

Electronic Supporting Information

Copper (II) triflate catalyzed three-component reaction for the synthesis of 2,3-diarylquinoline derivatives using aryl amines, aryl aldehydes and styrene oxides

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Title page	S1
Crystal Data and Structure Refinement for Compound 5e	S2
Copies of ¹ H NMR, ¹³ C NMR and HRMS spectra of all the Compounds	S3–S74

The left image is an ORTEP diagram of compound 5e, showing the crystal structure with thermal ellipsoids at the 50% probability level. The structure is a complex polycyclic molecule with various functional groups, including carboxylate (COO), hydroxyl (OH), and a fluorine atom (F1). The right image is a chemical structure of compound 5e, which is a 2,6-diphenyl-4-methoxy-1H-benzimidazole derivative. The structure is color-coded: the benzimidazole core is blue, the phenyl rings are red, and the methoxy group is green. The label '5e' is placed below the nitrogen atom.

Identification code	Compound 5c
Empirical formula	C ₂₂ H ₁₆ FNO
Formula weight	329.12
Temperature	296 K
Wavelength	0.71073
Radiation type	MoK α
Radiation source	'fine-focus sealed tube'
Crystal system	Monoclinic
Space group	P 2 ₁ /c
Cell length	A = 13.9206 (6), b = 9.0995(4), c = 14.8399(6)
Cell Angle	α = 90, β = 116.476(1), γ = 90
Cell Volume	1682.63(12)
Density	1.3
Completeness to theta	0.999-28.489
Absorption correction	multi-scan
Refinement method	Full
Index ranges	-18 $\leq$ h $\leq$ 18, -12 $\leq$ k $\leq$ 12, -19 $\leq$ l $\leq$ 19
Reflection number	83679
Theta range	1.634-28.489
Cell formula units Z	1
CCDC no.	2040858

¹H NMR spectrum of compound: 4a

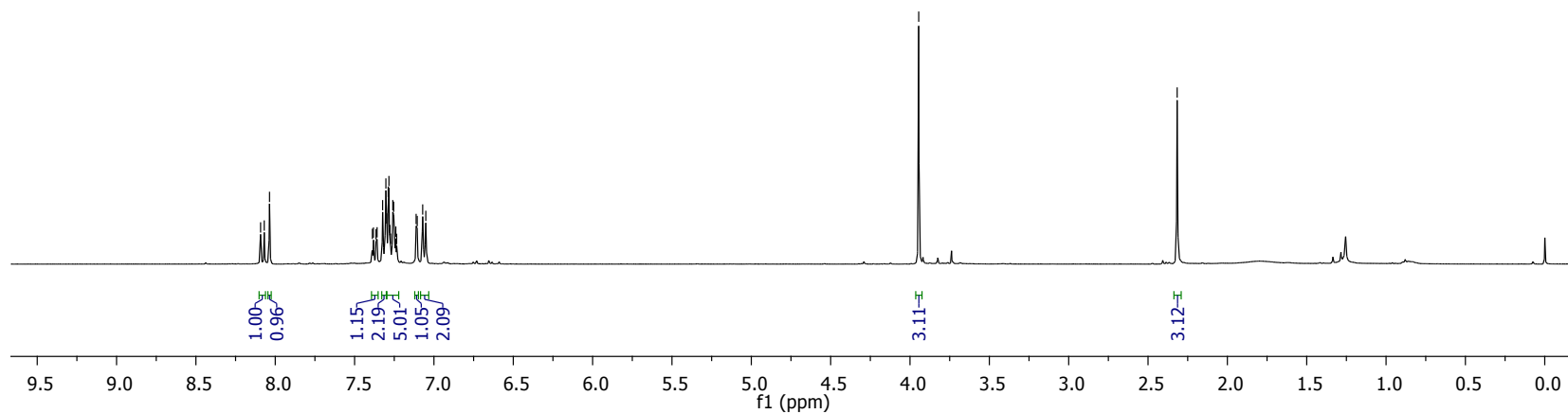
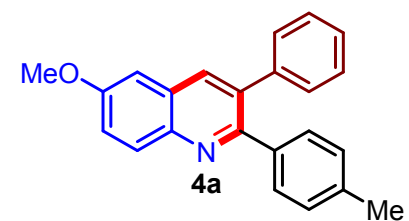
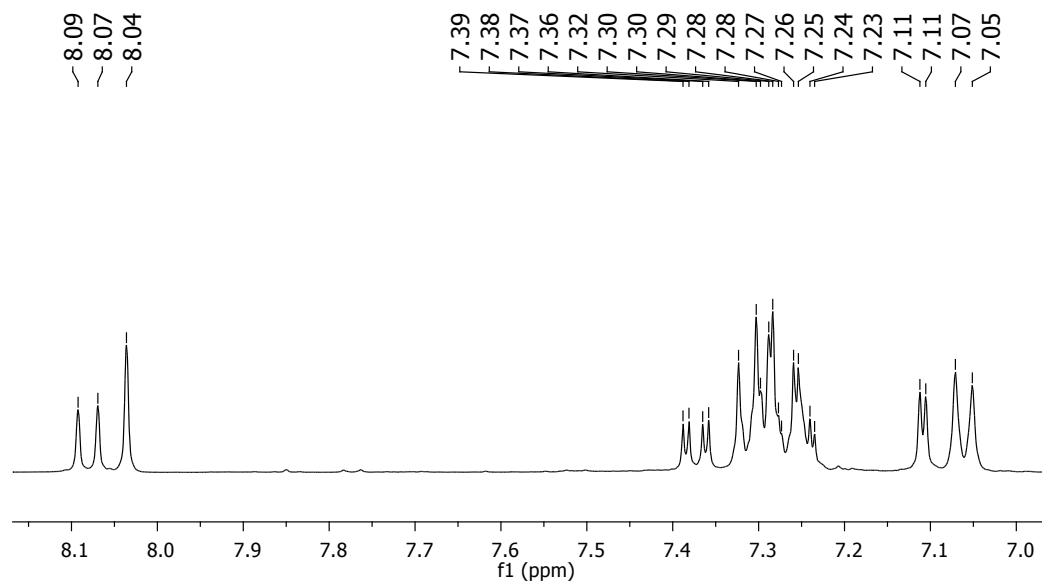
ATK-SA-4-OME-A-1H
ATK-SA-4-OME-A-1H

8.09
8.07
8.04
7.39
7.38
7.37
7.36
7.32
7.30
7.30
7.29
7.28
7.28
7.27
7.26
7.25
7.24
7.23
7.11
7.11
7.07
7.05

8.09
8.07
8.04
7.39
7.38
7.37
7.36
7.32
7.30
7.30
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7.07
7.05

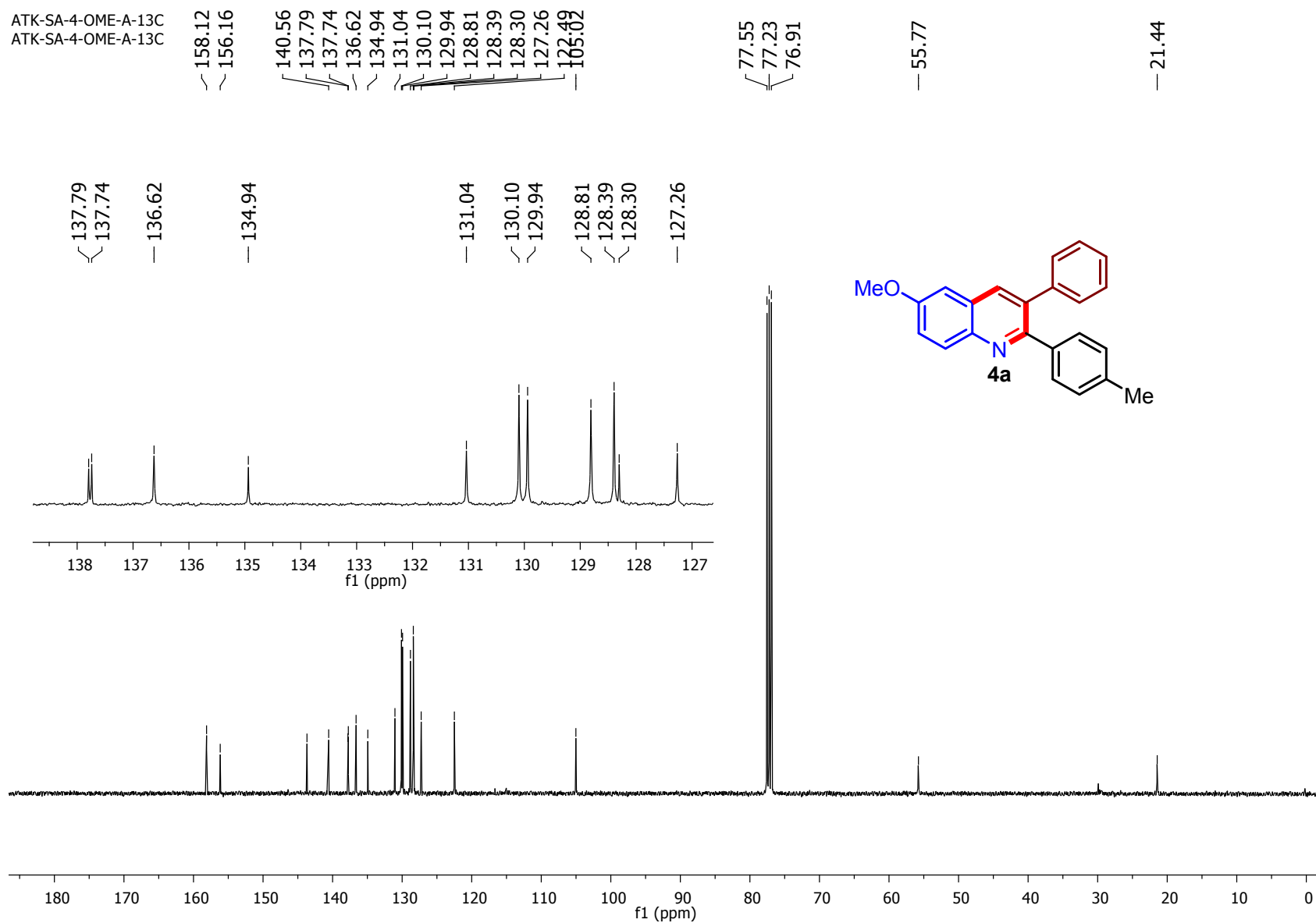
— 3.95

— 2.32



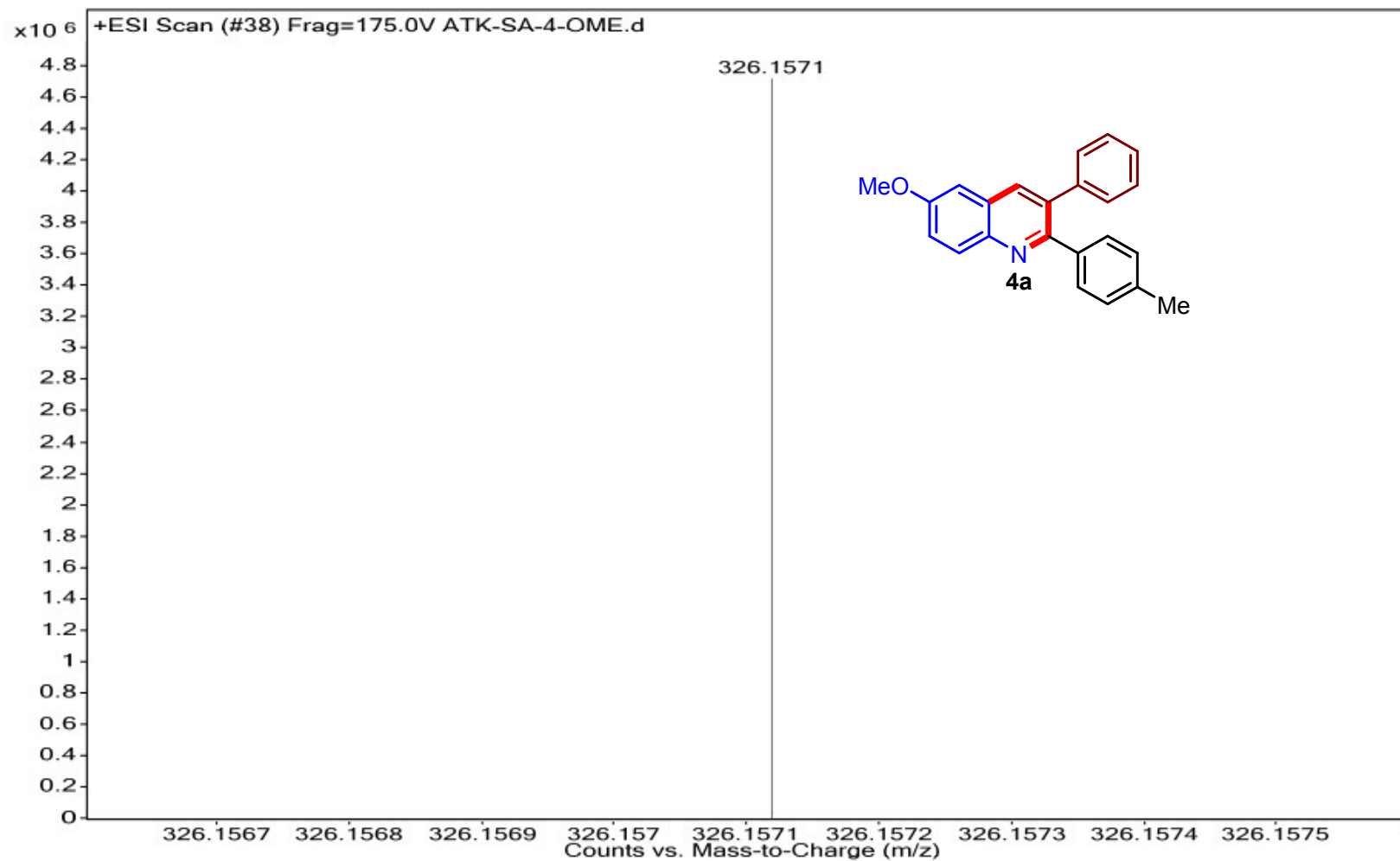
¹³CNMR spectrum of compound: 4a

ATK-SA-4-OME-A-13C
ATK-SA-4-OME-A-13C



HRMS spectrum of compound: 4a

Sample Name	SAMPLE 36	Position	P2-D4	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-4-OME.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	8/9/2019 6:10:27 PM



¹H NMR spectrum of compound: 4b

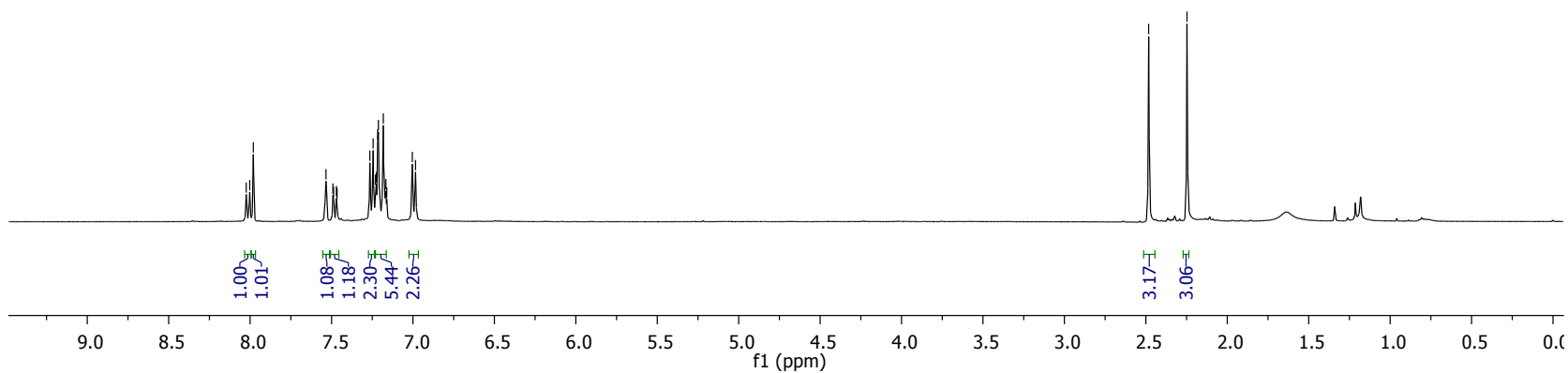
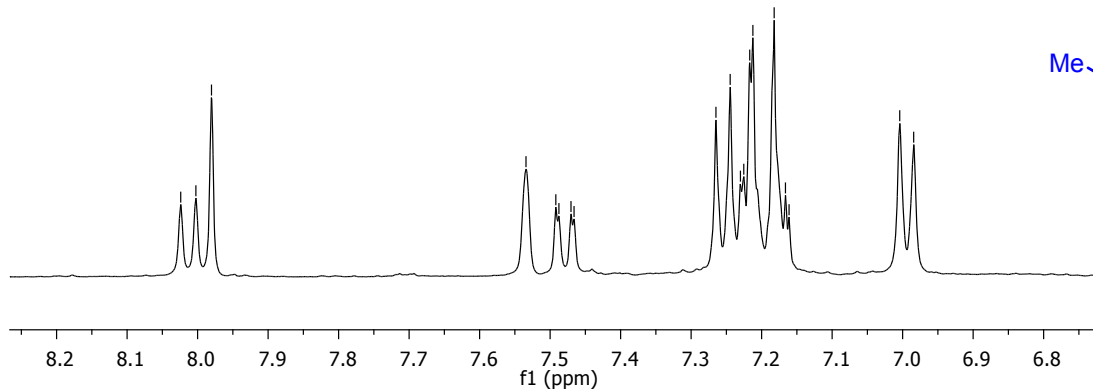
ATK-SA-4-ME-1H
ATK-SA-4-ME-1H

8.02
8.00
7.98
7.53
7.49
7.49
7.47
7.47
7.26
7.24
7.23
7.23
7.22
7.21
7.18
7.17
7.16
7.00
6.98

2.48
2.25

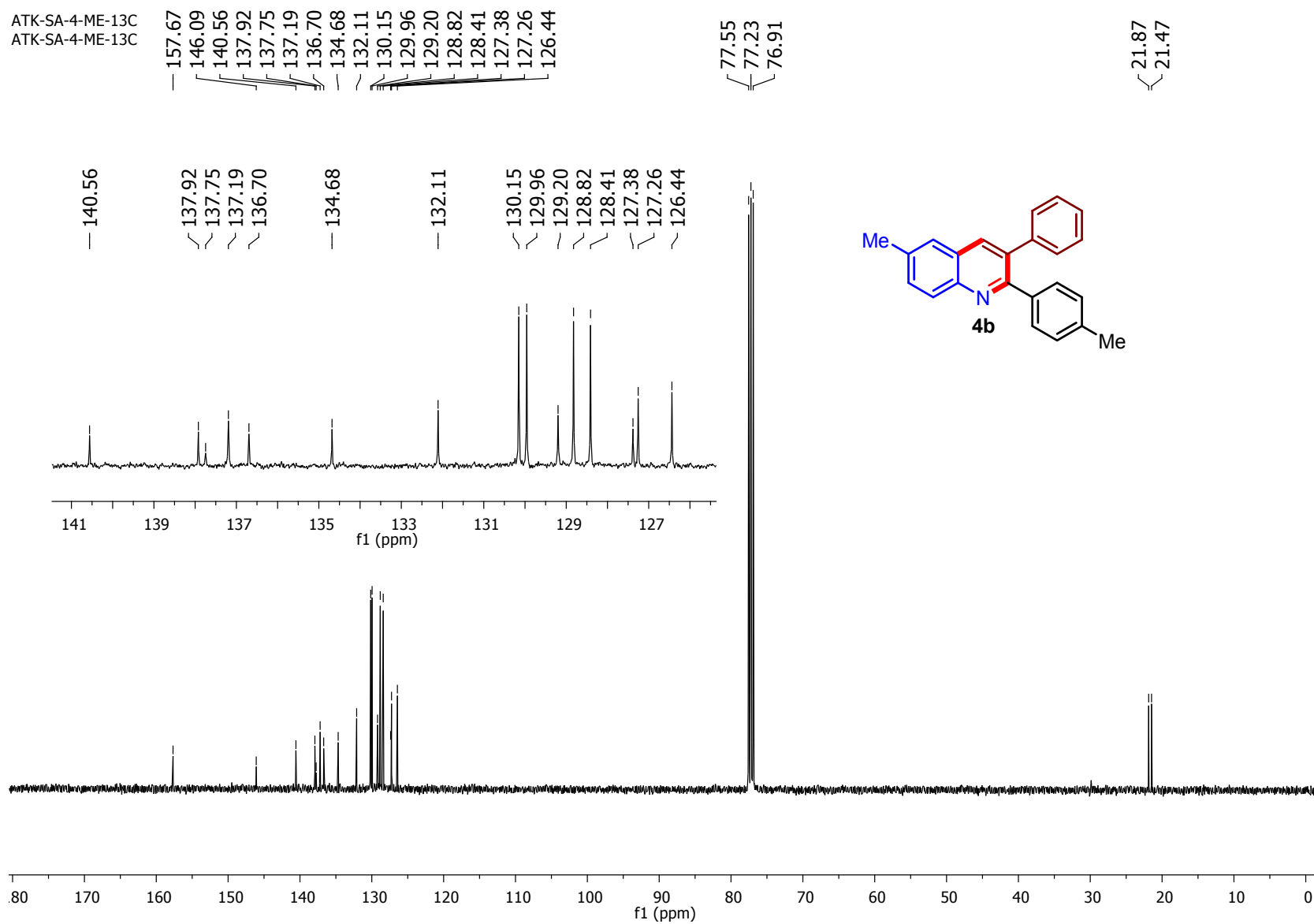
8.02
8.00
7.98

7.53
7.49
7.49
7.47
7.47
7.26
7.24
7.23
7.23
7.22
7.21
7.18
7.00
6.98



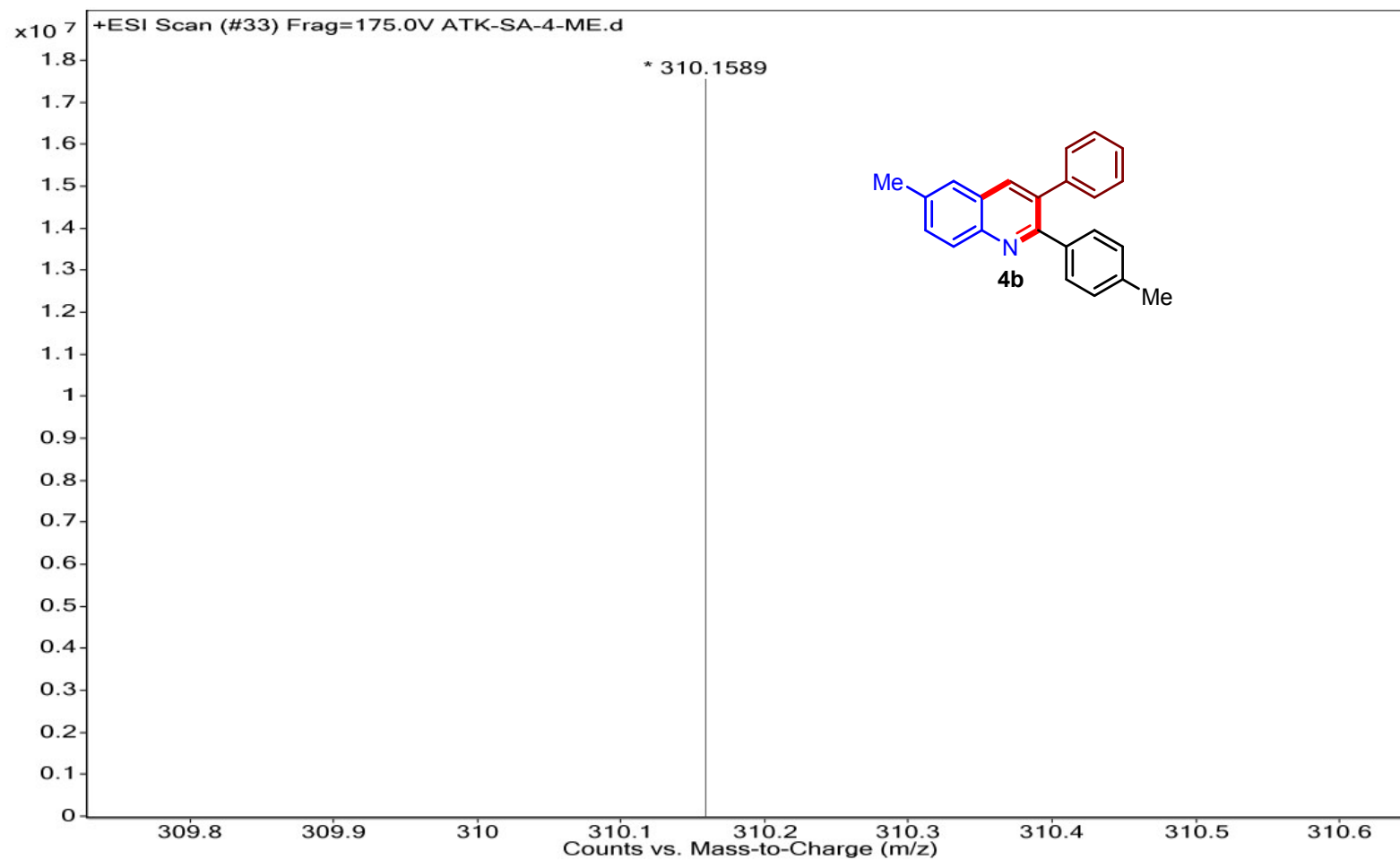
¹³CNMR spectrum of compound: 4b

ATK-SA-4-ME-13C
ATK-SA-4-ME-13C



MRMS spectrum of compound: 4b

Sample Name	SAMPLE	Position	P2-C11	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-4-ME.d	ACQ Method	ESI ALS 100-800.m	Comment		Acquired Time	8/1/2019 5:56:15 PM



¹H NMR spectrum of compound: 4c

ATK-UM-1-18-1H
ATK-UM-1-18-1H

8.03
8.01
7.98
7.52
7.50
7.48
7.25
7.23
7.20
7.20
7.19
7.18
7.18
7.16
7.15
7.14
6.98
6.96

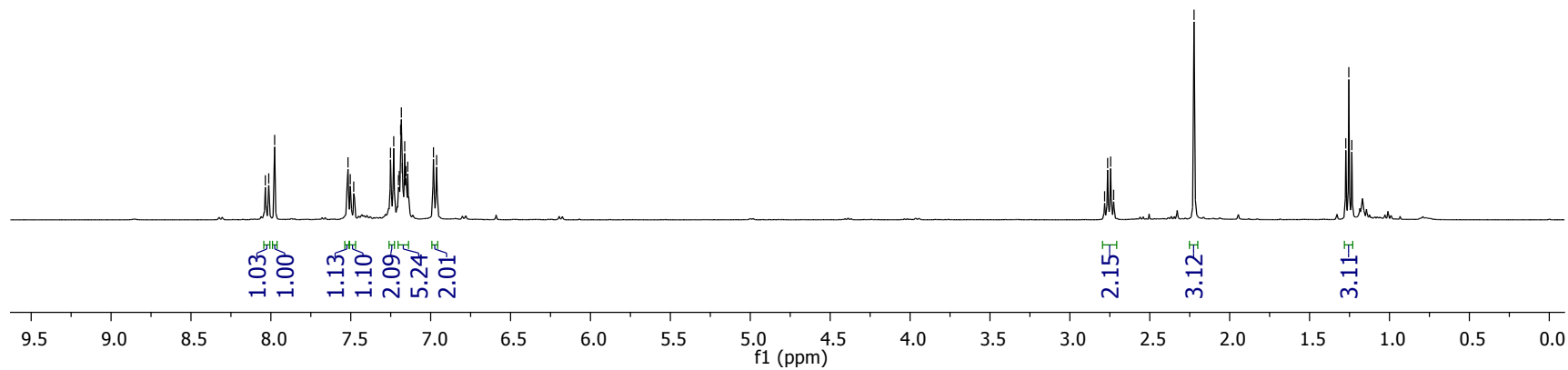
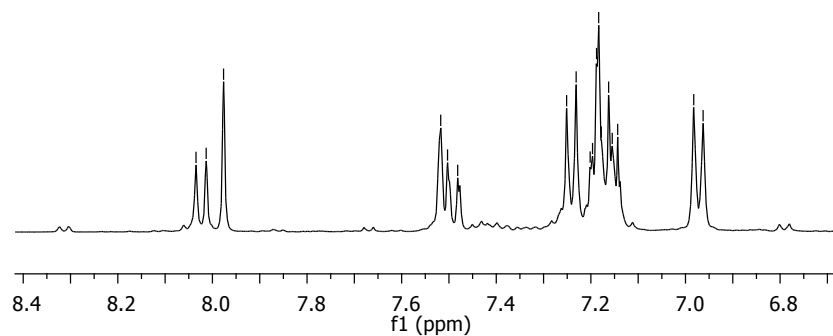
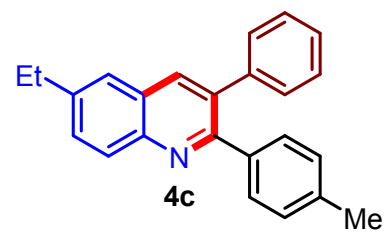
2.78
2.76
2.74
2.73
— 2.22

