

Supporting Information

K₂CO₃ catalyzed regioselective synthesis of thieno[2,3-*b*]thiochromen-4-one oximes: Access to the corresponding Amine and Nitroso derivatives

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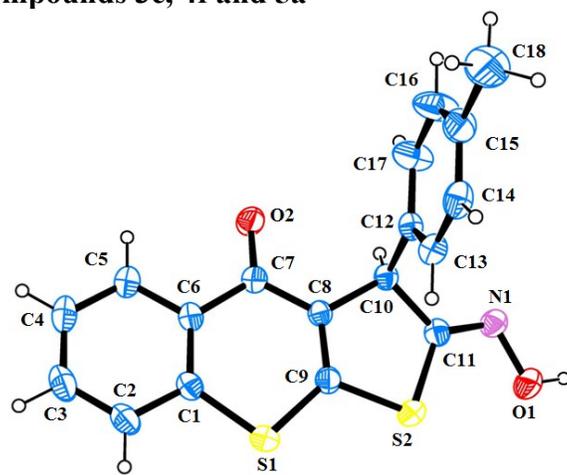
^bPresent address: Vice-Chancellor, Aliah University, IIA/27, New Town, Kolkata-700 156, West Bengal, India.

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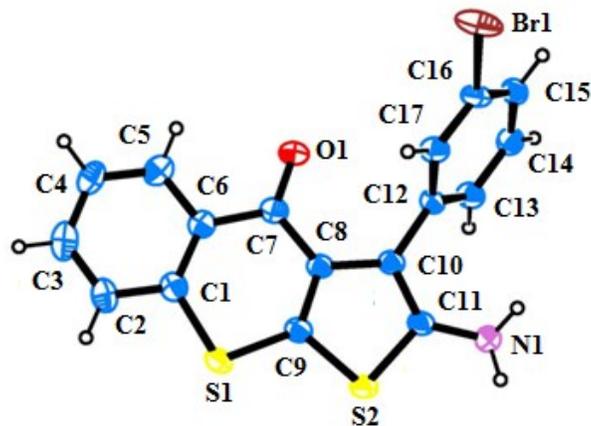
I. General Information and Methods

^1H and ^{13}C NMR spectra were recorded on 400 MHz, 600 MHz and 100 MHz, 150 MHz spectrometer TMS as internal reference; chemical shifts (δ scale) are reported in parts per million (ppm). ^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 b s (broad singlet). IR spectra were recorded in KBr. HRMS spectra were recorded using ESI and APCI (TOF) mode. The X-ray crystal structures were determined with a diffractometer. Complete crystallographic data of **3c** (CCDC no.1454211), **4f** (CCDC no.1454212) and **5a** (CCDC no.1454213) 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).

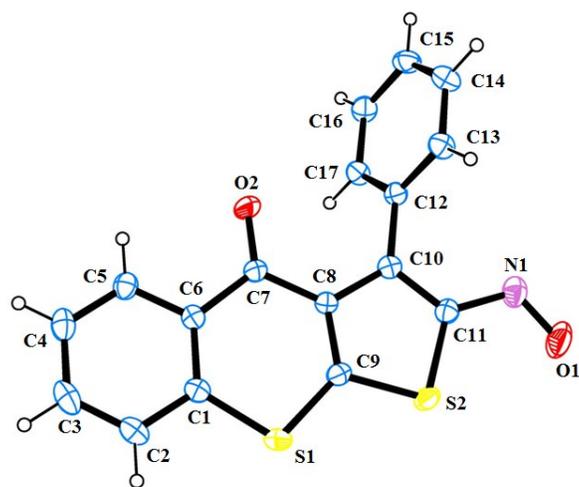
2. X-ray Structure of Compounds 3c, 4f and 5a



(3c)



(4f)



(5a)

Figure 1. 30% probability of ORTEP ellipsoids of compounds **3c**, **4f** and **5a**

3. Crystal Data and Structure Refinement for Compound 3c, 4f and 5a

Table S2 Data collection and refinement statistics for the compounds **3c**, **4f** and **5a**

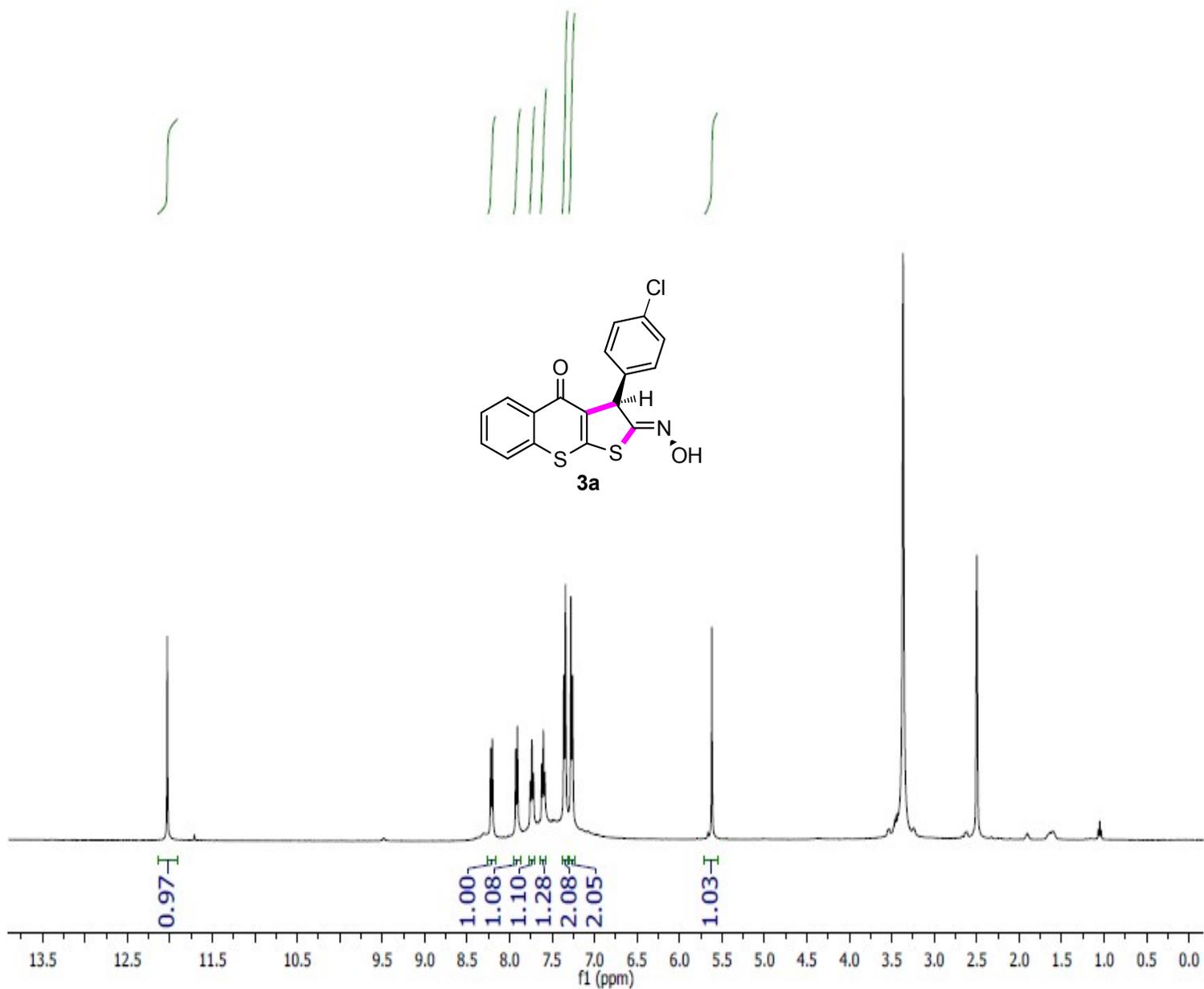
Entry	Identification code	Compound 3c	Compound 4f	Compound 5a
01	Empirical formula	C18 H13 N O2 S2	C17 H10 Br N O S2	C17 H9 N O2 S2
02	Formula weight	339.41	388.28	323.37
03	Temperature	296(2) K	296(2) K	296(2) K
04	Wavelength	0.71073	0.71073	0.71073
05	Radiation type	Mo K α	Mo K α	Mo K α
06	Radiation source	Fine-focus sealed tube	Fine-focus sealed tube	Fine-focus sealed tube
07	Crystal system	Monoclinic	Monoclinic	Monoclinic
08	Space group	P21/c	P21/c	P21/c
09	Cell length	a 8.1398(3) b 12.3213(4) c 16.5028(5)	a 18.1202(5) b 12.7017(3) c 14.3420(4)	a 6.3128(3) b 18.0467(9) c 12.6157(5)
10	Cell Angle	α 90 β 102.686(2) δ 90	α 90 β 113.1330(10) δ 90	α 90.00 β 96.132(4) δ 90.00
11	Cell Volume	1614.71(9)	3035.51(14)	1429.03(11)
12	Density	1.387	1.686	1.495
13	Completeness to theta	28.56° / 99.8%	28.42° / 100%	28.70° / 99.9%
14	Absorption correction	multi-scan	multi-scan	multi-scan
15	Refinement method	Full-matrix least-squares on F2	Full-matrix least-squares on F2	Full-matrix least-squares on F2

16	Index ranges	-10<=h<=10, -16<=k<=16, -22<=l<=22	-24<=h<=24, -17<=k<=17, -19<=l<=19	-5<=h<=8, -24<=k<=19, -16<=l<=17
17	Reflection number	4102	7634	3698
18	Theta range	3.38-28.56	3.22-28.42	3.25-28.70
19	Cell formula units Z	4	8	4
20	CCDC no	1454211	1454212	1454213

4. Copies of ^1H NMR, ^{13}C NMR and HRMS spectra of all Compounds

^1H NMR spectra of compound: 3a

KM-NS-PI-4Cl-R-1H
KM-NS-PI-4Cl-R-1H



¹³CNMR spectra of compound: 3a

KM-NS-PI-4Cl-R-13C
KM-NS-PI-4Cl-R-1H

—172.82

~152.56

~149.43

139.18

135.26

132.03

131.77

130.21

130.09

129.15

128.56

128.39

127.92

126.95

—53.53

40.14

39.93

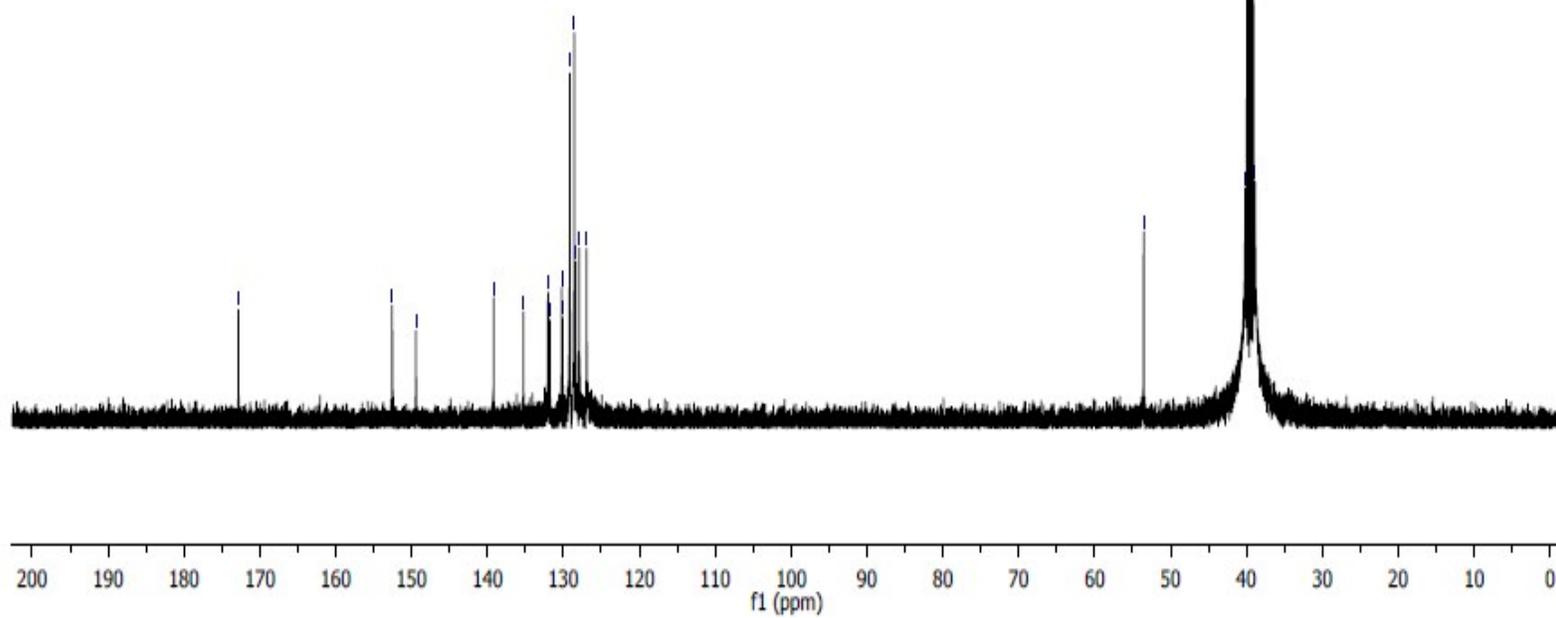
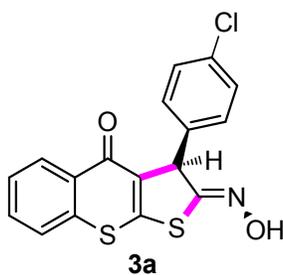
39.71

39.50

39.29

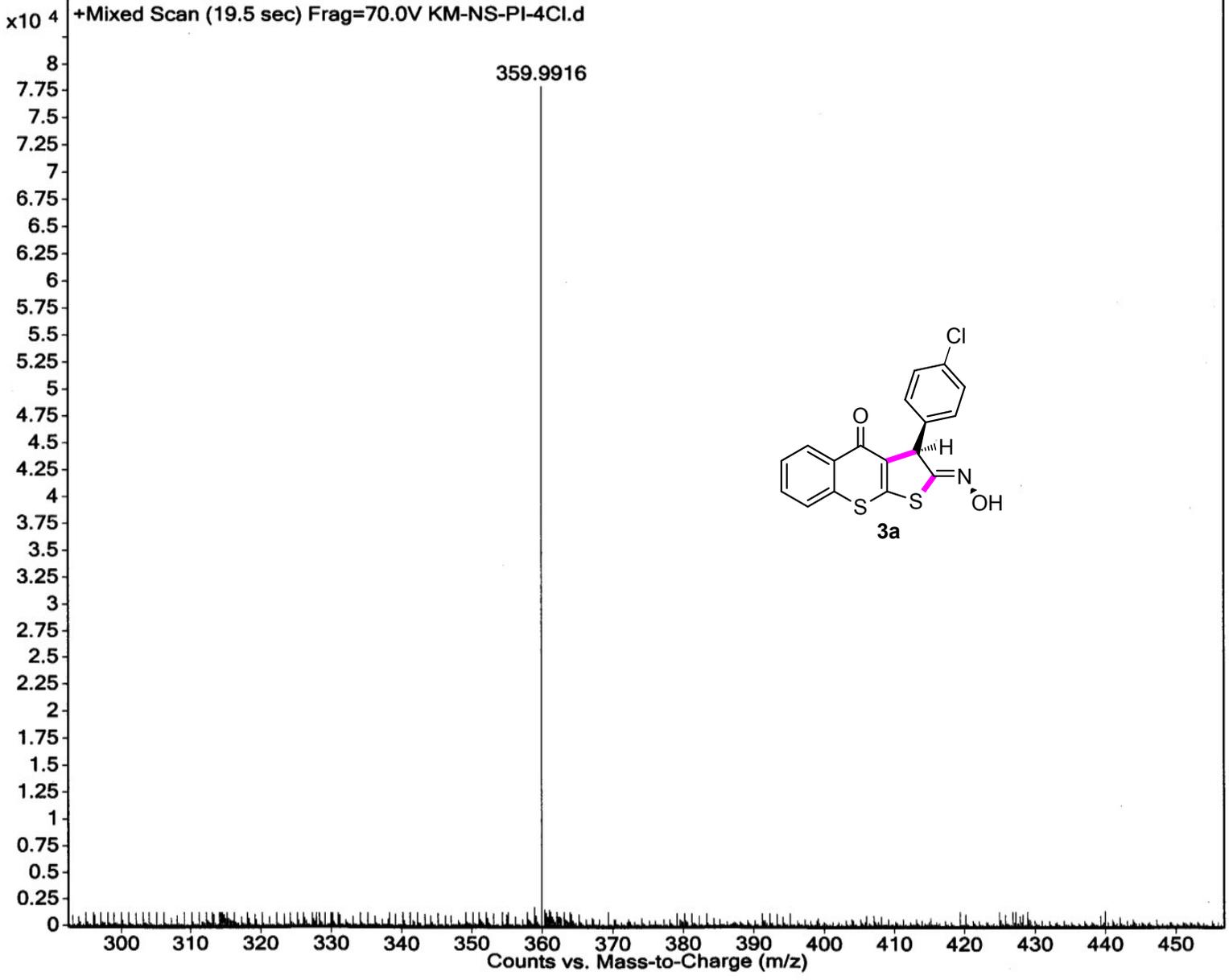
39.08

38.86



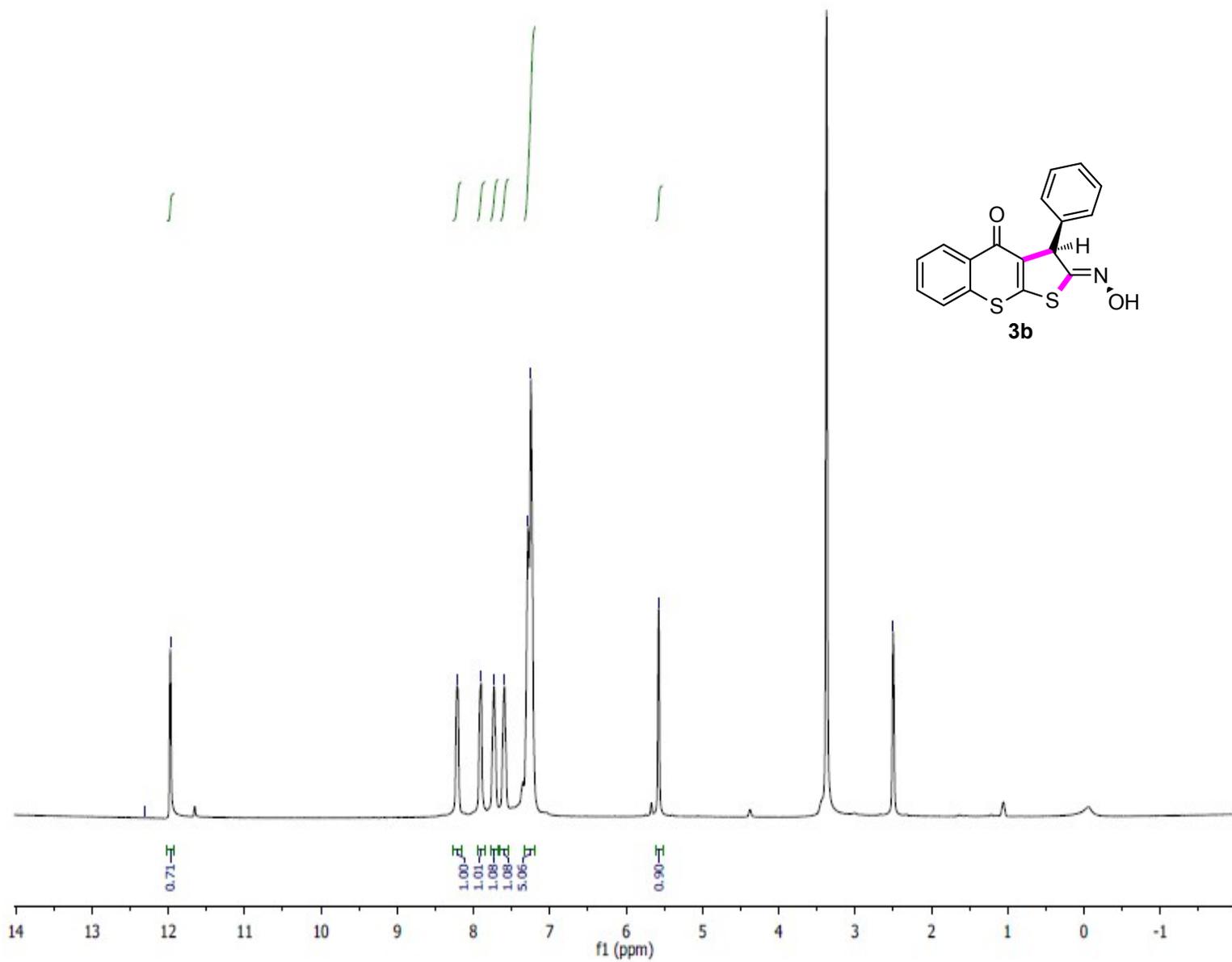
HRMS spectra of compound: 3a

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 compound: 3b

KM-NS-PI-BEN-1H
KM-NS-PI-BEN-1H

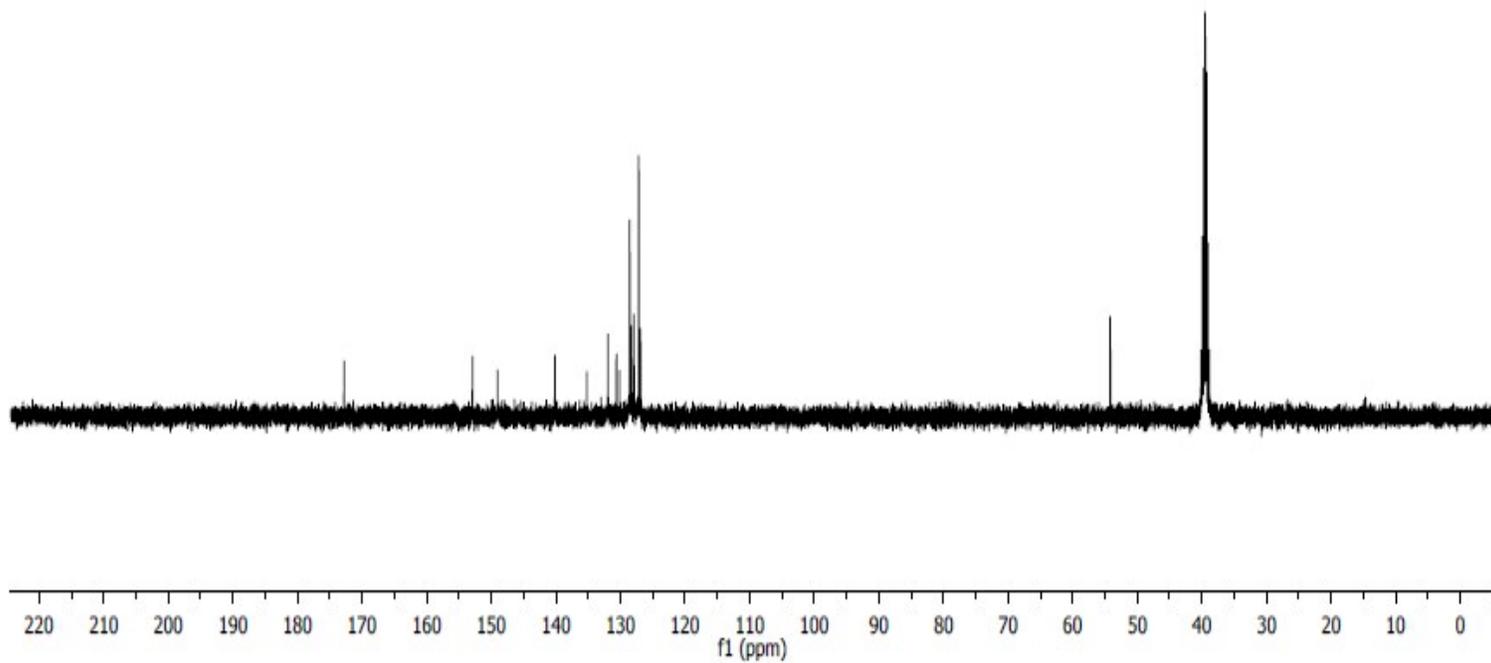
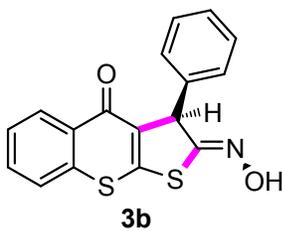


¹³CNMR spectra of compound: 3b

KM-NS-PI-BEN-13C-1
KM-NS-PI-BEN-13C

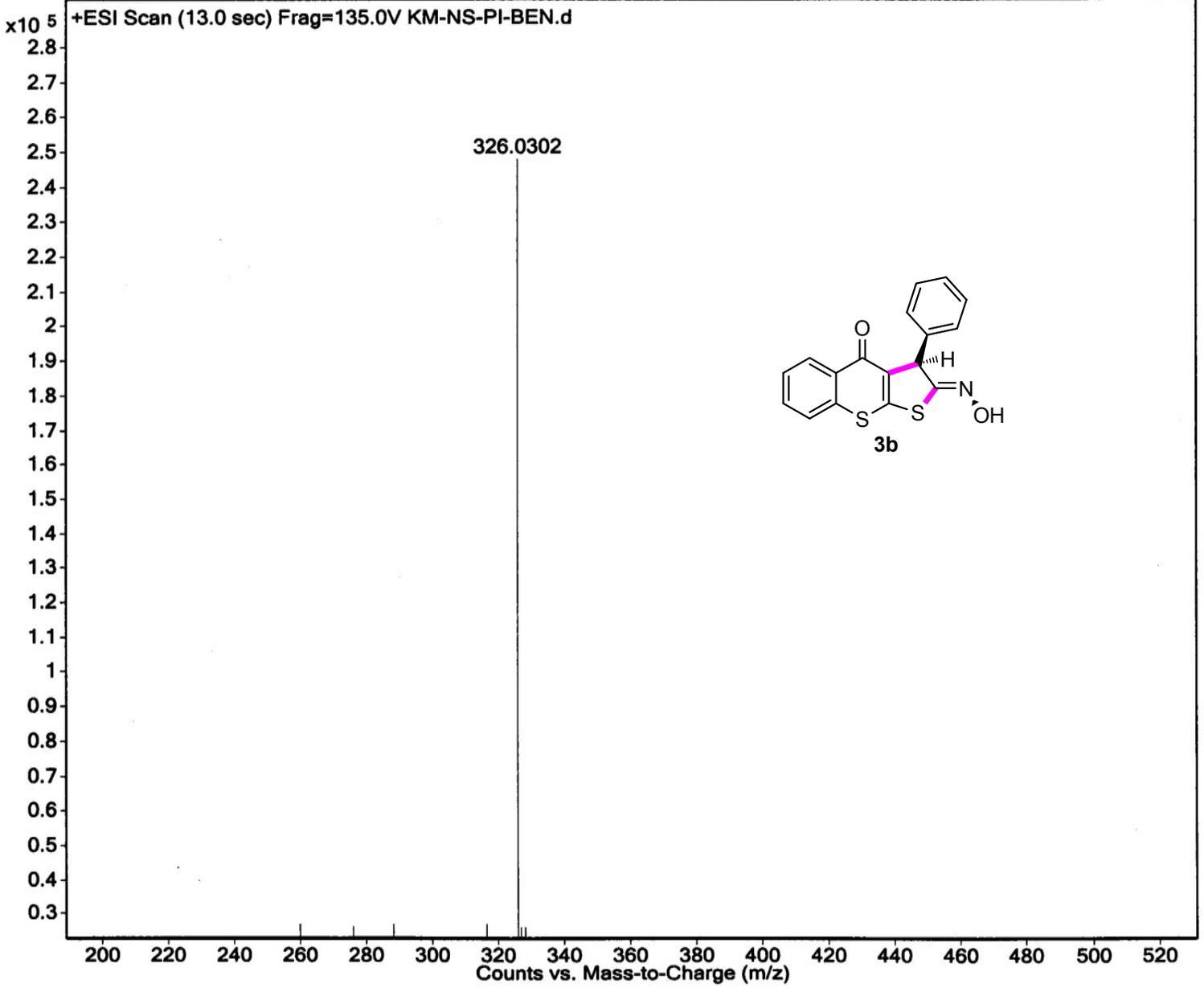
172.78
152.90
149.03
140.15
135.19
131.94
130.63
130.12
128.57
128.31
127.92
127.17
126.90

54.19
40.13
39.92
39.71
39.50
39.29
39.08
38.87



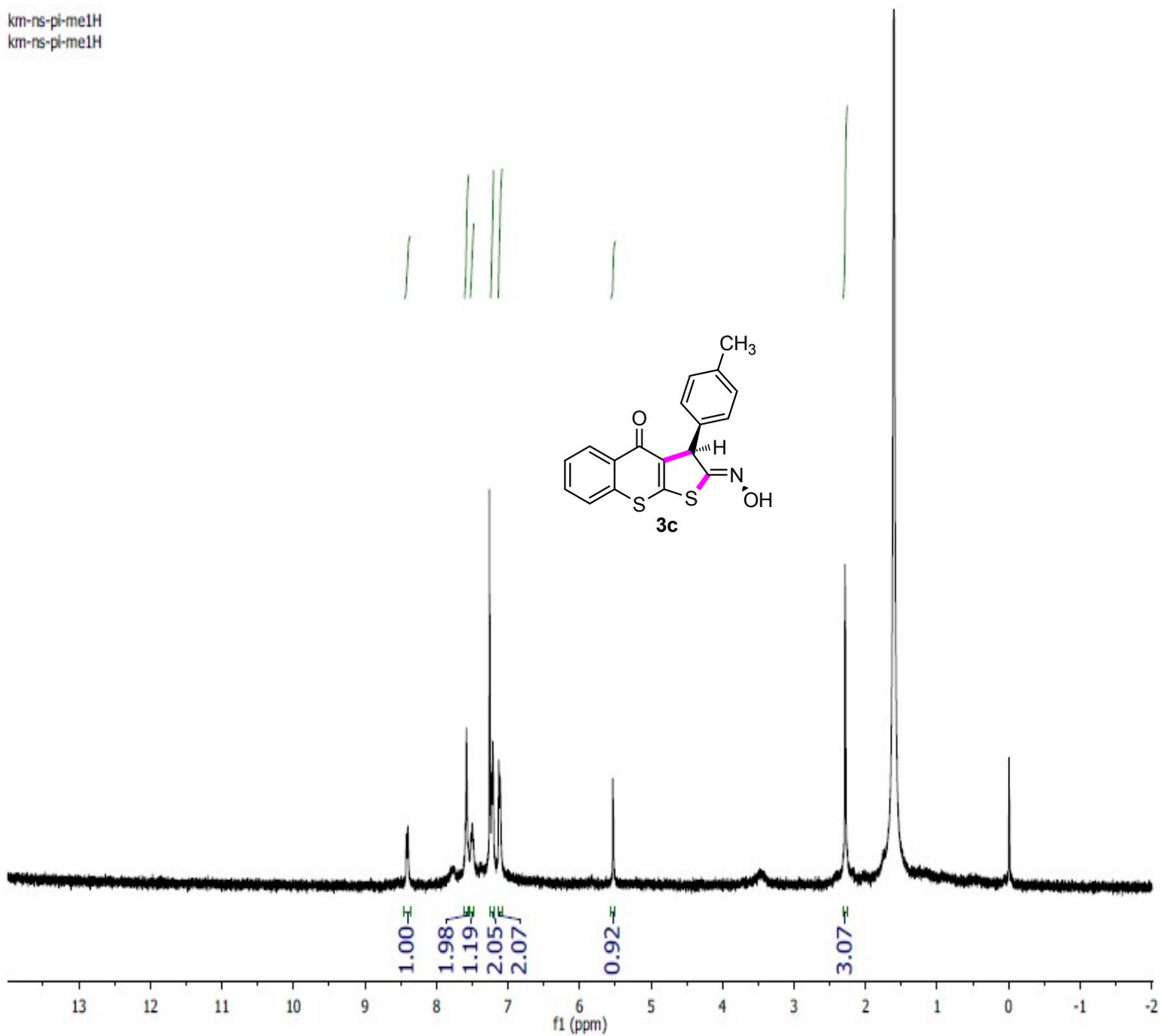
HRMS spectra of compound: 3b

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Inj Vol	InjPosition	SampleType	IRM Calibration Status
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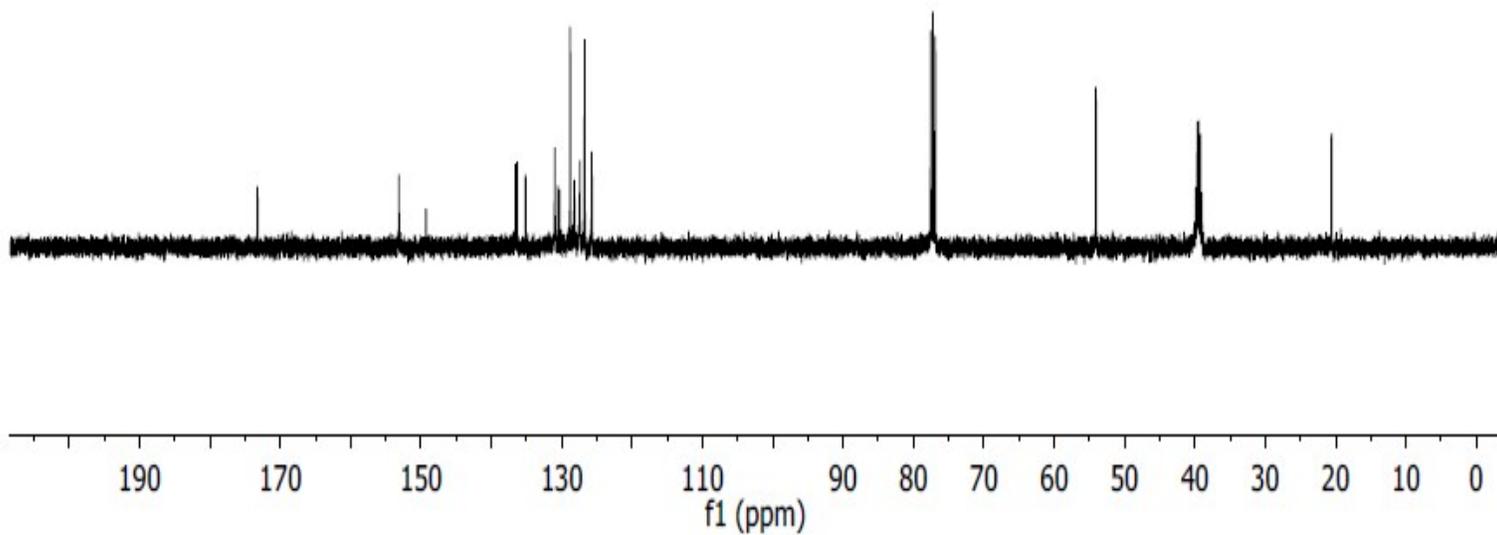
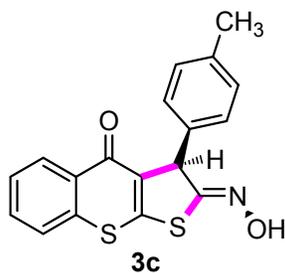
¹H NMR spectra of compound: 3c

km-ns-pl-me1H
km-ns-pl-me1H



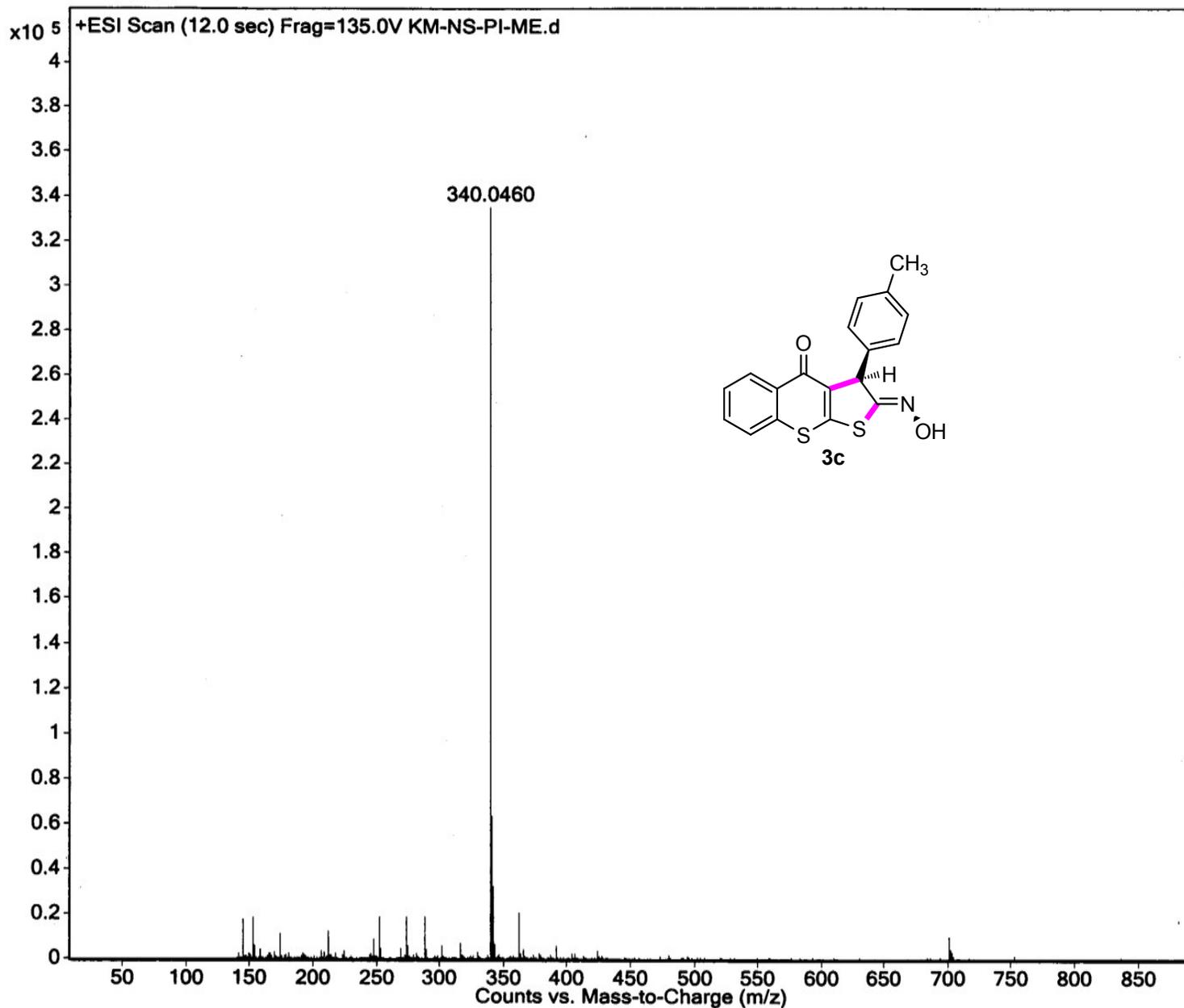
¹³CNMR spectra of compound: 3c

KM-NS-PI-1R-13C
KM-NS-PI-1R-13C



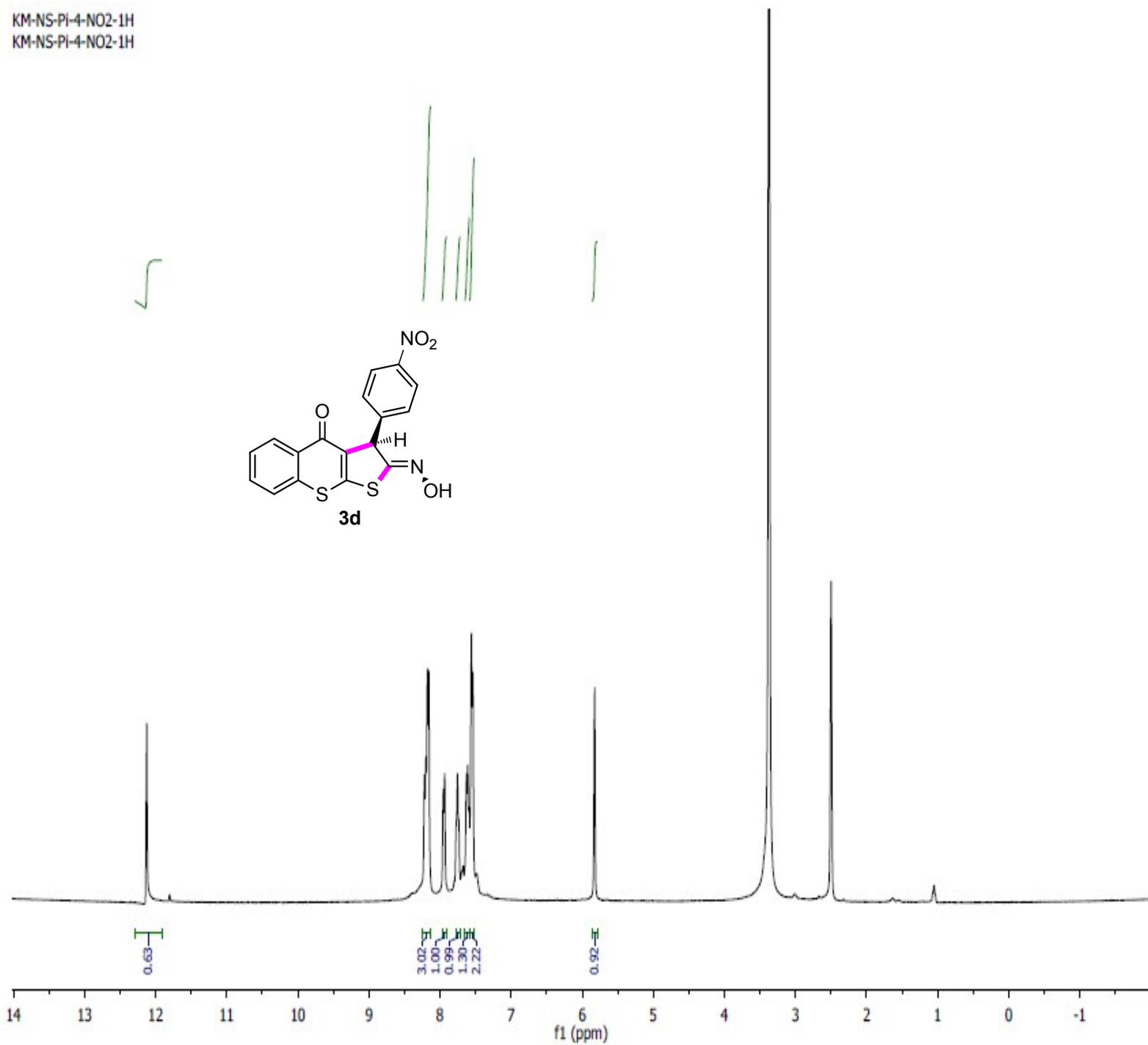
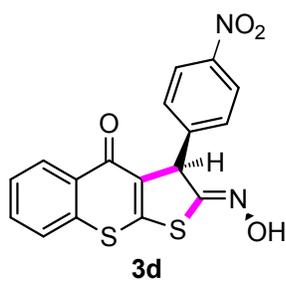
HRMS spectra of compound: 3c

Sample Name	KM-NS-PI-ME	Position	Vial 1	Instrument Name	Instrument 1	User Name	
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¹H NMR spectra of compound: 3d

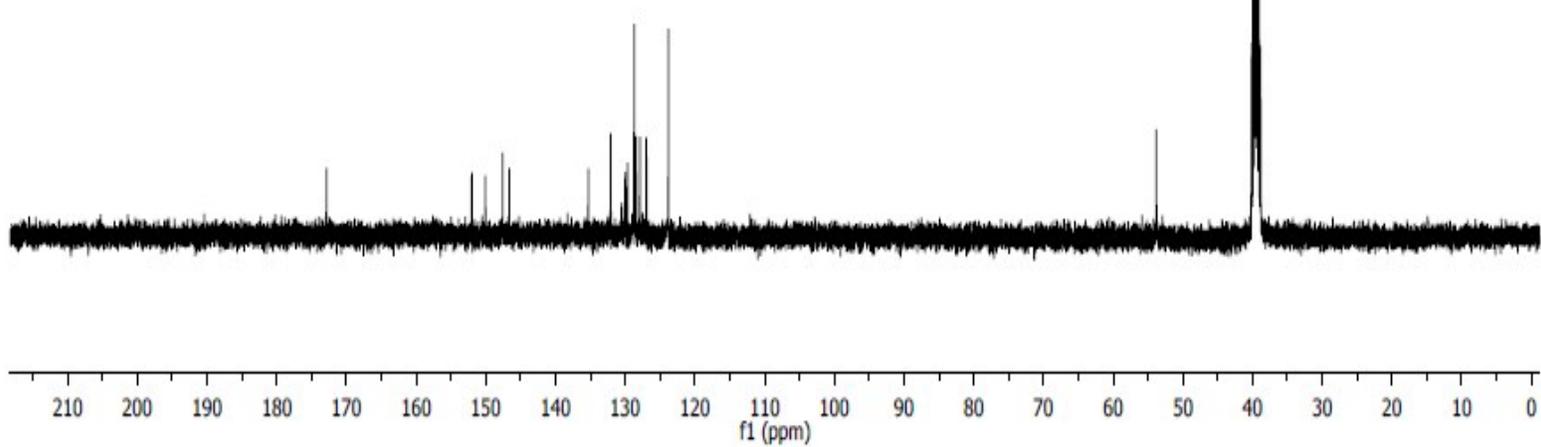
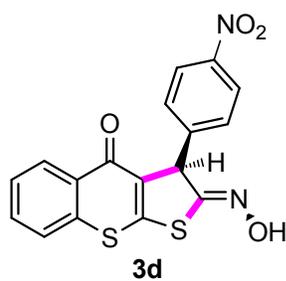
KM-NS-PI-4-NO2-1H
KM-NS-PI-4-NO2-1H



¹³CNMR spectra of compound: 3d

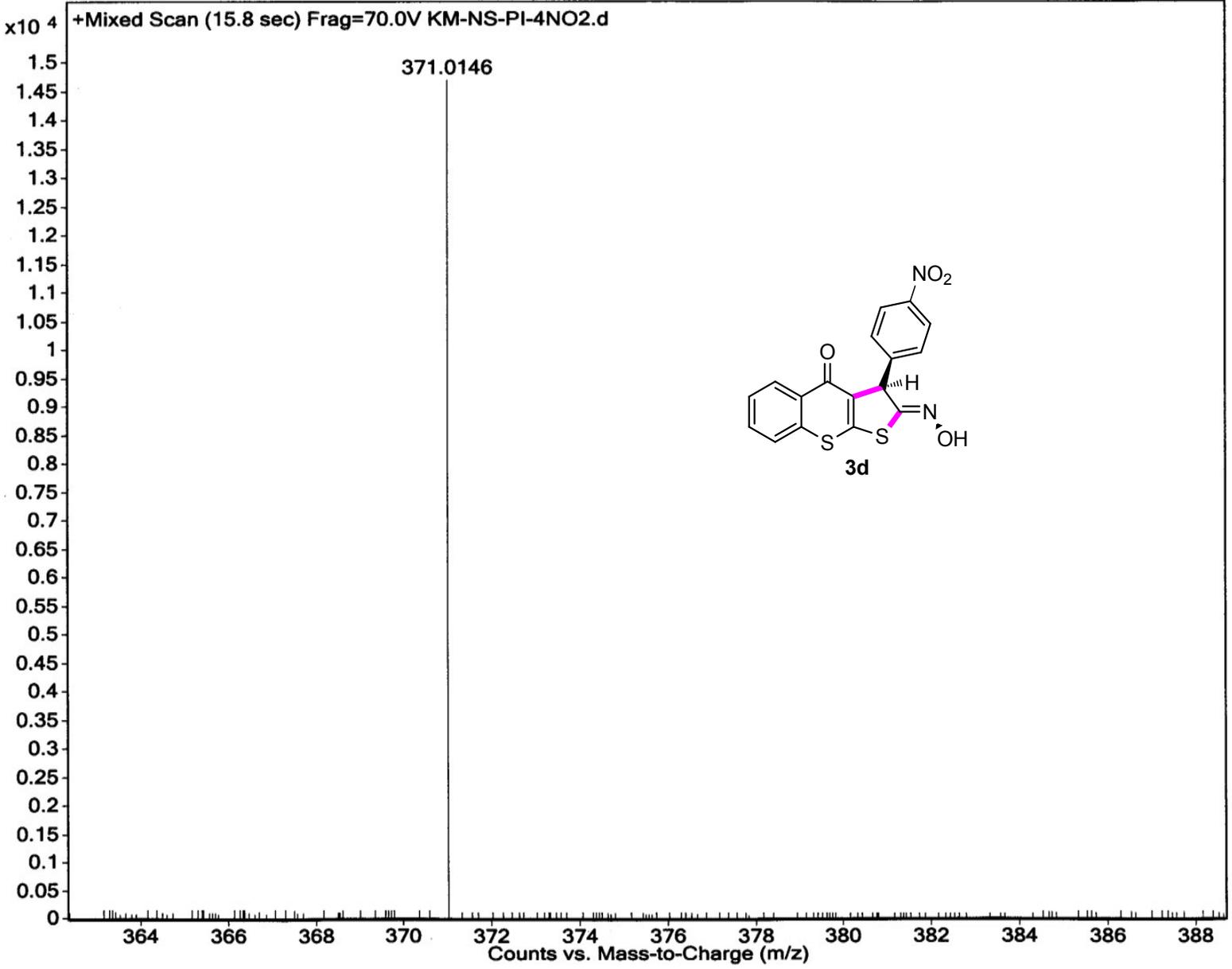
KM-NS-PI-4-NO2-13C
KM-NS-PI-4-NO2-13C

—172.83
152.01
150.05
147.57
146.62
135.28
132.07
130.00
129.68
128.71
128.42
127.88
126.95
123.79
53.81
40.12
39.92
39.71
39.50
39.29
39.08
38.88



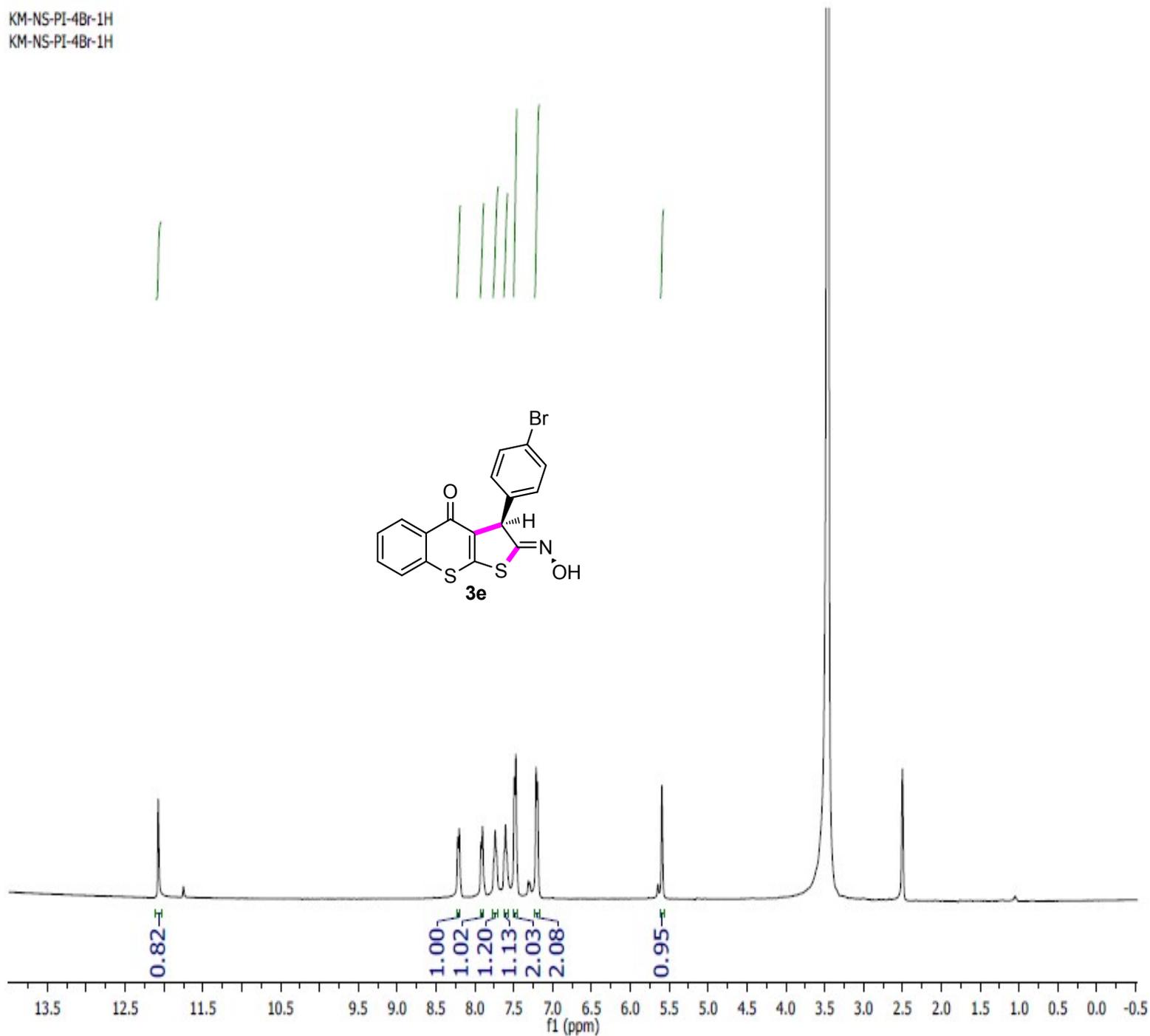
HRMS spectra of compound: 3d

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Data Filename	ACQ Method	Comment	Acquired Time



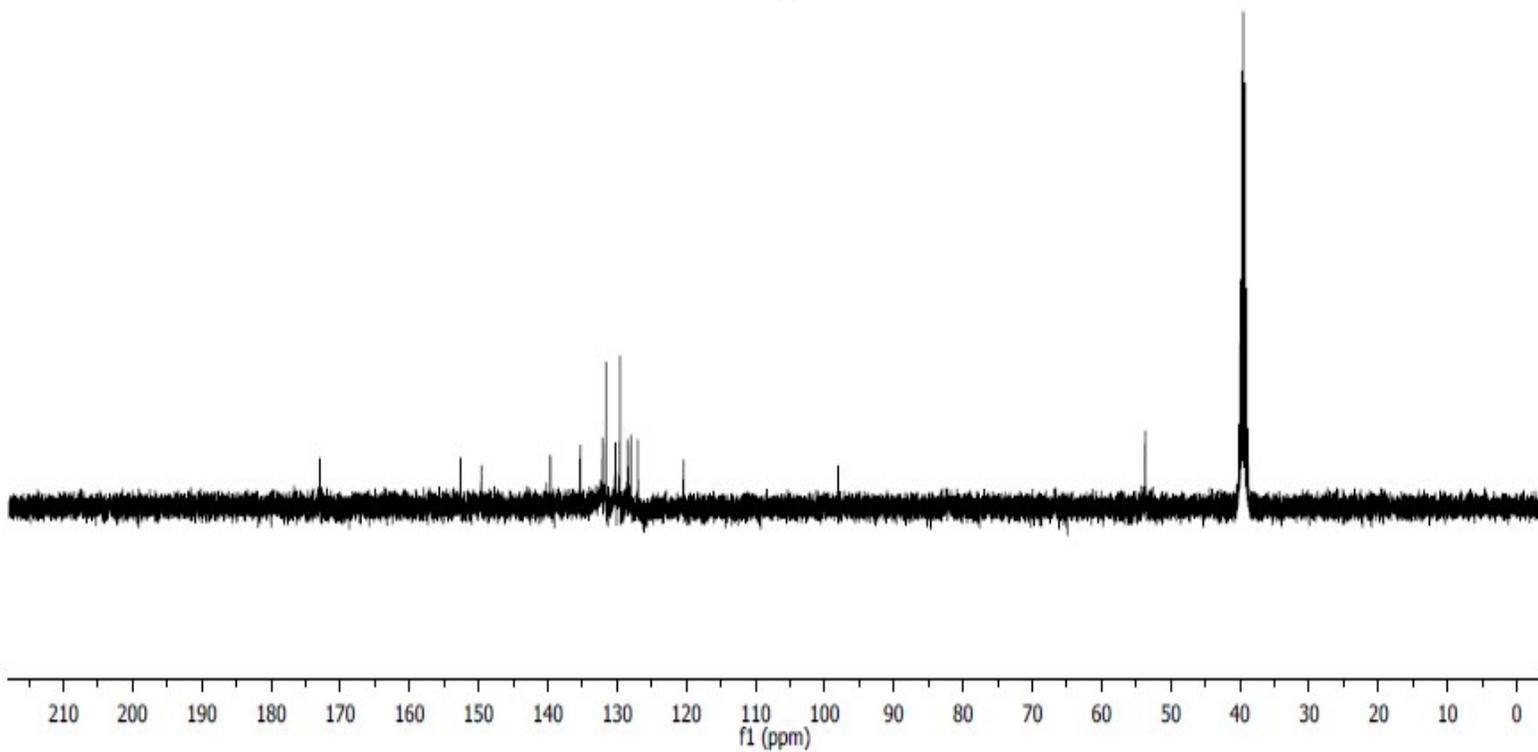
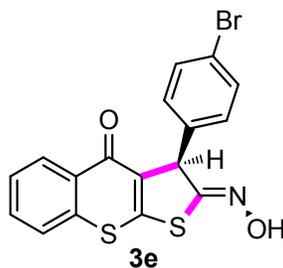
¹H NMR spectra of compound: 3e

