

Electronic Supporting Information

Synthesis of vinyl sulfides and thioethers *via* hydrothiolation reaction of 4-hydroxydithiocoumarin and arylacetylenes/styrenes†

Santa Mondal, Sabina Yashmin and Abu Taleb Khan*

Department of Chemistry, Indian Institution of Technology, Guwahati, Guwahati – 781039, India

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

Content

1. General Information and Methods

2. Copies of ¹H NMR, ¹³C NMR and HRMS spectra of all Compounds

1. General Information and Methods

¹H and ¹³C NMR spectra were recorded on 400 MHz and 500 MHz NMR 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), *q* (quartet) and *m* (multiplet). IR spectra were recorded in KBr pellet. HRMS spectra were recorded using ESI and APCI (TOF) mode.

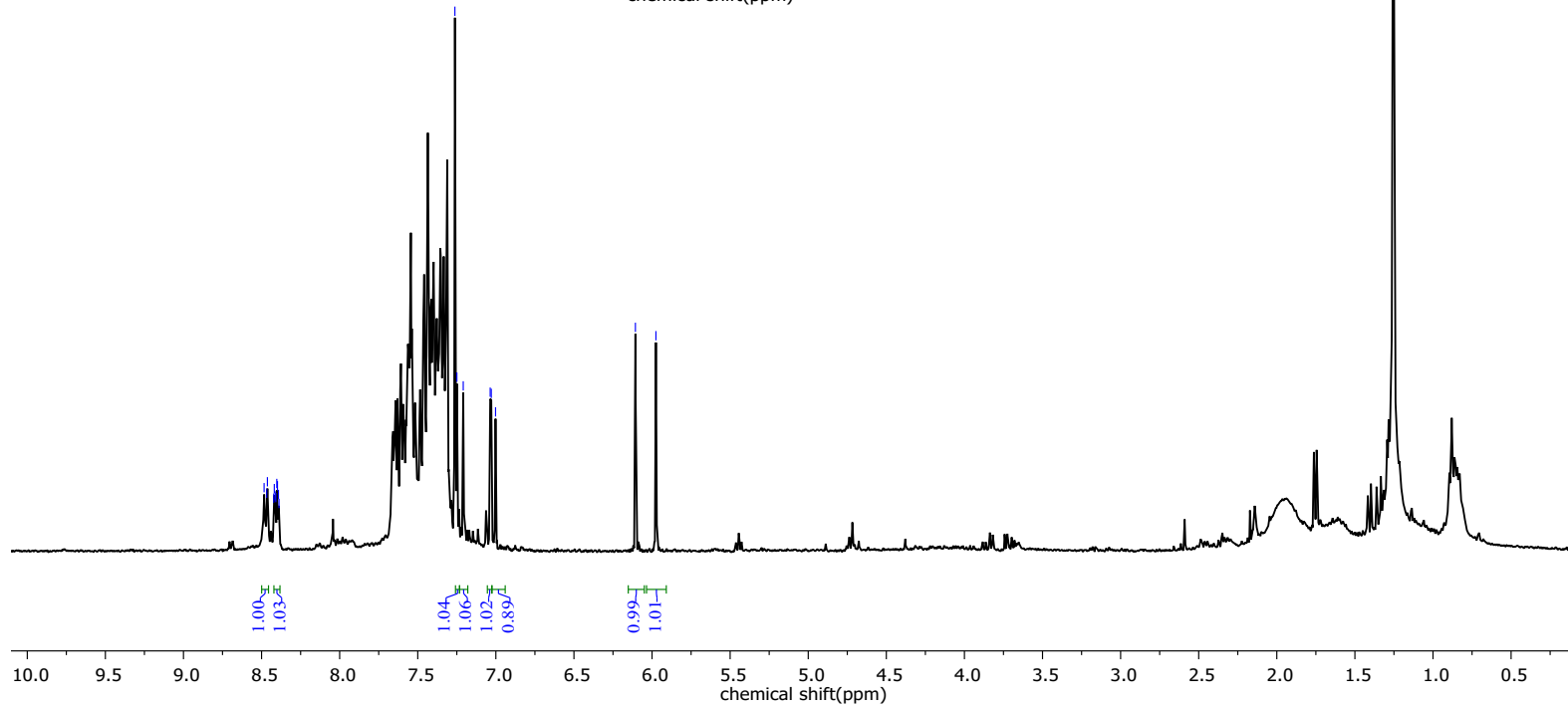
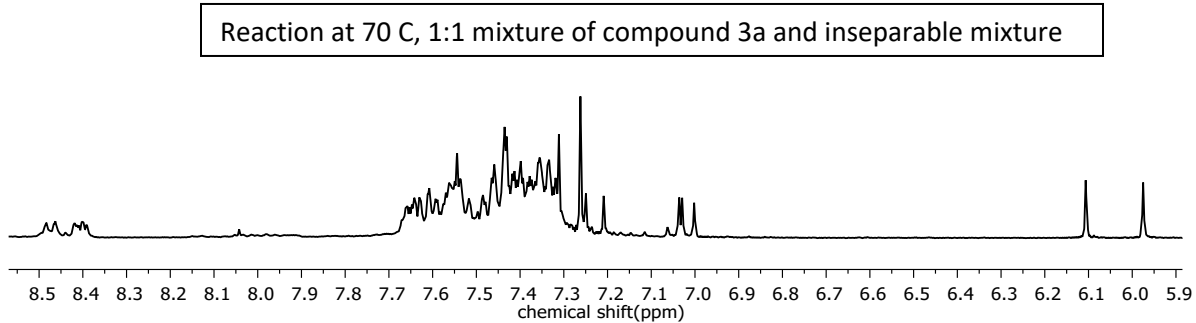
2. Copies of ^1H NMR, ^{13}C NMR and HRMS spectra of all Compounds

^1H NMR of optimization Table 1, entry 2

SM-42I2-1-1H.1.fid
SM-42I2-1-1H

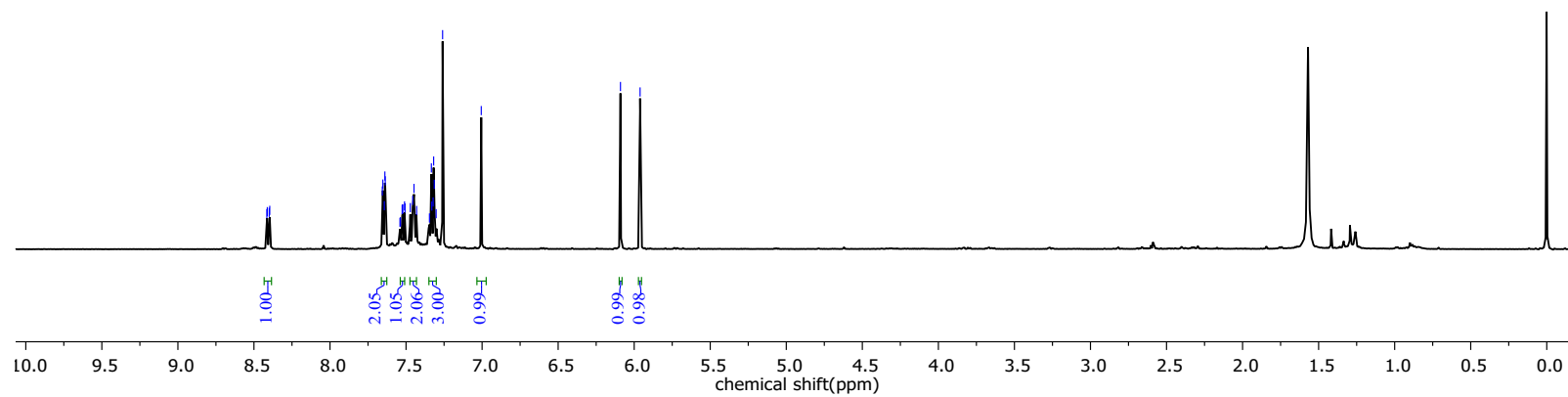
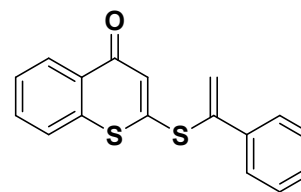
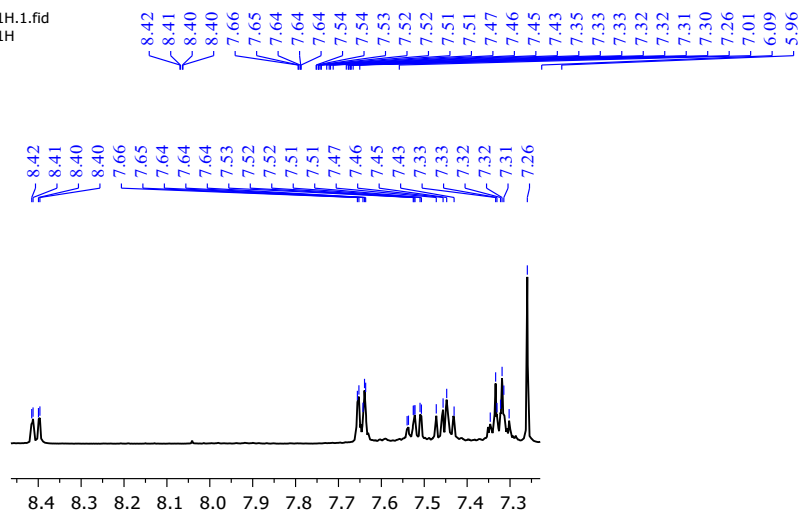
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8.41
8.40
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8.39
8.39
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7.04
7.03
7.00
6.11
5.98

Reaction at 70 C, 1:1 mixture of compound 3a and inseparable mixture



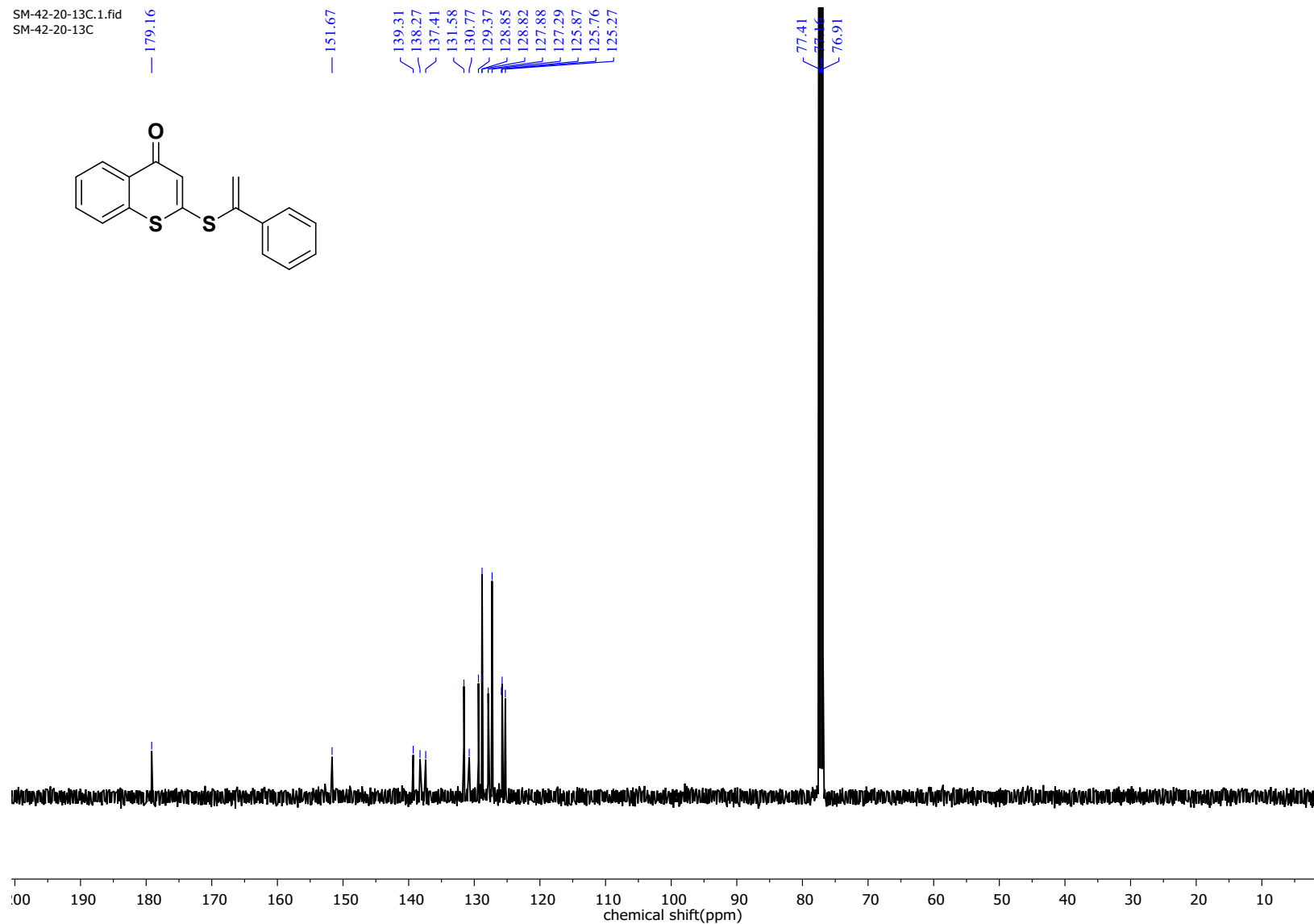
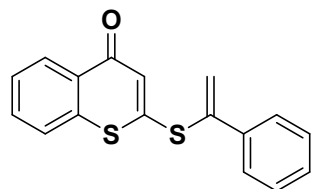
¹H NMR of compound3a

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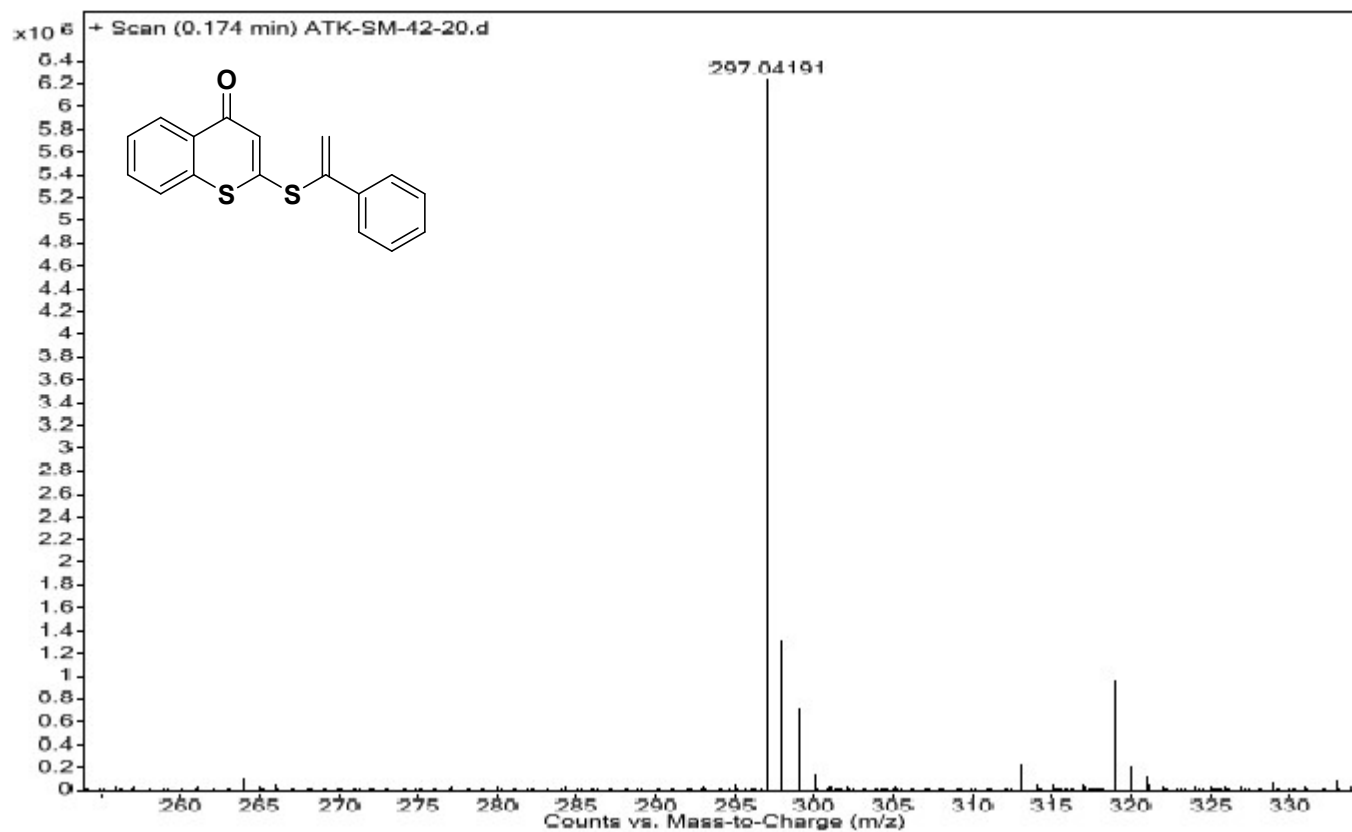
¹³C NMR of compound 3a

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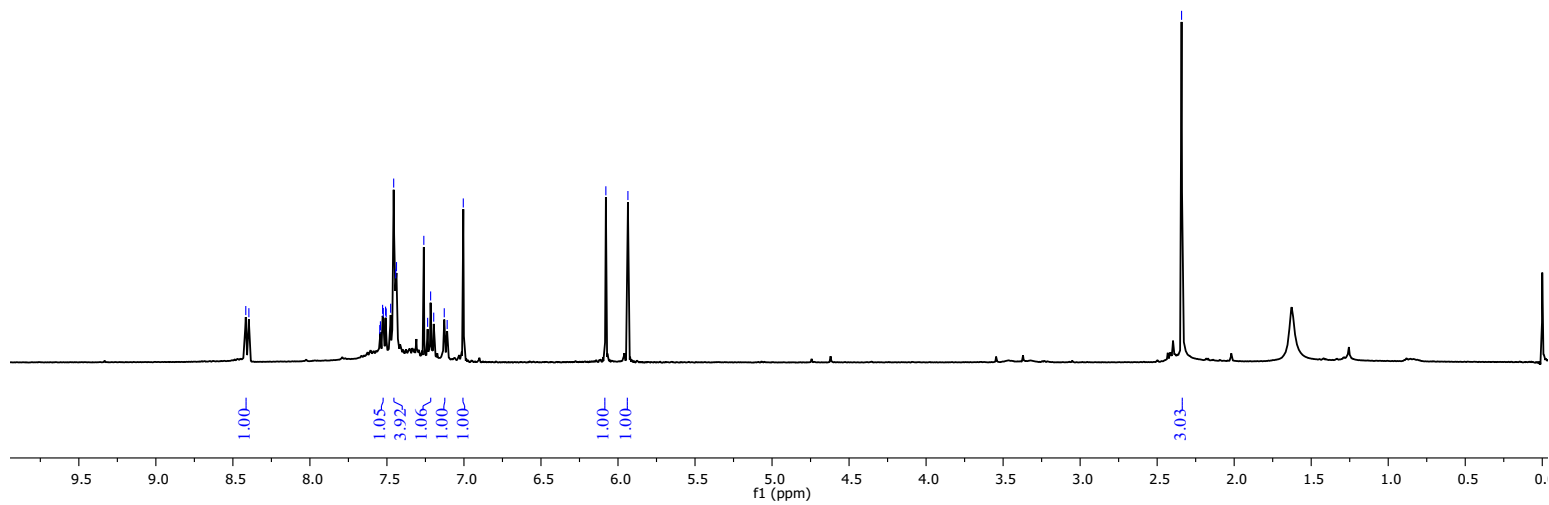
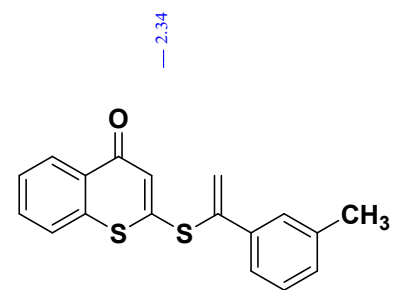
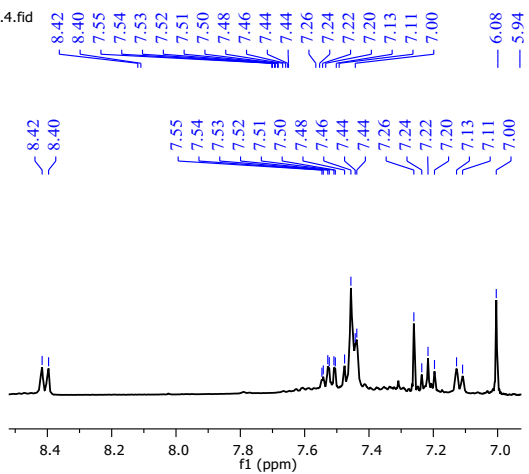
HRMS of compound 3a

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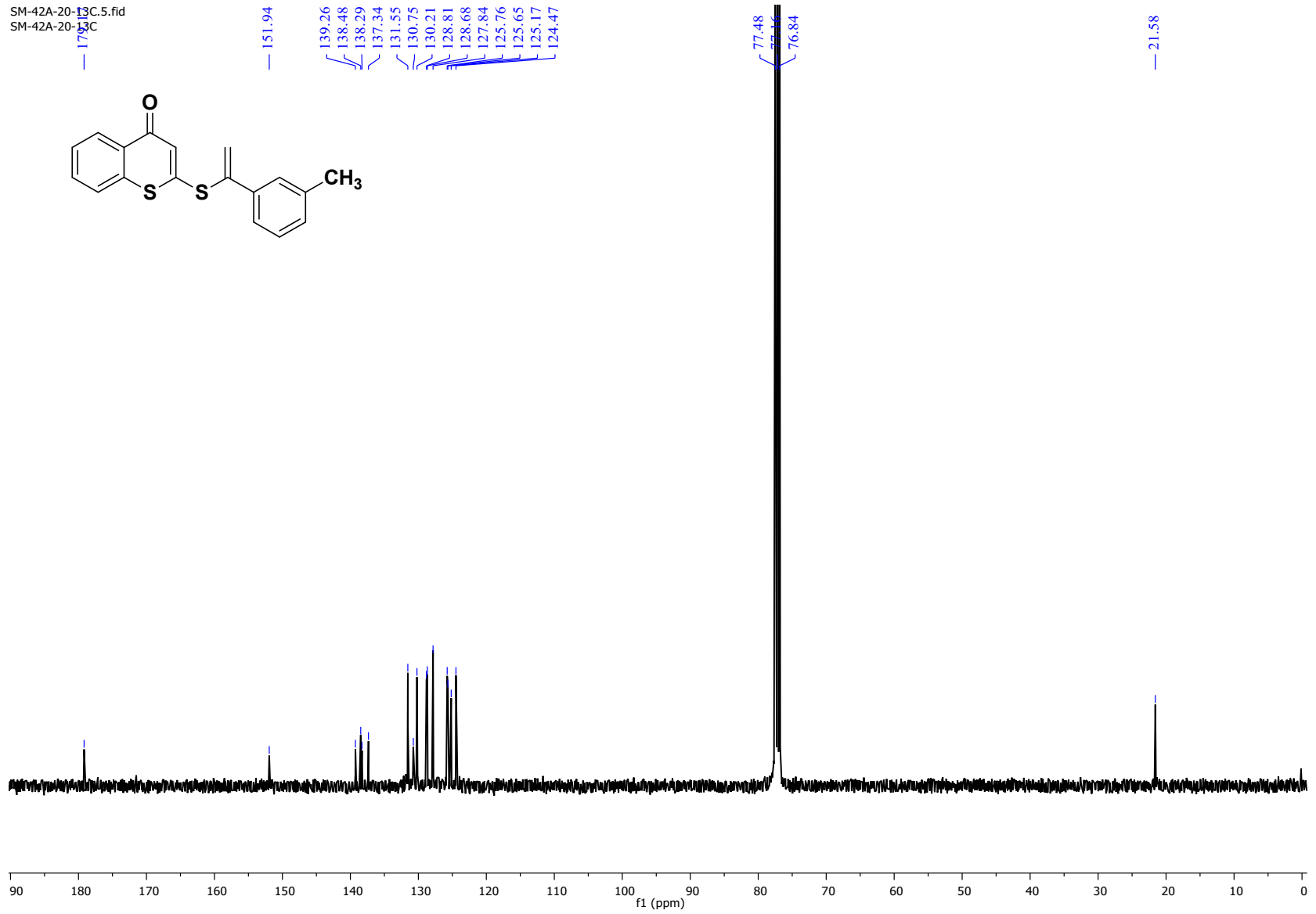
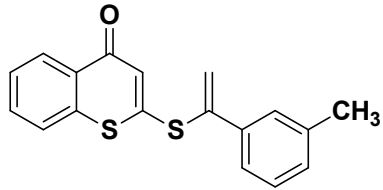
¹H NMR of compound 3b

SM-42A-20-1H.4.fid
SM-42A-20-1H



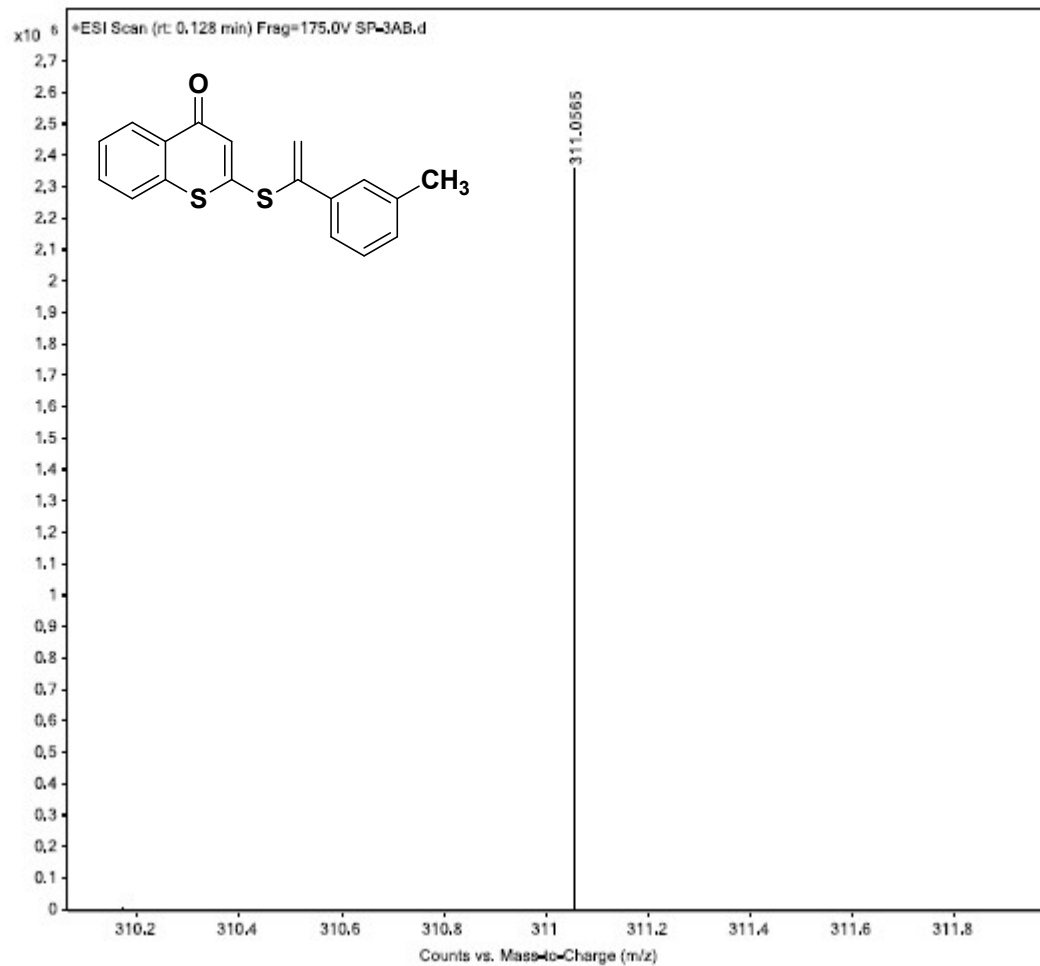
¹³C NMR of compound 3b

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SM-42A-20-13C



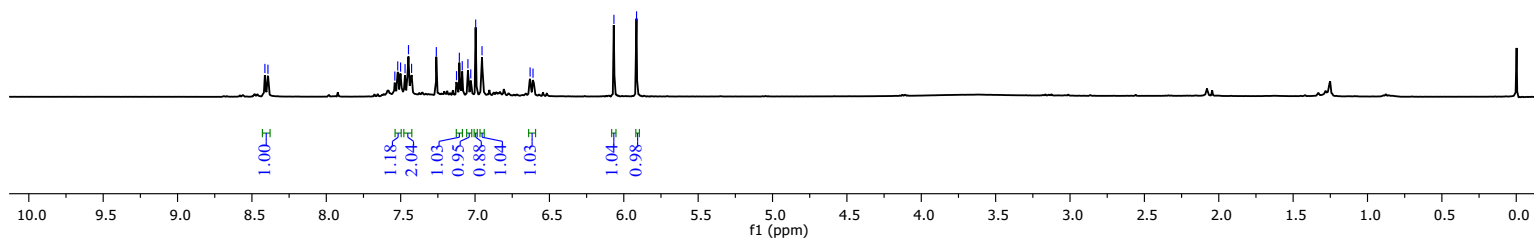
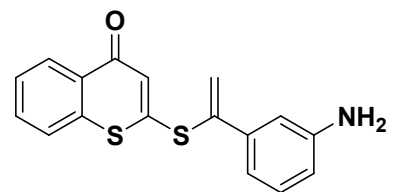
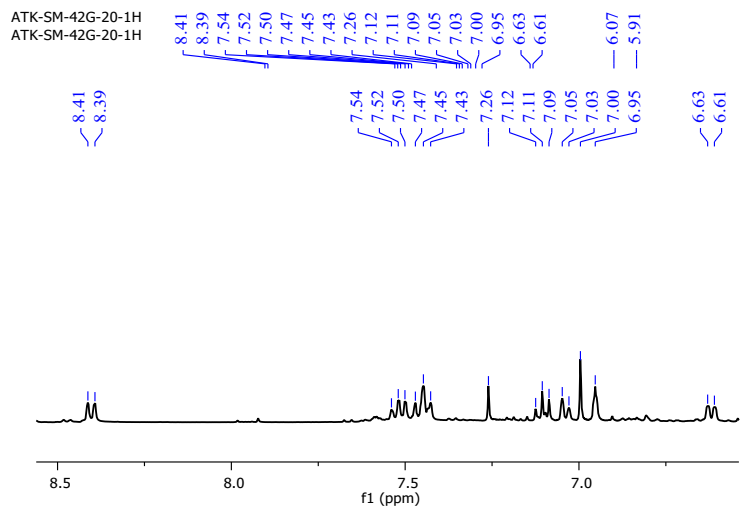
HRMS of compound 3b

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Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SP-3AB.d
ACQ Method	ESI ALS 100-1000,m	Comment		Acquired Time	11-09-2021 09:51:52 (UTC+05:30)



¹H NMR of compound 3c

ATK-SM-42G-20-1H
ATK-SM-42G-20-1H



¹³C NMR of compound 3c

ATK-SM-42G-20-13C
ATK-SM-42G-20-13C

179.16

152.25

146.71

139.04

138.42

138.25

131.52

130.66

129.70

128.74

127.82

125.74

125.28

117.67

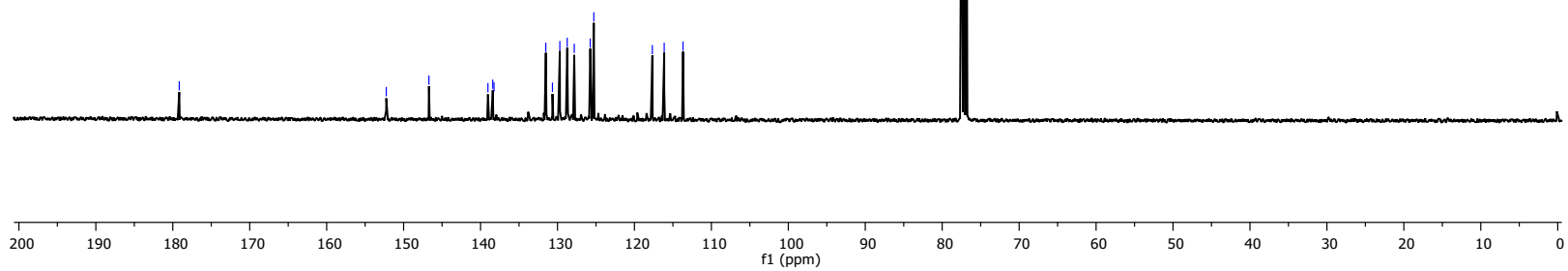
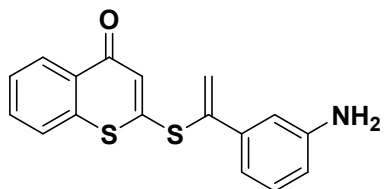
116.13

113.68

77.48

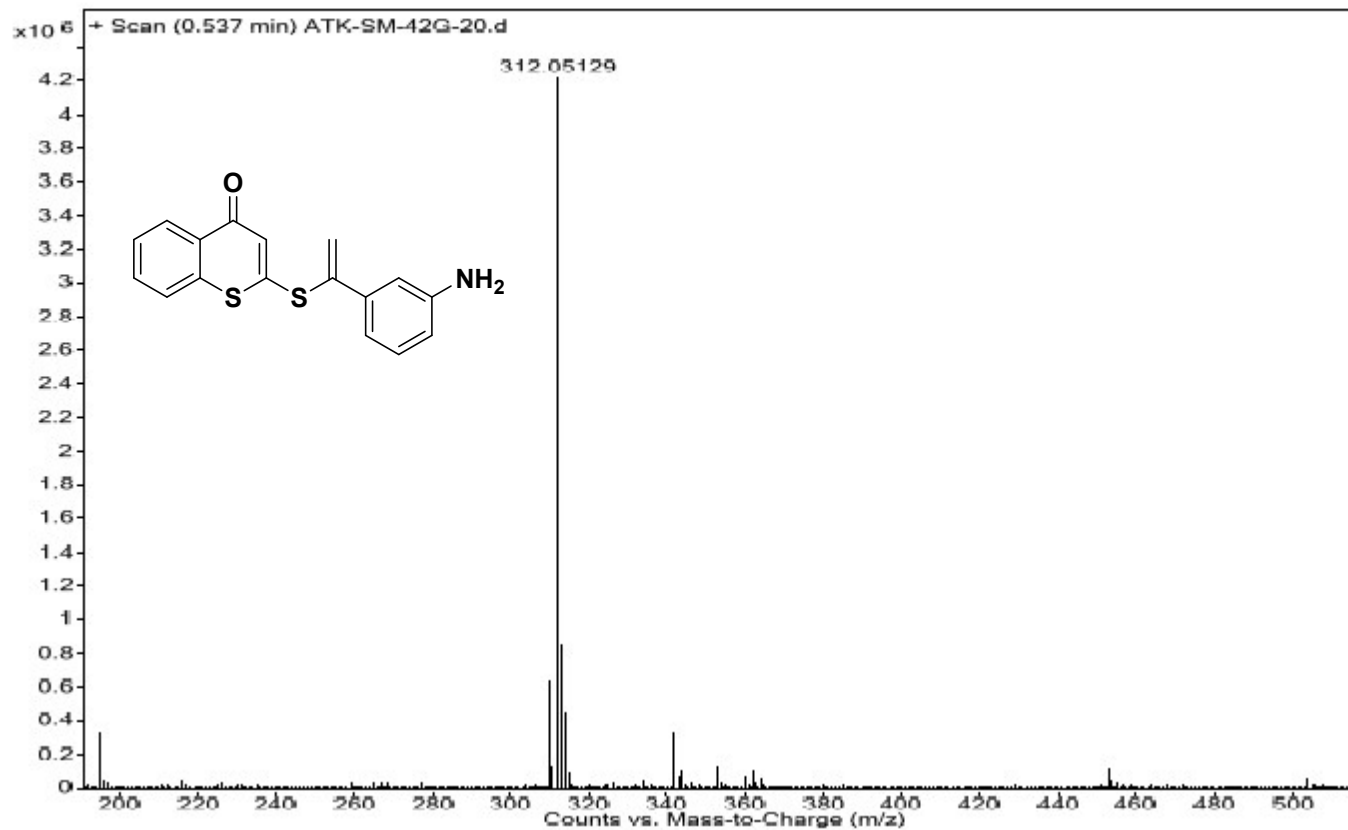
77.16

76.84



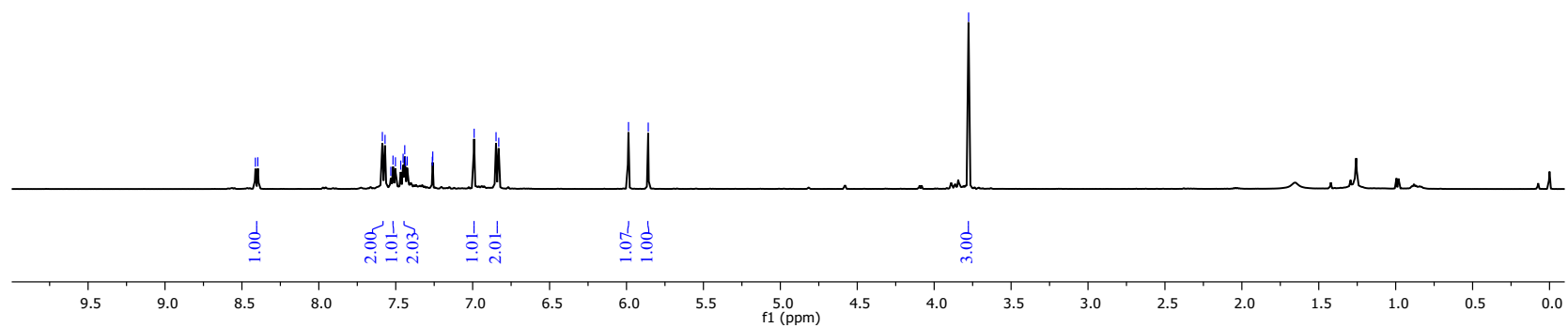
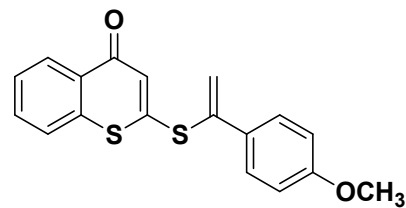
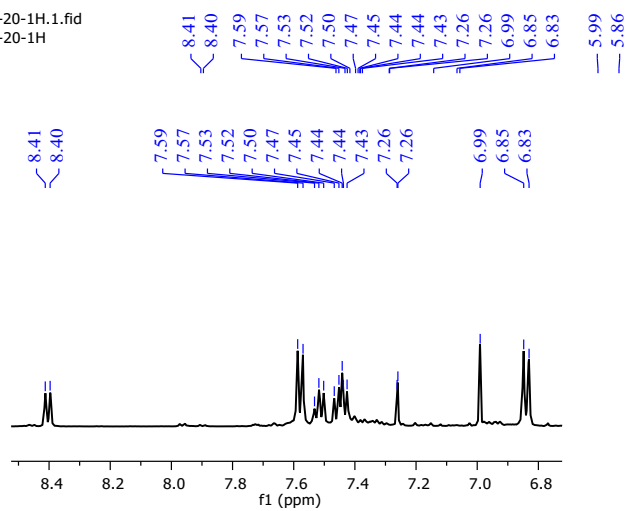
HRMS of compound 3c

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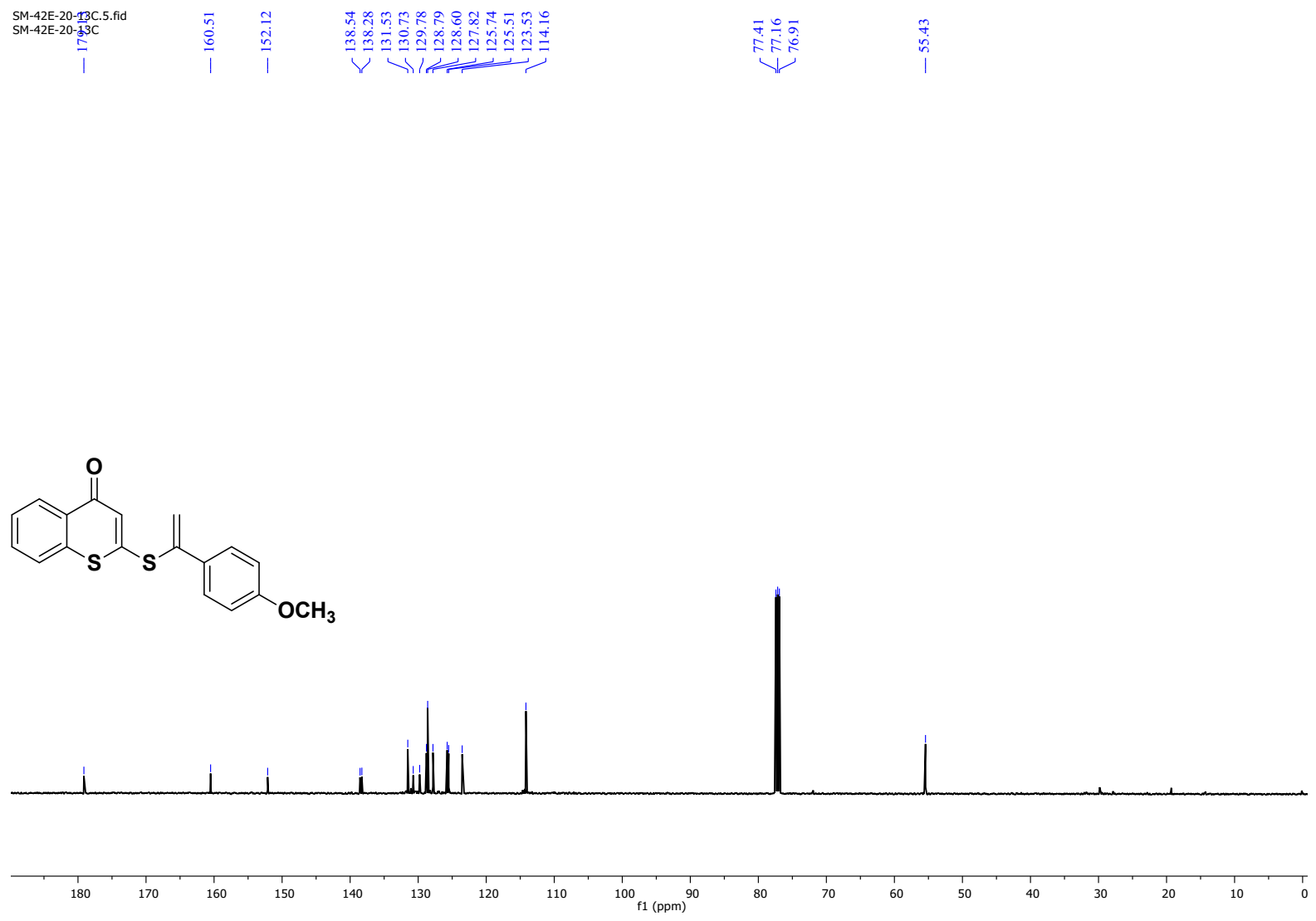
¹H NMR of compound 3d