1.27
1.25
1.24

8.03
8.01
7.98

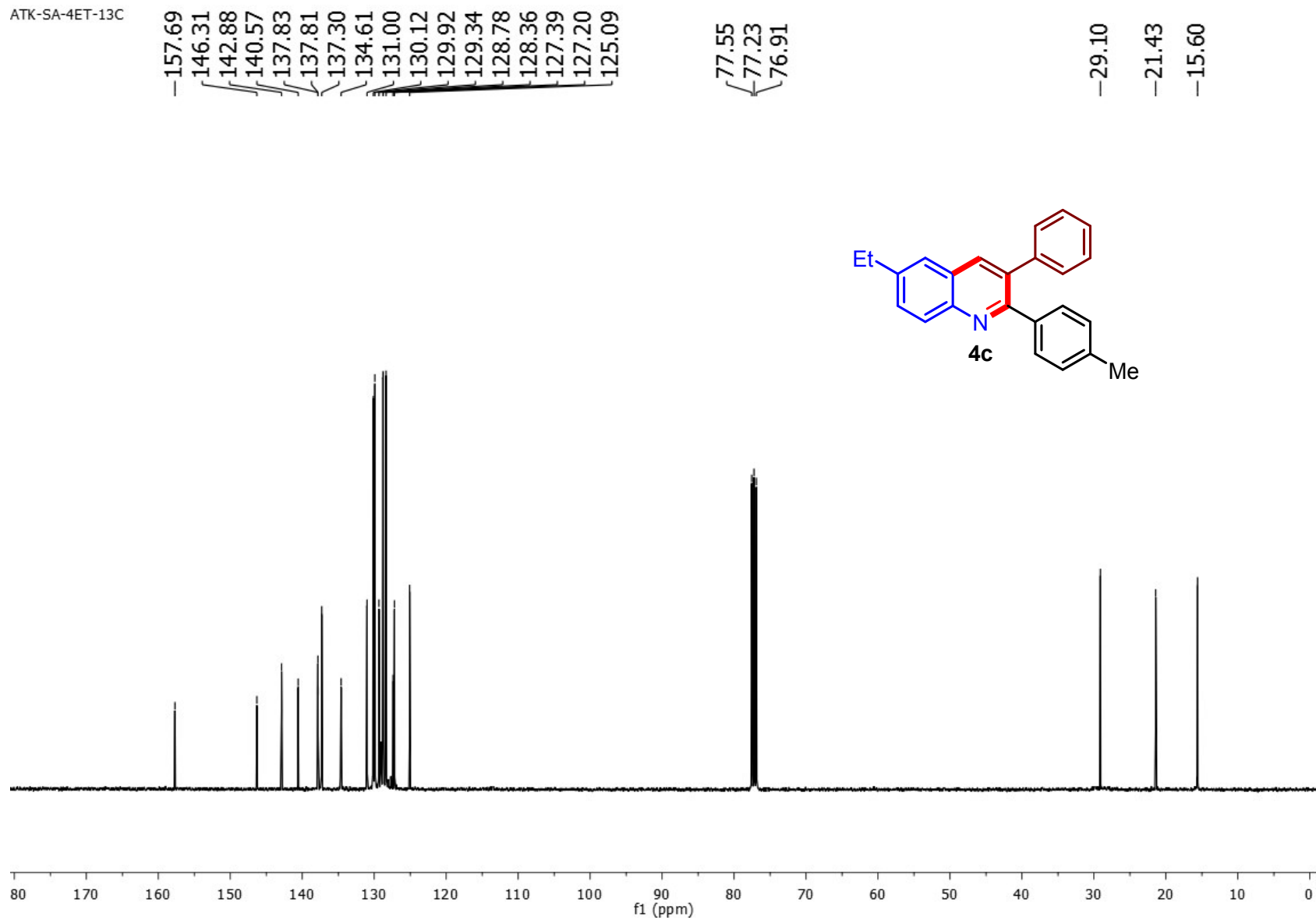
7.52
7.50
7.48

7.25
7.23
7.19
7.18
7.16
7.15
6.98
6.96



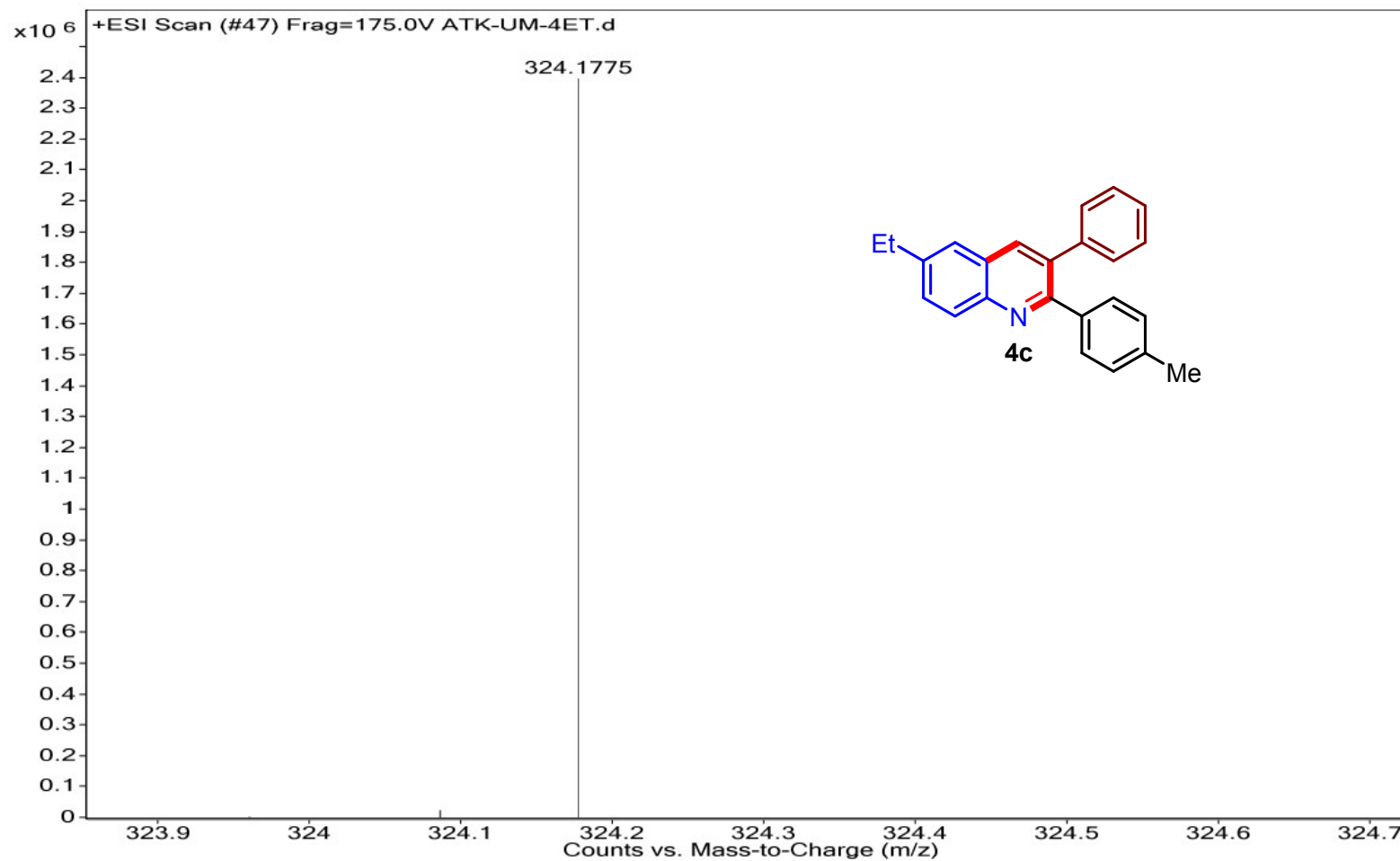
¹³CNMR spectrum of compound: 4c

ATK-SA-4ET-13C

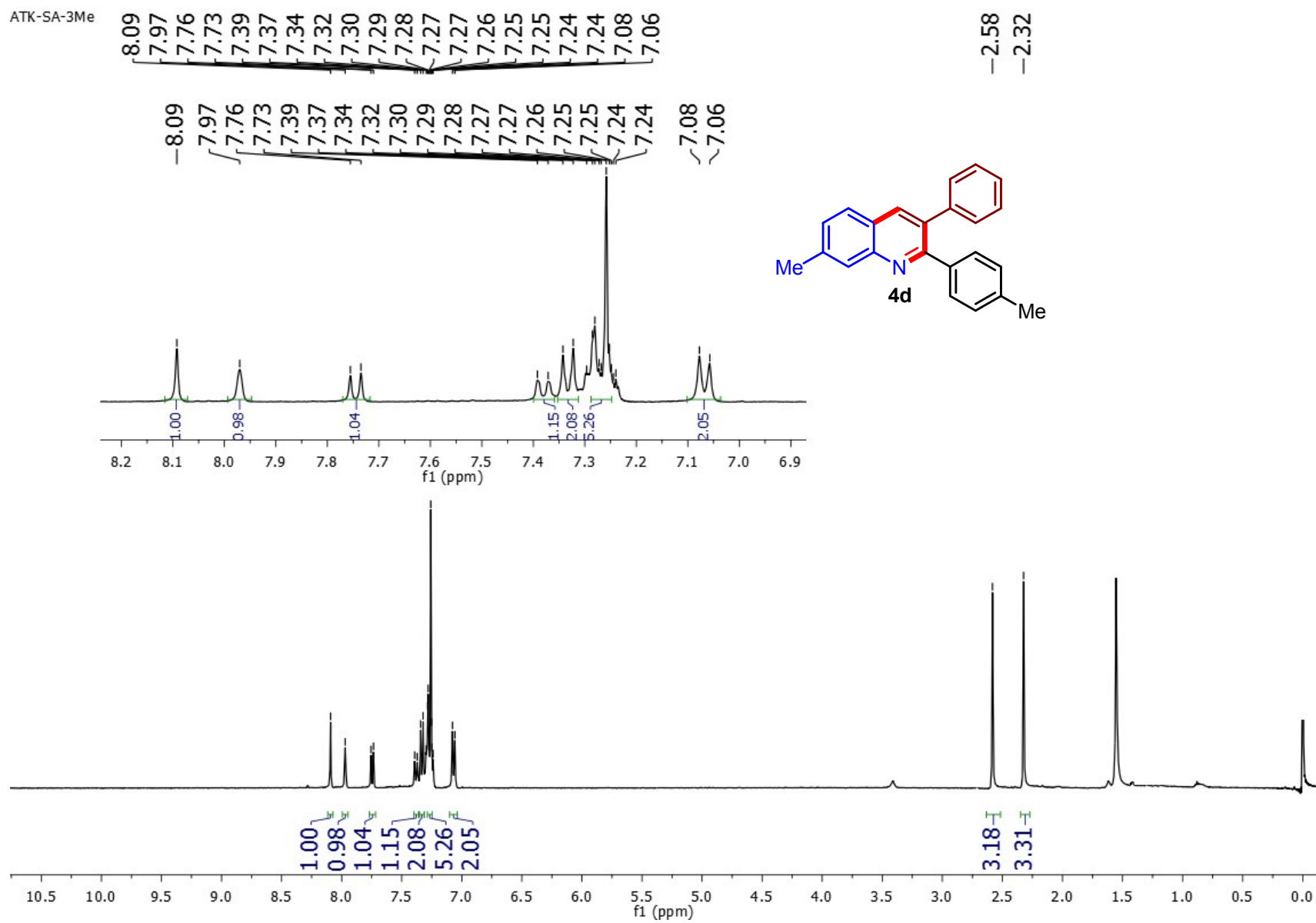


HRMS spectrum of compound: 4c

Sample Name	ATK-UM-4ET	Position	P1-D4	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-UM-4ET.d	ACQ Method	ESI ALS 200-700.m	Comment		Acquired Time	4/11/2019 12:17:54 PM

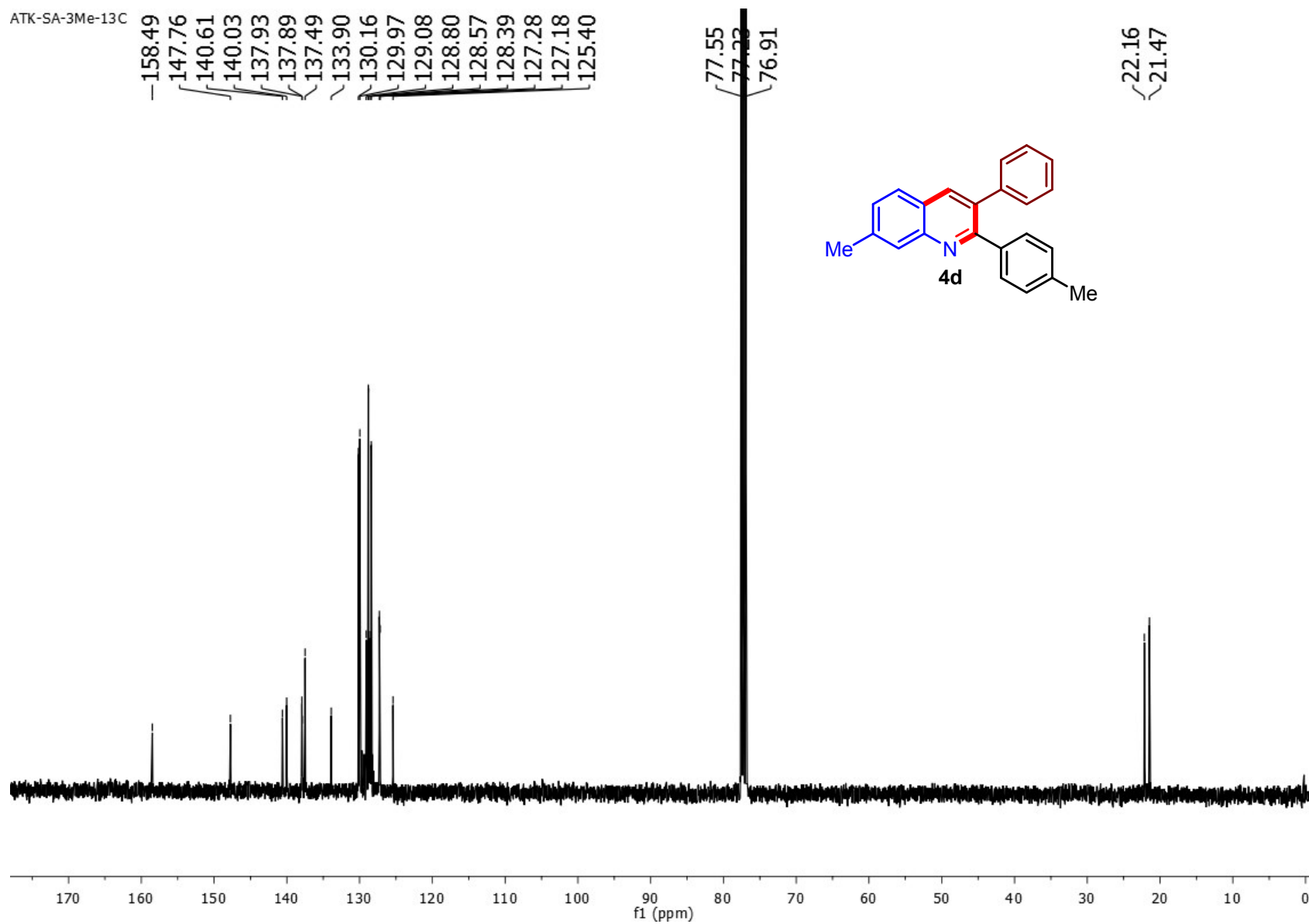


¹H NMR spectrum of compound: 4d



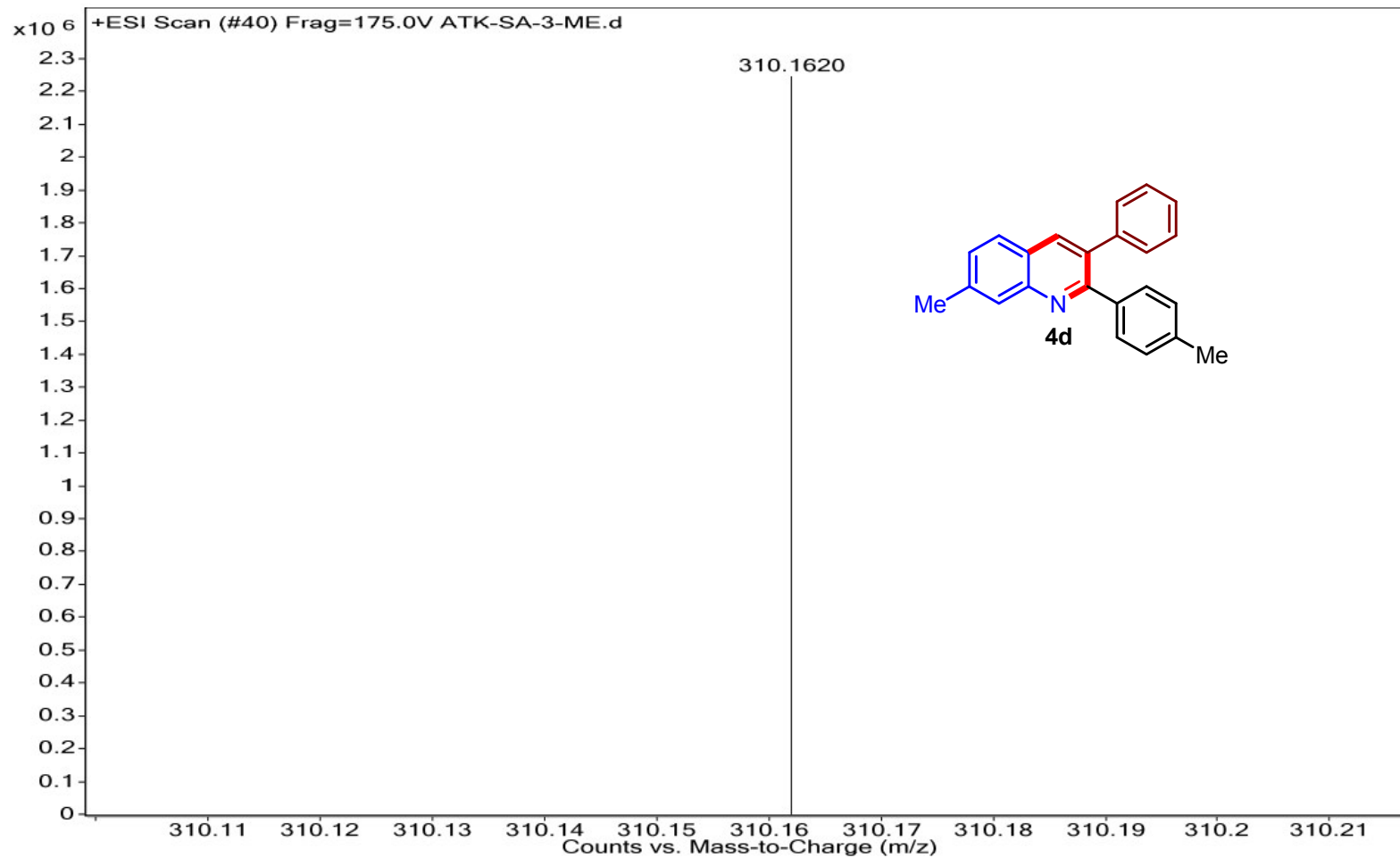
¹³CNMR spectrum of compound: 4d

ATK-SA-3Me-13C



HRMS spectrum of compound: 4d

Sample Name	SAMPLE 29	Position	P2-C8	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-3-ME.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	8/9/2019 6:04:33 PM

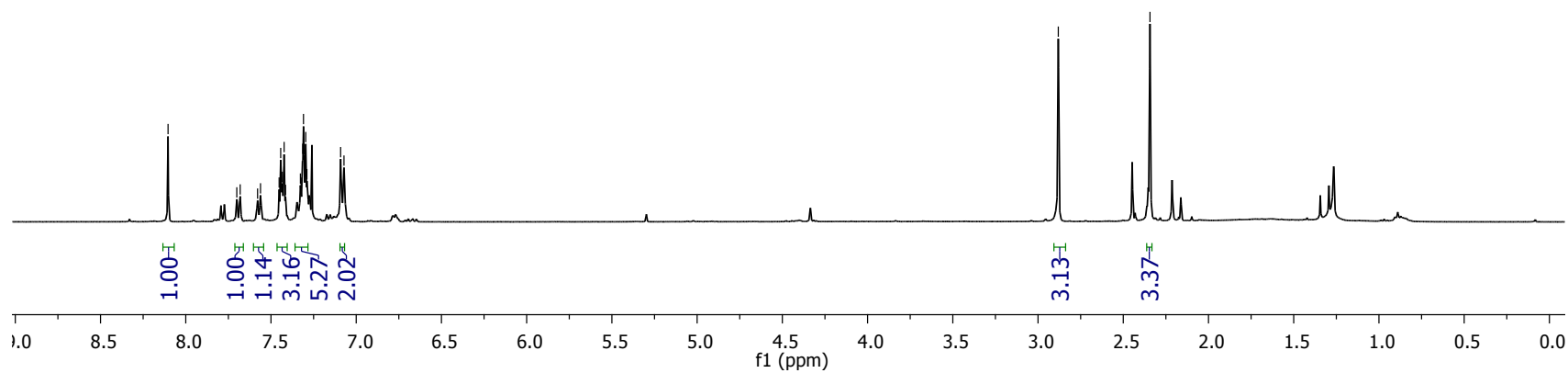
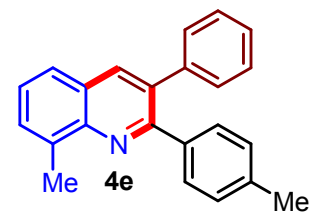
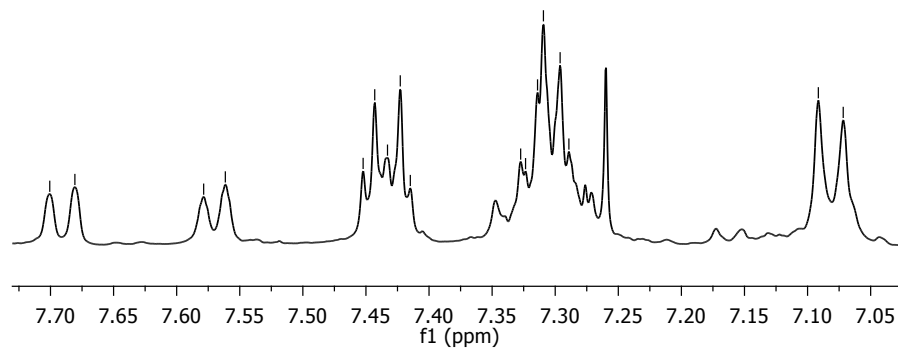


¹H NMR spectrum of compound: 4e

ATK-SA-2-ME-1H
ATK-SA-2-ME-1H

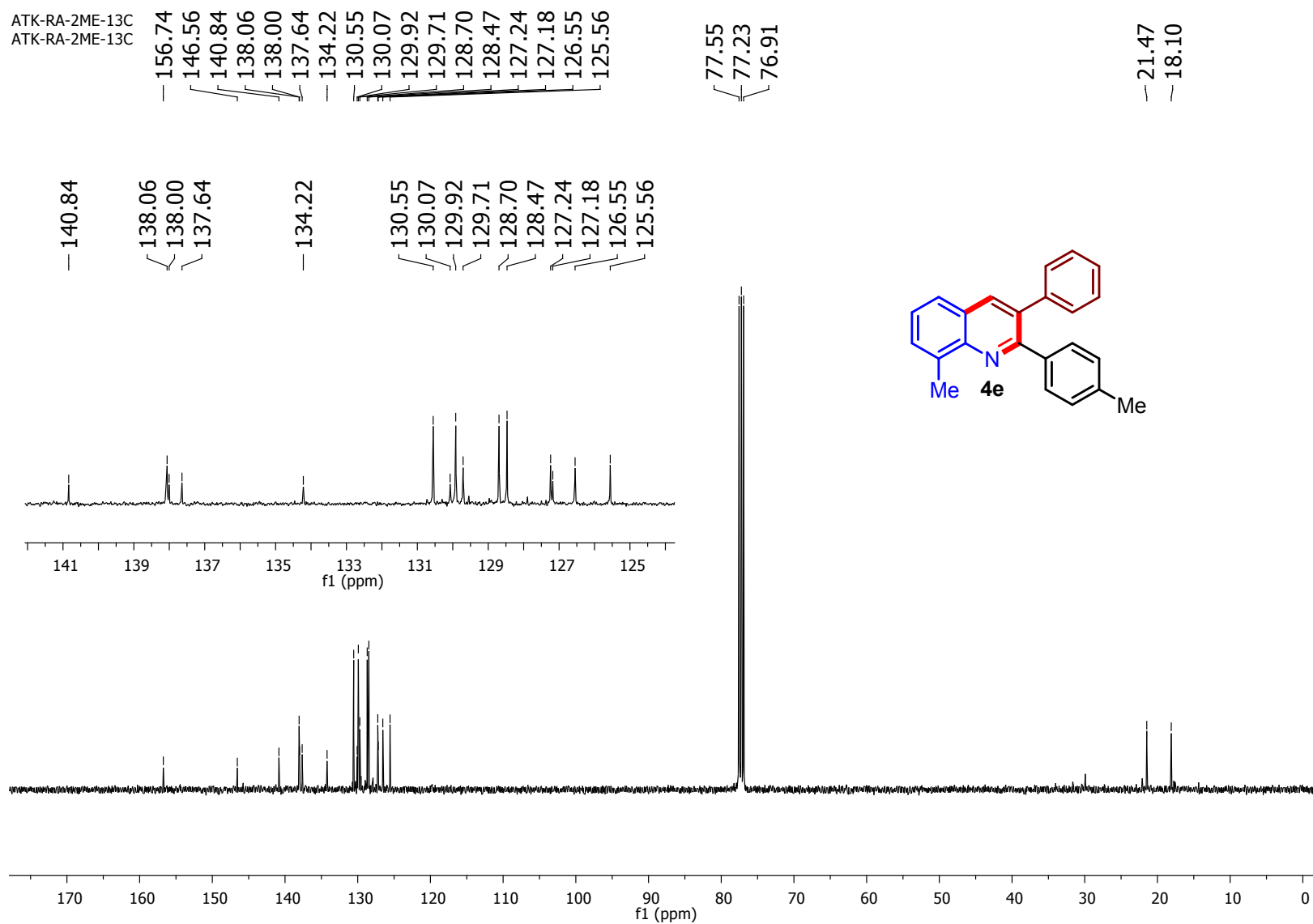
— 2.88
— 2.34

7.70
7.68
7.58
7.56
7.45
7.44
7.43
7.42
7.41
7.33
7.32
7.31
7.31
7.30
7.29
7.09
7.07



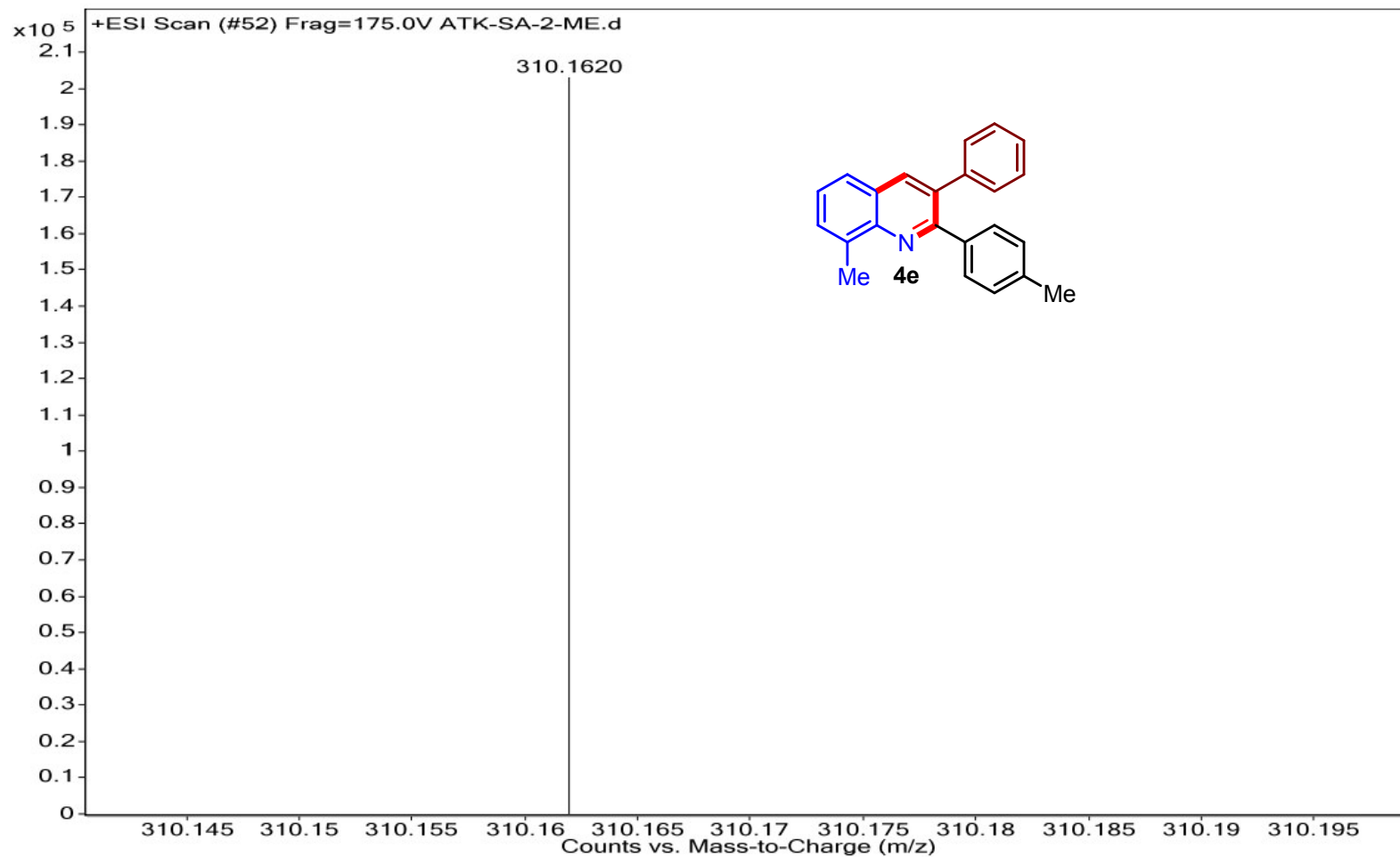
¹³CNMR spectrum of compound: 4e

ATK-RA-2ME-13C
ATK-RA-2ME-13C



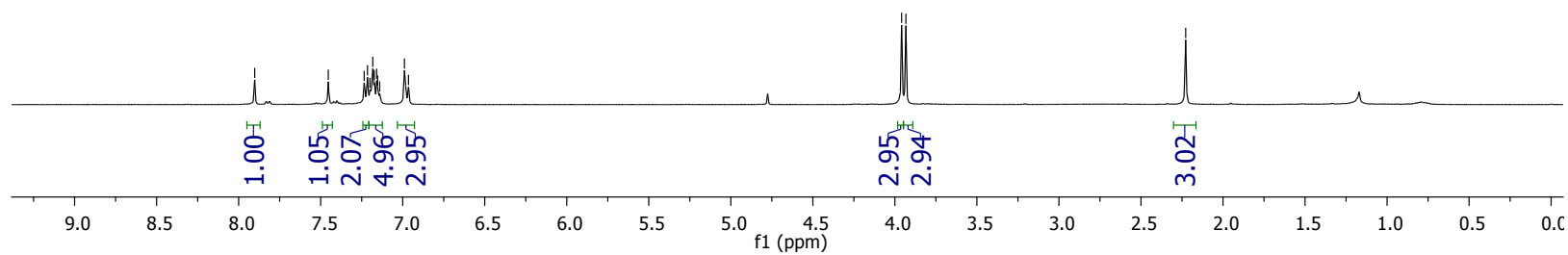
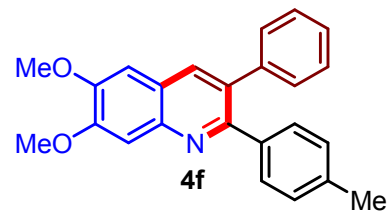
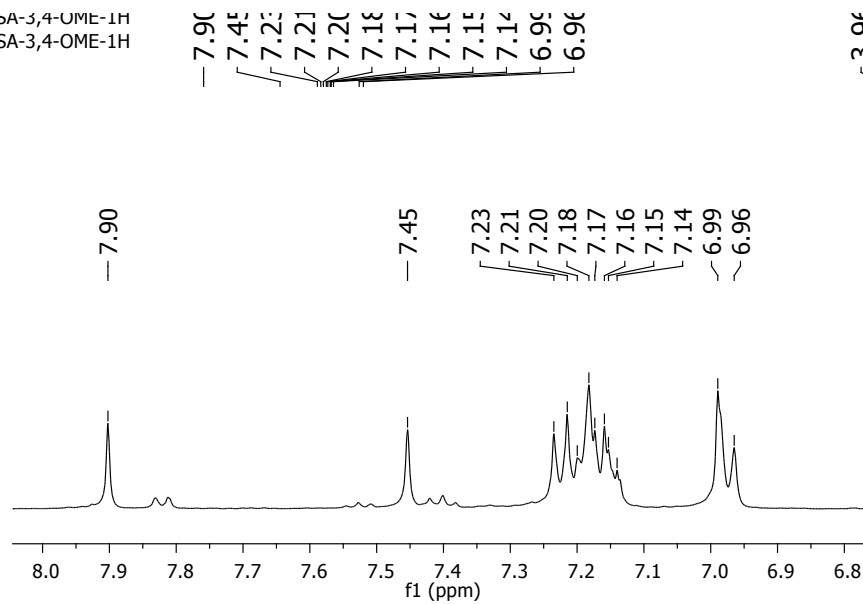
HRMS spectrum of compound: 4e

