

## Supporting Information

### One-pot three component regioselective synthesis of C1-functionalised 3-arylbenzo[*f*]quinoline

Radhakrishna Gattu, R. Sidick Basha, Prasanta Ray Bagdi and Abu T. Khan\*<sup>a,b</sup>

<sup>a</sup>*Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati 781 039, India  
Tel.: +91 361 2582305; Fax: +91 361 2582349*

<sup>b</sup>*Present address: Vice-Chancellor, Aliah University, IIA/27, New Town, Kolkata-700 156, West Bengal, India.*

*Email: atk@iitg.ernet.in (A. T. Khan)*

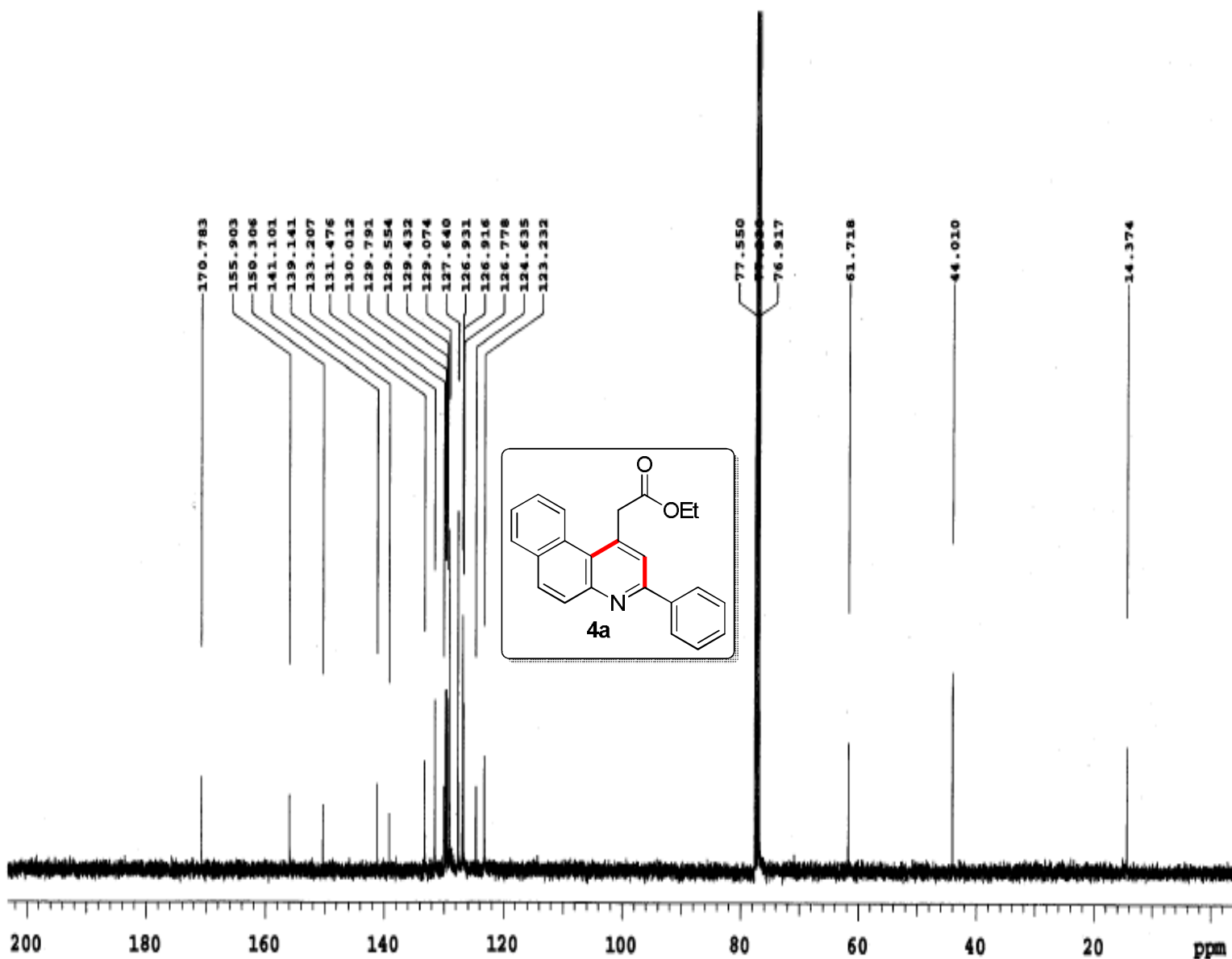
<i>Title page</i>	<b>1</b>
<i>Crystal Data and Structure Refinement for Compound 4g</i>	<b>2</b>
<i>Copies of <sup>1</sup>H NMR, <sup>13</sup>C NMR and HRMS spectra of all the Compounds</i>	<b>3-81</b>

**Table 3.** Crystal Data and Structure Refinement for Compound **4g**

Entry	Identification code	Compound <b>4g</b>
01	Empirical formula	C <sub>25</sub> H <sub>22</sub> F N O <sub>2</sub>
02	Formula weight	387.44
03	Temperature	293(2) K
04	Wavelength	0.71073
05	Radiation type	Mo K $\alpha$
06	Radiation source	'fine-focus sealed tube'
07	Crystal system	monoclinic
08	Space group	C2/c
09	Cell length	a 28.746 (3) b 10.589 (9) c 16.238 (15)
10	Cell Angle	$\alpha$ 90.0 $\beta$ 123.742 (6) $\delta$ 90.0
11	Cell Volume	4110.3 (7)
12	Density	1.252
13	Absorption correction	multi-scan
14	Refinement method	Full-matrix least-squares on F <sup>2</sup>
15	Index ranges	-33 $\leq$ h $\leq$ 30, -10 $\leq$ k $\leq$ 11, -16 $\leq$ l $\leq$ 17
16	Reflection number	12686
17	Theta range	1.70-24.24
18	Cell formula units Z	8
19	CCDC no	1434638



<sup>13</sup>C NMR spectra of compound 4a



PULSE SEQUENCE

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
2920 repetitions

OBSERVE C13, 100.5425817

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

DATA PROCESSING

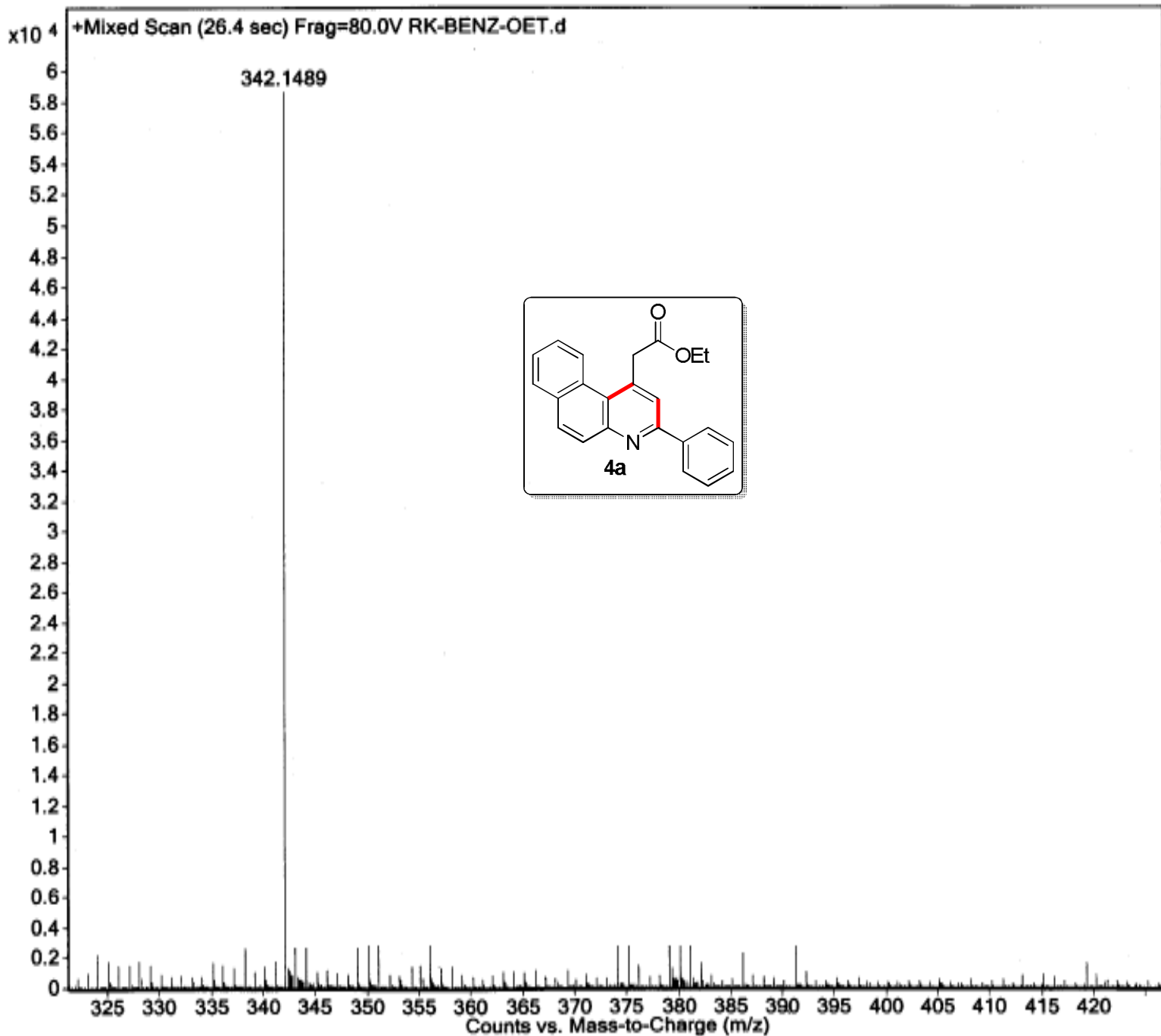
Line broadening 0.5 Hz  
FT size 65536  
Total time 112 minutes

RK-BEMZ-OET-13C

Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: RK-BEMZ-OET-13C  
Mercury-400 \*IITG-NMR\*

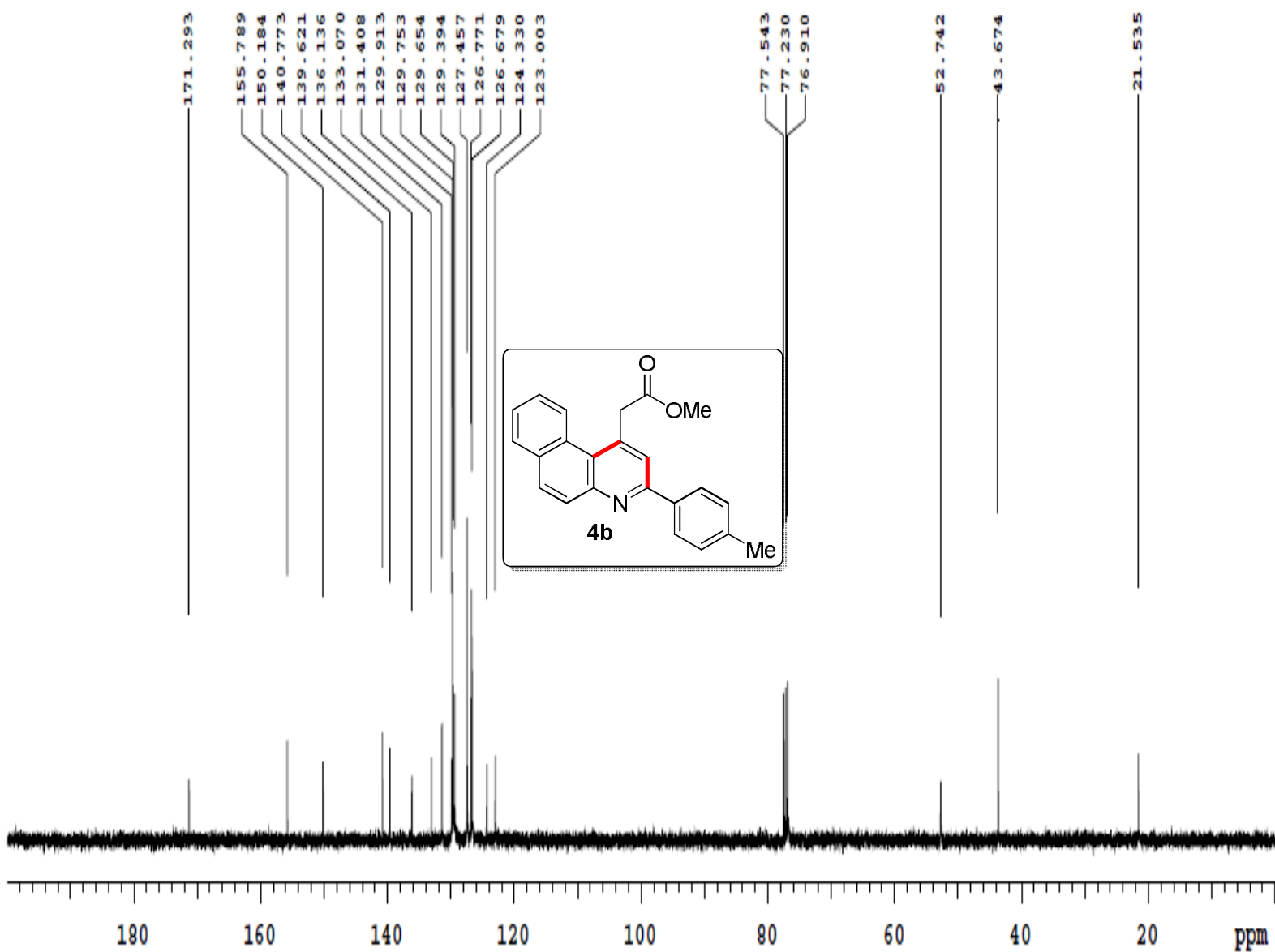
*HRMS spectra of compound 4a*

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





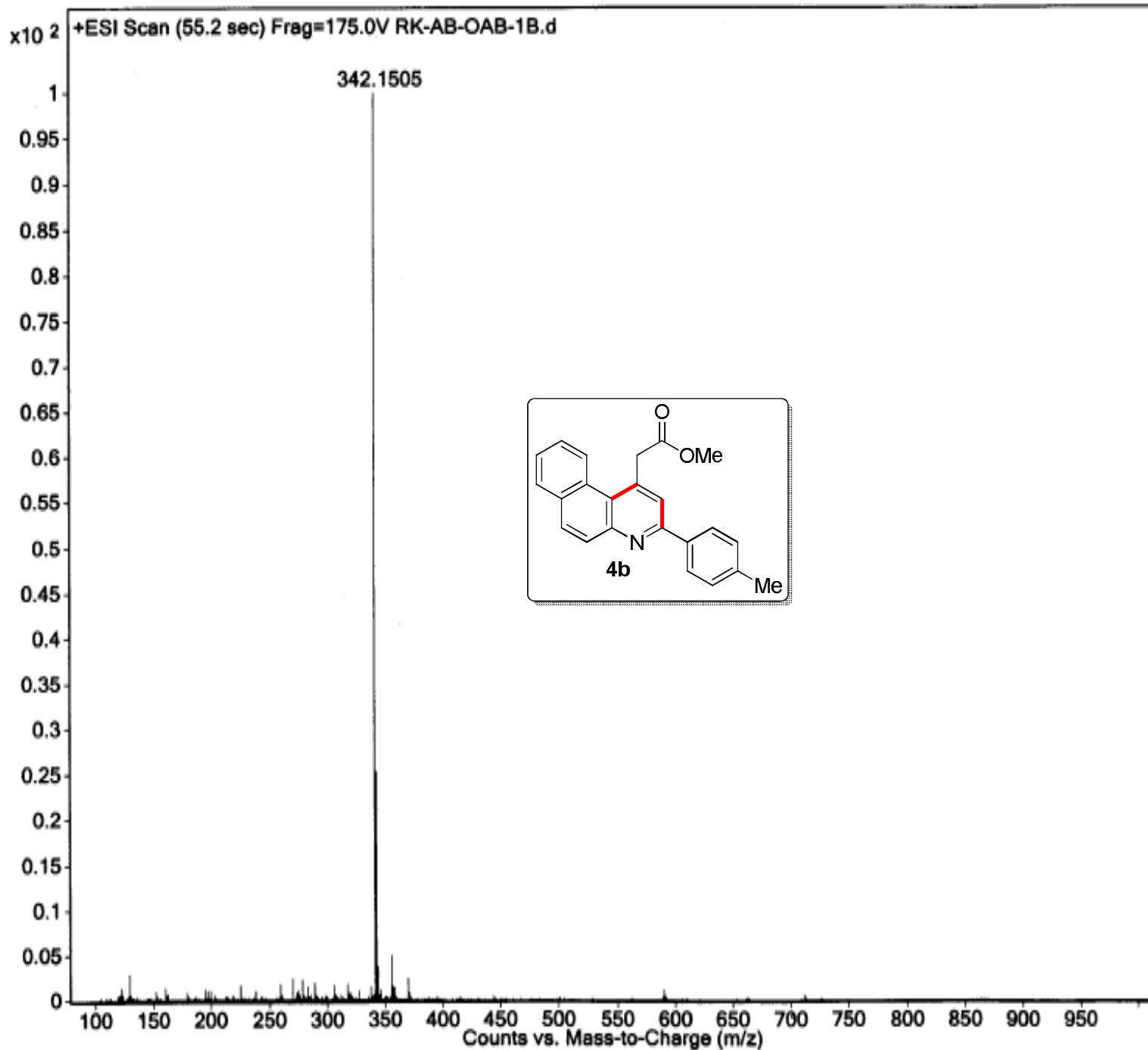
*<sup>13</sup>C NMR spectra of compound 4b*



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 90 repetitions	<b>OBSERVE</b> c13, 100.5425086 <b>DECOUPLE</b> H1, 399.0529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 3 minutes	<b>RK-ME-OME-1B-13C</b> Solvent: cdcl3 Temp. 25.0 c / 290.1 K Operator: chem File: RK-ME-OME-1B-13C Mercury-400 "IITG-NMR"
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HRMS spectra of compound 4b

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





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

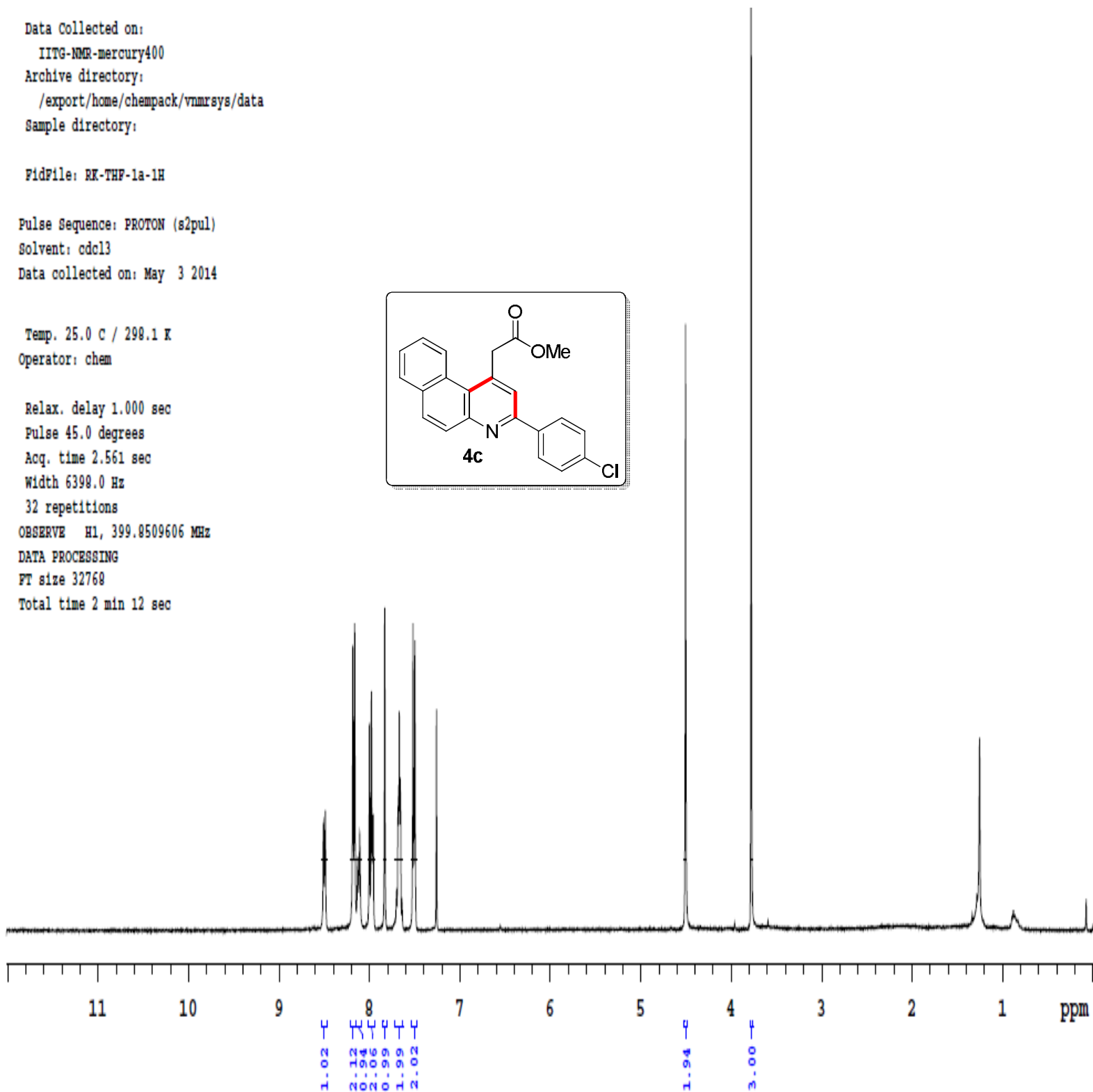
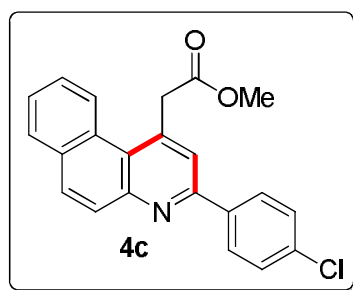
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
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Sample directory:

FidFile: RK-THF-1a-1H

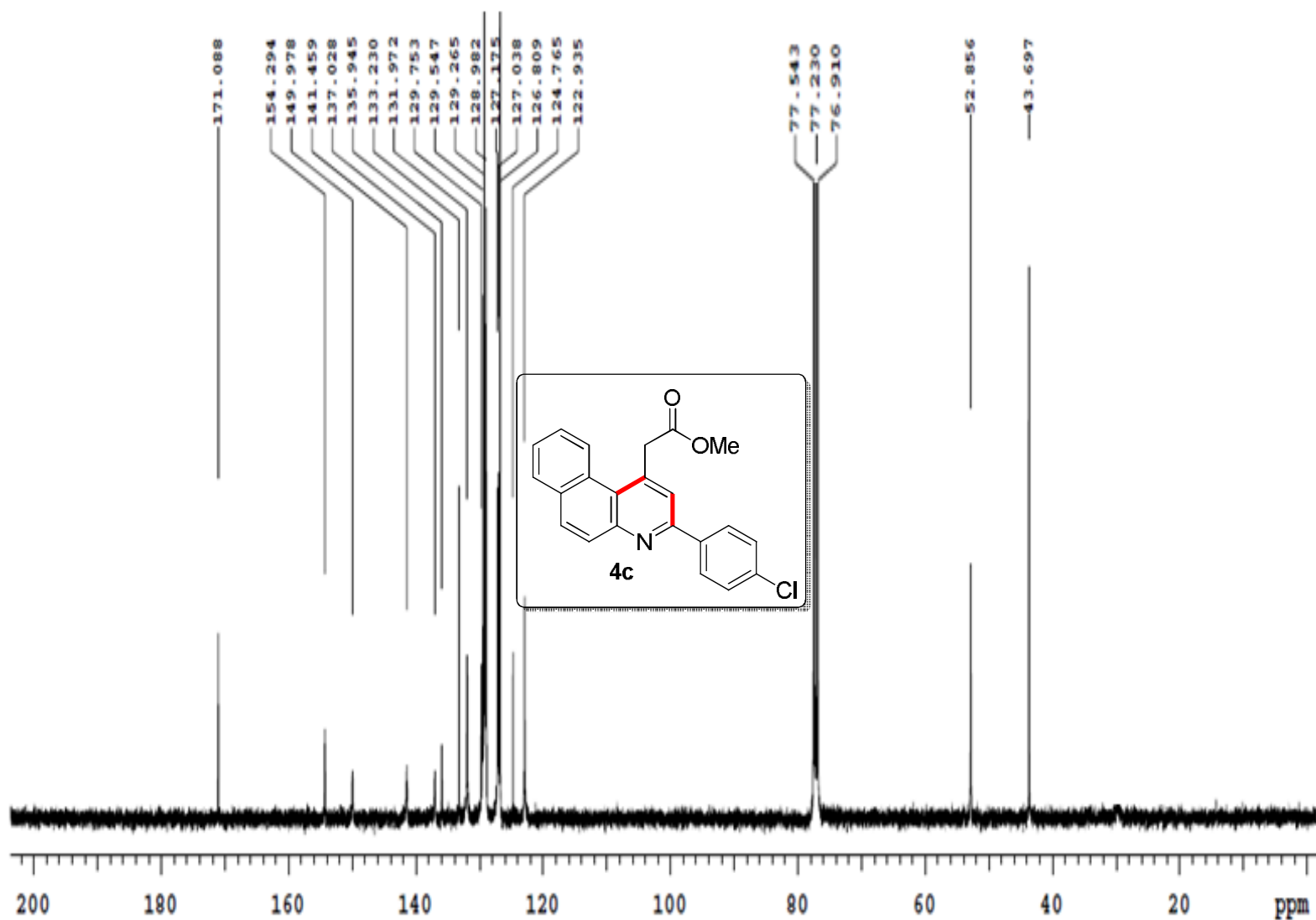
Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: May 3 2014

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, 399.8509606 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



*<sup>13</sup>C NMR spectra of compound 4c*



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
15000 repetitions

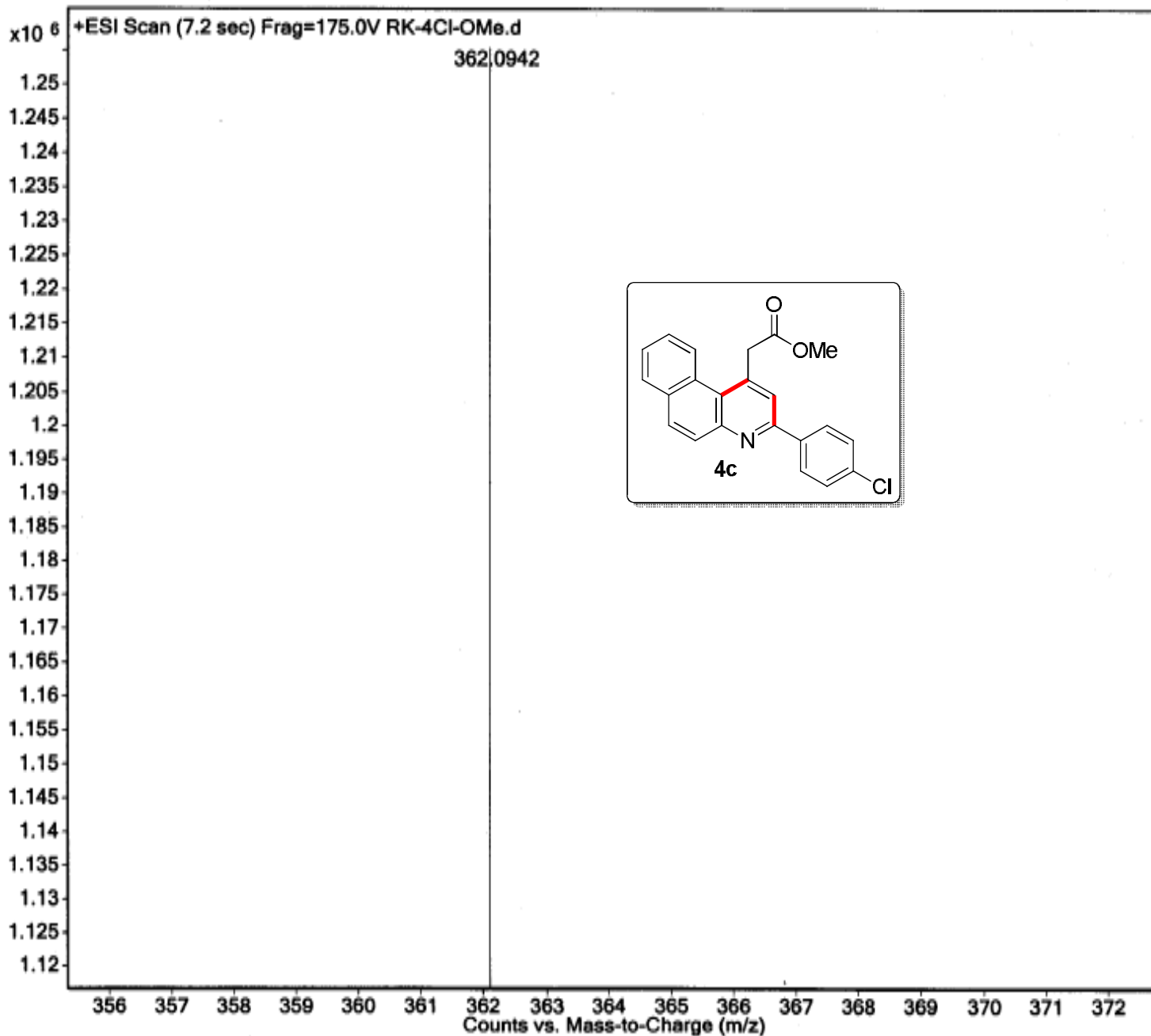
OBSERVE C13, 100.5425824  
DECOUPLE W1, 399.8529994  
Power 42 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 9.6 hours

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

HRMS spectra of compound 4c

Sample Name	RK-4Cl-OMe	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-4Cl-OMe.d	ACQ Method		Comment		Acquired Time	11/11/2014 11:54:46 AM

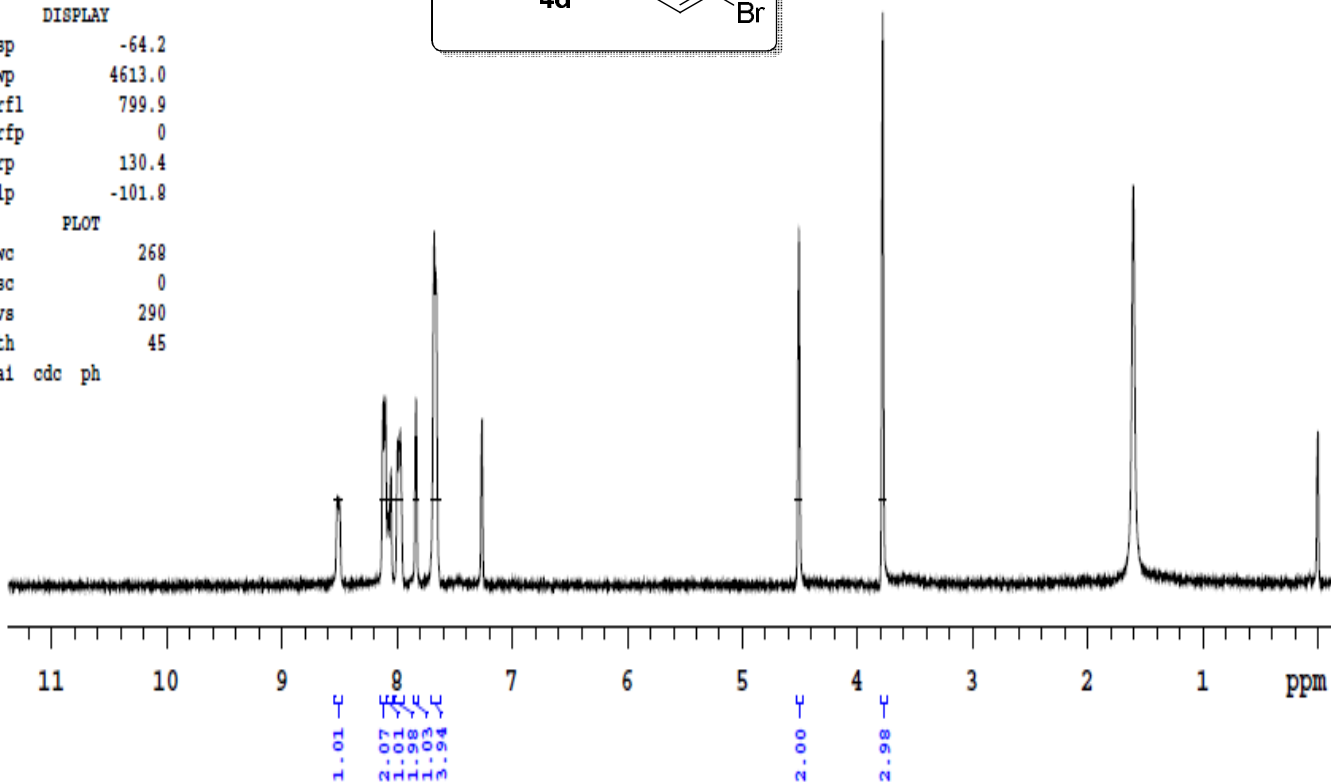
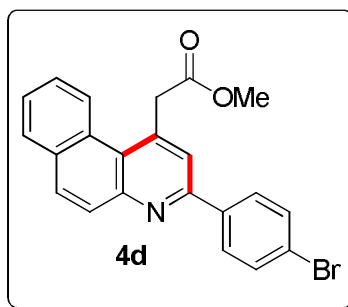


*<sup>1</sup>H NMR spectra of compound 4d*

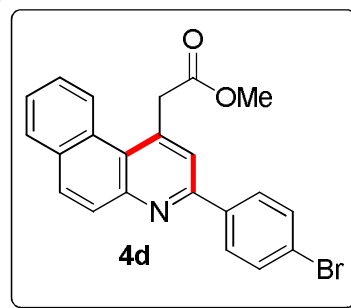
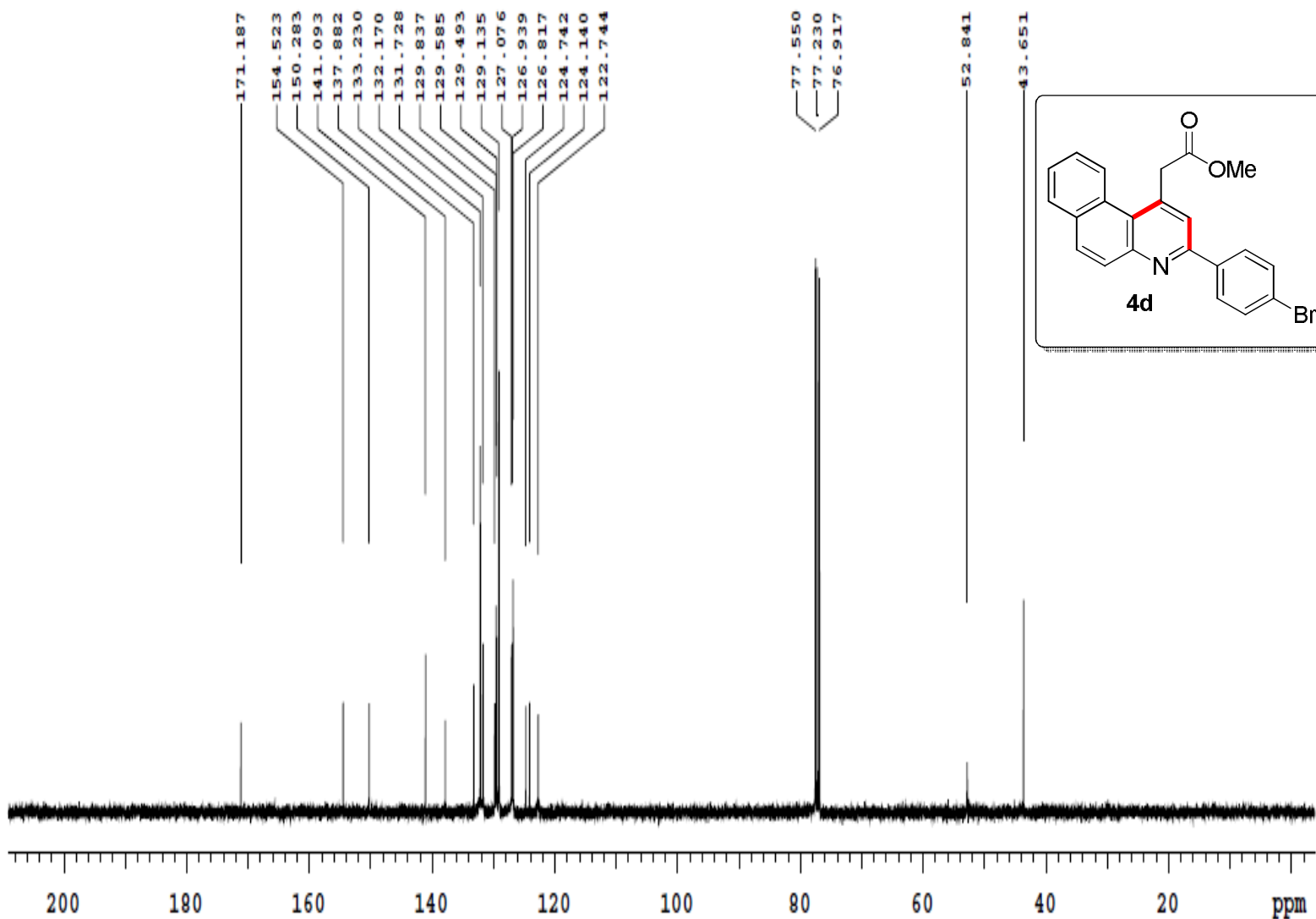
RK\_4Br\_ome\_1H

expl PROTON

SAMPLE		PRESATURATION	
date	Sep 19 2014	satmode	n
solvent	cdcl3	wet	n
file	/home/chem/da-	SPECIAL	
ta/ATK/Radha/RK_4B-	r_ome_1H.fid	temp	25.0
		gain	30
ACQUISITION		spin	not used
sw	6398.0	hst	0.008
at	2.561	pw90	16.300
np	32768	alfa	10.000
fb	3600	FLAGS	
bs	4	il	n
di	1.000	in	n
nt	32	dp	y
ct	32	hs	nn
TRANSMITTER		PROCESSING	
tn	H1	fn	not used
sfrq	399.853	DISPLAY	
tof	363.1	sp	-64.2
tpwr	58	wp	4613.0
pw	8.150	rfl	799.9
DECOUPLER		rfp	0
dn	C13	rp	130.4
dof	0	lp	-101.8
dm	nnn	PLOT	
decwave	g	wc	268
dpwr	40	sc	0
dmf	17100	vs	290
		th	45
		ai	cdc ph



*<sup>13</sup>C NMR spectra of compound 4d*



PULSE SEQUENCE  
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
1000 repetitions