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SM-42E-20-1H



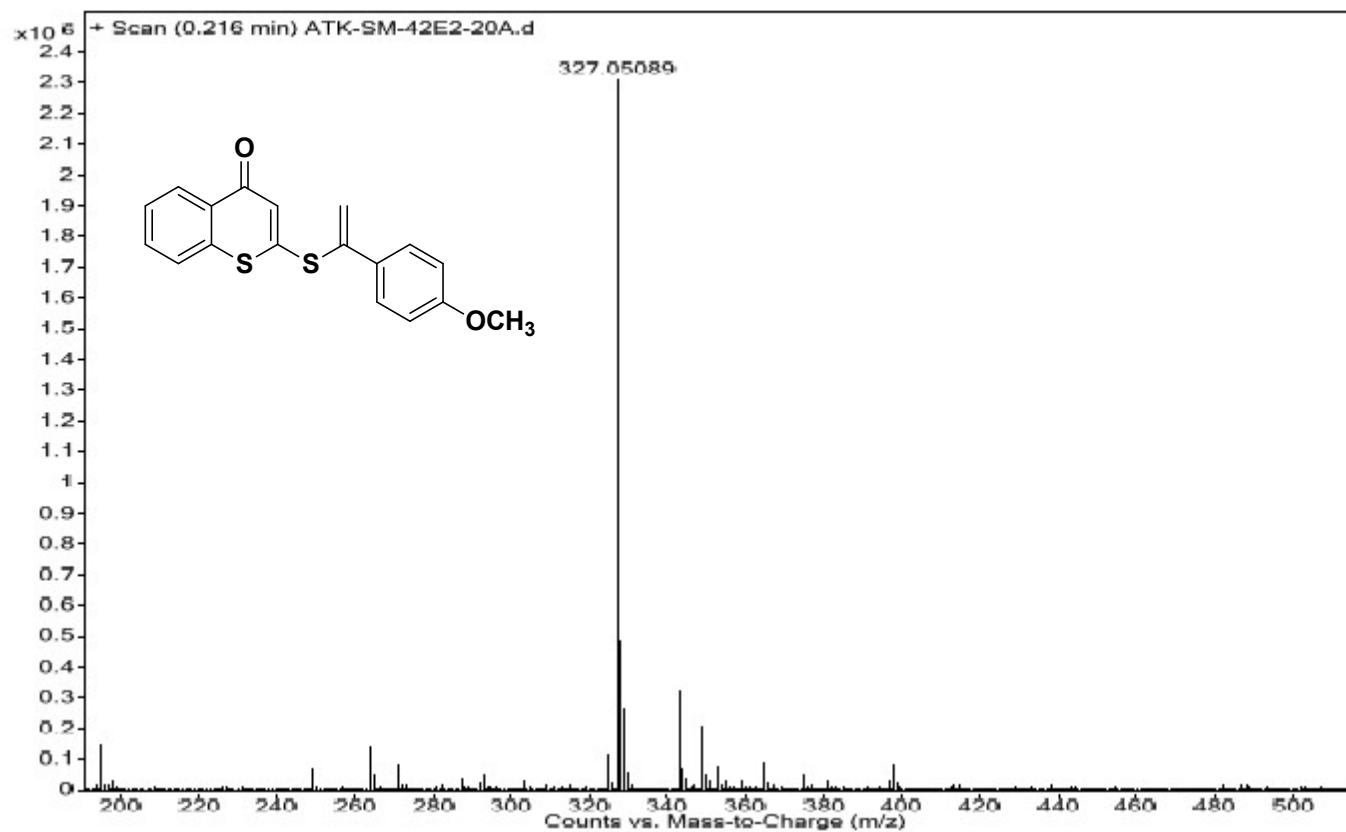
¹³C NMR of compound 3d

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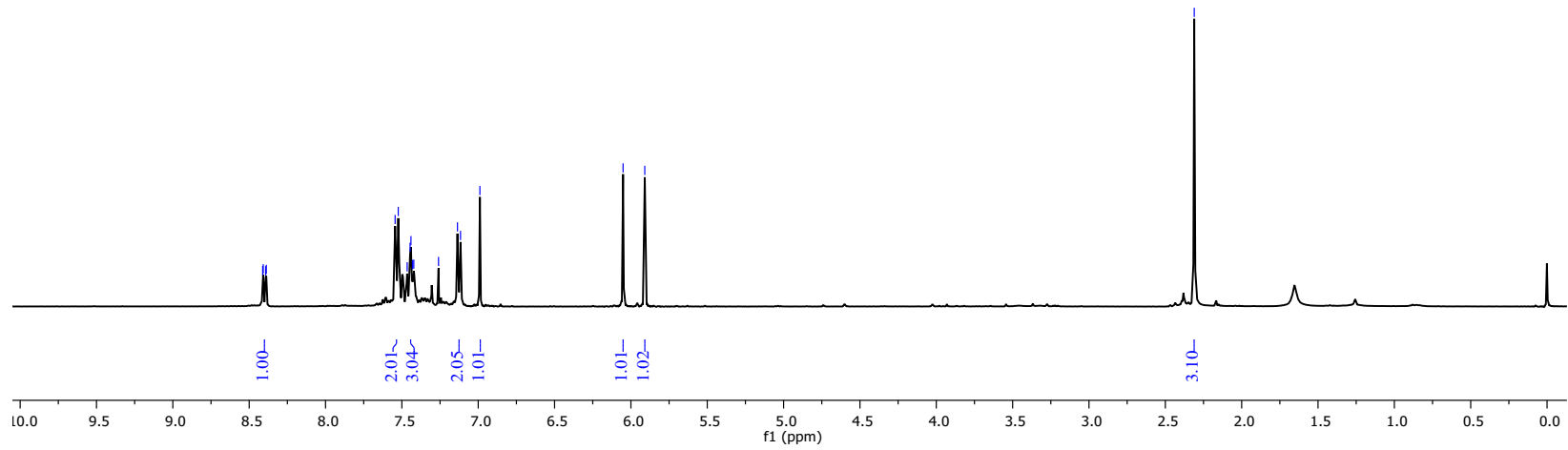
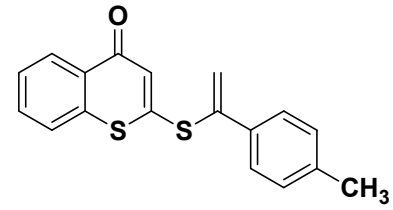
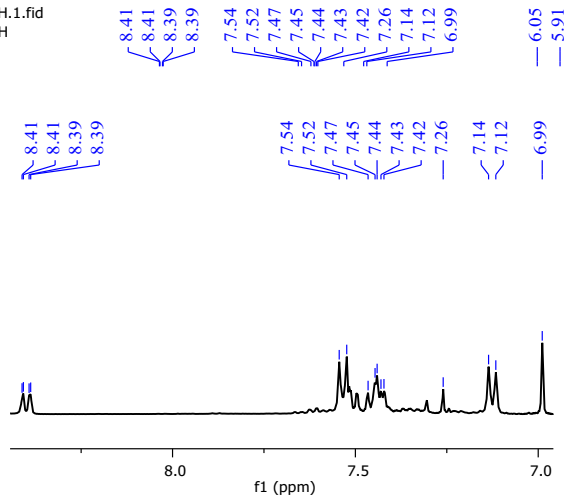
HRMS of compound 3d

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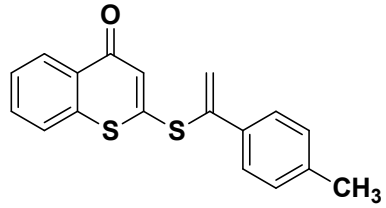
¹H NMR of compound 3e

SM-42F2-19-1H.1.fid
SM-42F2-19-1H



¹³C NMR of compound 3e

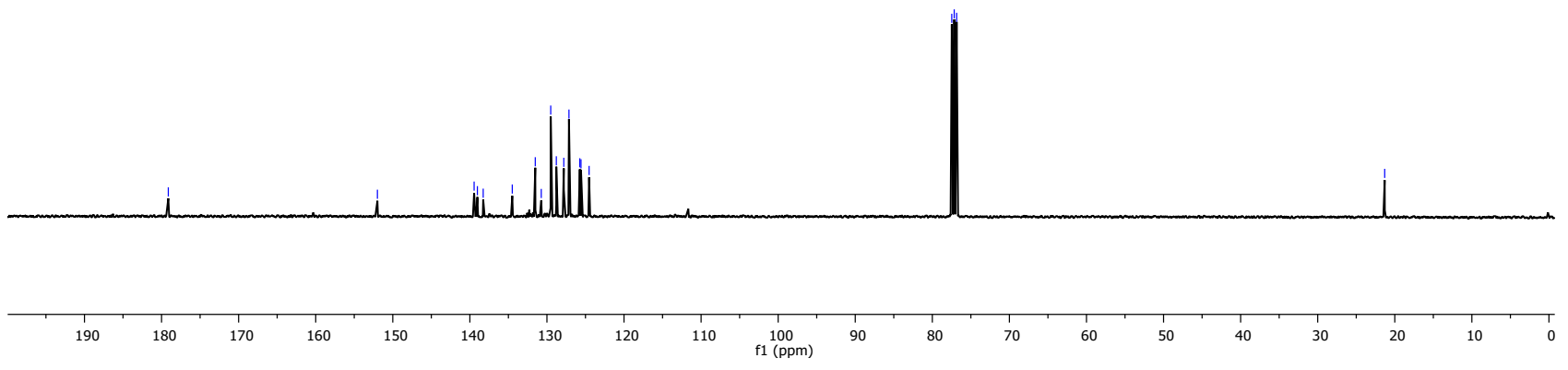
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SM-42F2-19-13C



179.12
152.00
139.45
139.02
138.27
134.50
131.51
130.74
129.51
128.78
127.81
127.14
125.74
125.58
124.53

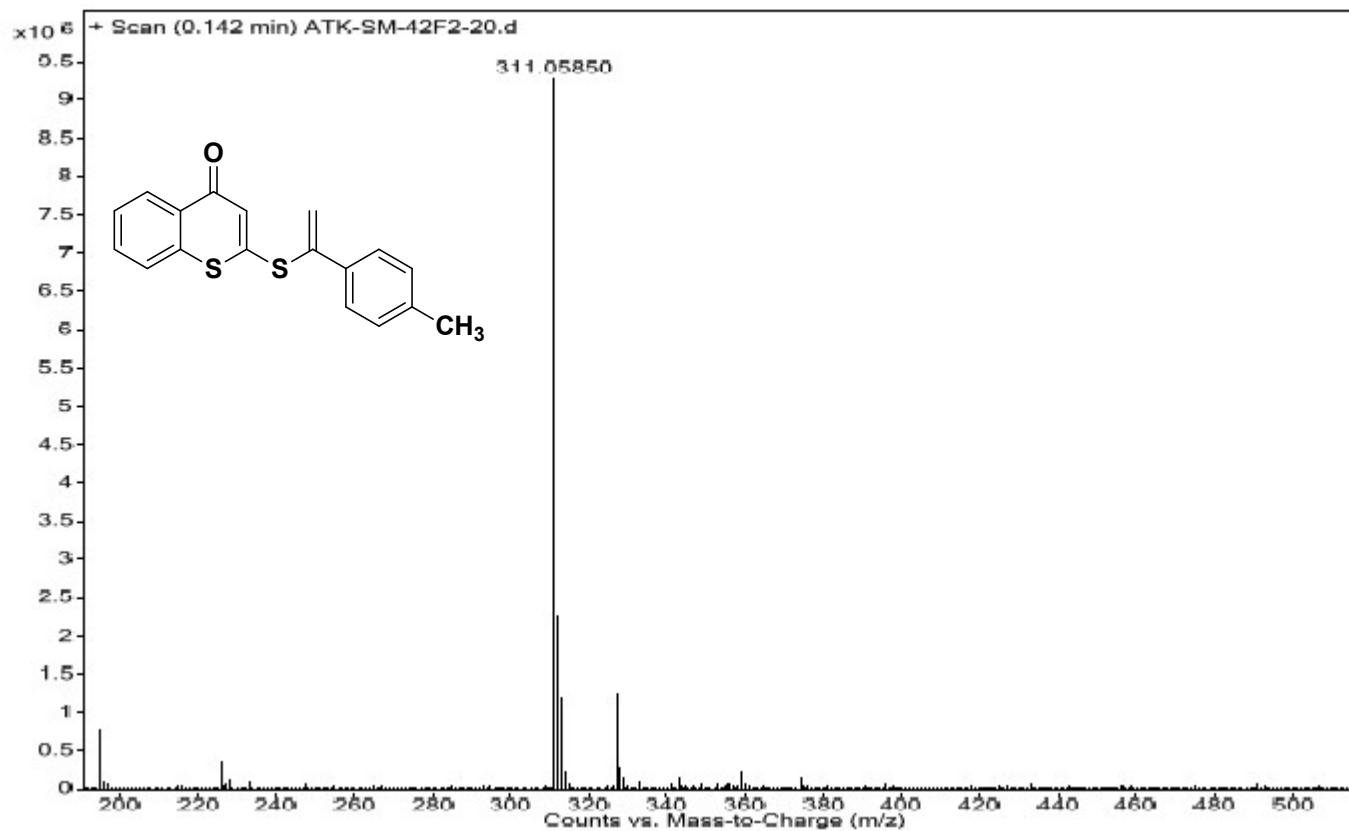
77.48
77.16
76.84

21.31



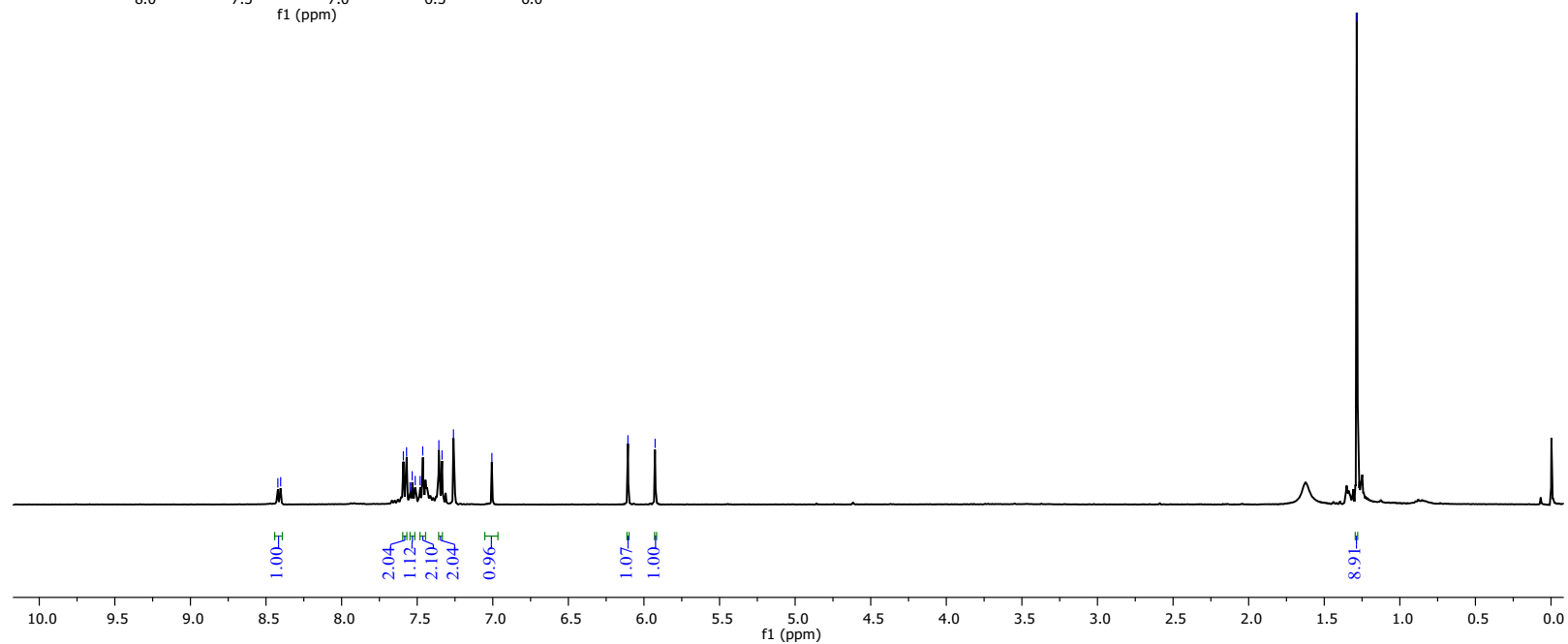
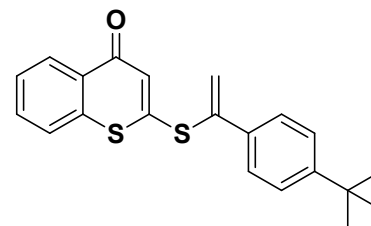
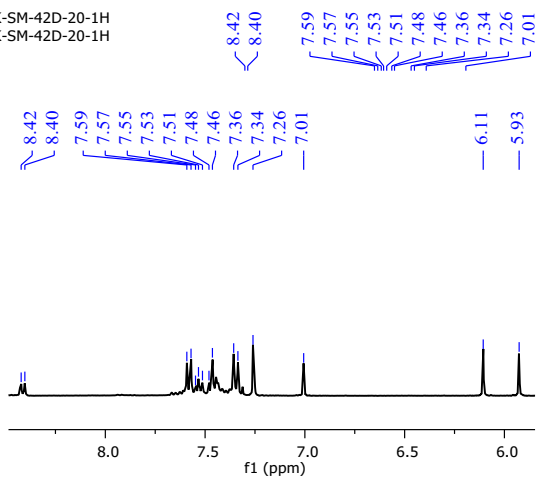
HRMS of compound 3e

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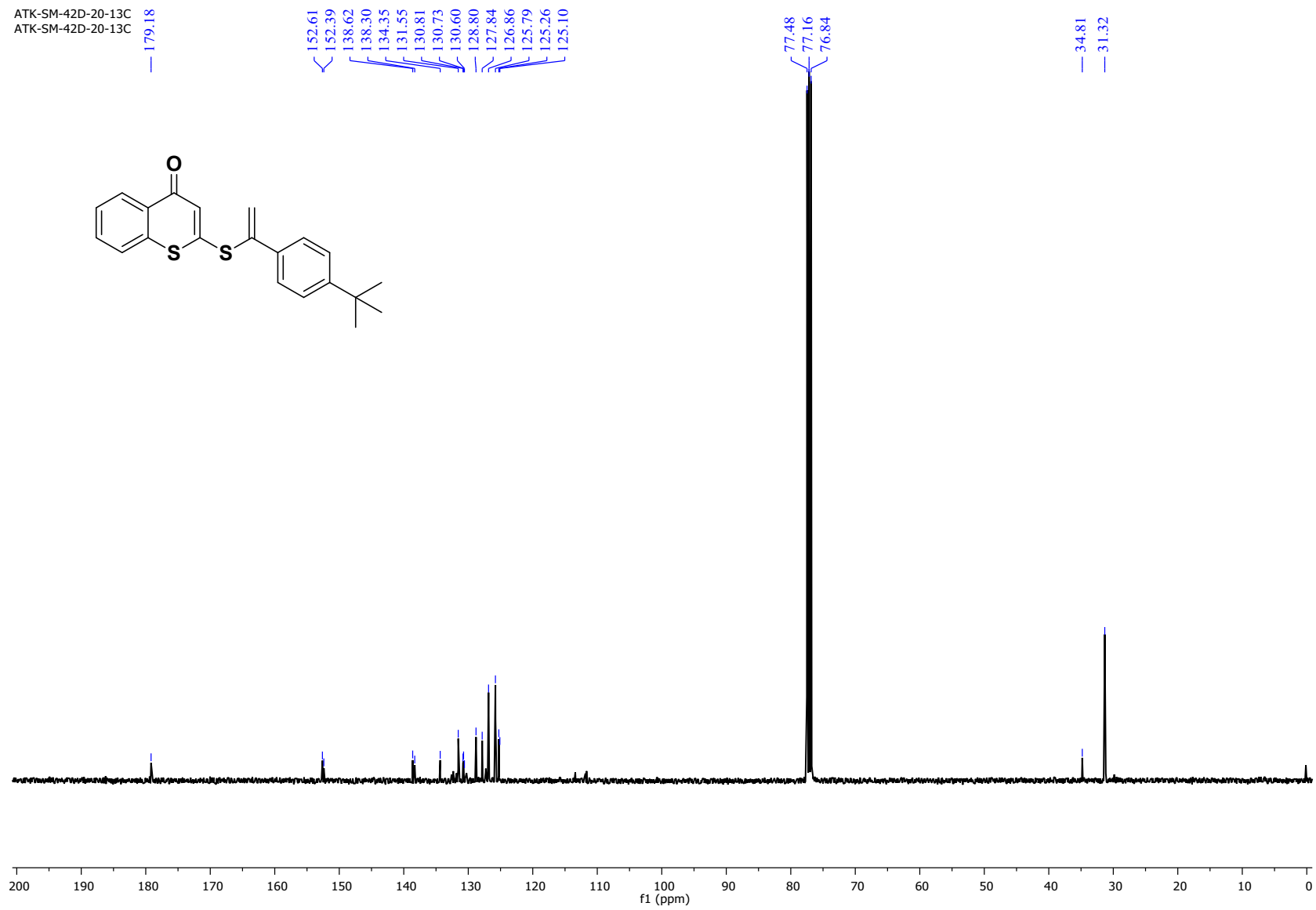
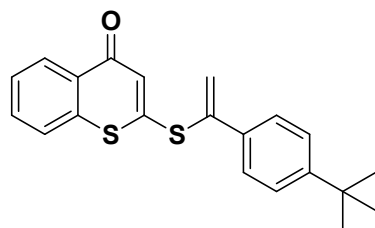
¹H NMR of compound 3f

ATK-SM-42D-20-1H
ATK-SM-42D-20-1H



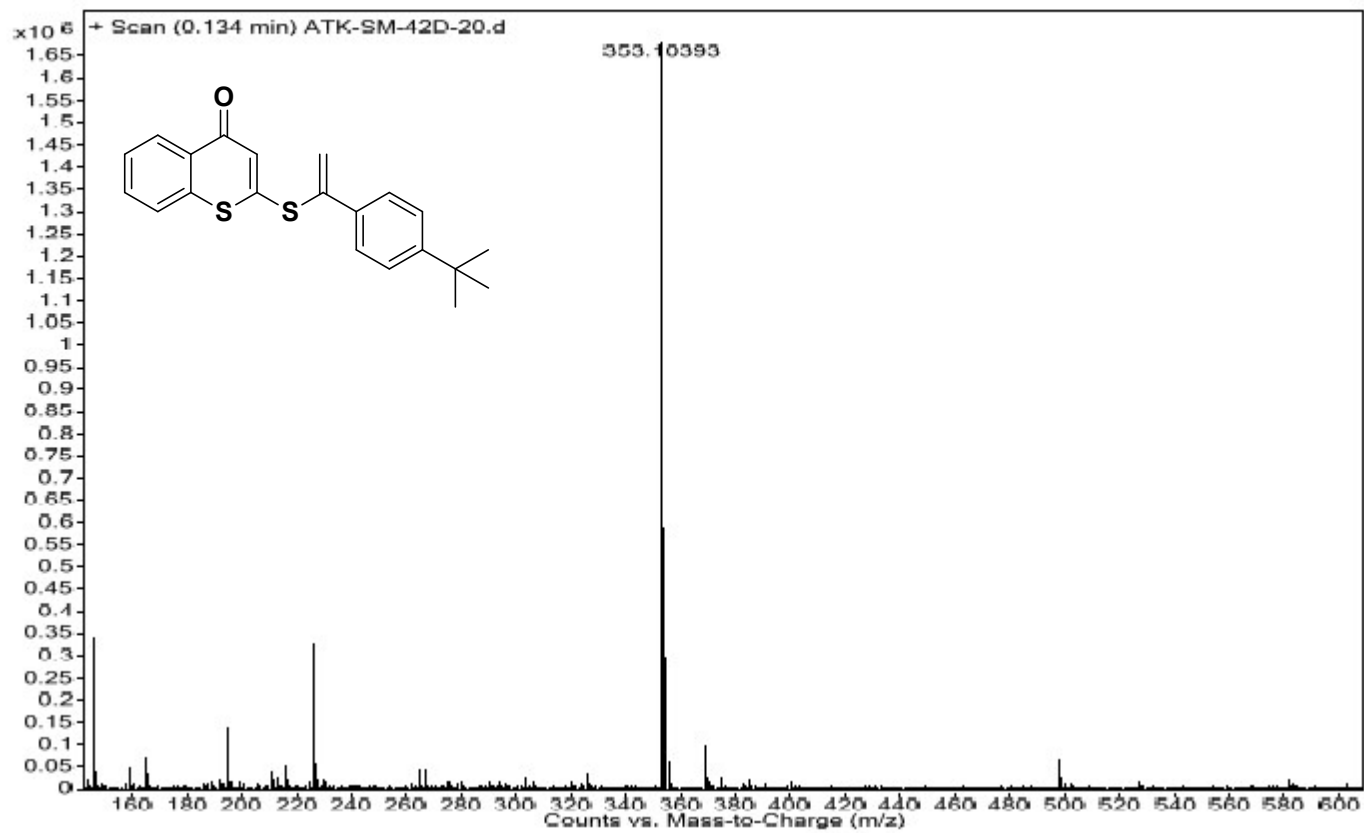
¹³C NMR of compound 3f

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ATK-SM-42D-20-13C



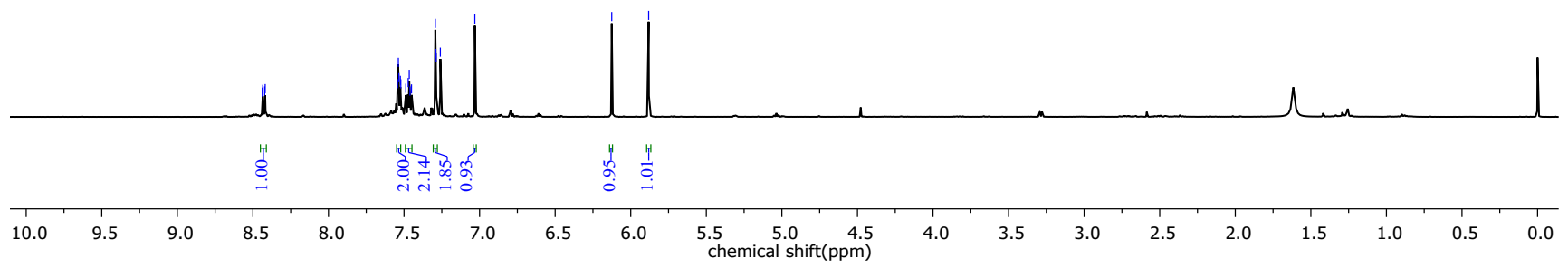
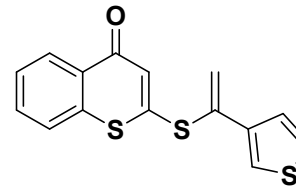
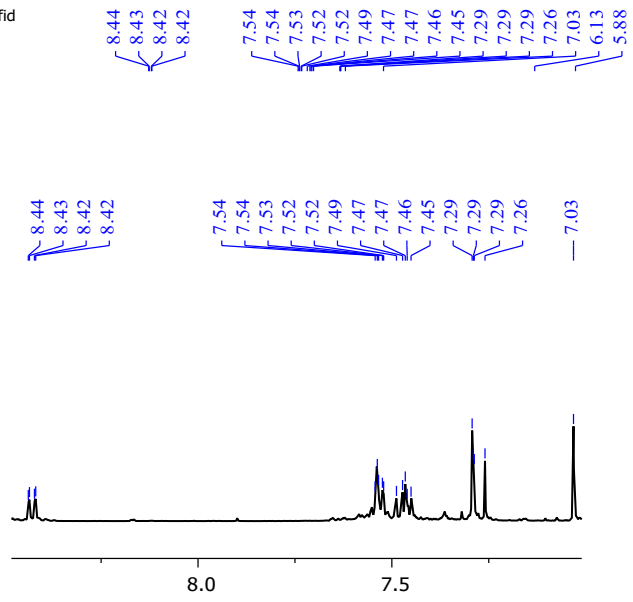
HRMS of compound 3f

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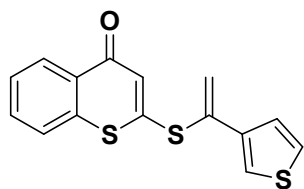


¹H NMR of compound 3g

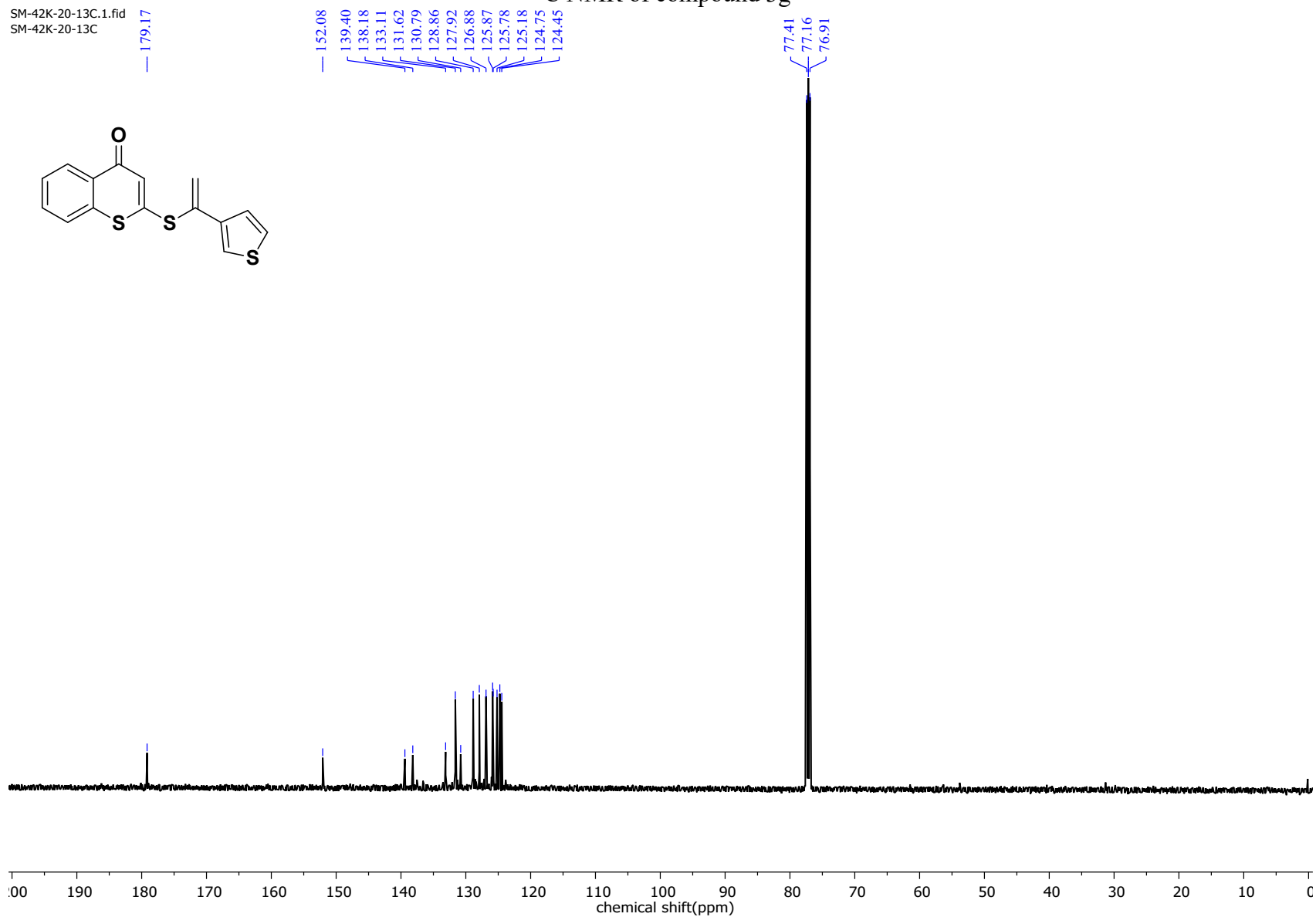
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SM-42K-20-1H



SM-42K-20-13C.1.fid
SM-42K-20-13C

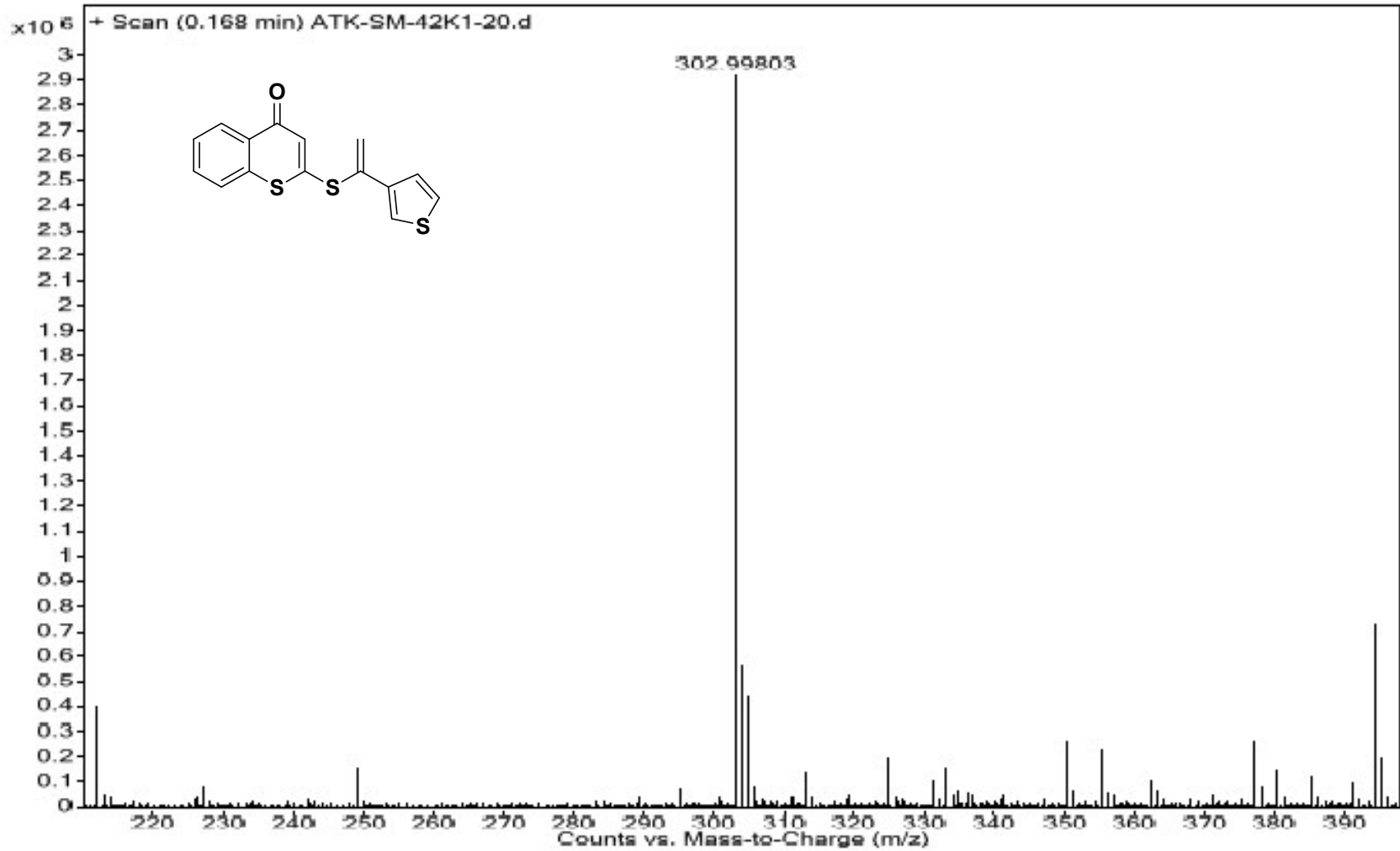


¹³C NMR of compound 3g

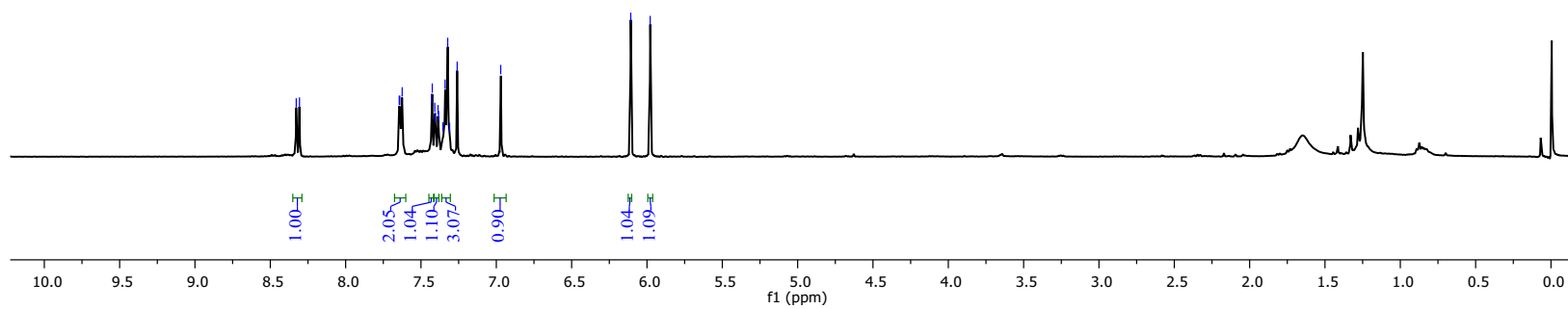
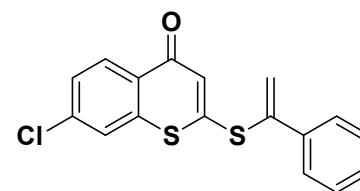
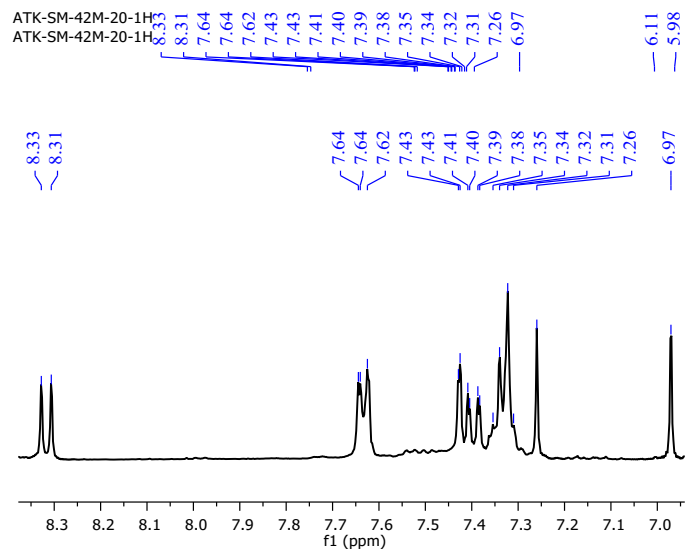