KM-NS-PI-4Br-1H
KM-NS-PI-4Br-1H



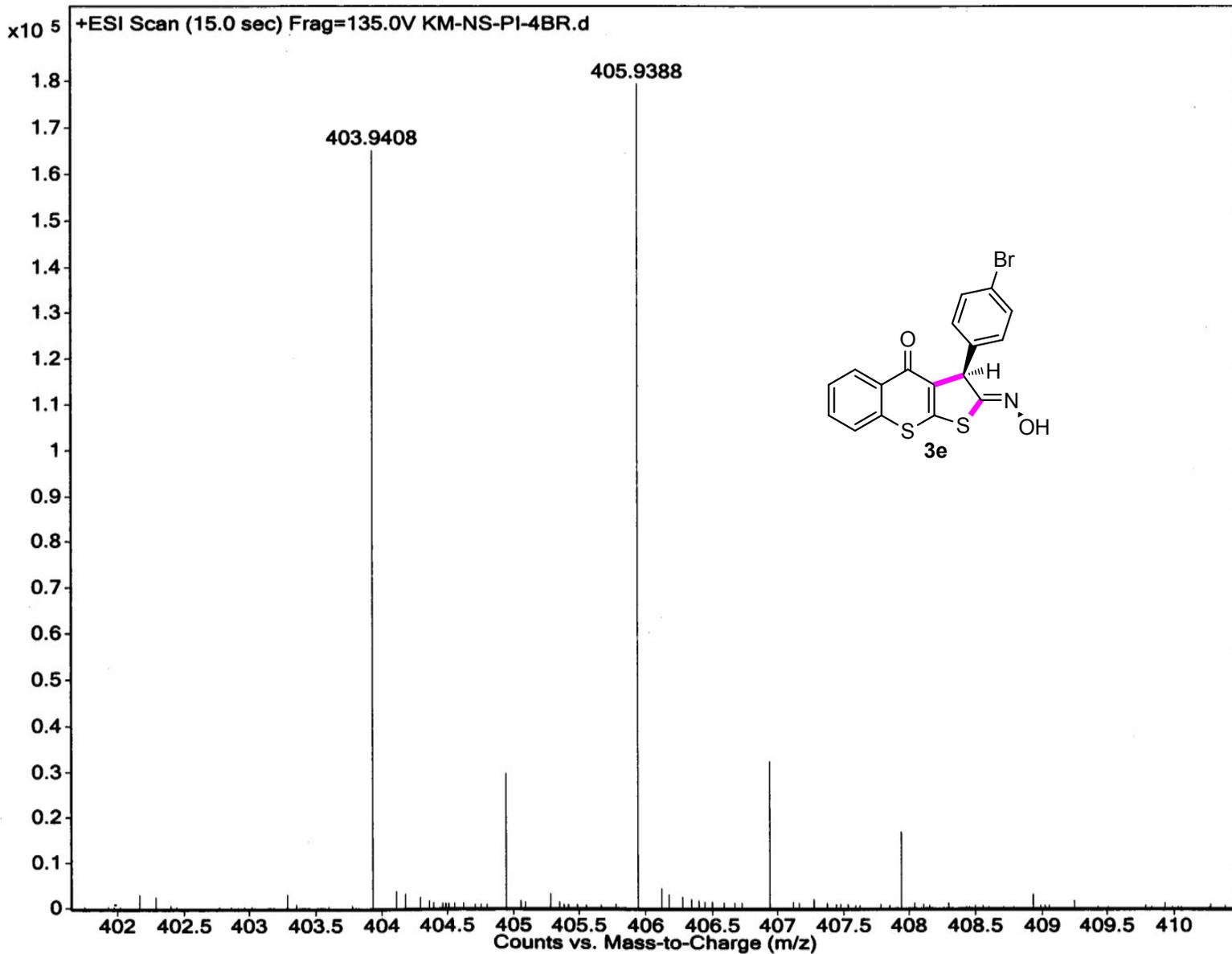
¹³CNMR spectra of compound: 3e

KM-NS-4Br-13C
KM-NS-4Br-13C



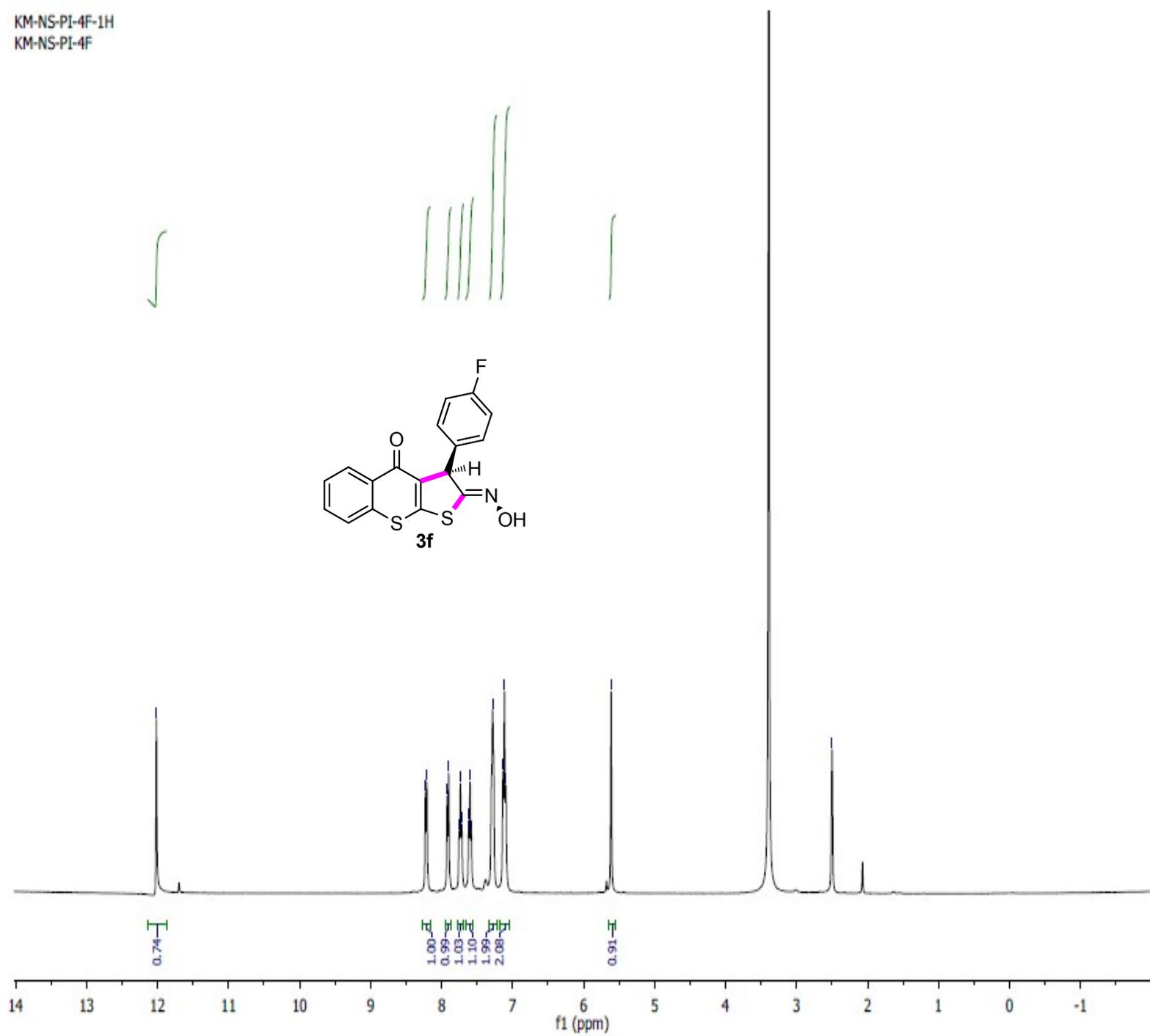
HRMS spectra of compound: 3e

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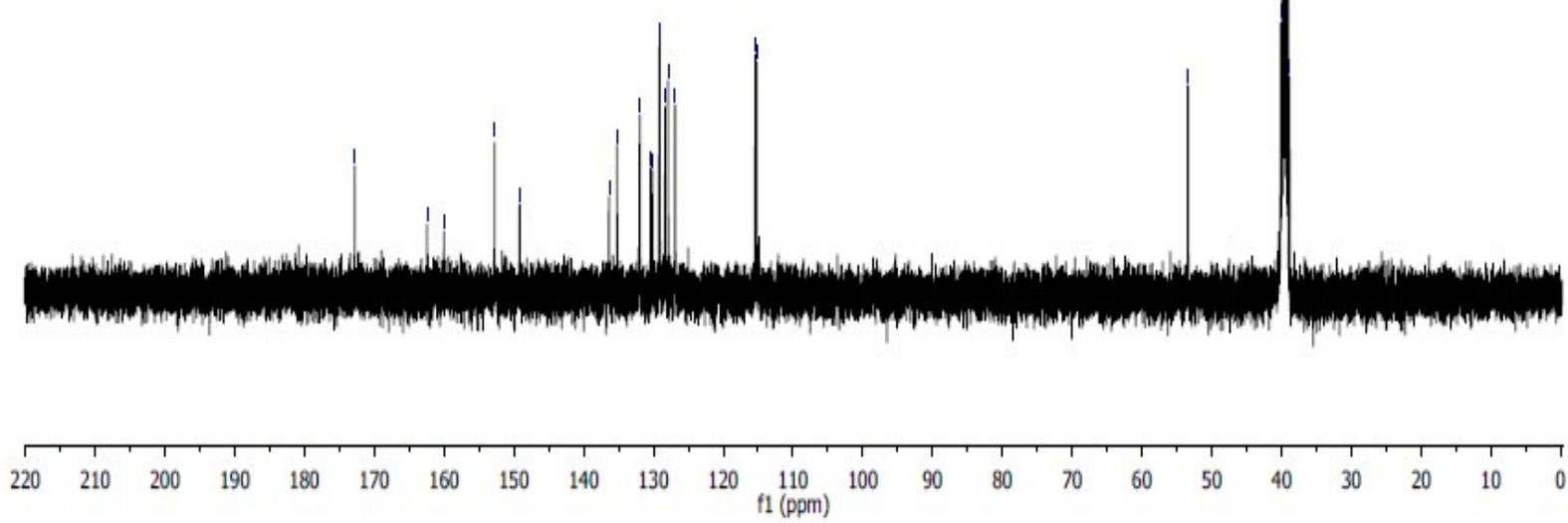
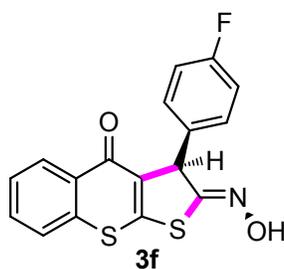
¹H NMR spectra of compound: 3f

KM-NS-PI-4F-1H
KM-NS-PI-4F



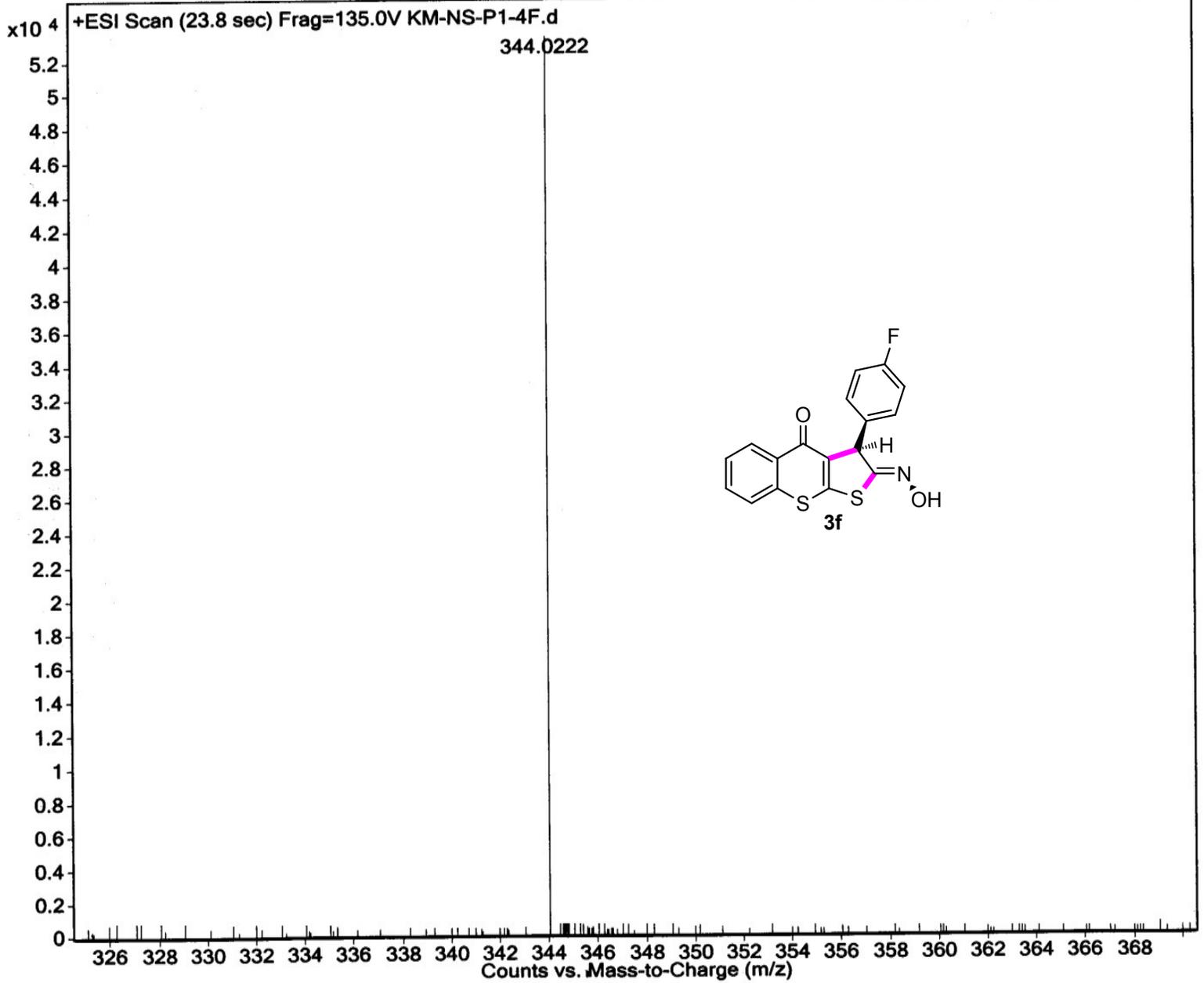
¹³CNMR spectra of compound: 3f

KM-NS-PI-4F-13C
KM-NS-PI-4F-13C



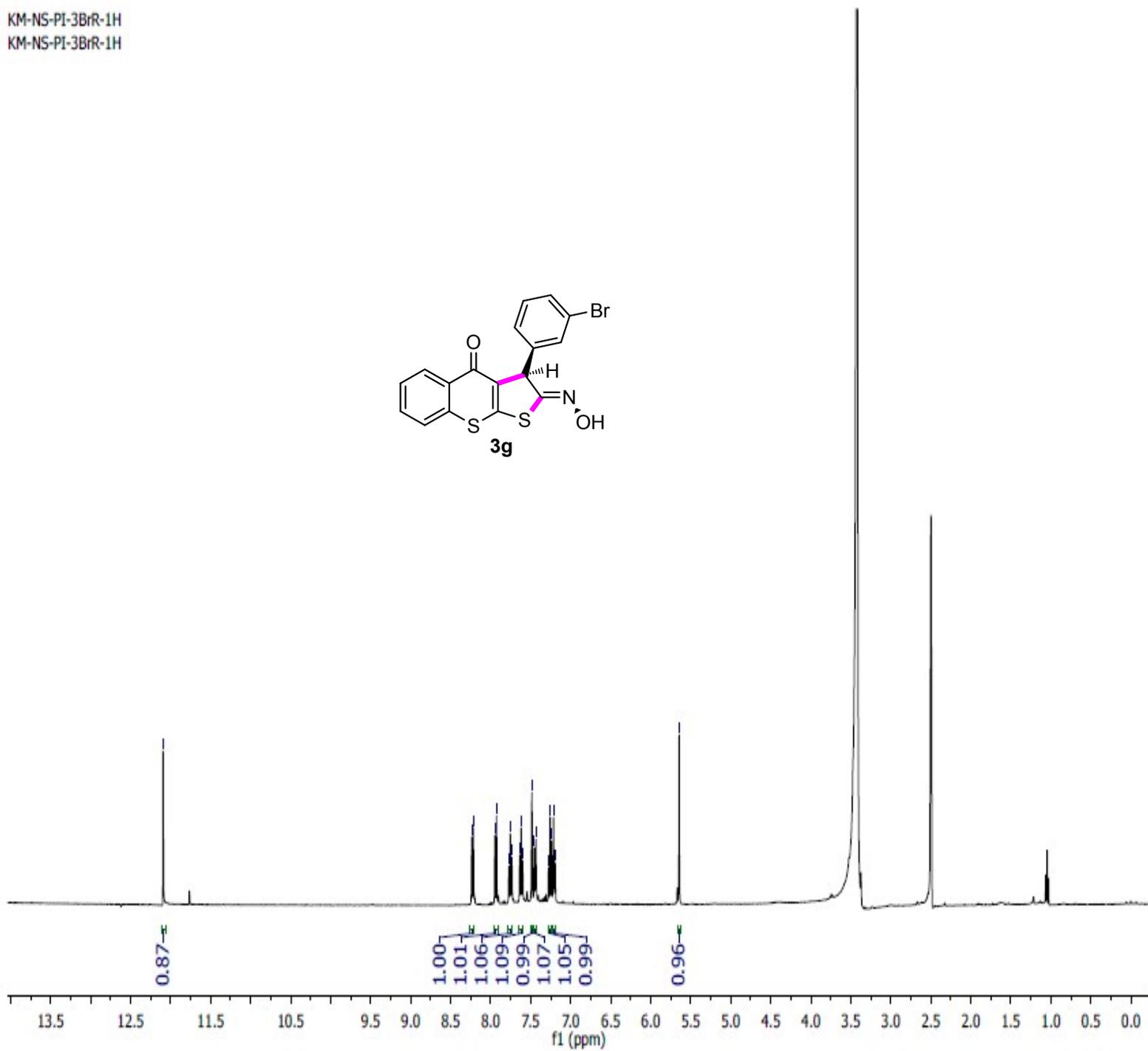
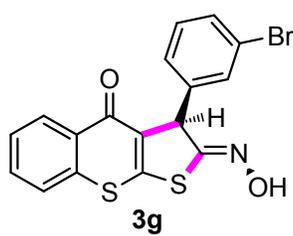
HRMS spectra of compound: 3f

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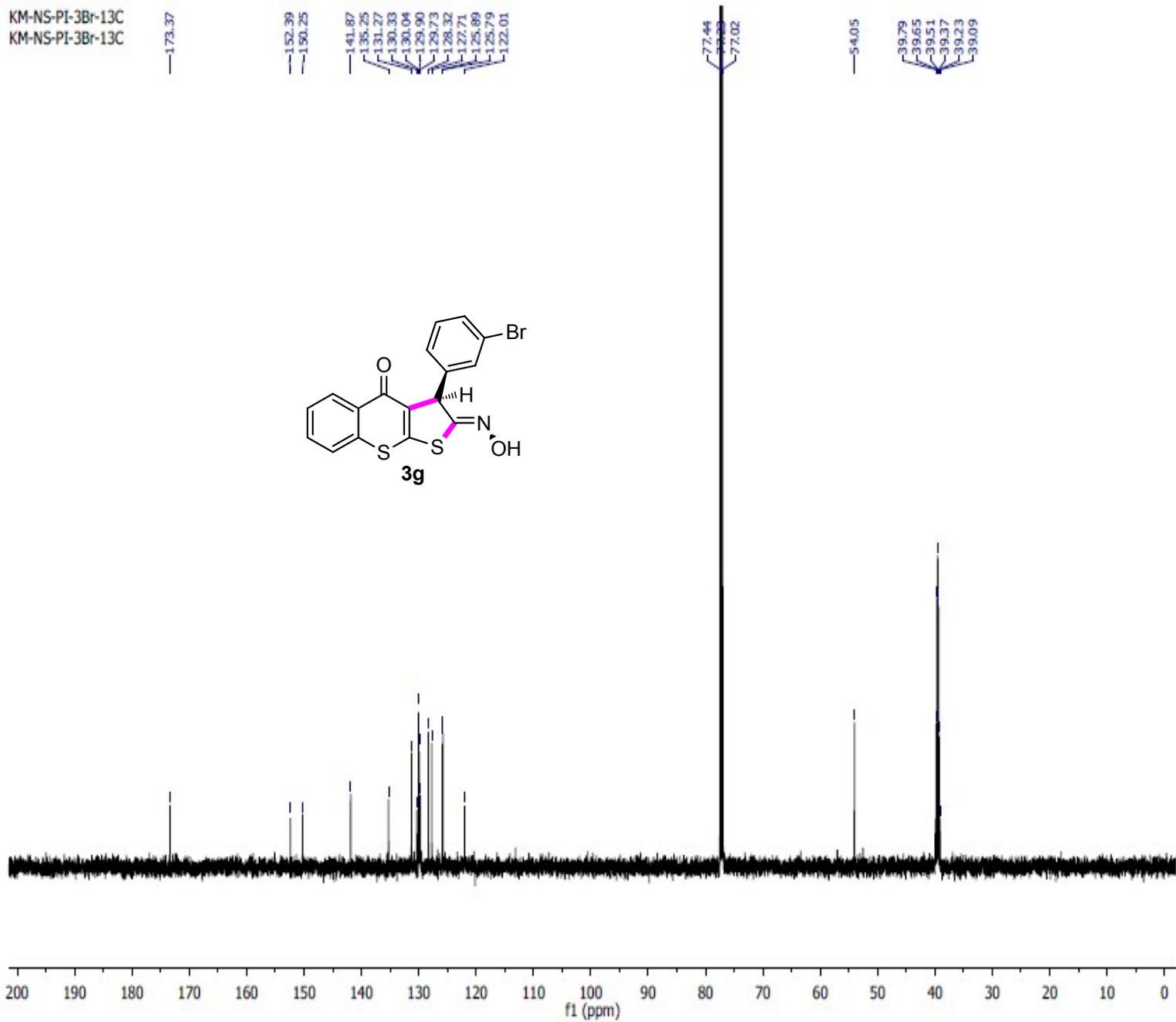
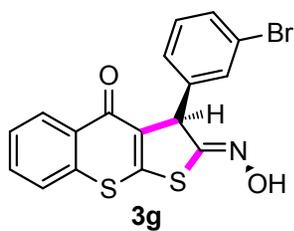
¹H NMR spectra of compound: 3g

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KM-NS-PI-3BrR-1H



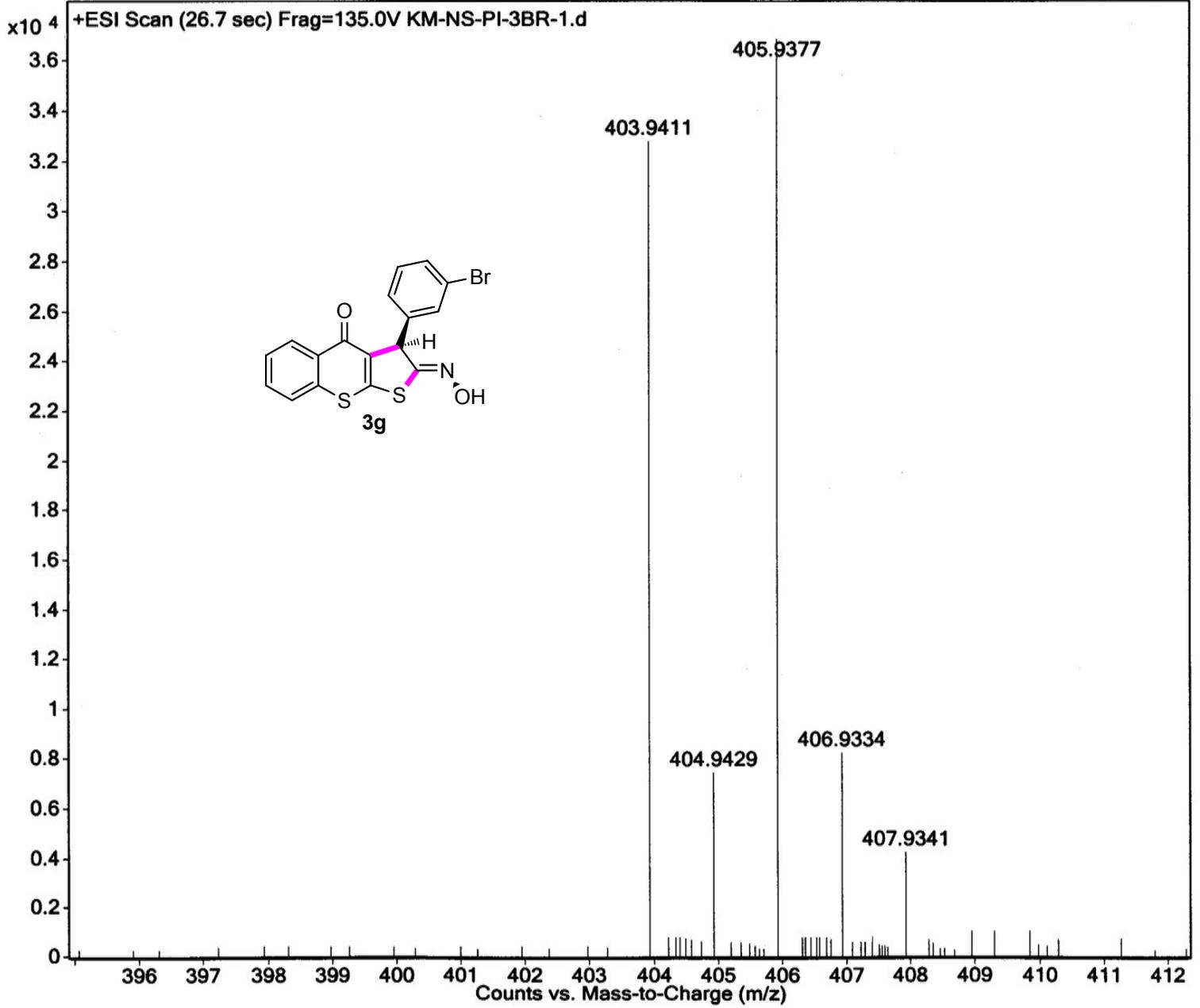
¹³CNMR spectra of compound: 3g

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KM-NS-PI-3Br-13C



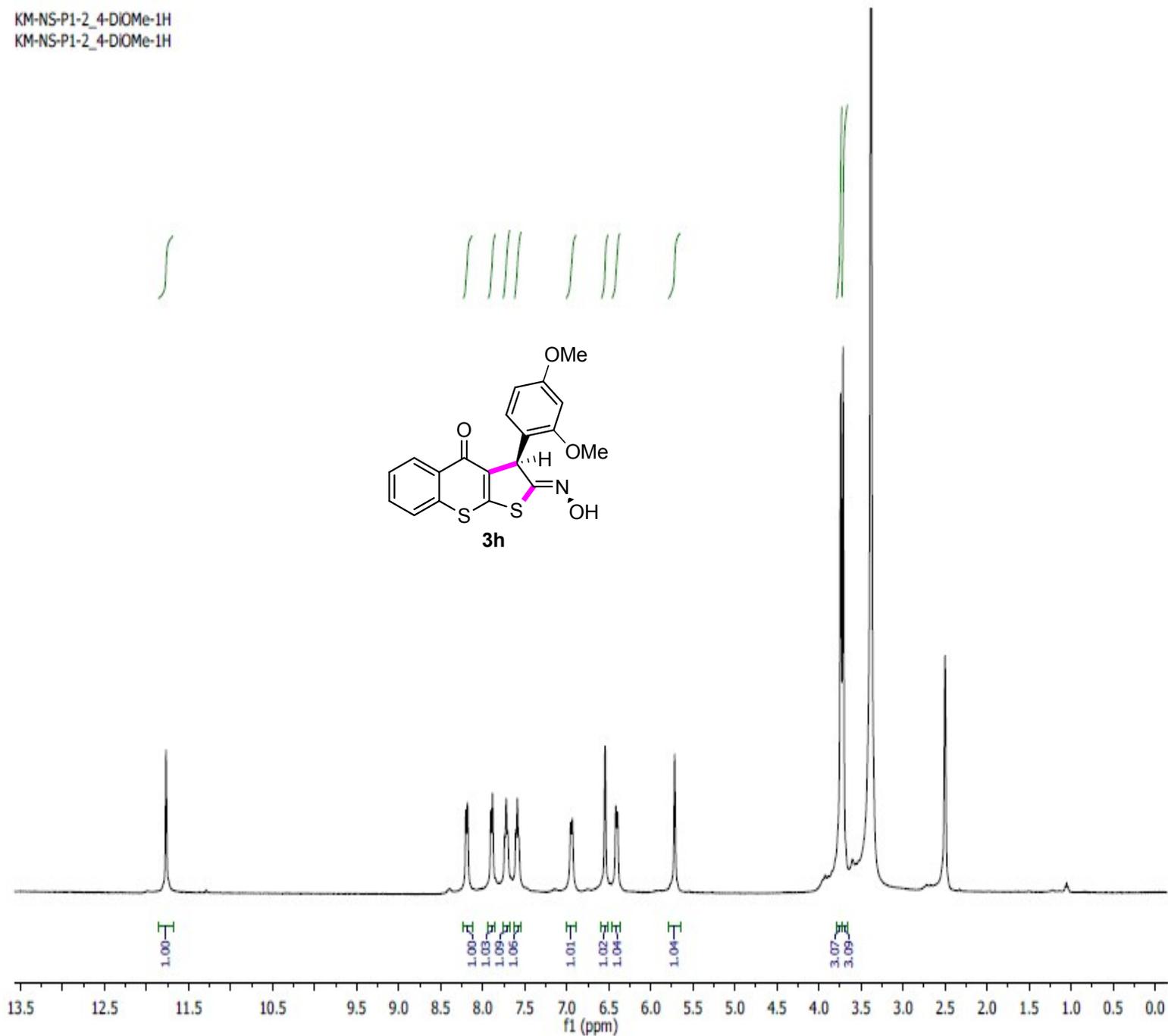
HRMS spectra of compound: 3g

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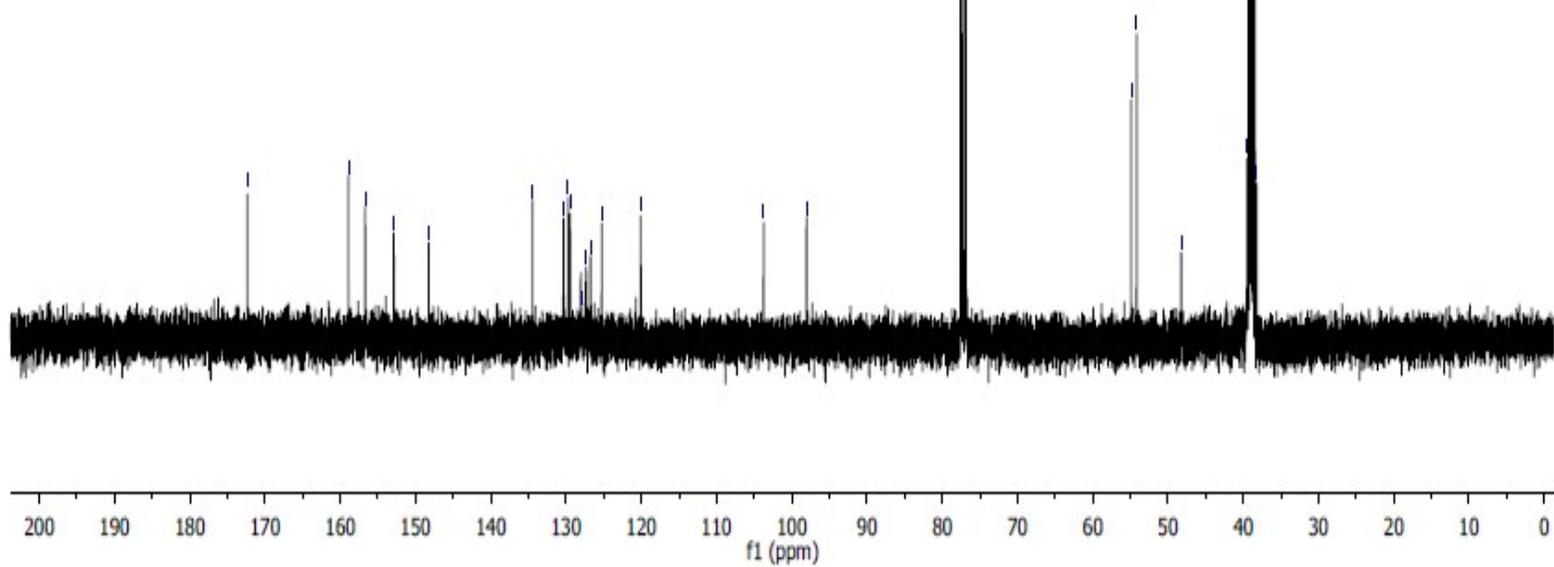
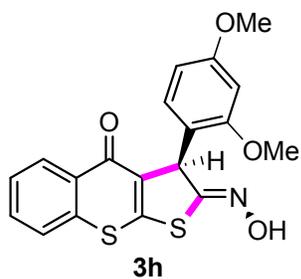
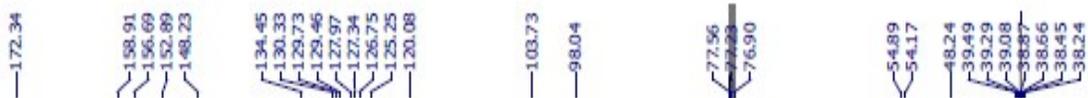
¹H NMR spectra of compound: 3h

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KM-NS-P1-2_4-DIOMe-1H



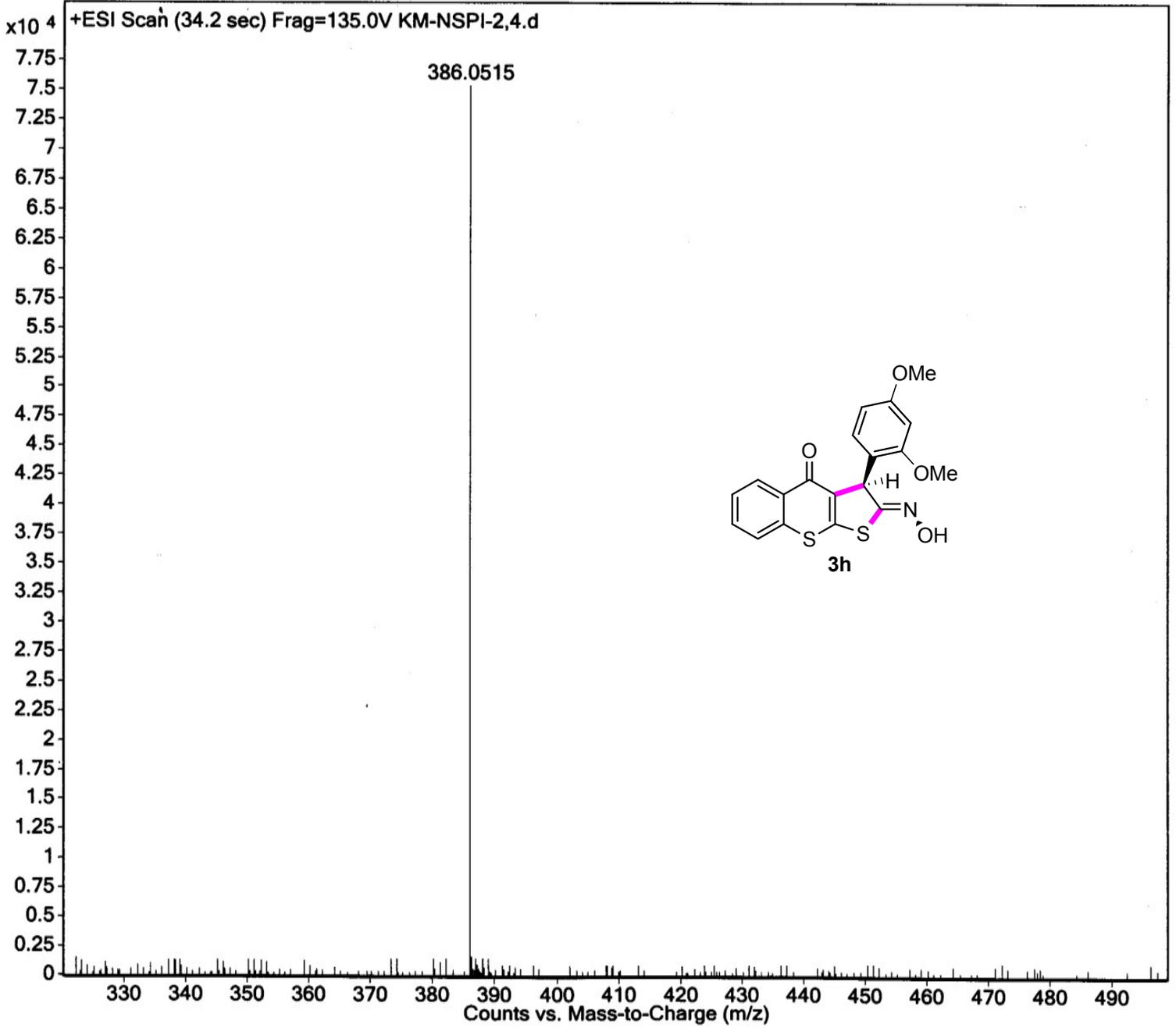
¹³CNMR spectra of compound: 3h

KM-NS-PI-2-13C
KM-NS-PI-2-13C



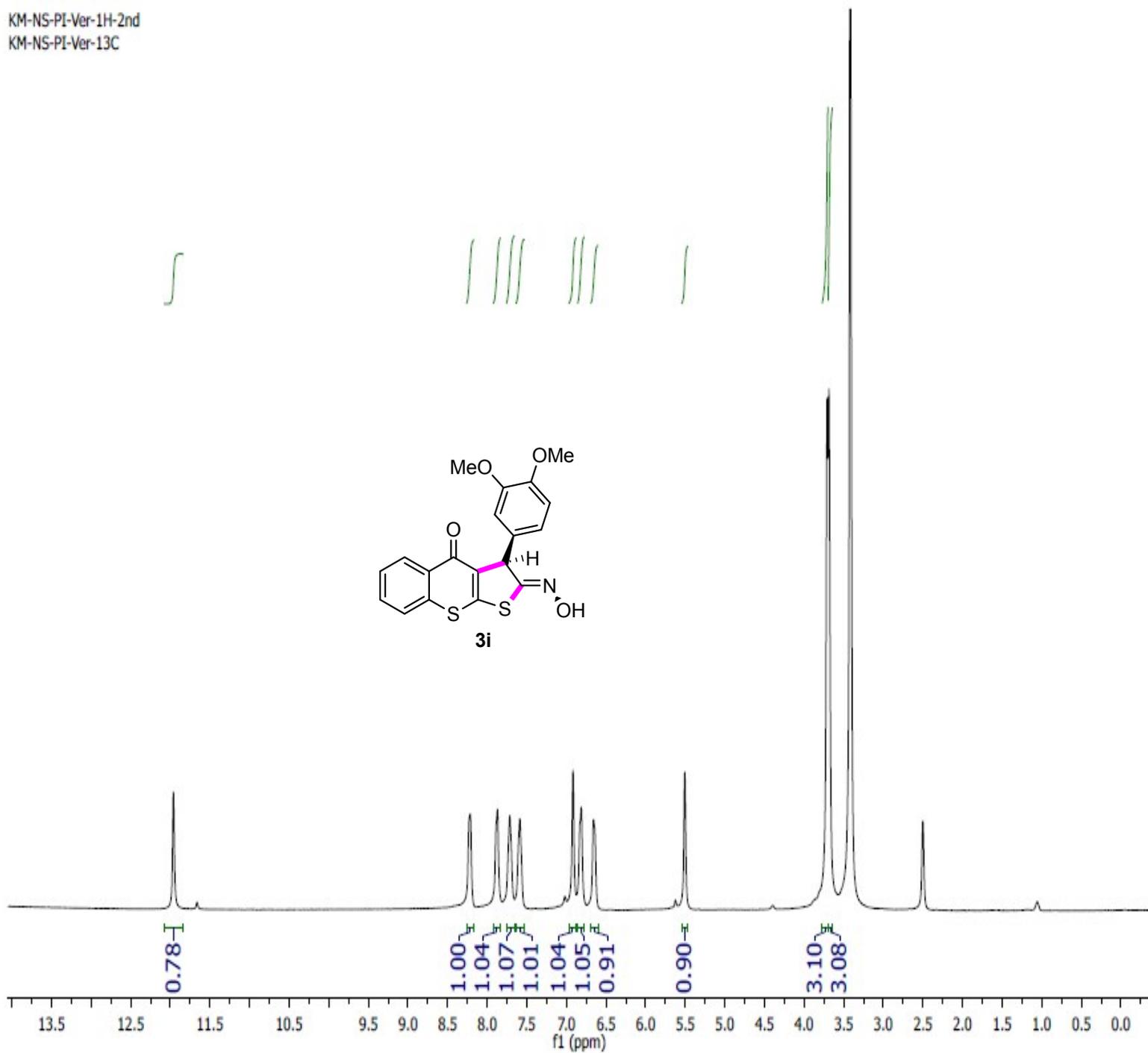
HRMS spectra of compound: 3h

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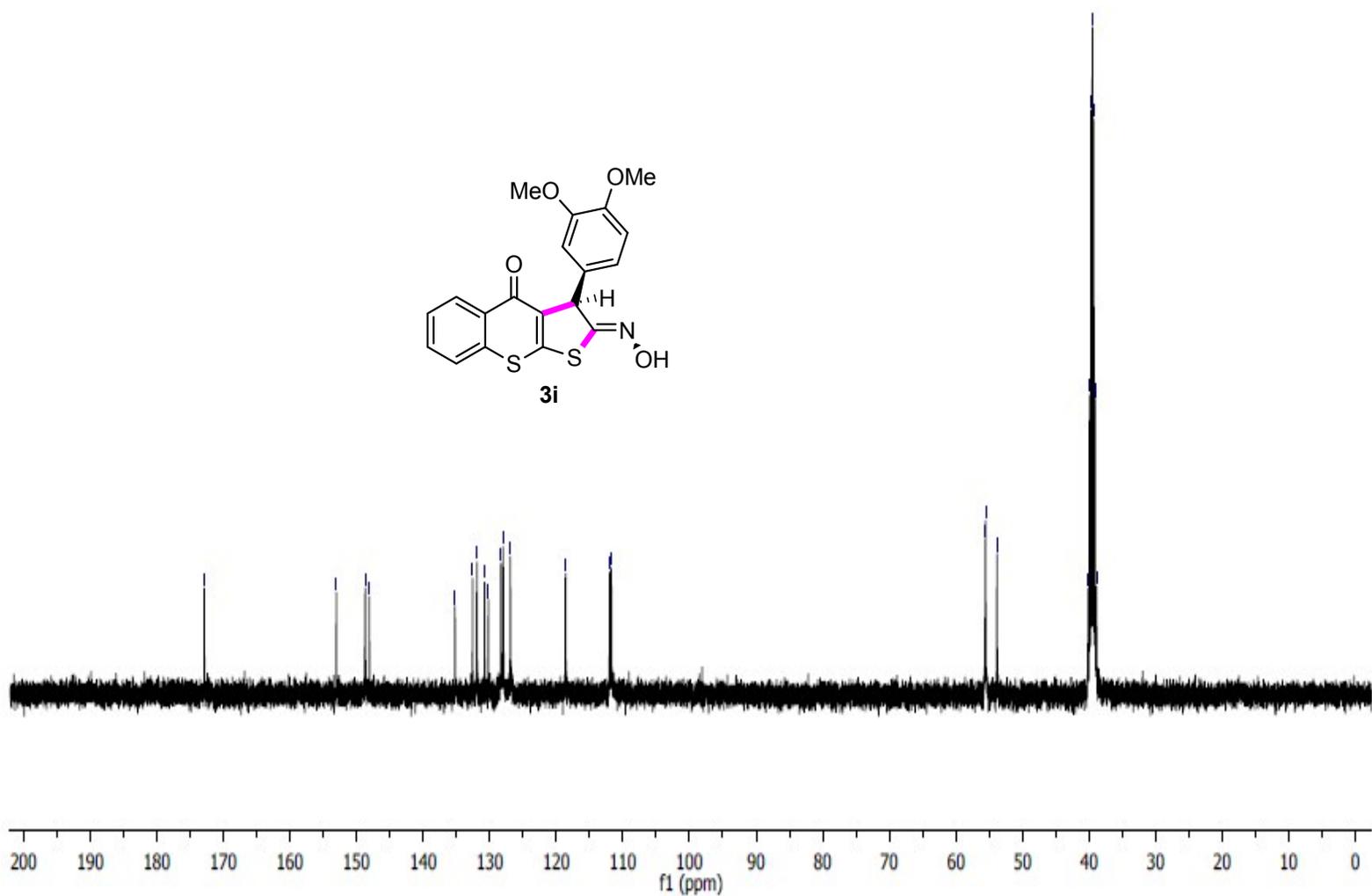
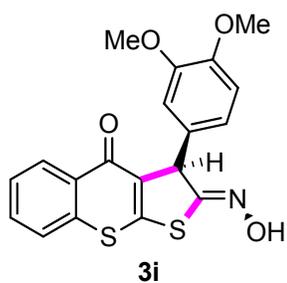
¹HNMR spectra of compound: 3i

KM-NS-PI-Ver-1H-2nd
KM-NS-PI-Ver-13C



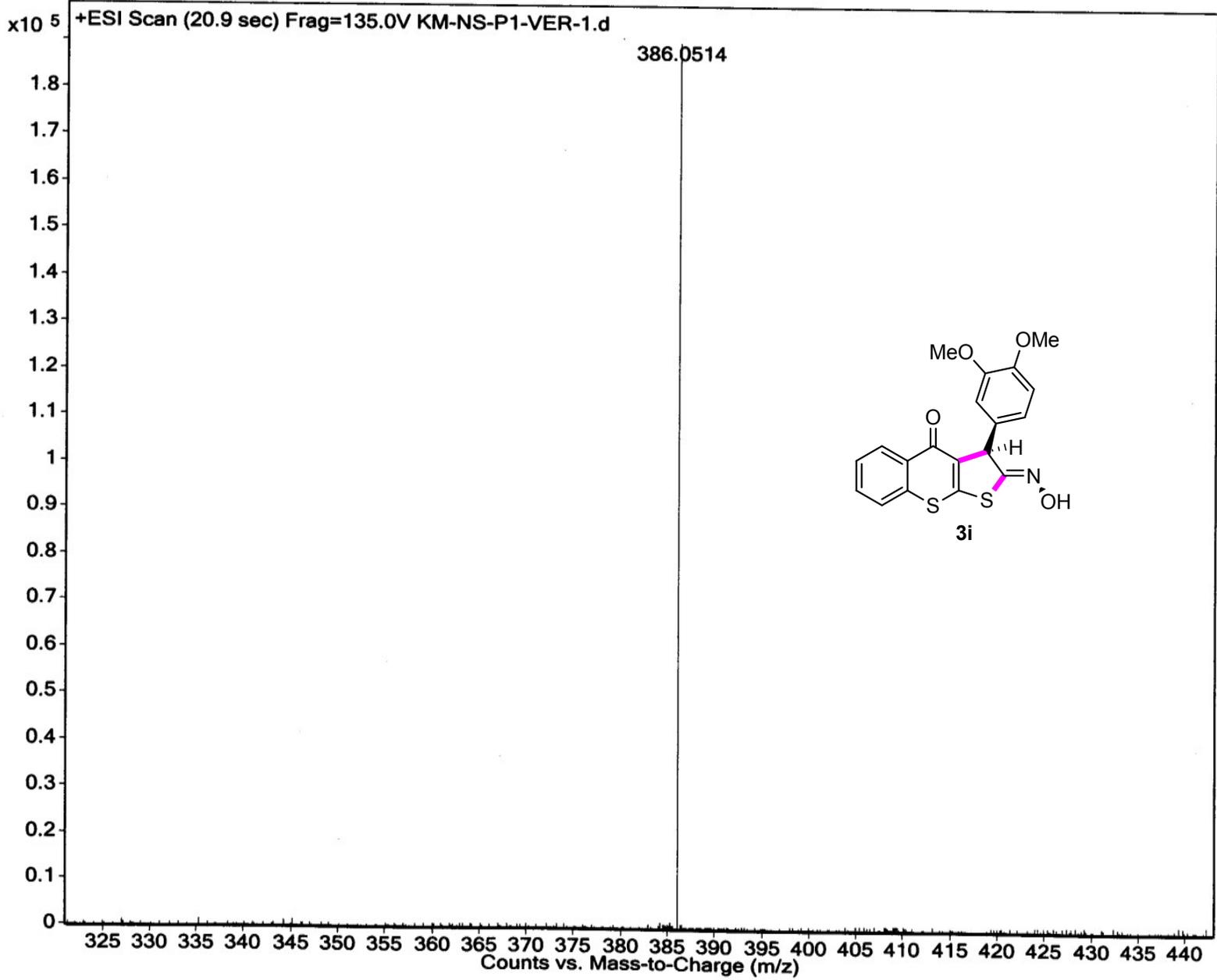
¹³CNMR spectra of compound: 3i

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KM-NS-PI-Ver-13C



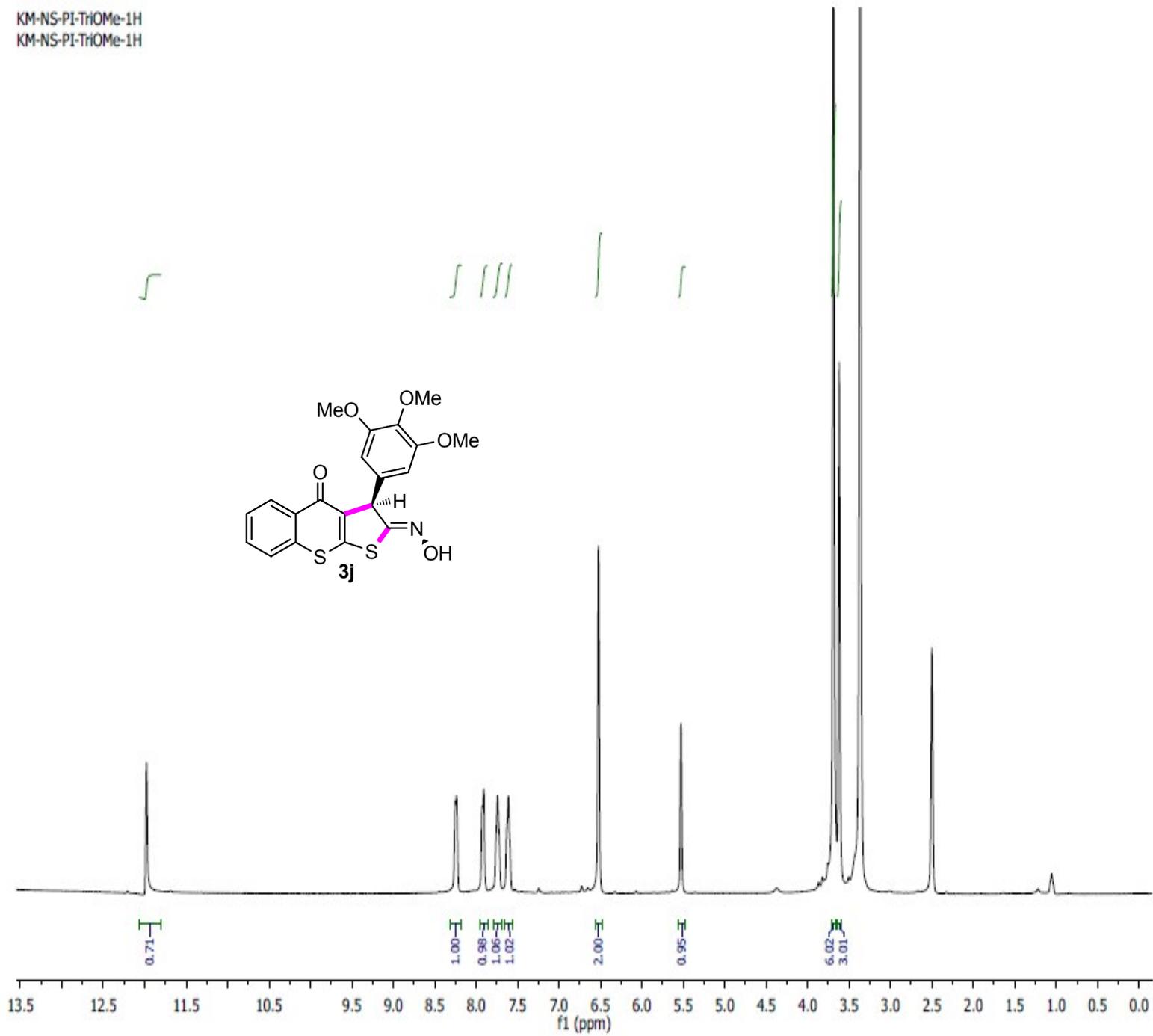
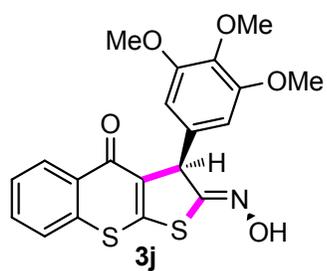
HRMS spectra of compound: 3i

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



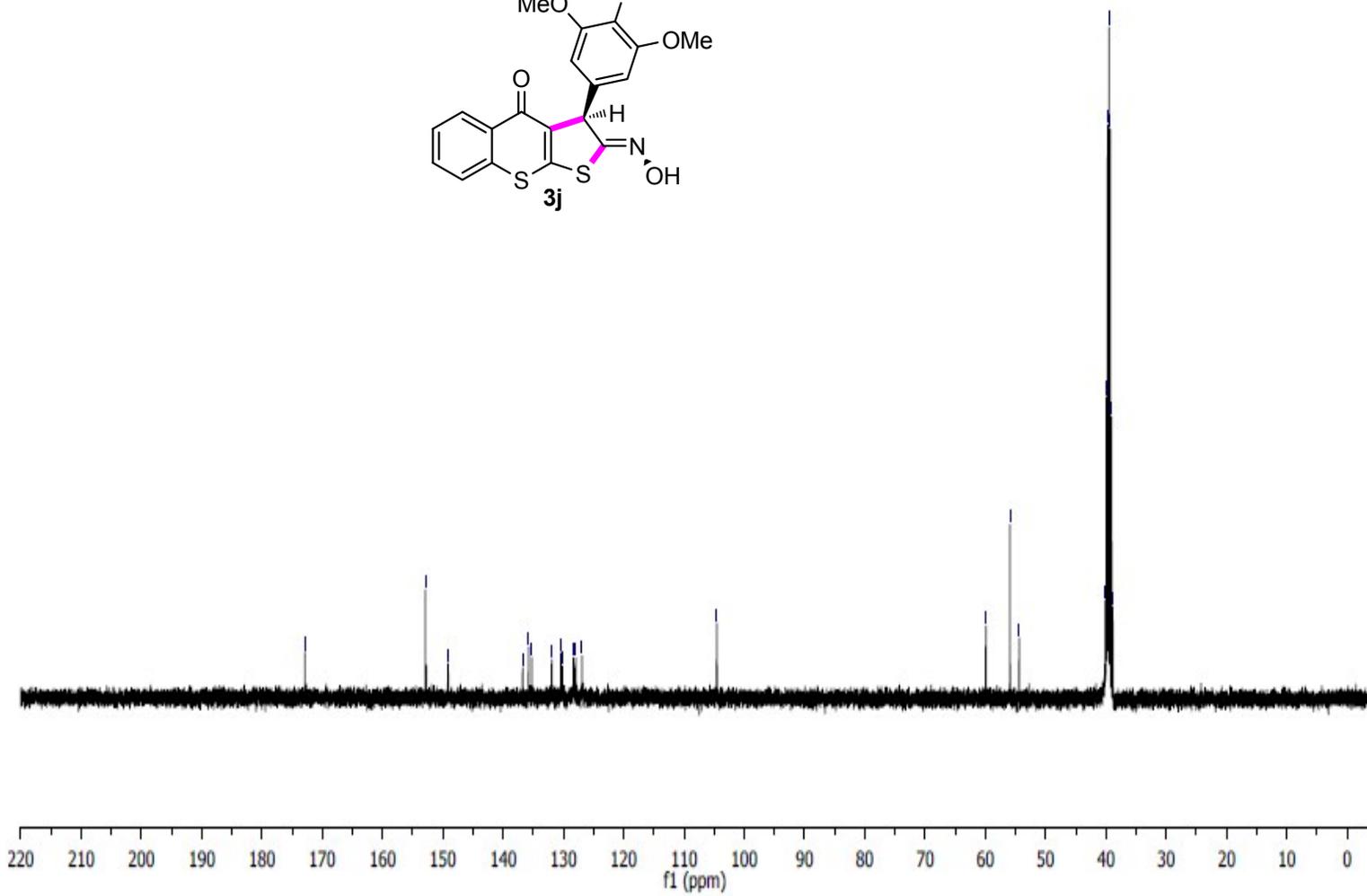
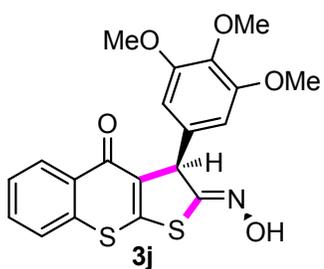
¹H NMR spectra of compound: 3j