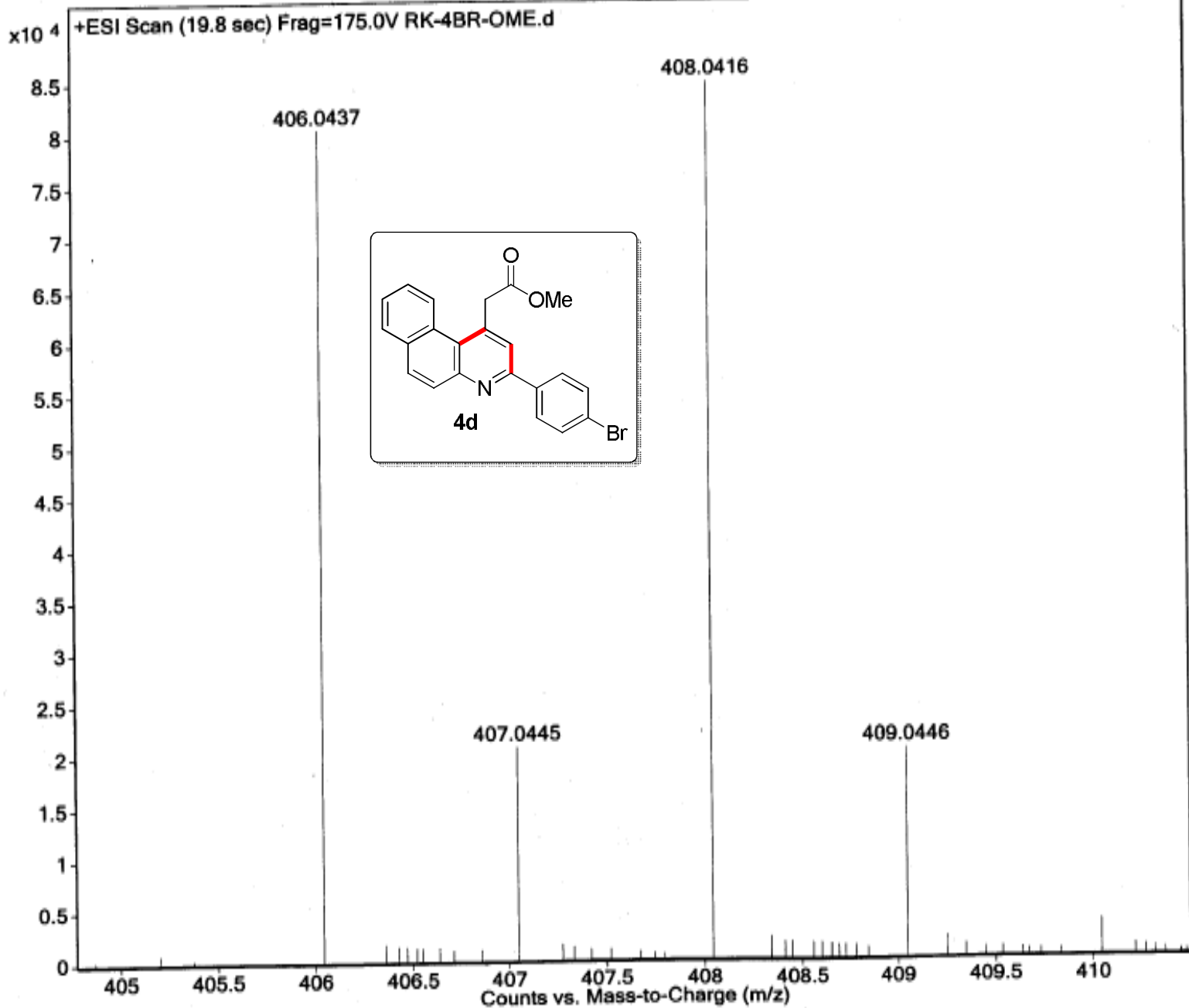
OBSERVE C13, 100.5425040  
DECOUPLE H1, 399.0529994  
Power 42 dB  
continuously on  
WALTZ-16 modulated

DATA PROCESSING  
Line broadening 0.5 Hz  
FT size 65536  
Total time 30 minutes

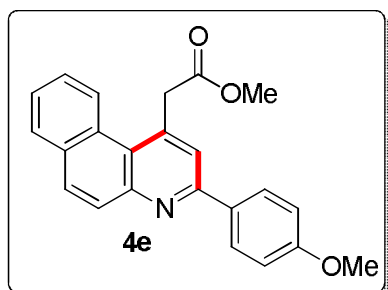
UGRD-93-03-13C  
Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: Rk-4Br-OMe-13C  
Mercury-400 "IITG-NMR"

HRMS spectra of compound 4d

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



*<sup>1</sup>H NMR spectra of compound 4e*

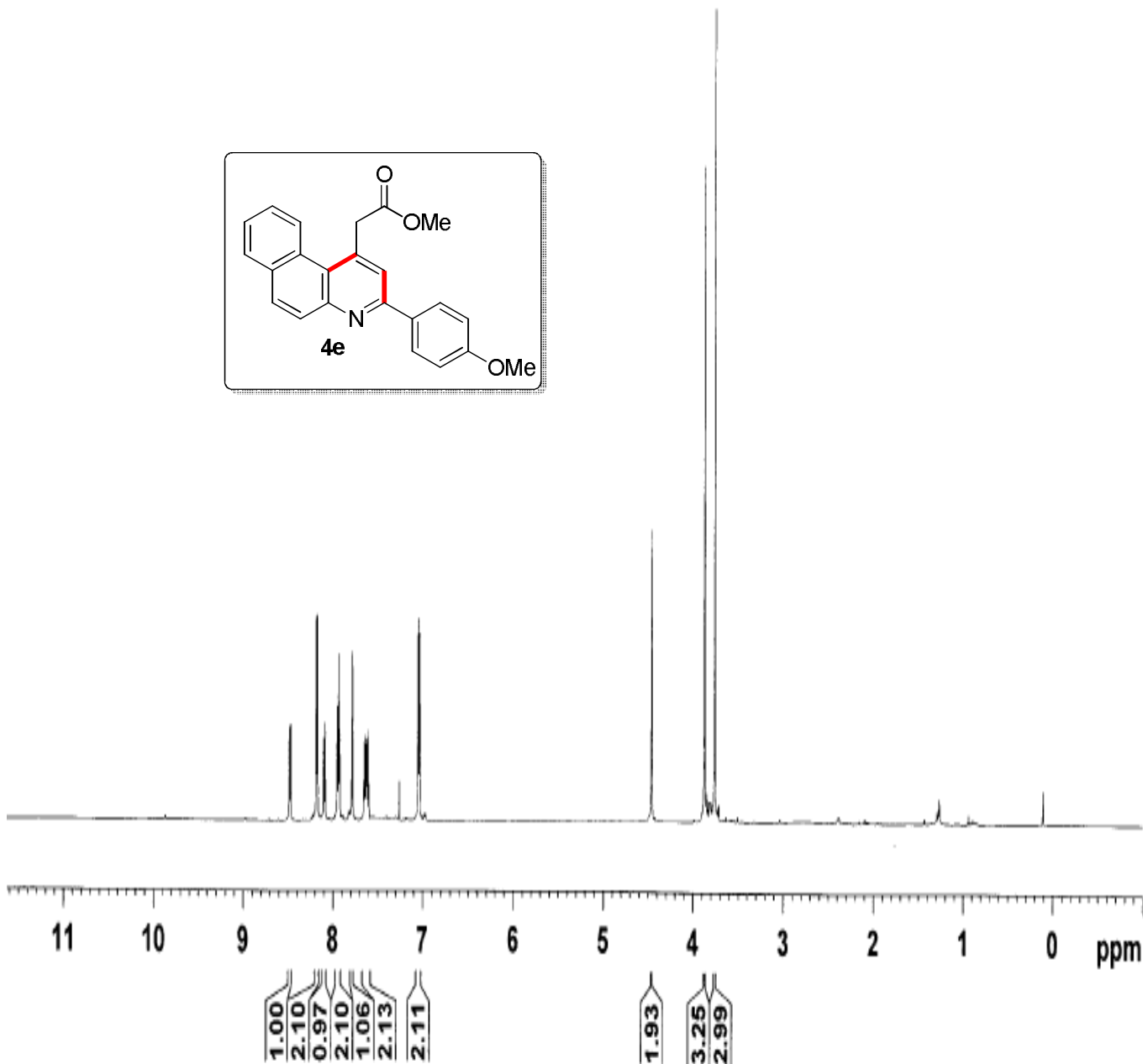


Current Data Parameters  
NAME BK-OMe-OMe-1H  
EXPNO 1  
PROCNO 1

F2 = Acquisition Parameters  
Date\_ 20141208  
Time 15.05  
INSTRUM spect  
PROBHD 5 mm EBBQ BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 34.76  
DW 41.600 usec  
DE 6.50 usec  
TE 298.4 K  
D1 1.00000000 sec  
TD0 1

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

F2 = Processing parameters  
SI 16384  
SF 600.1370148 MHz  
WDW EN  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



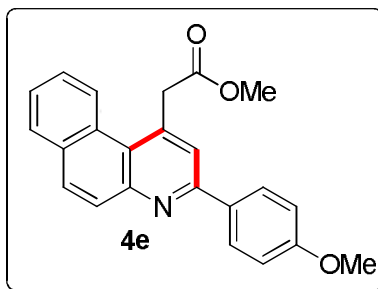
<sup>13</sup>C NMR spectra of compound 4e



171.22  
 161.08  
 155.26  
 149.96  
 140.96  
 132.99  
 131.84  
 131.50  
 131.25  
 129.89  
 129.40  
 128.97  
 126.79  
 126.72  
 126.61  
 124.06  
 122.66  
 114.40  
 77.44  
 77.23  
 77.02  
 55.53  
 52.72  
 43.65

Current Data Parameters  
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 EXPNO 1  
 PROCNO 1

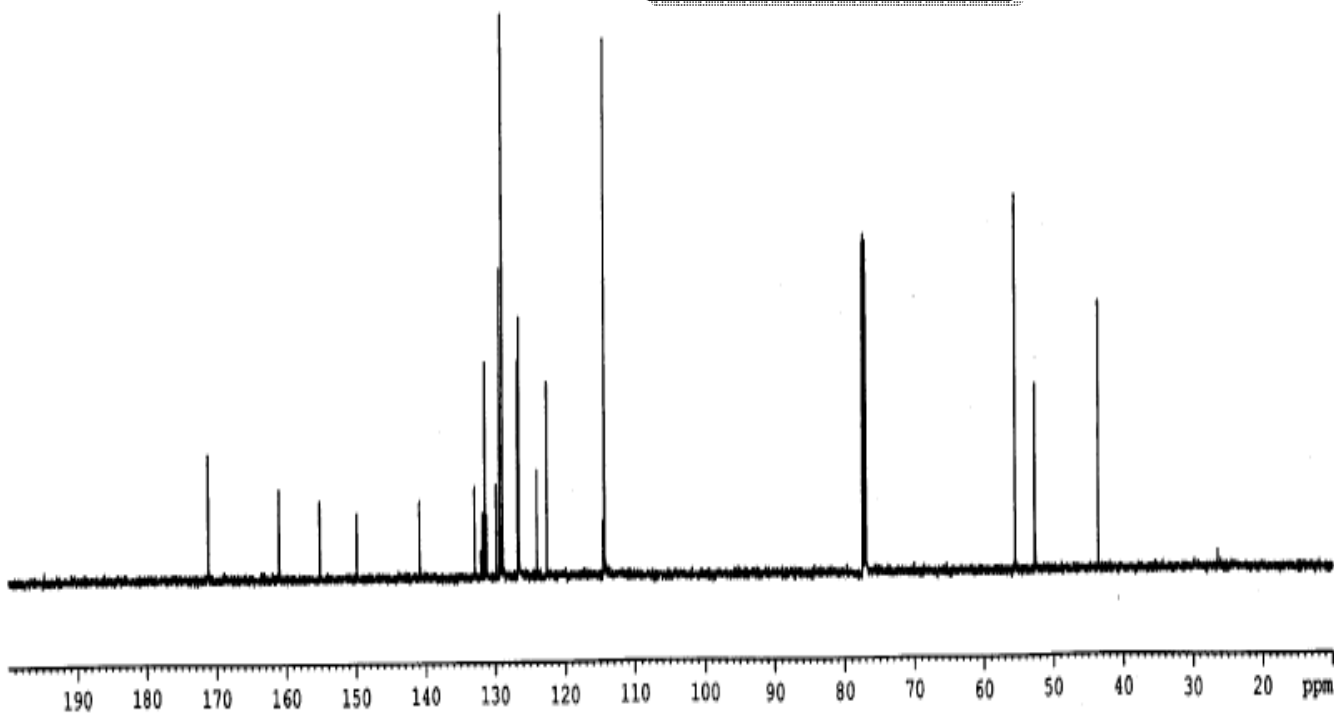
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 TD 32768  
 SOLVENT CDCl3  
 NS 118  
 DS 2  
 SMH 36057.691 Hz  
 FIDRES 1.100393 Hz  
 AQ 0.4543829 sec  
 RG 200.18  
 DM 13.867 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1



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

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

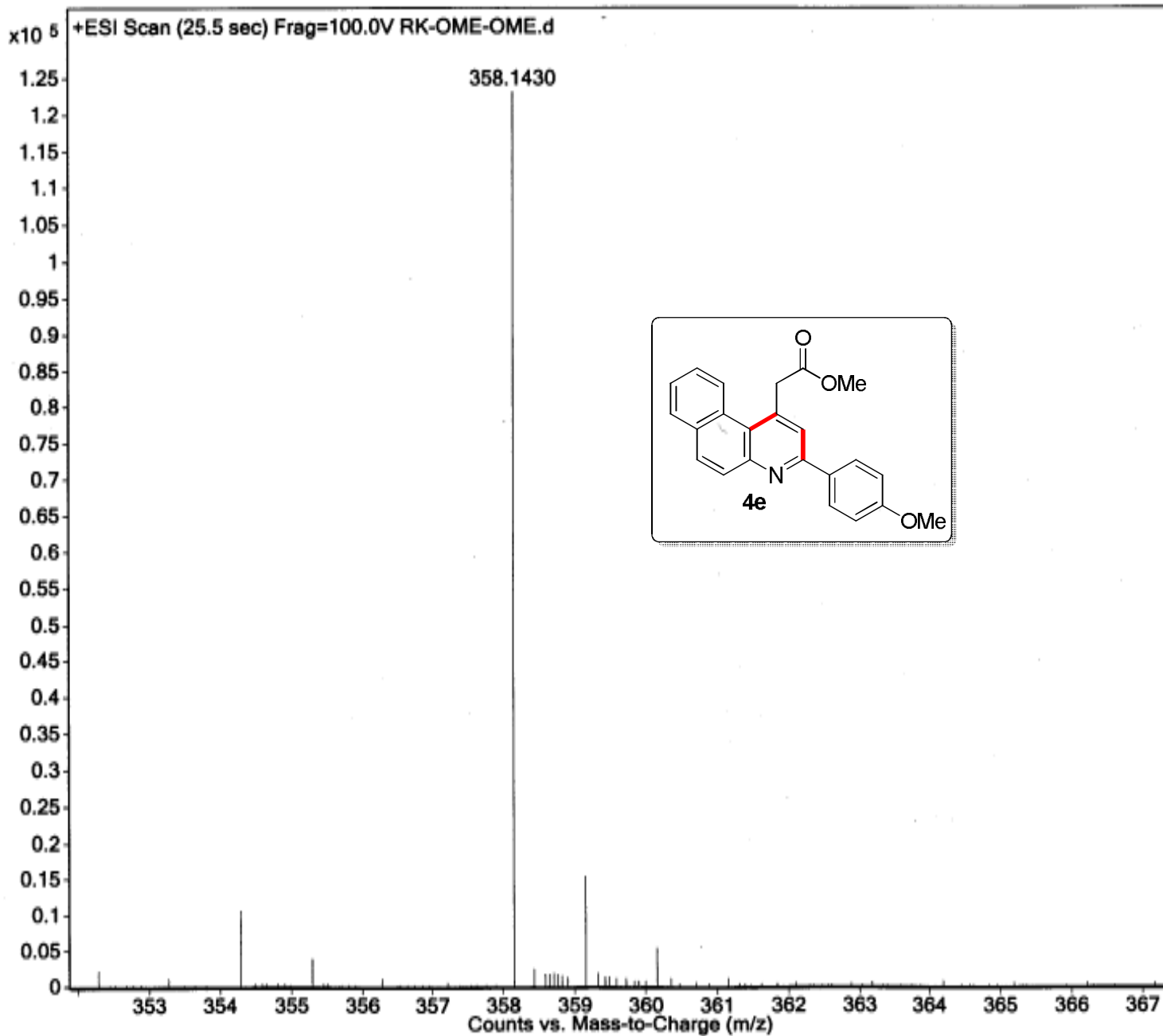
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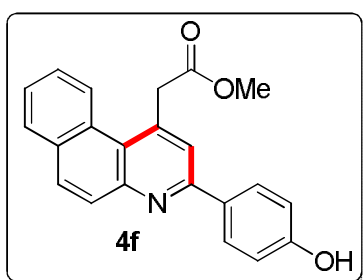


HRMS spectra of compound 4e

Sample Name	RK-OME-OME	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-OME-OME.d	ACQ Method		Comment		Acquired Time	12/10/2014 11:33:51 AM



*<sup>1</sup>H NMR spectra of compound 4f*

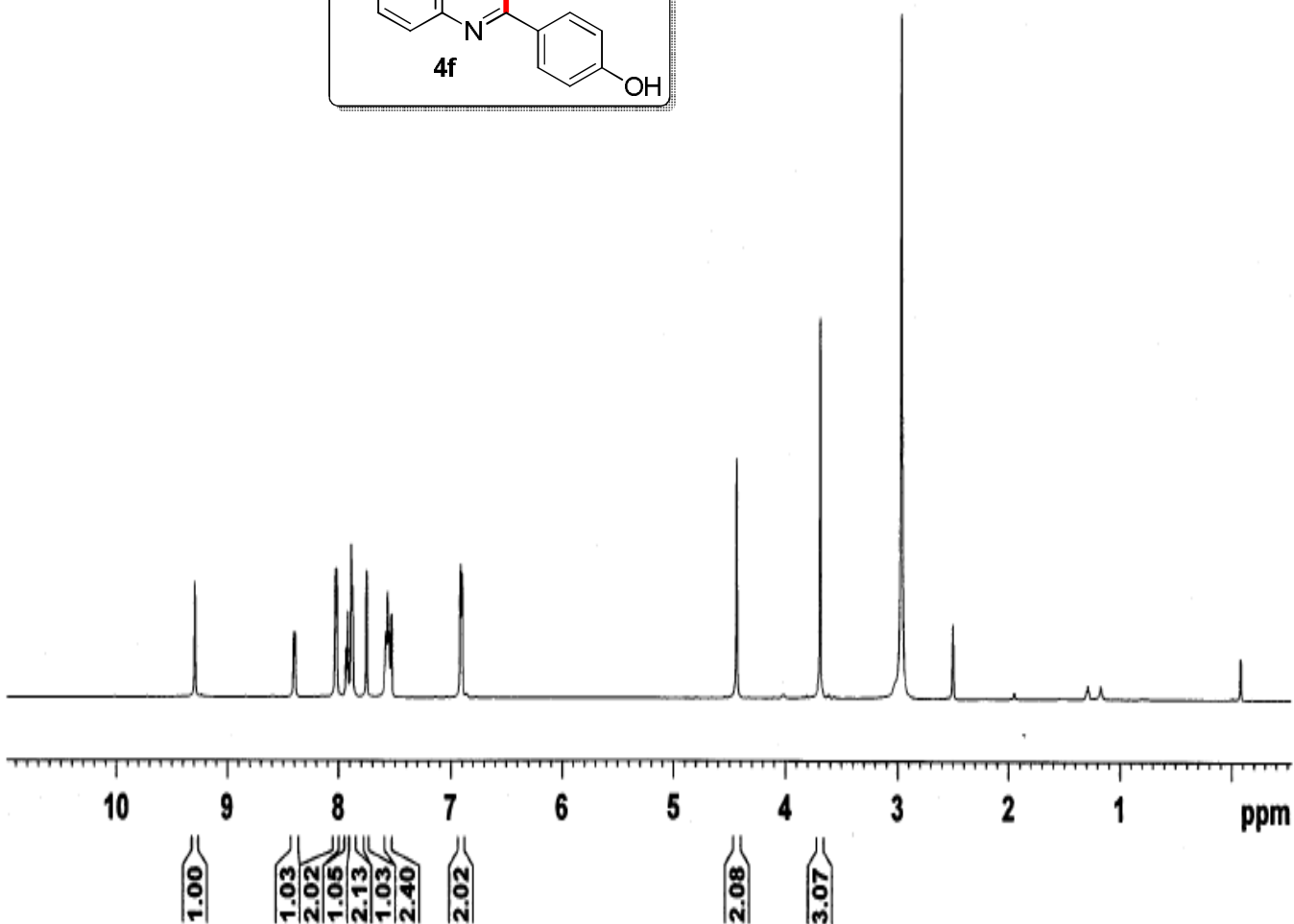


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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20141007  
Time 10.58  
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 1.3631488 sec  
RG 113  
DW 41.600 usec  
DE 6.50 usec  
TE 299.0 K  
D1 1.00000000 sec  
TDO 1

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

F2 - Processing parameters  
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SF 600.1728581 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C NMR spectra of compound 4f



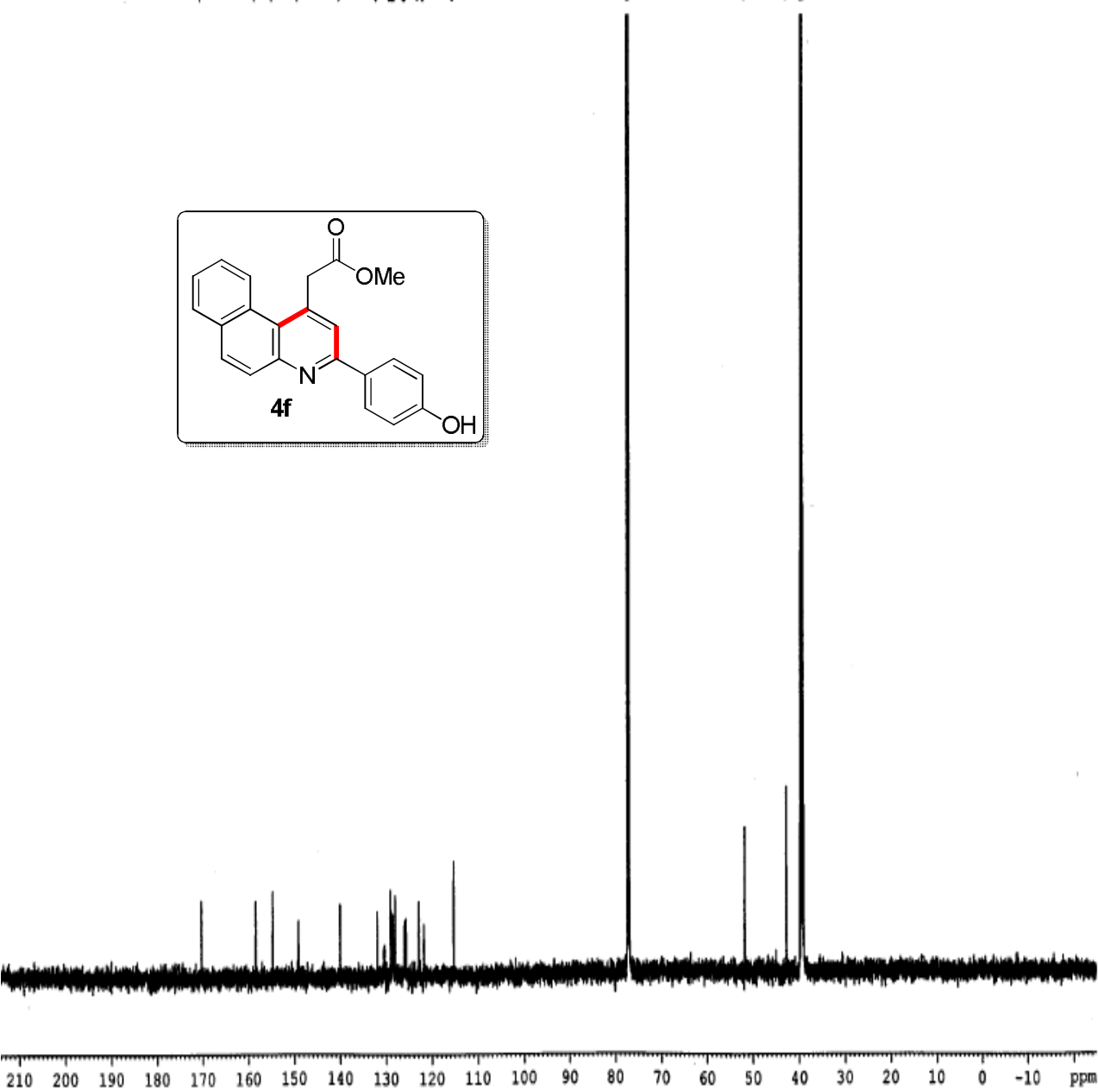
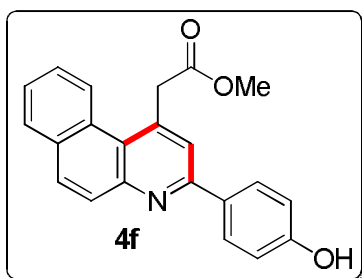
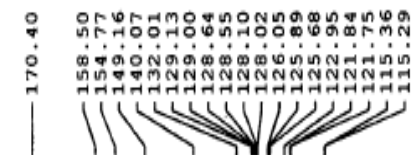
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PROCNO 1

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PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 383  
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 299.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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NUC1 13C  
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PLW1 95.00000000 W

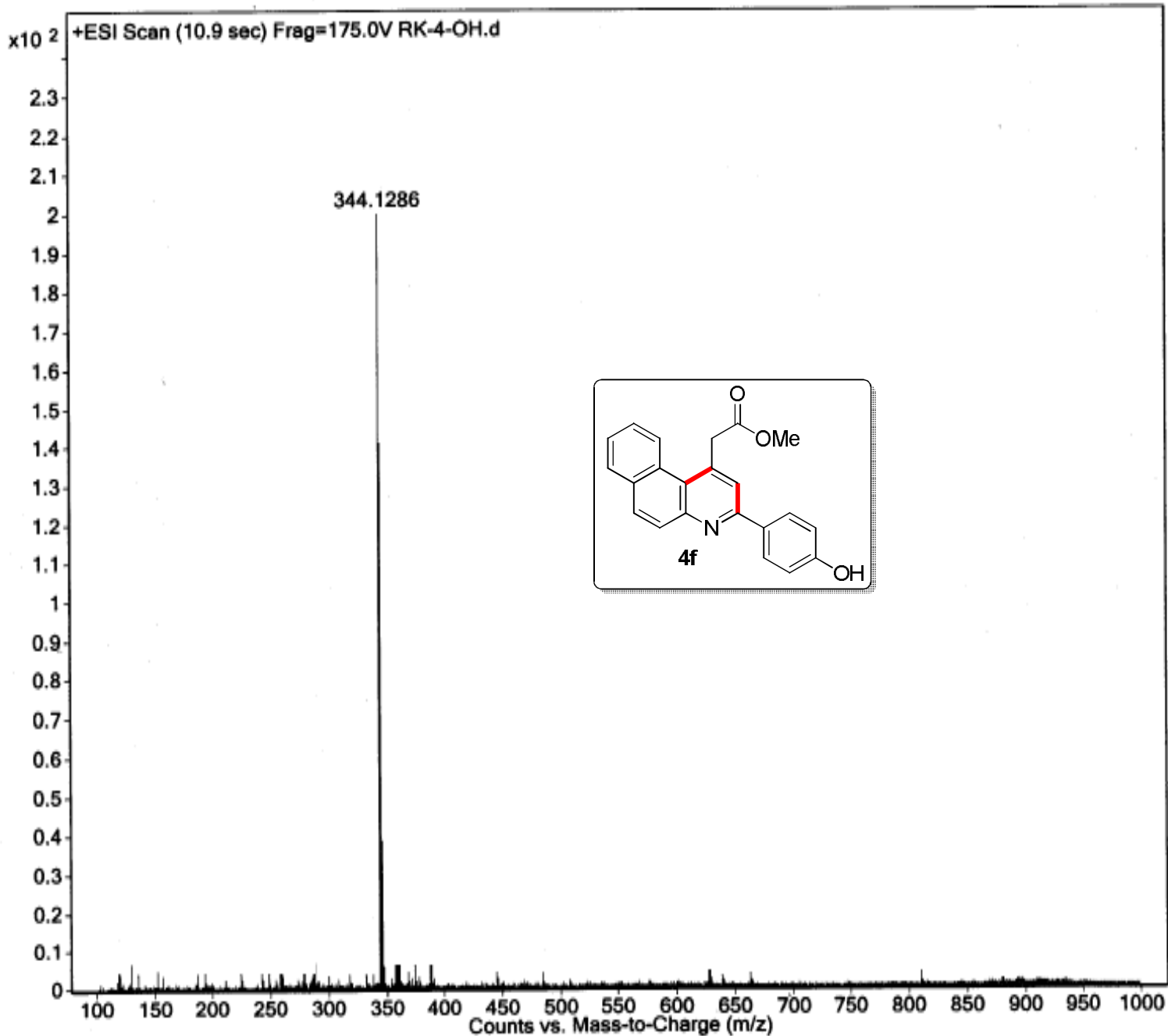
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NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9136798 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



*HRMS spectra of compound 4f*

Sample Name	RK-4-OH	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-4-OH.d	ACQ Method		Comment		Acquired Time	10/30/2014 11:47:22 AM



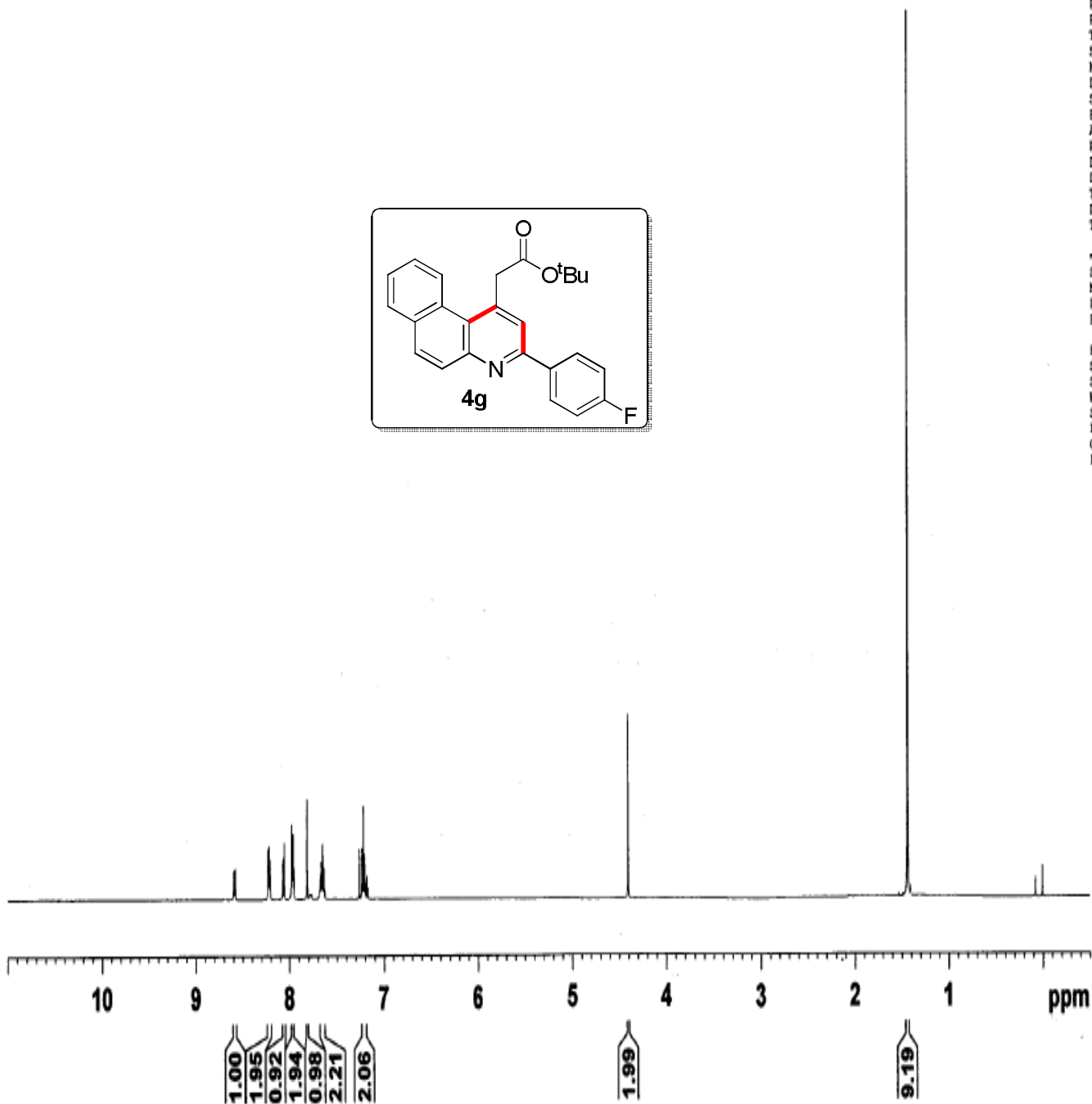
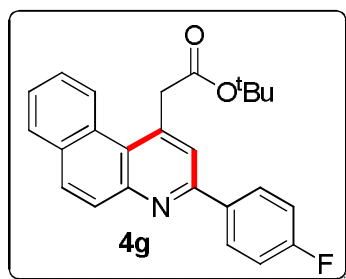
*<sup>1</sup>H NMR spectra of compound 4g*

Current Data Parameters  
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EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140930  
Time 13.08  
INSTRUM spect  
PROBHD 5 mm VABBO 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  
DM 41.600 usec  
DE 6.50 usec  
TE 298.5 K  
D1 1.00000000 sec  
TDO 1

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

F2 - Processing parameters  
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WDW EM  
LN 0.30 Hz  
GB  
PC 1.00



*<sup>13</sup>C NMR spectra of compound 4g*

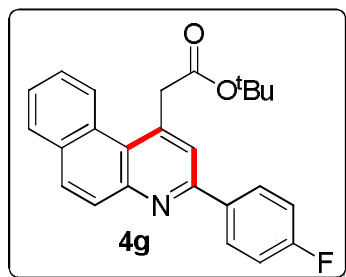


169.49  
165.18  
163.53  
154.12  
133.47  
133.14  
131.19  
131.13  
130.27  
130.09  
129.73  
129.57  
129.33  
128.31  
127.32  
127.24  
127.18  
127.01  
126.65  
124.83  
123.61  
116.30  
116.16  
115.64  
115.50

82.56  
77.45  
77.23  
77.03

45.56

29.22



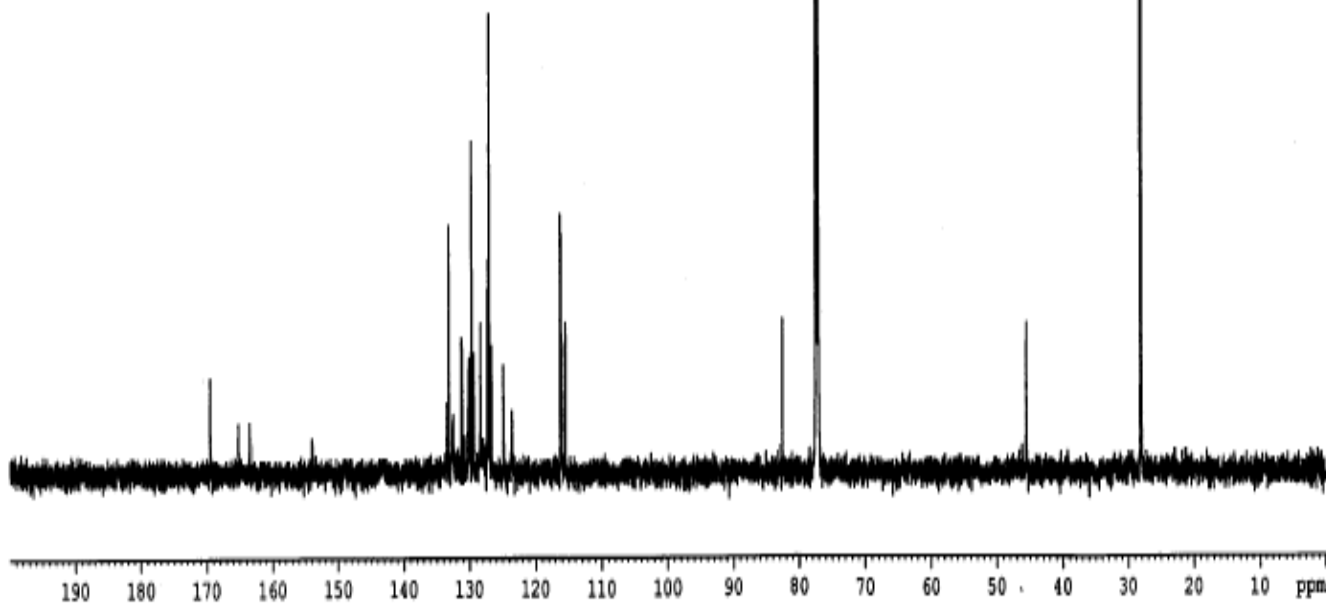
Current Data Parameters  
NAME *AN-4F-CBu-Final-13C*  
EXFNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20141205  
Time 13.13  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 2077  
DS 2  
SWH 3607.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
RW 13.867 usec  
DE 6.50 usec  
TE 299.4 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLM1 95.0000000 W