HRMS of compound 3g

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¹H NMR of compound 3h



¹³C NMR of compound 3h

ATK-SM-42M-20-13C
ATK-SM-42M-20-13C

178.28

151.77

139.47

138.85

138.32

137.17

130.34

129.46

129.04

128.86

128.51

127.23

125.84

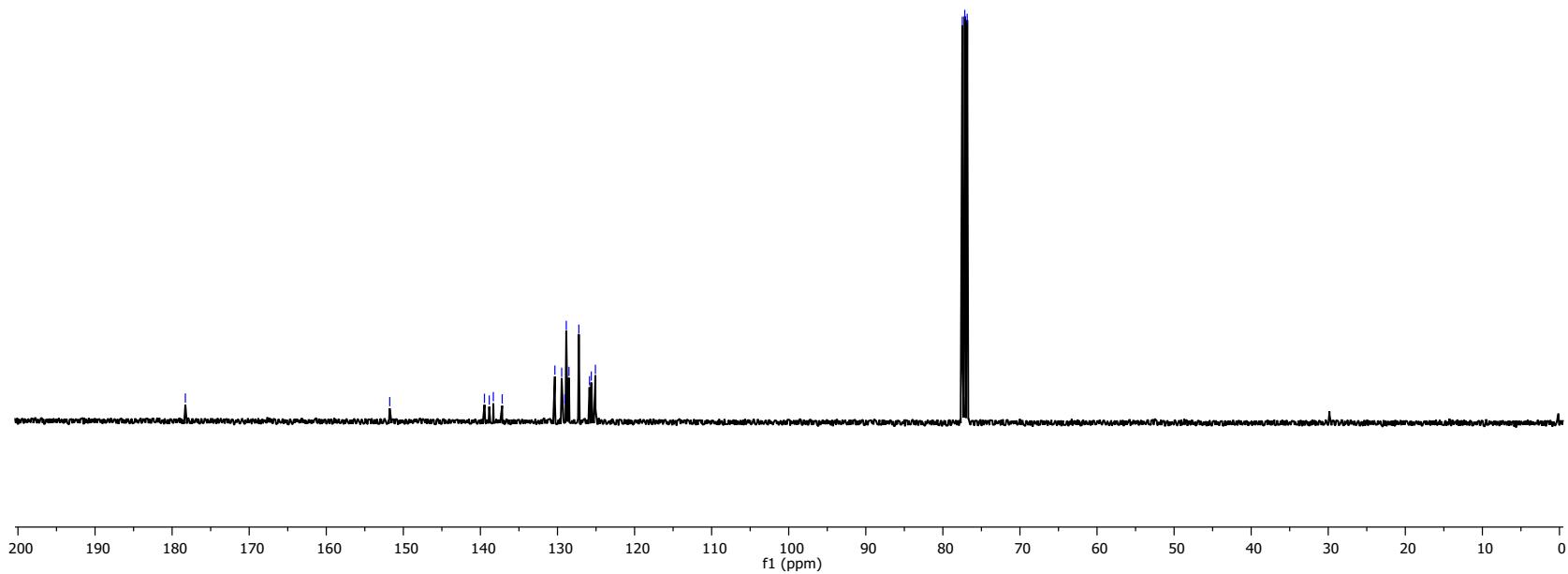
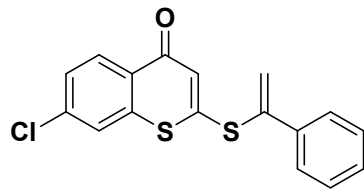
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125.08

77.48

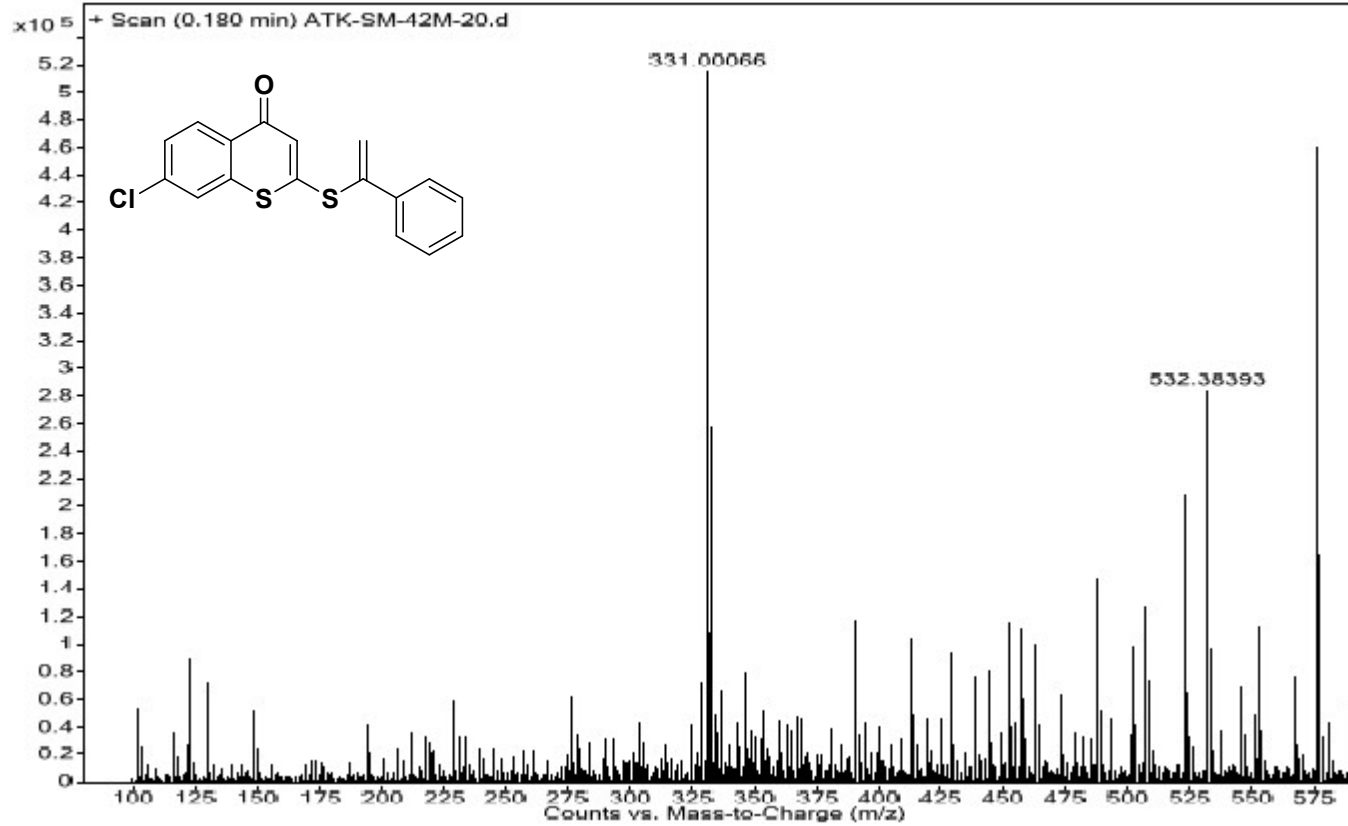
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76.84



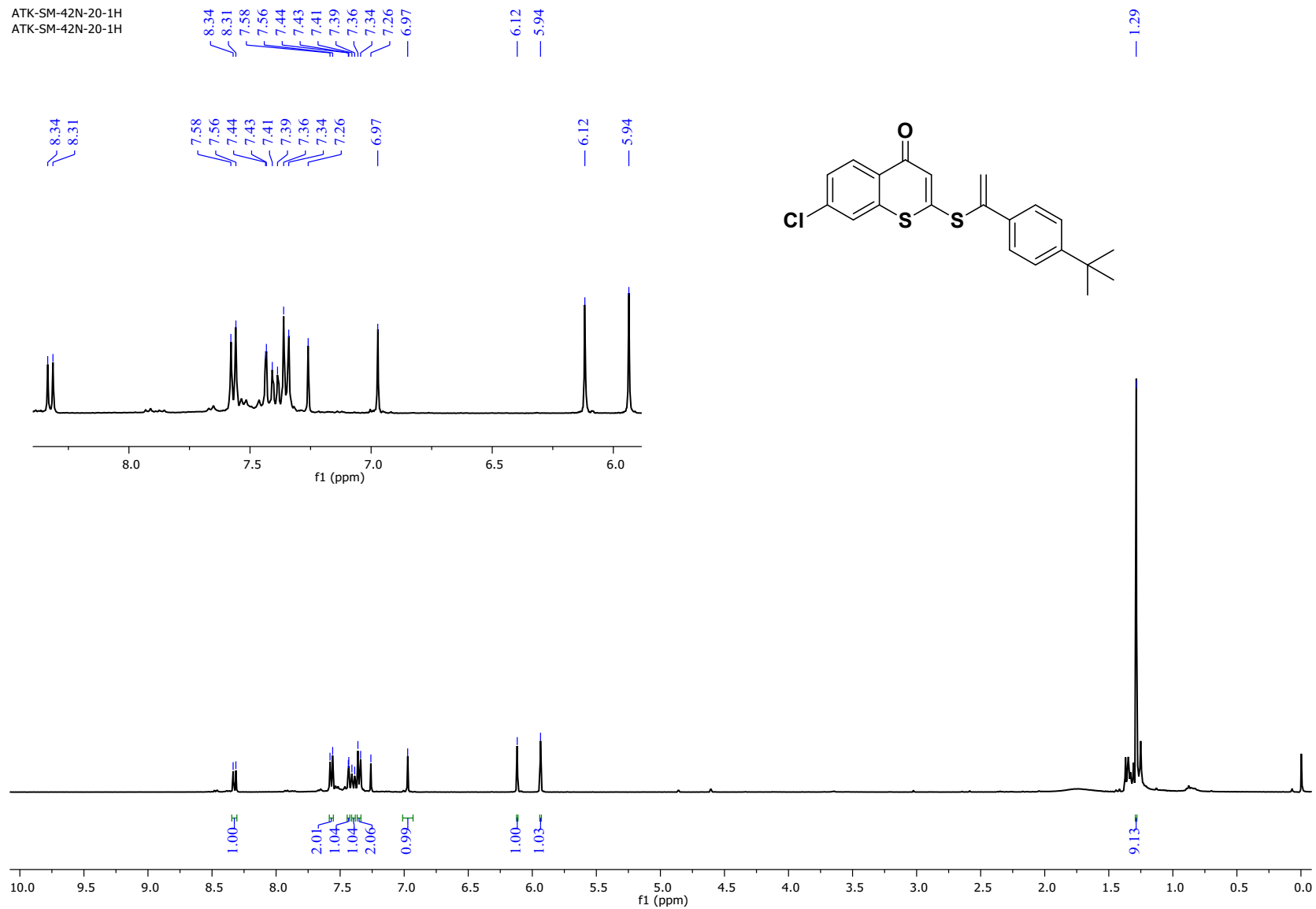
HRMS of compound 3h

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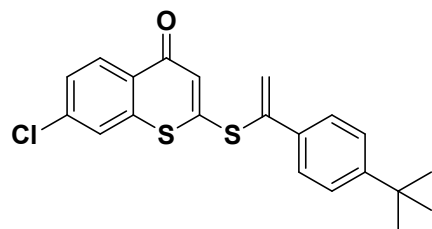
¹H NMR of compound 3i

ATK-SM-42N-20-1H
ATK-SM-42N-20-1H



¹³C NMR of compound 3i

ATK-SM-42N-20-13C
ATK-SM-42N-20-13C



178.29

152.72

152.36

139.53

138.31

138.27

134.19

130.32

129.07

128.46

126.82

125.84

125.52

125.14

125.08

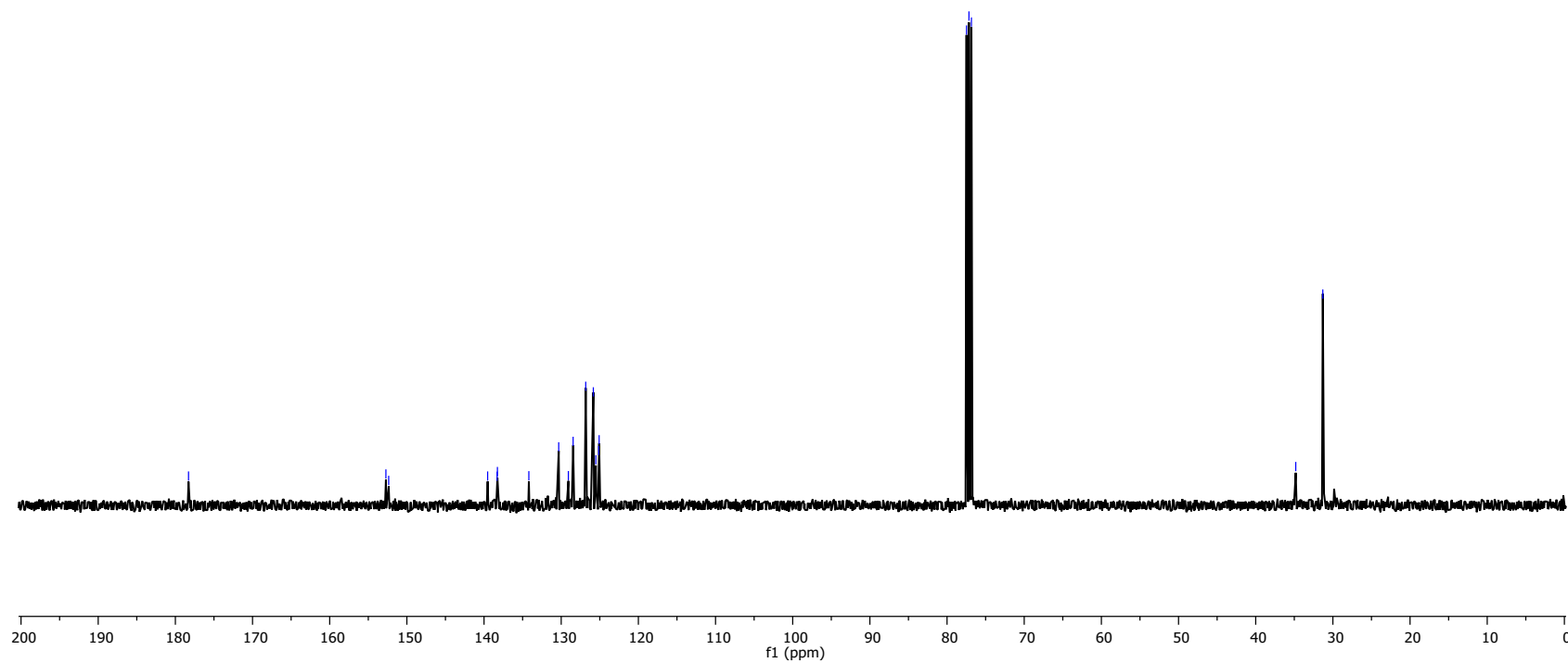
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77.16

76.84

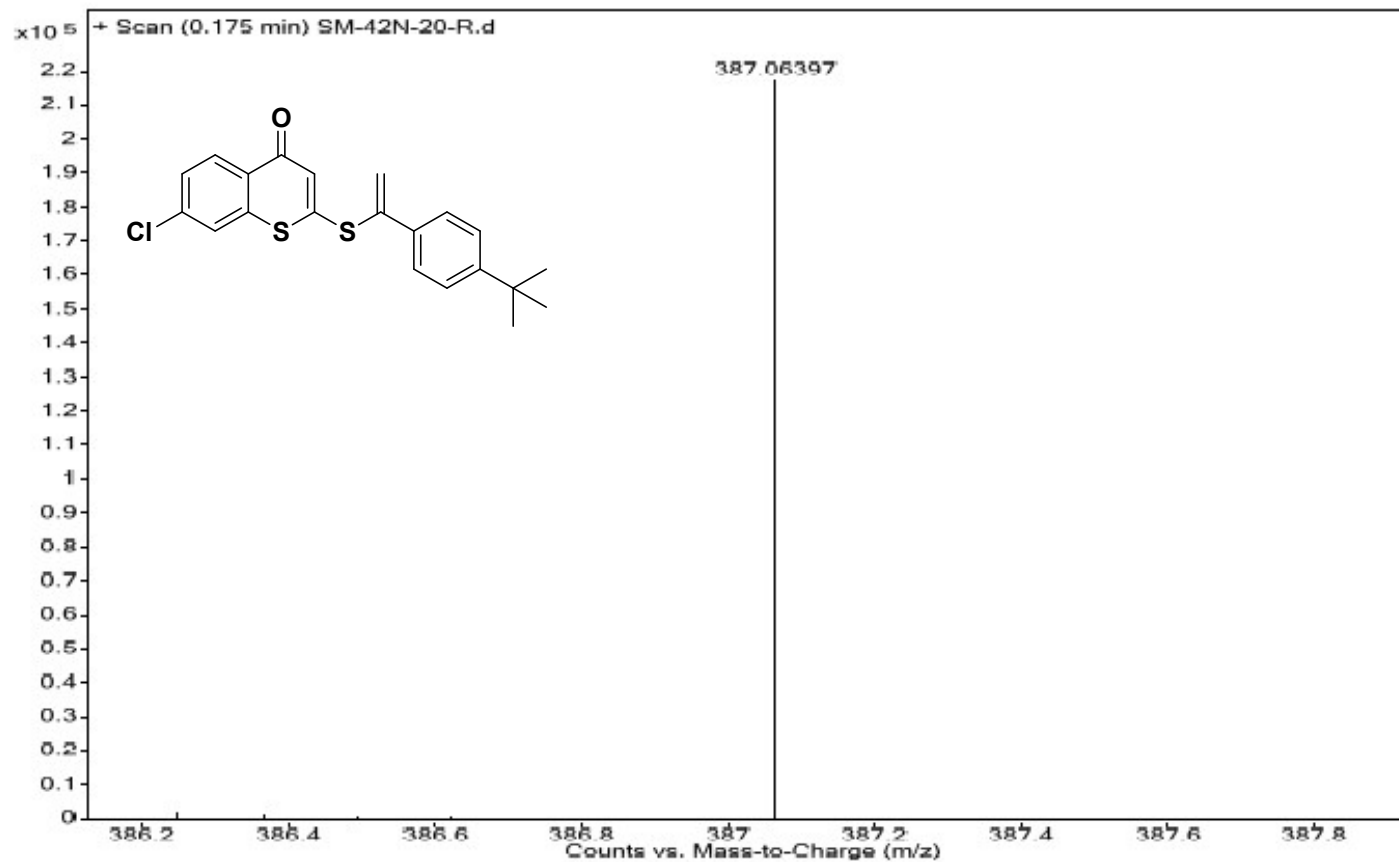
34.81

31.31



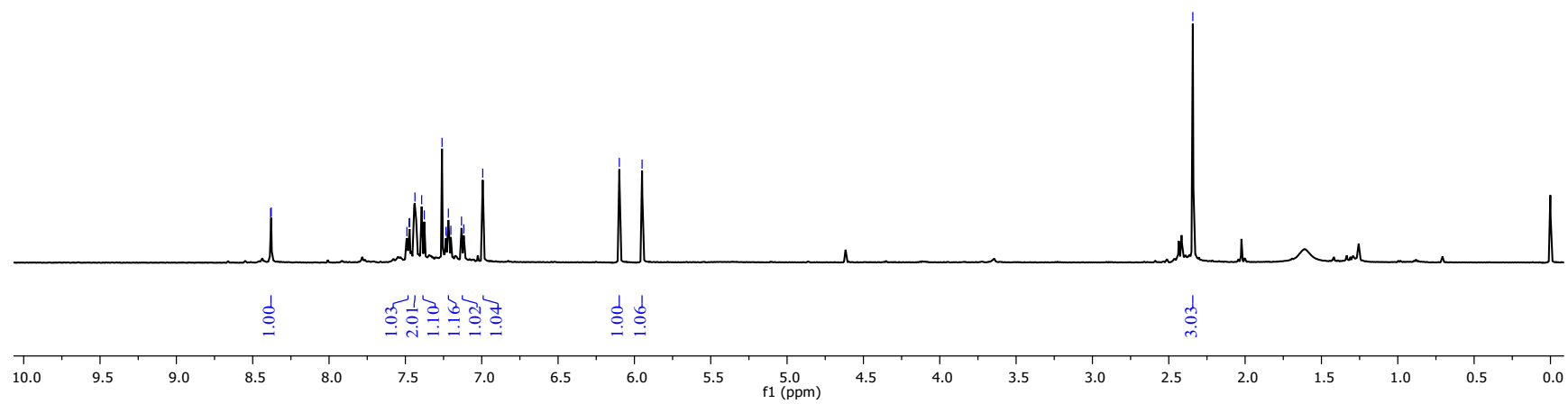
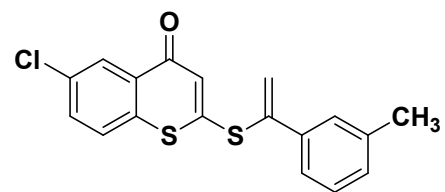
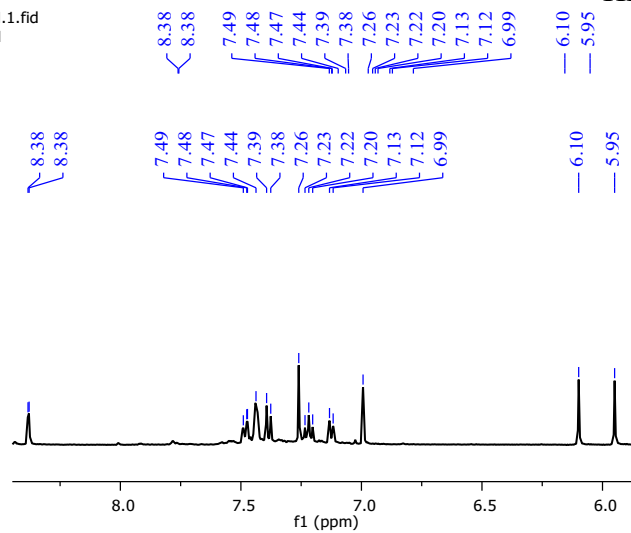
HRMS of compound 3i

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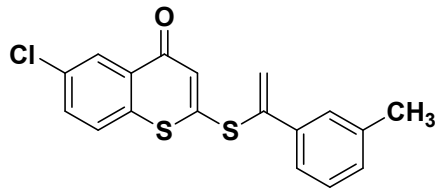
¹HNMR of compound 3j

SM-420-20-1H.1.fid
SM-420-20-1H



¹³C NMR of compound 3j

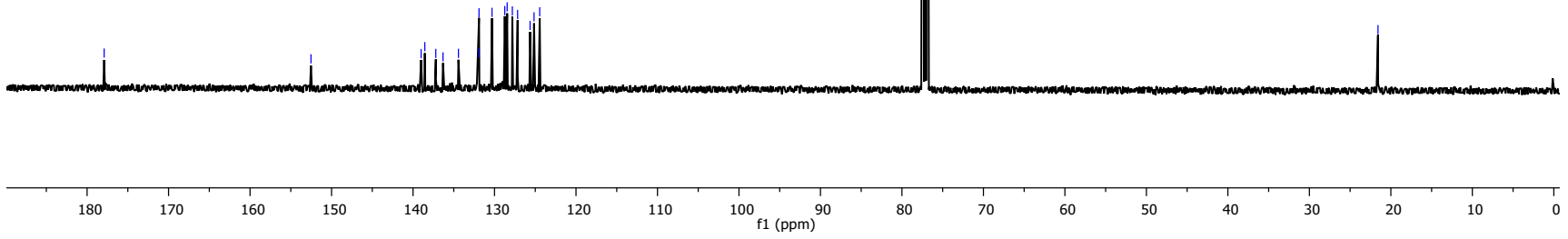
SM-420-20-13C.1.fid
SM-420-20-13C



152.52
139.01
138.55
137.20
136.32
134.43
131.96
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128.74
128.45
127.81
127.17
125.63
125.15
124.45

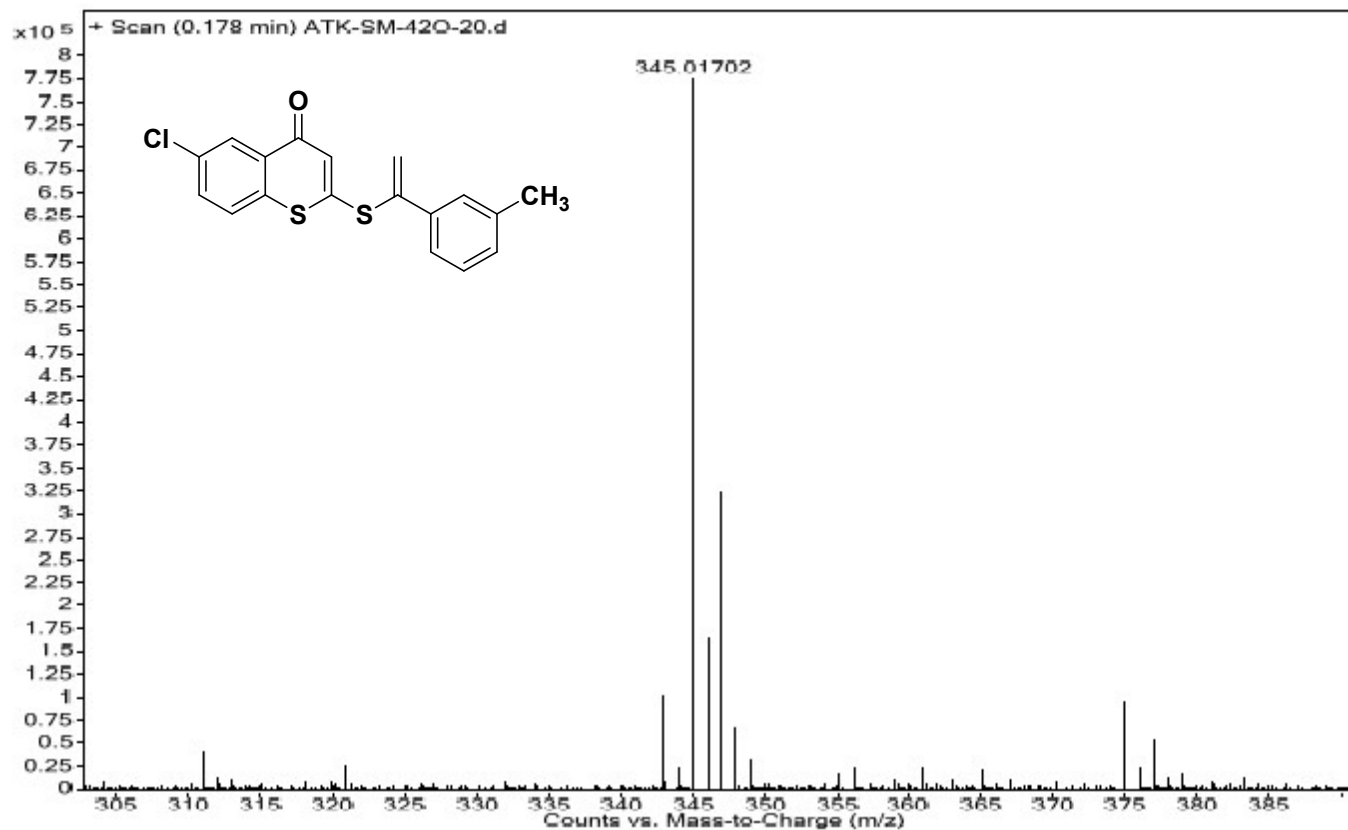
77.41
77.16
76.91

21.58



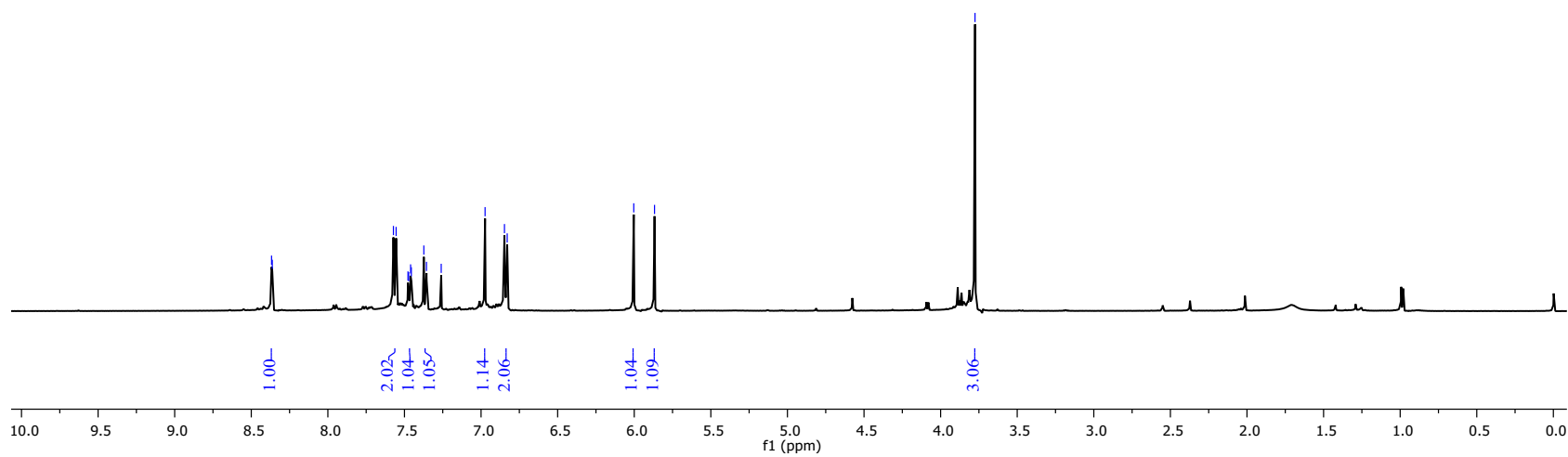
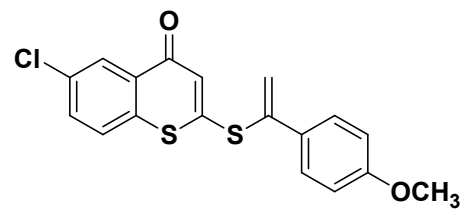
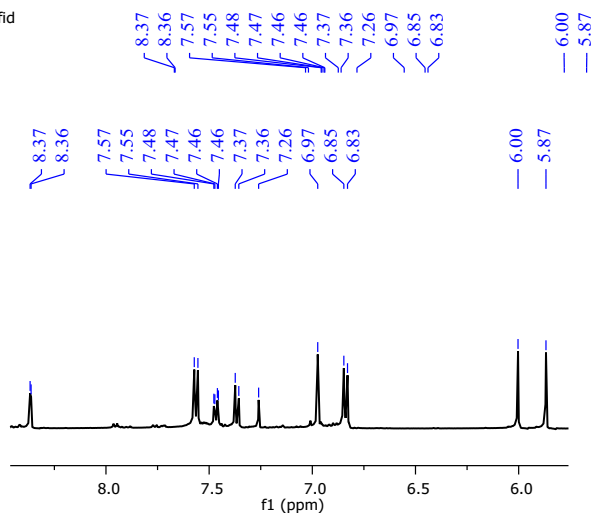
HRMS of compound 3j

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¹H NMR of compound 3k

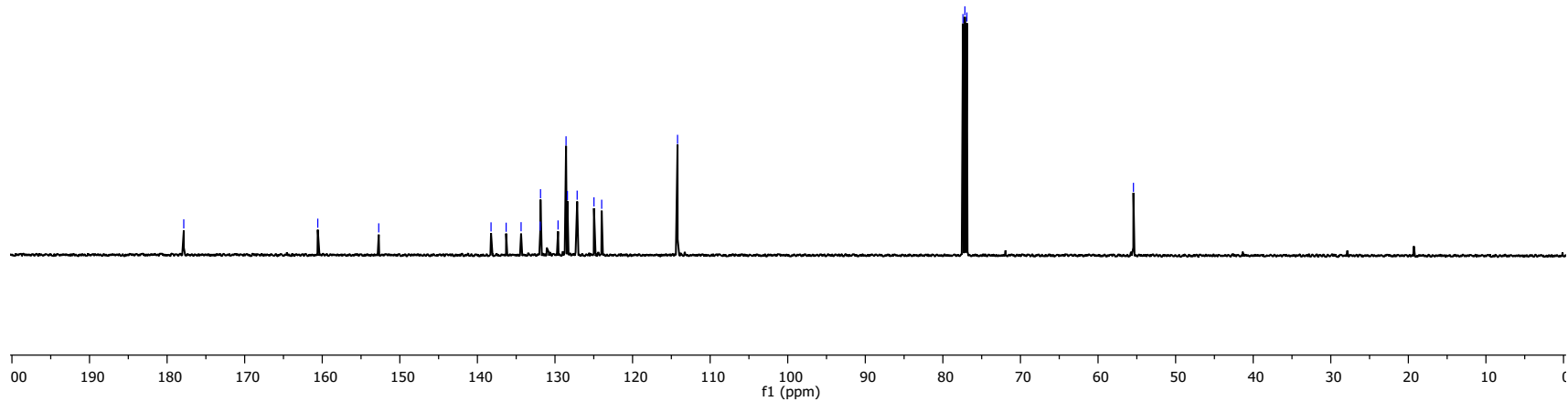
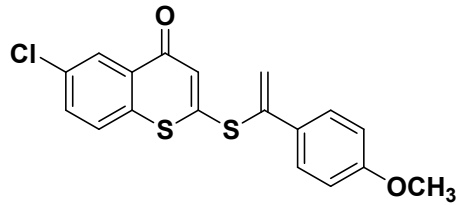
SM-42Q-1H.4.fid
SM-42Q-1H



¹³C NMR of compound 3k

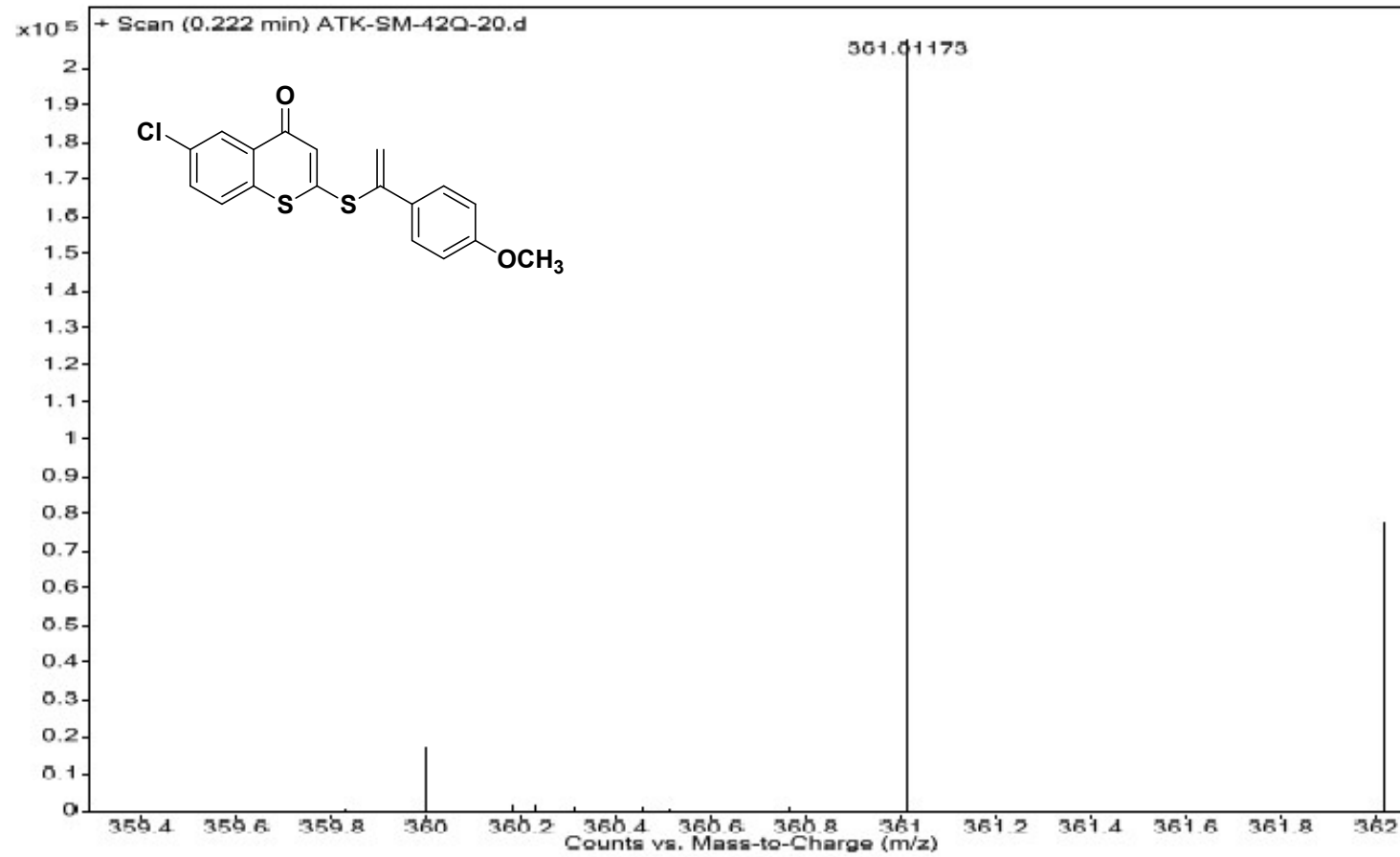
SM-42Q-20-1H.1.fid
SM-42Q-20-1H

- 177.85
- 160.58
- 152.72
- 138.24
- 136.30
- 134.37
- 131.90
- 131.86
- 129.60
- 128.57
- 128.40
- 127.14
- 124.97
- 123.98
- 114.20
- 77.41
- 77.16
- 76.91
- 55.44



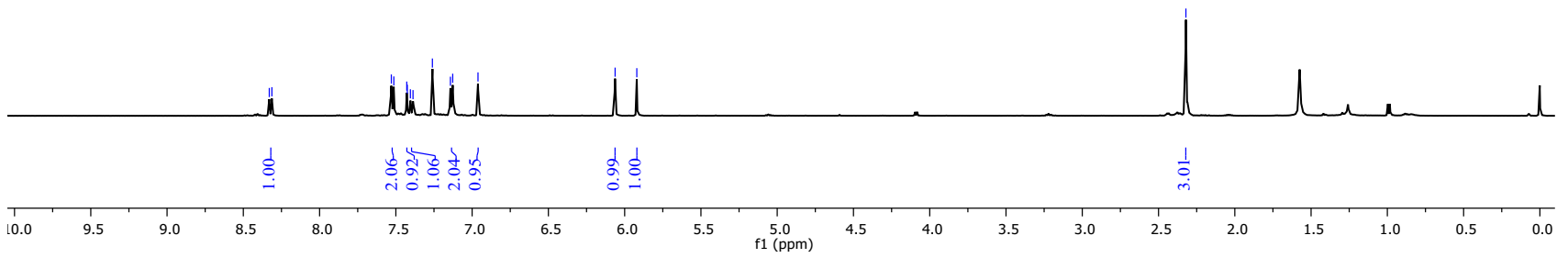
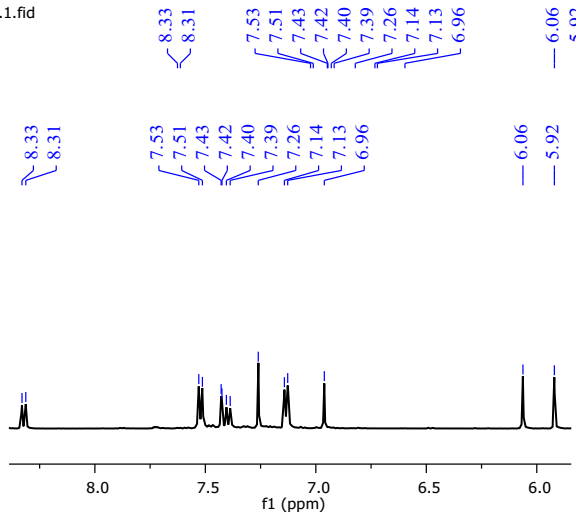
HRMS of compound 3k

Sample Name	SAMPLE 2	Position	P1-B6	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SM-42Q-20.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/4/2021 11:07:06 AM