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KM-NS-PI-ThOMe-1H



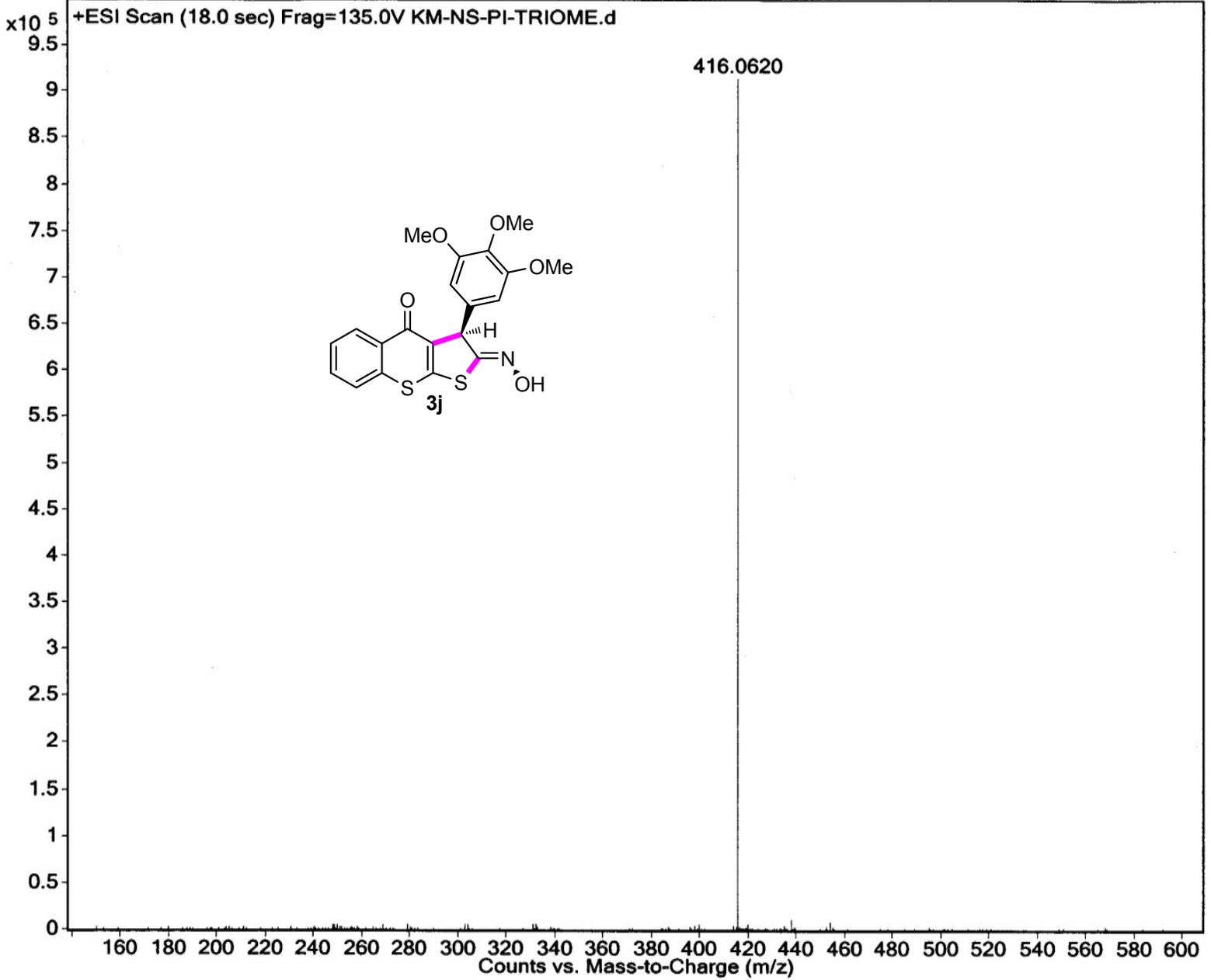
¹³CNMR spectra of compound: 3j

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RK-4CL-N1-TBCH-13C



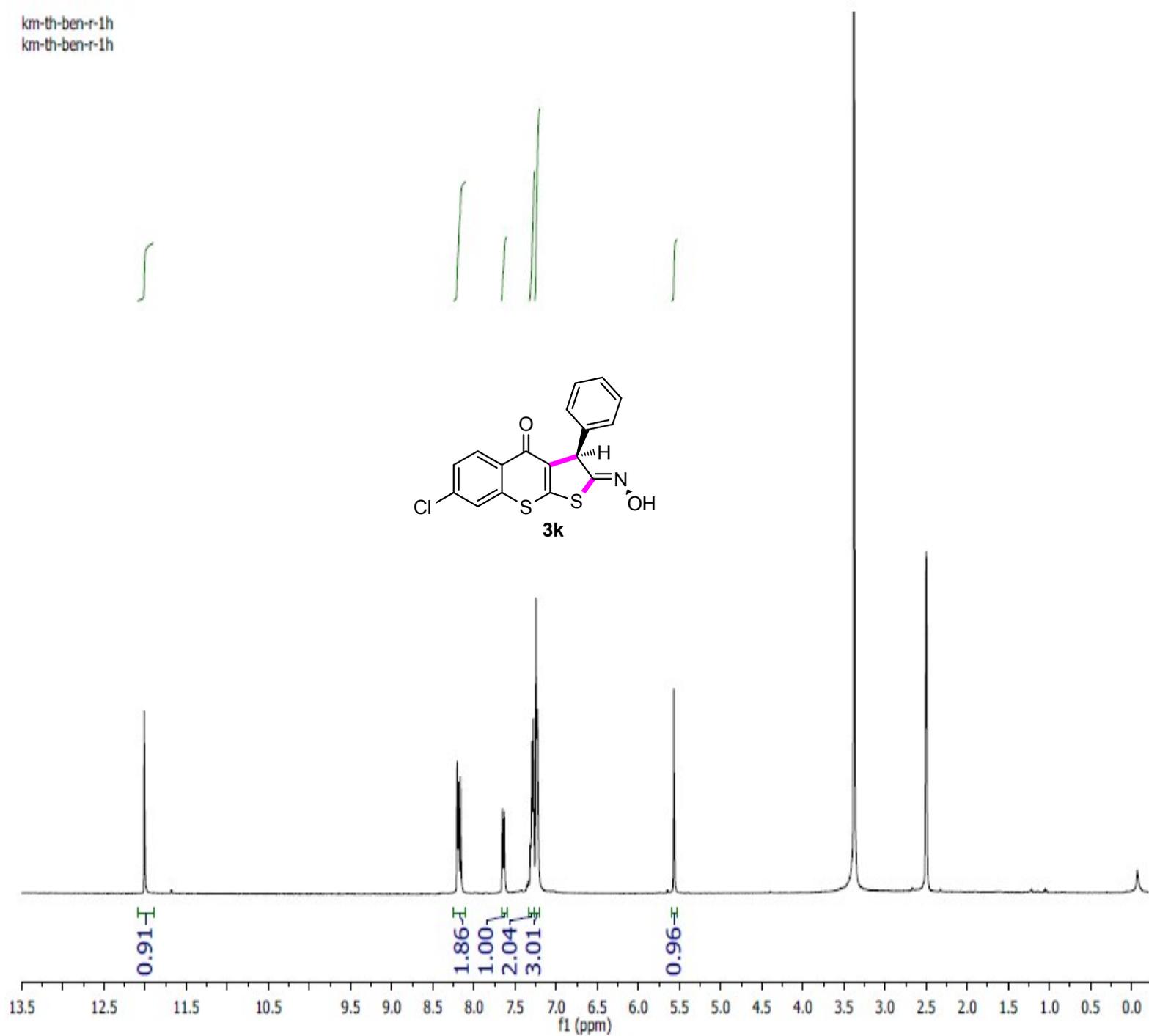
HRMS spectra of compound: 3j

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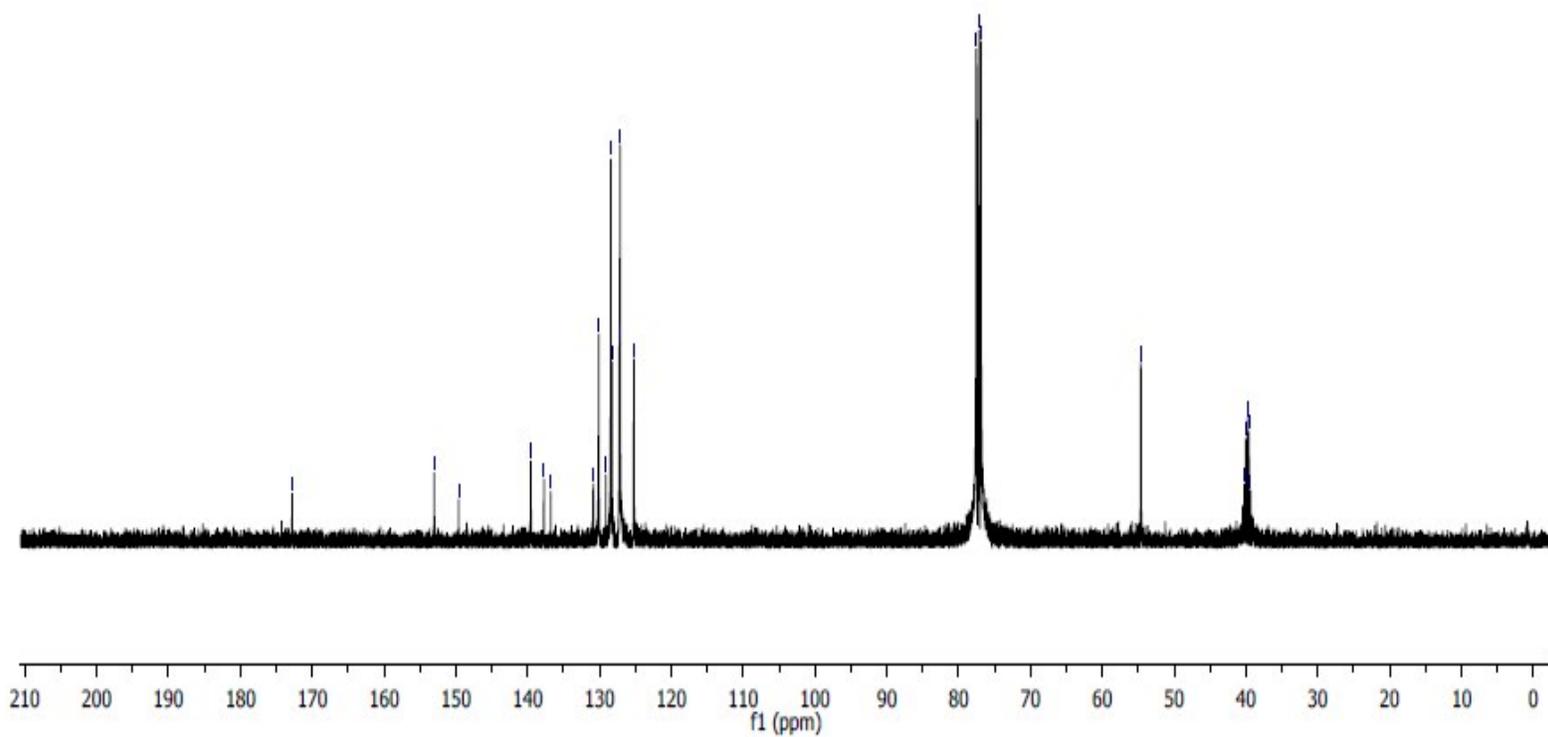
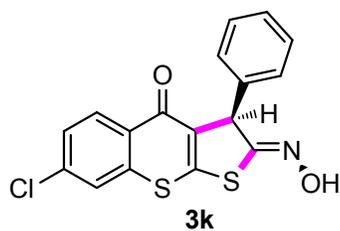
¹H NMR spectra of compound: 3k

km-th-ben-r-1h
km-th-ben-r-1h



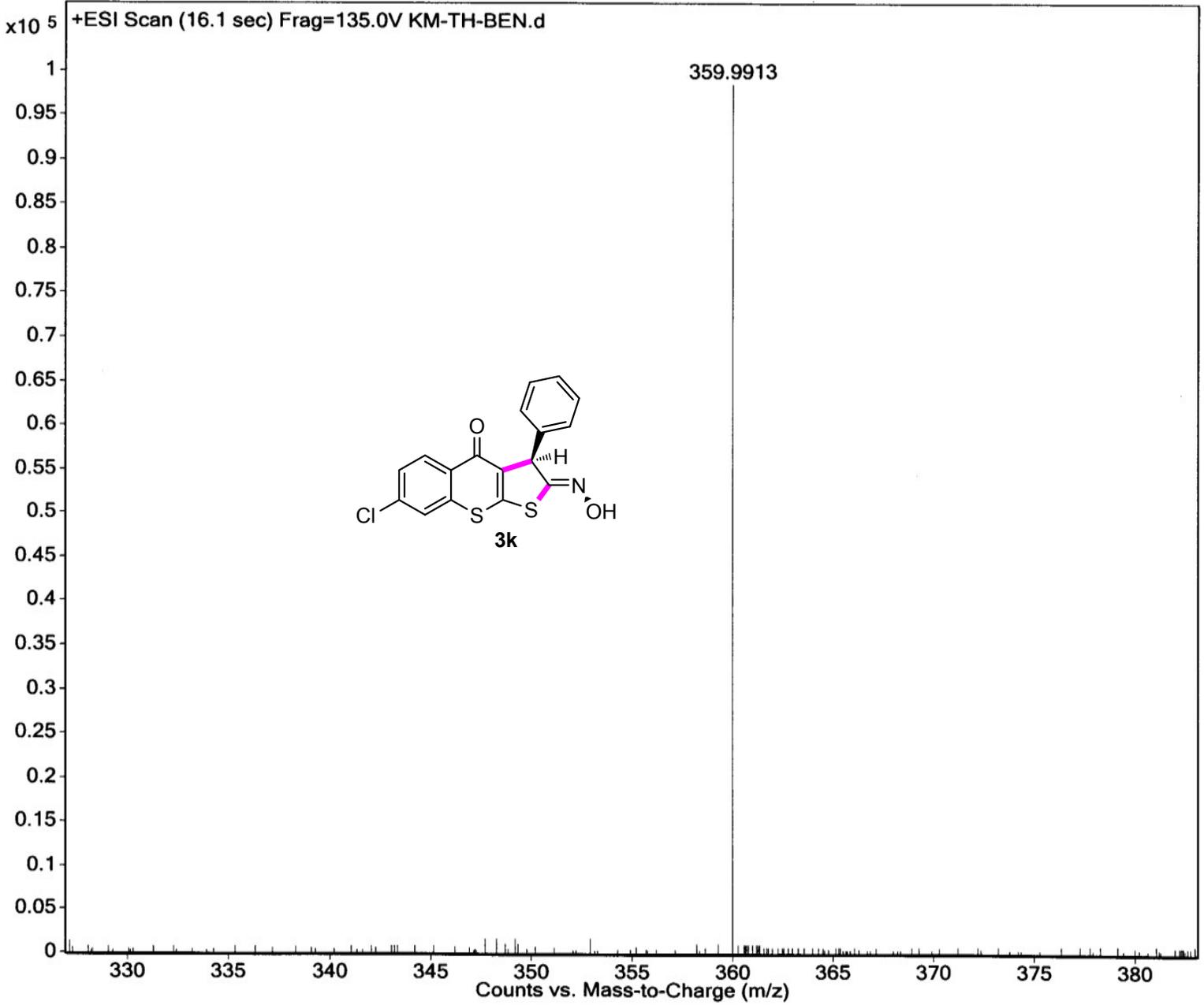
¹³CNMR spectra of compound: 3k

km-th-ben-r-13c
km-th-ben=13c



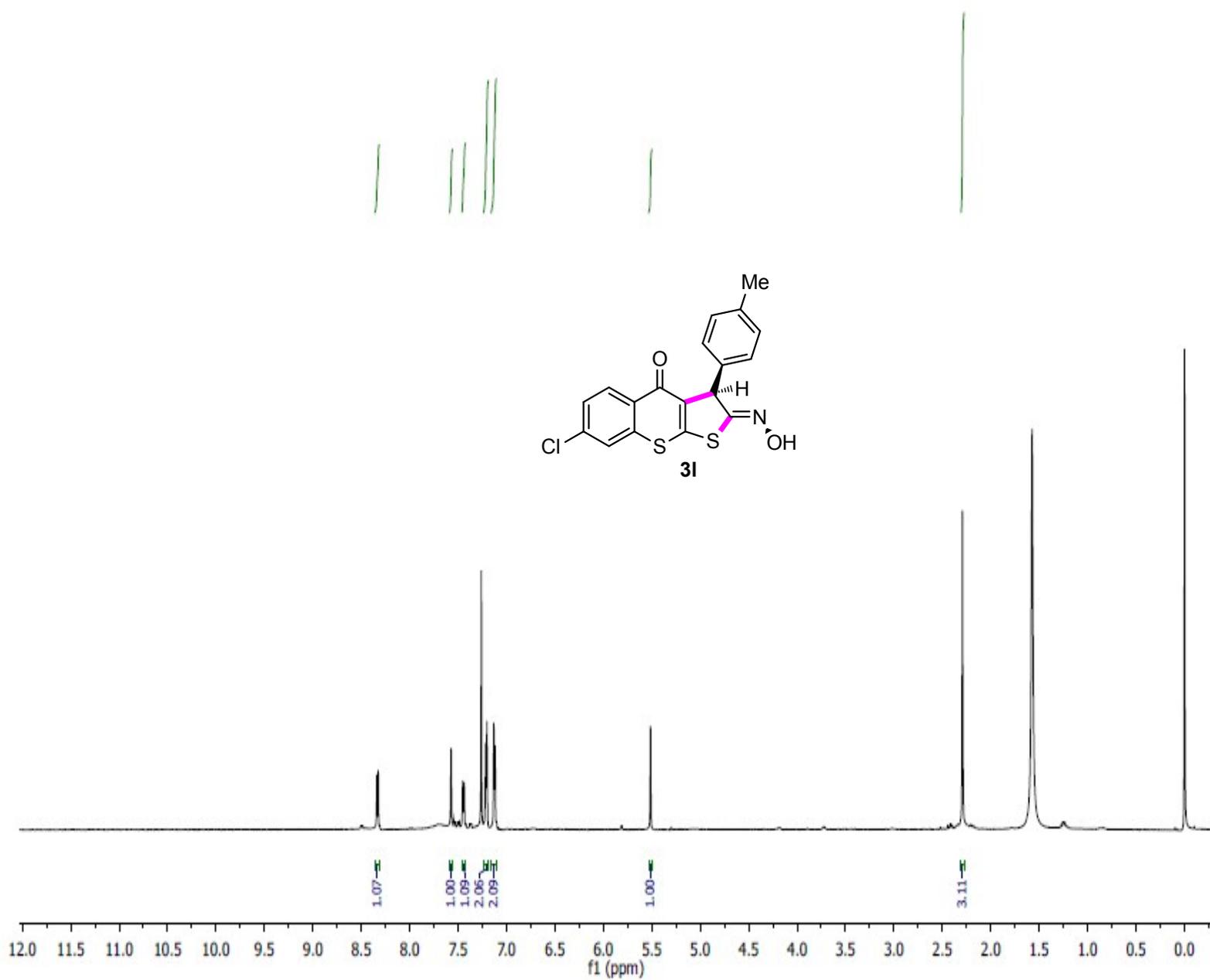
HRMS spectra of compound: 3k

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



¹HNMR spectra of compound: 3I

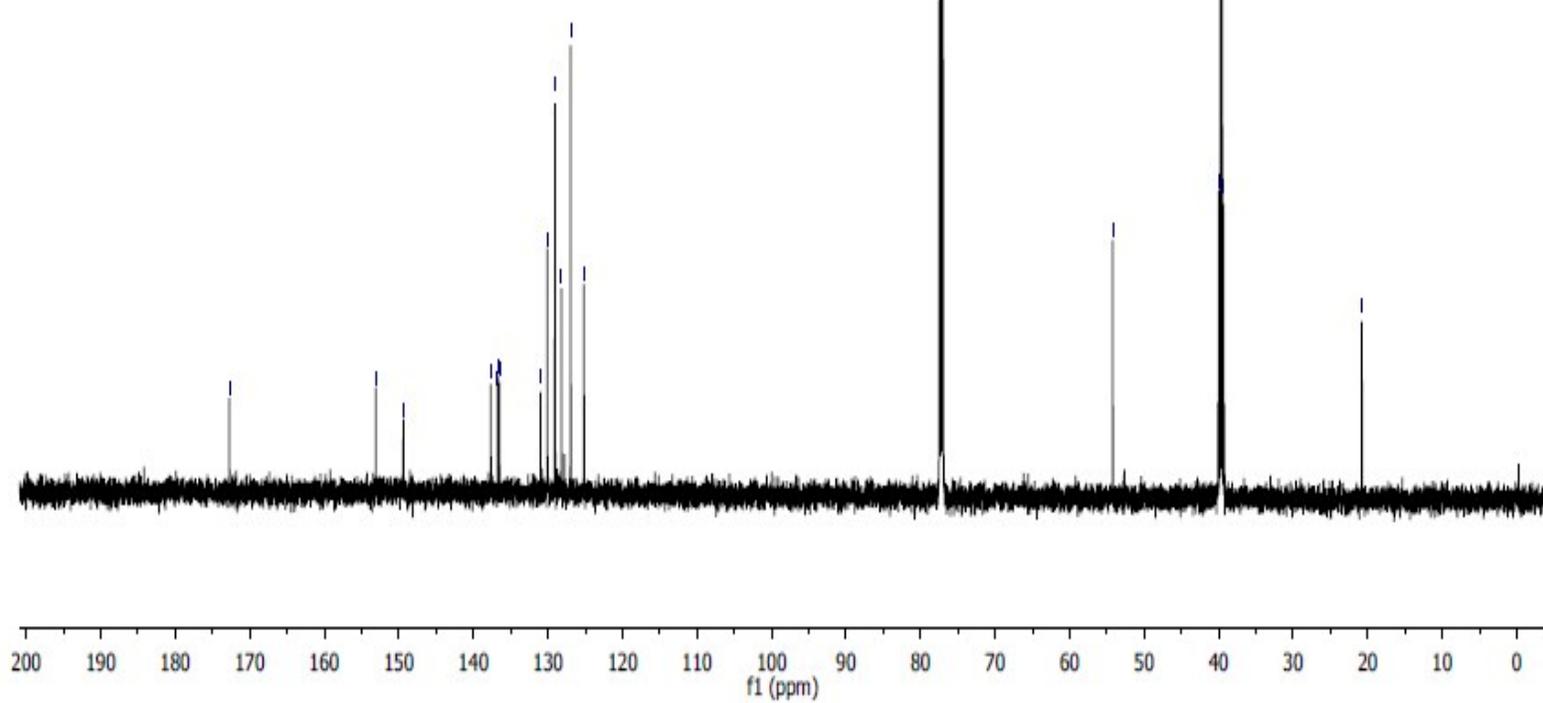
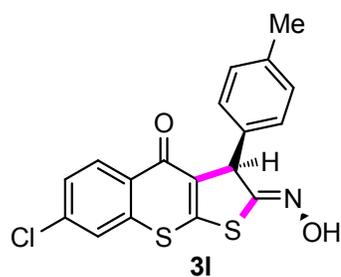
KM-TH-Me-1H
KM-TH-Me-1H



¹³CNMR spectra of compound: 3I

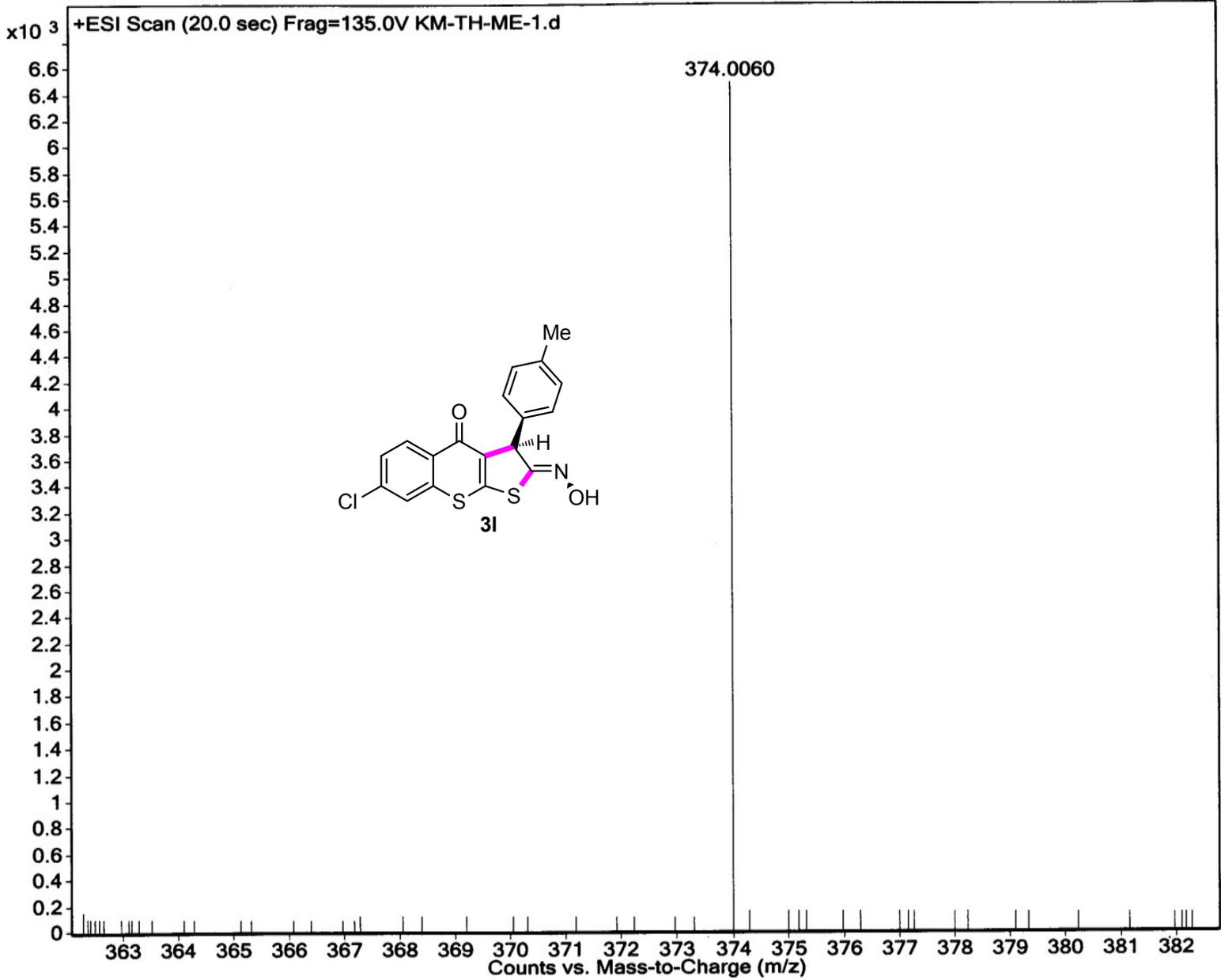
KM-TH-ME-13C
KM-TH-ME-13C

—172.75
—153.11
—149.39
137.66
136.76
136.73
136.50
130.99
130.08
129.06
128.19
126.95
125.17
77.44
77.02
76.63
54.22
39.94
39.80
39.66
39.52
39.38
20.79



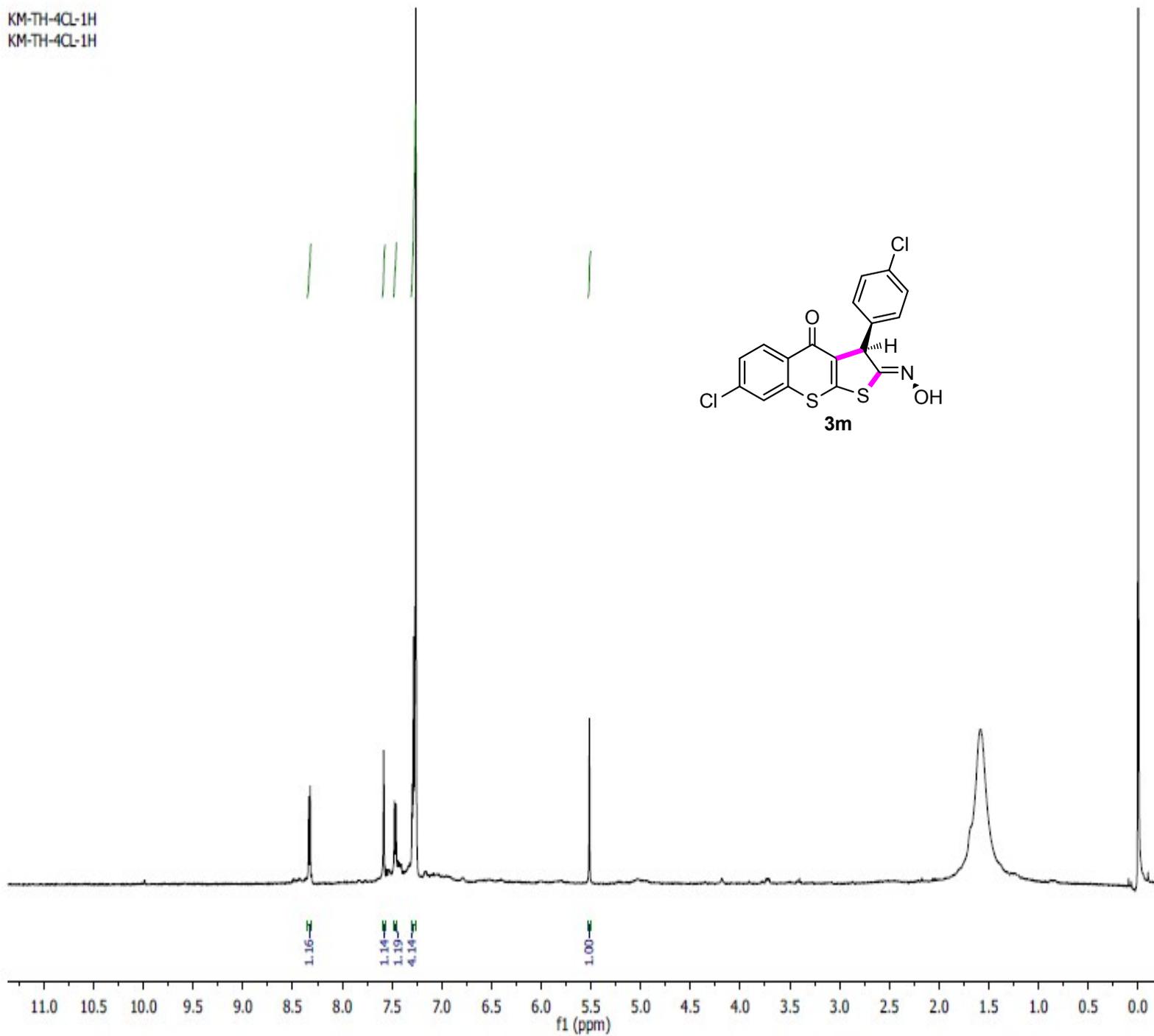
HRMS spectra of compound: 3l

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 compound: 3m

KM-TH-4CL-1H
KM-TH-4CL-1H



¹³CNMR spectra of compound: 3m

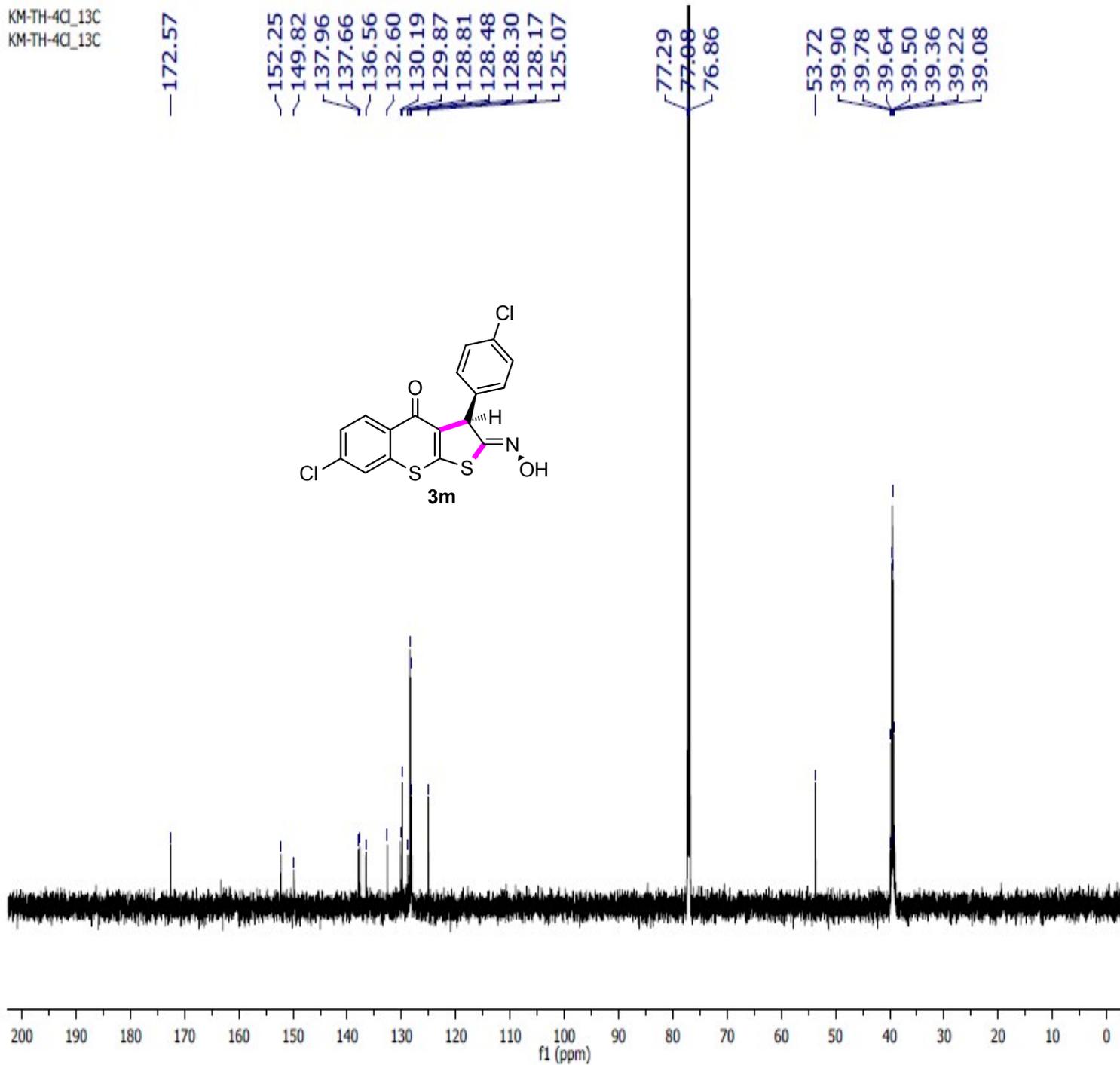
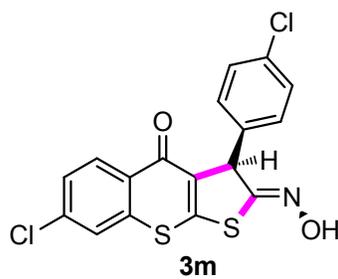
KM-TH-4Cl_13C
KM-TH-4Cl_13C

—172.57

~152.25
~149.82
137.96
137.66
136.56
132.60
130.19
129.87
128.81
128.48
128.30
128.17
125.07

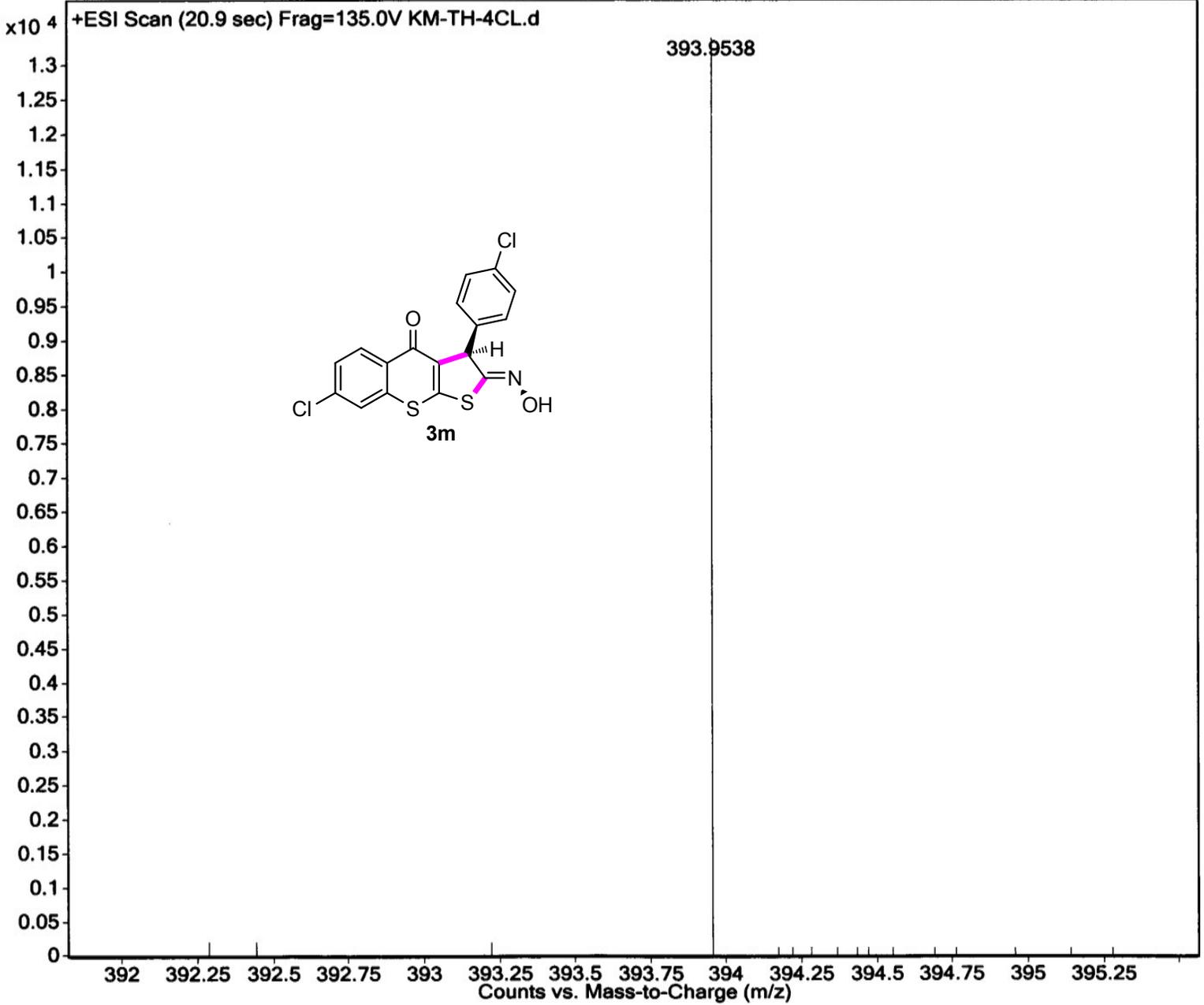
77.29
77.08
76.86

—53.72
39.90
39.78
39.64
39.50
39.36
39.22
39.08



HRMS spectra of compound: 3m

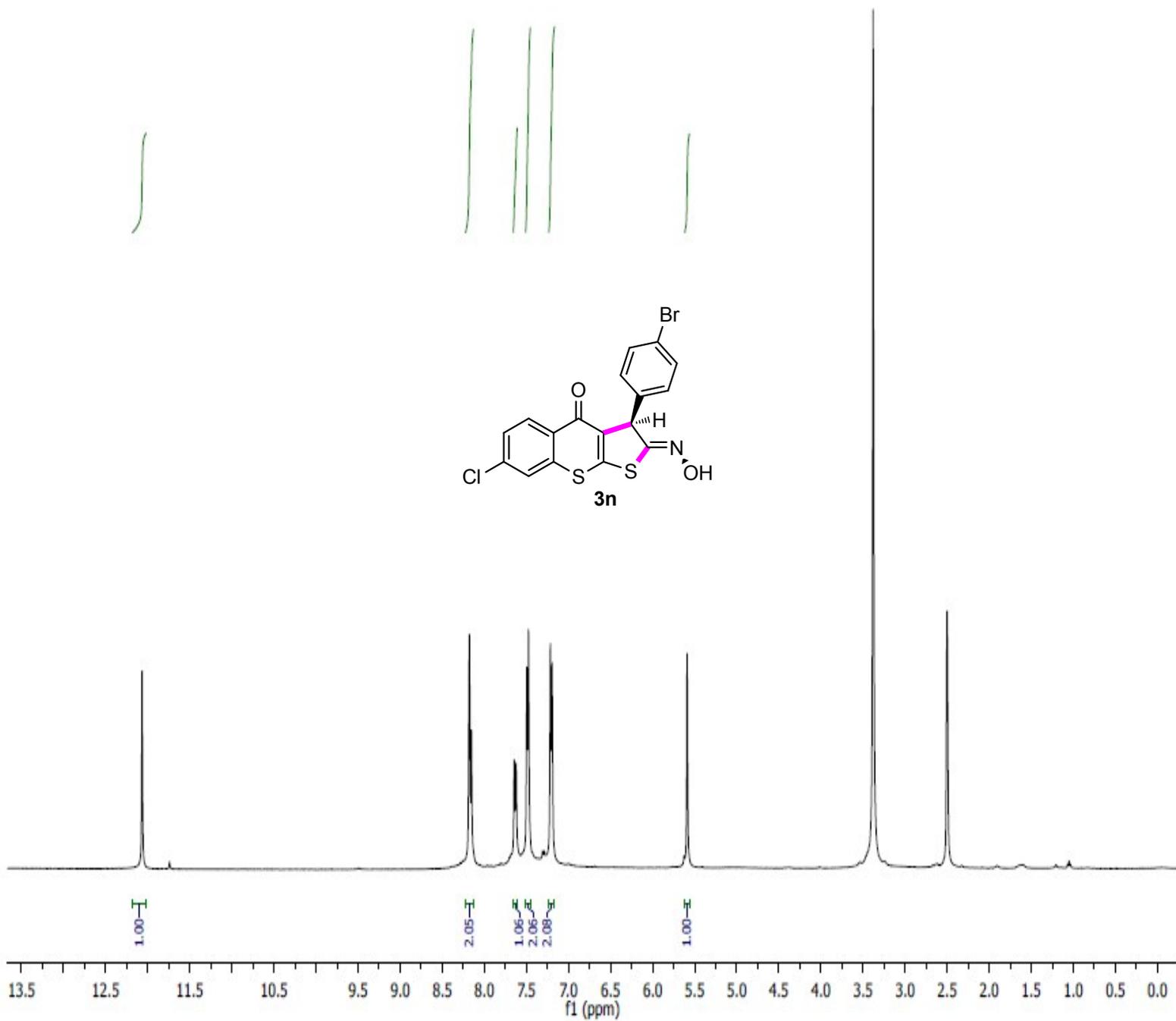
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



¹H NMR spectra of compound: 3n

KM-TH-4BR-1H

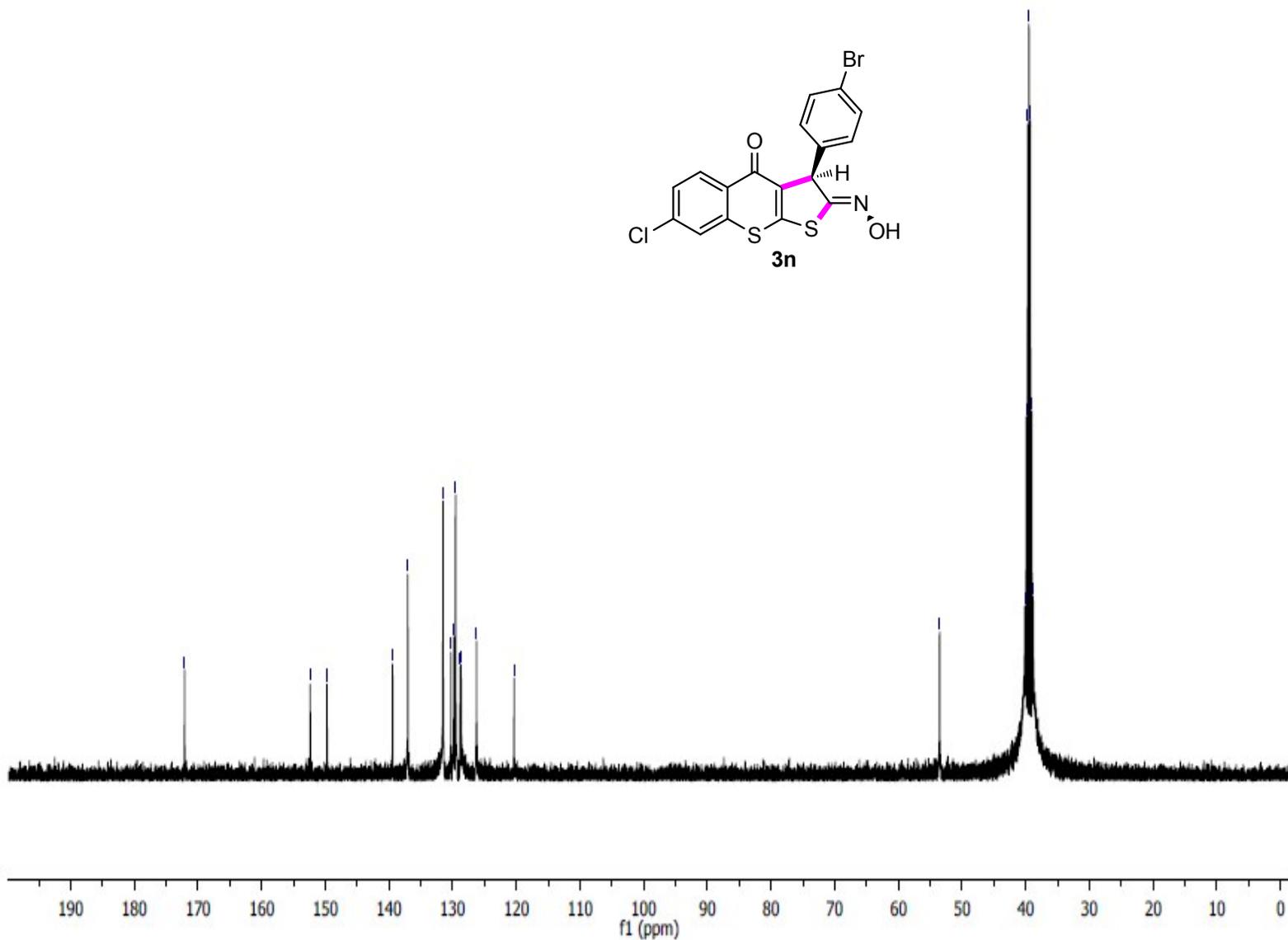
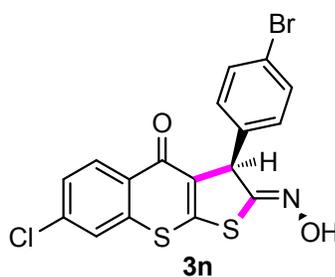
KM-TH-4BR-1H



¹³CNMR spectra of compound: 3n

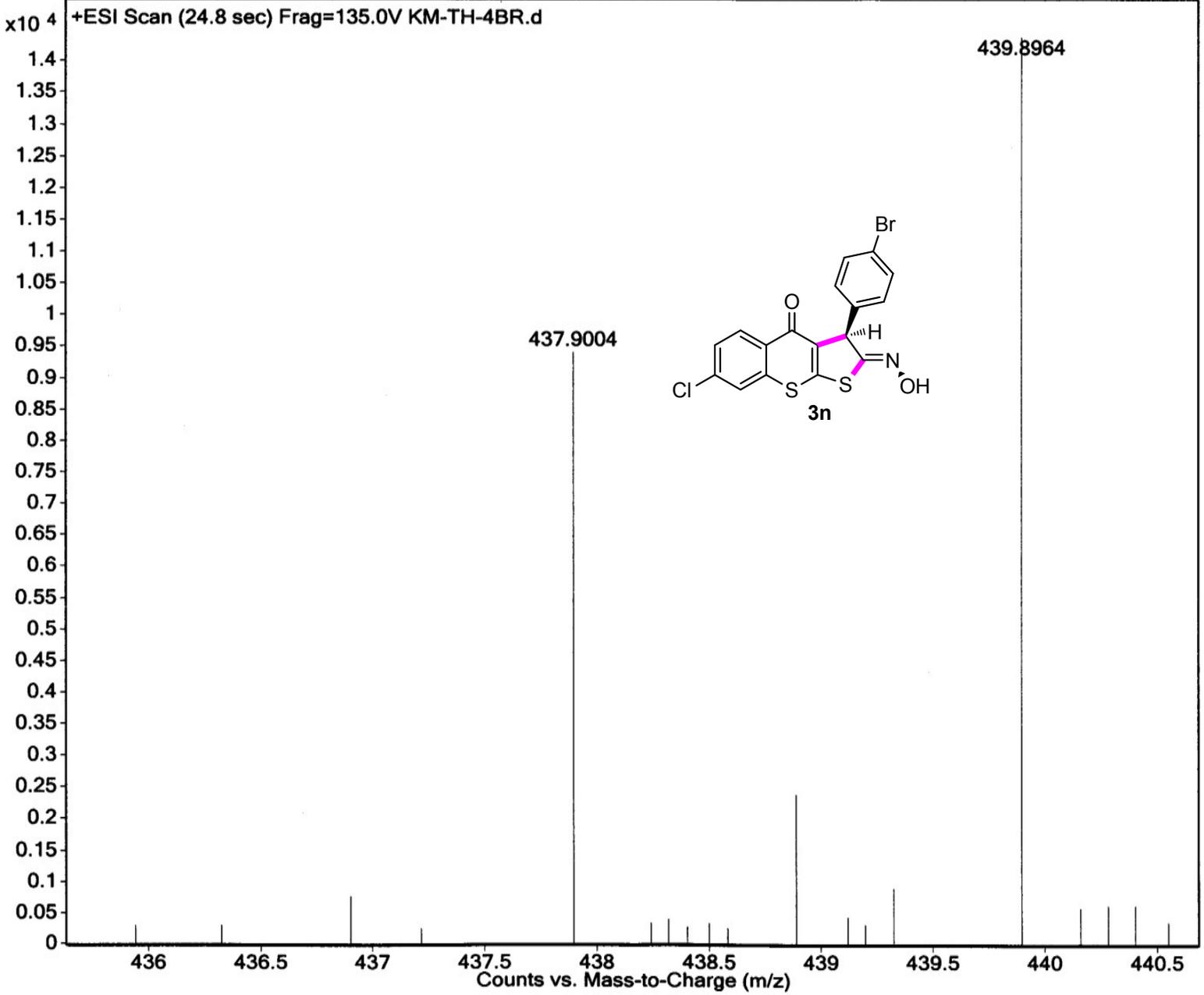
km-th-4br-13c
km-th-4br-13c

—172.12
—152.38
—149.75
—139.45
—137.06
—131.52
—130.29
—129.80
—129.56
—128.85
—128.69
—126.26
—120.37
—53.53
—40.15
—39.93
—39.71
—39.50
—39.29
—39.08
—38.87



