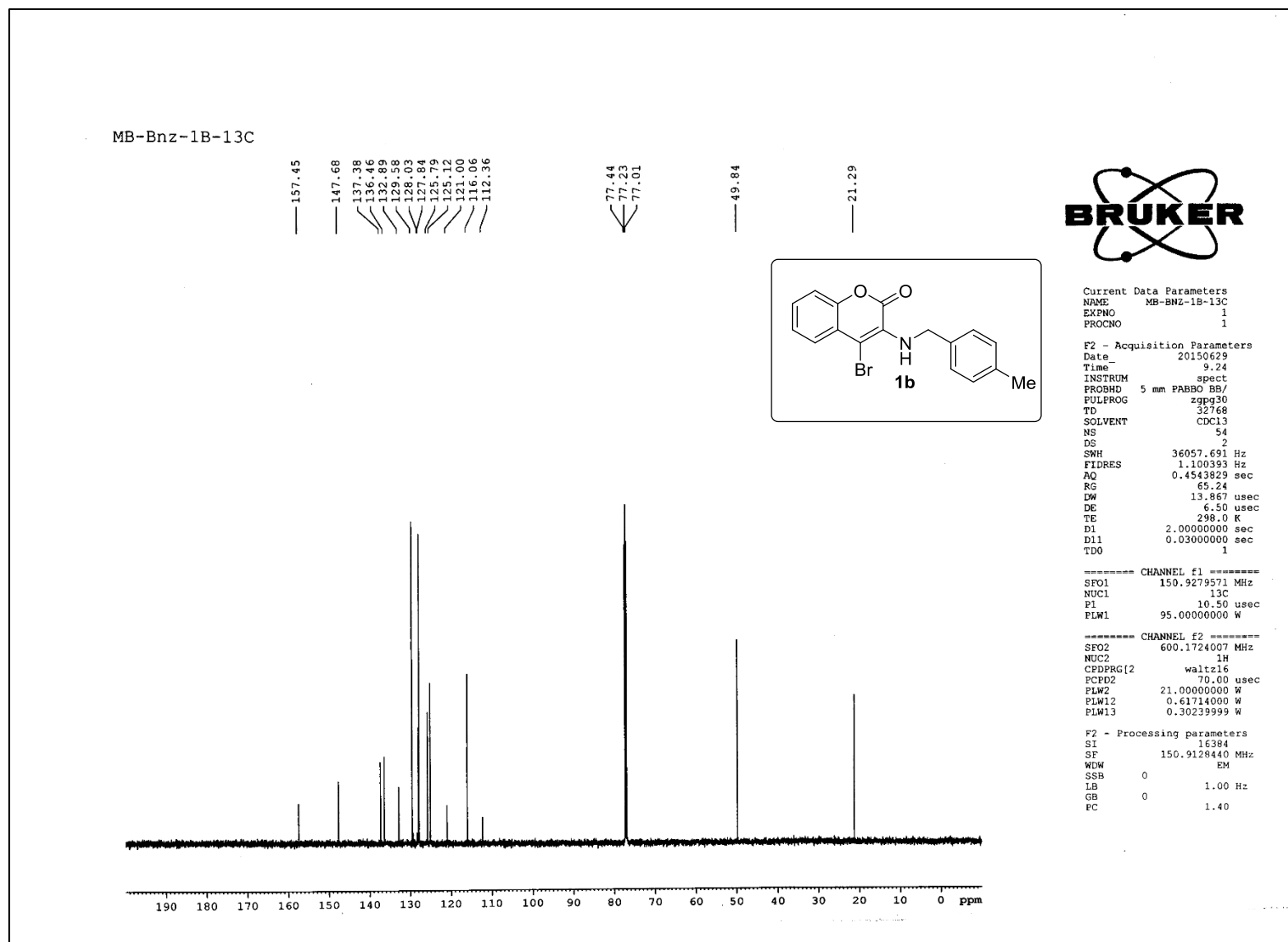
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¹H NMR spectra of **1b**



¹³C NMR spectra of **1b**



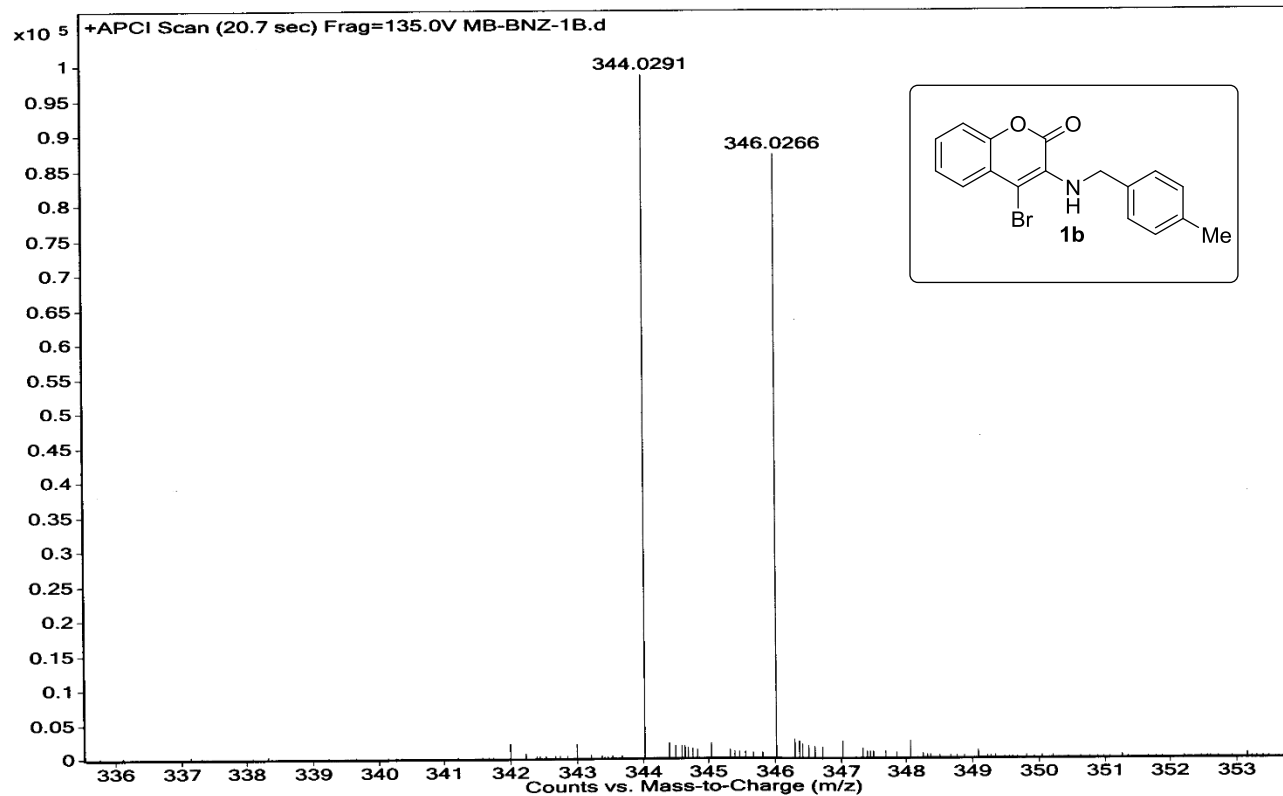
HRMS Spectra of **1b**

Sample Name
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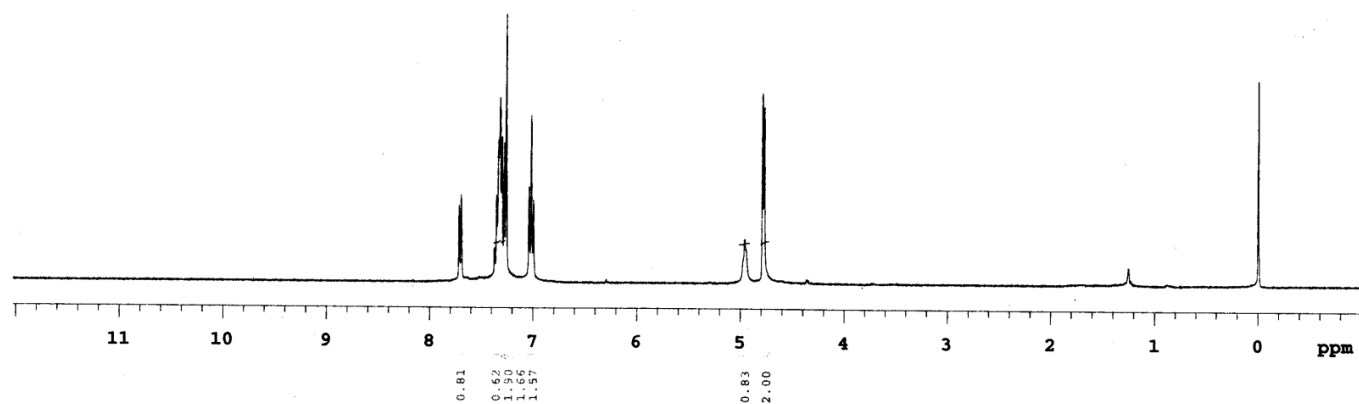
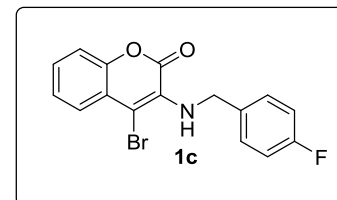
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Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



¹H NMR spectra of **1c**



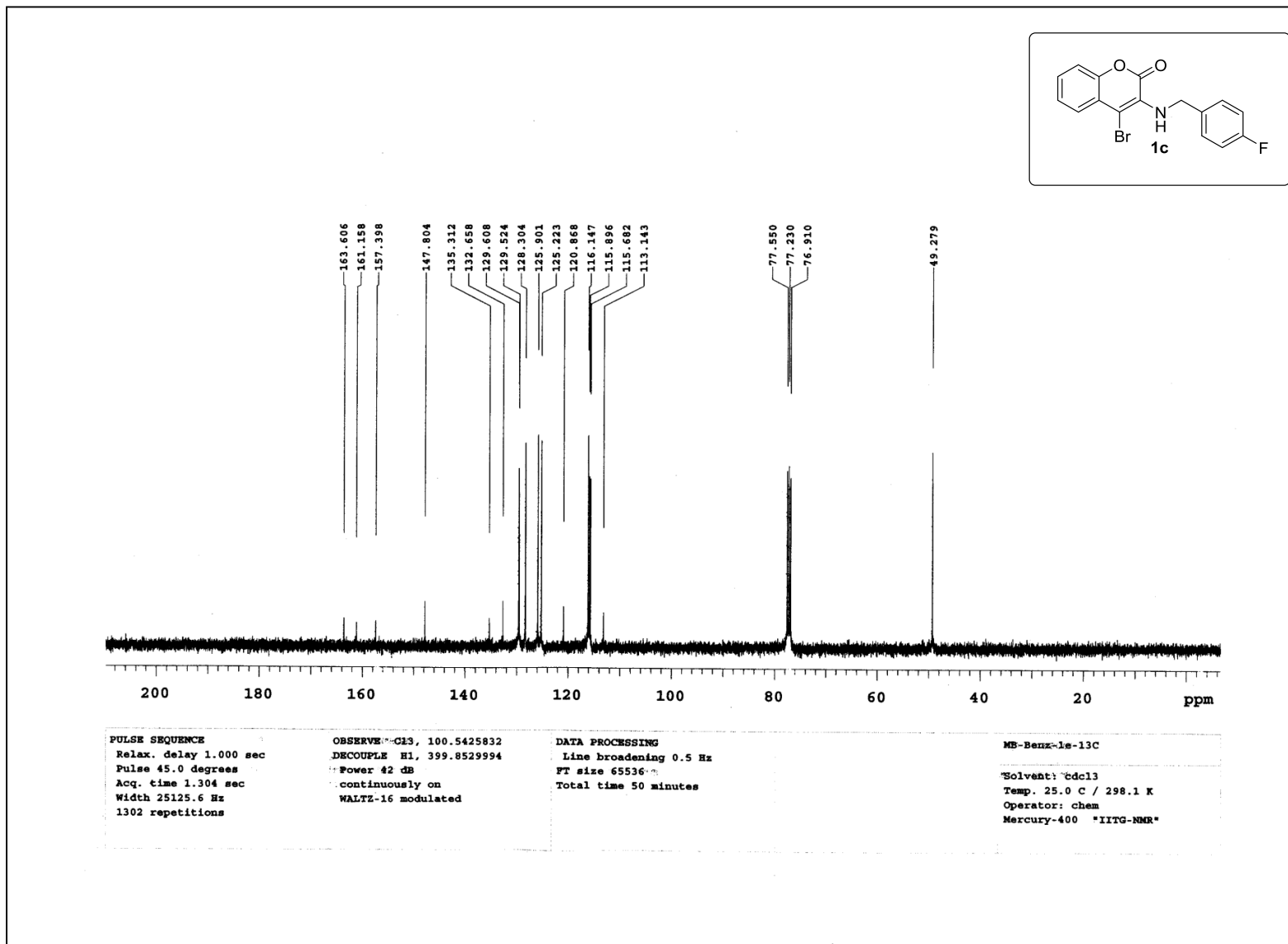
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Acq. time 2.561 sec
Width 6398.0 Hz
64 repetitions

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EXPNO: 1
PROCNO: 1
F2: 399.8509634

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Total time 3 minutes

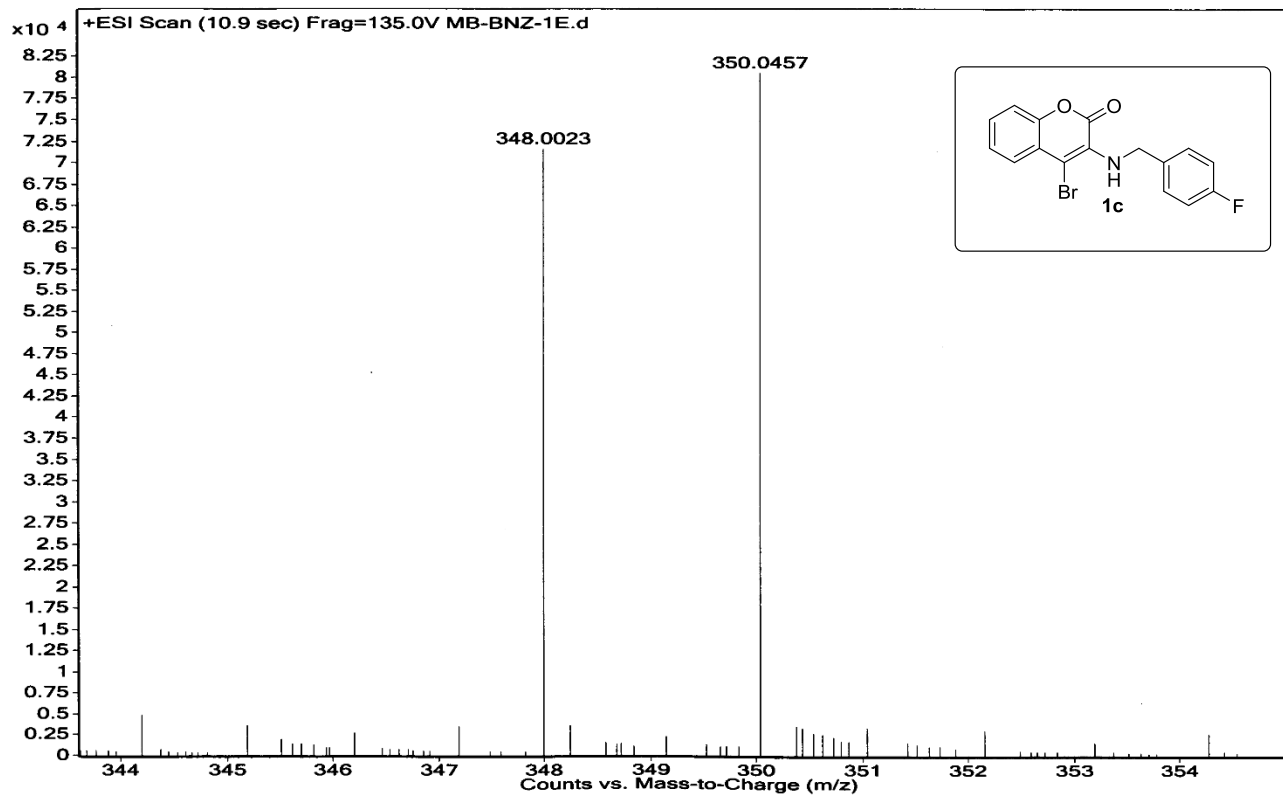
NAME: 1c
Solvent: DMSO-d6
Temp. 25.0°C / 298.1 K
Operator: chem
File: MS-Benz-1E-1H
Mercury-400 "IITG-NMR"

¹³C NMR spectra of **1c**

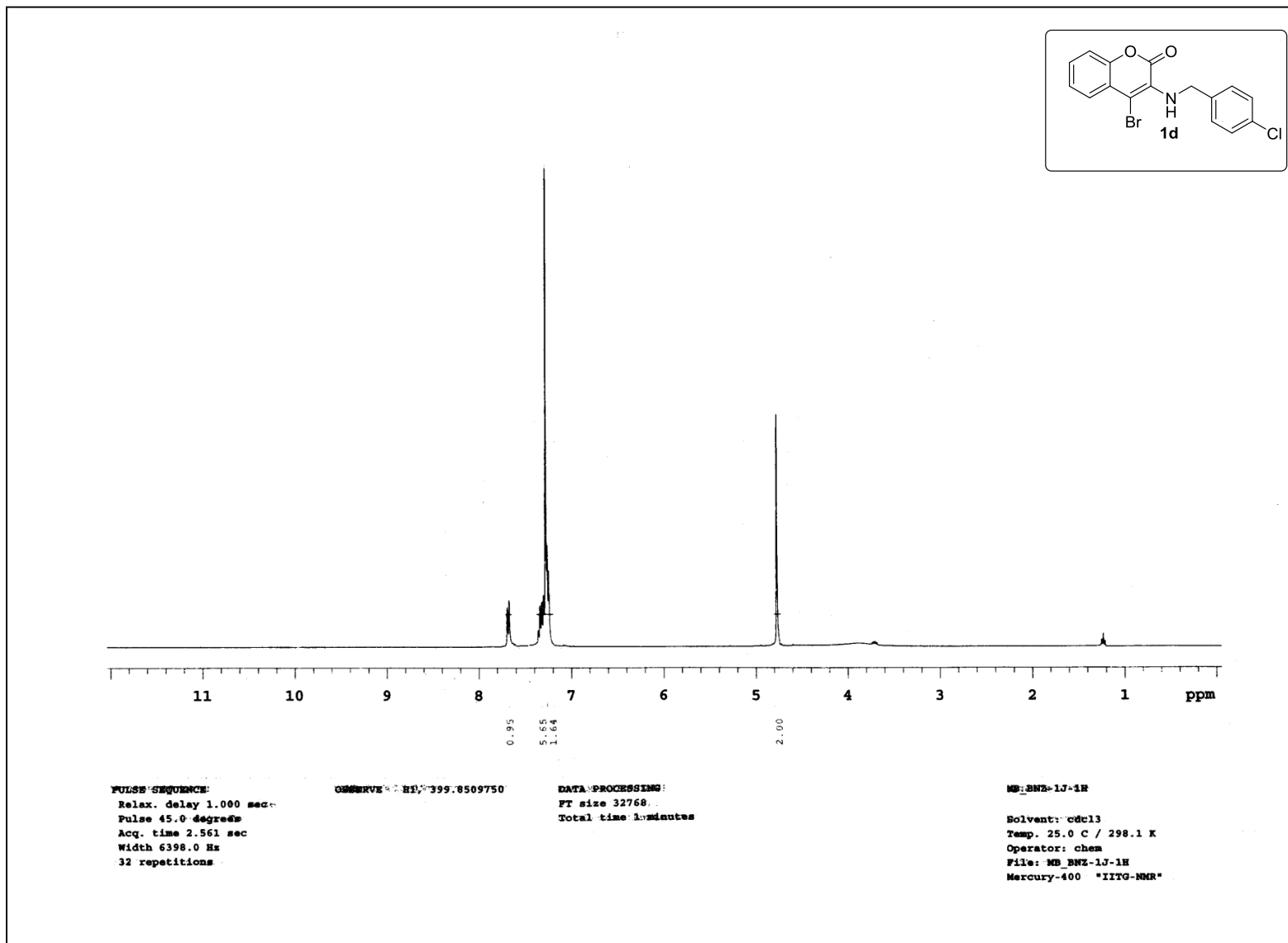


HRMS spectra of 1c

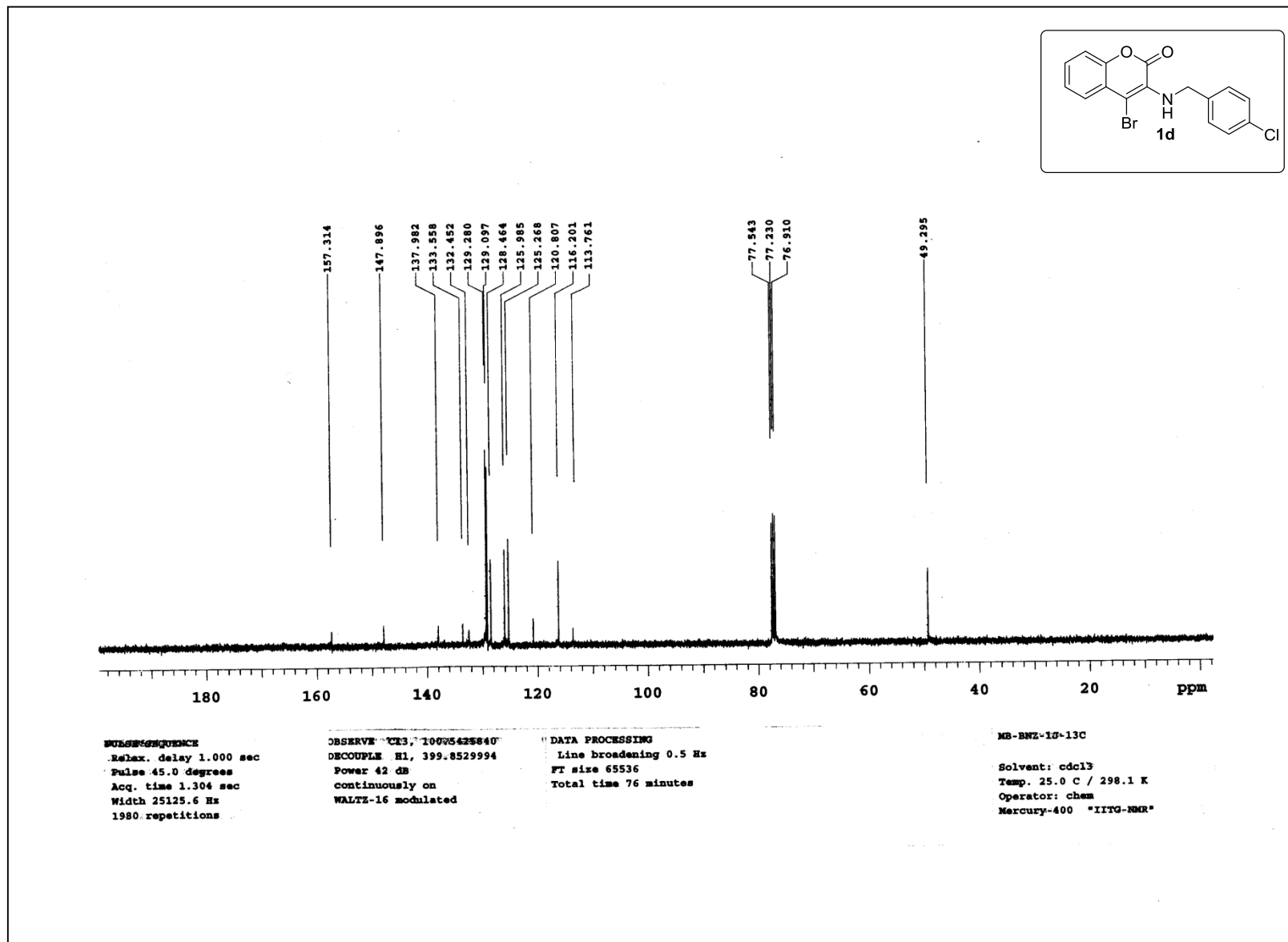
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¹H NMR spectra of **1d**

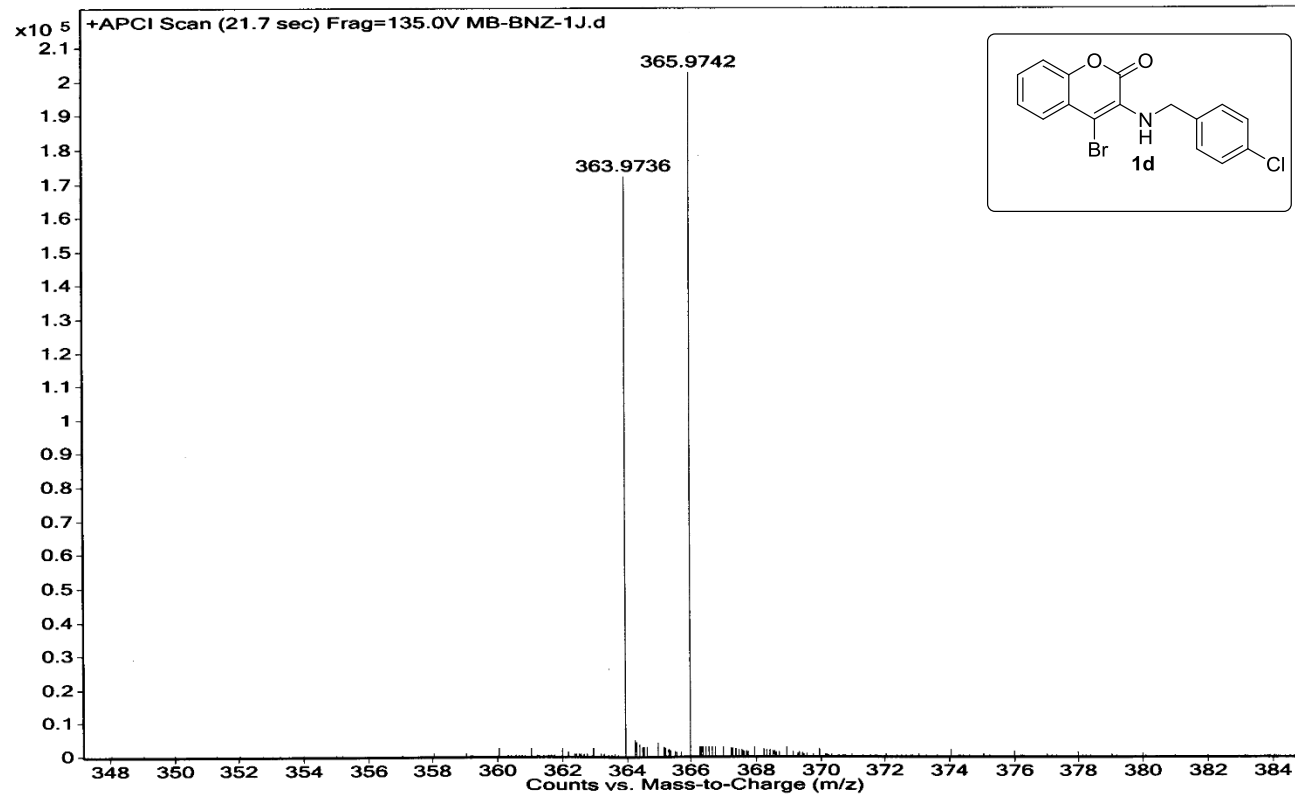


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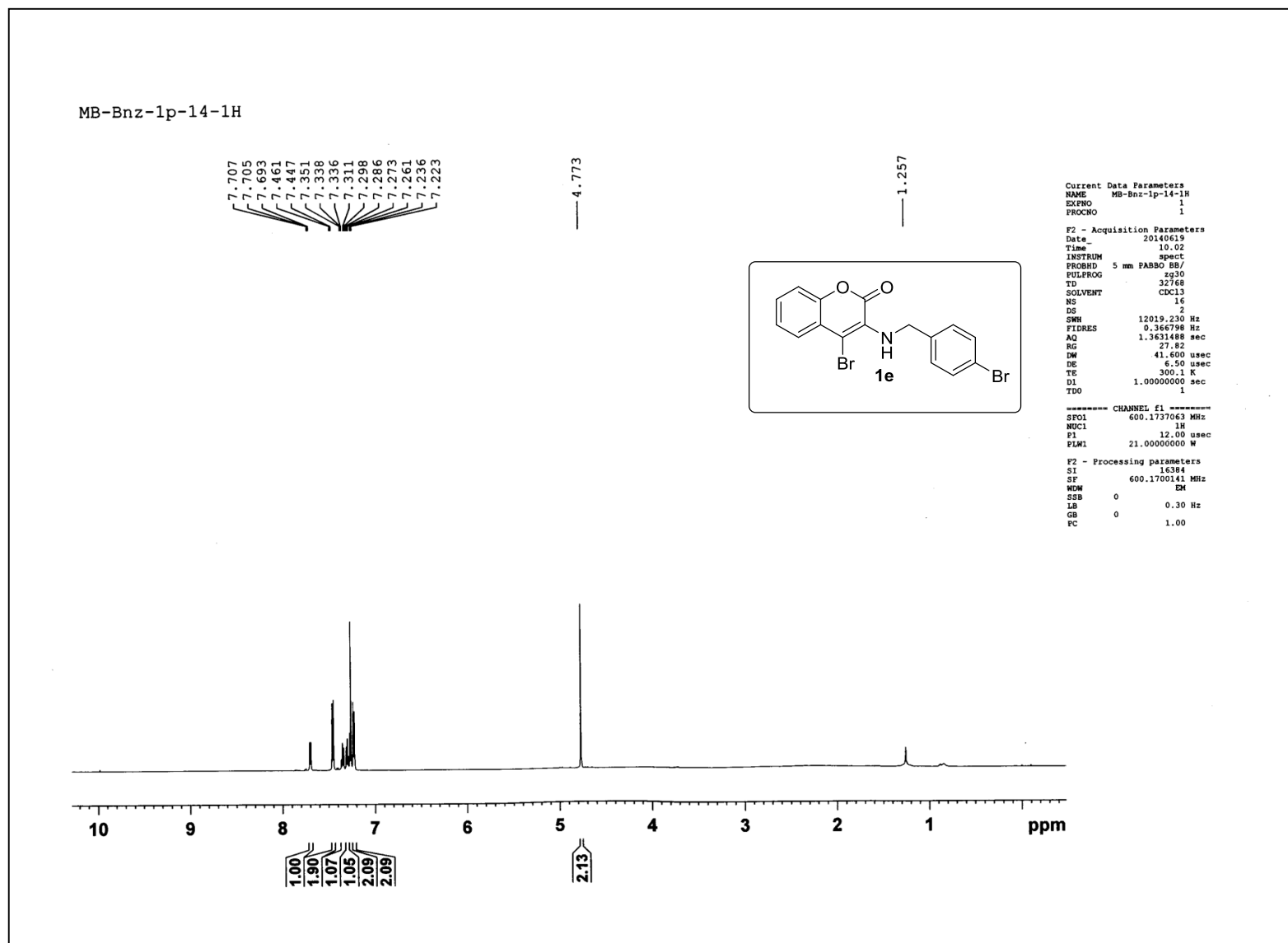


HRMS Spectra of **1d**

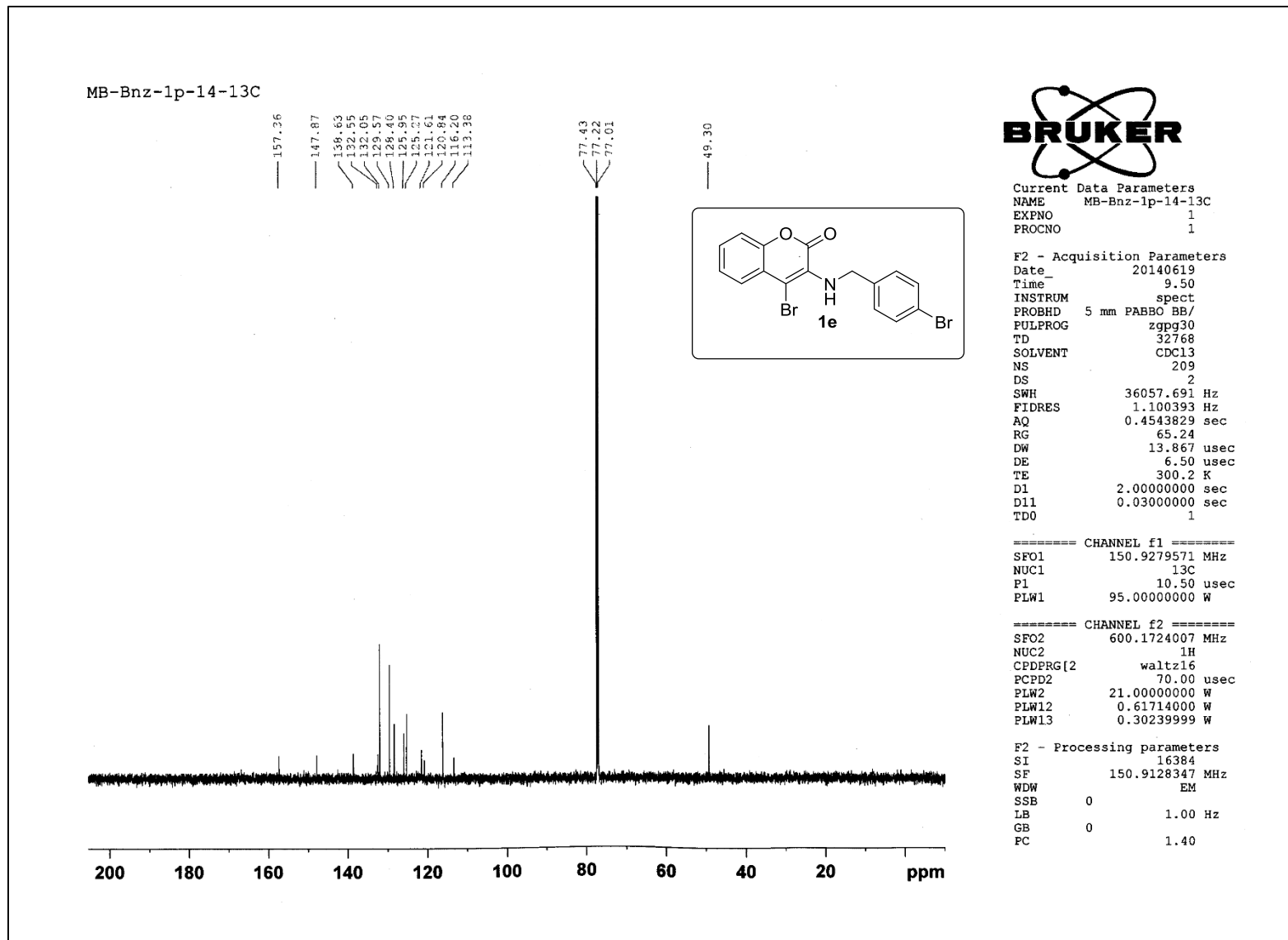
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¹H NMR spectra of **1e**

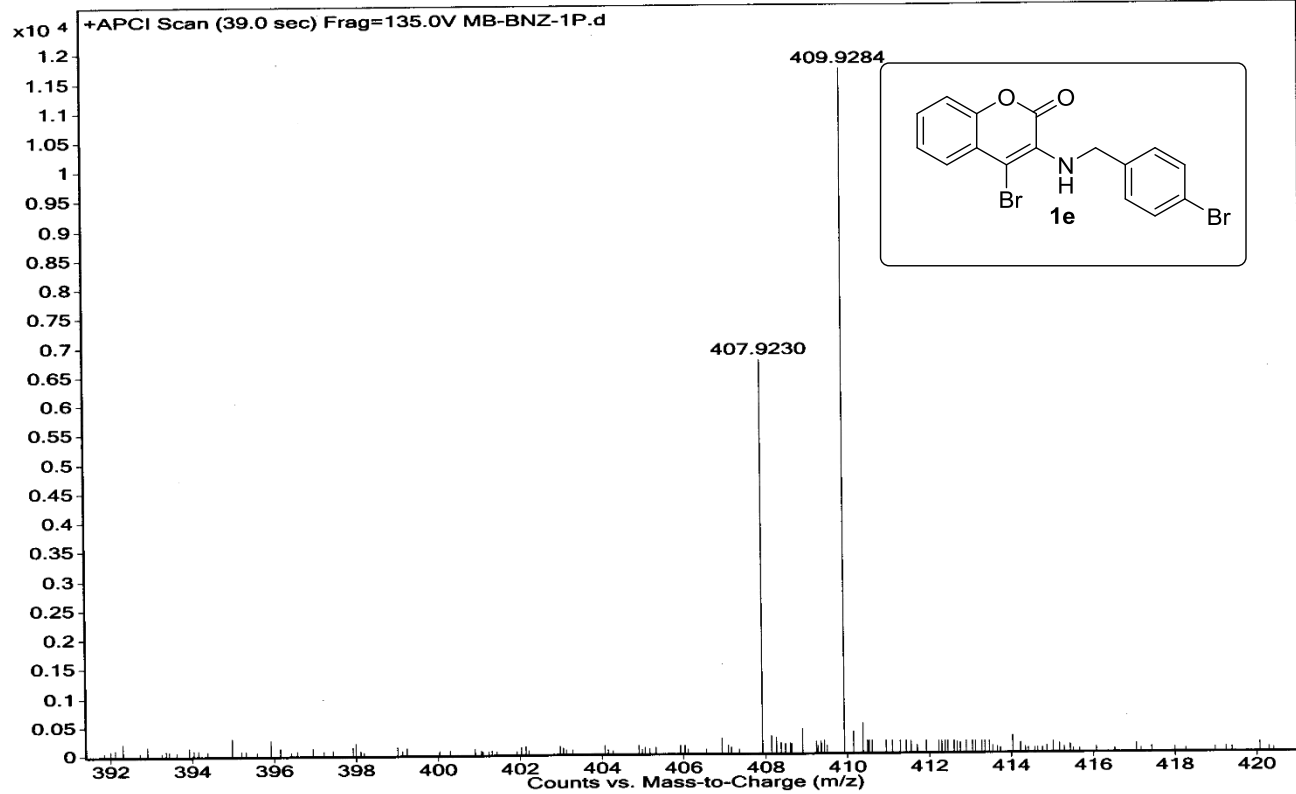


¹³C NMR spectra of **1e**

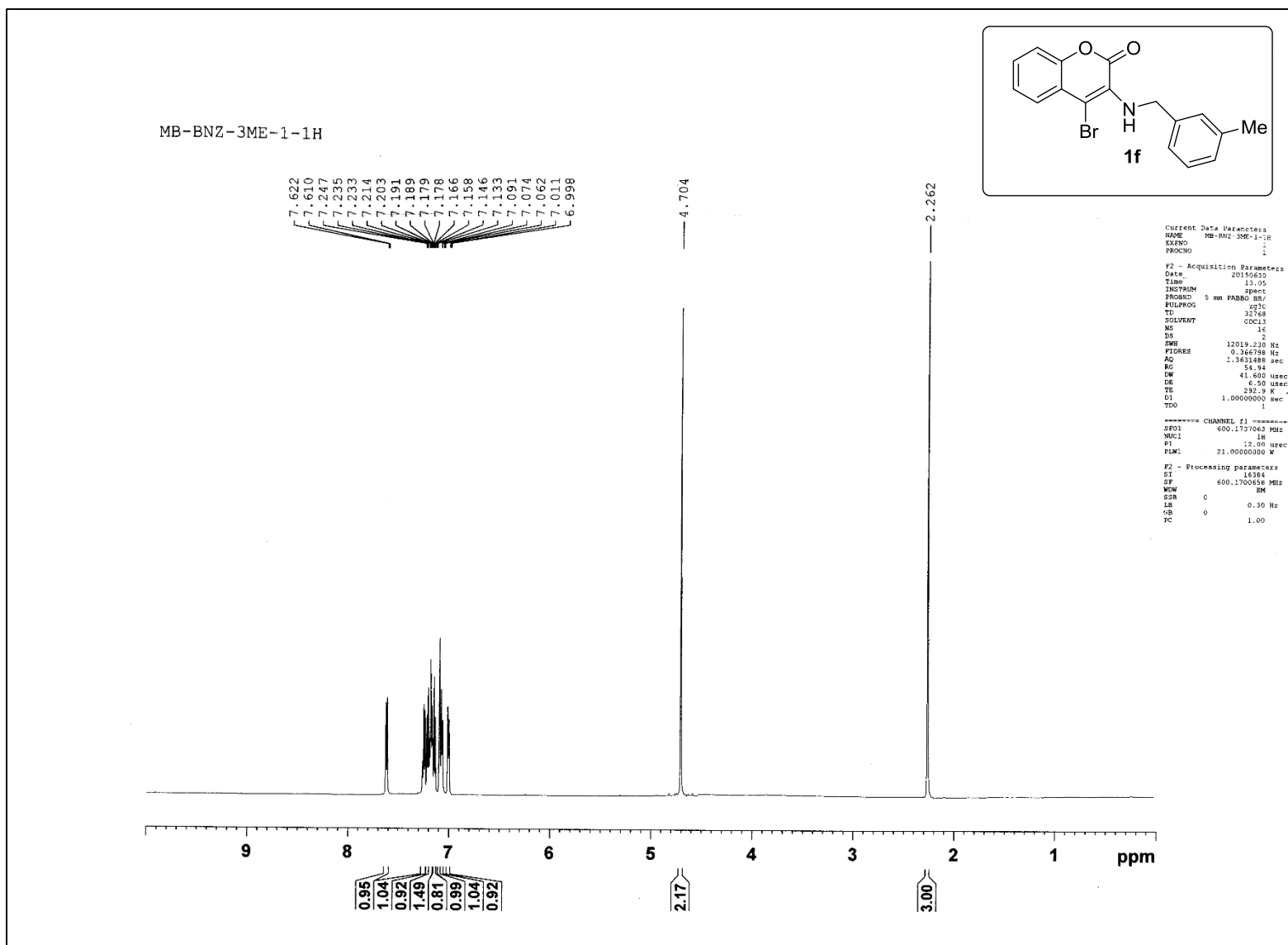


HRMS Spectra of 1e

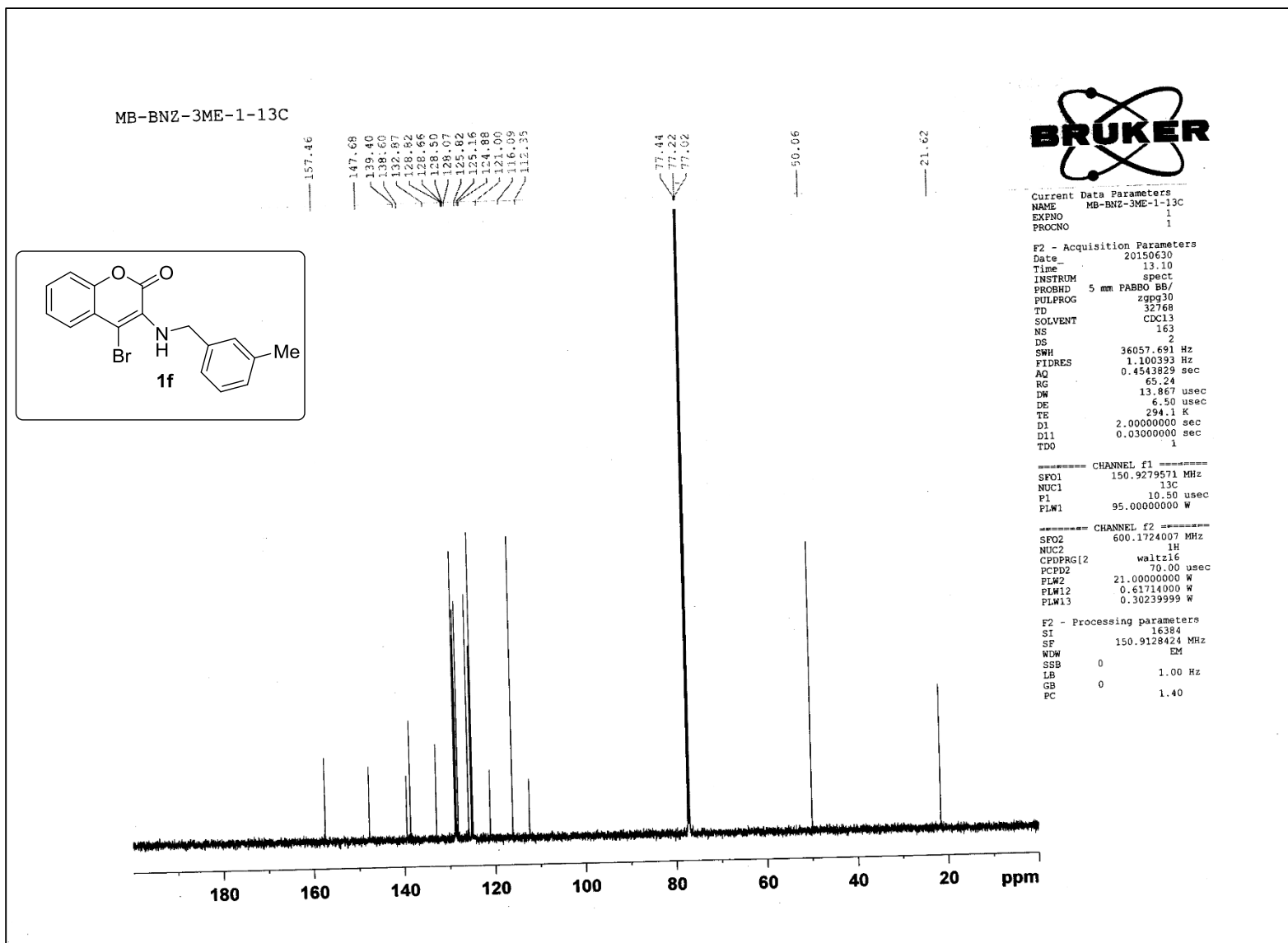
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Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



H1 NMR Spectra of 1f

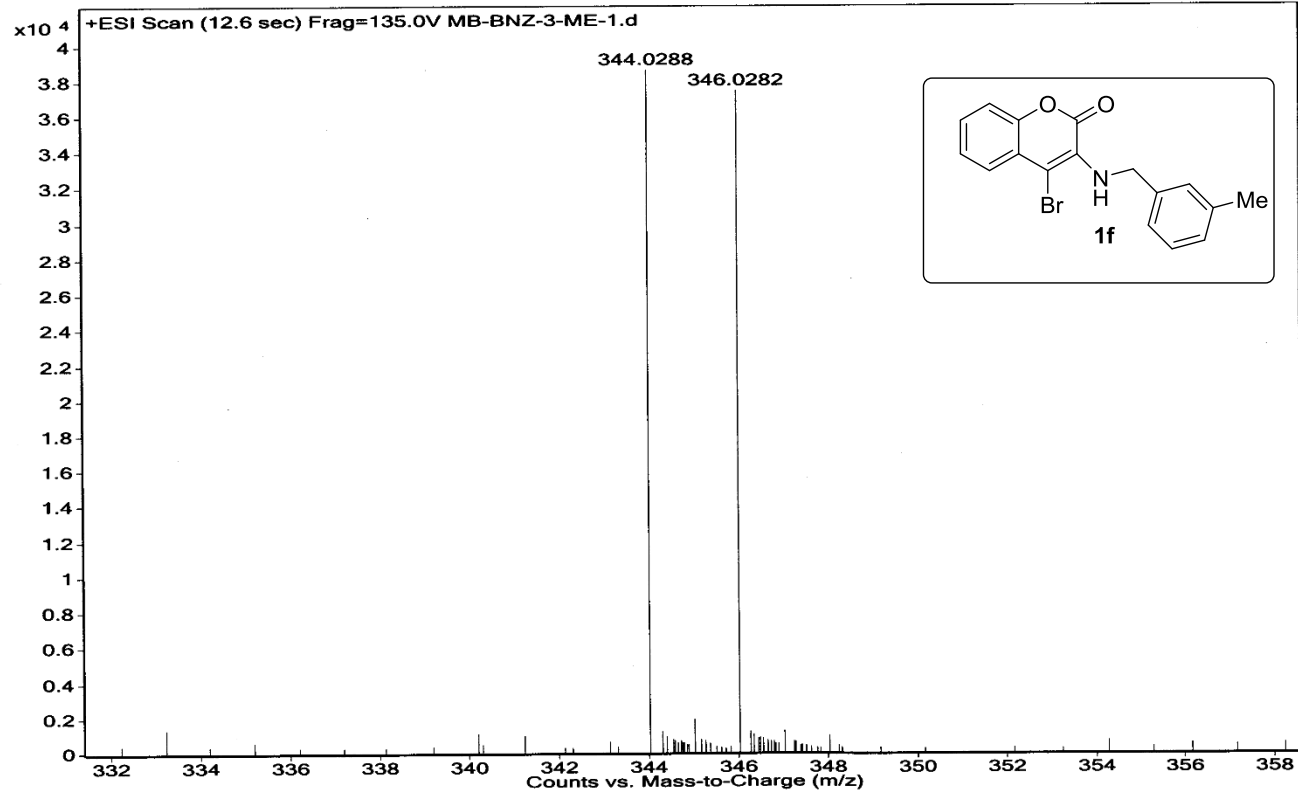


¹³C NMR spectra of **1f**

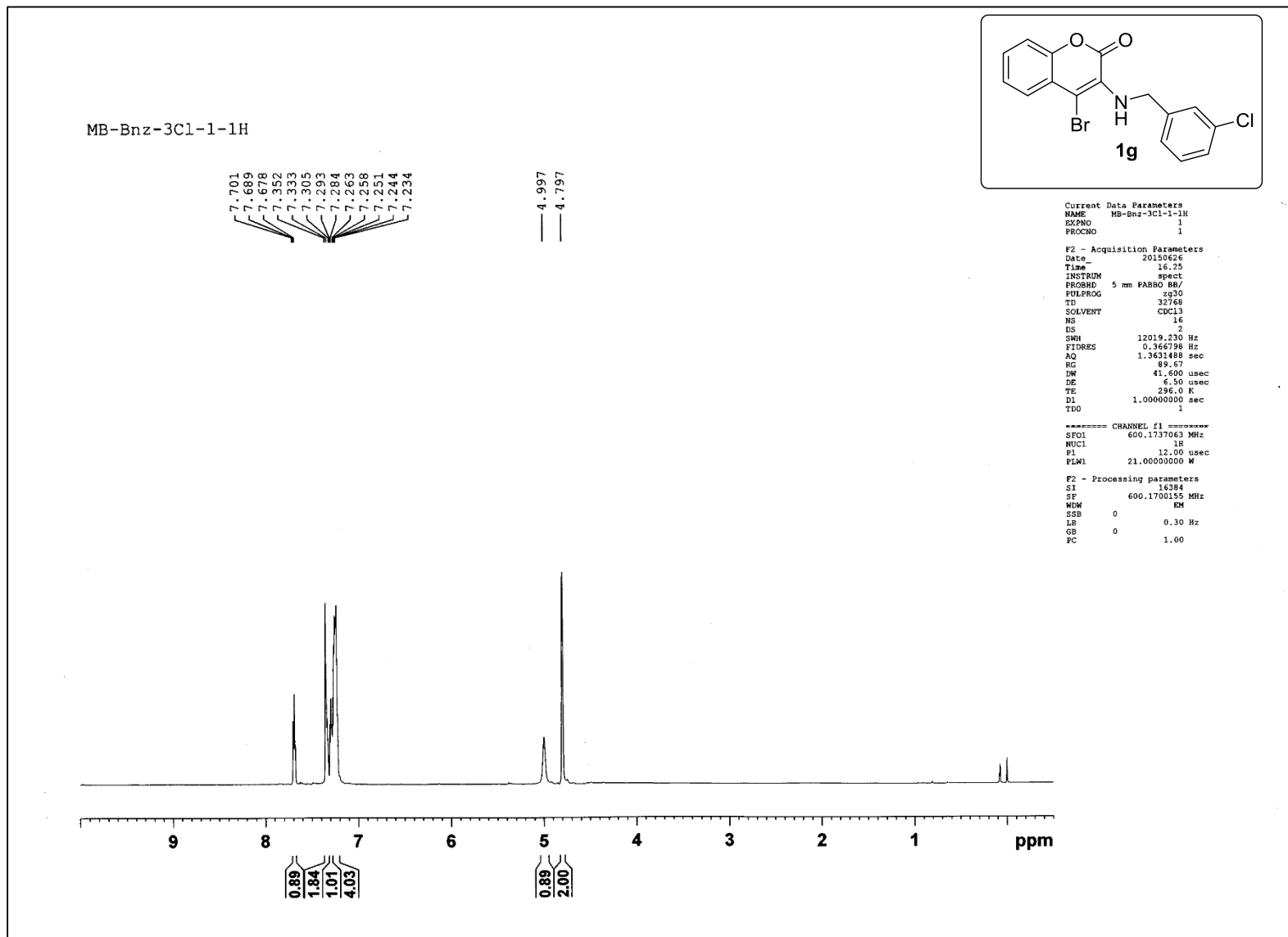


HRMS Spectra of **1f**

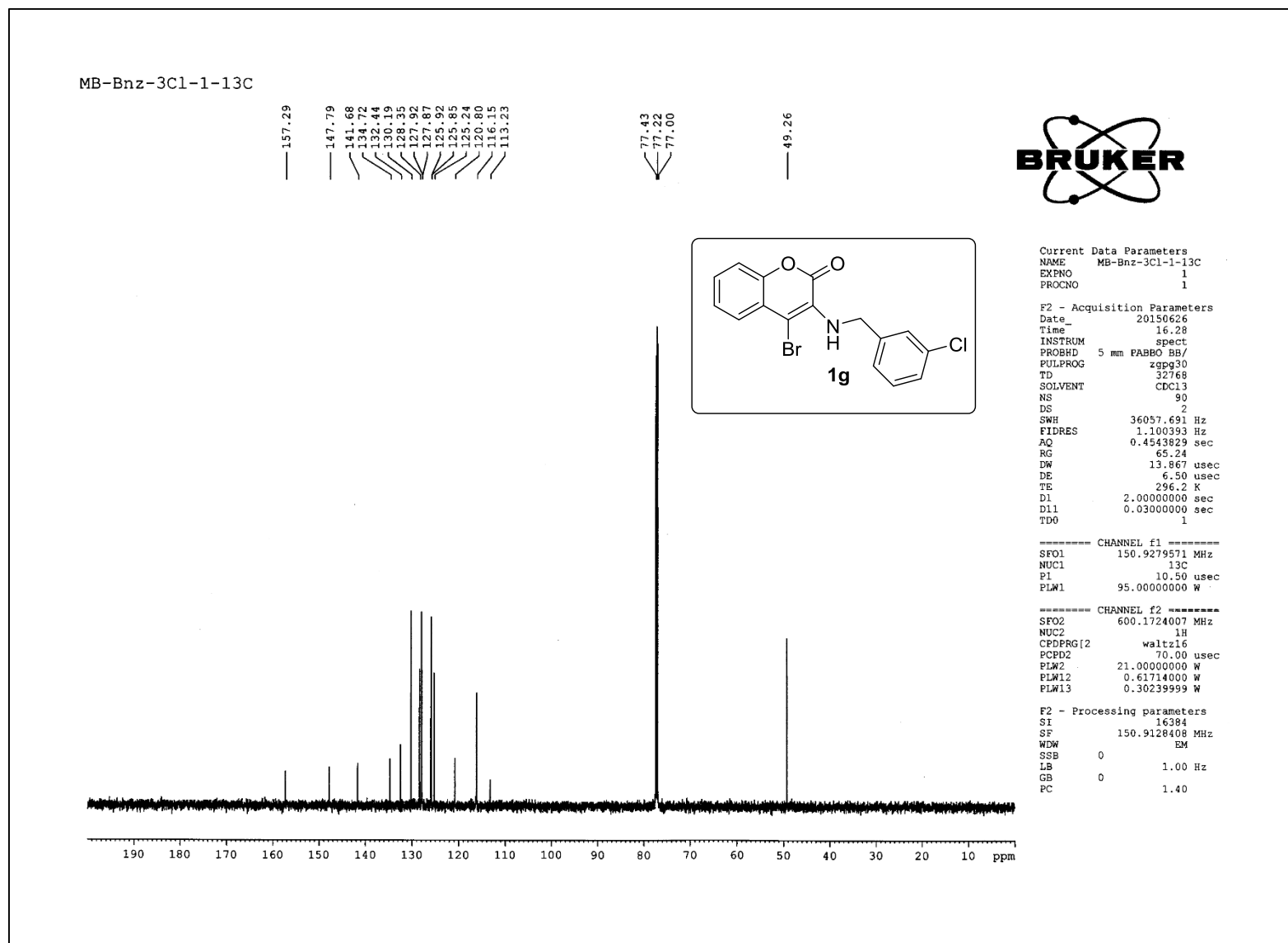
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¹H NMR spectra of **1g**