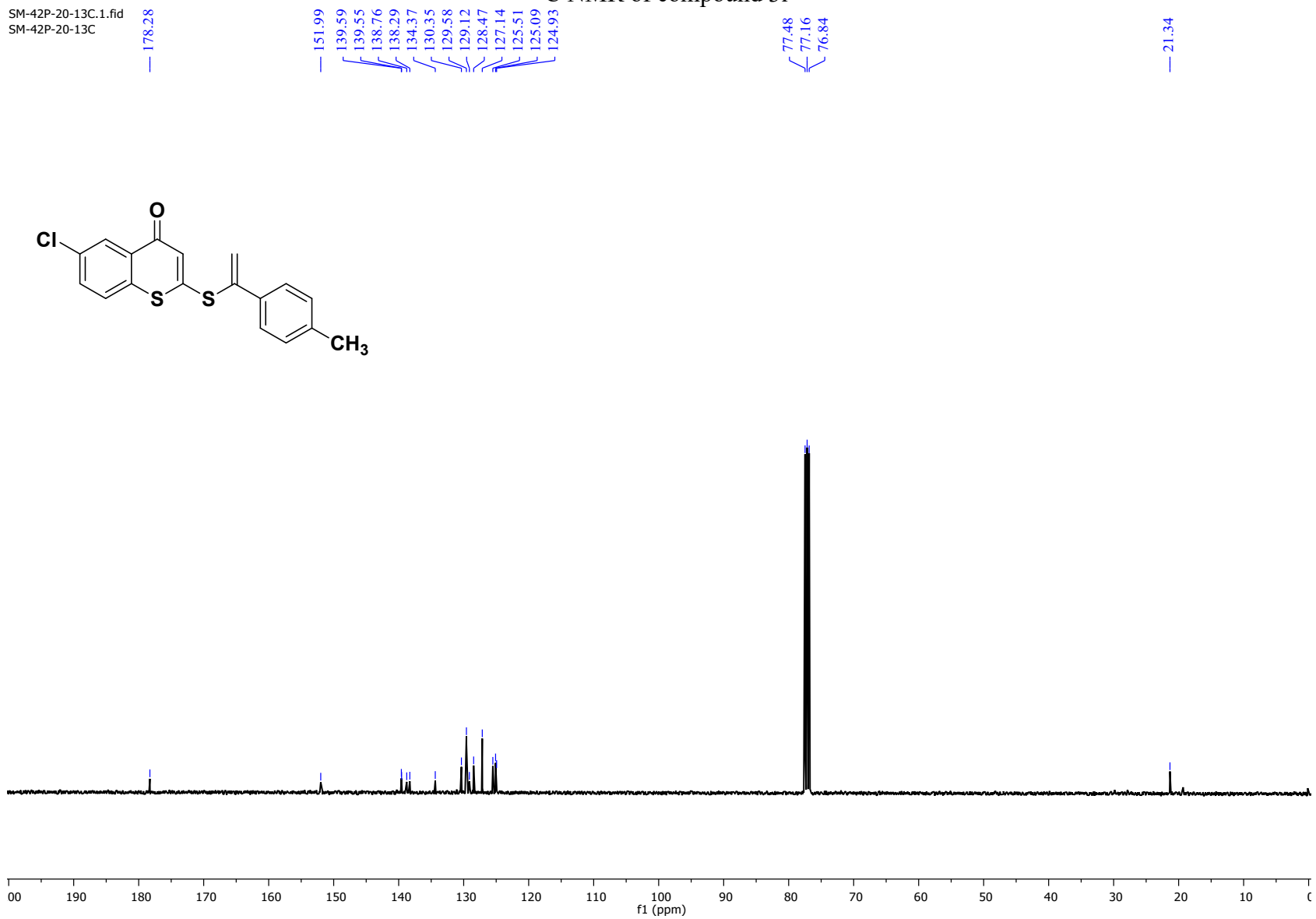
SM-42P-20-1H.1.fid
SM-42P-20-1H

¹H NMR of compound 31



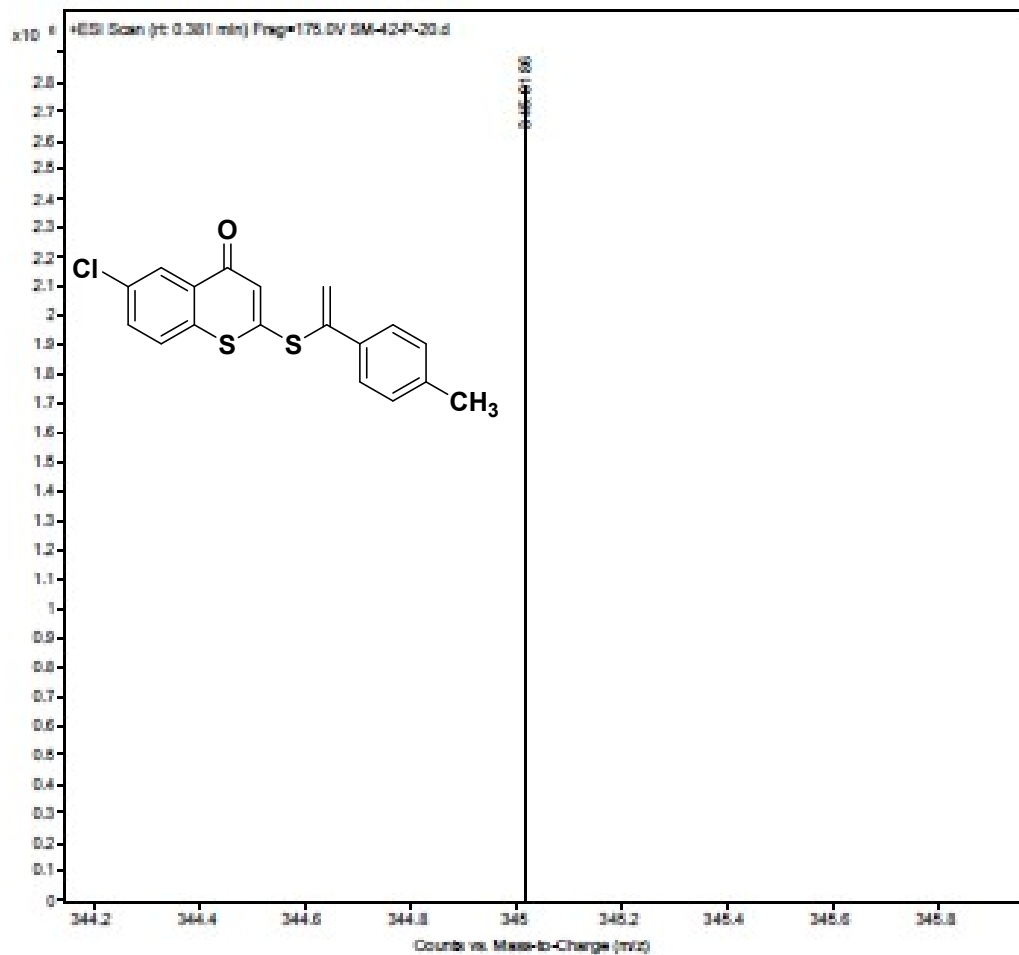
SM-42P-20-13C.1.fid
SM-42P-20-13C

¹³C NMR of compound 31



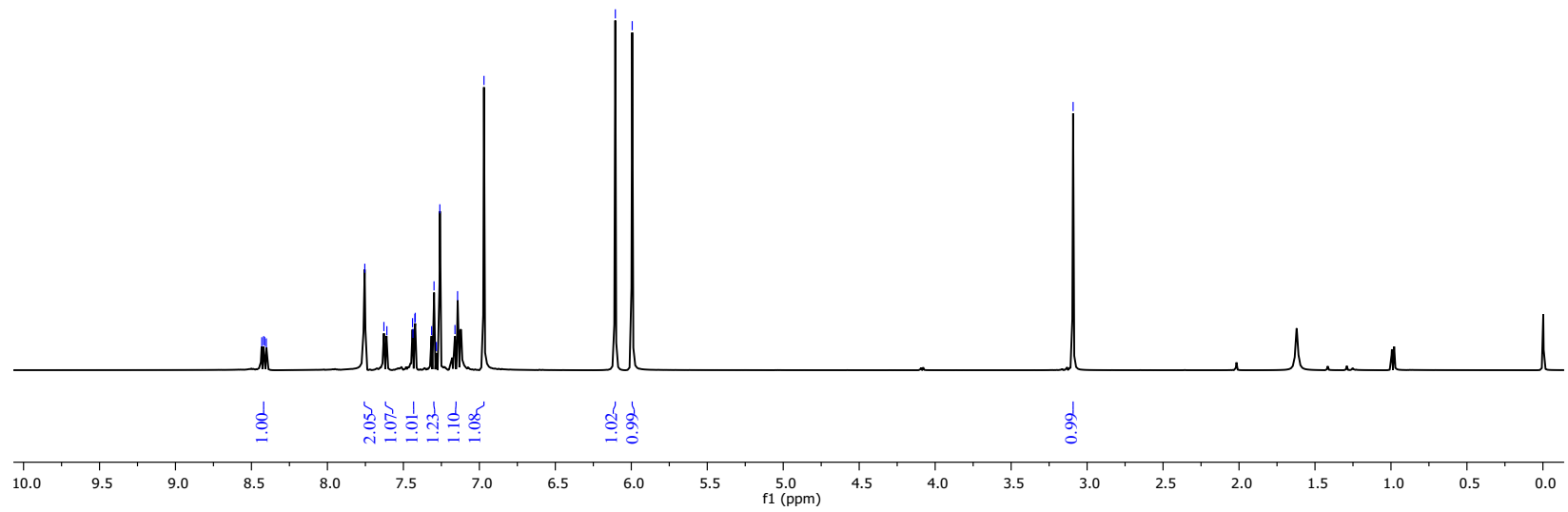
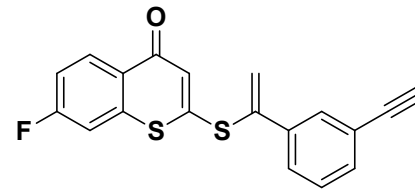
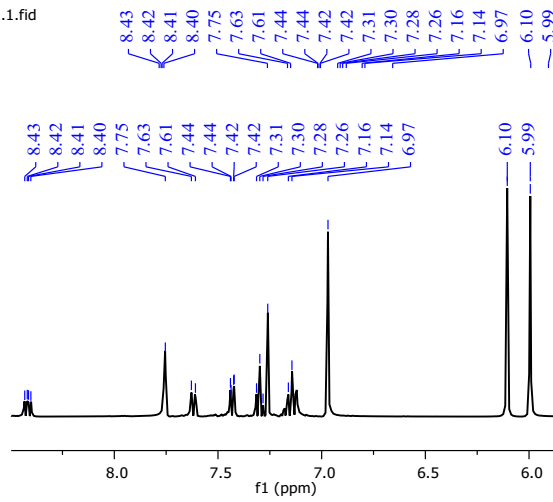
HRMS of compound 31

Sample Name	SM-42-P-20	Position	P1-C5	Instrument Name	Instrument 1
User Name		Inj Vol	20	Inj Position	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SM-42-P-20.d
ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	17-Feb-21 03:18:06 PM (UTC+05:30)



¹H NMR of compound 3m

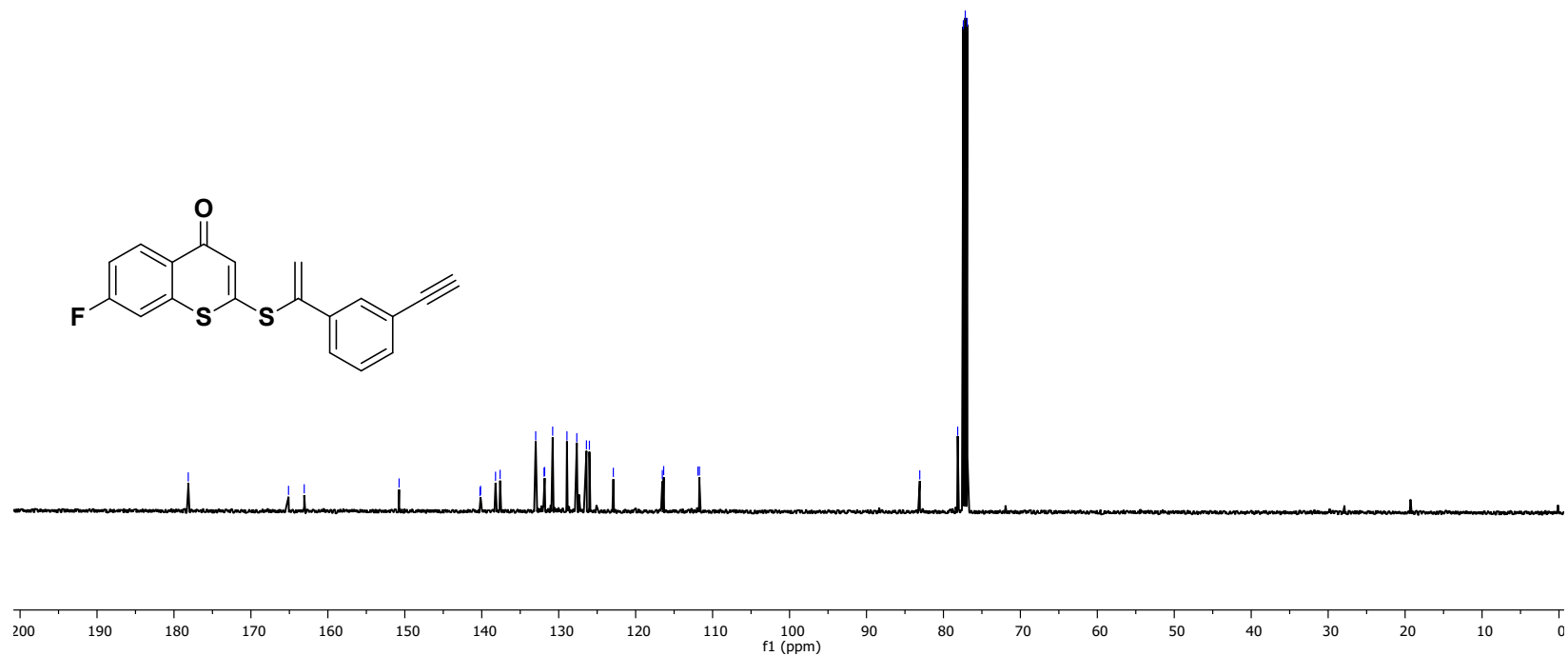
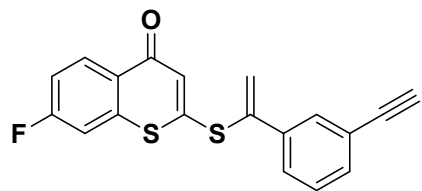
SM-42S-20-1H.1.fid
SM-42S-20-1H



SM-42S-20-13C.1.fid
SM-42S-20-13C

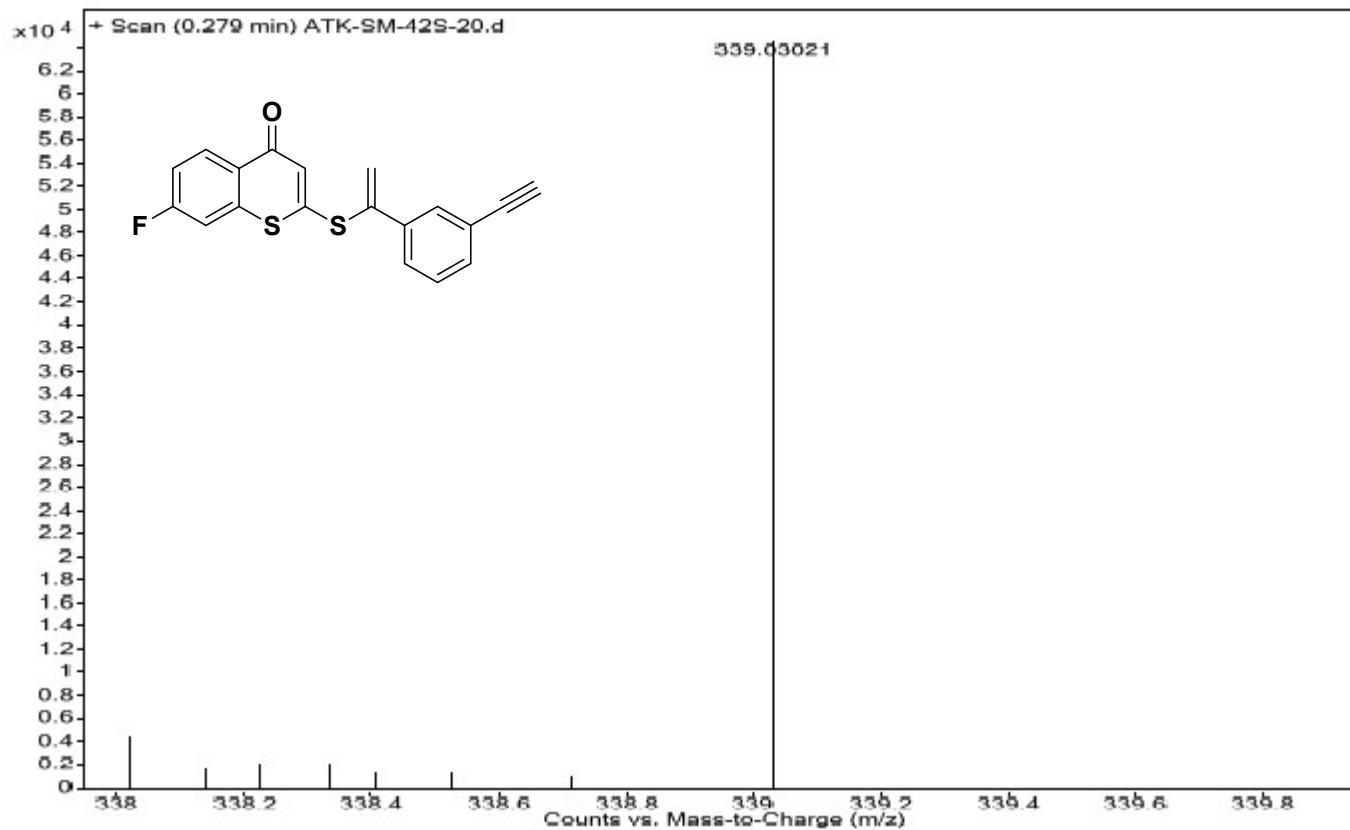
¹³C NMR of compound 3m

178.14
165.11
163.07
150.74
140.23
140.15
138.21
137.61
132.99
131.90
131.82
130.78
128.93
127.65
126.39
126.01
122.90
116.53
116.36
111.91
111.71
83.08
78.15
77.41
77.16
76.91



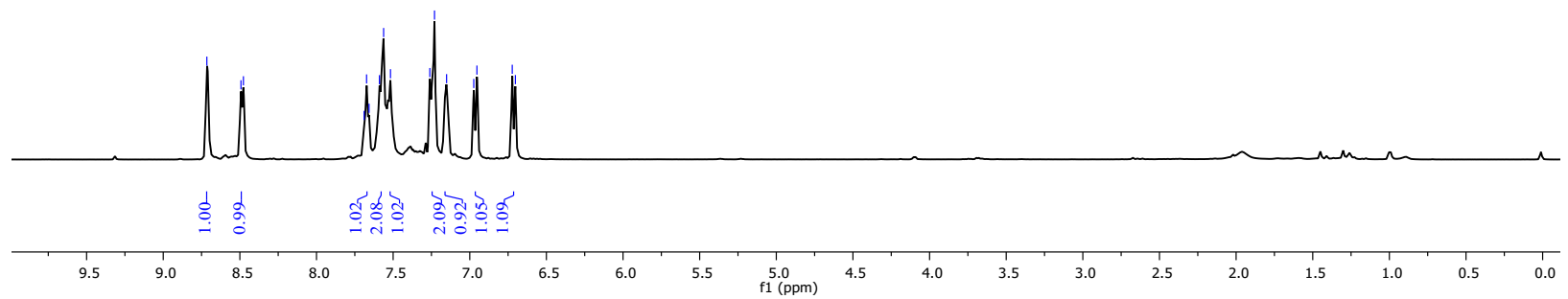
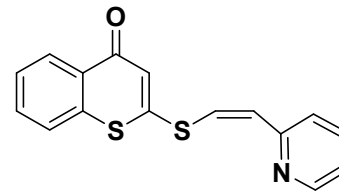
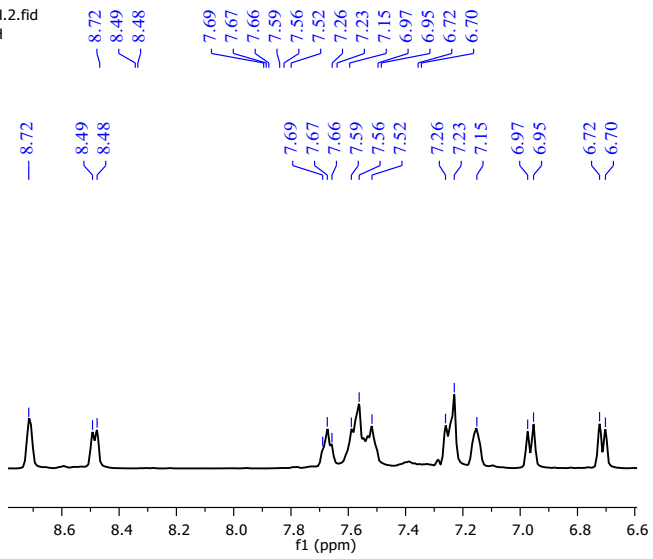
HRMS of compound 3m

Sample Name	SAMPLE 14	Position	P2-B5	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SM-42S-20.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/1/2021 7:18:05 PM



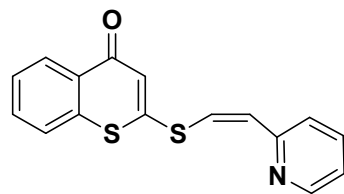
¹H NMR of compound 5a

SM-42LI-20-1H.2.fid
SM-42LI-20-1H



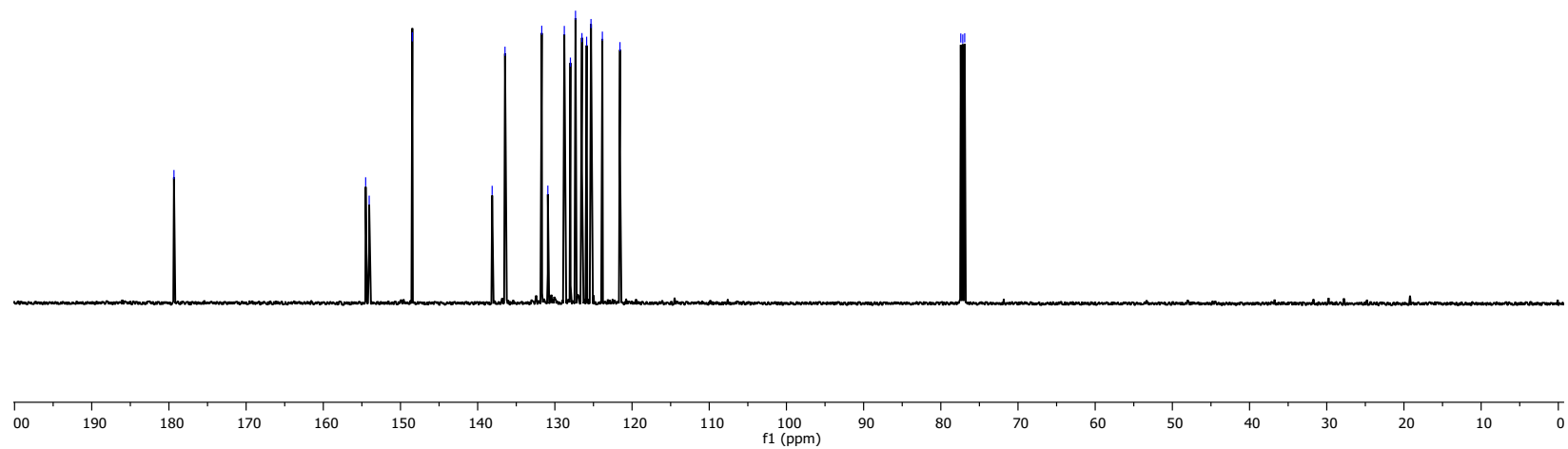
¹³C NMR of compound 5a

SM-42-LI-20-13C.1.fid
SM-42-LI-20-13C



179.35
154.51
154.06
148.47
138.12
136.46
131.70
130.91
128.78
127.99
127.33
126.49
125.88
125.32
123.85
121.56

77.41
77.16
76.91



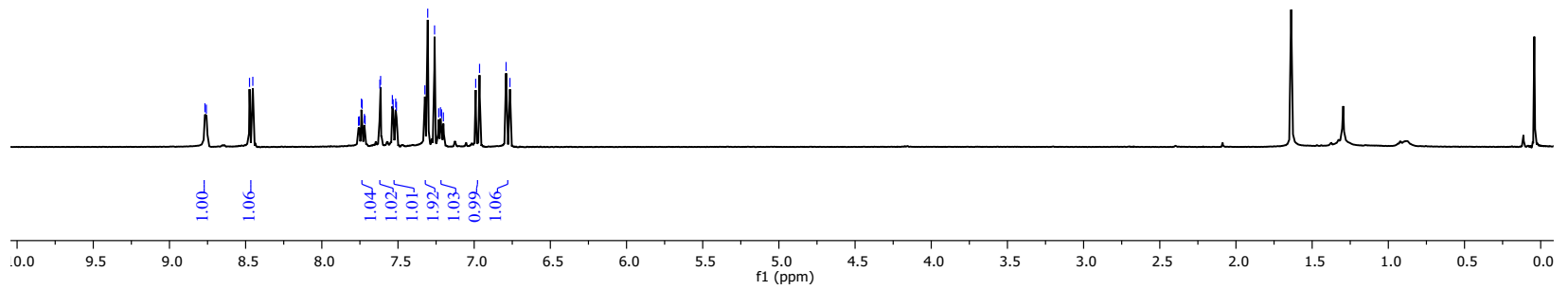
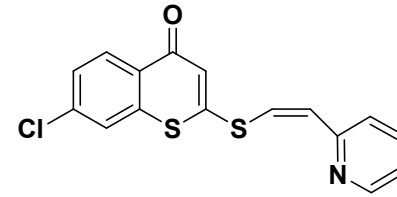
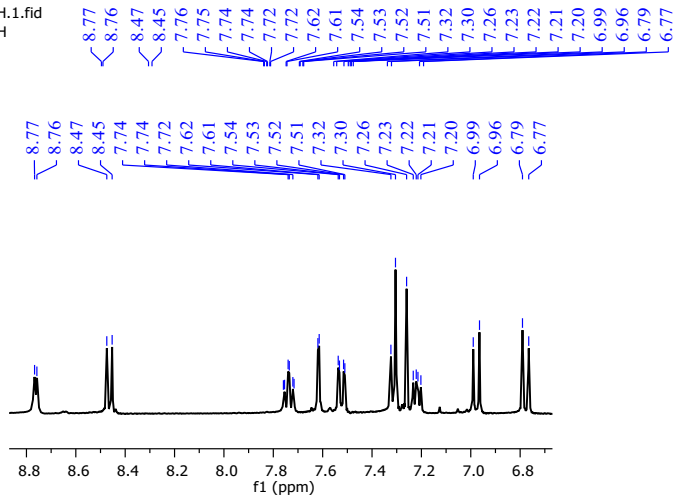
HRMS of compound 5a

Sample Name	SAMPLE 13	Position	P2-B4	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SM-42L1-20.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/1/2021 7:07:00 PM



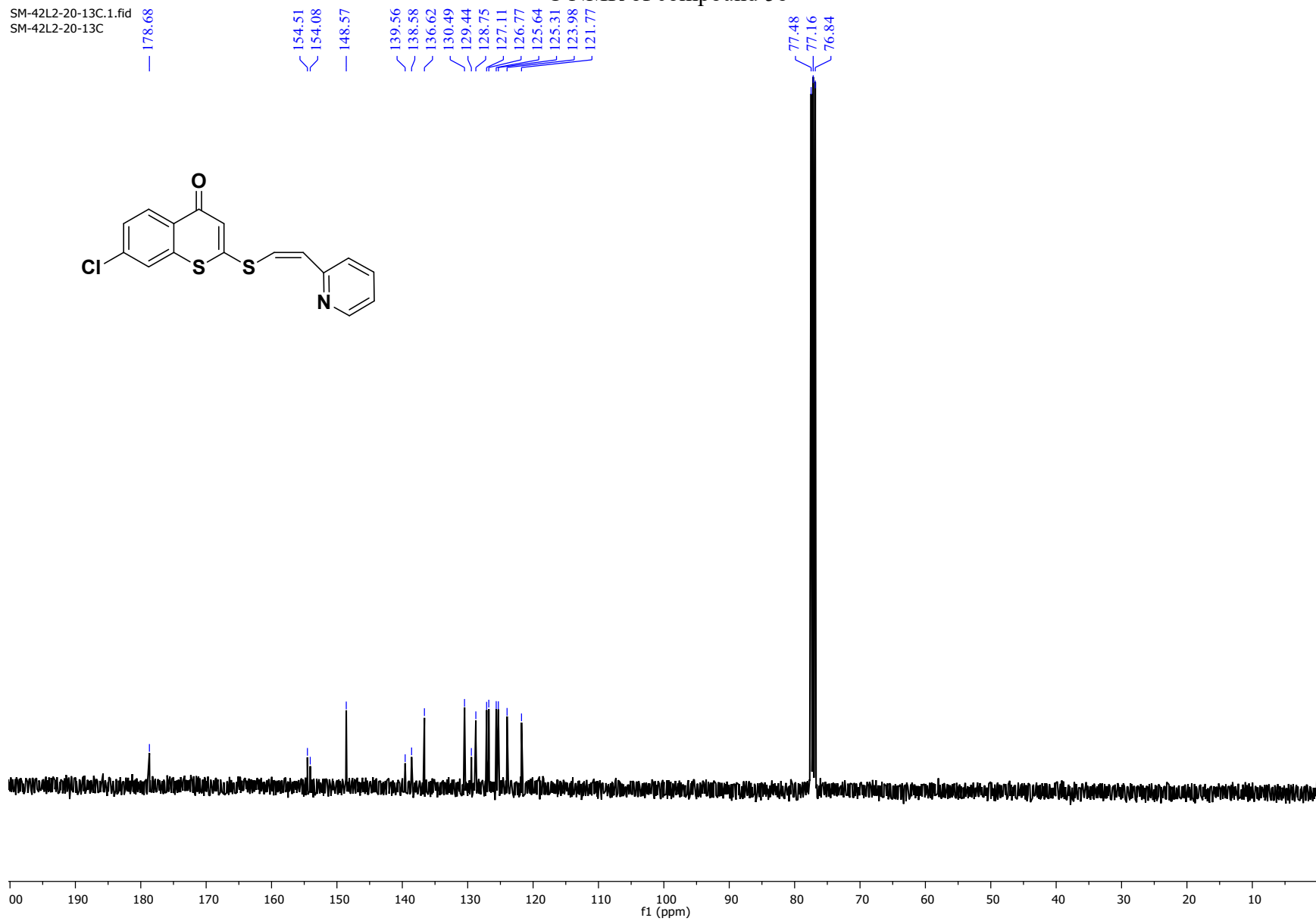
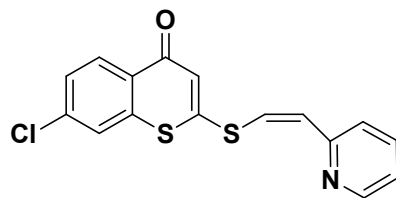
¹H NMR of compound 5b

SM-42L2-20-1H.1.fid
SM-42L2-20-1H



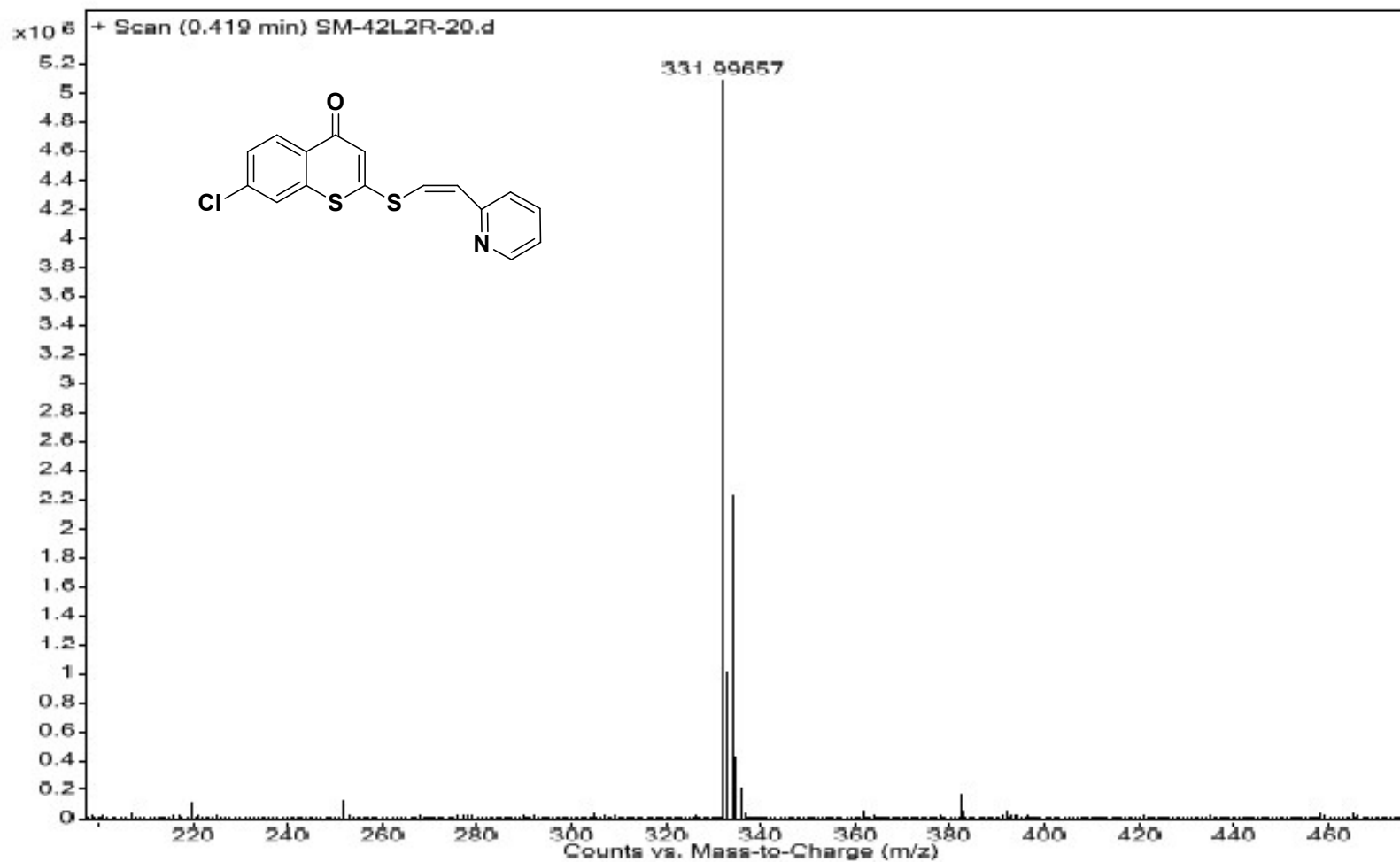
SM-42L2-20-13C.1.fid
SM-42L2-20-13C

¹³C NMR of compound 5b



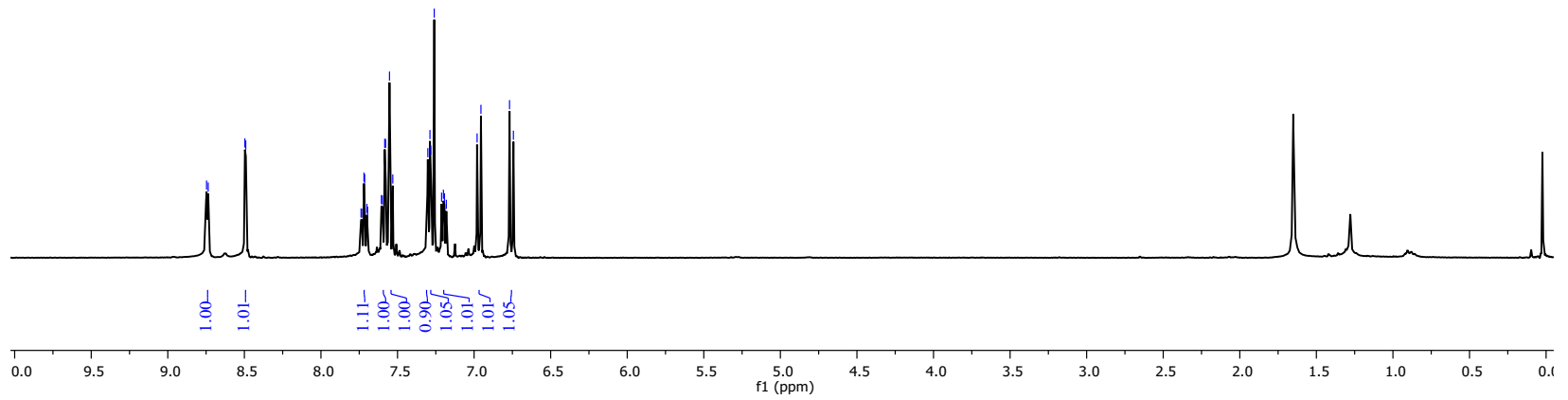
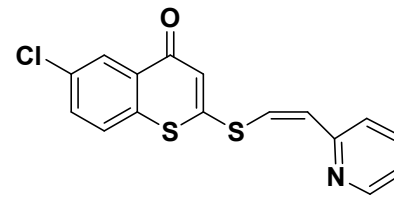
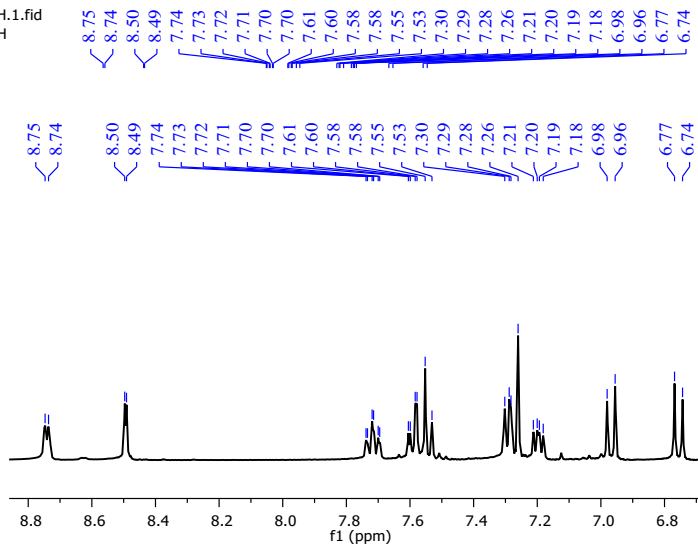
HRMS of compound 5b

Sample Name	SAMPLE	Position	P1-B11	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-42L2R-20.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/25/2021 12:15:35 PM



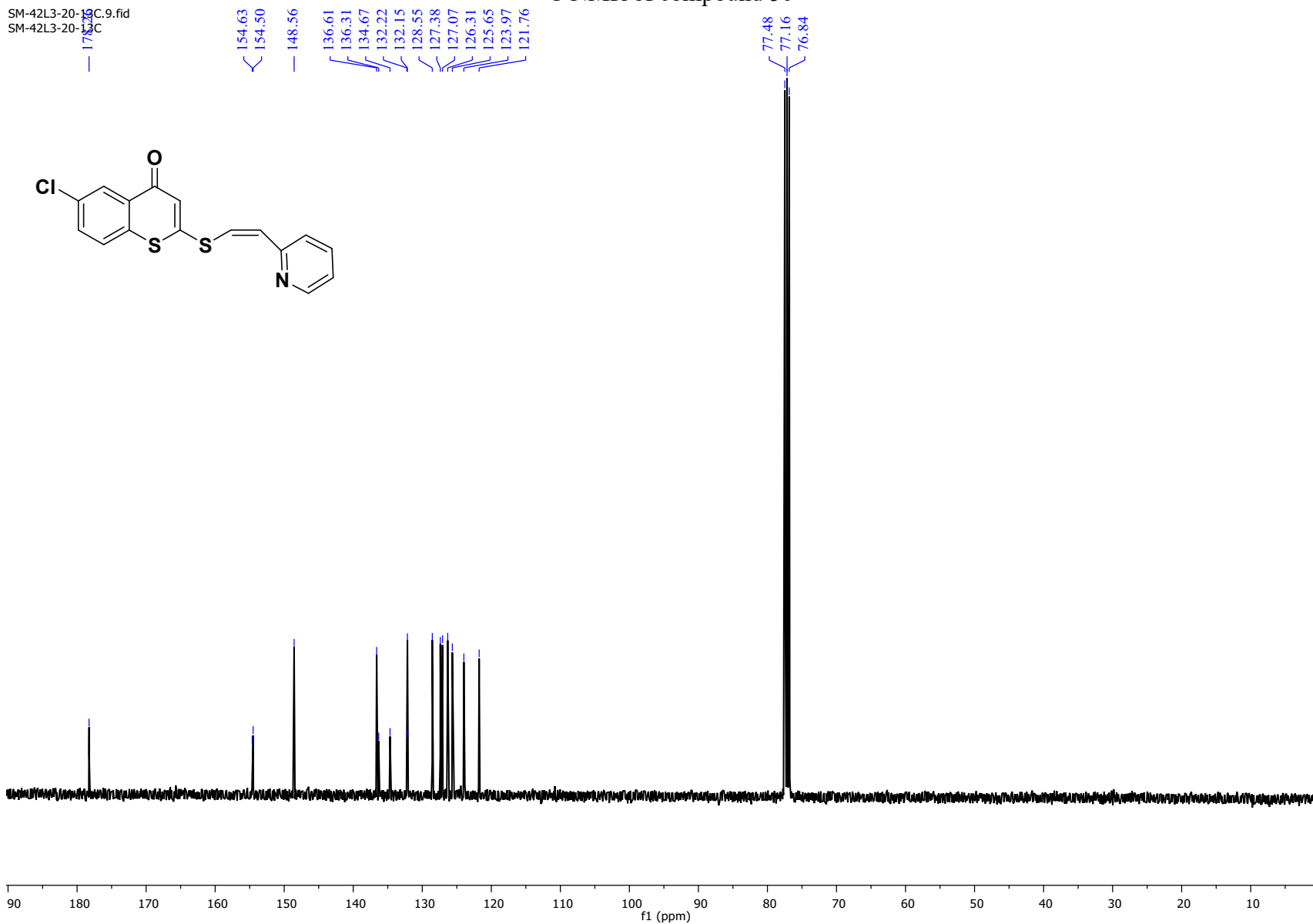
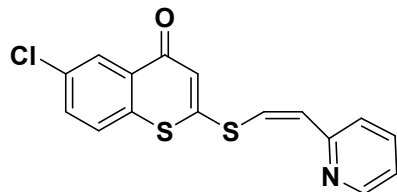
¹H NMR of compound 5c