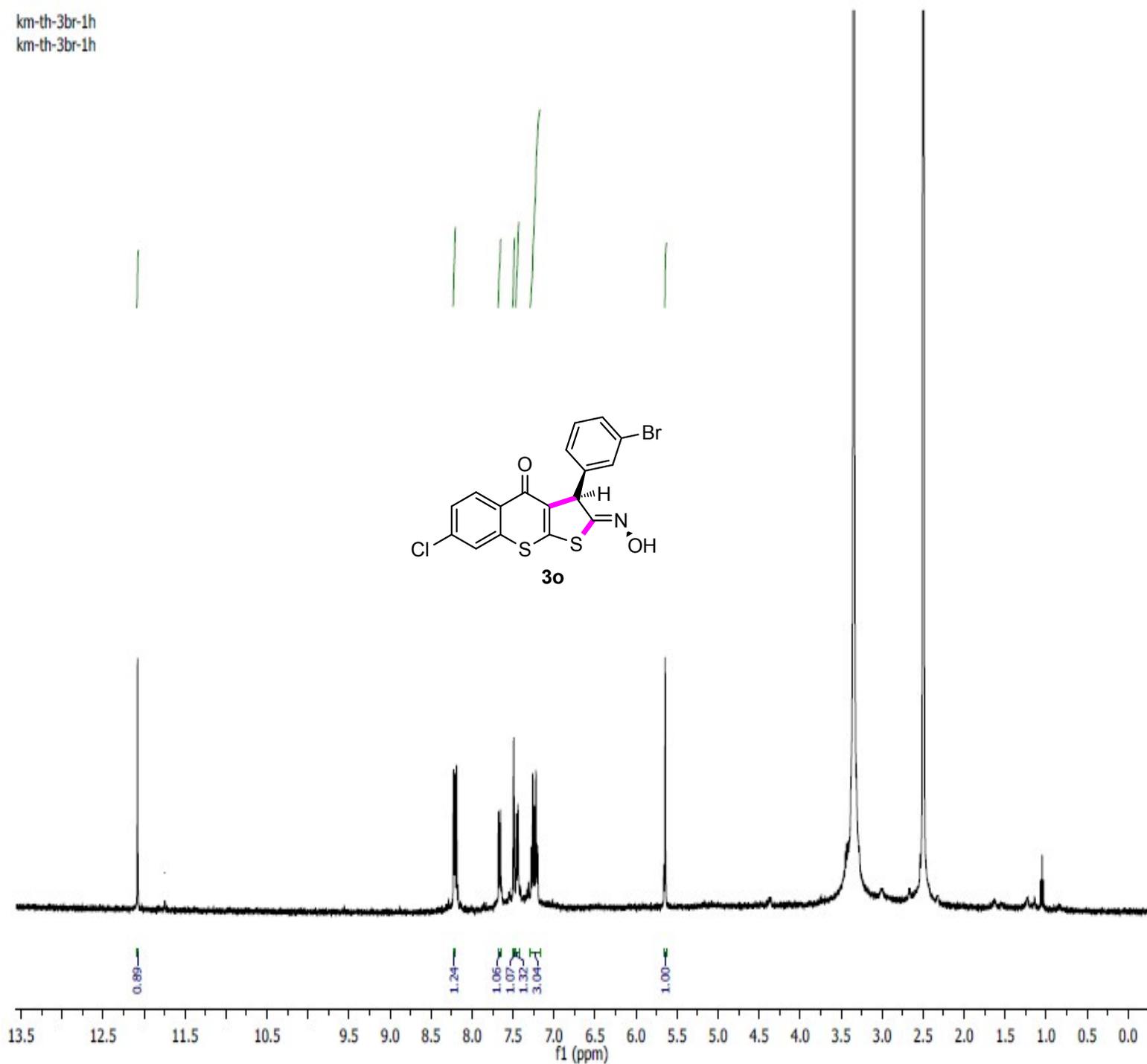
HRMS spectra of compound: 3n

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



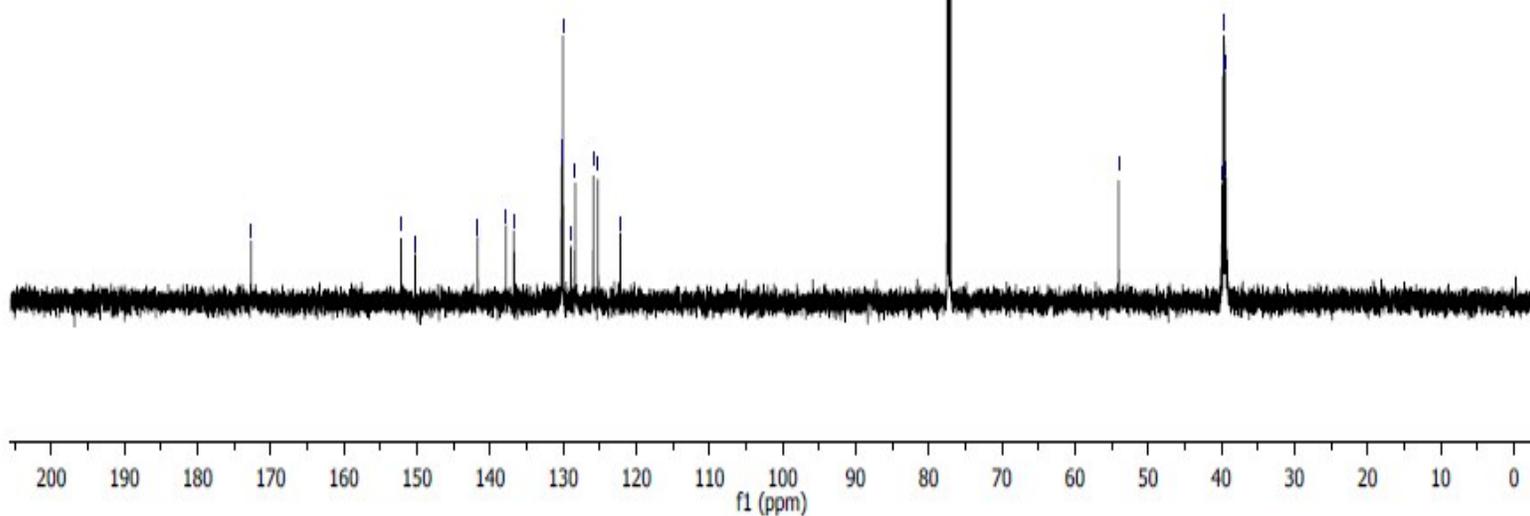
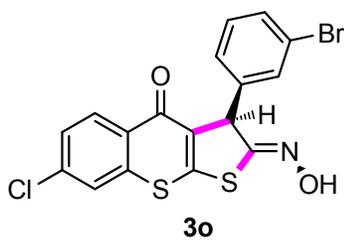
¹H NMR spectra of compound: 3o

km-th-3br-1h
km-th-3br-1h



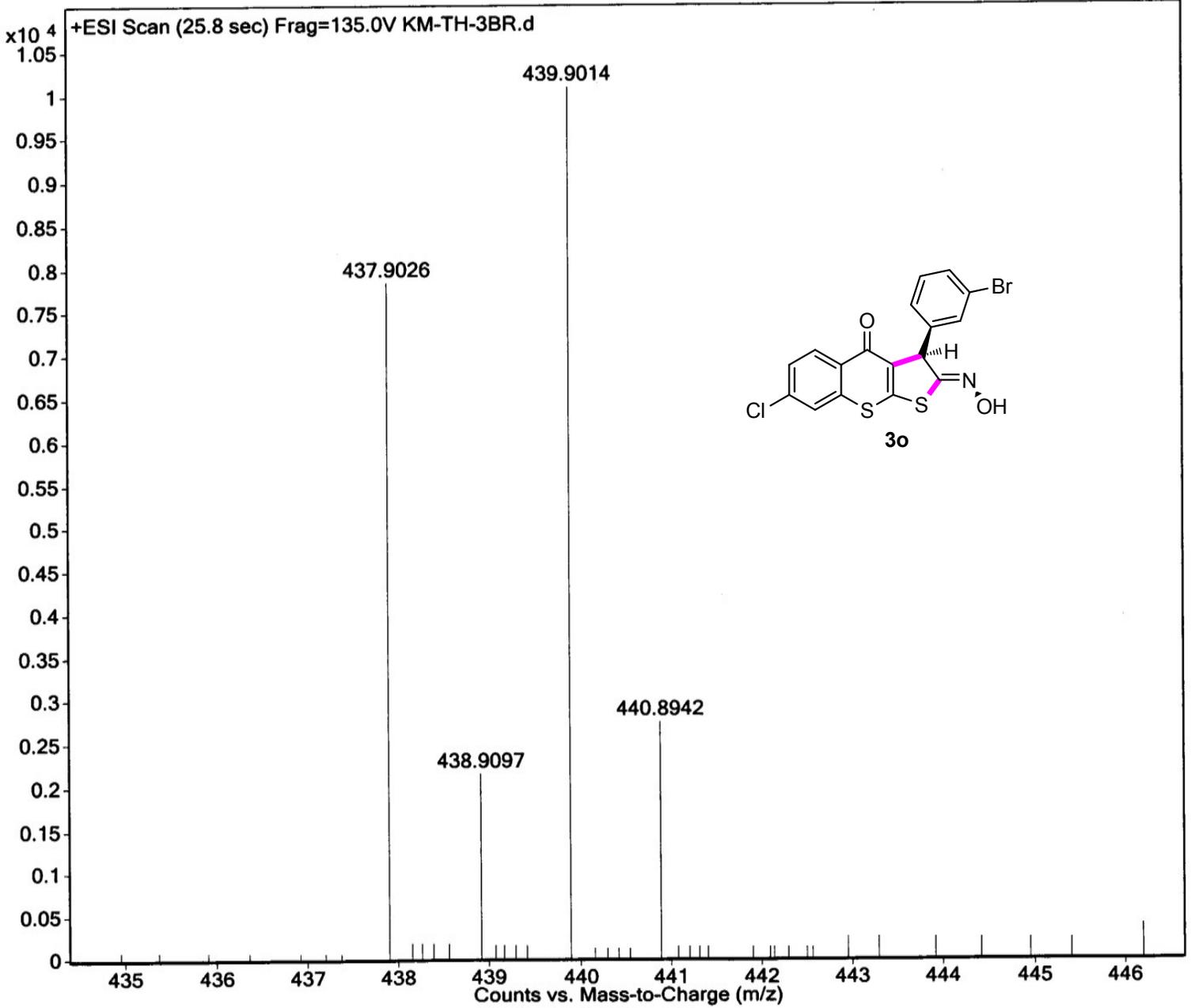
¹³CNMR spectra of compound: 3o

KM-TH-3BR_13C
KM-TH-3BR_13C



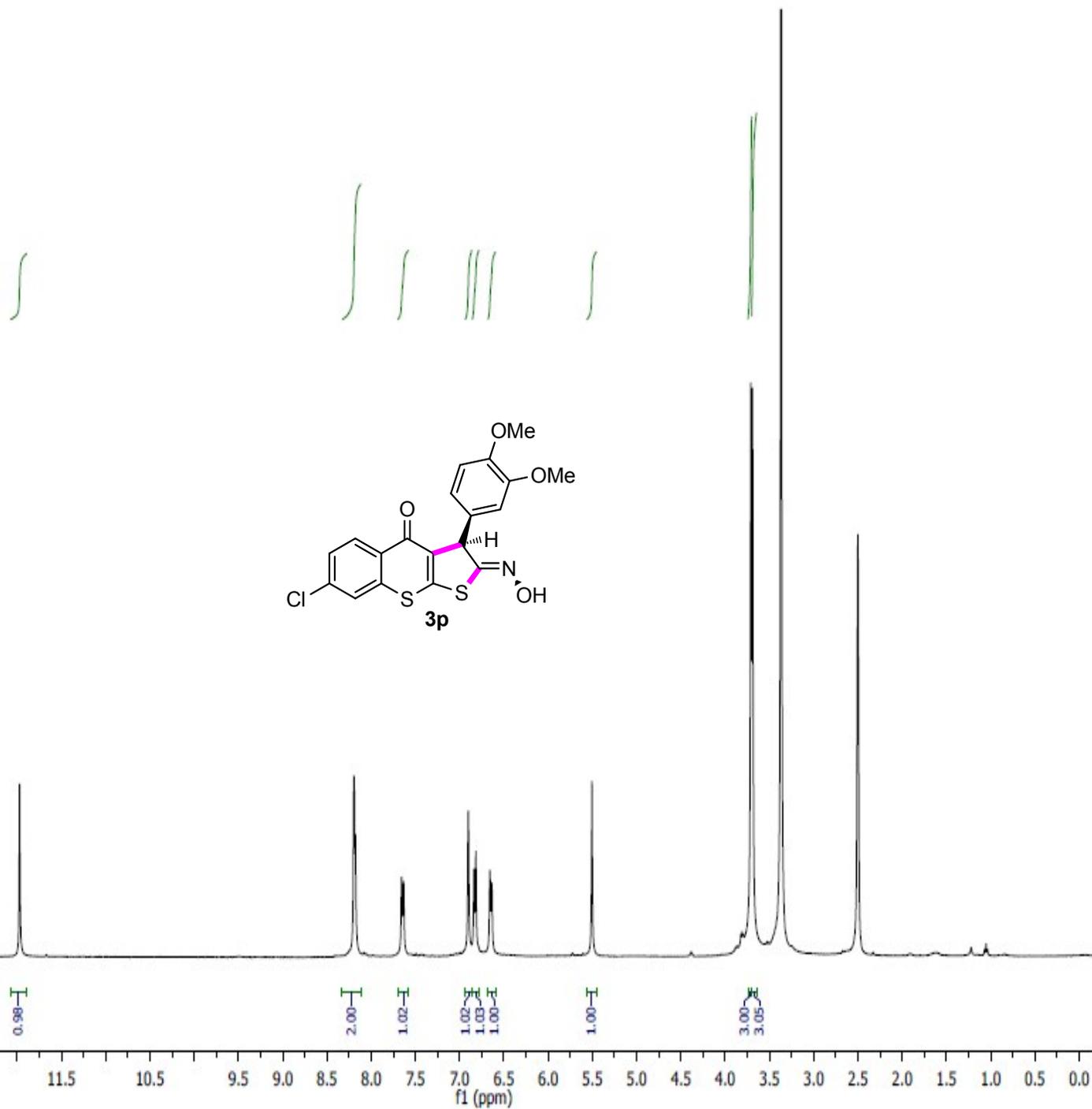
HRMS spectra of compound: 3o

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



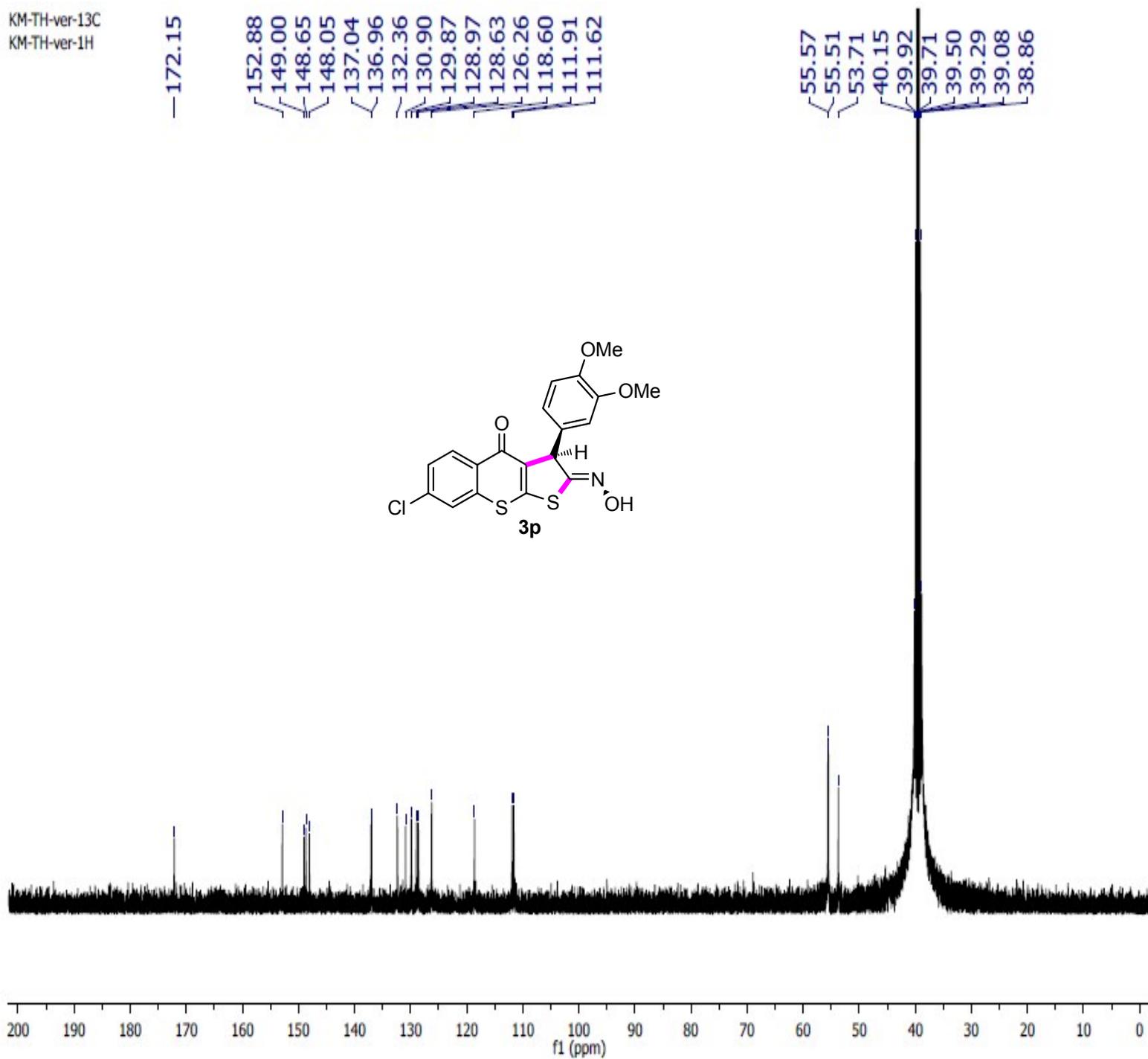
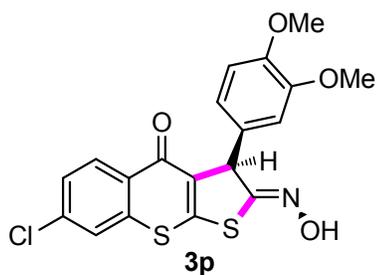
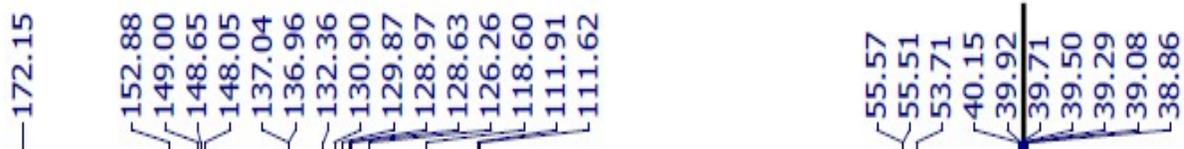
¹H NMR spectra of compound: 3p

KM-TH-ver-1H
KM-TH-ver-1H



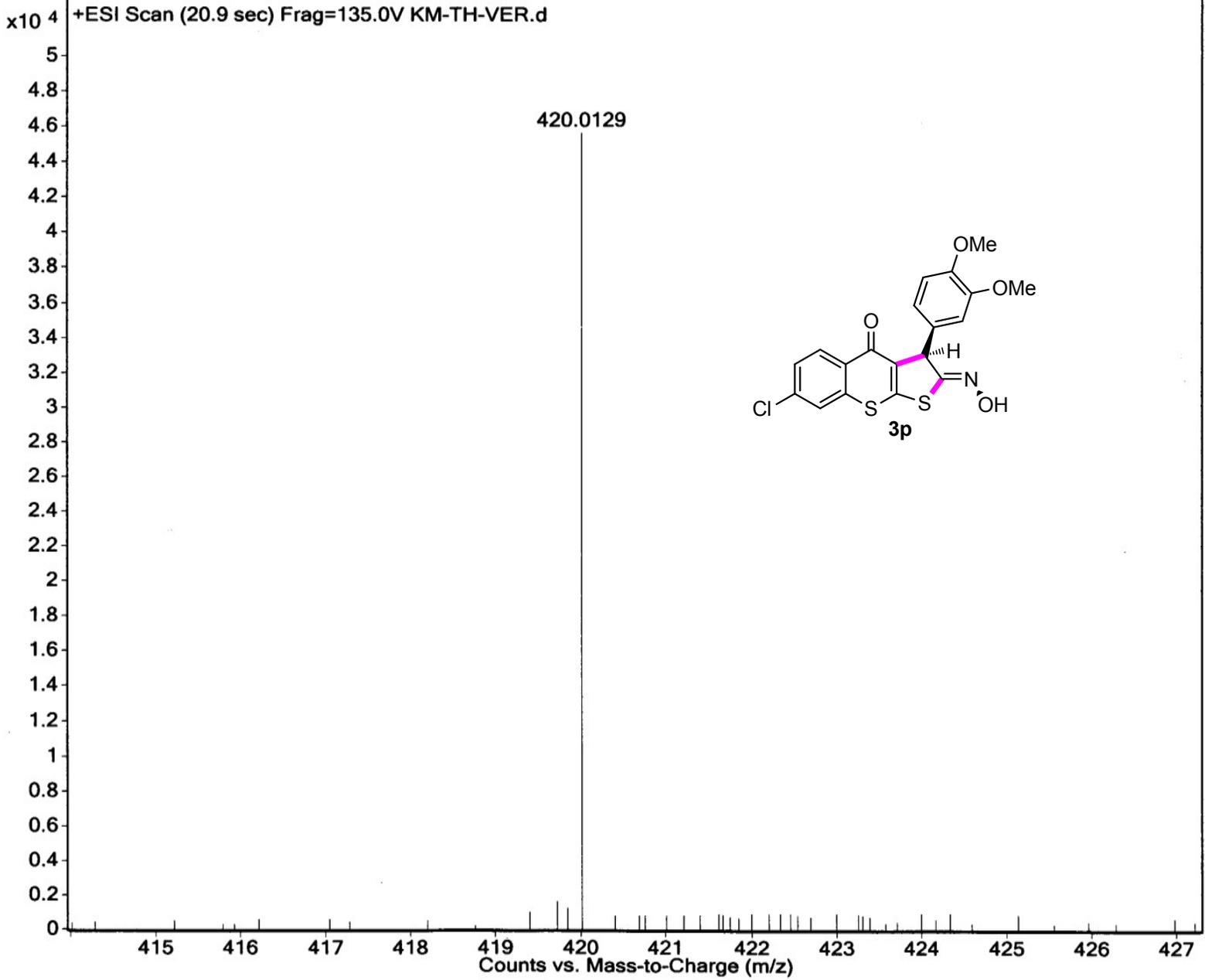
¹³CNMR spectra of compound: 3p

KM-TH-ver-13C
KM-TH-ver-1H



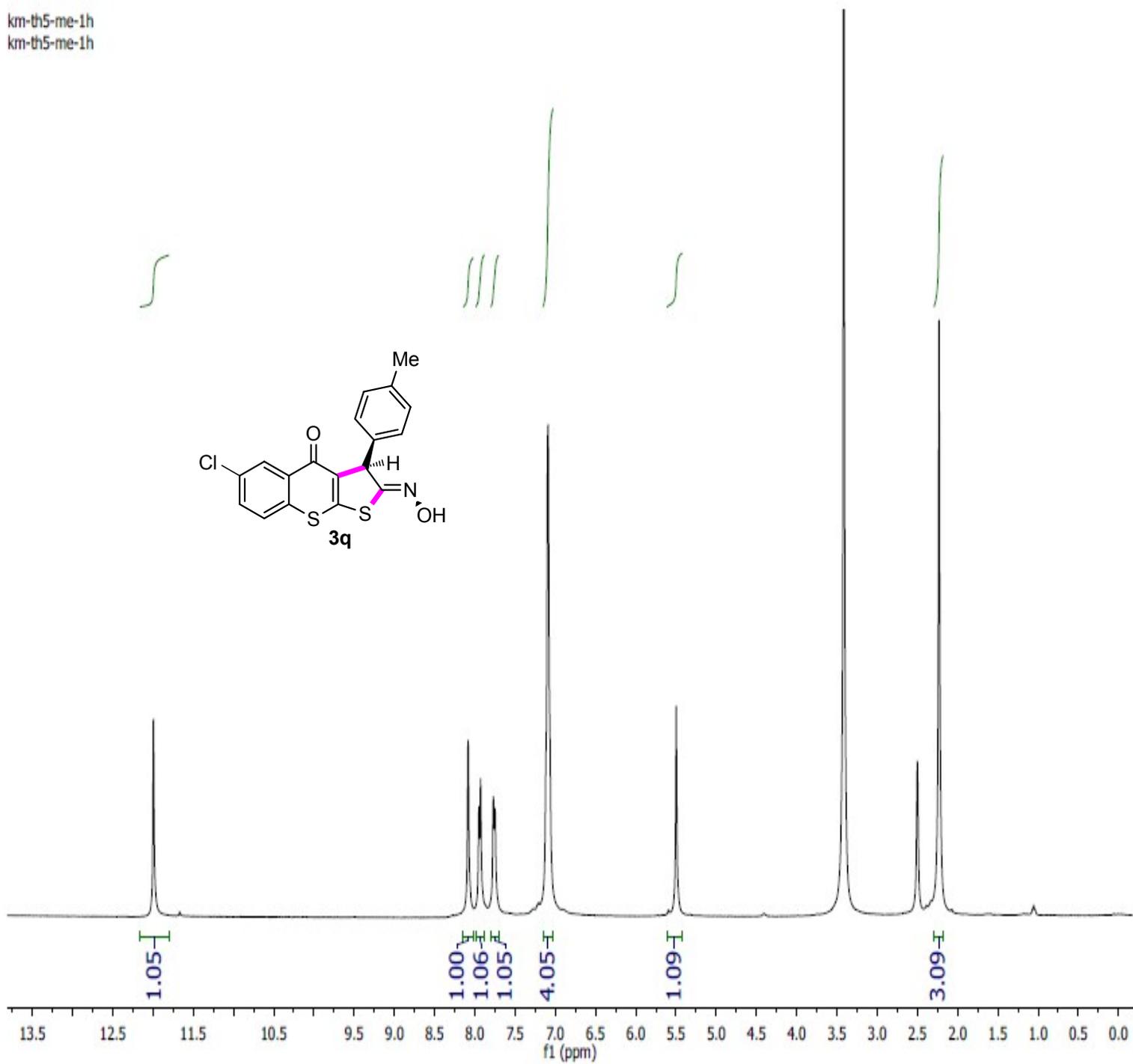
HRMS spectra of compound: 3p

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 compound: 3q

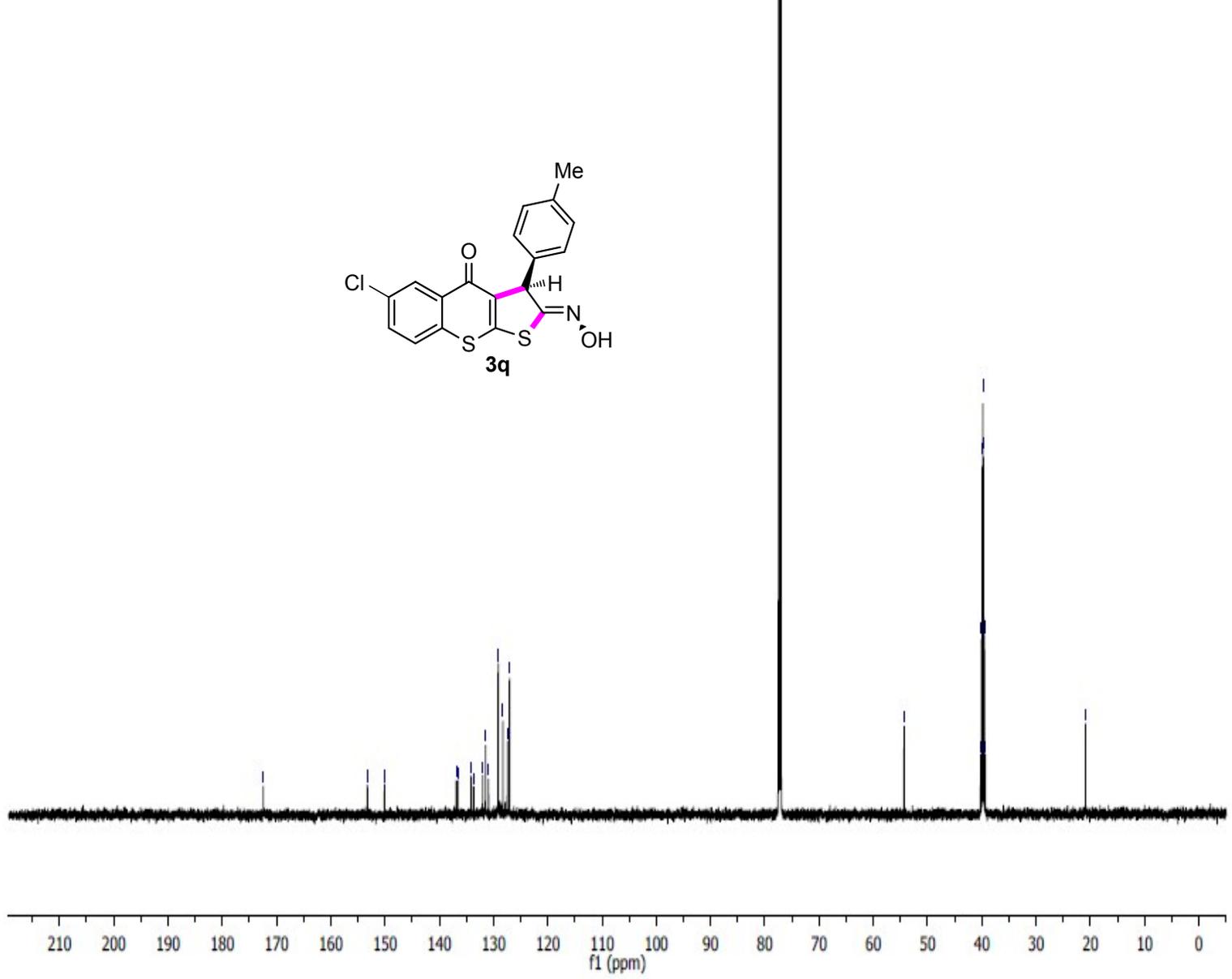
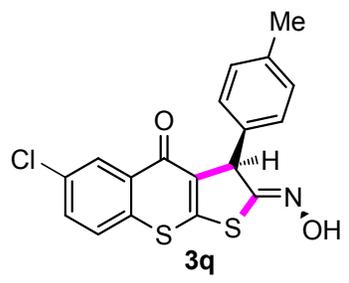
km-th5-me-1h
km-th5-me-1h



¹³CNMR spectra of compound: 3q

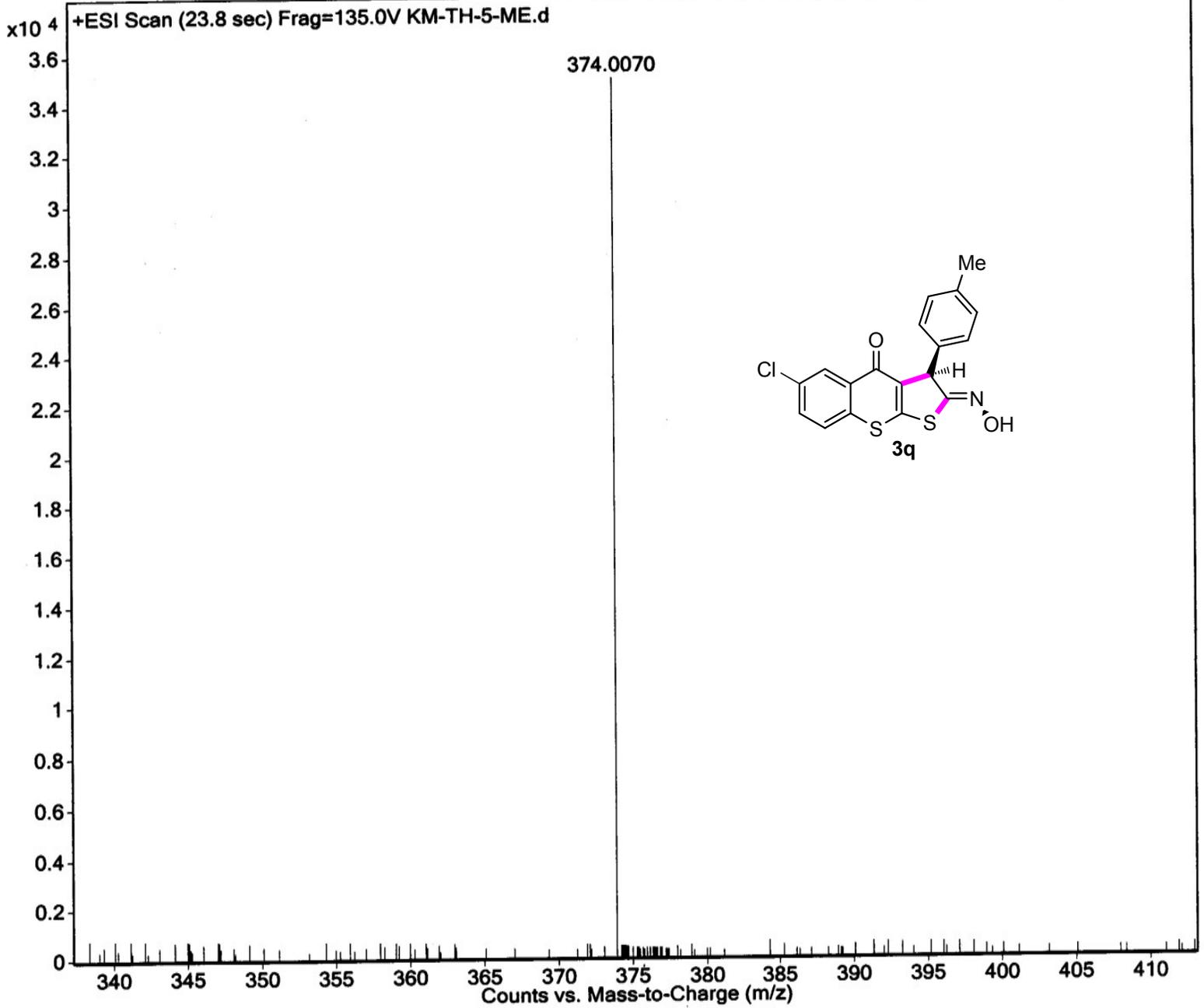
KM-TH-S-4ME-13C
KM-TH-S-4ME-13C

—172.44
—153.22
—150.08
—136.85
—136.55
—134.11
—133.66
—132.00
—131.47
—130.92
—129.14
—128.27
—127.42
—127.06
—77.44
—77.23
—77.02
—54.32
—40.08
—39.94
—39.80
—39.66
—39.52
—20.88

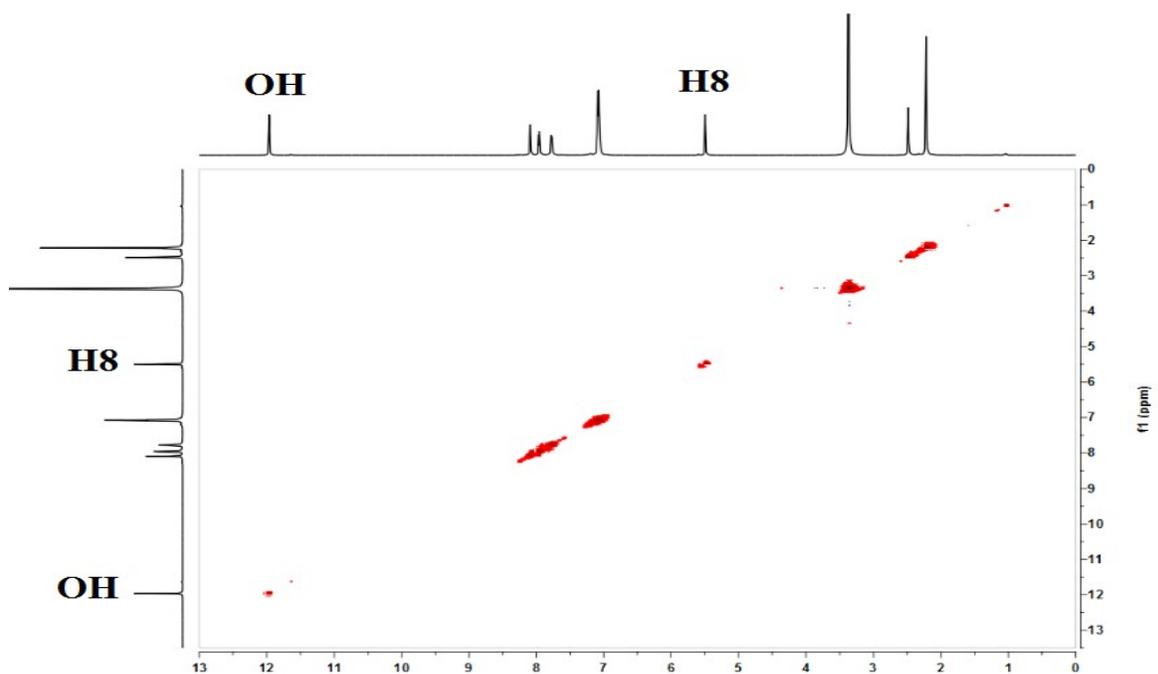


HRMS spectra of compound: 3q

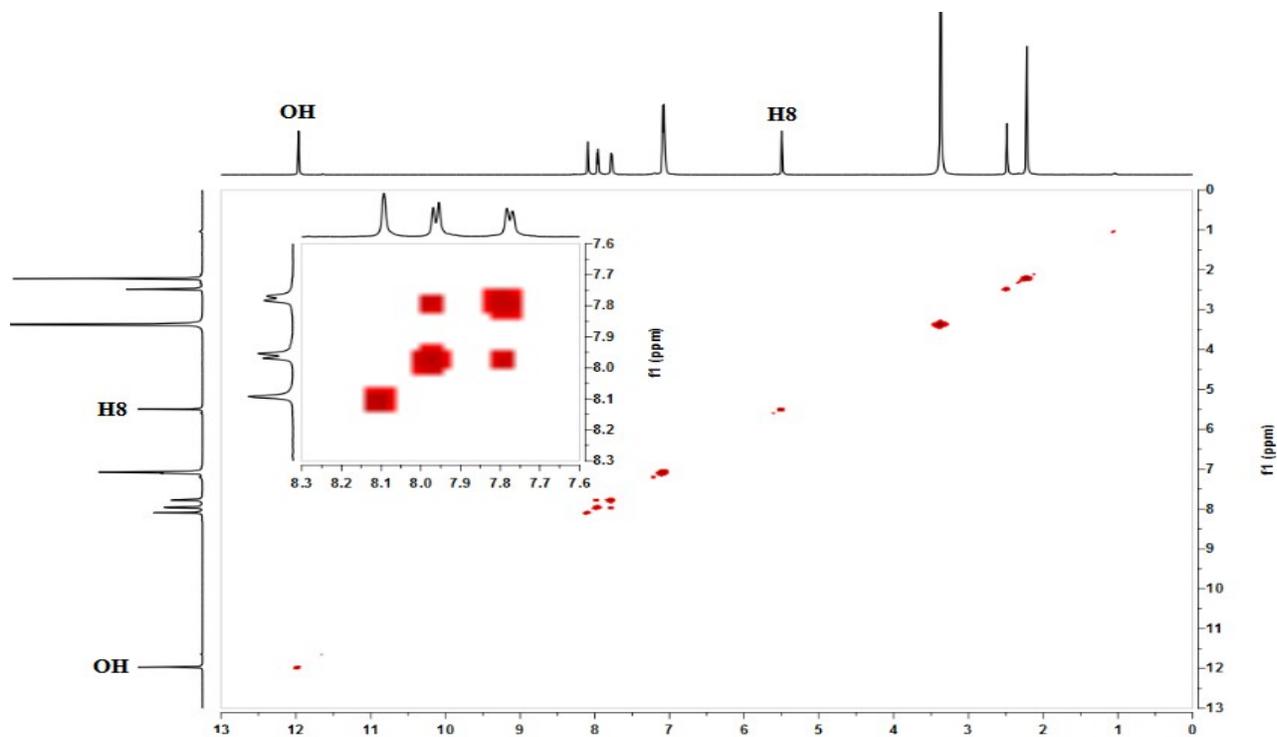
Sample Name	Position	Instrument Name	User Name
Inj Vol	InjPosition	SampleType	IRM Calibration Status
Data Filename	ACQ Method	Comment	Acquired Time



NOESY and COSY spectra of compound: 3q



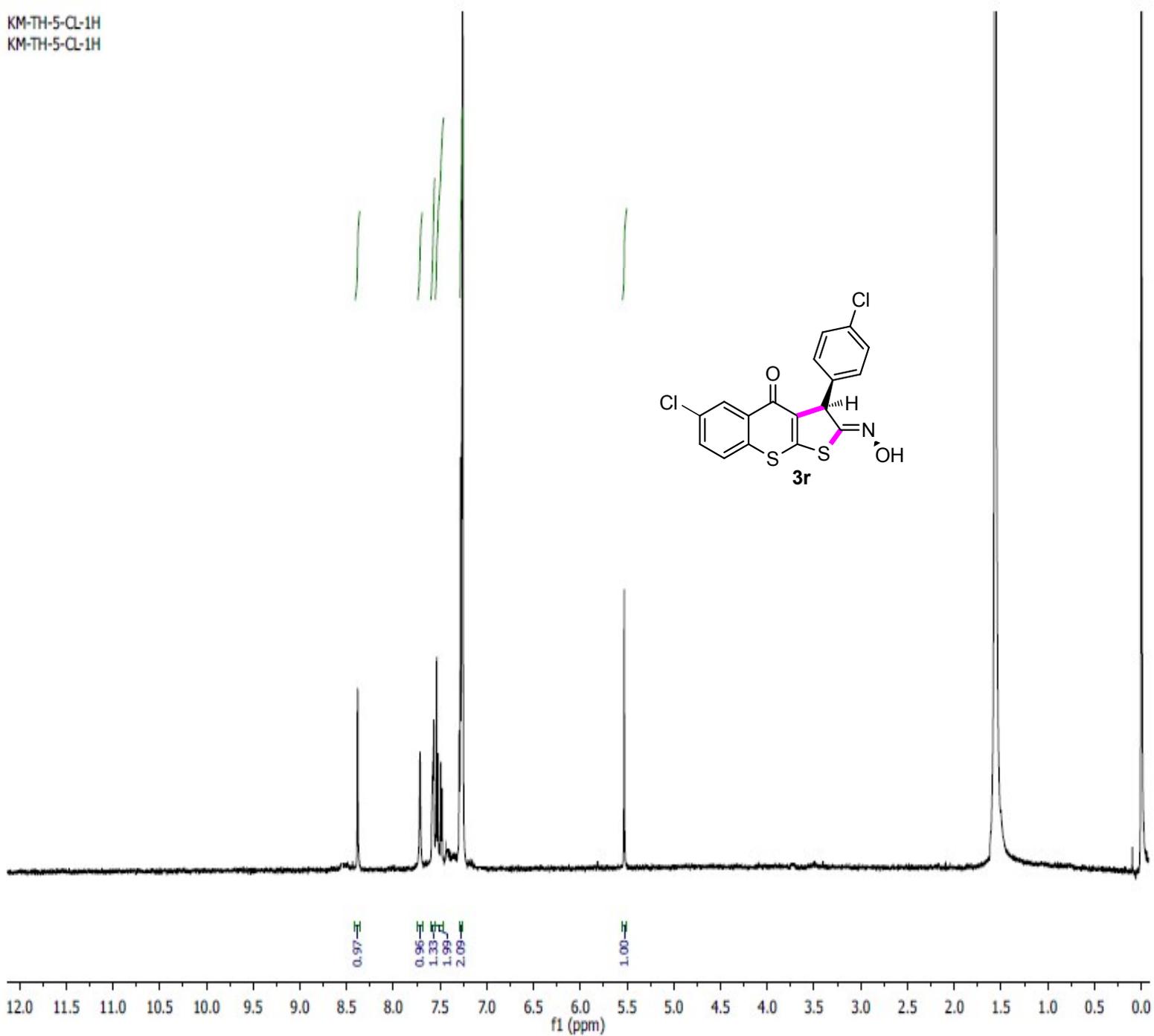
NOESY spectra



COSY spectra

¹H NMR spectra of compound: 3r

KM-TH-5-CL-1H
KM-TH-5-CL-1H



¹³CNMR spectra of compound: 3r

KM-TH-05-CL-13C
KM-TH-05-CL-13C

—172.37

—152.48
—150.63

—138.11

—134.20

—133.56

—132.84

—131.80

—131.57

—130.21

—128.70

—128.50

—128.13

—127.45

—77.44

—77.23

—77.02

—53.91

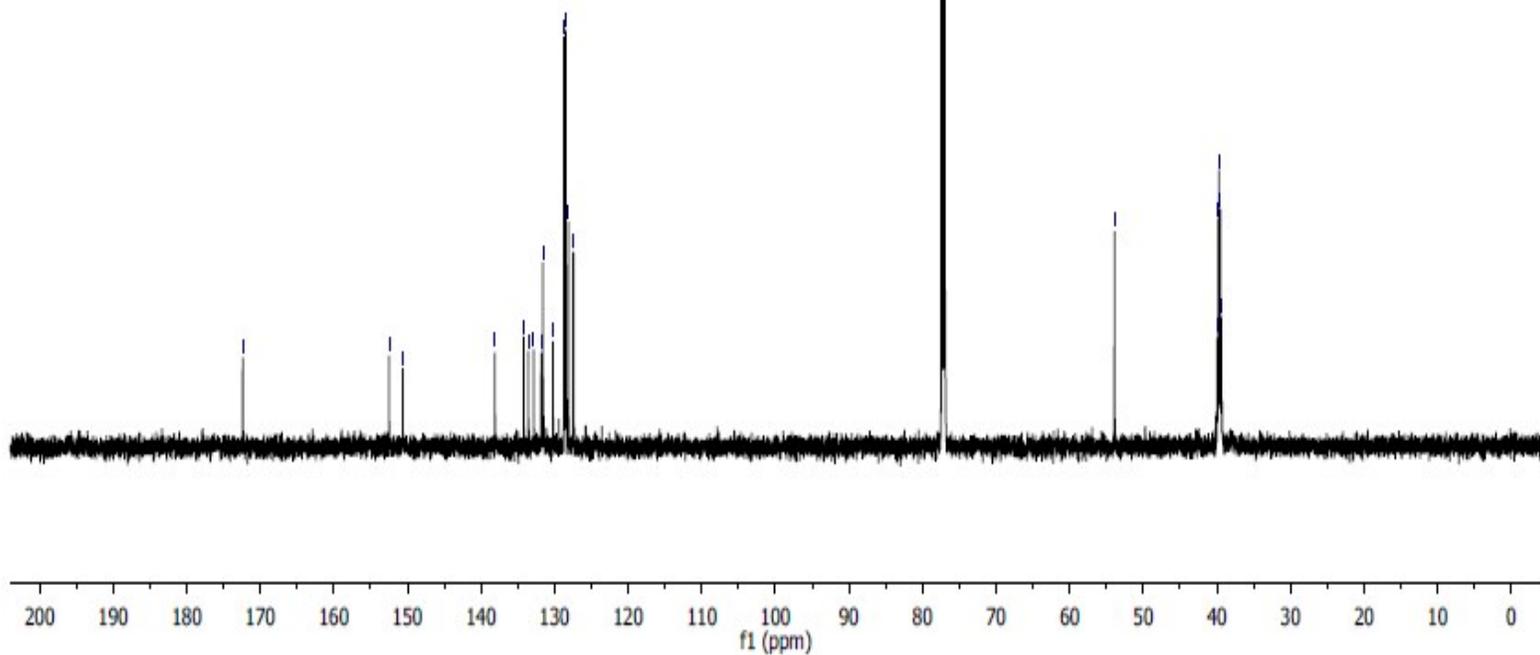
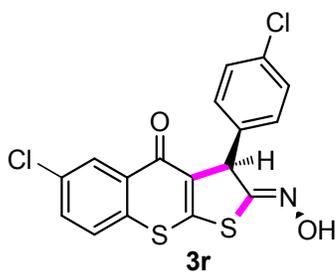
—39.96

—39.82

—39.68

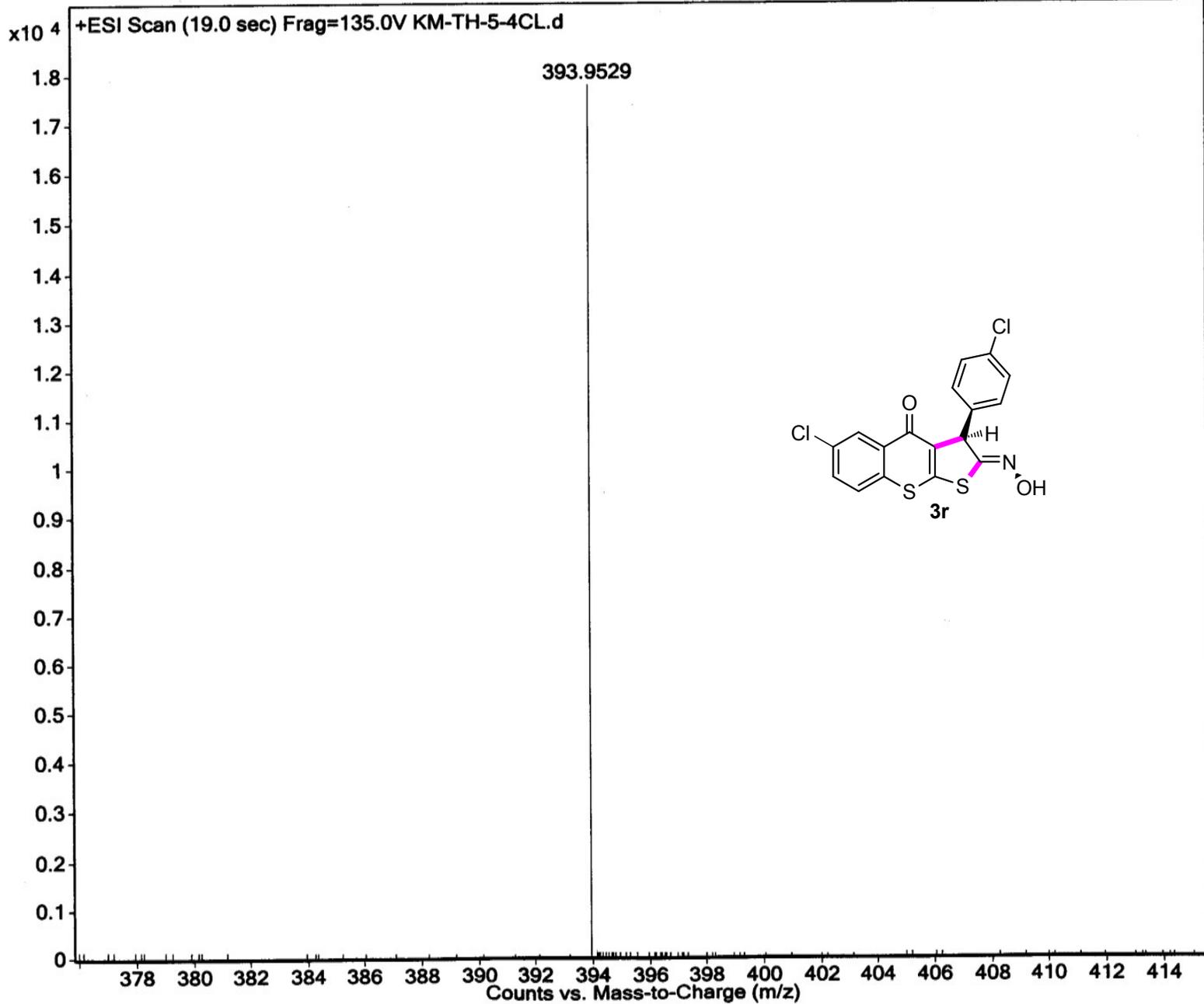
—39.54

—39.40



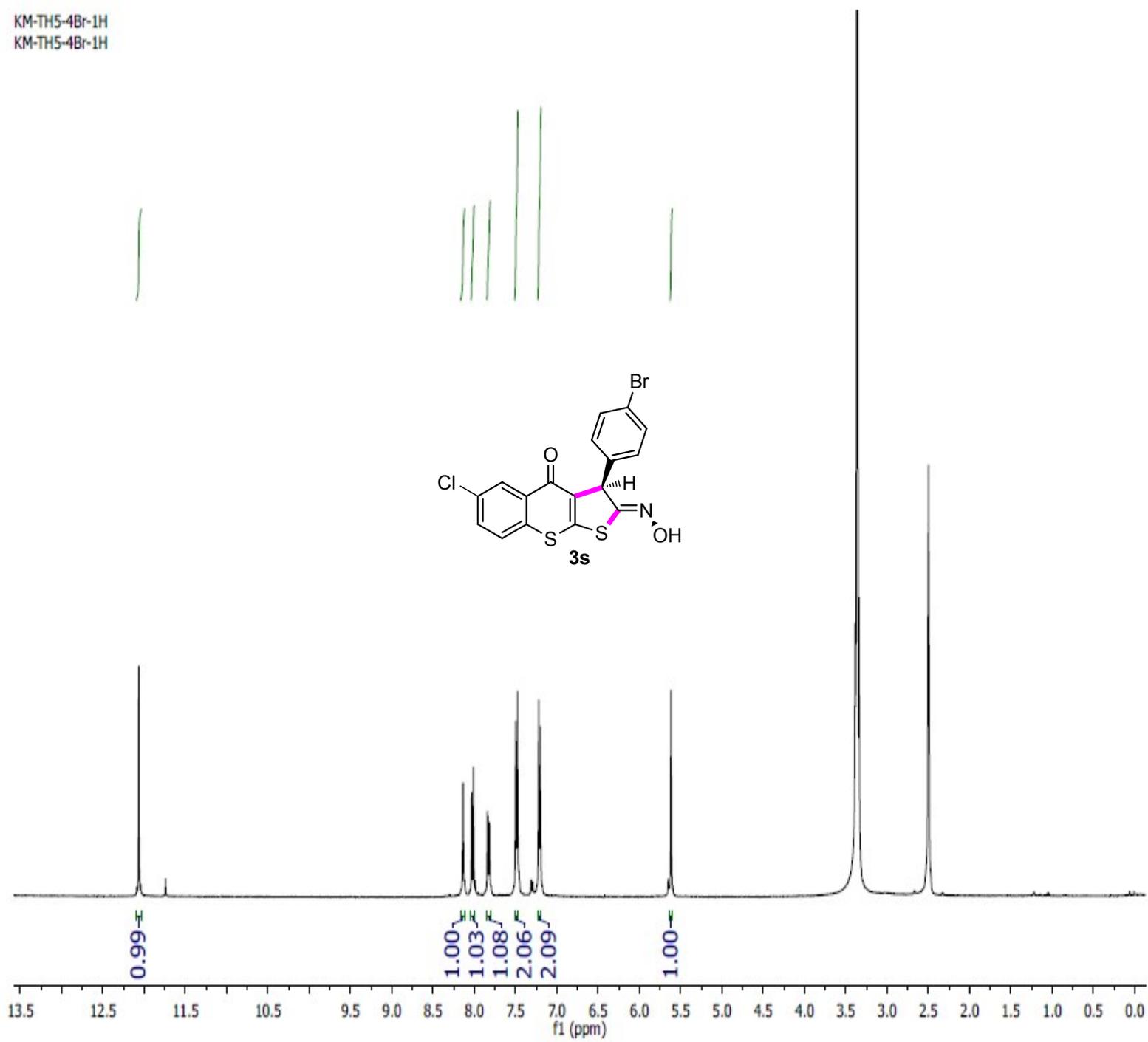
HRMS spectra of compound: 3r

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 compound: 3s

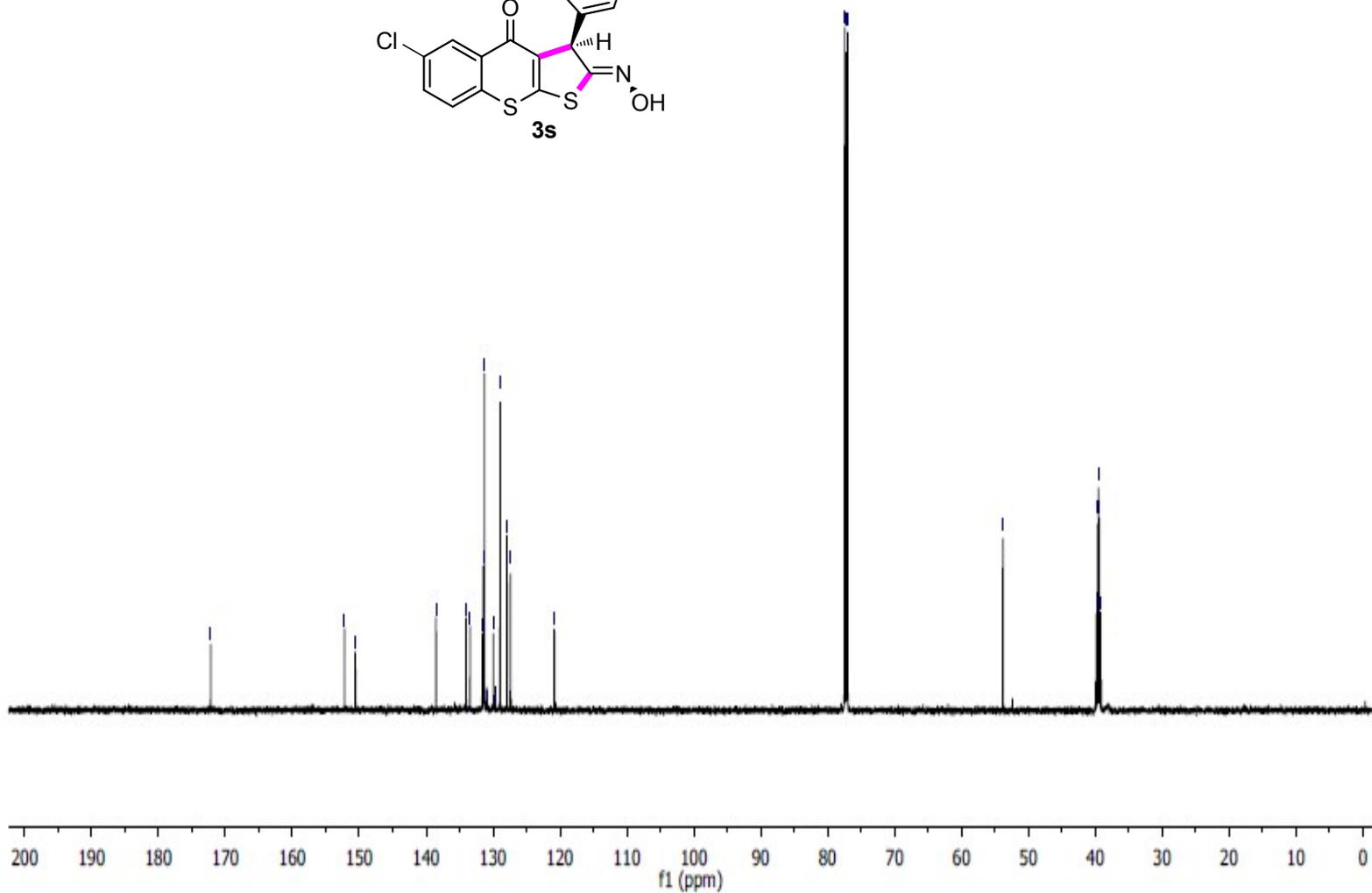
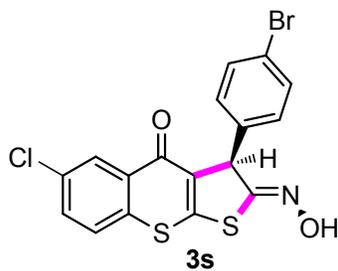
KM-TH5-4Br-1H
KM-TH5-4Br-1H



¹³CNMR spectra of compound: 3s

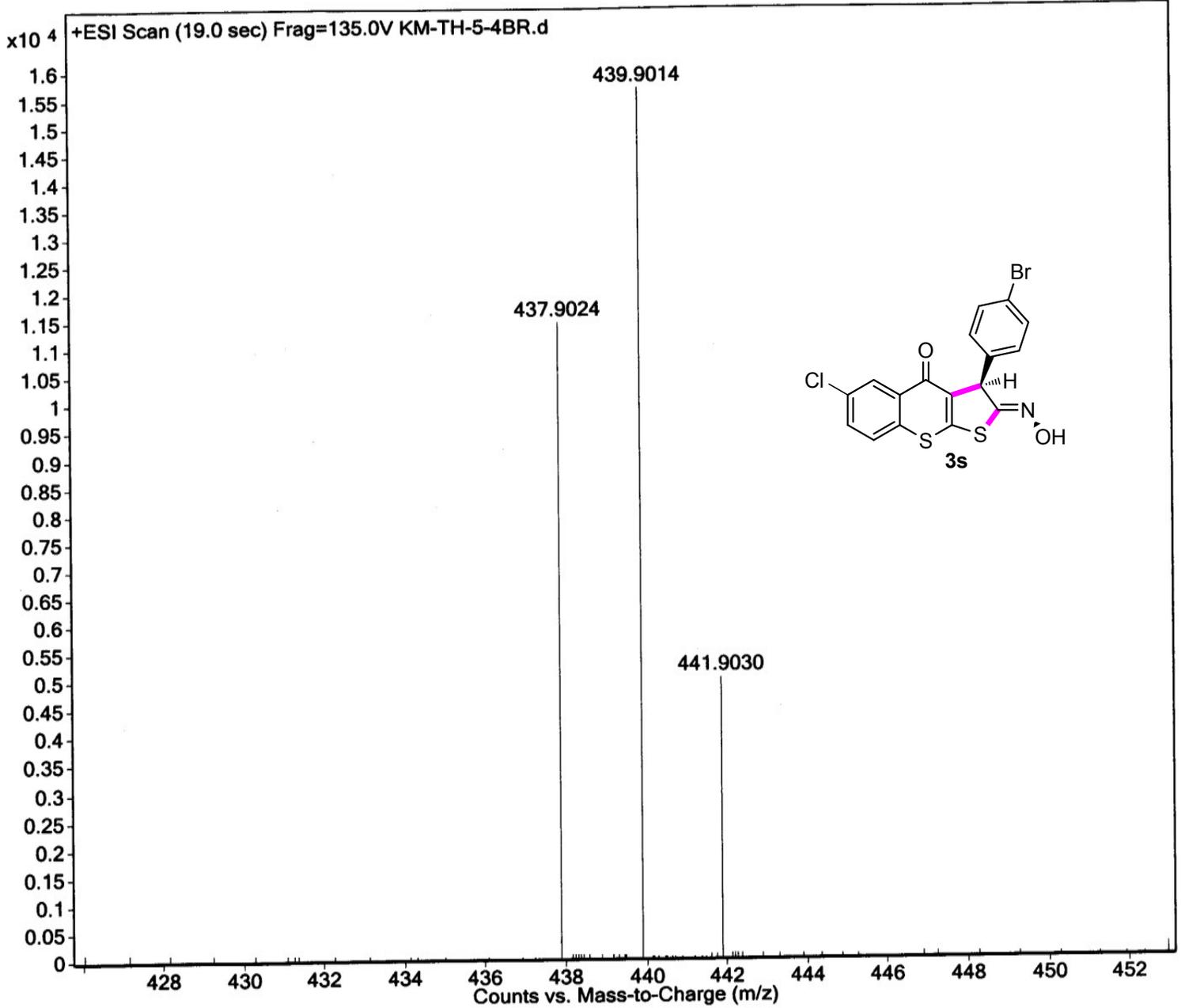
KM-TH-5-4BR-13C
KM-TH-5-4BR-13C

—172.19
—152.19
—150.58
—138.51
—134.02
—133.44
—131.61
—131.46
—131.29
—130.92
—129.96
—129.63
—128.93
—127.91
—127.40
—120.84
—77.44
—77.23
—77.02
—53.80
—39.80
—39.66
—39.52
—39.38
—39.24



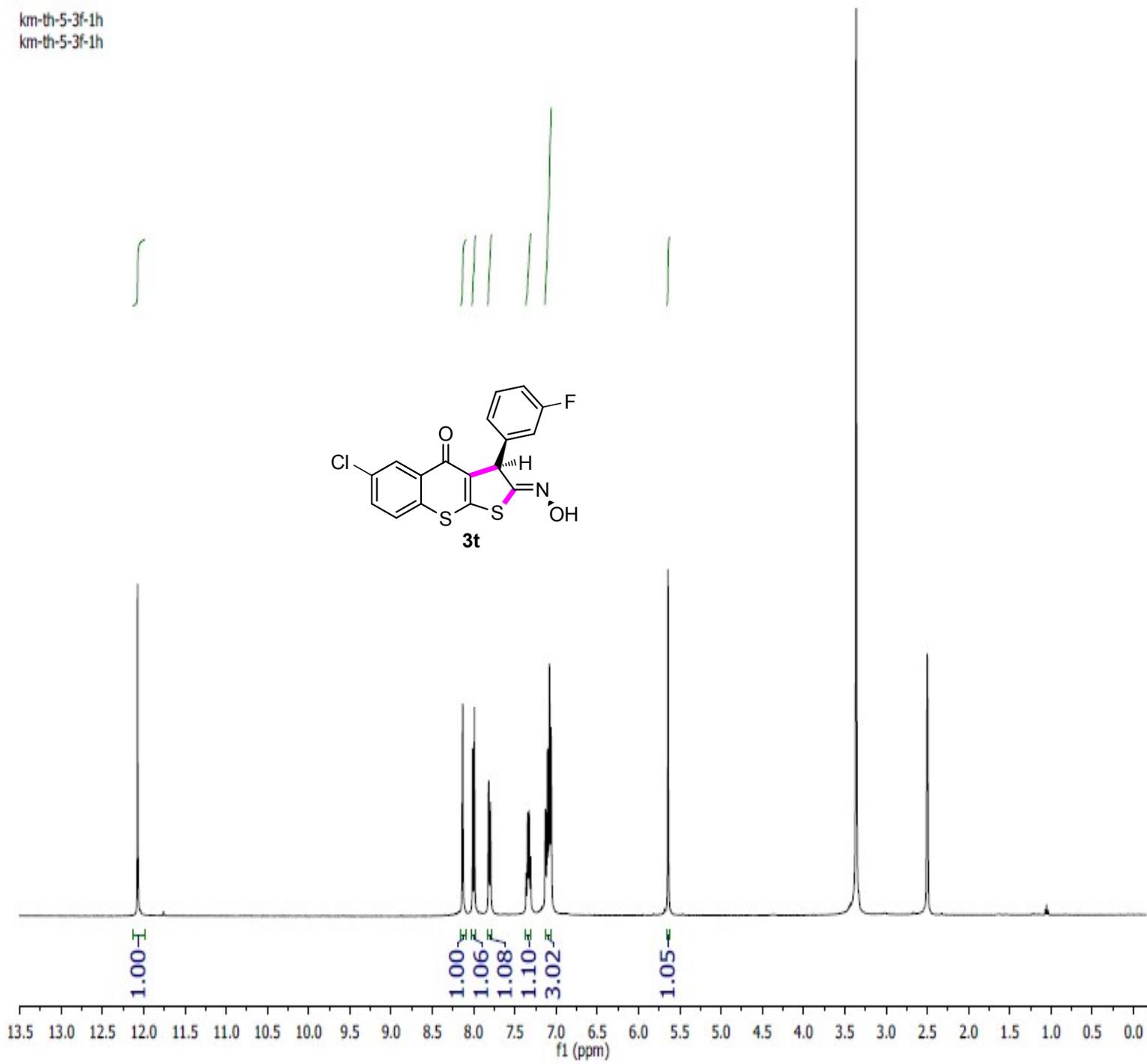
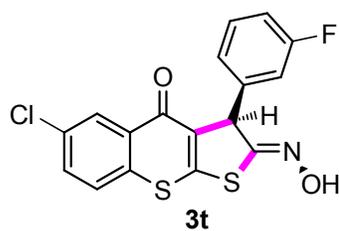
HRMS spectra of compound: 3s