Sample Name	SAMPLE 30	Position	P2-C9	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-2-ME.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	8/9/2019 6:14:19 PM



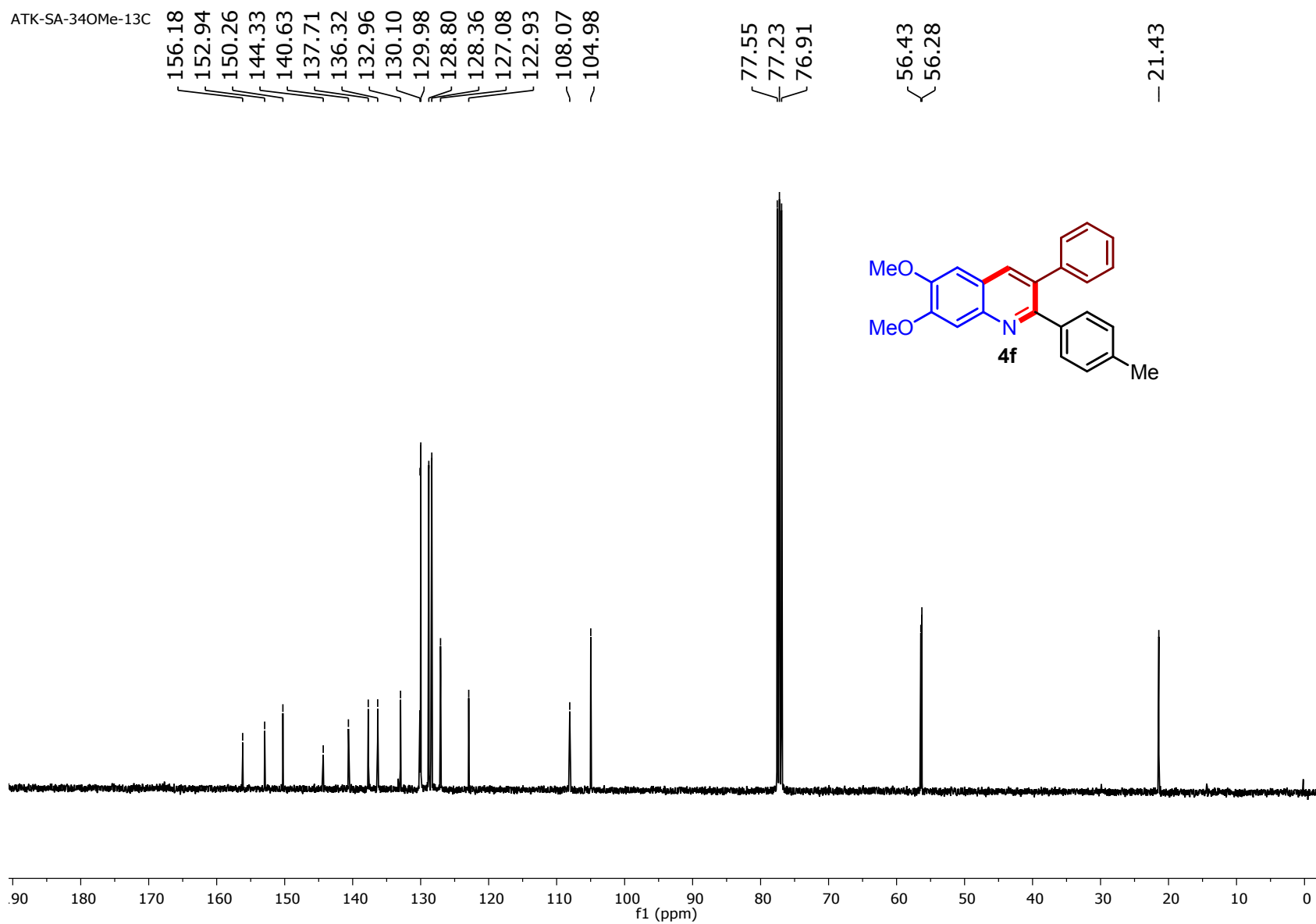
¹HNMR spectrum of compound: 4f

AIK-SA-3,4-OME-1H
ATK-SA-3,4-OME-1H



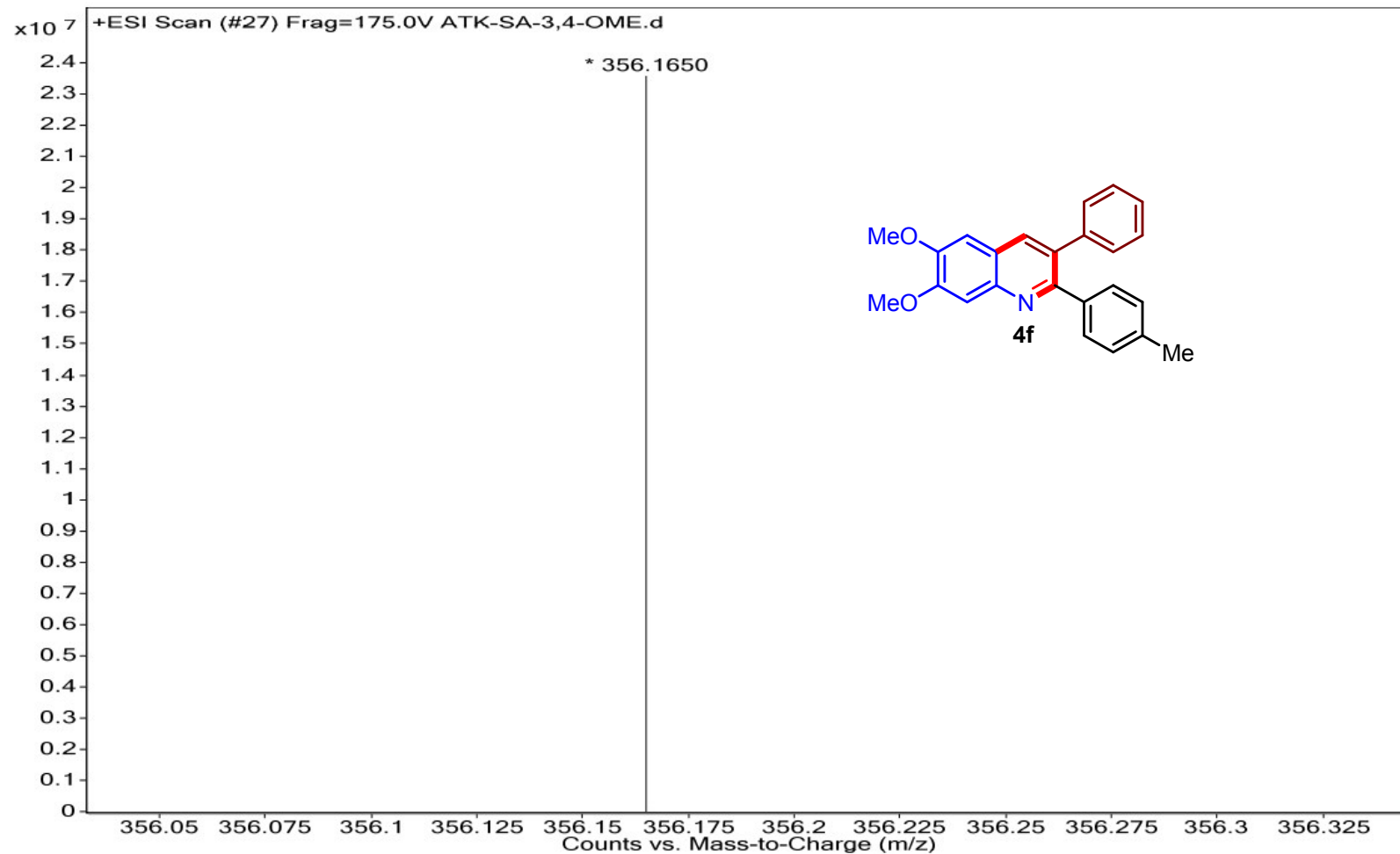
¹³CNMR spectrum of compound: 4f

ATK-SA-34OMe-13C



HRMS spectrum of compound: 4f

Sample Name	SAMPLE	Position	P2-C7	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-3,4-OME.d	ACQ Method	ESI ALS 100-800.m	Comment		Acquired Time	8/1/2019 5:48:48 PM

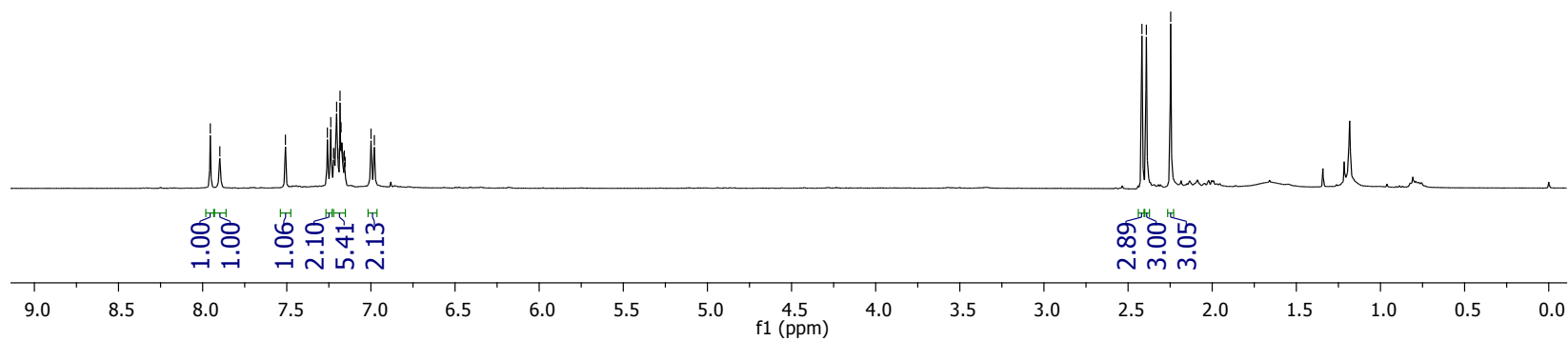
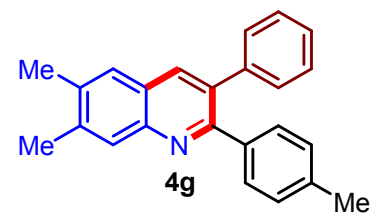
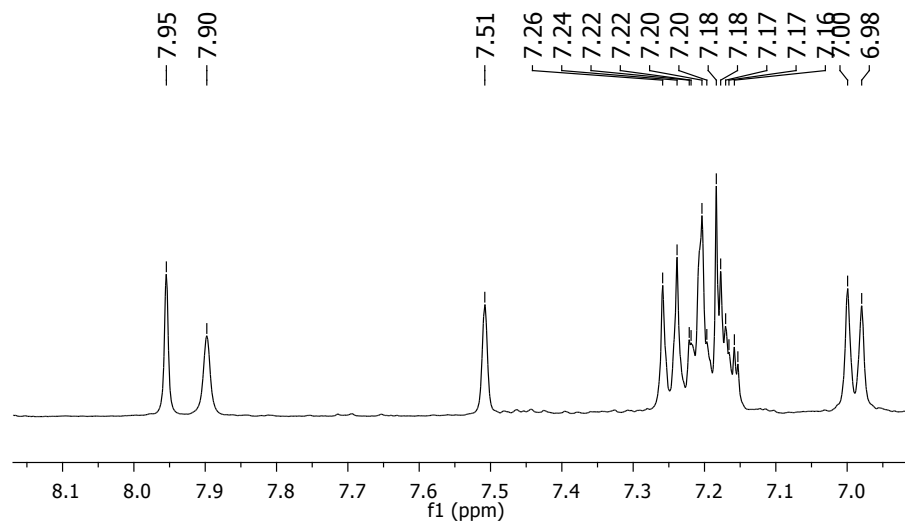


¹HNMR spectrum of compound: 4g

ATK-SA-3,4-ME-1H
ATK-SA-3,4-ME-1H

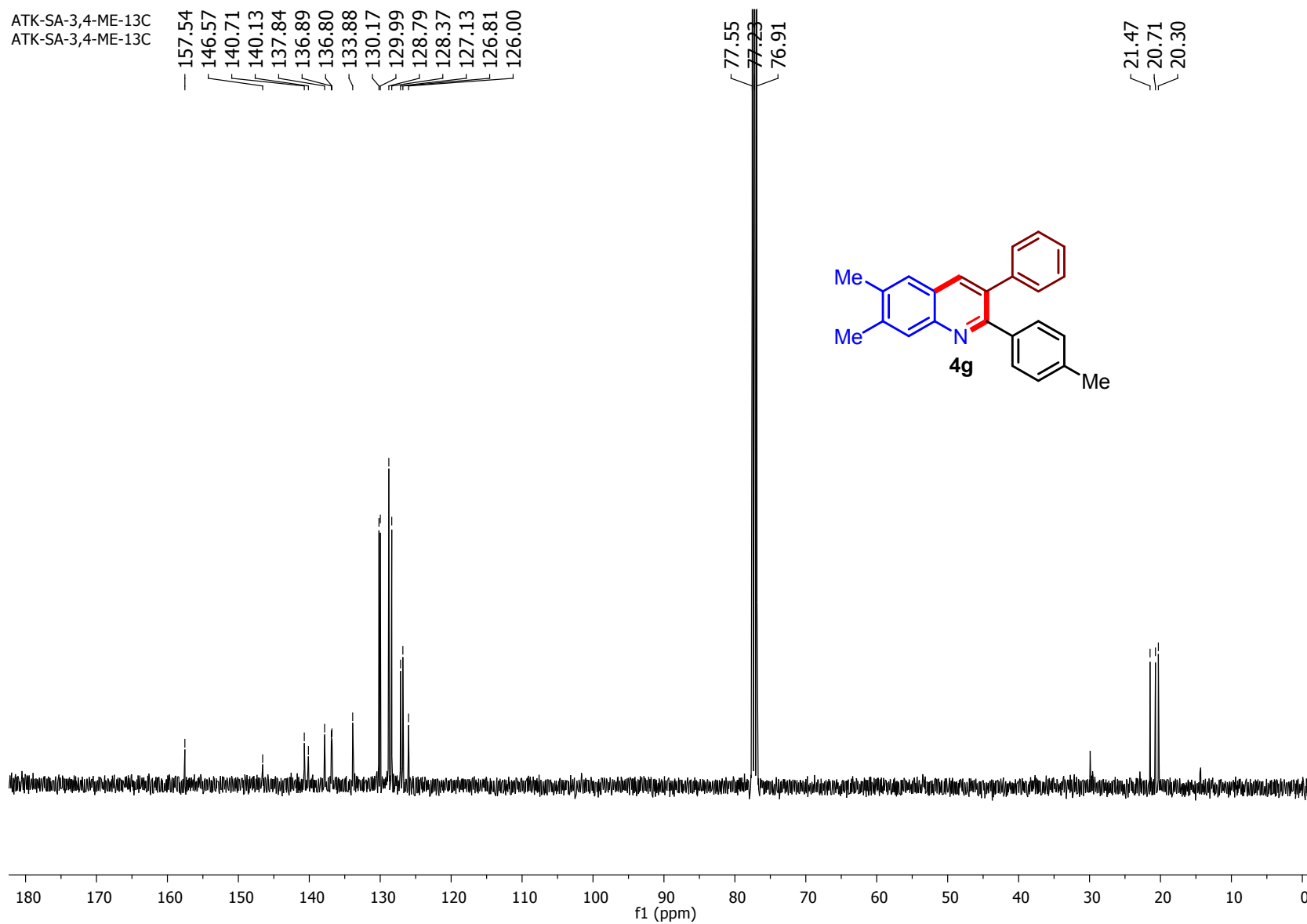
7.95
7.90
7.51
7.26
7.24
7.22
7.22
7.20
7.20
7.18
7.18
7.17
7.17
7.16
7.15
7.00
6.98

2.42
2.39
2.25



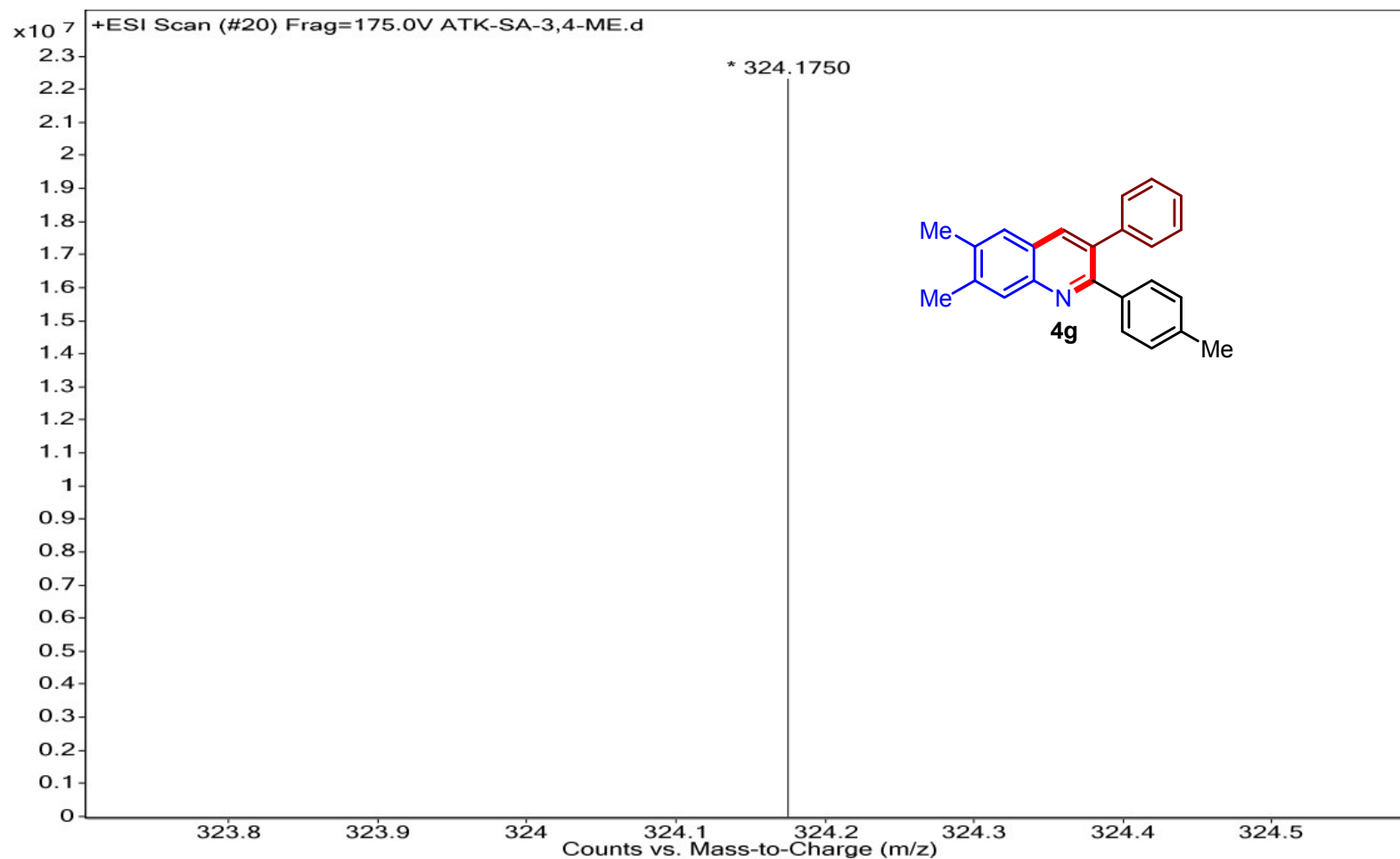
¹³CNMR spectrum of compound: 4g

ATK-SA-3,4-ME-13C
ATK-SA-3,4-ME-13C

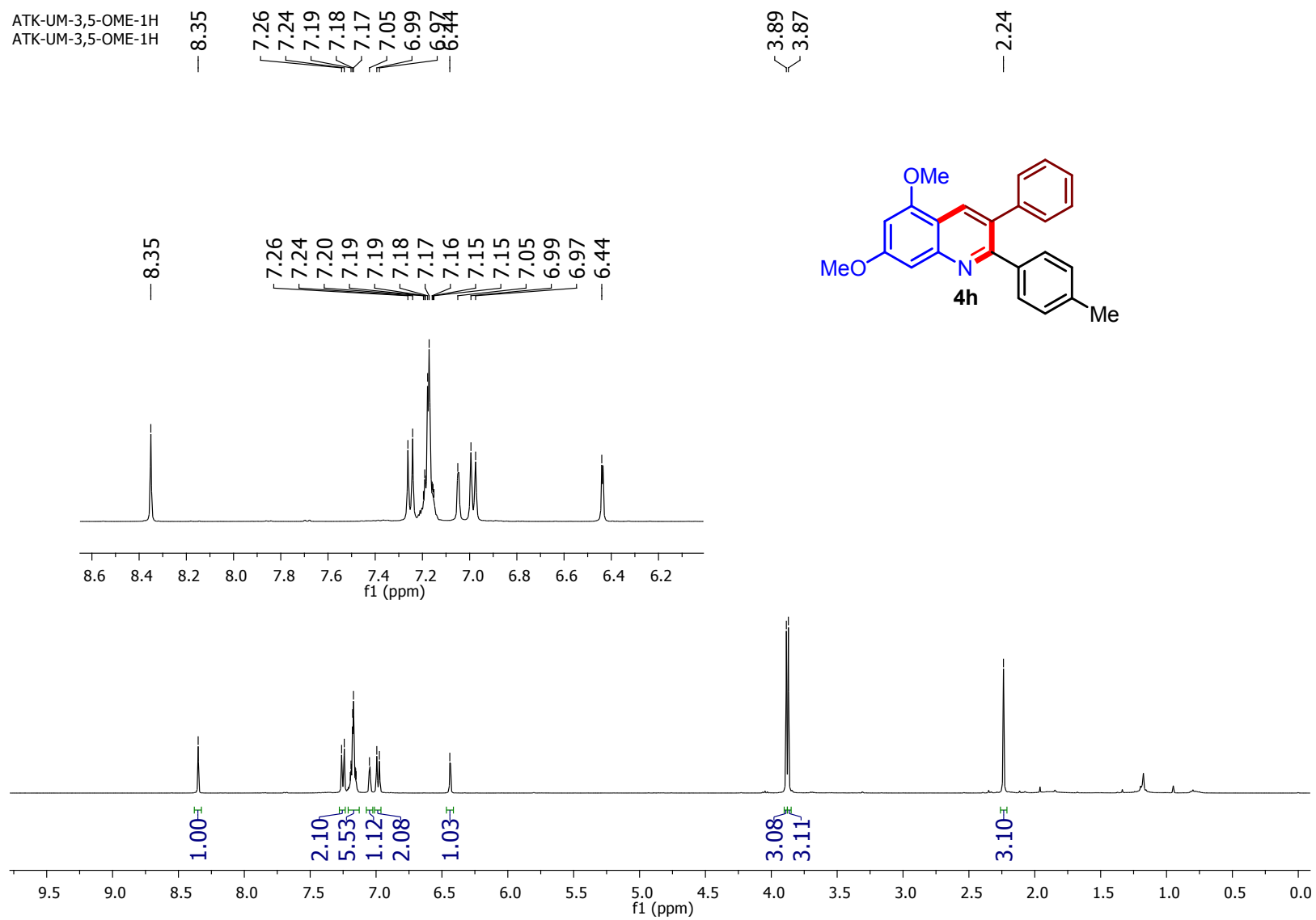


HRMS spectrum of compound: 4g

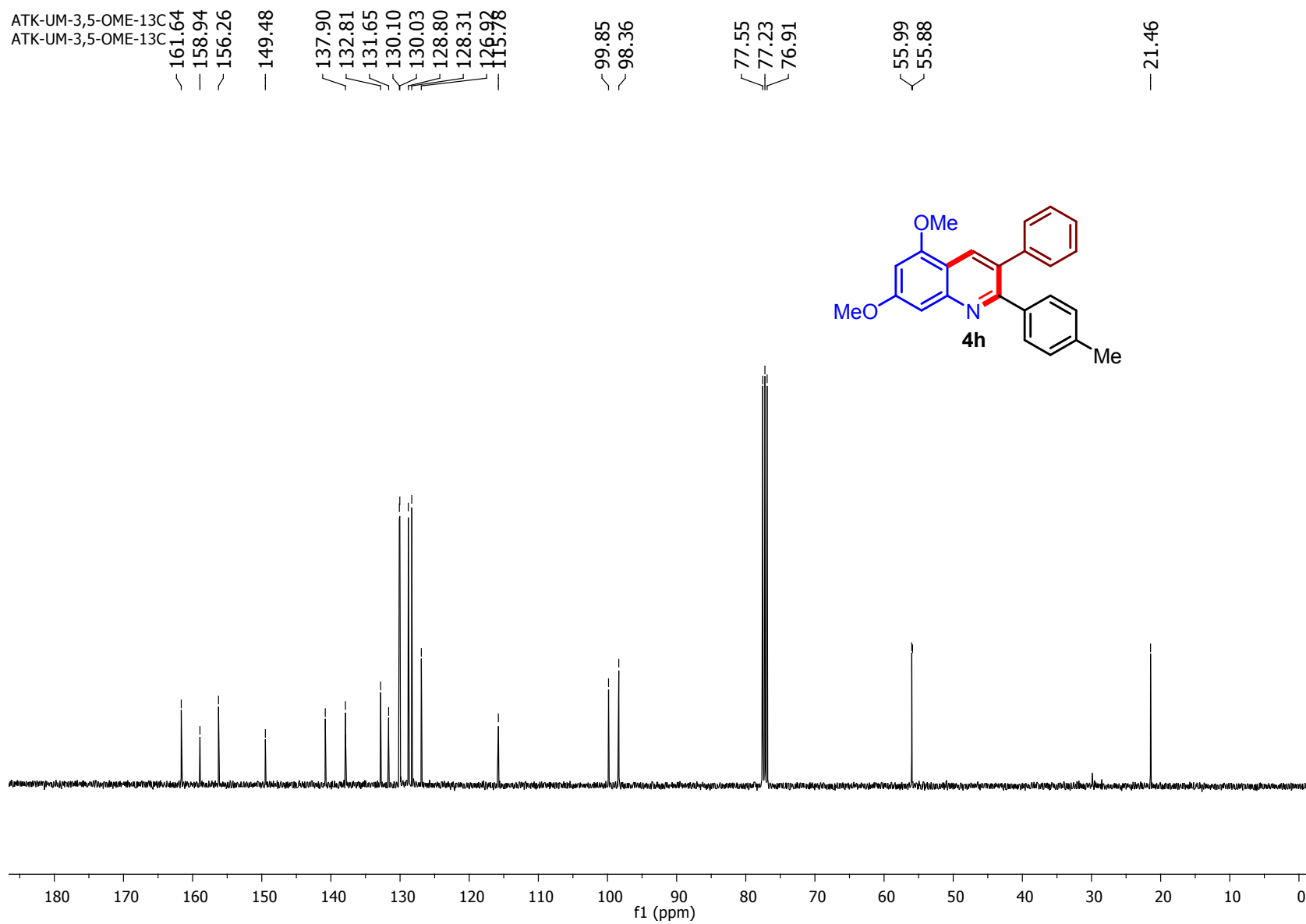
Sample Name	SAMPLE	Position	P2-C8	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-3,4-ME.d	ACQ Method	ESI ALS 100-800.m	Comment		Acquired Time	8/1/2019 5:50:41 PM