SM-42L3-20-1H.1.fid
SM-42L3-20-1H



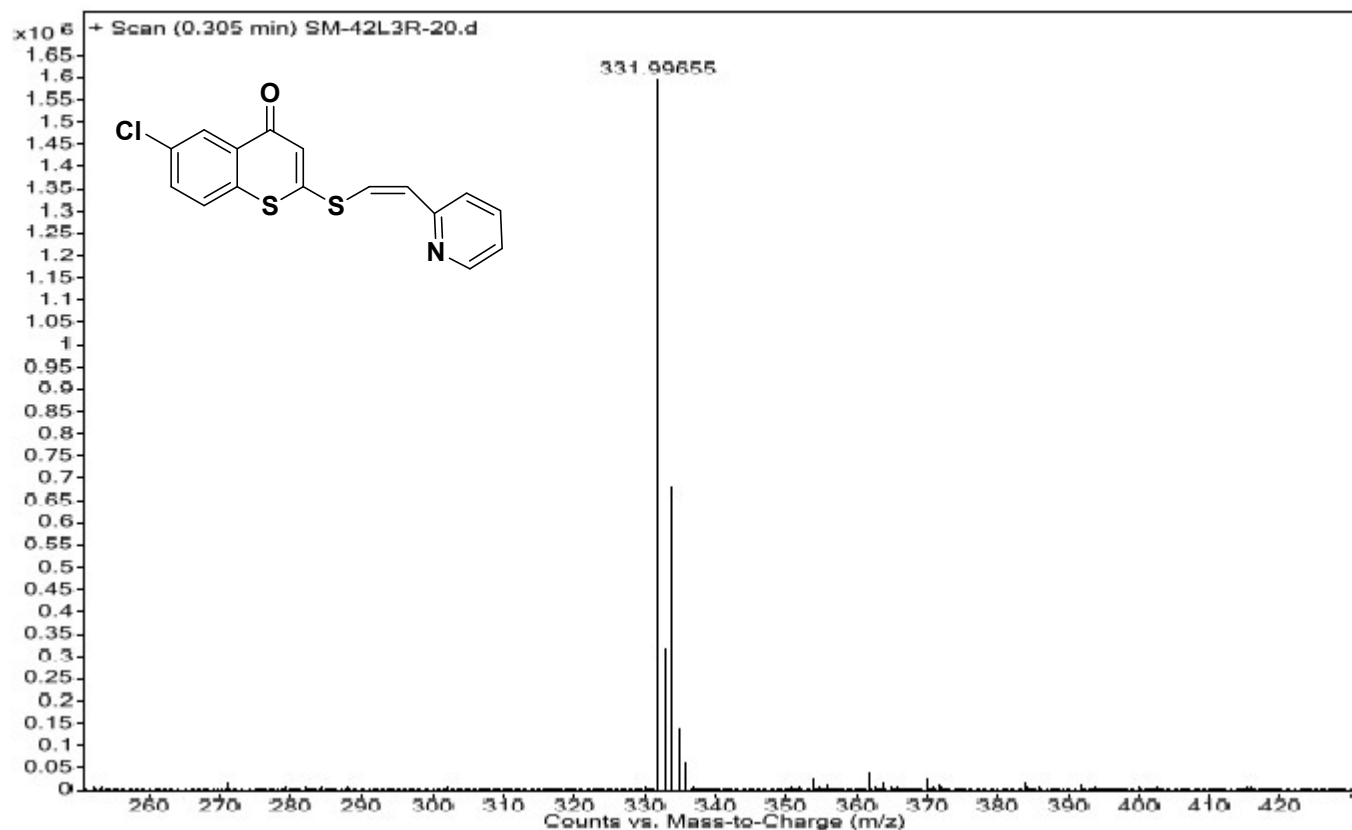
¹³C NMR of compound 5c

SM-42L3-20-13C.9.fid
SM-42L3-20-13C



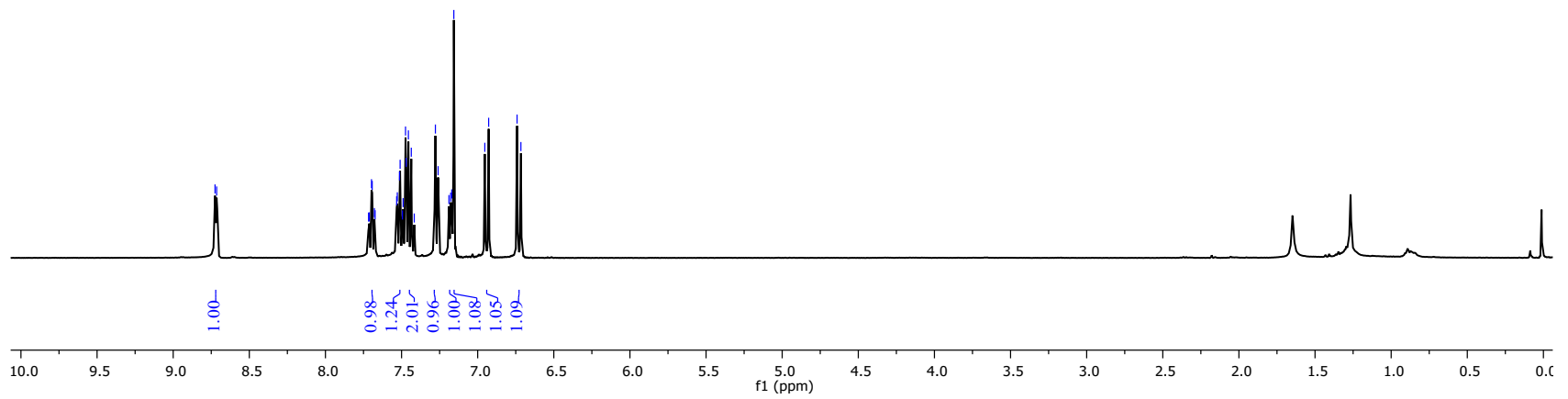
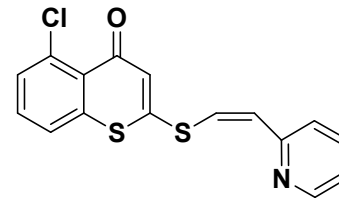
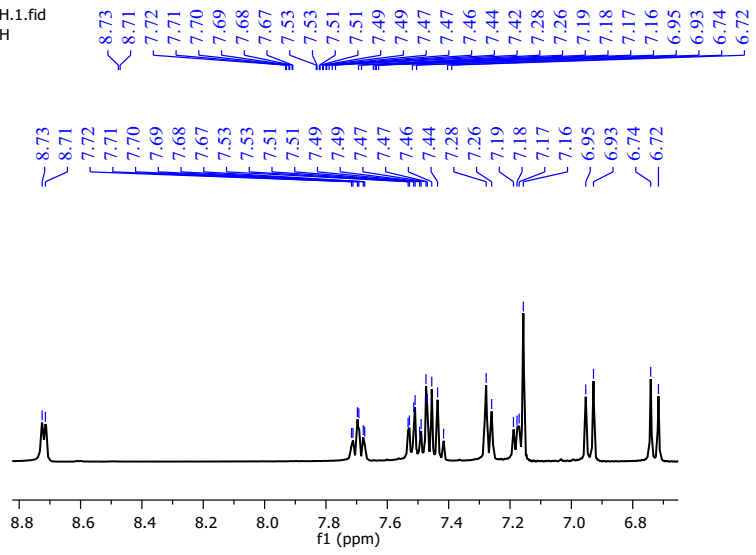
HRMS of compound 5c

Sample Name	SAMPLE	Position	P1-C2	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-42L3R-20.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/25/2021 12:17:30 PM



¹H NMR of compound 5d

SM-42L6-20-1H.1.fid
SM-42L6-20-1H

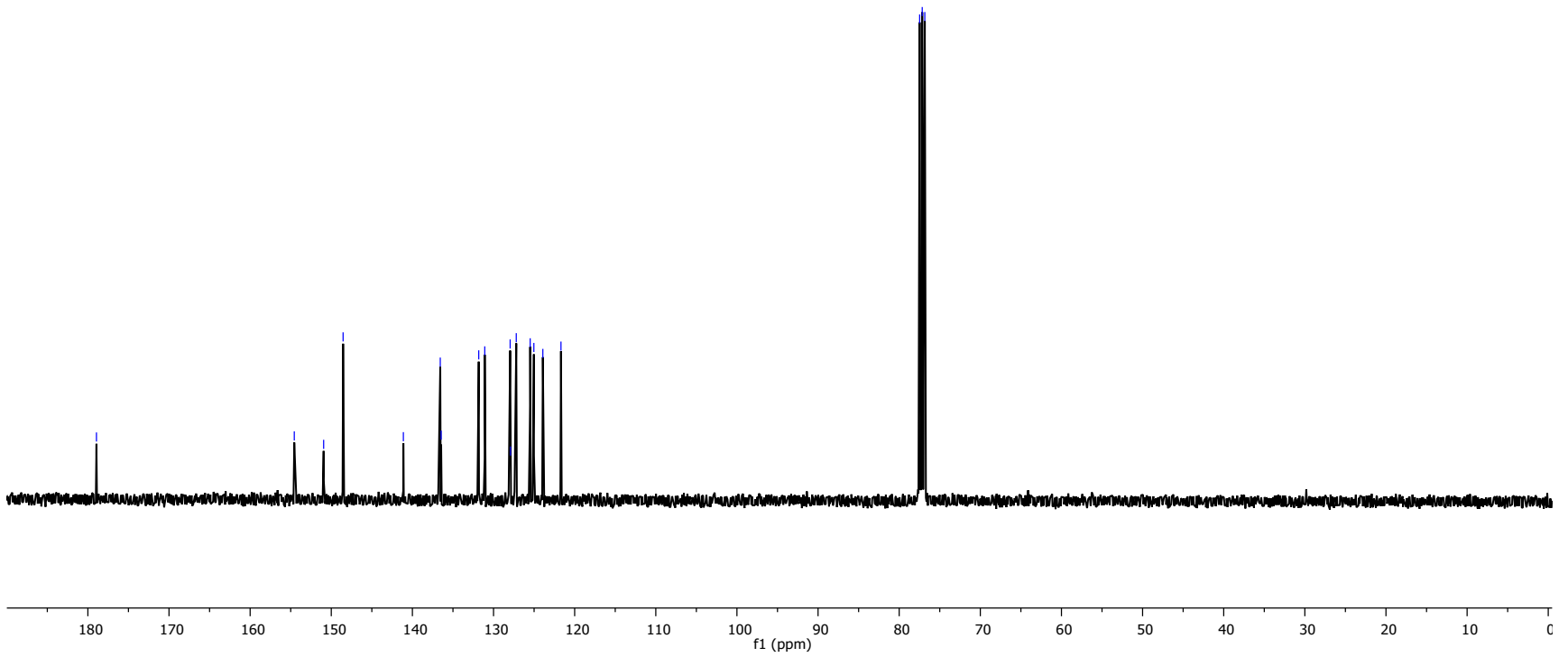
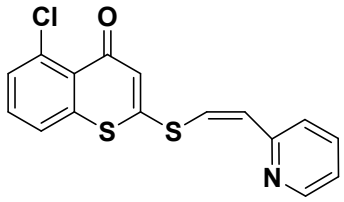


¹³C NMR of compound 5d

SM-42L6-2013C.1.fid
SM-42L6-2013C

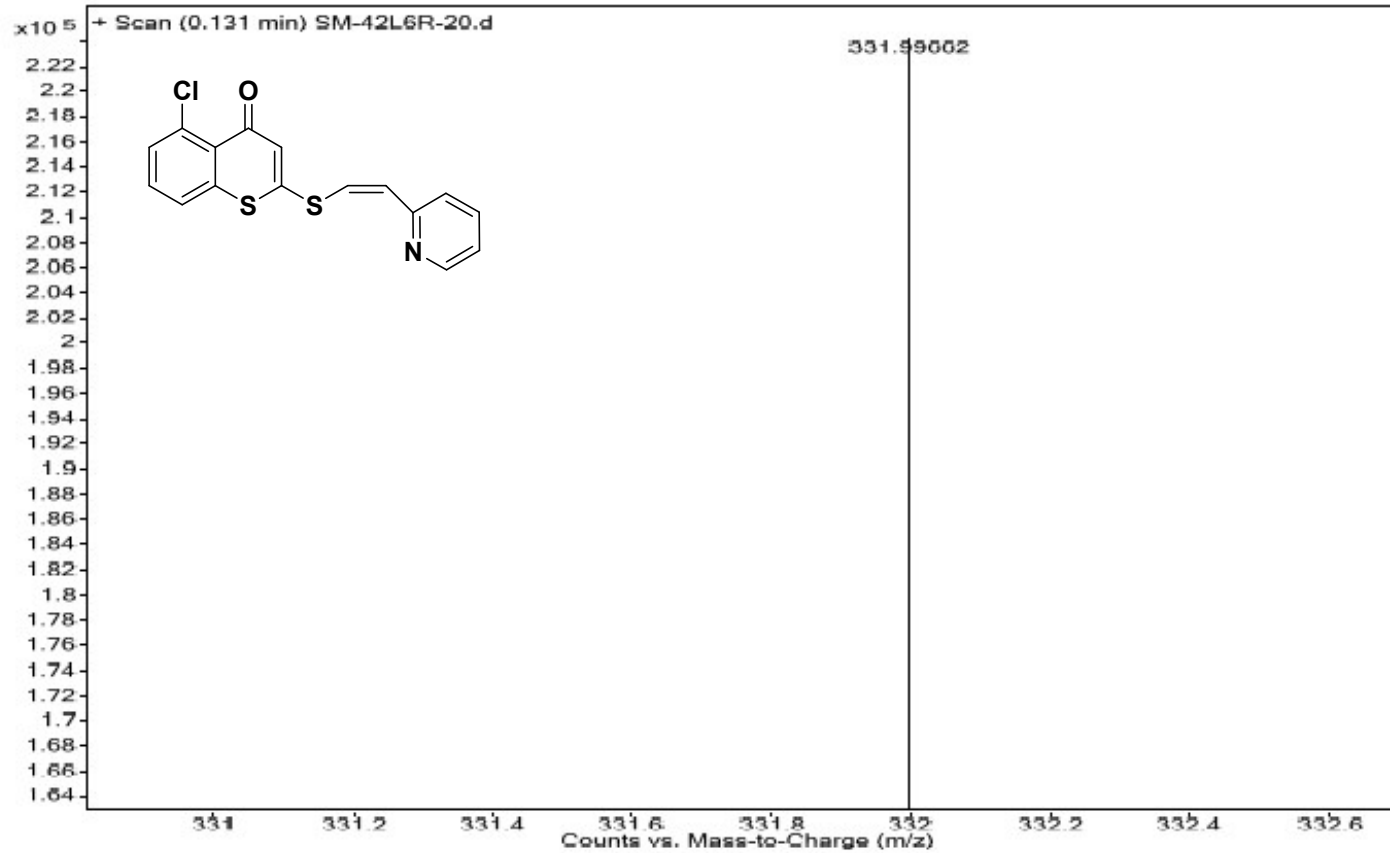
177.91
154.56
150.94
148.54
141.11
136.57
136.46
131.82
131.08
127.95
127.91
127.20
125.48
125.03
123.92
121.69

77.48
77.16
76.84



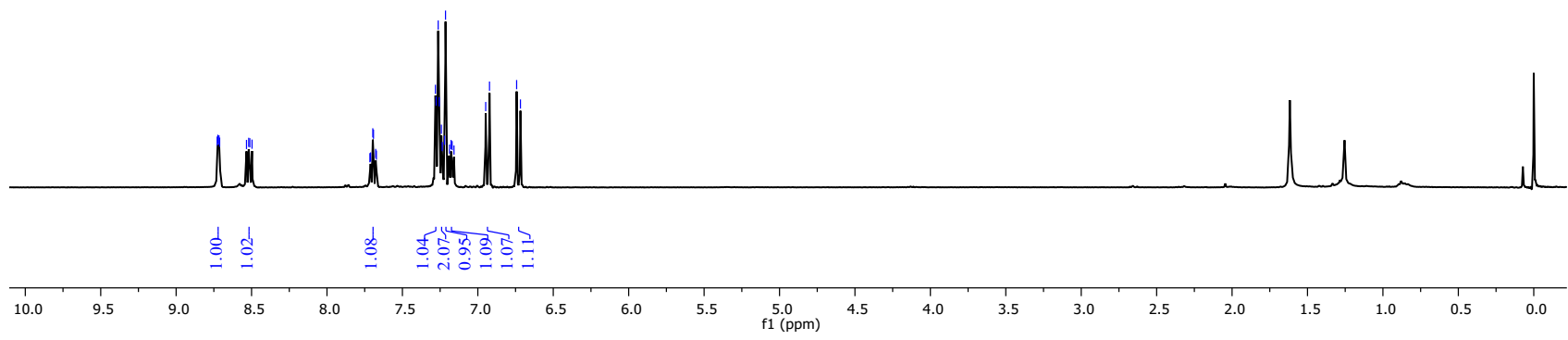
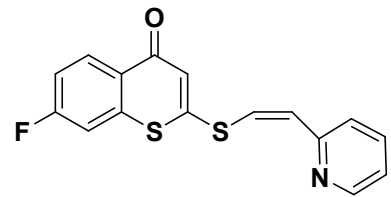
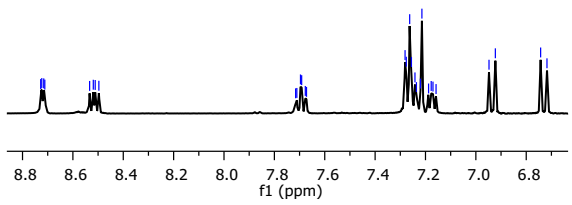
HRMS of compound 5d

Sample Name	SAMPLE	Position	P1-C5	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-42L6R-20.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/25/2021 12:23:15 PM



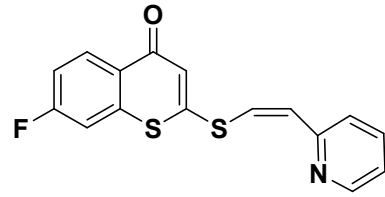
¹H NMR of compound 5e

SM-42L4-1H.1.fid
SM-42L4-1H

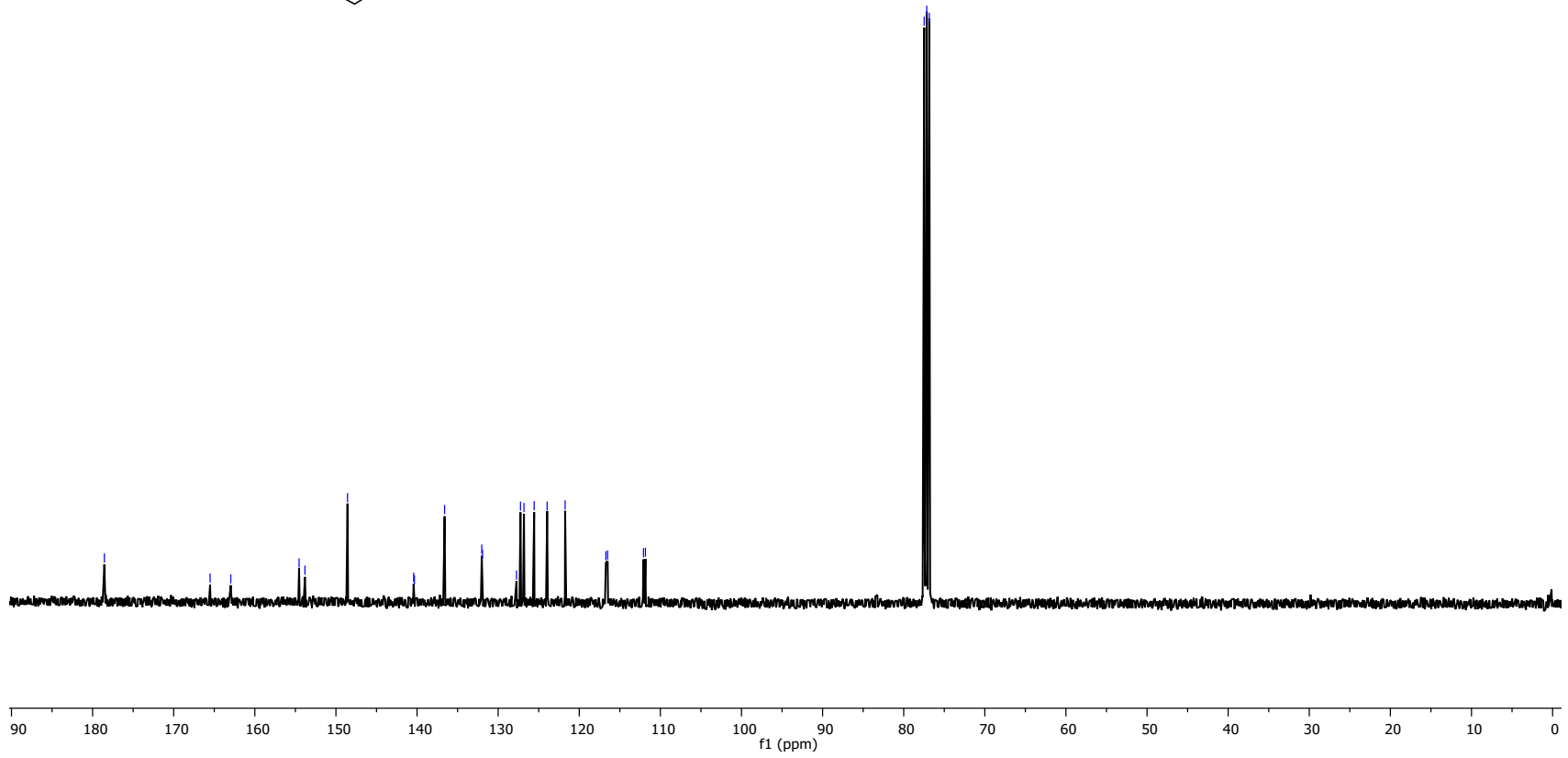


¹³C NMR of compound 5e

SM-42L4-20-13C.1.fid
SM-42L4-20-13C

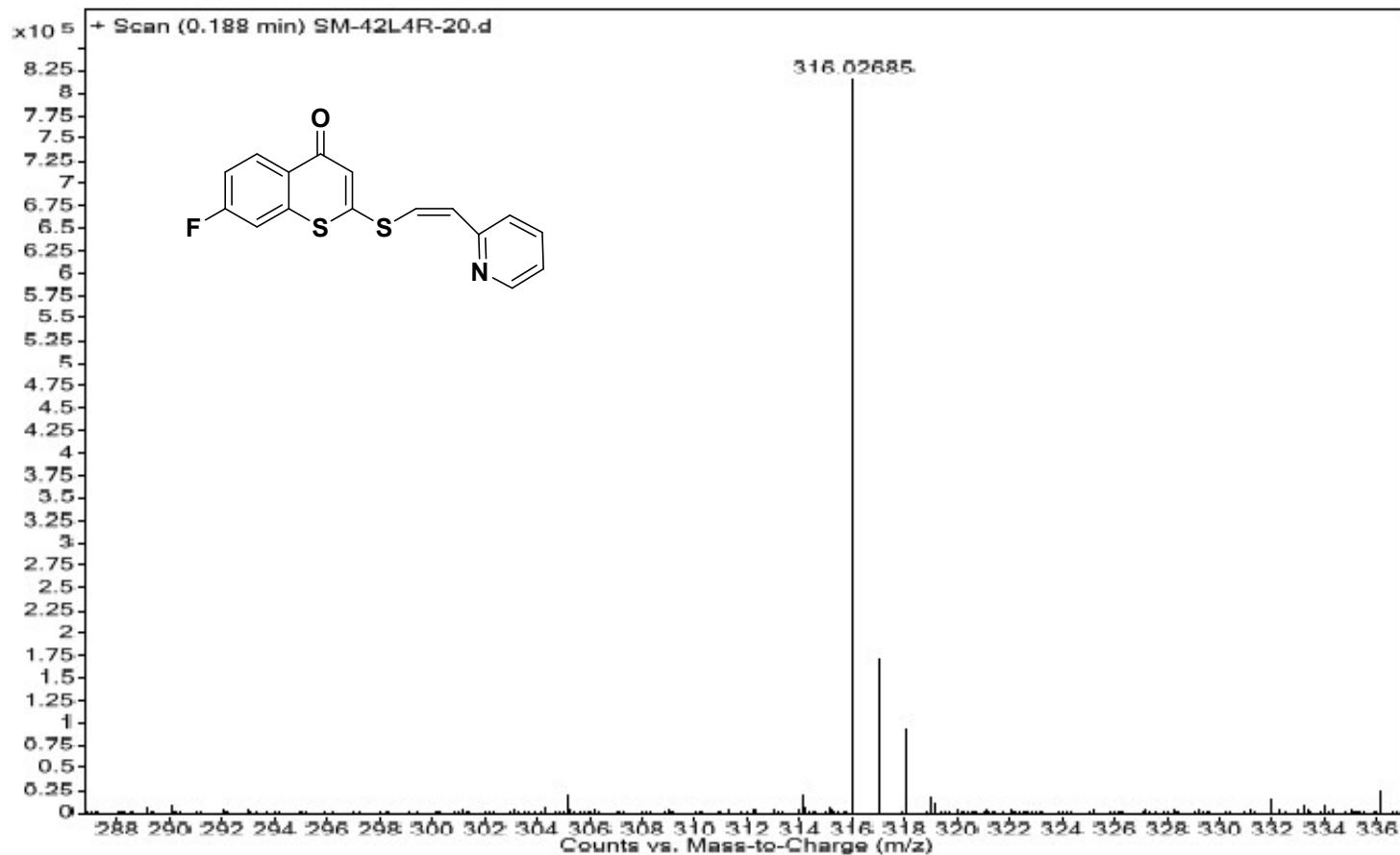


- 177.55
- 165.51
- 162.96
- 154.54
- 153.82
- 148.57
- 140.42
- 140.32
- 136.60
- 132.02
- 131.93
- 127.74
- 127.25
- 126.82
- 125.56
- 123.96
- 121.74
- 116.72
- 116.50
- 112.09
- 111.84
- 77.48
- 77.16
- 76.84



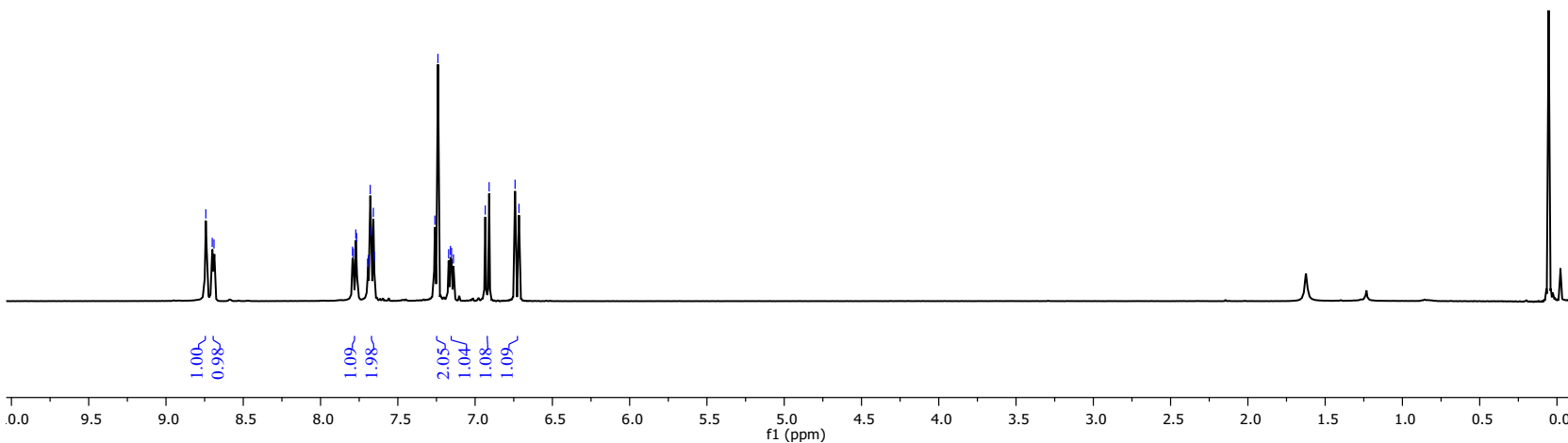
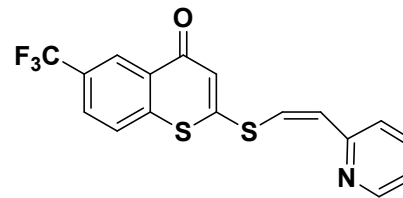
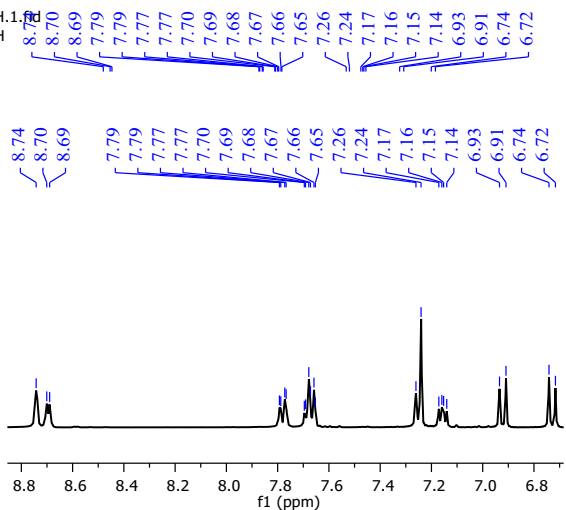
HRMS of compound 5e

Sample Name	SAMPLE	Position	P1-C3	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-42L4R-20.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/25/2021 12:19:30 PM



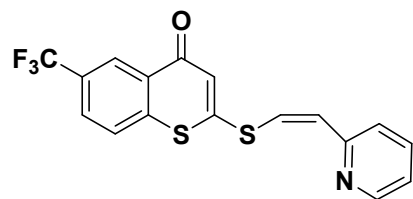
¹H NMR of compound 5f

SM-42L5-20-1H.1.0d
SM-42L5-20-1H

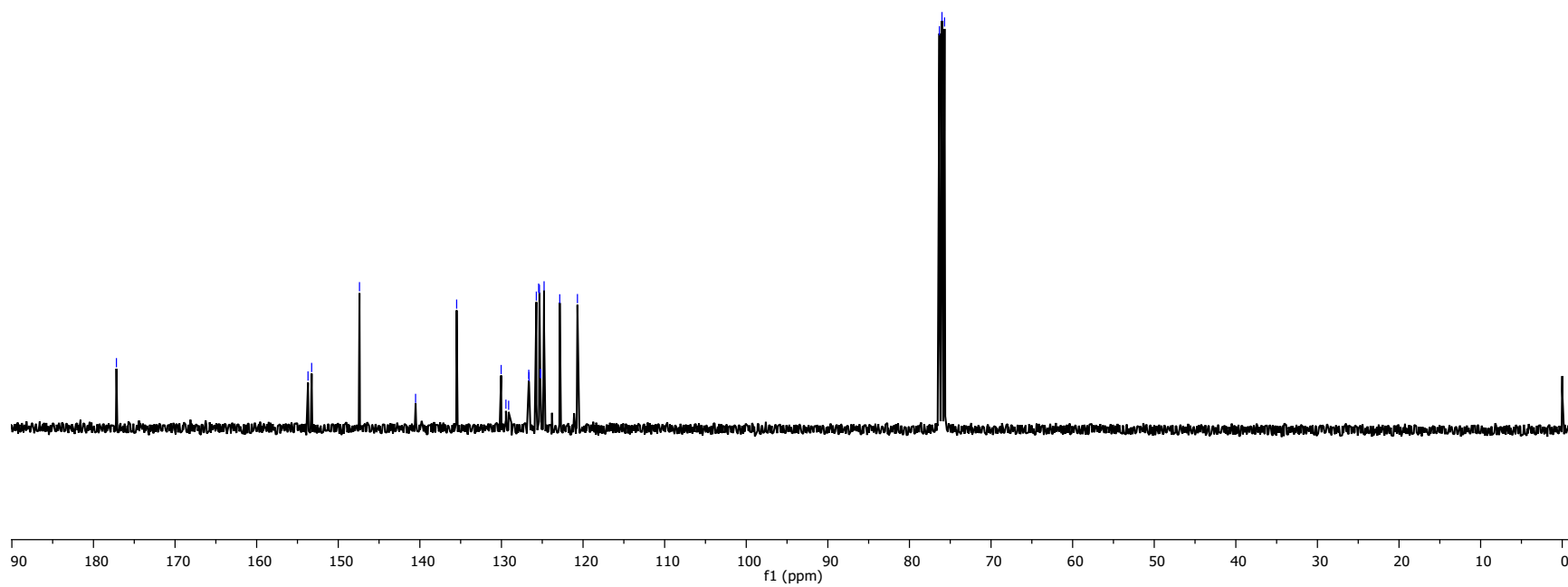


¹³C NMR of compound 5f

SM-42L5-20-13C.1.fid
SM-42L5-20-13C

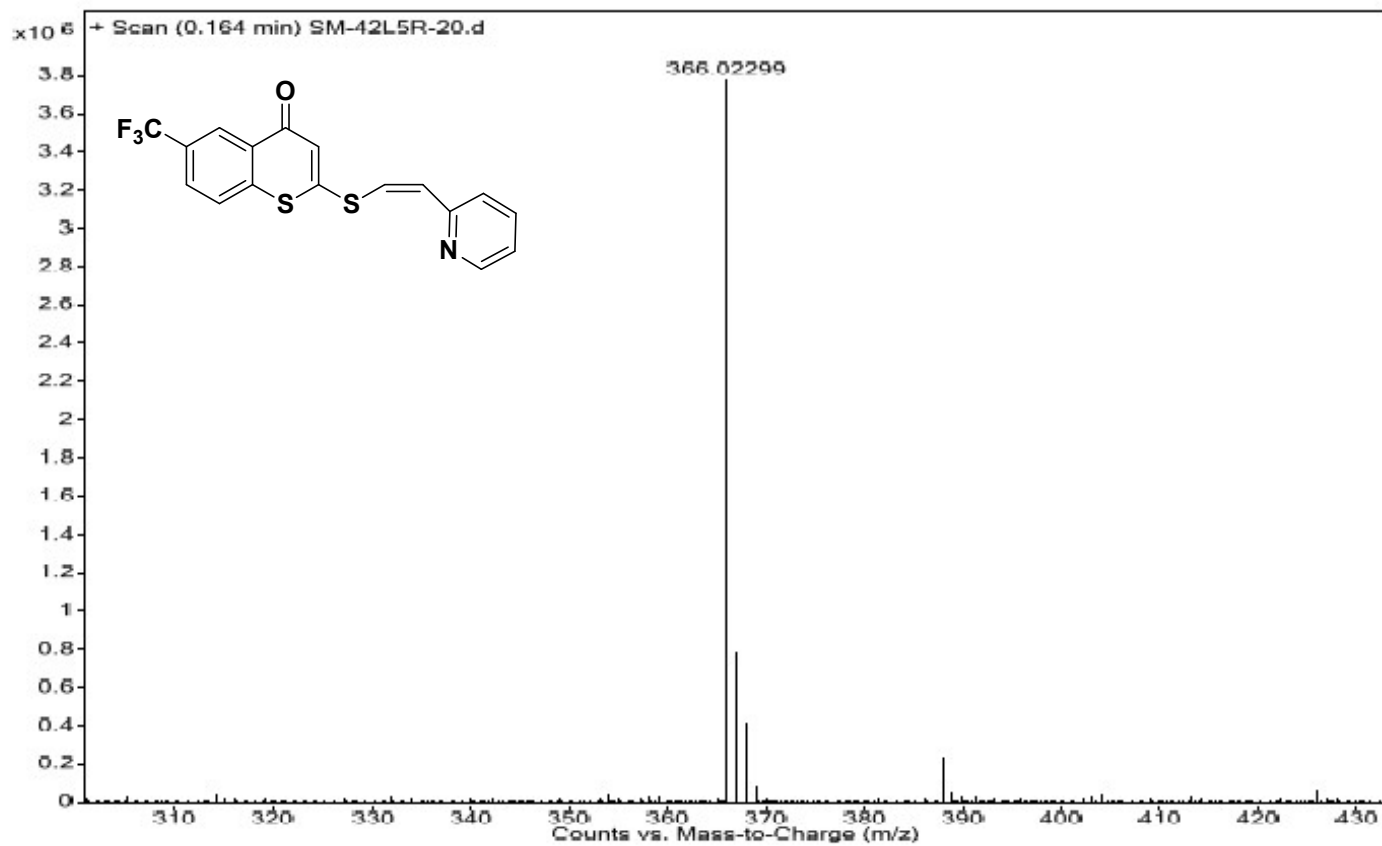


177.38
153.71
153.26
147.40
140.52
135.49
130.04
129.45
129.12
126.65
126.62
125.72
125.44
125.34
125.23
125.19
124.77
122.86
120.69
76.33
76.01
75.69



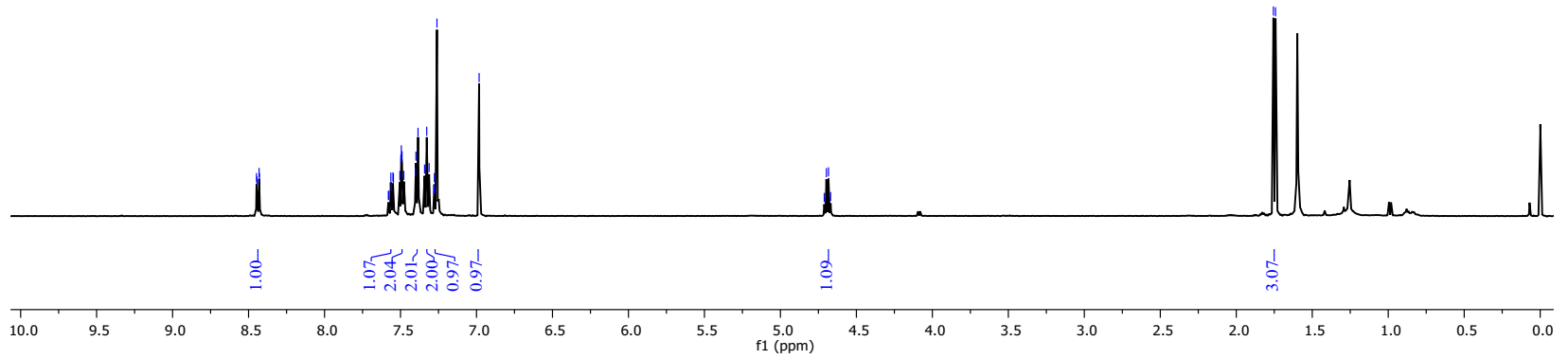
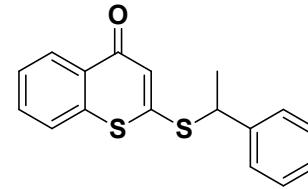
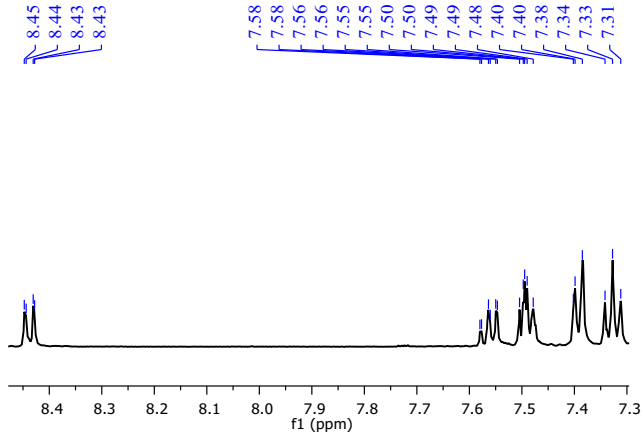
HRMS of compound 5f

Sample Name	SAMPLE	Position	P1-C4	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-42L5R-20.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/25/2021 12:21:22 PM