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



¹HNMR spectra of compound: 3t

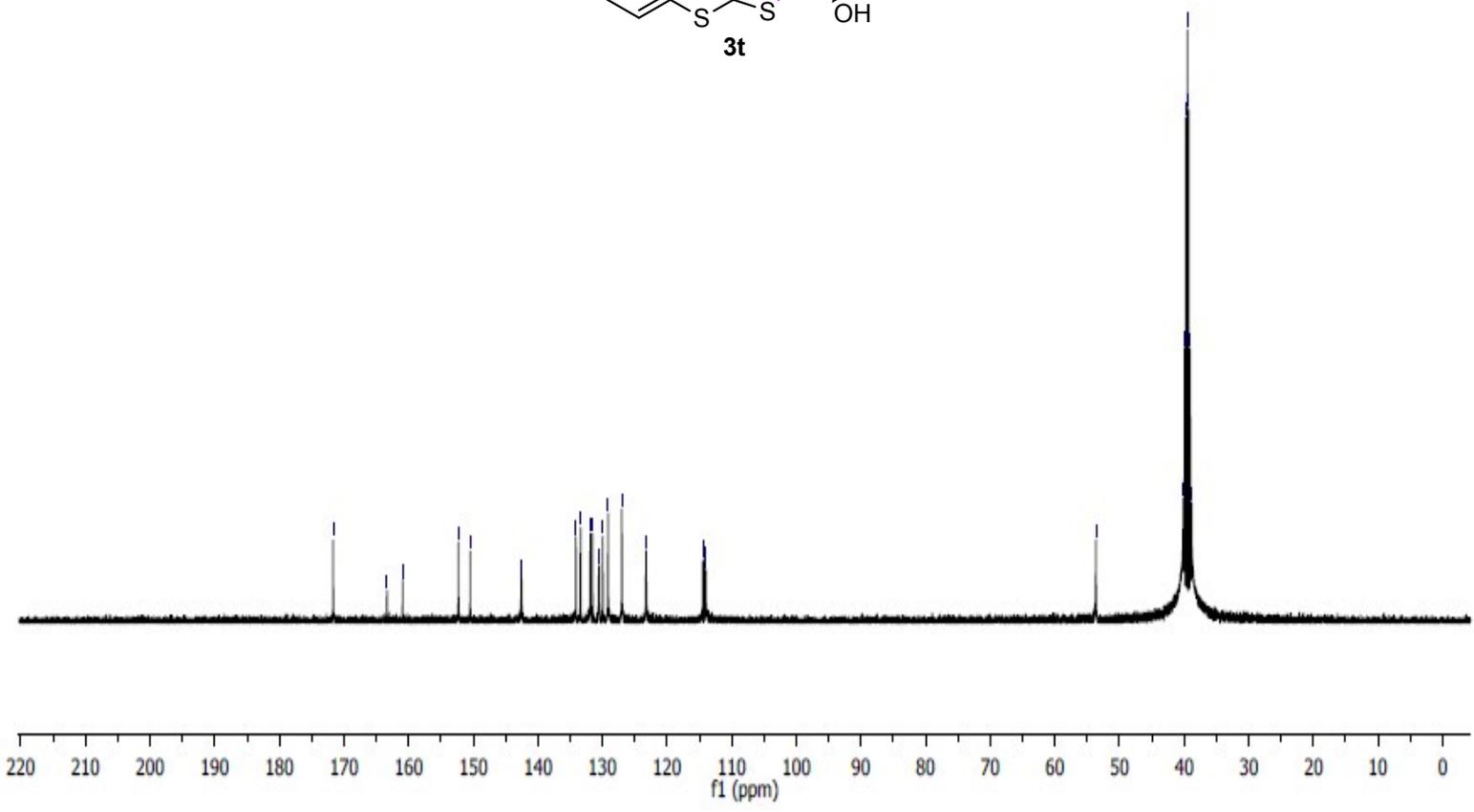
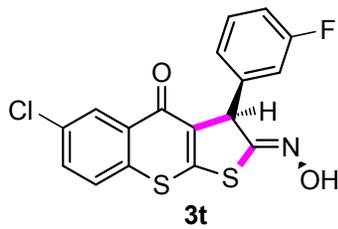
km-th-5-3f-1h
km-th-5-3f-1h



¹³CNMR spectra of compound: 3t

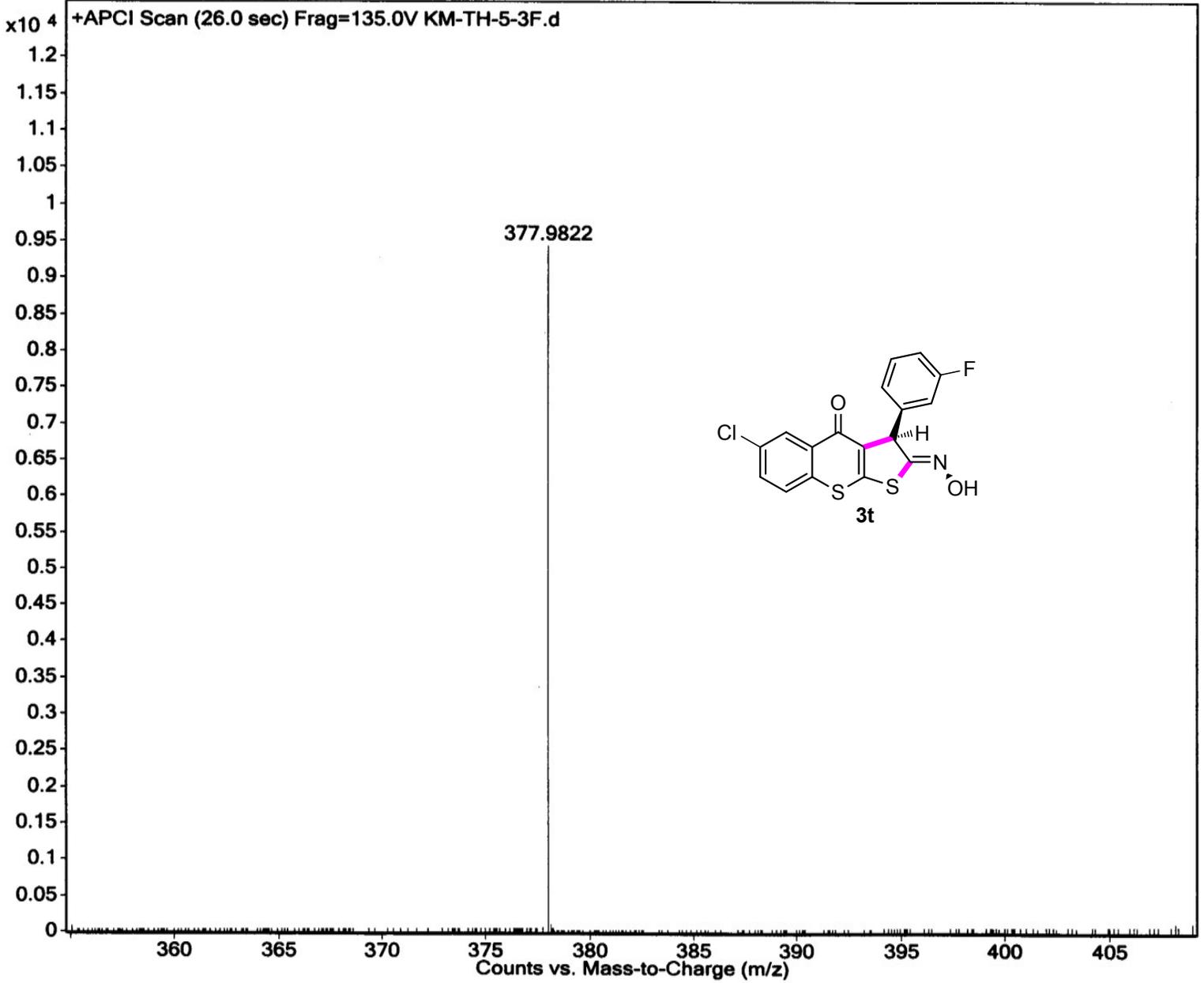
km-th-5-3f-13C
km-th-5-3f-1h

171.67
163.36
160.93
152.29
150.48
142.58
142.51
133.39
131.89
129.14
127.96
114.25
114.20
113.99
53.64
40.14
39.92
39.71
39.50
39.29
39.08
38.86



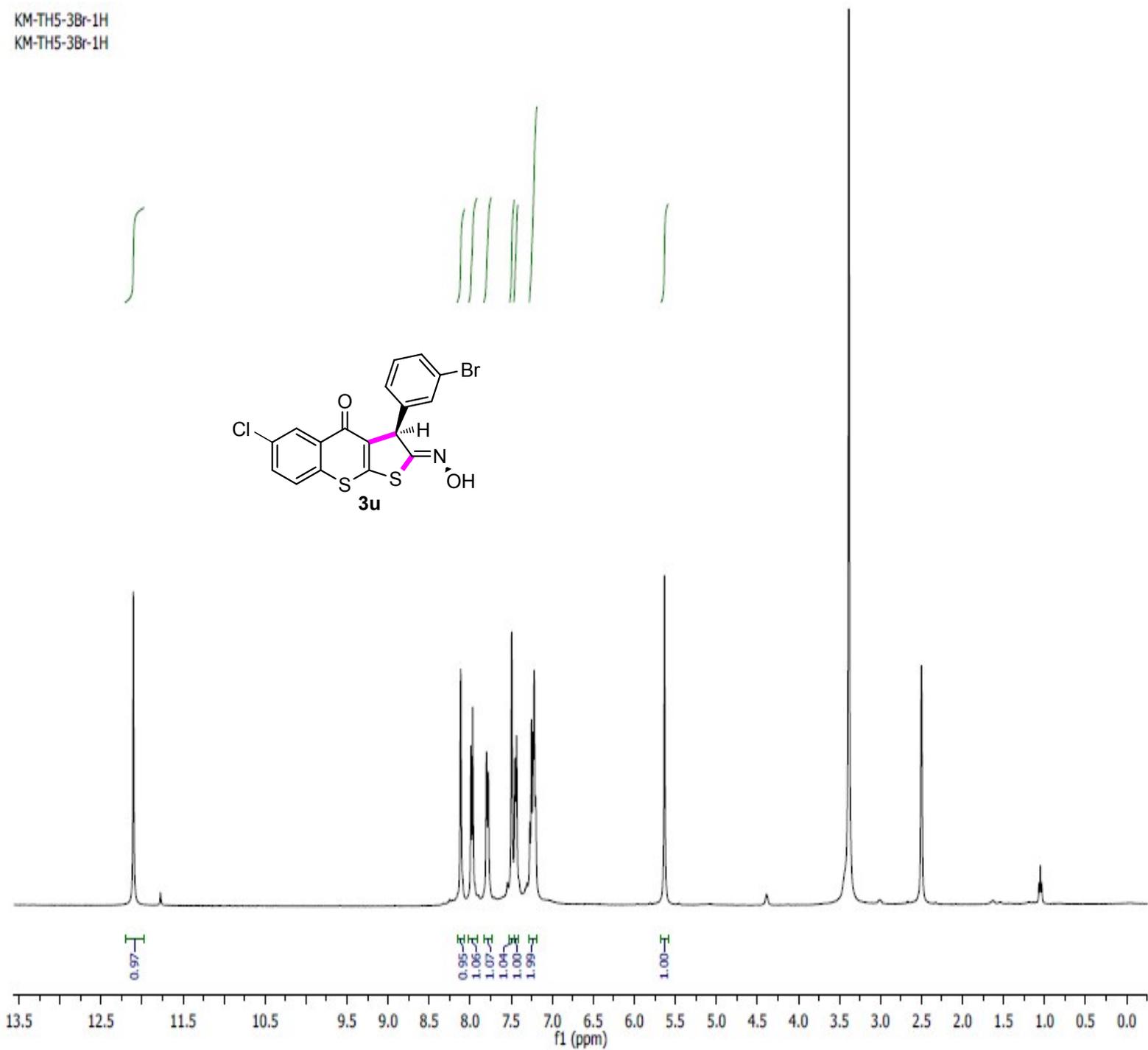
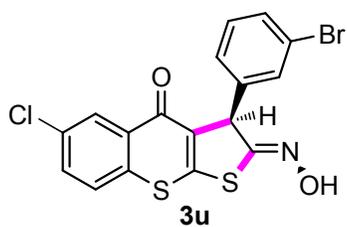
HRMS spectra of compound: 3t

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



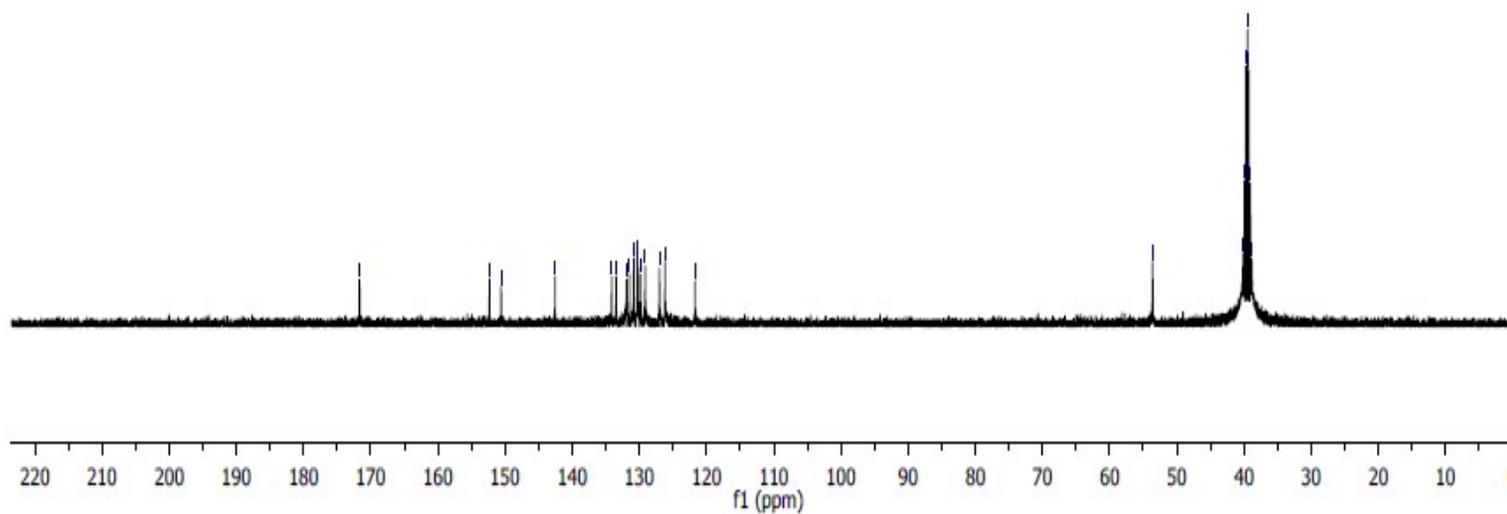
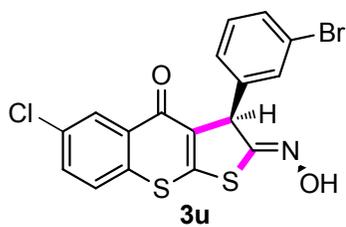
¹H NMR spectra of compound: 3u

KM-TH5-3Br-1H
KM-TH5-3Br-1H



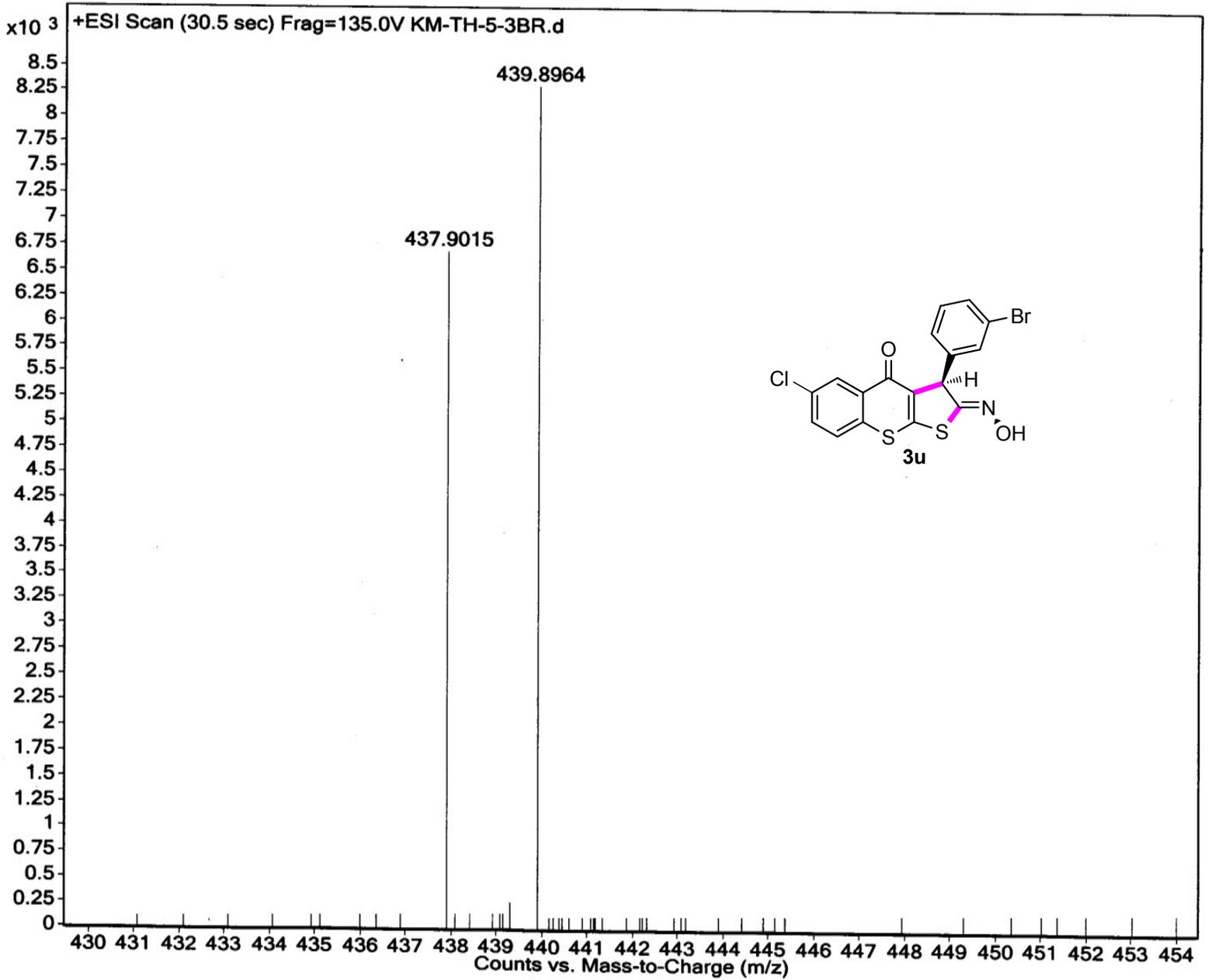
¹³CNMR spectra of compound: 3u

k-th-5-3br-13c
k-th-5-3br-13c



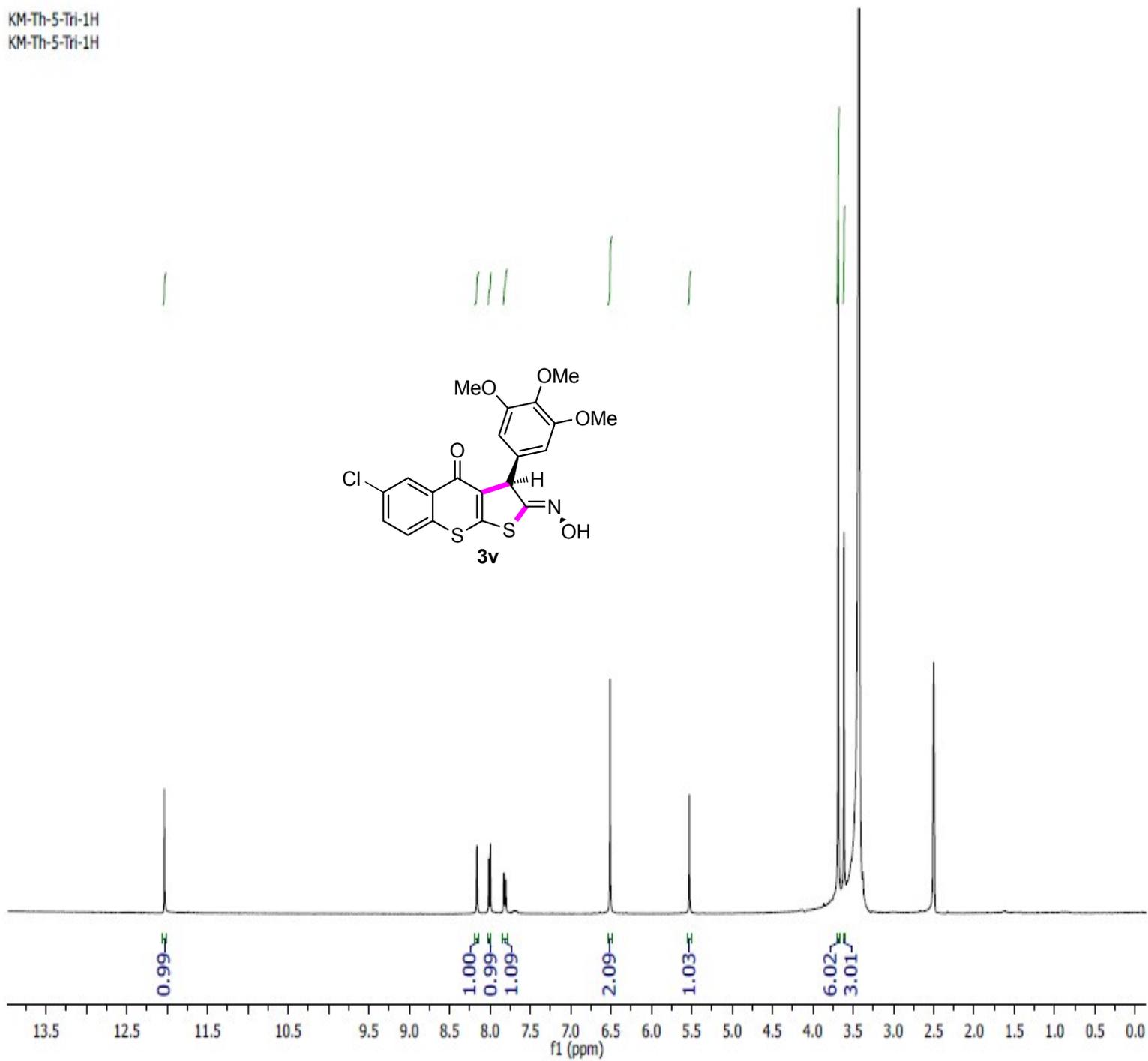
HRMS spectra of compound: 3u

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 compound: 3v

KM-Th-5-Tri-1H
KM-Th-5-Tri-1H



¹³CNMR spectra of compound: 3v

KM-TH-5-TR-OME_13C
KM-TH-5-TR-OME_13C

172.64

153.13

150.43

137.08

135.25

134.38

133.70

132.01

131.68

130.72

128.41

127.52

104.37

77.44

77.23

77.02

60.55

55.98

54.90

40.25

40.12

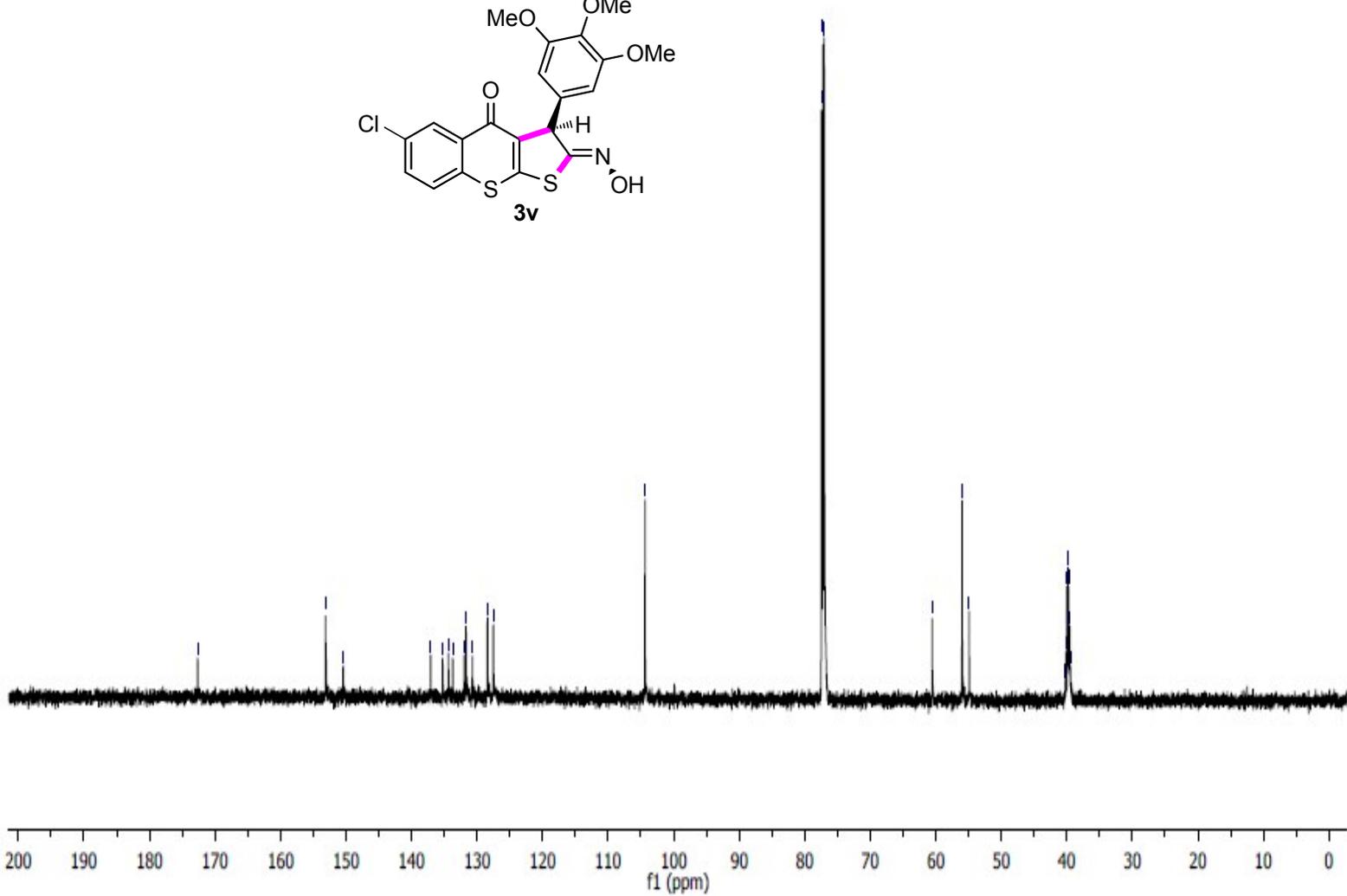
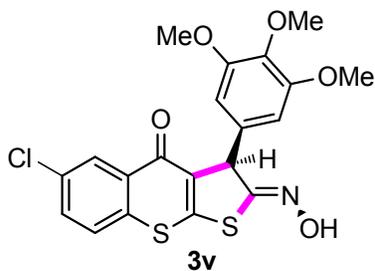
39.98

39.84

39.70

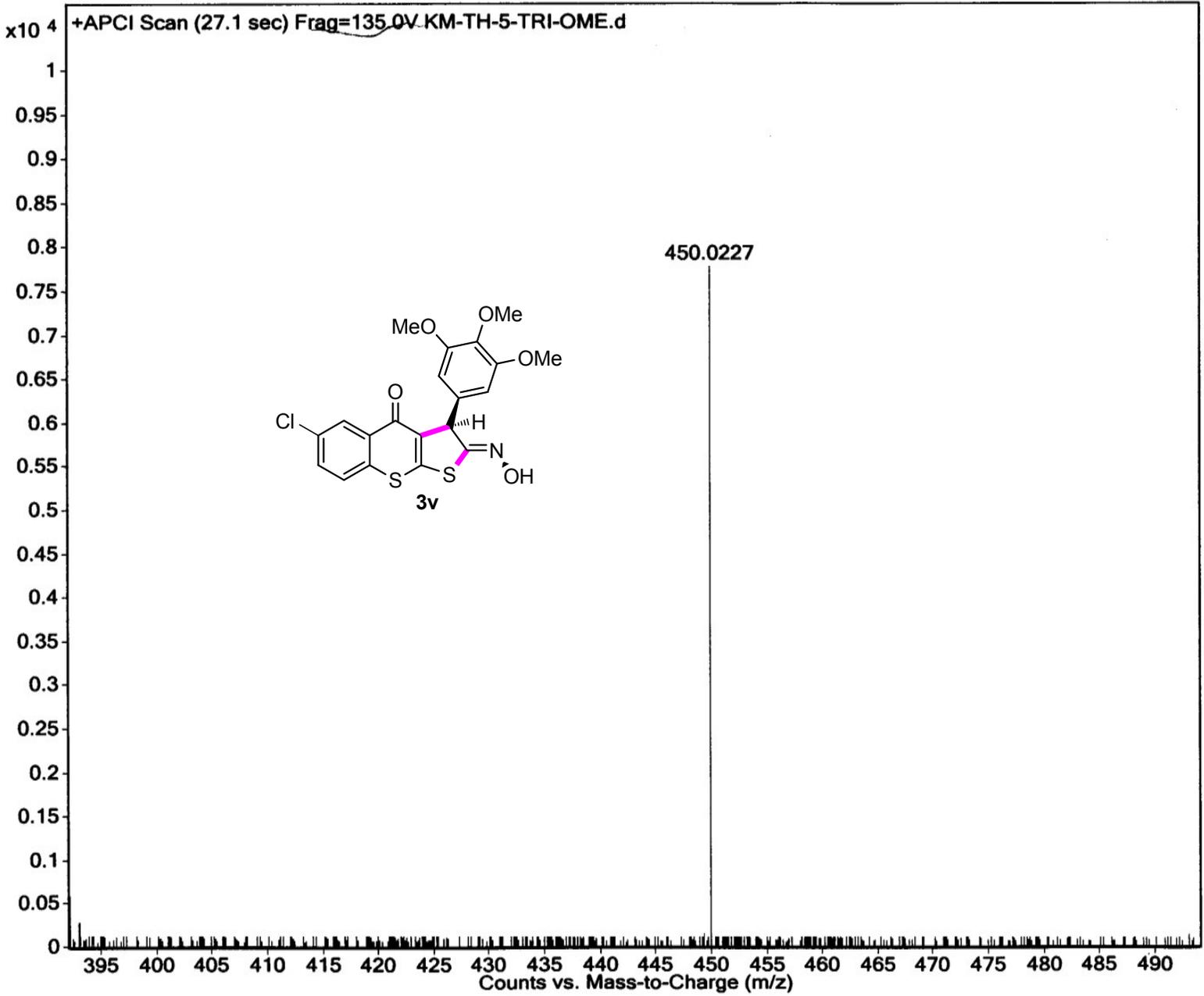
39.56

39.42



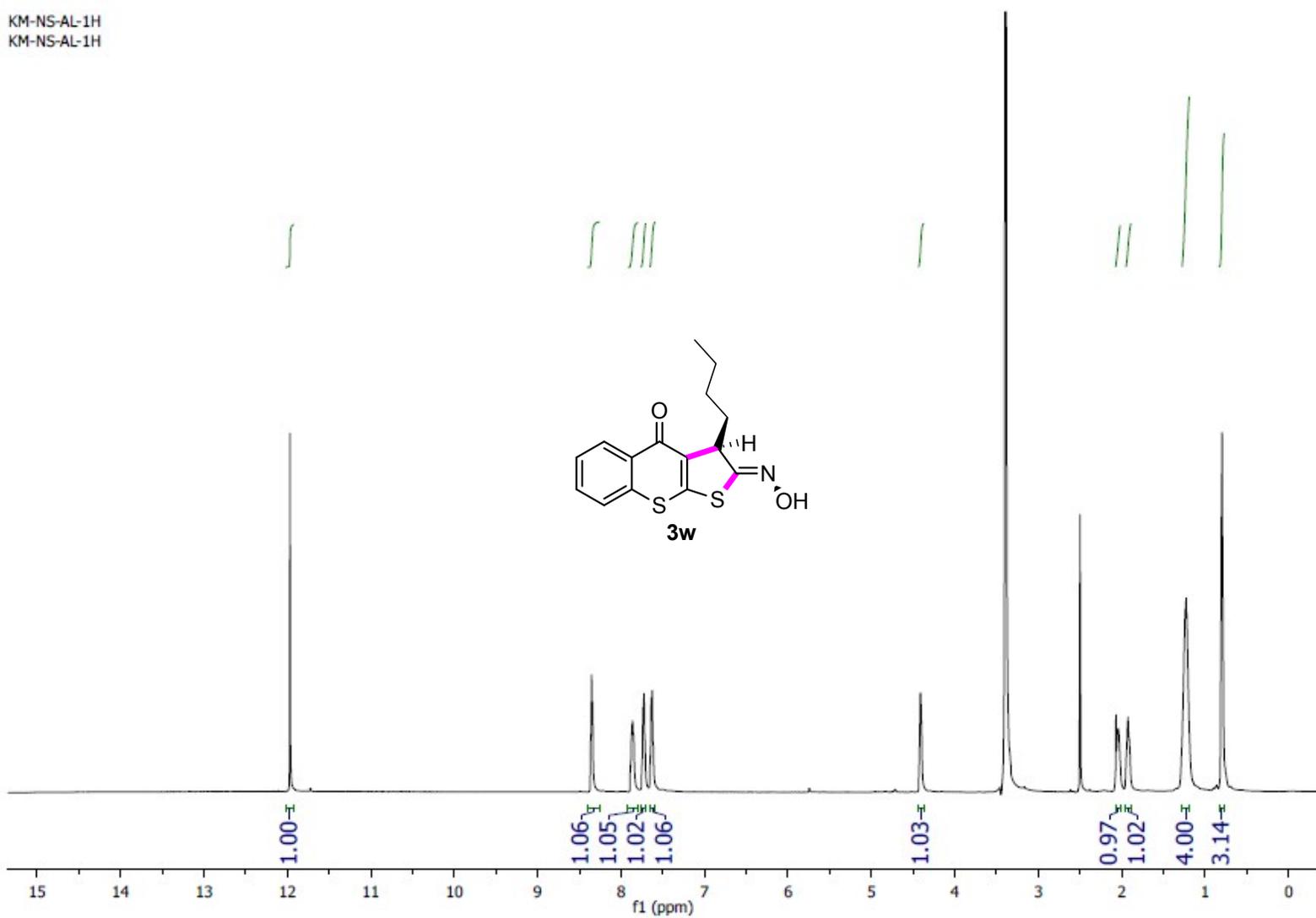
HRMS spectra of compound: 3v

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 compound: 3w

KM-NS-AL-1H
KM-NS-AL-1H



¹³CNMR spectra of compound: 3w

2017-06-05aa
KM-NS-AL

—173.37

—153.18

—148.20

—135.23

—131.88

—130.44

—130.05

—128.31

—128.08

—126.82

—49.13

—40.34

—40.06

—39.78

—39.50

—39.22

—38.94

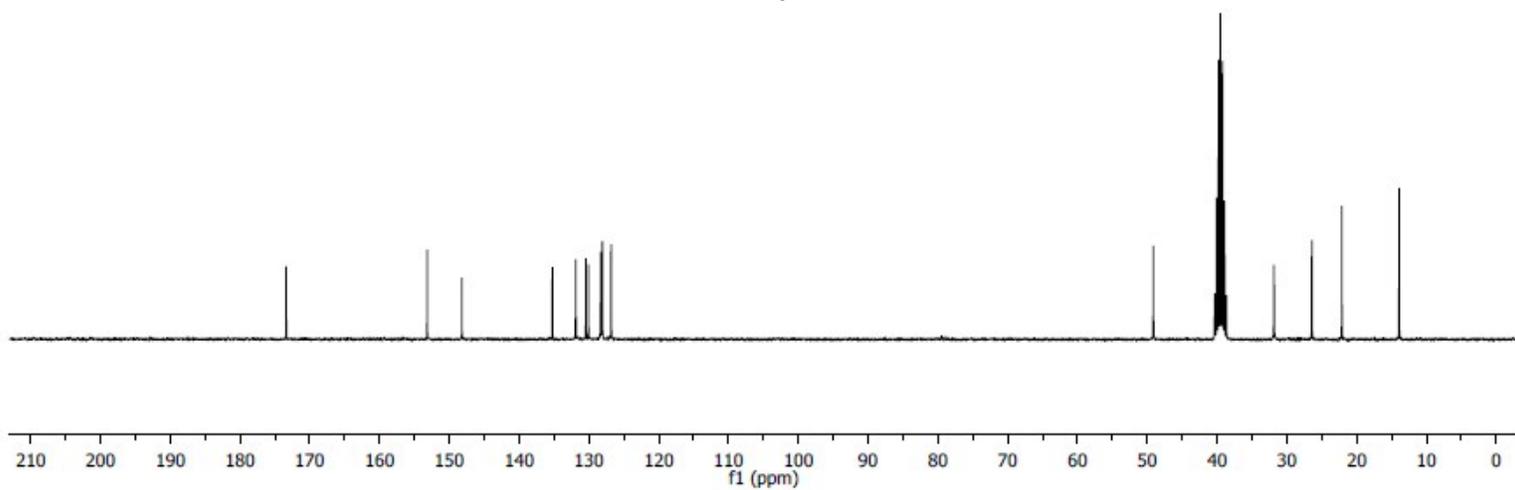
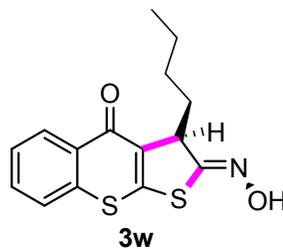
—38.66

—31.84

—26.42

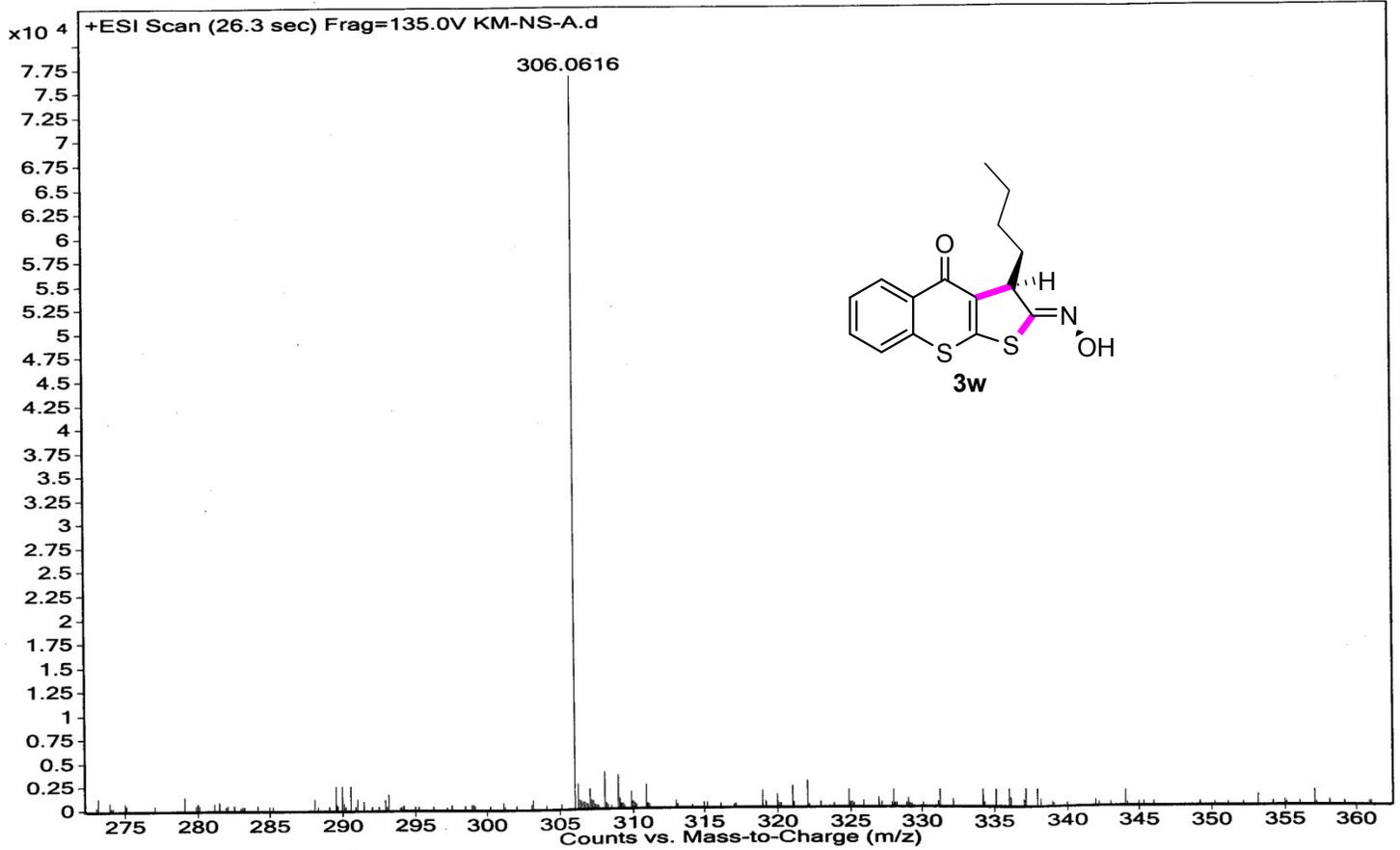
—22.12

—13.91



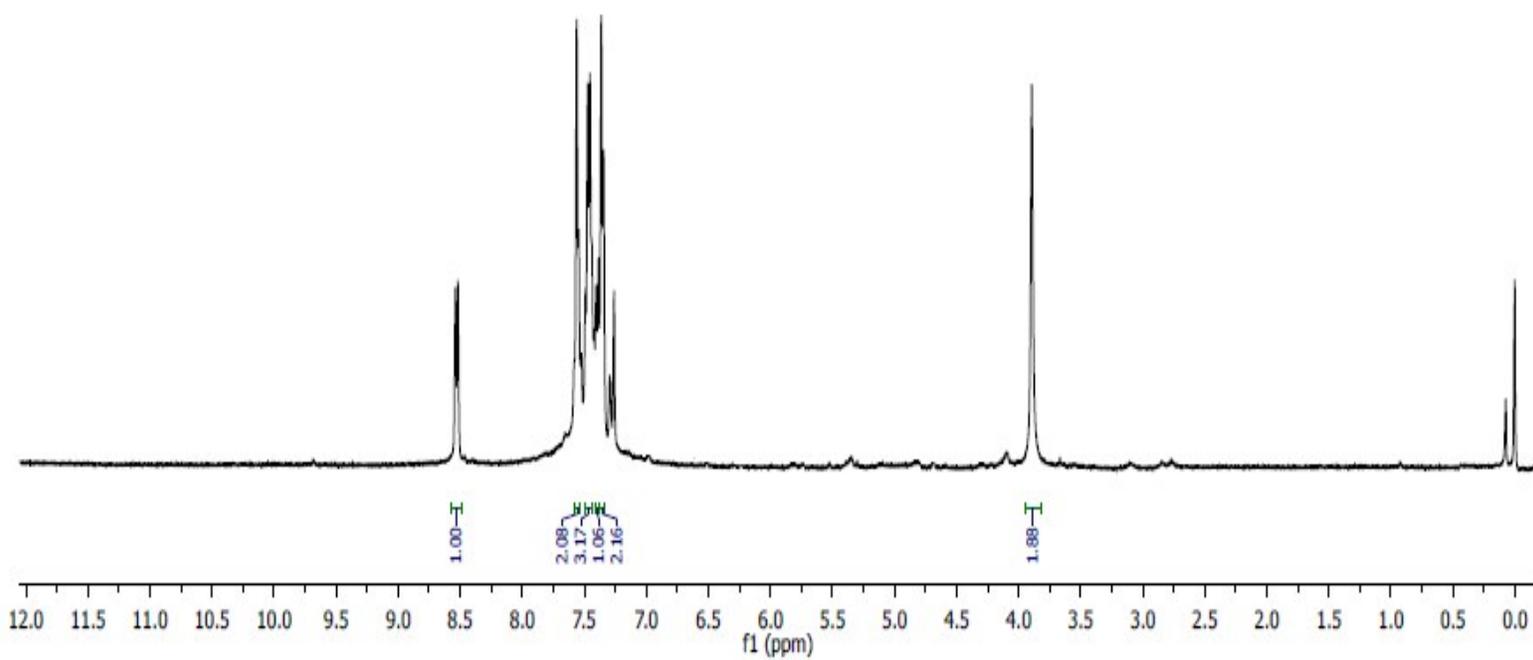
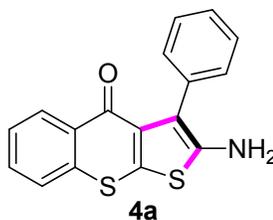
HRMS spectra of compound: 3w

Sample Name	KM-NS-A	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	KM-NS-A.d	ACQ Method		Comment		Acquired Time	5/23/2017 3:49:11 PM



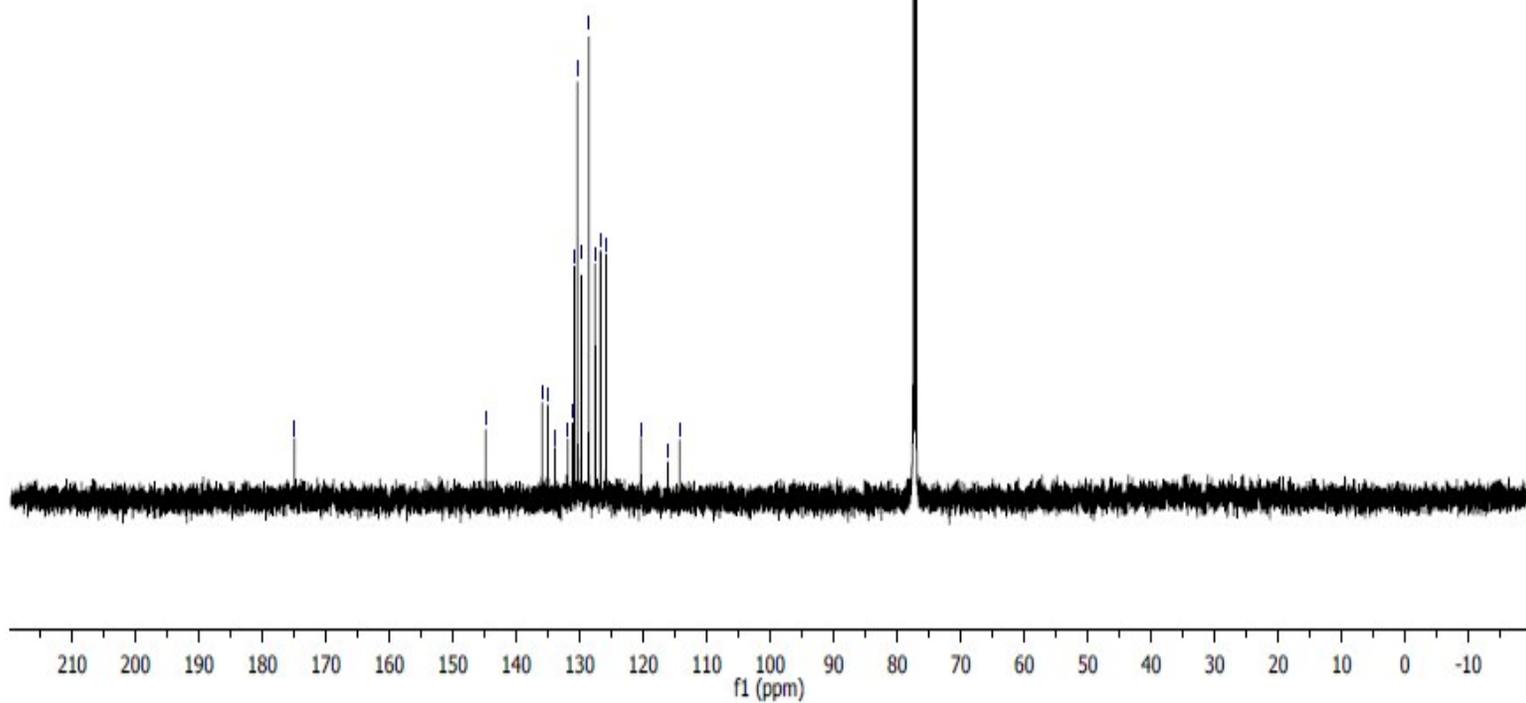
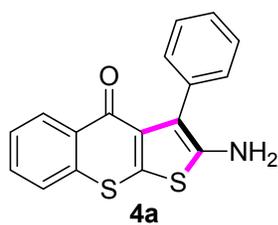
¹H NMR spectra of compound: 4a

KM-BR-Ben-1H
KM-BR-Ben-1H



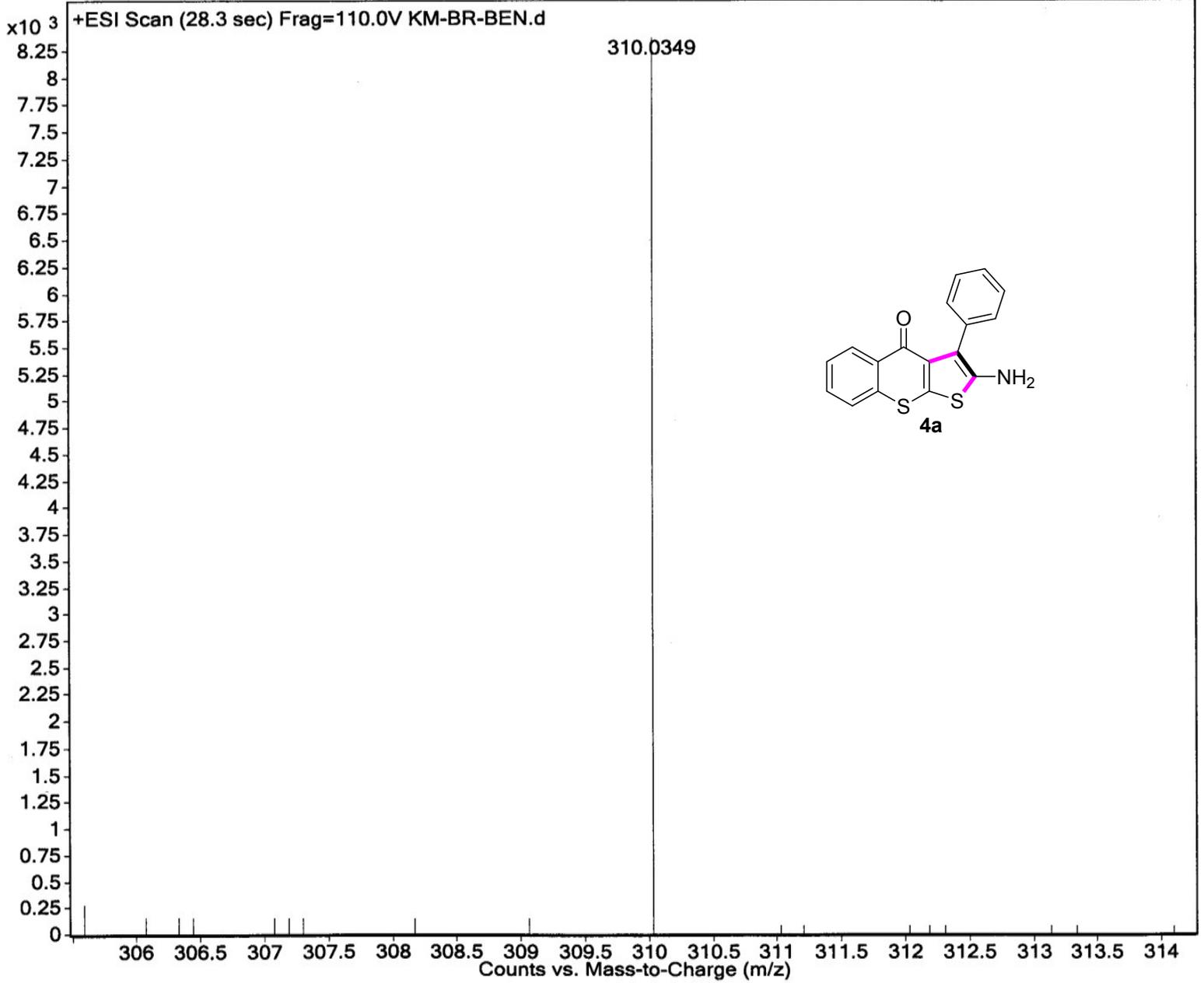
¹³CNMR spectra of compound: 4a

KM-BR-BEN-13C
KM-BR-BEN-13C



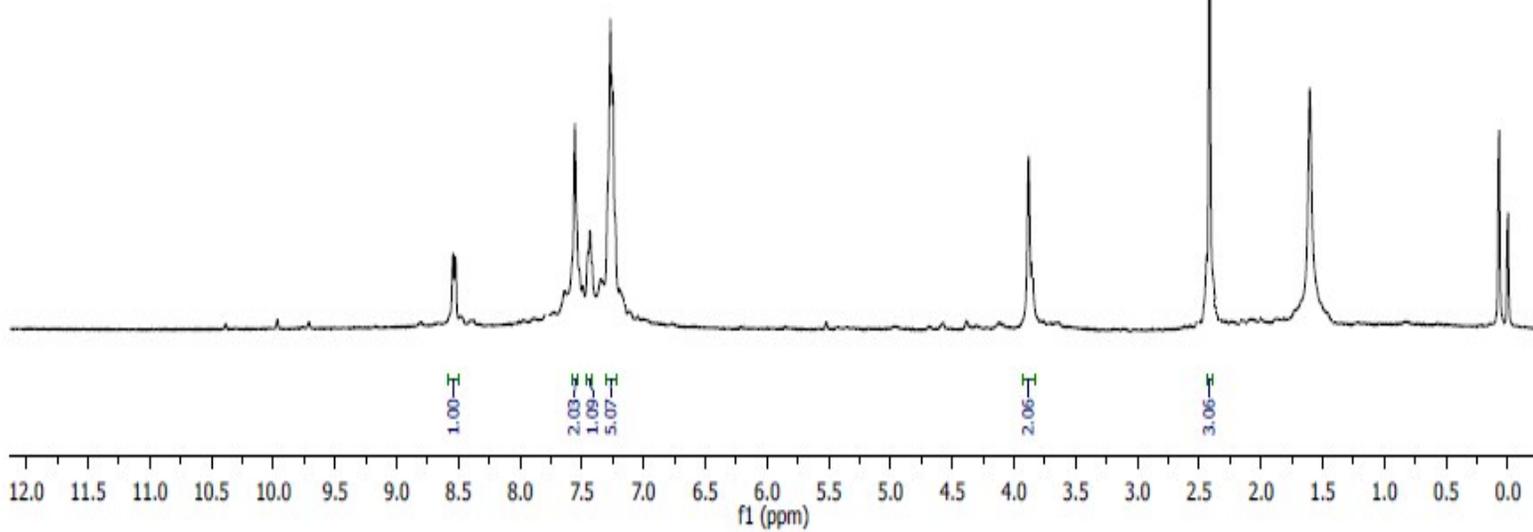
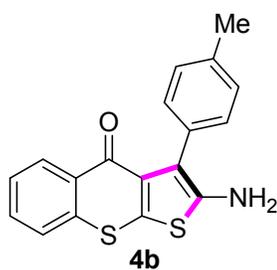
HRMS spectra of compound: 4a