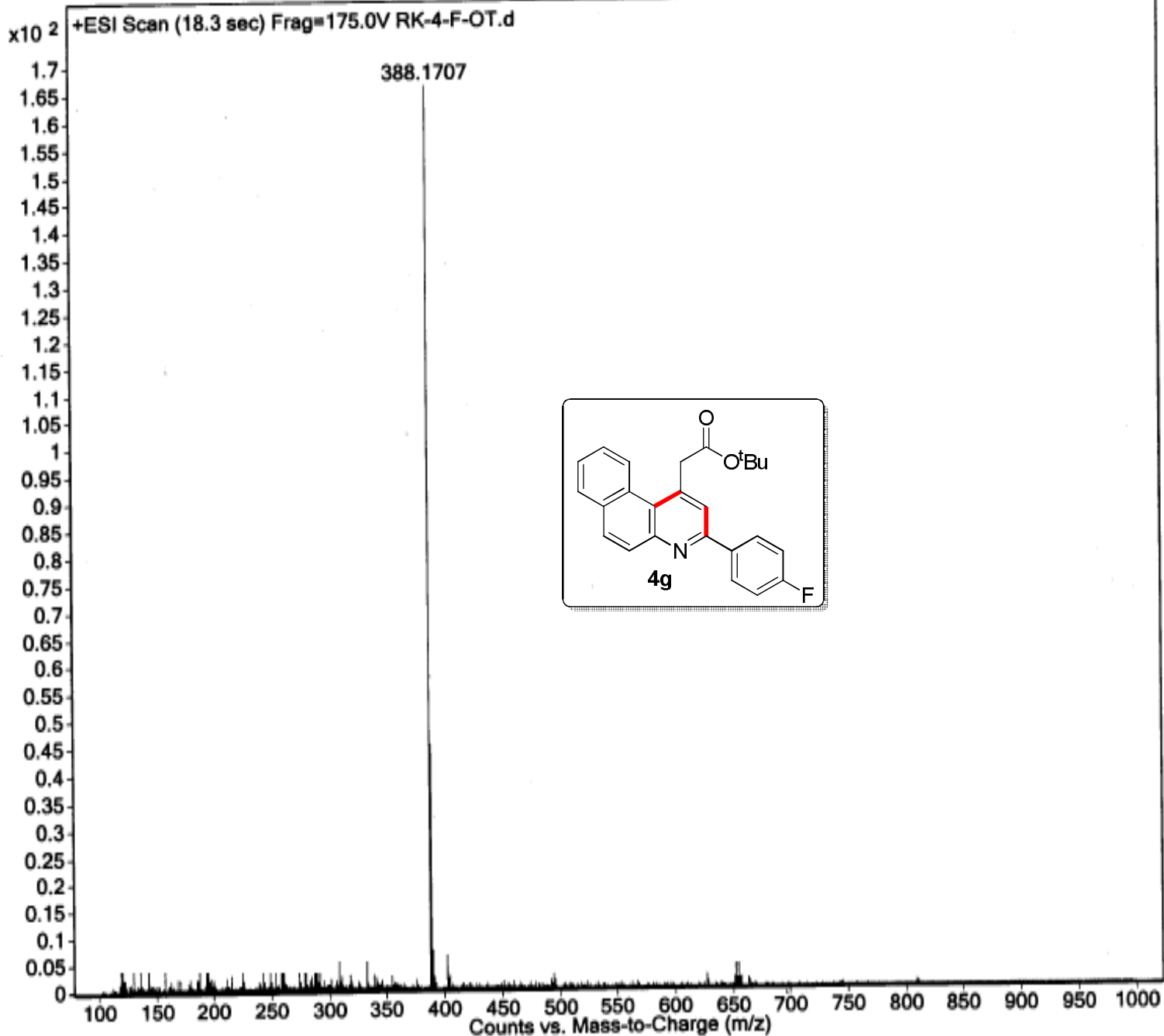
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PCPD2 70.00 usec  
PLM2 21.0000000 W  
PLM3 0.61714000 W  
PLM3 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128345 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



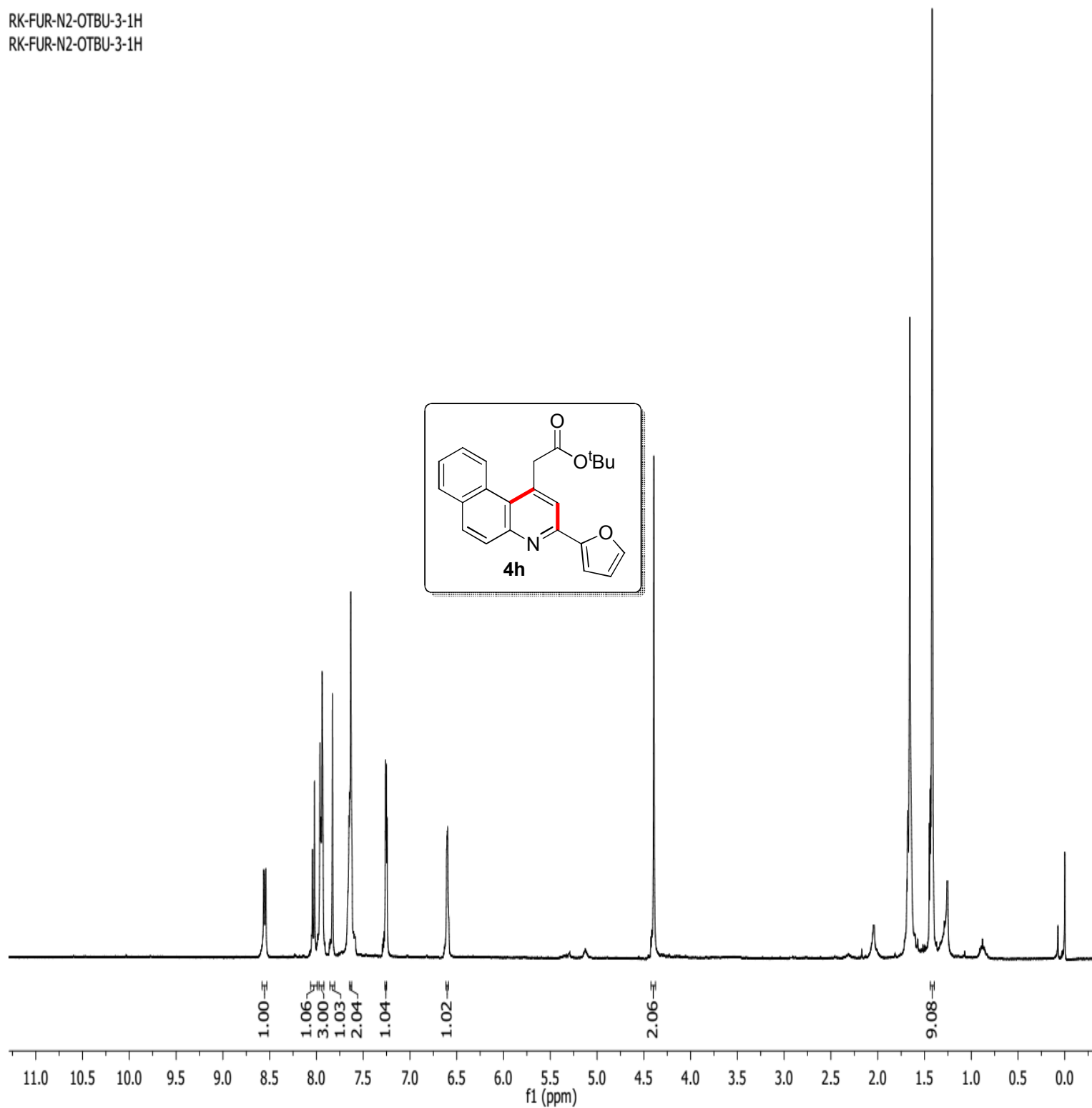
HRMS spectra of compound 4g

Sample Name	RK-4-F-OT	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-4-F-OT.d	ACQ Method		Comment		Acquired Time	10/30/2014 11:48:52 AM



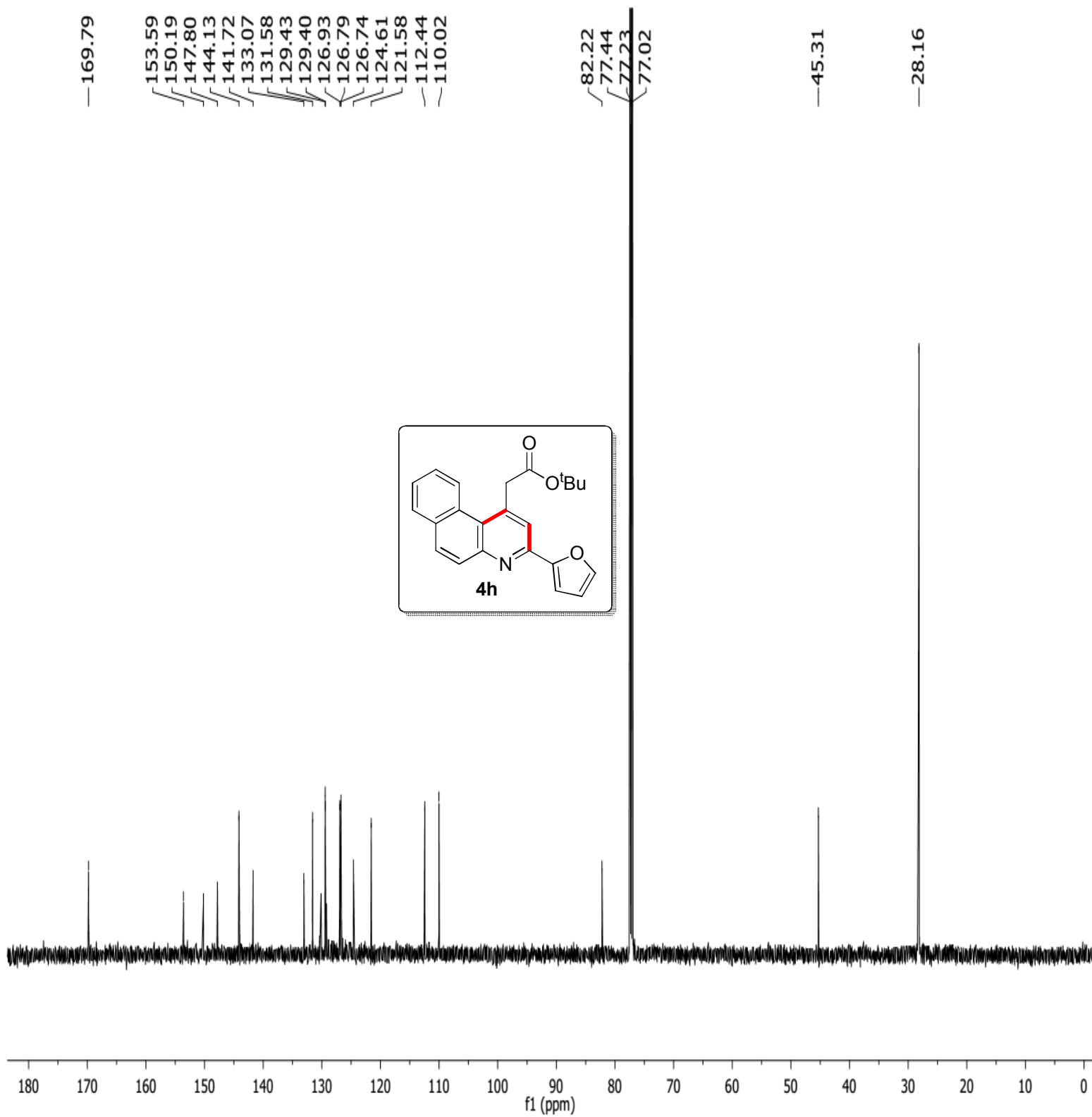
*<sup>1</sup>H NMR spectra of compound 4h*

RK-FUR-N2-OTBU-3-1H  
RK-FUR-N2-OTBU-3-1H



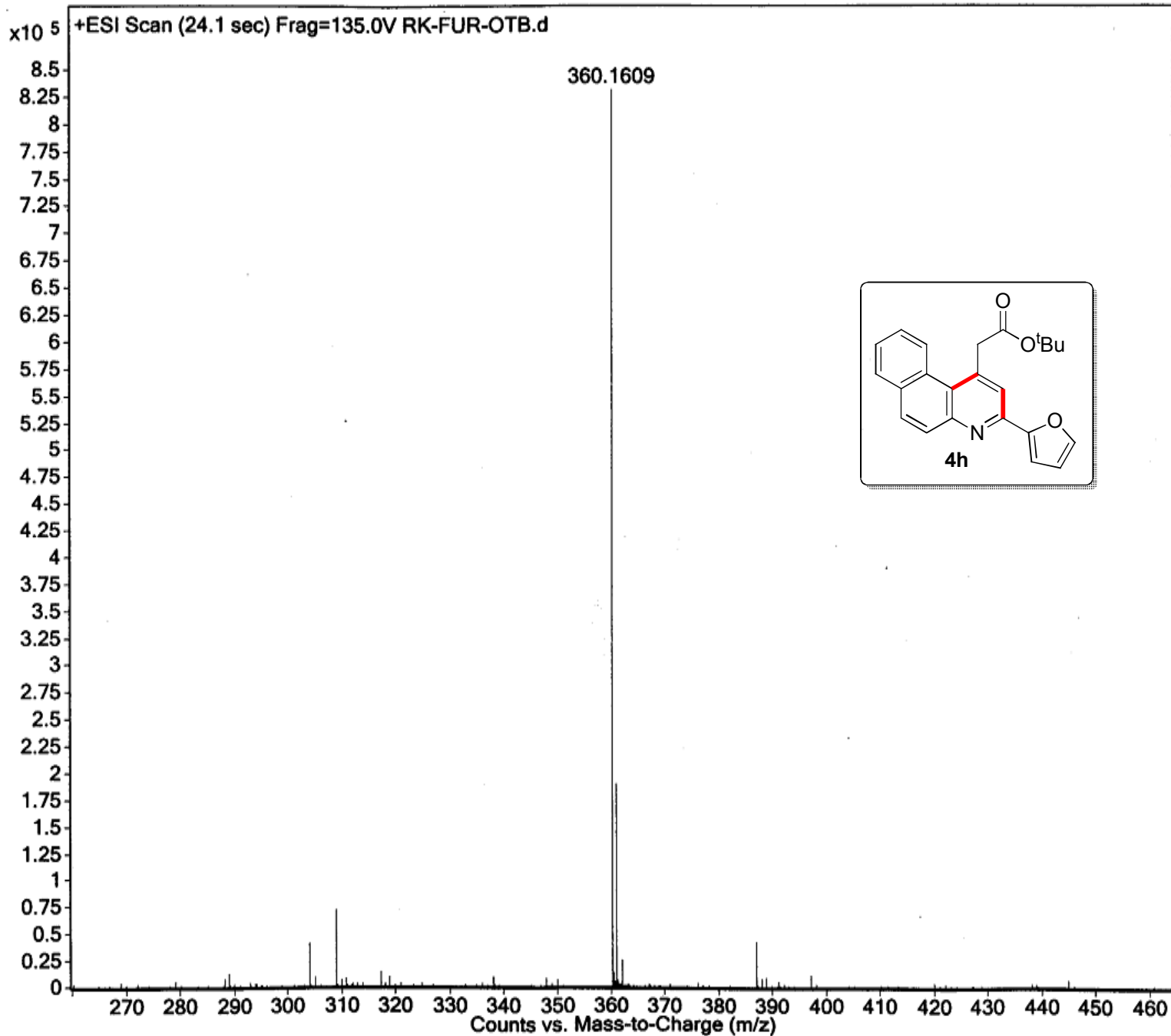


*<sup>13</sup>C NMR spectra of compound 4h*



HRMS spectra of compound 4h

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Some Ions Missed
Data Filename	RK-FUR-OTB.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



*<sup>1</sup>H NMR spectra of compound 4i*

RK-34-3C-14

Sample Name:

RK-34-3C-14

Data Collected on:

IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: RK-34-3C-14

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: May 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

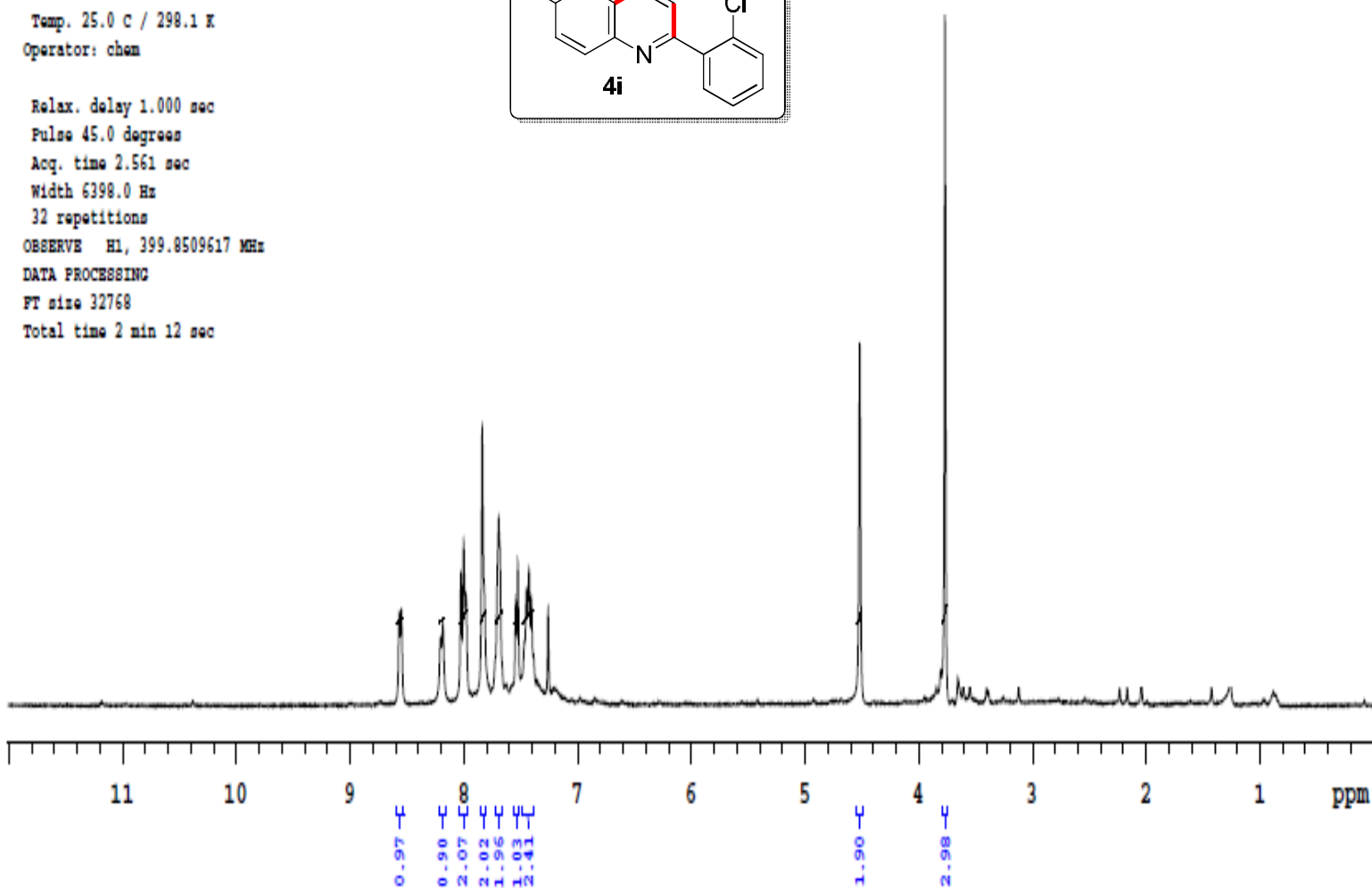
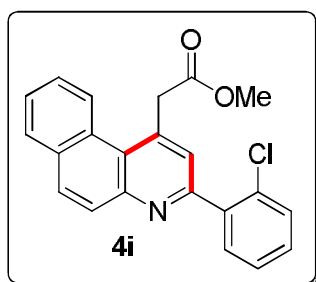
32 repetitions

OBSERVE H1, 399.8509617 MHz

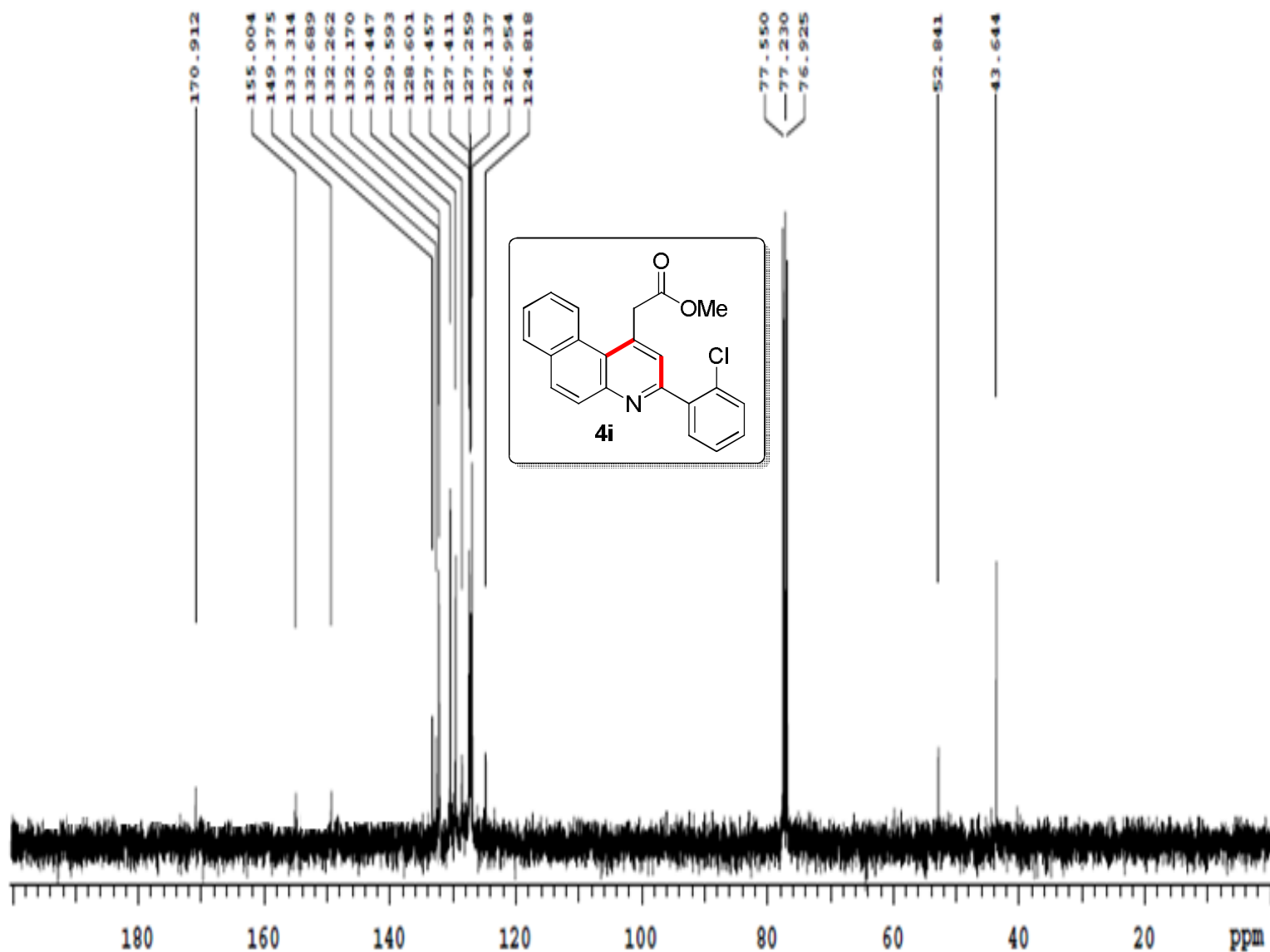
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



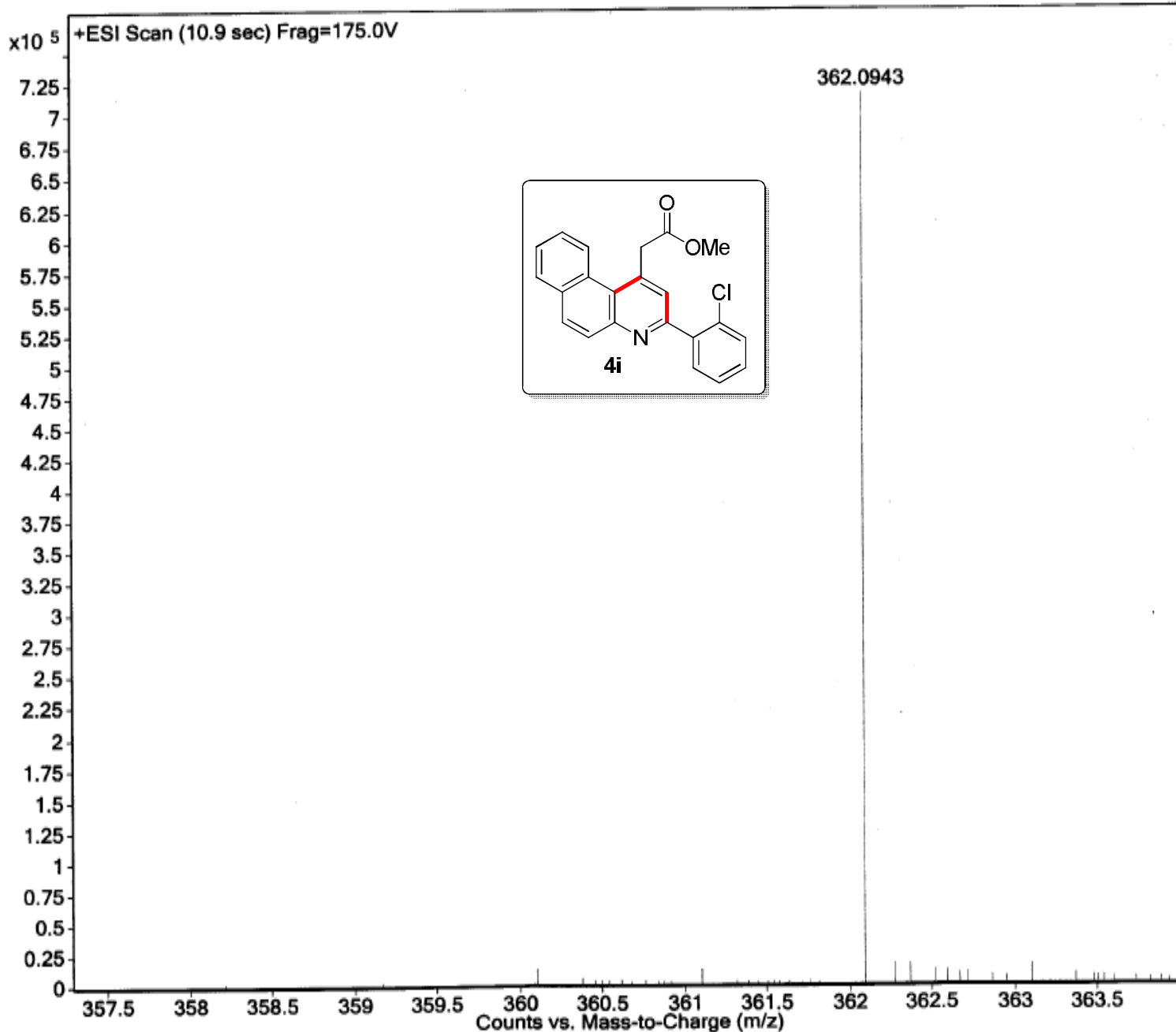
*<sup>13</sup>C NMR spectra of compound 4i*



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 0.652 sec Width 25125.6 Hz 500 repetitions	<b>OBSERVE</b> C13, 100.5425840 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 32768 Total time 15 minutes	<b>RK-34-3C-14</b>  Solvent: cdcl3 Temp. 25.0 c / 298.1 K Operator: chem File: RK-34-3C-14-13C Mercury-400 *IITC-NMR*
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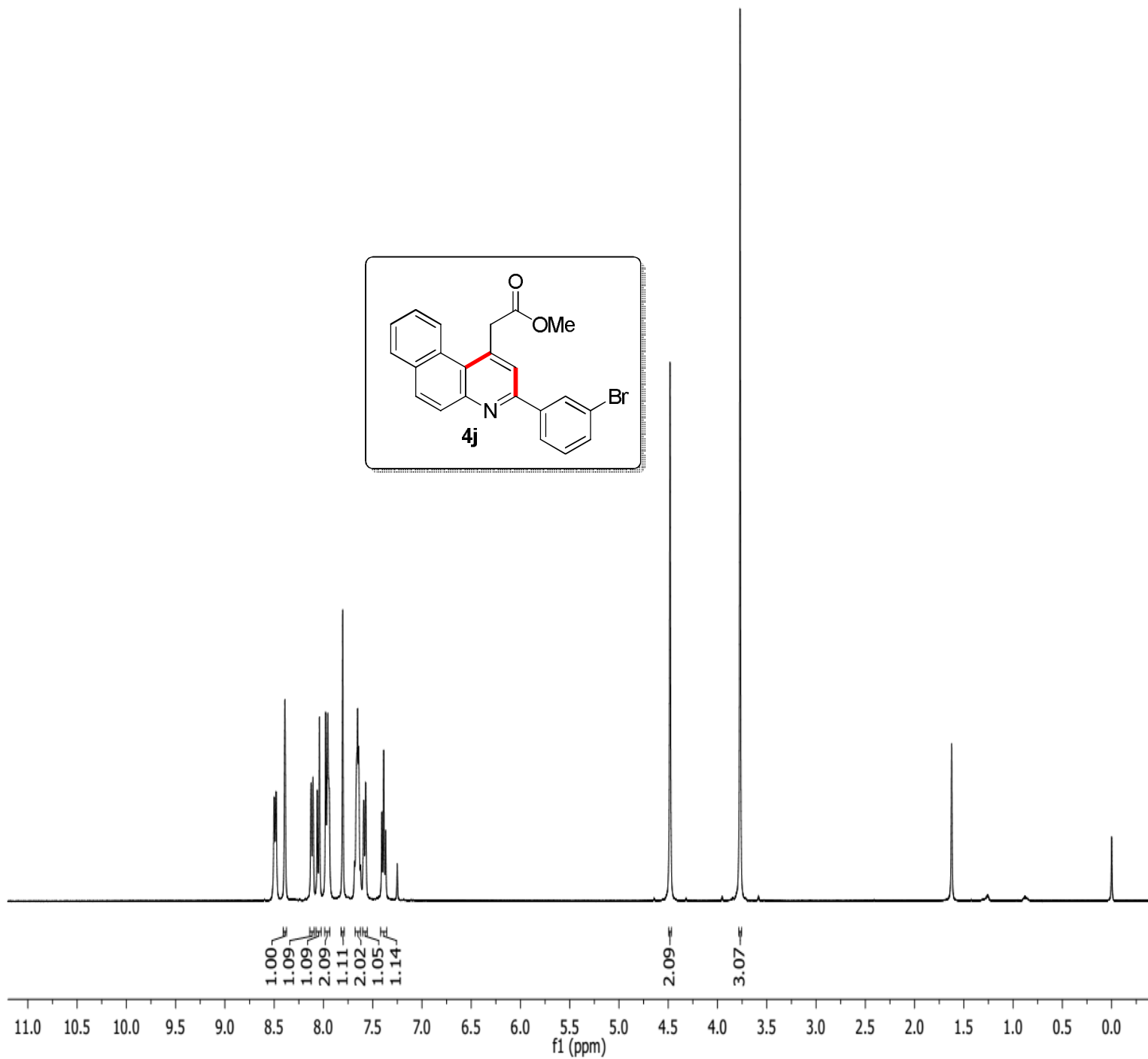
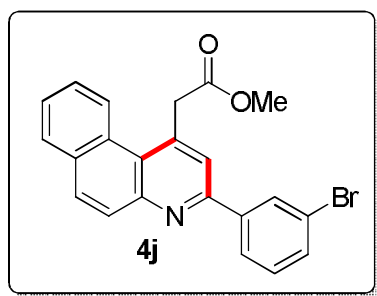
HRMS spectra of compound 4i

Sample Name	RK-2Cl-OEt	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-2Cl-OEt.d	ACQ Method		Comment		Acquired Time	11/11/2014 12:00:24 PM



*<sup>1</sup>H NMR spectra of compound 4j*

RK-3BR-OME-N2-1H-2  
RK-3BR-OME-N2-1H-2



*<sup>13</sup>C NMR spectra of compound 4j*

RK-3BR-OME-N2-13C  
RK-3BR-OME-N2-13C  
—171.14

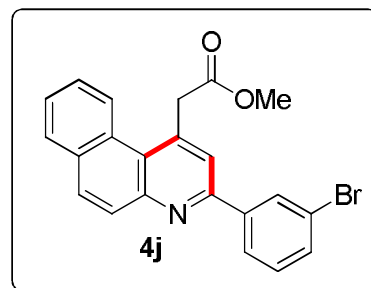
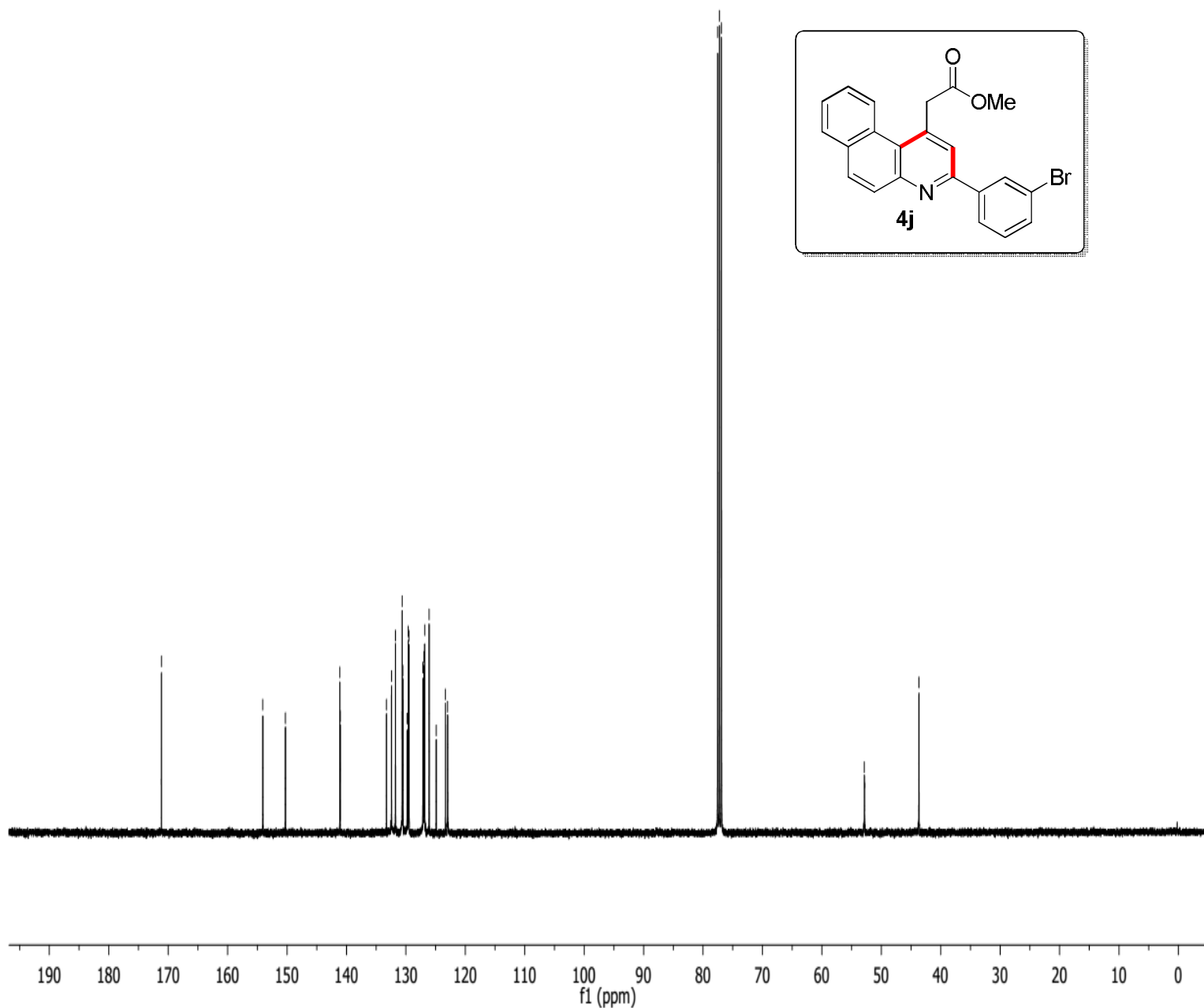
—154.08  
—150.28

141.13  
141.07  
133.27  
132.42  
131.76  
130.63  
130.52  
129.79  
129.62  
129.49  
127.14  
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126.10  
124.90  
123.35  
122.98

77.55  
77.23  
76.91

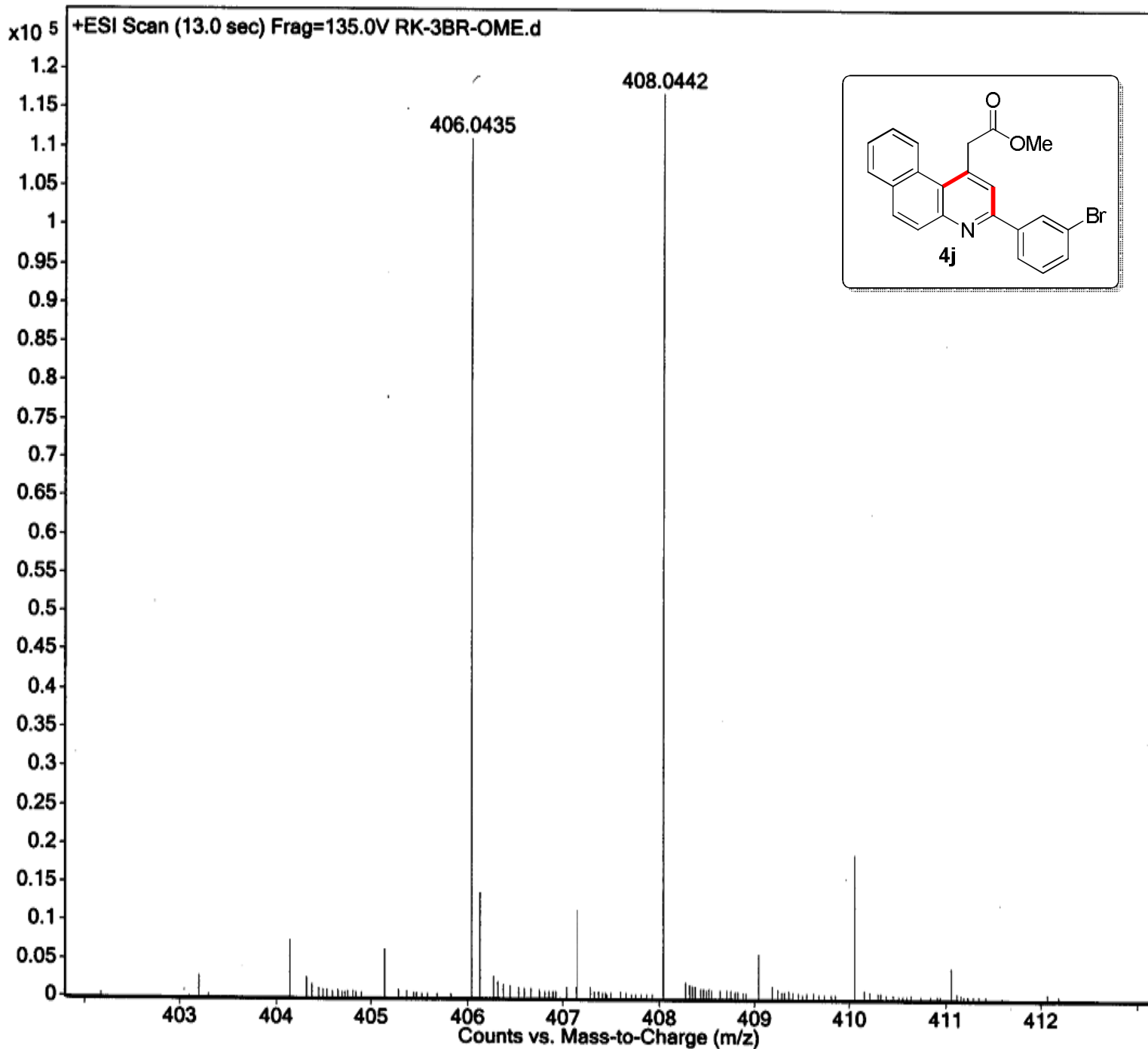
—52.86

—43.67



HRMS spectra of compound 4j

Sample Name	RK-3BR-OME	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	RK-3BR-OME.d	ACQ Method		Comment		Acquired Time	12/4/2015 5:16:34 PM