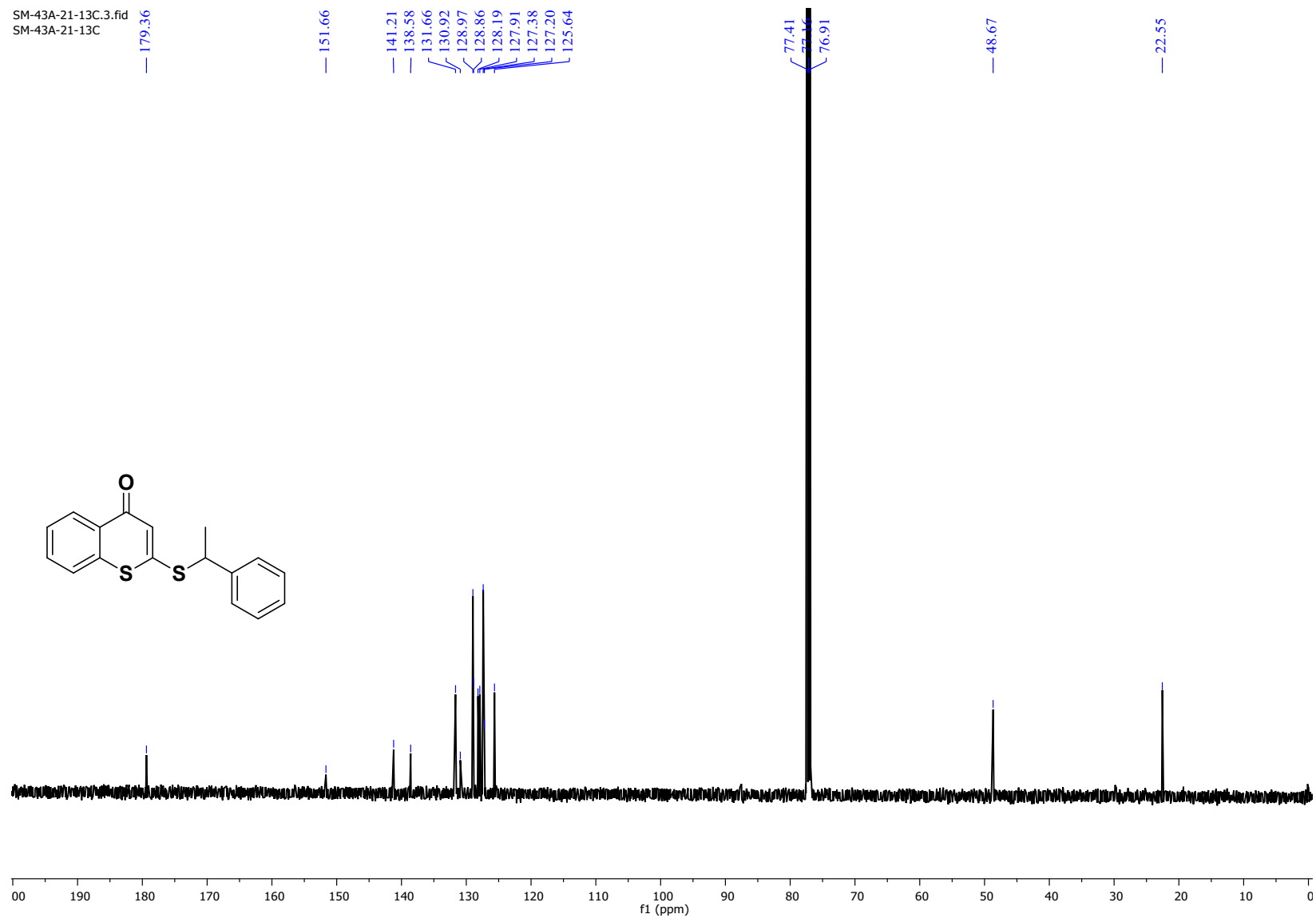
¹H NMR of compound 7a

SM-43A-21-1H.1.fid
SM-43A-21-1H



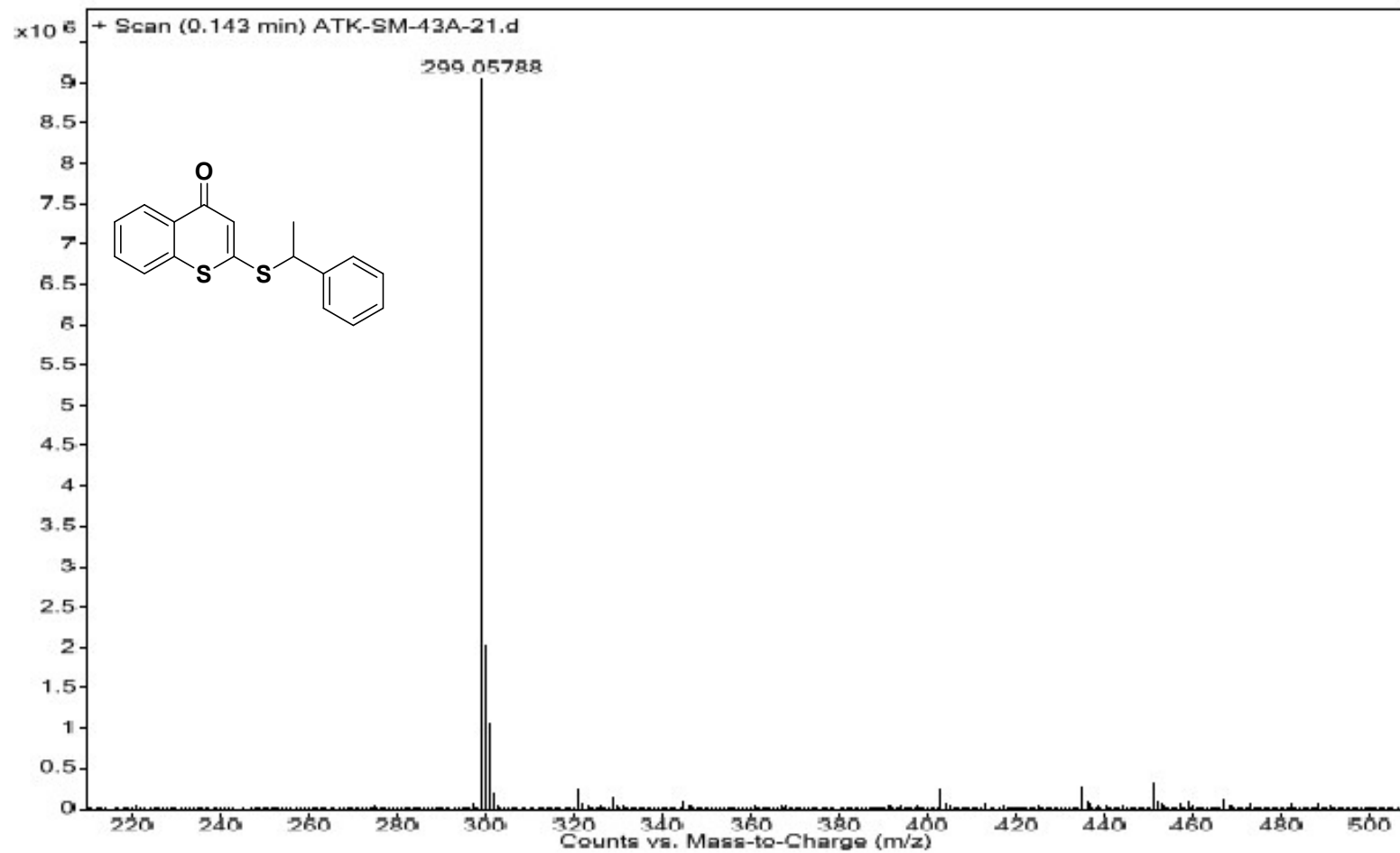
¹³C NMR of compound 7a

SM-43A-21-13C.3.fid
SM-43A-21-13C



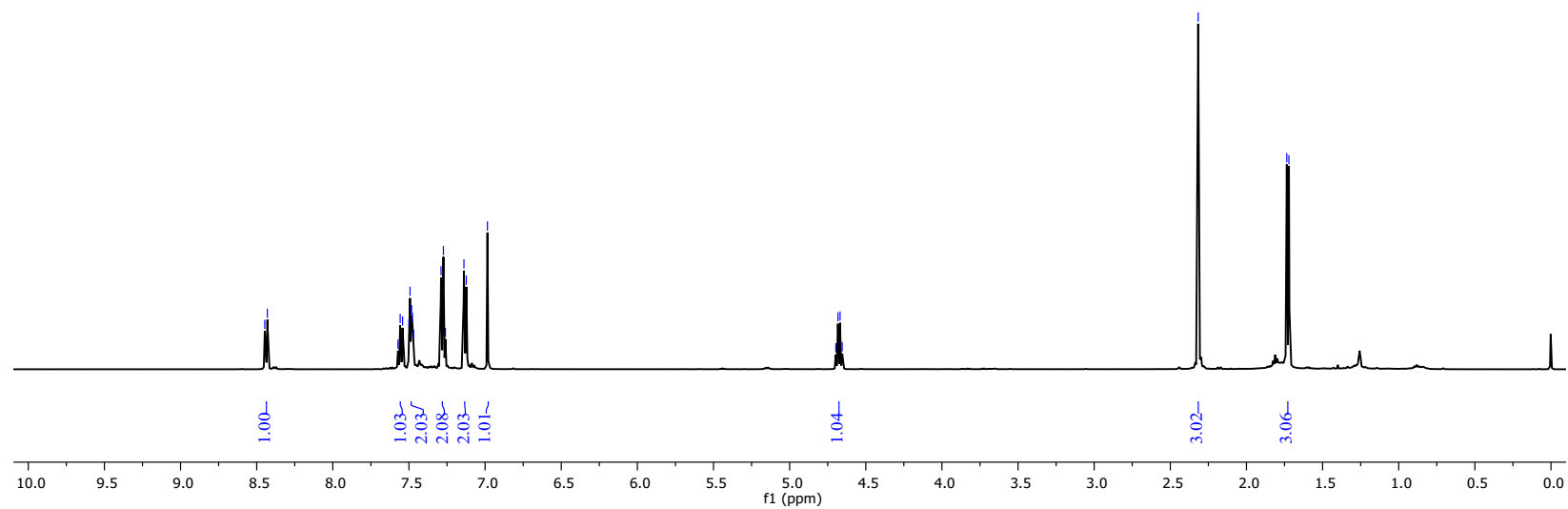
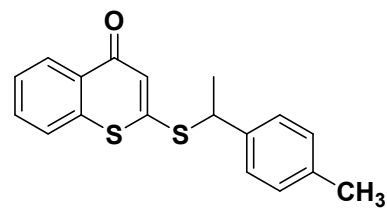
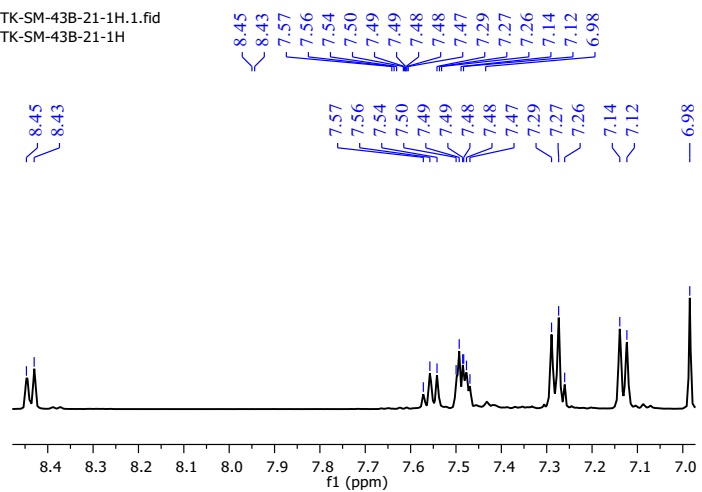
HRMS of compound 7a

Sample Name	SAMPLE	Position	P2-A4	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SM-43A-21.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/4/2021 4:33:06 PM



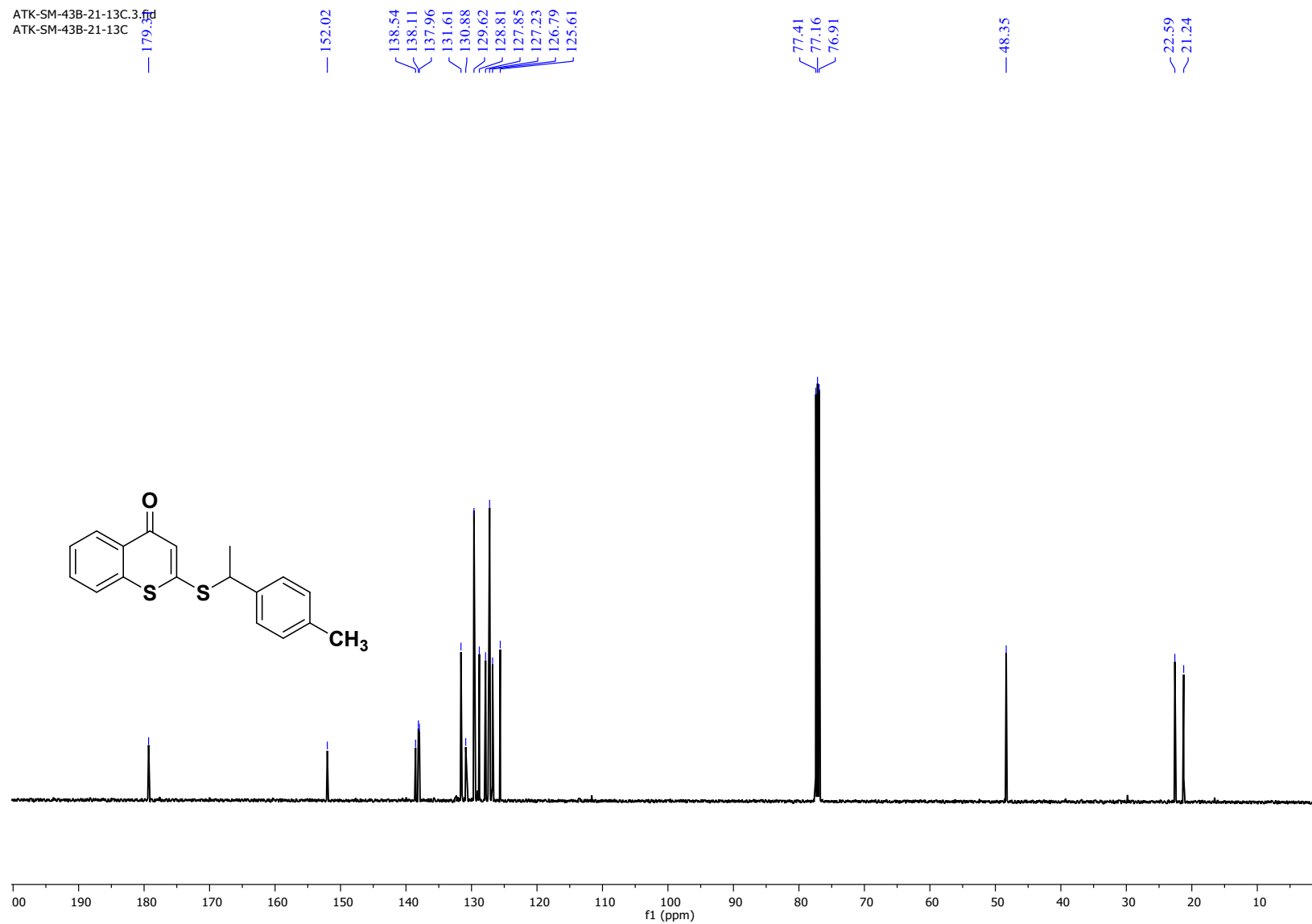
¹H NMR of compound 7b

ATK-SM-43B-21-1H.1.fid
ATK-SM-43B-21-1H



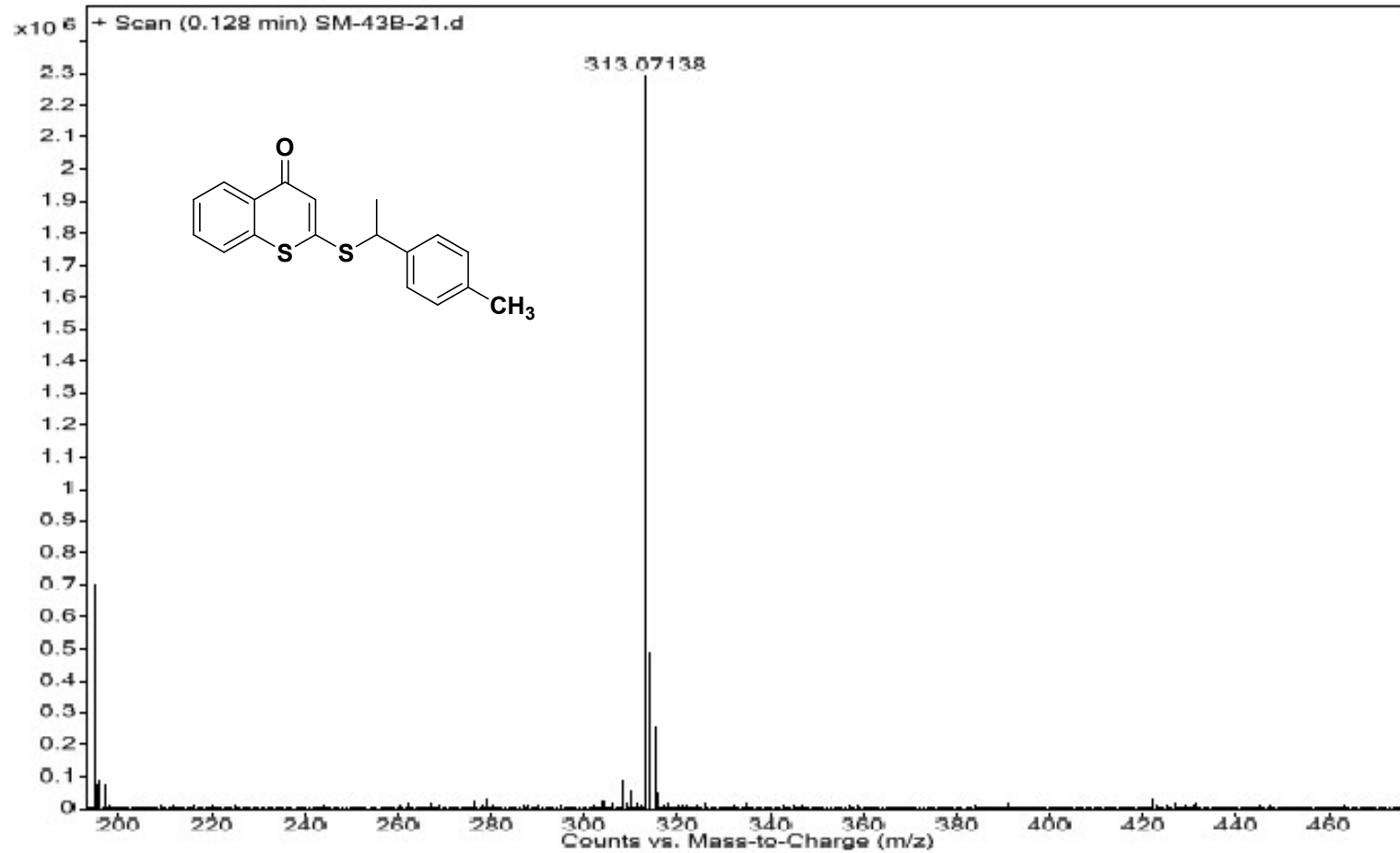
¹³C NMR of compound 7b

ATK-SM-43B-21-13C.3.fid
ATK-SM-43B-21-13C



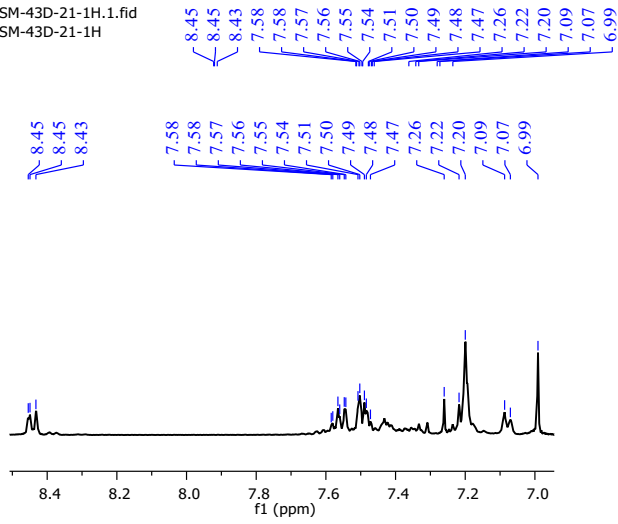
HRMS of compound 7b

Sample Name	SAMPLE 21	Position	P1-B7	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-43B-21.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/11/2021 12:43:44 PM



¹H NMR of compound 7c

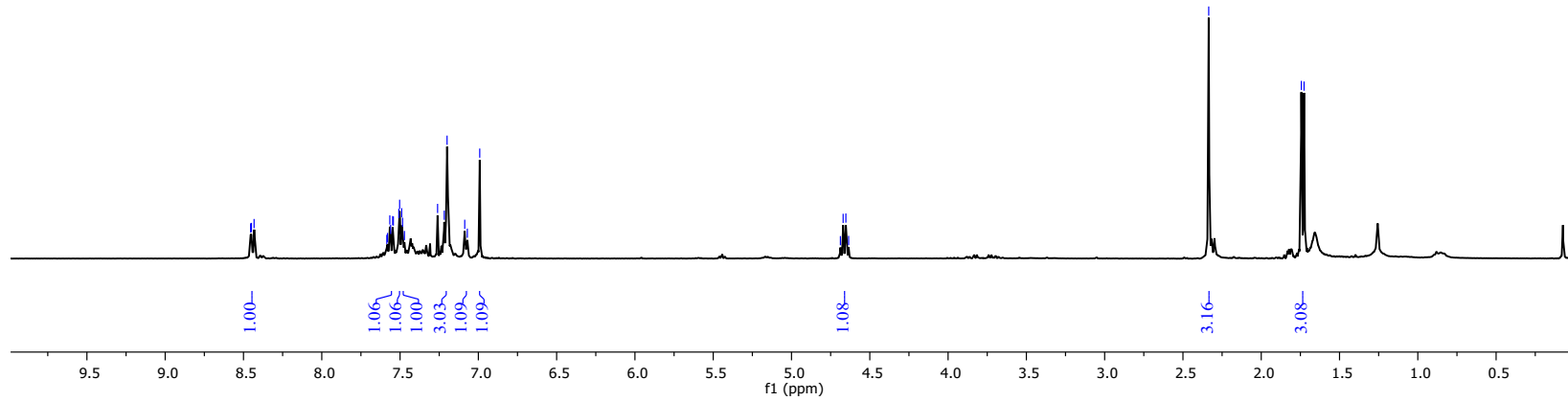
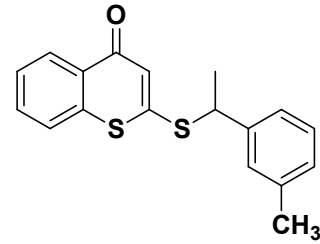
ATK-SM-43D-21-1H.1.fid
ATK-SM-43D-21-1H



4.69
4.67
4.65
4.64

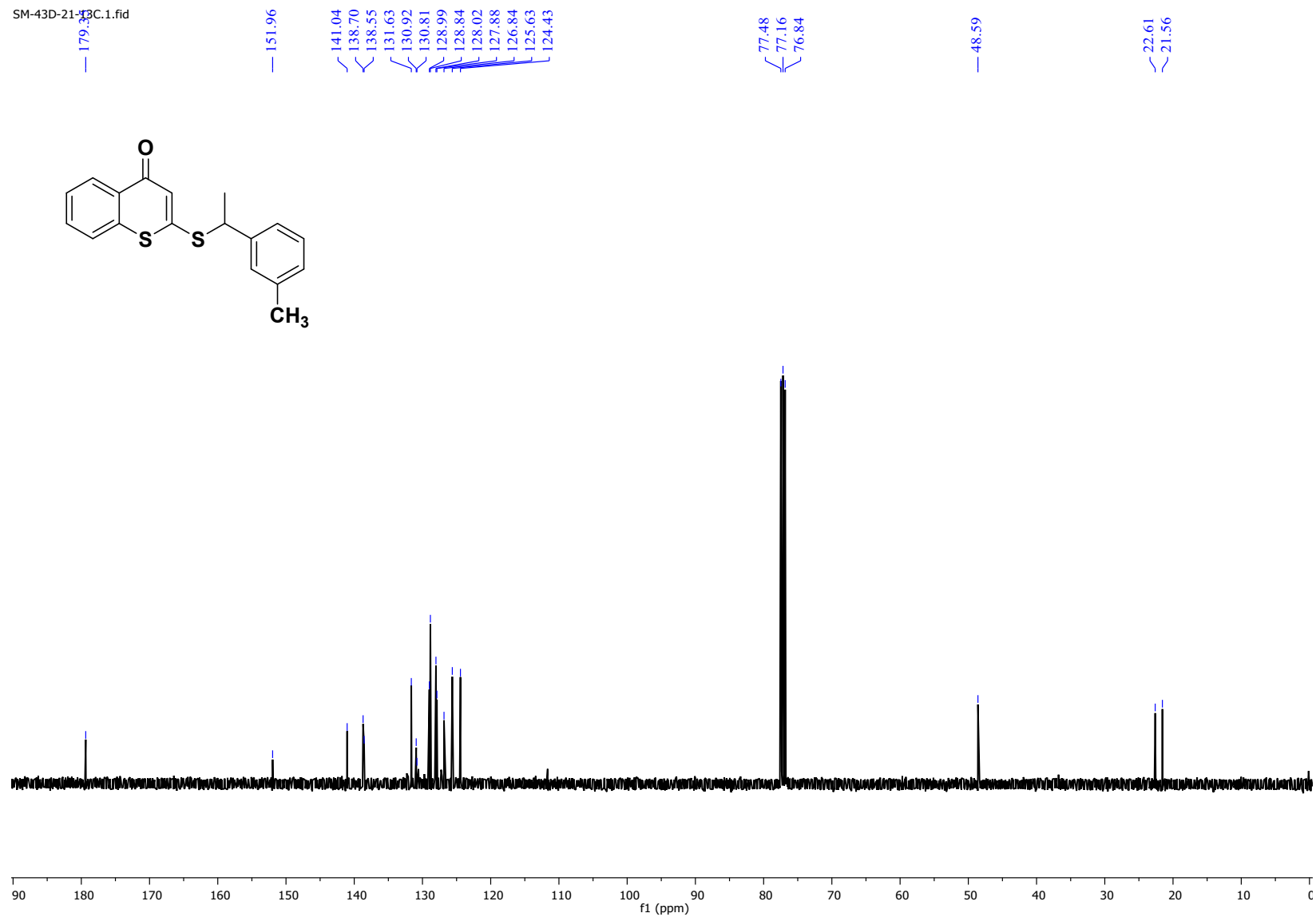
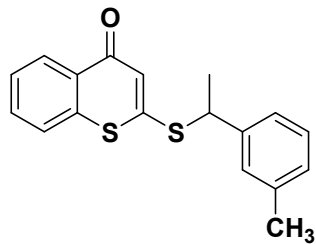
2.34

1.74
1.73



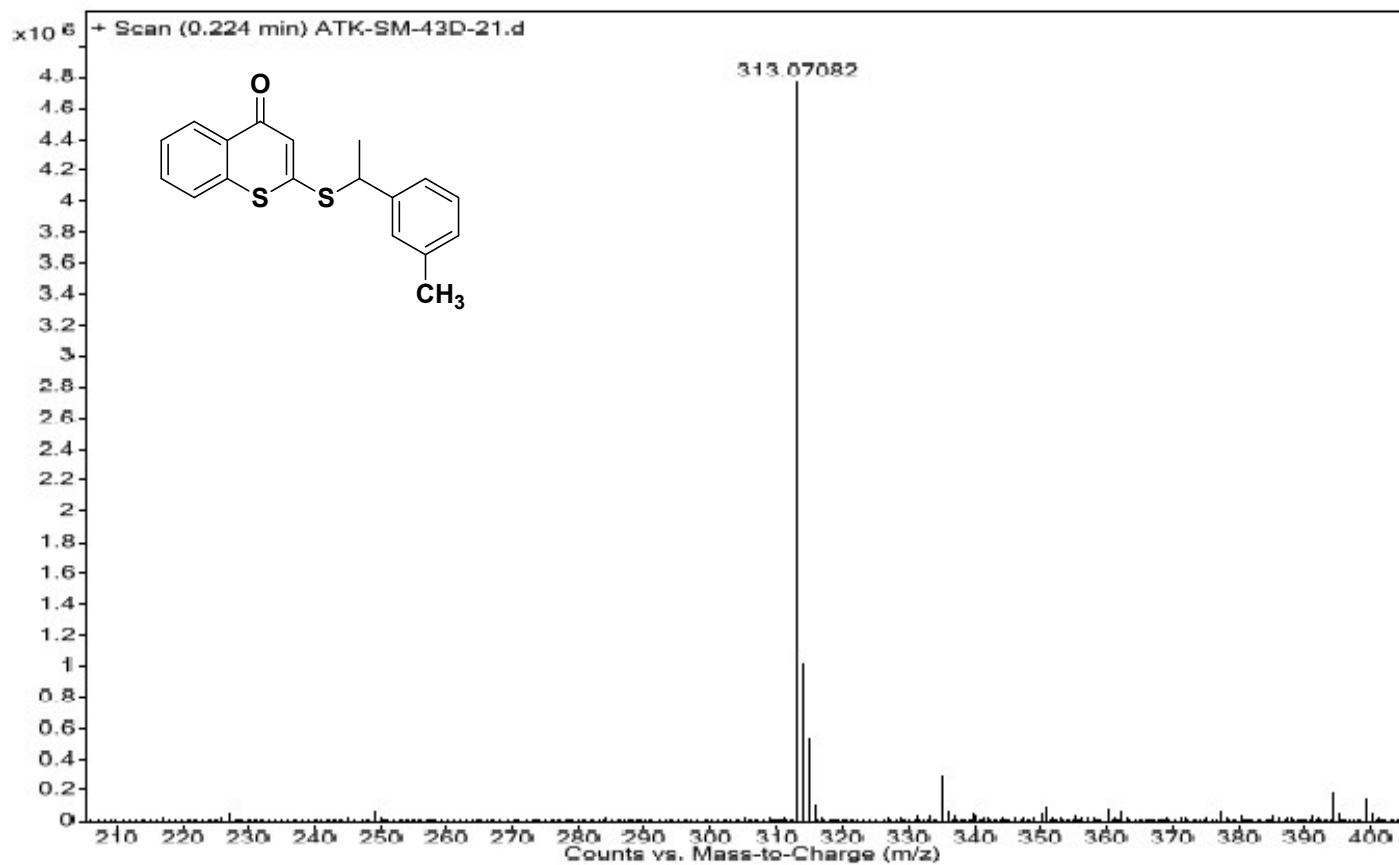
¹³C NMR of compound 7c

SM-43D-21-13C.1.fid



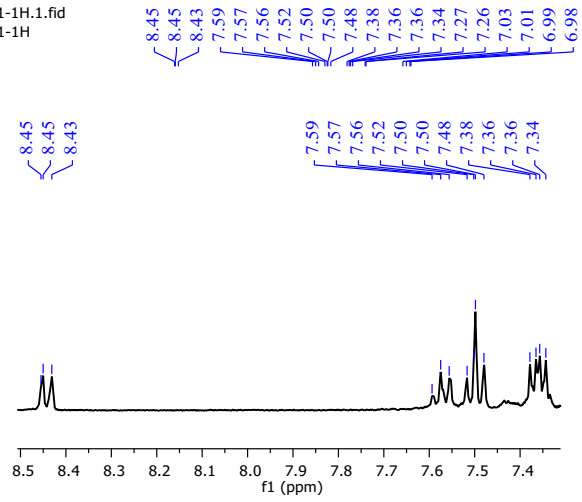
HRMS of compound 7c

Sample Name	SAMPLE 11	Position	P2-A11	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SM-43D-21.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	1/25/2021 6:55:47 PM



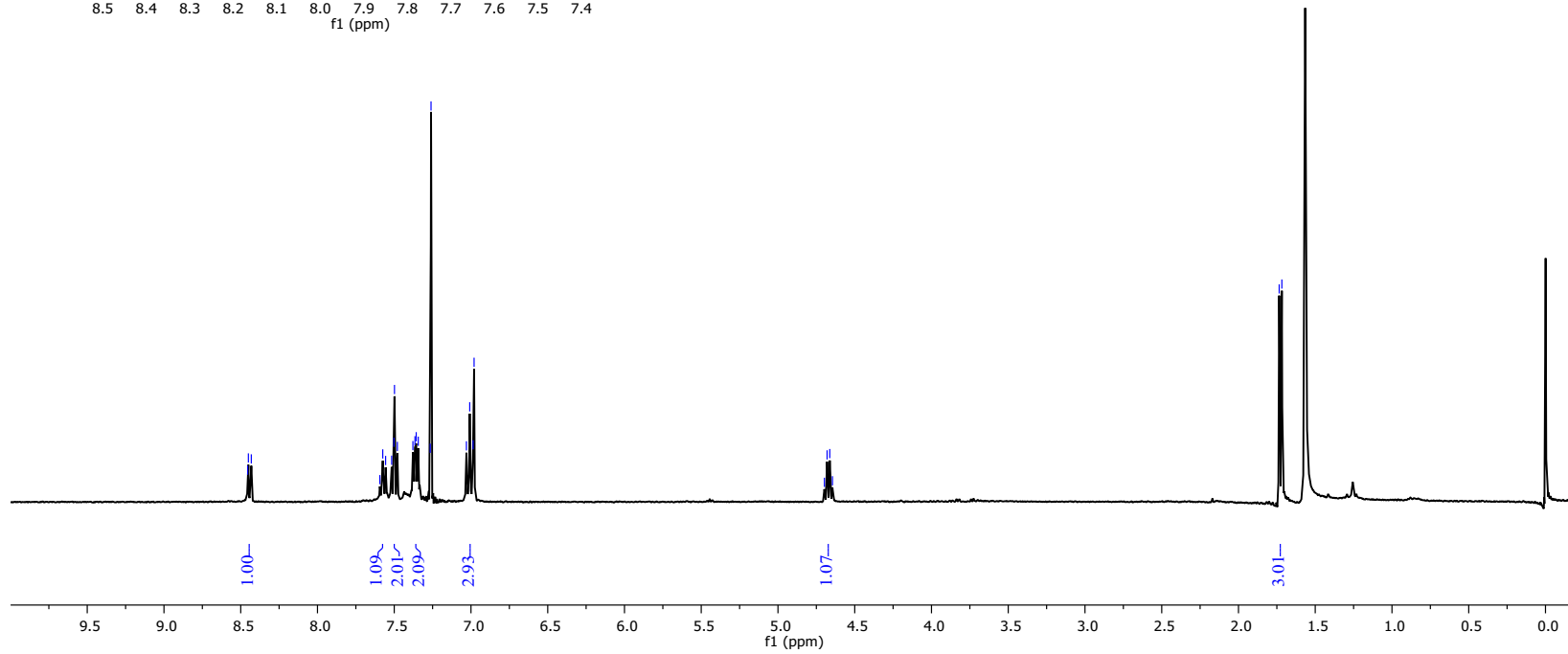
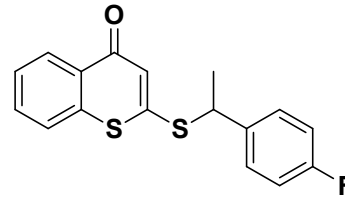
¹H NMR of compound 7d

SM-43E-21-1H.1.fid
SM-43E-21-1H



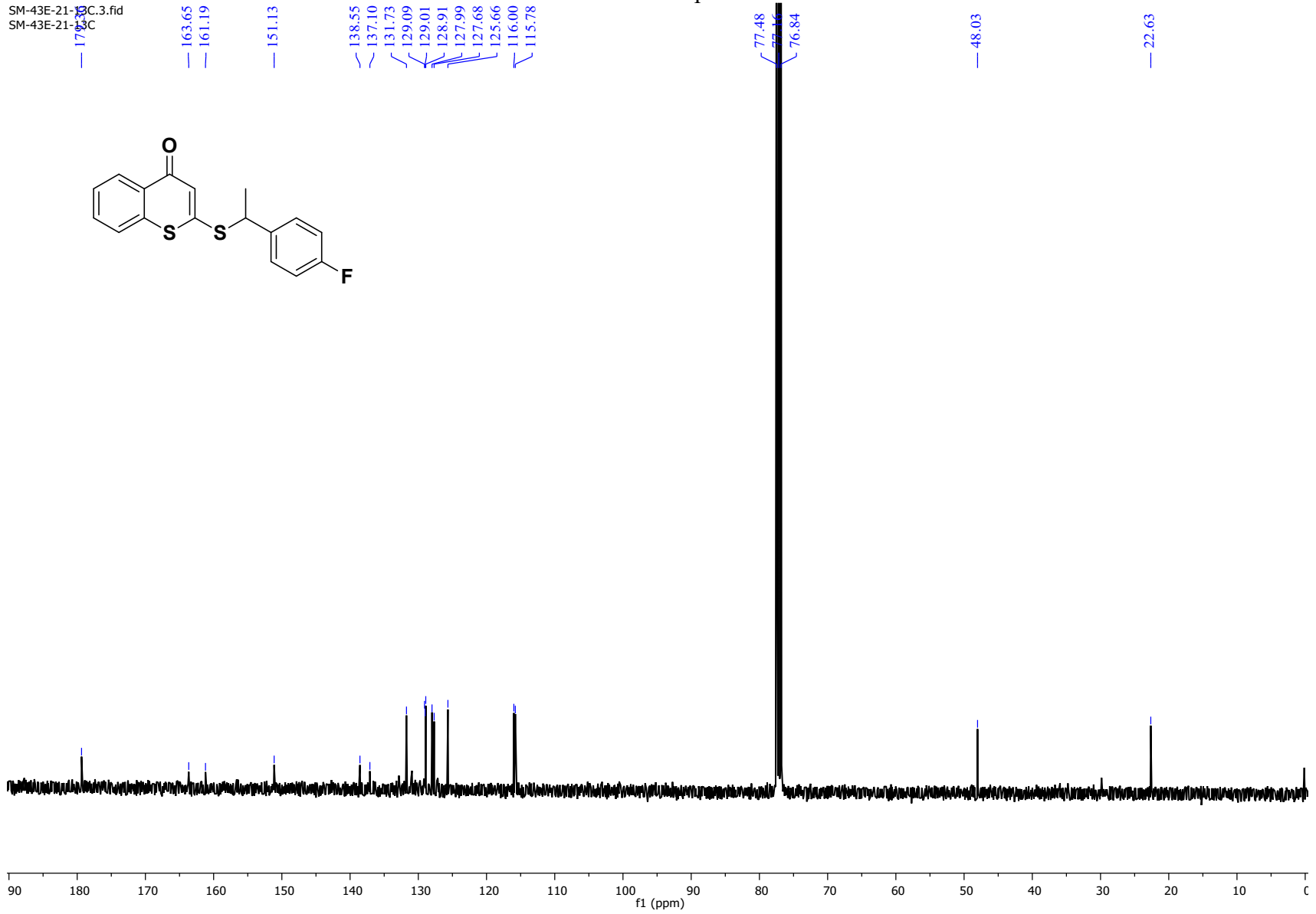
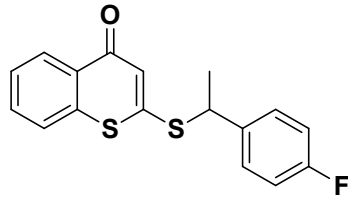
4.70
4.68
4.66
4.65

1.73
1.72



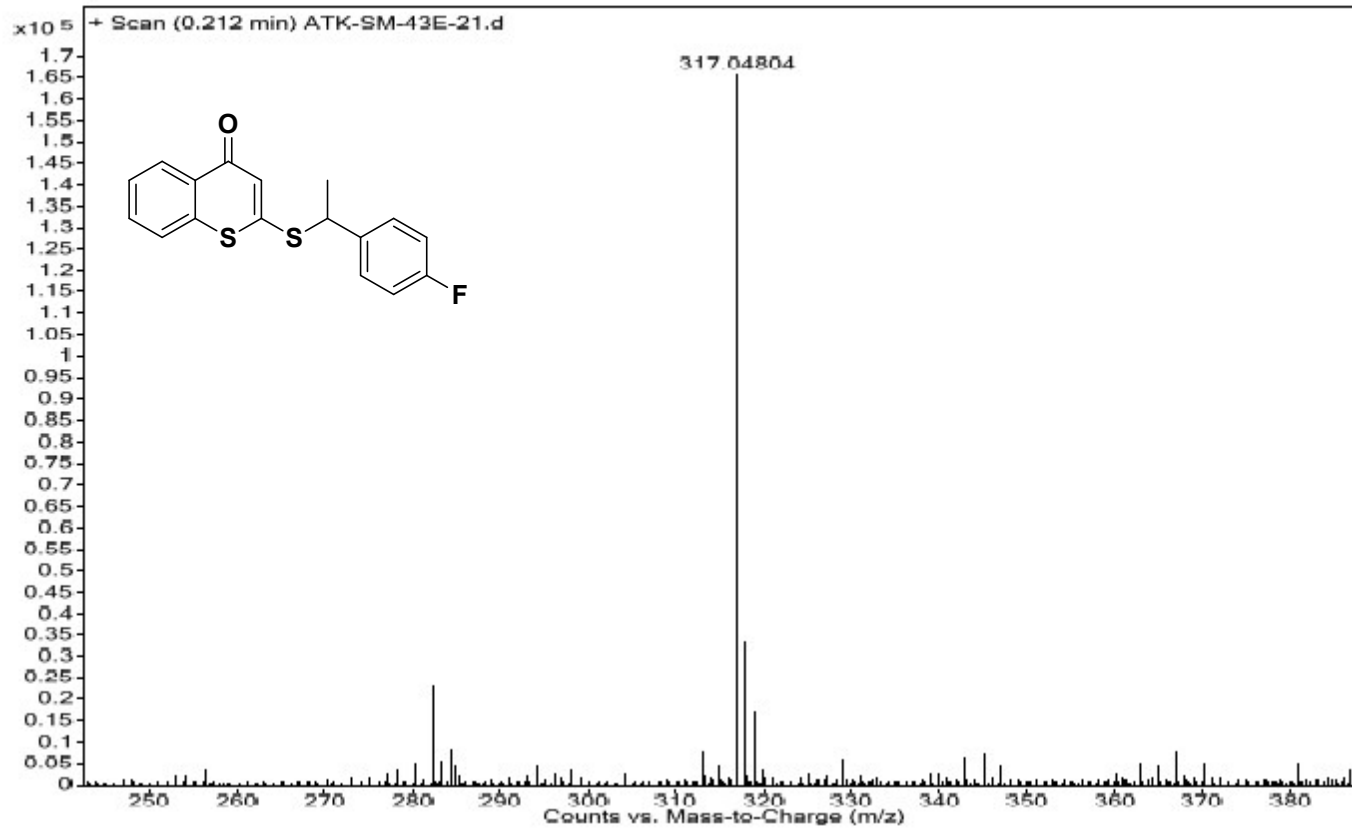
¹³C NMR of compound 7d

SM-43E-21-13 C.3.fid
SM-43E-21-13 C



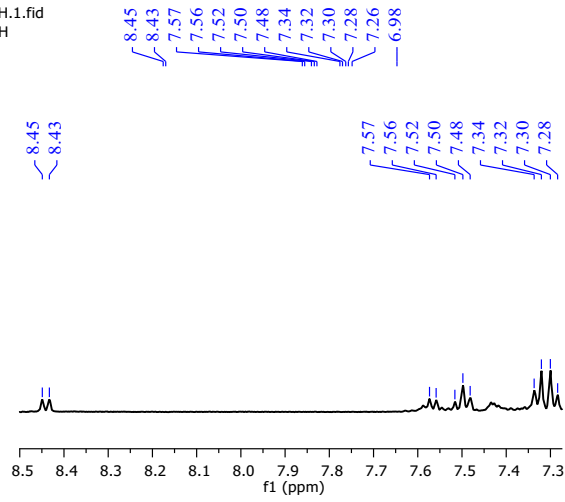
HRMS of compound 7d

Sample Name	SAMPLE 11	Position	P1-A9	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SM-43E-21.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/18/2021 2:10:04 PM