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



¹H NMR spectra of compound: 4b

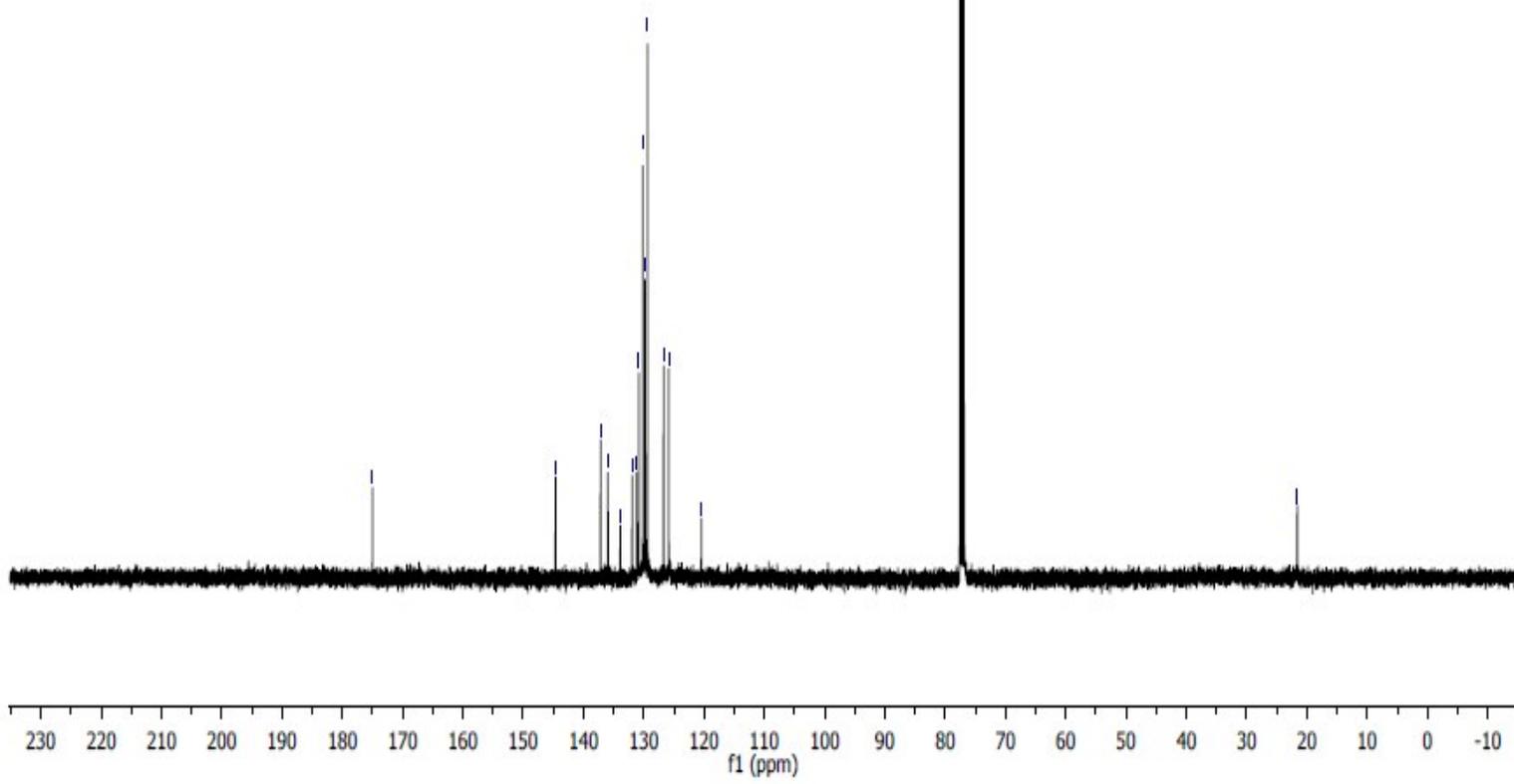
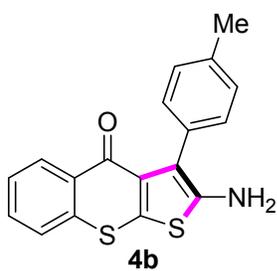
KM-BRMe-1H
KM-BRMe-1H



¹³CNMR spectra of compound: 4b

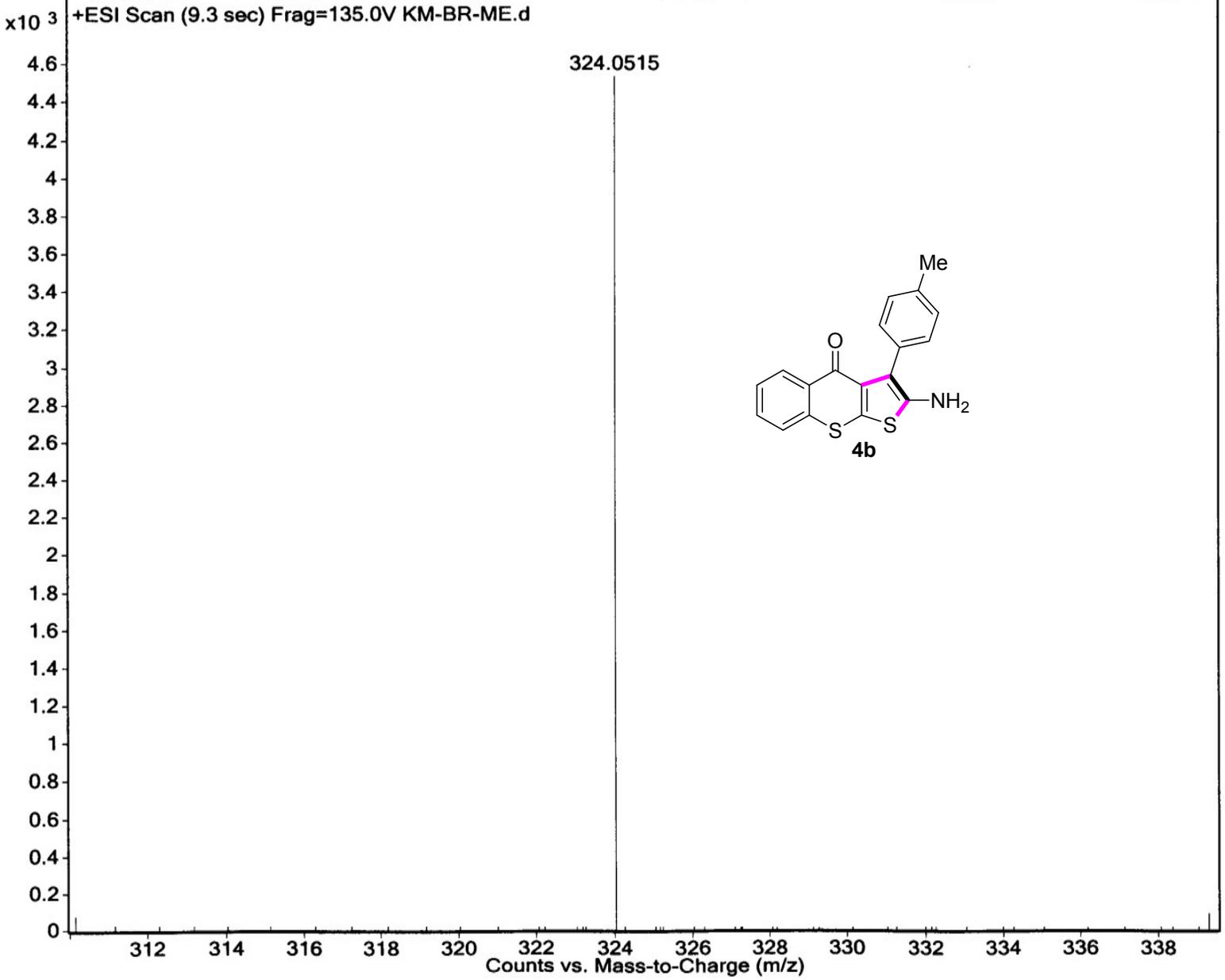
km-br-me-13c
km-br-me-13c

—175.00
144.64
137.16
135.94
133.89
131.91
131.17
130.83
130.16
129.77
129.37
126.70
125.86
120.45
77.55
77.23
76.91
—21.59



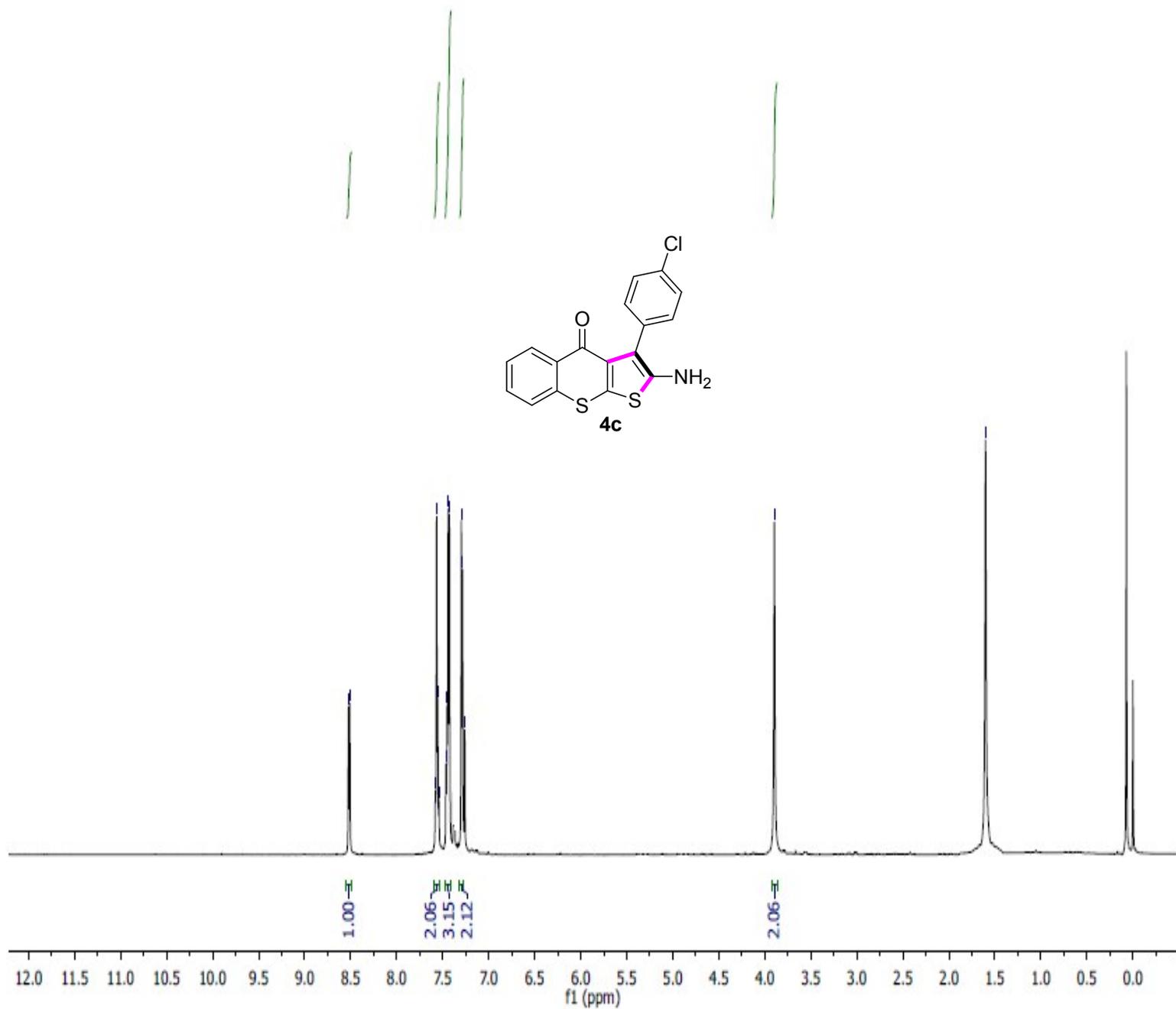
HRMS spectra of compound: 4b

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

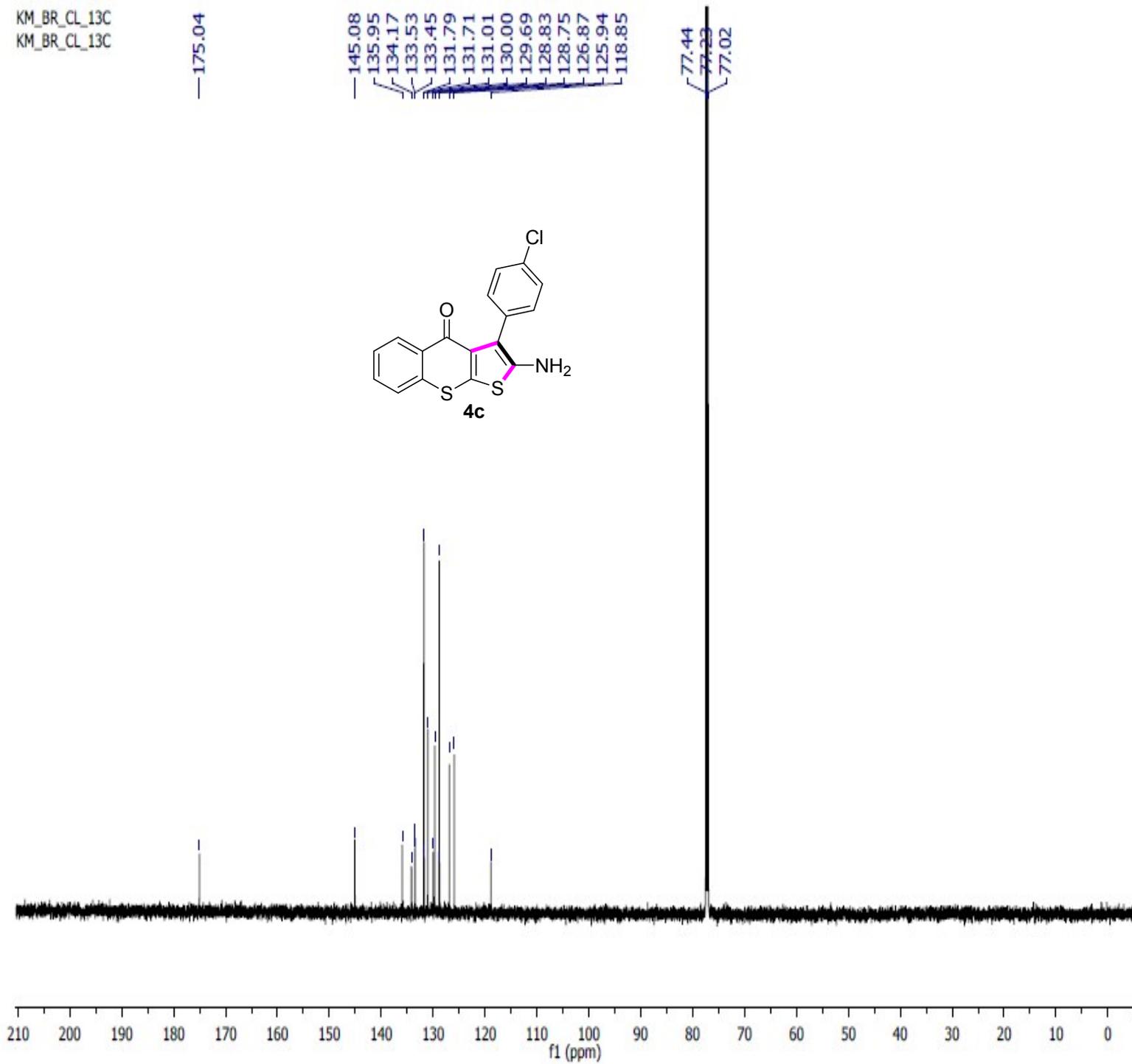


¹HNMR spectra of compound: 4c

KM-Br-Cl-1H
KM-Br-Cl-1H

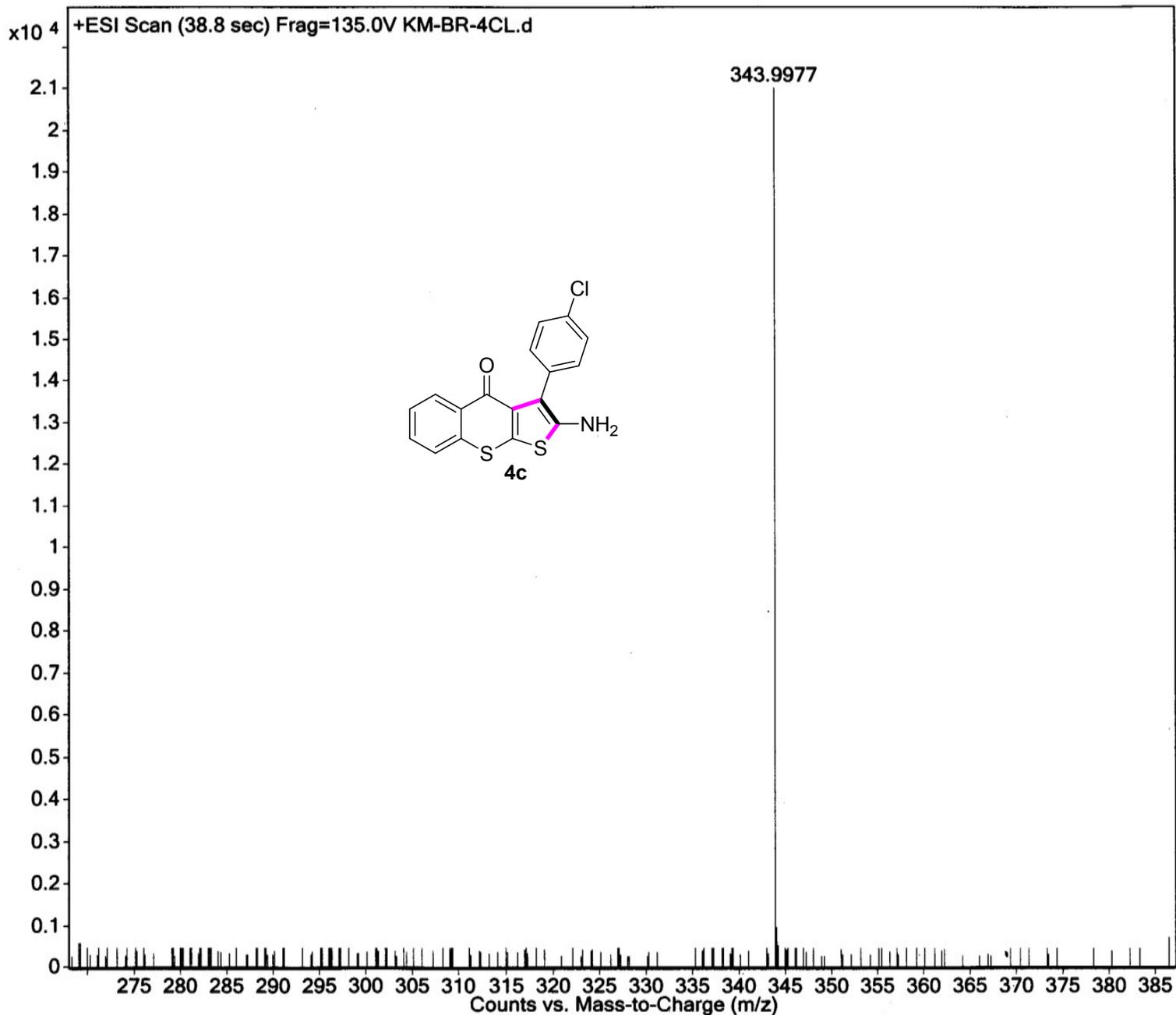


¹³CNMR spectra of compound: 4c



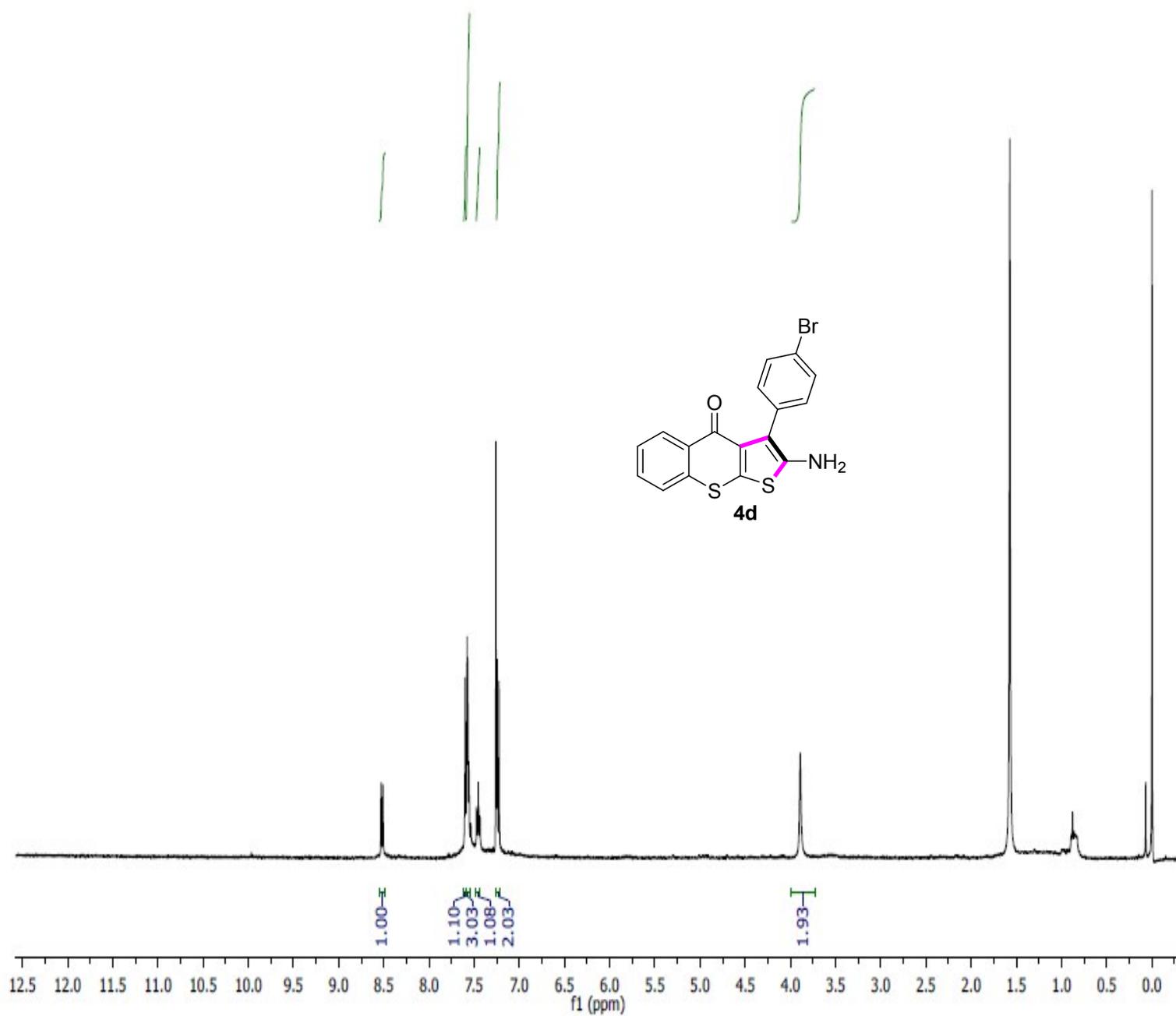
HRMS spectra of compound: 4c

Sample Name	KM-BR-4CL	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	KM-BR-4CL.d	ACQ Method		Comment		Acquired Time	2/3/2016 11:25:30 AM



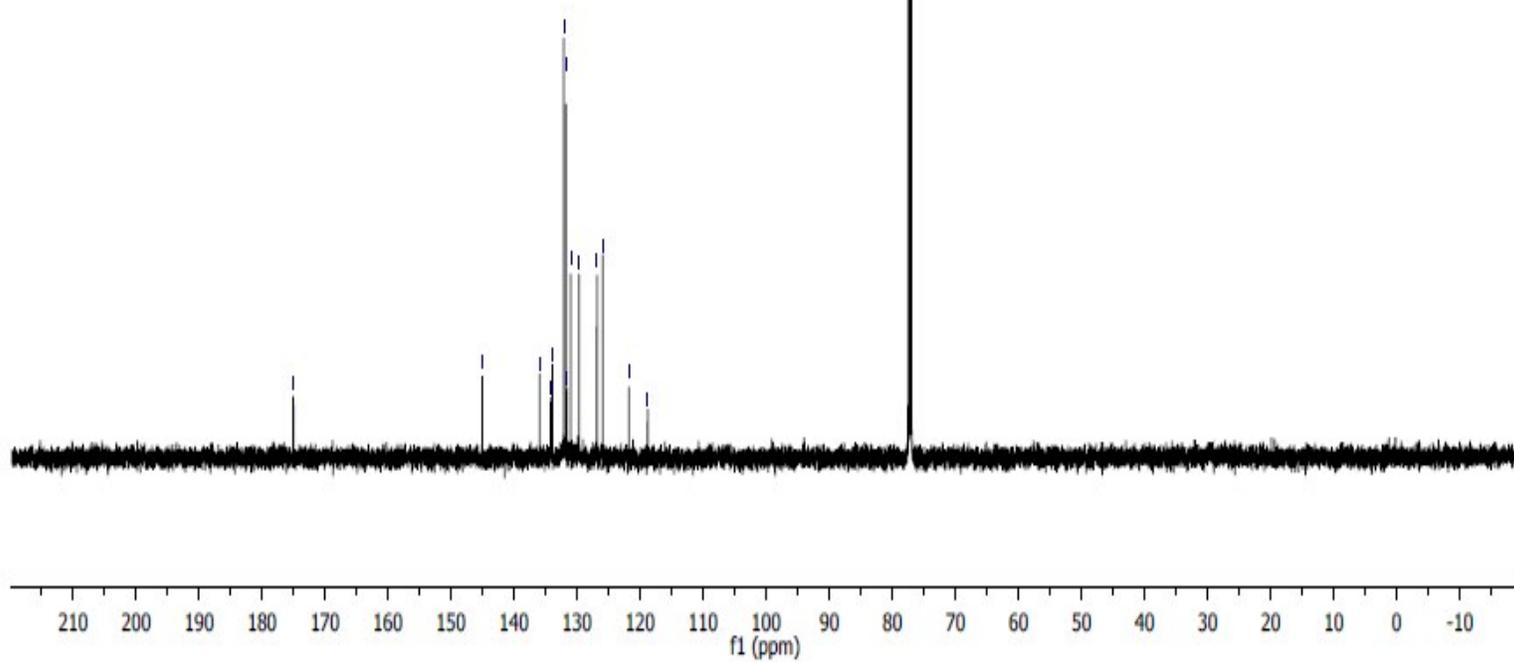
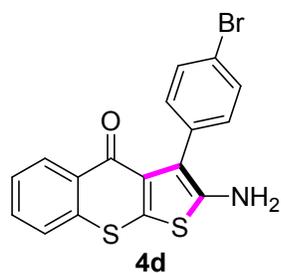
¹H NMR spectra of compound: 4d

KM-BR-4Br-1H
KM-BR-4Br-1H



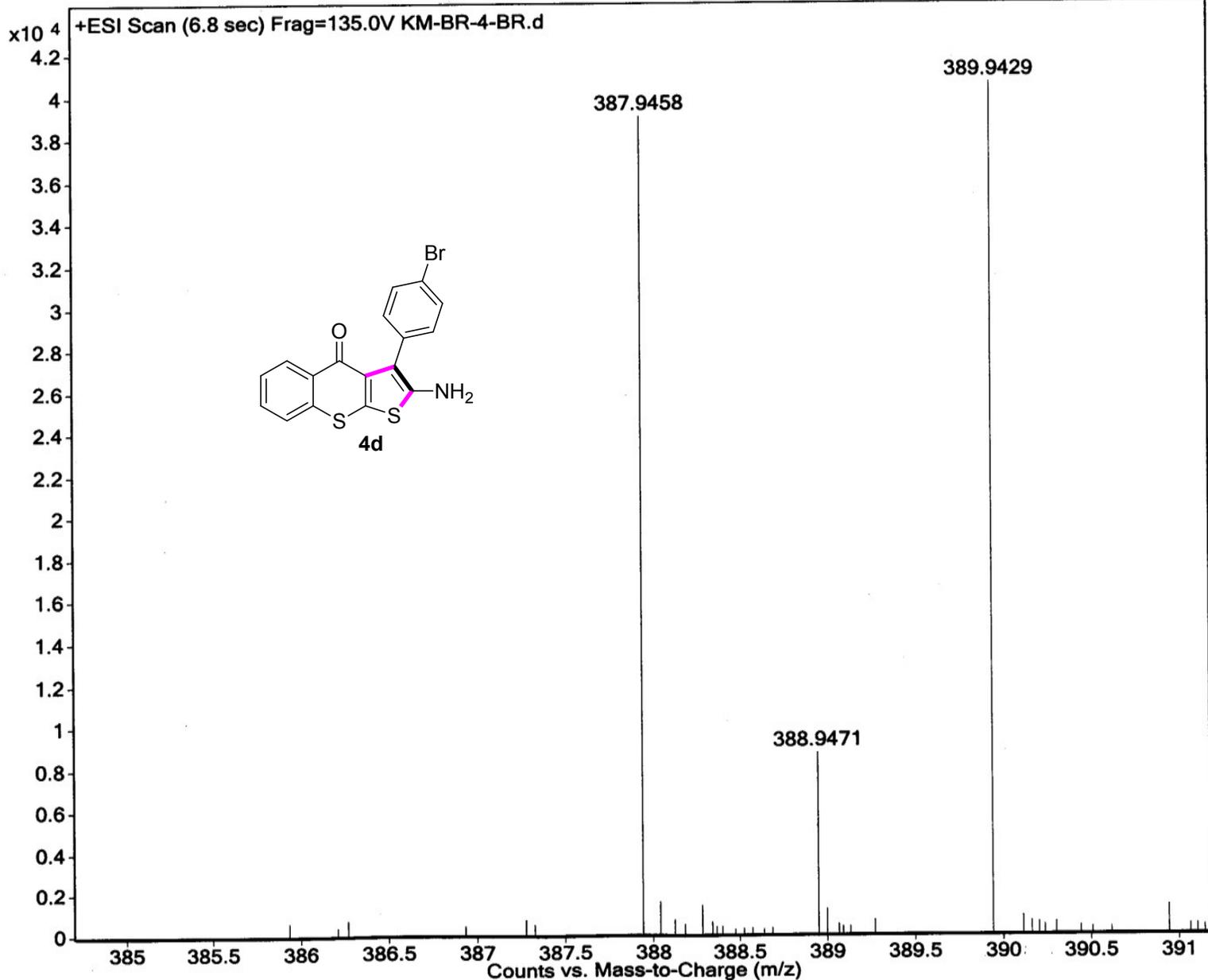
¹³CNMR spectra of compound: 4d

KM-BR-4Br-13C
KM-BR-4Br-13C



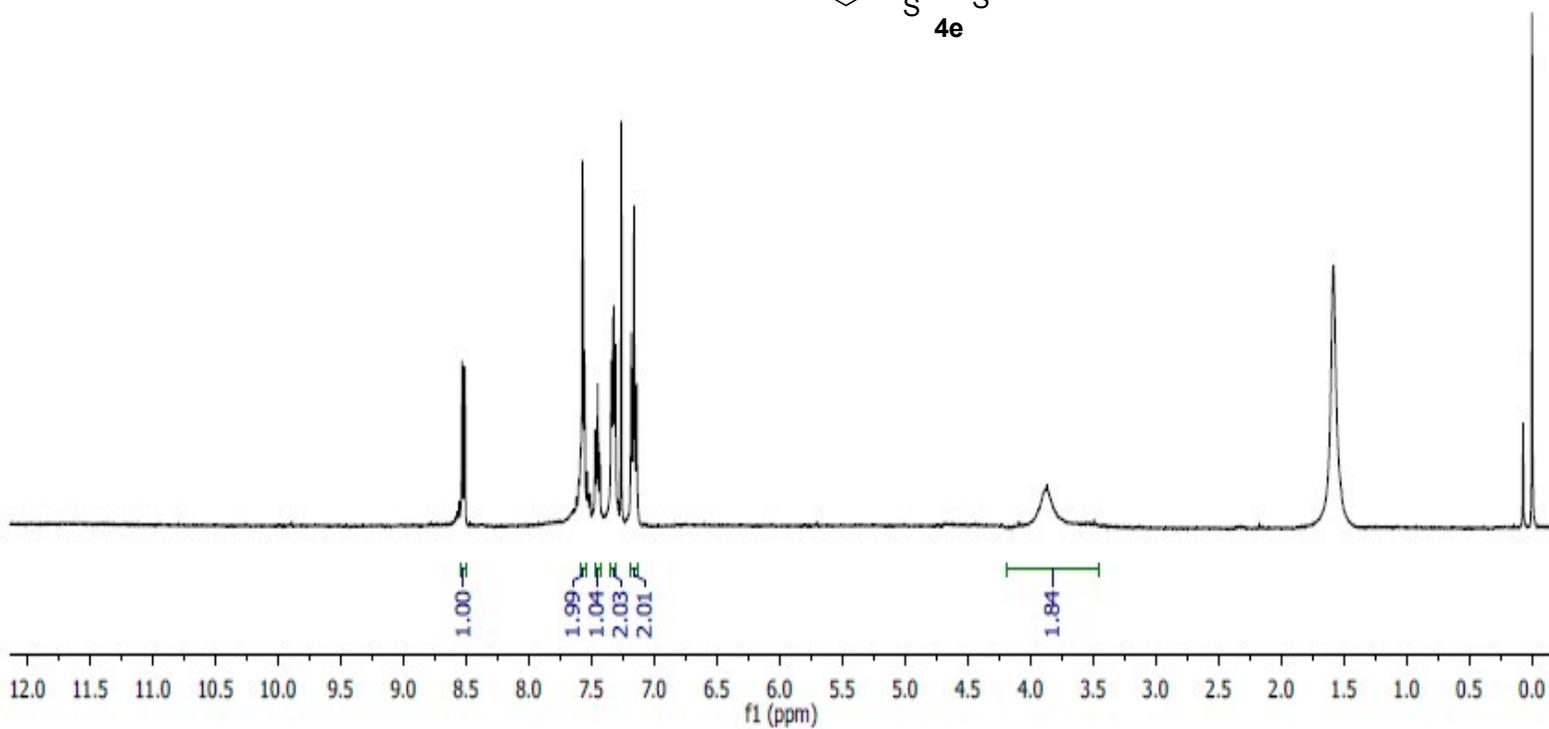
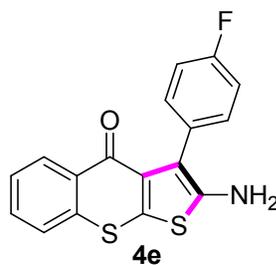
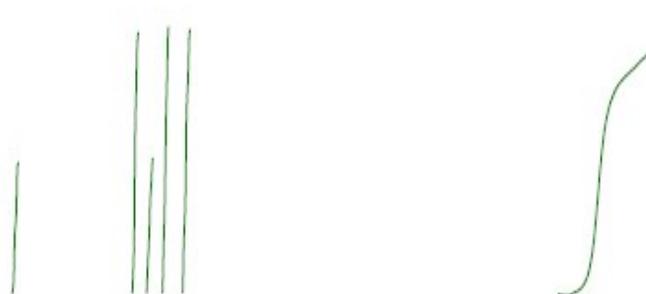
HRMS spectra of compound: 4d

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	KM-BR-4-BR.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹HNMR spectra of compound: 4e

km-br-4f-1h
km-br-4f-13c



¹³CNMR spectra of compound: 4e

KM-BR-4F_13C
KM-BR-4F_13C

— 175.08

~ 163.18

~ 161.55

— 144.97

— 135.96

— 134.06

— 132.12

— 132.07

— 131.81

— 131.08

— 130.99

— 129.71

— 126.84

— 125.94

— 119.24

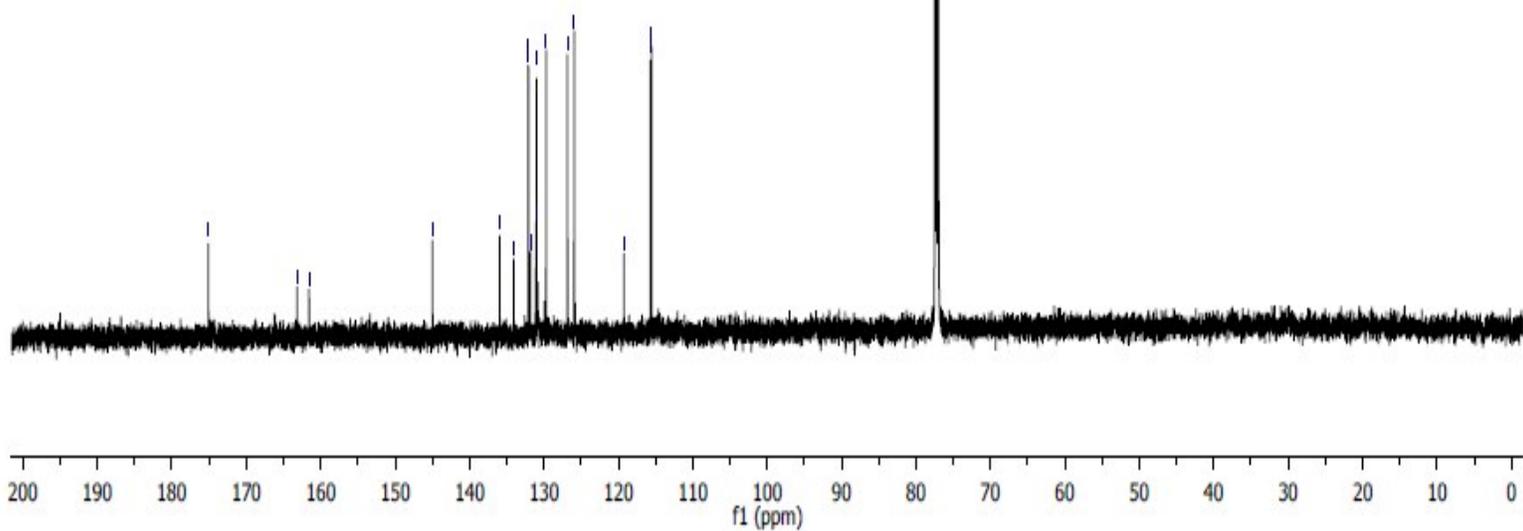
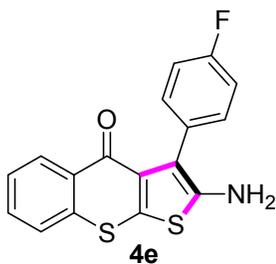
— 115.69

— 115.55

— 77.44

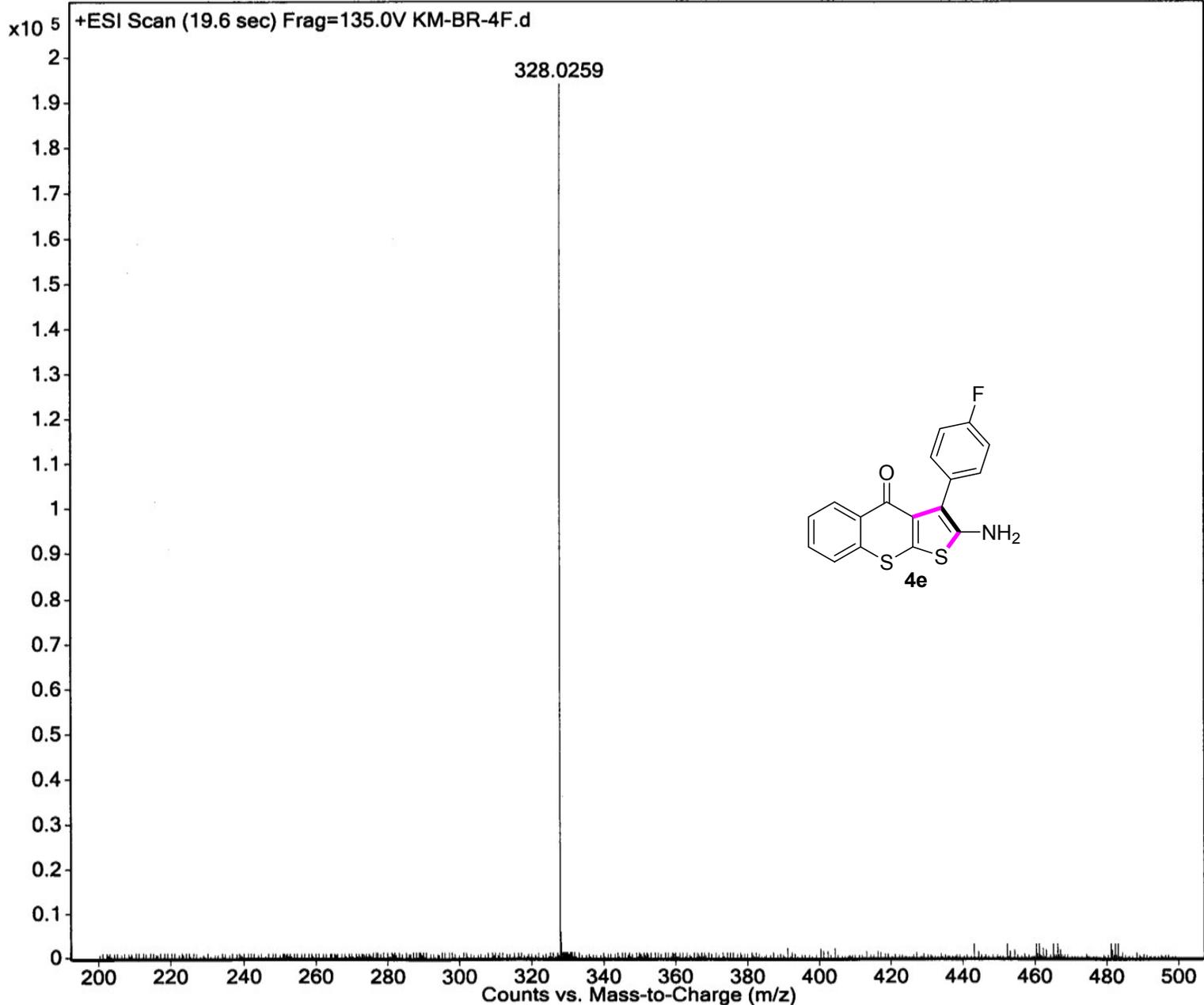
— 77.23

— 77.02



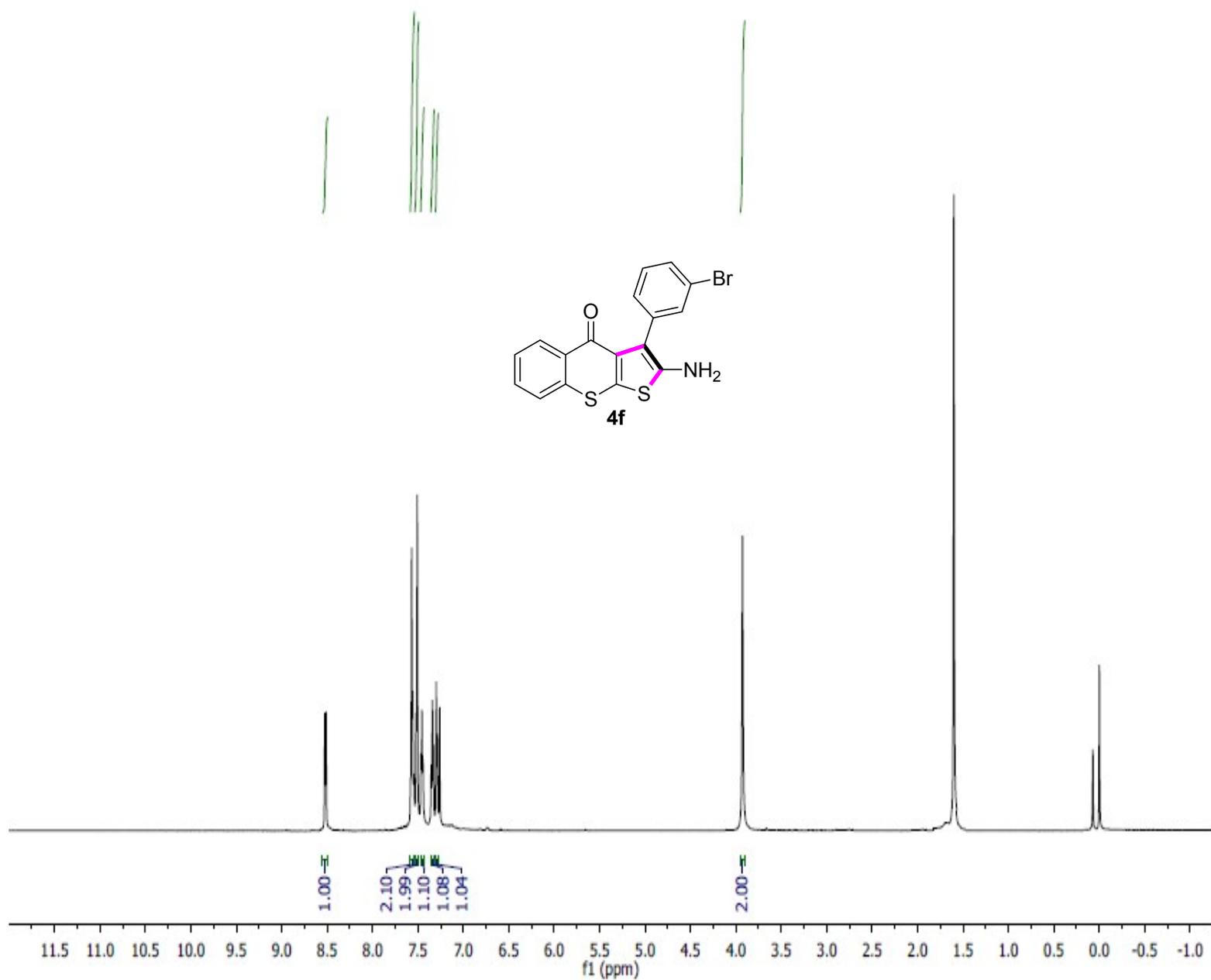
HRMS spectra of compound: 4e

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



¹H NMR spectra of compound: 4f

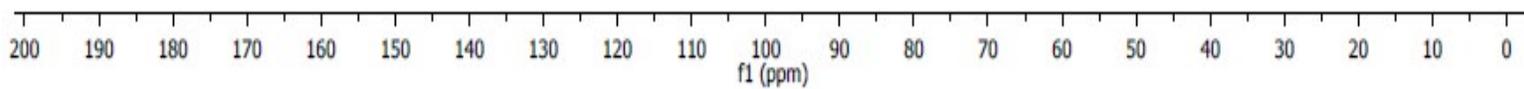
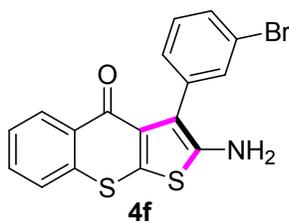
KM-N-3BR-1H
KM-N-3BR-1H



¹³CNMR spectra of compound: 4f

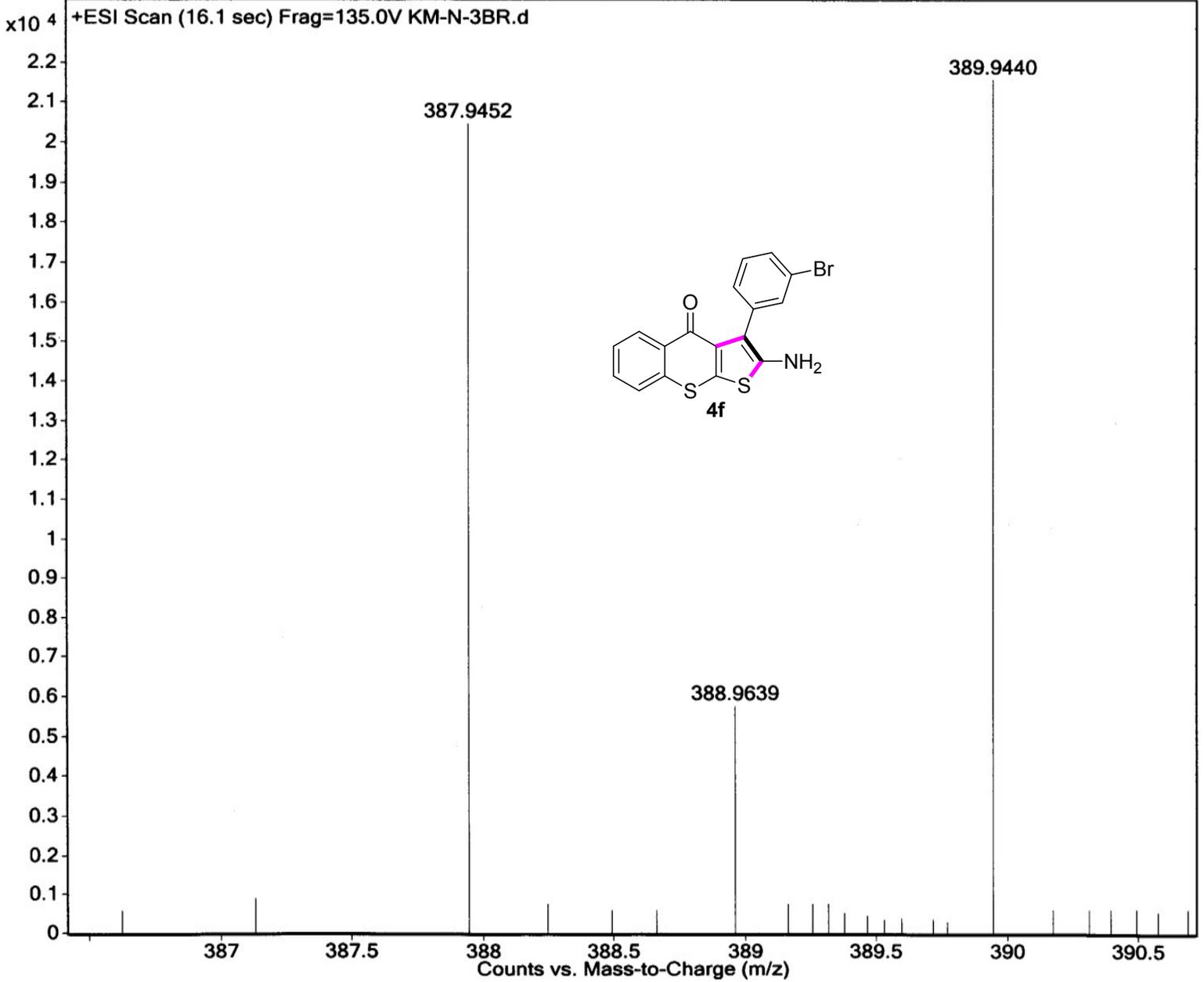
KM-N-3BR-13C
KM-N-3BR-13C

—174.92
145.37
137.16
135.91
134.03
133.10
131.68
131.02
130.96
130.64
130.02
129.71
129.40
126.87
125.94
122.52
118.48
77.44
77.23
77.02



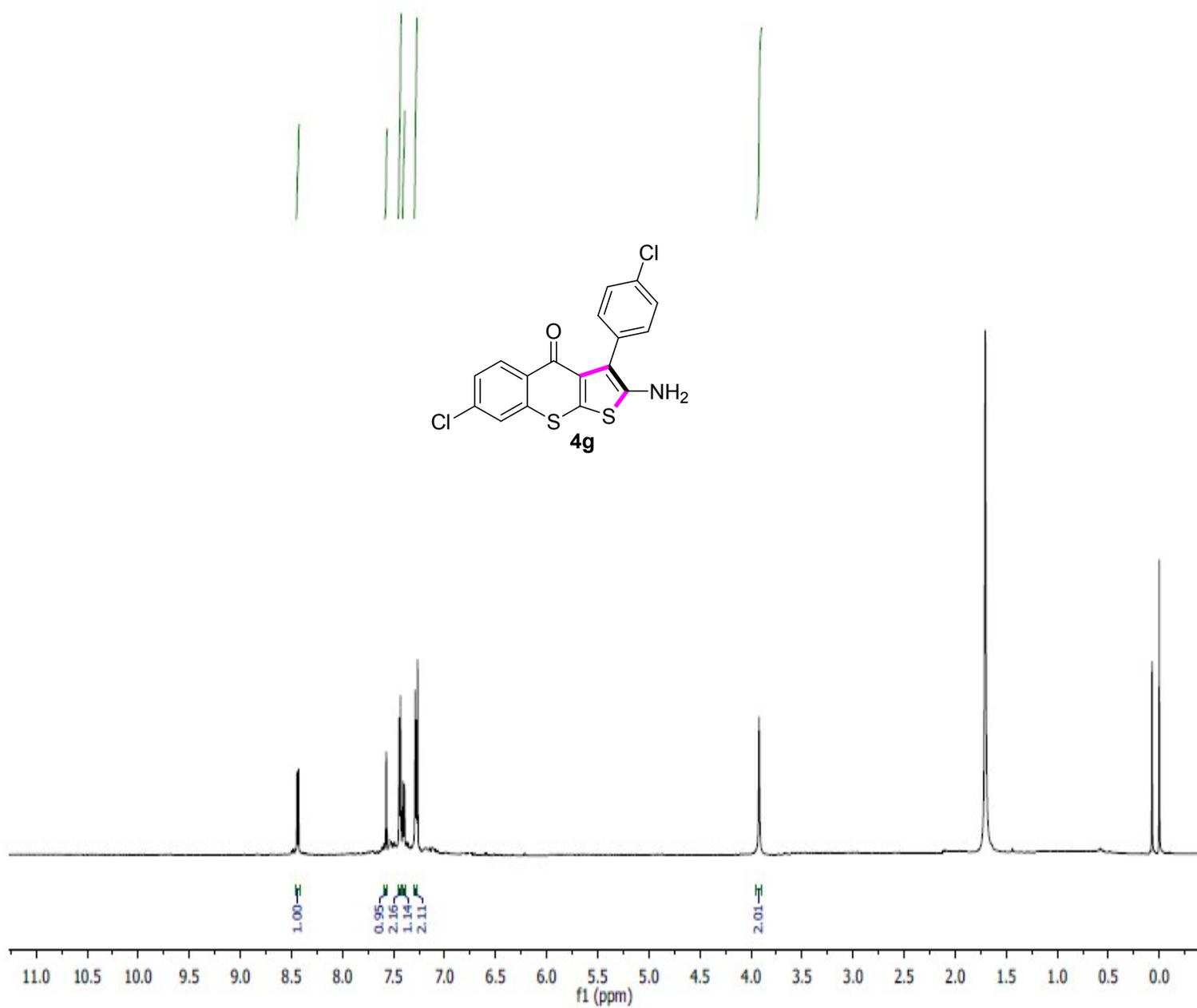
HRMS spectra of compound: 4f

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 compound: 4g

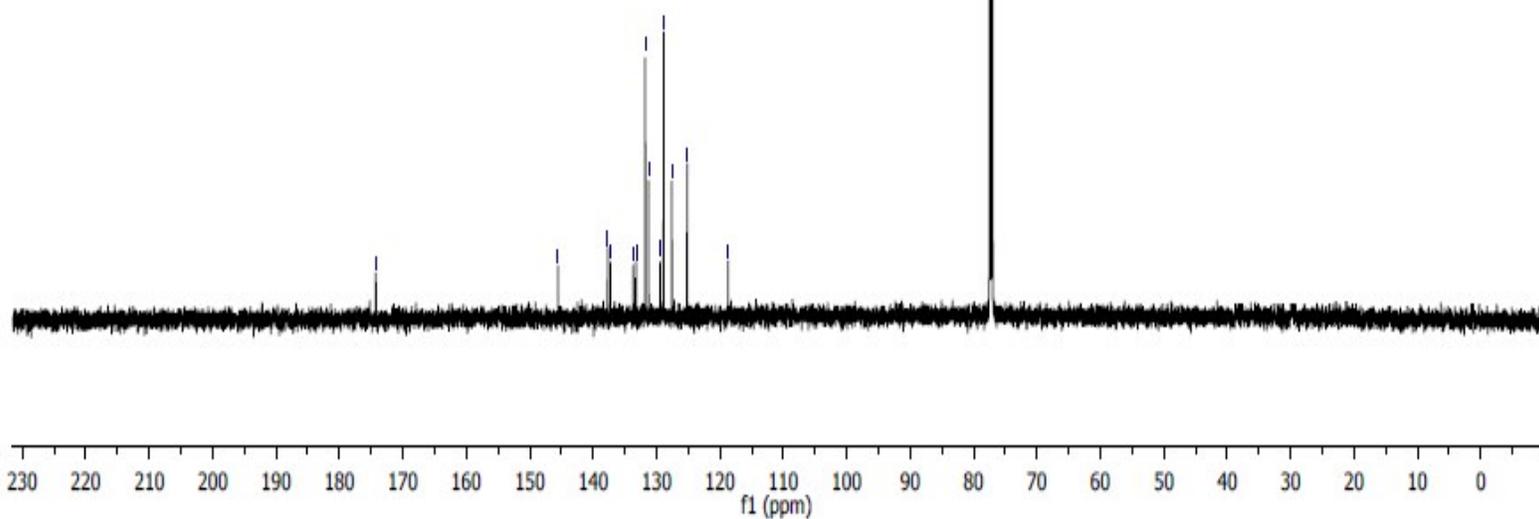
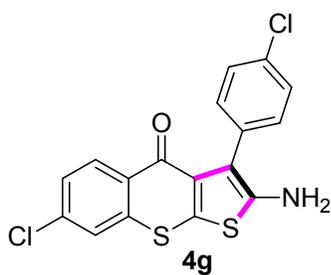
KM-N-4CL-1H
KM-N-4CL-1H