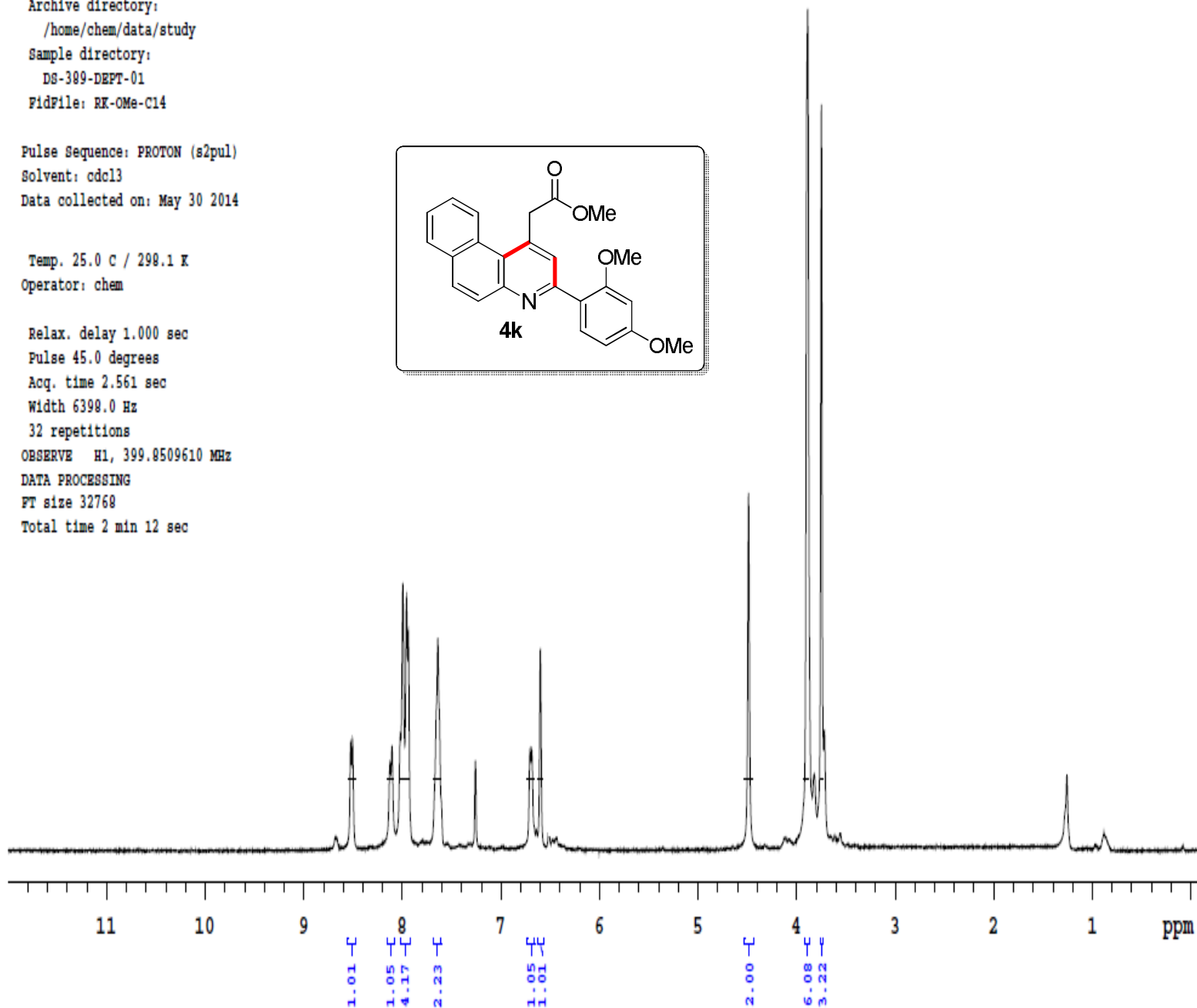
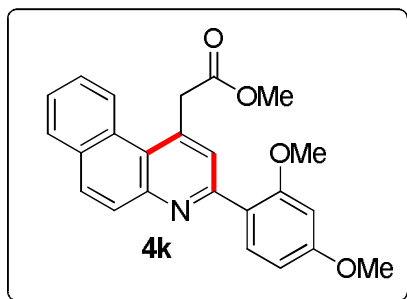
# *<sup>1</sup>H NMR spectra of compound 4k*

Sample Name:  
RK-OMe-C14  
Data Collected on:  
IITG-NMR-mercury400  
Archive directory:  
/home/chem/data/study  
Sample directory:  
DS-309-DEPT-01  
FidFile: RK-OMe-C14

Pulse Sequence: PROTON (s2pul)  
Solvent: cdcl3  
Data collected on: May 30 2014

Temp. 25.0 C / 298.1 K  
Operator: chem

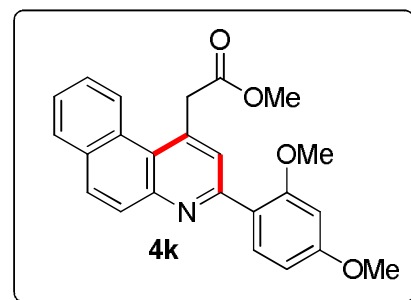
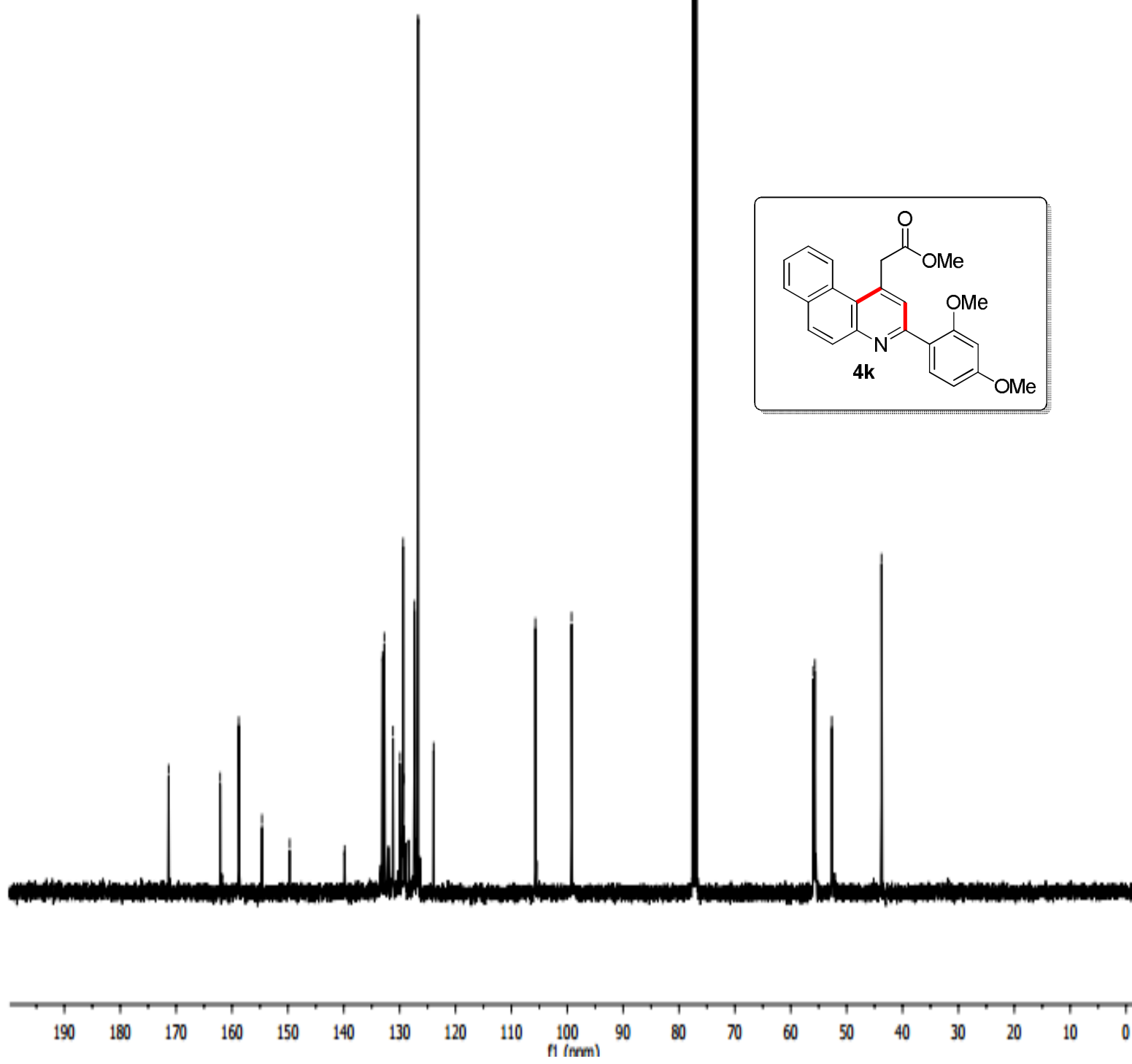
Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 2.561 sec  
Width 6398.0 Hz  
32 repetitions  
OBSERVE H1, 399.8509610 MHz  
DATA PROCESSING  
FT size 32768  
Total time 2 min 12 sec



*<sup>13</sup>C NMR spectra of compound 4k*

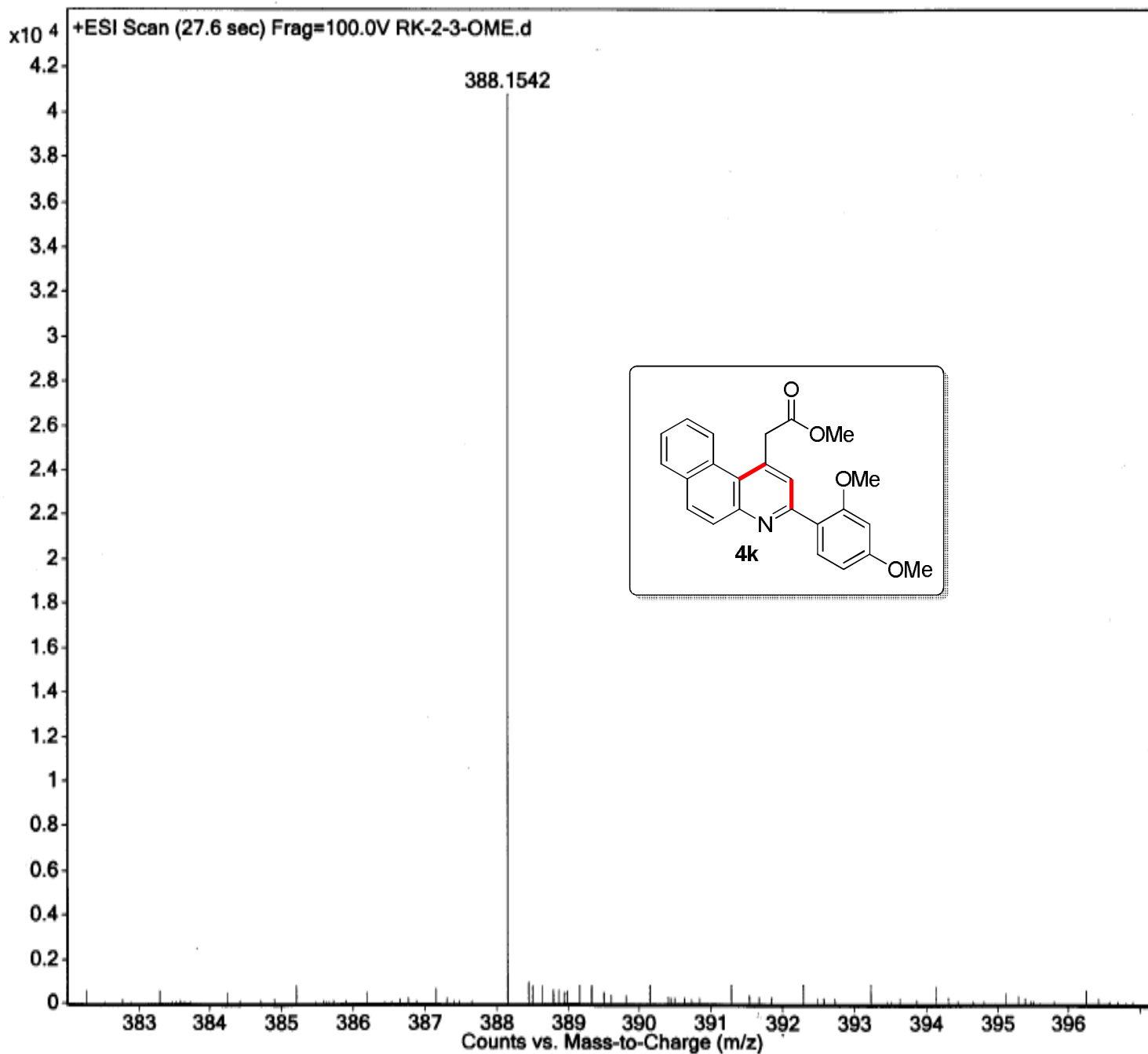
RK-OMe-C14-13C  
RK-OMe-C14-13C

— 177.34  
— 162.13  
— 158.79  
— 154.64  
— 149.68  
— 139.83  
— 133.04  
— 132.74  
— 131.20  
— 128.95  
— 128.38  
— 127.25  
— 126.71  
— 123.91  
— 105.70  
— 99.23  
77.55  
77.33  
76.91  
55.94  
55.70  
52.96  
— 43.76



HRMS spectra of compound 4k

Sample Name	RK-2-3-OME	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-2-3-OME.d	ACQ Method		Comment		Acquired Time	12/9/2014 4:05:57 PM



*<sup>1</sup>H NMR spectra of compound 4l*

RK-NAP-SAL-OALL-1A-1H

Sample Name:

RK-NAP-SAL-OALL-1A-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

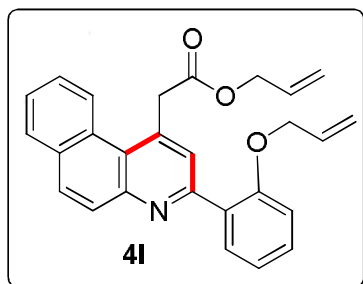
Sample directory:

FidFile: PROTON

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Dec 20 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

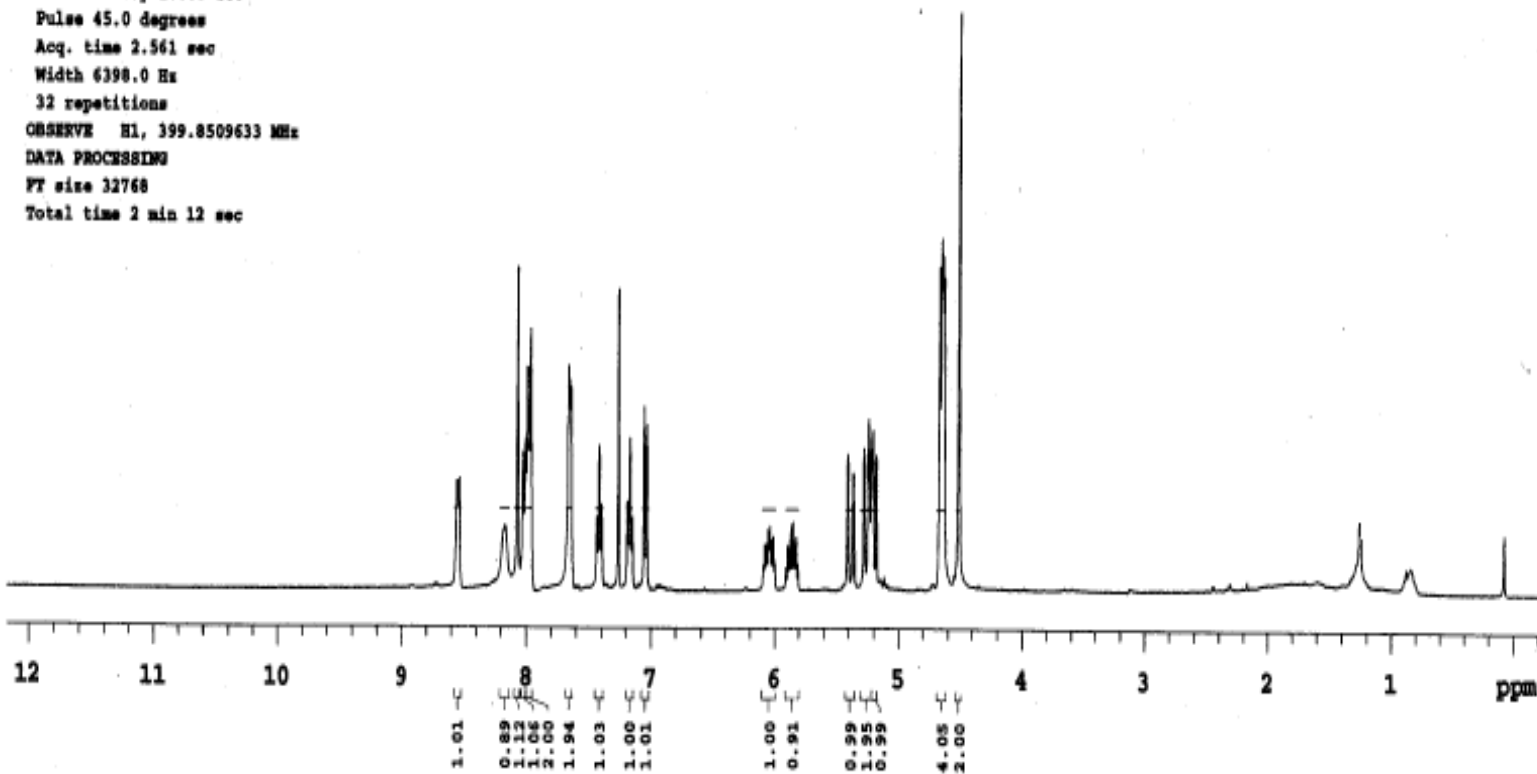
32 repetitions

OBSERVE H1, 399.8509633 MHz

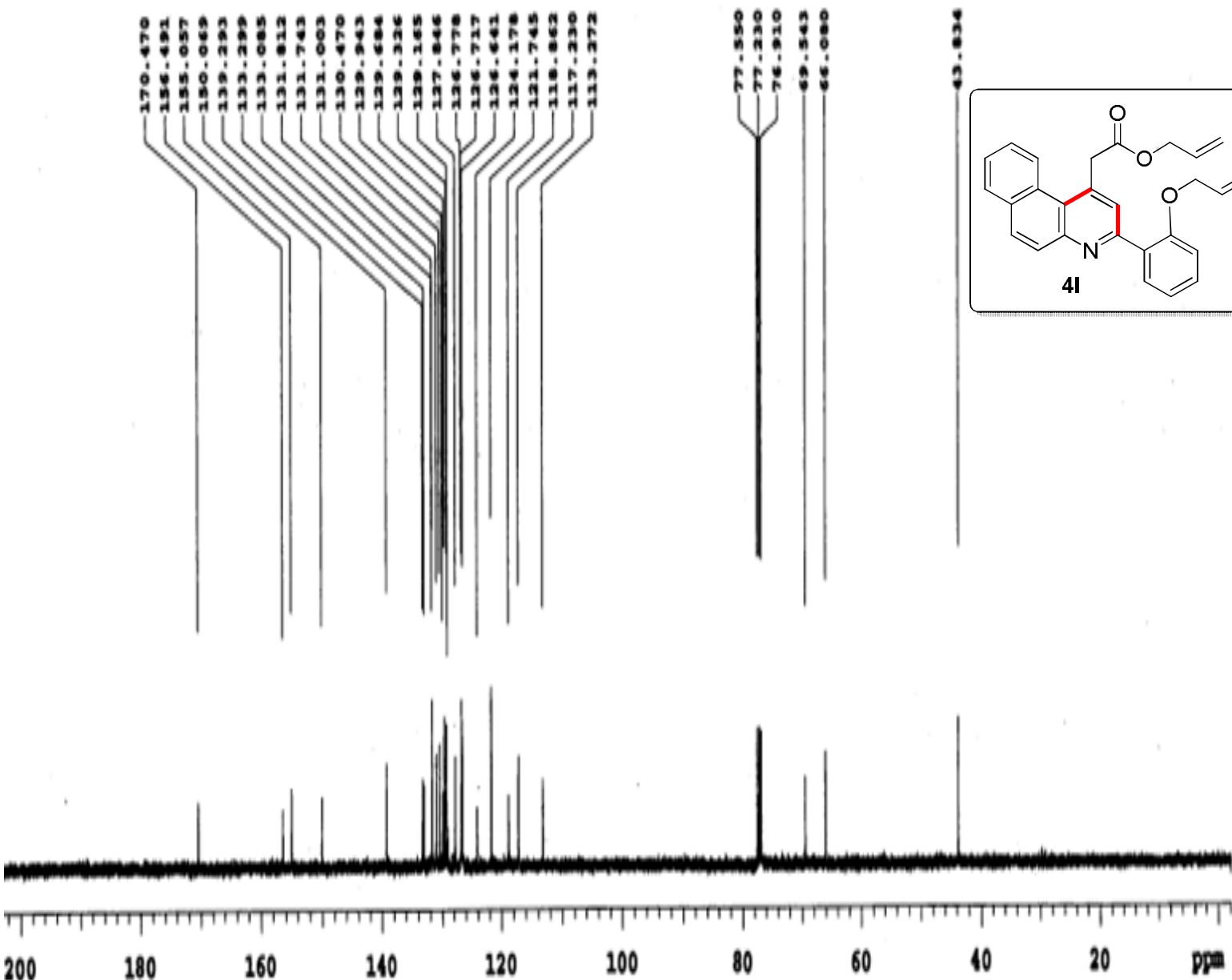
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



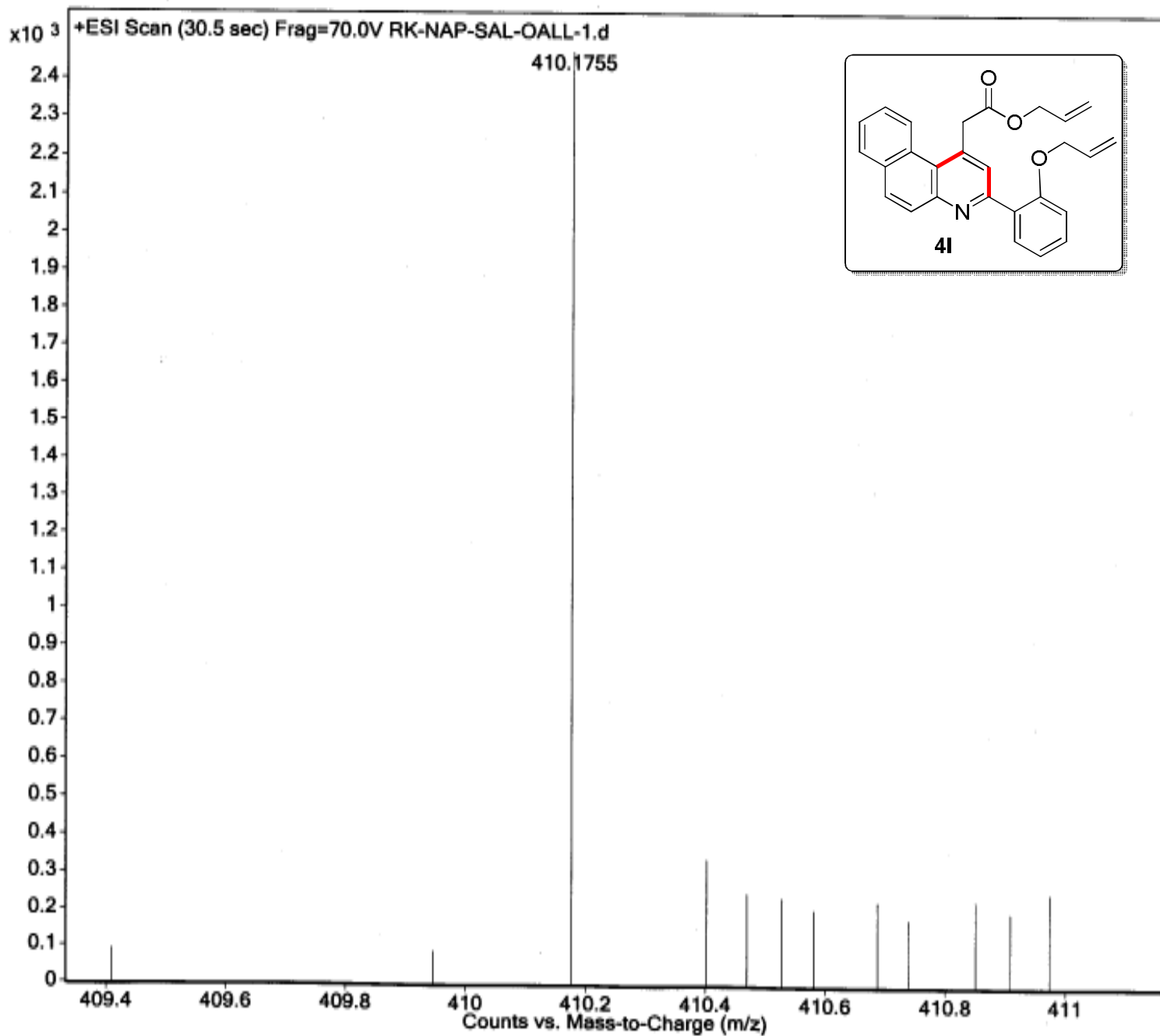
*<sup>13</sup>C NMR spectra of compound 4I*



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 130 repetitions	<b>OBSERVE</b> C13, 100.5425932 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 5 minutes	EK-MAP-SAL-CALL-3-13C
			Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 *IITG-NMR*

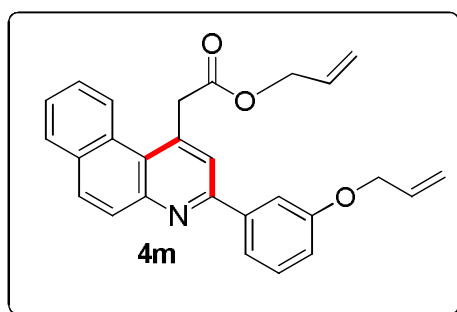
### HRMS spectra of compound 4l

Sample Name	RK-NAP-SAL-OALL-1	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-NAP-SAL-OALL-1.d	ACQ Method		Comment		Acquired Time	12/31/2014 3:25:38 PM



*<sup>1</sup>H NMR spectra of compound 4m*

RK-30H-N2

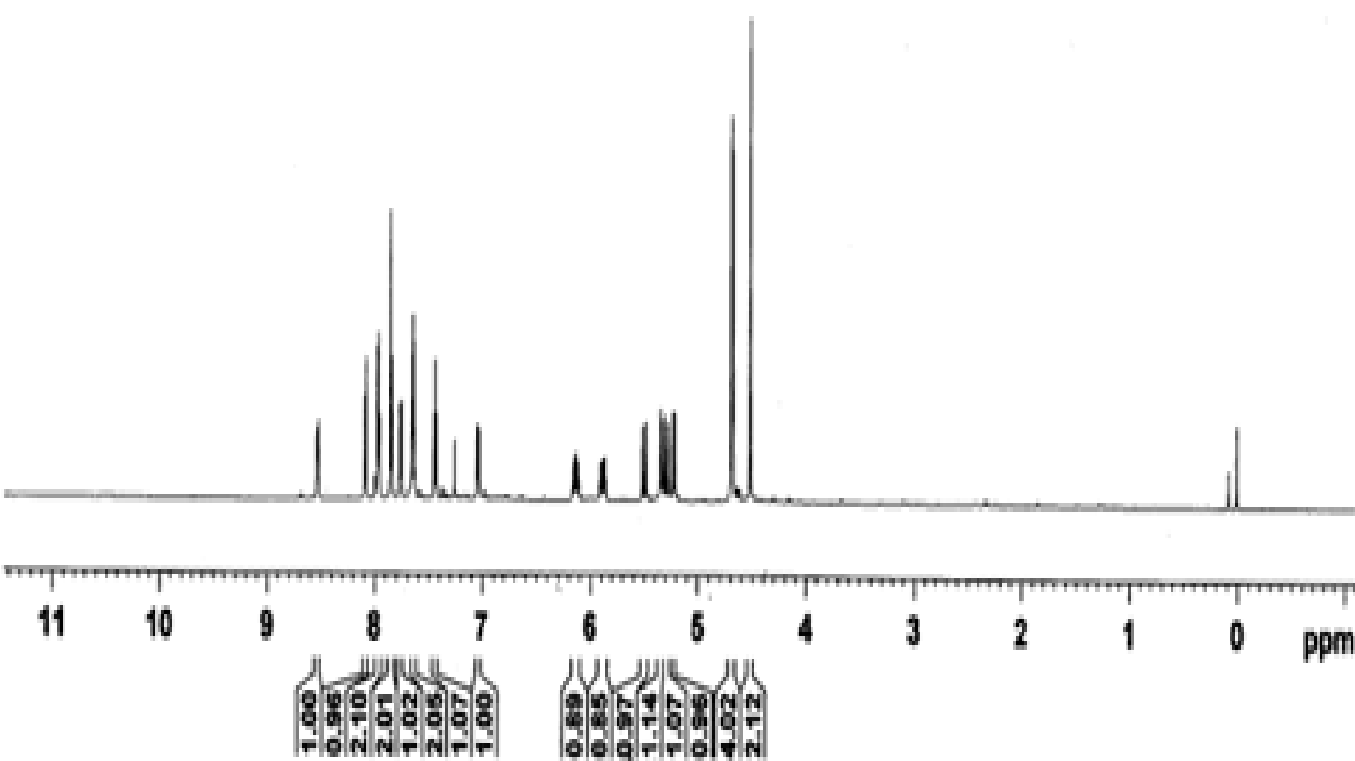


Current Data Parameters  
Date: 08-08-02  
Time: 1  
Pulse: 1

F1 - Acquisition Parameters  
Date\_: 08/08/02  
Time: 11.58  
Instrum: spect  
PROBHD: 5 mm HBBB QNP  
PULPROG: zgpg30  
TD: 65536  
SOLVENT: CDCl3  
NS: 18  
DS: 2  
SWH: 12000.200 Hz  
FIDRES: 0.340700 Hz  
AQ: 1.1411400 sec  
RG: 48.00  
SN: 61.400 sec  
IN: 4.00 sec  
TE: 297.2 K  
D1: 1.0000000 sec  
TAD: 1

===== CHANNEL F1 =====  
NUC1: 13C-125MHz  
PULP1: 18  
PC1: 15.00 sec  
PL1: 0.0000000 Hz

F1 - Processing parameters  
SI: 32768  
SF: 600.1370000 MHz  
WDW: EM  
SSB: 0  
LB: 0.20 Hz  
GB: 0  
PC: 1.00



<sup>13</sup>C NMR spectra of compound 4m

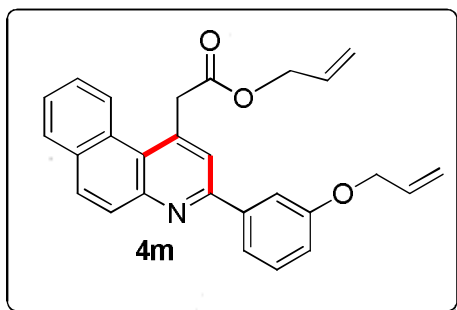
RK-30H-N2\_13C



170.42  
159.38  
155.56  
150.21  
140.85  
140.50  
133.51  
132.21  
131.81  
131.51  
130.03  
129.92  
129.74  
129.43  
129.95  
126.88  
126.84  
124.58  
123.29  
120.22  
119.12  
117.97  
116.25  
113.77

77.44  
77.22  
77.02  
68.17  
66.25

43.64



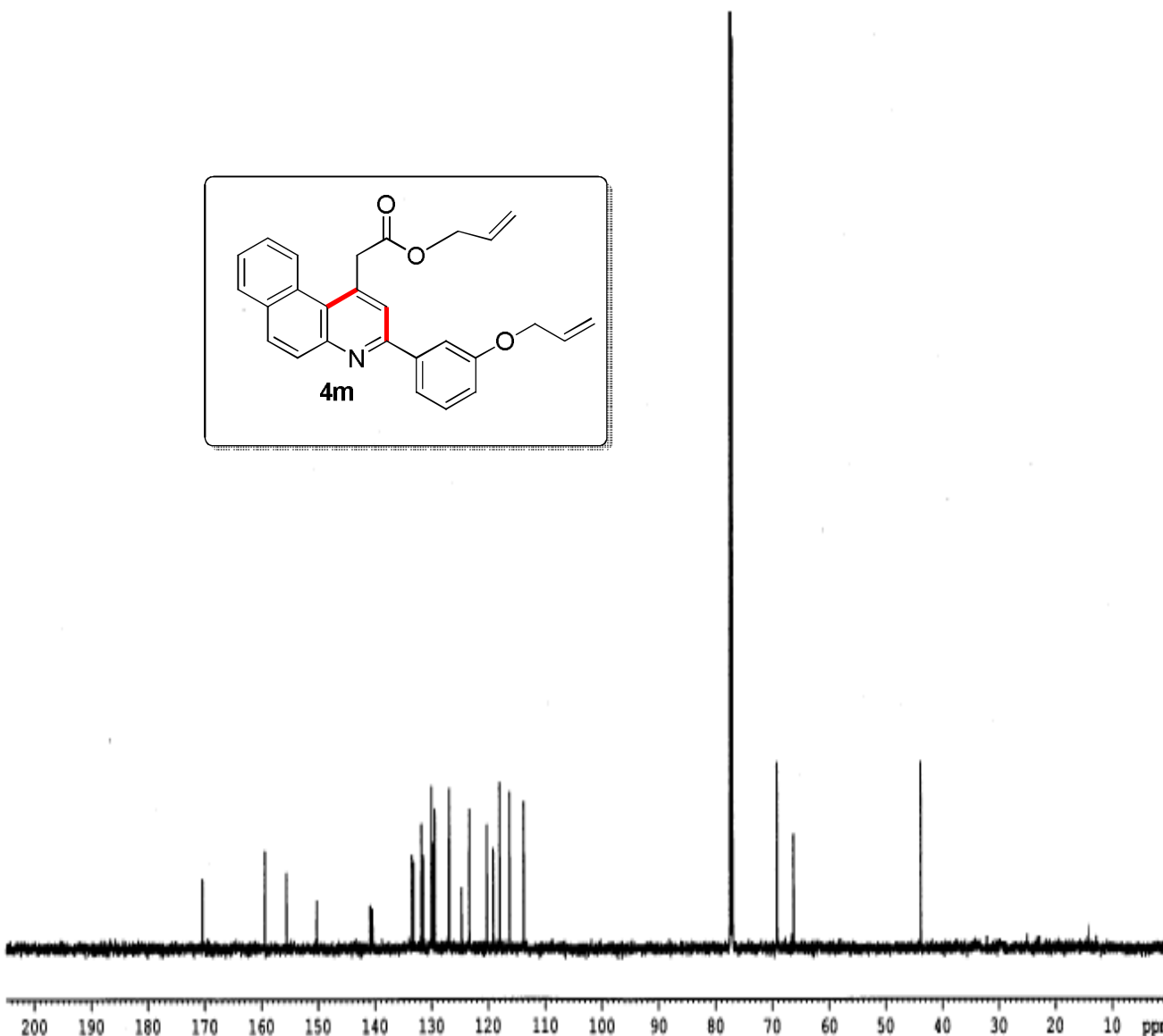
Current Data Parameters  
NAME RK-30H-N2\_13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150226  
Time 16.30  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 182  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DM 13.867 usec  
DE 6.50 usec  
TE 298.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

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

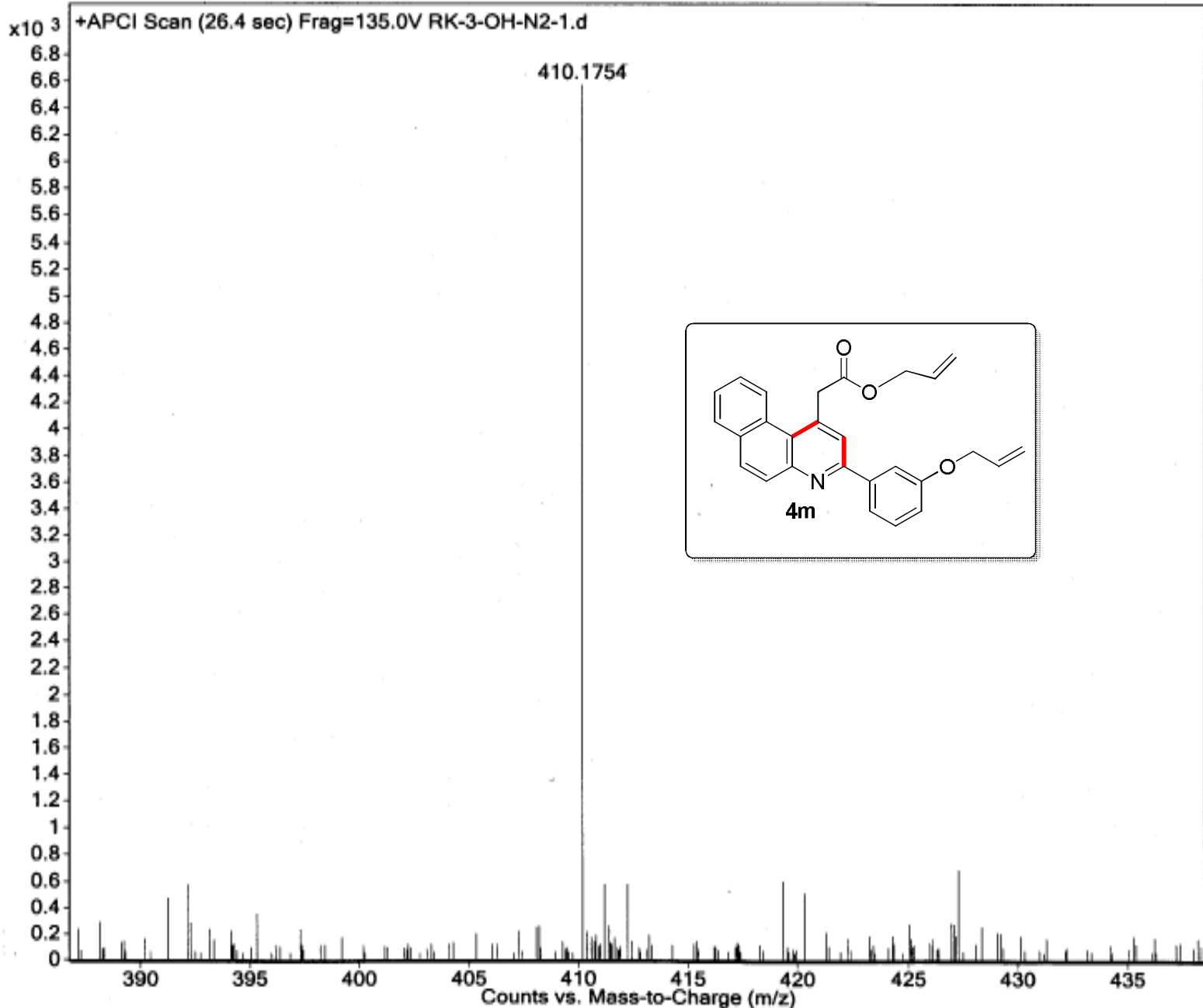
F2 - Processing parameters  
SI 16384  
SF 150.9128380 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