¹³C NMR spectra of **1g**



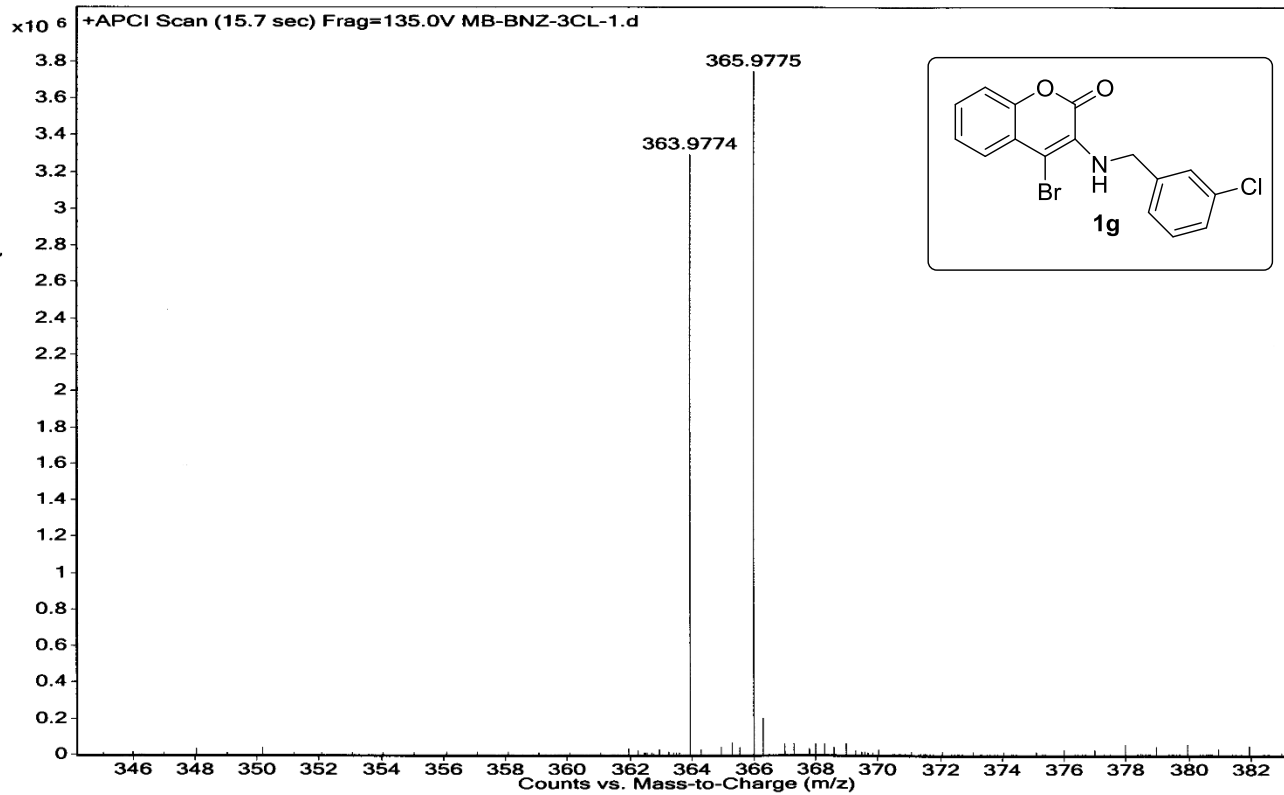
HRMS Spectra of **1g**

Sample Name
Inj Vol
Data Filename

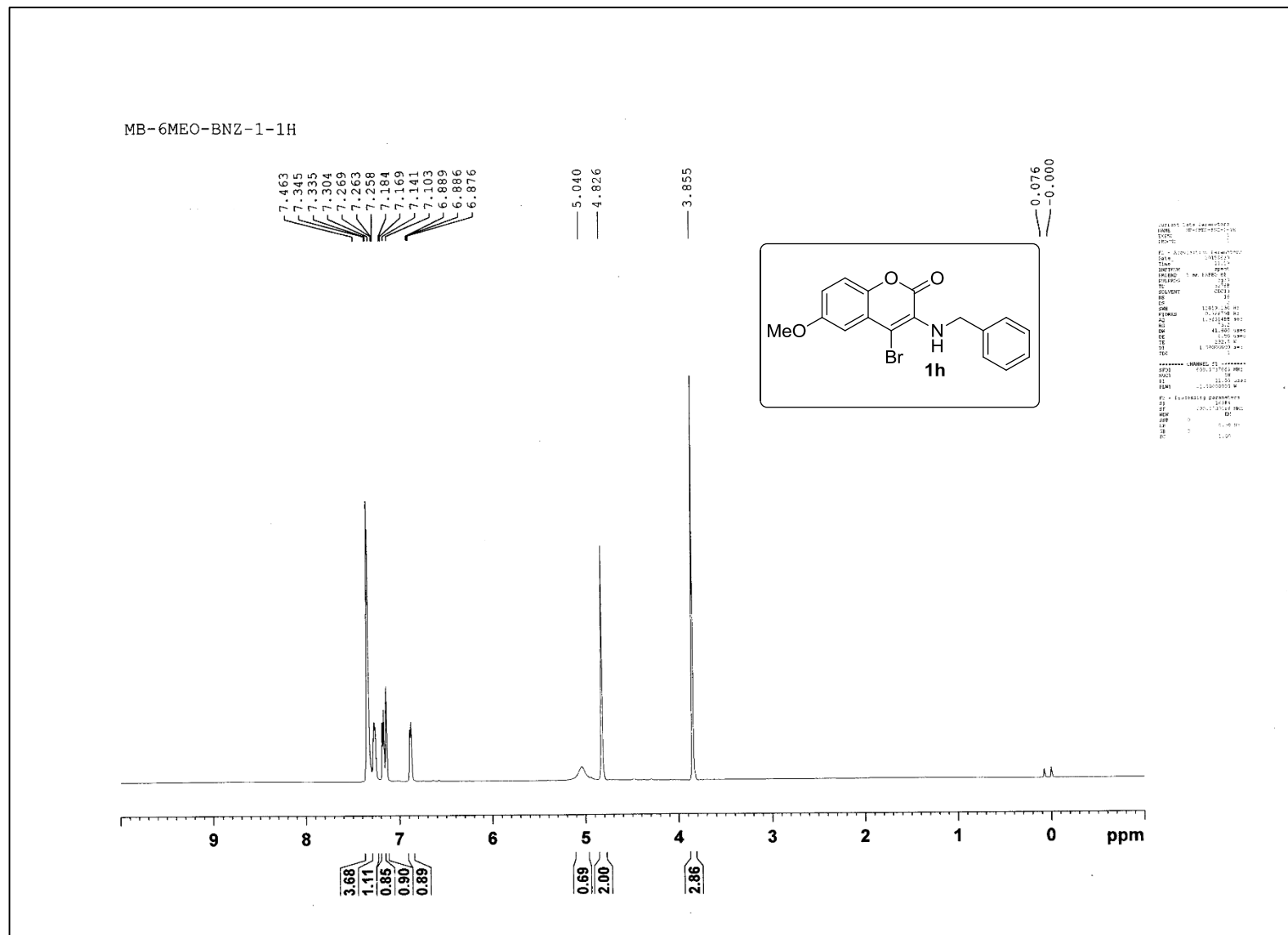
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Instrument Name
SampleType
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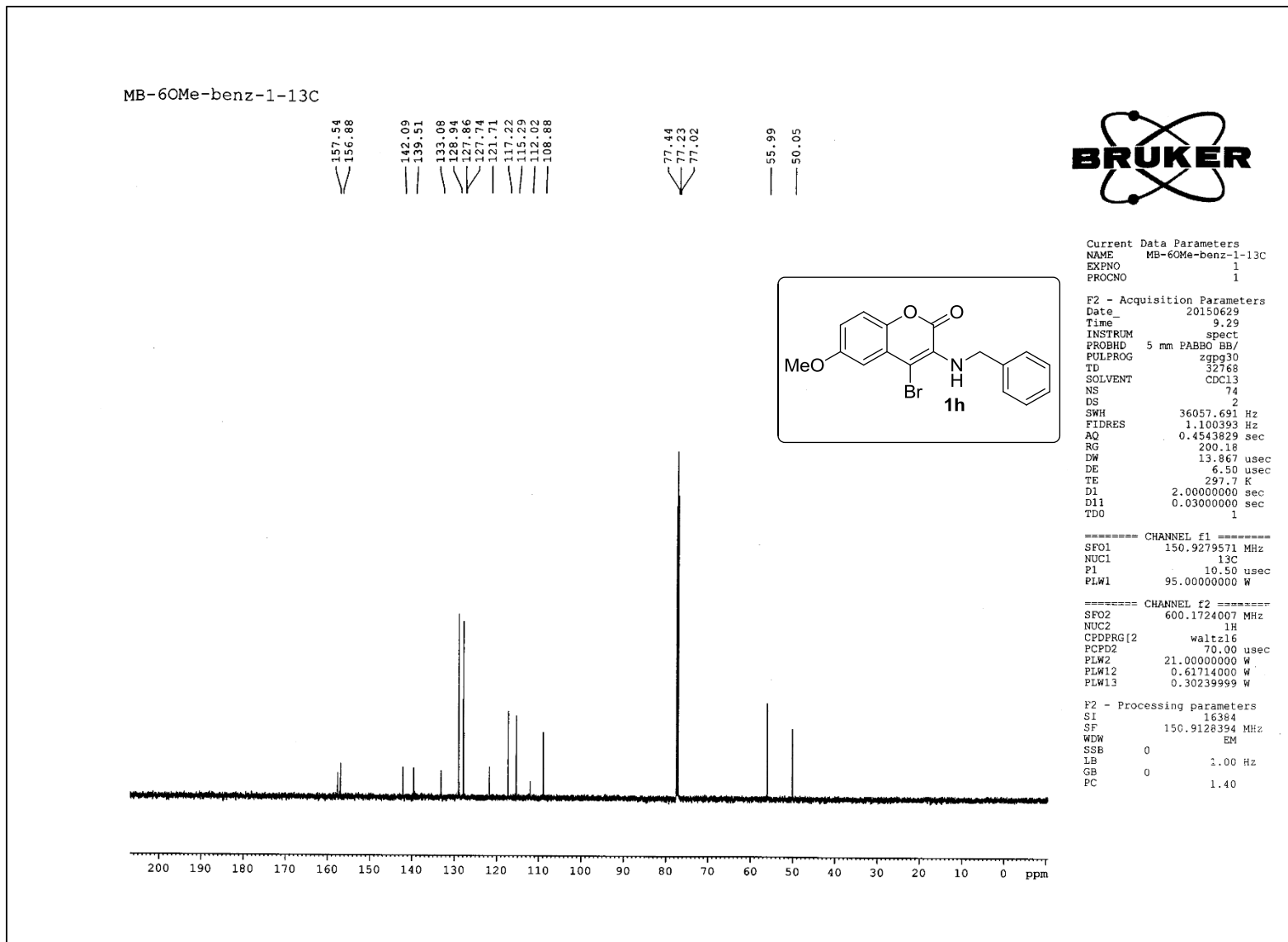
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¹H NMR spectra of **1h**

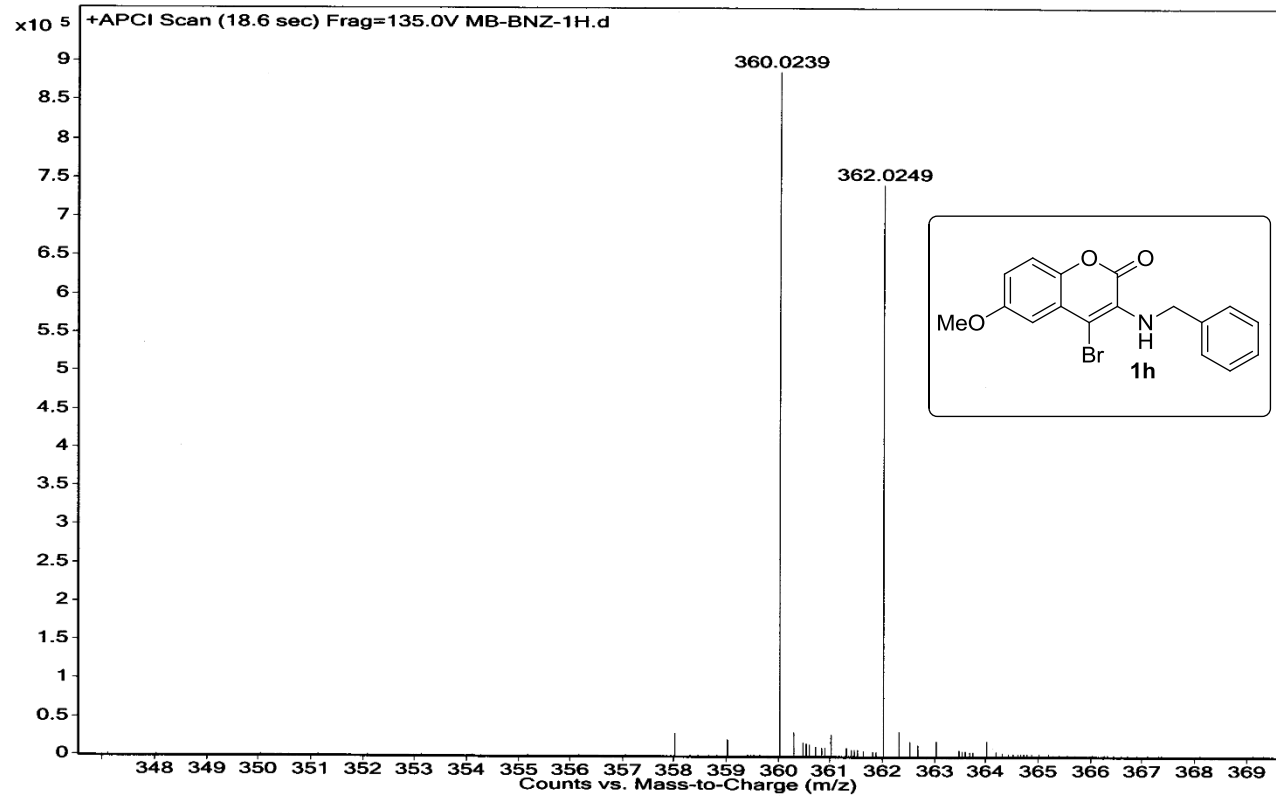


¹³C NMR of spectra of **1h**

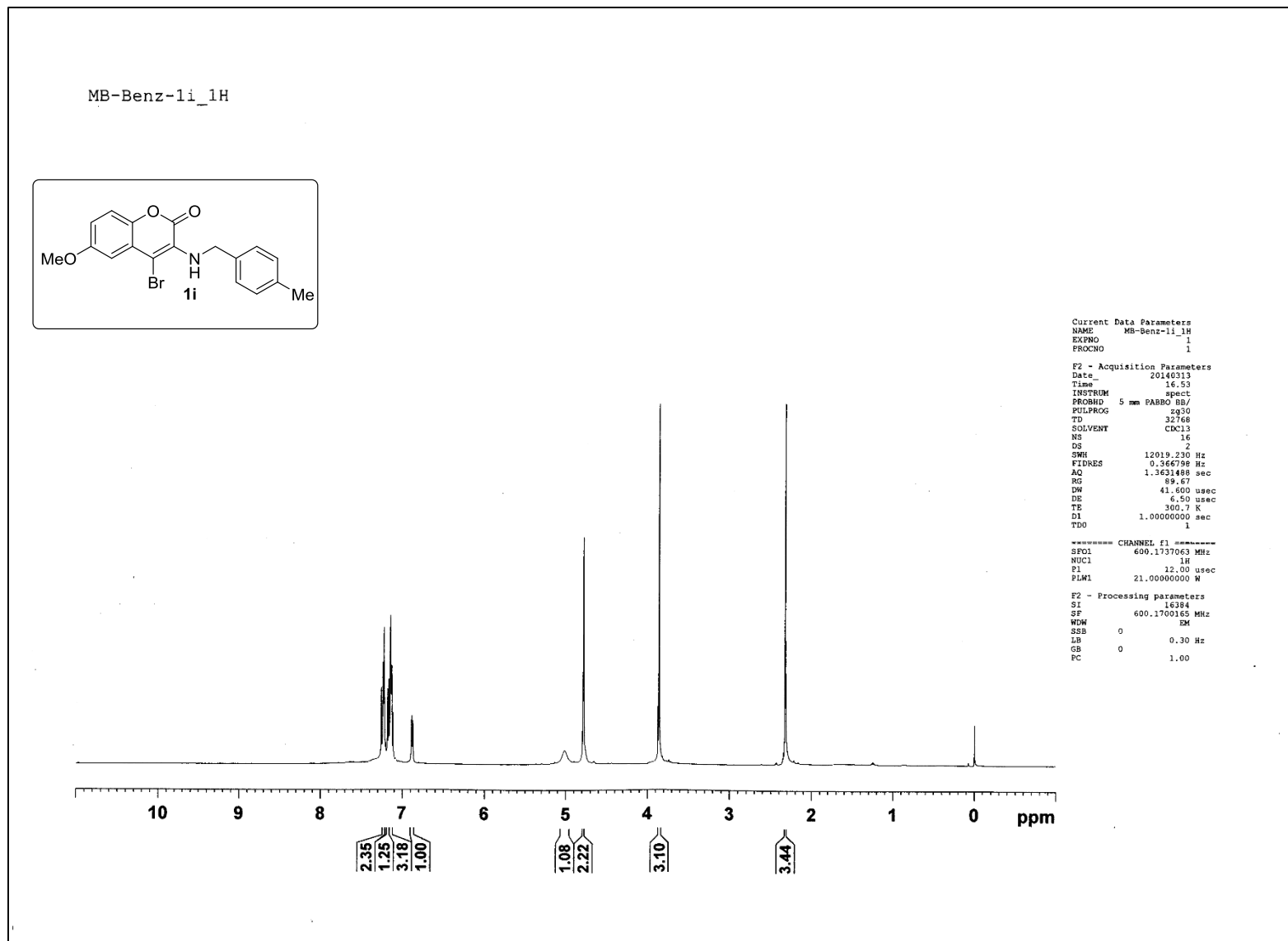


HRMS spectra of **1h**

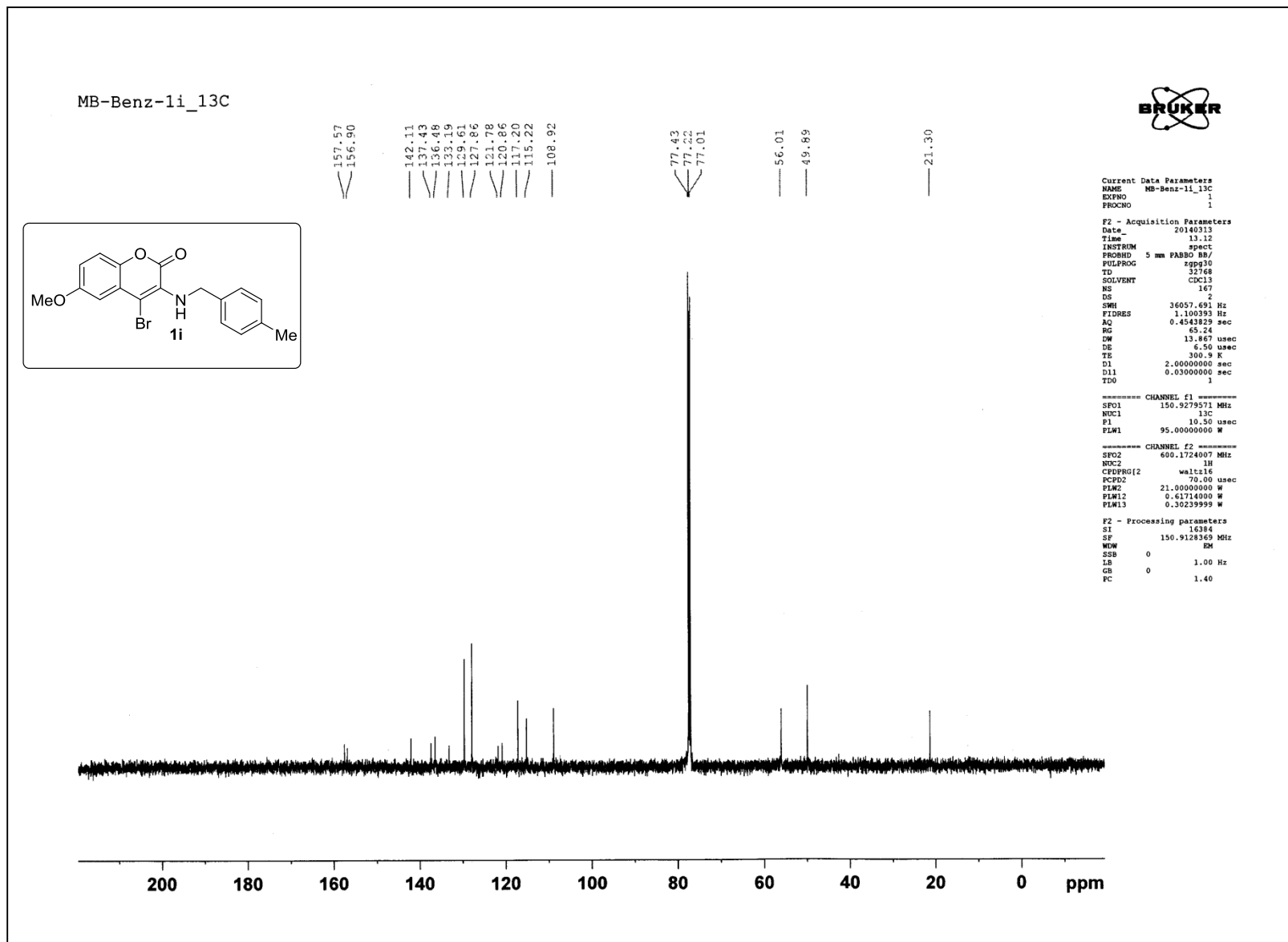
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Data Filename	ACQ Method	Comment	Acquired Time



¹H NMR spectra of **1i**

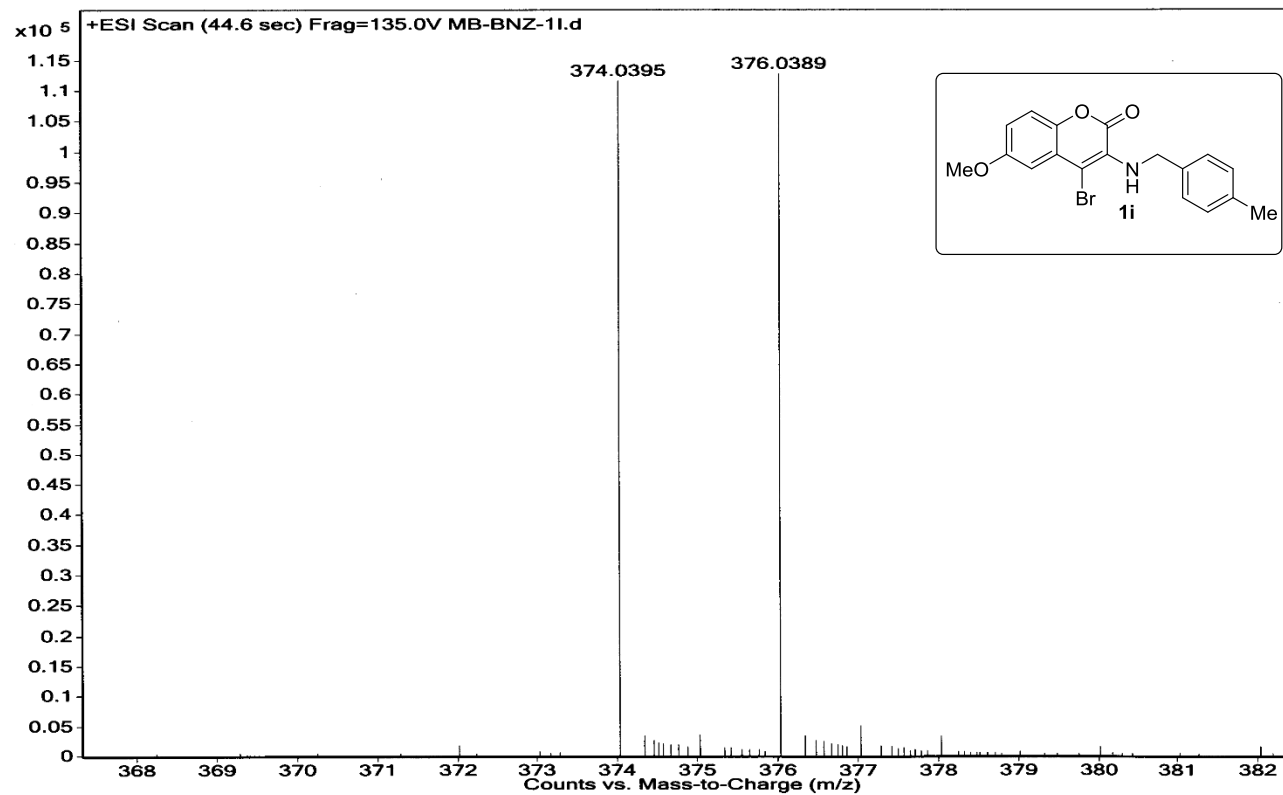


¹³C NMR spectra of **1i**

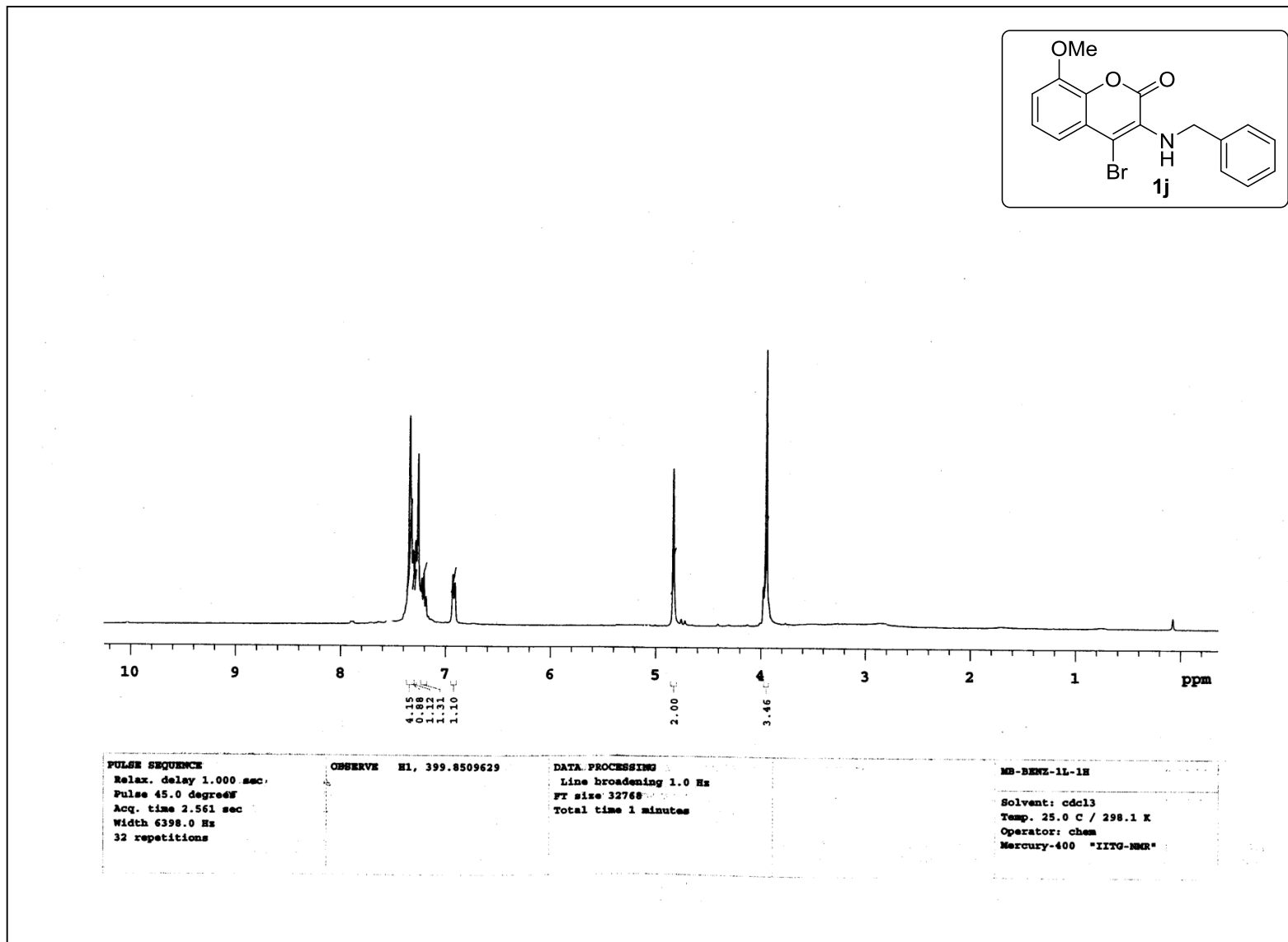


HRMS spectra of **1i**

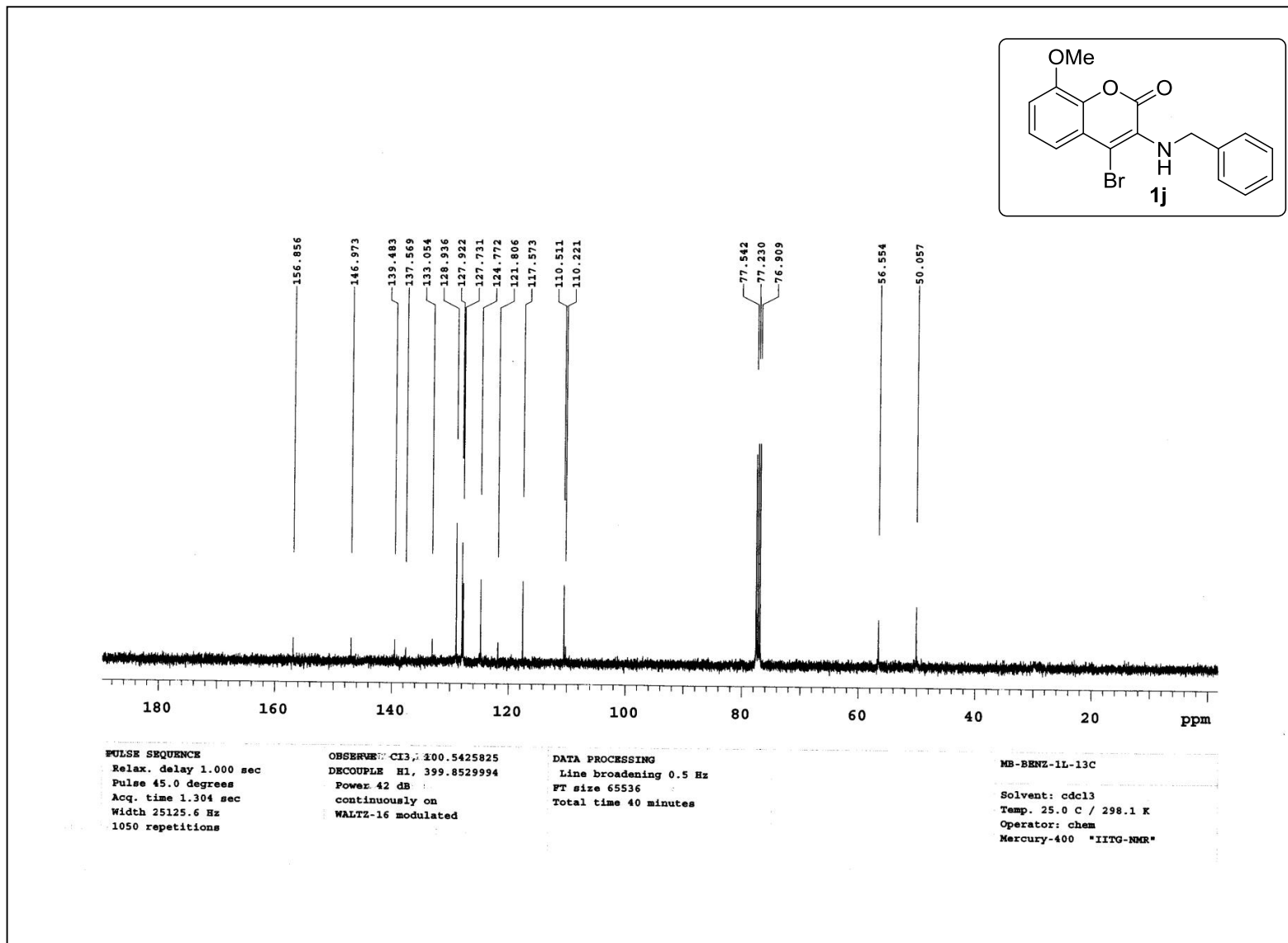
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^1H NMR spectra of **1j**

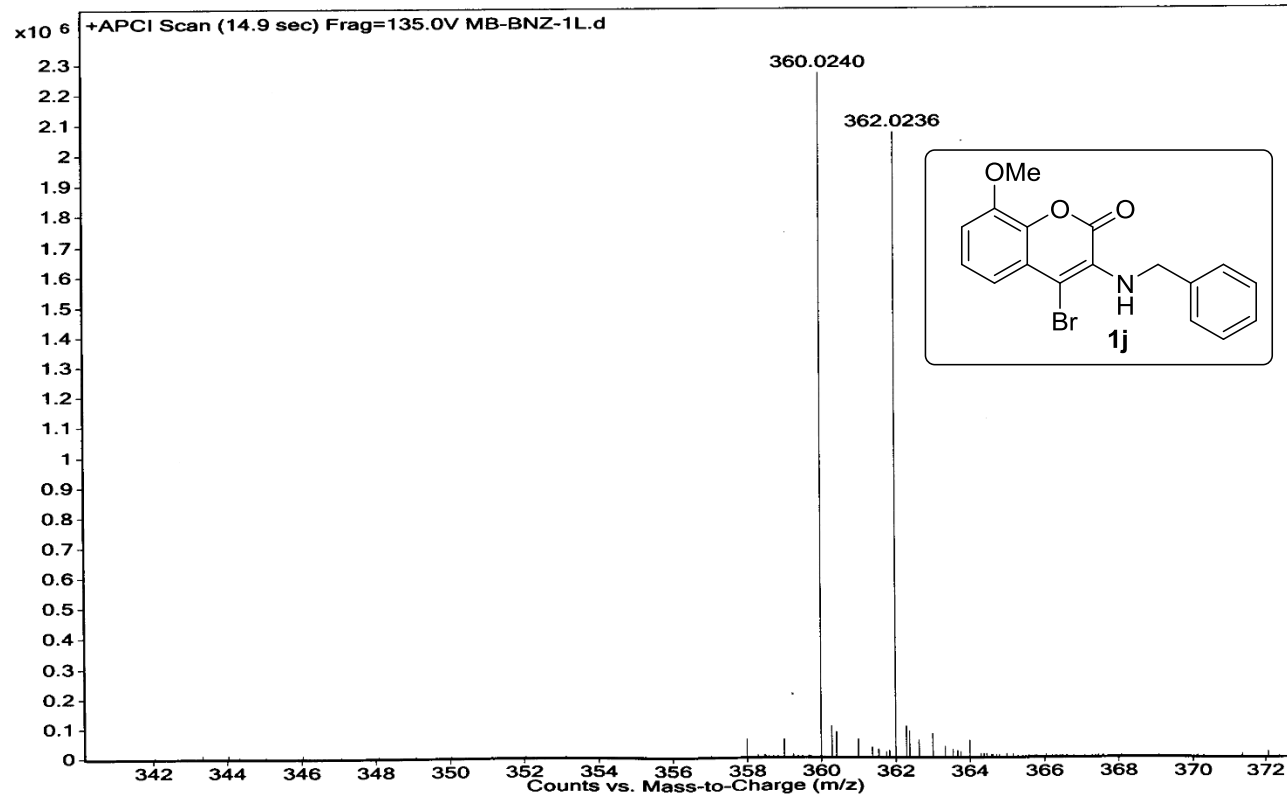


¹³C NMR spectra of **1j**

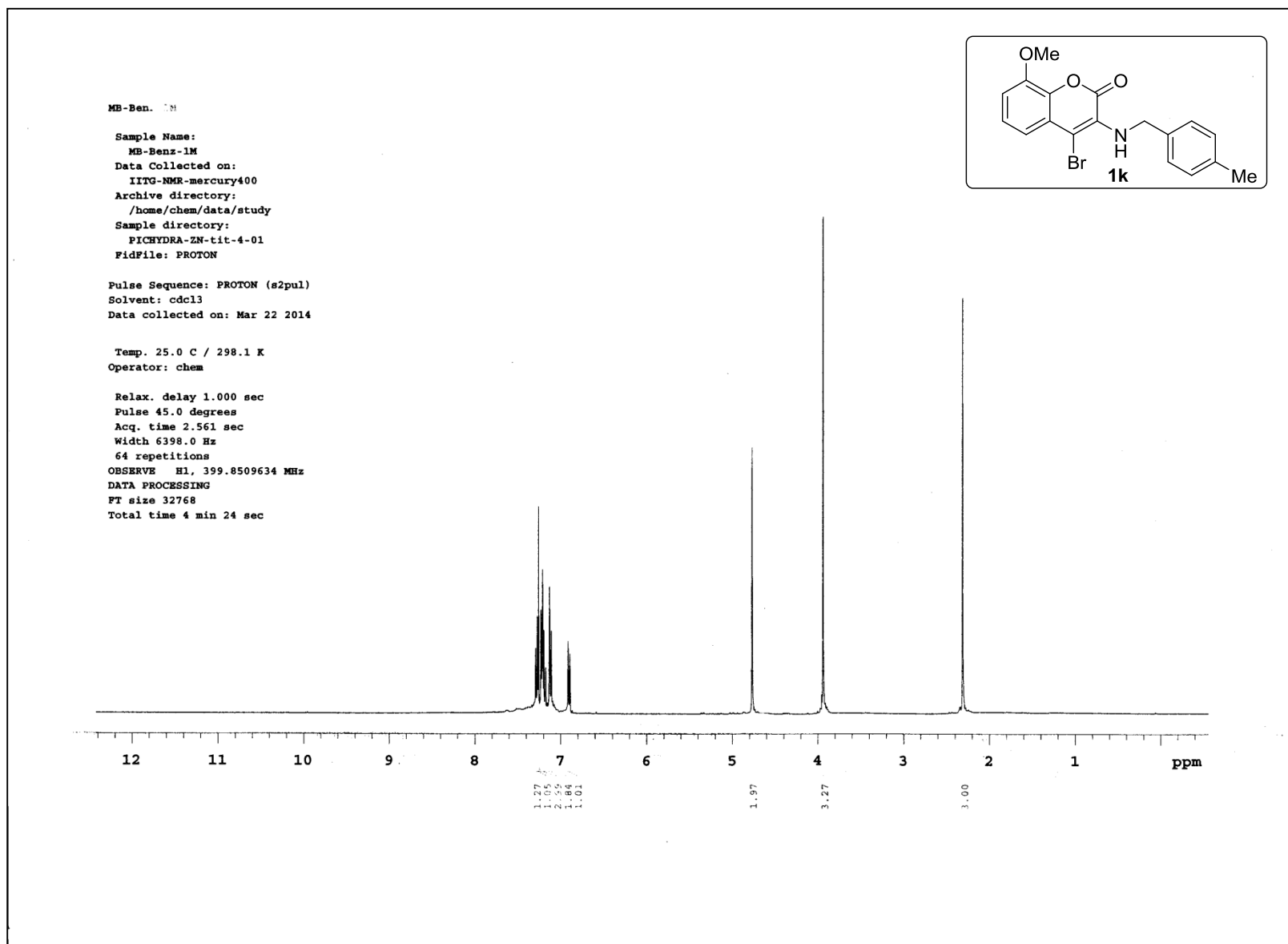


HRMS spectra of 1j

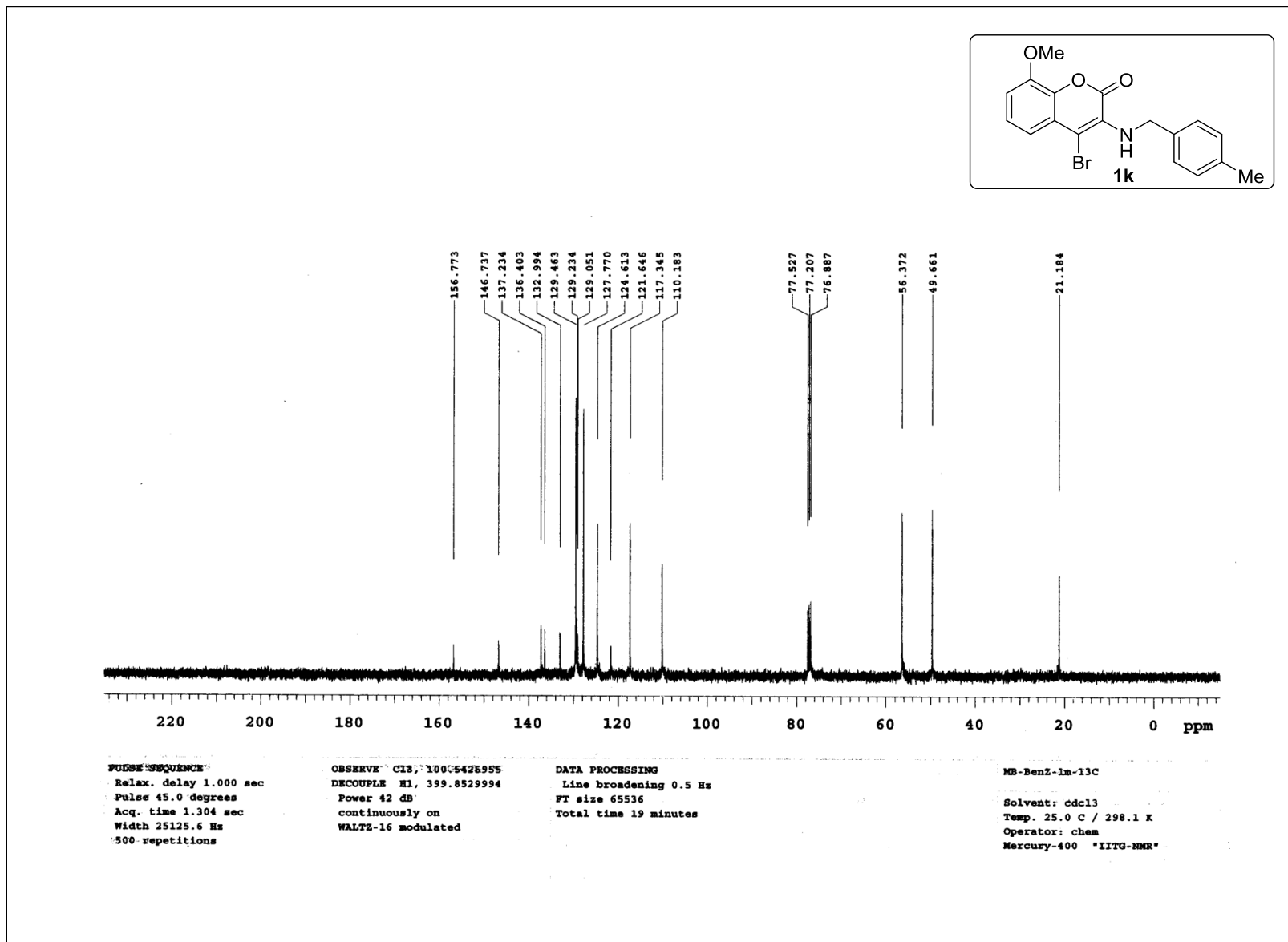
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



¹H NMR spectra of **1k**



¹³C NMR spectra of **1k**



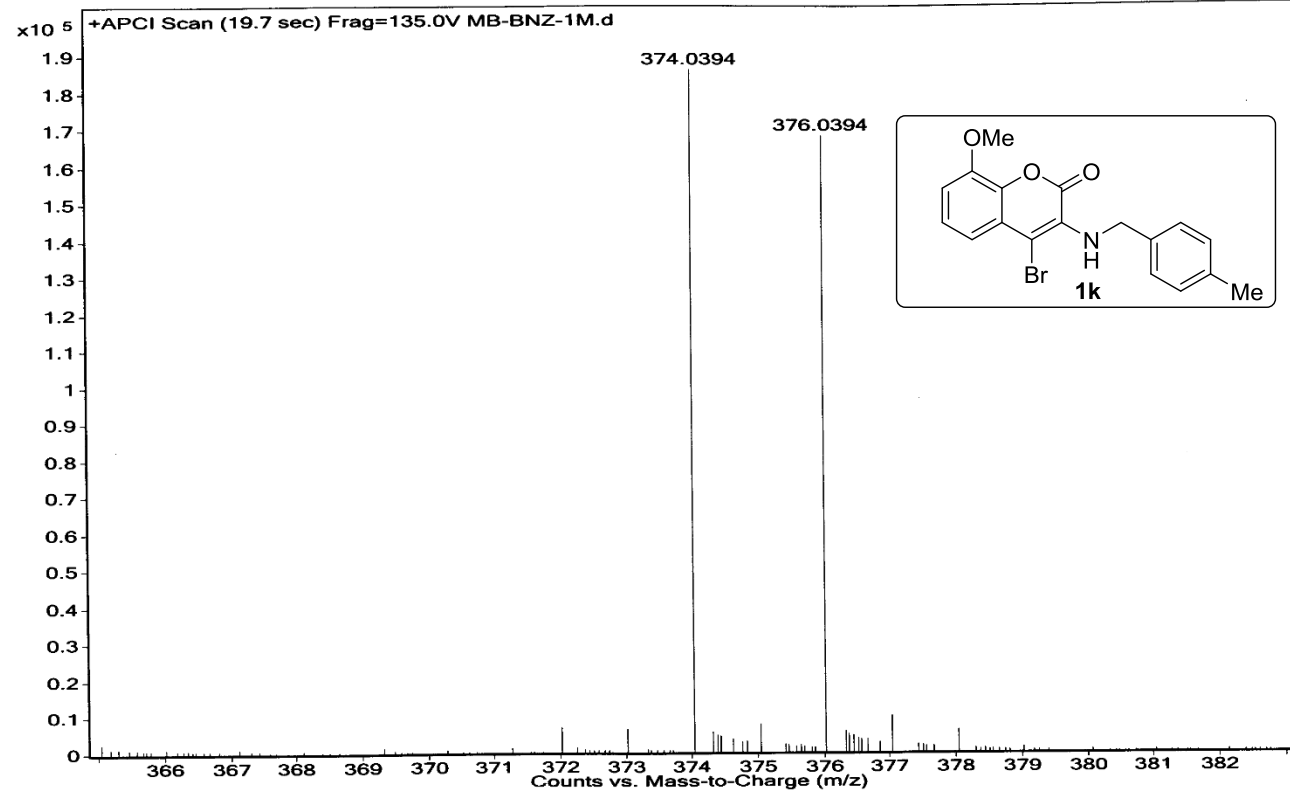
HRMS spectra of **1k**

Sample Name
Inj Vol
Data Filename

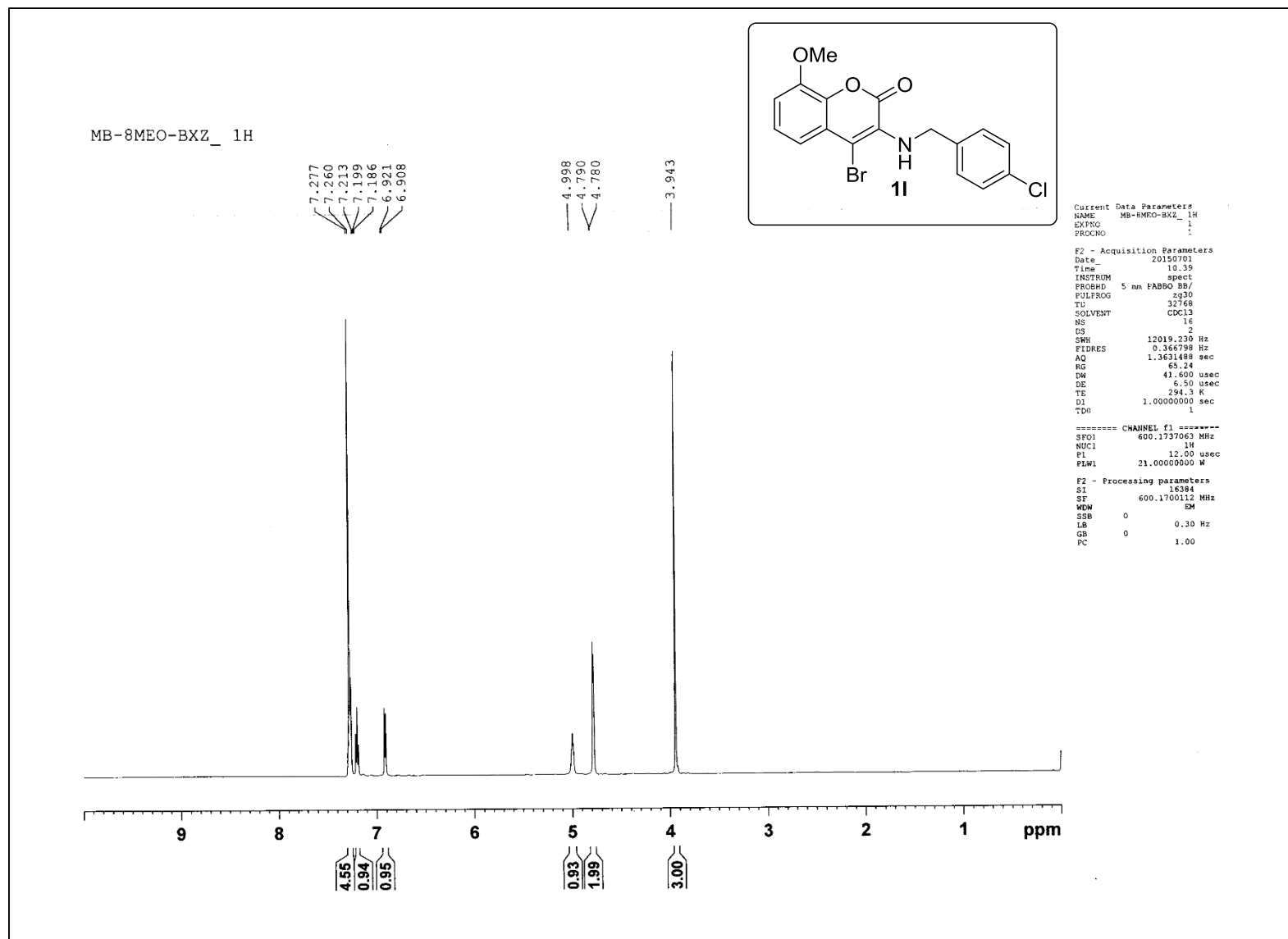
Position
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ACQ Method

Instrument Name
SampleType
Comment

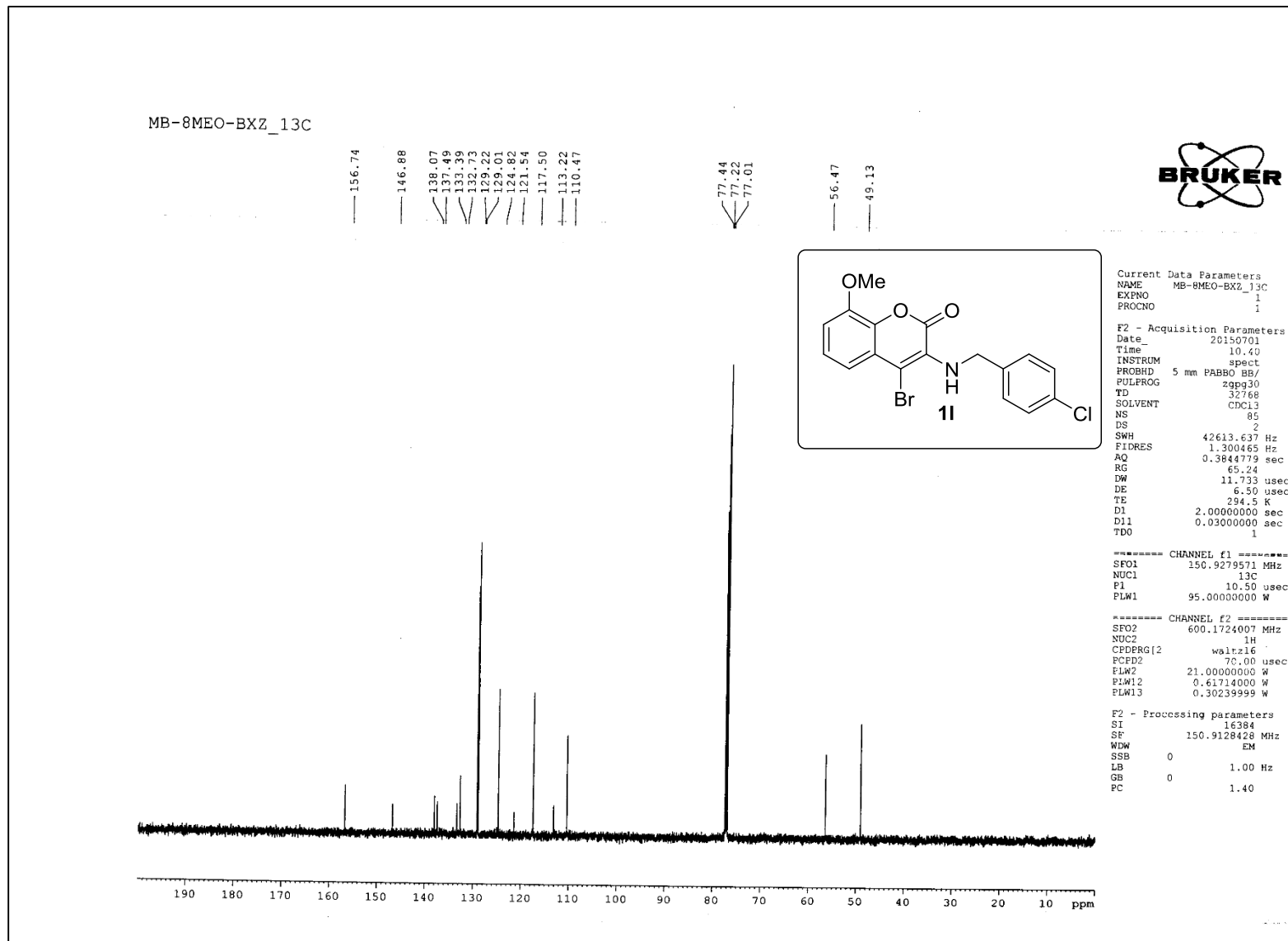
User Name
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Acquired Time