¹³CNMR spectra of compound: 4g

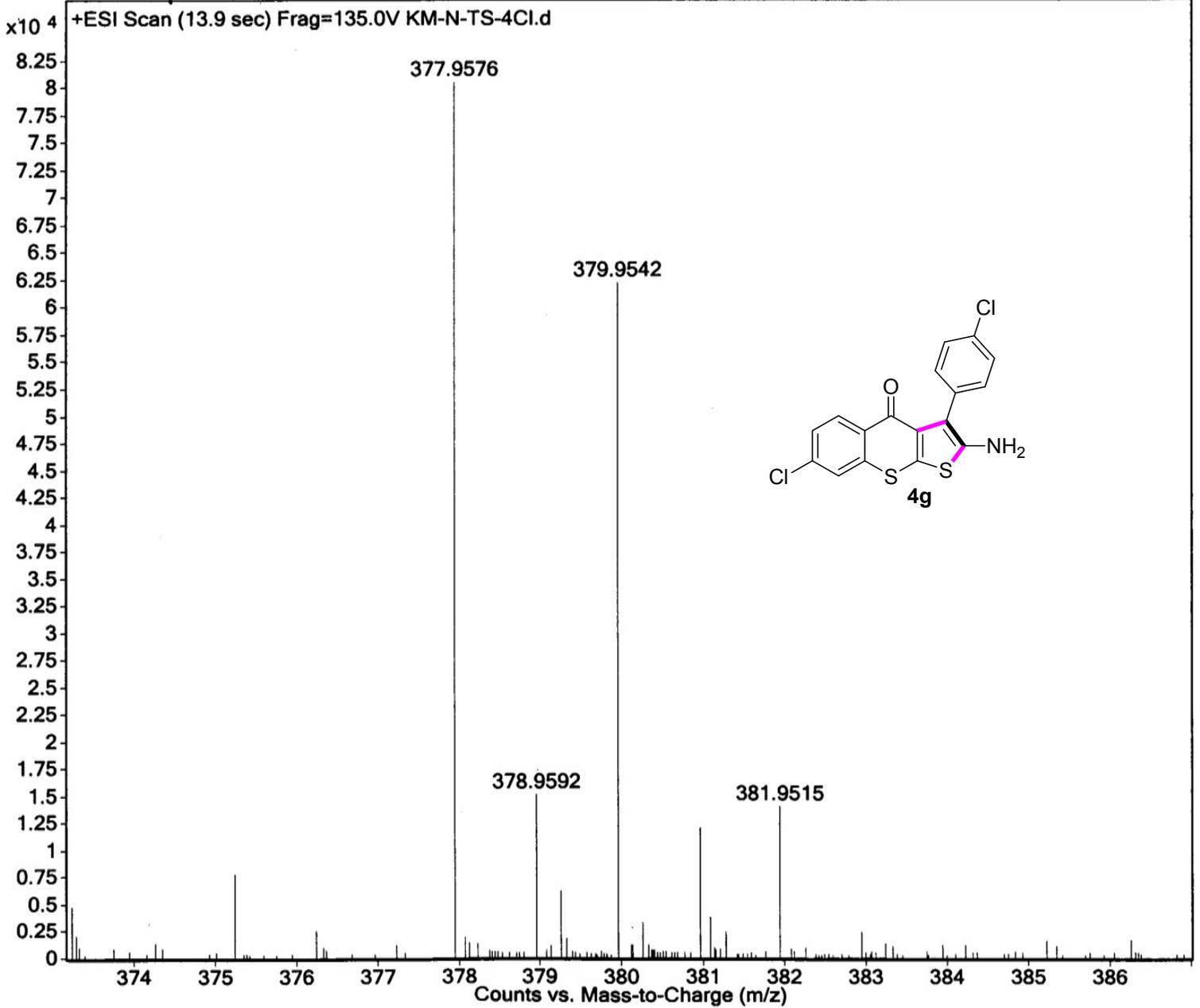
KM-NTH-4CL-13C
KM-NTH-4CL-13C

—174.26
145.54
137.71
137.28
133.67
133.19
131.77
131.23
129.41
128.89
127.58
125.18
118.72
77.44
77.23
77.02



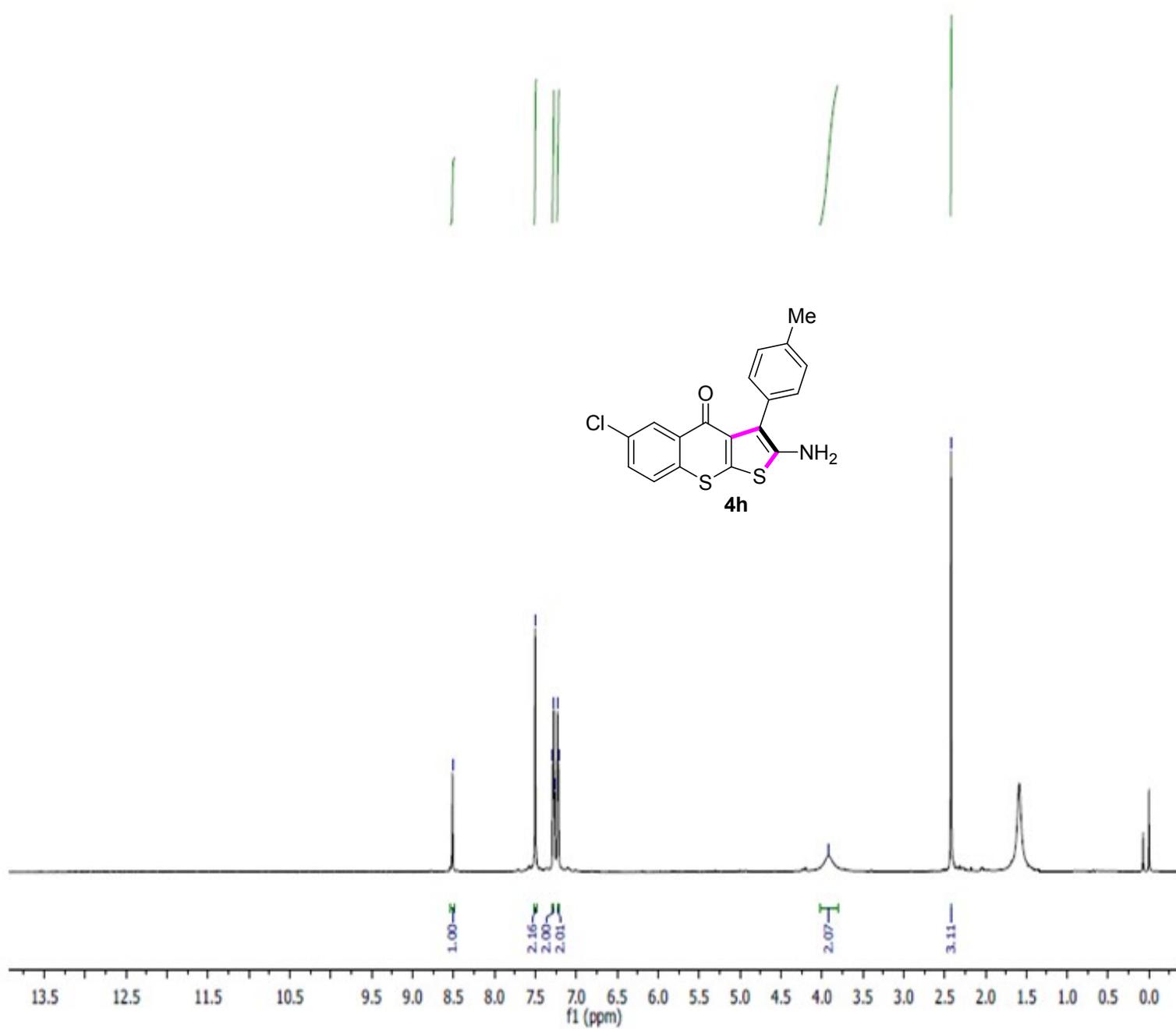
HRMS spectra of compound: 4g

Sample Name	KM-N-TS-4Cl	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	KM-N-TS-4Cl.d	ACQ Method		Comment		Acquired Time	2/9/2016 10:51:01 AM



¹H NMR spectra of compound: 4h

KM-N5-Me-1H
KM-N5-Me-1H



¹³CNMR spectra of compound: 4h

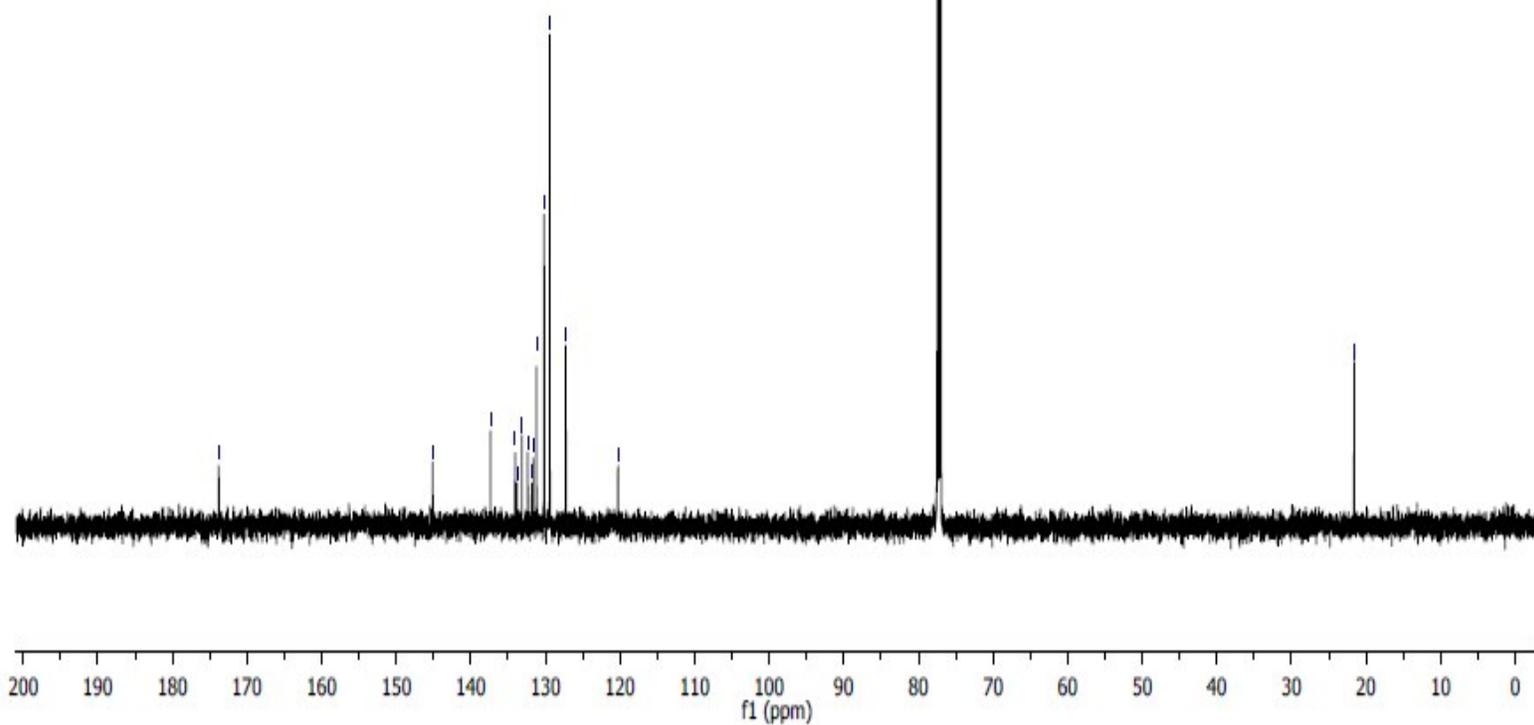
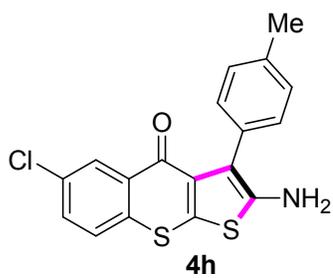
KM-N5-Me-13C
KM-N5-Me-13C

—173.78

145.11
137.36
134.07
133.80
133.15
132.36
131.81
131.61
131.19
130.17
129.41
127.27
120.27

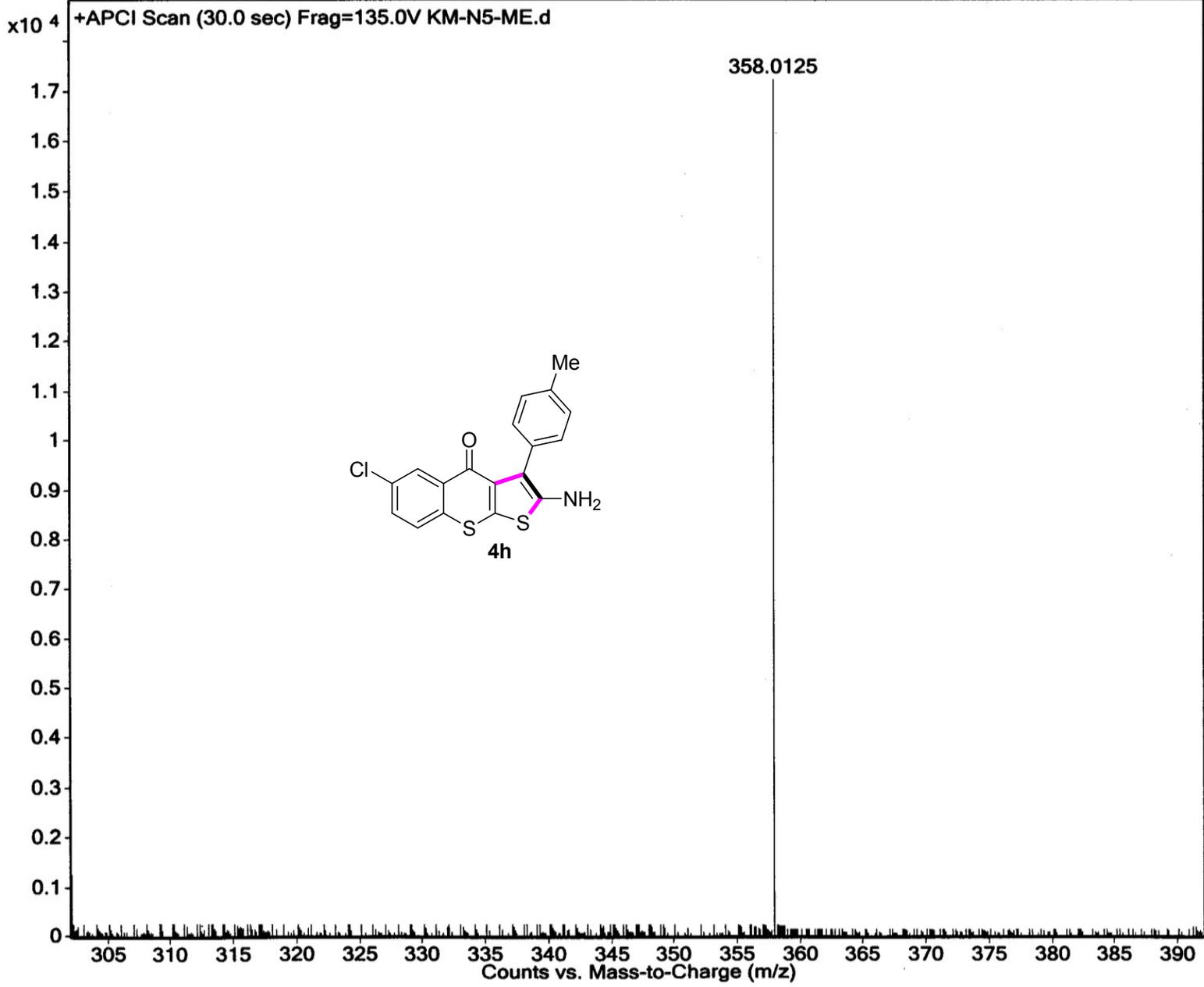
77.44
77.23
77.02

—21.59



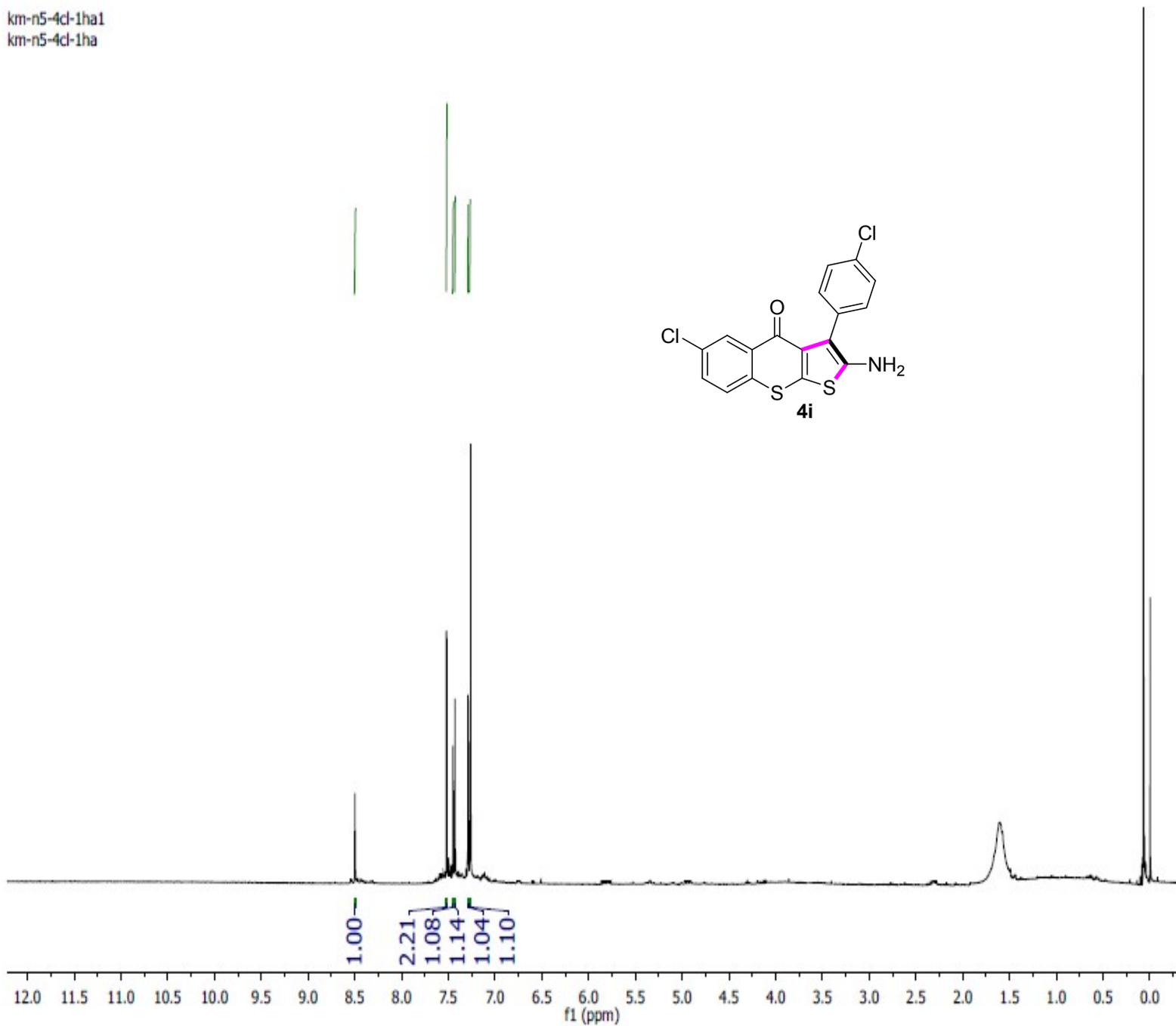
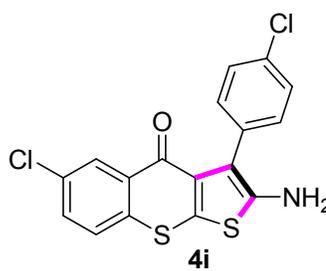
HRMS spectra of compound: 4h

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



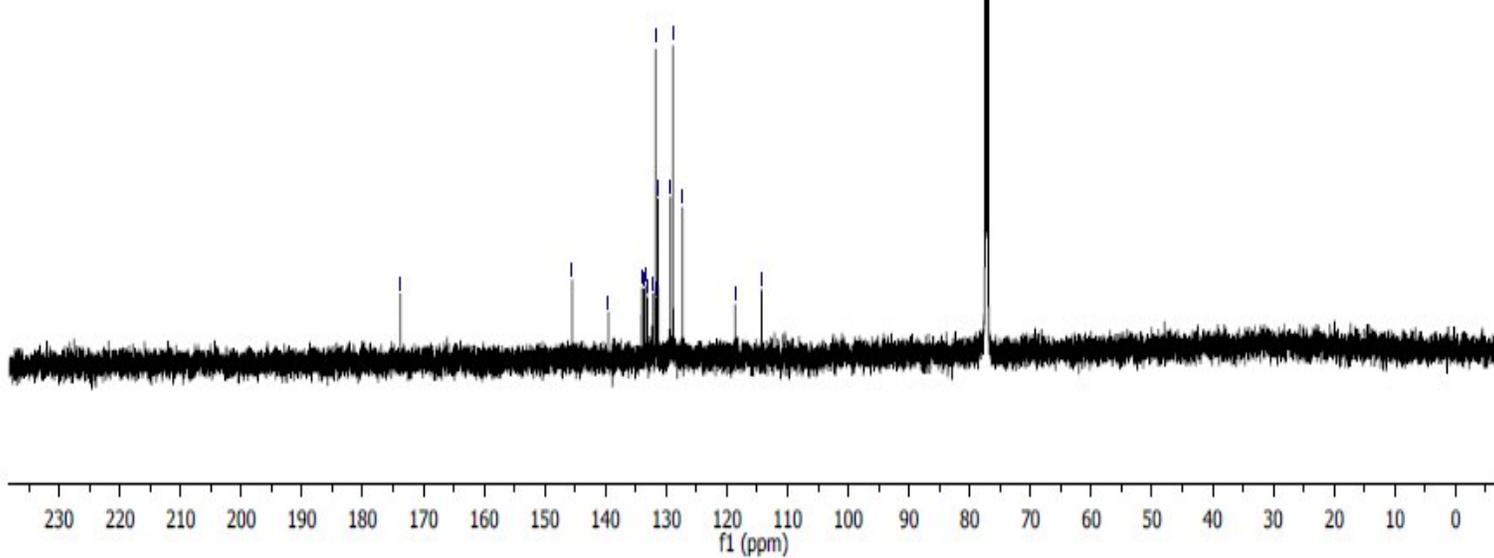
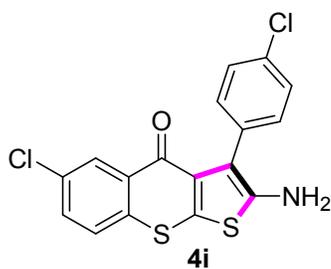
¹HNMR spectra of compound: 4i

km-n5-4cl-1ha1
km-n5-4cl-1ha



¹³CNMR spectra of compound: 4i

KM-5N-4C-13C
KM-5N-4C-13C



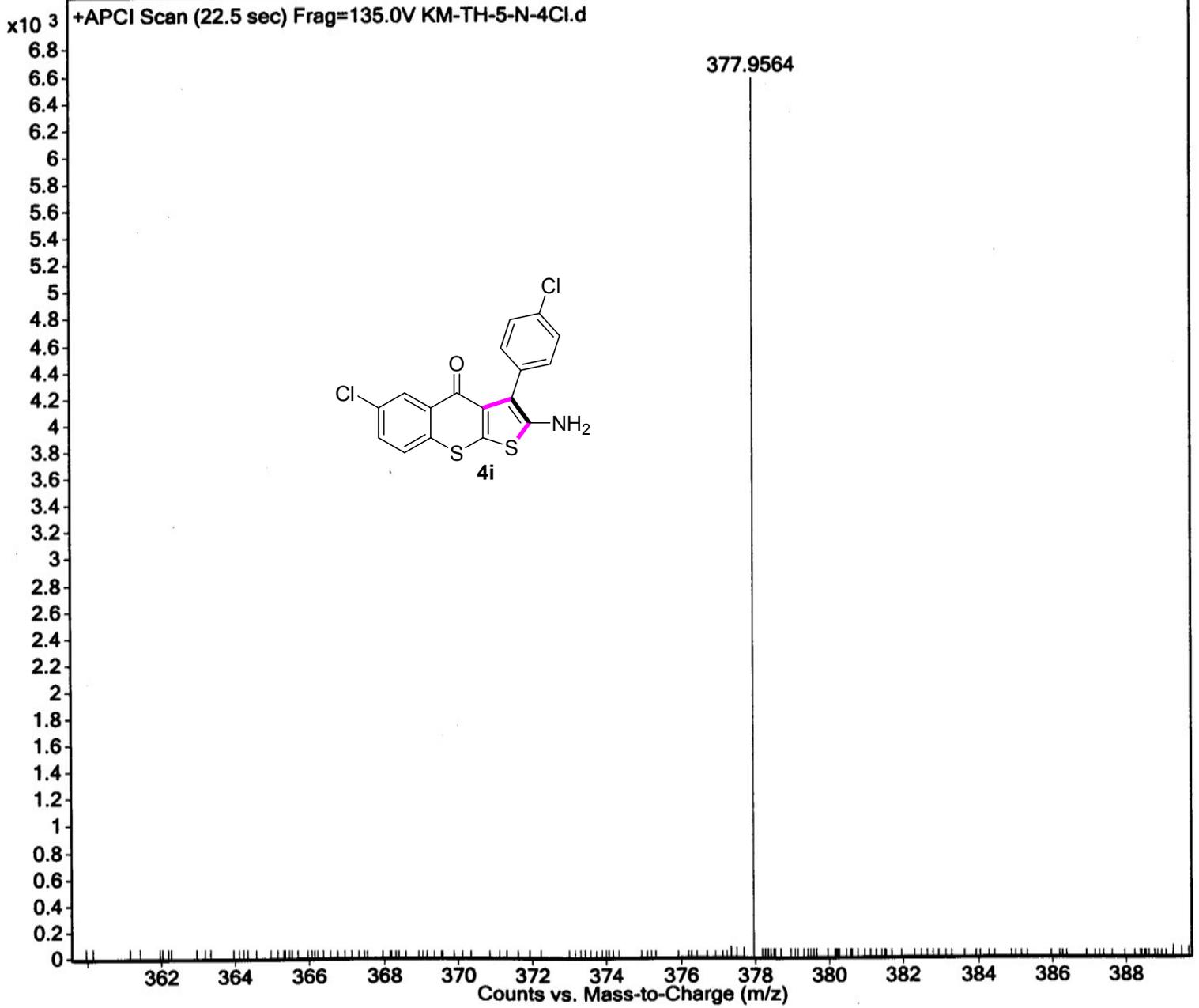
HRMS spectra of compound: 4i

Sample Name
Inj Vol
Data Filename

Position
InjPosition
ACQ Method

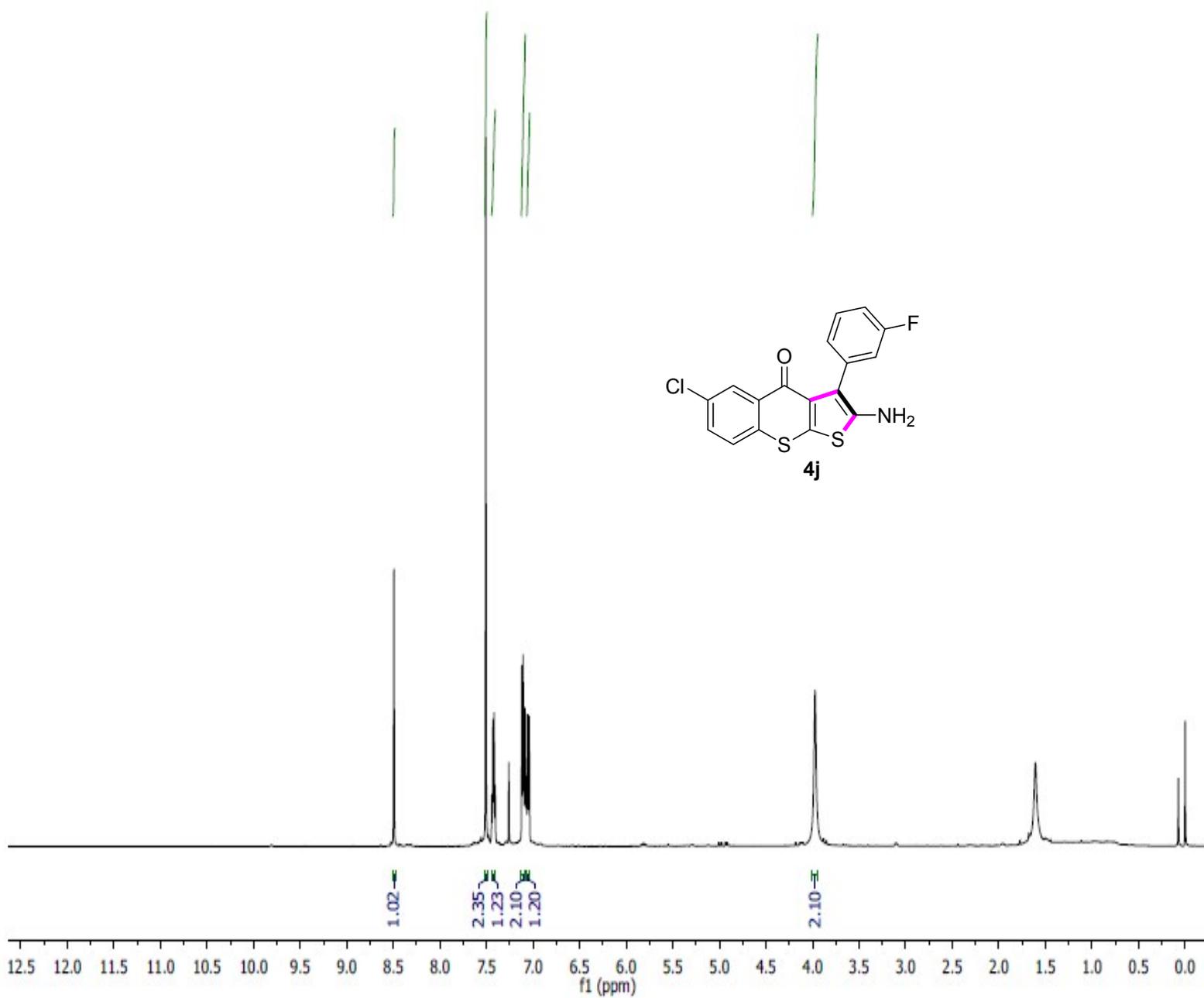
Instrument Name
SampleType
Comment

User Name
IRM Calibration Status
Acquired Time



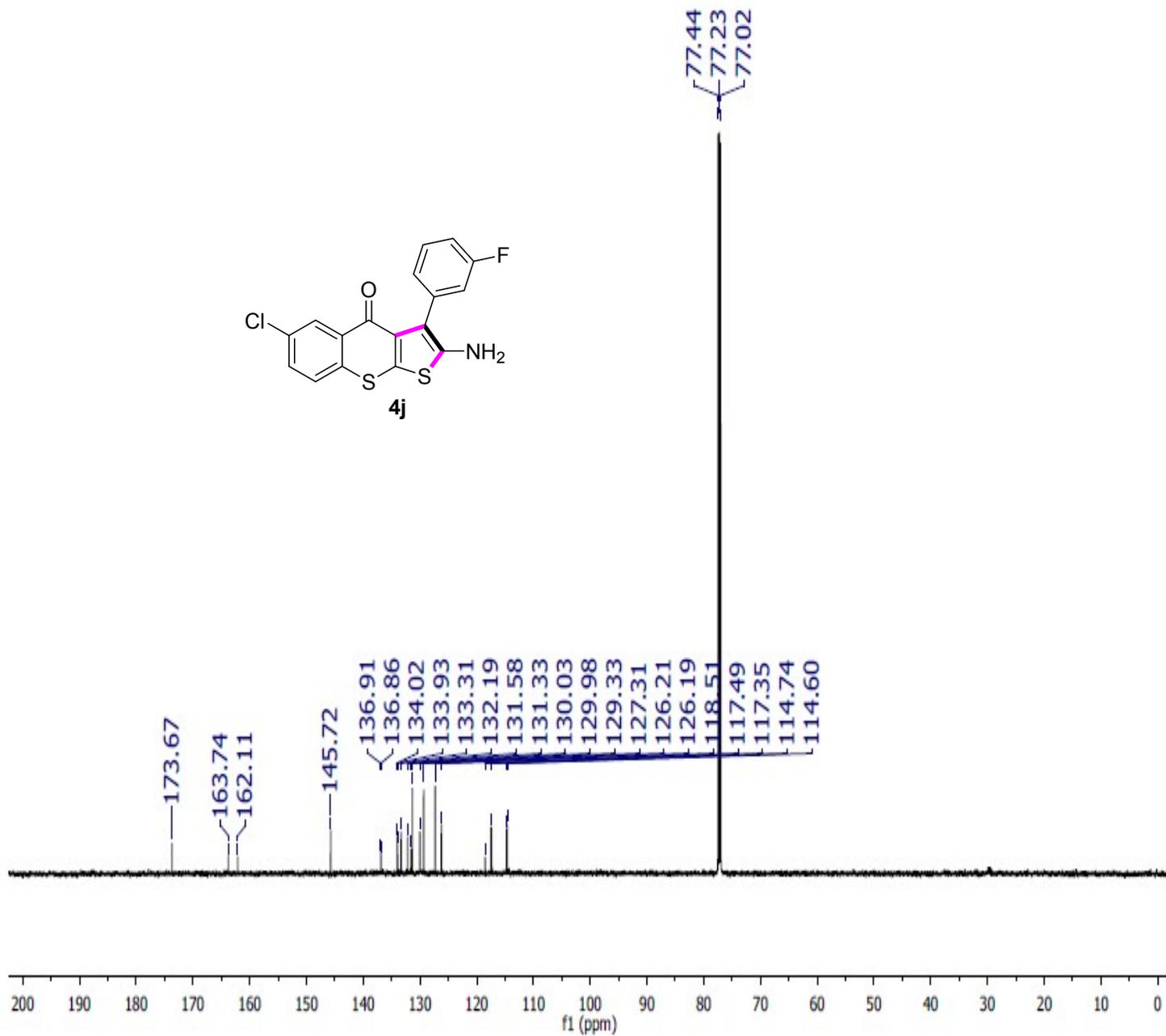
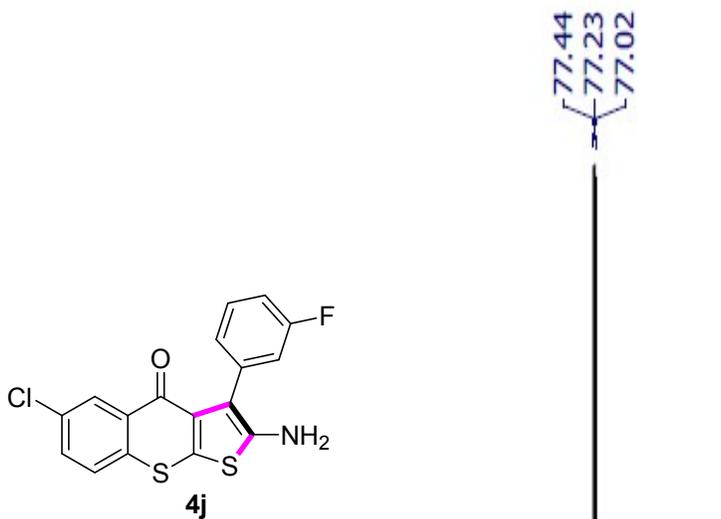
¹HNMR spectra of compound: 4j

KM-N-5-3F-1H
KM-N-5-3F-1H



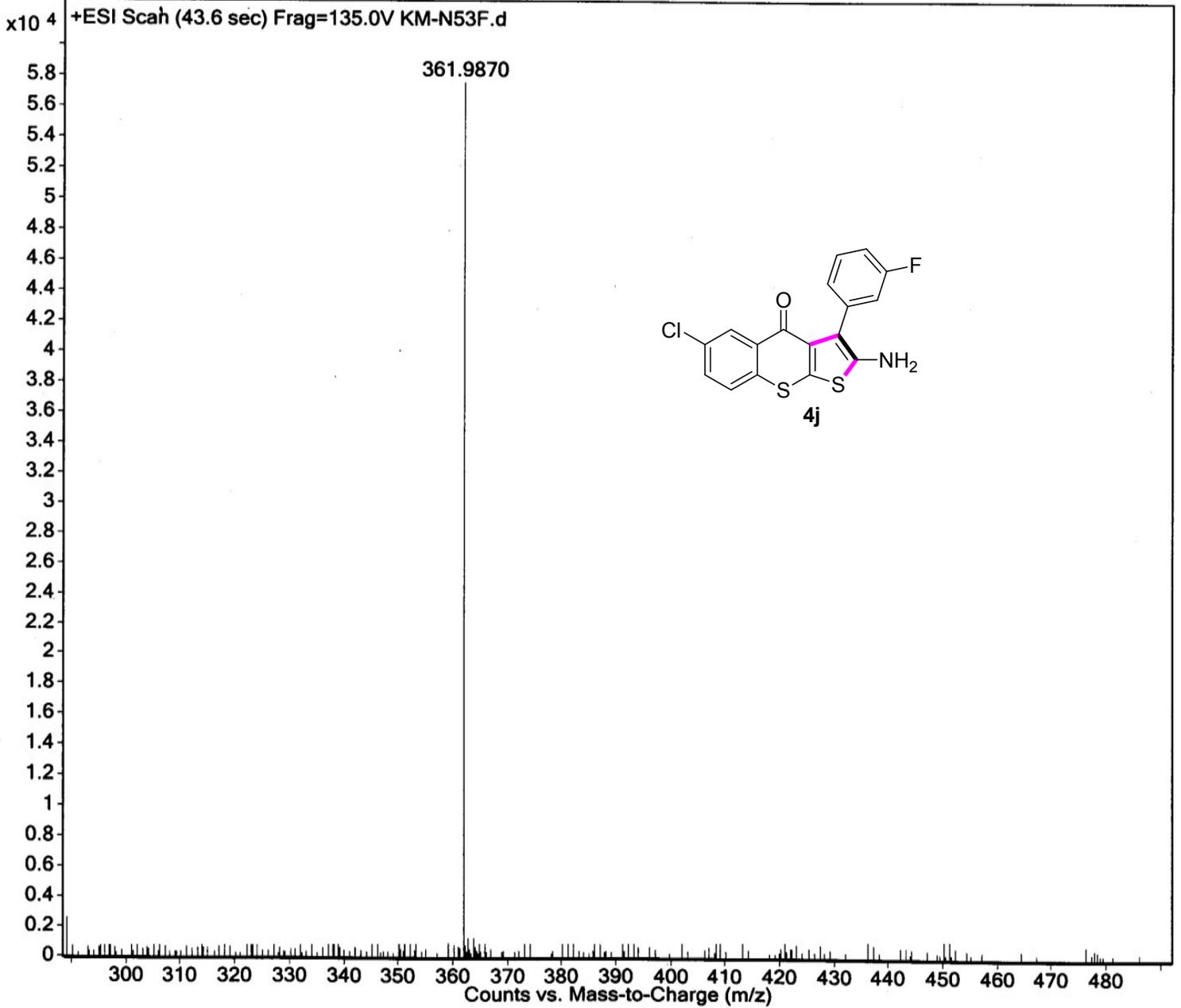
¹³CNMR spectra of compound: 4j

KM_N_5_3F_13C
KM_N_5_3F_13C



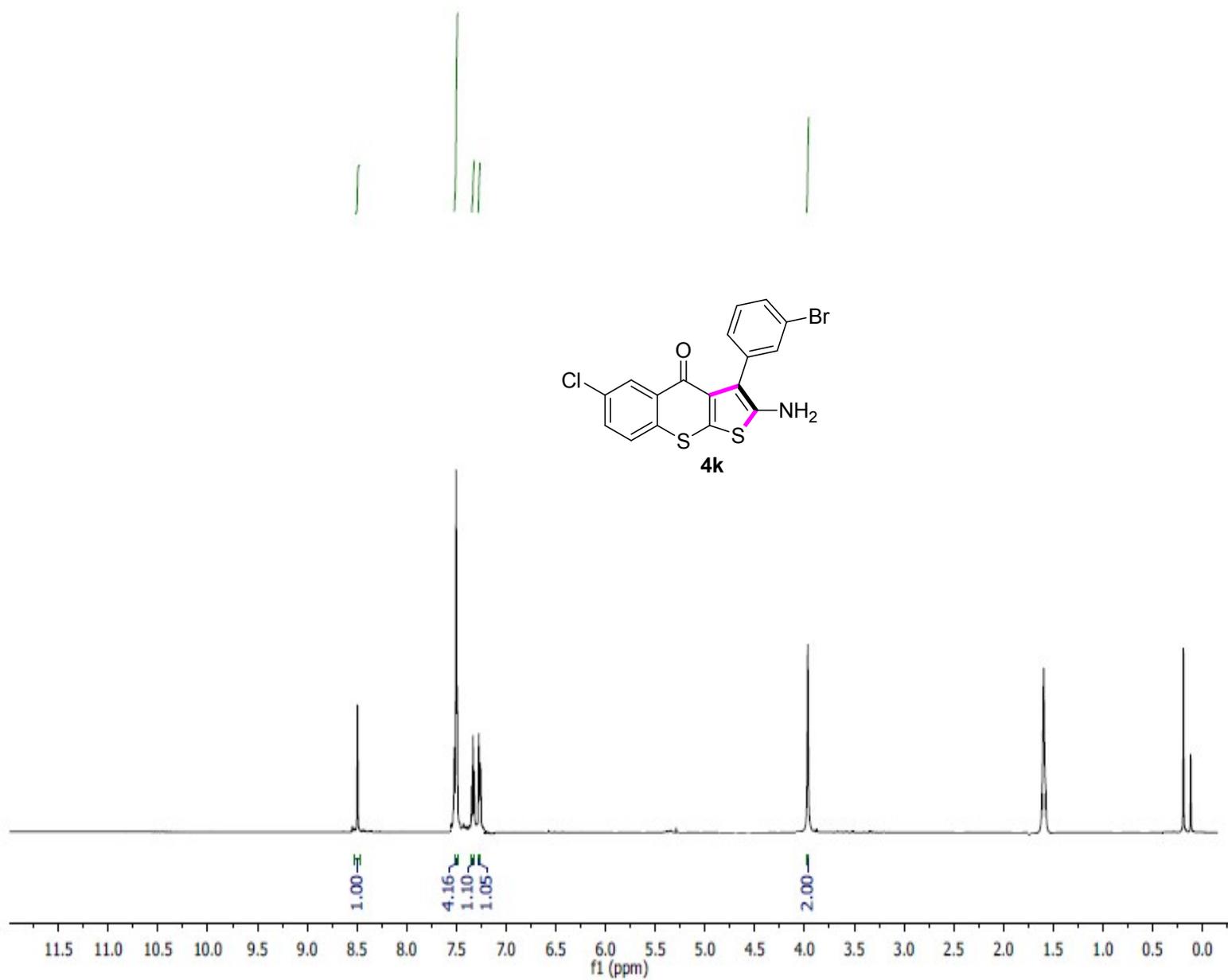
HRMS spectra of compound: 4j

Sample Name	KM-N53F	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	KM-N53F.d	ACQ Method		Comment		Acquired Time	2/3/2016 4:07:53 PM



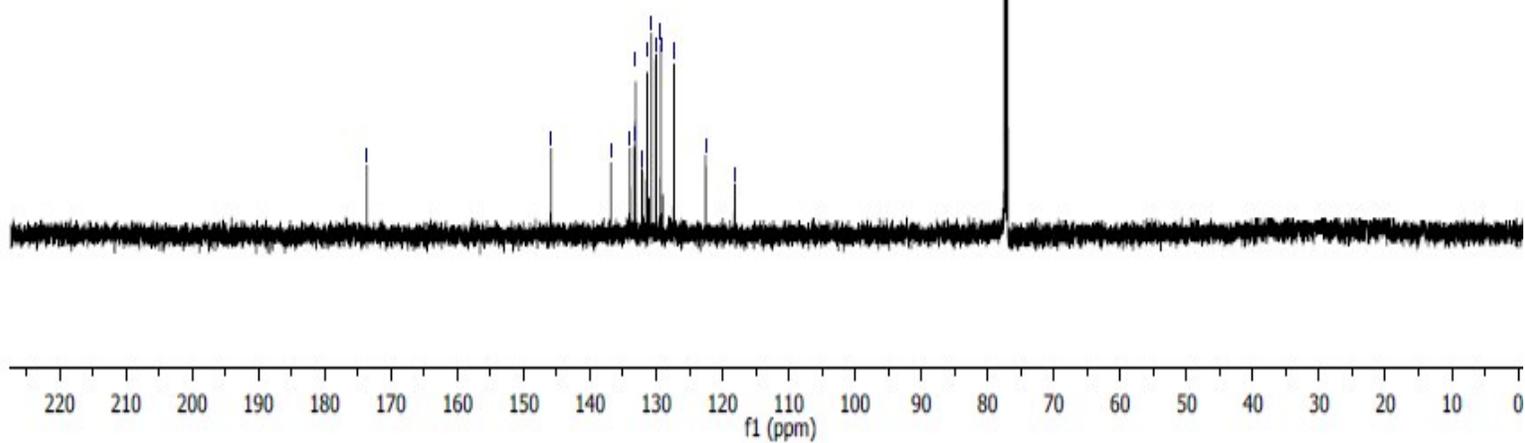
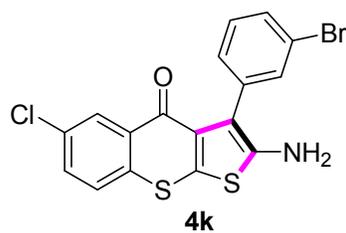
¹HNMR spectra of compound: 4k

KM-N-5-3Br-1H
KM-N-5-3Br-1H



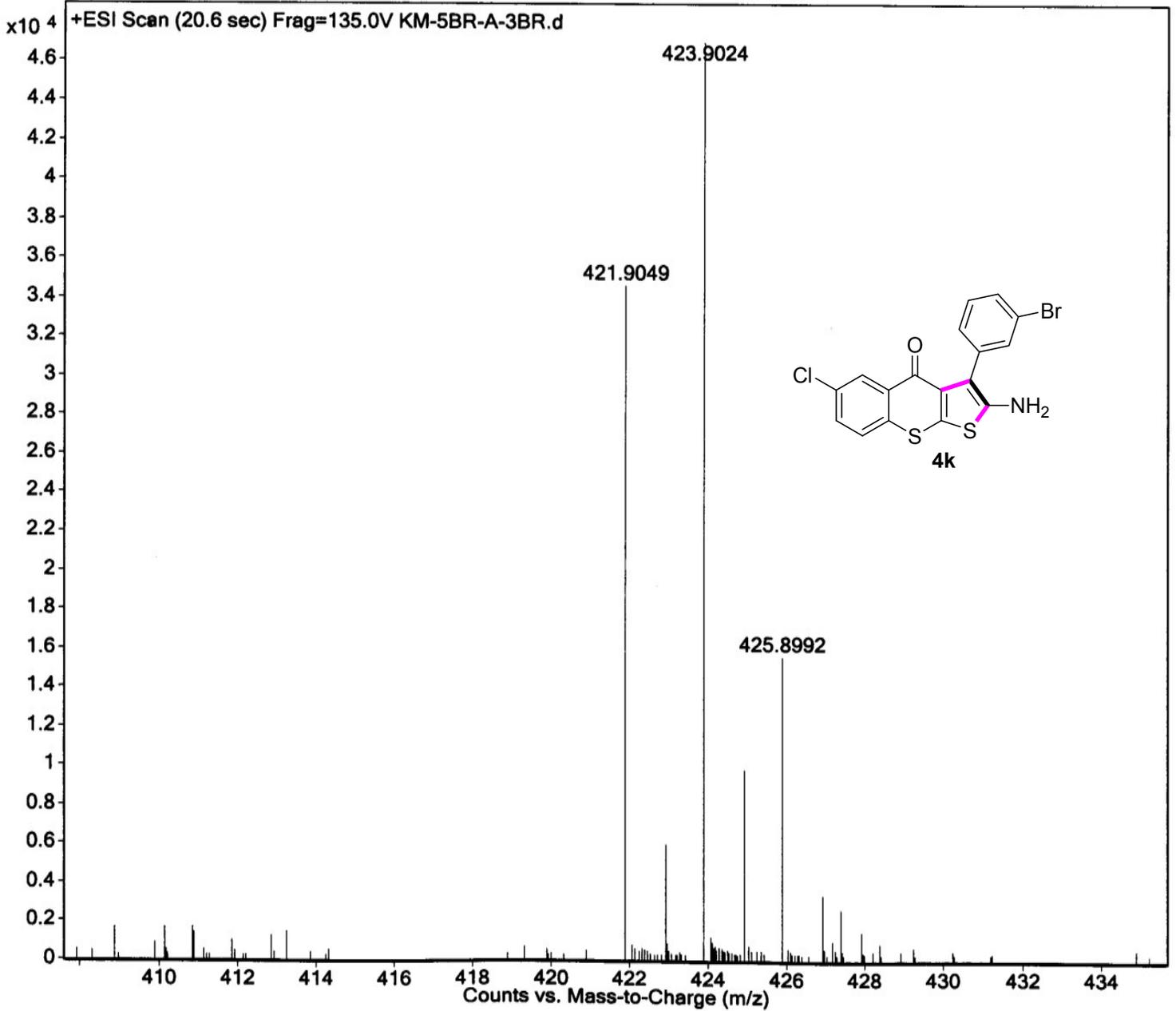
¹³CNMR spectra of compound: 4k

KM-N-5-3Br-13C
KM-N-5-3Br-13C



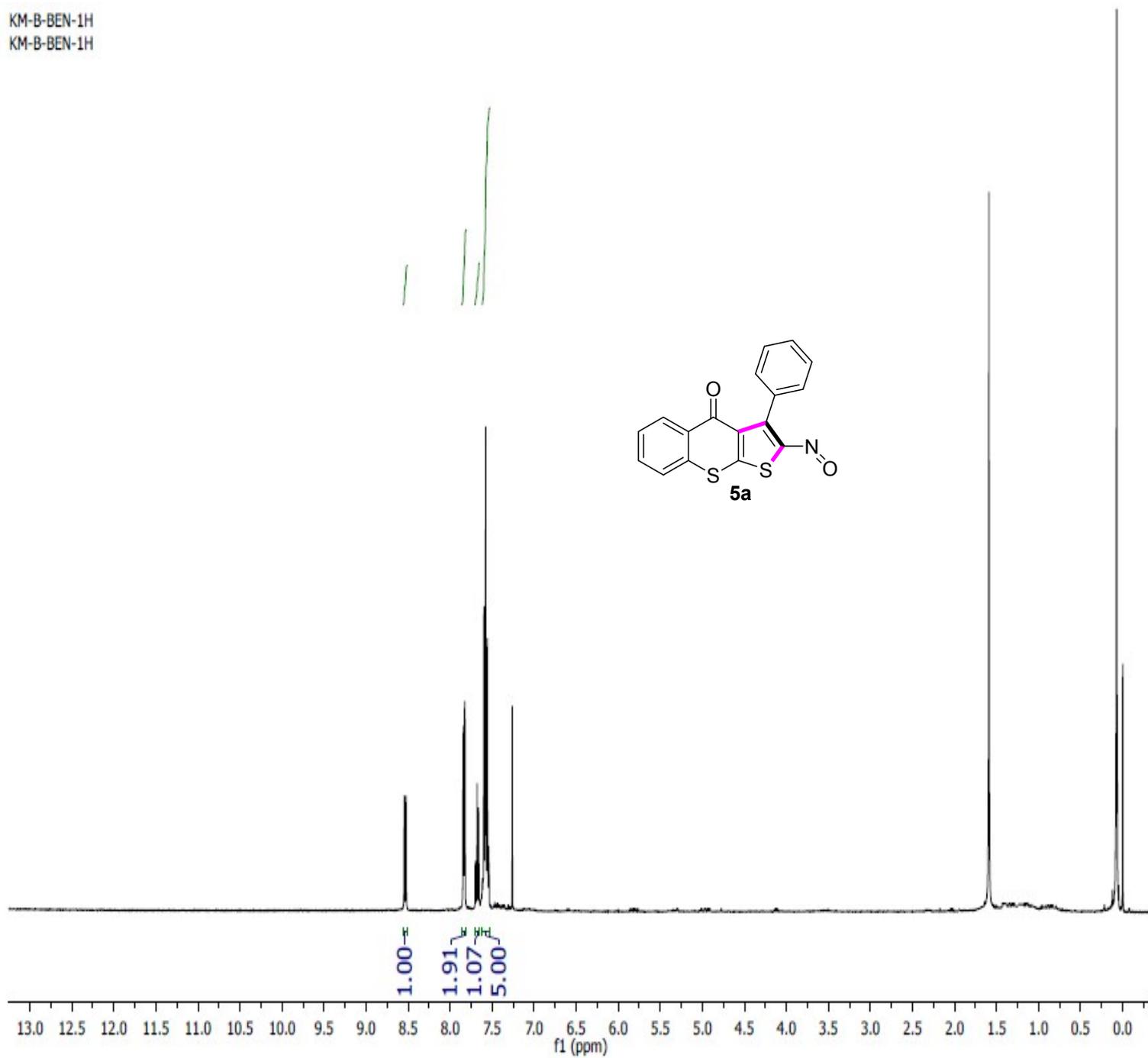
HRMS spectra of compound: 4k

Sample Name	KM-5BR-A-3BR	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	KM-5BR-A-3BR.d	ACQ Method		Comment		Acquired Time	6/3/2016 12:11:18 PM



¹H NMR spectra of compound: 5a

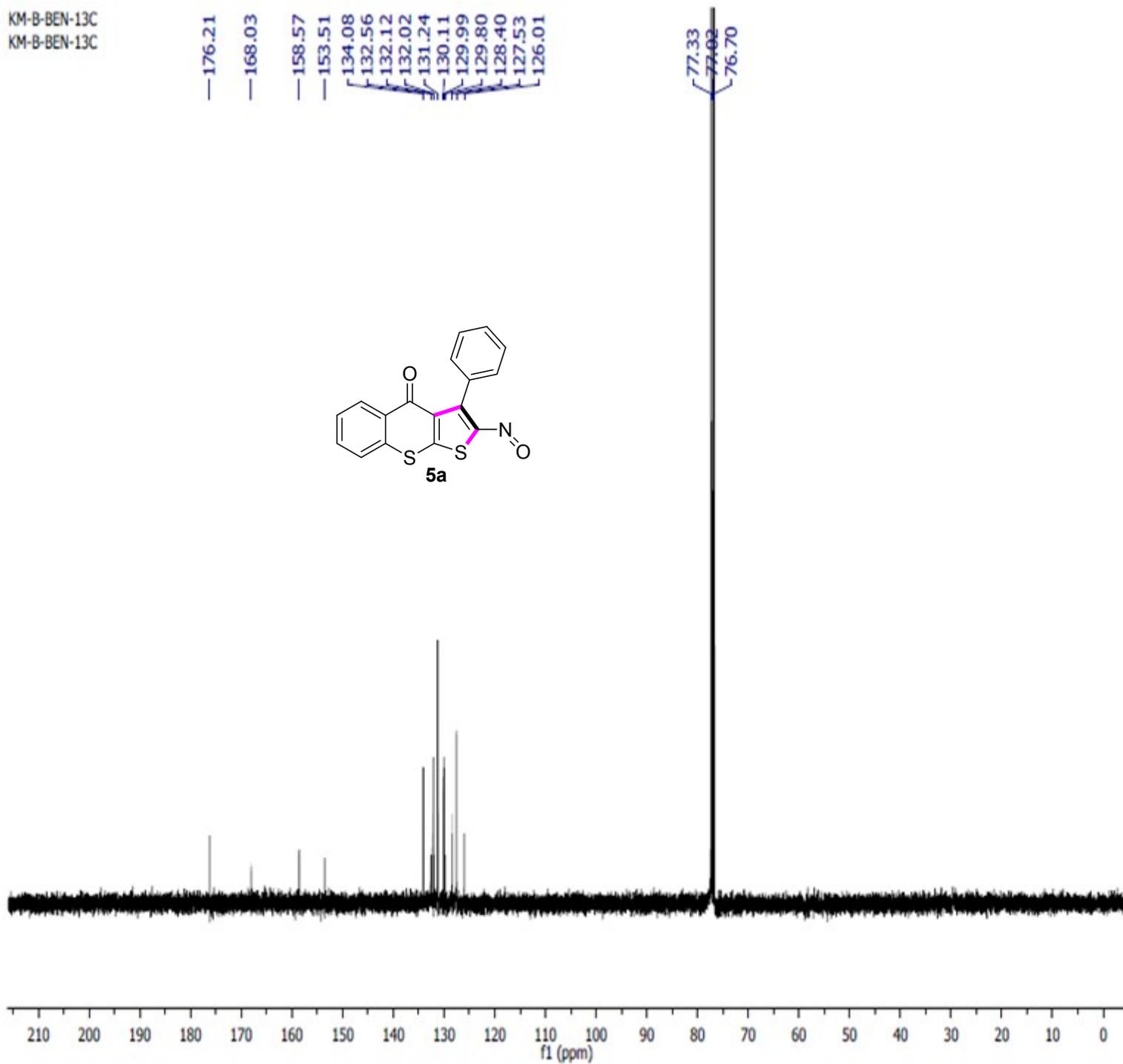
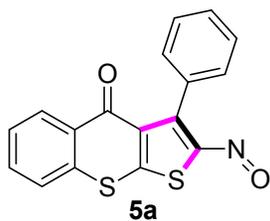
KM-B-BEN-1H
KM-B-BEN-1H



¹³CNMR spectra of compound: 5a

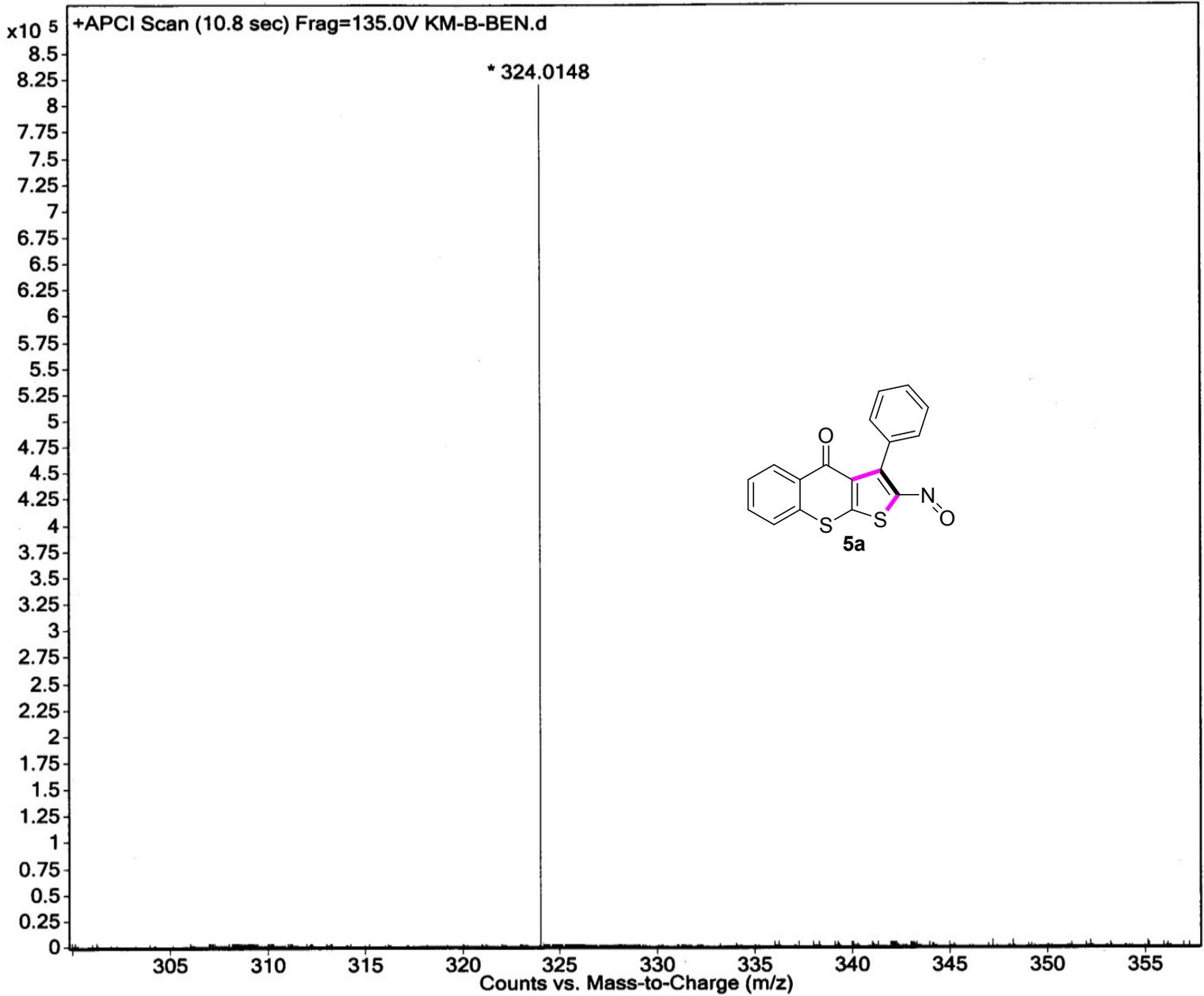
KM-B-BEN-13C
KM-B-BEN-13C

—176.21
—168.03
—158.57
—153.51
134.08
132.56
132.12
132.02
131.24
130.11
129.99
129.80
128.40
127.53
126.01
77.33
77.02
76.70