HRMS spectra of compound 4m

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



# *<sup>1</sup>H NMR spectra of compound 4n*

RK-ME-OBT-1H

Sample Name:

RK-ME-OBT-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/home/chem/data/study

Sample directory:

LR-Karanjin\_COBY-2-01

Fidfile: RK-ME-OBT-1H

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 16 2014

Temp. 25.0 C / 298.1 K

Operator: chem

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

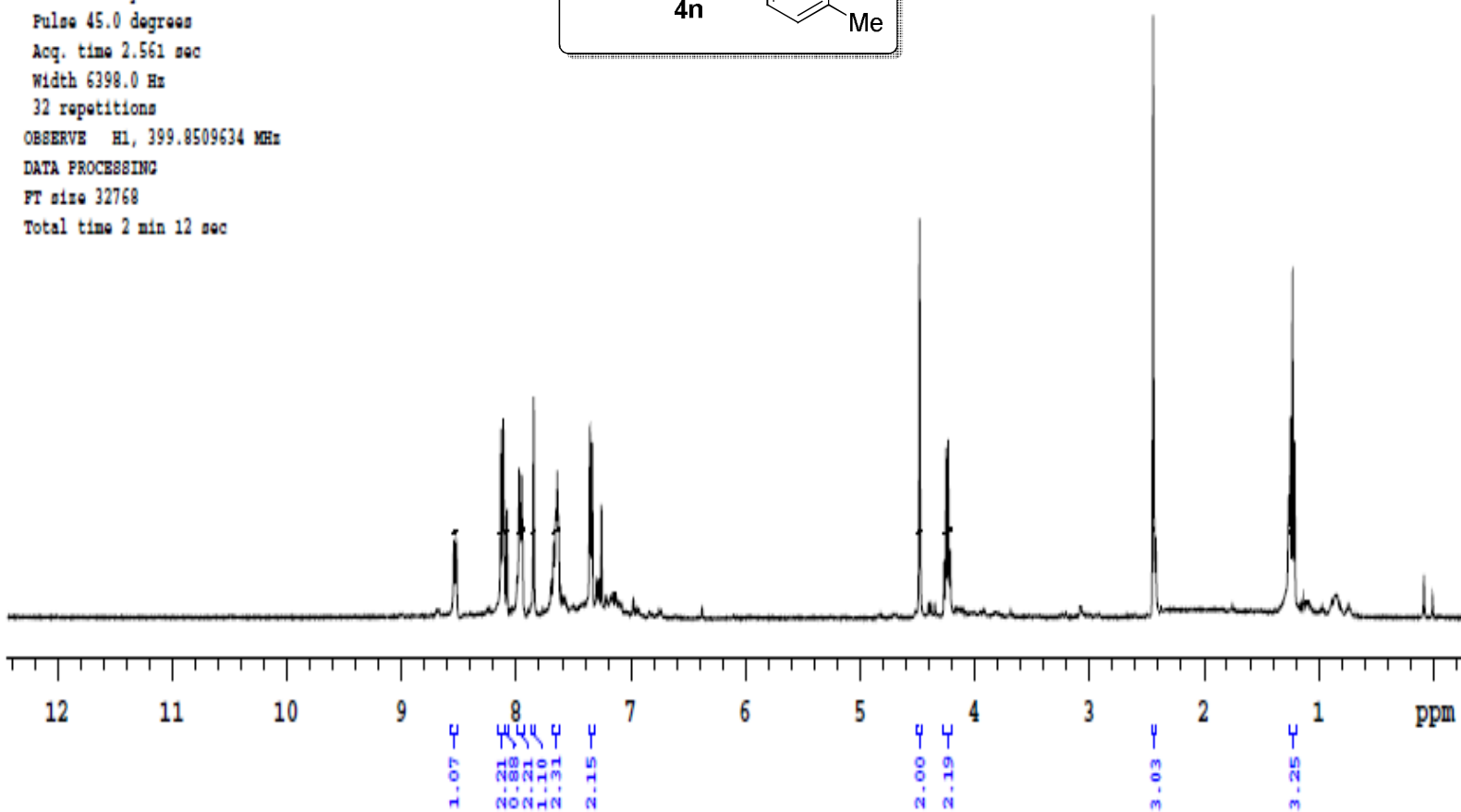
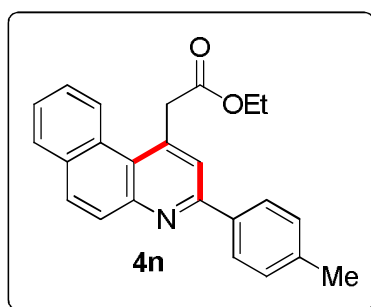
32 repetitions

OBSERVE H1, 399.8509634 MHz

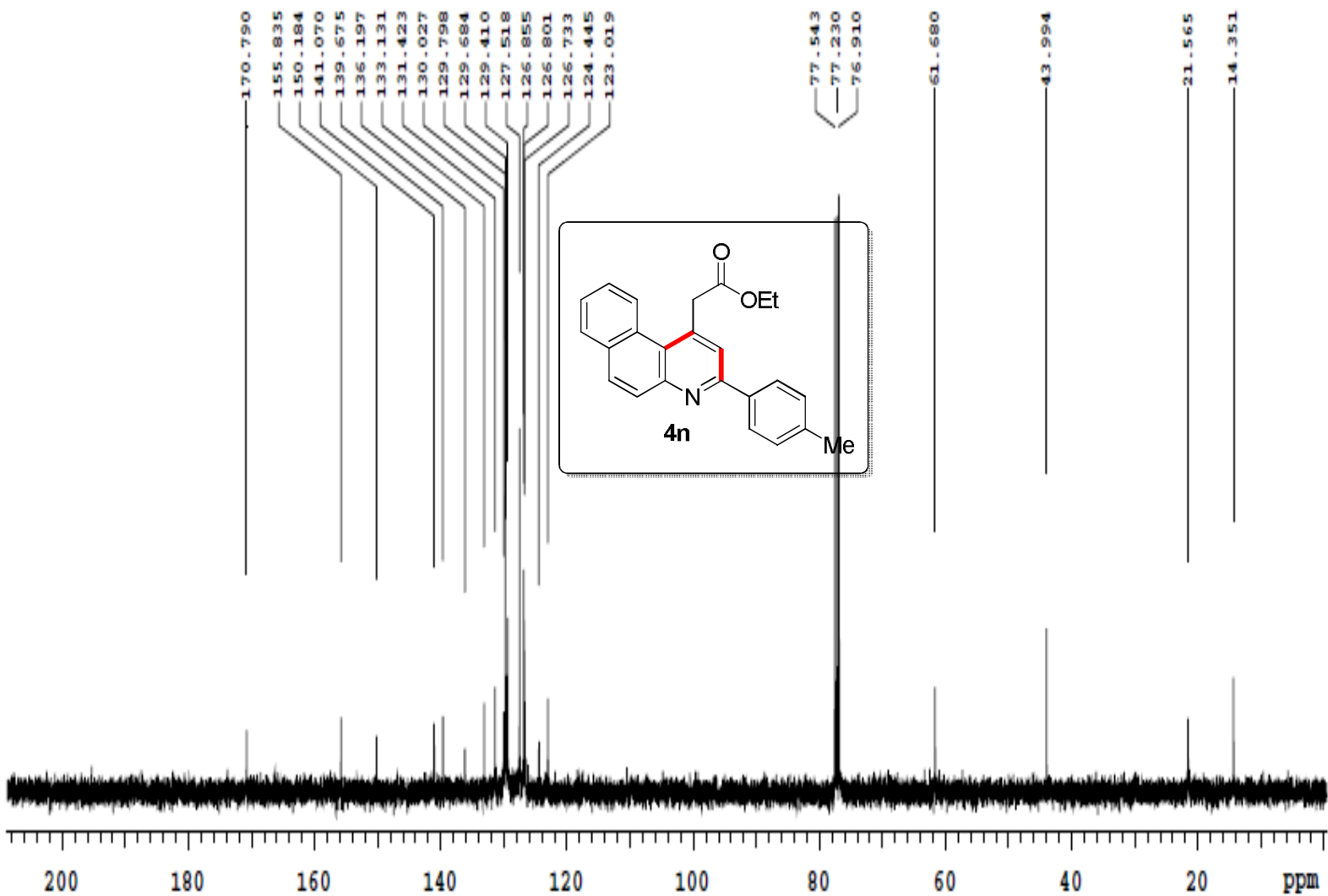
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



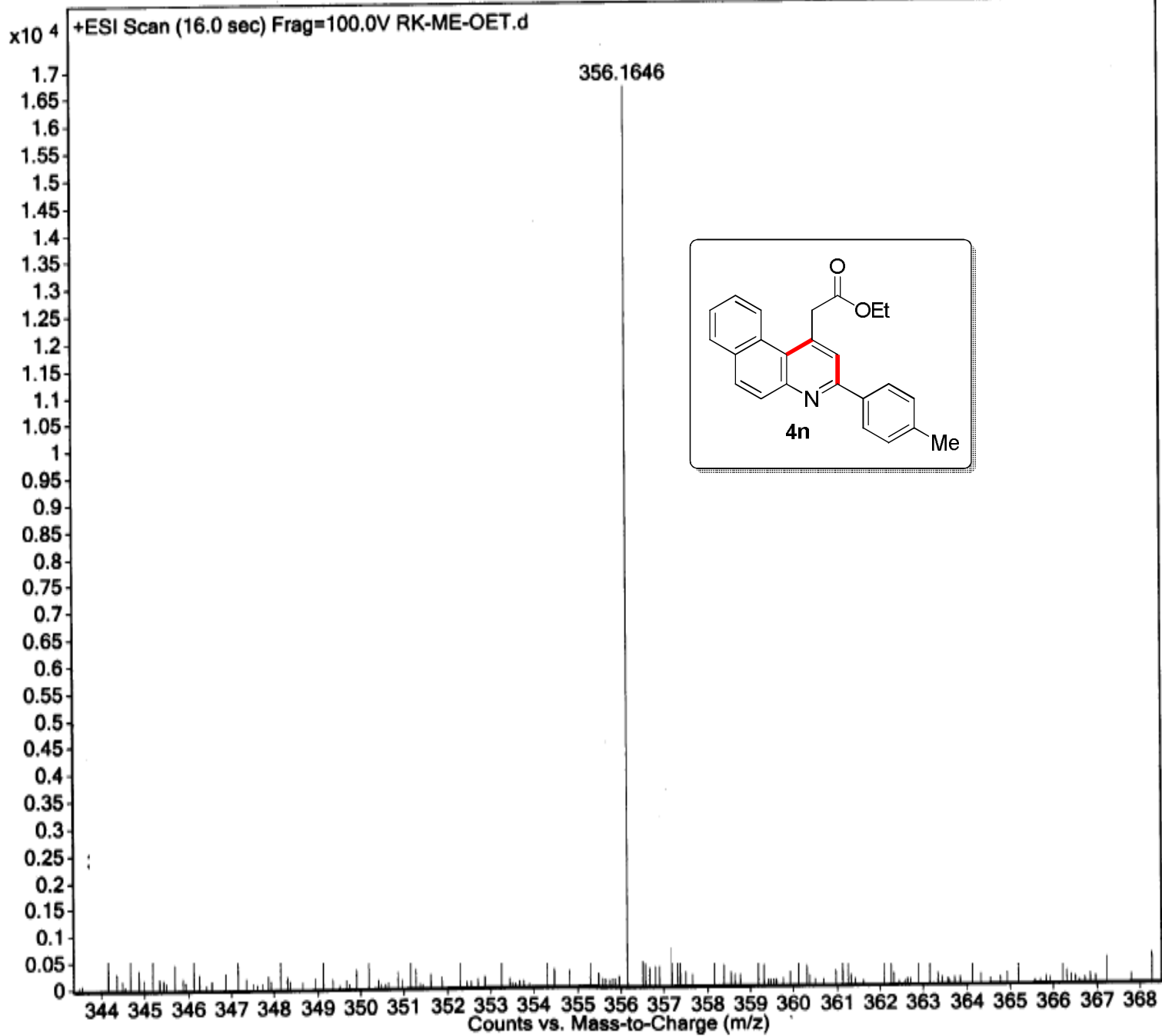
*<sup>13</sup>C NMR spectra of compound 4n*



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 780 repetitions	<b>OBSERVE</b> C13, 100.5425832 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 29 minutes	<b>RK-ME-OBT-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: RK-ME-OBT-13C Mercury-400 *IITG-NMR*
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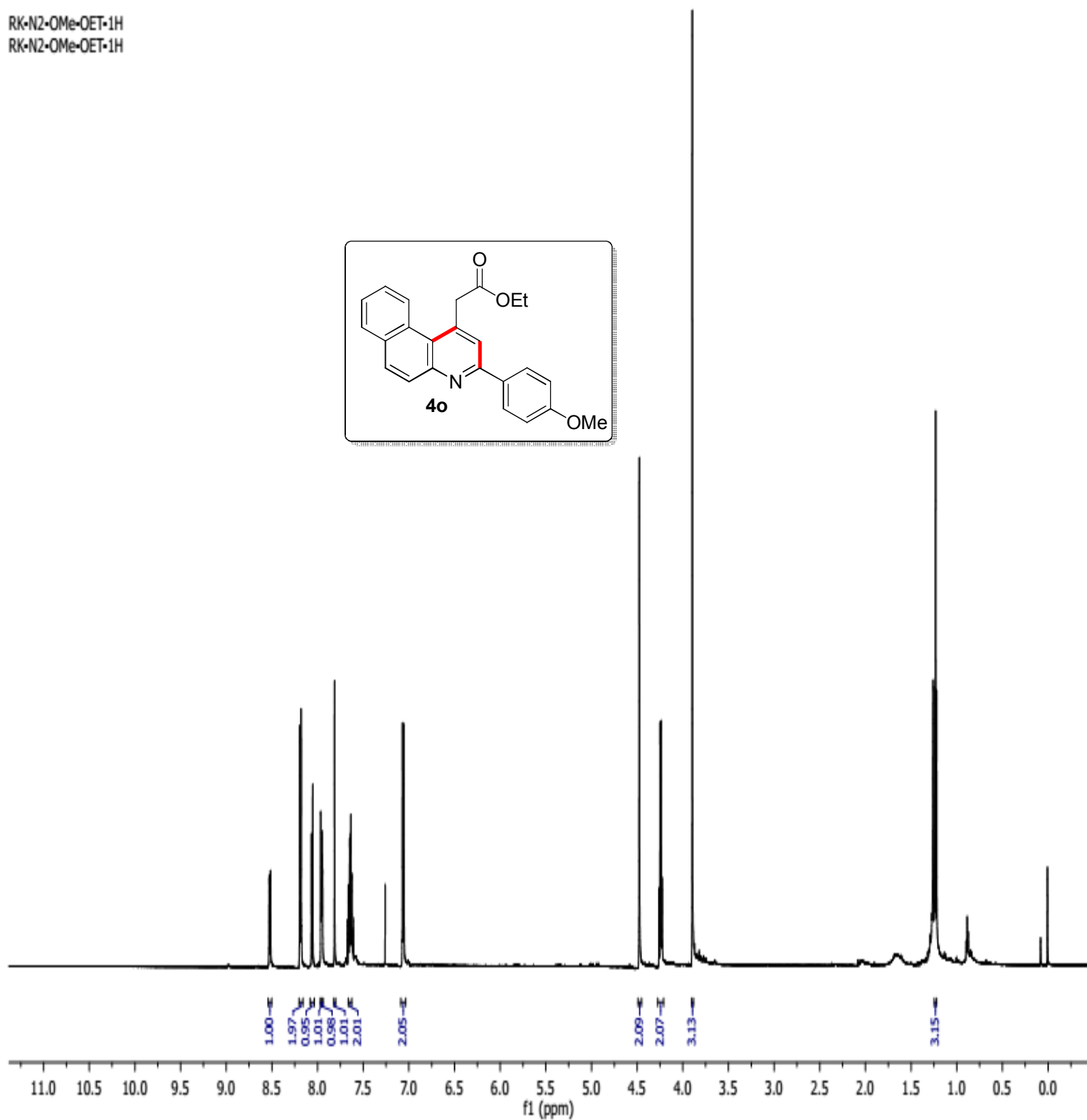
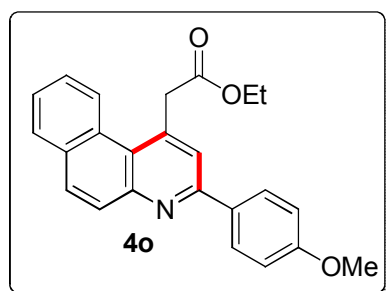
HRMS spectra of compound 4n

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



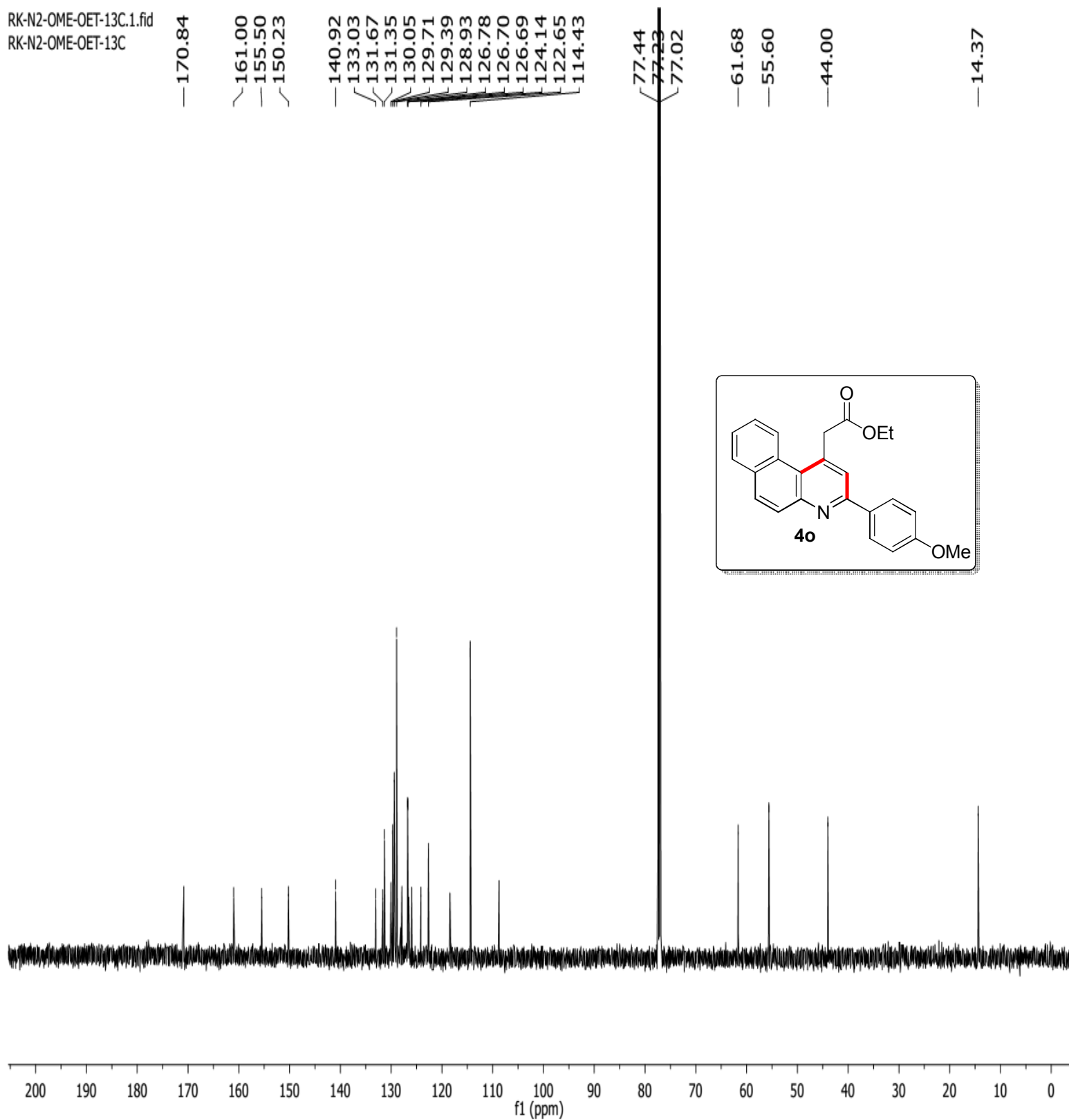
*<sup>1</sup>H NMR spectra of compound 4o*

RK-N2-OMe-OEt-1H  
RK-N2-OMe-OEt-1H



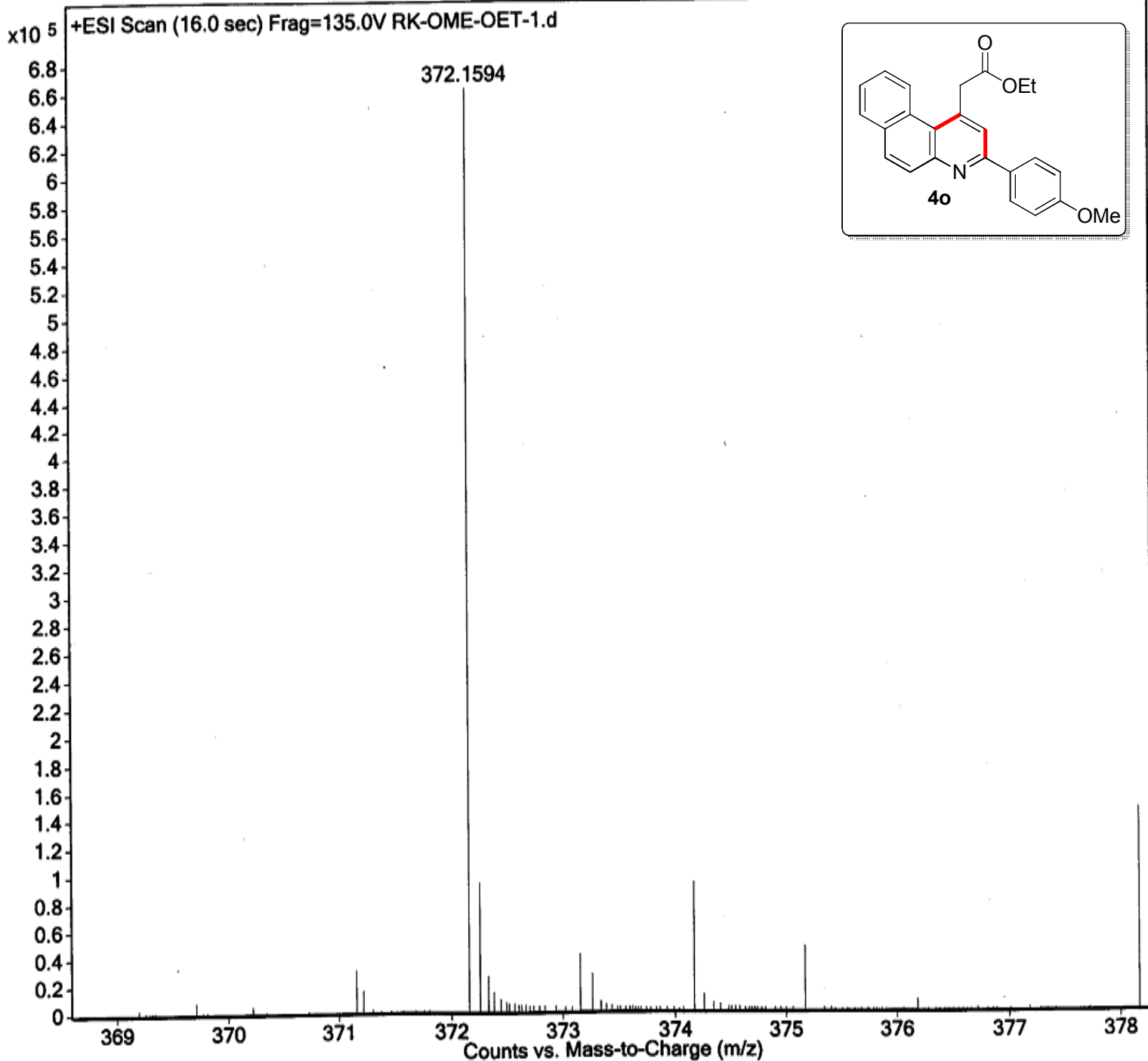
*<sup>13</sup>C NMR spectra of compound 4o*

RK-N2-OME-OET-13C.1.fid  
RK-N2-OME-OET-13C



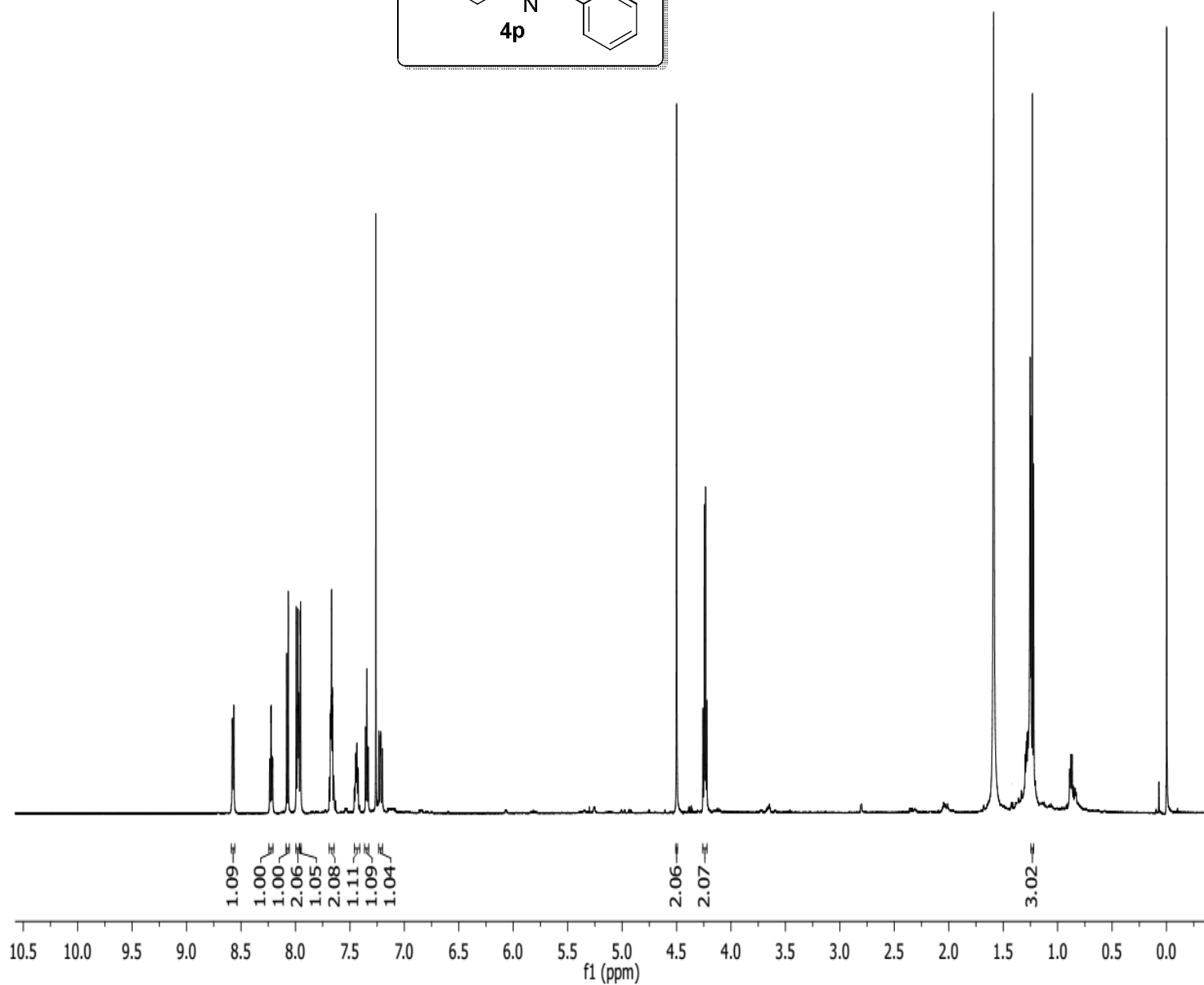
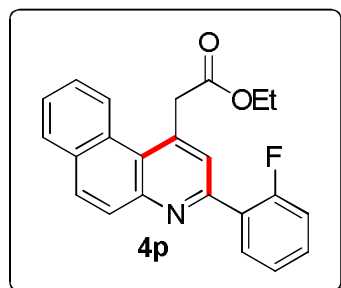
HRMS spectra of compound 4o

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Some Ions Missed
Data Filename	RK-OME-OET-1.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



*<sup>1</sup>H NMR spectra of compound 4p*

RK-N2-2F-OET-1H  
RK-N2-2F-OET-1H

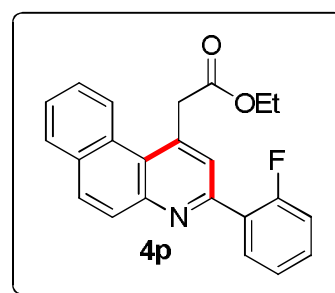




*<sup>13</sup>C NMR spectra of compound 4p*

RK-2F-OEt-13C.1.fid  
RK-2F-OEt-13C

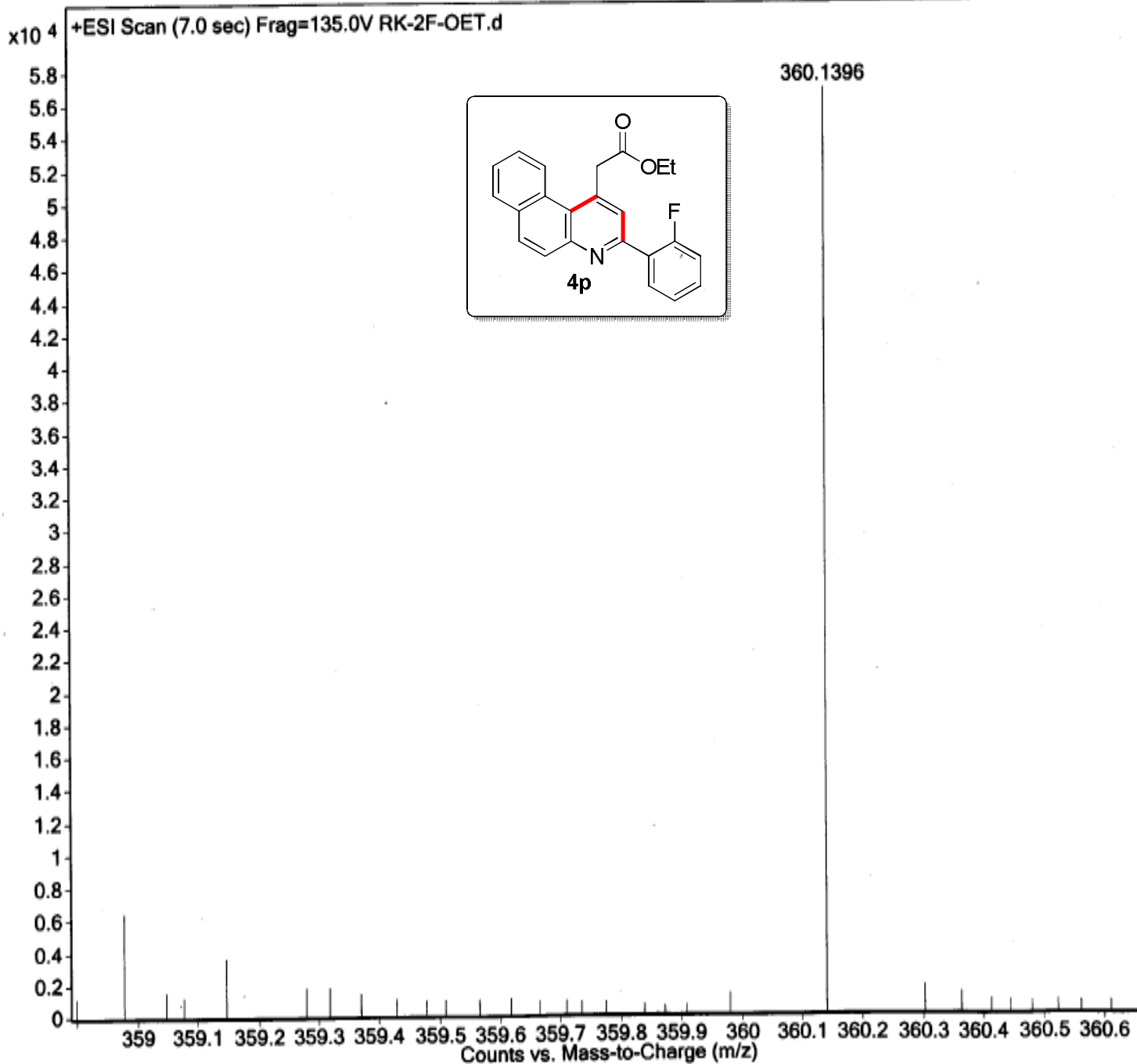
—170.73  
~161.89  
~160.23  
~152.22  
~150.24  
—140.73  
133.27  
131.64  
131.62  
131.51  
131.07  
131.02  
129.93  
129.61  
129.43  
127.09  
127.05  
126.85  
124.94  
124.91  
124.75  
116.56  
116.41  
77.44  
77.23  
77.02  
—61.73  
—44.00  
—14.33



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0  
f1 (ppm)

HRMS spectra of compound 4p

Sample Name	RK-2F-OET	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	RK-2F-OET.d	ACQ Method		Comment		Acquired Time	12/4/2015 5:18:19 PM



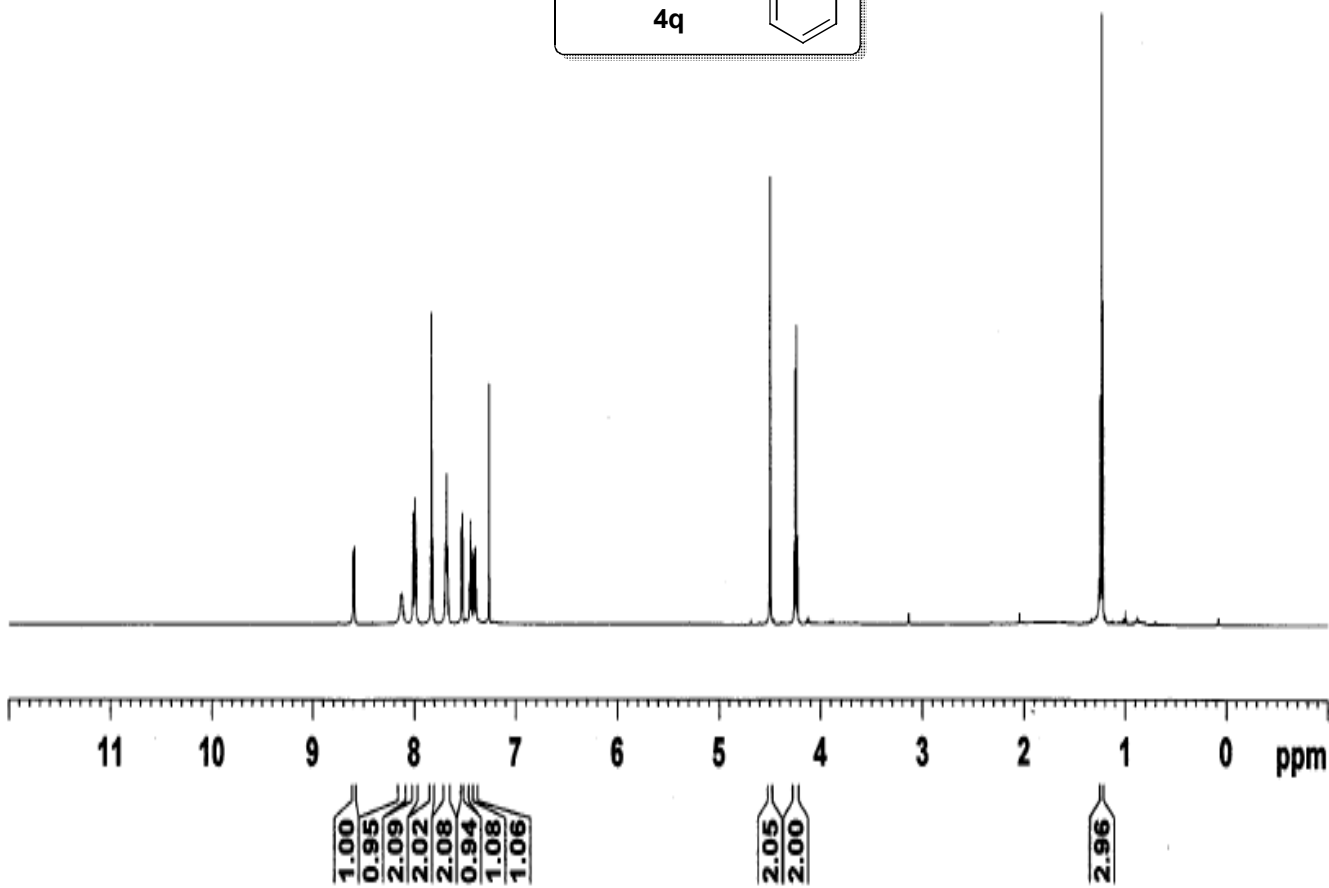
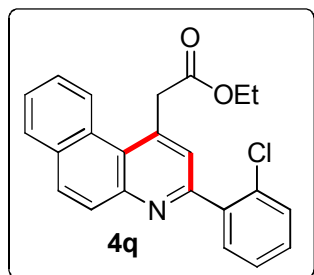
*<sup>1</sup>H NMR spectra of compound 4q*