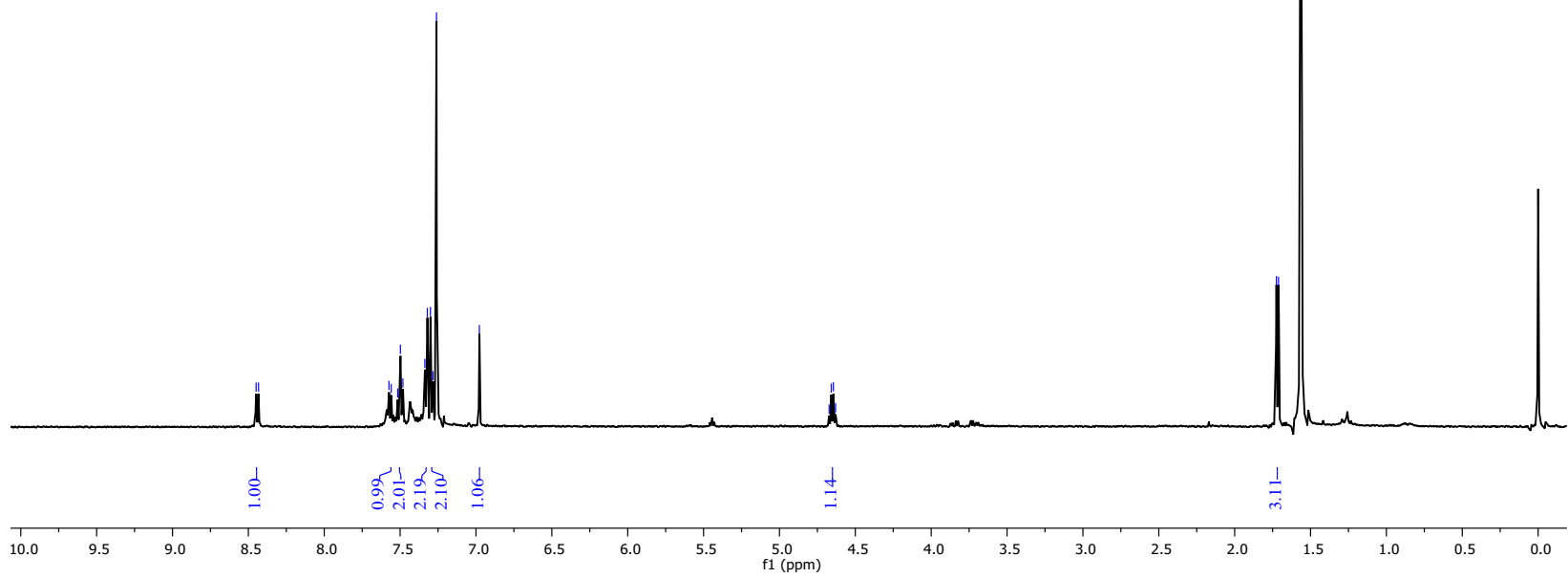
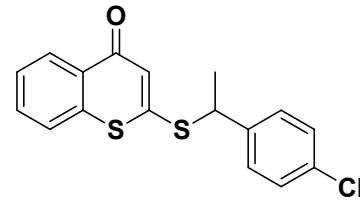
¹H NMR of compound 7e

SM-43F-21-1H.1.fid
SM-43F-21-1H



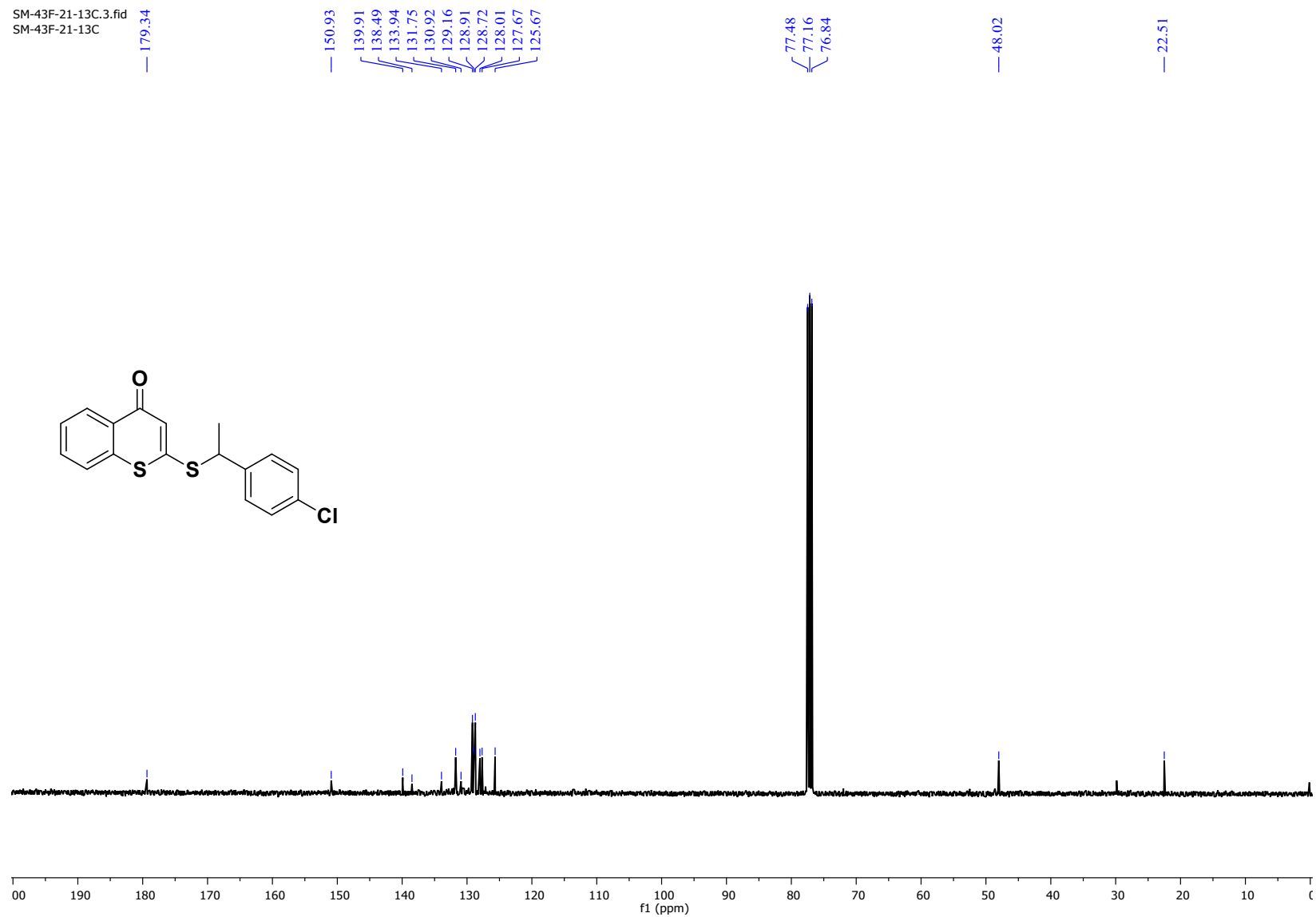
4.67
4.66
4.64
4.63

1.72
1.71



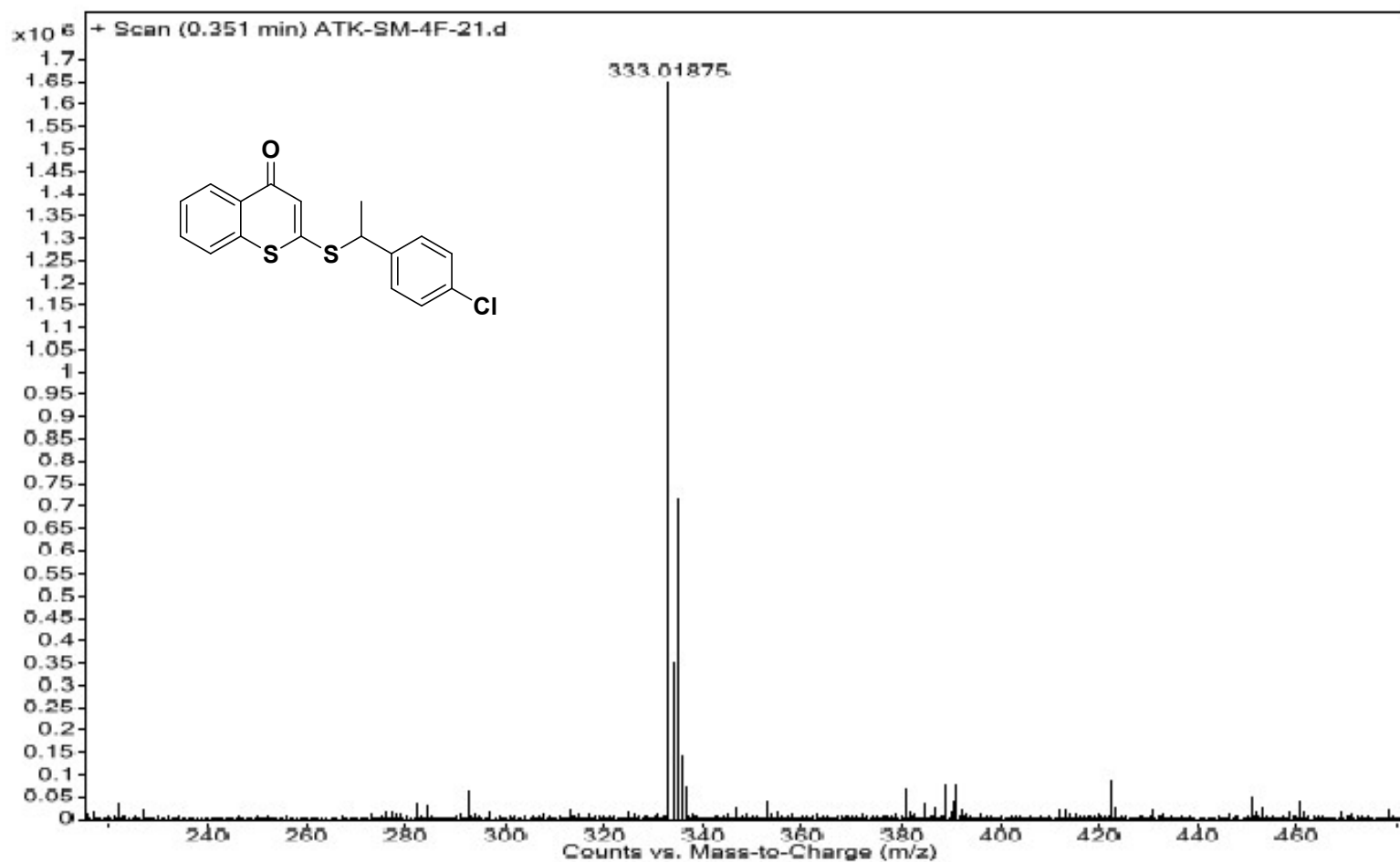
¹³C NMR of compound 7e

SM-43F-21-13C.3.fid
SM-43F-21-13C



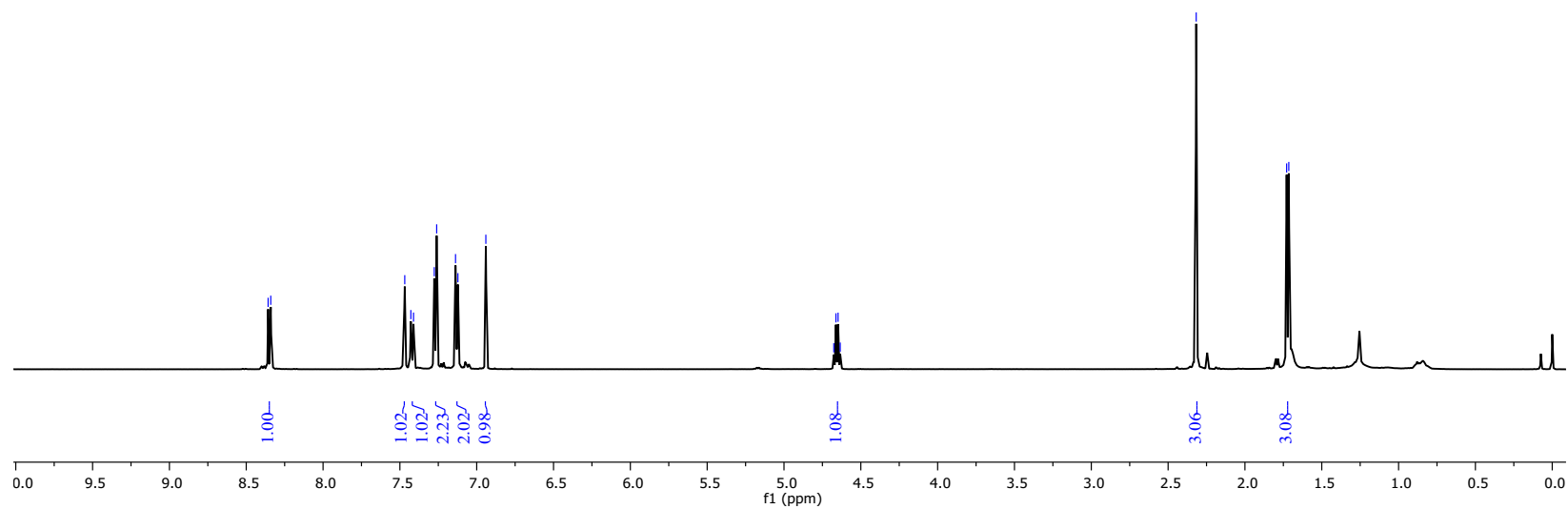
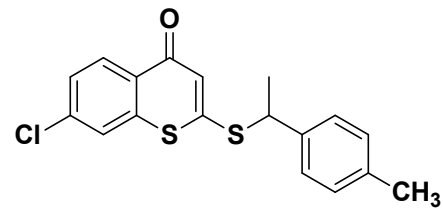
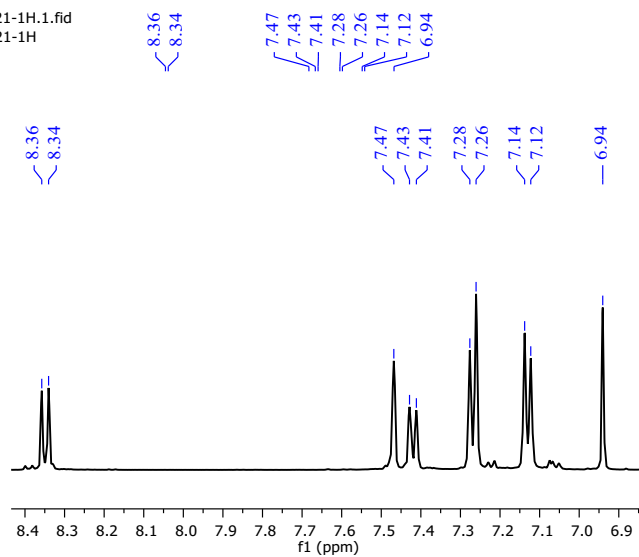
HRMS of compound 7e

Sample Name	SAMPLE 12	Position	P1-A10	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SM-4F-21.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/18/2021 2:19:32 PM



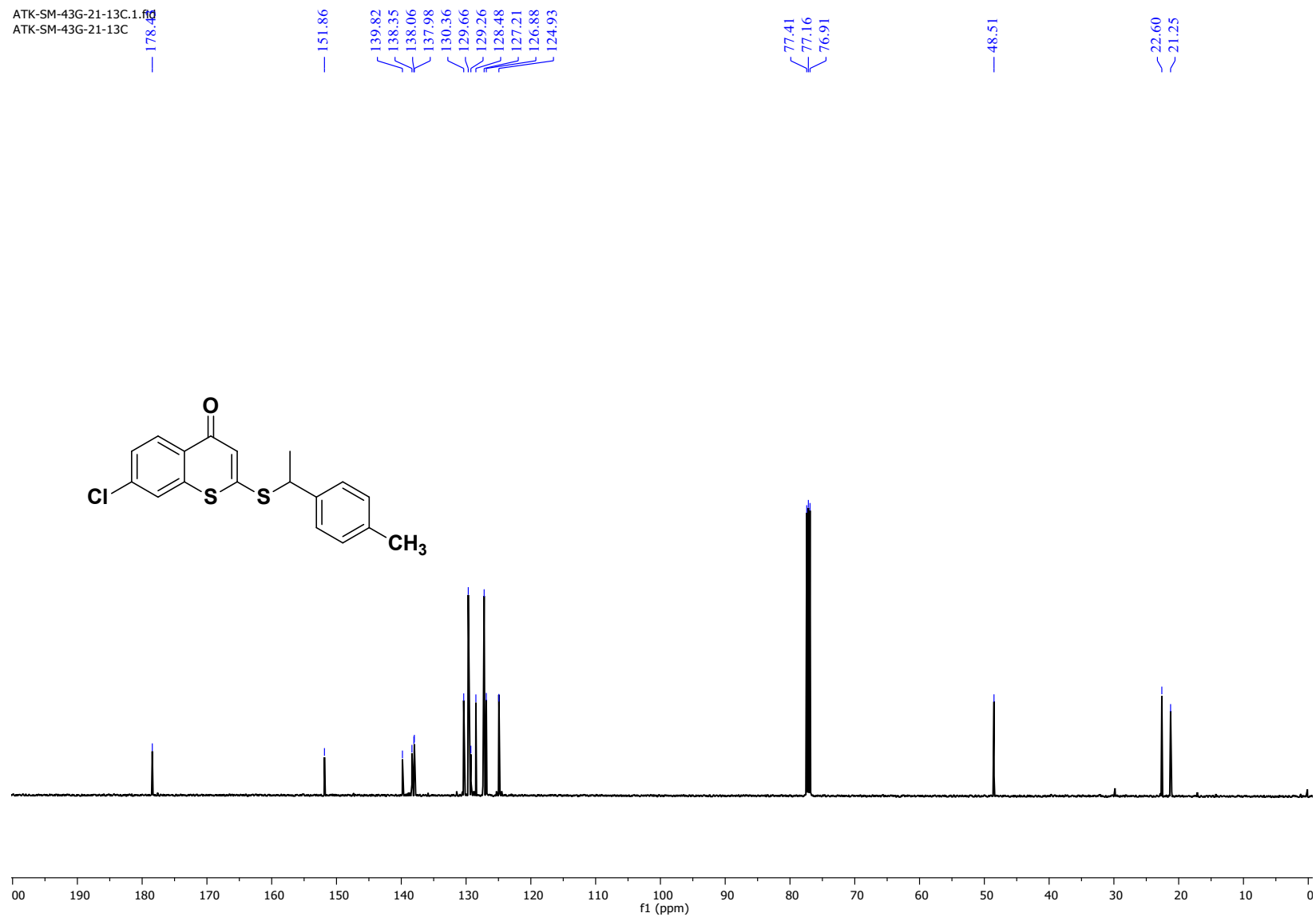
¹H NMR of compound 7f

ATK-SM-43G-21-1H.1.fid
ATK-SM-43G-21-1H



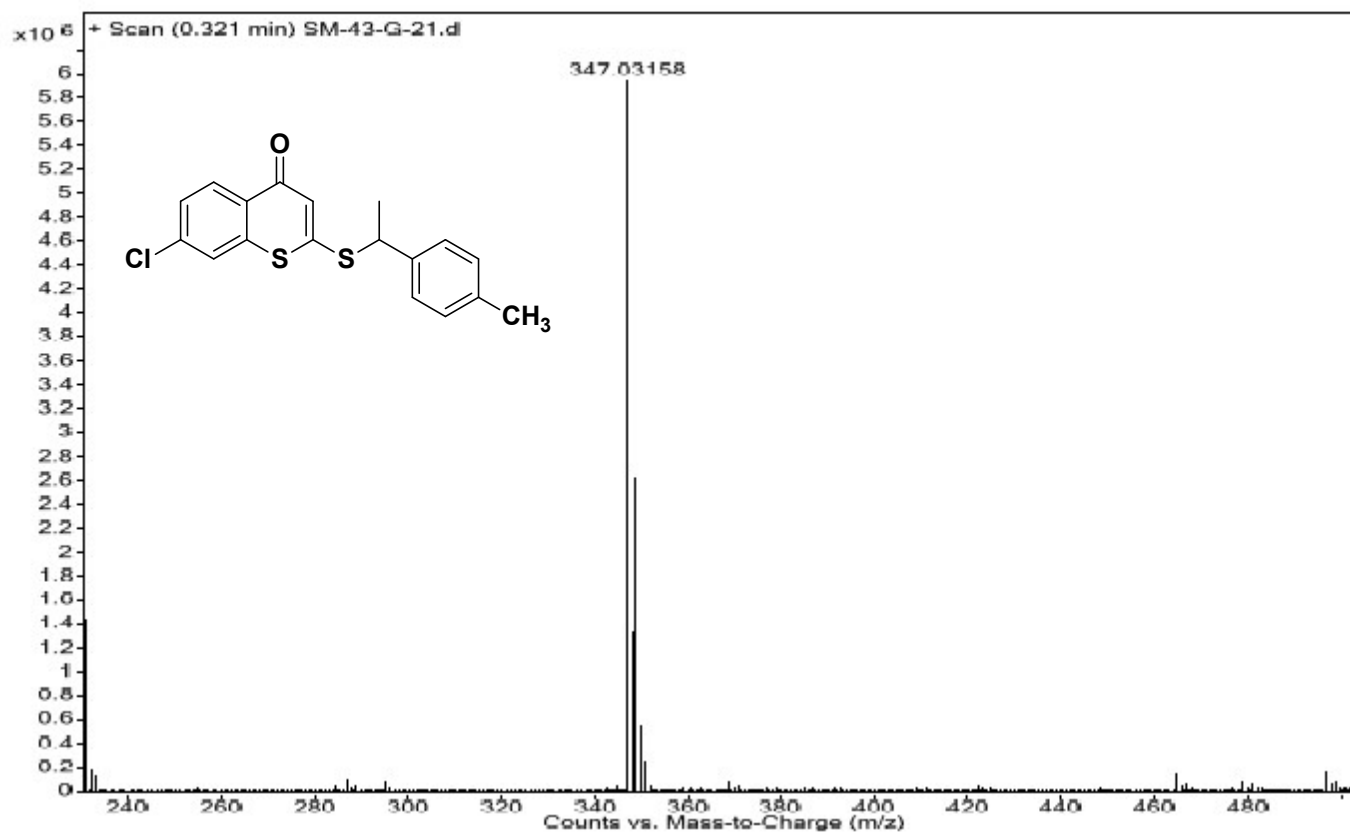
¹³C NMR of compound 7f

ATK-SM-43G-21-13C.1.fg
ATK-SM-43G-21-13C



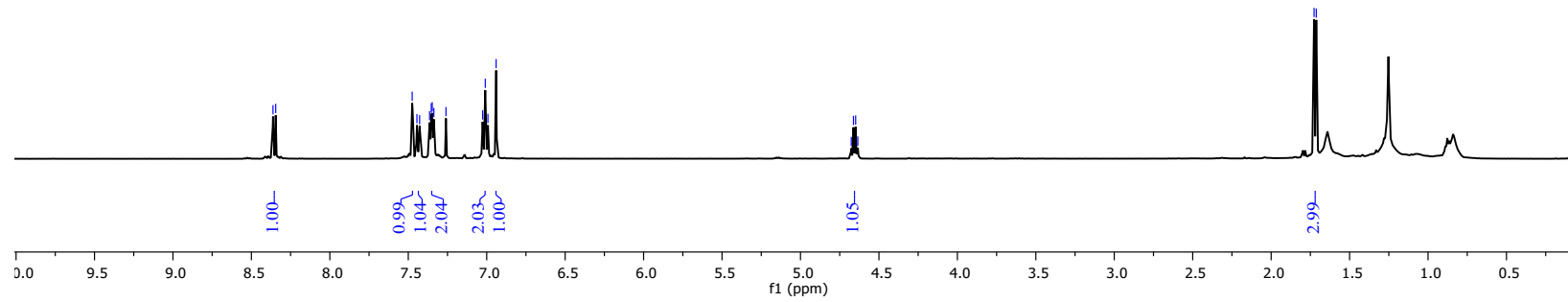
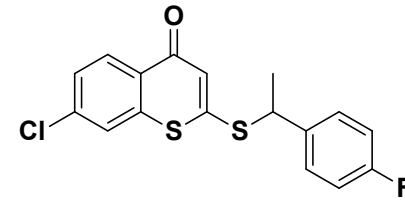
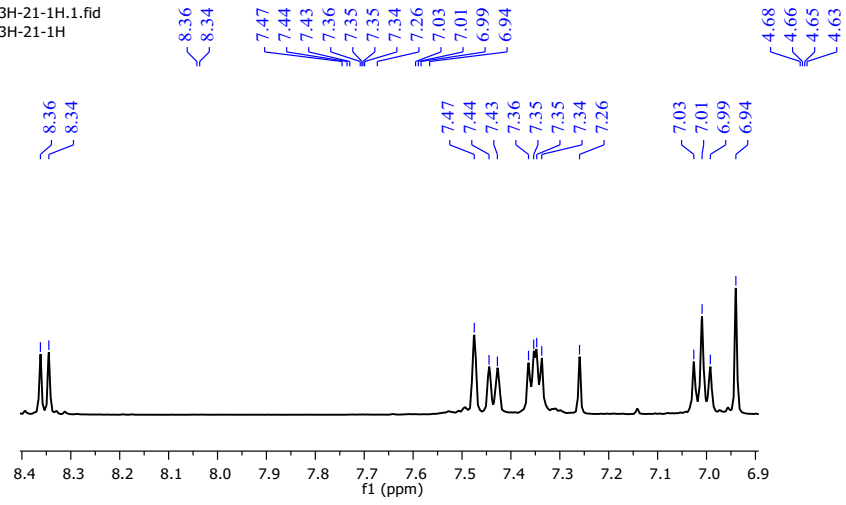
HRMS of compound 7f

Sample Name	SAMPLE	Position	P2-A8	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-43-G-21.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/18/2021 5:06:44 PM



¹H NMR of compound 7g

ATK-SM-43H-21-1H.1.fid
ATK-SM-43H-21-1H



¹³C NMR of compound 7g

SM-43H-21-13C.1.fid
SM-43H-21-13C

178.48

163.40

161.43

151.09

139.78

138.52

136.90

136.87

130.42

129.23

129.05

129.00

128.99

128.63

127.63

124.98

116.02

115.85

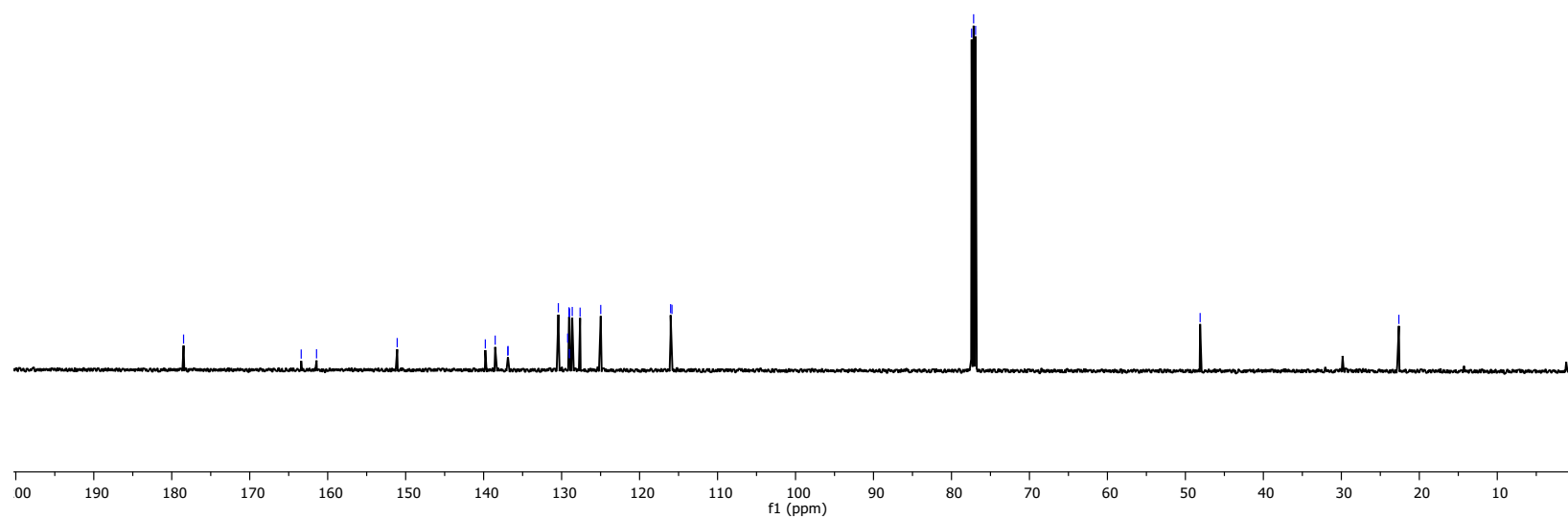
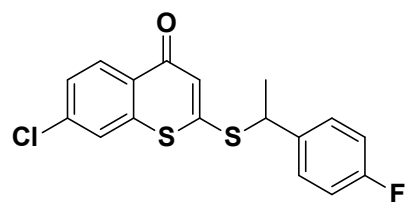
77.41

77.16

76.91

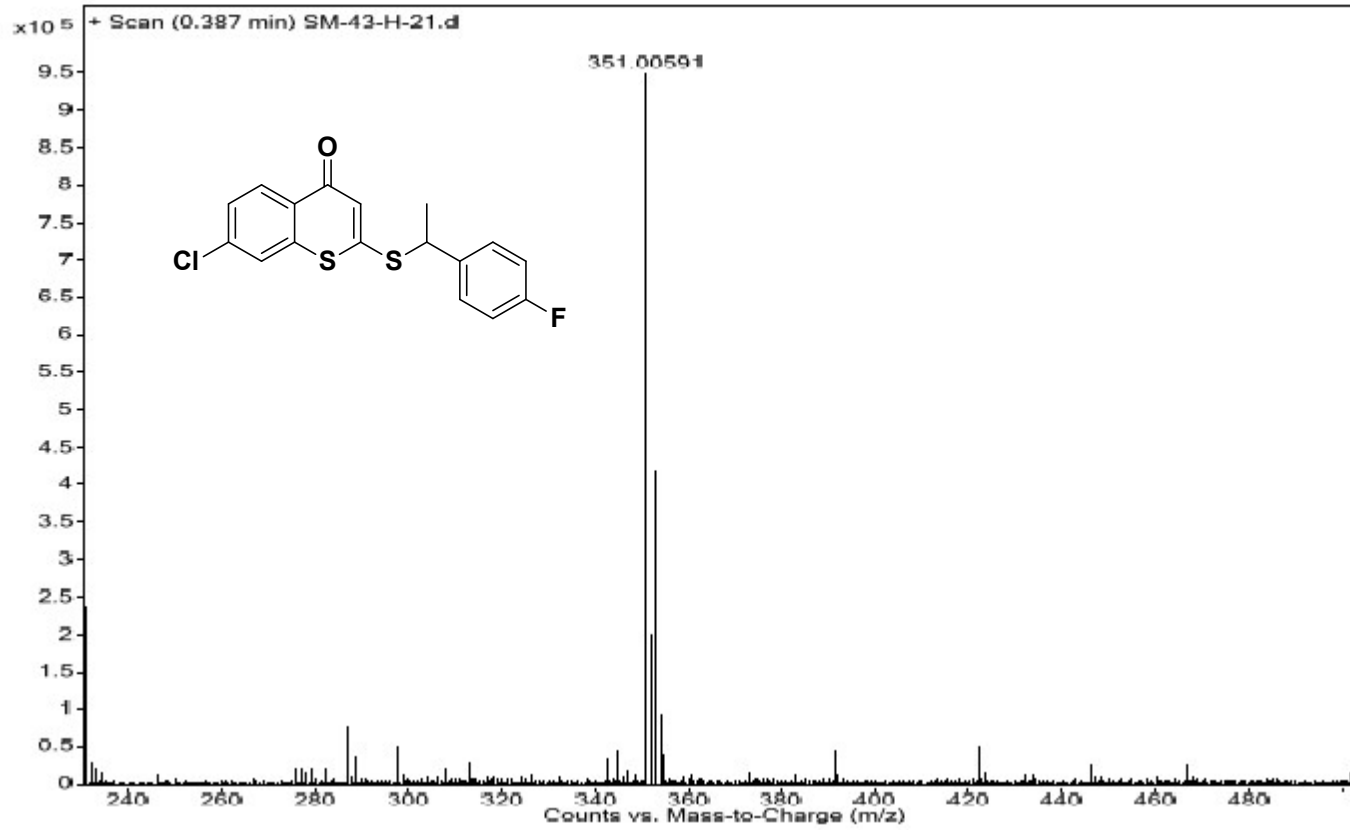
48.11

22.62



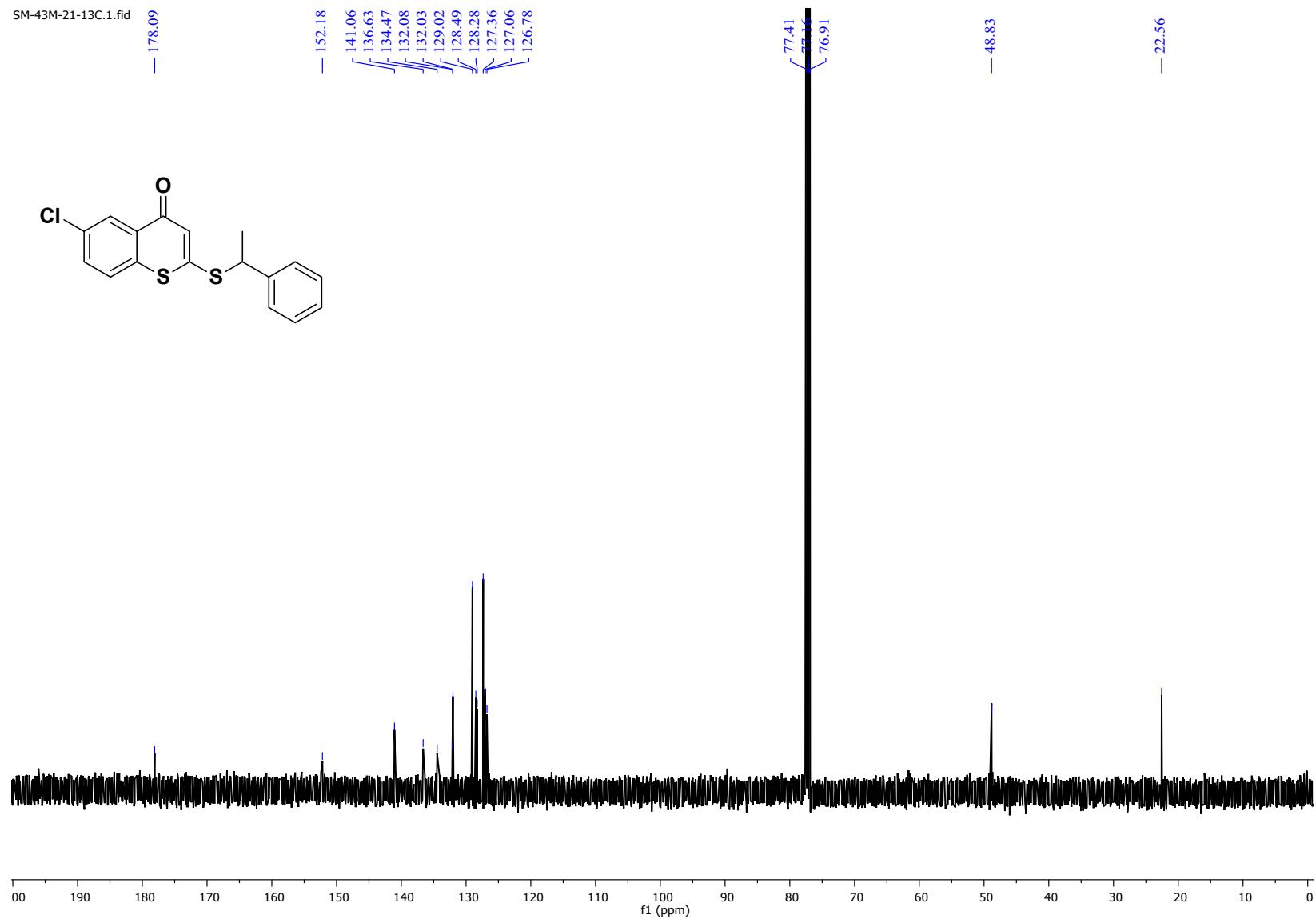
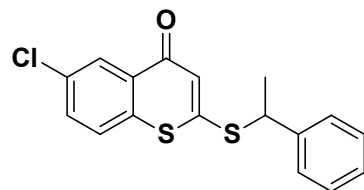
HRMS of compound 7g

Sample Name	SAMPLE	Position	P2-A9	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-43-H-21.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/18/2021 5:17:40 PM



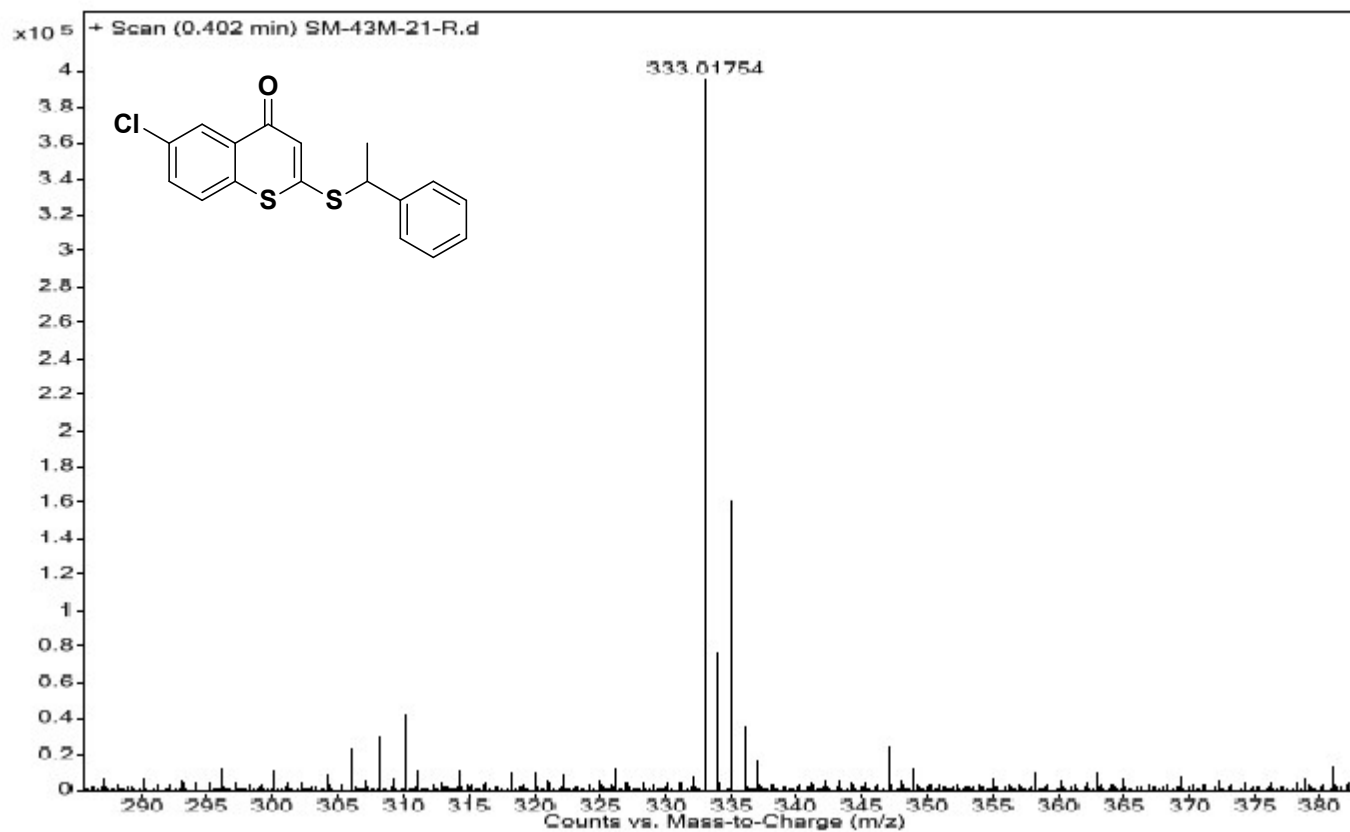
¹³C NMR of compound 7h

SM-43M-21-13C.1.fid



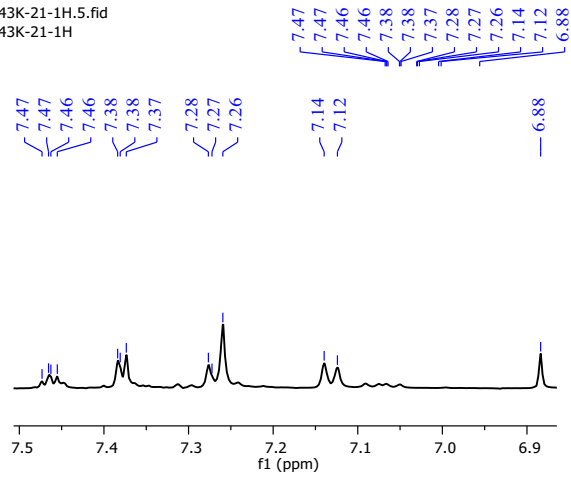
HRMS of compound 7h

Sample Name	WASH	Position	P1-A6	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-43M-21-R.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/19/2021 12:36:52 PM