¹HNMR spectrum of compound: 4h

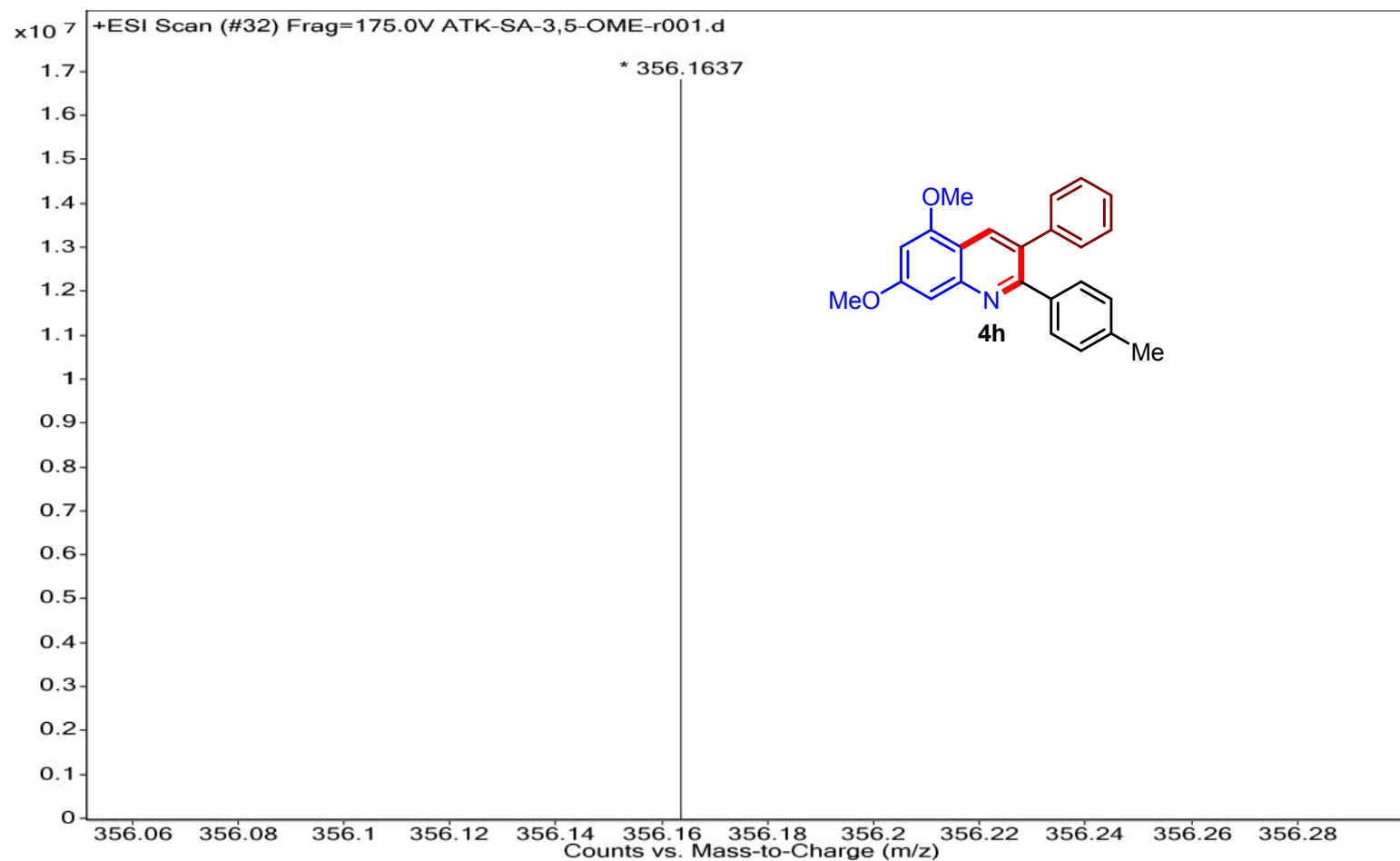


¹³CNMR spectrum of compound: 4h



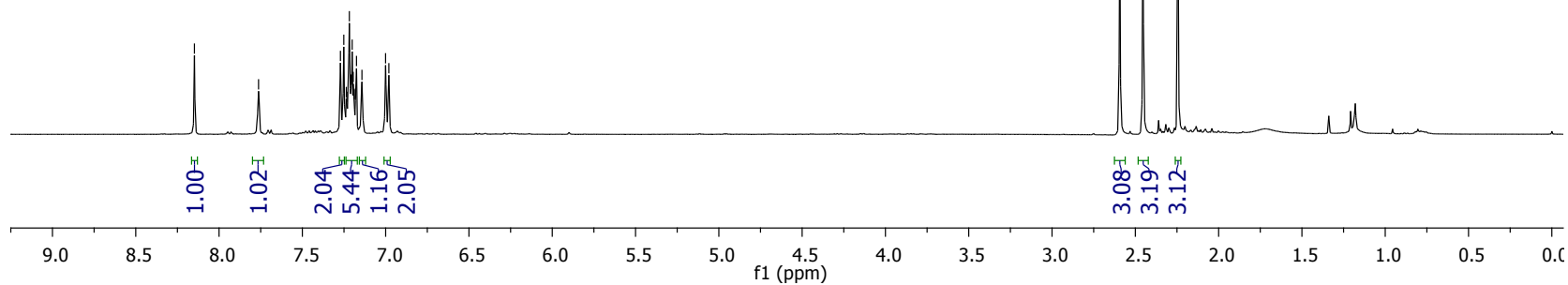
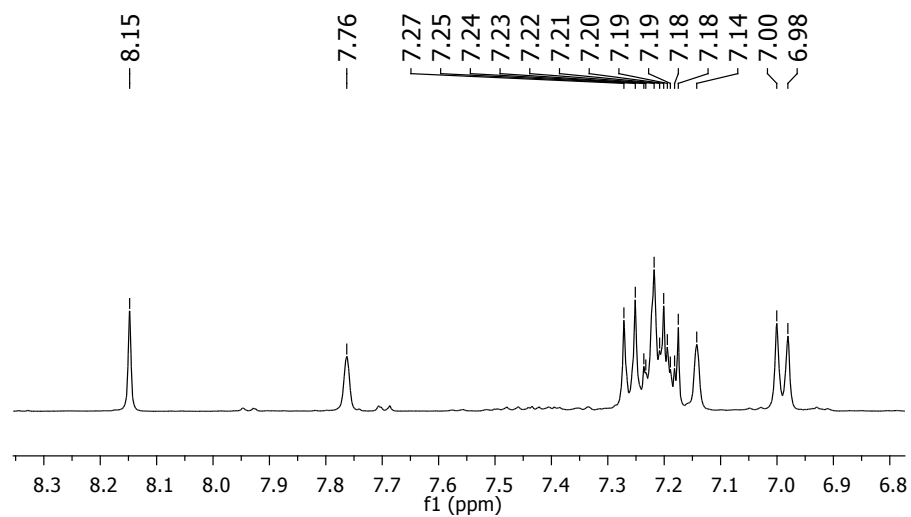
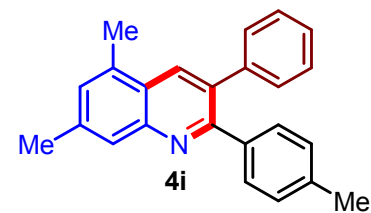
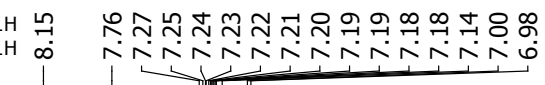
HRMS spectrum of compound: 4h

Sample Name	SAMPLE	Position	P2-C6	Instrument Name	Instrument 1	User Name	
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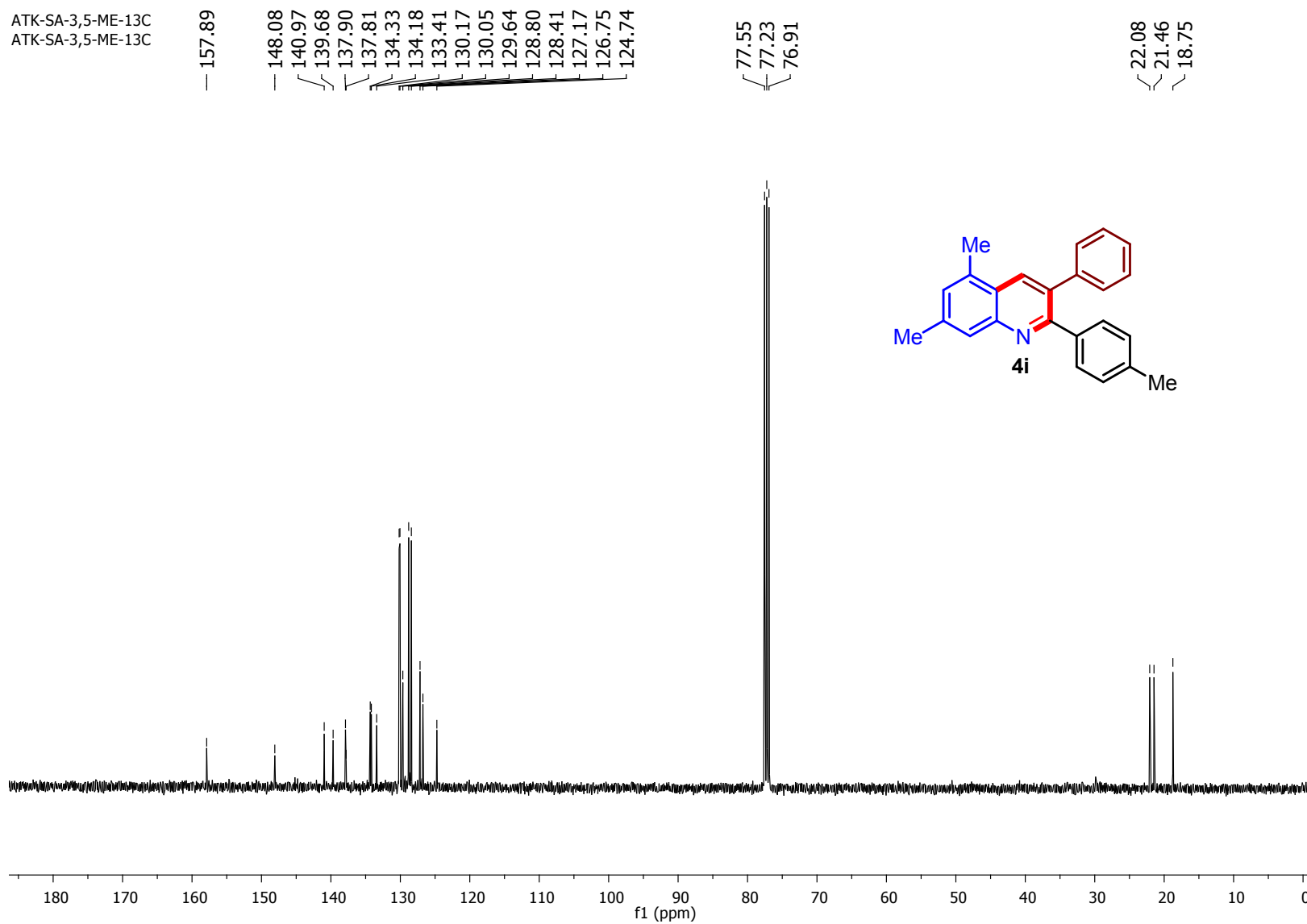
¹HNMR spectrum of compound: 4i

ATK-SA-3,5-ME-1H
ATK-SA-3,5-ME-1H



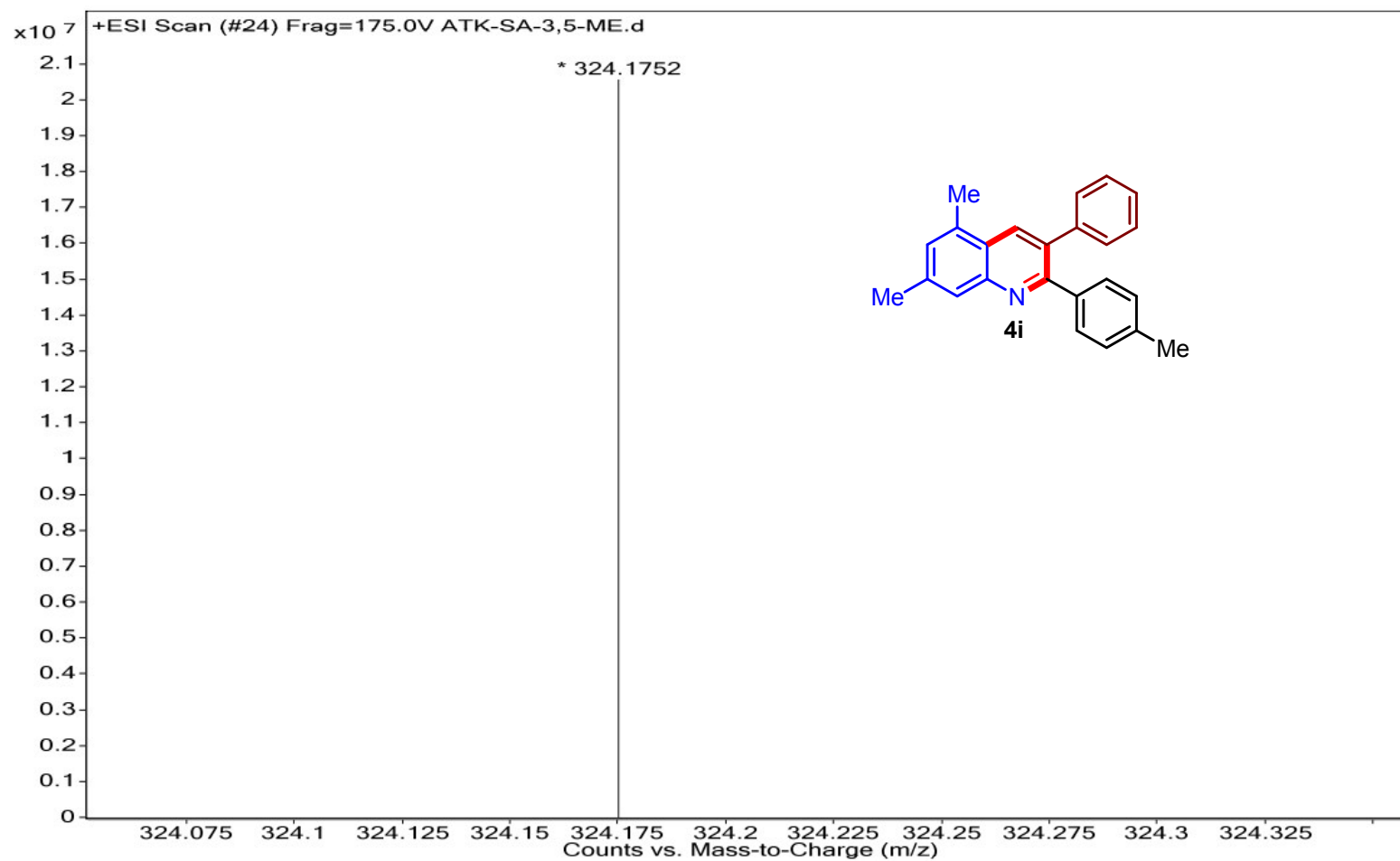
¹³CNMR spectrum of compound: 4i

ATK-SA-3,5-ME-13C
ATK-SA-3,5-ME-13C



HRMS spectrum of compound: 4i

Sample Name	SAMPLE	Position	P2-C9	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-3,5-ME.d	ACQ Method	ESI ALS 100-800.m	Comment		Acquired Time	8/1/2019 5:52:31 PM



¹HNMR spectrum of compound: 4j

ATK-SA-3,4,5-OMe-1H
ATK-SA-3,4,5-OMe-1H

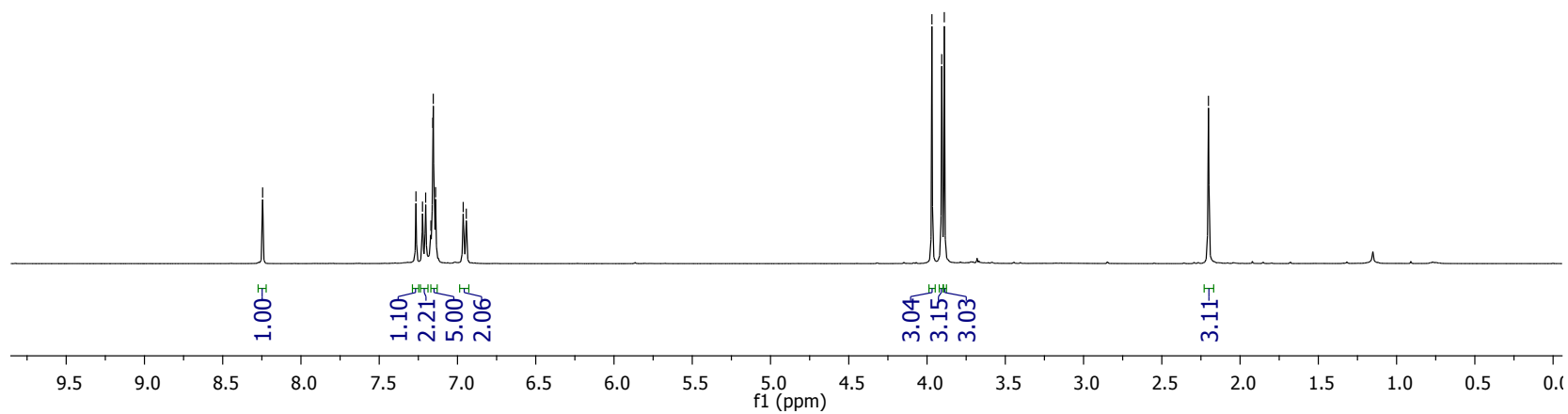
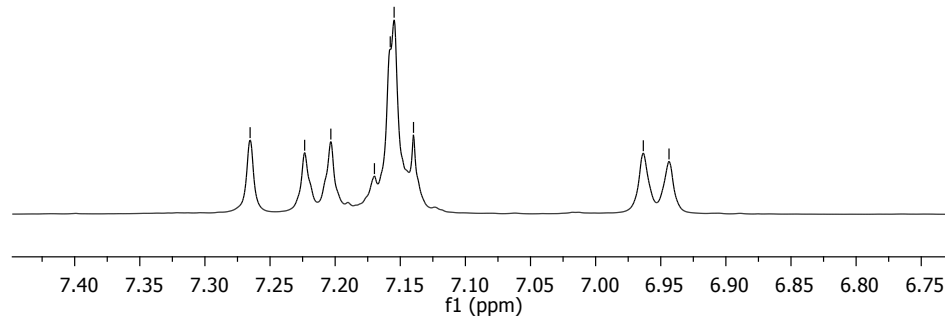
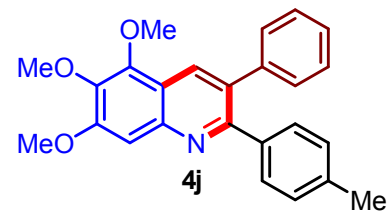
8.24
7.27
7.22
7.20
7.17
7.16
7.15
7.14
6.96
6.94

3.97
3.91
3.89

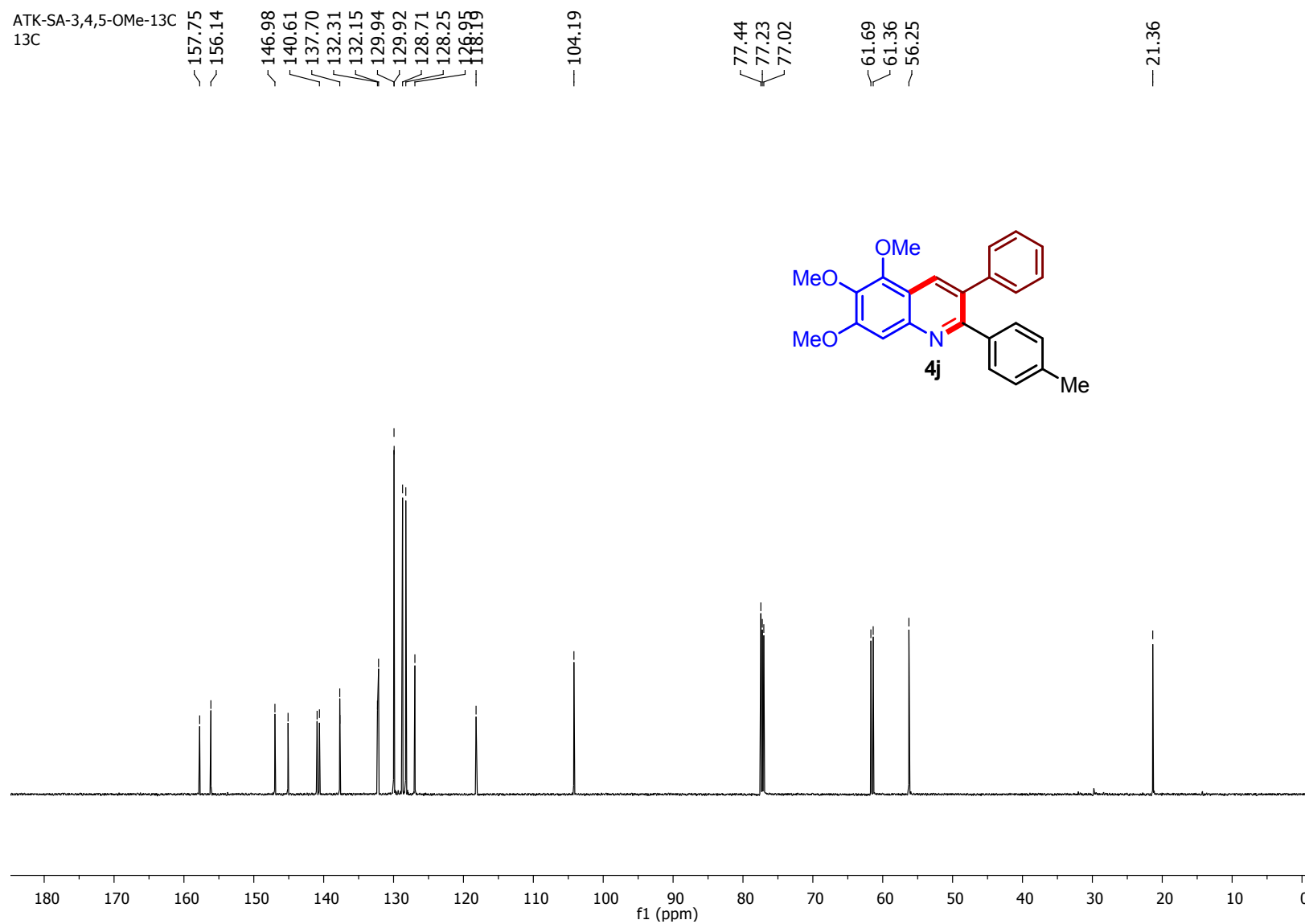
2.20

7.27
7.22
7.20
7.17
7.16
7.15
7.14

6.96
6.94

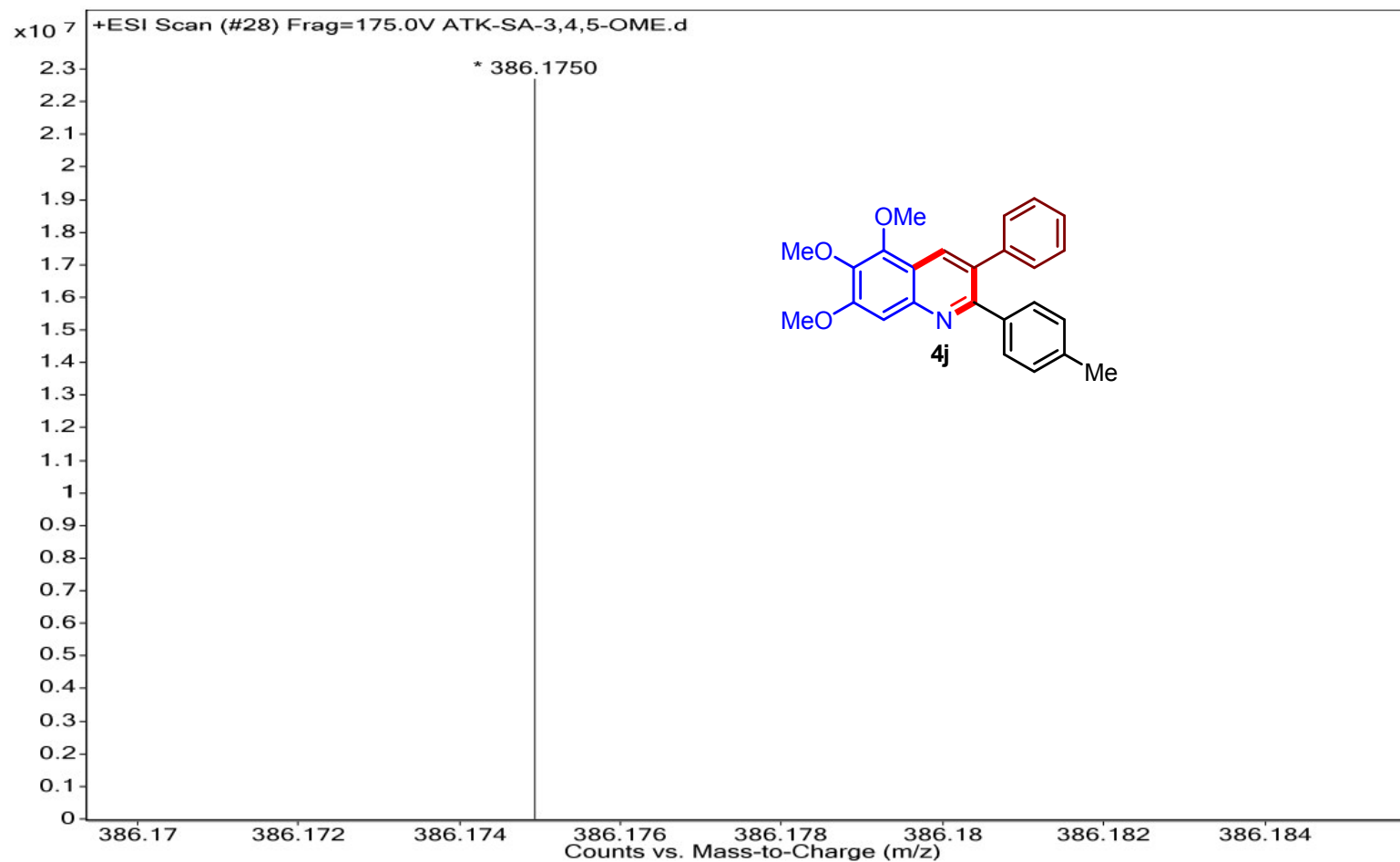


^{13}C NMR spectrum of compound: 4j



HRMS spectrum of compound: 4j

Sample Name	SAMPLE	Position	P2-C10	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-3,4,5-OME.d	ACQ Method	ESI ALS 100-800.m	Comment		Acquired Time	8/1/2019 5:54:24 PM



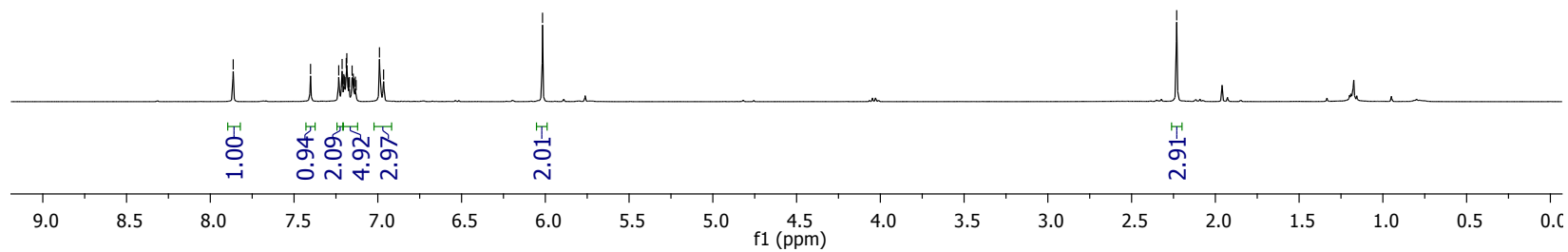
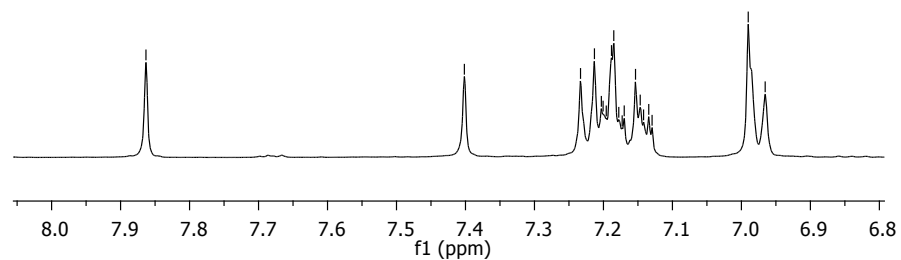
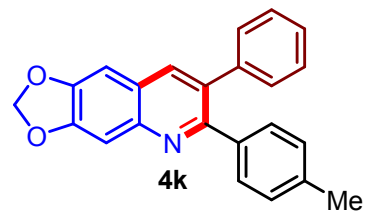
¹HNMR spectrum of compound: 4k

ATK-UM-SES-1H
ATK-UM-SES-1H

7.86
7.40
7.23
7.21
7.20
7.19
7.19
7.15
7.15
6.99
6.82

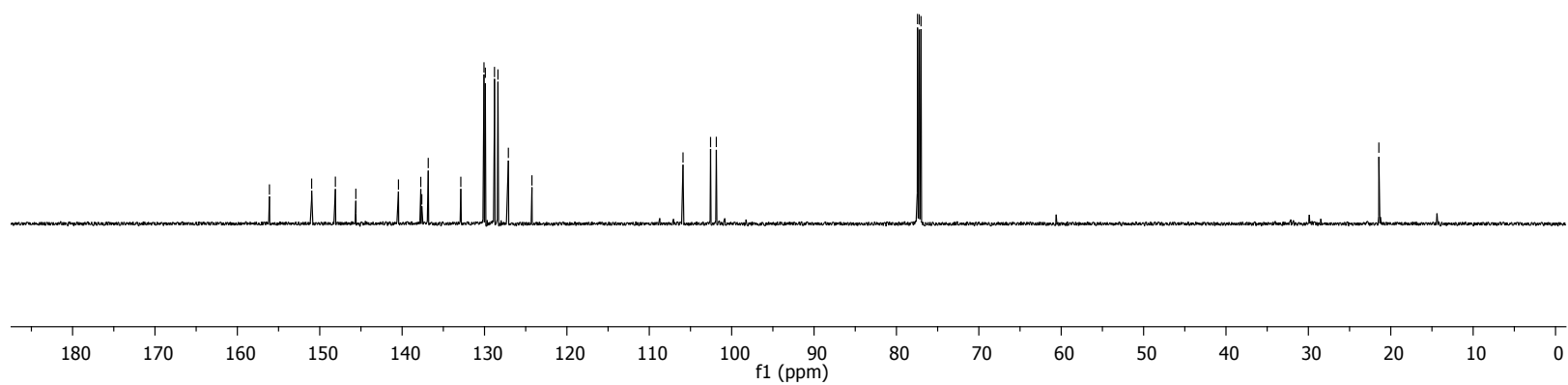
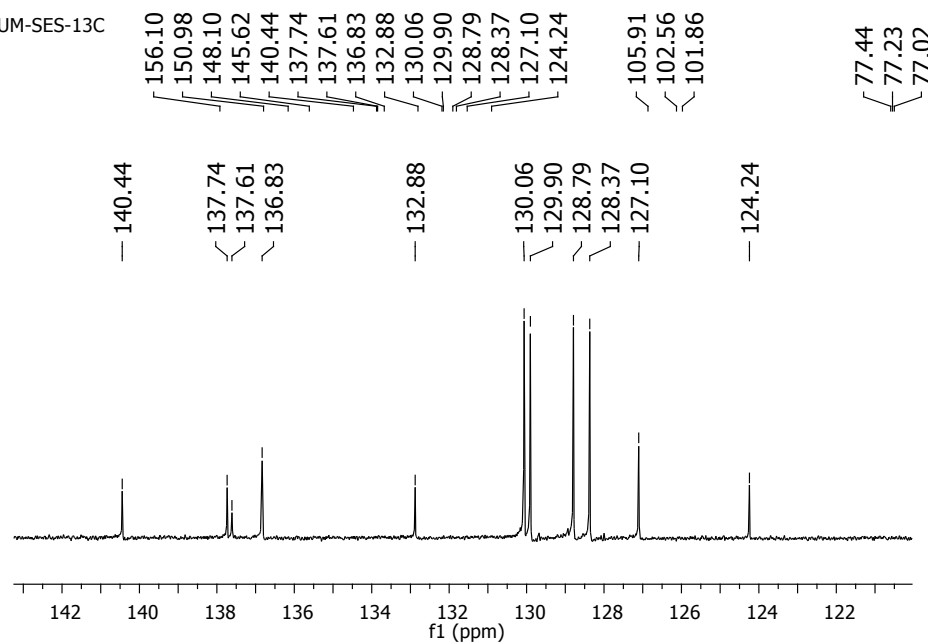
2.23