Current Data Parameters  
NAME RK-2Cl-ORL-LHA  
EXFNO 1  
PROCNO 1

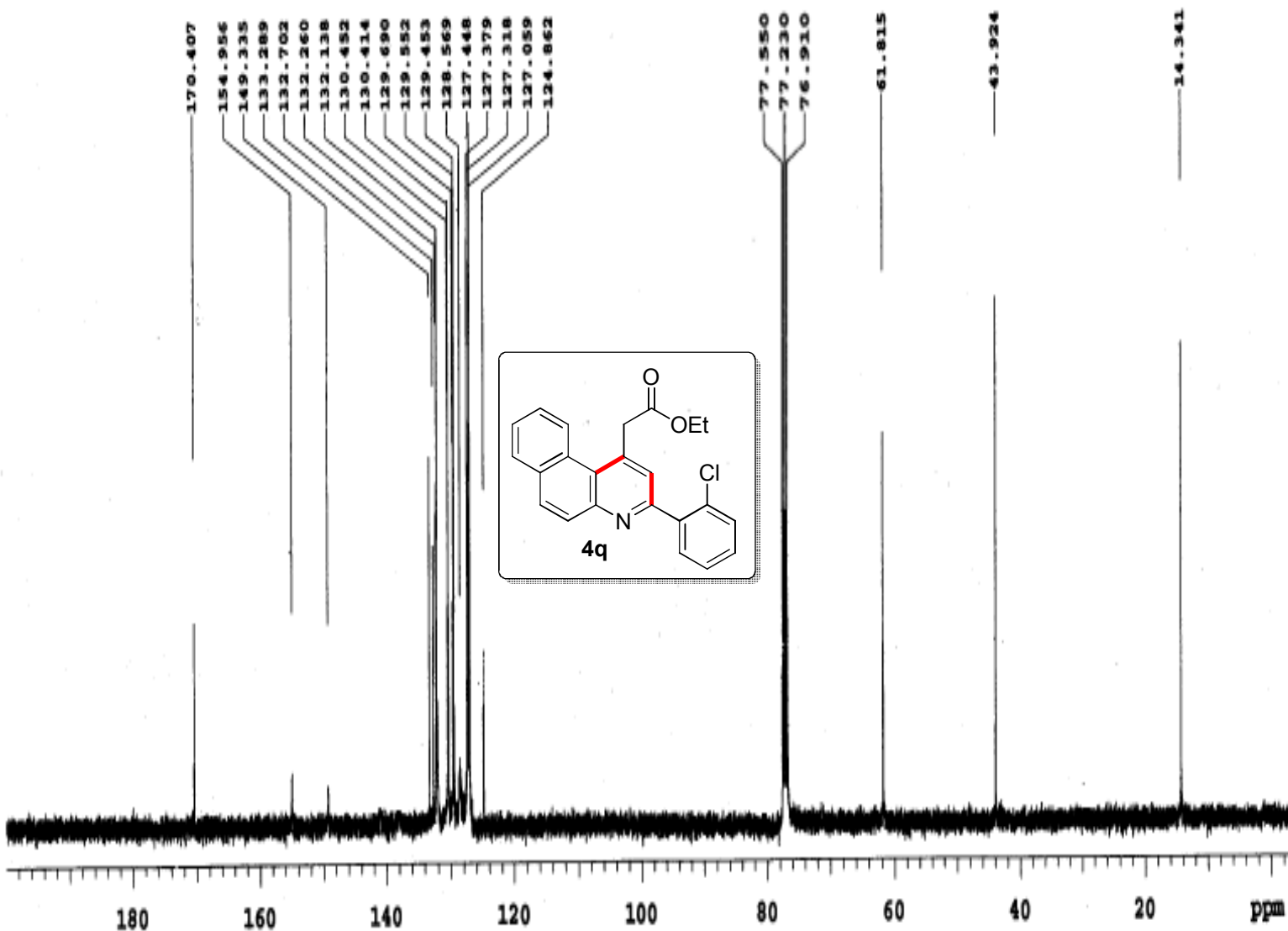
F2 - Acquisition Parameters  
Date\_ 20141209  
Time\_ 13.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 89.67  
DM 41.600 usec  
DE 6.50 usec  
TR 298.4 K  
D1 1.00000000 sec  
TDO 1

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

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



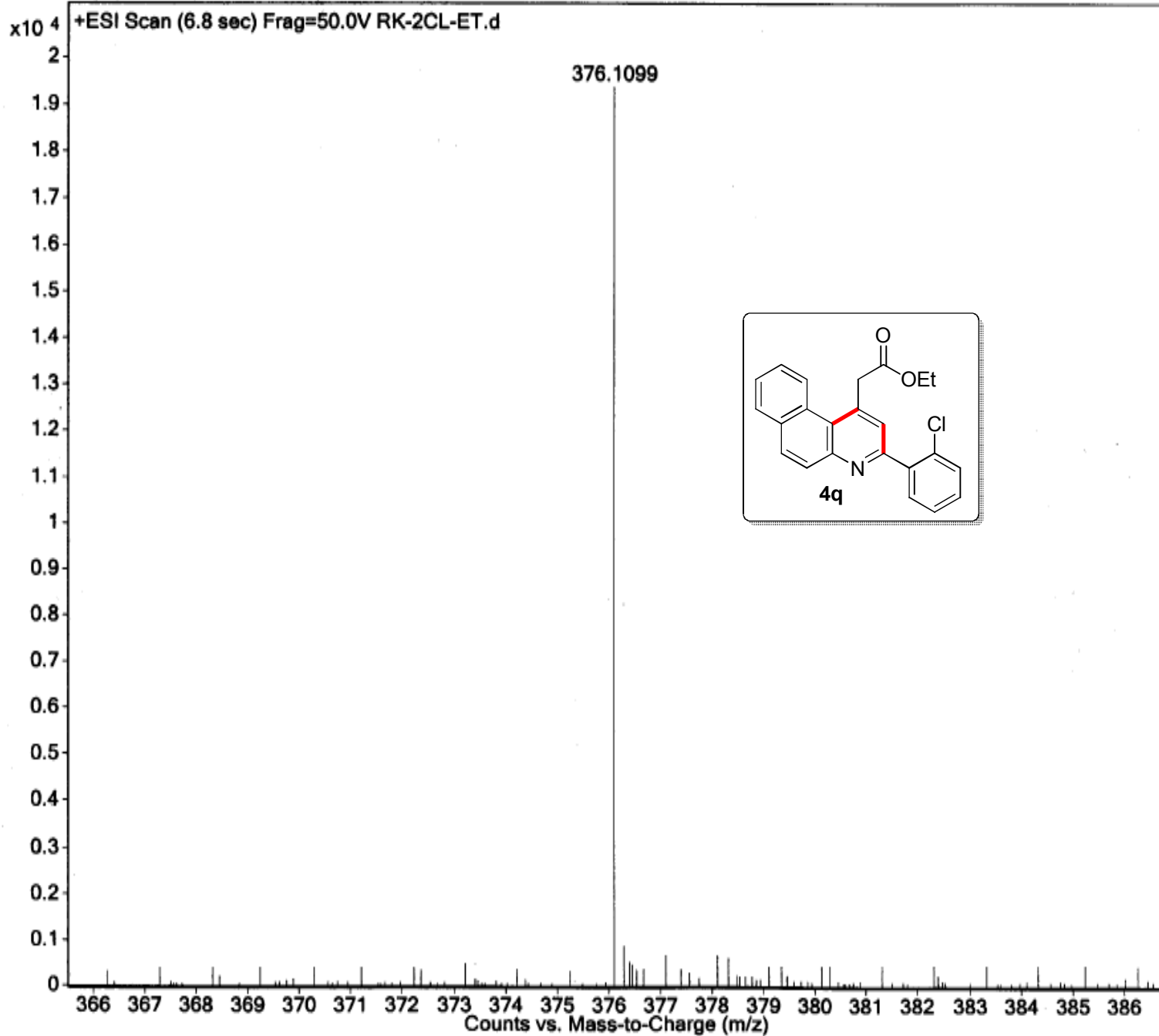
*<sup>13</sup>C NMR spectra of compound 4q*



<p><b>PULSE SEQUENCE</b>                  Relax. delay 1.000 sec                  Pulse 45.0 degrees                  Acq. time 1.304 sec                  Width 25125.6 Hz                  12710 repetitions</p>	<p><b>OBSERVE</b> C13, 100.5425849  <b>DECOUPLE</b> H1, 399.8529994                  Power 42 dB                  continuously on                  WALTZ-16 modulated</p>	<p><b>DATA PROCESSING</b>                  Line broadening 0.5 Hz                  FT size 65536                  Total time 8.1 hours</p>	<p><b>EX-2CL-ET-13C</b>                  Solvent: cdcl3                  Temp. 25.0 C / 298.1 K                  Operator: chem                  File: EX-2CL-ET-13C                  Mercury-400 "IITG-MMR"</p>
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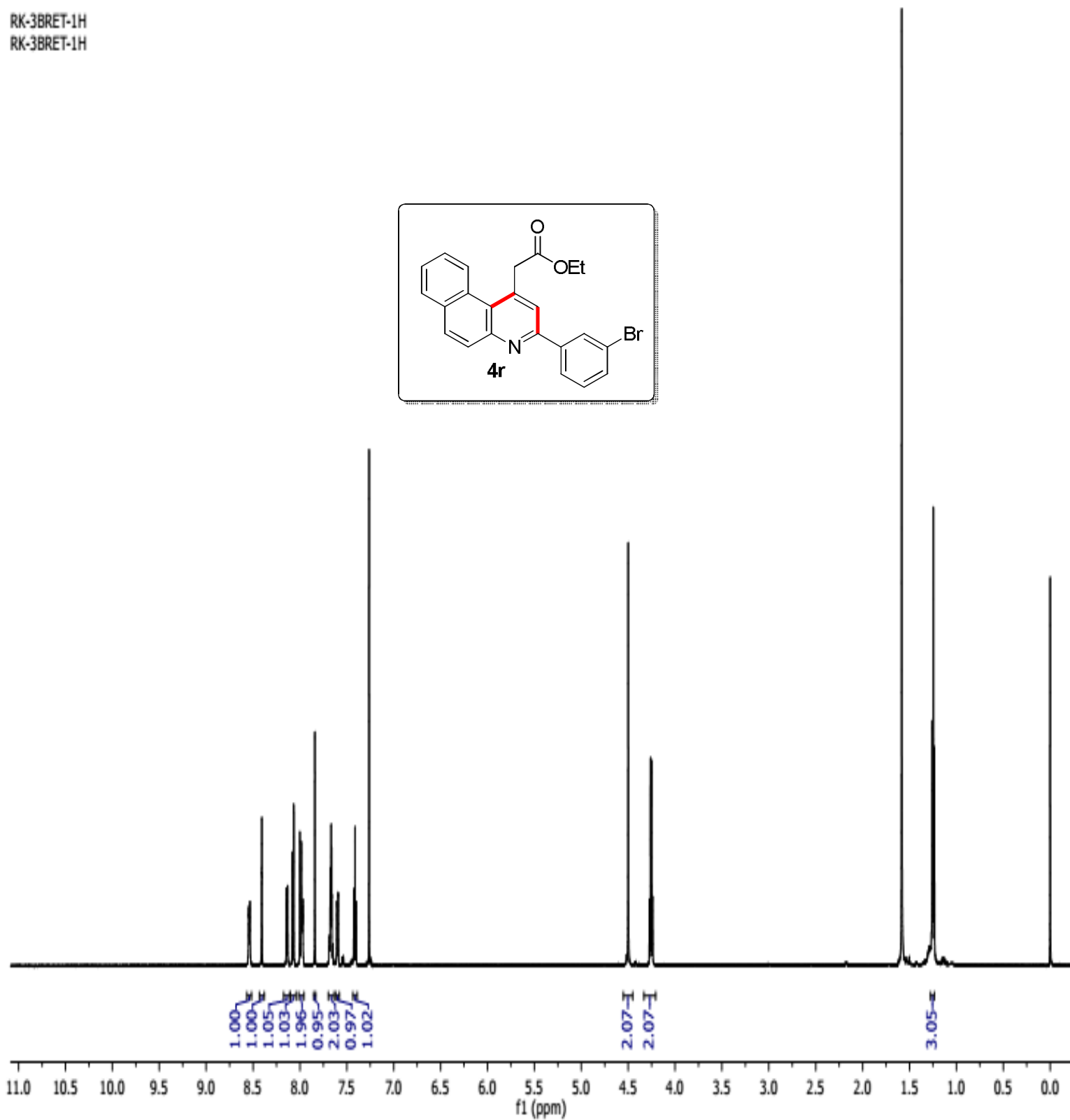
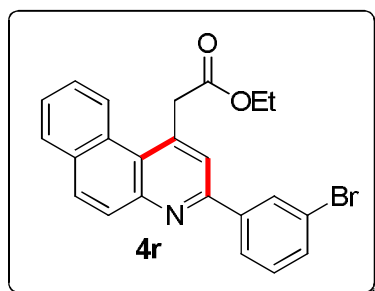
HRMS spectra of compound 4q

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

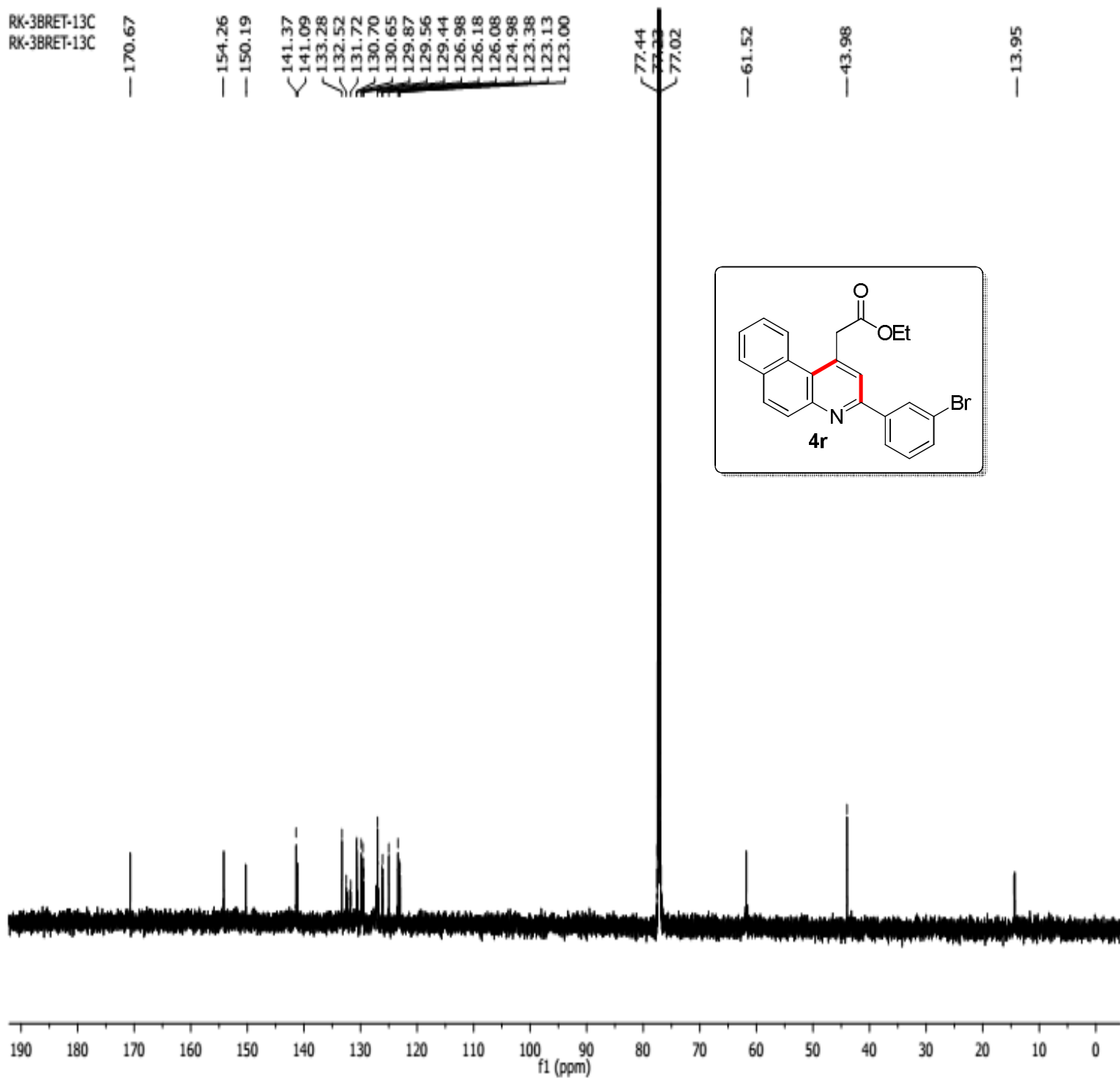


*<sup>1</sup>H NMR spectra of compound 4r*

RK-3BRET-1H  
RK-3BRET-1H

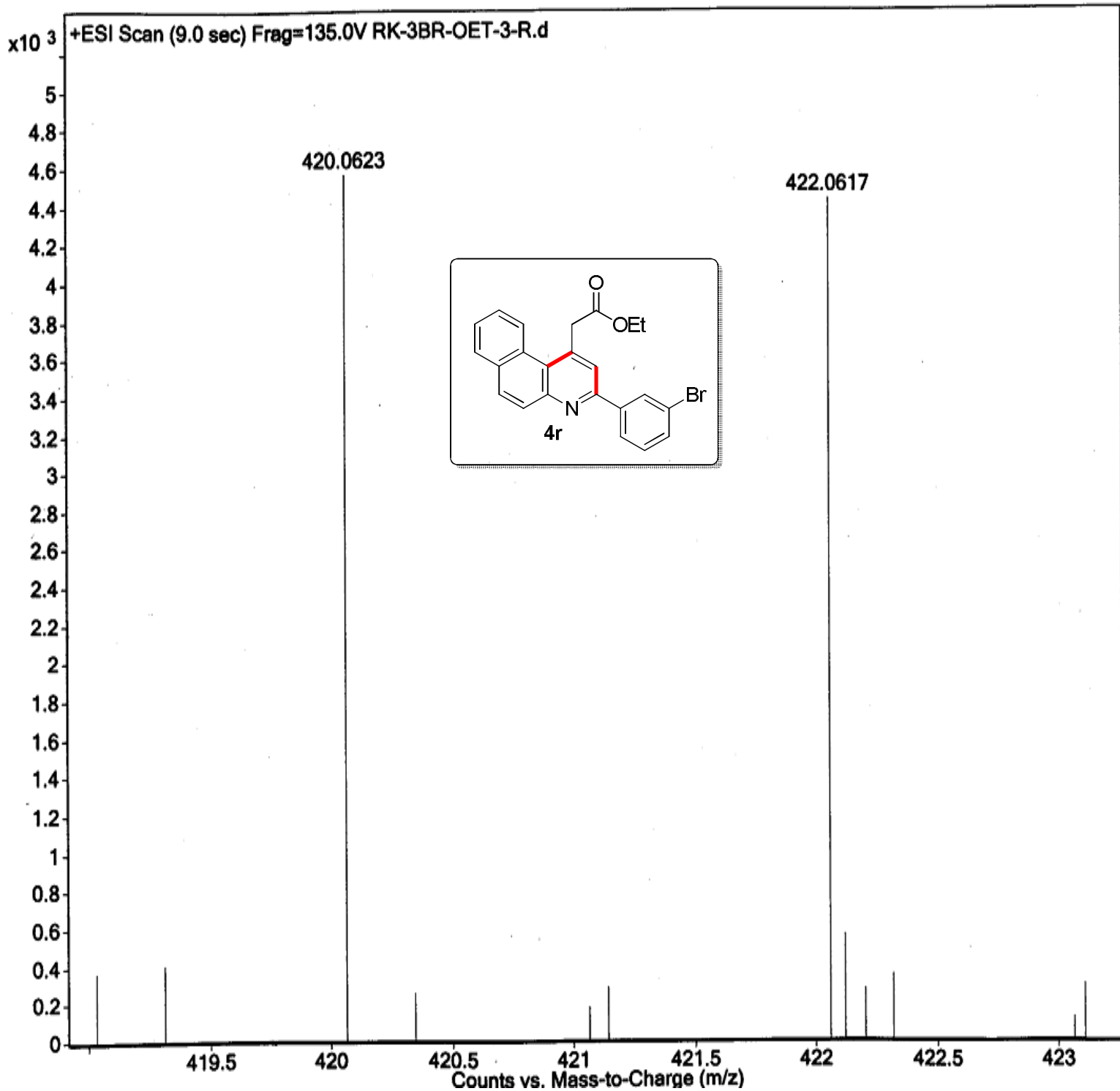


*<sup>13</sup>C NMR spectra of compound 4r*



HRMS spectra of compound 4r

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	RK-3BR-OET-3-R.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable





# <sup>1</sup>H NMR spectra of compound 4s

RK-ME -OALL-1B-1H

Sample Name:

RK-ME -OALL-1B-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: RK-ME -OALL-1B-1H

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 14 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

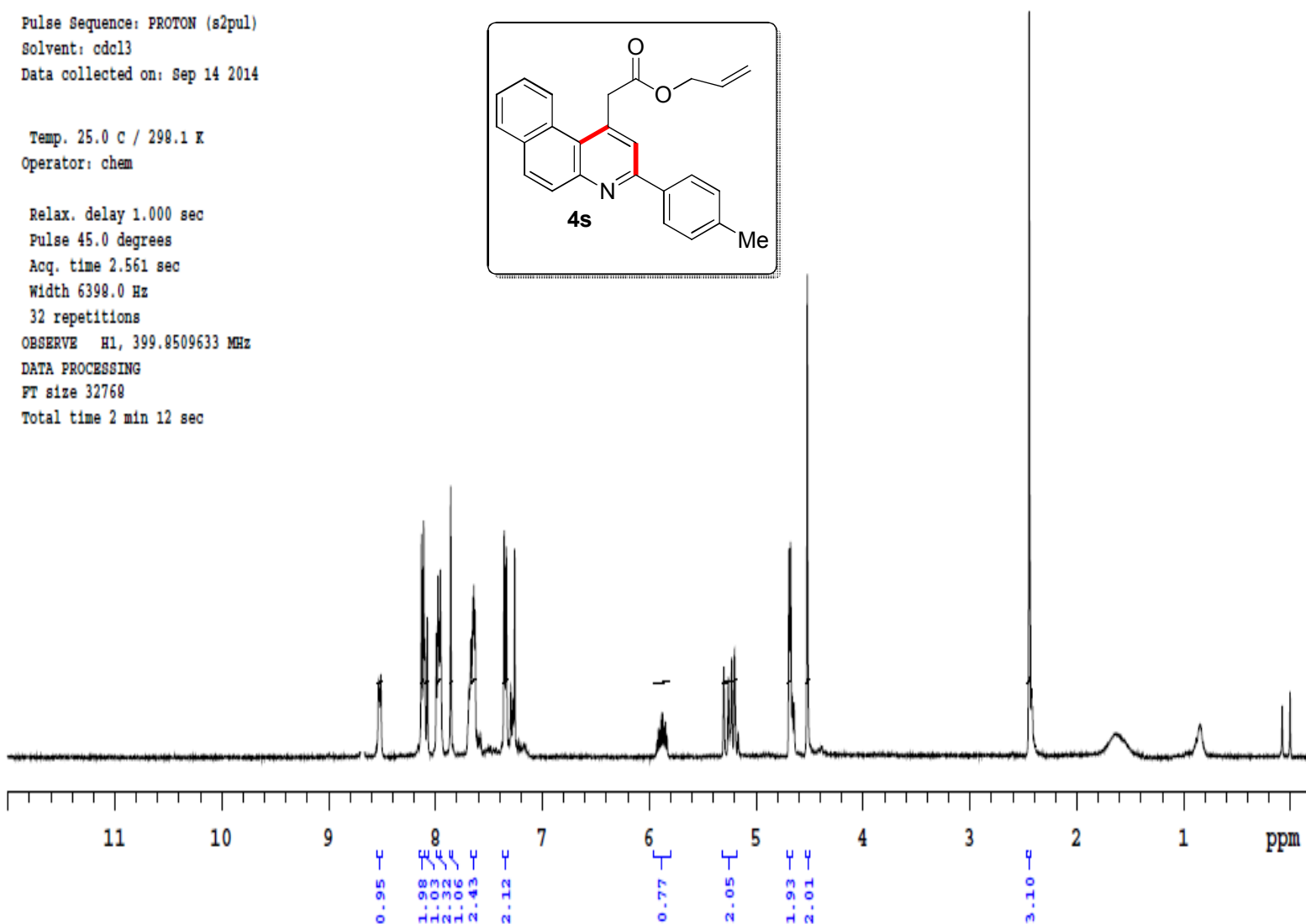
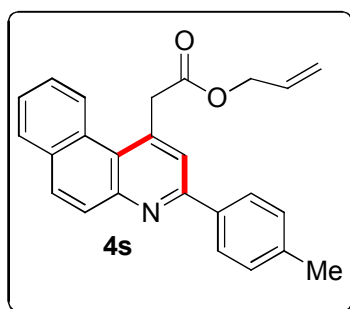
32 repetitions

OBSERVE H1, 399.8509633 MHz

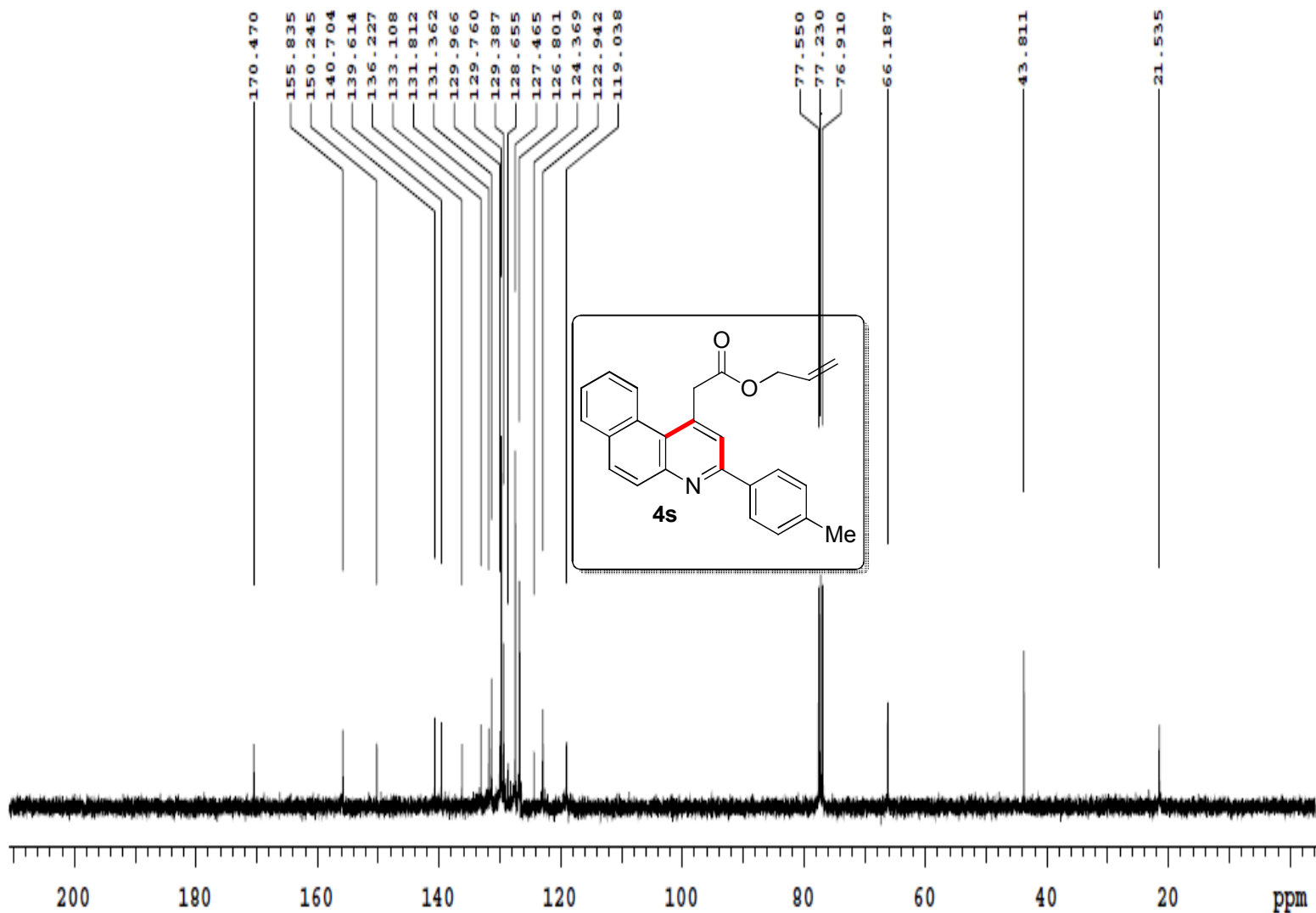
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



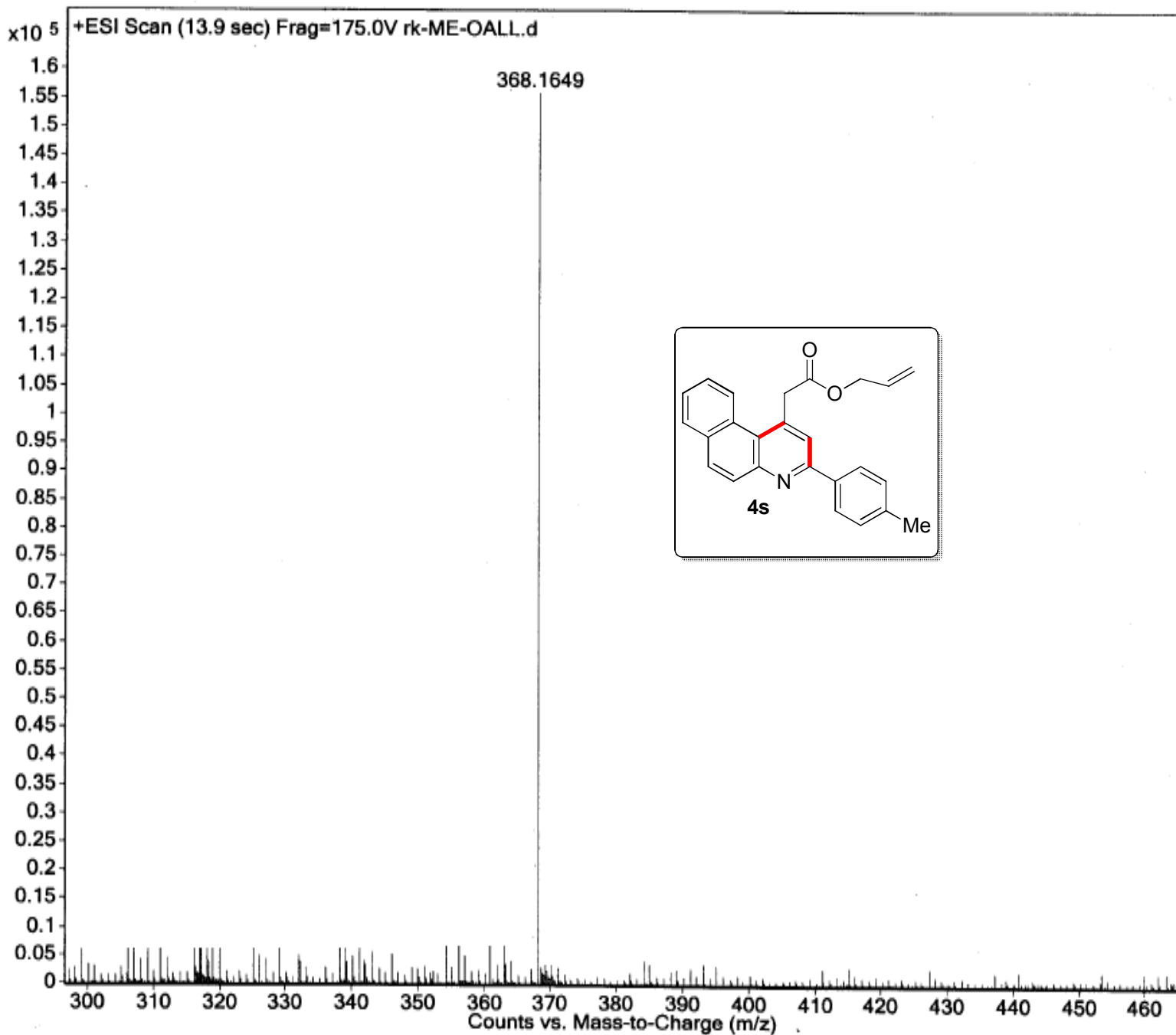
*<sup>13</sup>C NMR spectra of compound 4s*



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 490 repetitions	<b>OBSERVE</b> c13, 100.5425970 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 18 minutes	RK-ME_-OALL-1B-13c  Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem File: RK-ME_-OALL-1B-13c Mercury-400 "IITG-NMR"
---	--	--	--

HRMS spectra of compound 4s

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



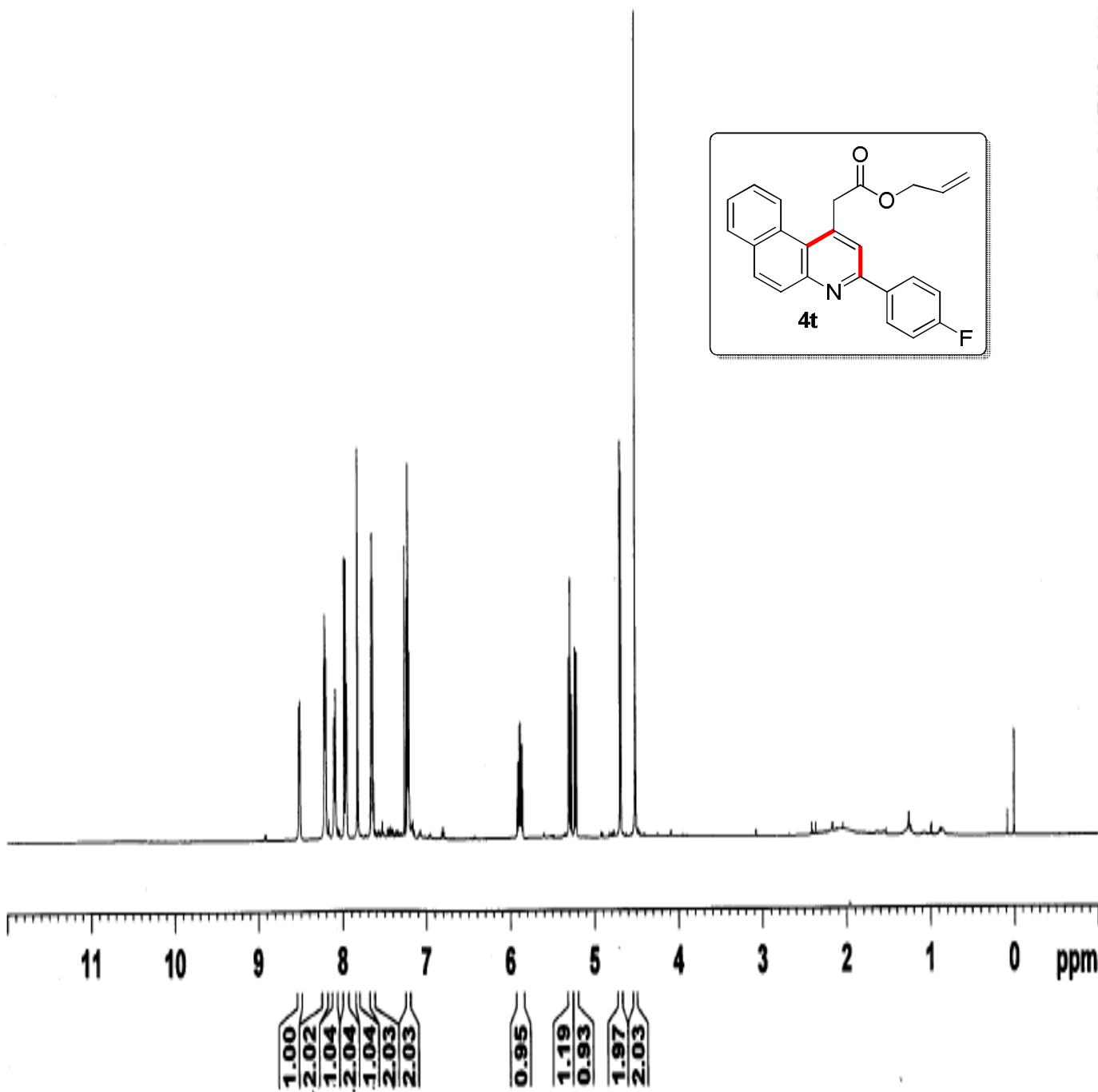
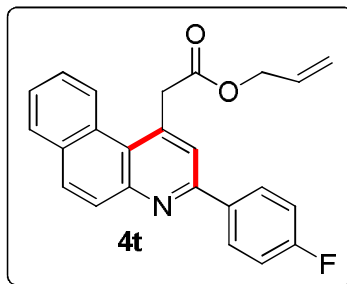
*<sup>1</sup>H NMR spectra of compound 4t*

Current Data Parameters  
NAME NR-4F-QALL-1H  
EXPRO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20140929  
Time 16.53  
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  
DM 41.600 usec  
DE 6.50 usec  
TE 297.8 K  
D1 1.00000000 sec  
TDO 1

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

F2 - Processing parameters  
SI 16384  
SF 600.1700150 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



<sup>13</sup>C NMR spectra of compound 4t

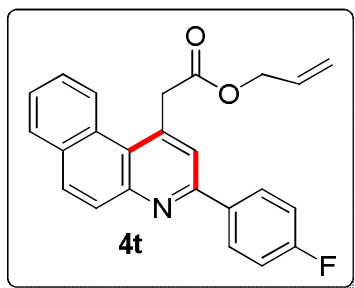


170.33  
164.91  
163.26  
154.61  
150.02  
141.26  
133.17  
131.81  
131.77  
129.81  
129.58  
129.53  
129.50  
129.32  
127.04  
126.95  
126.84  
124.52  
122.88  
119.17  
116.08  
115.94