¹H NMR spectra of **11**

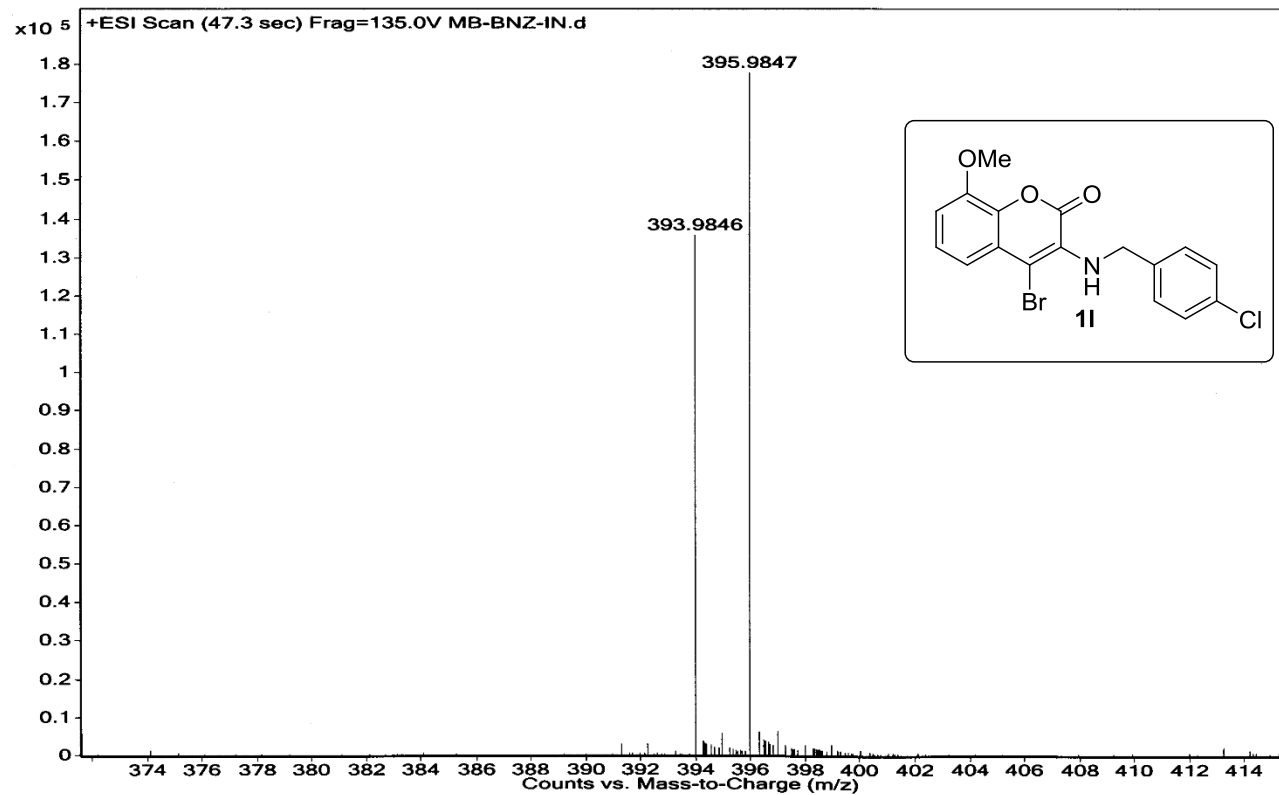


¹³C NMR spectra of 11



HRMS spectra of **1l**

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Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BNZ-IN.d	ACQ Method		Comment		Acquired Time	8/13/2015 3:09:52 PM



¹H NMR spectra of **1m**

MB-Benz-1C-1H

Sample Name:

MB-Benz-1C-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/home/chem/data/study

Sample directory:

DS_382_am-01

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 23 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

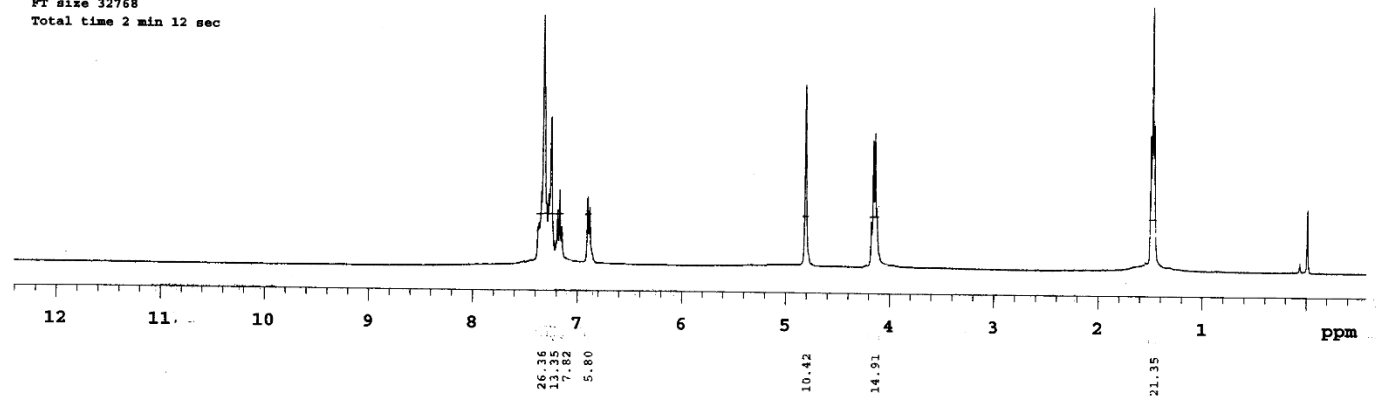
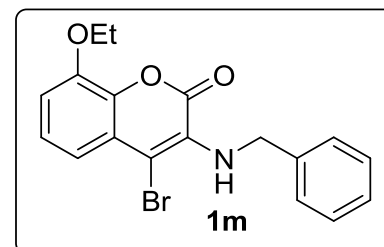
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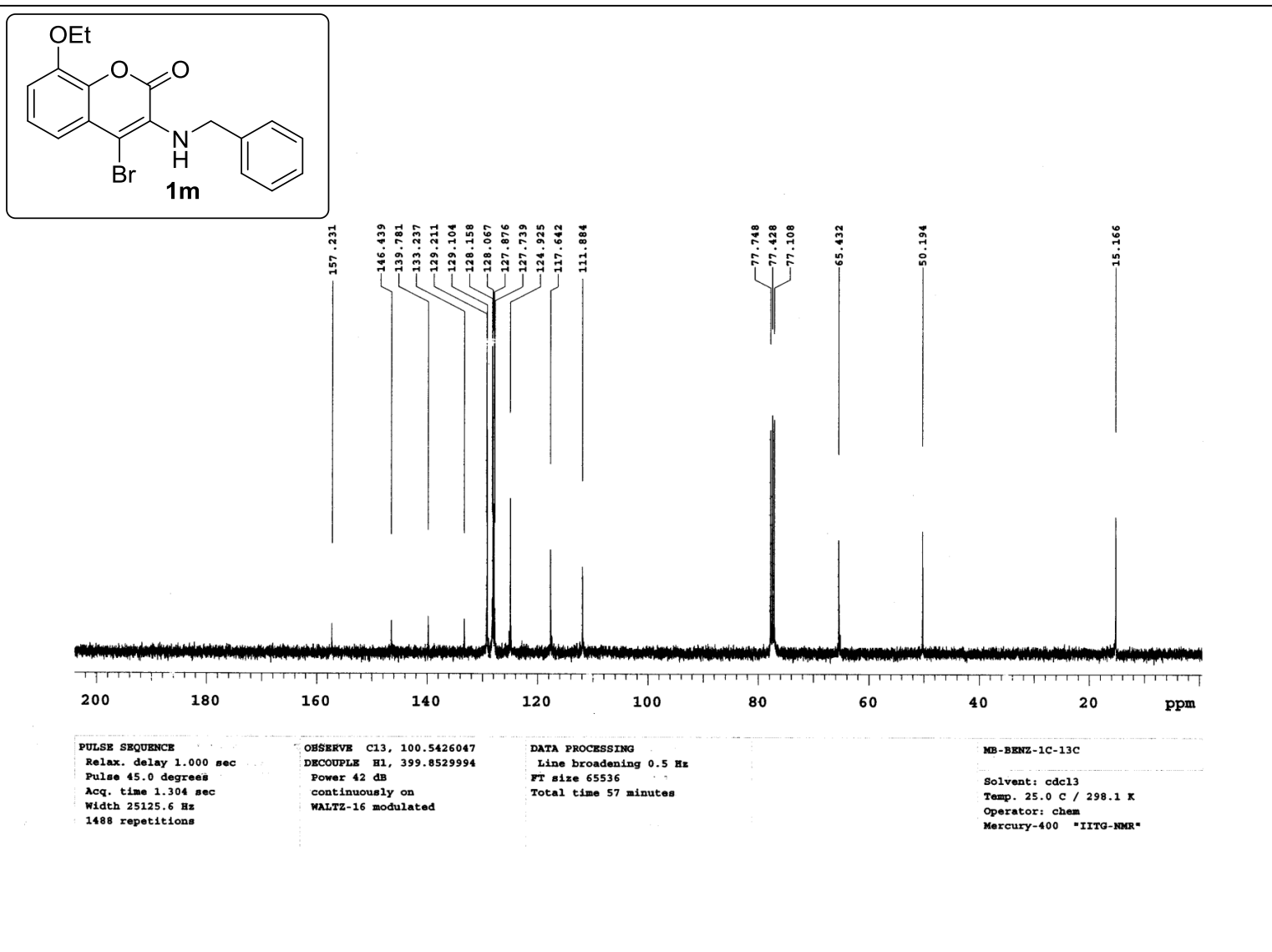
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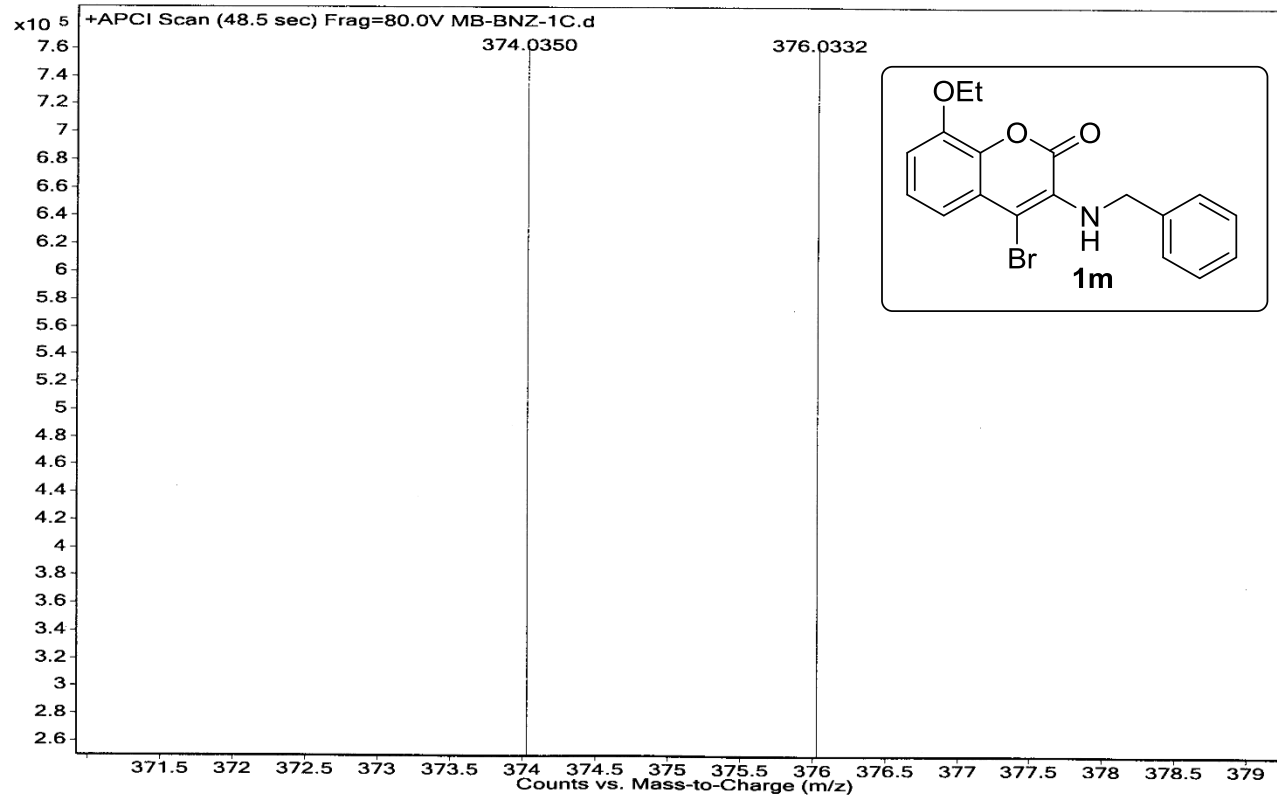


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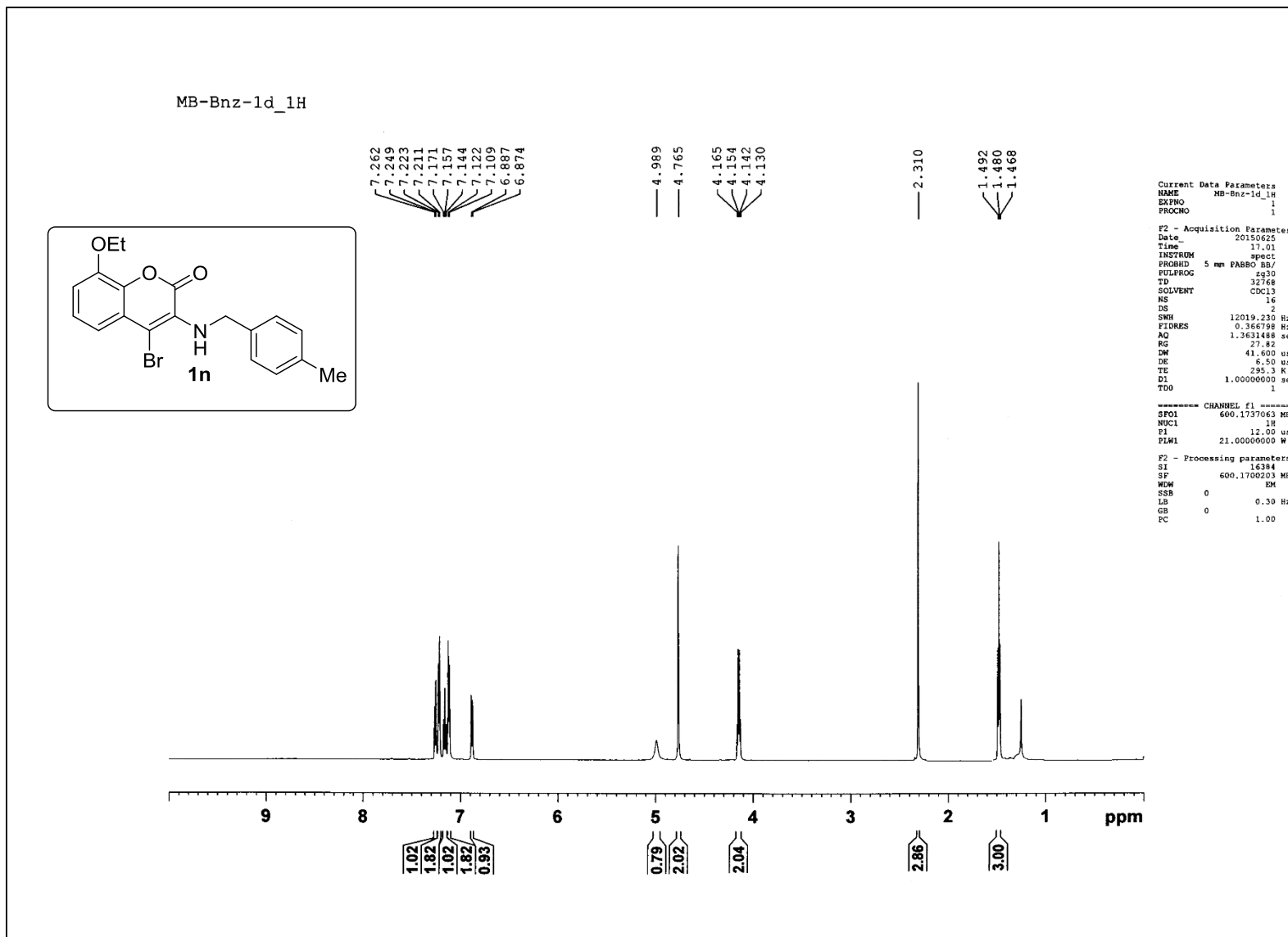


HRMS spectra of **1m**

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



¹H NMR spectra of 1n



¹³C NMR spectra of **1n**

MB-Bnz-1d_13C

157.05
146.21
137.69
137.33
136.52
133.09
129.57
127.86
124.69
121.84
117.40
112.56
111.56

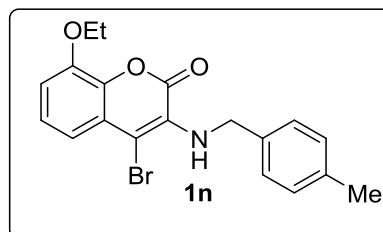
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77.23
77.02

65.18

49.78

21.29

14.97



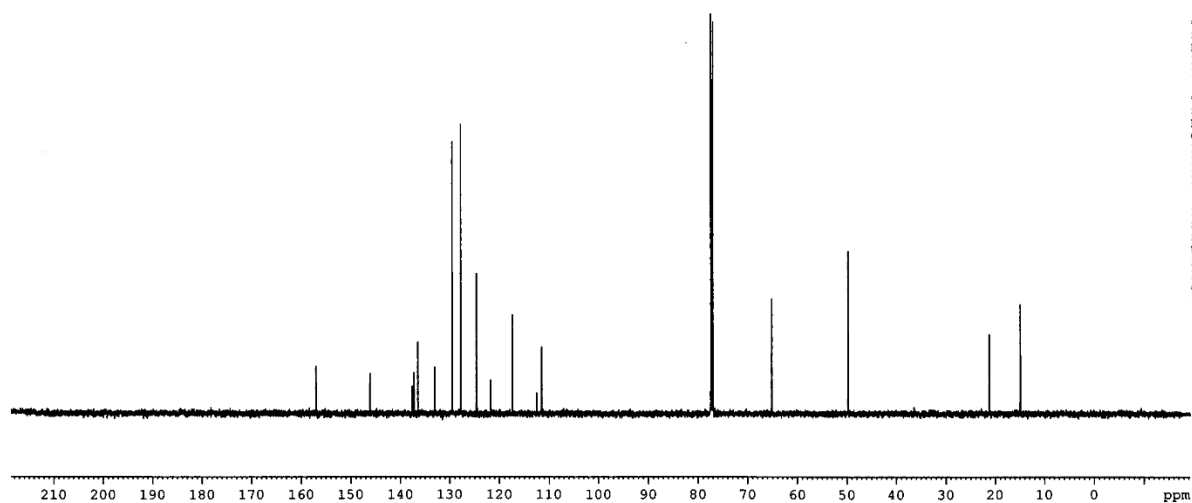
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PULPROG zgpg30
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SOLVENT CDCl3
NS 70
DS 2
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 65.24
DW 13.867 usec
DE 6.50 usec
TE 296.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

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NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

===== CHANNEL f2 =====
SF02 600.1724007 MHz
NUC2 1H
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PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.61714000 W
PLW13 0.30239999 W

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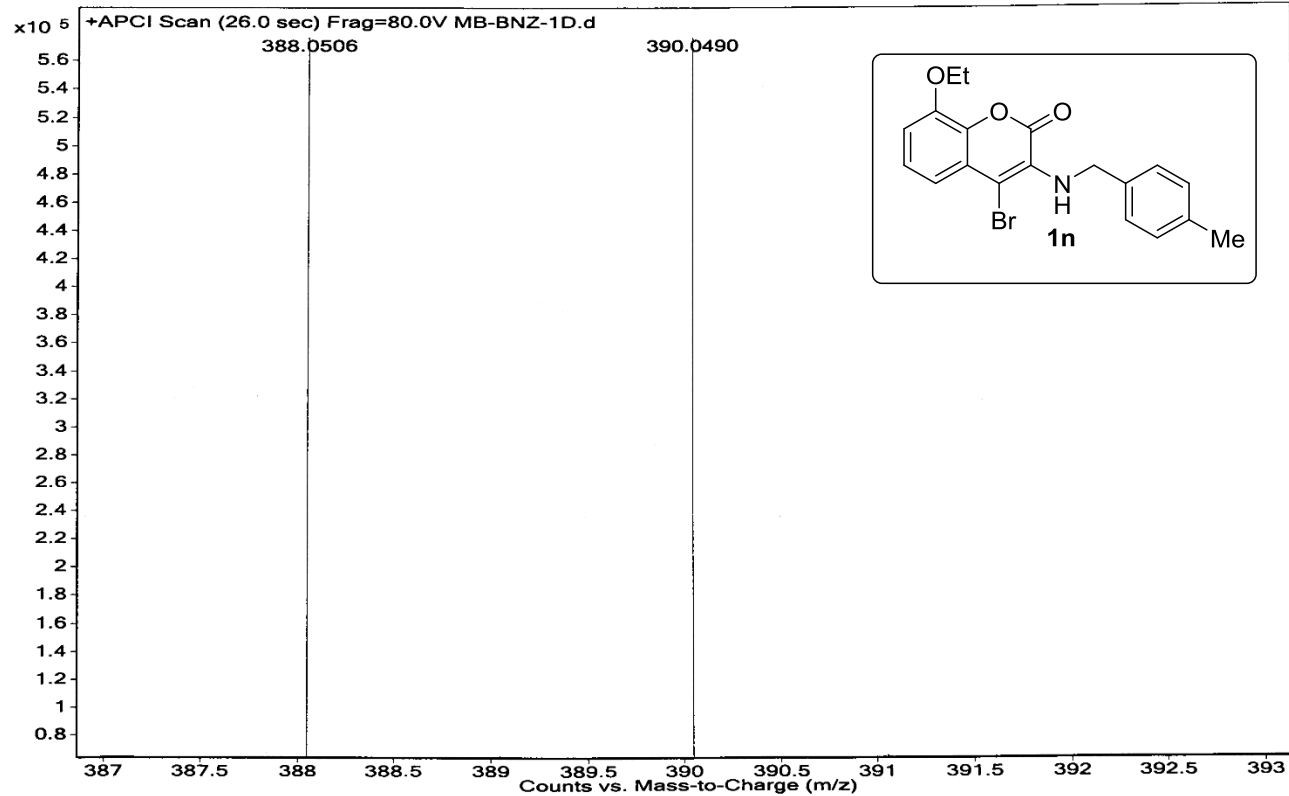
HRMS spectra of **1n**

Sample Name
Inj Vol
Data Filename

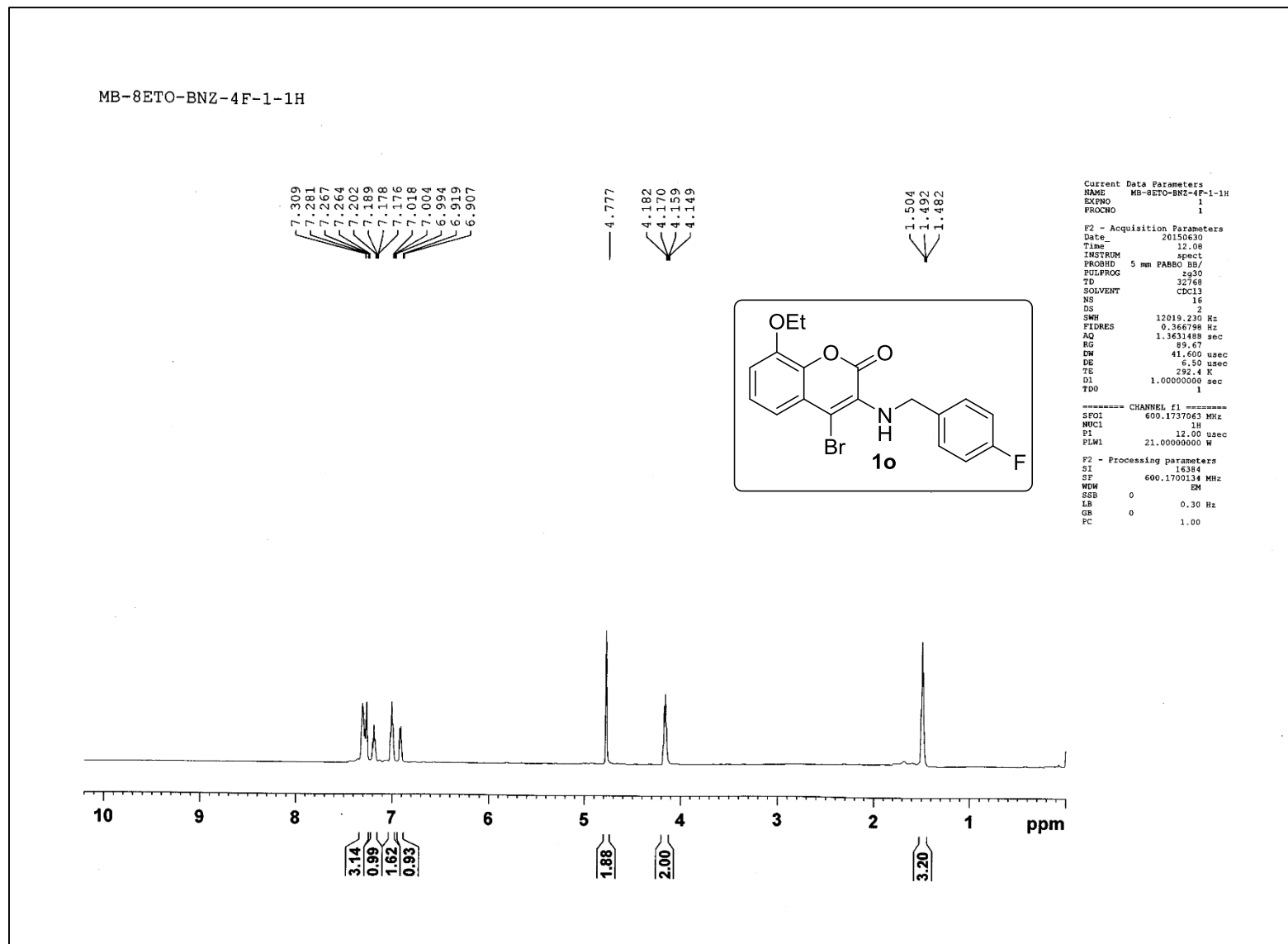
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ACQ Method

Instrument Name
SampleType
Comment

User Name
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Acquired Time

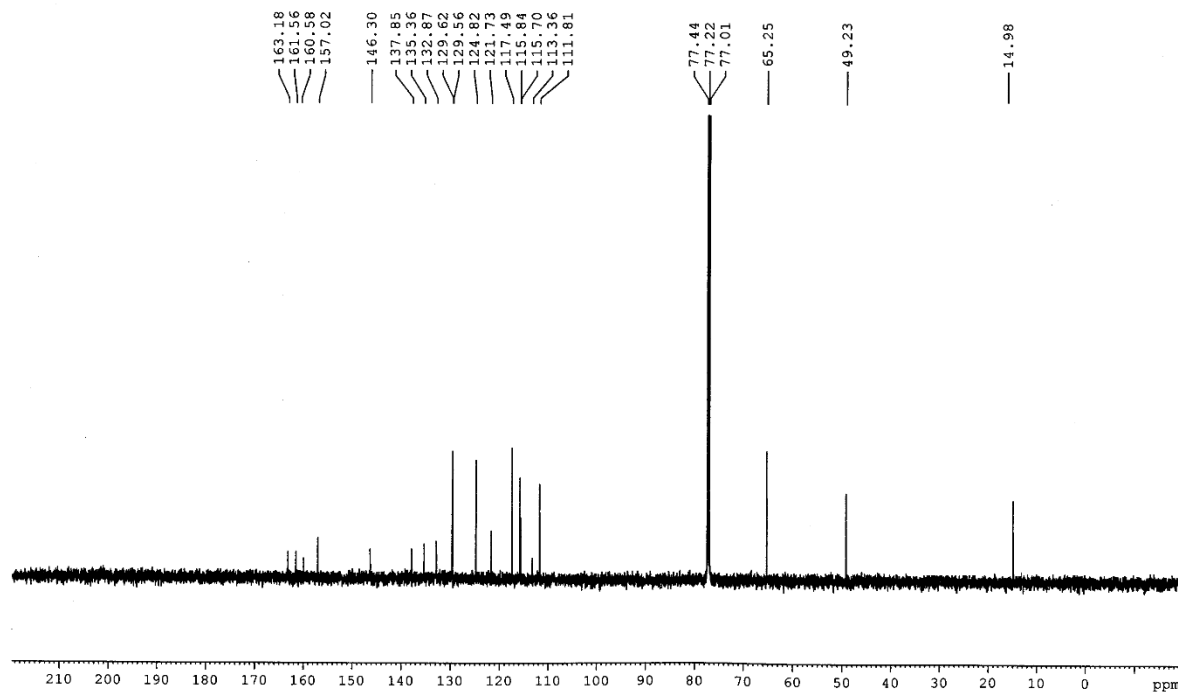
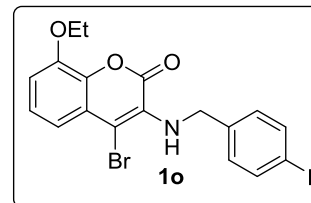


¹H NMR spectra of **1o**



¹³C NMR spectra of **1o**

MB-8EtO-Bnz-4F-13C



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PROCNO    1

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DS         2
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FIDRES     1.100393 Hz
AQ         0.4543829 sec
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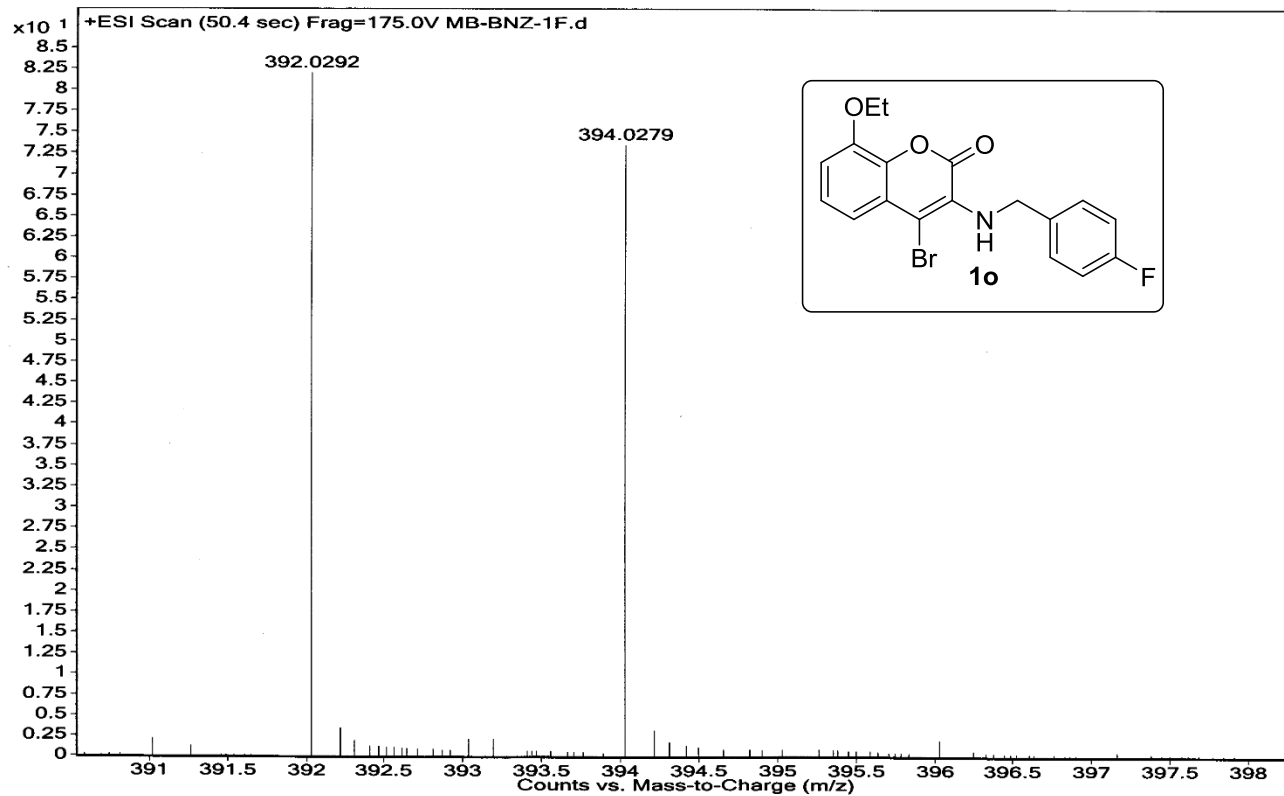
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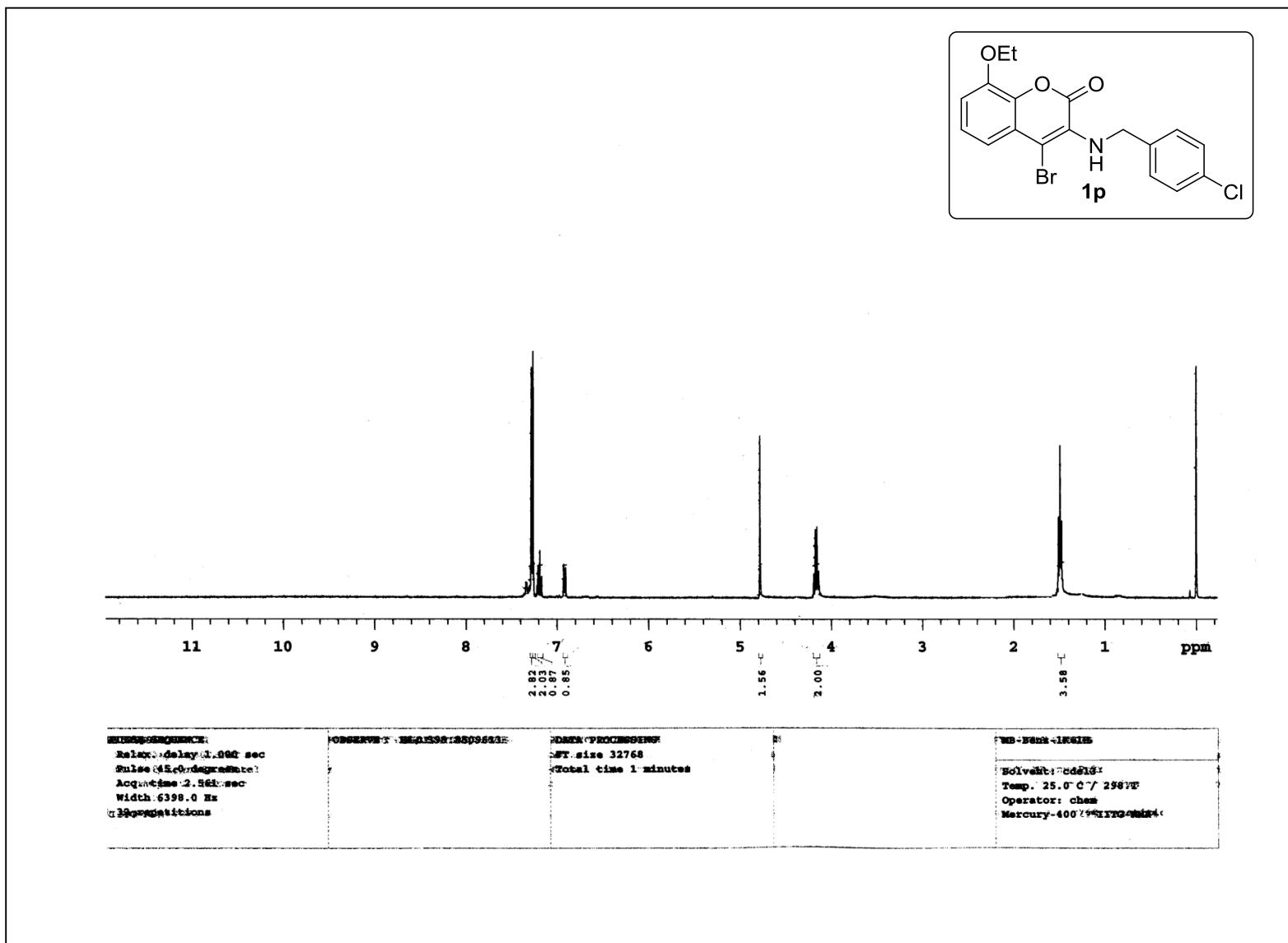
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HRMS spectra Of **1o**

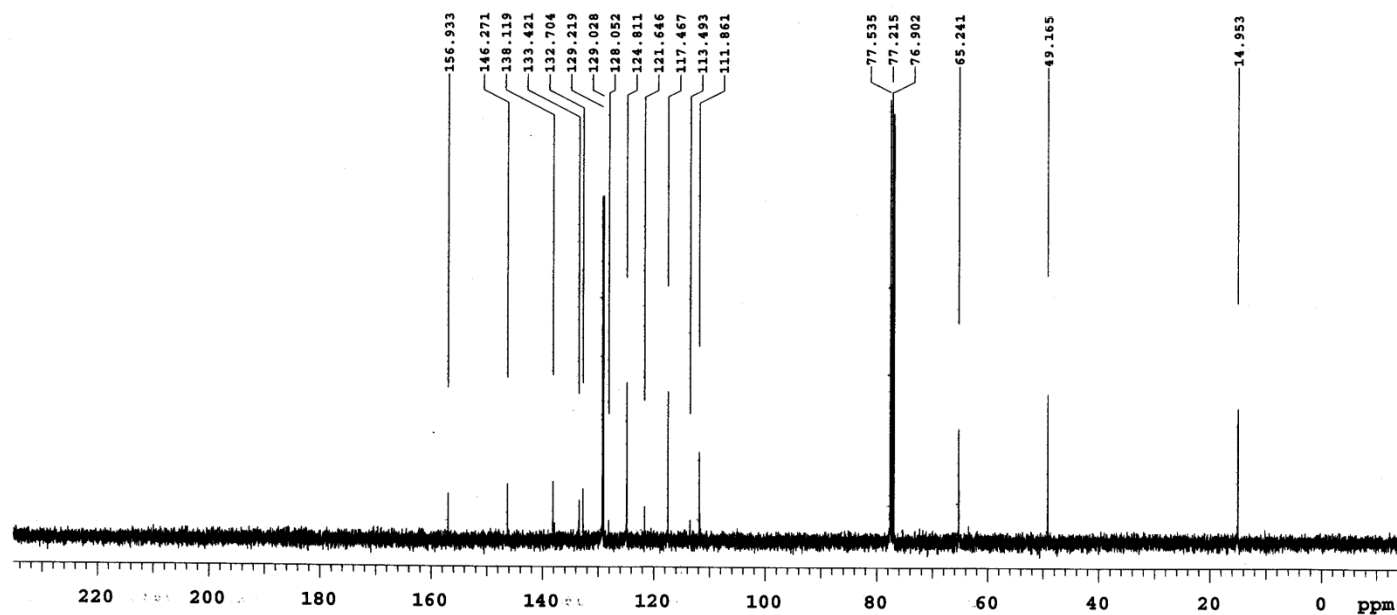
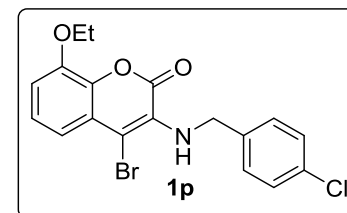
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



H¹NMR spectra of **1p**



¹³C NMR spectra of **1p**



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degree Acq. time 1.304 sec Width 25125.6 Hz 670 repetitions	OBSERVE C13, 100.5425847 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 25 minutes	MS-Benz-1K-13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*
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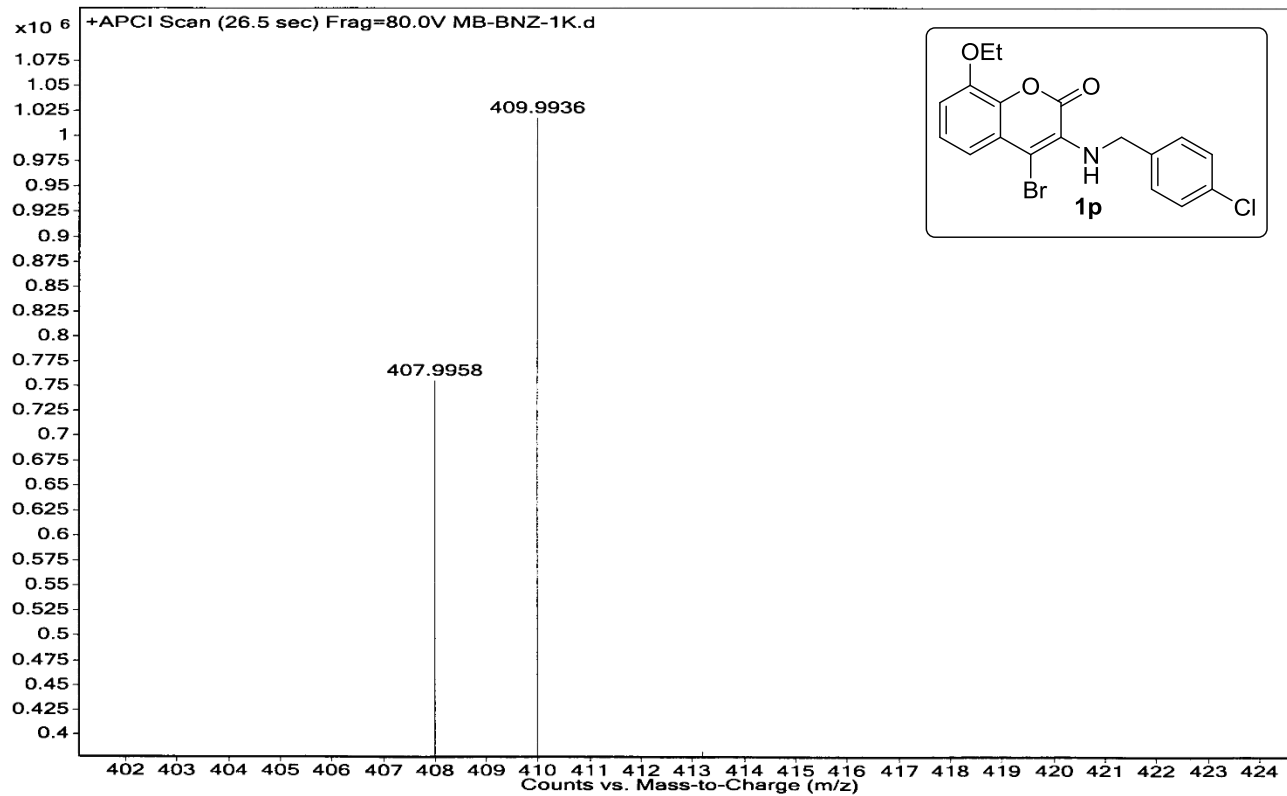
HRMS spectra of 1p

Sample Name
Inj Vol
Data Filename

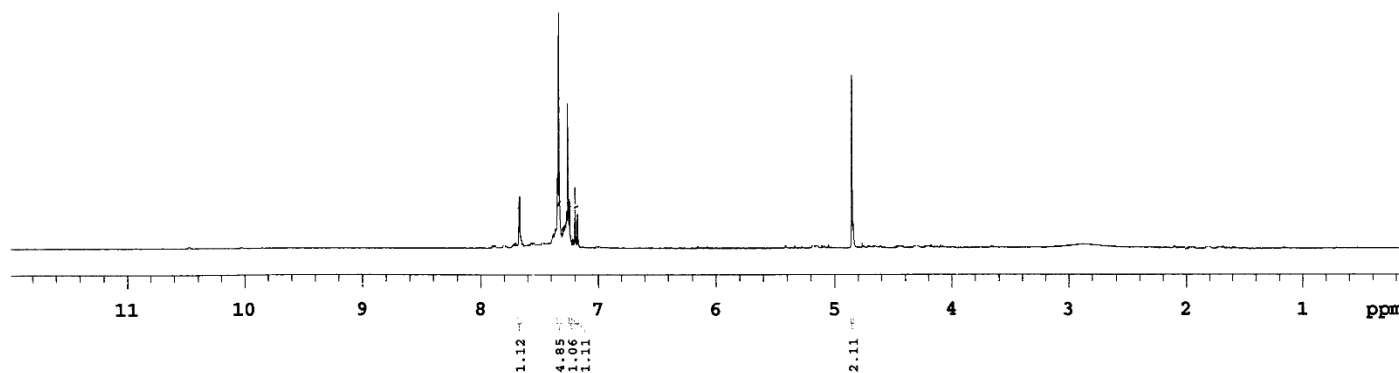
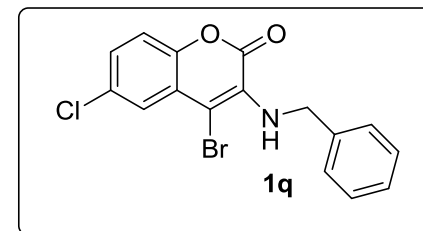
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



¹H NMR spectra of **1q**



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

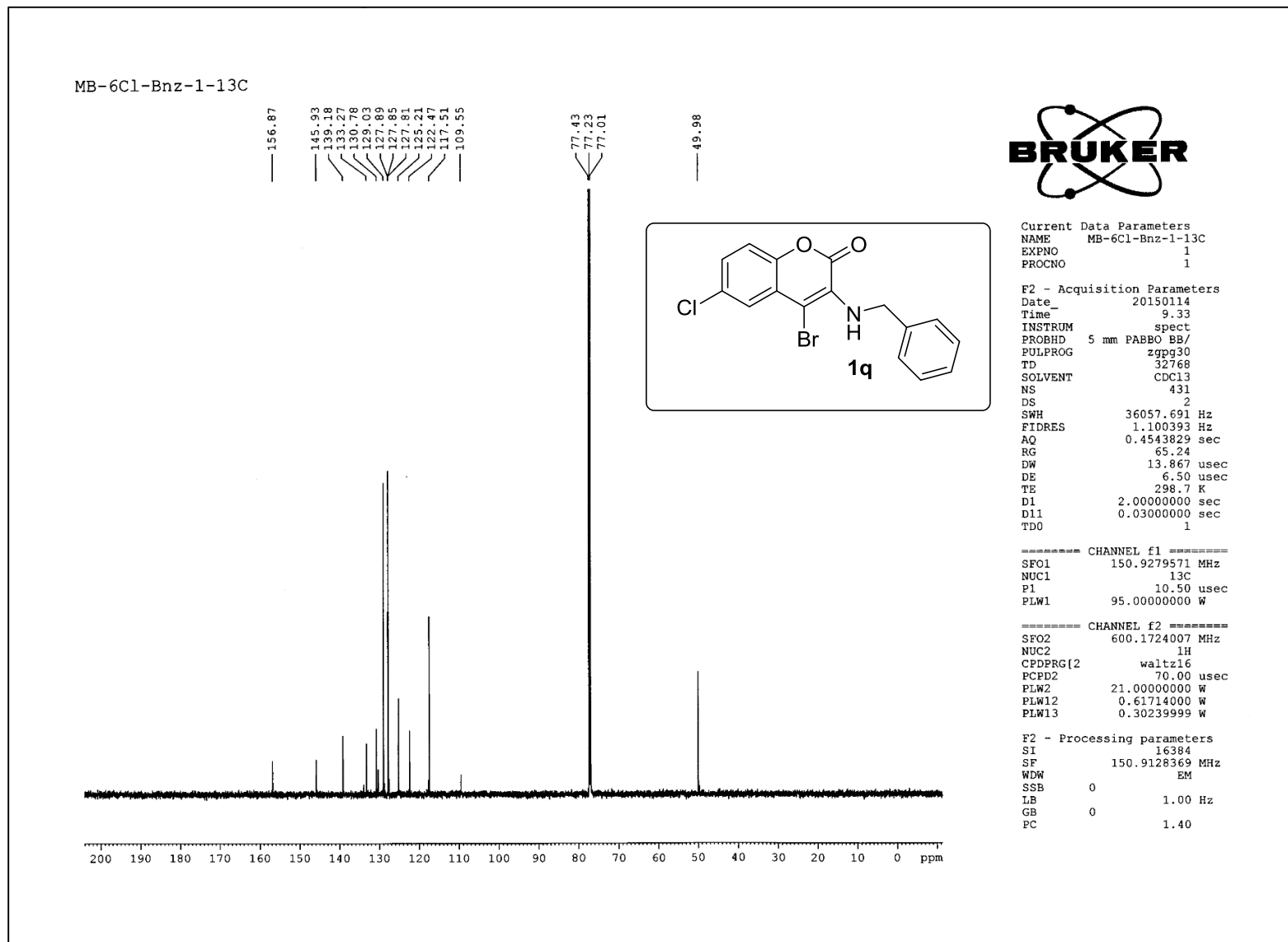
OBSERVE H1, 399.8509633

DATA PROCESSING
FT size 32768
Total time 1 minutes

MB-6-Cl-Bnz-1-1H

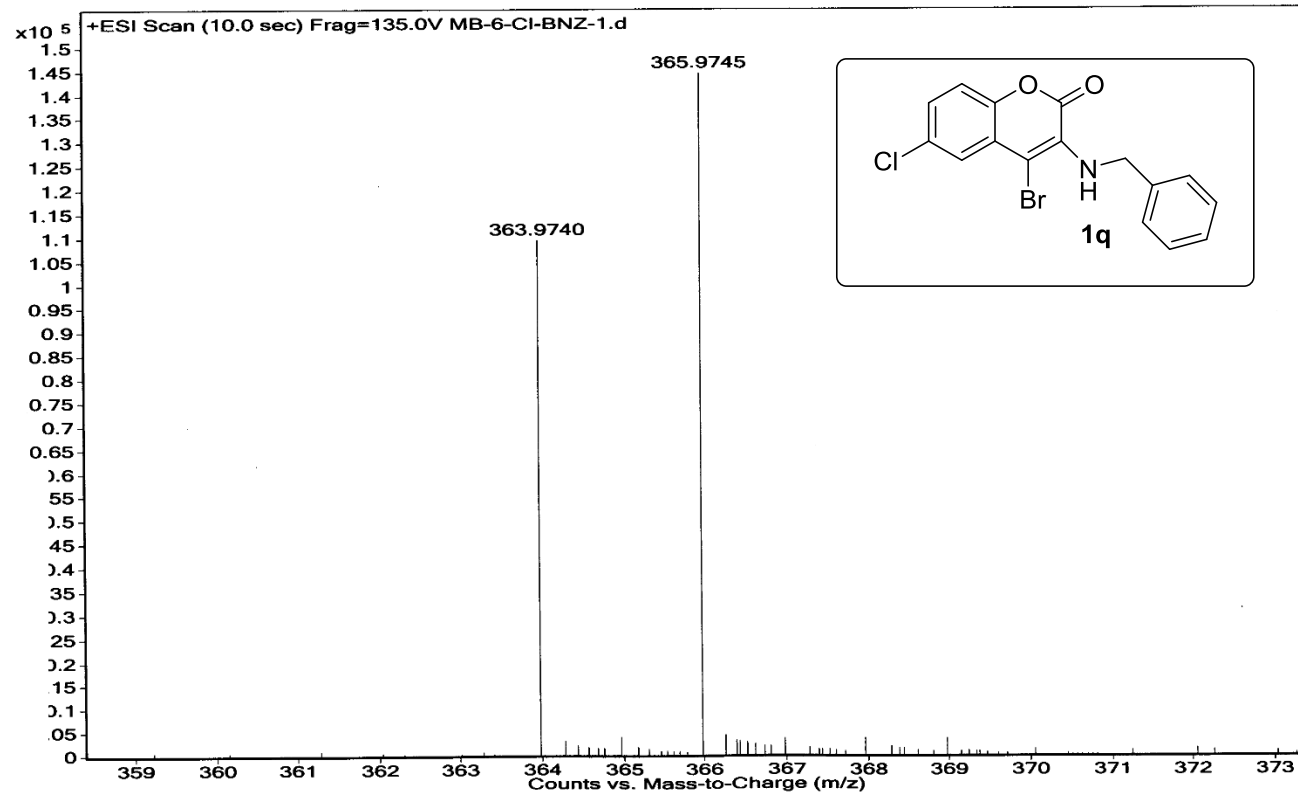
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: chem
File: MB-6-Cl-Bnz-1-1H
Mercury-400 "IITG-NMR"

¹³C NMR spectra of **1q**



HRMS spectra of **1q**

Sample Name	MB-6-Cl-BNZ-1	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-6-Cl-BNZ-1.d	ACQ Method		Comment		Acquired Time	8/13/2015 3:16:31 PM



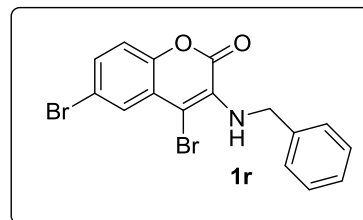
¹H NMR Spectra of **1r**

MB-6Br-Bnz-1-14-1H

7.824
7.820
7.407
7.403
7.393
7.389
7.346
7.341
7.337
7.259
7.136
7.122

4.857

-U.UU3



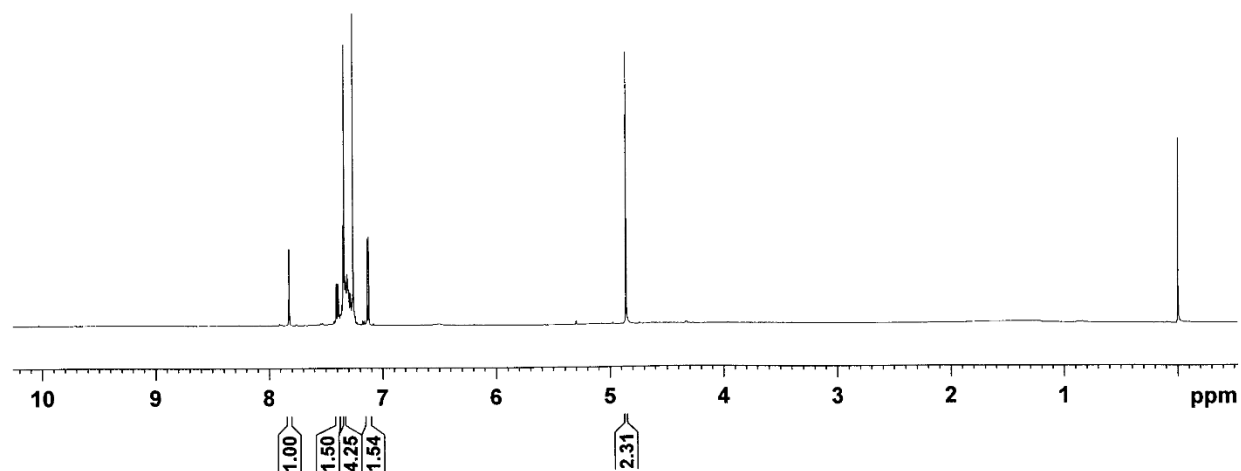
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Current Data Parameters
NAME      MB-6Br-Bnz-1-14-1H
EXPNO     1
PROCNO    1