HRMS spectra of compound: 5a

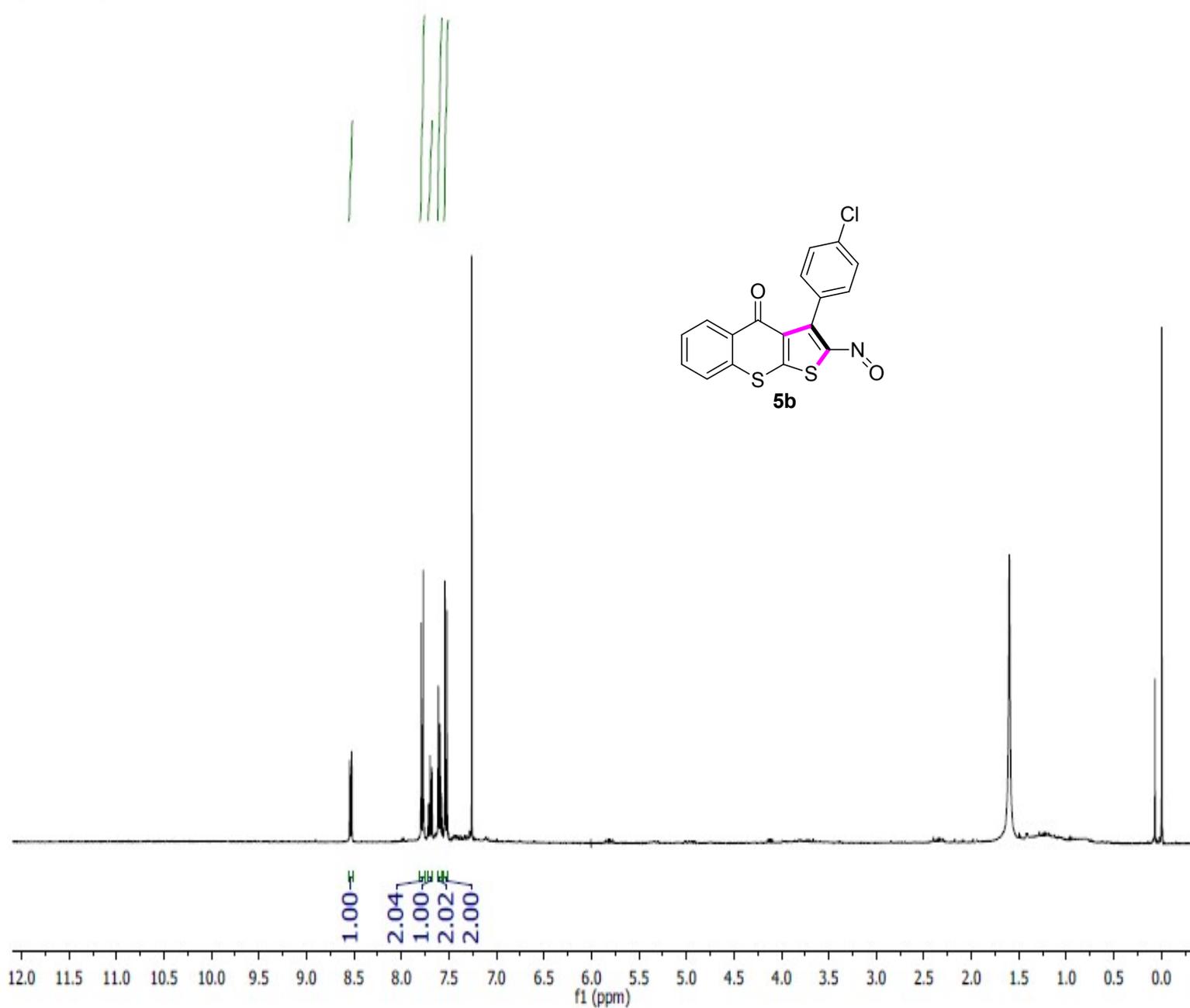
Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	KM-B-BEN.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹HNMR spectra of compound: 5b

km-b-r-4d-1h

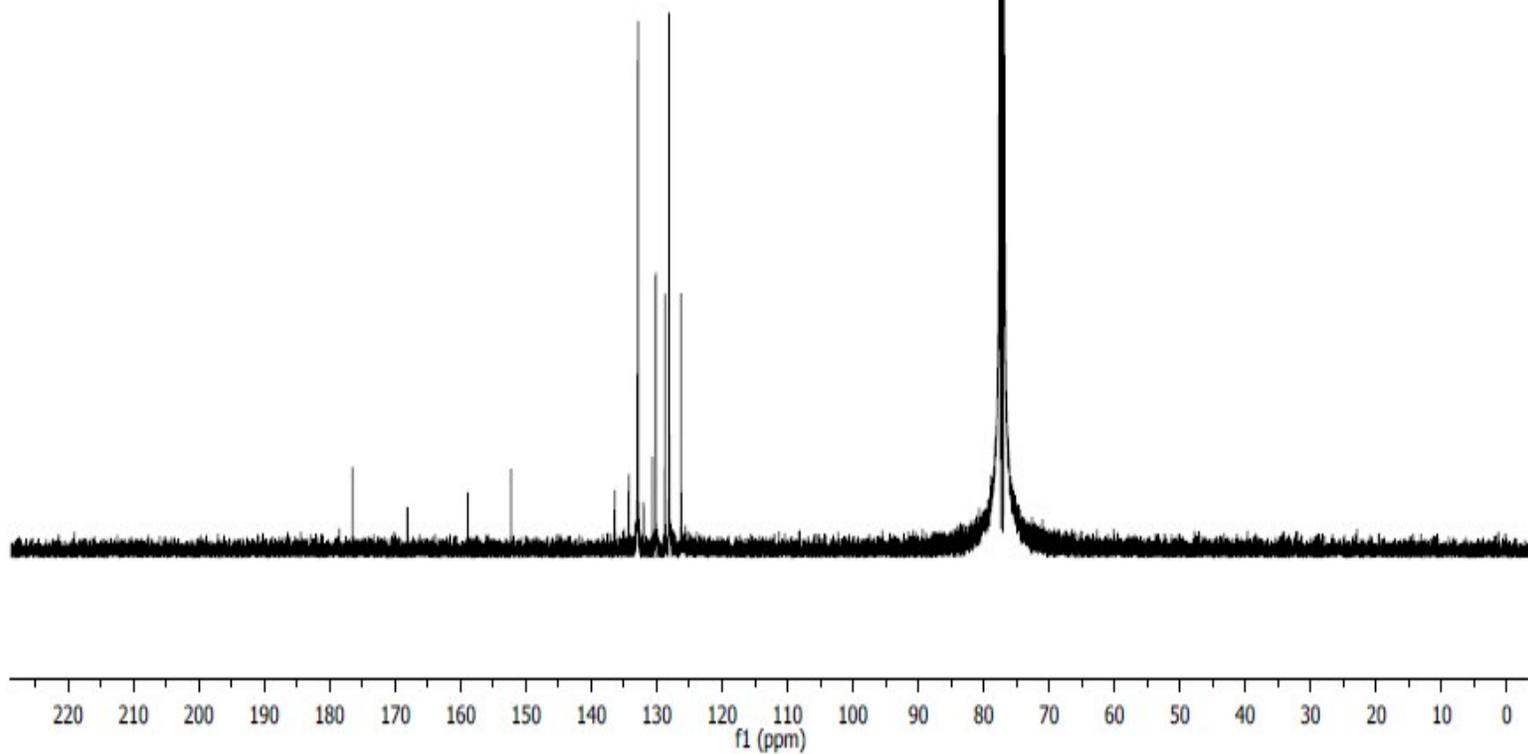
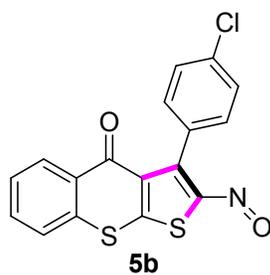
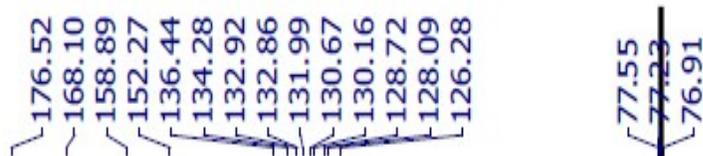
km-b-r-4d-1h



¹³CNMR spectra of compound: 5b

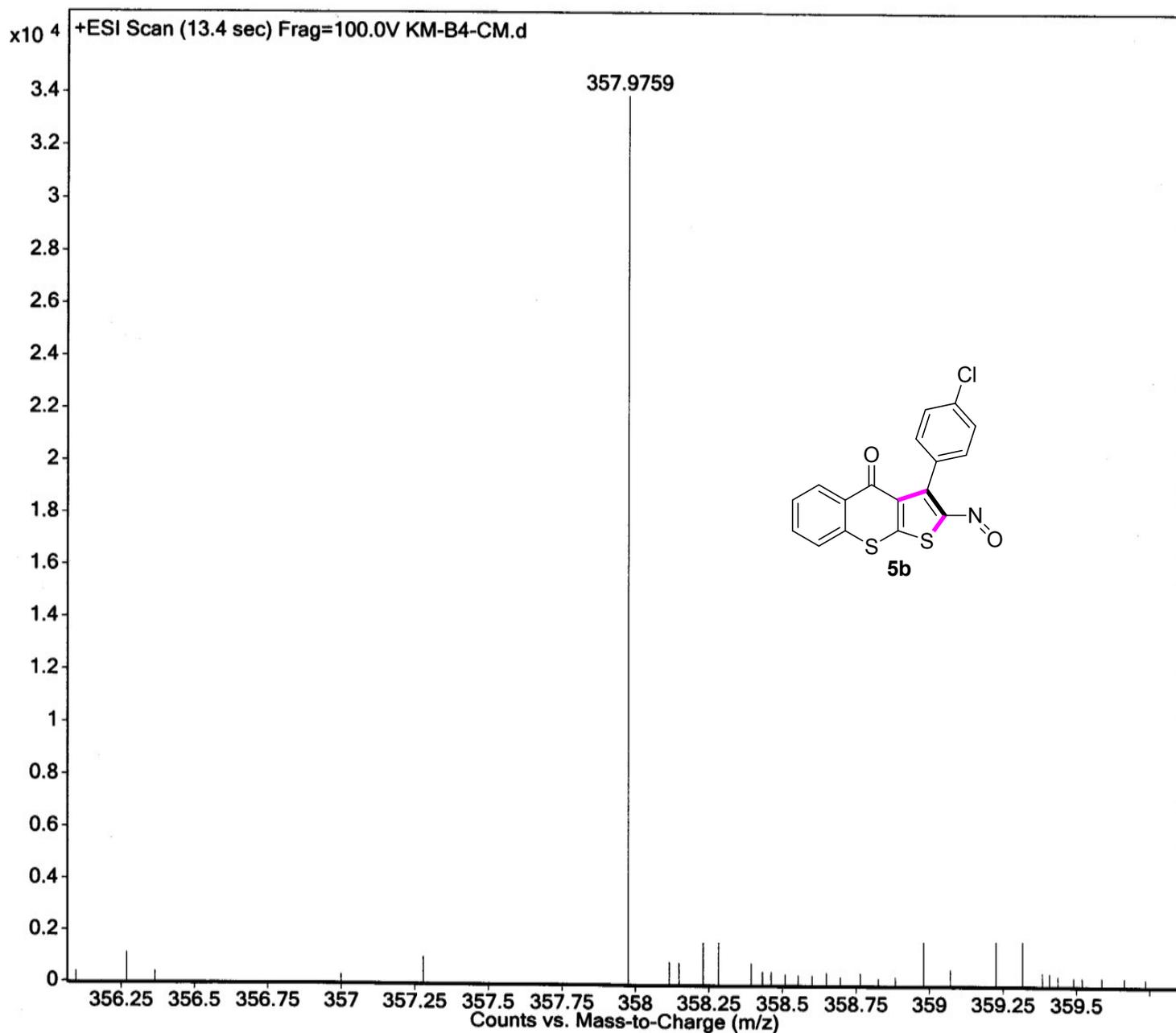
km-b-r-4c-13c

km-b-r-4c-1h



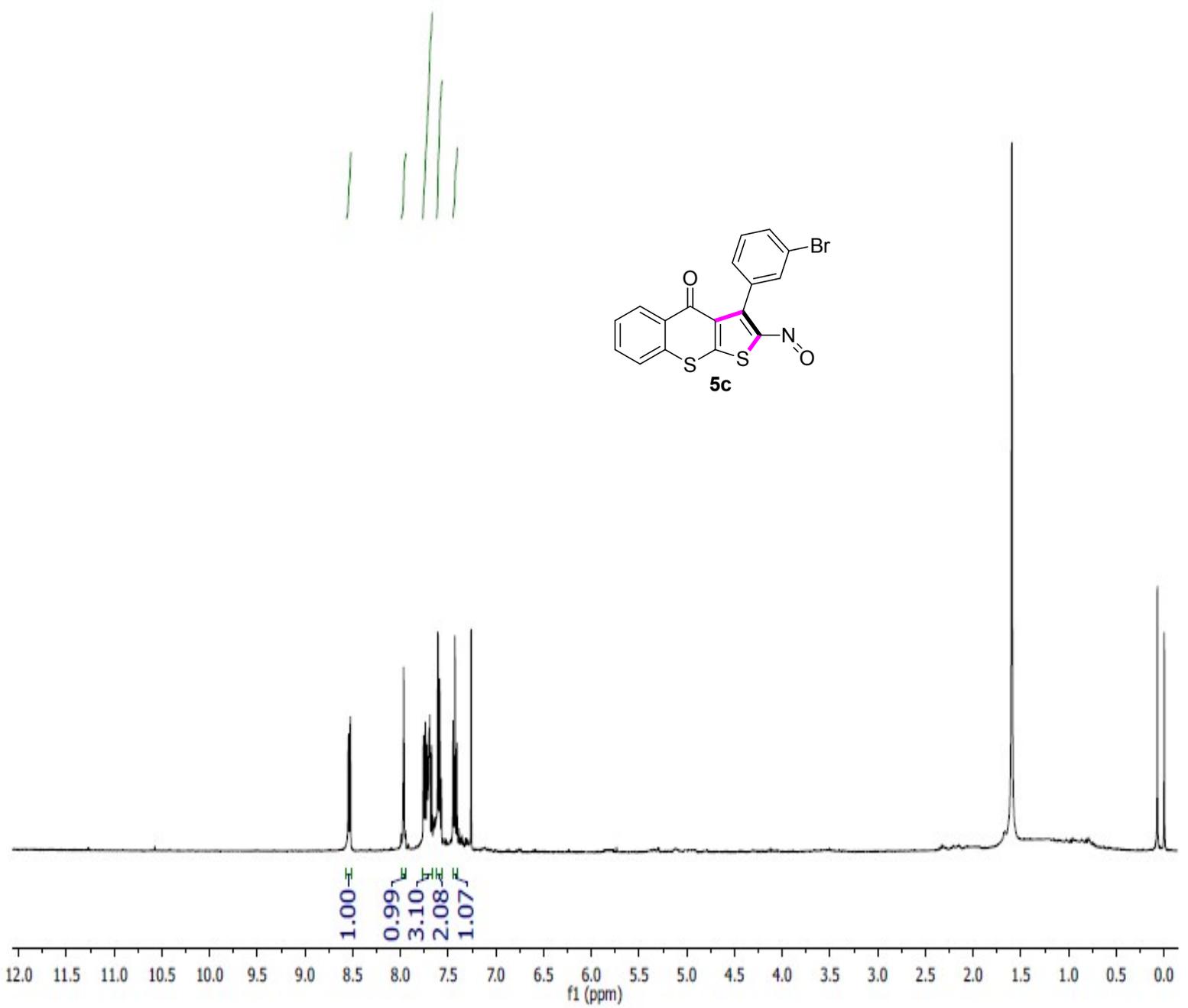
HRMS spectra of compound: 5b

Sample Name	KM-B4-CM	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	KM-B4-CM.d	ACQ Method		Comment		Acquired Time	2/16/2016 10:54:51 AM



¹H NMR spectra the compound: 5d

KM_B_3Br-1H
KM_B_3Br-1H

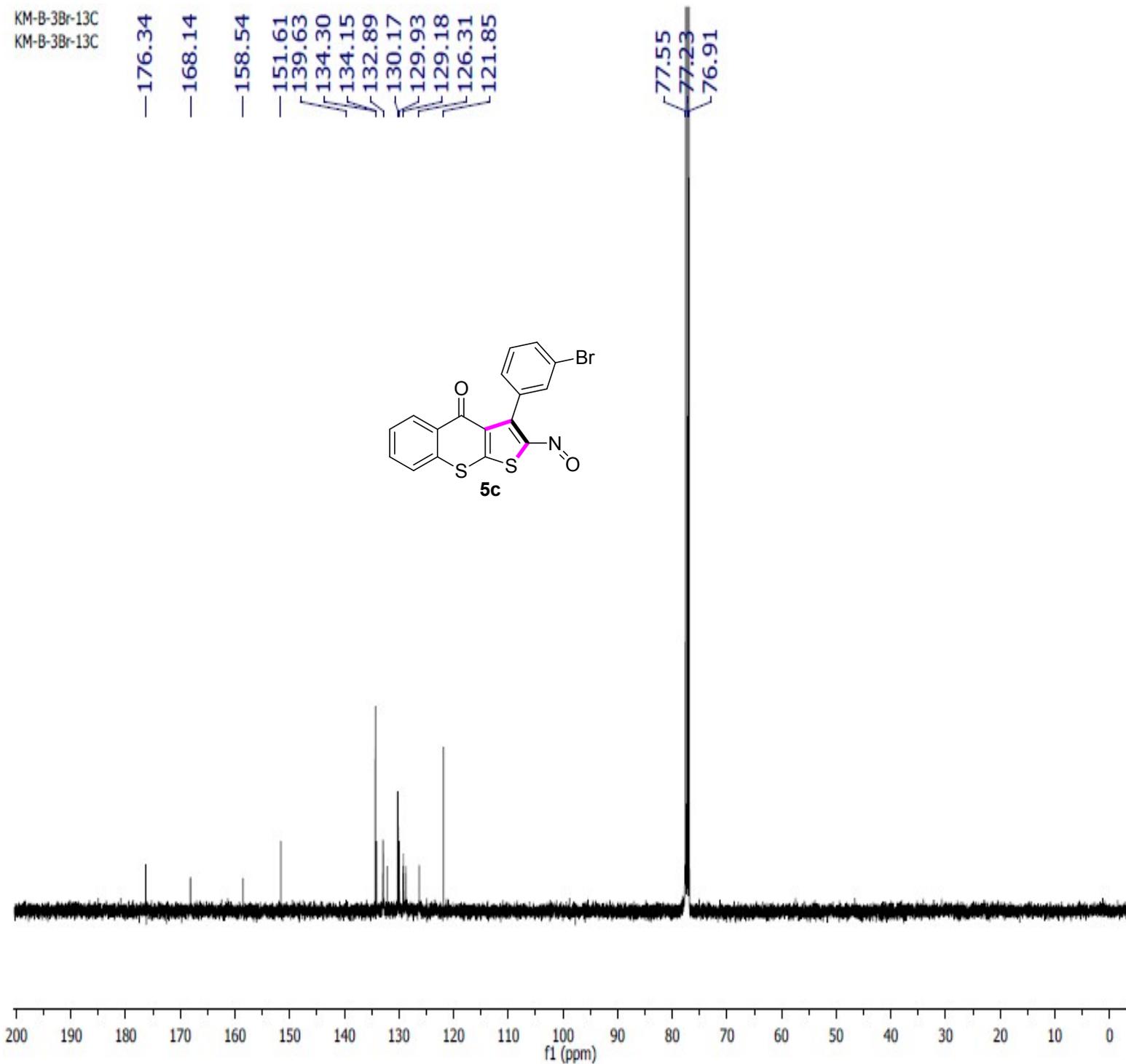
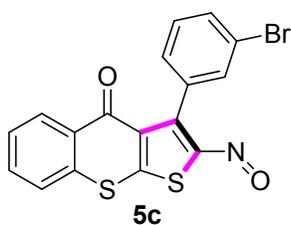


¹³CNMR spectra of compound: 5c

KM-B-3Br-13C
KM-B-3Br-13C

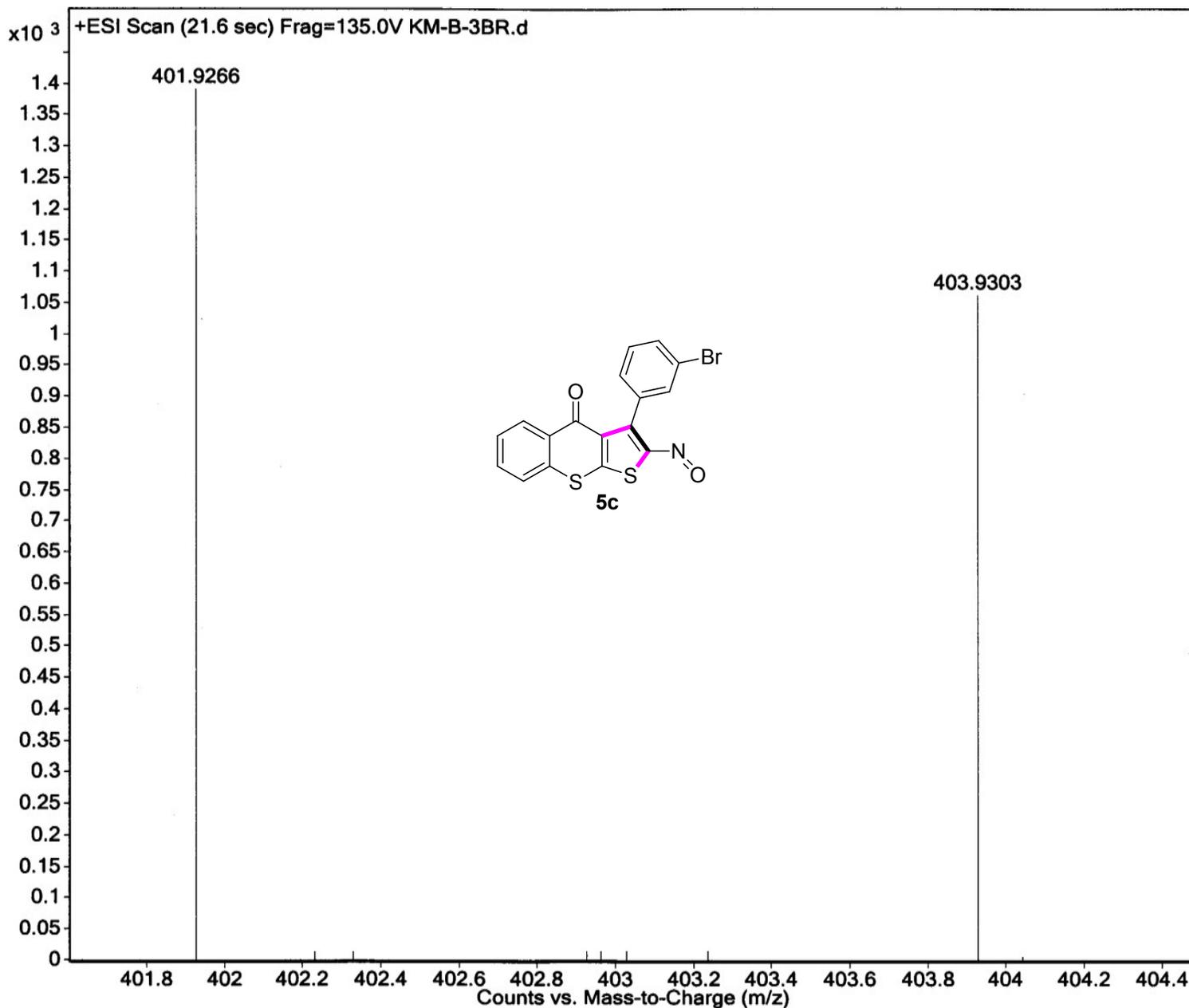
— 176.34
— 168.14
— 158.54
— 151.61
139.63
134.30
134.15
132.89
130.17
129.93
129.18
126.31
121.85

77.55
77.23
76.91



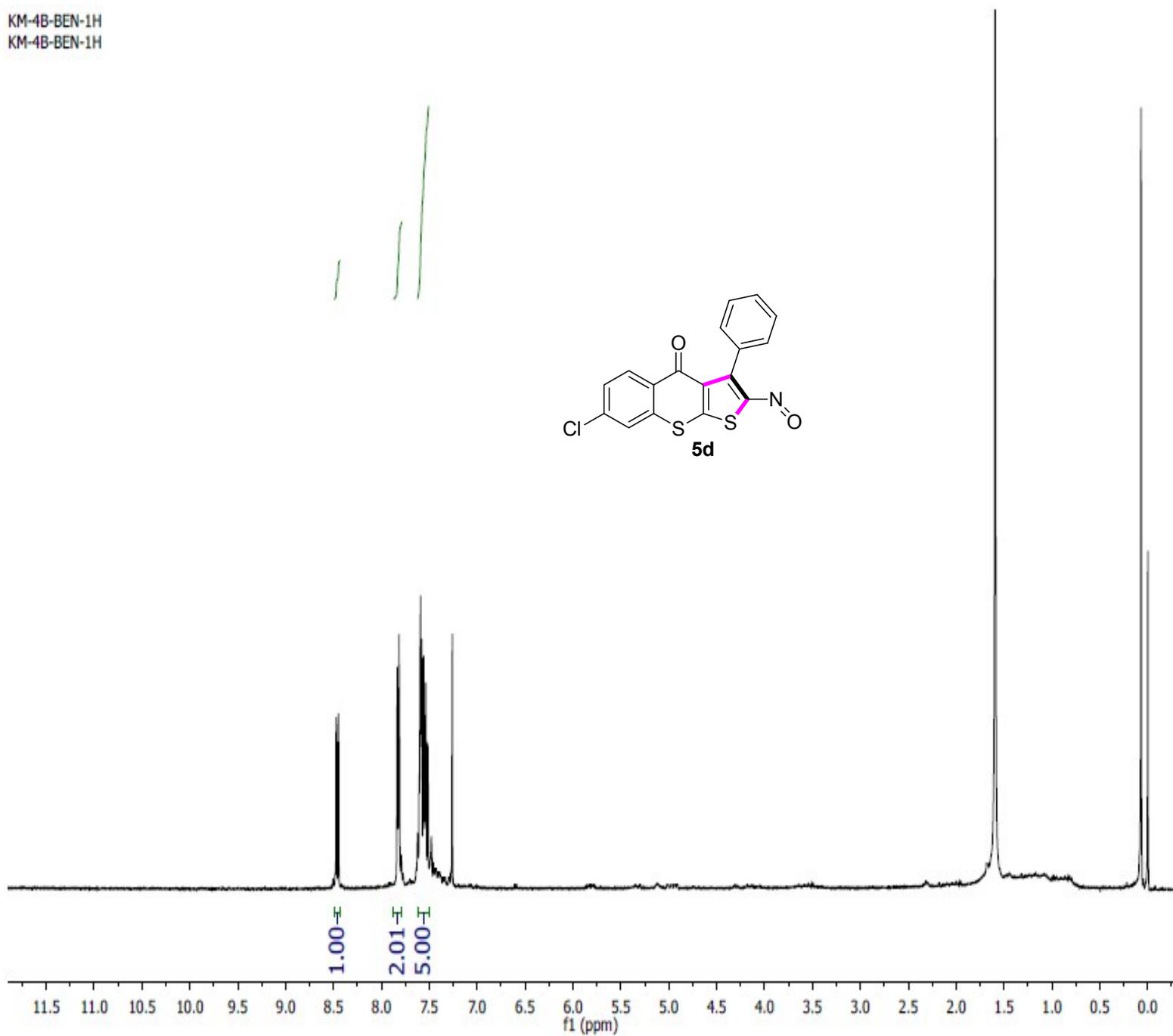
HRMS spectra of compound: 5c

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	All Ions Missed
Data Filename	KM-B-3BR.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



¹H NMR spectra the compound: 5d

KM-4B-BEN-1H
KM-4B-BEN-1H

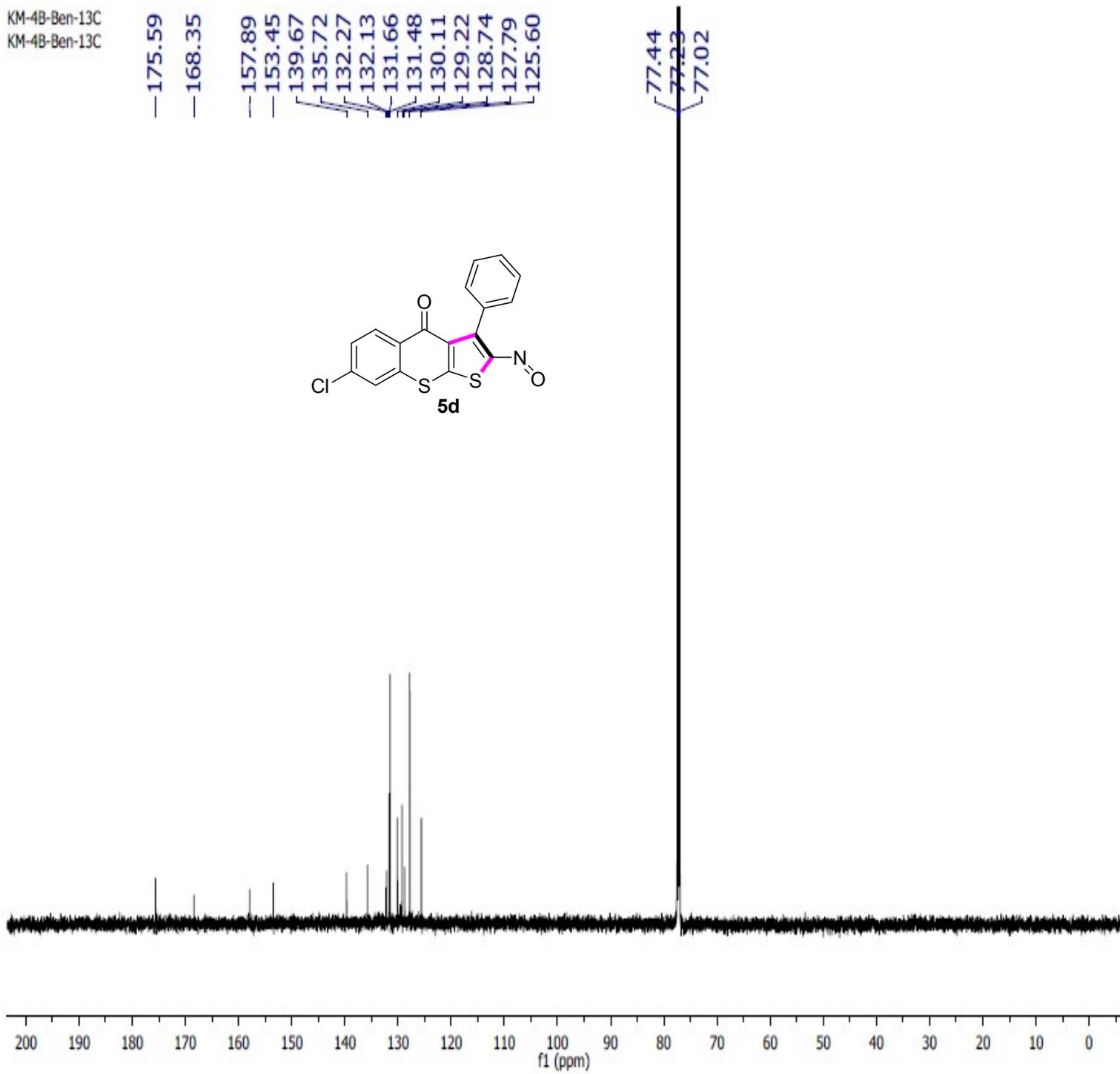
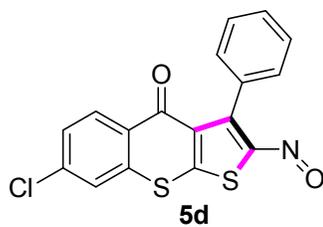


¹³CNMR spectra of compound: 5d

KM-4B-Ben-13C
KM-4B-Ben-13C

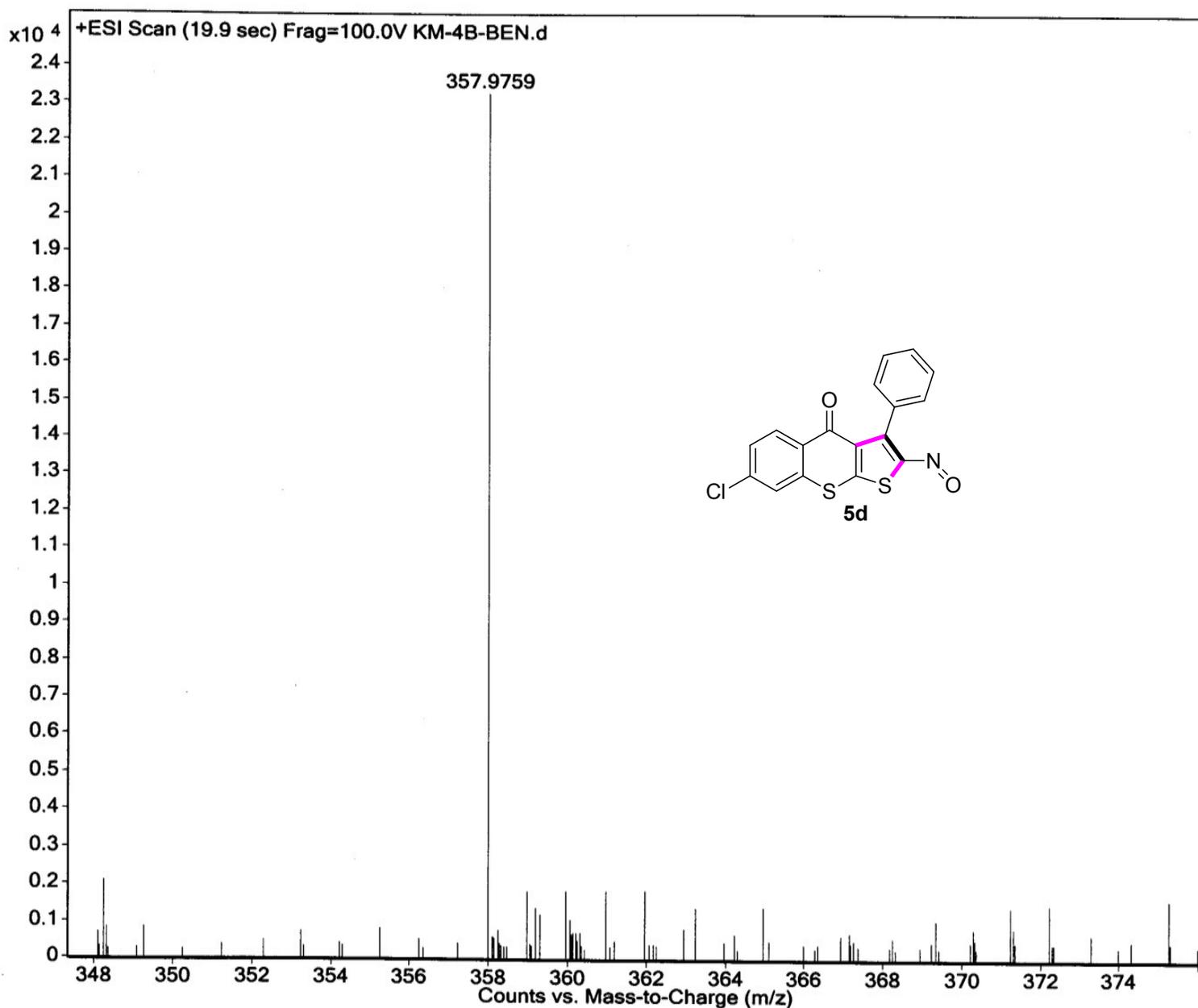
— 175.59
— 168.35
— 157.89
— 153.45
— 139.67
— 135.72
— 132.27
— 132.13
— 131.66
— 131.48
— 130.11
— 129.22
— 128.74
— 127.79
— 125.60

{ 77.44
{ 77.23
{ 77.02



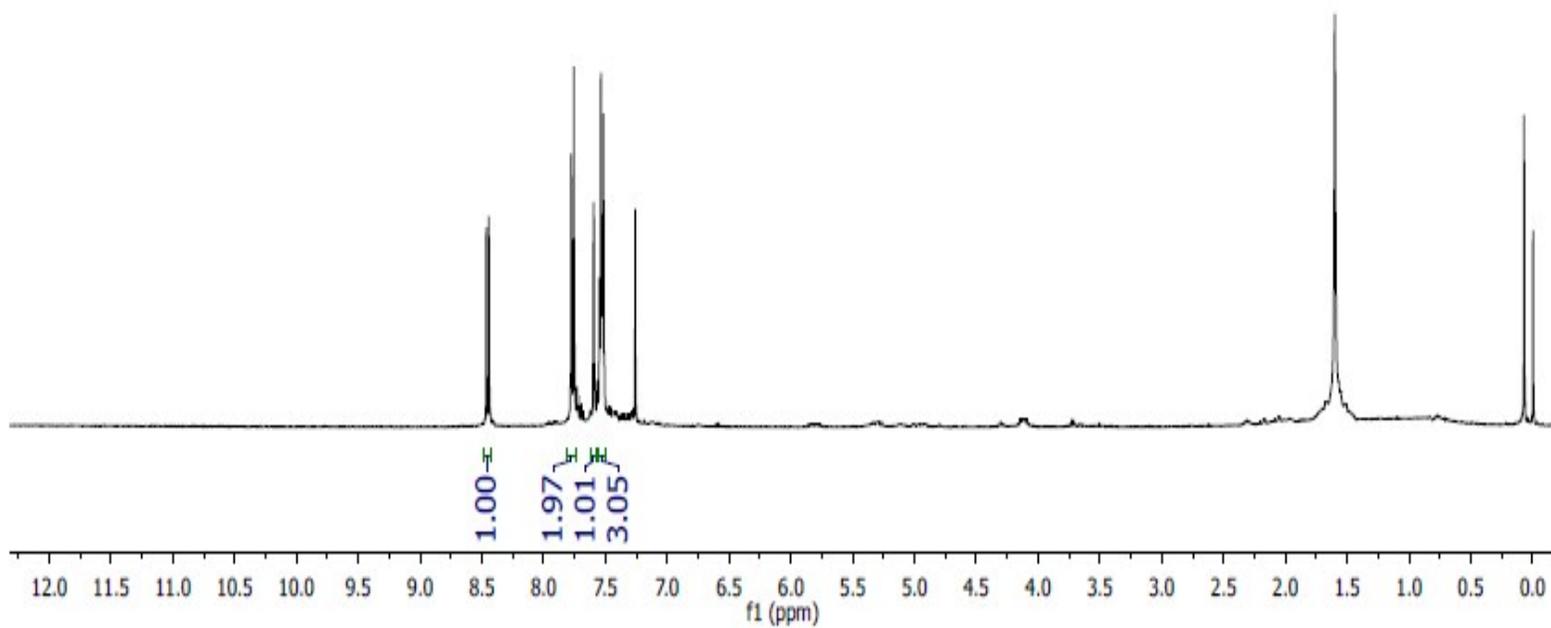
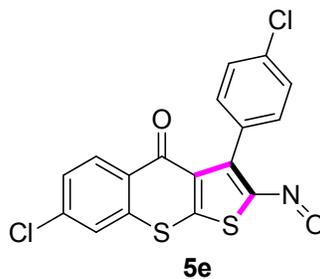
HRMS spectra of compound: 5d

Sample Name	KM-4B-BEN	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	KM-4B-BEN.d	ACQ Method		Comment		Acquired Time	2/16/2016 11:03:29 AM



¹H NMR spectra of compound: 5e

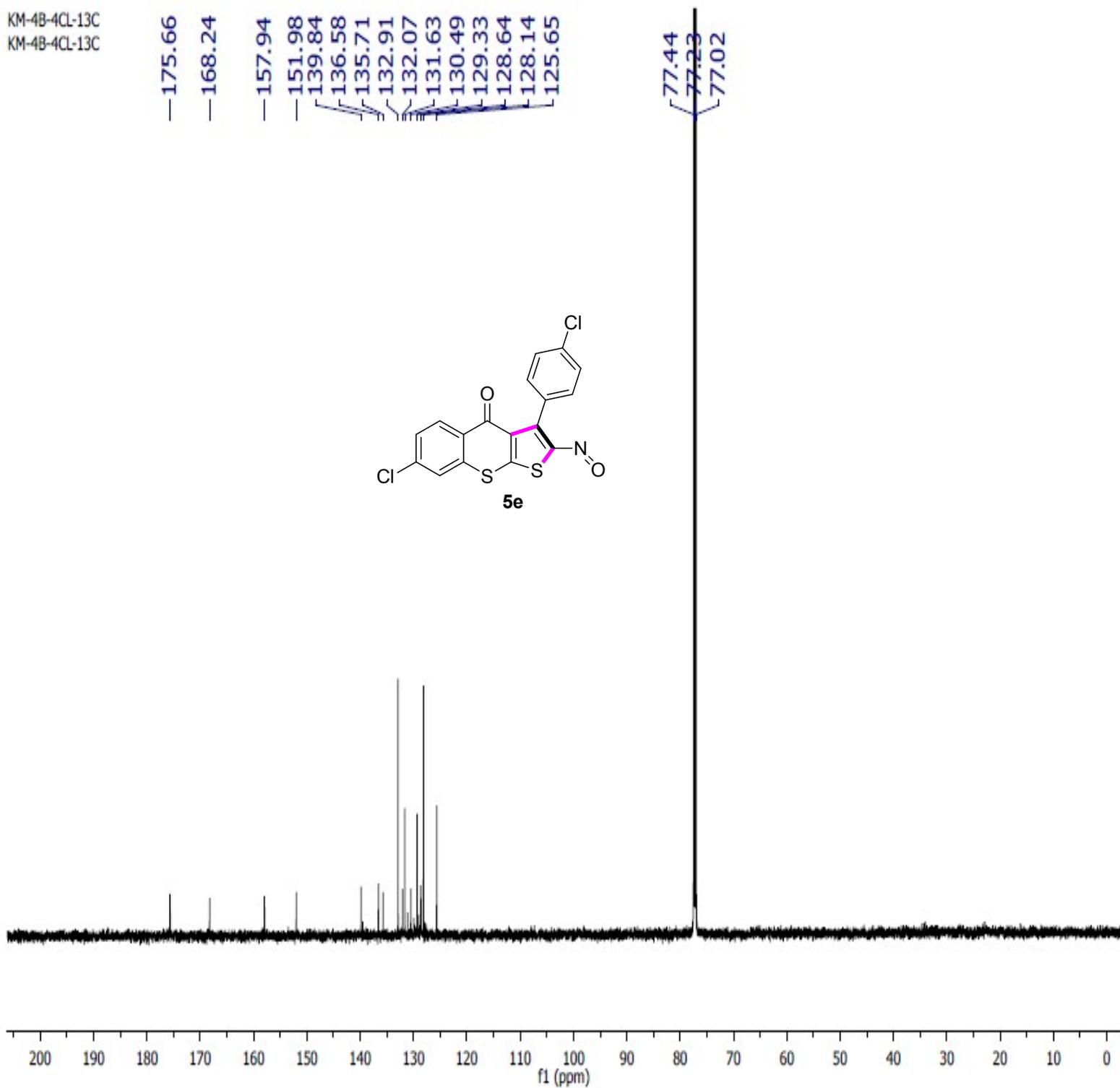
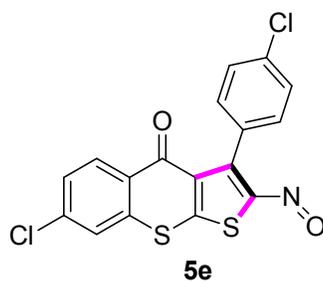
KM-4B-4CL-1H
KM-4B-4CL-1H



¹³CNMR spectra of compound: 5e

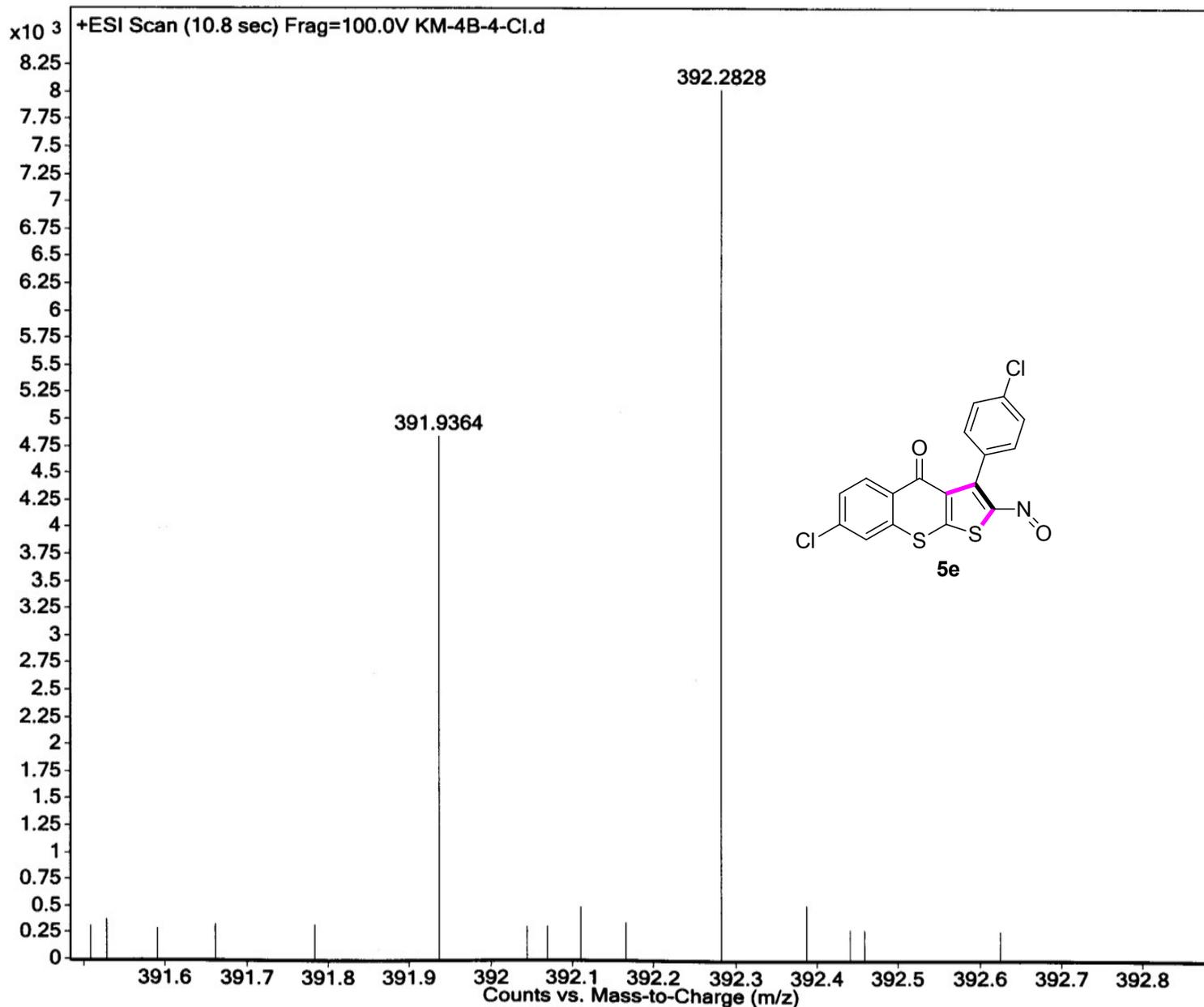
KM-4B-4Cl-13C
KM-4B-4Cl-13C

— 175.66
— 168.24
— 157.94
— 151.98
139.84
136.58
135.71
132.91
132.07
131.63
130.49
129.33
128.64
128.14
125.65
77.44
77.23
77.02



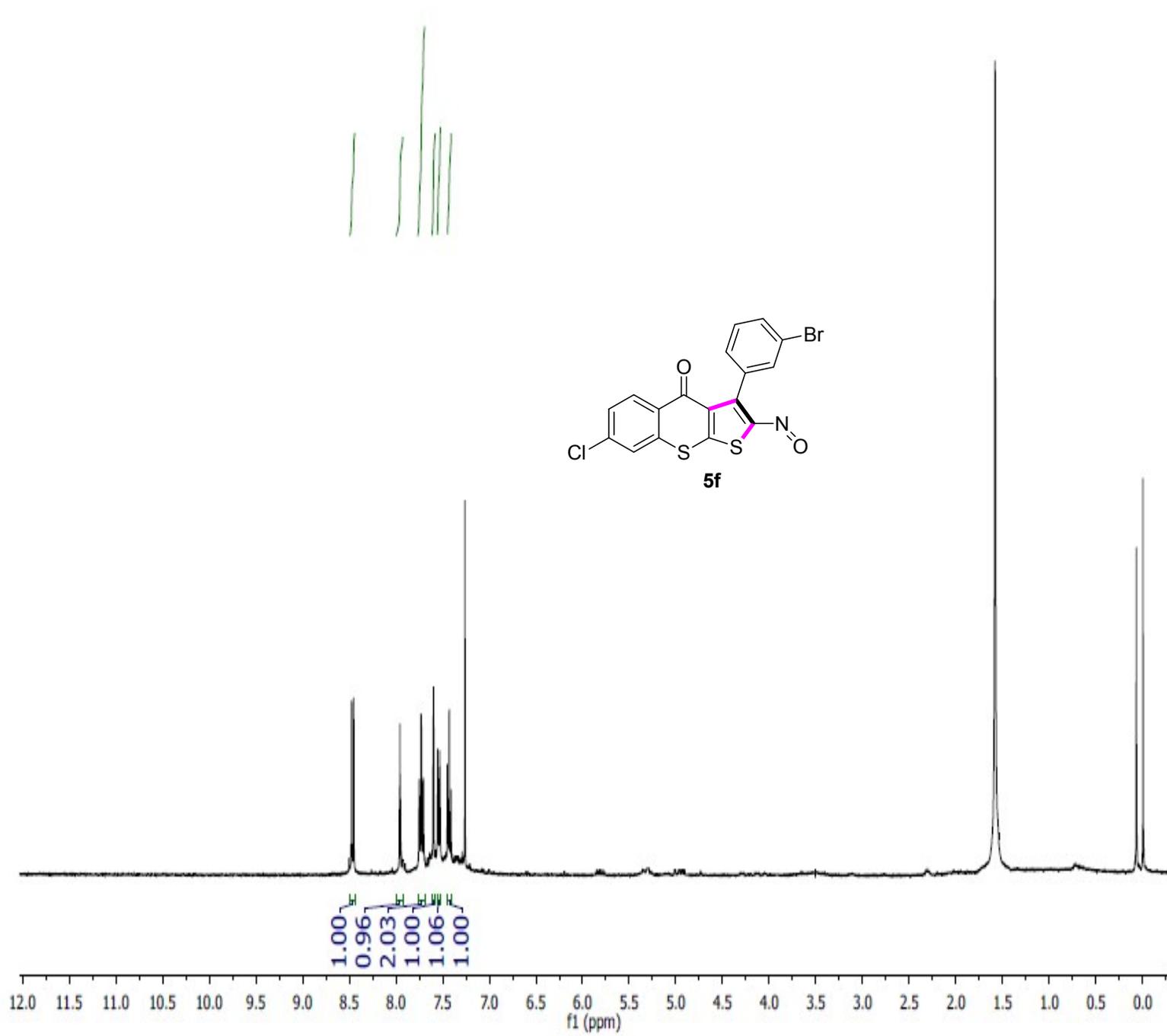
HRMS spectra of compound: 5e

Sample Name	KM-4B-4-Cl	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	KM-4B-4-Cl.d	ACQ Method		Comment		Acquired Time	2/16/2016 10:59:54 AM



¹H NMR spectra of compound: 5f

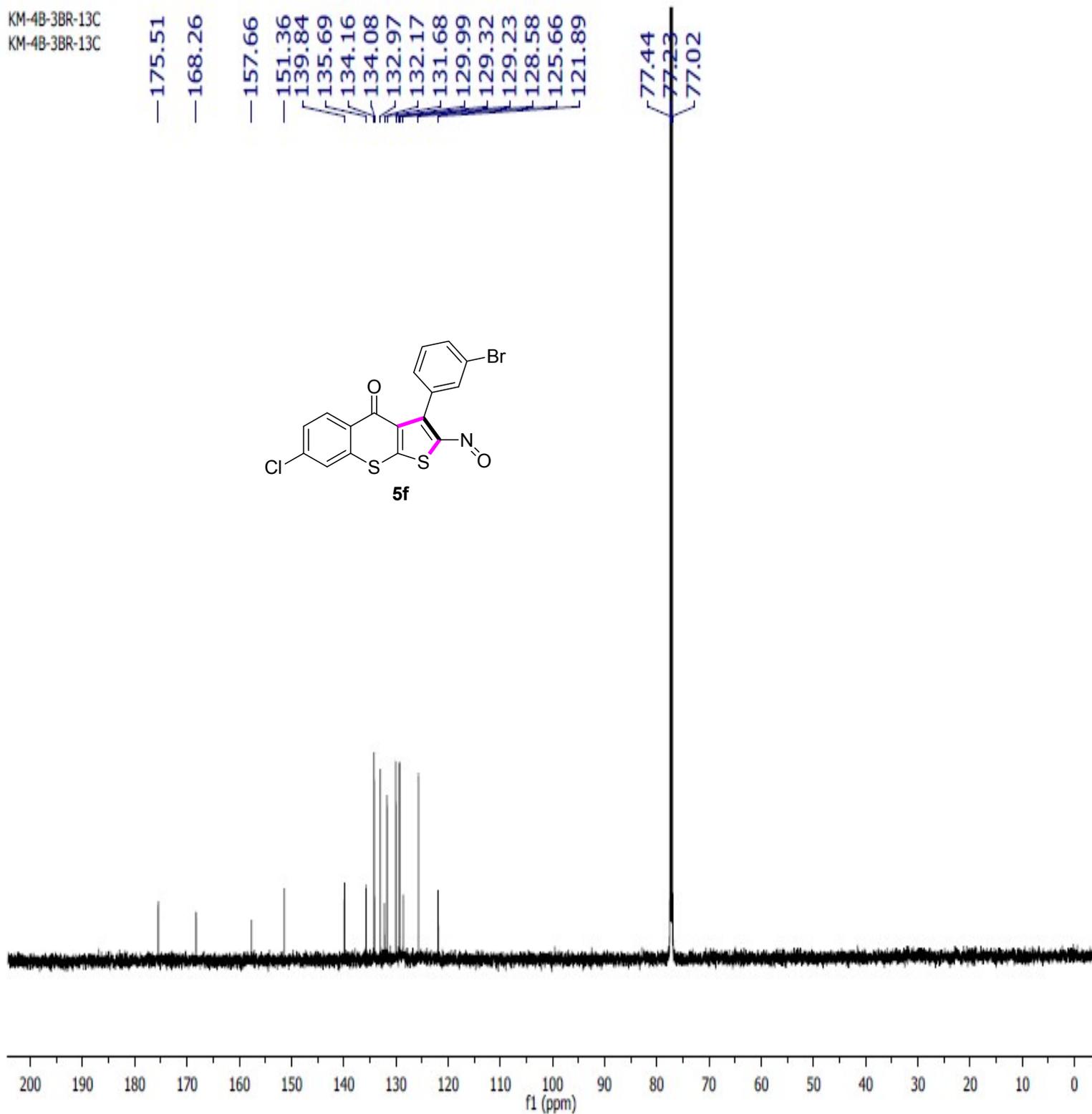
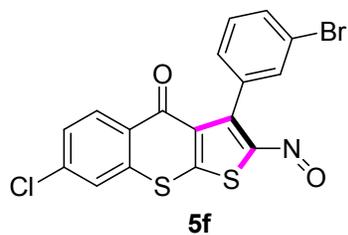
KM-4B-3Br-1H
KM-4B-3Br-1H



¹³CNMR spectra of compound: 5f

KM-4B-3BR-13C
KM-4B-3BR-13C

— 175.51
— 168.26
— 157.66
— 151.36
— 139.84
— 135.69
— 134.16
— 134.08
— 132.97
— 132.17
— 131.68
— 129.99
— 129.32
— 129.23
— 128.58
— 125.66
— 121.89
— 77.44
— 77.23
— 77.02



HRMS spectra of compound: 5f

Sample Name	KM-4B-A-3BR	Position	Vial 1	Instrument Name	Instrument 1	User Name	
Inj Vol	0	InjPosition		SampleType	Sample	IRM Calibration Status	All Ions Missed
Data Filename	KM-4B-A-3BR.d	ACQ Method		Comment		Acquired Time	6/3/2016 12:09:38 PM