77.44  
77.23  
77.01

66.29

43.81



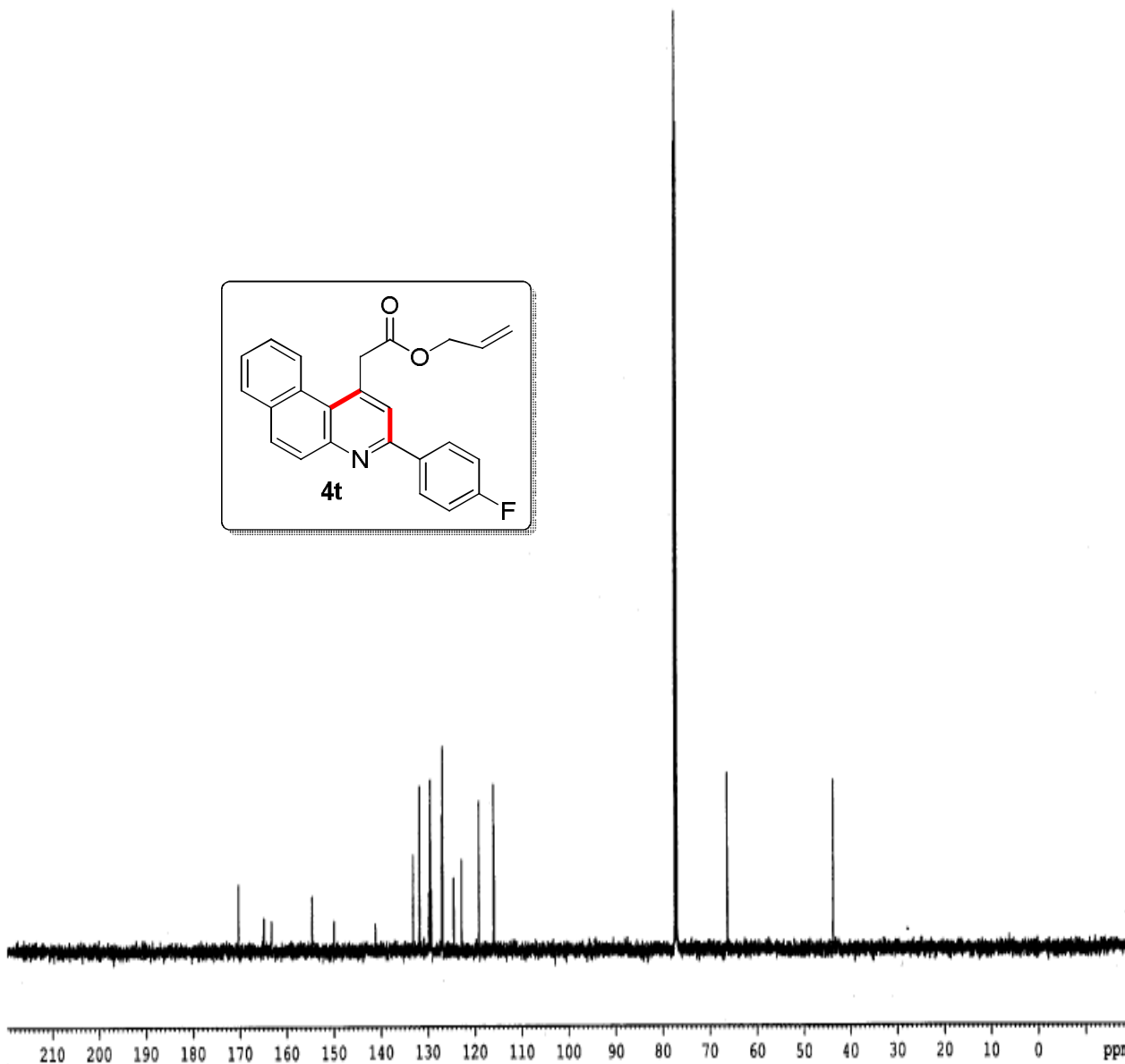
Current Data Parameters  
NAME RK-4F-QALL 13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20141001  
Time 11.19  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 108  
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 299.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

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

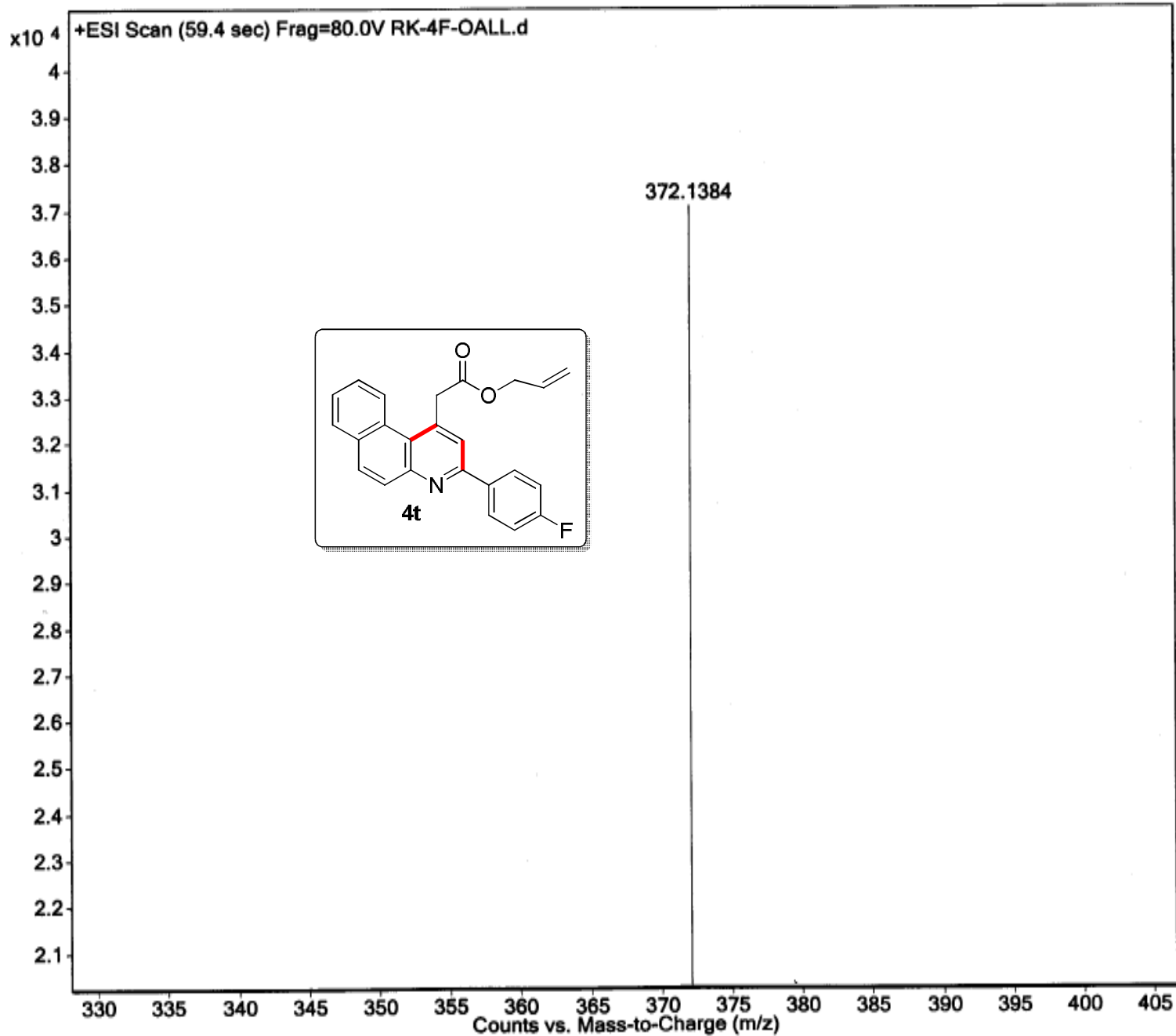
----- CHANNEL f2 -----  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG2 waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128392 MHz  
MDW EM  
SBB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



*HRMS spectra of compound 4t*

Sample Name	RK-4F-OALL	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-4F-OALL.d	ACQ Method		Comment		Acquired Time	12/4/2014 11:55:49 AM



# *<sup>1</sup>H NMR spectra of compound 4u*

RK-OMe-OALL-1H

Sample Name:

RK-OMe-OALL-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

/export/home/chempack/vnmrsys/data

Sample directory:

FidFile: RK-OMe-OALL-1H

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Sep 19 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 6390.0 Hz

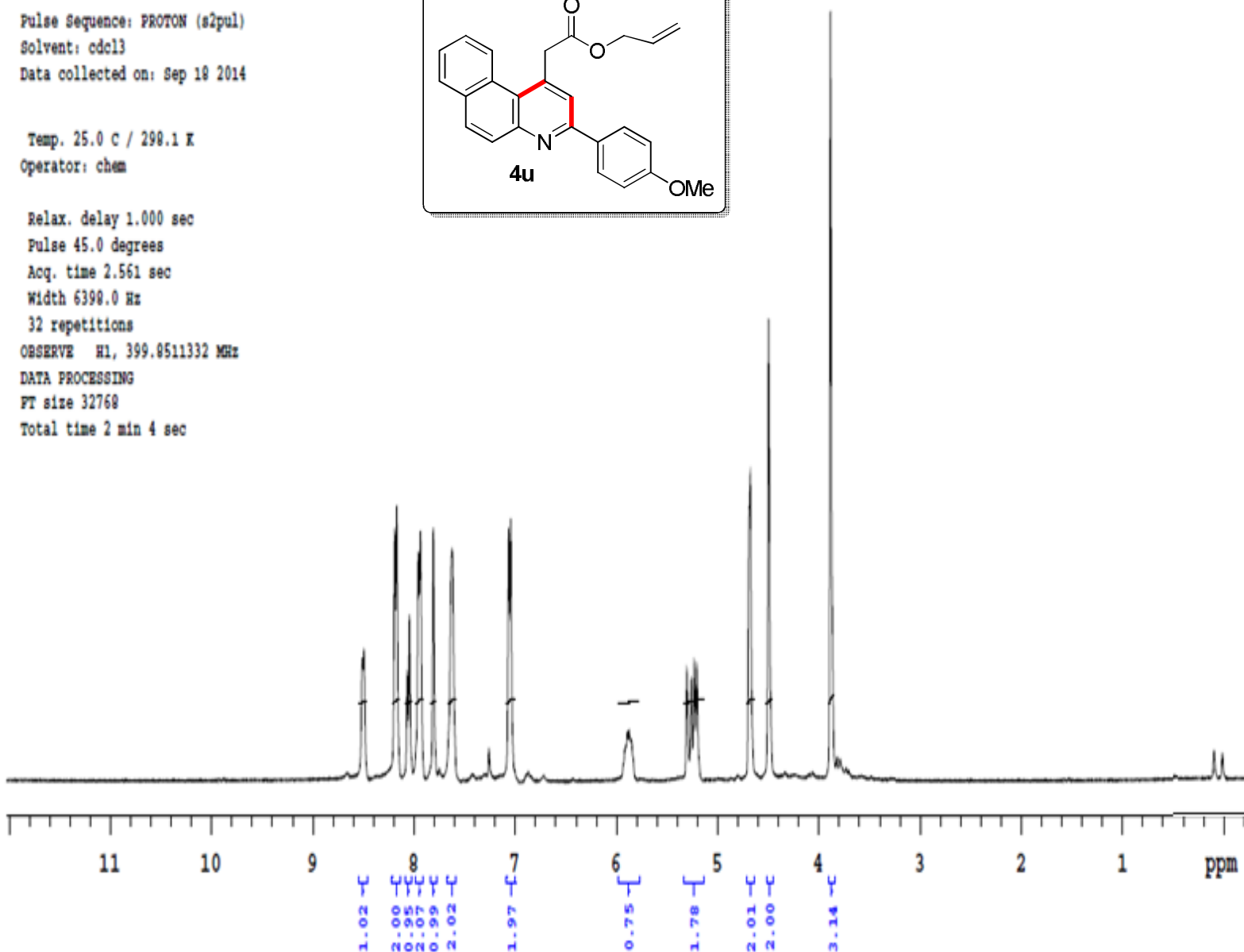
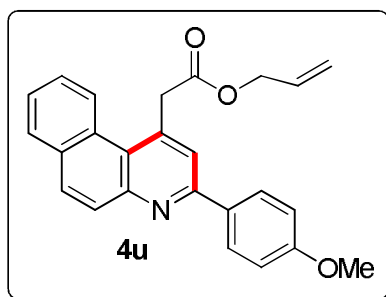
32 repetitions

OBSERVE H1, 399.8511332 MHz

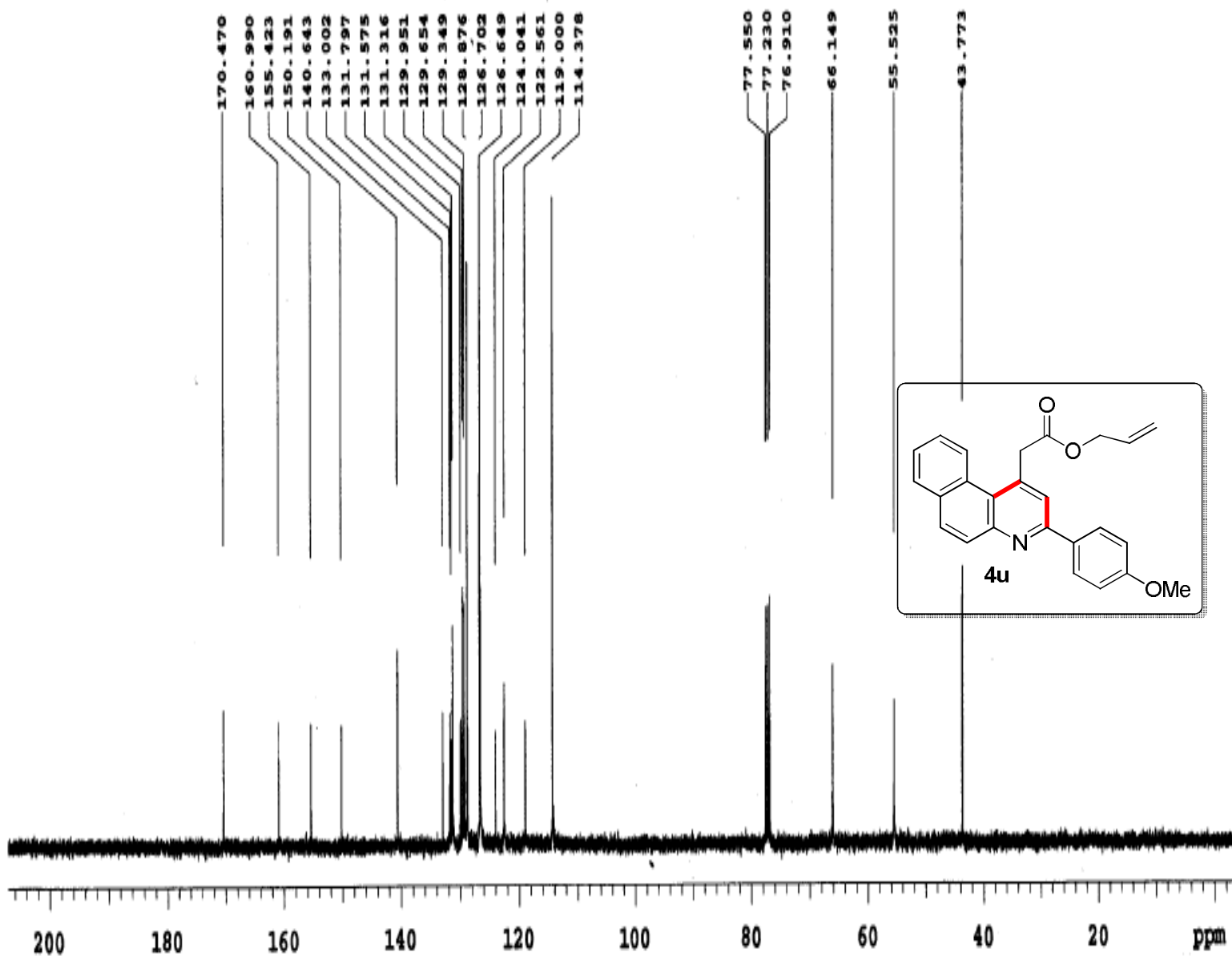
DATA PROCESSING

FT size 32768

Total time 2 min 4 sec



*<sup>13</sup>C NMR spectra of compound 4u*

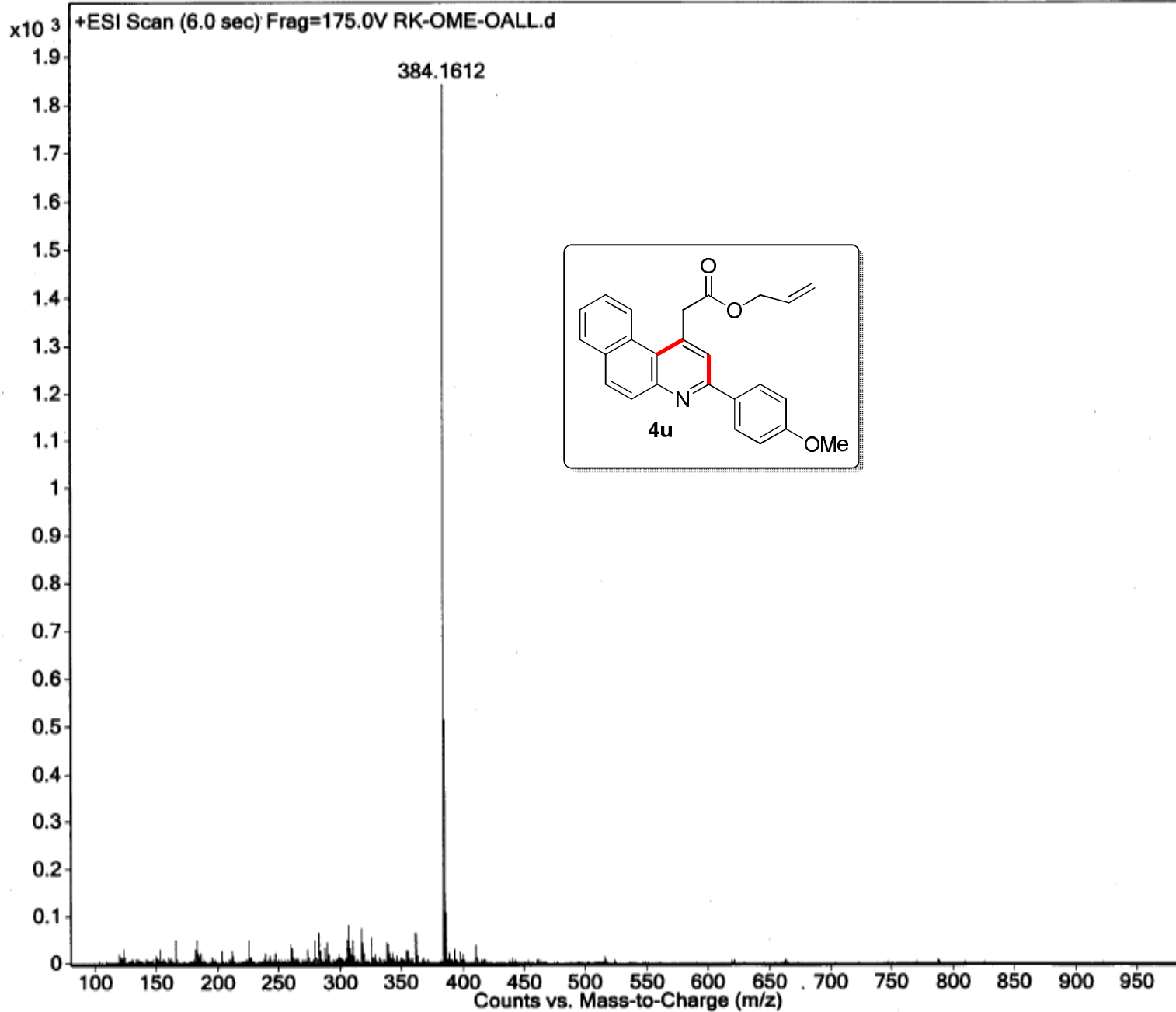


<p><b>PULSE SEQUENCE</b>                  Relax. delay 1.000 sec                  Pulse 45.0 degrees                  Acq. time 1.304 sec                  Width 25125.6 Hz                  550 repetitions</p>	<p><b>OBSERVE</b> c13, 100.5425901  <b>DECOUPLE</b> H1, 399.8529994                  Power 42 dB                  continuously on                  WALTZ-16 modulated</p>	<p><b>DATA PROCESSING</b>                  Line broadening 0.5 Hz                  FT size 65536                  Total time 21 minutes</p>	<p><b>RK-4-OMe-QALL-13C</b>                  Solvent: cdcl3                  Temp. 25.0 C / 298.1 K                  Operator: chem                  File: RK-4-OMe-QALL-13C                  Mercury-400 *IITG-NMR*</p>
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HRMS spectra of compound 4u

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

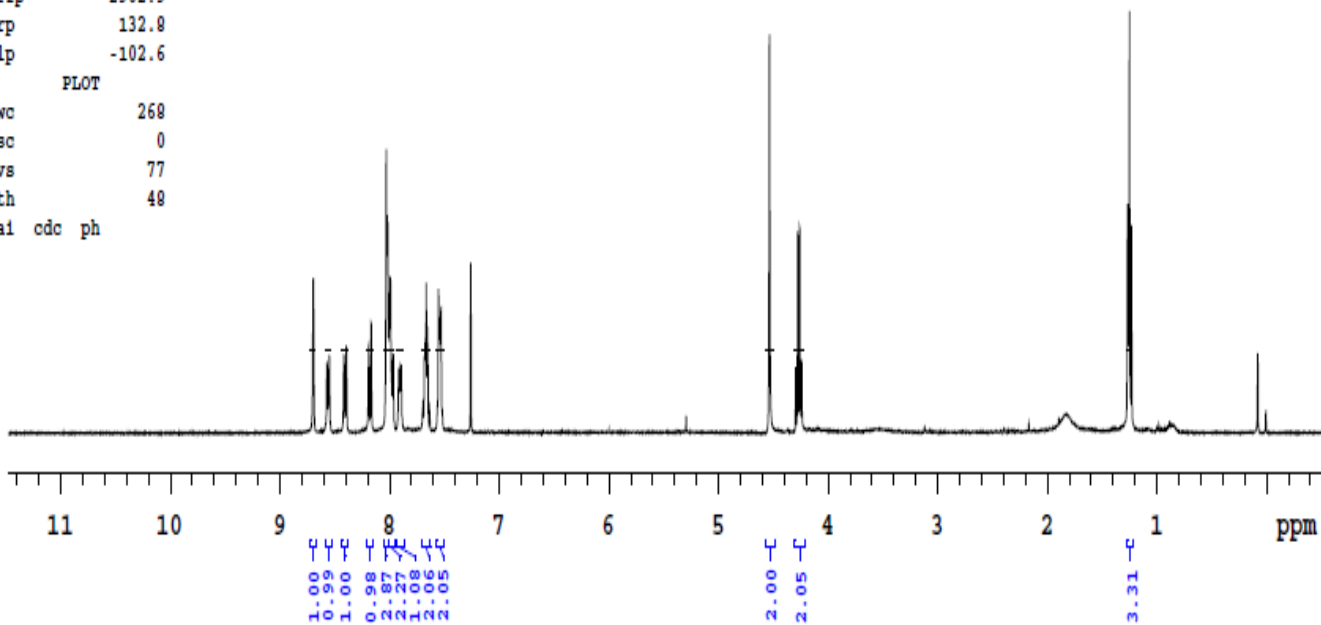
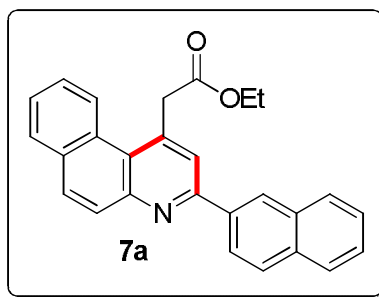


*<sup>1</sup>H NMR spectra of compound 7a*

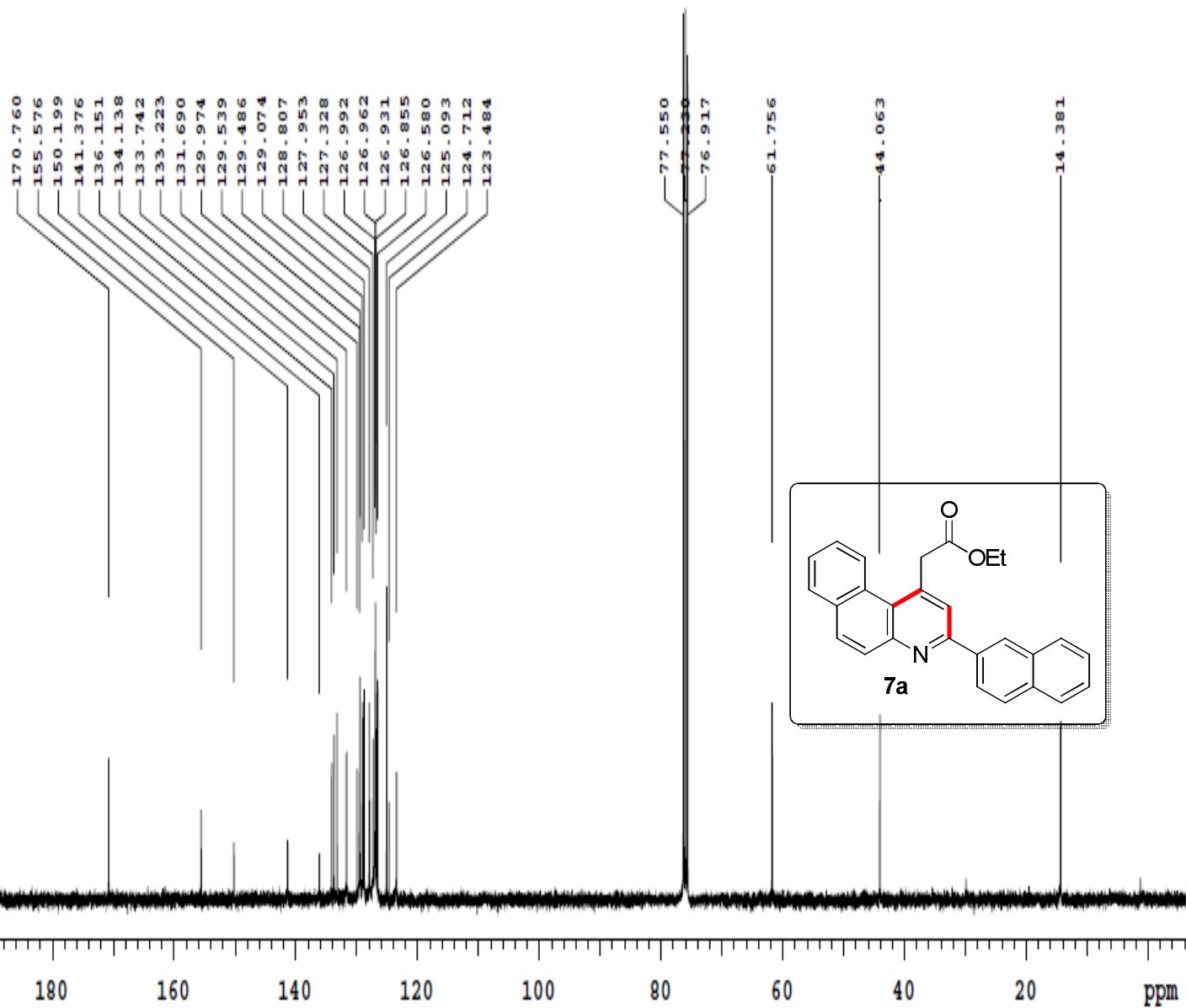
EK-NAP-NAP-OET-1H

exp2 PROTON

SAMPLE		PRESATURATION	
date	Oct 20 2014	satmode	n
solvent	cdcl3	wet	n
file	exp	SPECIAL	
ACQUISITION		temp	25.0
sw	6398.0	gain	30
at	2.561	spin	not used
np	32768	hst	0.008
fb	3600	pw90	16.300
bs	4	alfa	10.000
dl	1.000	FLAGS	
nt	32	il	n
ct	32	in	n
TRANSMITTER		dp	y
tn	H1	hs	nn
sfrq		399.853	PROCESSING
tof	363.1	fn	not used
tpwr	58	DISPLAY	
pw	8.150	sp	-219.1
DECOUPLER		wp	4806.7
dn	c13	rfl	3703.1
dof	0	rpf	2902.9
dm	nnn	rp	132.8
decwave	g	lp	-102.6
dpwr	40	PLOT	
dmf	17100	wc	268
		sc	0
		vs	77
		th	48
		ai	cdc ph



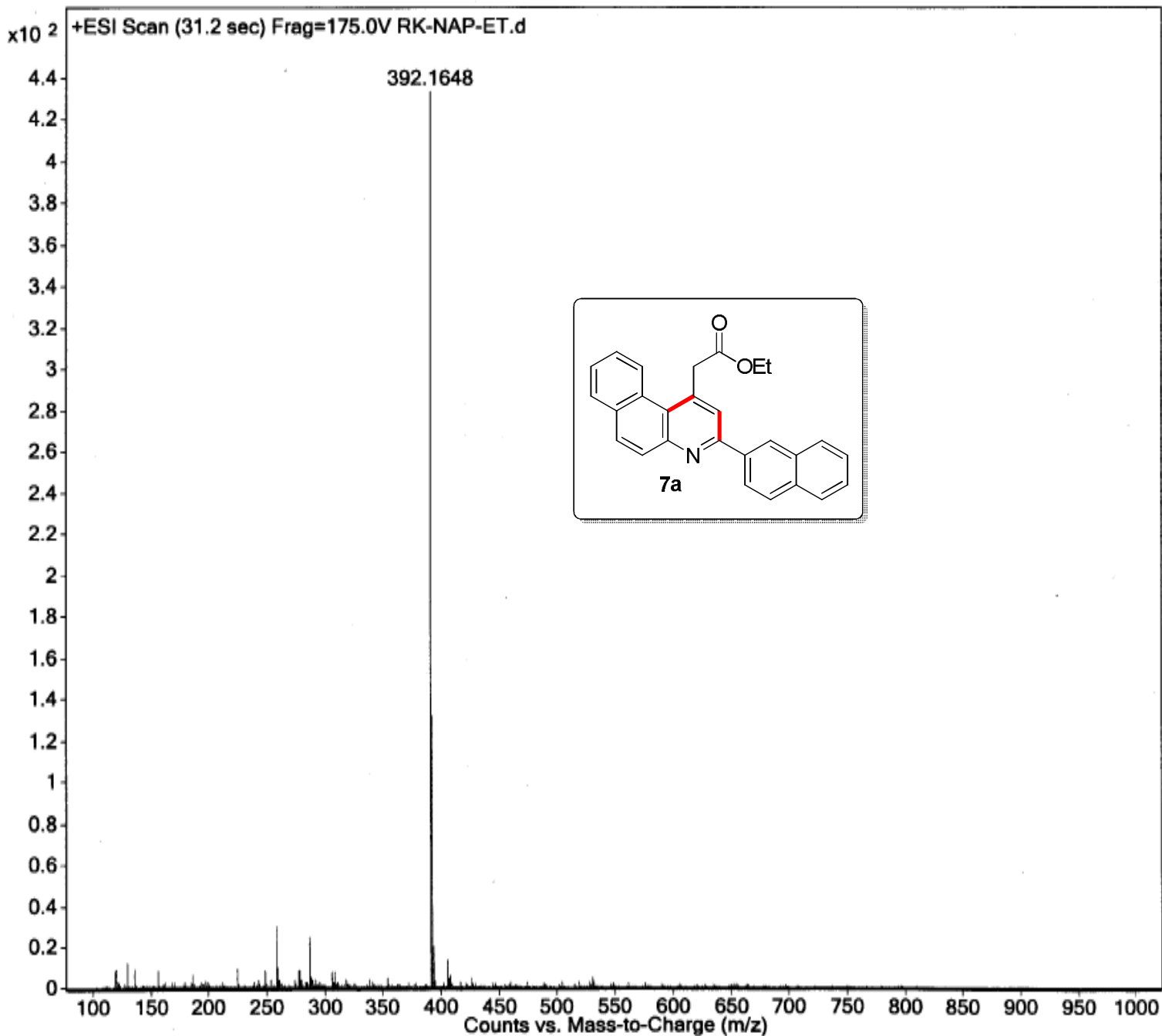
*<sup>13</sup>C NMR spectra of compound 7a*



<b>PULSE SEQUENCE</b> Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.304 sec Width 25125.6 Hz 6700 repetitions	<b>OBSERVE</b> C13, 100.5425932 <b>DECOUPLE</b> H1, 399.8529994 Power 42 dB continuously on WALTZ-16 modulated	<b>DATA PROCESSING</b> Line broadening 0.5 Hz FT size 65536 Total time 4.3 hours	<b>RK-NAP-NAP-OET-13C</b> Solvent: cdcl3 Temp. 25.0 C / 298.1 K Operator: chem Mercury-400 "IITG-NMR"
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*HRMS spectra of compound 7a*

Sample Name	RK-NAP-ET	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-NAP-ET.d	ACQ Method		Comment		Acquired Time	10/30/2014 11:50:24 AM



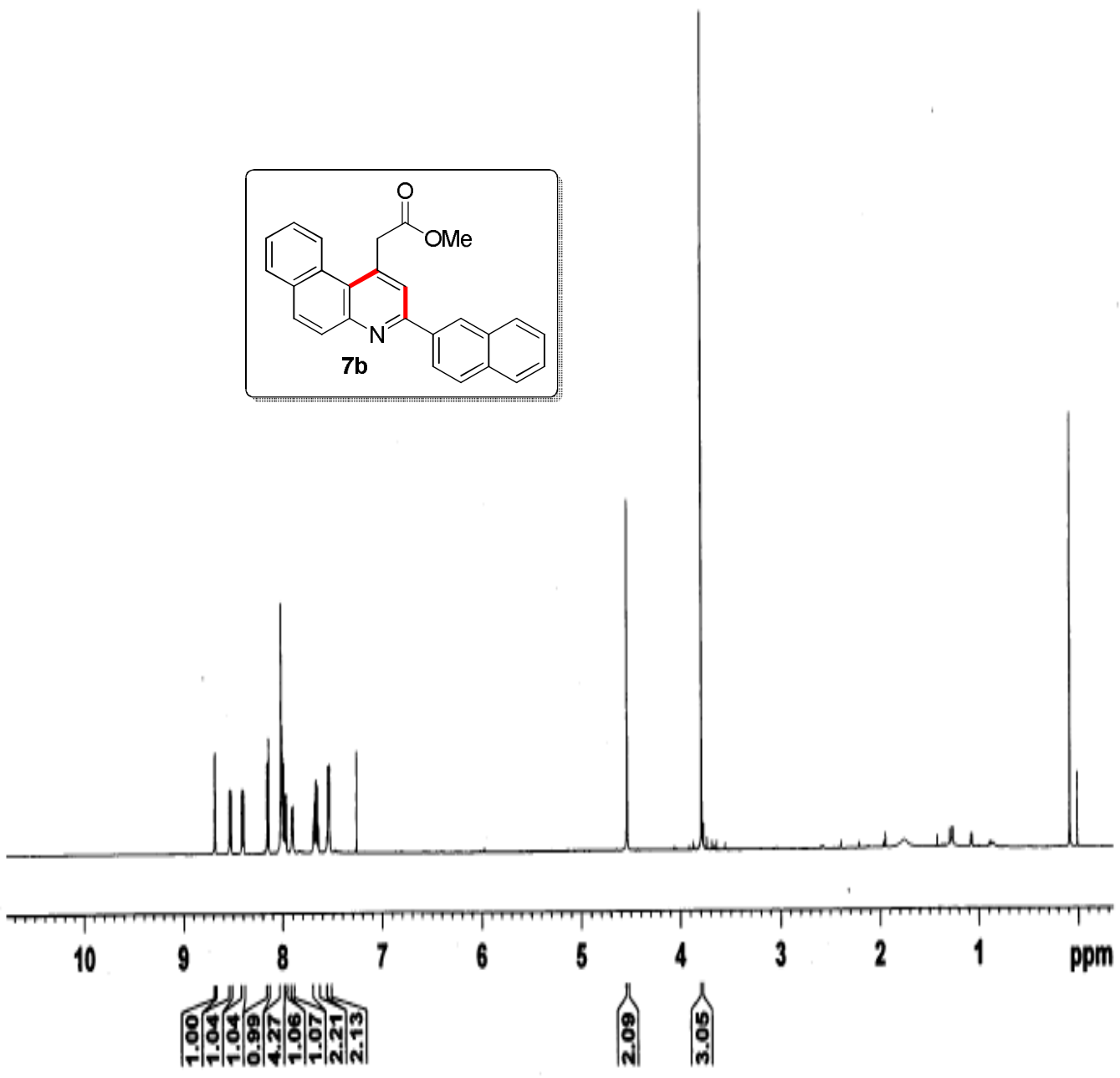
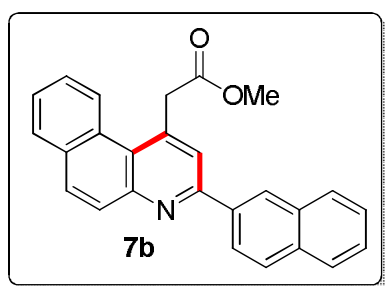
*<sup>1</sup>H NMR spectra of compound 7b*

Current Data Parameters  
NAME BK-MAP-OMe-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20141010  
Time 10.27  
INSTRUM spect  
PROBHD 5 mm F400 BBO/  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 33.2  
IN 41.620 usec  
DE 6.30 usec  
TE 299.0 K  
DI 1.0000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 600.137063 MHz  
NUC1 1H  
P1 12.00 usec  
PLW1 21.0000000 W

F2 - Processing parameters  
SI 16384  
SF 600.137063 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



*<sup>13</sup>C NMR spectra of compound 7b*



171.29  
155.64  
150.34  
141.00  
136.26  
134.11  
133.73  
133.23  
131.63  
129.93  
129.67  
129.48  
128.04  
128.78  
127.94  
127.23  
126.97  
126.93  
126.89  
126.81  
125.56  
124.08  
123.63  
123.43

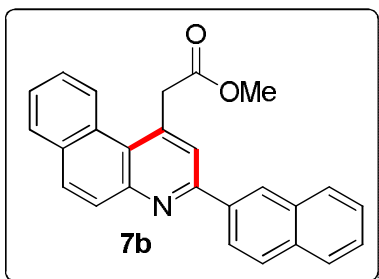
77.43  
77.22  
77.01

52.83

43.76

Current Data Parameters  
NAME RK-NAP-OMe-13C  
EXPNO 1  
PROCNO 1

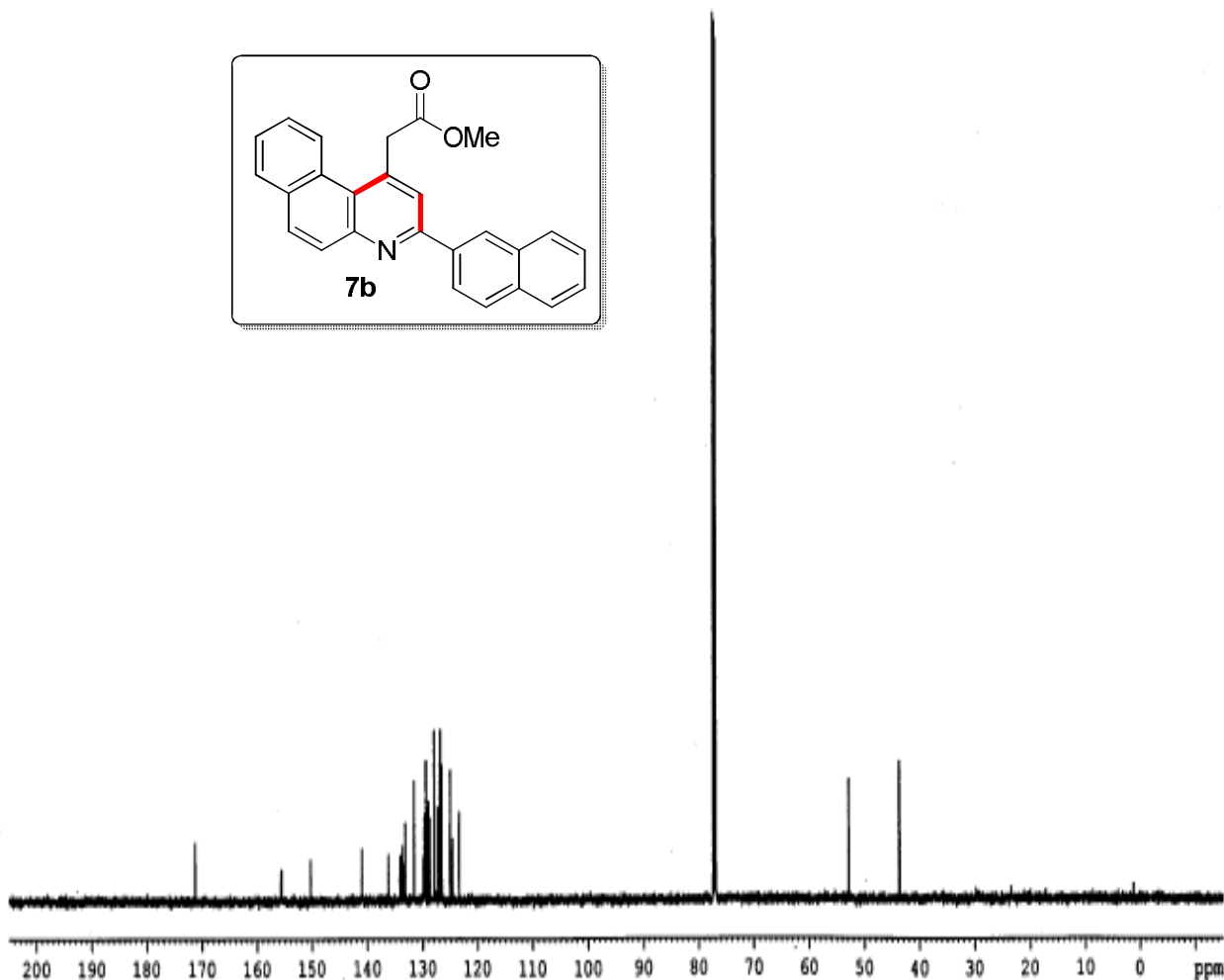
F2 - Acquisition Parameters  
Date\_ 20141010  
Time 10.33  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 184  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DW 13.867 usec  
DE 6.50 usec  
TE 299.8 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1