7.86
7.40
7.23
7.21
7.20
7.20
7.19
7.19
7.15
7.15
6.99
6.97



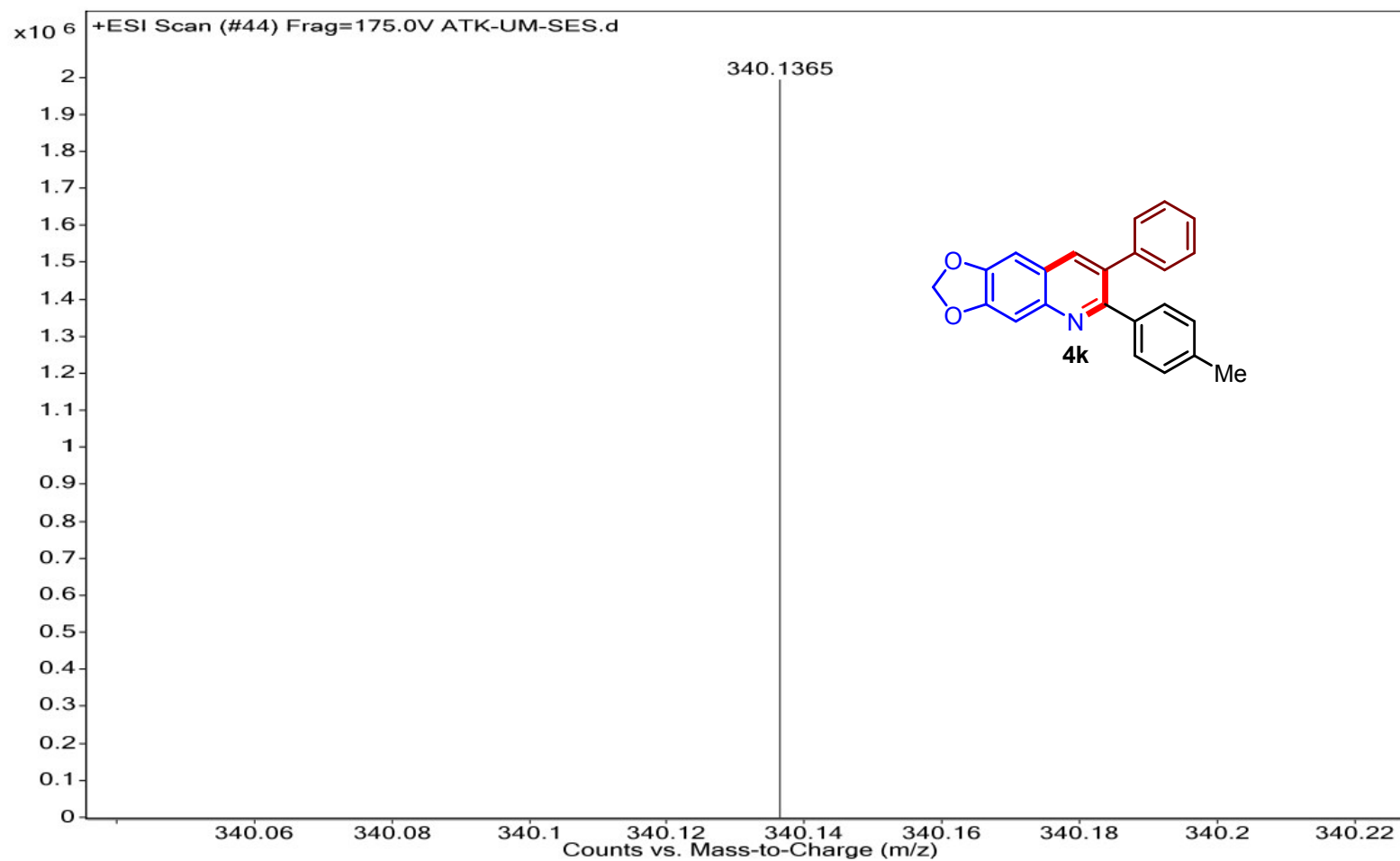
¹³CNMR spectrum of compound: 4k

ATK-UM-SES-13C
13C



HRMS spectrum of compound: 4k

Sample Name	ATK-UM-SES	Position	P1-D5	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-UM-SES.d	ACQ Method	ESI ALS 200-700.m	Comment		Acquired Time	4/11/2019 12:19:46 PM



¹HNMR spectrum of compound: 4I

ATK-SA-5-IND-1H
ATK-SA-5-IND-1H

7.97
7.92
7.55
7.26
7.24
7.22
7.20
7.19
7.18
7.17
7.00
6.98

3.07
3.05
3.03
3.01
2.99
2.24
2.14
2.12
2.10
2.09
2.07

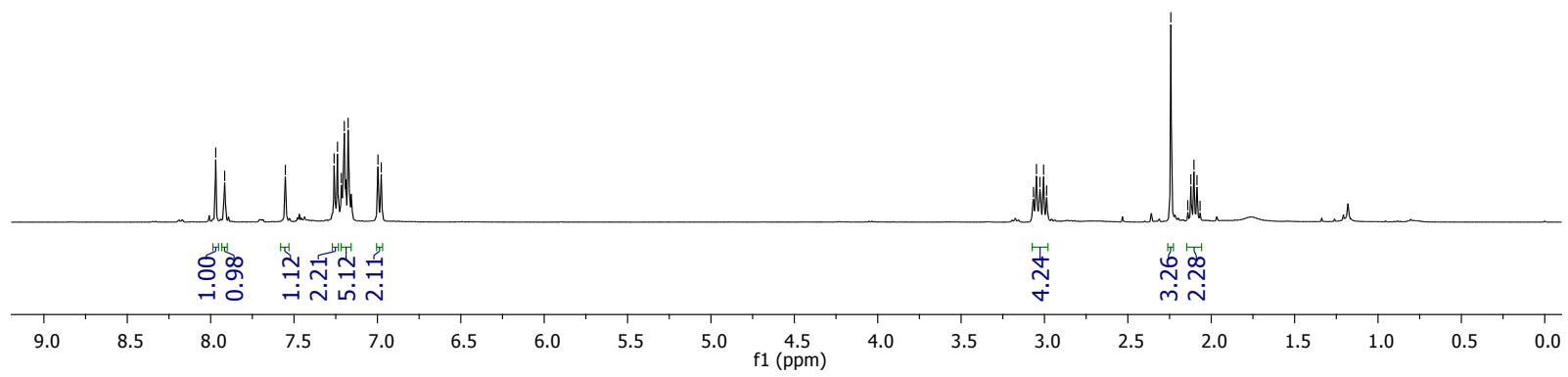
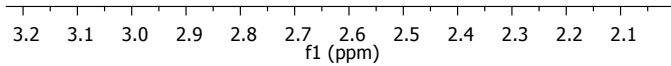
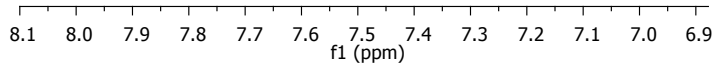
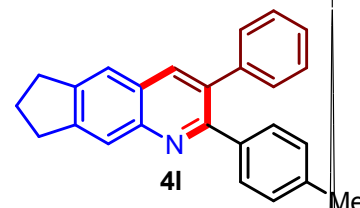
7.97
7.92

7.55

7.26
7.24
7.22
7.20
7.19
7.18
7.17
7.00
6.98

3.07
3.05
3.03
3.01
2.99

2.24
2.14
2.12
2.10
2.09
2.07



¹³CNMR spectrum of compound: 4l

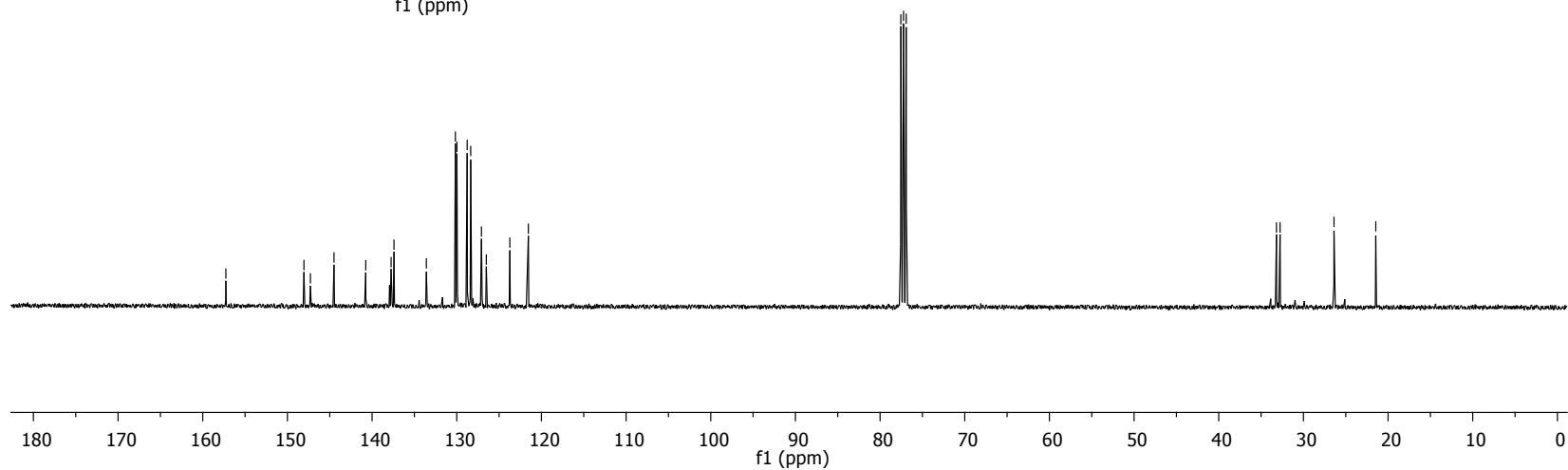
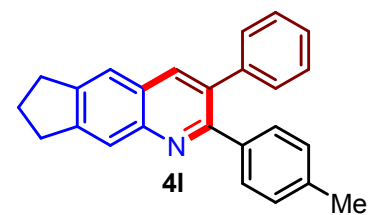
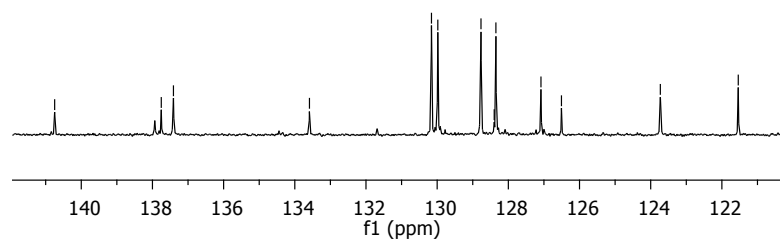
ATK-SA-5-INP-13C
ATK-SA-5-INP-13C

157.21
148.01
147.21
144.51
140.71
137.71
137.41
133.51
130.11
129.91
128.71
128.41
128.31
127.01
126.51
123.71
121.51

77.55
77.23
76.91

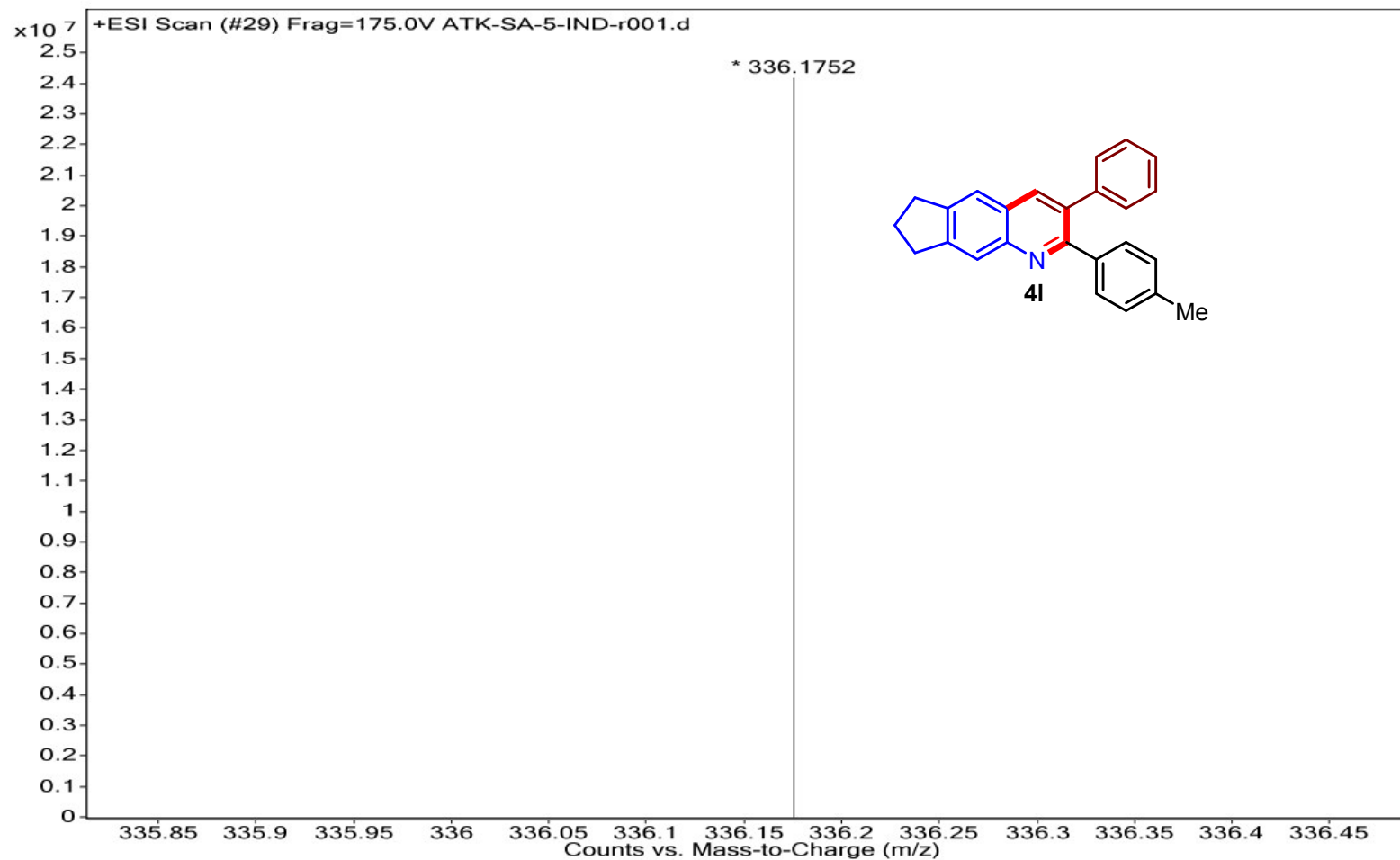
33.18
32.76
26.39
21.45

140.75
137.75
137.41
133.59
130.16
129.98
128.77
128.40
128.35
127.08
126.51
123.73
121.54

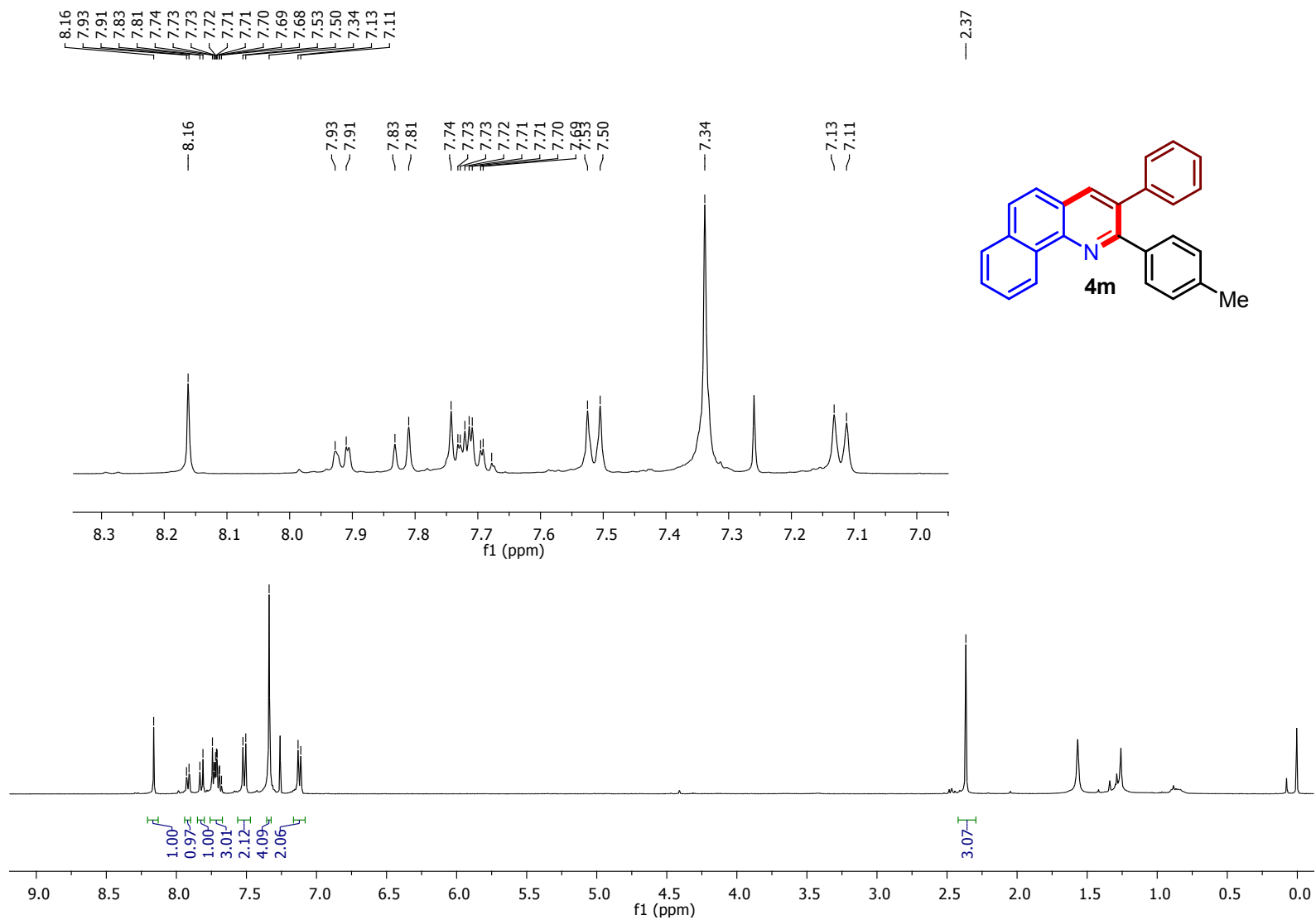


HRMS spectrum of compound: 4l

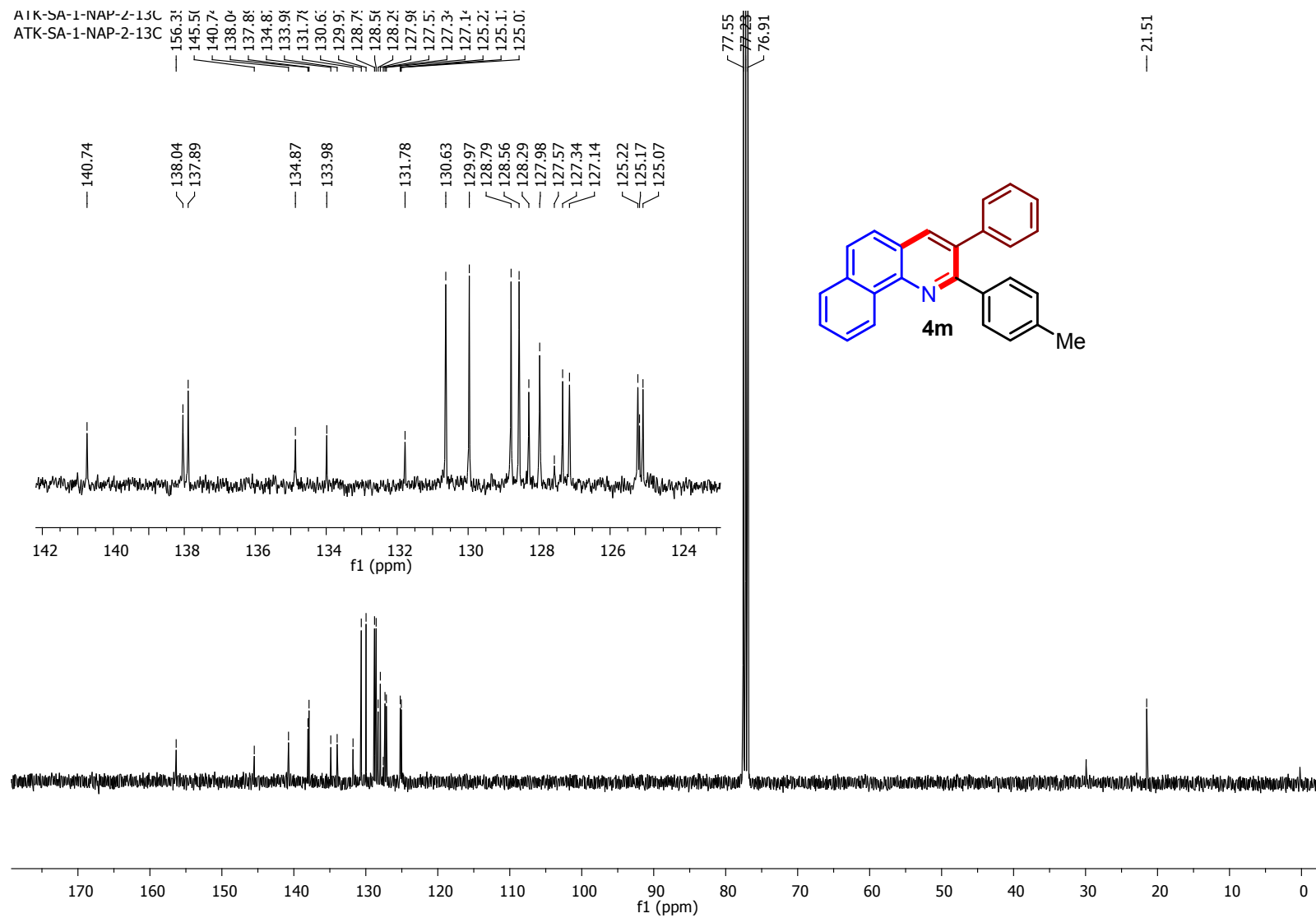
Sample Name	SAMPLE	Position	P2-D2	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-5-IND-r001.d	ACQ Method	ESI ALS 100-800.m	Comment		Acquired Time	8/1/2019 5:58:06 PM



¹H NMR spectrum of compound: 4m

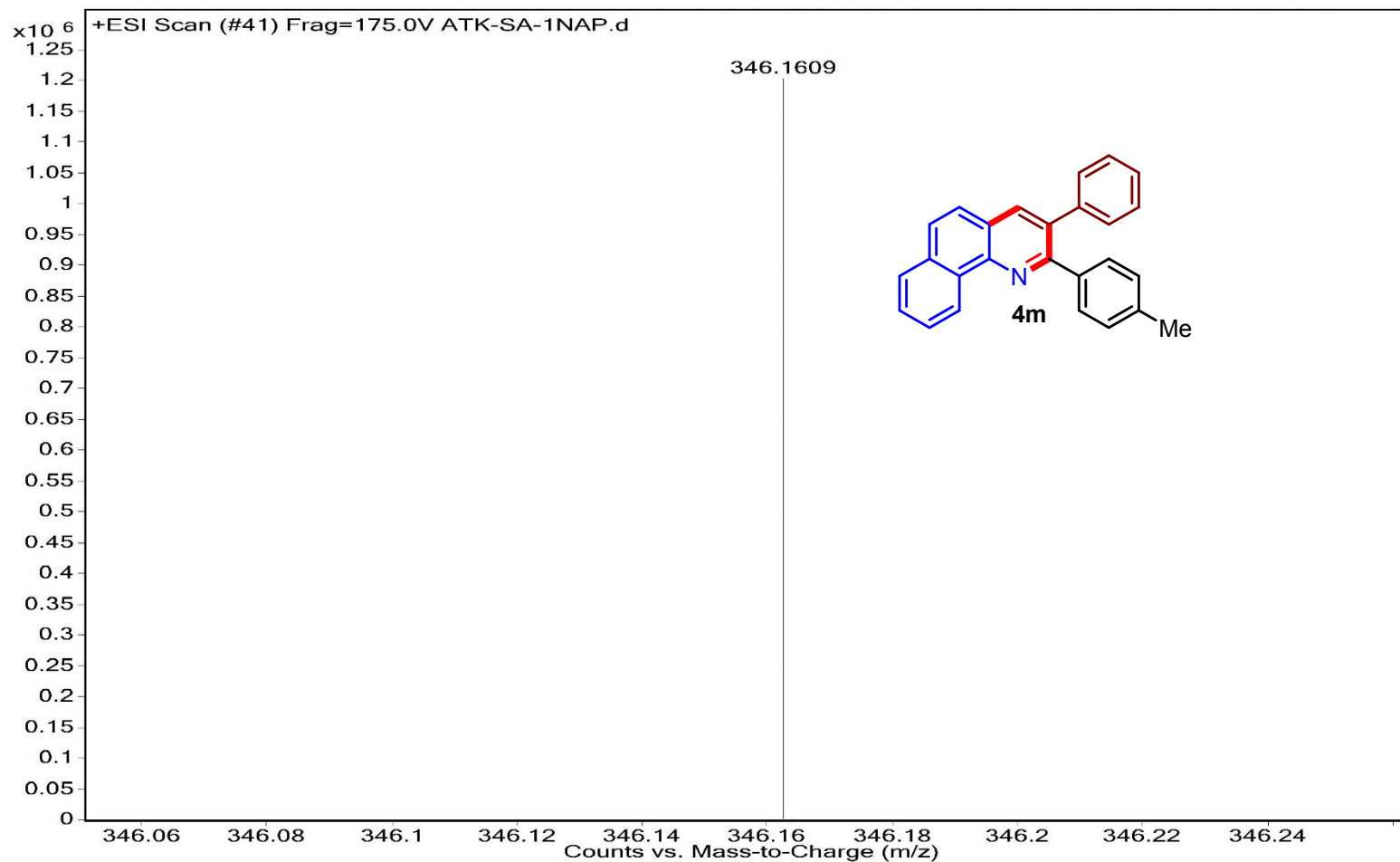


¹³CNMR spectrum of compound: 4m

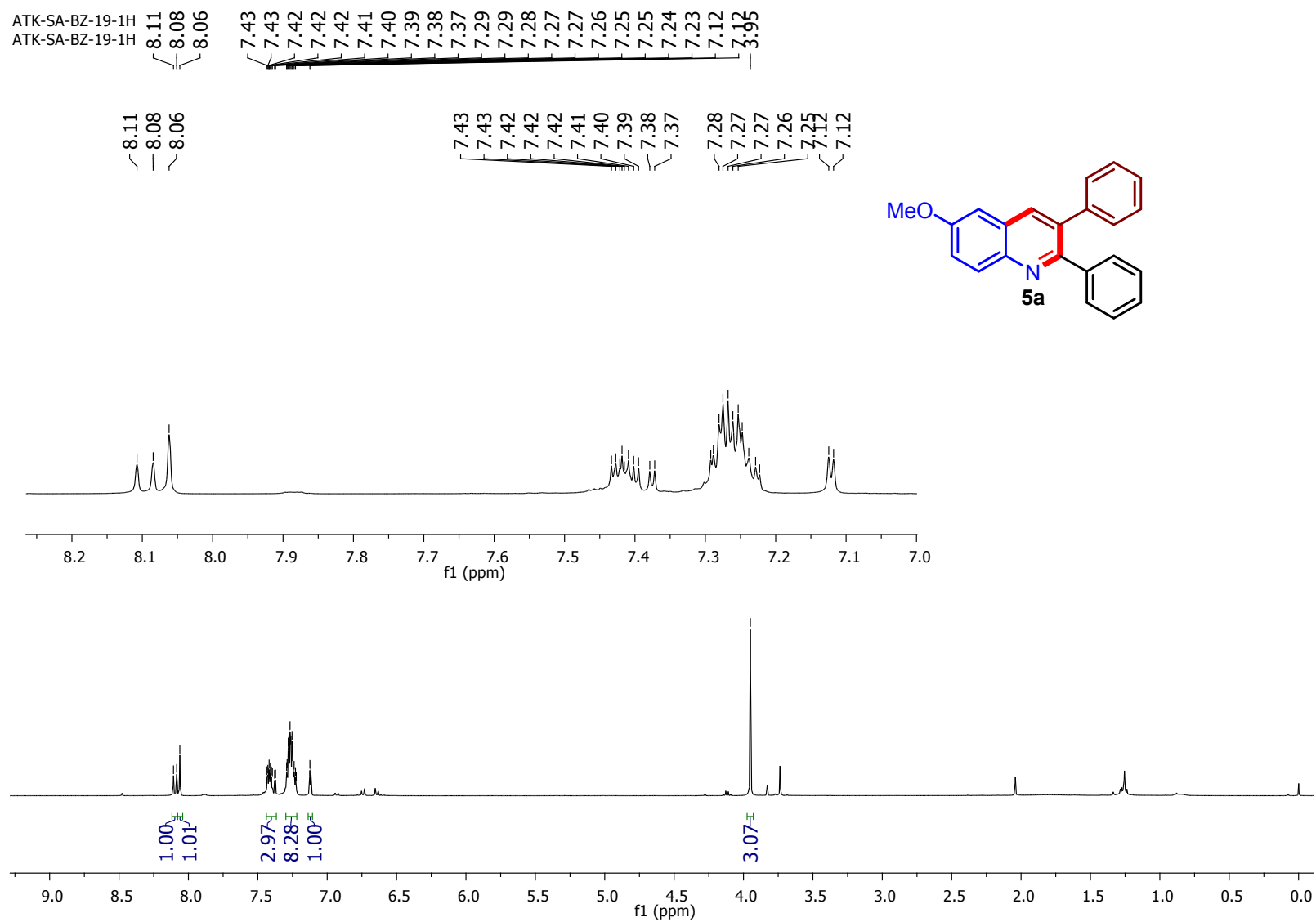


HRMS spectrum of compound: 4m

Sample Name	ATK-SA-1NAP	Position	P1-D7	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-2NAP.d	ACQ Method	ESI ALS 200-700.m	Comment		Acquired Time	4/11/2019 12:23:34 PM