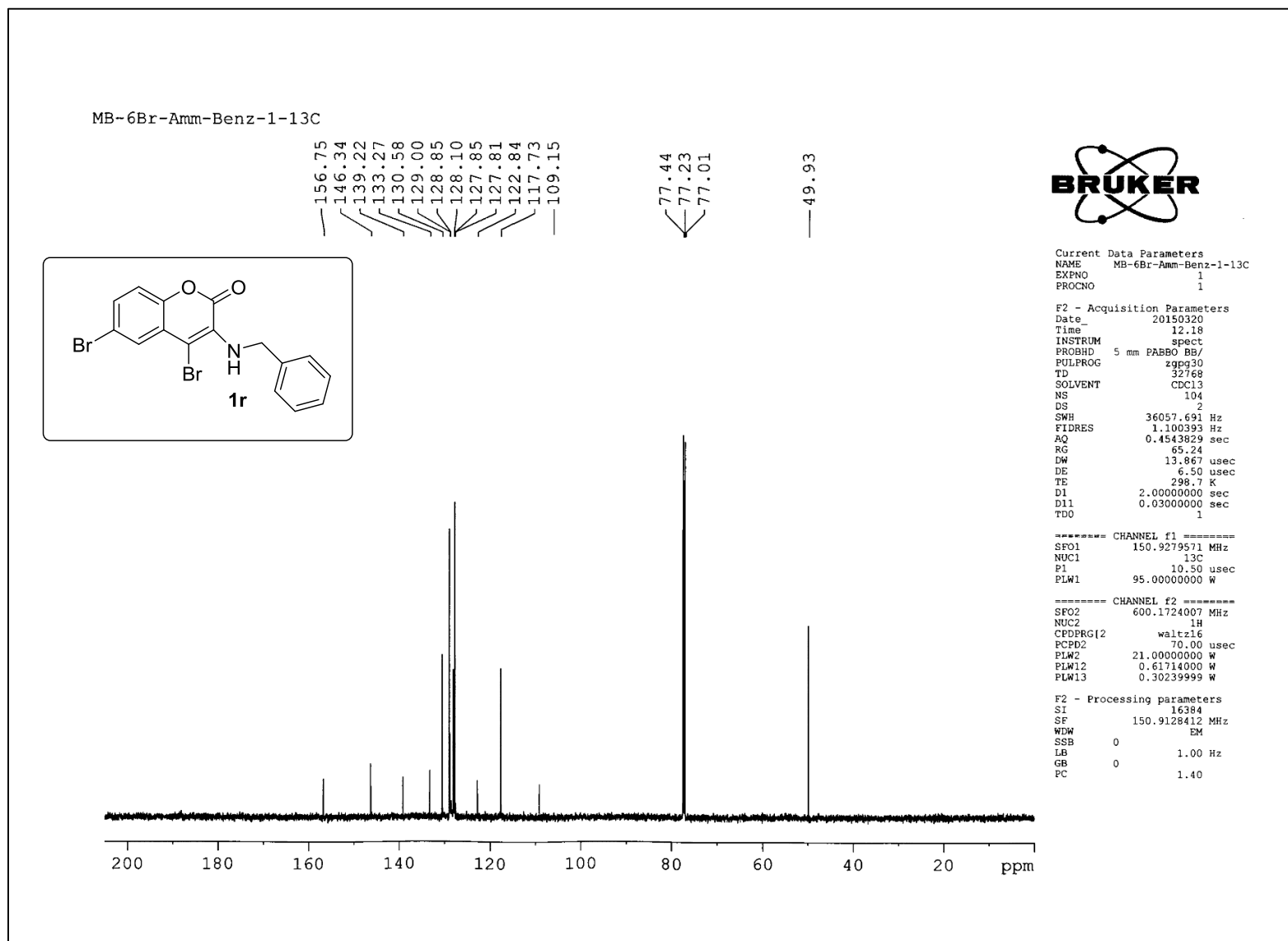
F2 - Acquisition Parameters
Date_     20150409
Time      10.34
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zg30
TD         32768
SOLVENT    CDCl3
NS         16
DS         2
SWH        12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         143.33
DW         41.600 usec
DE         6.50 usec
TE         297.1 K
D1         1.00000000 sec
TD0        1

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

F2 - Processing parameters
SI         16384
SF         600.1700155 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

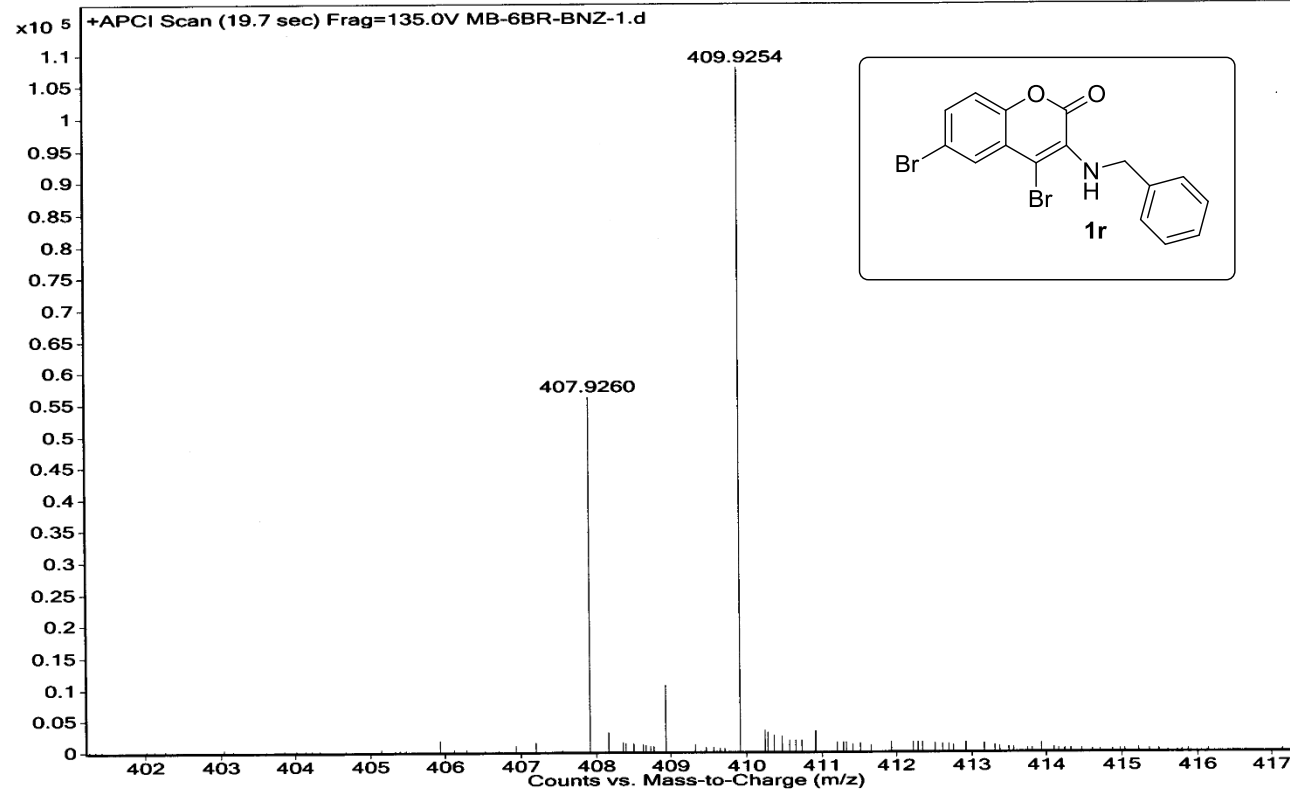


¹³C NMR spectra of **1r**



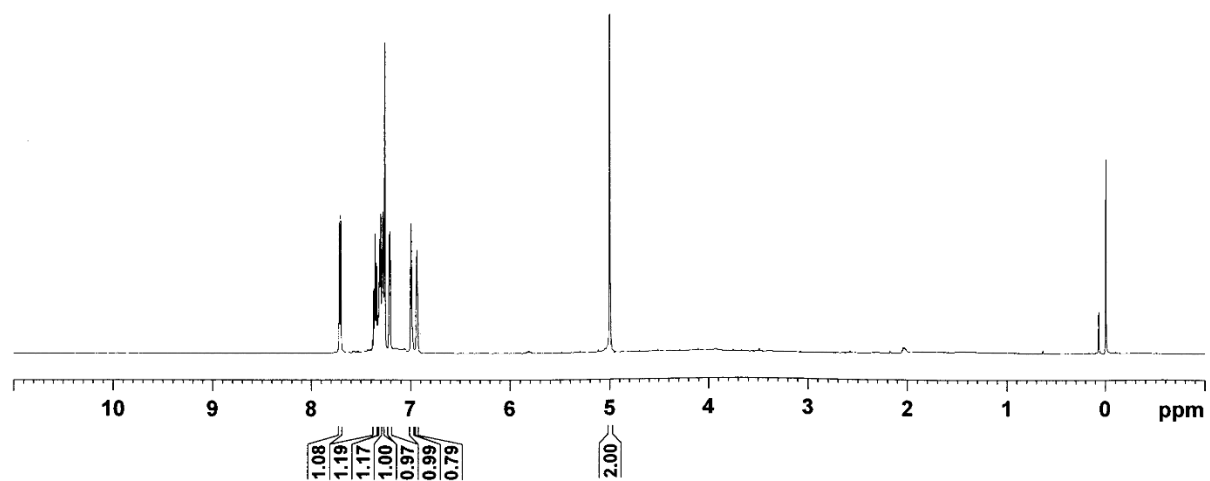
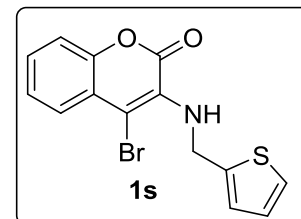
HRMS spectra of 1r

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



¹H NMR spectra of **1s**

MB-BNZ-THIO-1-1H



```

Current Data Parameters
NAME      MB-BNZ-Thio-1-1H
EXPNO     1
PROCNO    1

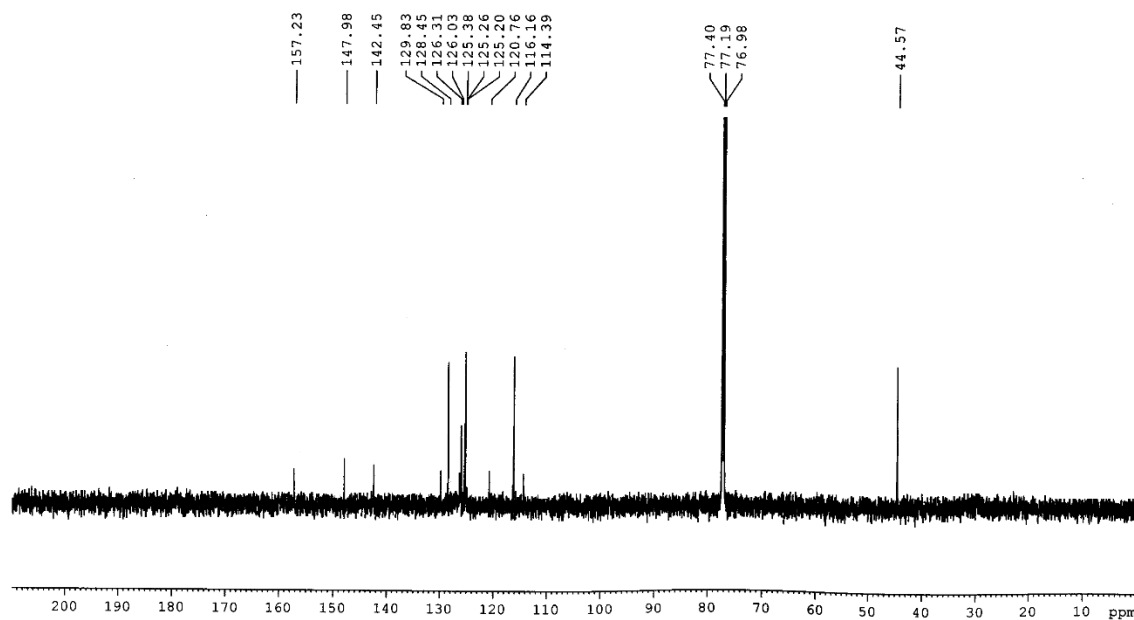
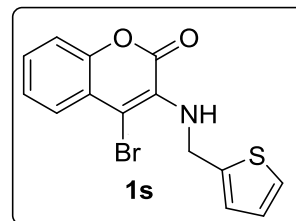
F2 - Acquisition Parameters
Date_     20150819
Time      11.05
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zg30
TD         32768
SOLVENT    CDCl3
NS         16
DS         2
SWH         12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.363488 sec
RG         40.22
DW         41.600 usec
DE         6.50 usec
TE         294.2 K
D1         1.00002000 sec
TDO        1

===== CHANNEL f1 =====
SFO1       600.1737063 MHz
NUC1       1H
P1         12.00 usec
PLM1       21.00000000 W

F2 - Processing parameters
SI         16384
SF         600.1700151 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

¹³C NMR spectra of **1s**

MB_BNZ_THIO-1_13C



```

Current Data Parameters
NAME      MB_BNZ_THIO-1_13C
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20150820
Time      11.57
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zgpg30
TD         32768
SOLVENT    CDCl3
NS         525
DS         2
SWH         42613.637 Hz
FIDRES     1.300465 Hz
AQ         0.3844775 sec
RG         200.18
DW         11.733 usec
DE         6.50 usec
TE         294.7 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1

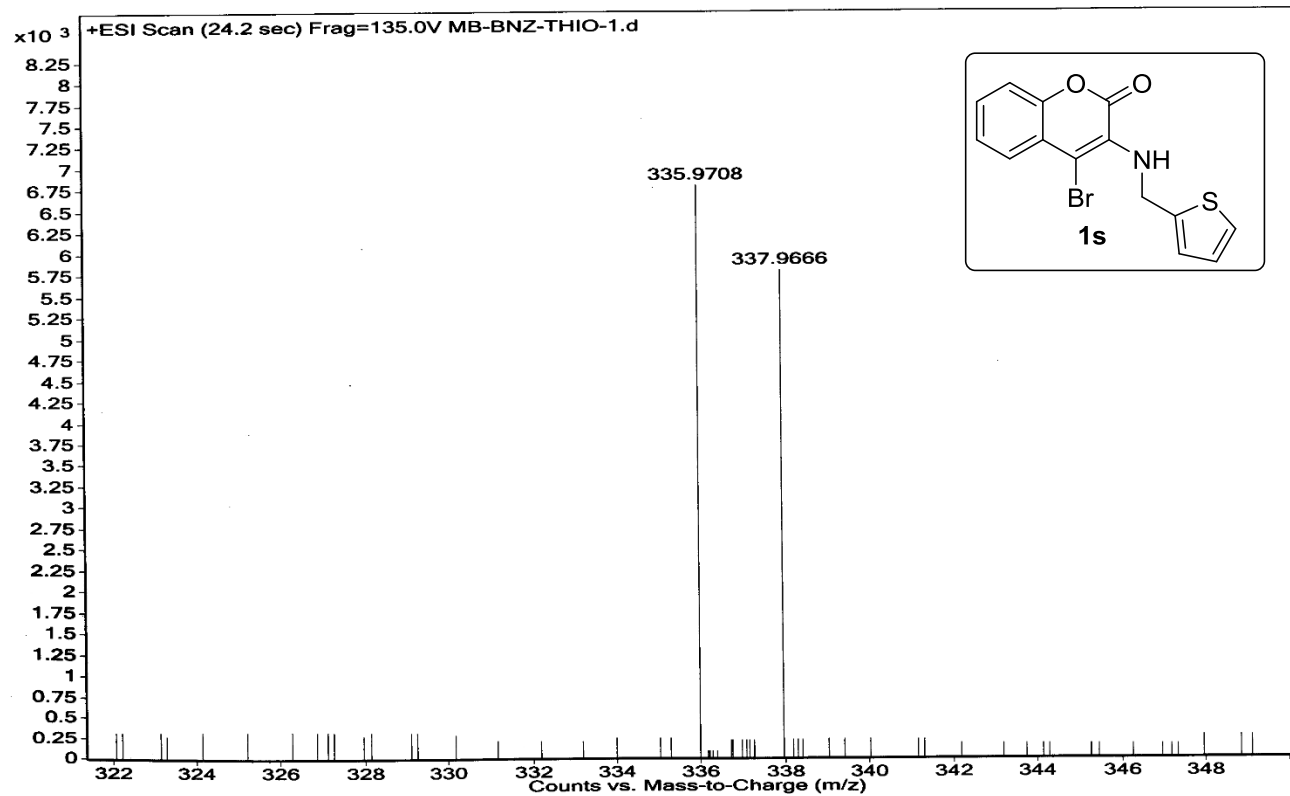
===== CHANNEL f1 =====
SFO1      150.9279971 MHz
NUC1       13C
P1         10.50 usec
PLW1      95.00000000 W

===== CHANNEL f2 =====
SFO2      600.1724007 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      70.00 usec
PLW2      21.00000000 W
PLW12     0.61714000 W
PLW13     0.30239999 W

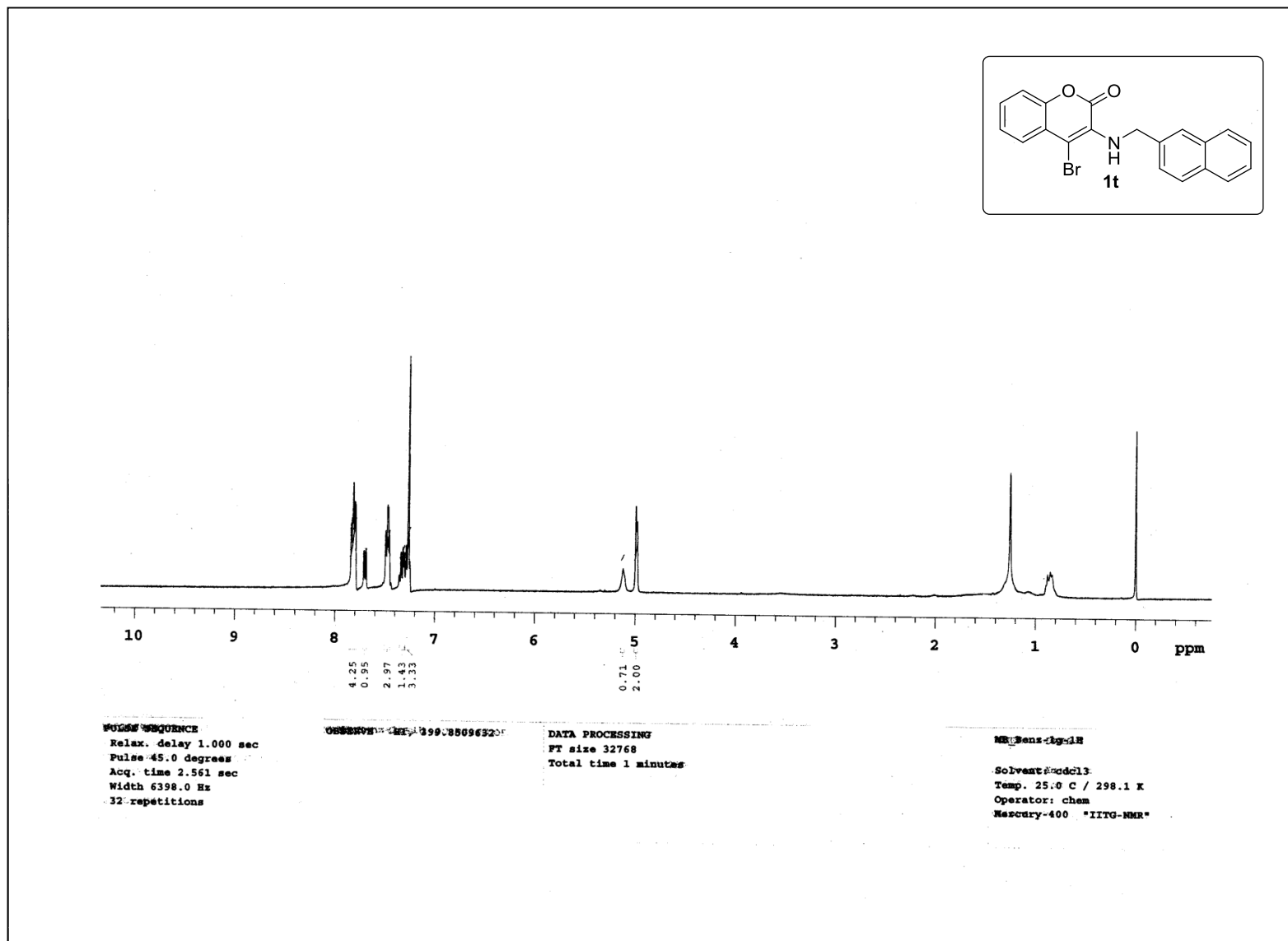
F2 - Processing parameters
SI         16384
SF         150.9128416 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```

HRMS spectra of 1s

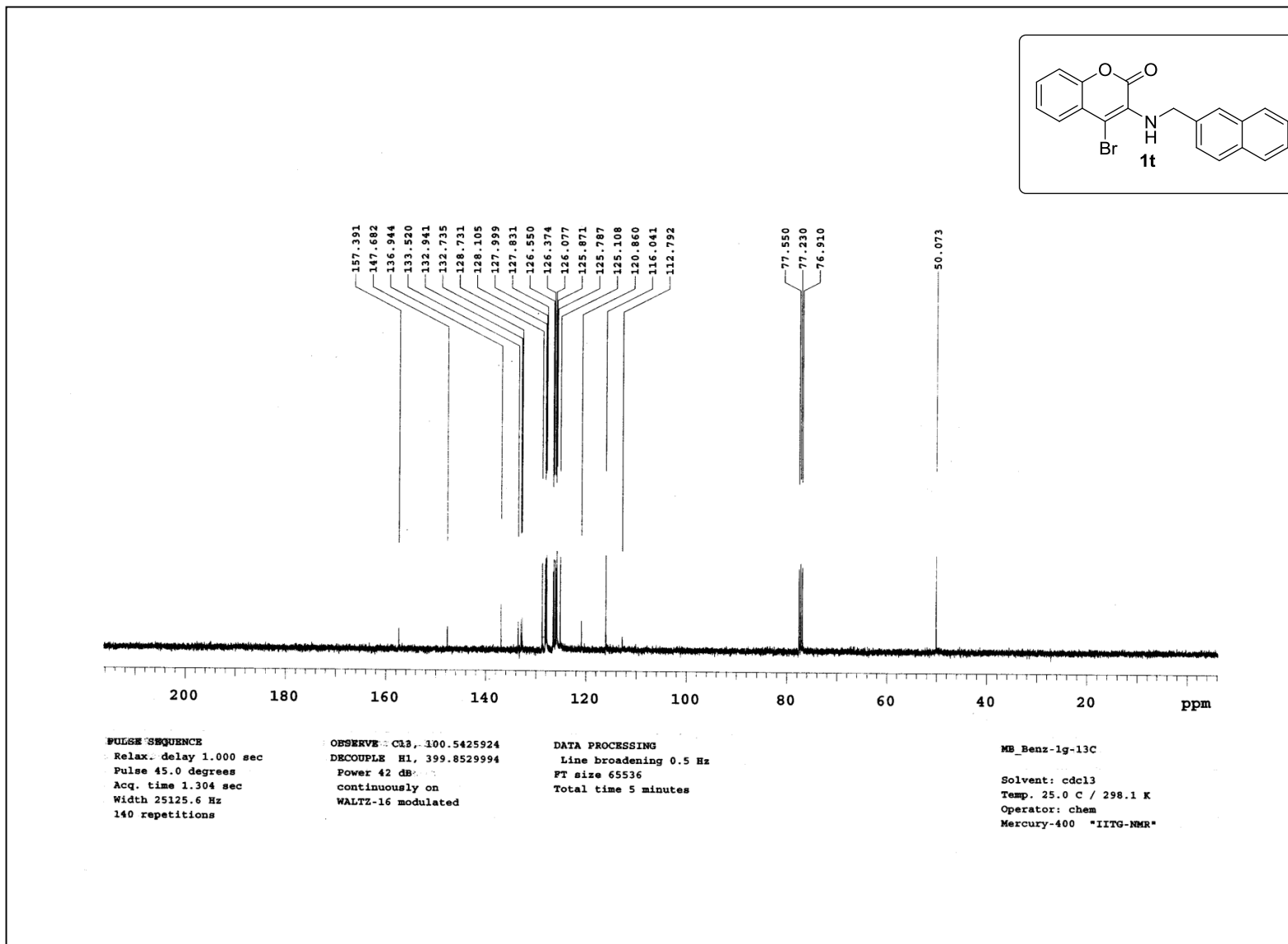
Sample Name	MB-BNZ-THIO-1	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BNZ-THIO-1.d	ACQ Method		Comment		Acquired Time	8/14/2015 11:36:00 AM



¹H NMR spectra of **1t**

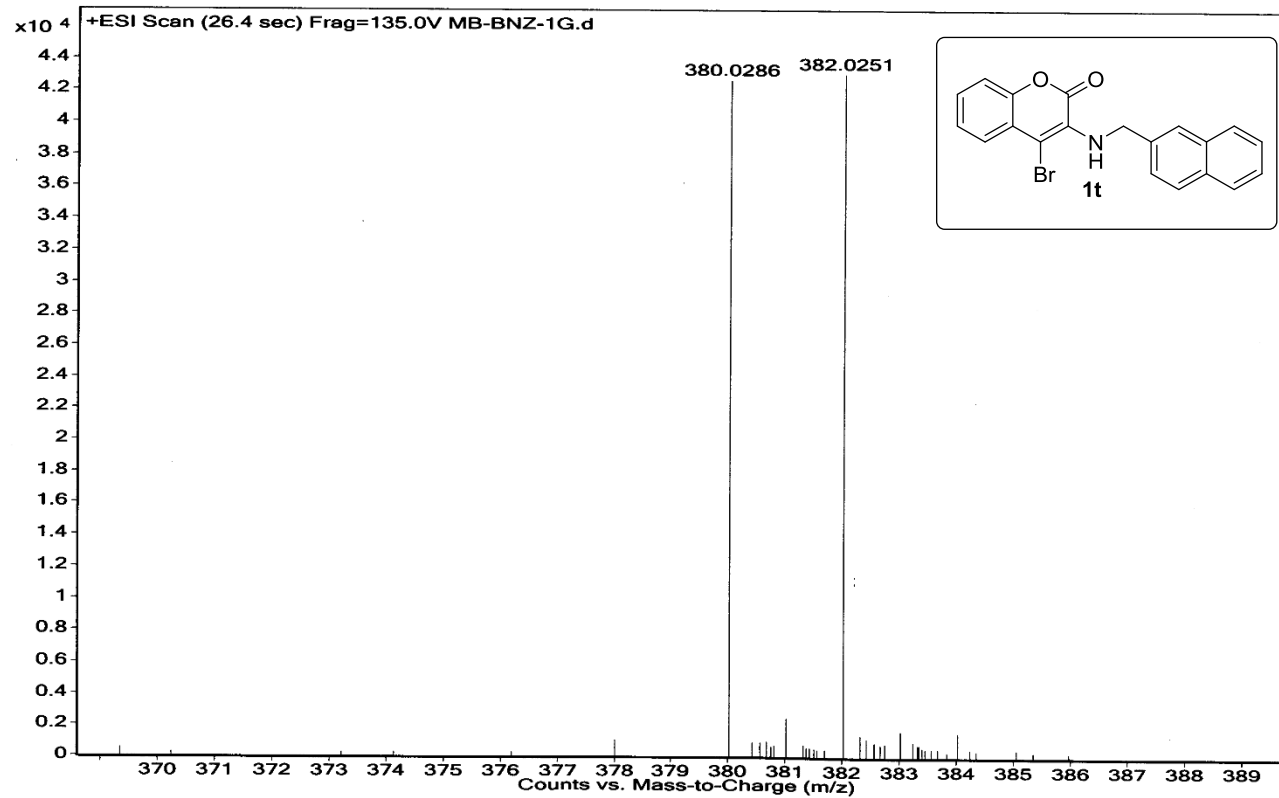


¹³C NMR spectra of **1t**

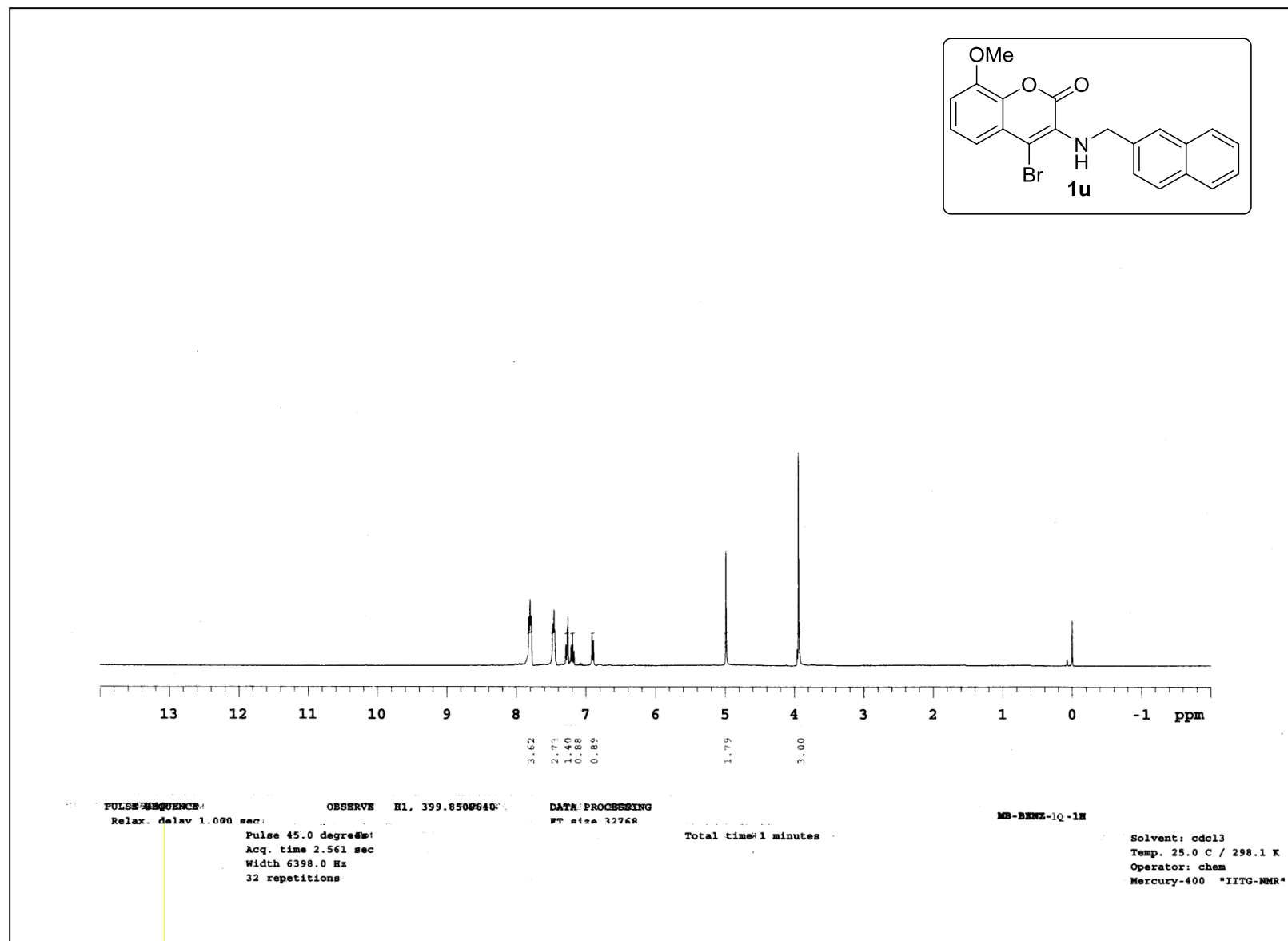


HRMS spectra of 1t

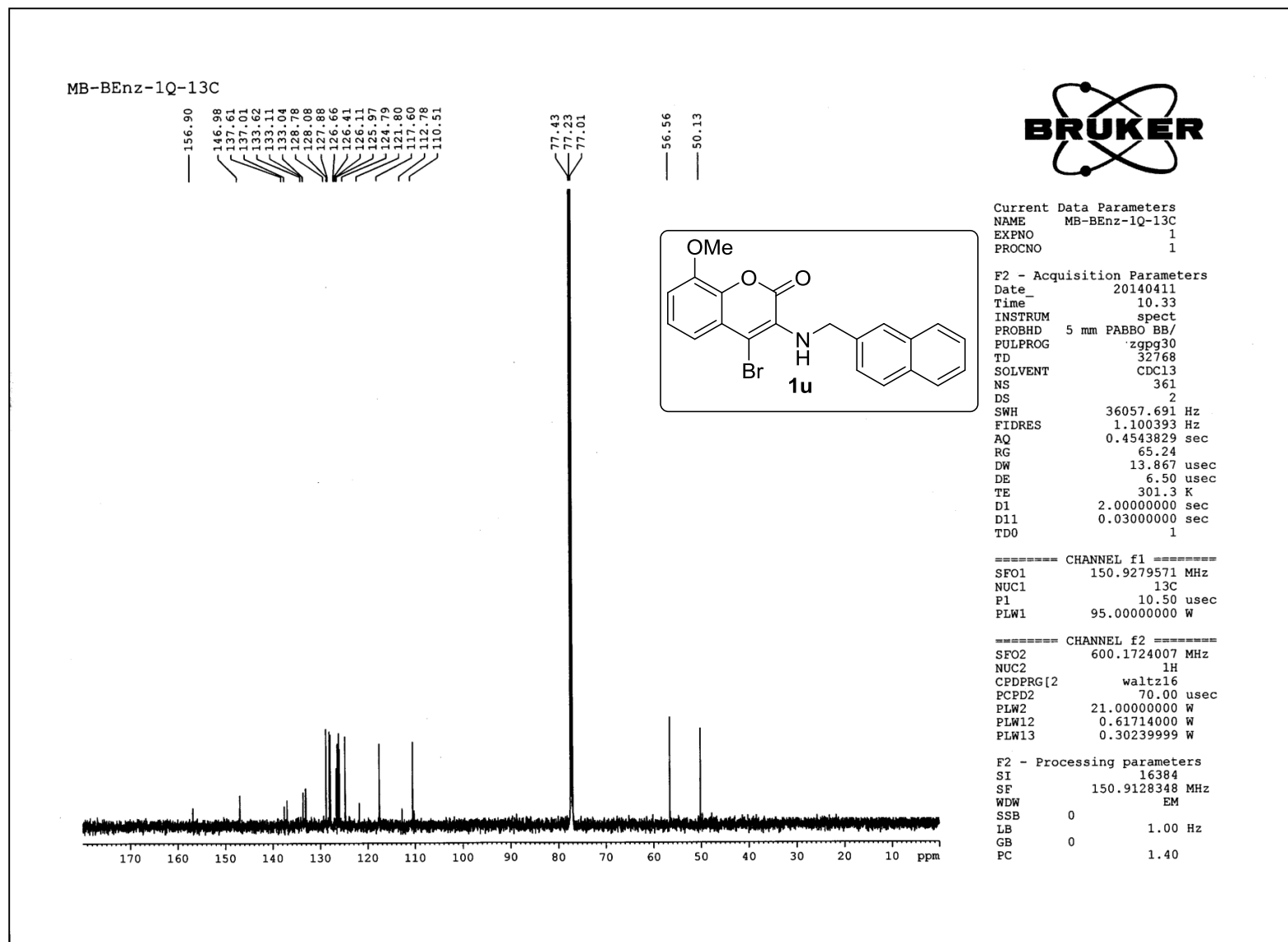
Sample Name	MB-BNZ-1G	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BNZ-1G.d	ACQ Method		Comment		Acquired Time	8/13/2015 3:11:54 PM



H¹ NMR spectra of **1u**



¹³C NMR spectra of **1u**



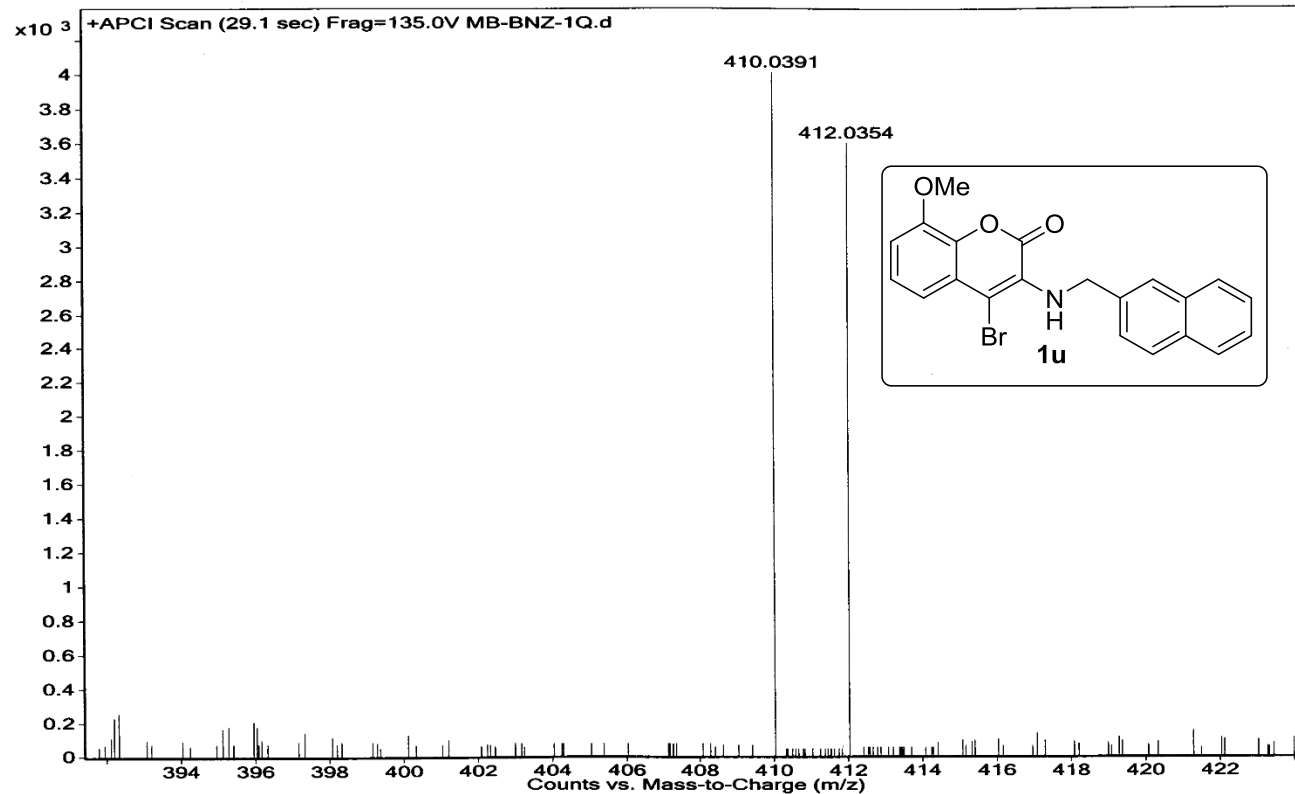
HRMS spectra of **1u**

Sample Name
Inj Vol
Data Filename

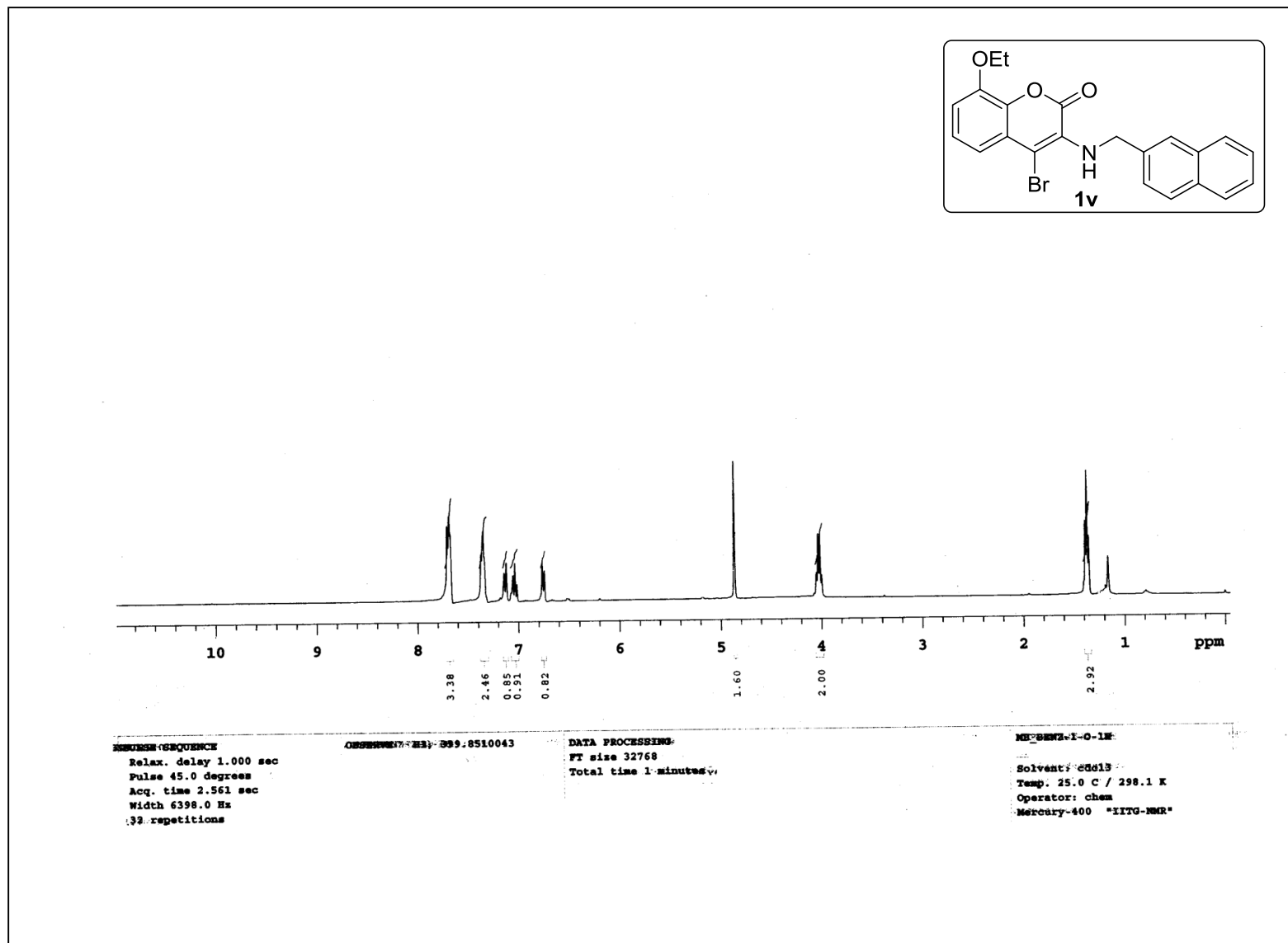
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

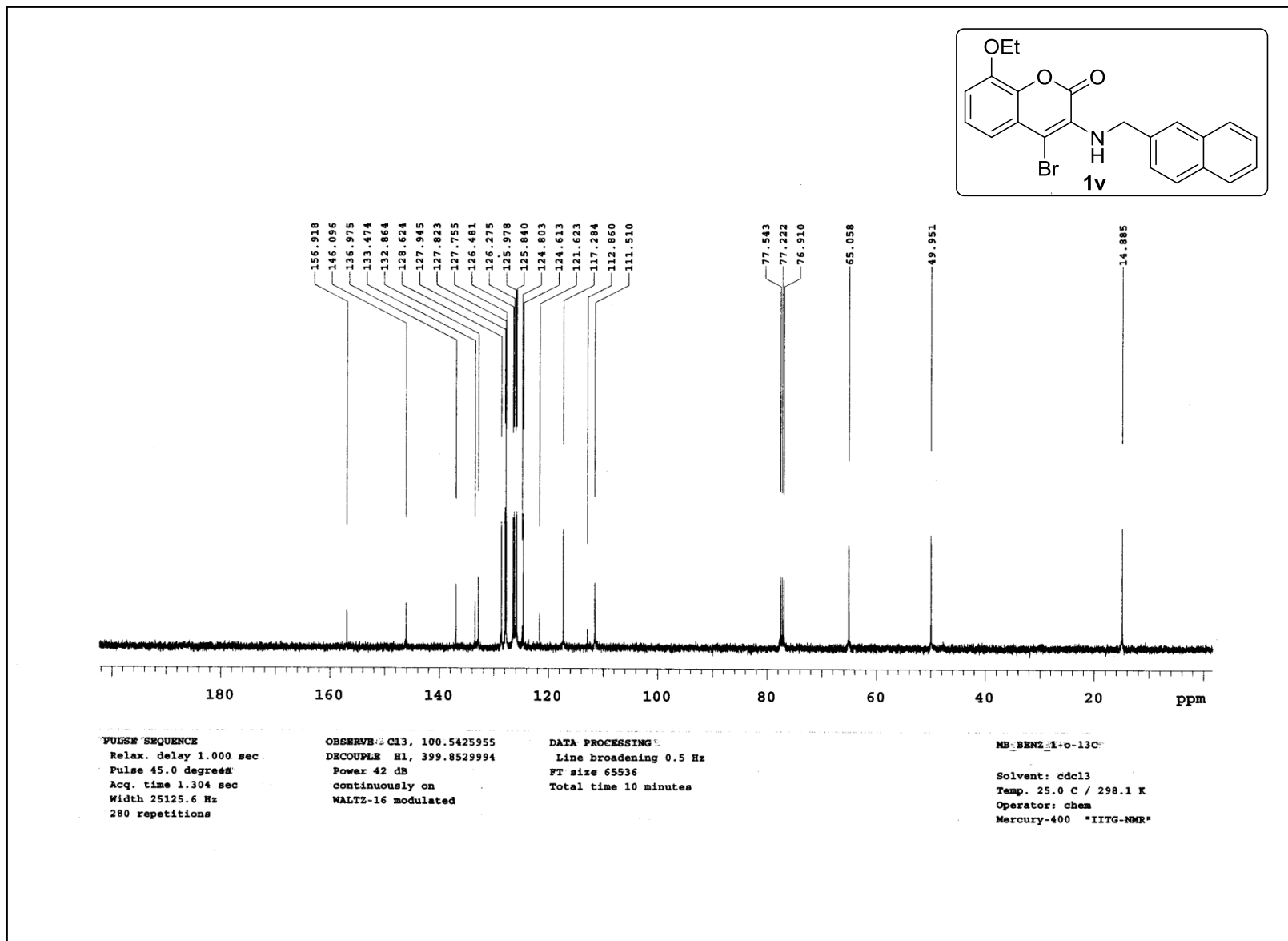
User Name
IRM Calibration Status
Acquired Time



^1H NMR spectra of **1v**

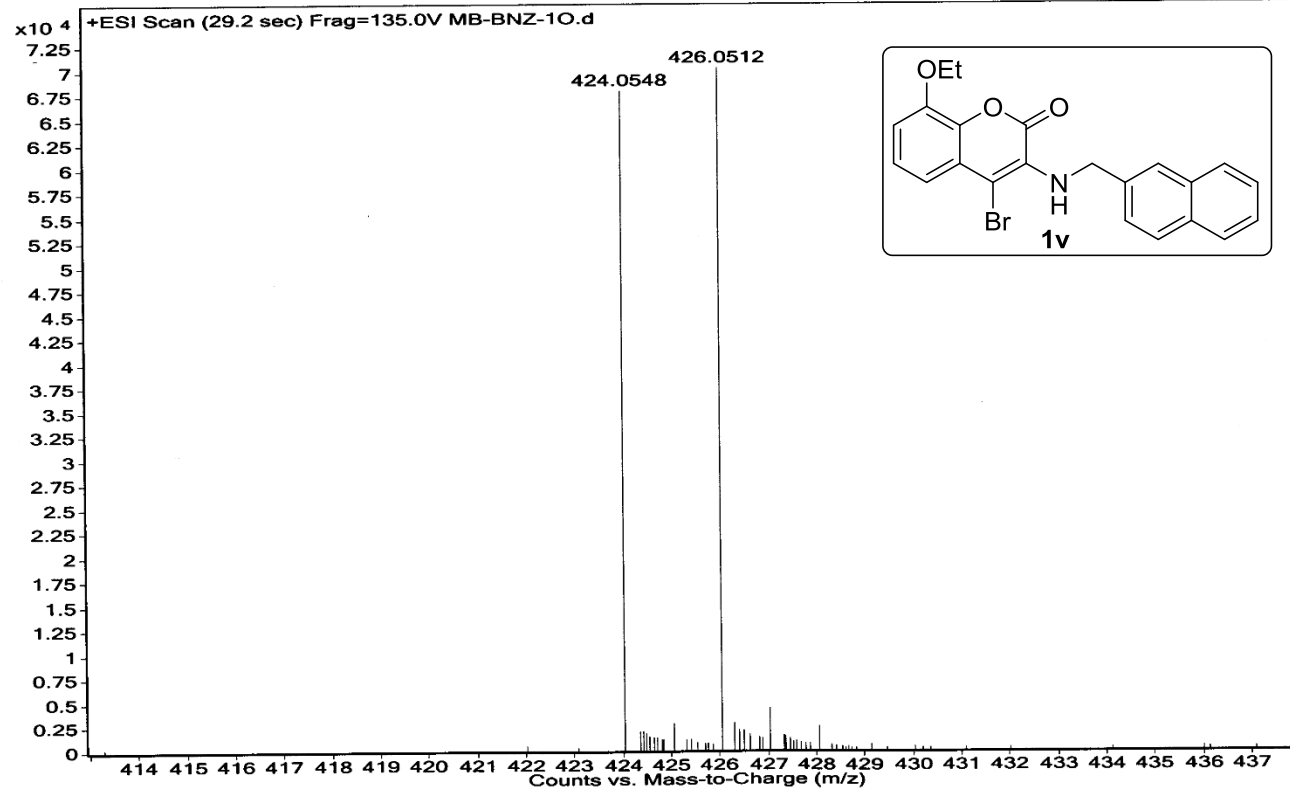


¹³C NMR spectra of **1v**



HRMS spectra of **1v**

Sample Name	MB-BNZ-10	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BNZ-10.d	ACQ Method		Comment		Acquired Time	8/13/2015 3:13:29 PM



¹H NMR spectra of **2a**

MS-BT-1-14-1H

Sample Name:

MS-BT-1-14-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Feb 21 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

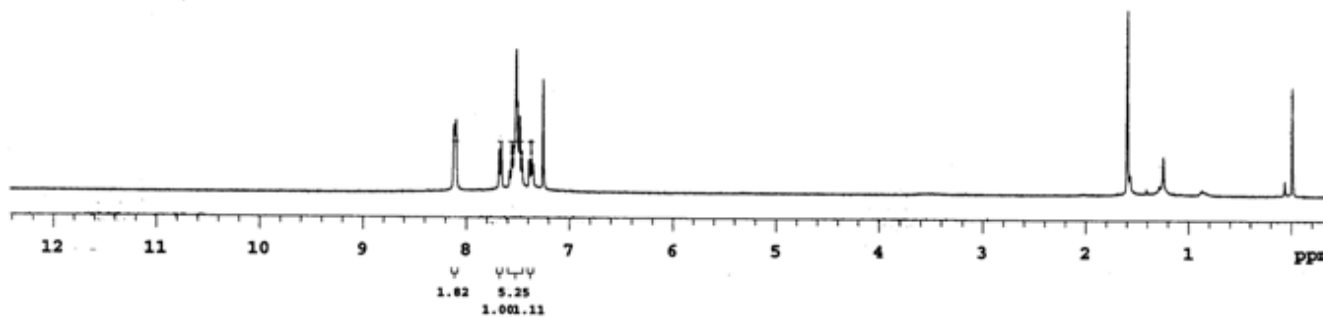
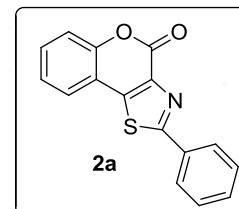
64 repetitions