¹H NMR of compound of 7i

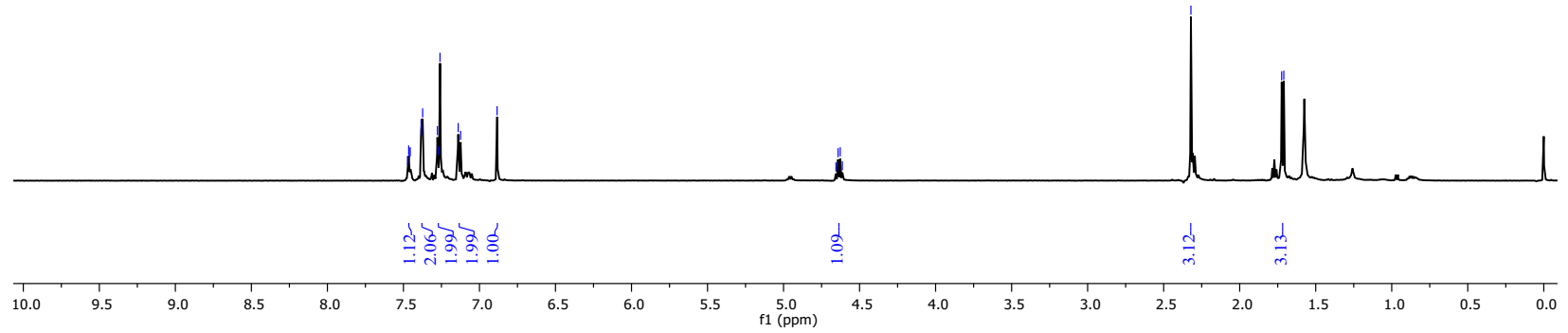
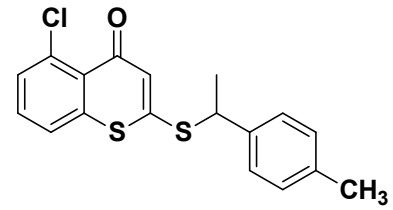
SM-43K-21-1H.5.fid
SM-43K-21-1H



4.66
4.64
4.63
4.61

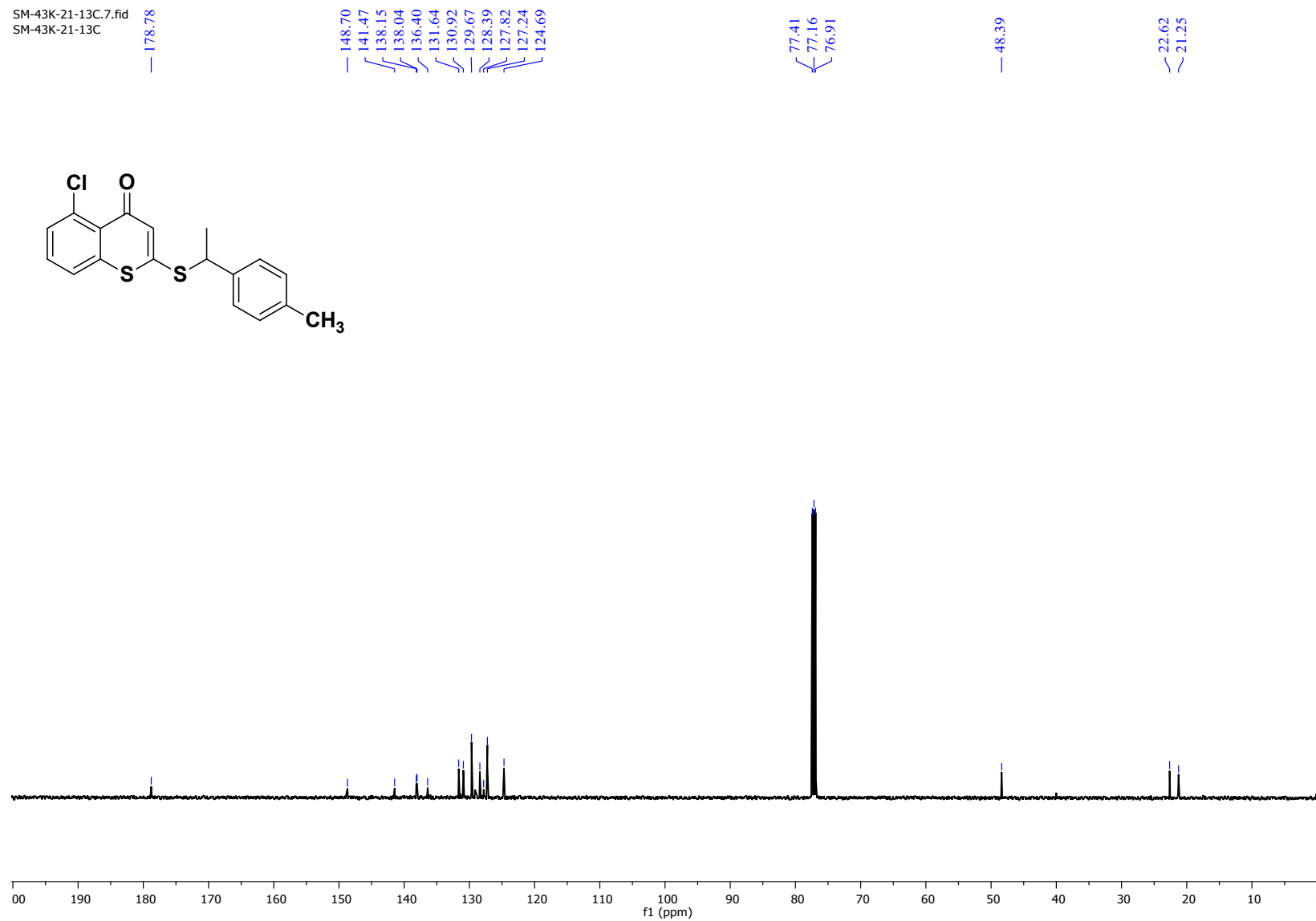
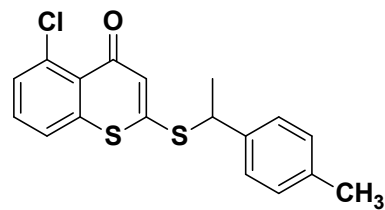
2.32

1.72
1.71



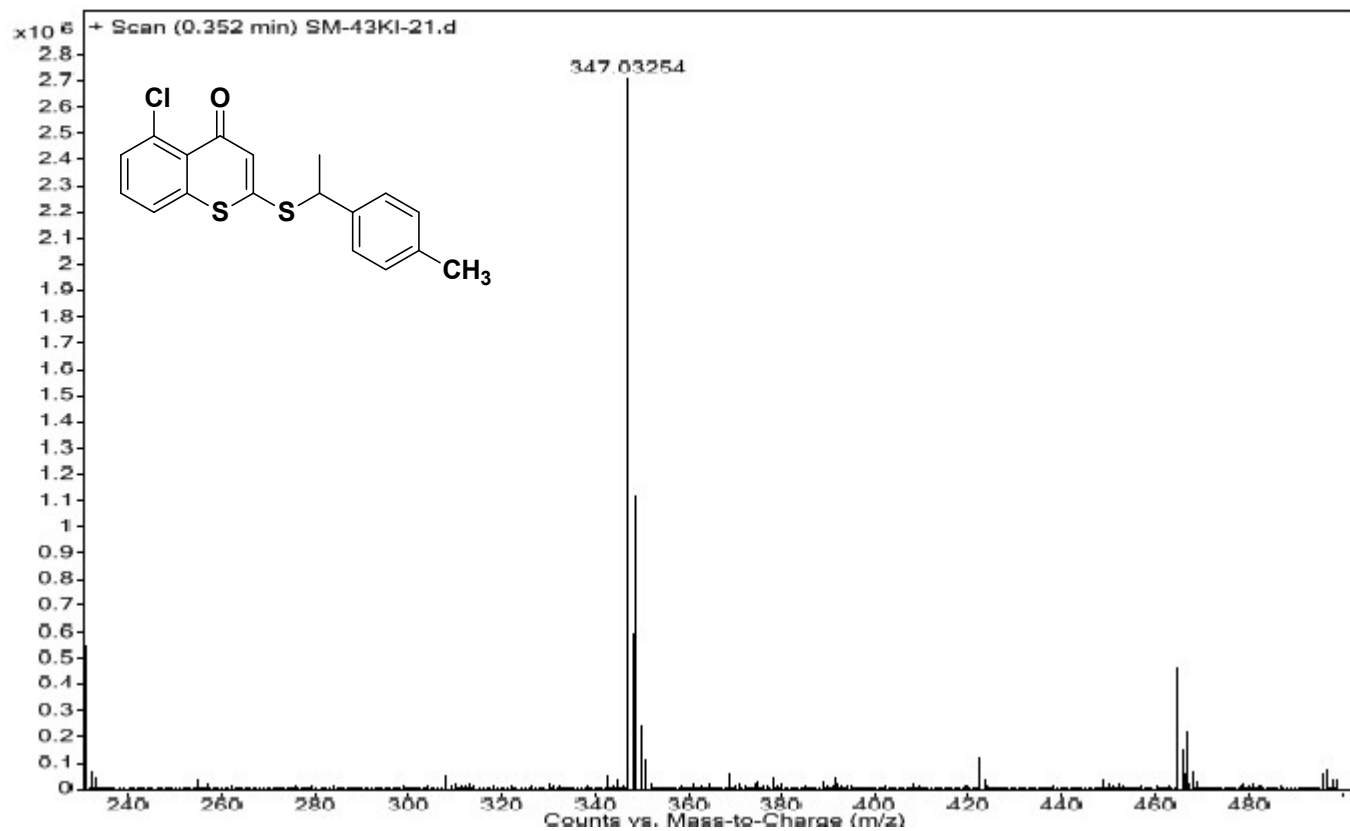
¹³C NMR of compound 7i

SM-43K-21-13C.7.fid
SM-43K-21-13C



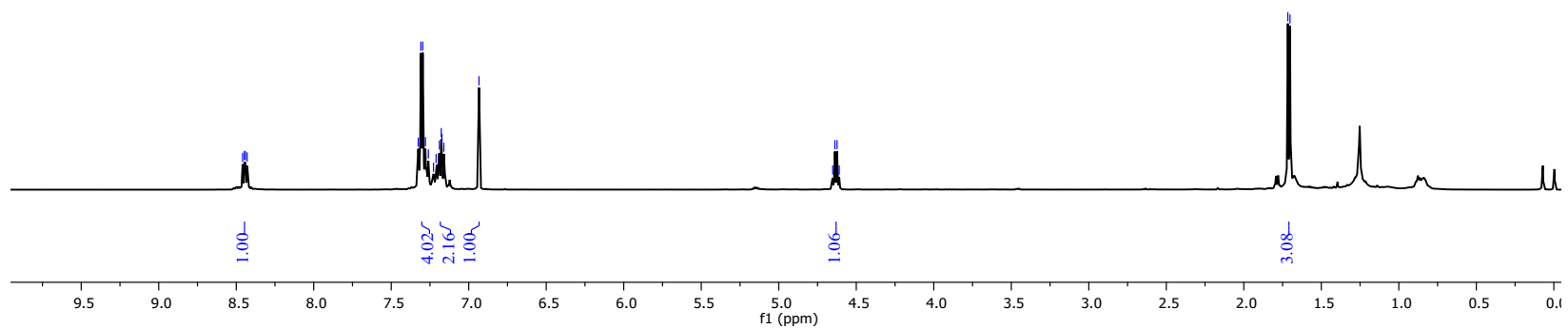
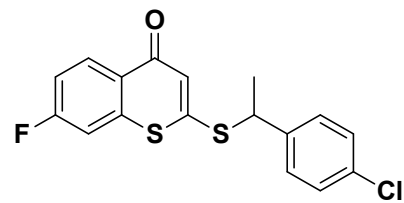
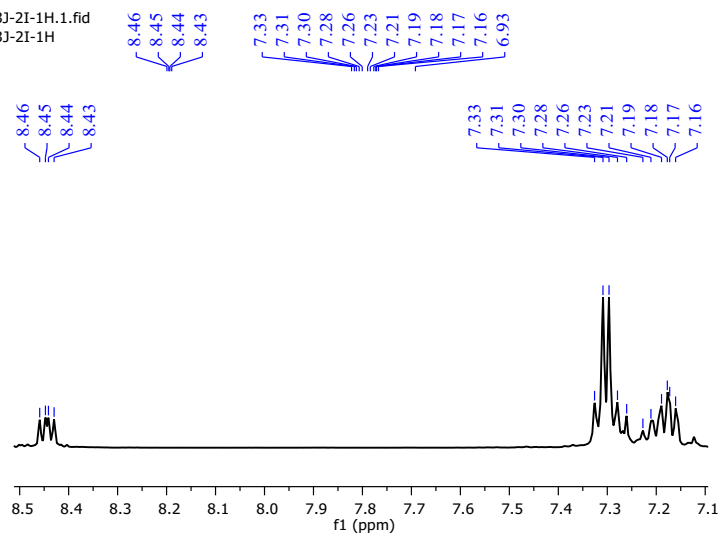
HRMS of compound 7i

Sample Name	SAMPLE 22	Position	P1-B8	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-43KI-21.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/11/2021 12:45:34 PM



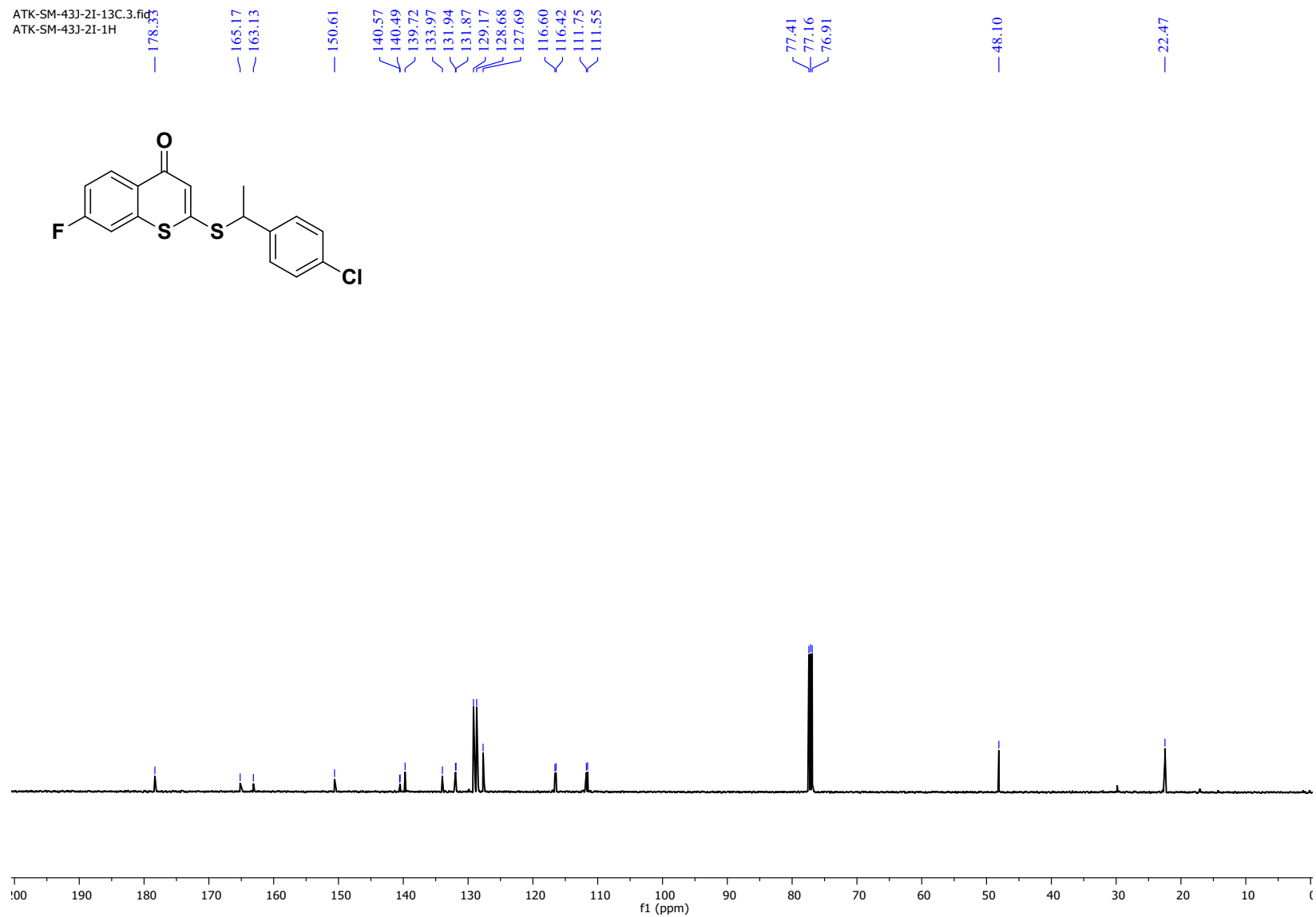
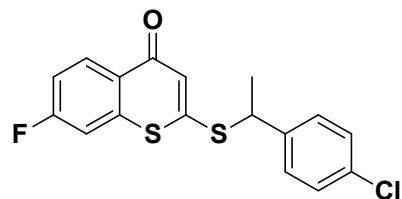
¹H NMR of compound 7j

ATK-SM-43J-2I-1H.1.fid
ATK-SM-43J-2I-1H



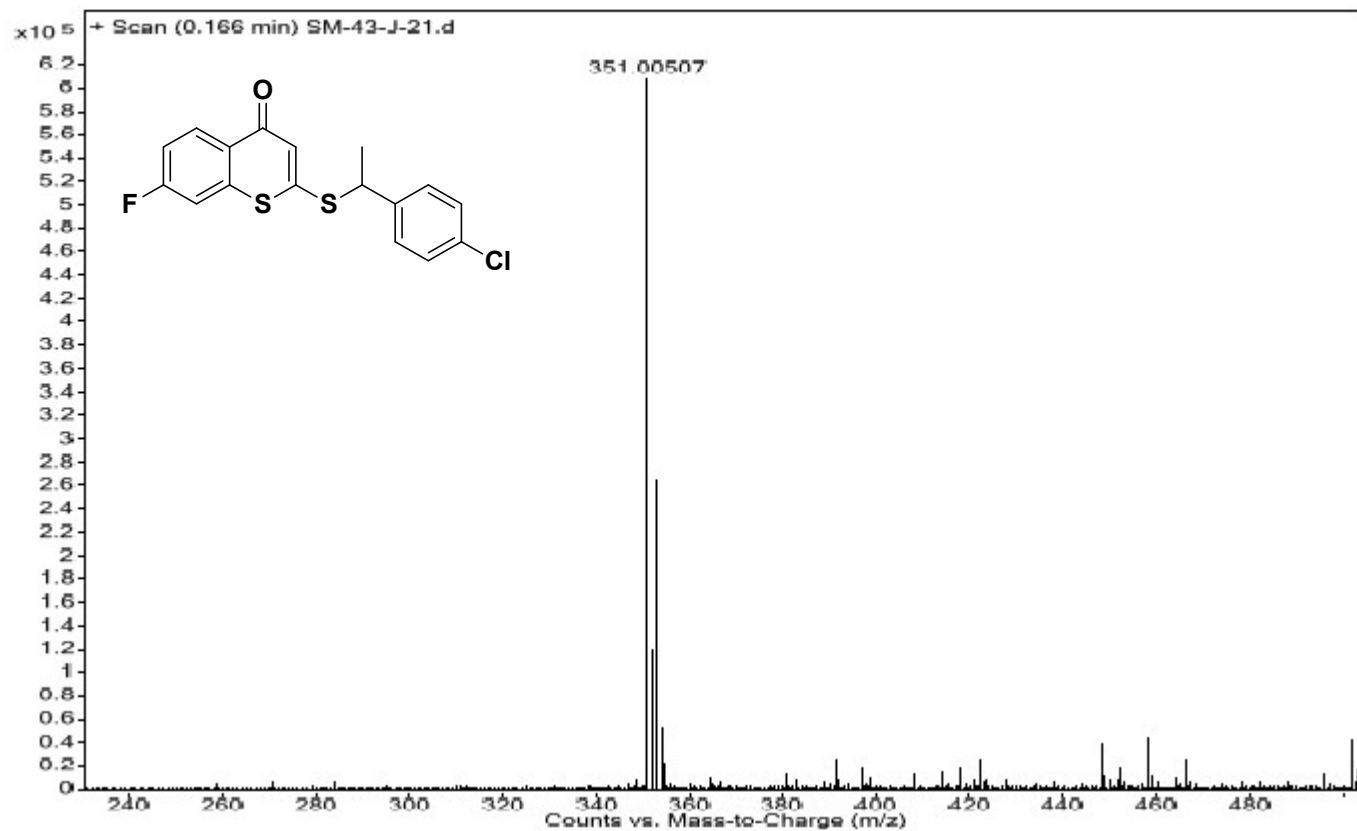
¹³C NMR of compound 7j

ATK-SM-43J-2I-13C.3.fid
ATK-SM-43J-2I-1H



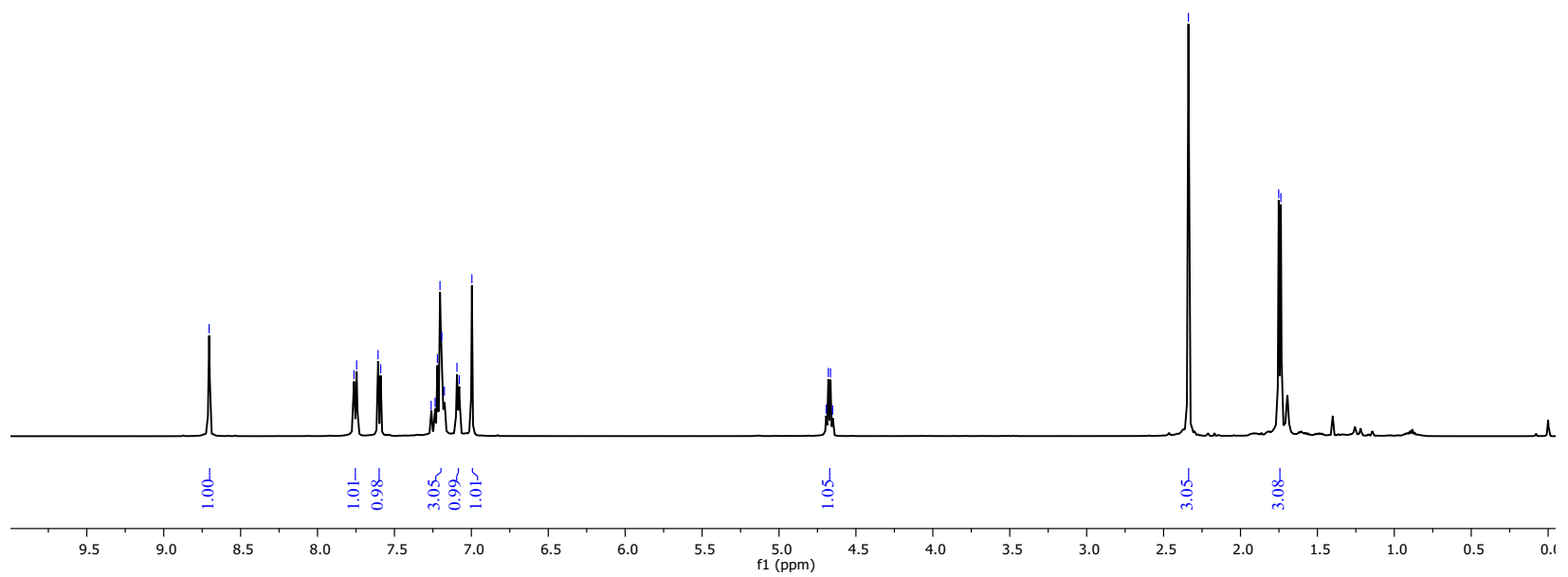
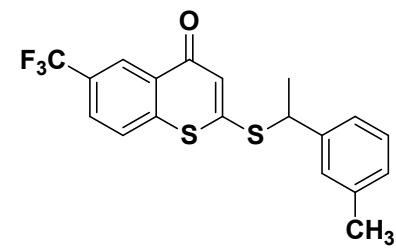
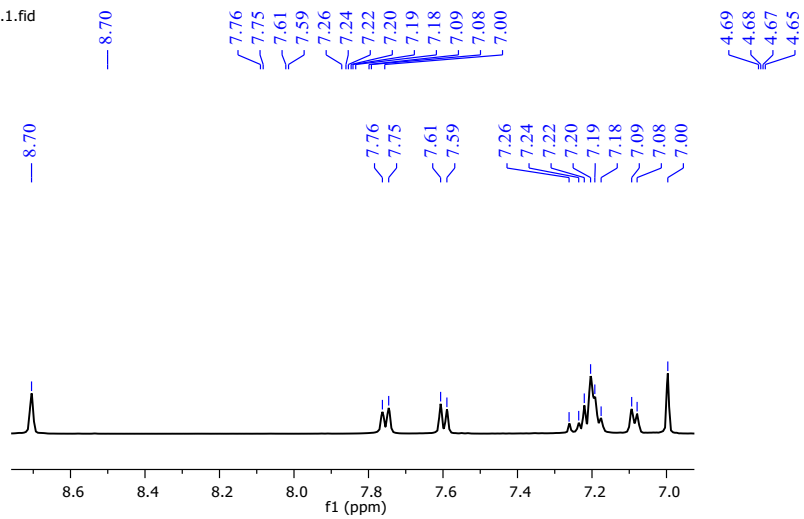
HRMS of compound 7j

Sample Name	SAMPLE	Position	P2-A10	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-43-J-21.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/18/2021 5:28:35 PM



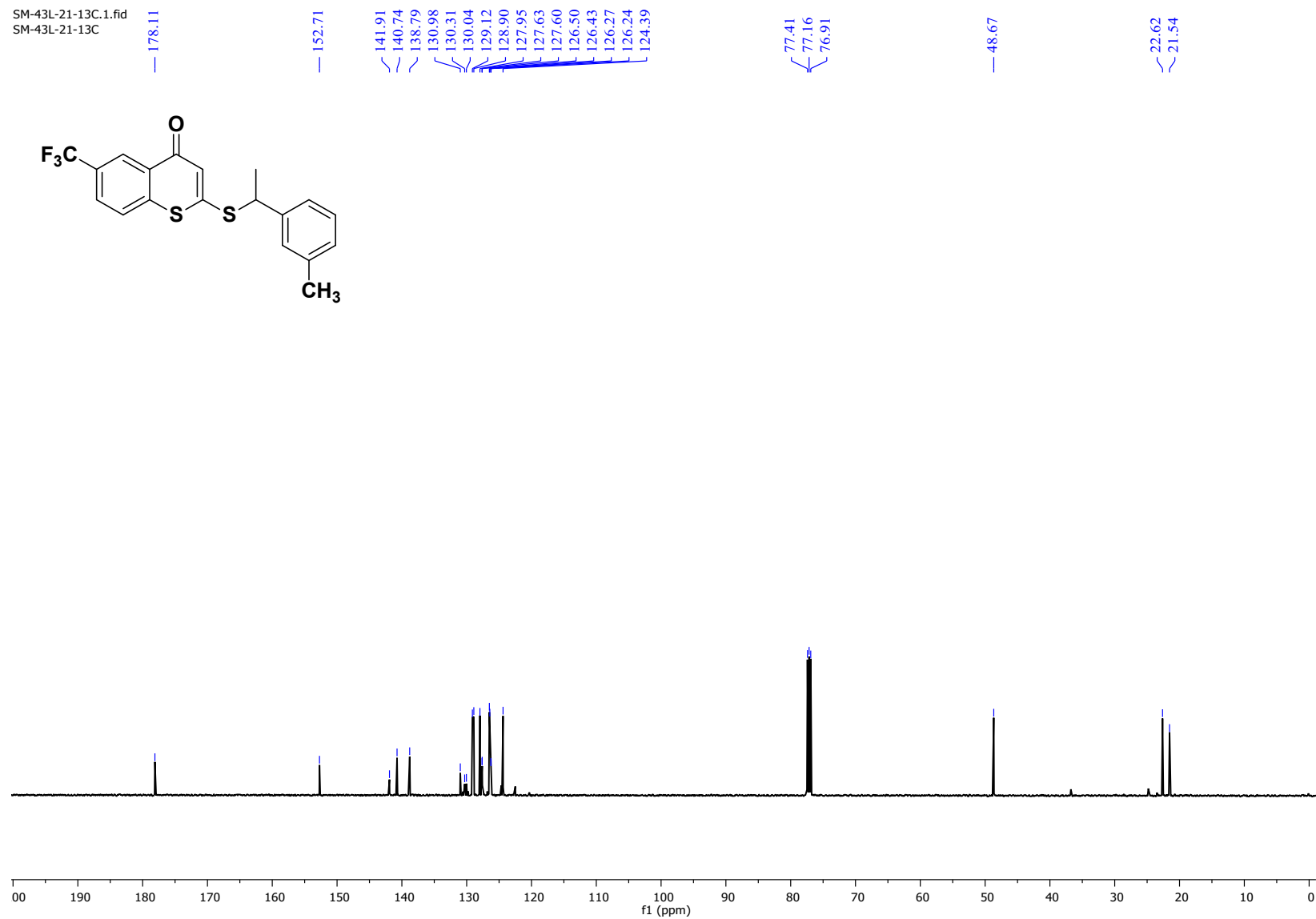
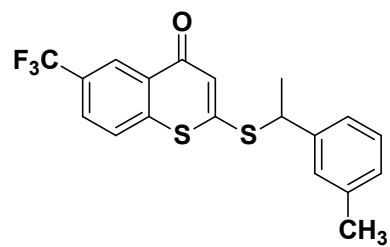
¹H NMR of compound 7k

SM-43L-21-1H.1.fid
SM-43L-21-1H



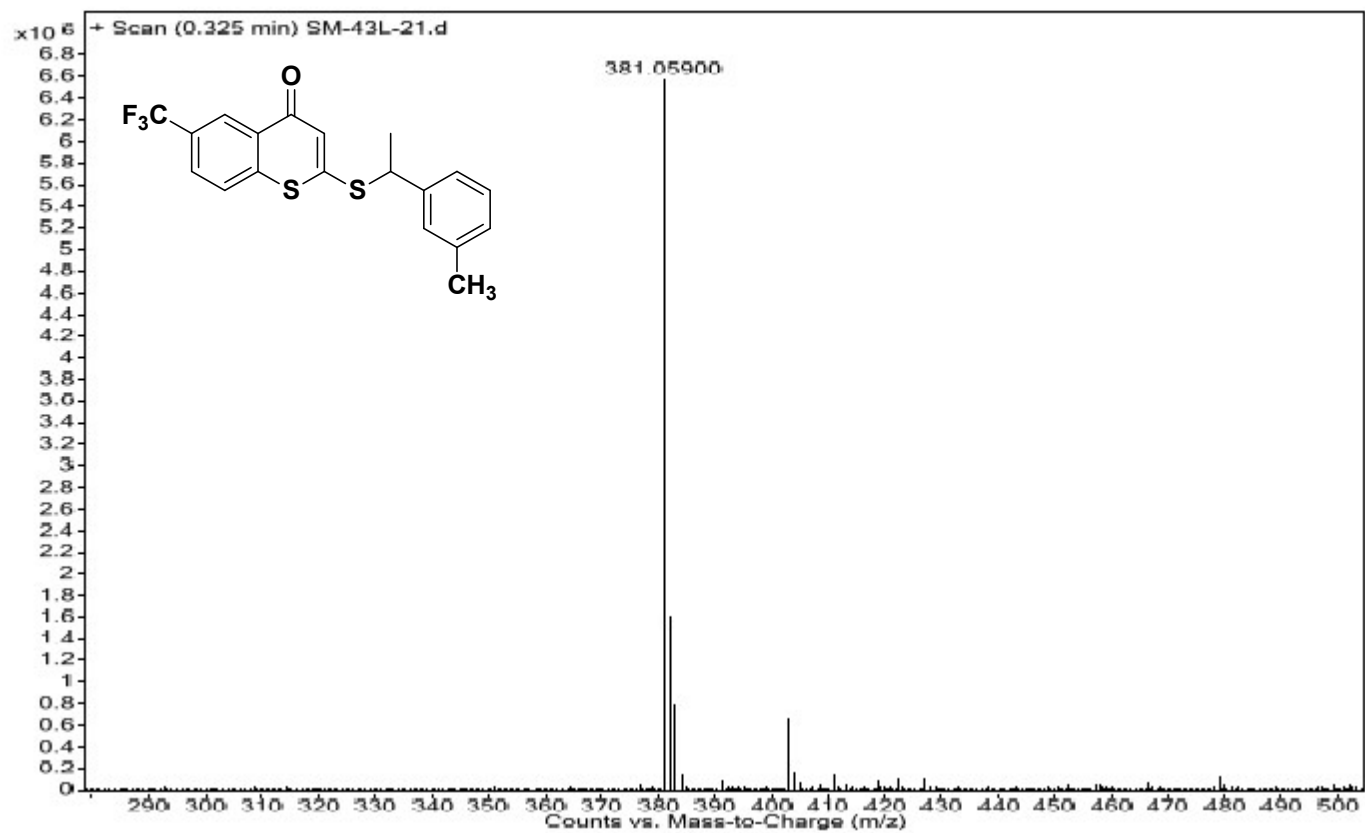
¹³C NMR of compound 7k

SM-43L-21-13C.1.fid
SM-43L-21-13C

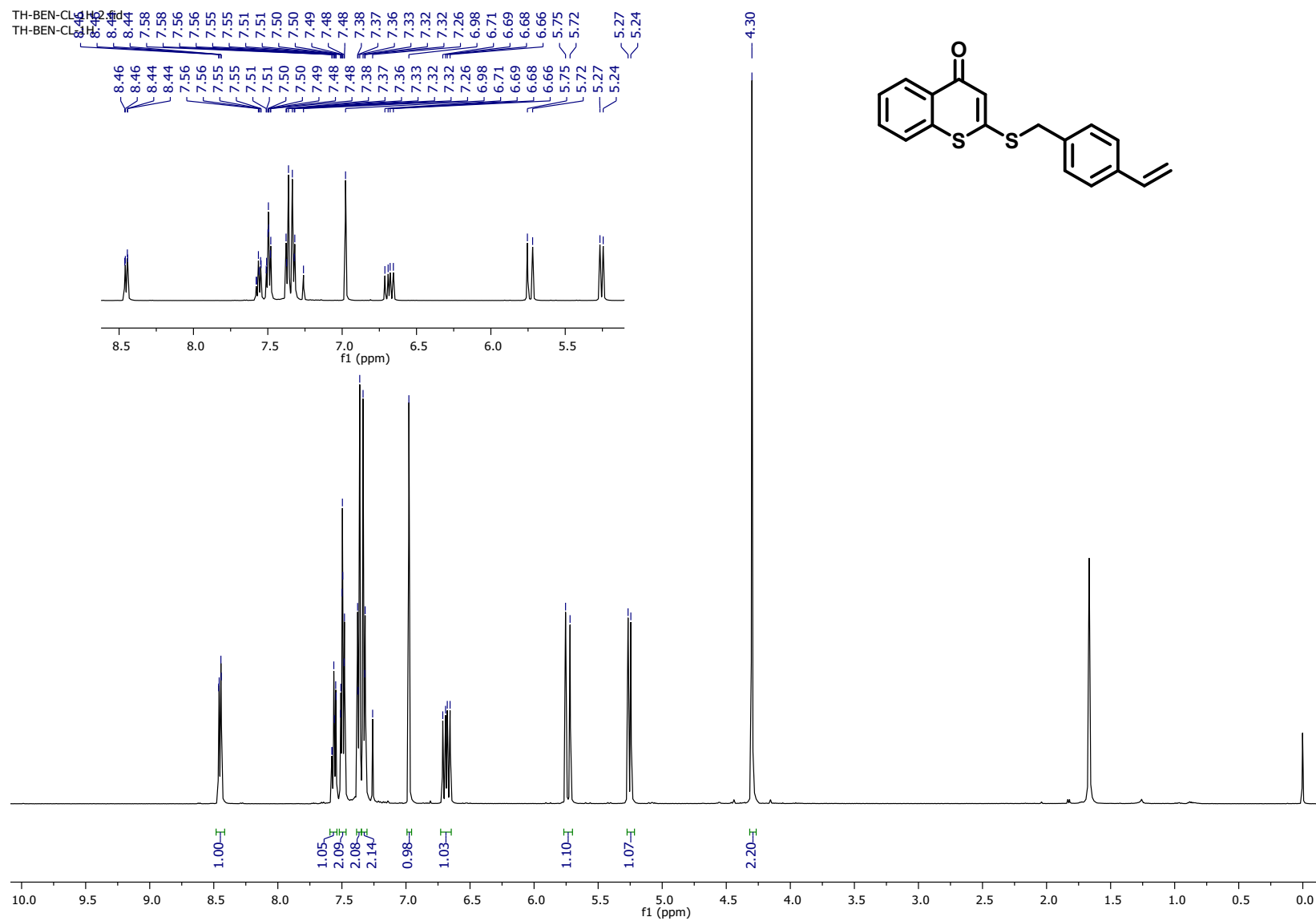


HRMS of compound 7k

Sample Name	WASH	Position	P1-A5	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SM-43L-21.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	2/19/2021 12:35:03 PM

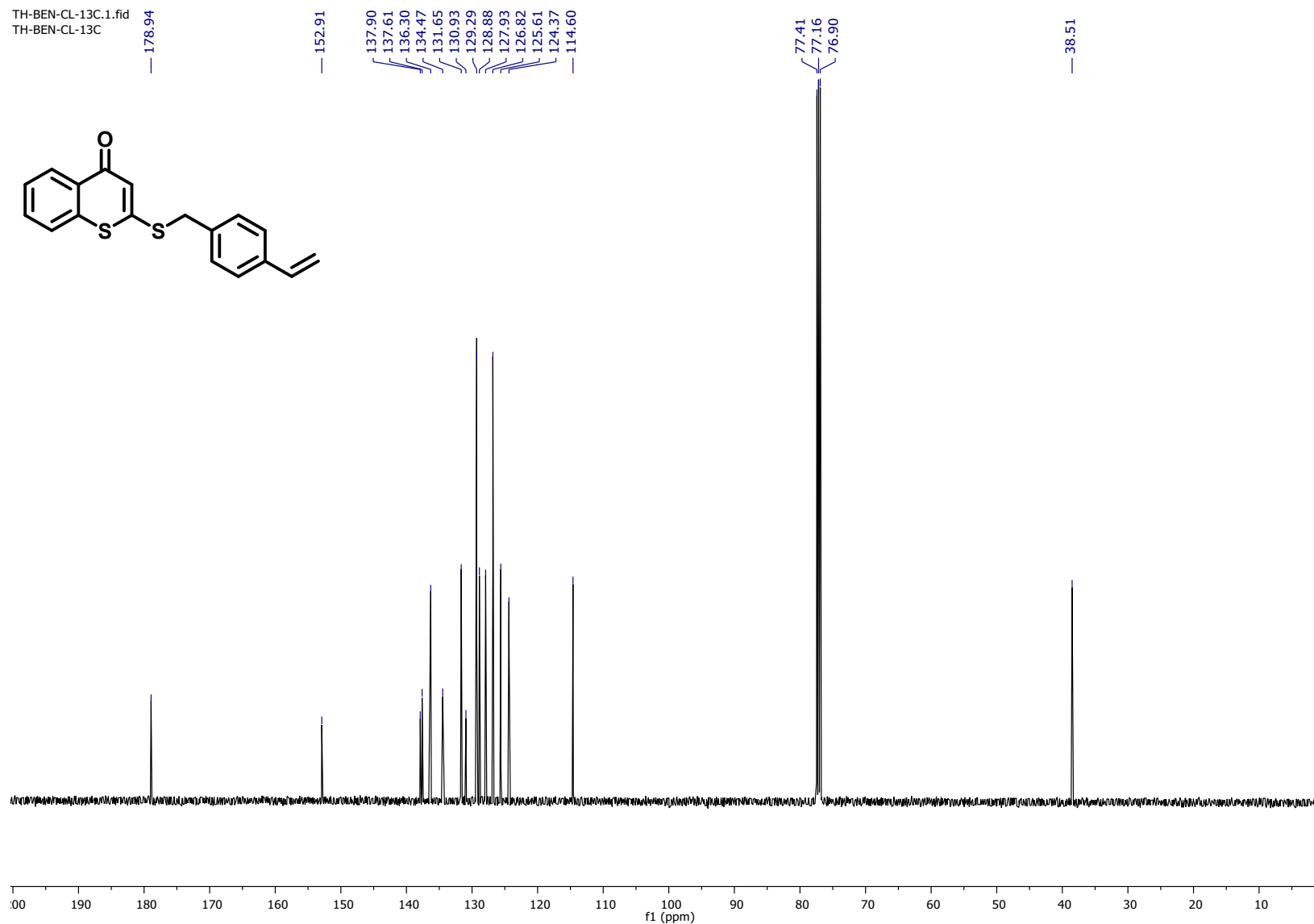
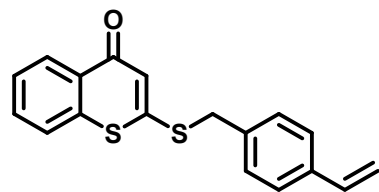


¹H NMR of 2-((4-vinylbenzyl)thio)-4*H*-thiochromen-4-one



¹³C NMR of 2-((4-vinylbenzyl)thio)-4*H*-thiophen-4-one

TH-BEN-CL-13C.1.fid
TH-BEN-CL-13C



HRMS of 2-((4-vinylbenzyl)thio)-4*H*-thiochromen-4-one

Sample Name
User Name
Sample Type
ACQ Method

WASH

Sample

ESI ALS 100-1000,m

Position

Inj Vol

IRM Calibration Status

Comment

P2-B11

20

Success

Instrument Name

InjPosition

Data Filename

Acquired Time

Instrument 1

TH-Ber-CL.d

31-Aug-21 07:07:18 PM (UTC+05:30)