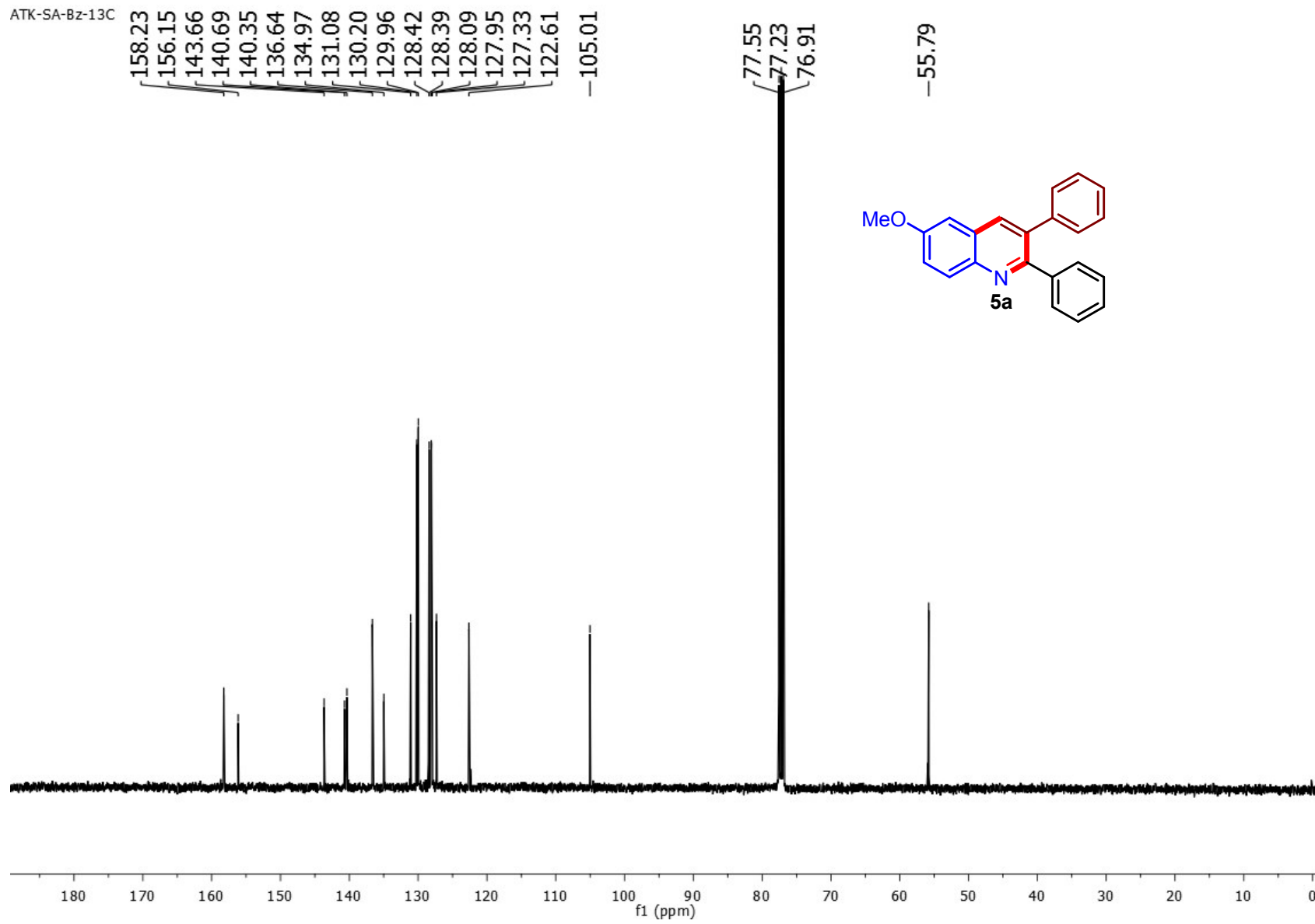


¹HNMR spectrum of compound: 5a



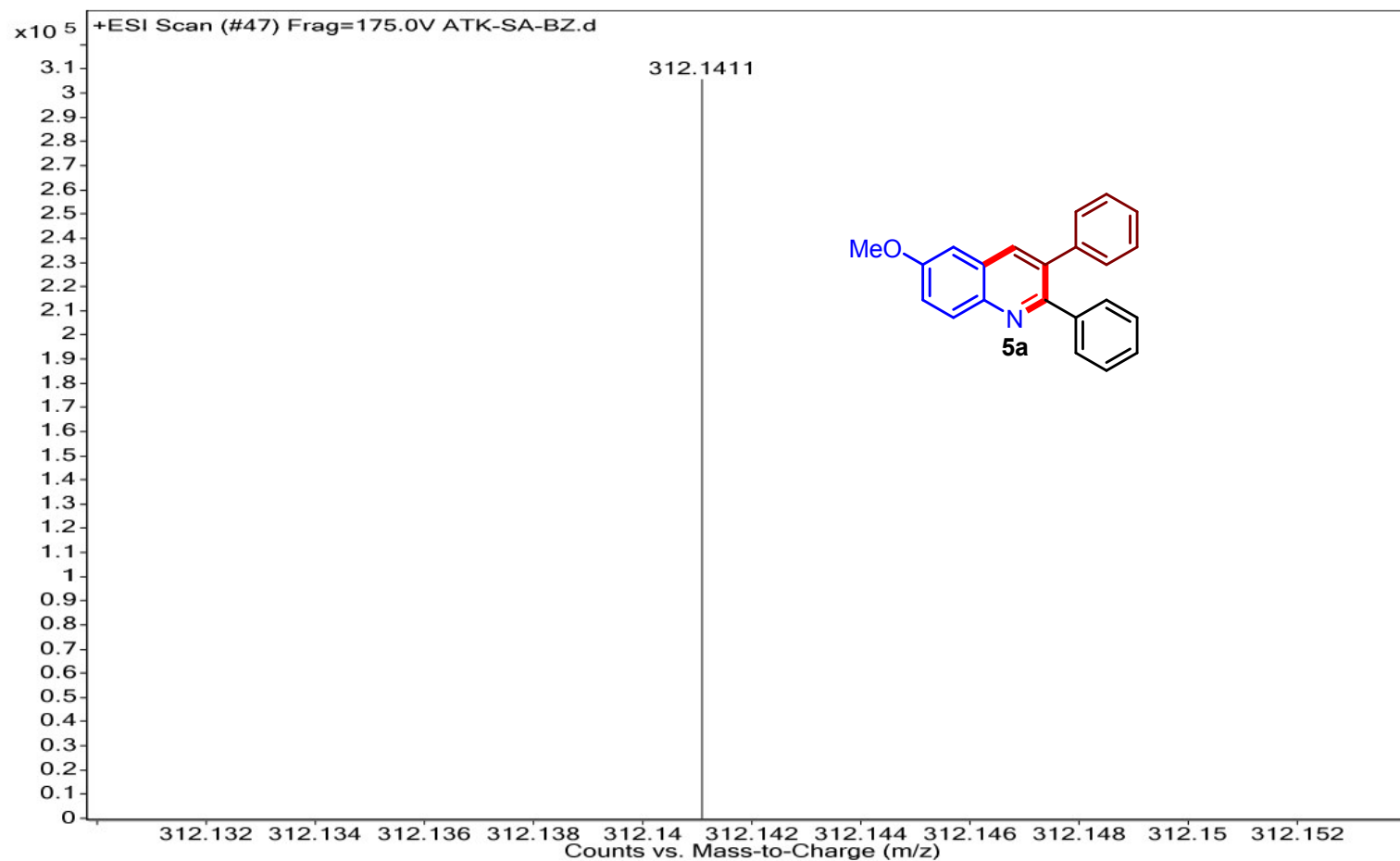
¹³CNMR spectrum of compound: 5a

ATK-SA-Bz-13C

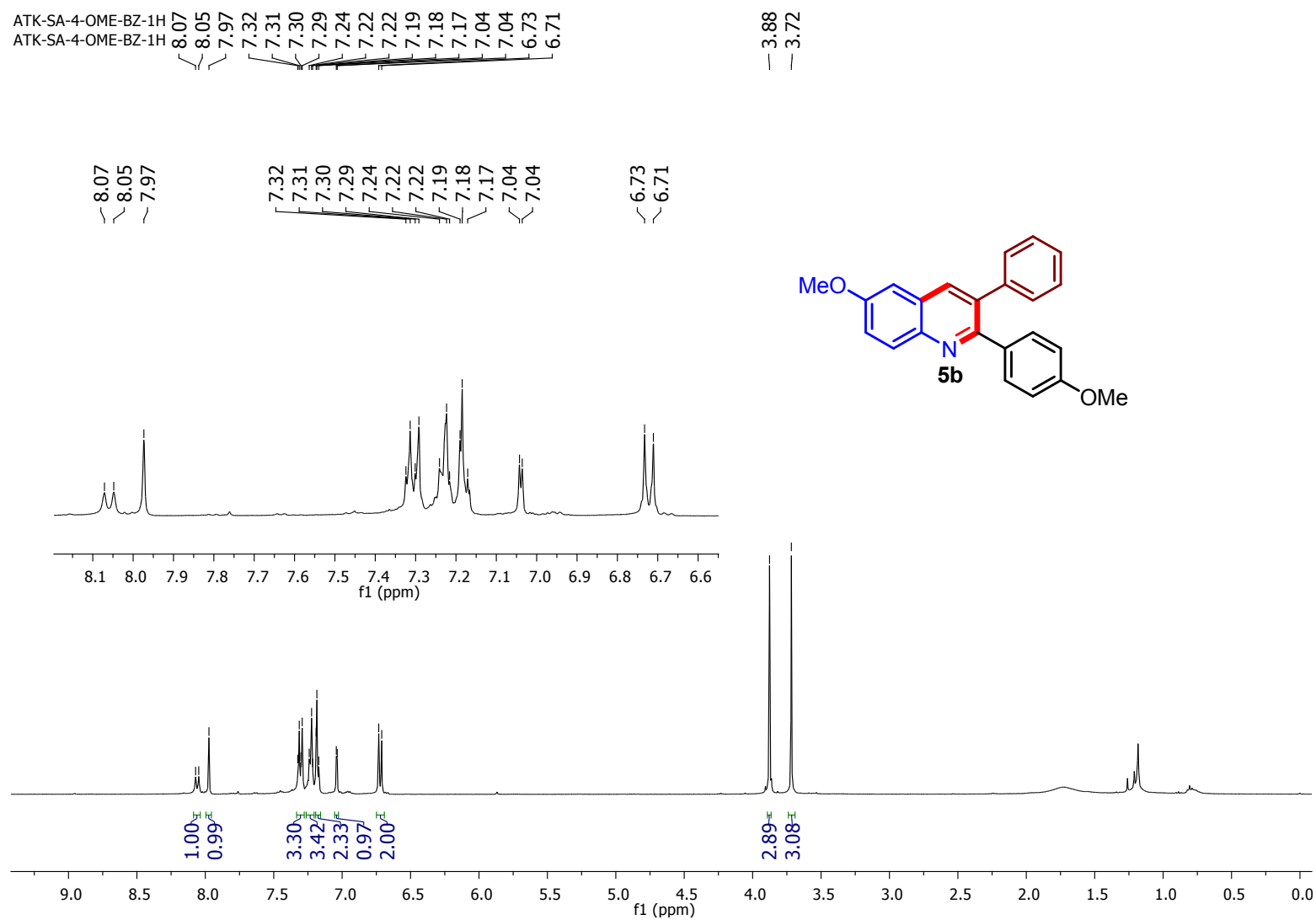


HRMS spectrum of compound: 5a

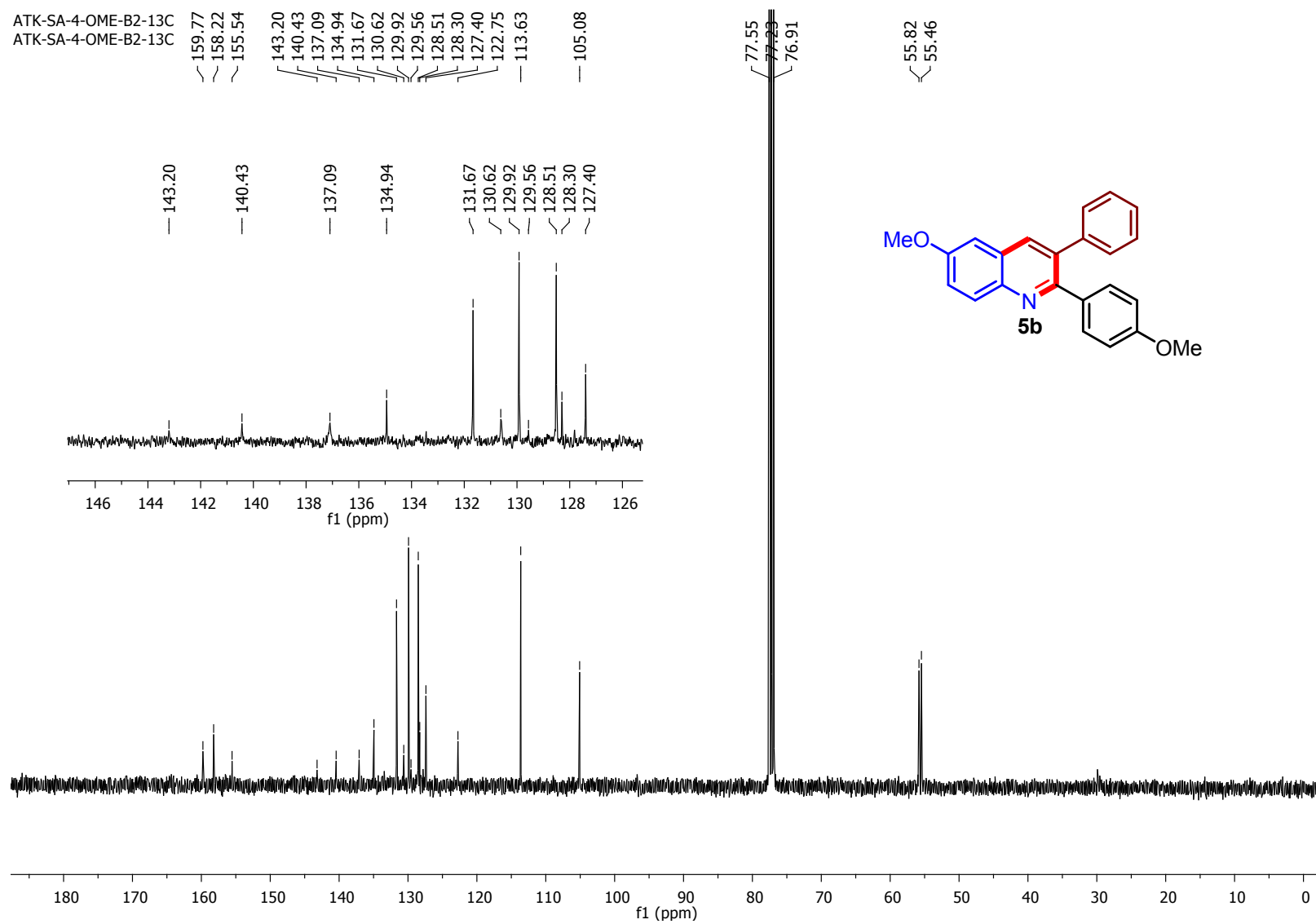
Sample Name	SAMPLE 34	Position	P2-D2	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-BZ.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	8/9/2019 6:12:22 PM



¹HNMR spectrum of compound: 5b

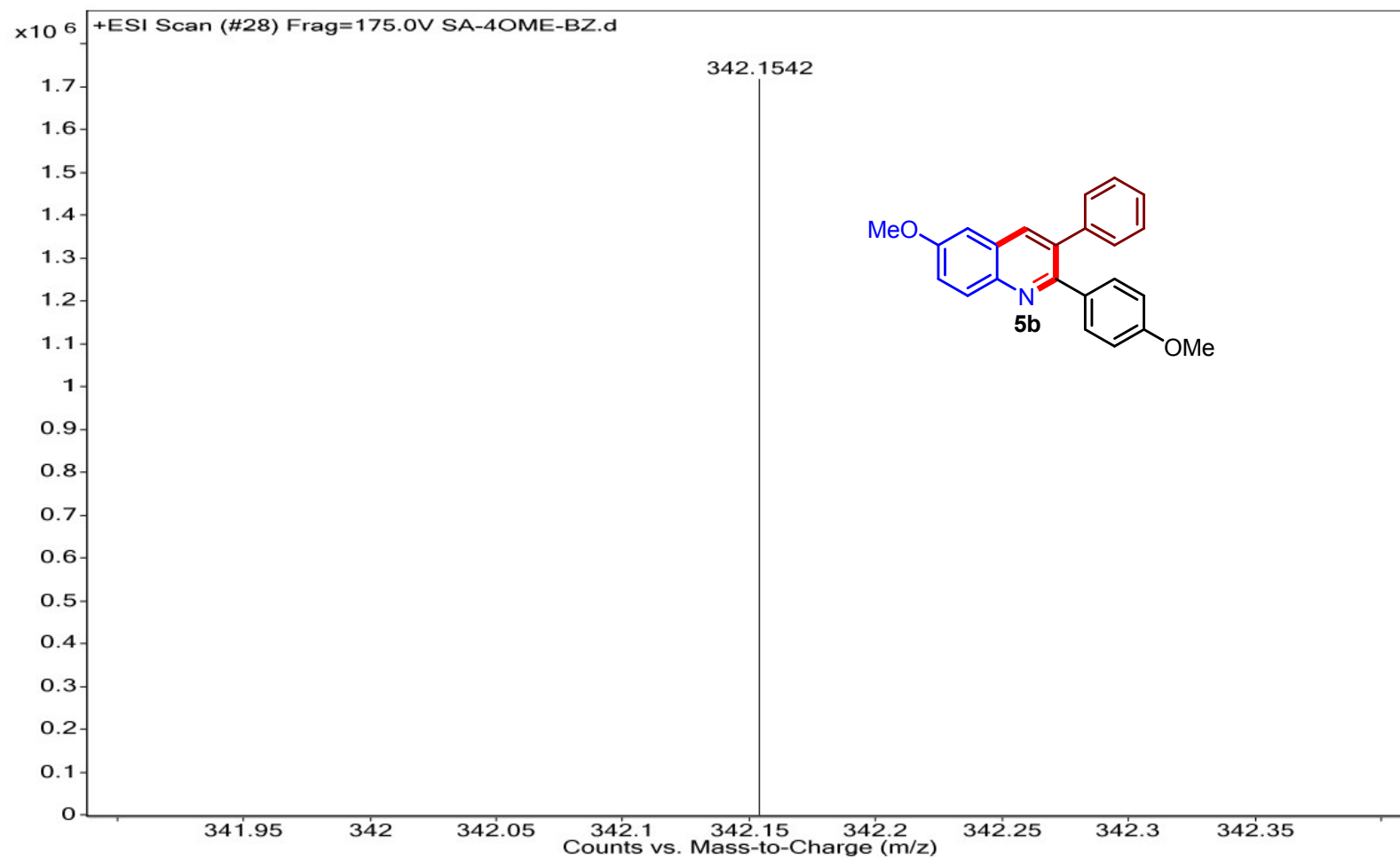


¹³CNMR spectrum of compound: 5b

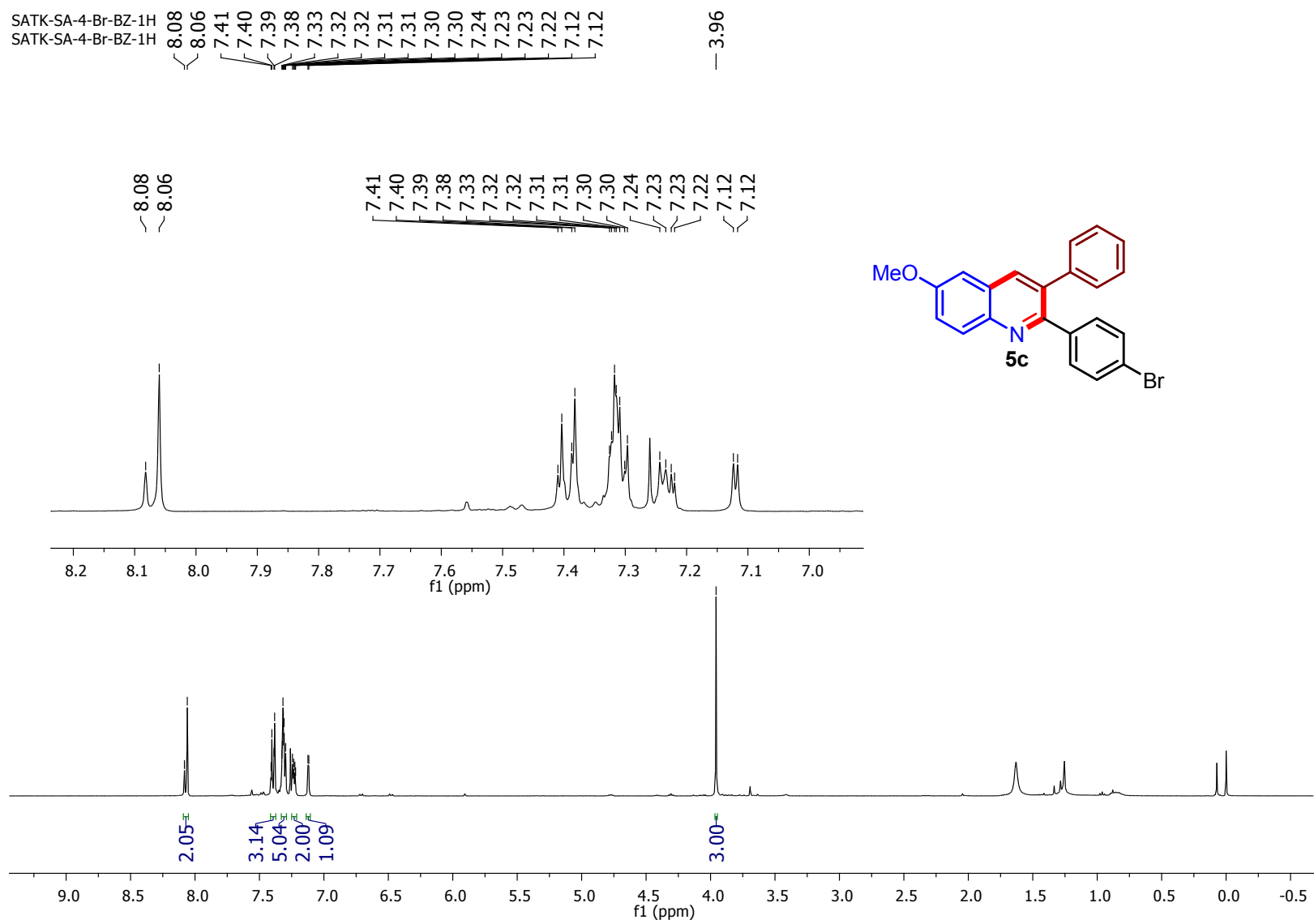


HRMS spectrum of compound: 5b

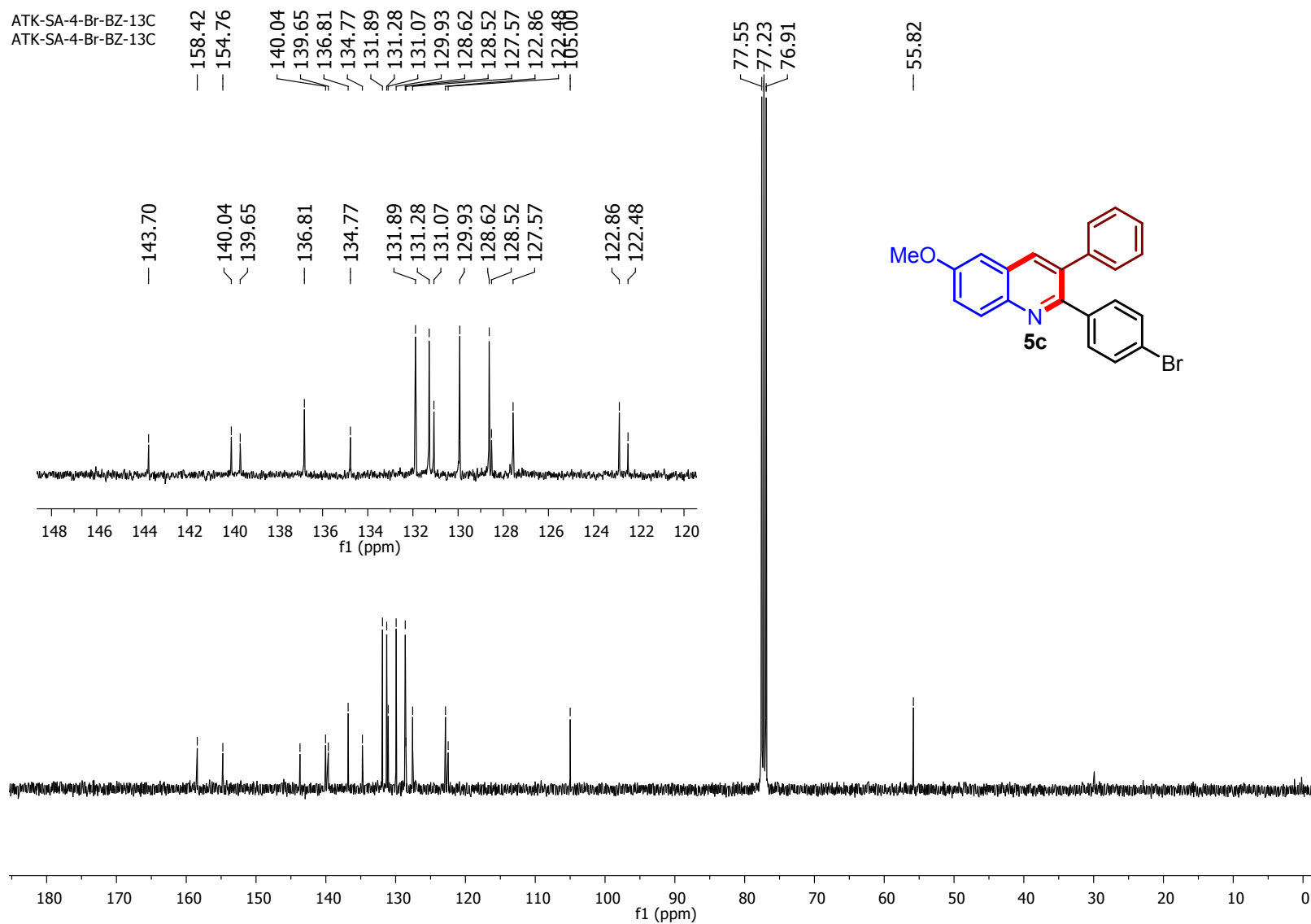
Sample Name	SAMPLE	Position	P1-F6	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-4OME-BZ.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/6/2020 6:17:47 PM



¹HNMR spectrum of compound: 5c

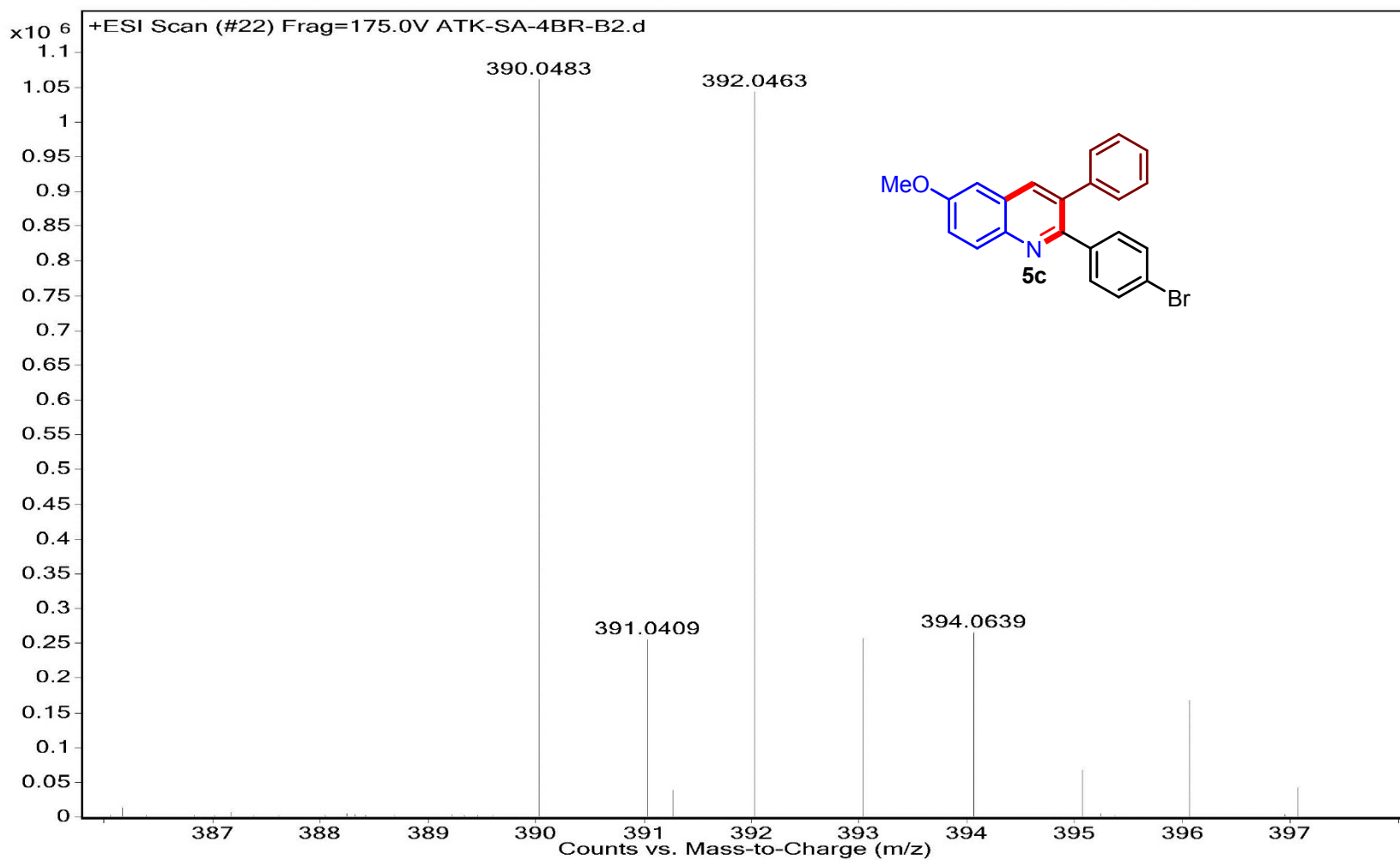


¹³CNMR spectrum of compound: 5c



HRMS spectrum of compound: 5c

Sample Name	SAMPLE 21	Position	P1-D4	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-4BR-B2.d	ACQ Method	ESI ALS 100-600.m	Comment		Acquired Time	10/29/2019 5:12:51 PM