OBSERVE H1, 399.8509606 MHz

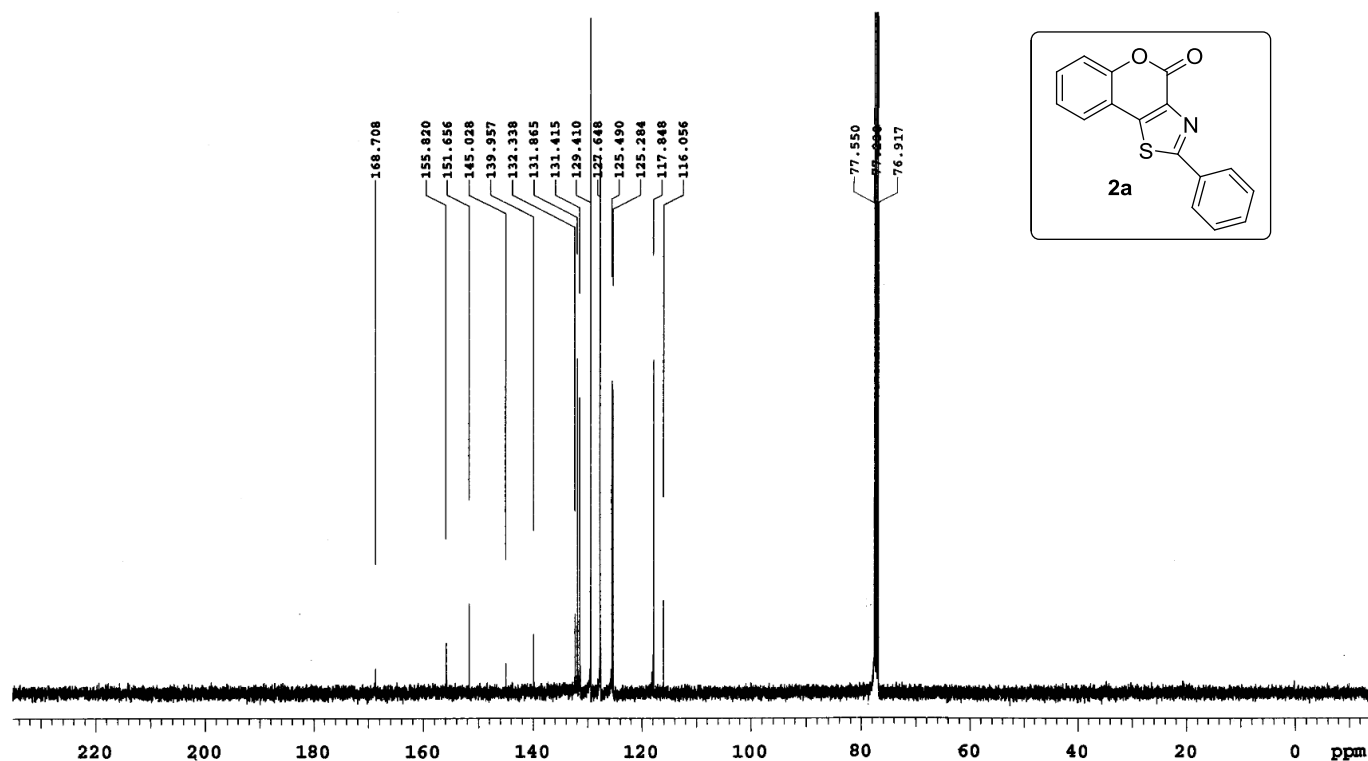
DATA PROCESSING

FT size 32768

Total time 4 min 24 sec



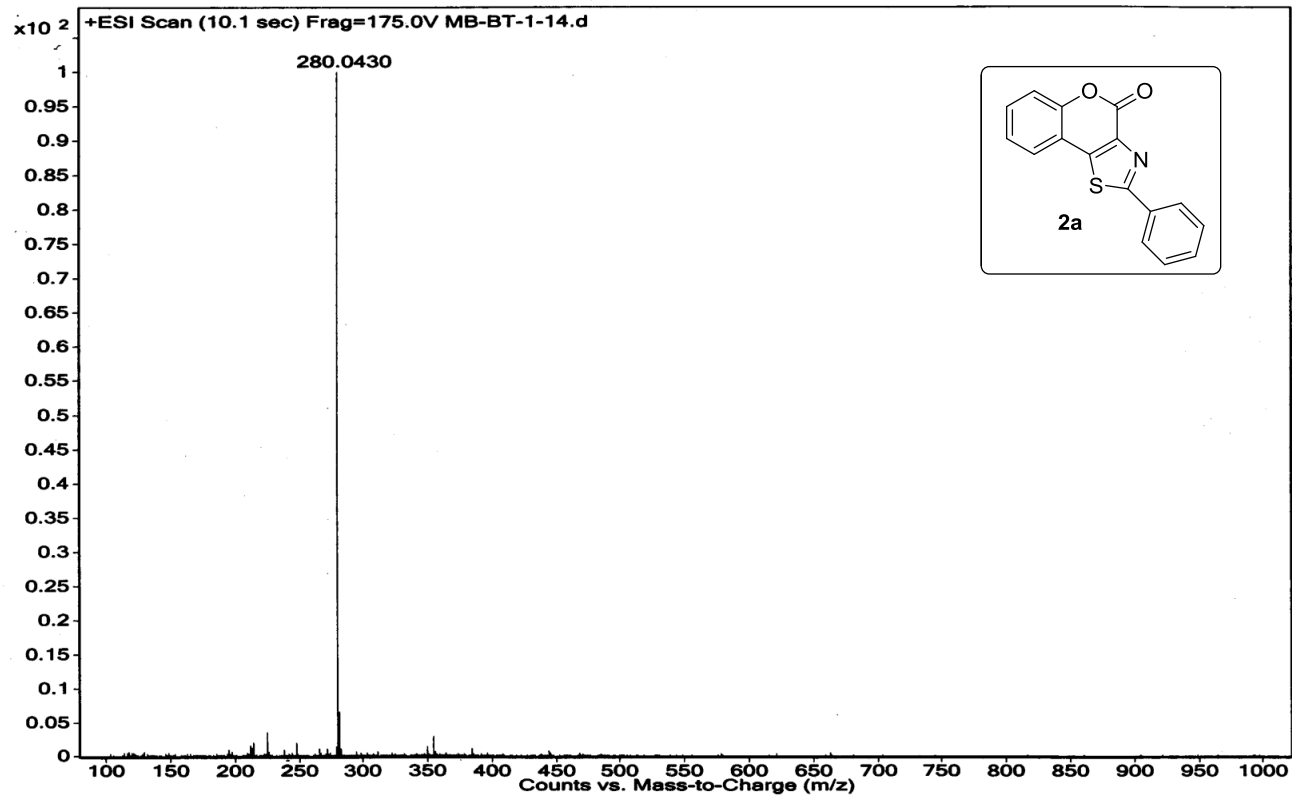
¹³C NMR of 2a



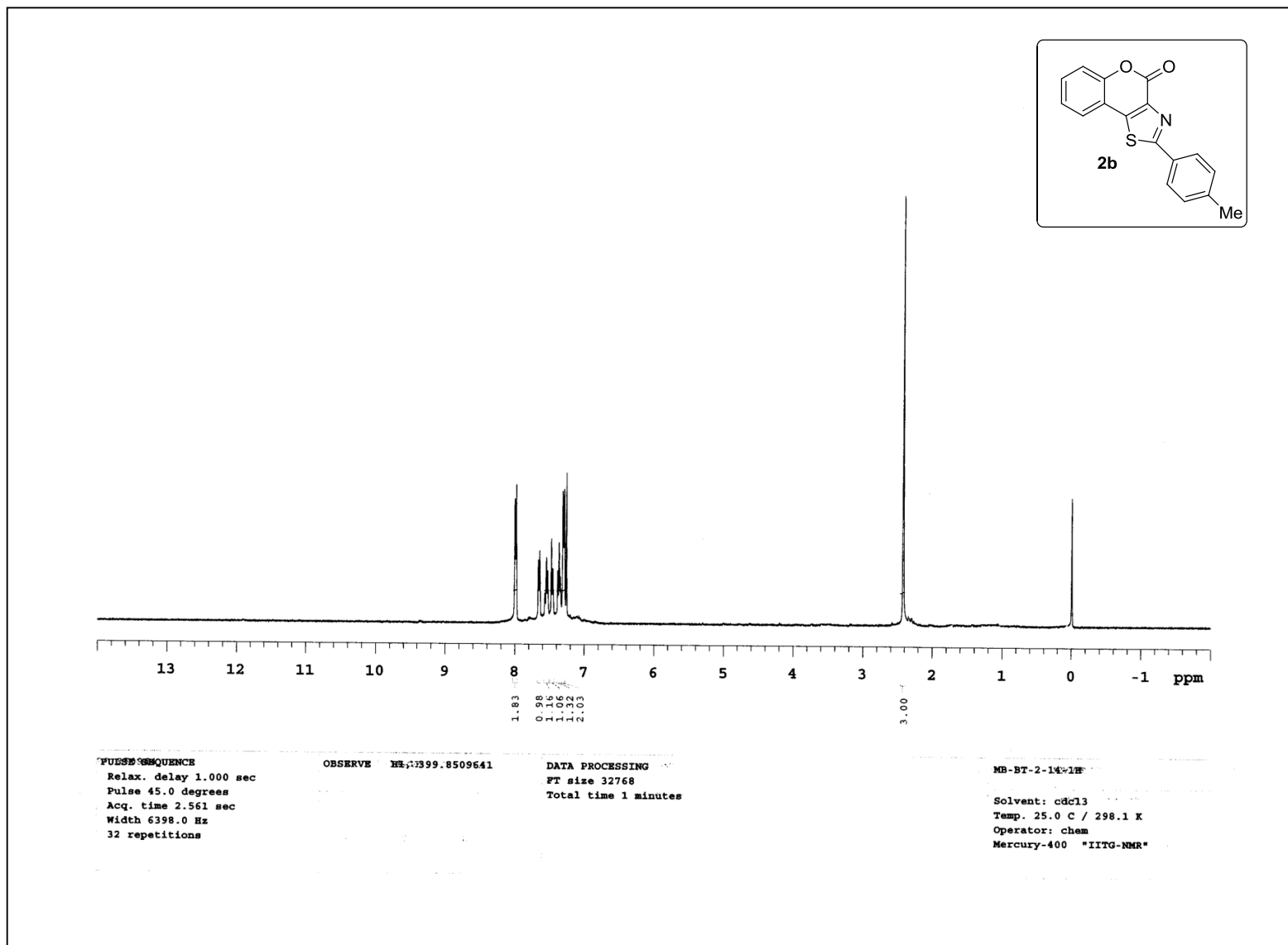
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 5484 repetitions	OBSERVE C13, 100.5425824 DECOUPLE H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 3.5 hours	MB-B-1-1-14-13C Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: MB-B-1-1-14-13C Mercury-400 "IITG-NMR"
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HRMS Spectra of 2a

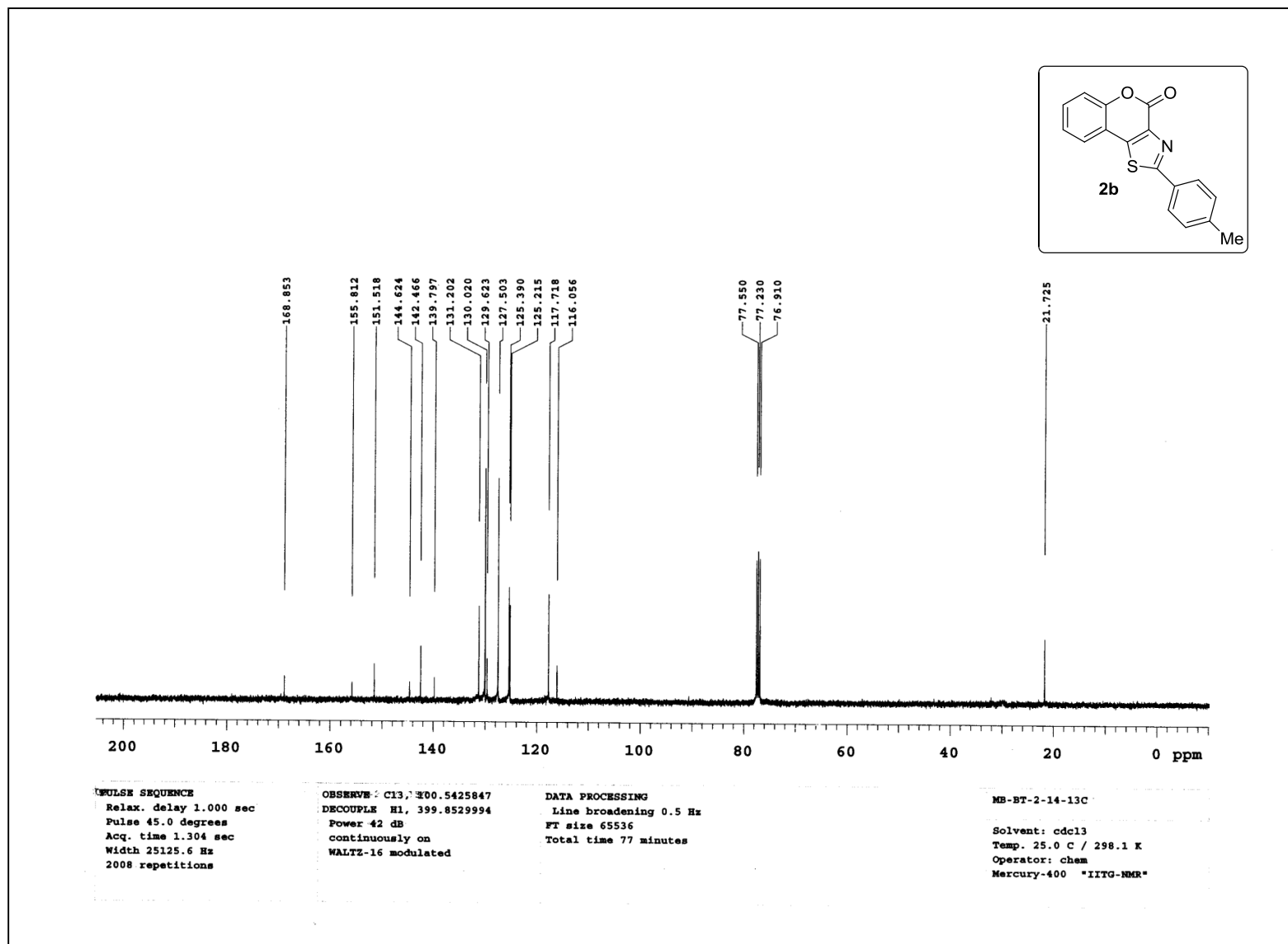
Sample Name	MB-BT-1-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-1-14.d	ACQ Method		Comment		Acquired Time	5/6/2014 2:46:43 PM



H¹NMR spectra of **2b**

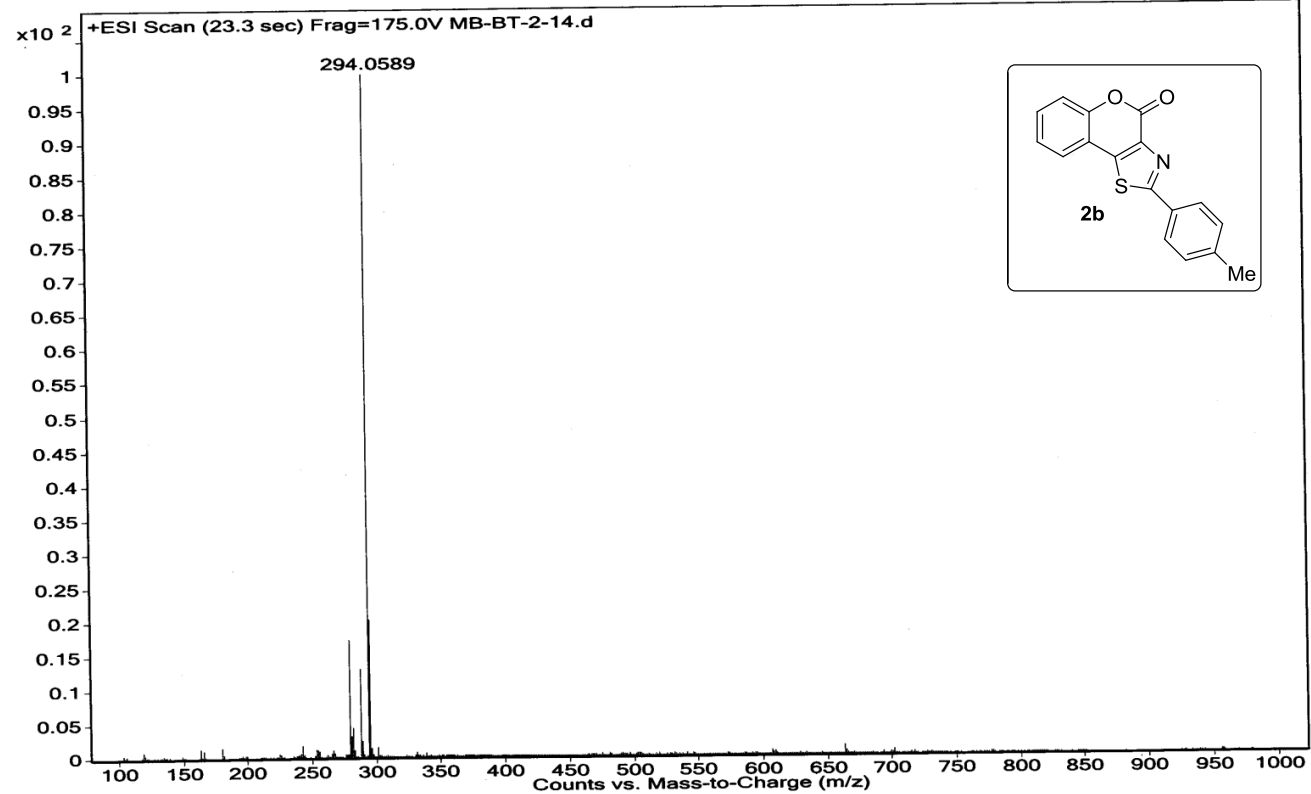


¹³C NMR spectra of **2b**

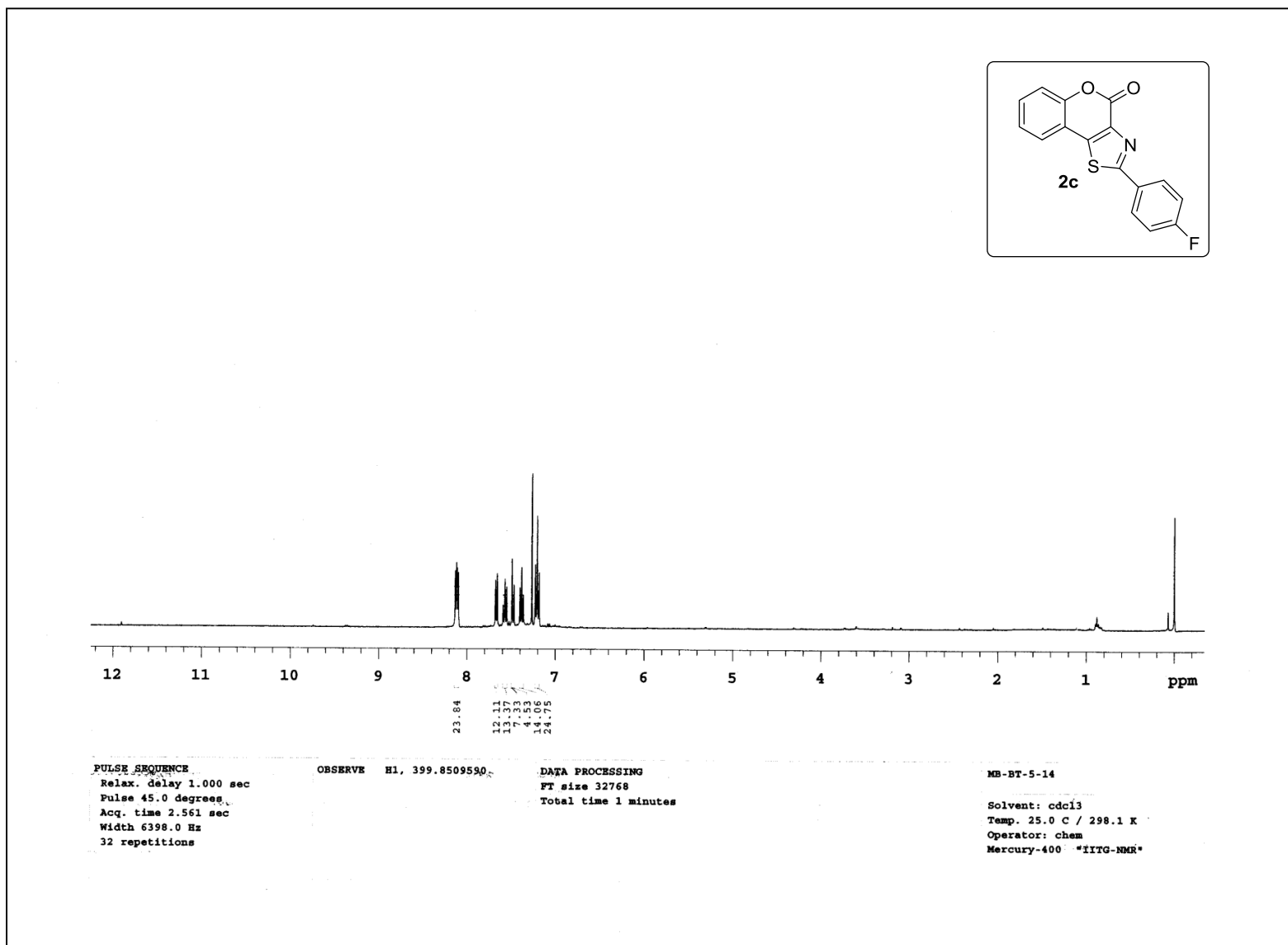


HRMS Spectra of 2b

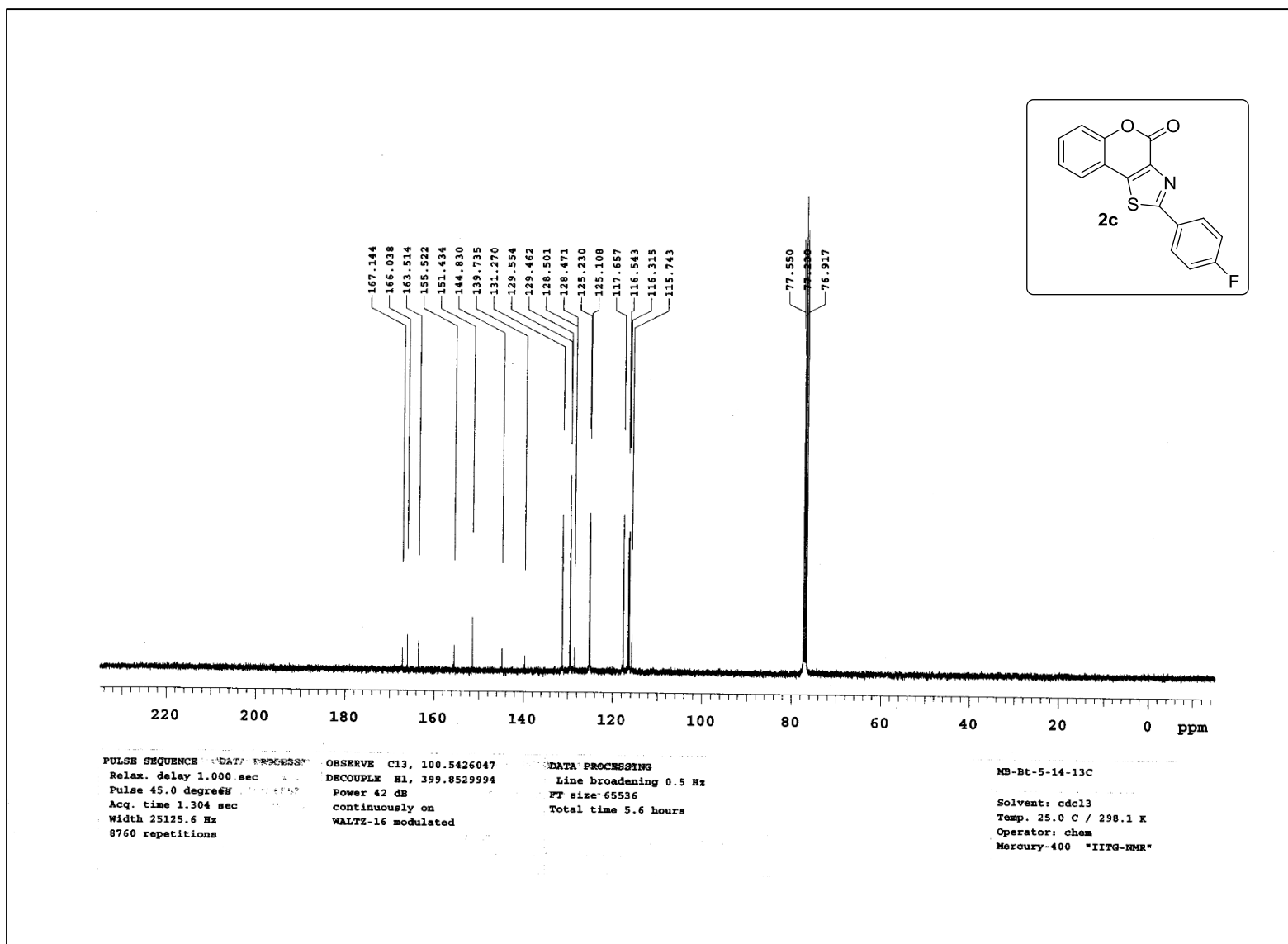
Sample Name	MB-BT-2-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-2-14.d	ACQ Method		Comment		Acquired Time	5/6/2014 2:48:07 PM



¹H NMR spectra of **2c**

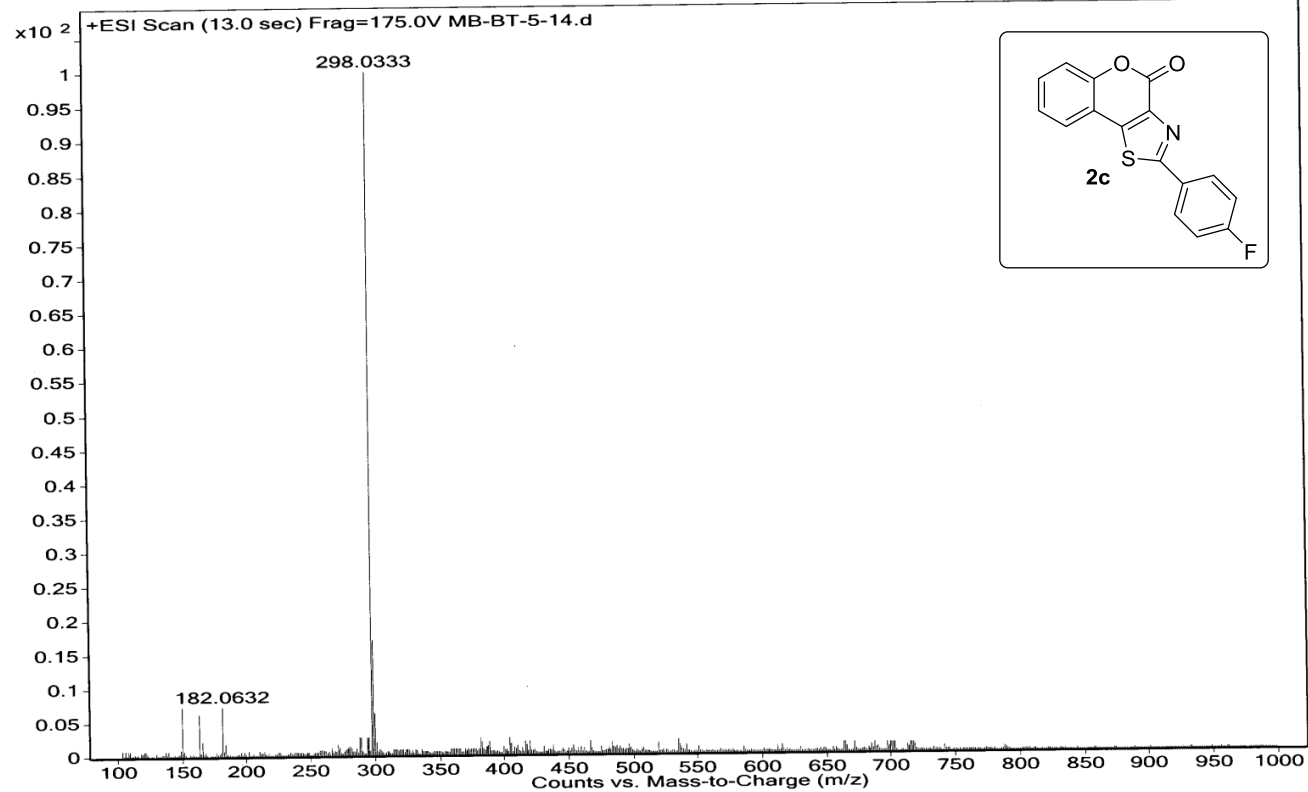


¹³C NMR spectra of **2c**

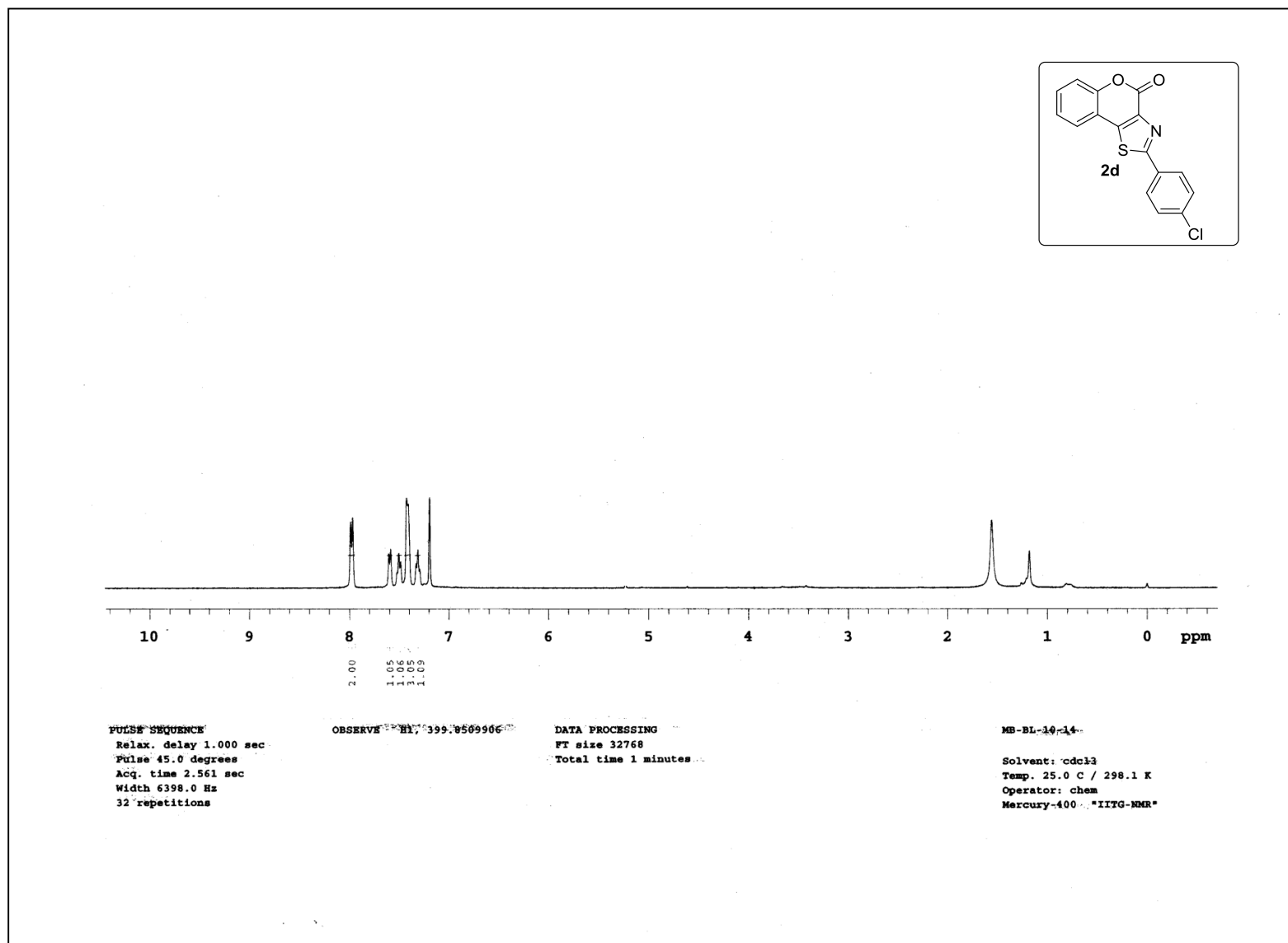


HRMS spectra of **2c**

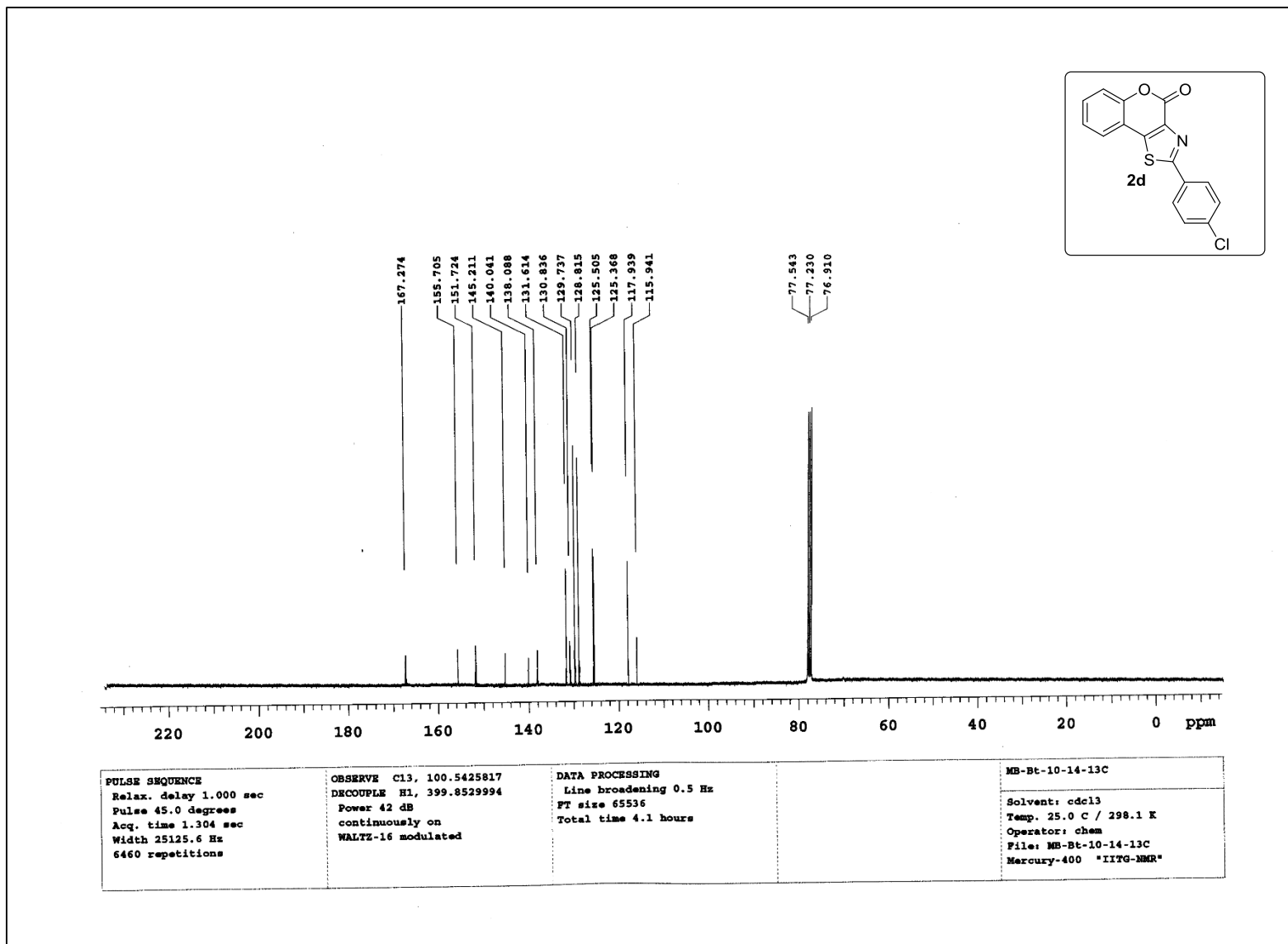
Sample Name	MB-BT-5-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-5-14.d	ACQ Method		Comment		Acquired Time	5/6/2014 2:52:23 PM



^1H NMR spectra of **2d**

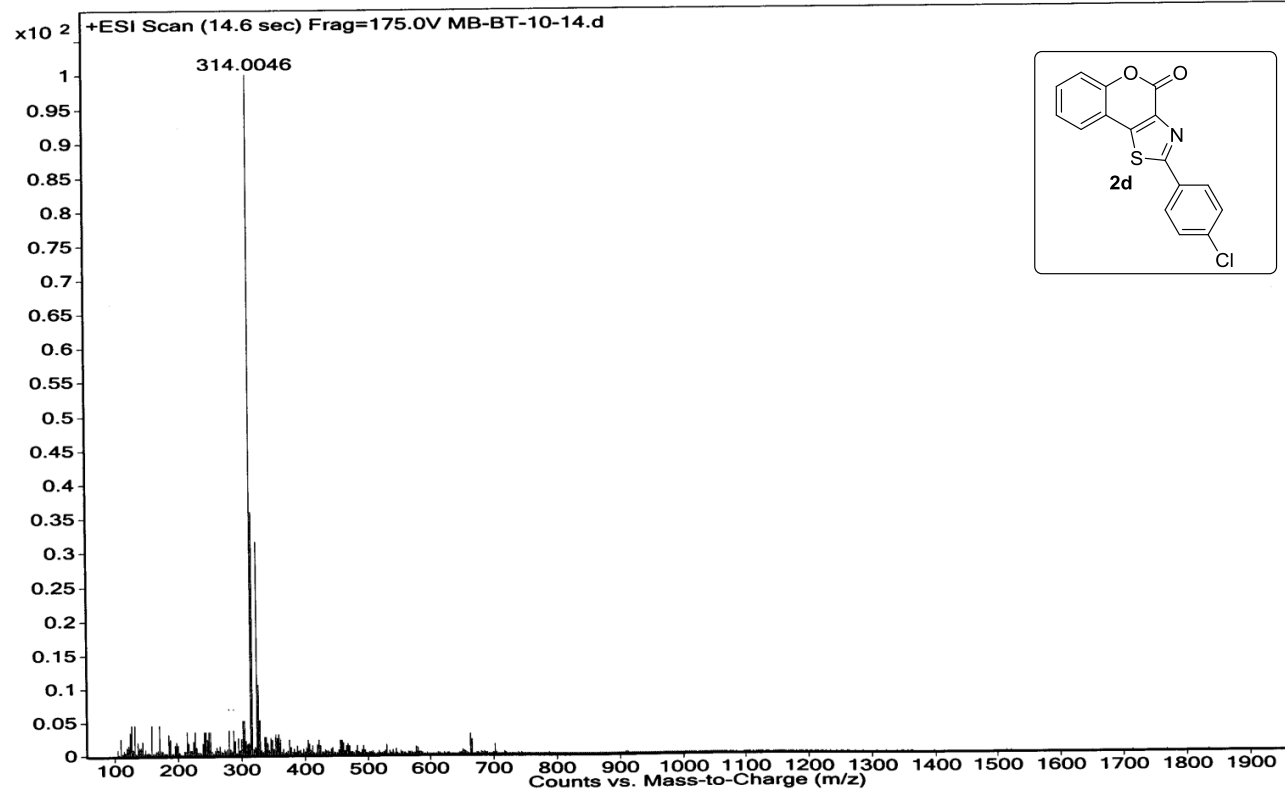


¹³C NMR spectra of **2d**



HRMS spectra of 2d

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-BT-10-14.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



^1H NMR spectra of **2e**

Sample Name:
MB-Bt-17-14-1H
Data Collected on:
IITG-NMR-mercury400
Archive directory:

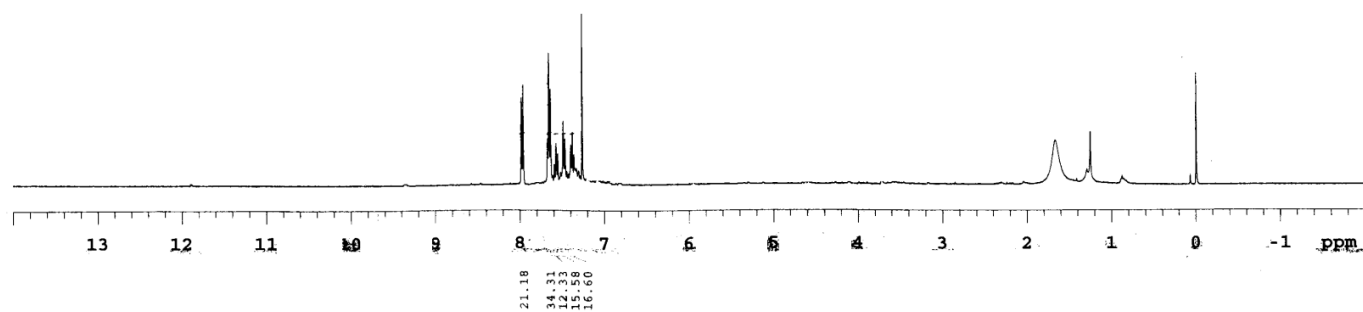
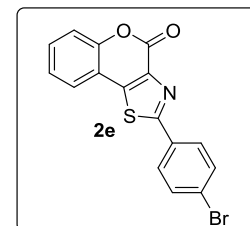
Sample directory:

FidFile: MB-Bt-17-14-1H

Pulse Sequence: PROTON (s2pul)
Solvent: cdcl3
Data collected on: Jun 18 2014

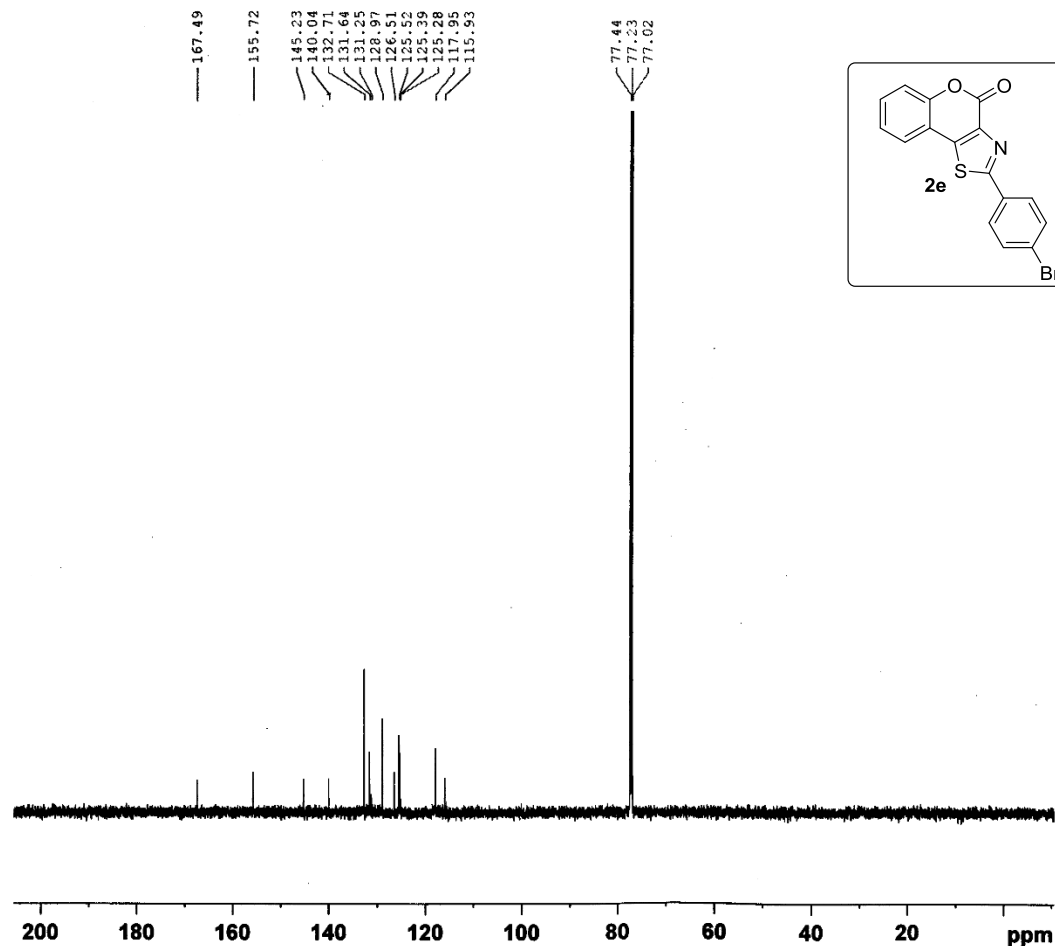
Temp. 25.0 C / 298.1 K
Operator: chem

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.561 sec
Width 6398.0 Hz
64 repetitions
OBSERVE H1, 399.8509641 MHz
DATA PROCESSING
FT size 32768
Total time 4 min 24 sec



¹³C NMR spectra of **2e**

MB-Bt-17-14-13C



Current Data Parameters
NAME MB-Bt-17-14-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140619
Time_ 9.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 407
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 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

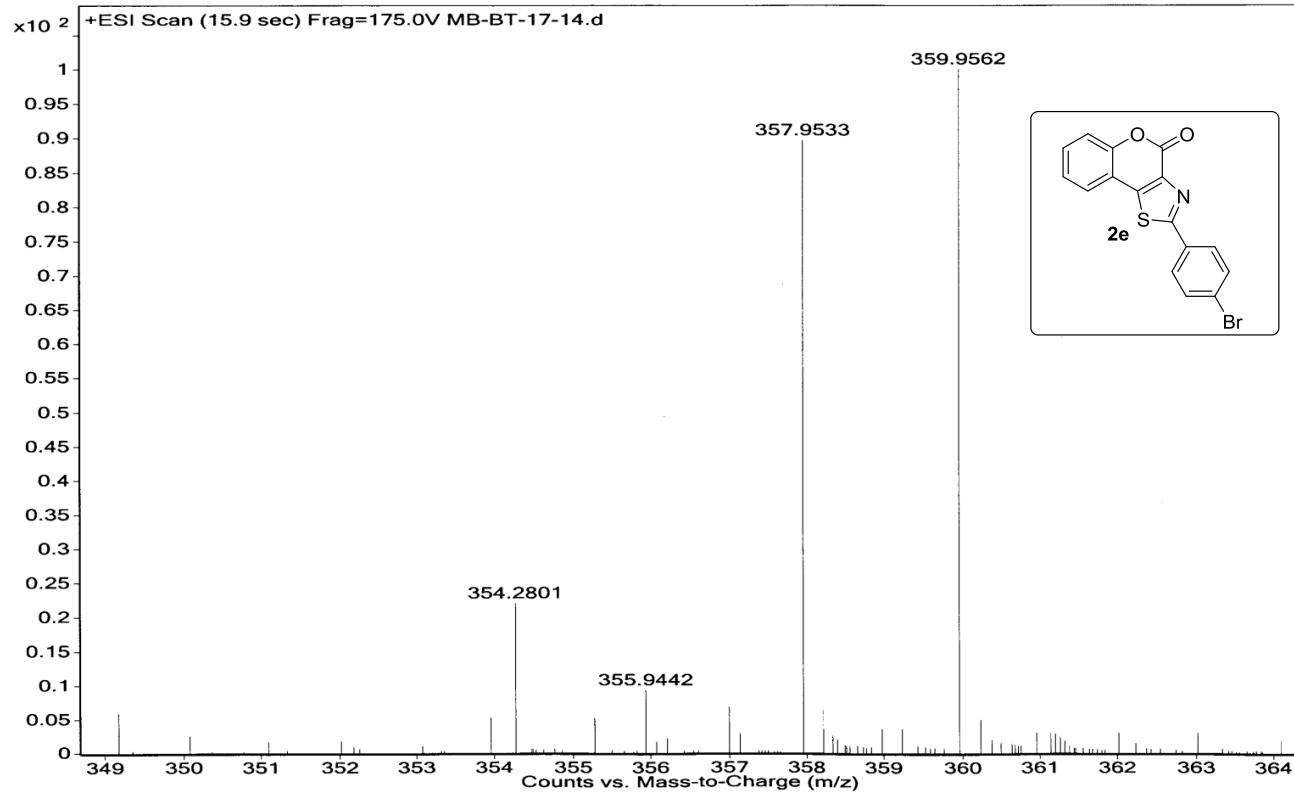
===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

===== 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

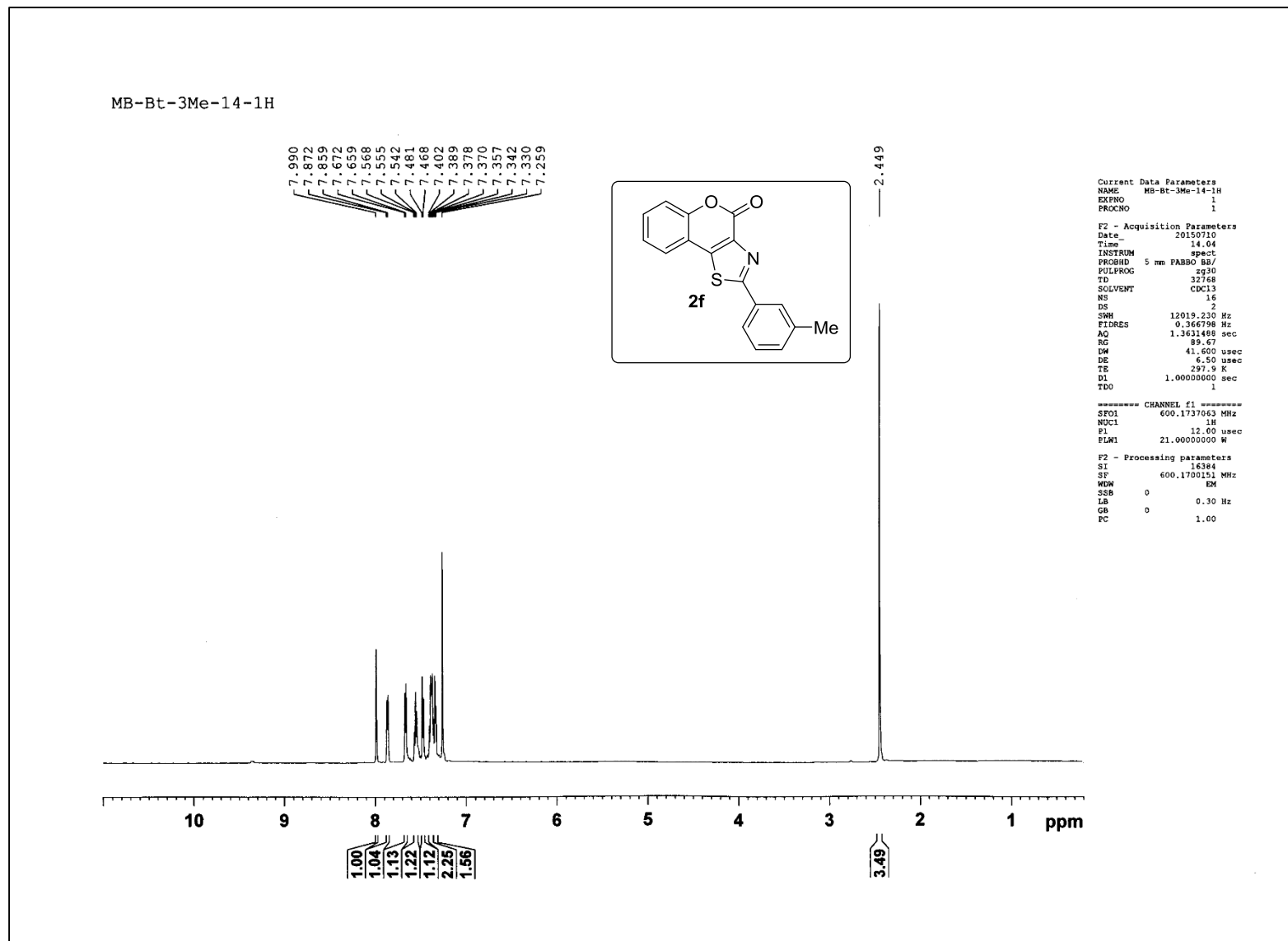
F2 - Processing parameters
SI 16384
SF 150.9128347 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectra of **2e**

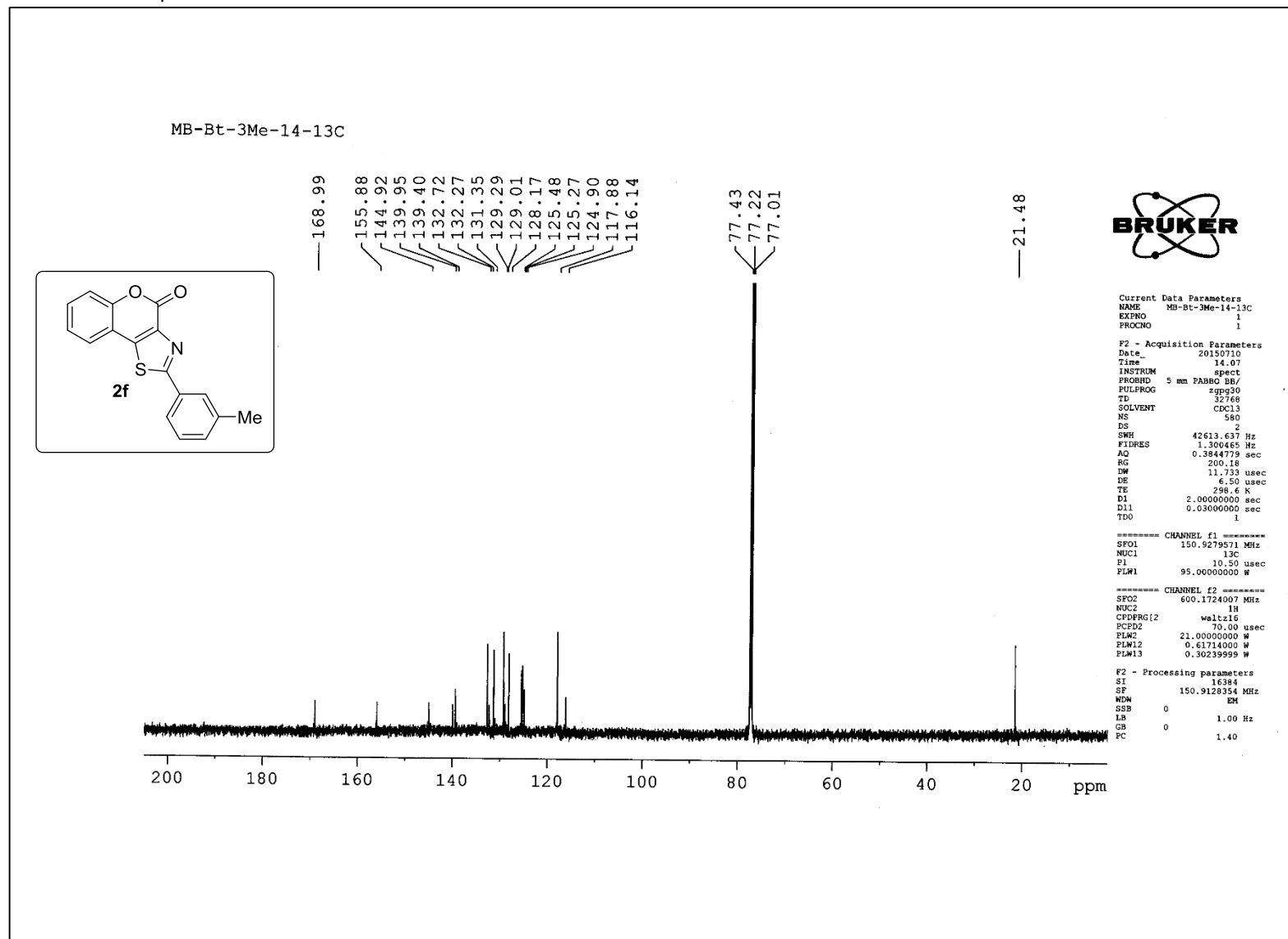
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