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

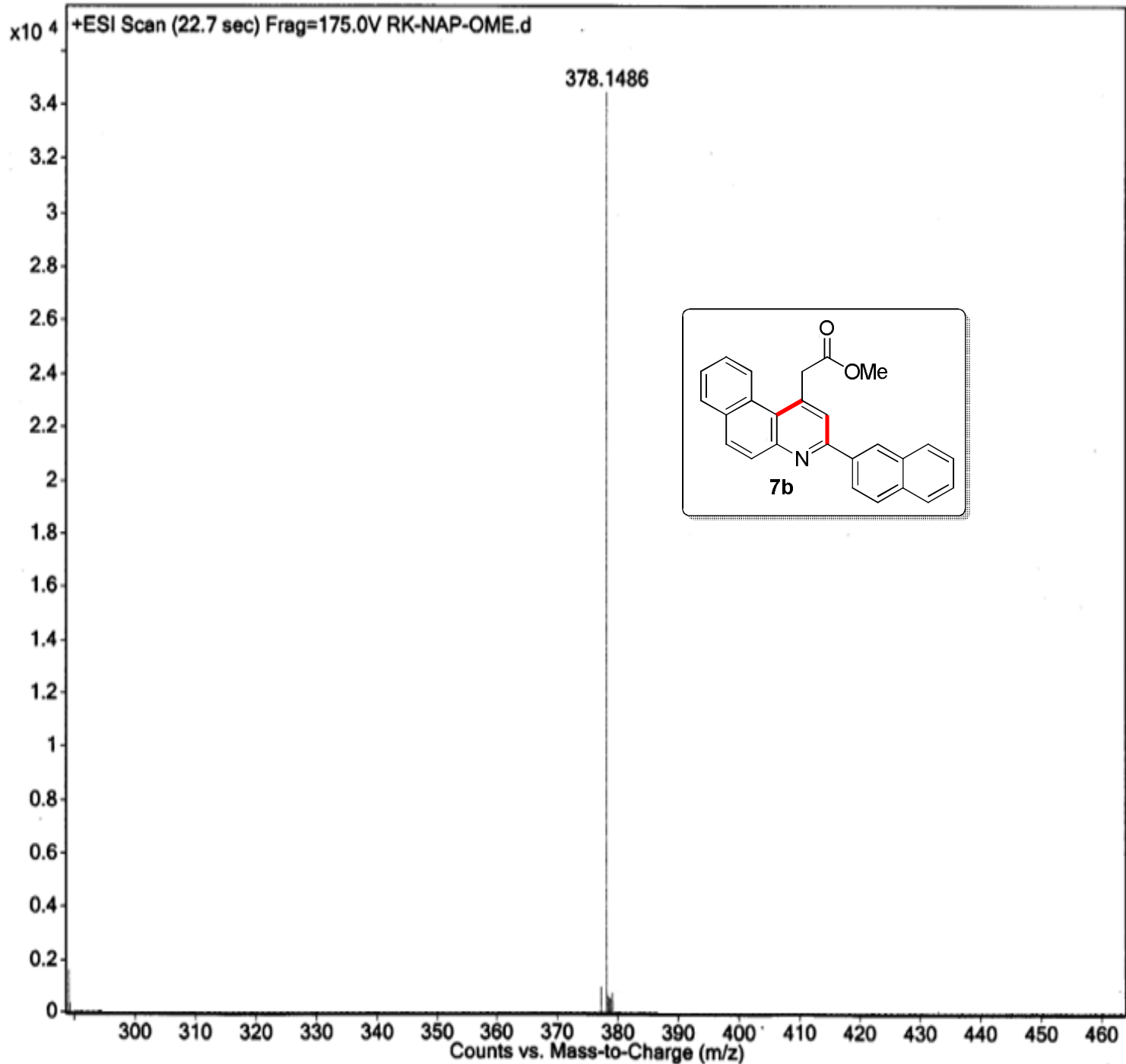
----- CHANNEL f2 -----  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG12 walzr16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9128391 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



*HRMS spectra of compound 7b*

Sample Name	RK-NAP-OME	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-NAP-OME.d	ACQ Method		Comment		Acquired Time	10/15/2014 12:25:35 PM

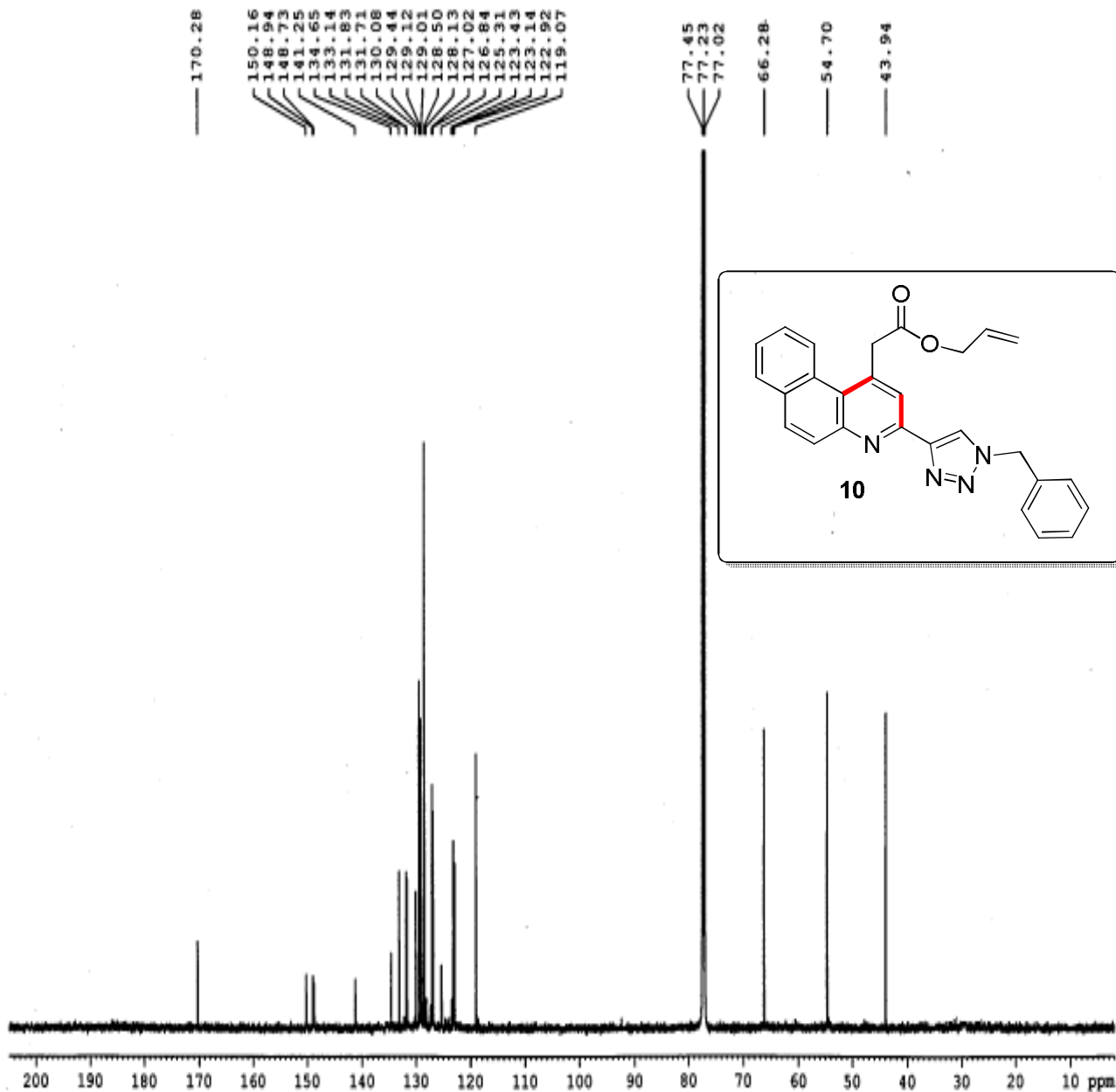






*<sup>13</sup>C NMR spectra of compound 10*

RK-TRi-Bn-OA11-13C



Current Data Parameters  
NAME RK-TRi-Bn-OA11-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150316  
Time 17.32  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 32768  
SOLVENT CDCl3  
NS 15000  
DS 2  
SMH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 200.18  
DM 13.867 usec  
DE 6.50 usec  
TE 297.6 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

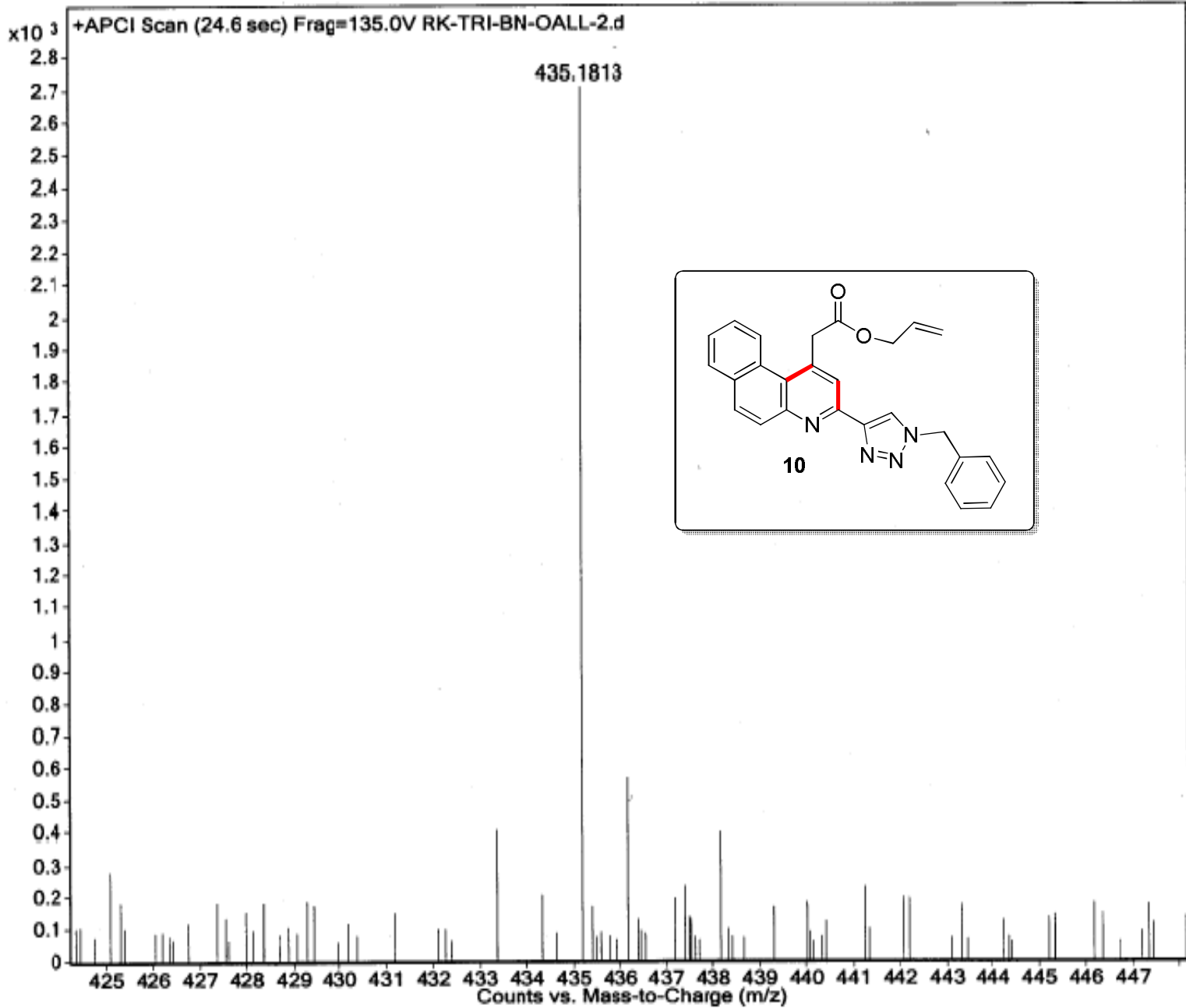
----- CHANNEL #1 -----  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

----- CHANNEL #2 -----  
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 150.9128327 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

HRMS spectra of compound 10

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



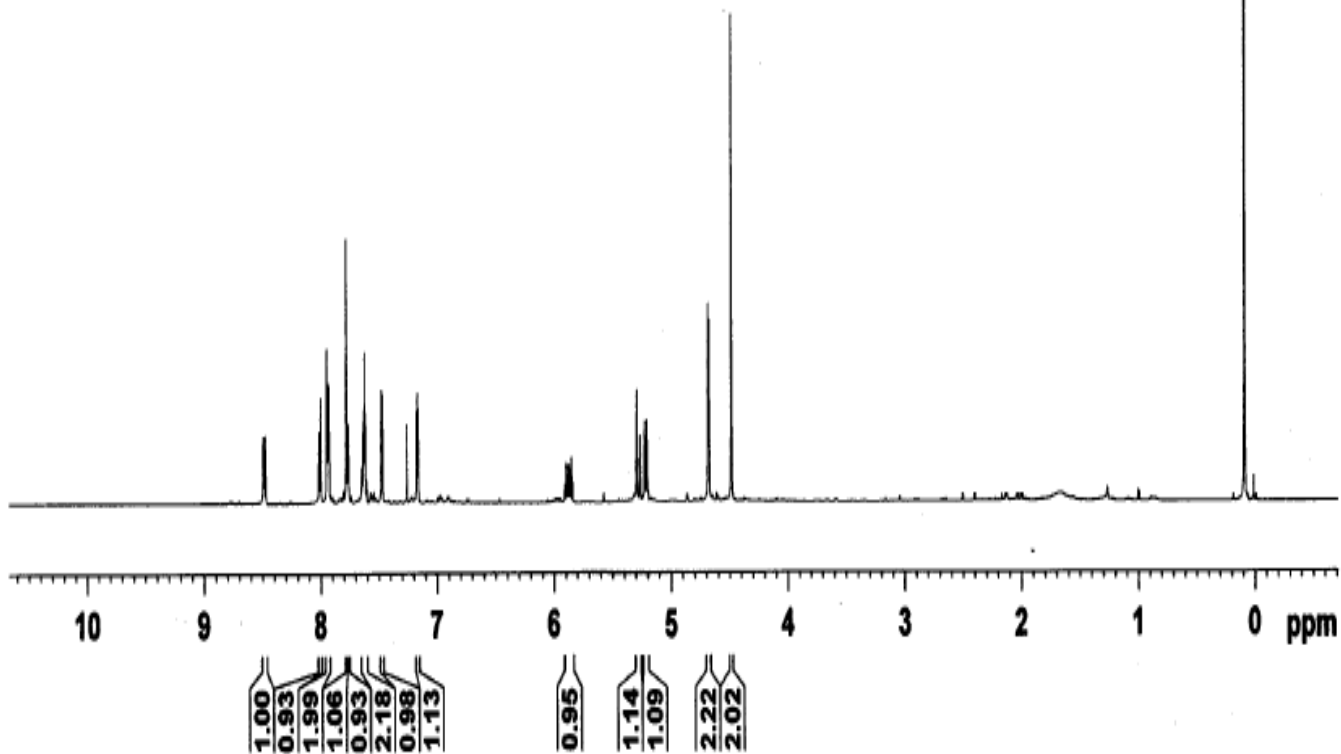
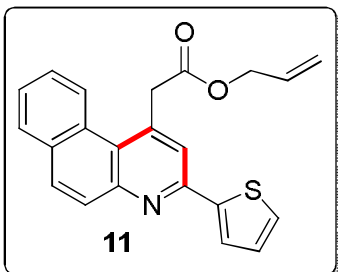
*<sup>1</sup>H NMR spectra of compound 11*

Current Data Parameters  
NAME NK-TWP-ALL-1H  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20141013  
Time 9.57  
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  
DM 41.600 usec  
DE 6.50 usec  
TE 299.7 K  
D1 1.00000000 sec  
TDO 1

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

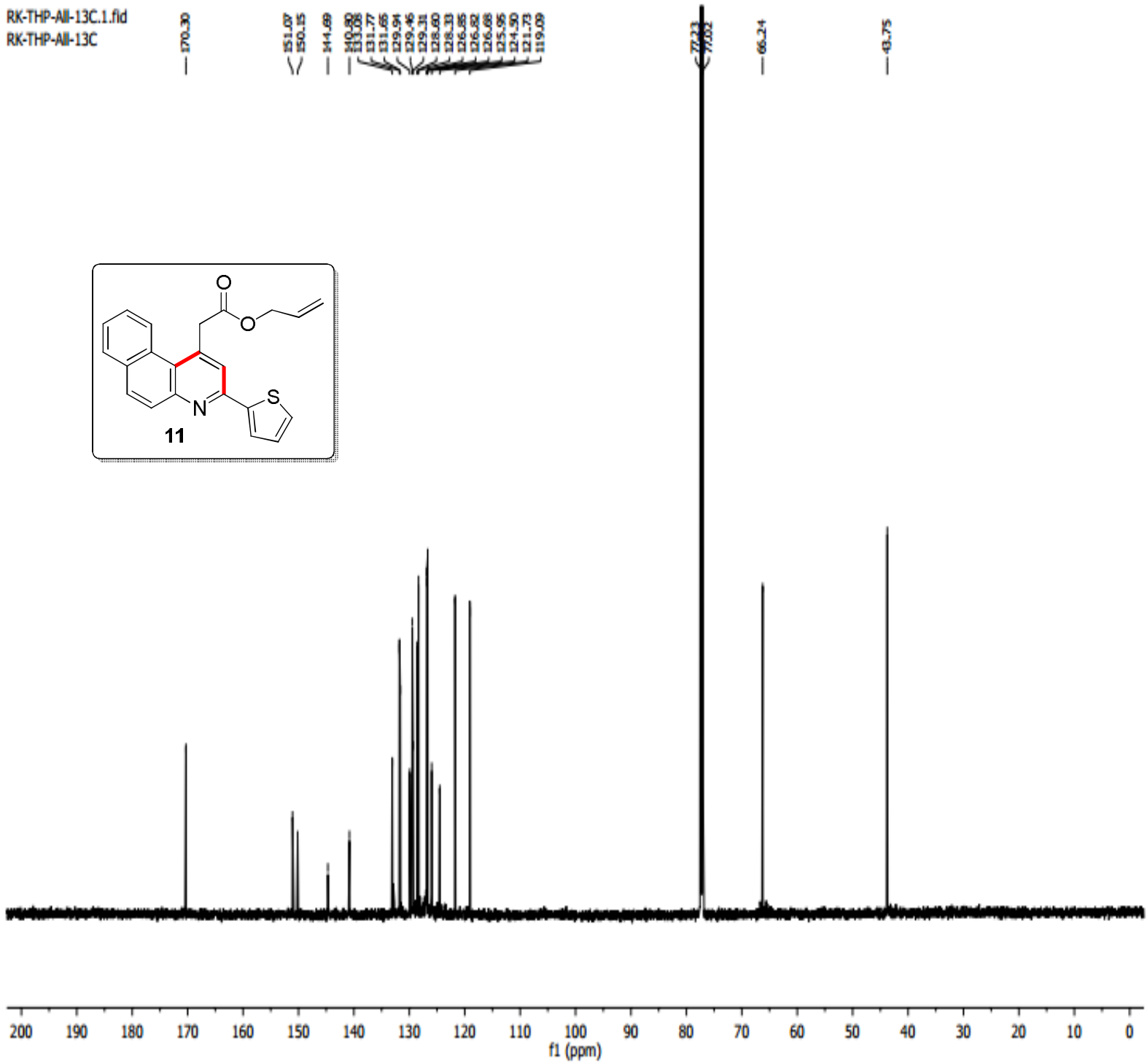
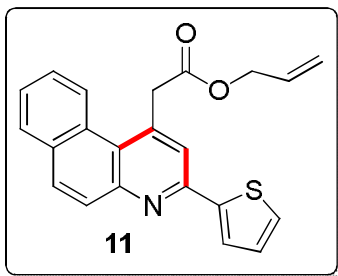
F2 - Processing parameters  
SI 16384  
SF 600.1700147 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



*<sup>13</sup>C NMR spectra of compound 11*

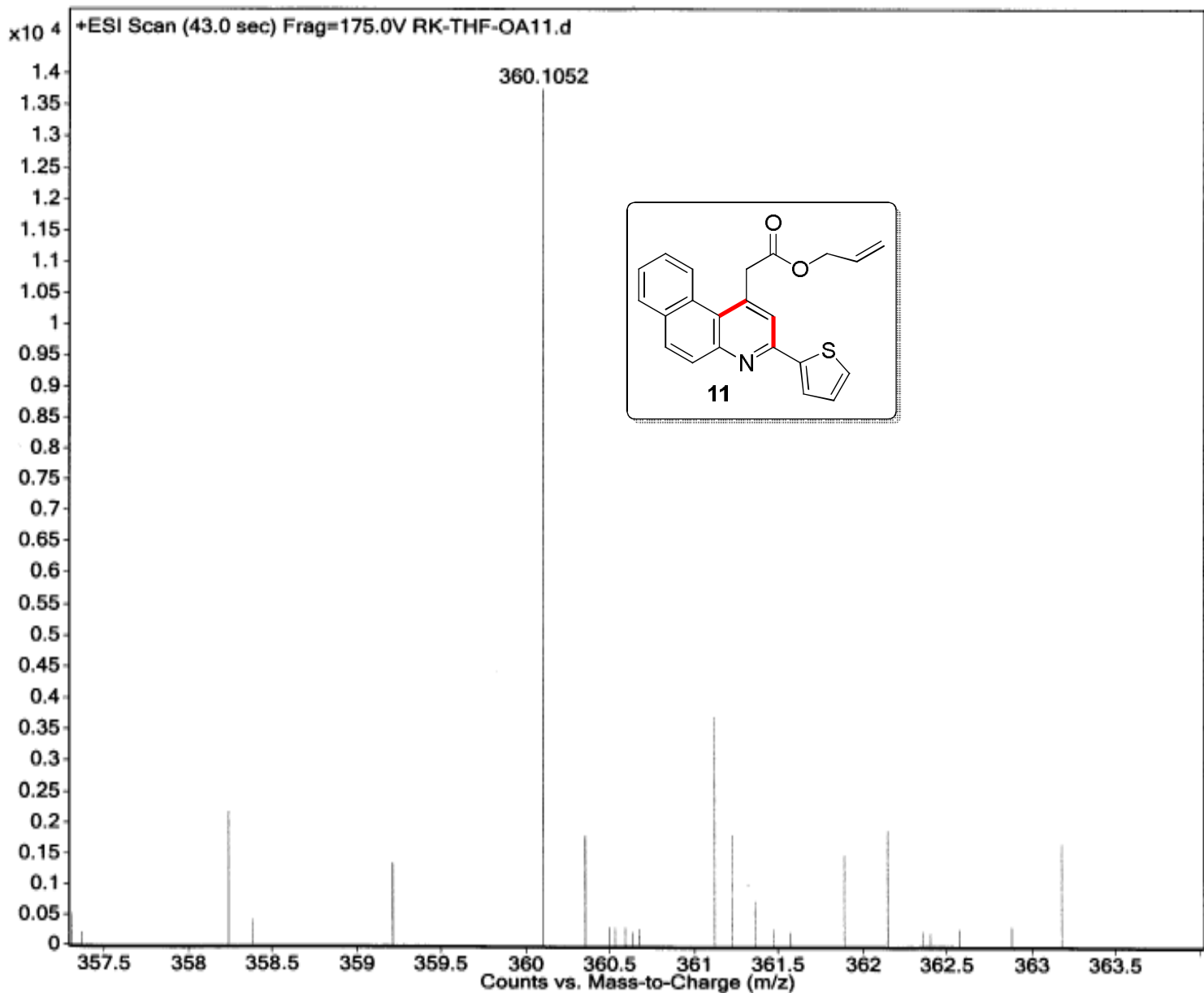
RK-THP-All-13C.1.fid  
RK-THP-All-13C

170.30  
151.07  
150.15  
144.69  
140.80  
139.78  
131.77  
131.65  
129.94  
129.46  
129.31  
128.60  
128.33  
126.85  
126.82  
126.68  
125.85  
124.90  
121.73  
119.09



### HRMS spectra of compound 11

Sample Name	RK-THF-OA11	Position	-1	Instrument Name	Instrument 1	User Name	
Inj Vol	-10	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RK-THF-OA11.d	ACQ Method		Comment		Acquired Time	10/15/2014 12:12:00 PM



*<sup>1</sup>H NMR spectra of compound 12*

RK-4OMe-ET-PRO-1H

Sample Name:

RK-4OMe-ET-PRO-1H

Data Collected on:

IITG-NMR-mercury400

Archive directory:

Sample directory:

FidFile: RK-4OMe-ET-PRO-1H

Pulse Sequence: PROTON (s2pul)

Solvent: cdcl3

Data collected on: Nov 4 2014

Temp. 25.0 C / 298.1 K

Operator: chen

Relax. delay 1.000 sec

Pulse 45.0 degrees

Acq. time 2.561 sec

Width 6398.0 Hz

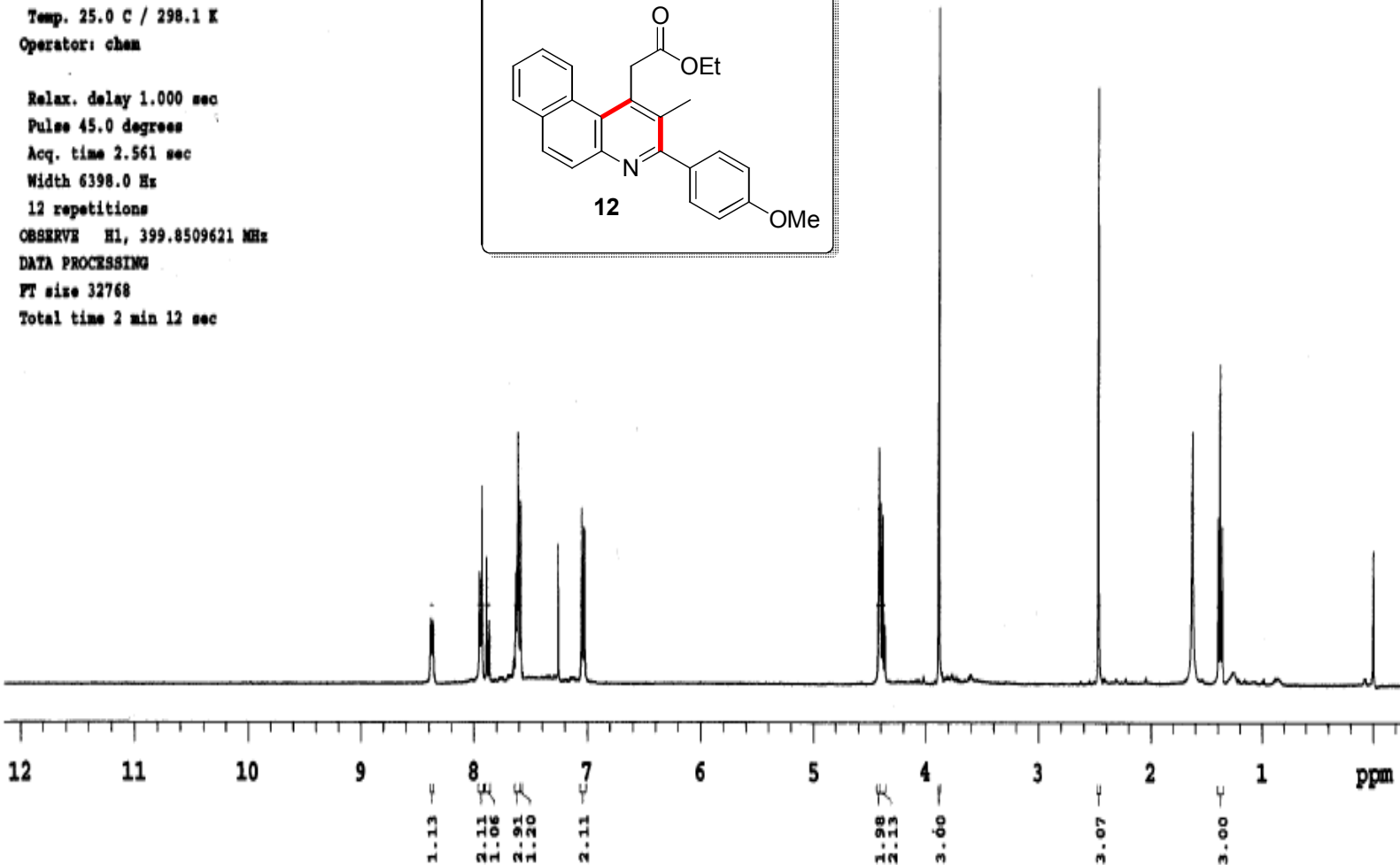
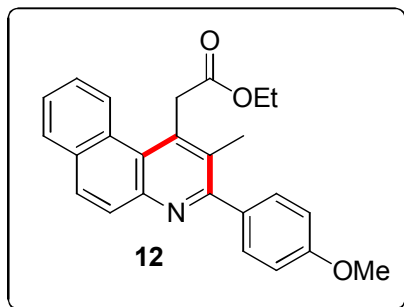
12 repetitions

OBSERVE H1, 399.8509621 MHz

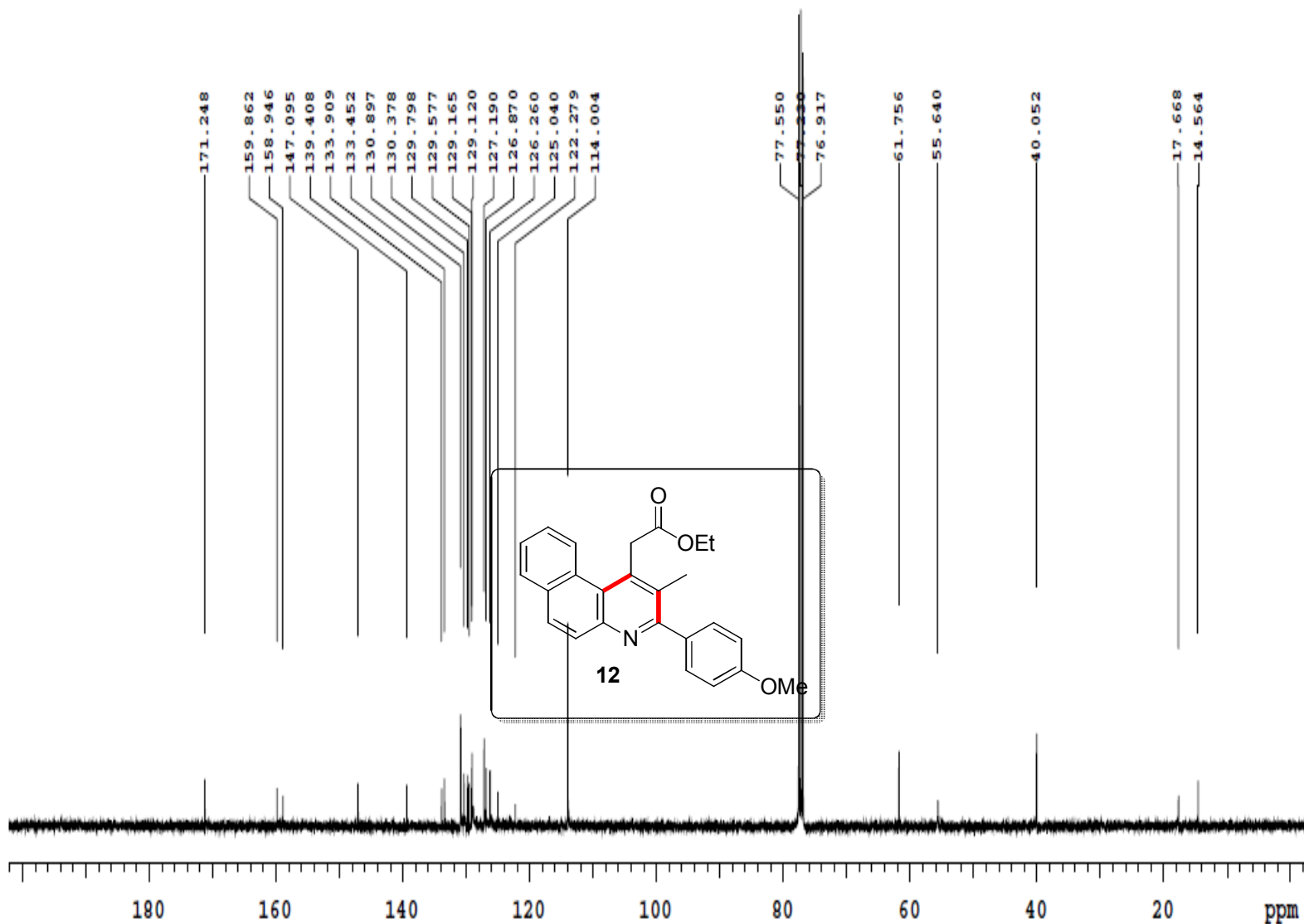
DATA PROCESSING

FT size 32768

Total time 2 min 12 sec



*<sup>13</sup>C NMR spectra of compound 12*



**PULSE SEQUENCE**

Relax. delay 1.000 sec  
Pulse 45.0 degrees  
Acq. time 1.304 sec  
Width 25125.6 Hz  
7100 repetitions

**OBSERVE C13, 100.5425809**

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

**DATA PROCESSING**

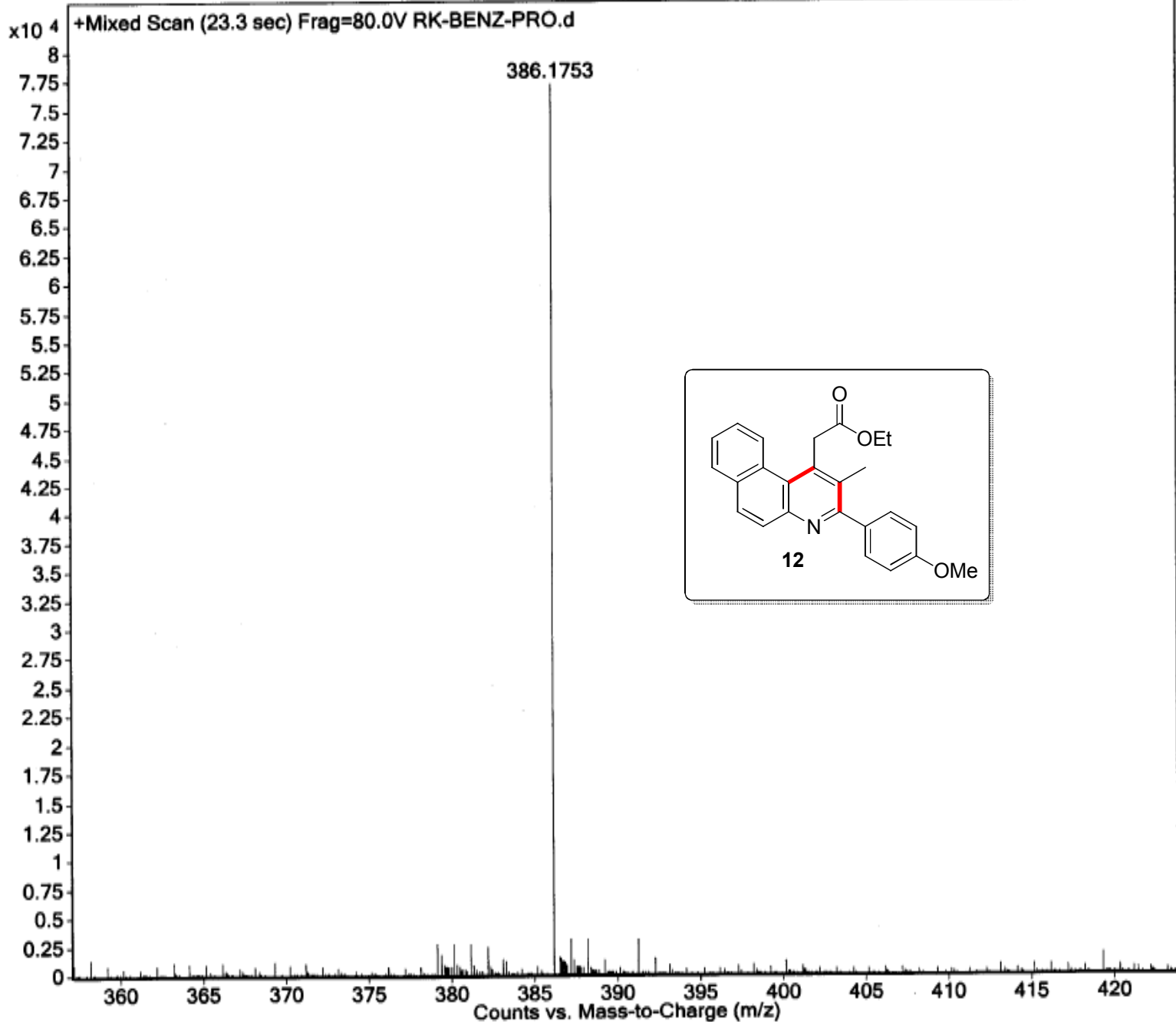
Line broadening 0.5 Hz  
FT size 65536  
Total time 4.5 hours

**RK-4OME-ET-PRO-13C**

Solvent: cdcl3  
Temp. 25.0 C / 298.1 K  
Operator: chem  
File: RK-4OME-ET-PRO-13c  
Mercury-400 "IITG-NMR"

HRMS spectra of compound 12

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





*Reaction monitoring after 10min for intermediate III of 4p*

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Some Ions Missed
Data Filename	RK-2F-RXN.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable