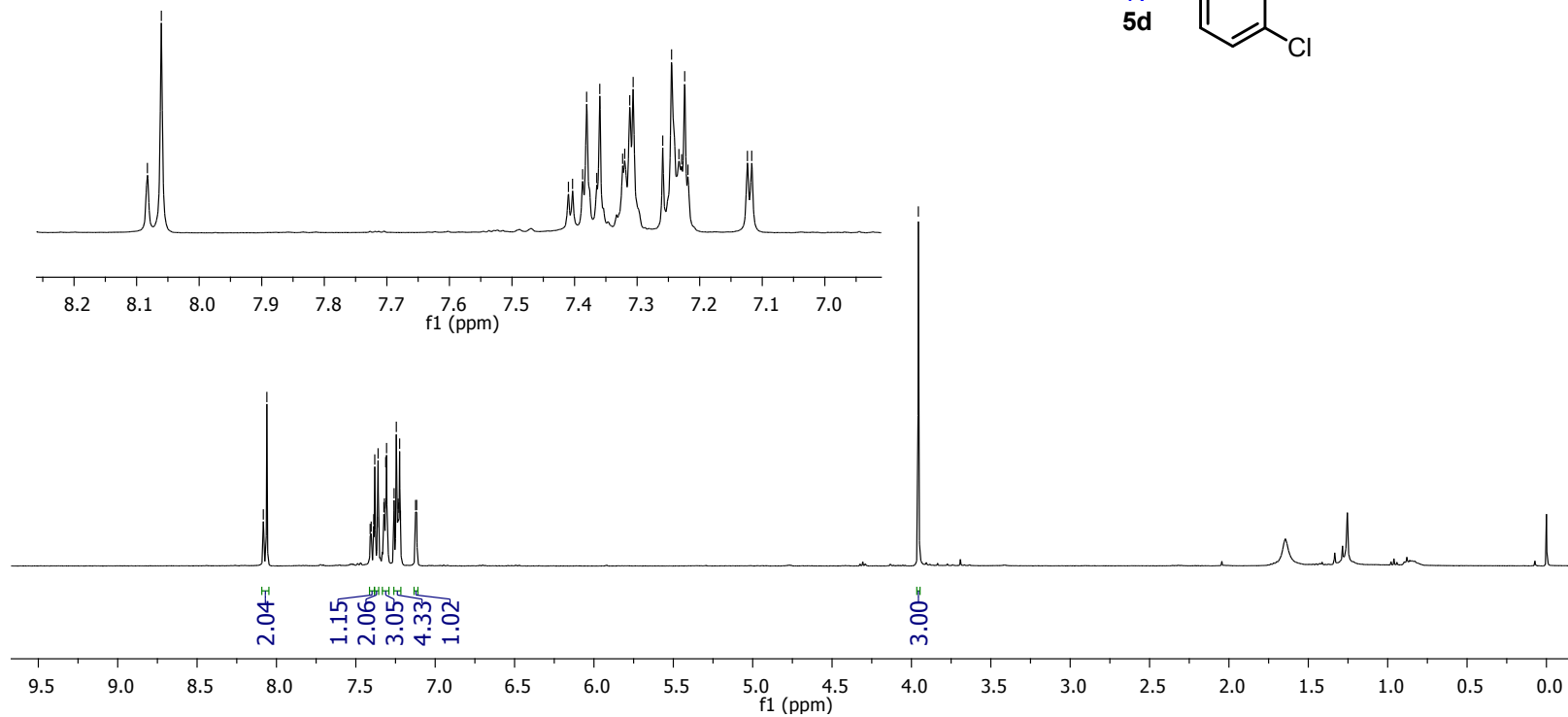
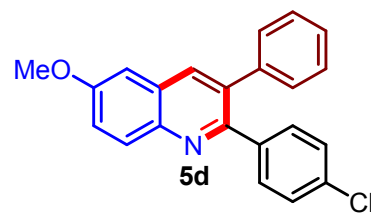
¹H NMR spectrum of compound: 5d

SATK-SA-4-Cl-BZ-A-1H
SATK-SA-4-Cl-BZ-A-1H

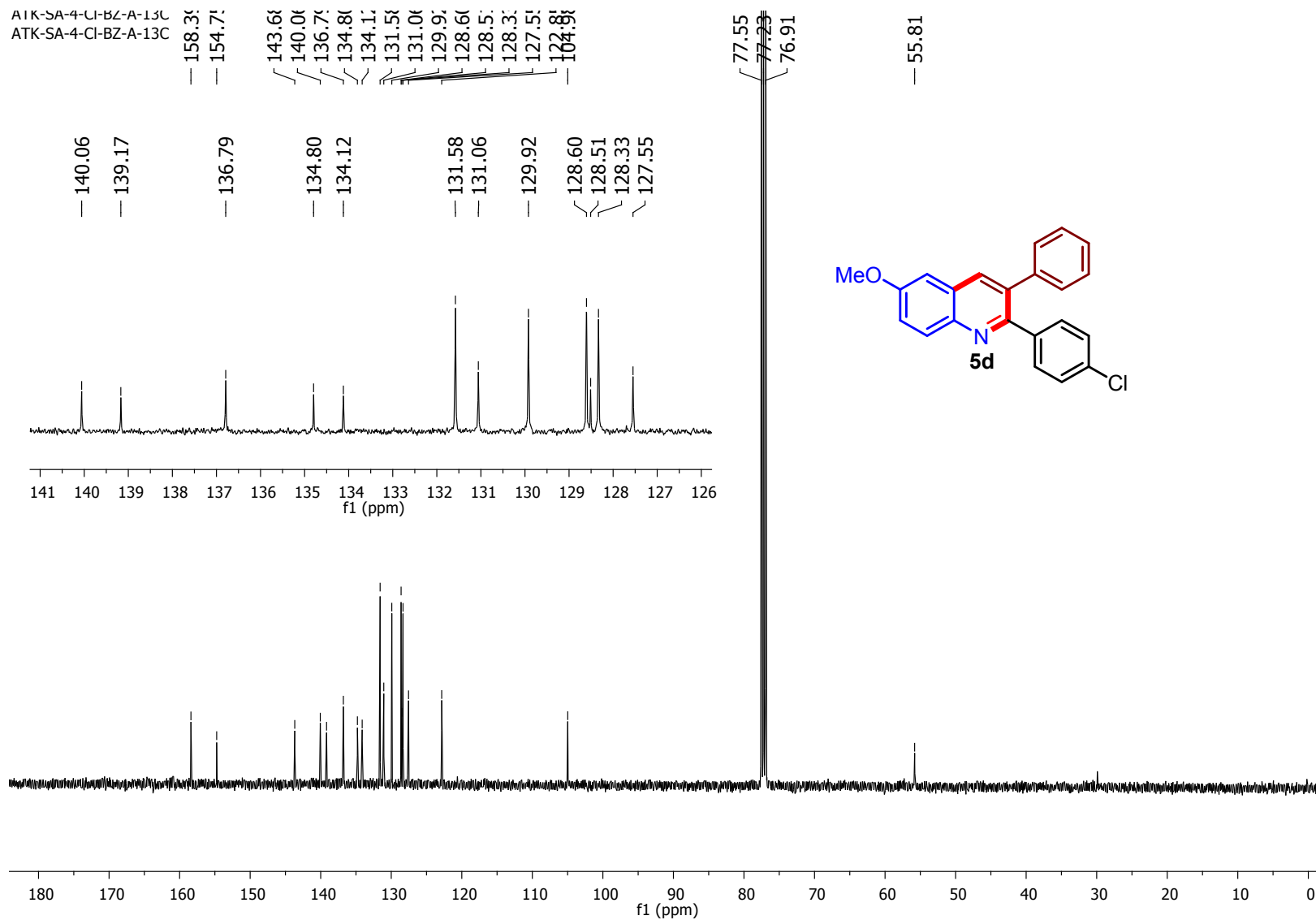
8.08
8.06
7.41
7.40
7.39
7.38
7.36
7.36
7.32
7.32
7.31
7.31
7.26
7.24
7.23
7.23
7.22
7.22
7.12
7.12
3.96

8.08
8.06

7.41
7.40
7.39
7.38
7.36
7.36
7.32
7.32
7.31
7.31
7.26
7.24
7.23
7.23
7.22
7.22
7.12
7.12

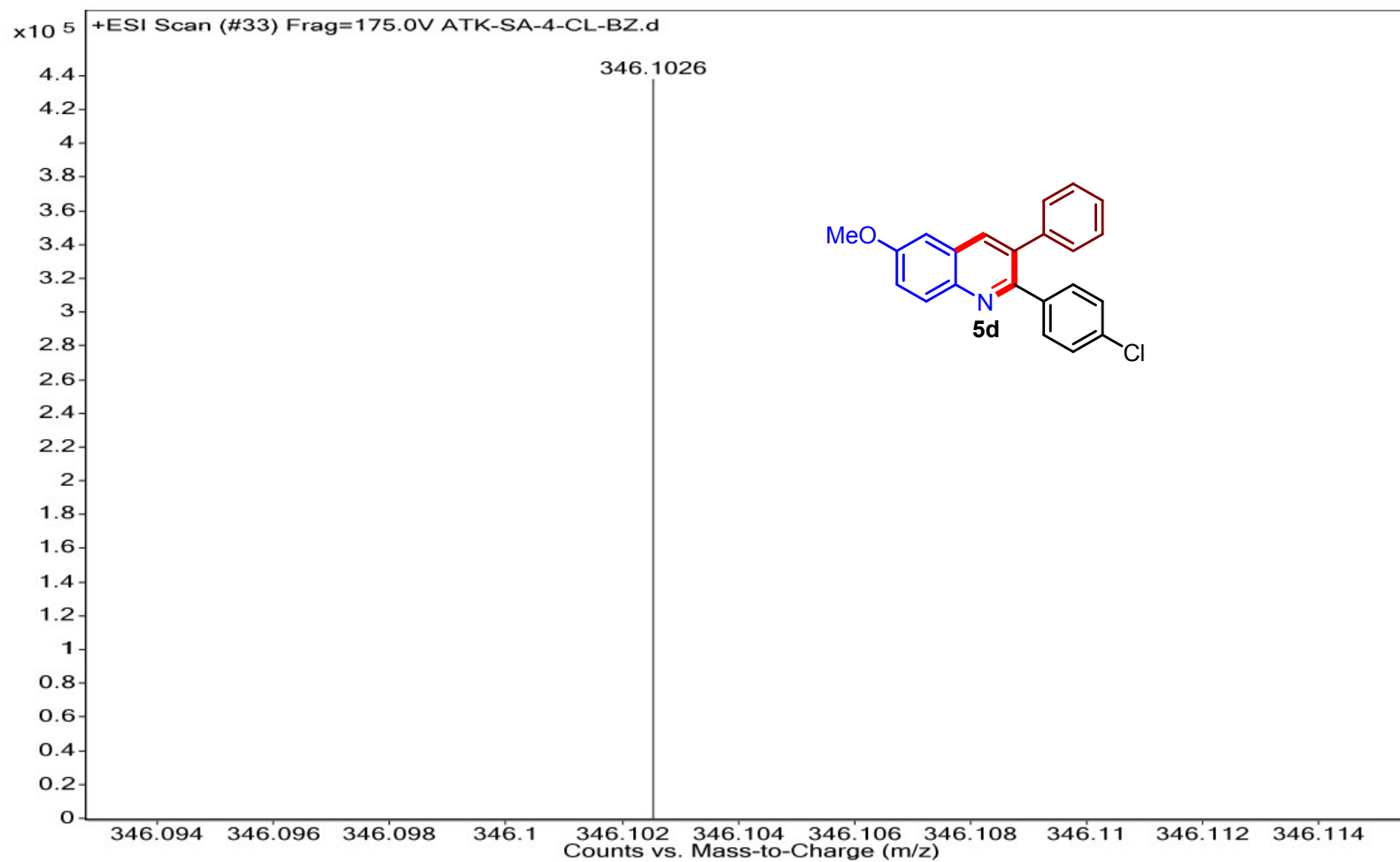


¹³CNMR spectrum of compound: 5d



HRMS spectrum of compound: 5d

Sample Name	SAMPLE 31	Position	P2-C10	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-4-CL-BZ.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	8/9/2019 6:08:28 PM



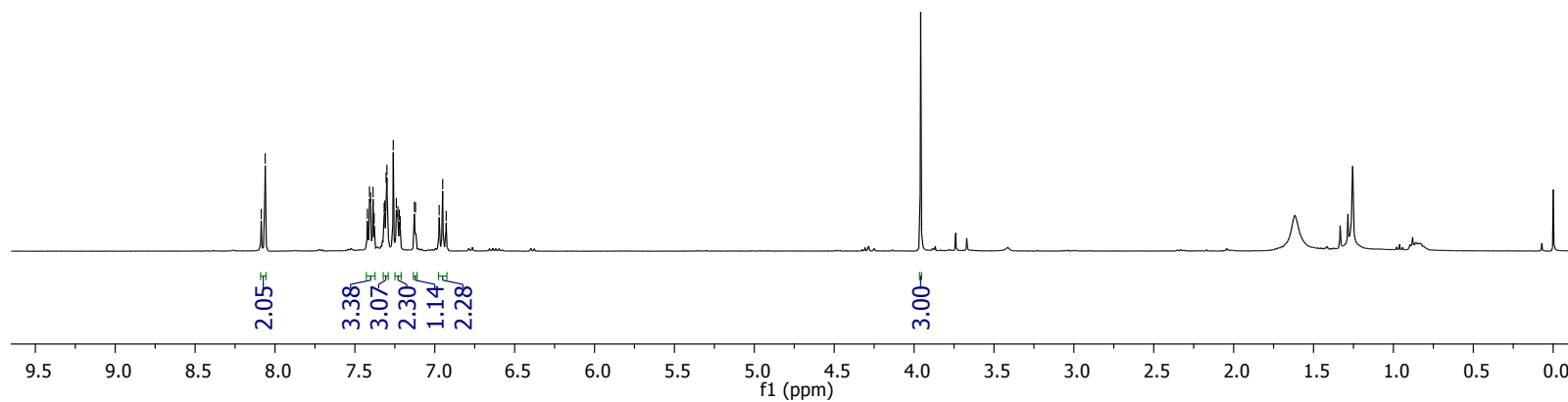
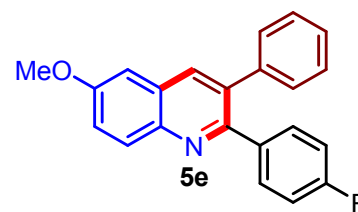
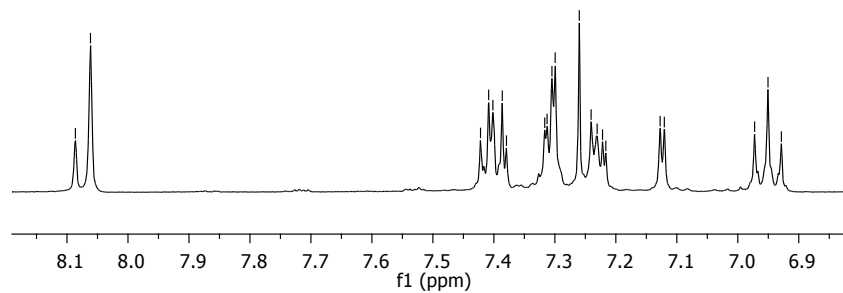
¹HNMR spectrum of compound: 5e

ATK-SA-4-F-BZ-A-1H
ATK-SA-4-F-BZ-A-1H

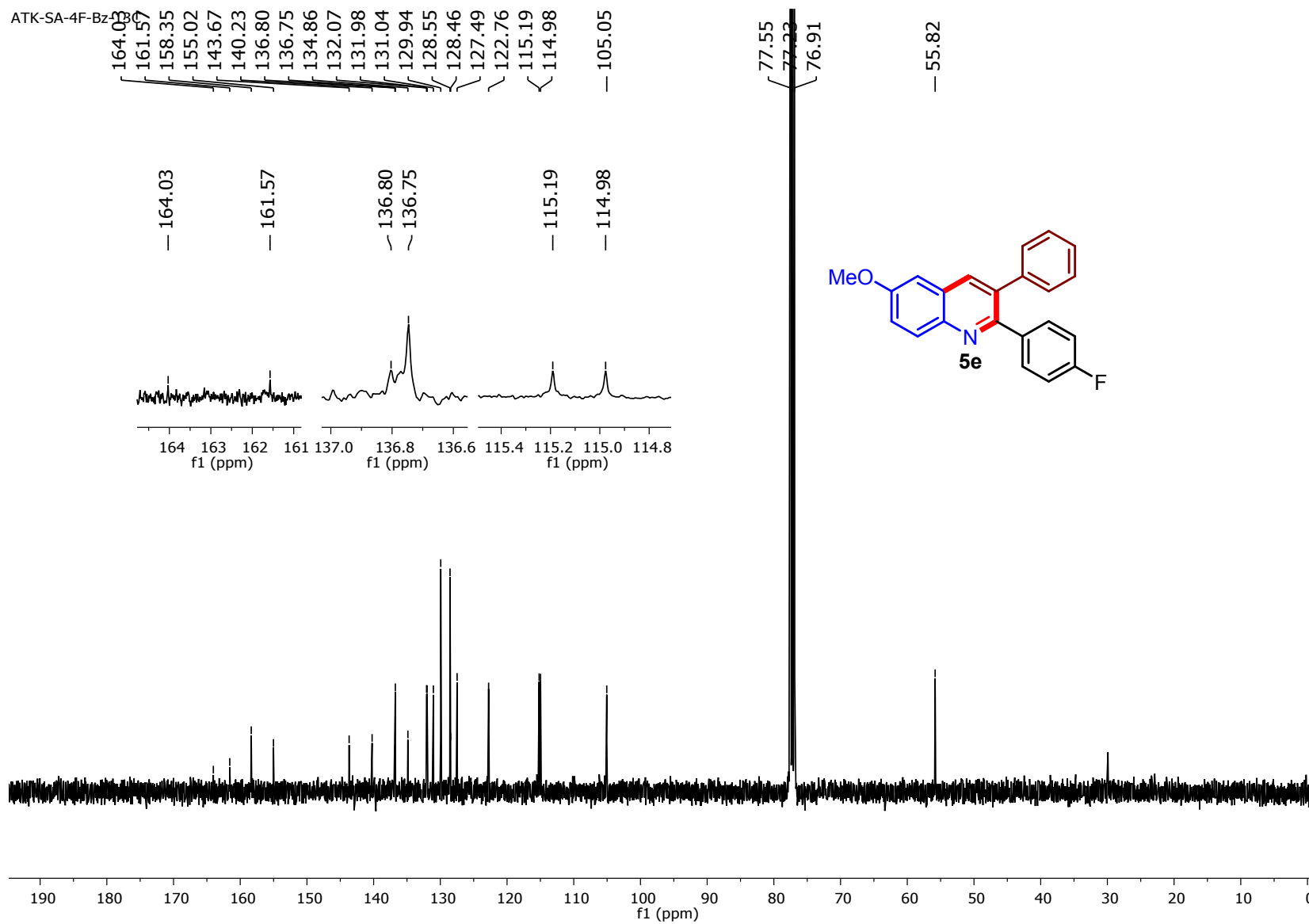
8.09
8.06
7.42
7.41
7.40
7.39
7.38
7.32
7.31
7.30
7.30
7.26
7.24
7.23
7.22
7.22
7.13
7.12
6.97
6.95
6.93

8.09
8.06

7.42
7.41
7.40
7.39
7.38
7.32
7.31
7.30
7.30
7.26
7.24
7.23
7.22
7.22
7.13
7.12
6.97
6.95
6.93

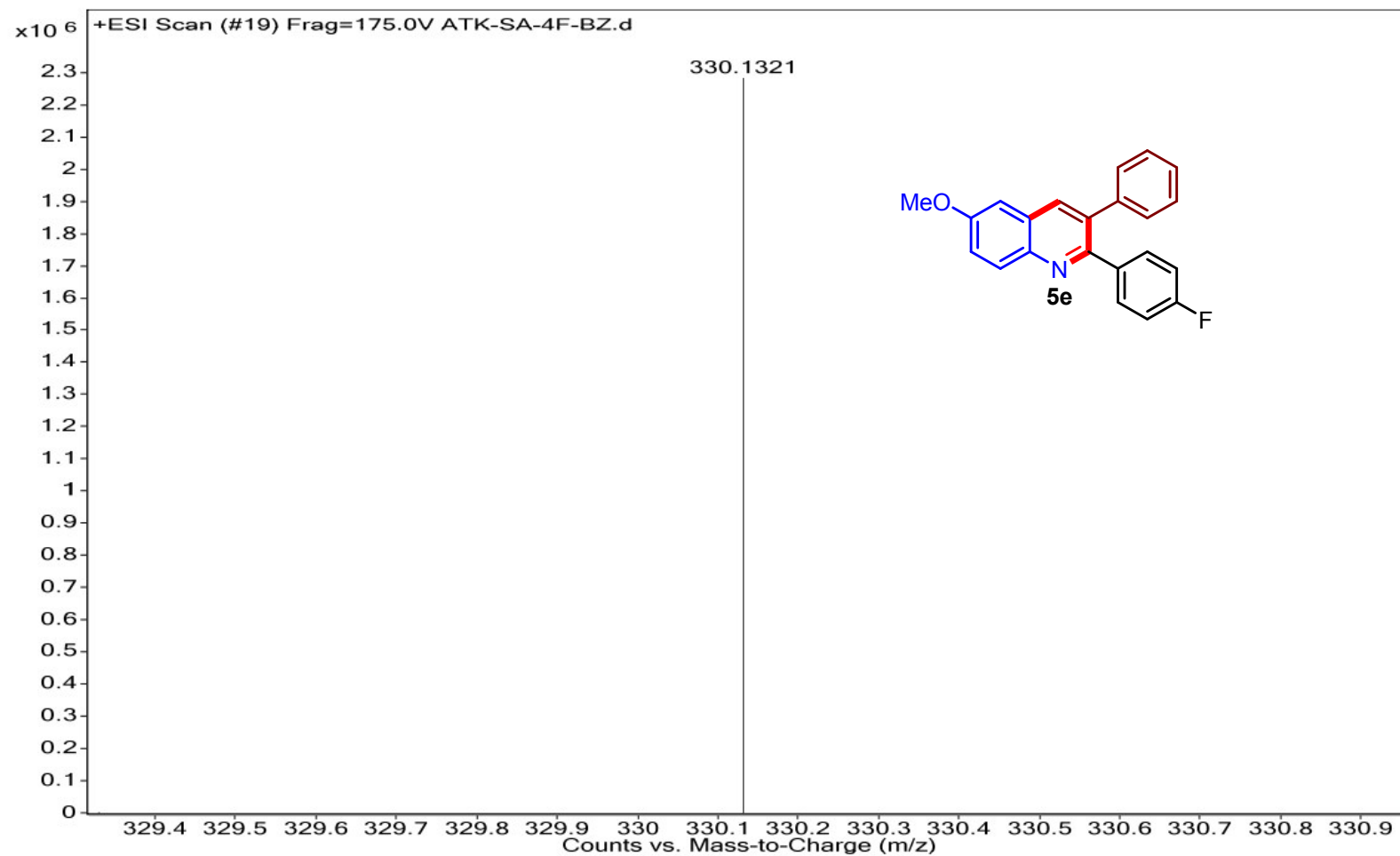


¹³CNMR spectrum of compound: 5e



HRMS spectrum of compound: 5e

Sample Name	SAMPLE 23	Position	P2-C5	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-4F-BZ.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	8/9/2019 6:06:32 PM



¹HNMR spectrum of compound: 5f

ATK-SA-3,4-OME-BZ-1H
ATK-SA-3,4-OME-BZ-1H

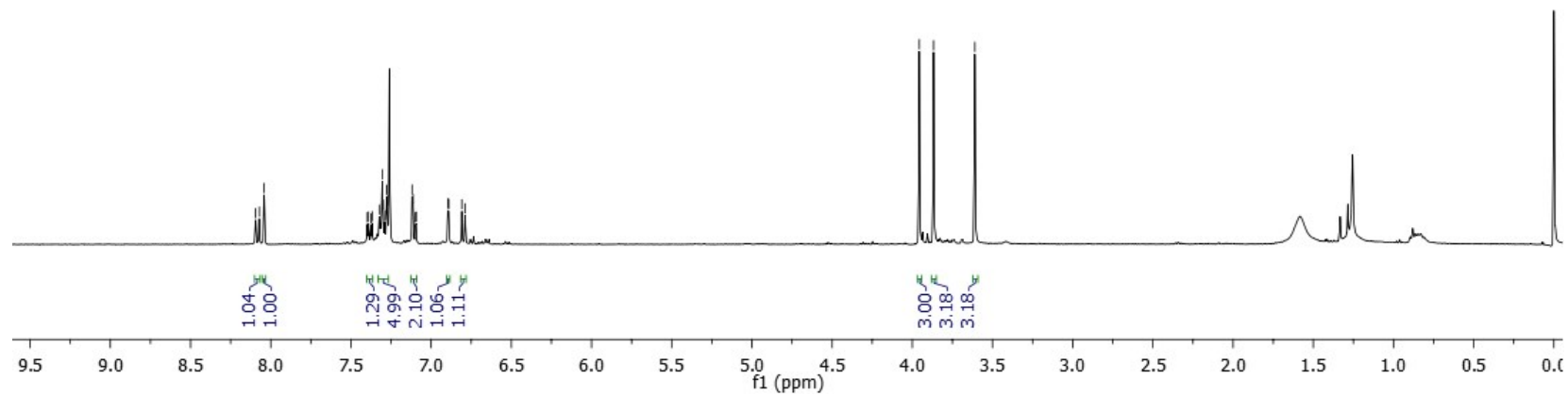
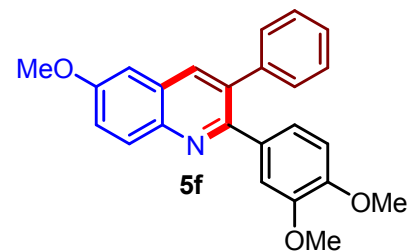
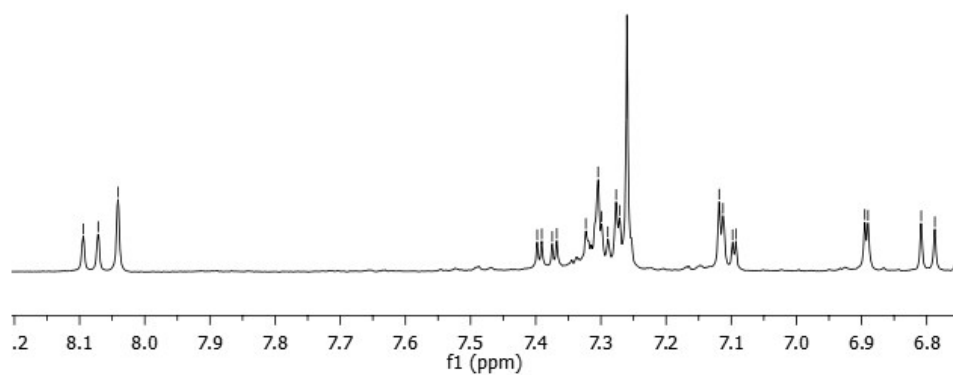
8.09
8.07
8.04
7.40
7.39
7.37
7.37
7.32
7.30
7.30
7.29
7.28
7.27
7.12
7.11
7.10
7.09
6.89
6.89
6.81
6.79

3.96
3.87
3.61

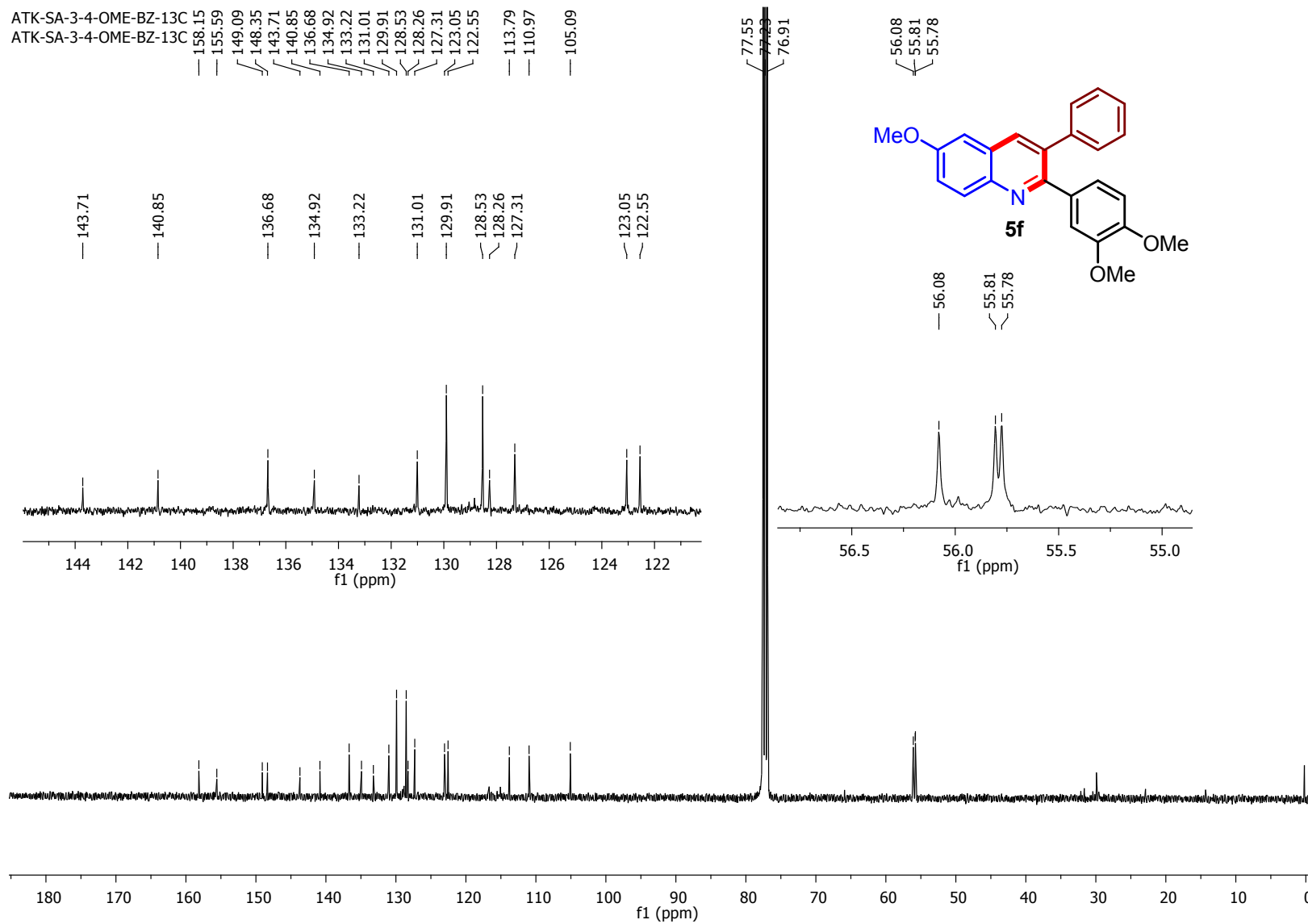
8.09
8.07
8.04

7.40
7.39
7.37
7.37
7.32
7.30
7.30
7.29
7.28
7.27
7.12
7.11
7.10
7.09

6.89
6.89
6.81
6.79

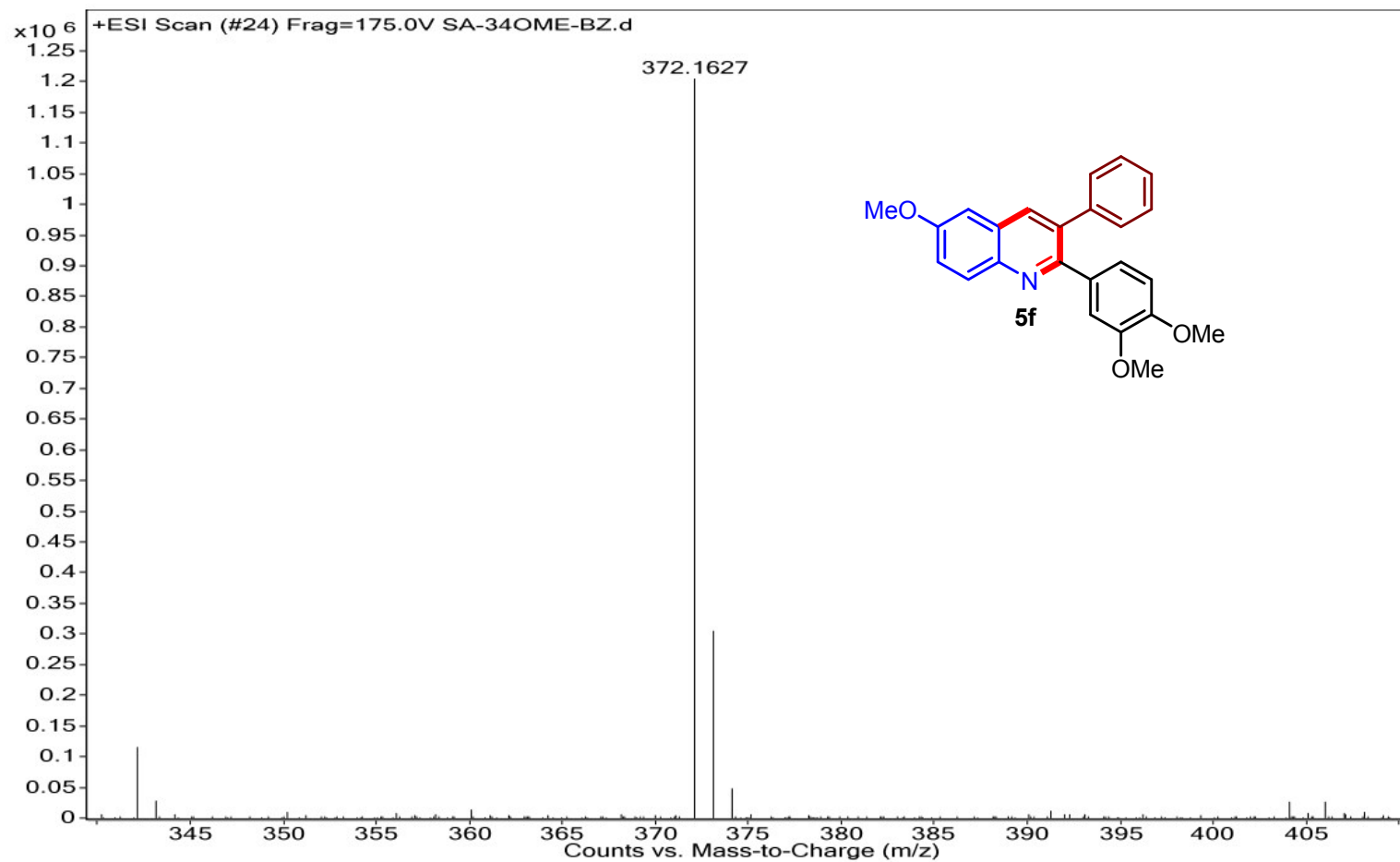


¹³CNMR spectrum of compound: 5f



HRMS spectrum of compound: 5f

Sample Name	SAMPLE	Position	P1-F2	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-34OME-BZ.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/6/2020 6:06:17 PM