¹H NMR spectra of **2f**

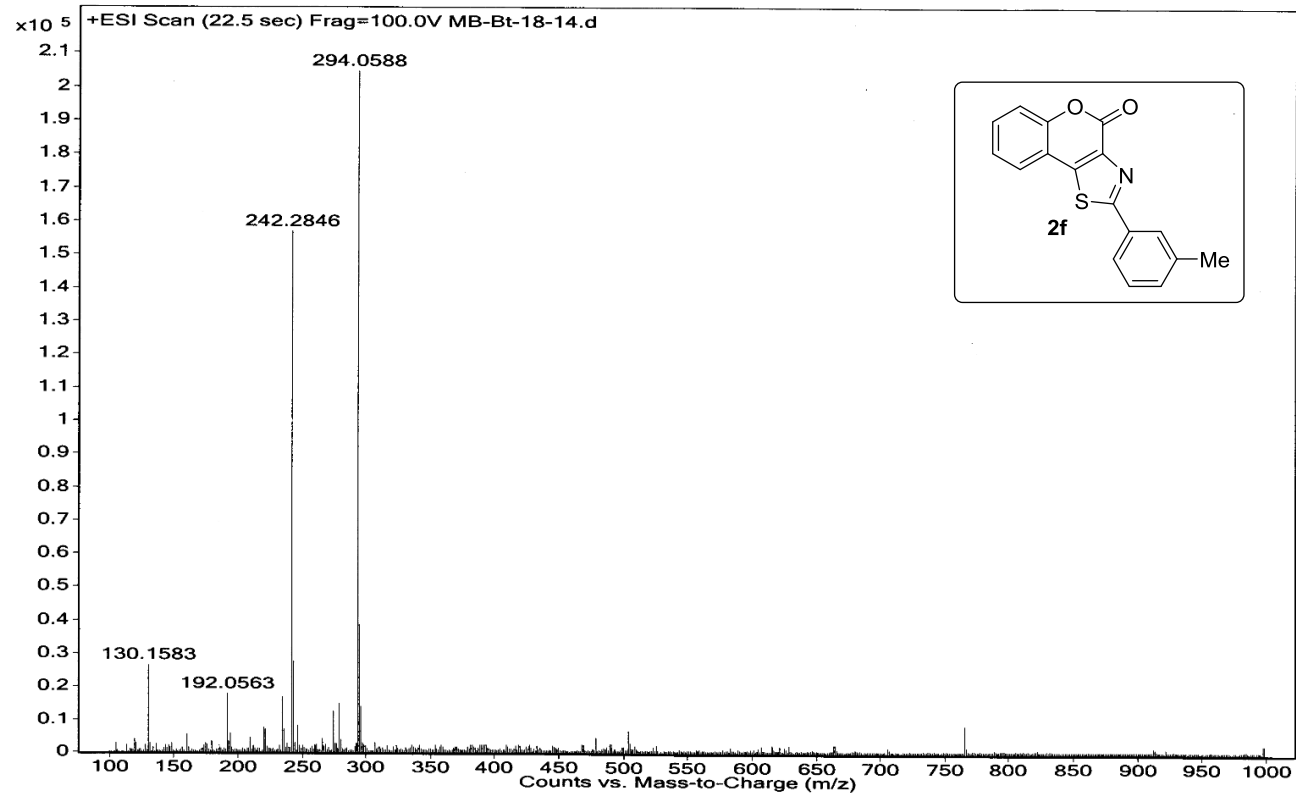


¹³C NMR spectra of **2f**

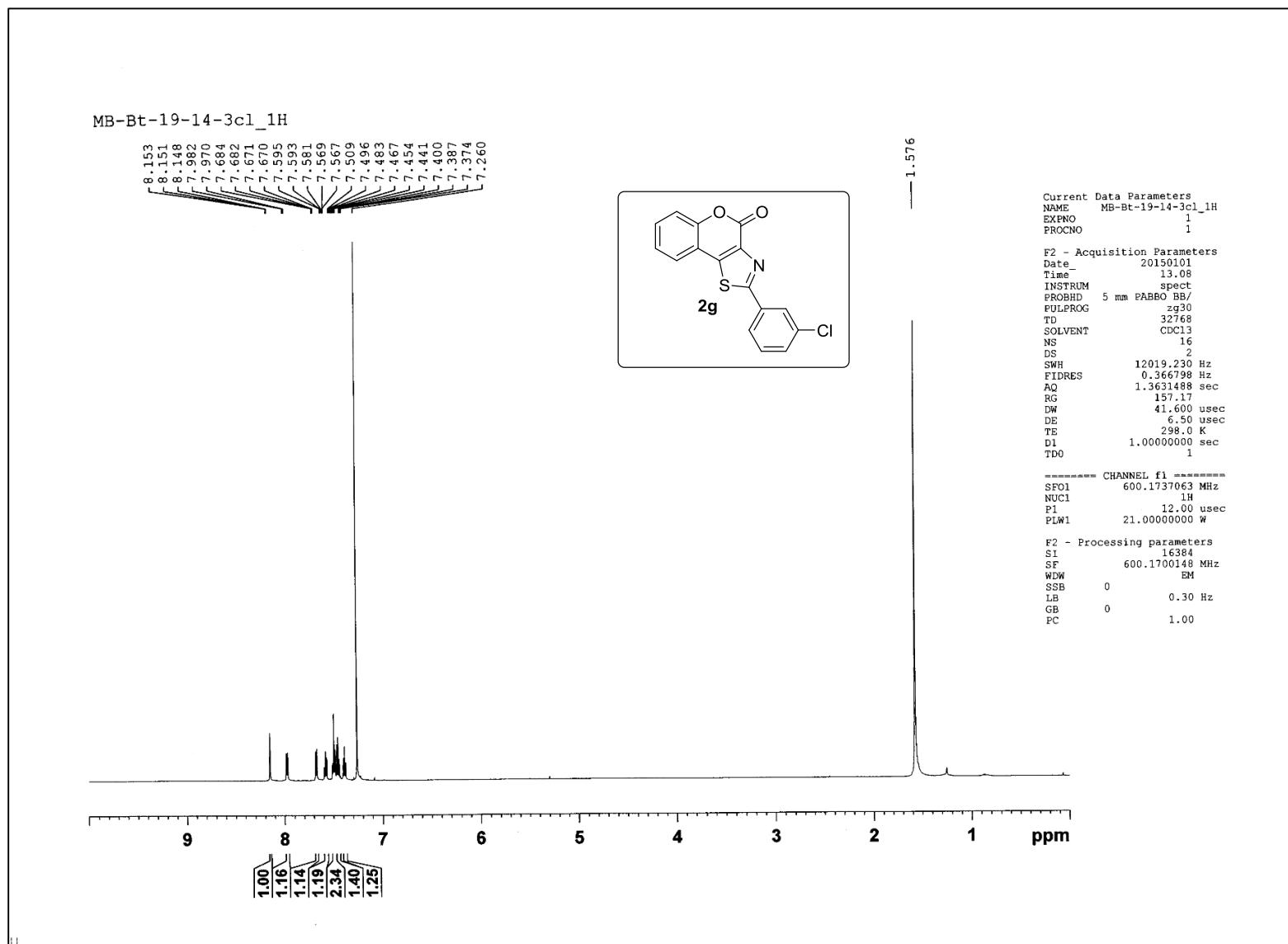


HRMS Spectra of 2f

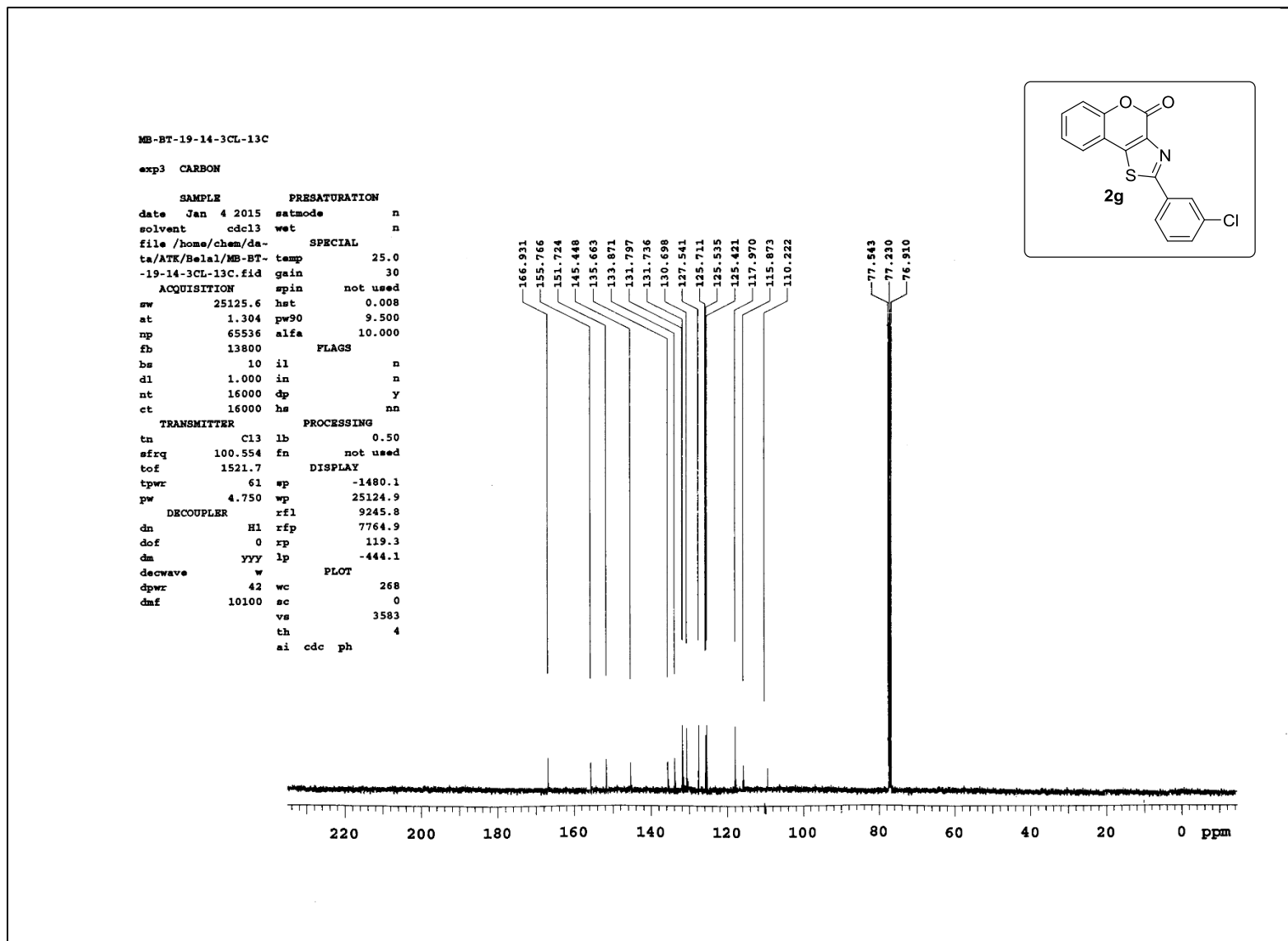
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-Bt-18-14.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H NMR Spectra of **2g**

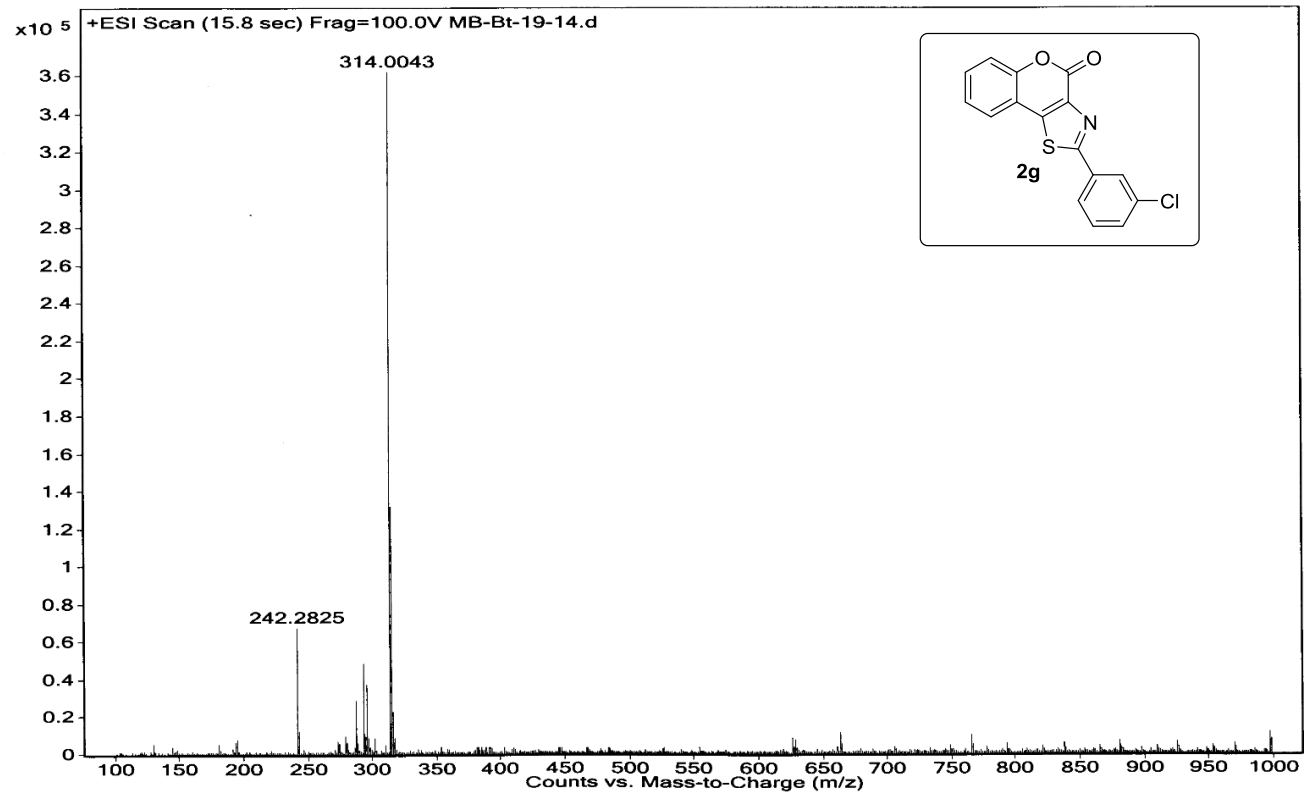


¹³C NMR spectra of **2g**



HRMS Spectra of 2g

Sample Name	MB-Bt-19-14	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-Bt-19-14.d	ACQ Method		Comment		Acquired Time	1/13/2015 11:03:24 AM



¹H NMR of 2h

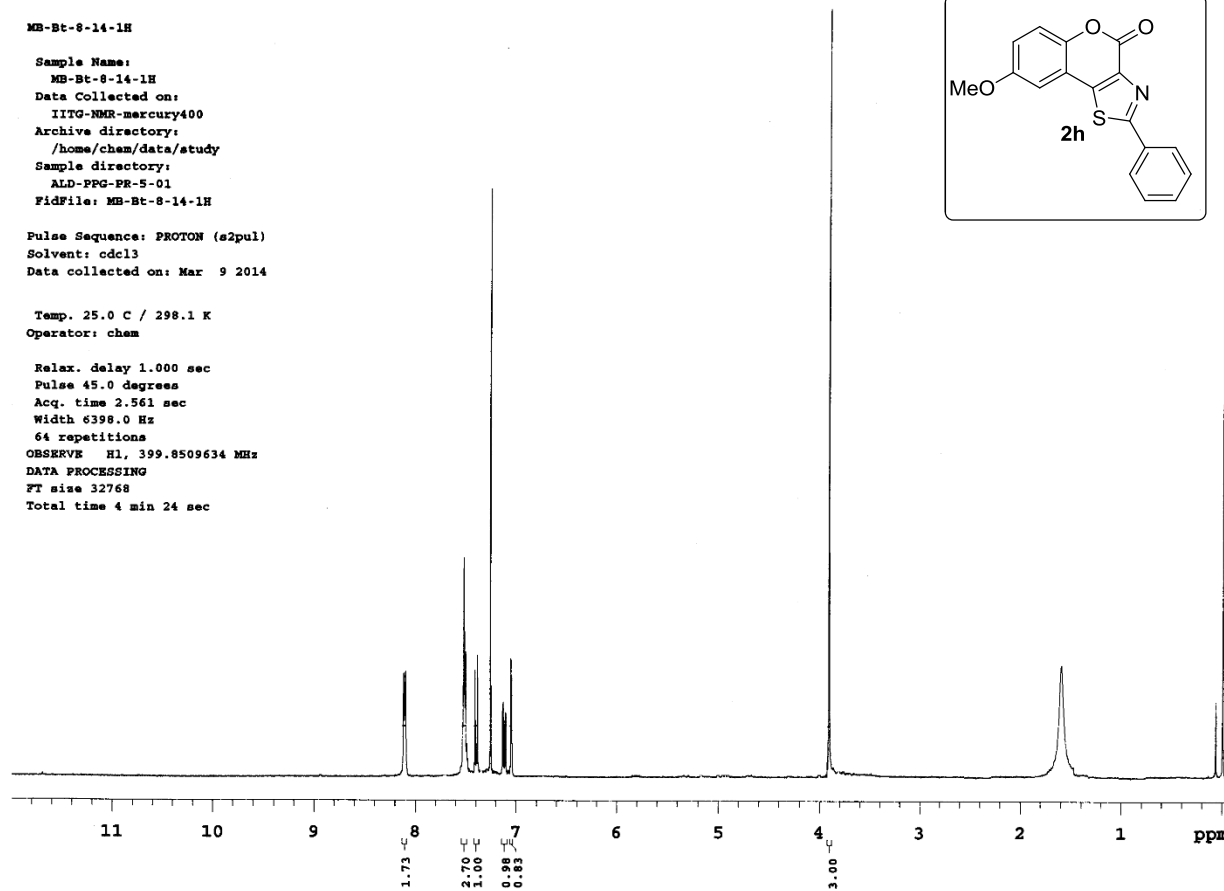
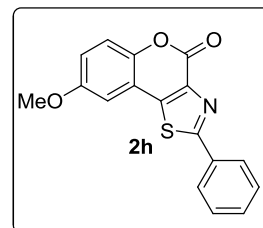
MB-Bt-8-14-1H

Sample Name:
MB-Bt-8-14-1H
Data Collected on:
IITG-NMR-mercury400
Archive directory:
/home/chem/data/study
Sample directory:
ALD-PPG-PR-5-01
FidFile: MB-Bt-8-14-1H

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

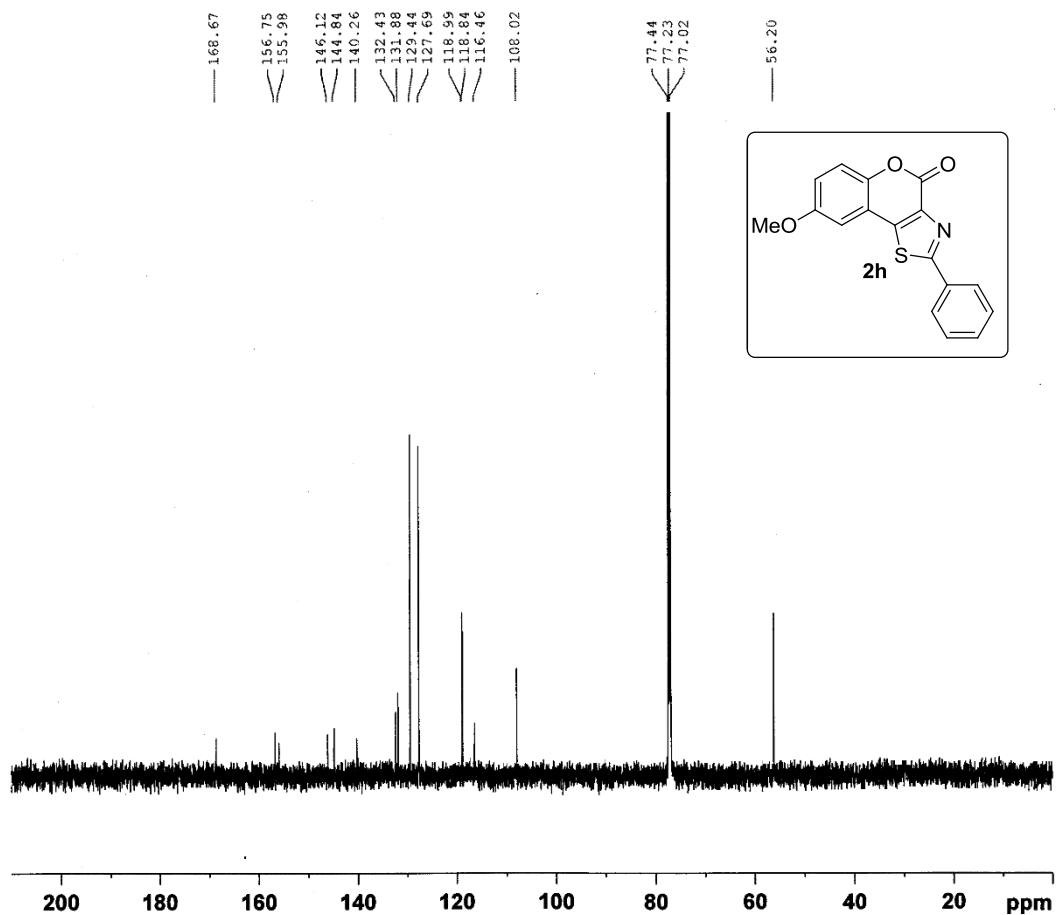
Temp. 25.0 C / 298.1 K
Operator: cham

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



¹³C NMR of 2h

MB-Bt-8-14-13C



Current Data Parameters
NAME MB-Bt-8-14-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140310
Time_ 10.23
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 781
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 300.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

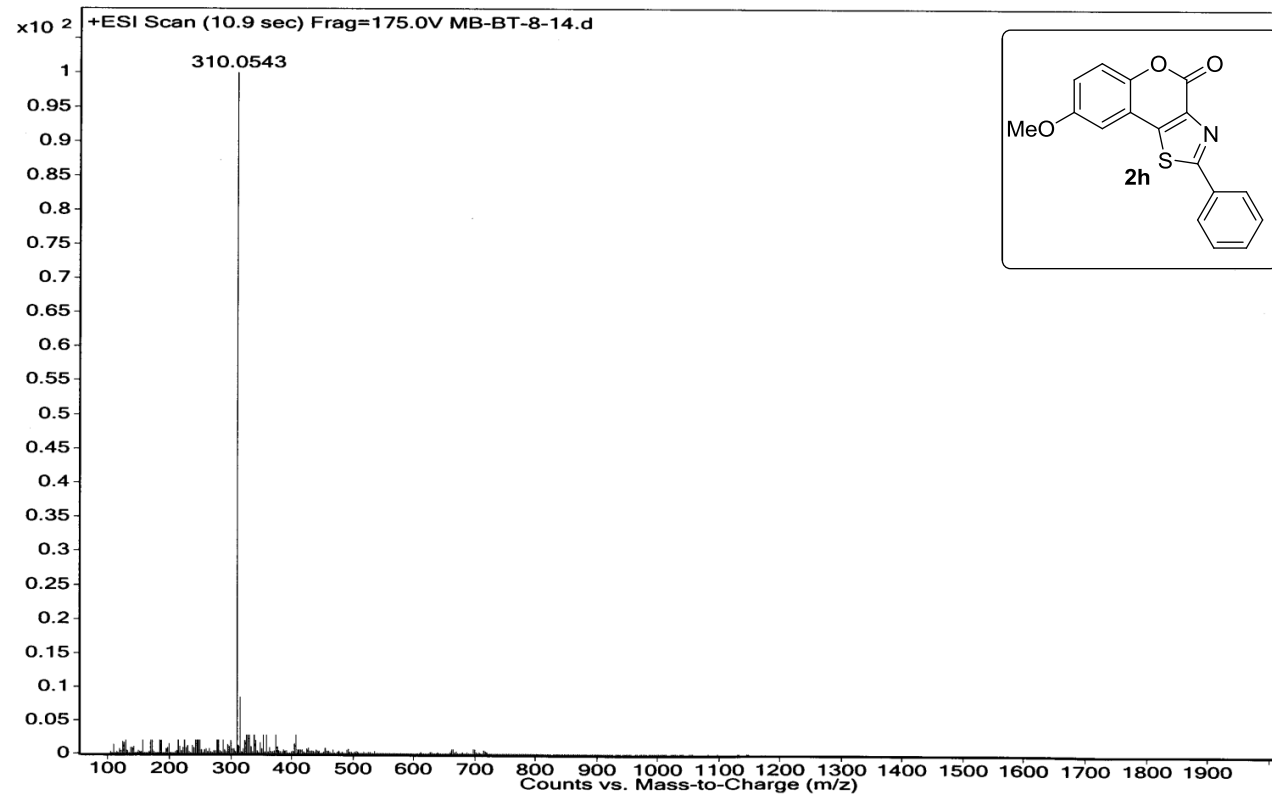
===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

===== 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 150.9128328 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectra of **2h**

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-BT-8-14.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H NMR spectra of **2i**

MB-Bt-9-14-1H

Sample Name:

MB-Bt-9-14-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 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

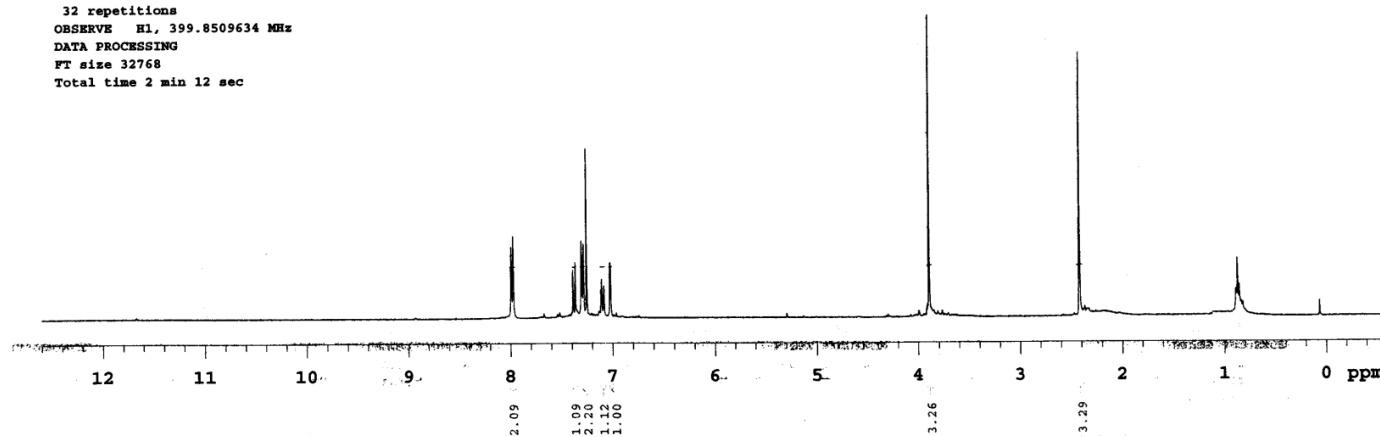
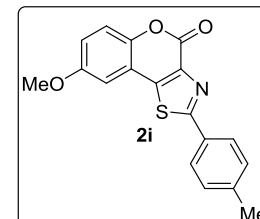
32 repetitions

OBSERVE H1, 399.8509634 MHz

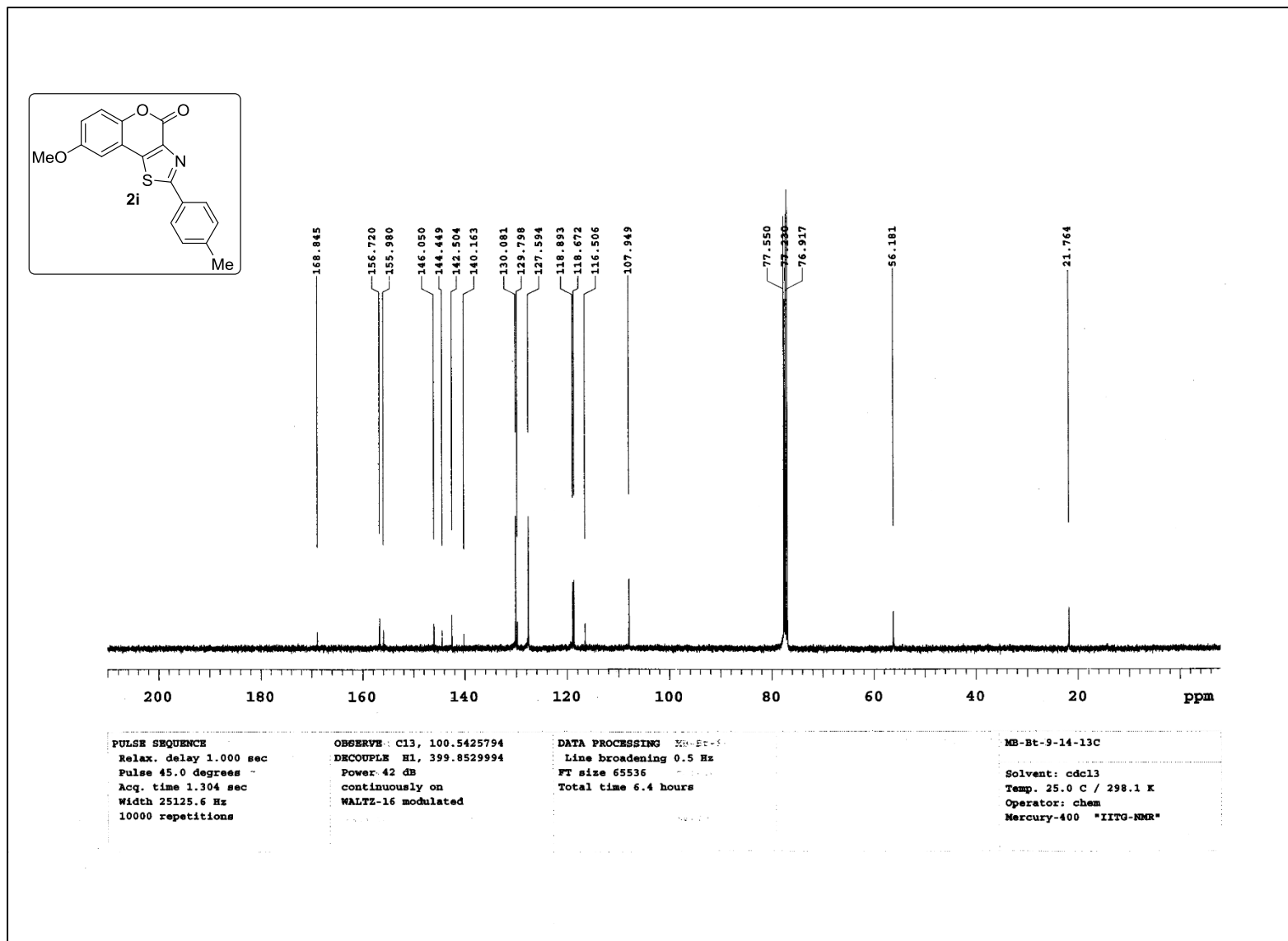
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec

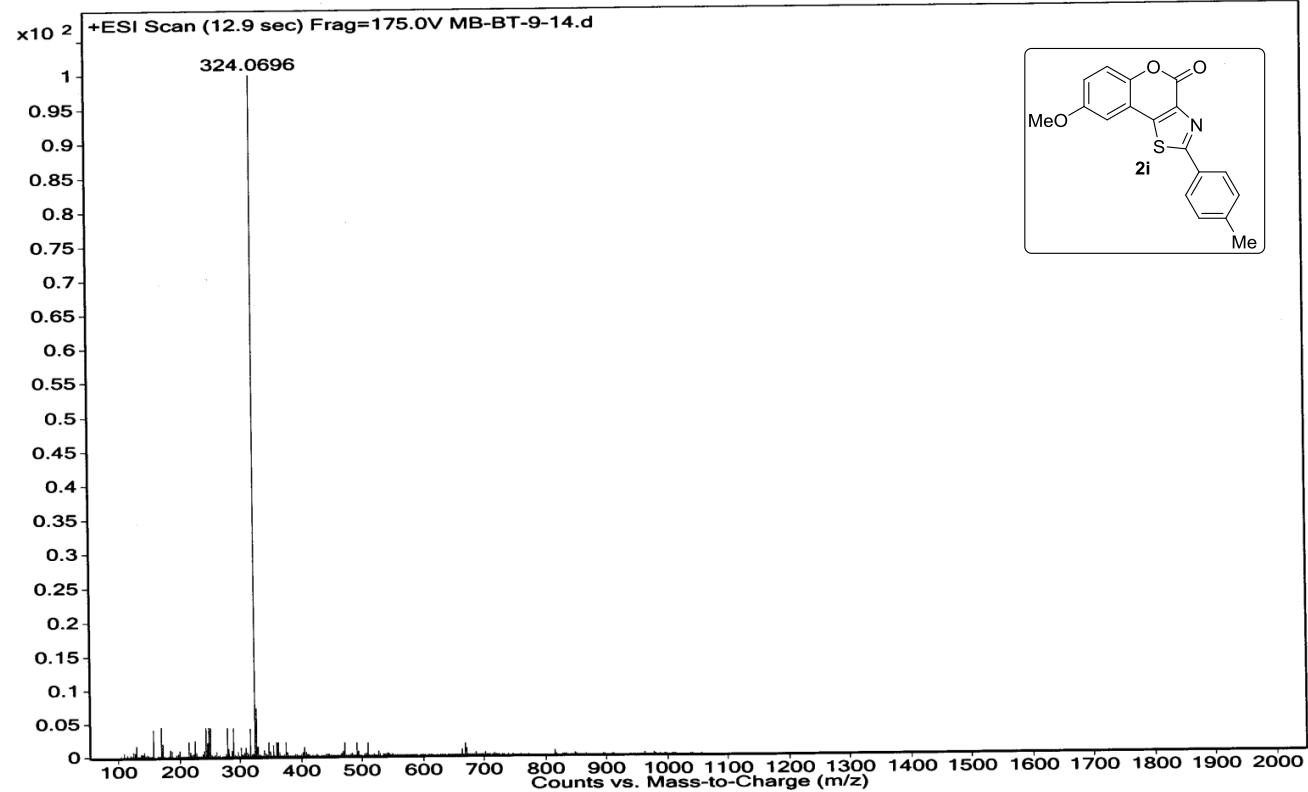


¹³C NMR spectra of **2i**



HRMS spectra of **2i**

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-BT-9-14.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H NMR spectra of **2j**

MB-Bt-12-14-1H

Sample Name:

MB-Bt-12-14-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/export/home/chempack/vnmrsvs/data

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 23 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

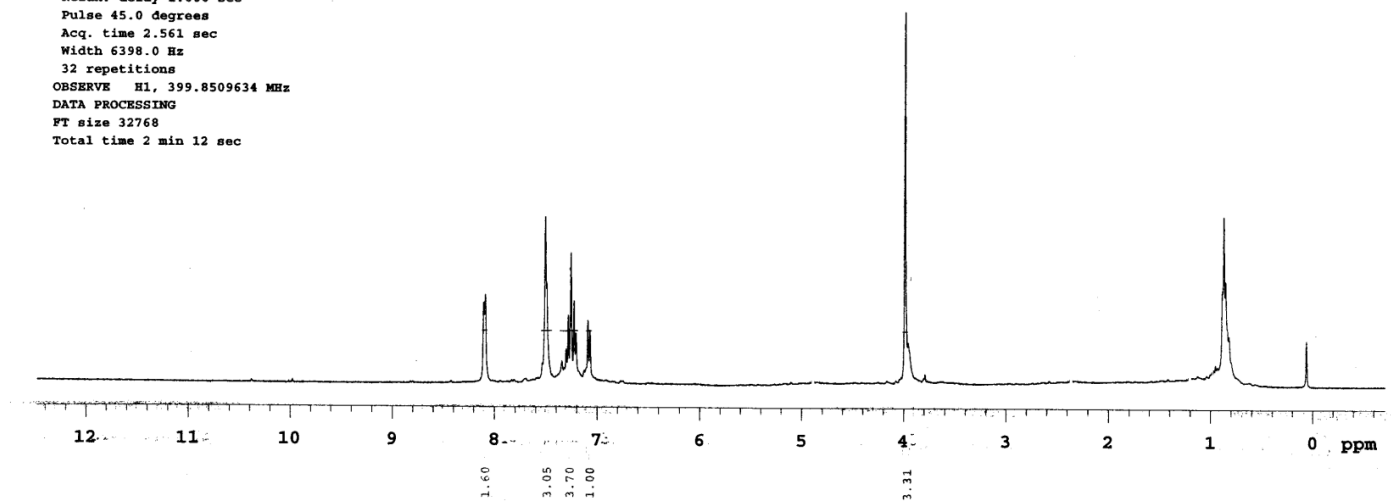
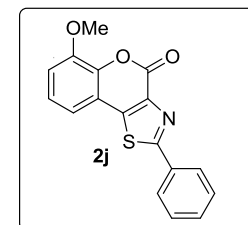
32 repetitions

OBSERVE H1, 399.8509634 MHz

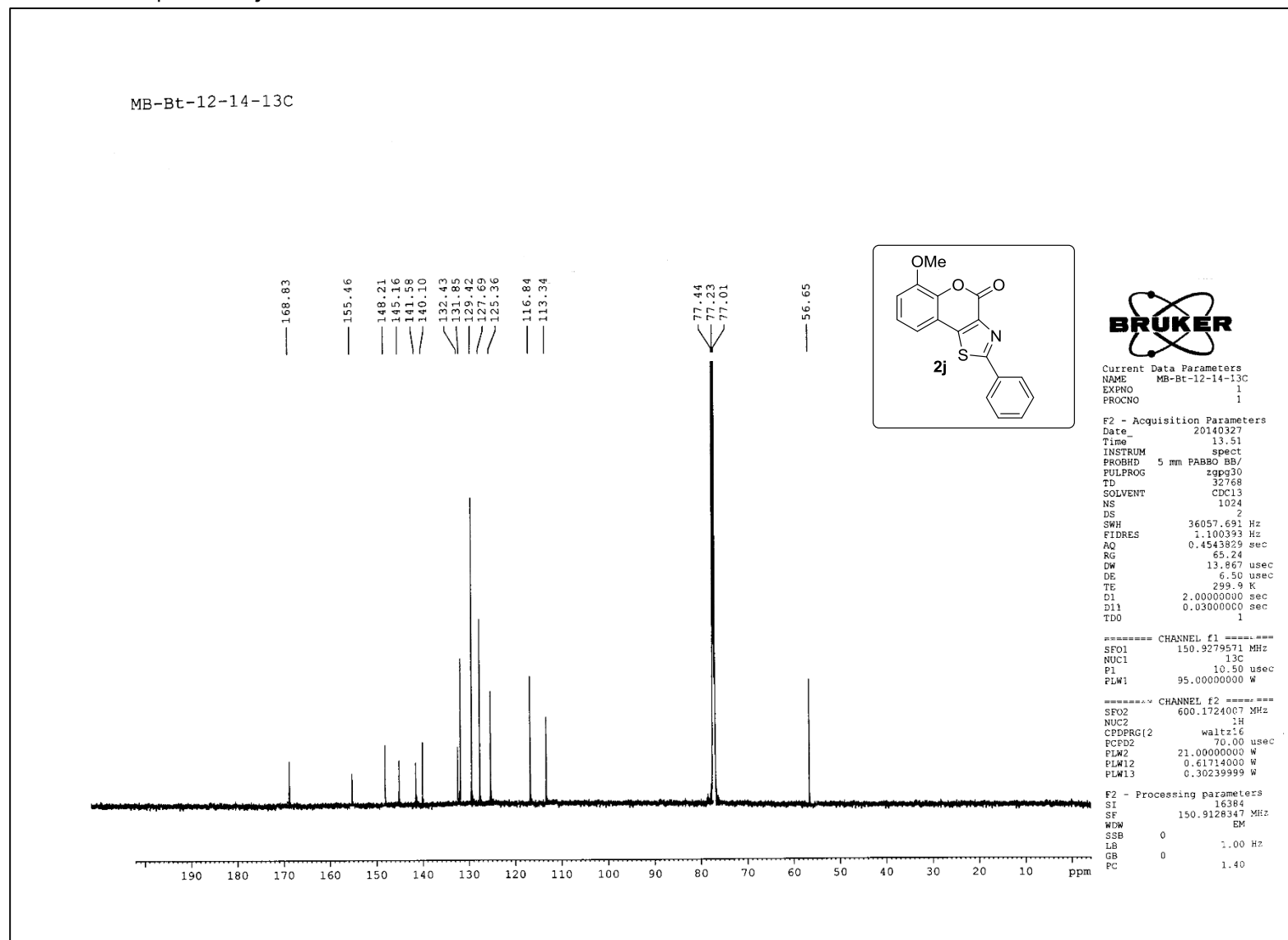
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec

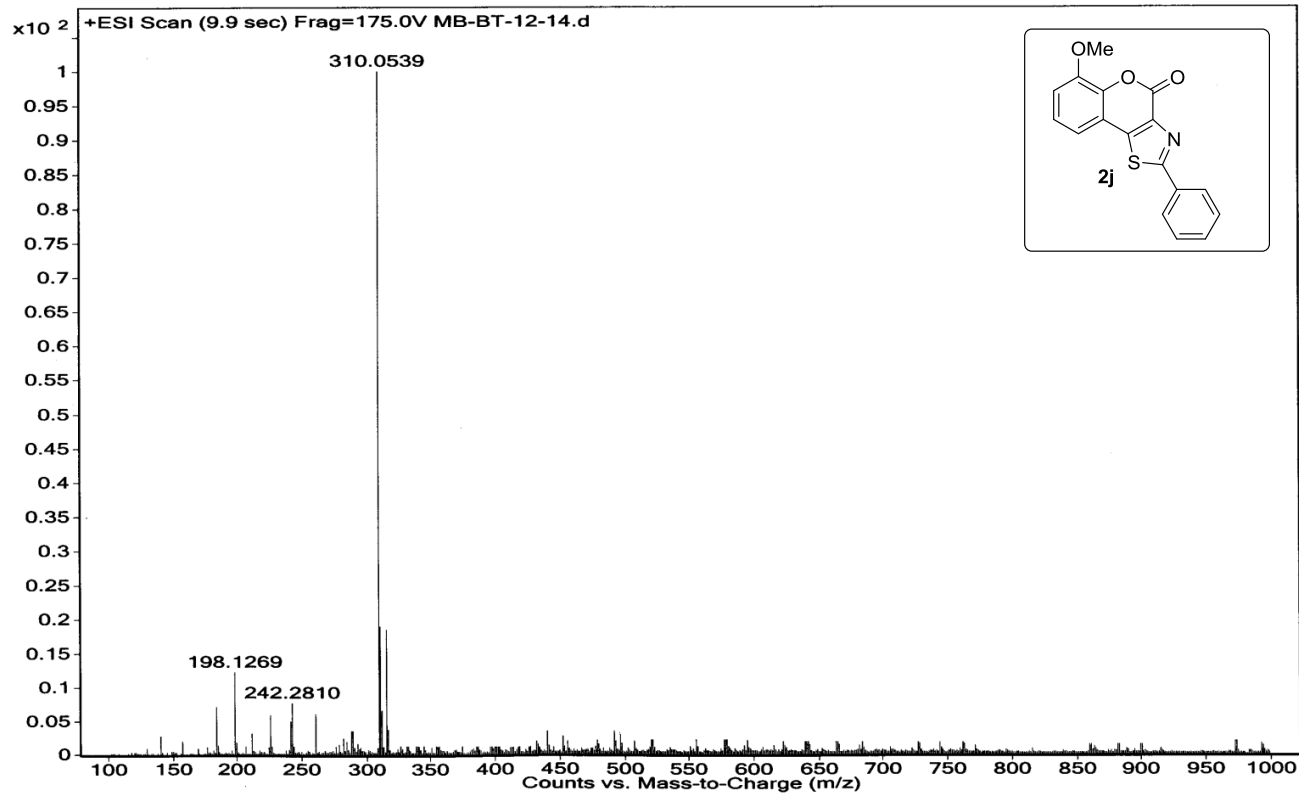


¹³C NMR spectra of 2j

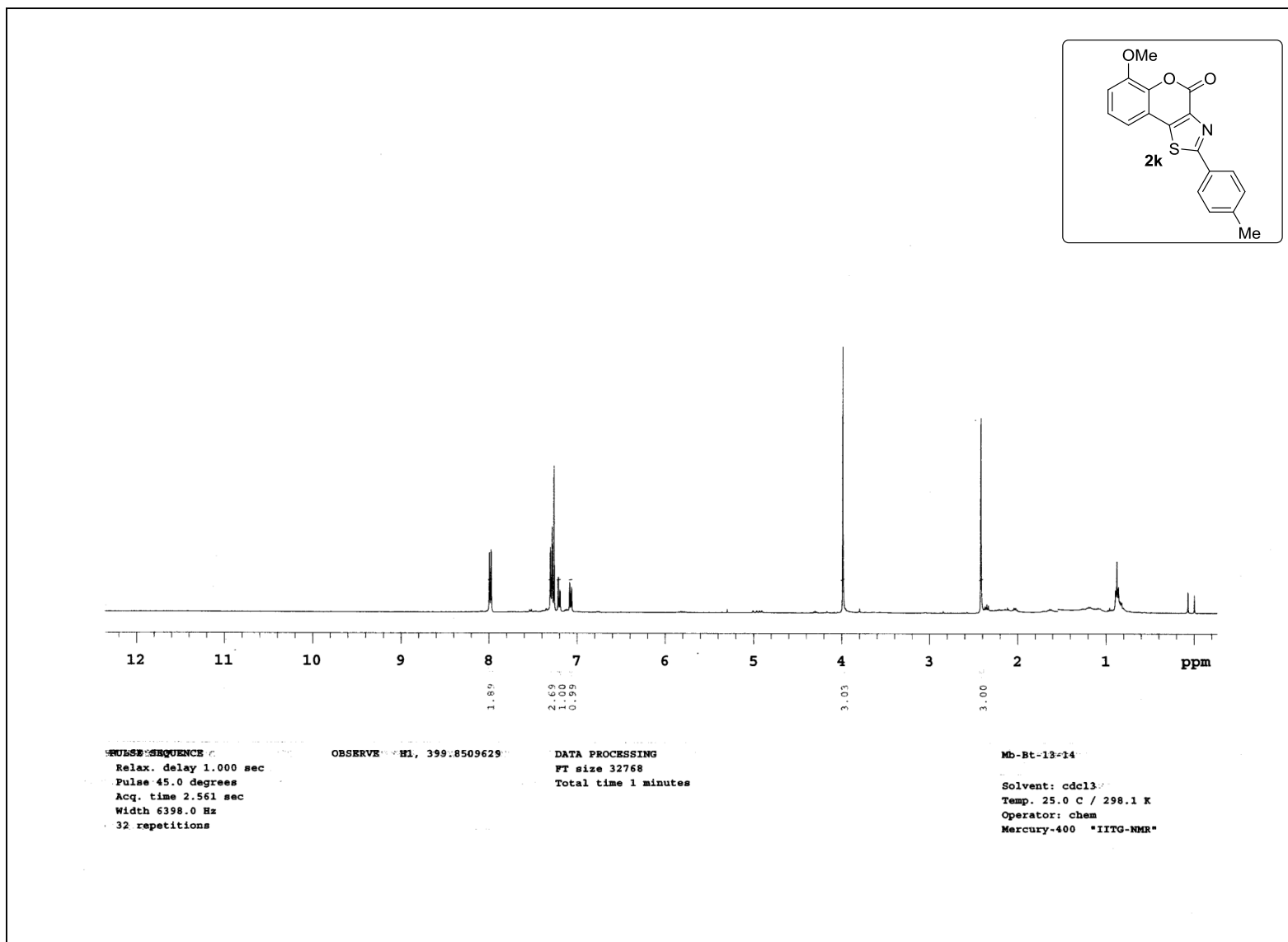


HRMS spectra of **2j**

Sample Name	MB-BT-12-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-12-14.d	ACQ Method		Comment		Acquired Time	5/13/2014 3:40:30 PM

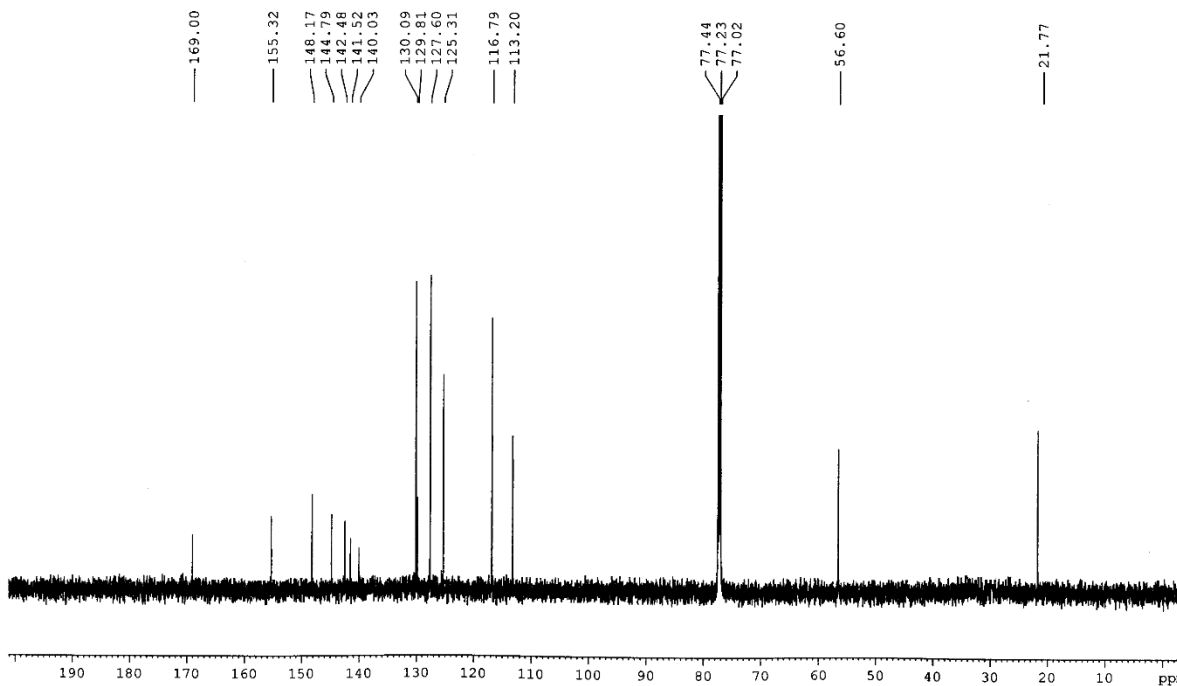
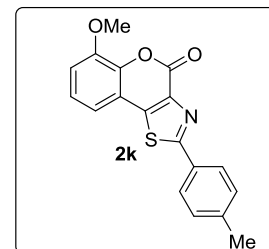


H¹ NMR spectra of **2k**



¹³C NMR spectra of **2k**

MB-BT-13-14_13C



Current Data Parameters
NAME MB-BT-13-14_13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140325
Time 18.43
INSTRUM spect
PROBHD 5 mm PABBO RB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 727
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 300.5 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

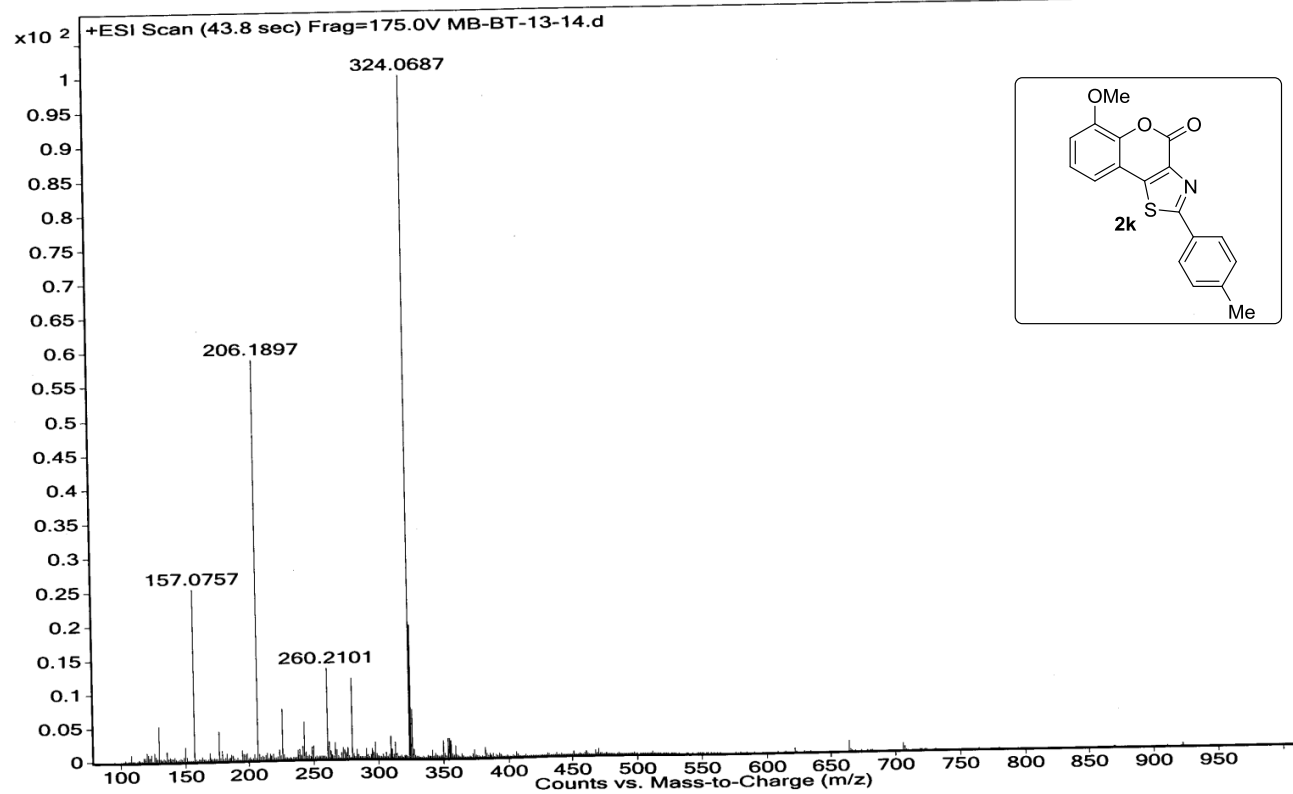
===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 70.00 usec
PLW2 21.00000000 W
PLW12 0.63714000 W
PLW13 0.30239999 W

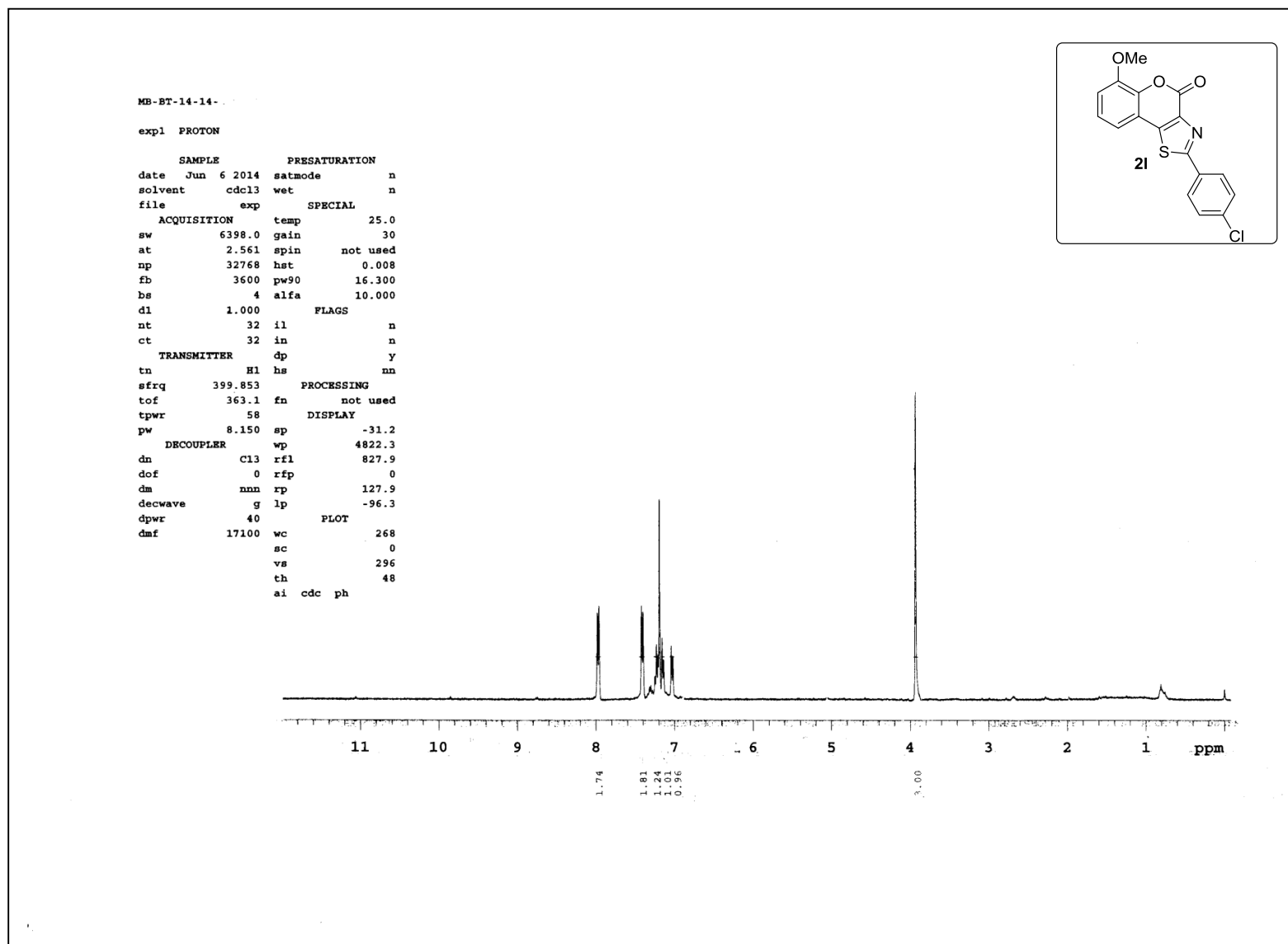
F2 - Processing parameters
SI 16384
SF 150.9128332 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectra of 2k

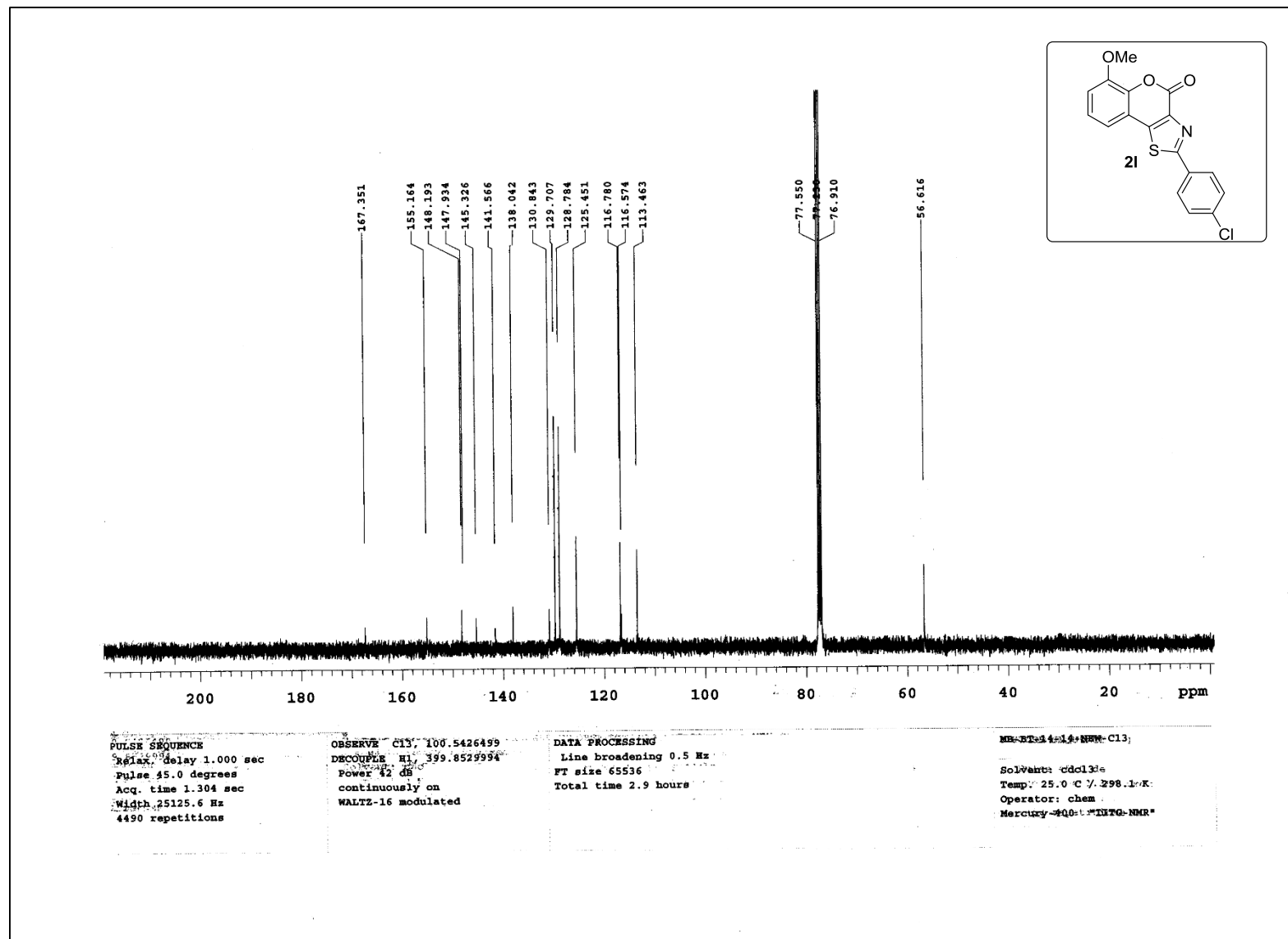
Sample Name	MB-BT-13-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-13-14.d	ACQ Method		Comment		Acquired Time	5/13/2014 3:35:40 PM



¹H NMR spectra of **2l**



¹³C NMR spectra of **21**



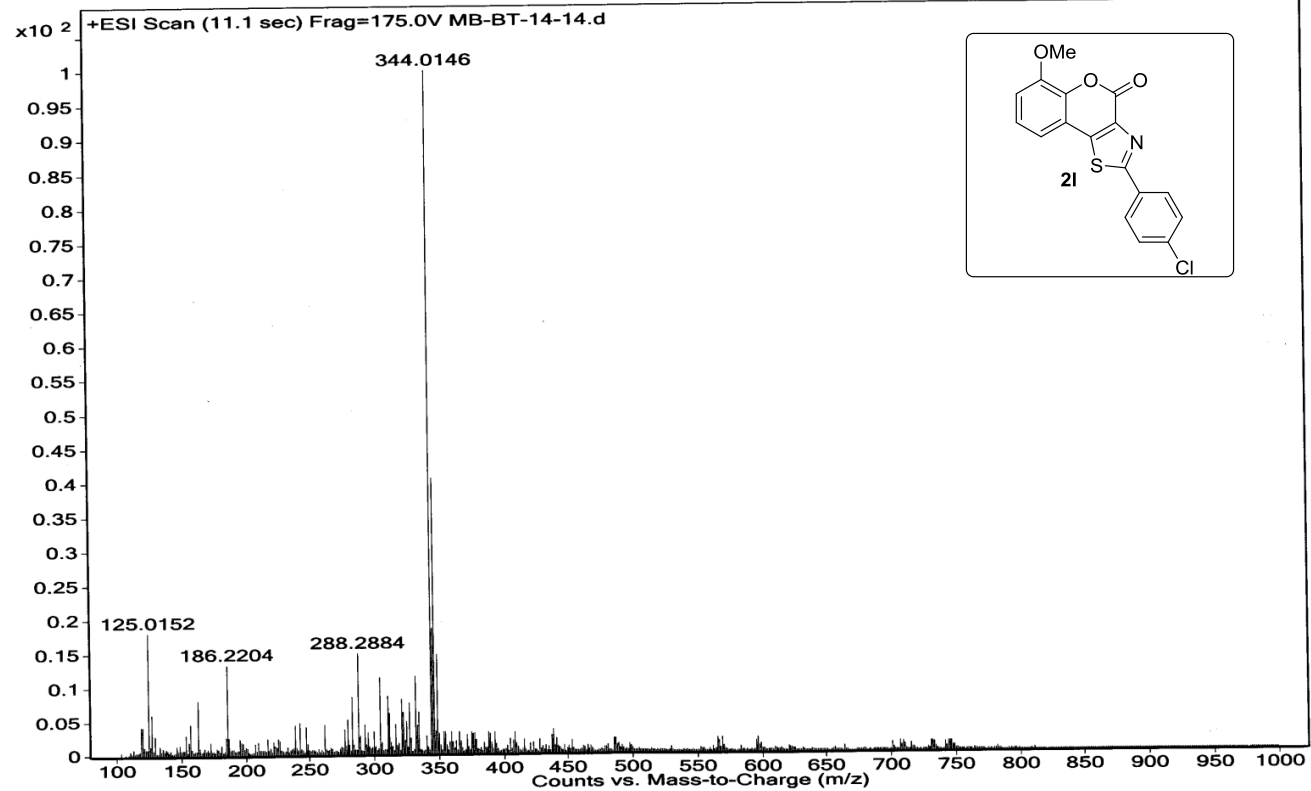
HRMS spectra of **2l**

Sample Name
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



H^1 NMR spectra of **2m**

MB-BT-3-14-1H

Sample Name:

MB-BT-3-14-1H

Data Collected on:

ITQ-NMR-mercury400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Mar 1 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

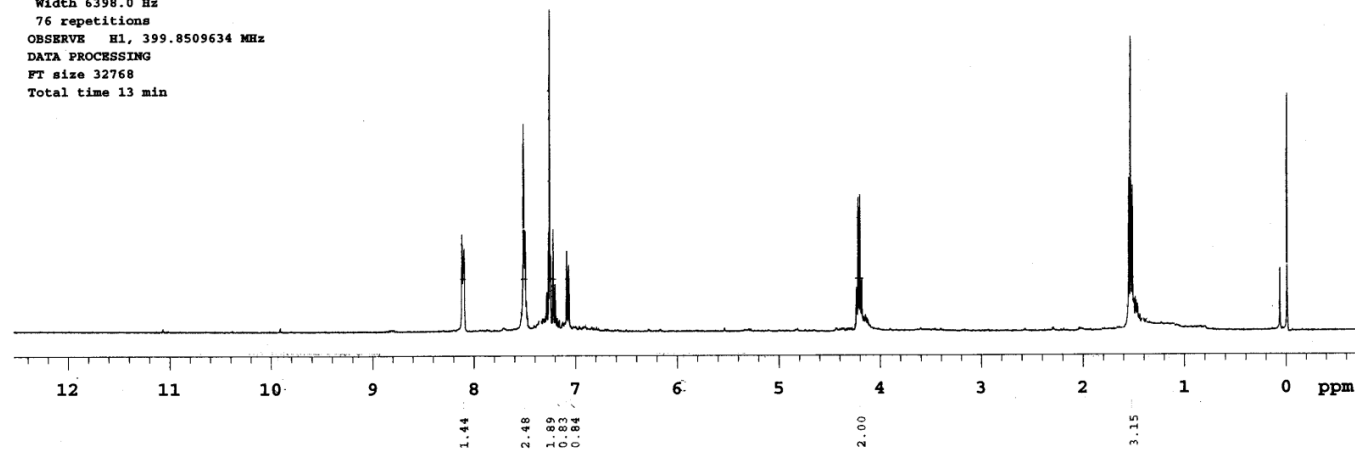
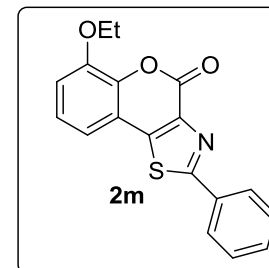
76 repetitions

OBSERVE H1, 399.8509634 MHz

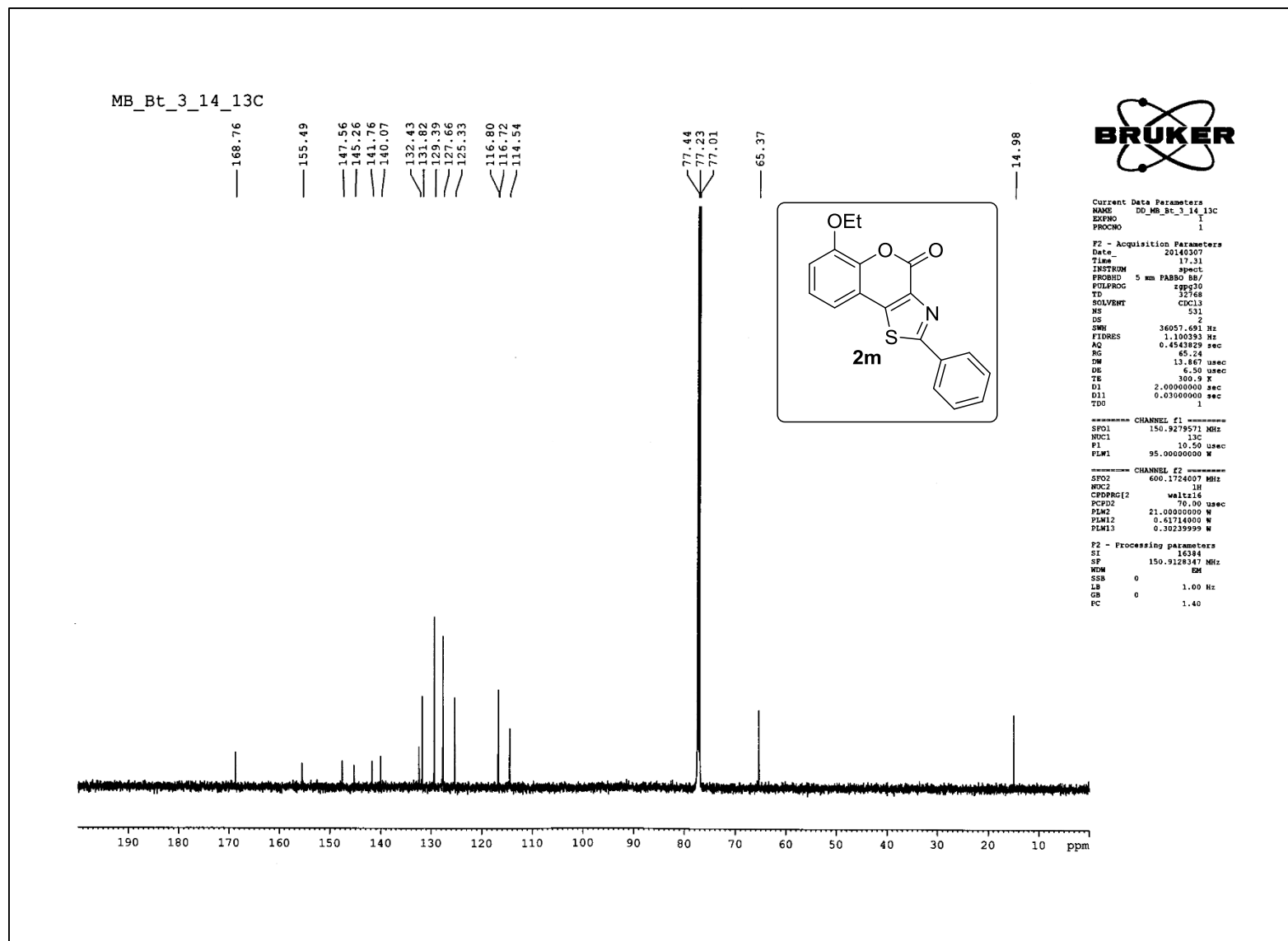
DATA PROCESSING

FT size 32768

Total time 13 min

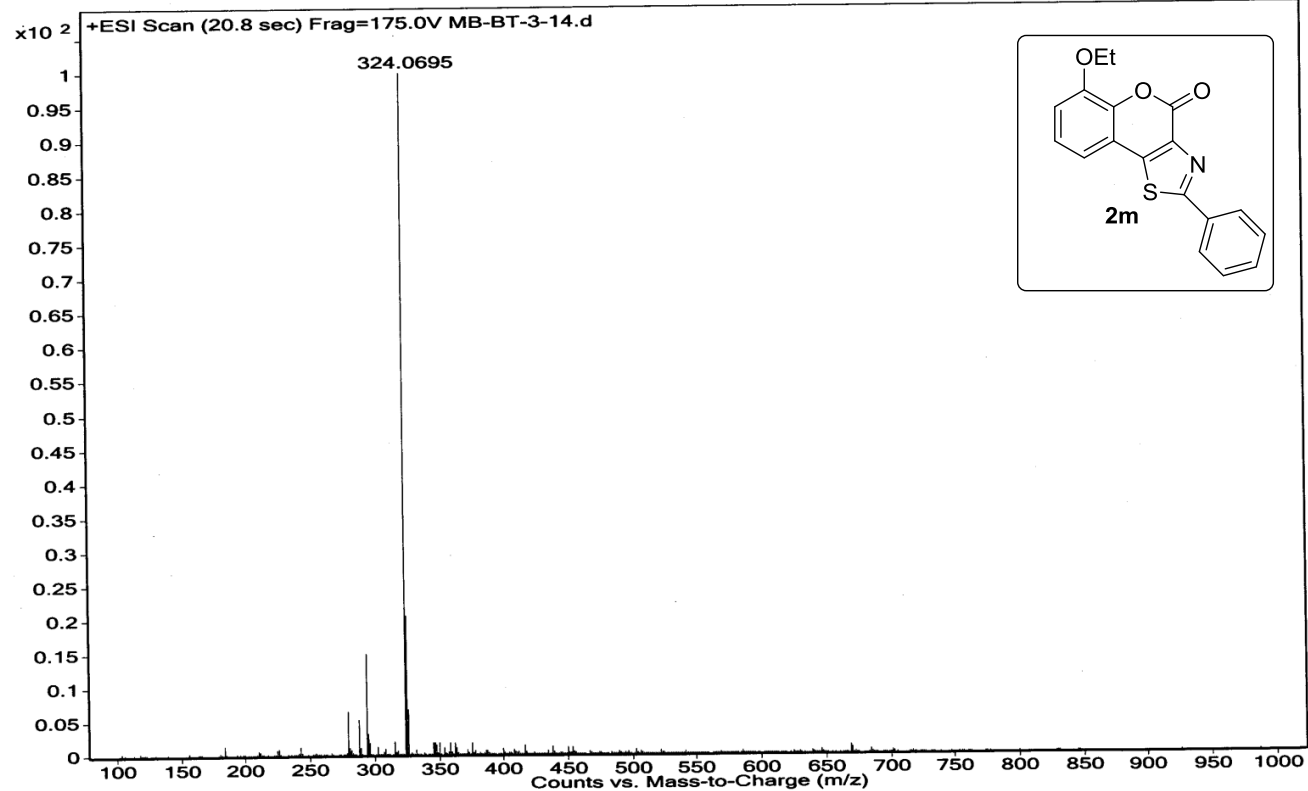


¹³C NMR spectra of **2m**

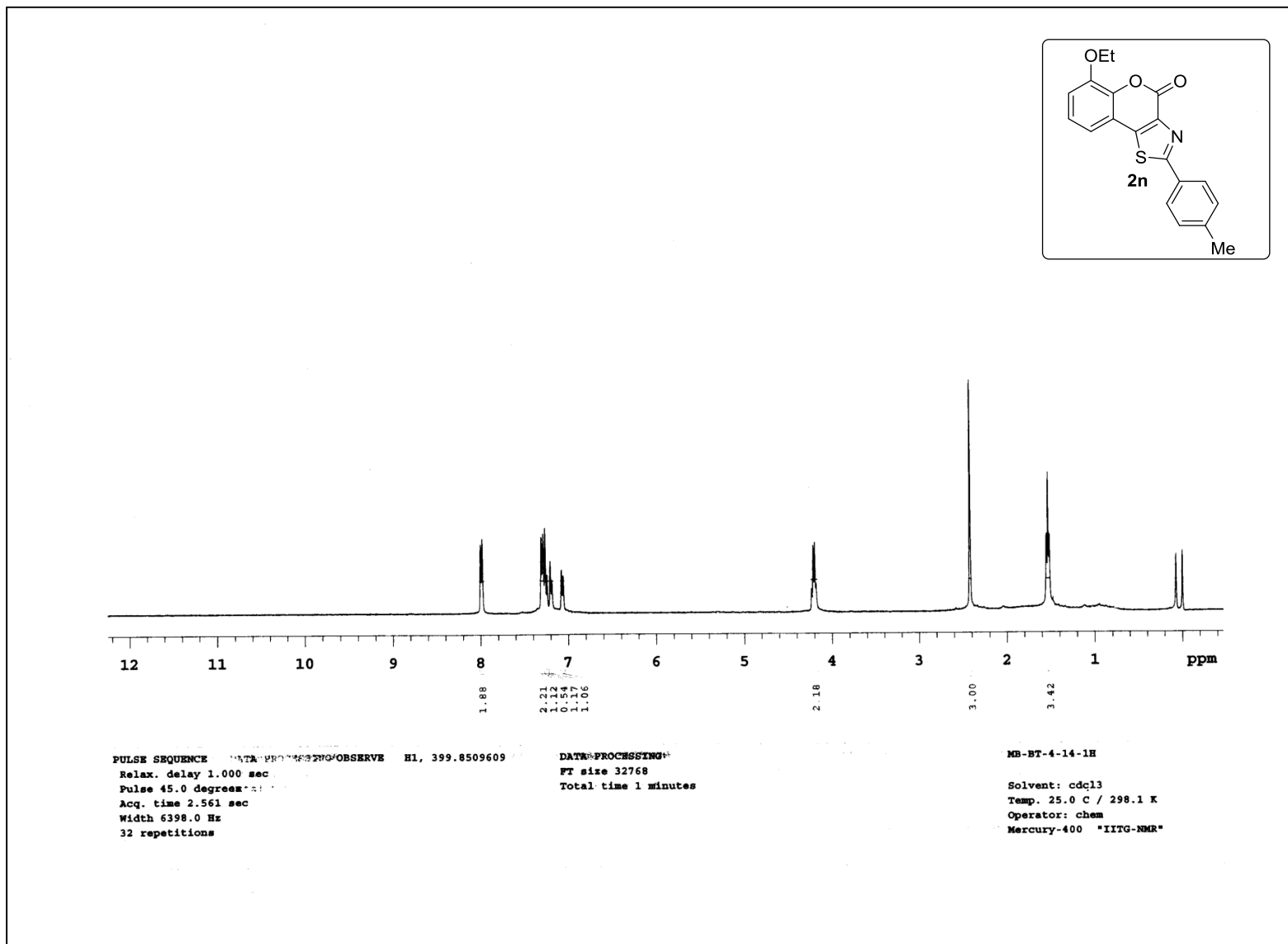


HRMS spectra of **2m**

Sample Name	MB-BT-3-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-3-14.d	ACQ Method		Comment		Acquired Time	5/6/2014 2:49:30 PM

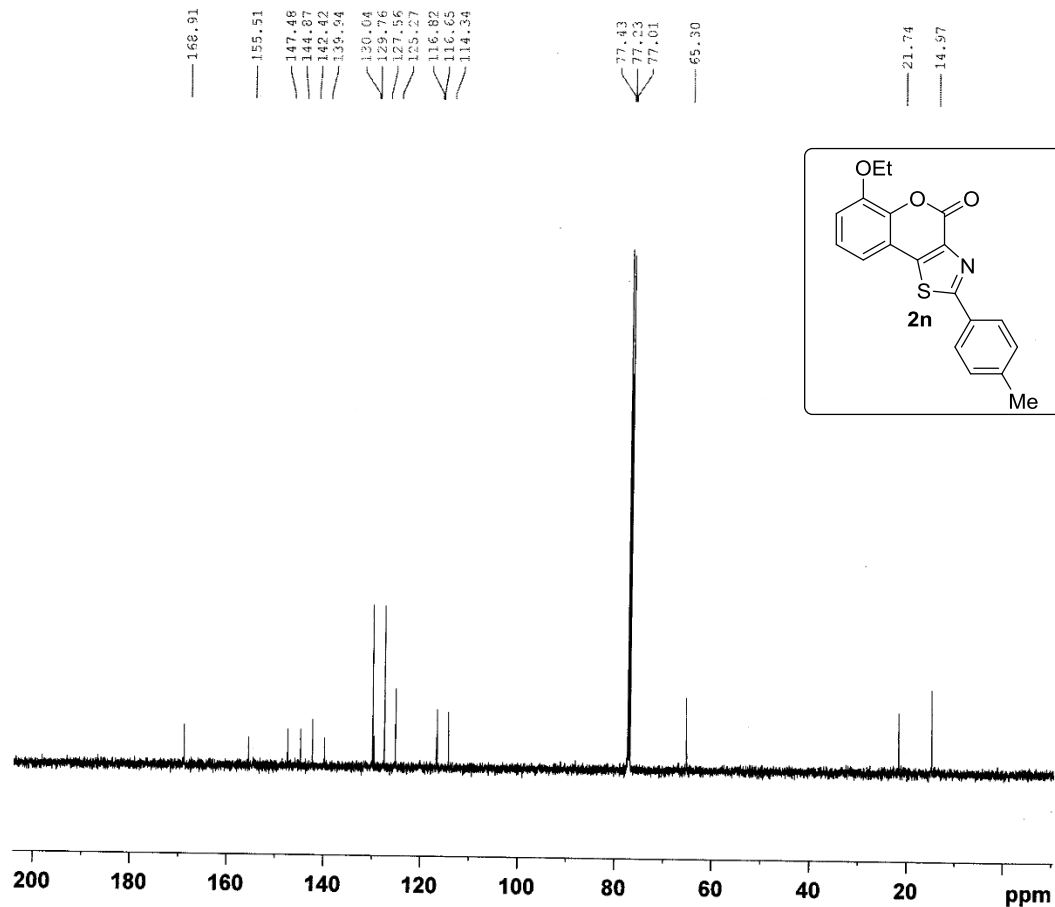


¹H NMR spectra of **2n**



¹³C NMR spectra of 2n

MB-BT-4-14-13C



Current Data Parameters
NAME MB-BT-4-14-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140307
Time 10.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 96
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

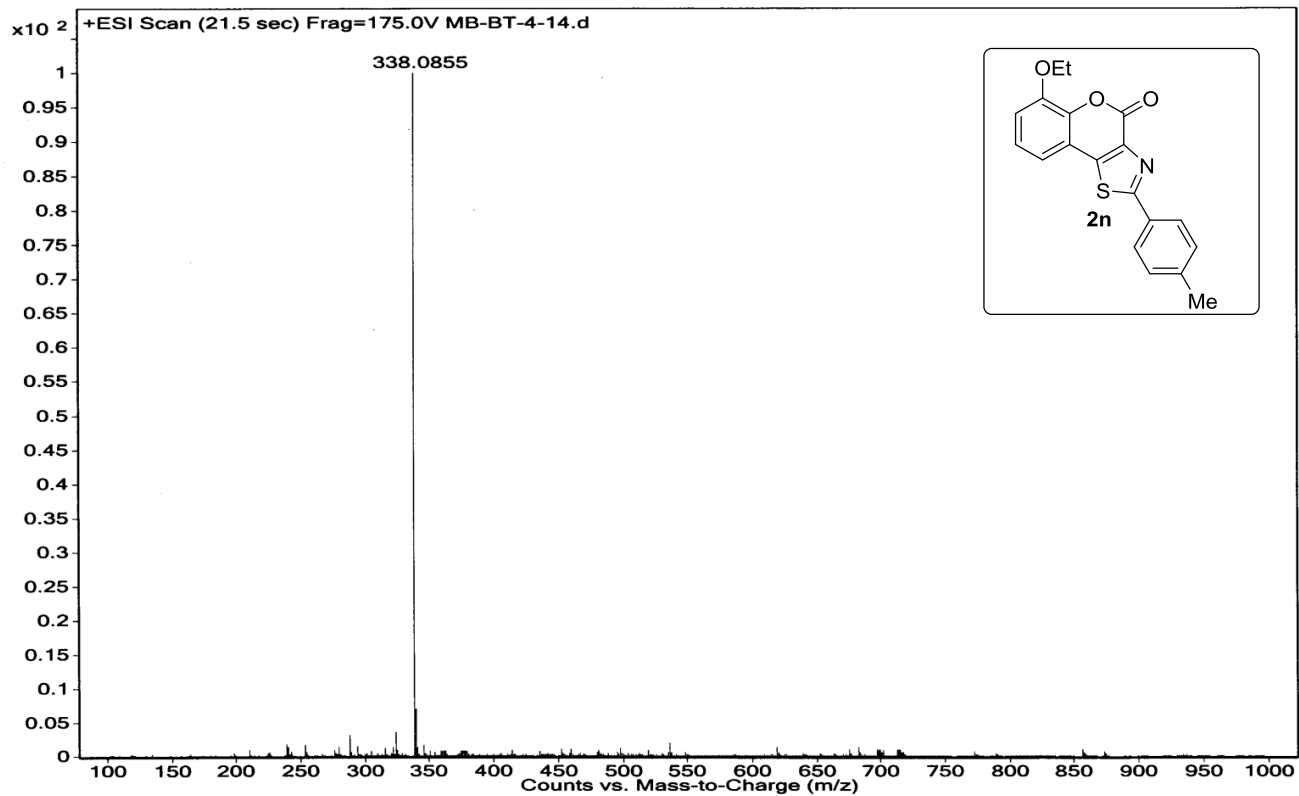
===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLW1 95.00000000 W

===== 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

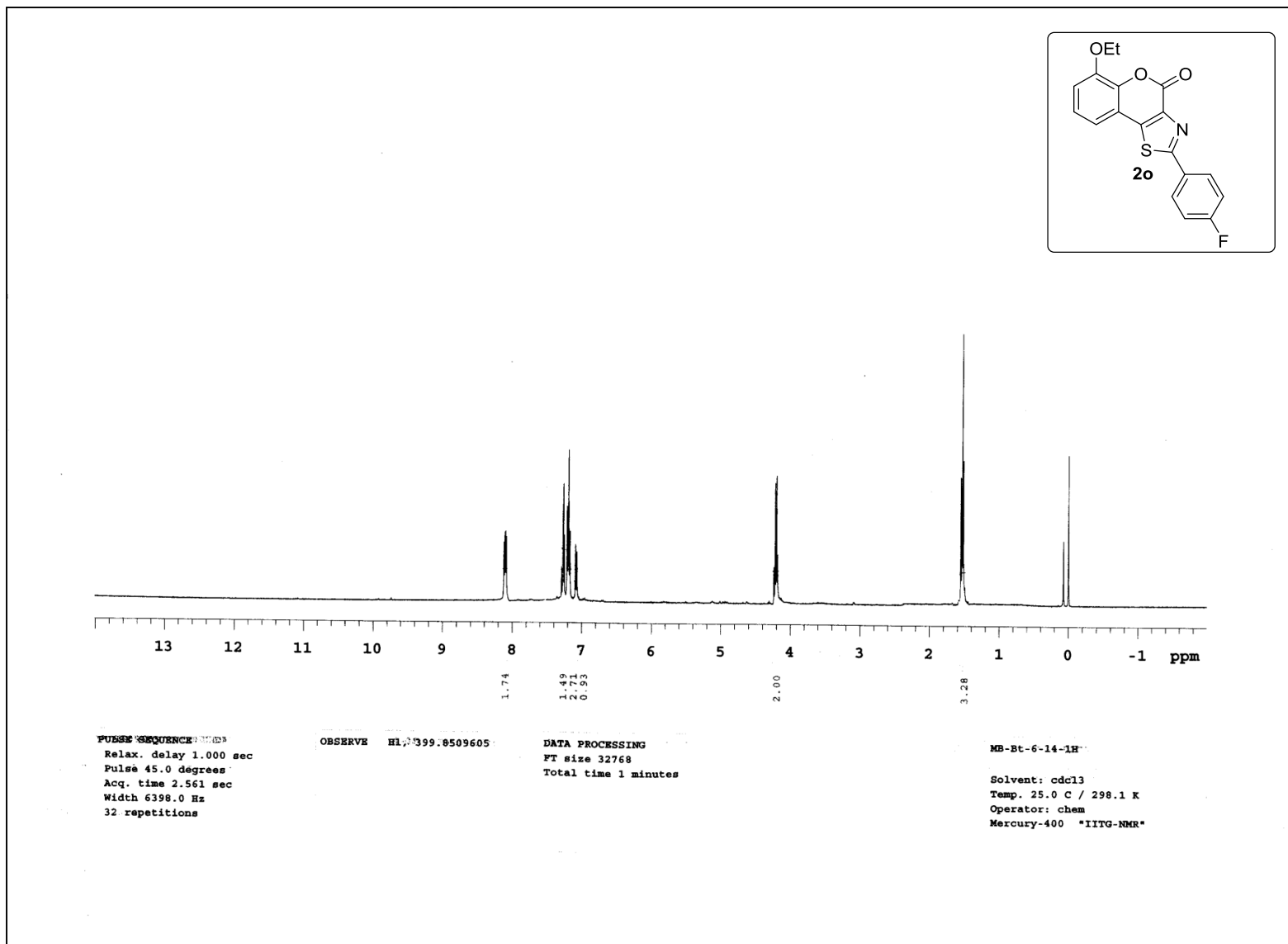
F2 - Processing parameters
SI 16384
SF 150.9128370 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectra of 2n

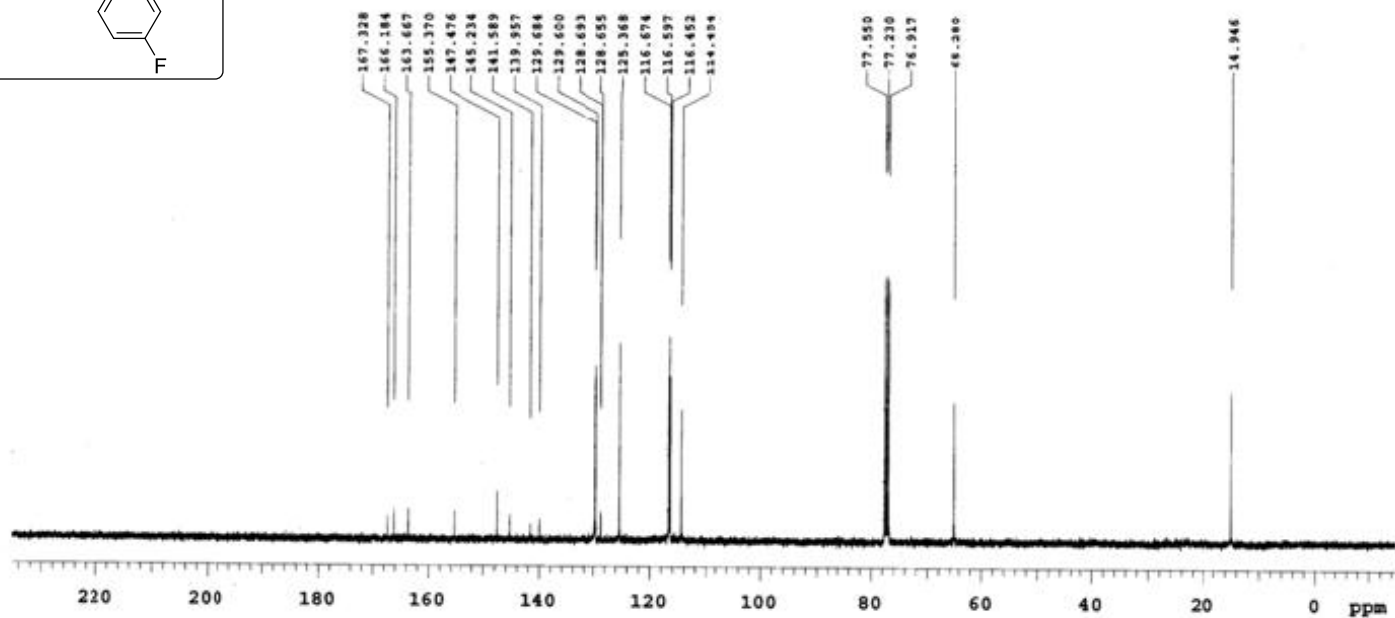
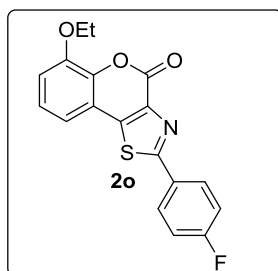
Sample Name	MB-BT-4-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-4-14.d	ACQ Method		Comment		Acquired Time	5/6/2014 2:50:57 PM



H¹ NMR spectra of **2o**



¹³C NMR spectra of **2o**



P00000000000000000000
 Relax. delay 1.000 sec
 Pulse 45.0 degrees
 Acq. time 1.304 sec
 Width 25125.6 Hz
 2540 repetitions

OBSERVE C13, 100.5425832
 DECOUPLE H1, 399.8529994
 Power 42 dB
 continuously on
 WALTZ-16 modulated

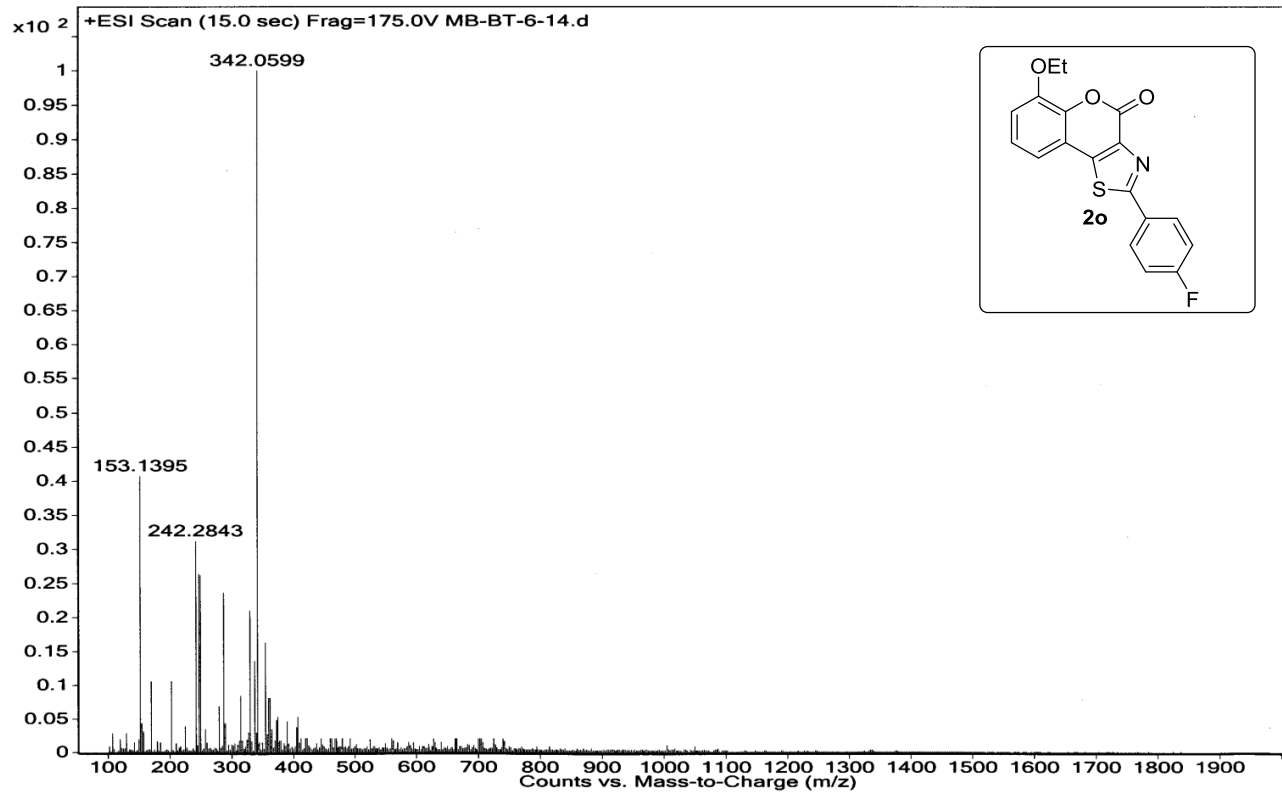
DATA PROCESSING
 line broadening 0.5 Hz
 FT size 65536
 Total time 97 minutes

MS-BT-6-14-13C

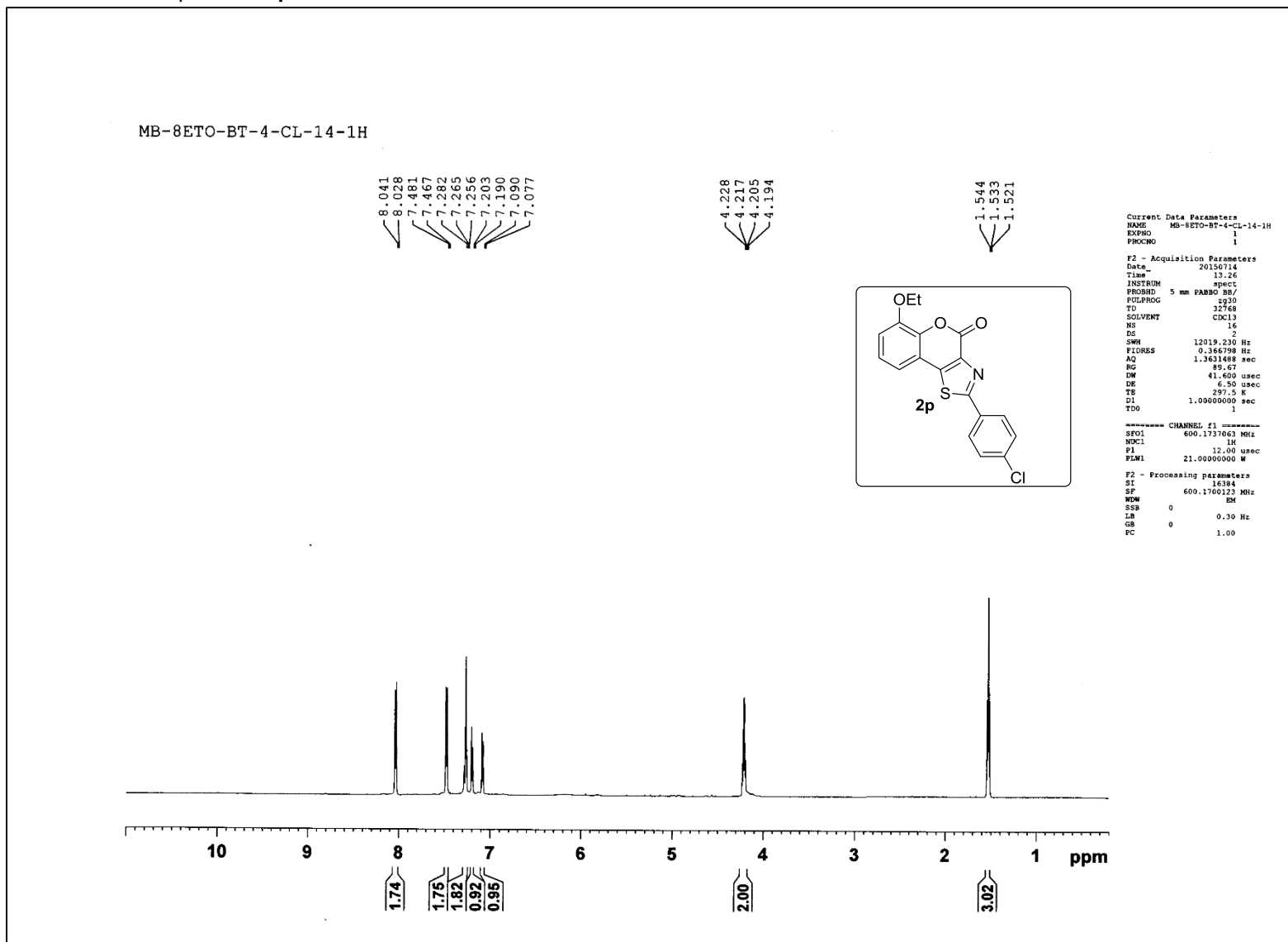
Solvent: cdcl3
 Temp. 25.0 C / 298.1 K
 Operator: chem
 Mercury-400 *IITG-NMR*

HRMS spectra of **2o**

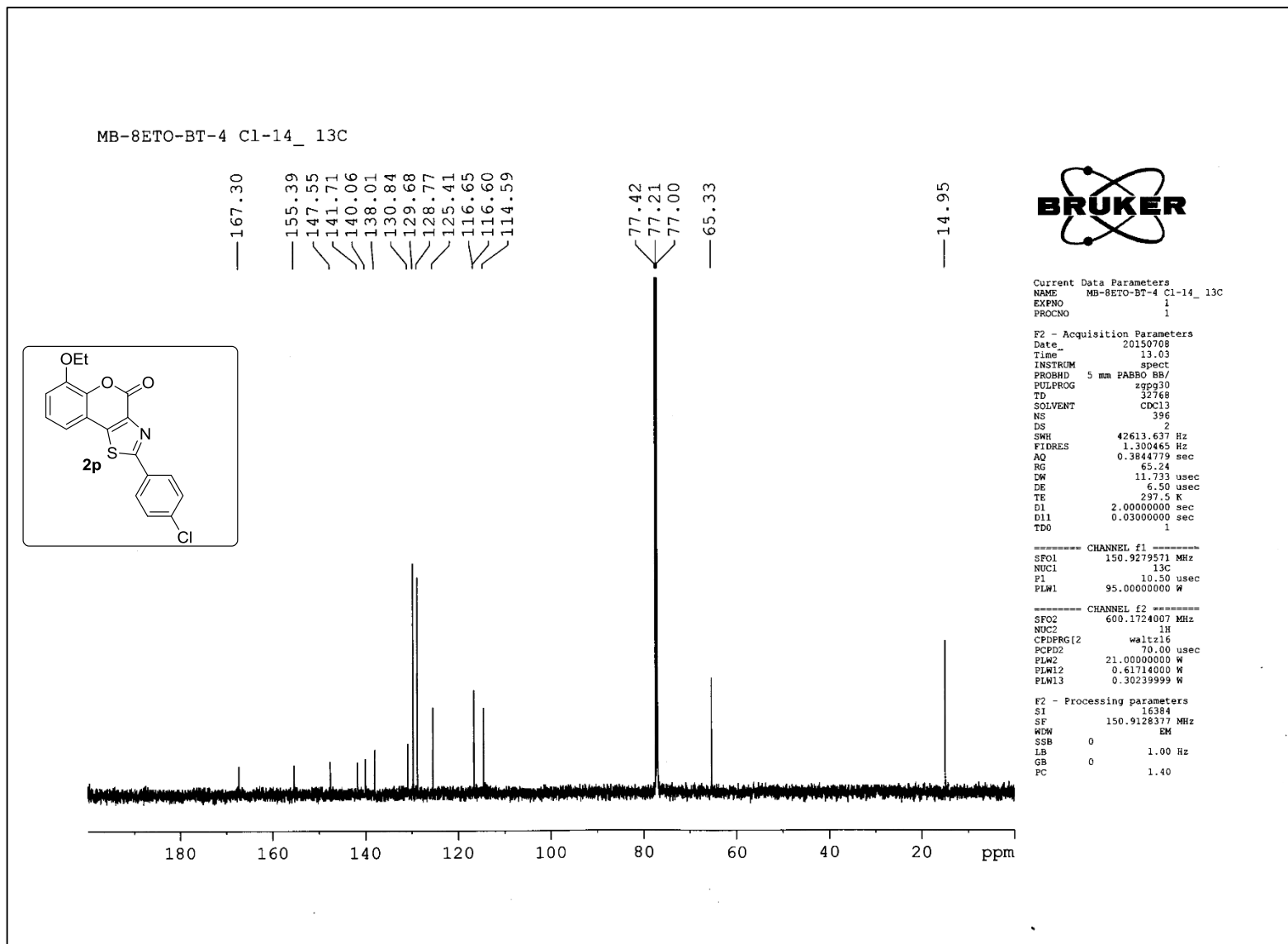
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-BT-6-14.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H NMR spectra of **2p**



¹³C NMR spectra of **2p**



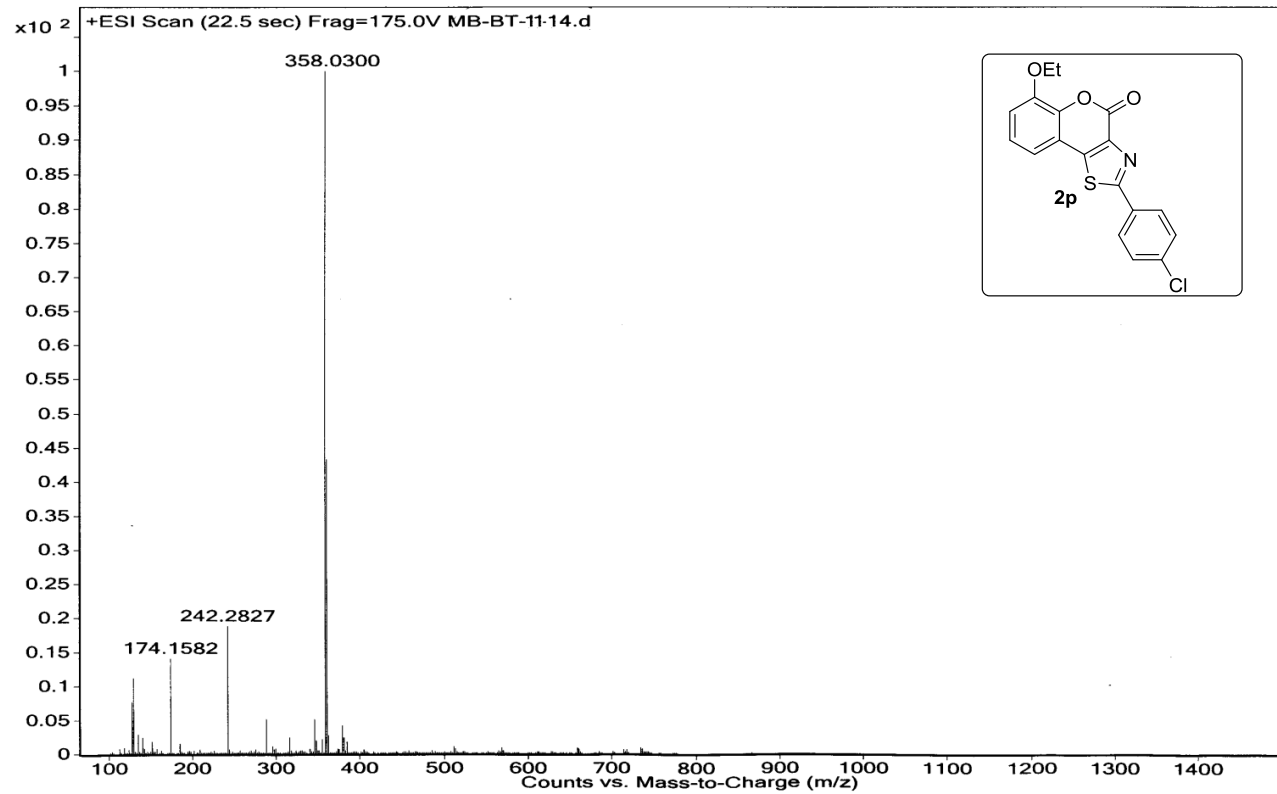
HRMS spectra of 2p

Sample Name
Inj Vol
Data Filename

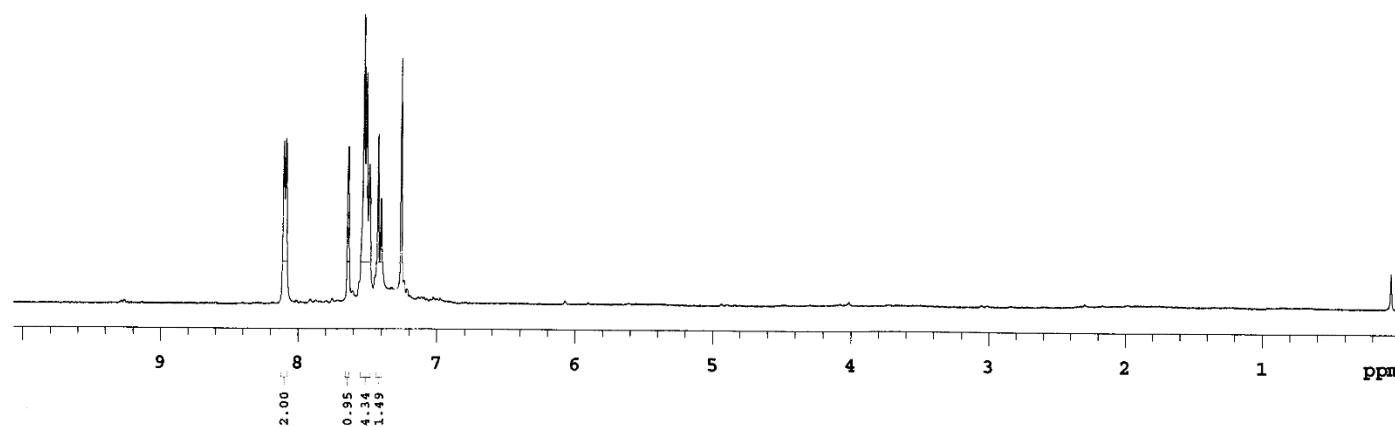
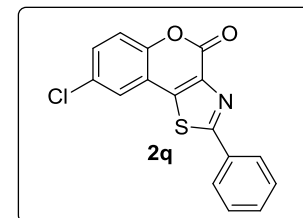
Position
InjPosition
ACQ Method

Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time

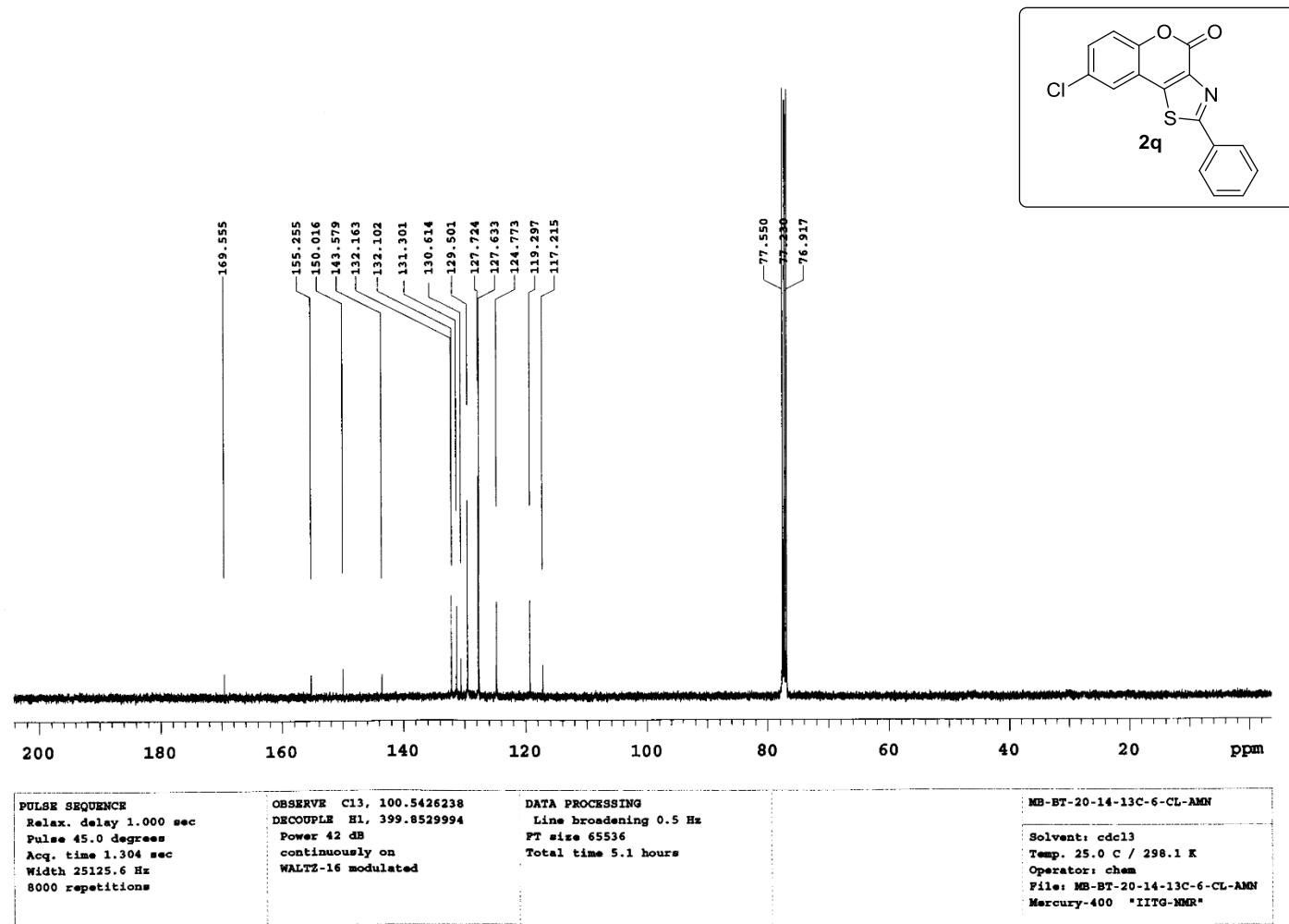


¹H NMR Spectra of **2q**



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.561 sec Width 6398.0 Hz 32 repetitions	OBSERVE H1, 399.8509637	DATA PROCESSING FT size 32768 Total time 1 minutes	MB-Bt-20-14-1H-6-Cl-amn Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: MB-Bt-20-14-1H-6-Cl-amn Mercury-400 "IITG-NMR"
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¹³C NMR spectra of **2q**



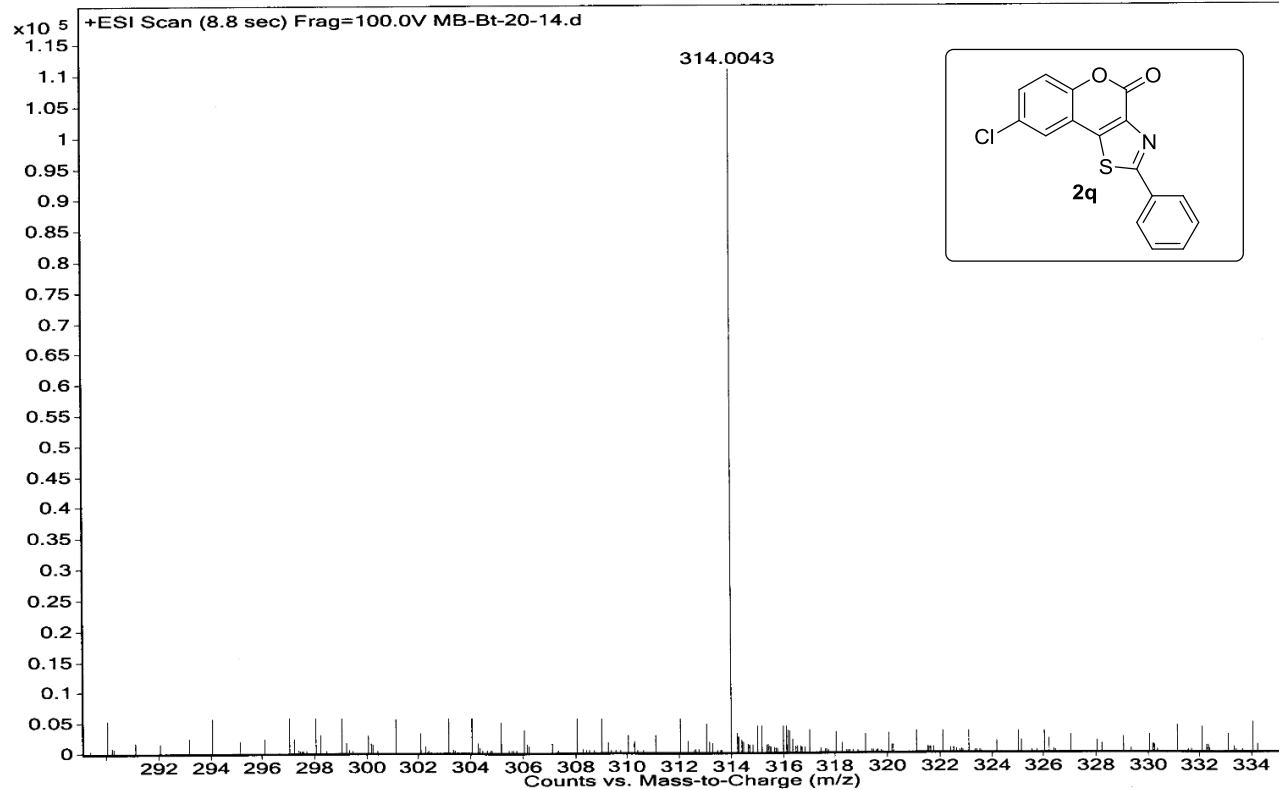
HRMS spectra of **2q**

Sample Name
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

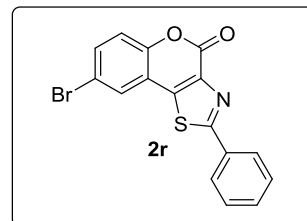
Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



¹H NMR Spectra of **2r**

MB-Bt-6Br-Amm-14_1H

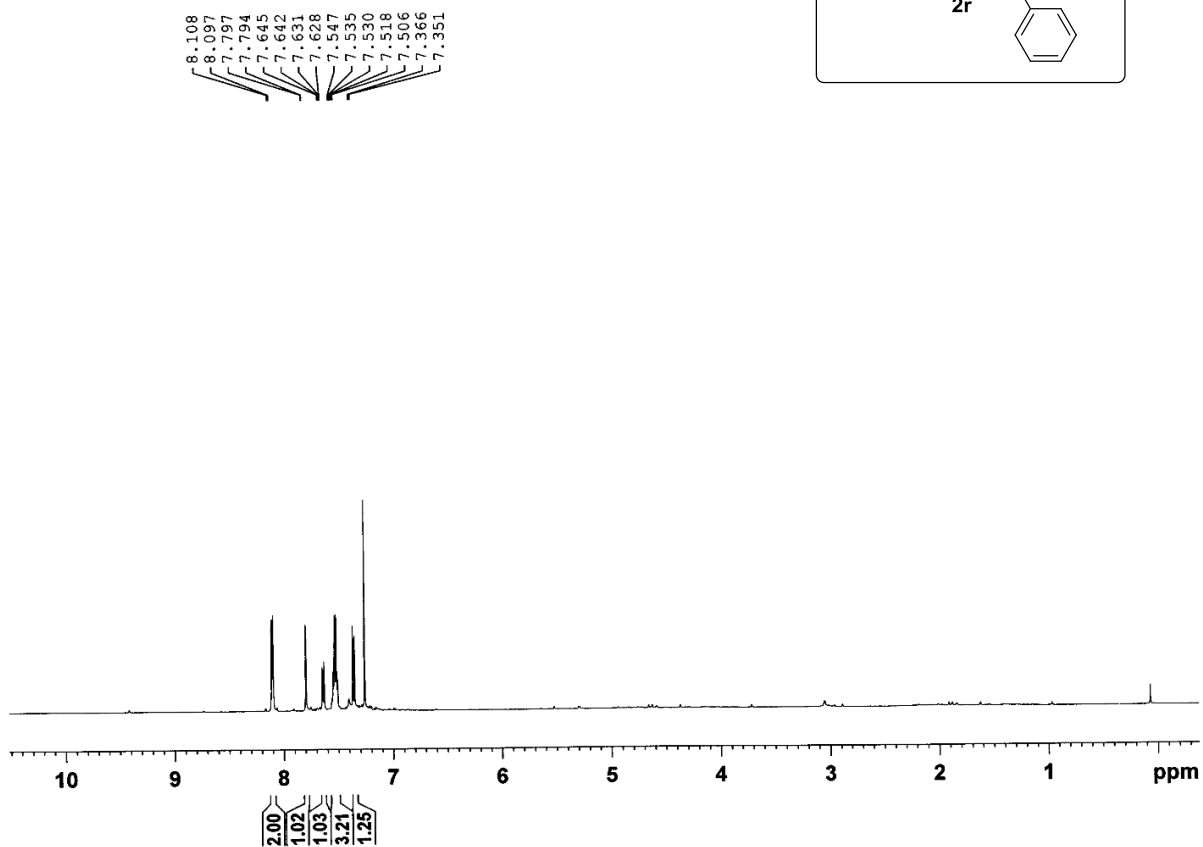


Current Data Parameters
NAME MB-Bt-6Br-Amm-14_1H
EXPNO 1
PROCNO 1

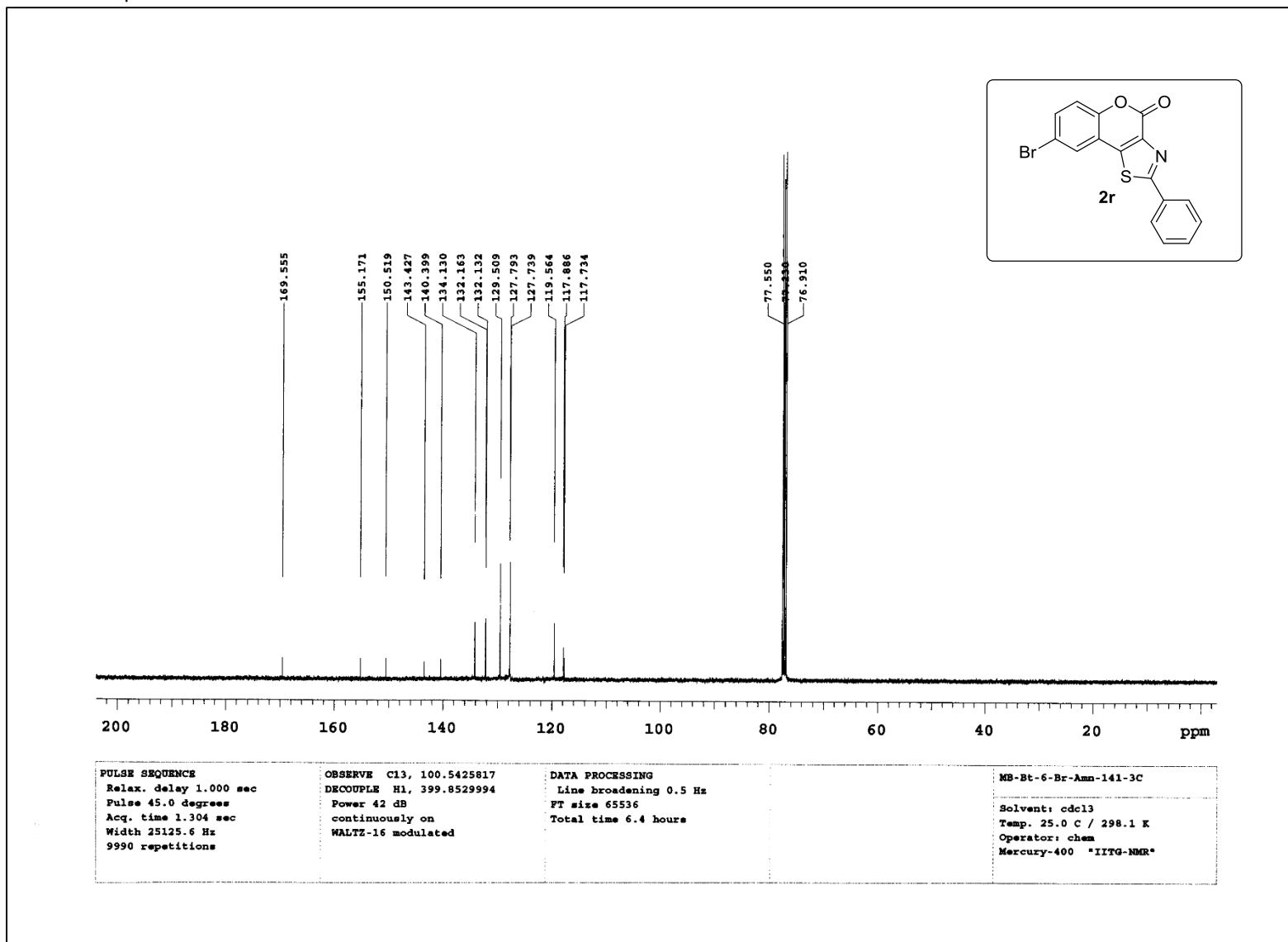
F2 - Acquisition Parameters
Date_ 20150325
Time 12.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3651488 sec
RG 143.33
DW 41.600 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 16384
SF 600.1700144 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

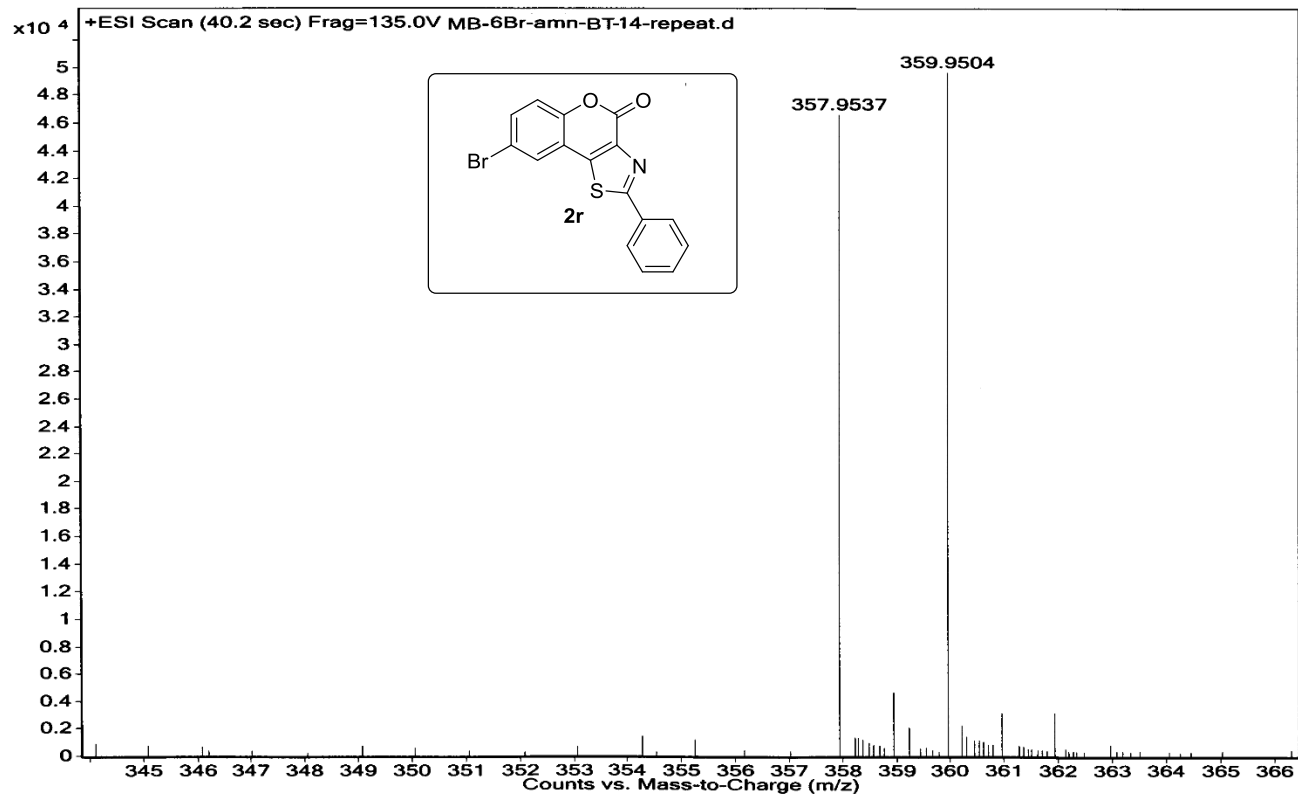


¹³C NMR spectra of 2r



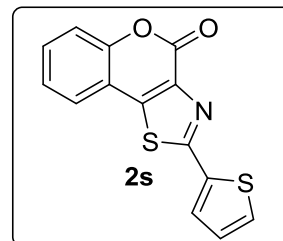
HRMS Spectra of 2r

Sample Name Inj Vol Data Filename	Position InjPosition ACQ Method	Instrument Name SampleType Comment	User Name IRM Calibration Status Acquired Time
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^1H NMR spectra of **2s**

MB-BT-THIO-14-1H



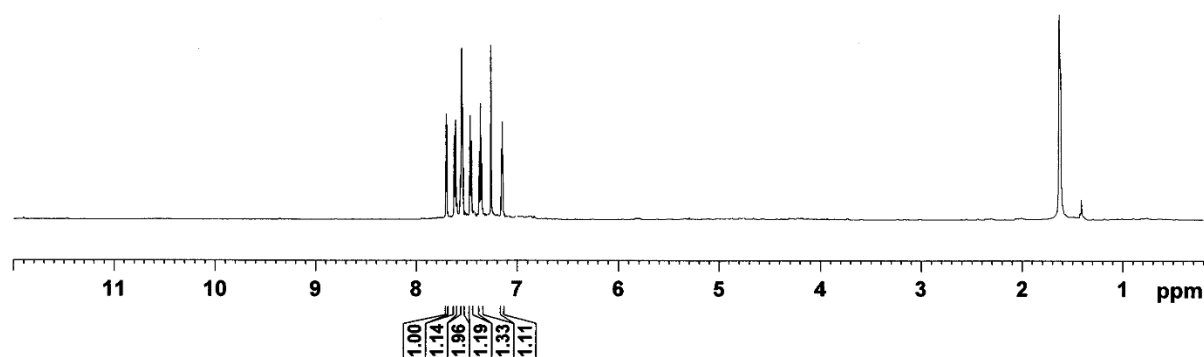
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Current Data Parameters
NAME      MB-BT-THIO-14-1H
EXPNO     1
PROCNO    1

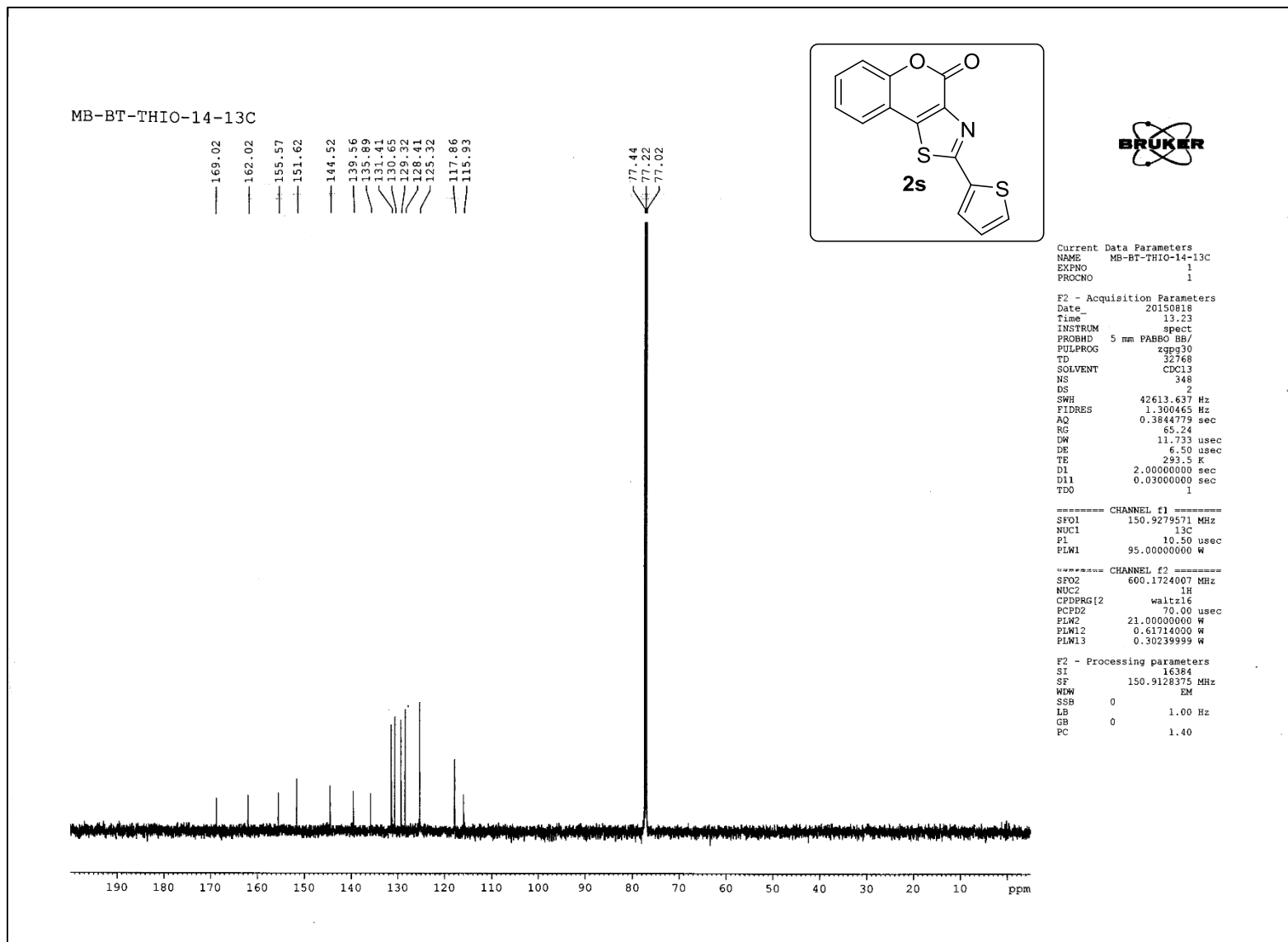
F2 - Acquisition Parameters
Date_     20150818
Time      13.20
INSTRUM    spect
PROBHD     5 mm PABBO BB/
PULPROG    zg30
TD         32768
SOLVENT    CDCl3
NS         16
DS         2
SWH         12019.230 Hz
FIDRES     0.366798 Hz
AQ         1.3631488 sec
RG         80.22
DW         41.600 usec
DE         6.50 usec
TE         292.7 K
D1         1.00000000 sec
TDO        1

===== CHANNEL f1 =====
SFO1       600.1737063 MHz
NUC1        1H
P1         12.00 usec
PL1        21.00000000 W

F2 - Processing parameters
SI         16384
SF         600.1700151 MHz
WDW         EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
    
```

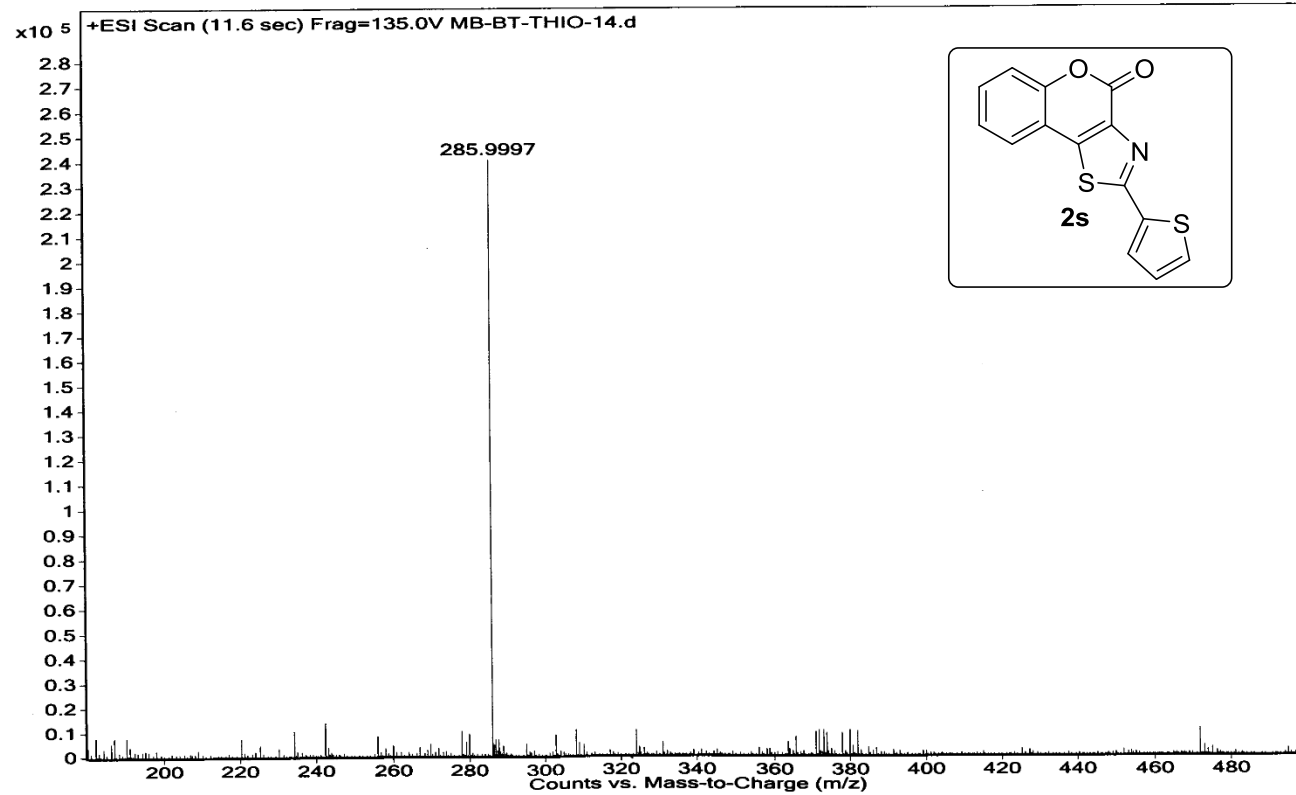


¹³C NMR spectra of **2s**

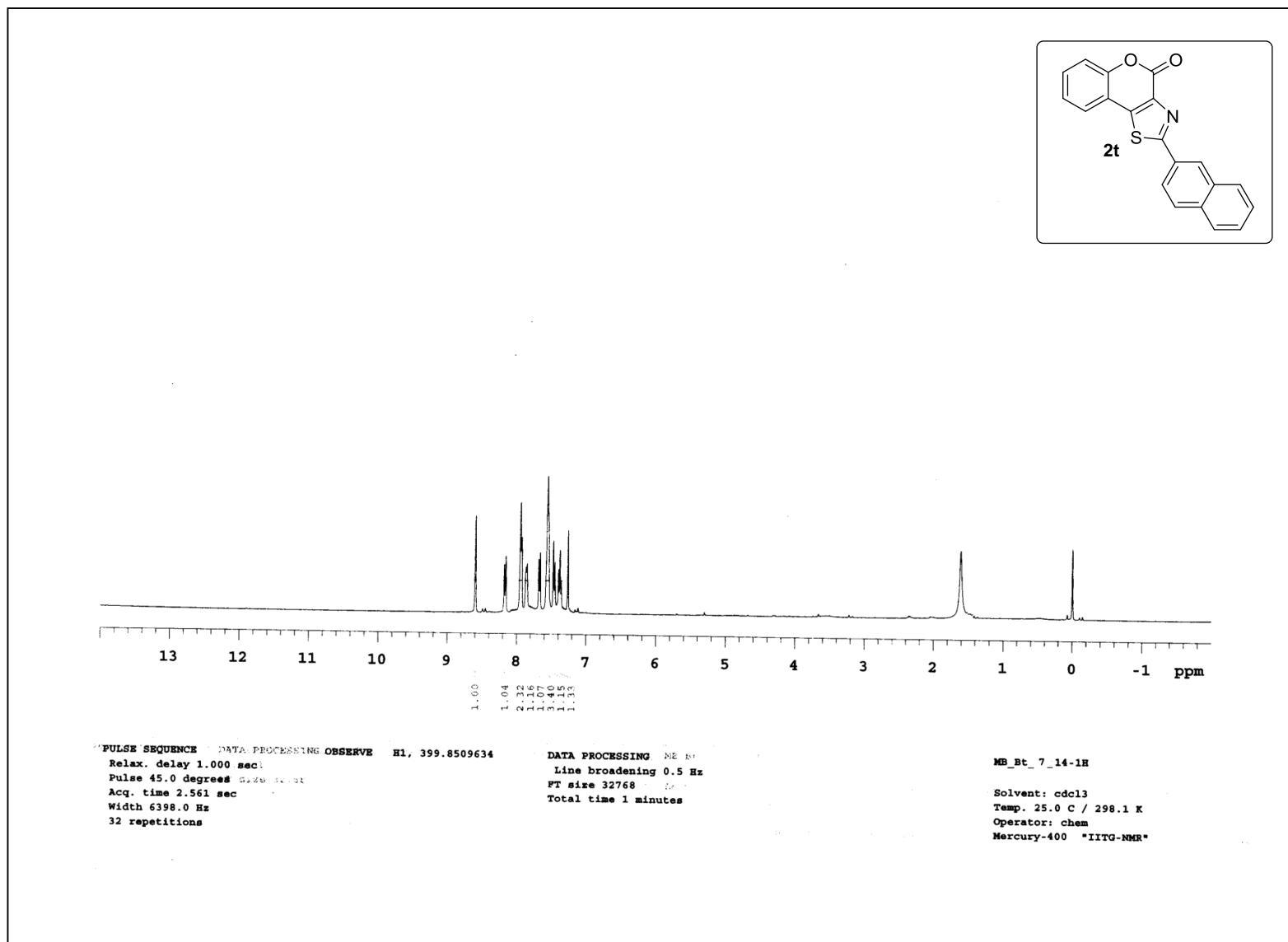


HRMS spectra of **2s**

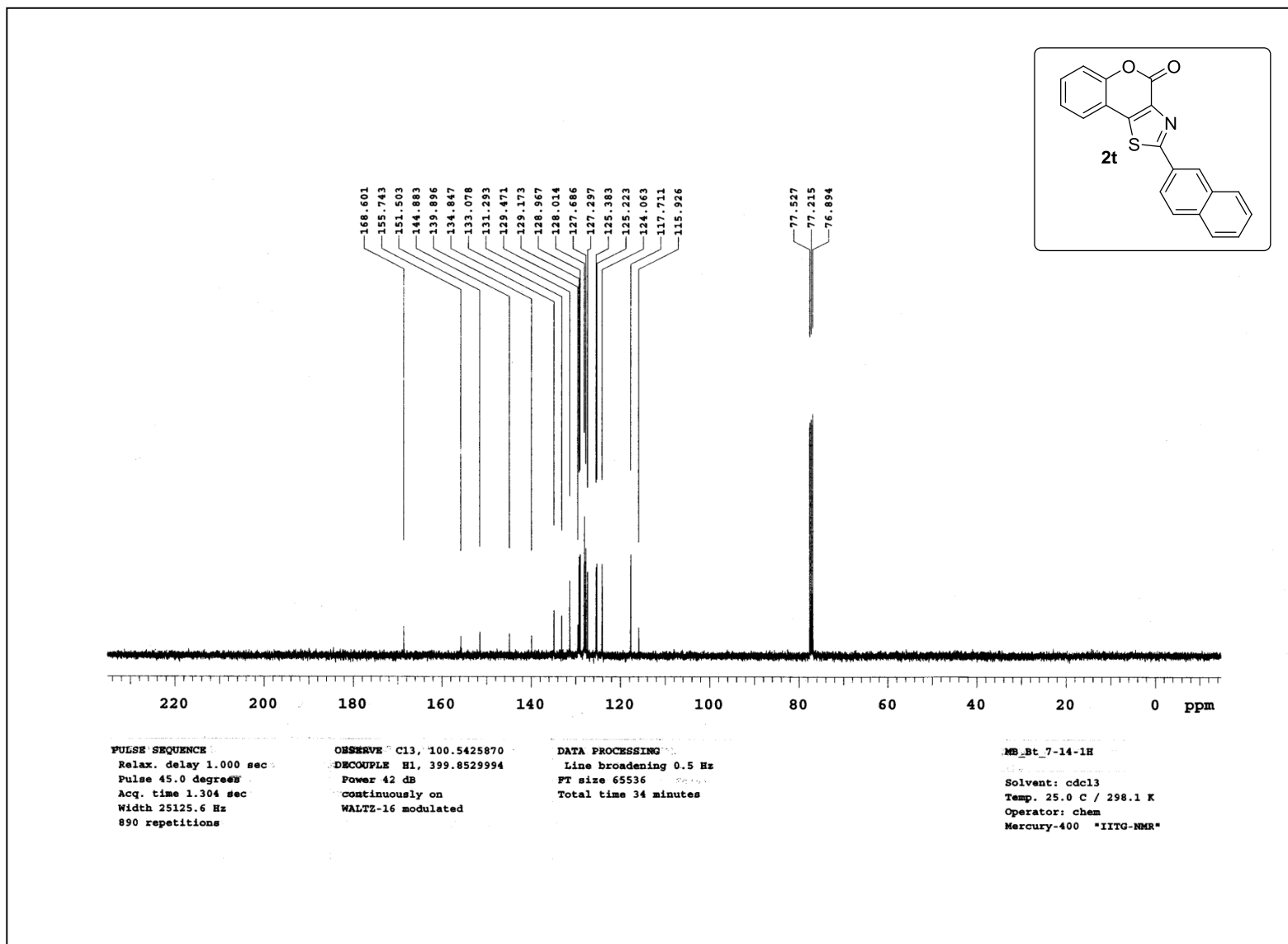
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-BT-THIO-14.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H NMR spectra of **2t**

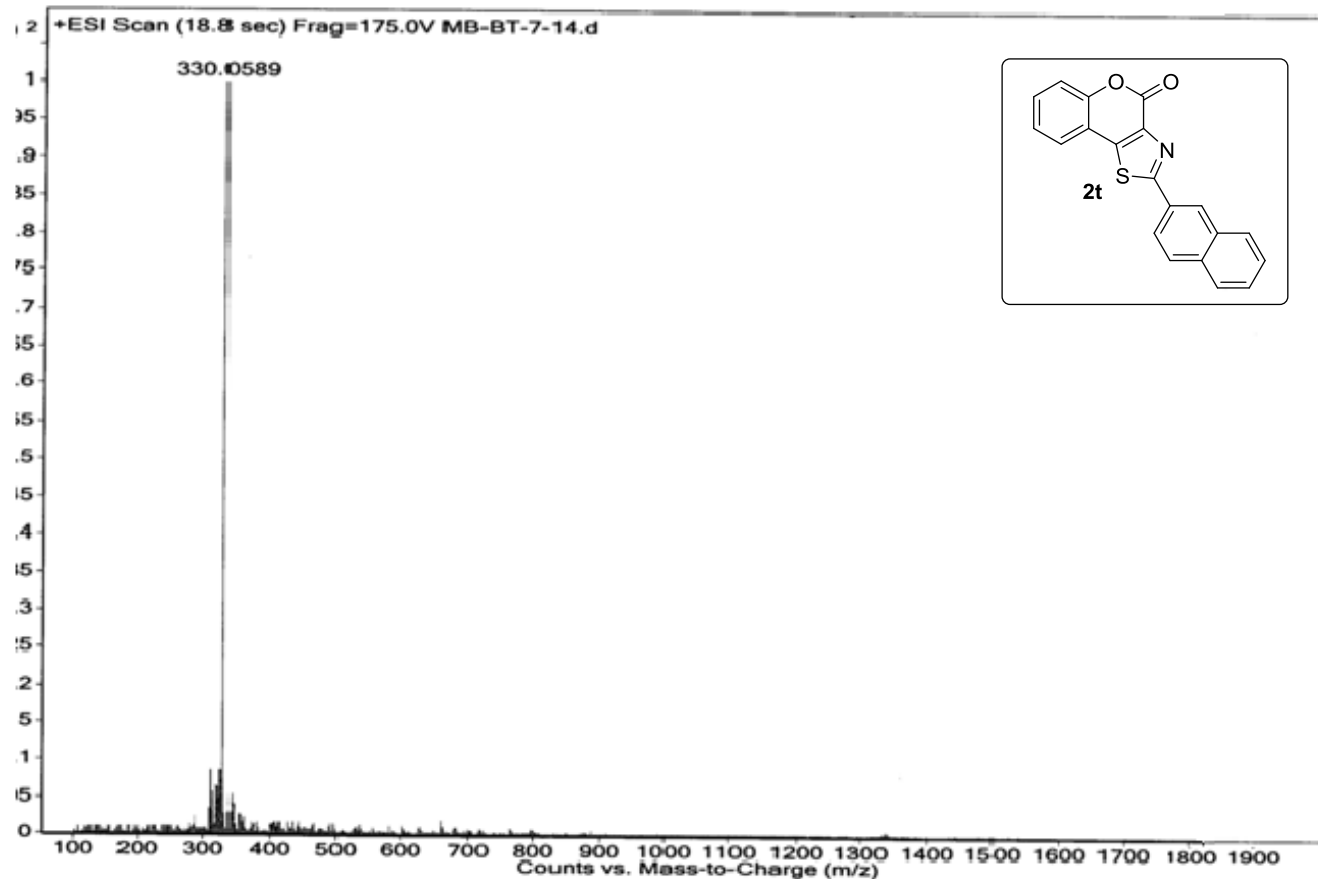


¹³C NMR spectra of **2t**



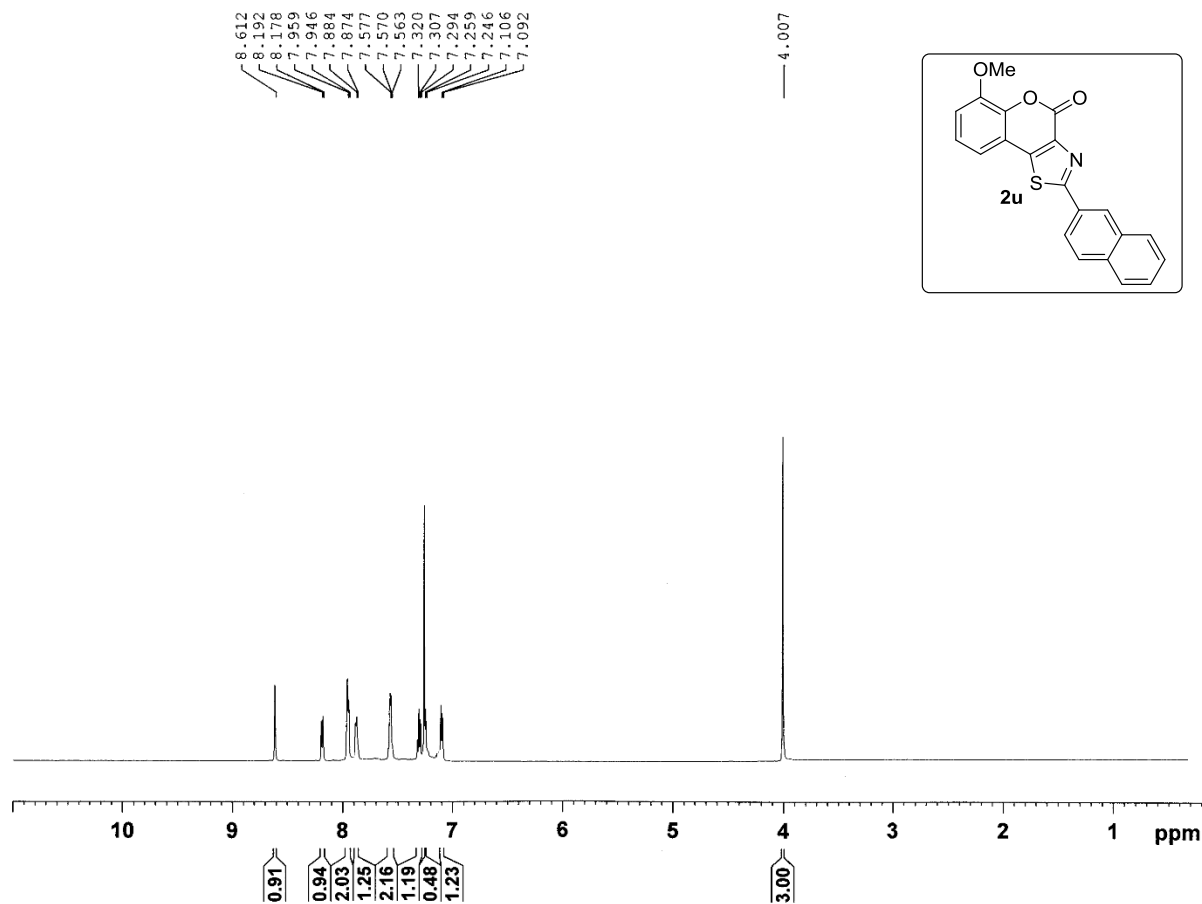
HRMS spectra of **2t**

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	MB-BT-7-14.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H NMR spectra of **2u**

MB-8MEO-BT-NAPH-14-1H



Current Data Parameters
NAME MB-8MEO-BT-NAPH-14-1H
EXPNO 1
PROCNO 1

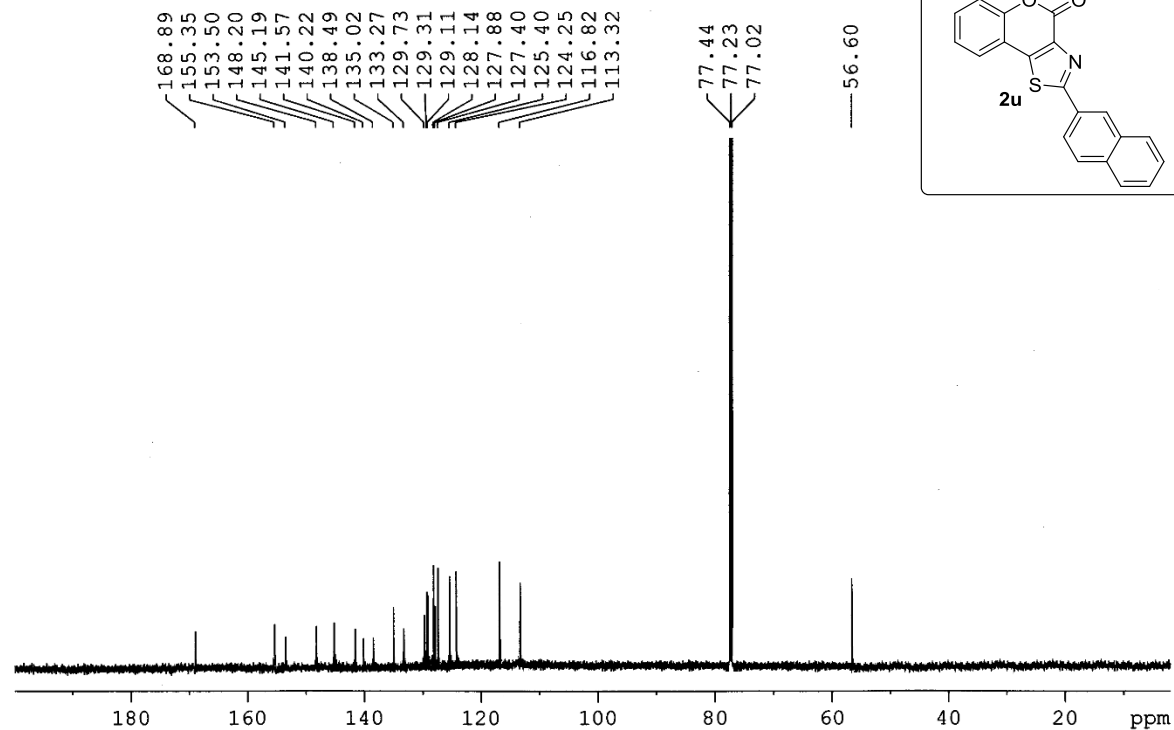
F2 - Acquisition Parameters
Date_ 20150706
Time 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3621488 sec
RG 39.36
DW 41.600 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 600.137063 MHz
NUC1 1H
P1 12.00 usec
PLW1 21.00000000 W

F2 - Processing parameters
SI 16384
SF 600.1700147 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectra of **2u**

MB-8MEO-BT-NAPTH-14-13C



BRUKER

Current Data Parameters
NAME MB-8MEO-BT-NAPTH-14-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Data 20150714
Time 8.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 933
DS 2
SWH 42613.637 Hz
FIDRES 1.300465 Hz
AQ 0.3848779 sec
RG 65.24
DW 11.733 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

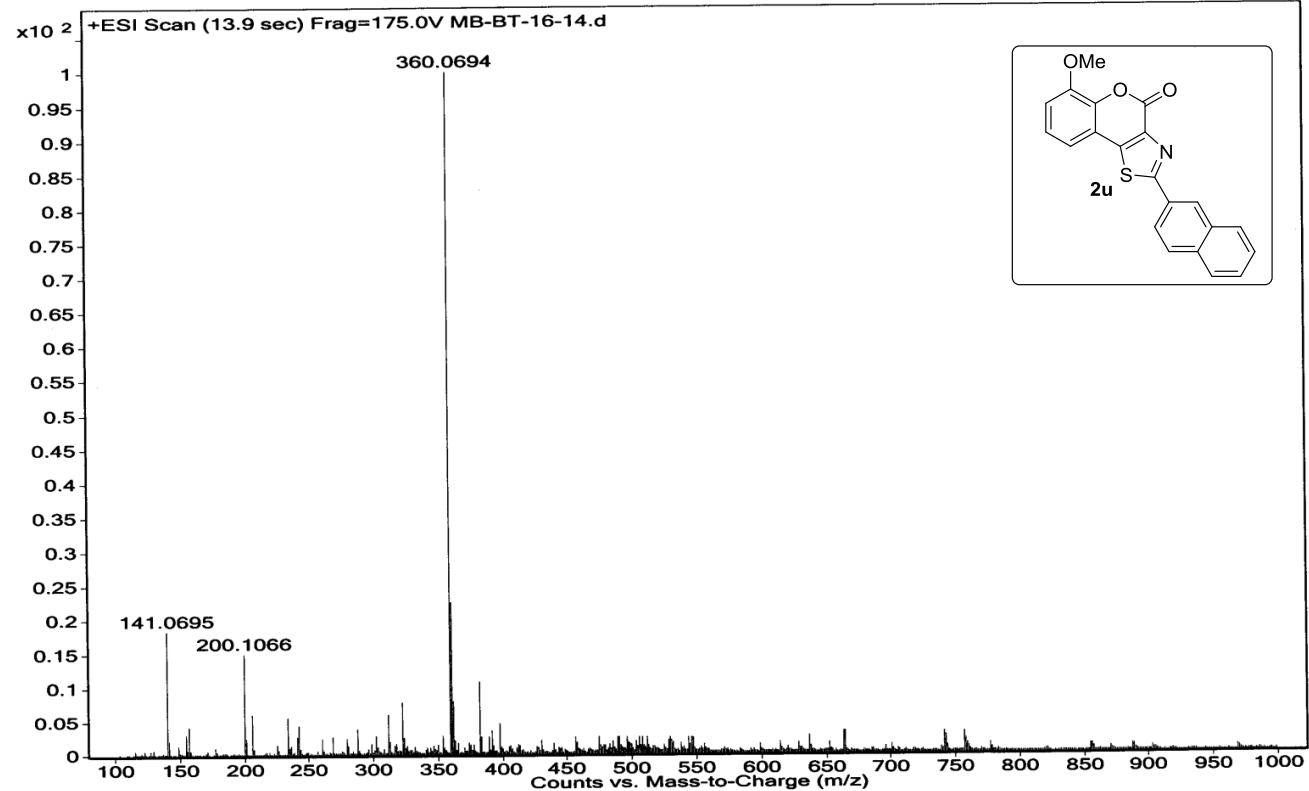
===== CHANNEL f1 =====
SFO1 150.9279571 MHz
NUC1 13C
P1 10.50 usec
PLM1 95.00000000 W

===== CHANNEL f2 =====
SFO2 600.1724007 MHz
NUC2 1H
CFDPRG2 waltz16
PCPD2 70.00 usec
PLM2 21.00000000 W
PLM12 0.41714000 W
PLM13 0.30239999 W

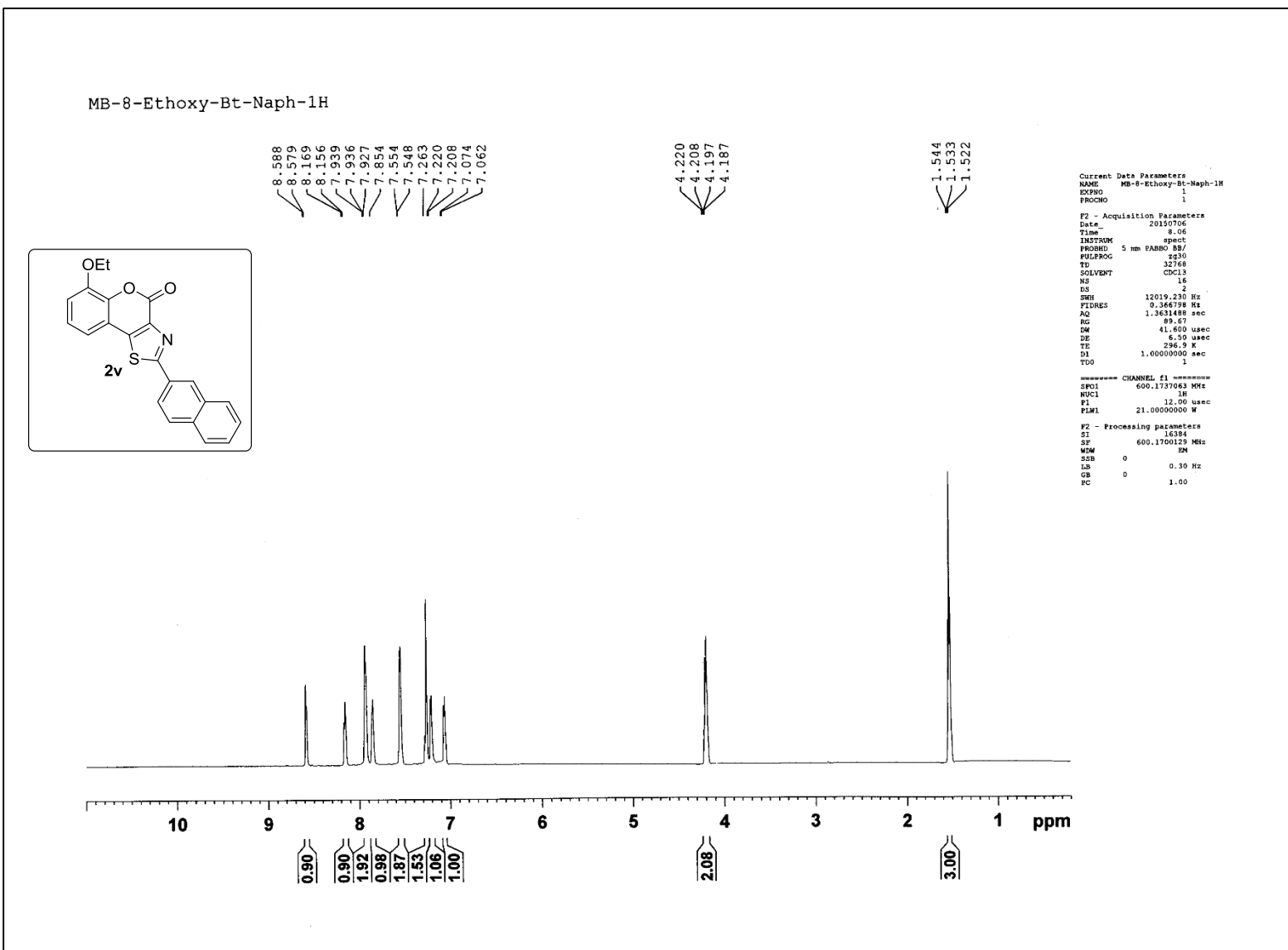
F2 - Processing parameters
SI 16384
SF 150.9126338 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HRMS spectra of **2u**

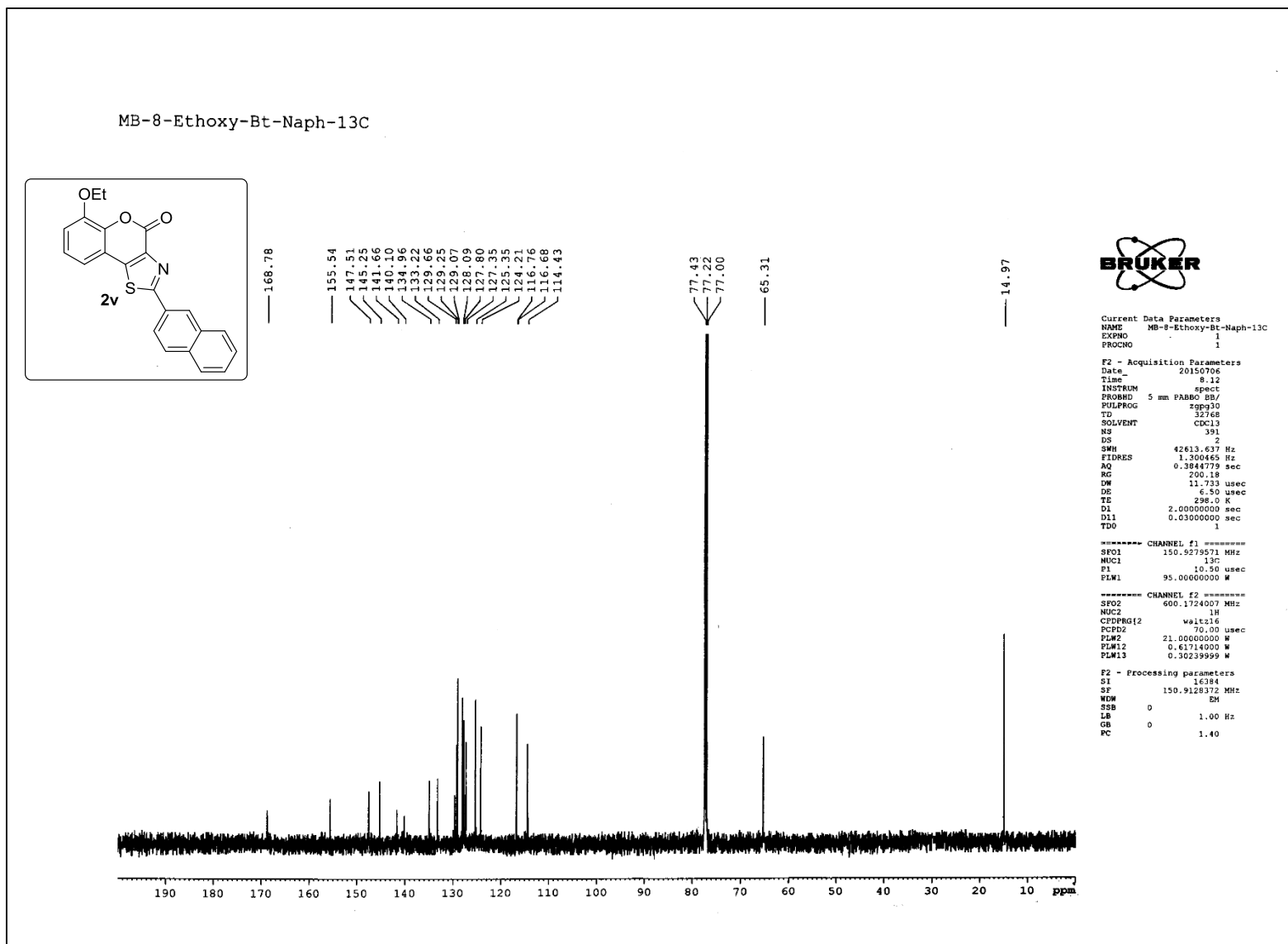
Sample Name	MB-BT-16-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-16-14.d	ACQ Method		Comment		Acquired Time	5/13/2014 3:37:29 PM



¹H NMR spectra of 2v



¹³C NMR spectra of **2v**



HRMS spectra of **2v**

Sample Name	MB-BT-15-14	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	MB-BT-15-14.d	ACQ Method		Comment		Acquired Time	5/13/2014 2:40:28 PM