¹HNMR spectrum of compound: 5g

ATK-SA-3,4,5-OMe-BZ-B-1H
ATK-SA-3,4,5-OMe-BZ-B-1H

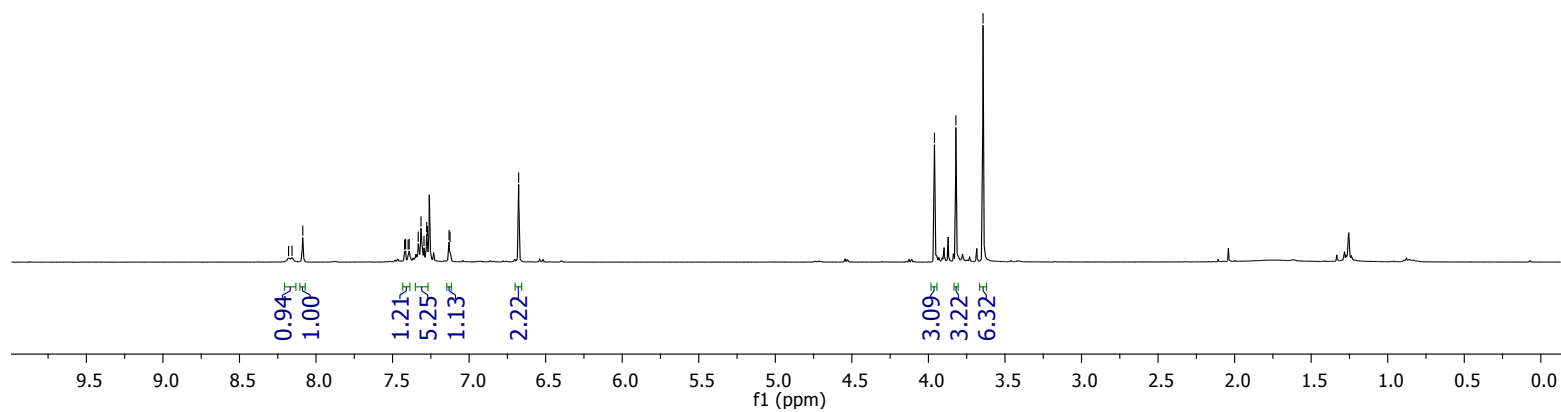
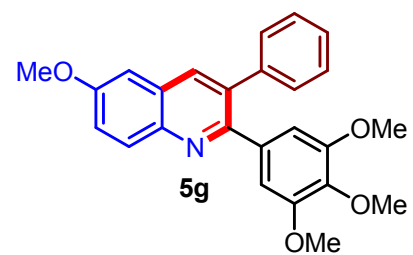
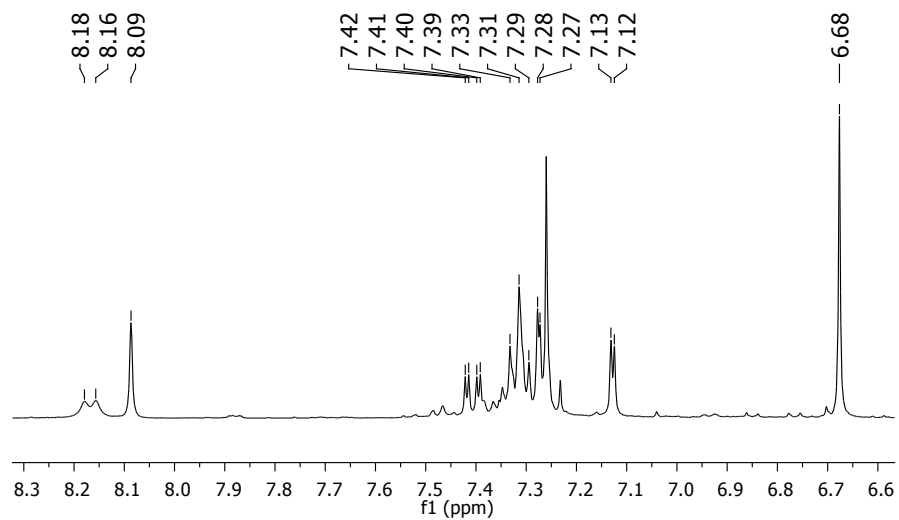
8.18
8.16
8.09
7.33
7.31
7.28
7.27
7.13
7.12

3.96
3.82
3.64

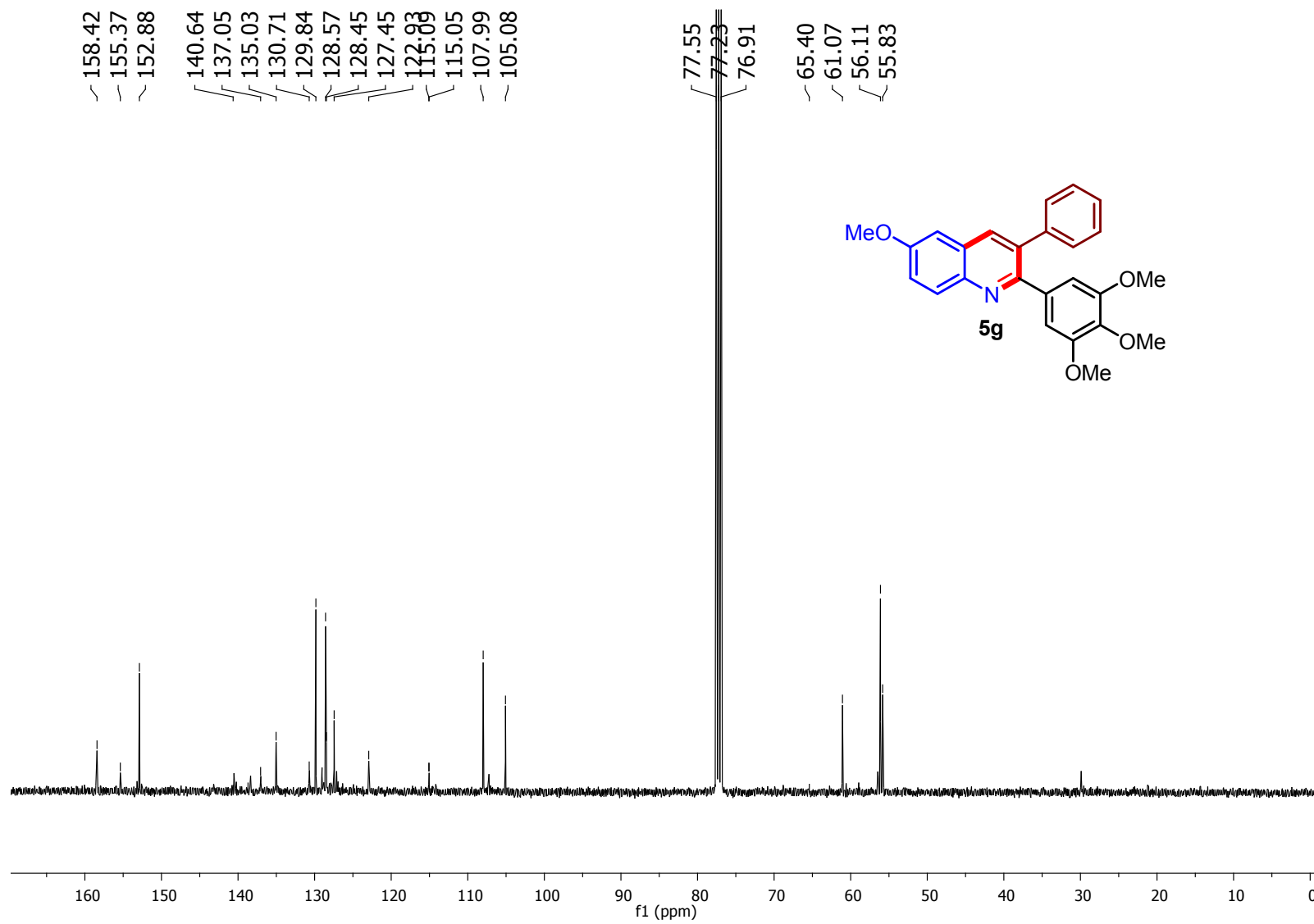
8.18
8.16
8.09

7.42
7.41
7.40
7.39
7.33
7.31
7.29
7.28
7.27
7.13
7.12

6.68

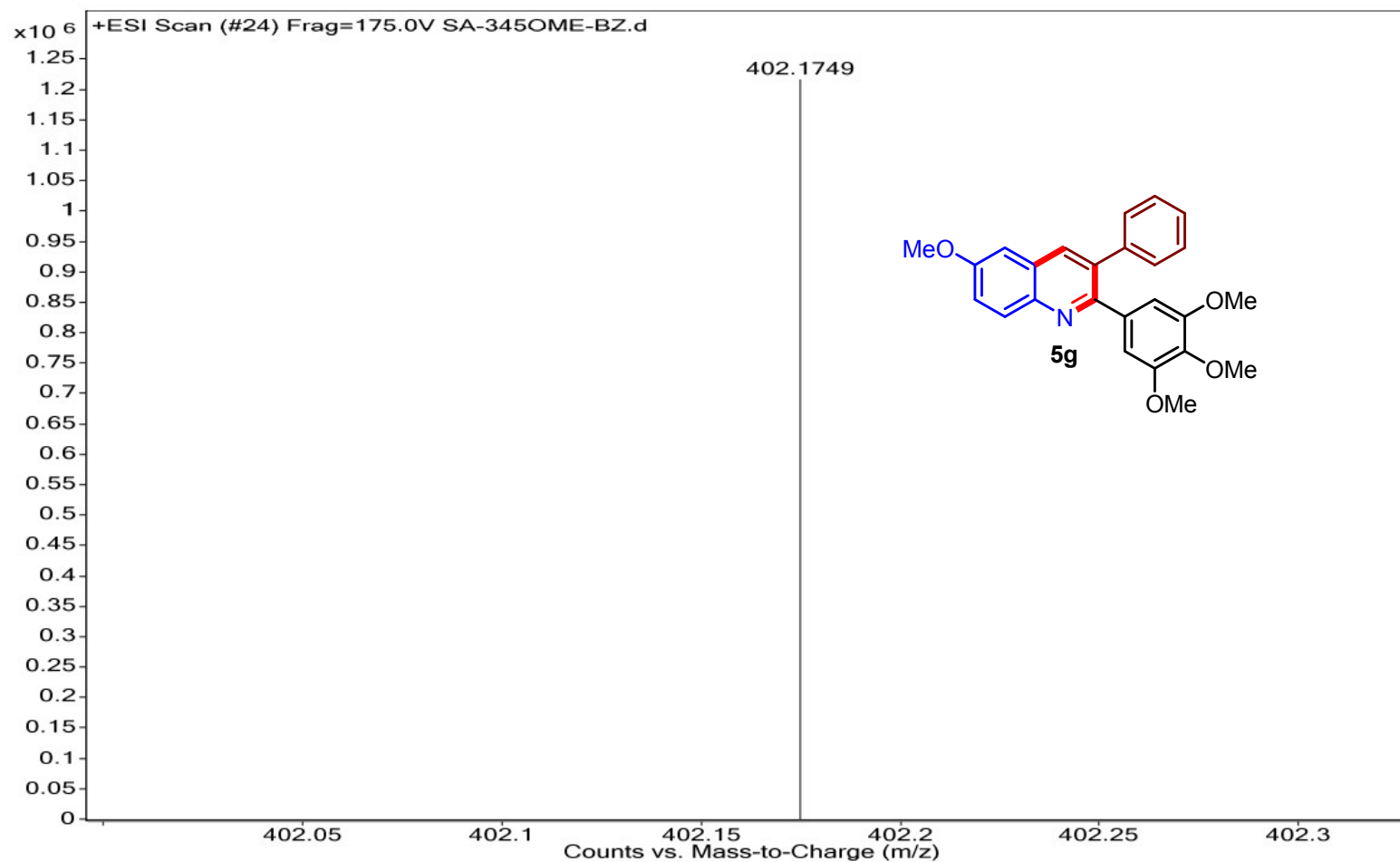


¹³CNMR spectrum of compound: 5g

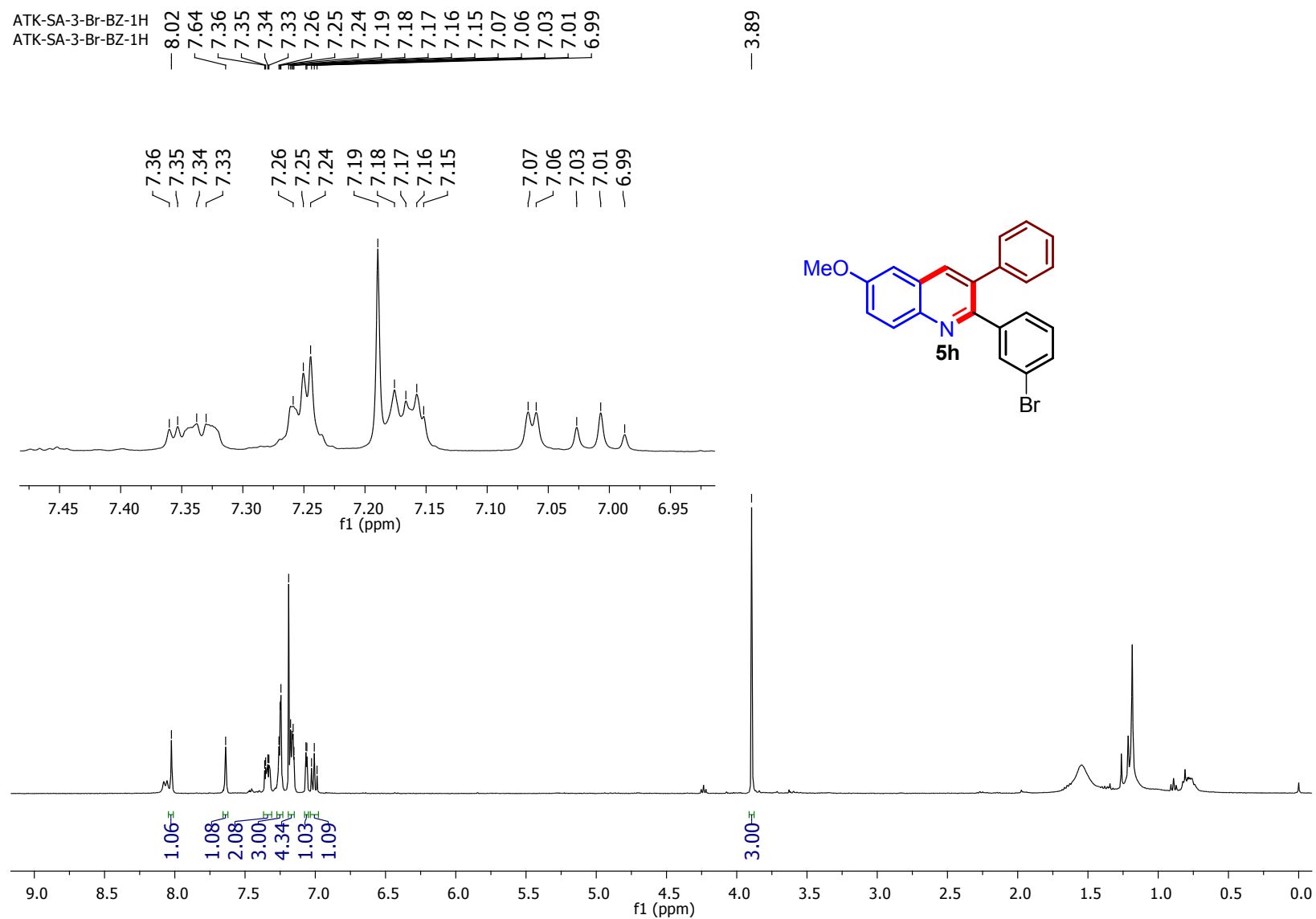


HRMS spectrum of compound: 5g

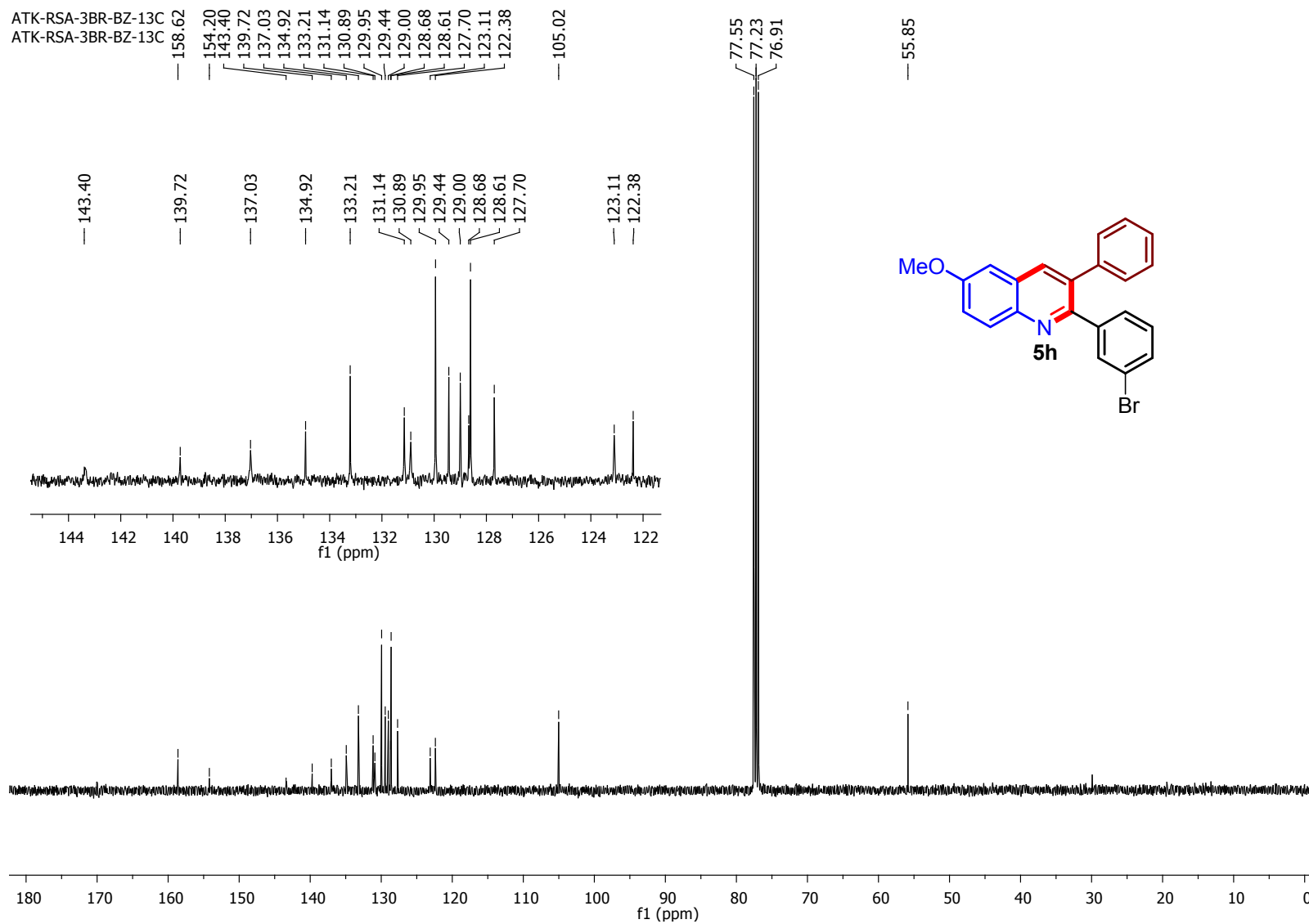
Sample Name	SAMPLE	Position	P1-F4	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-345OME-BZ.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/6/2020 6:11:57 PM



¹H NMR spectrum of compound: 5h

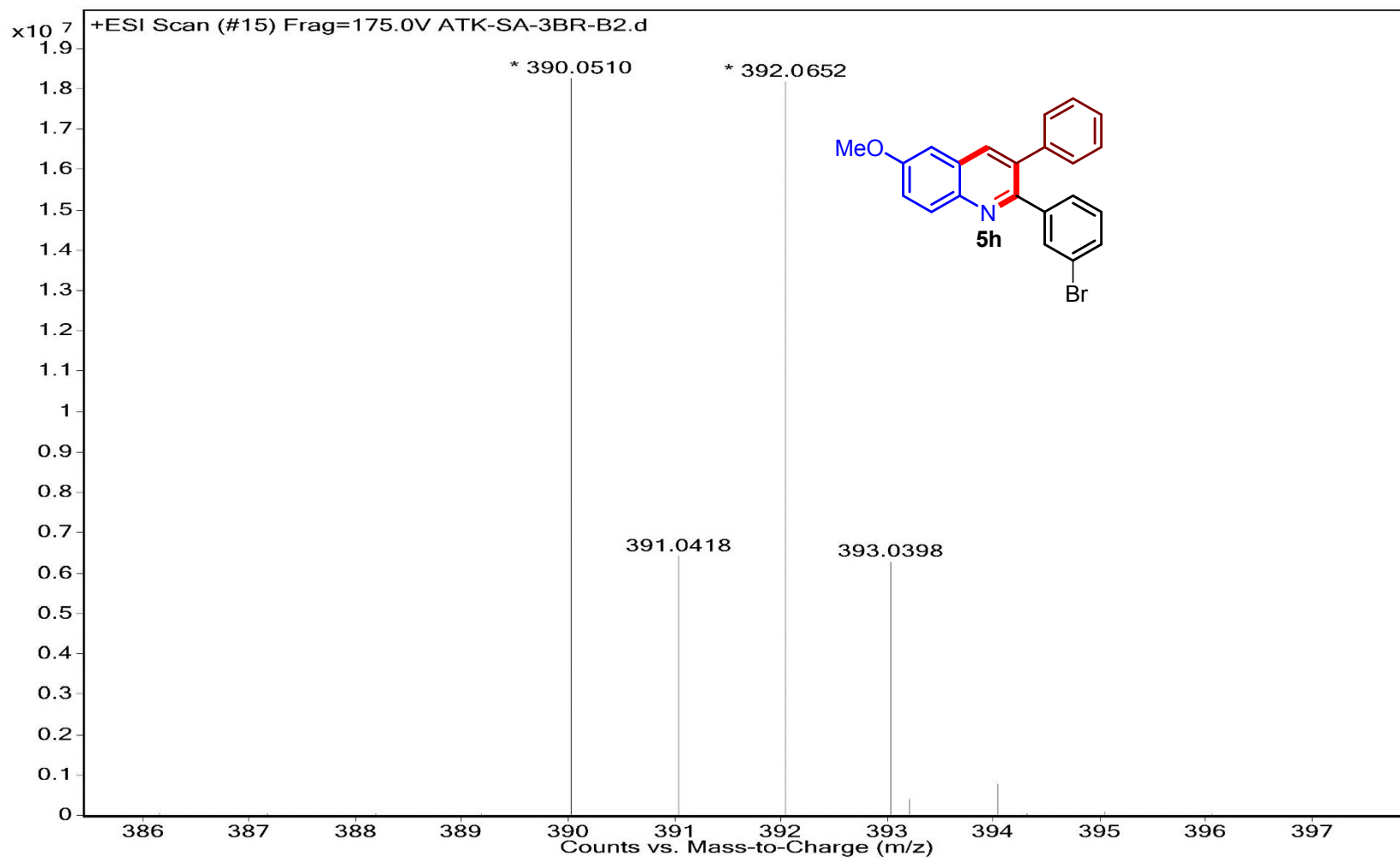


^{13}C NMR spectrum of compound: 5h

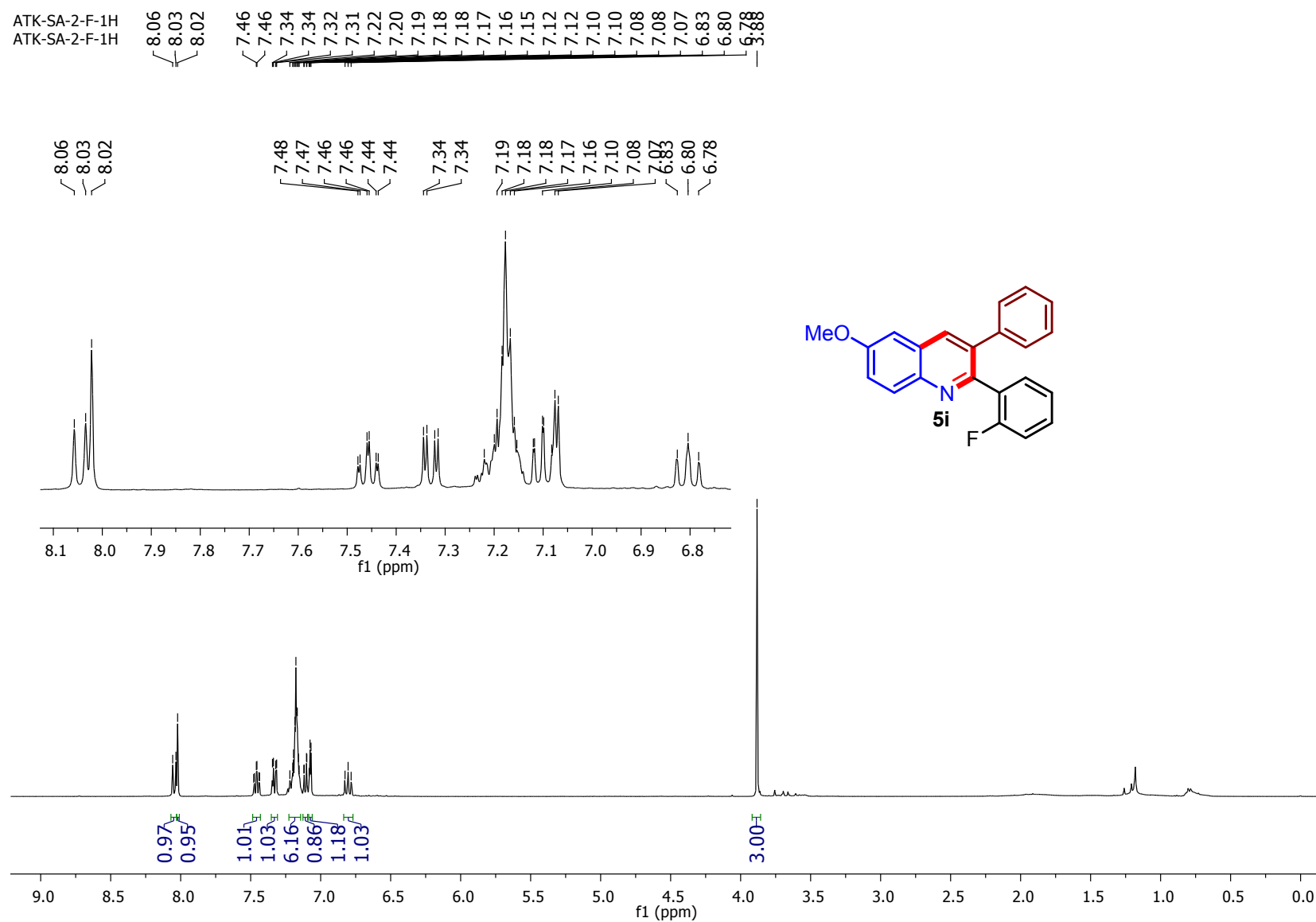


HRMS spectrum of compound: 5h

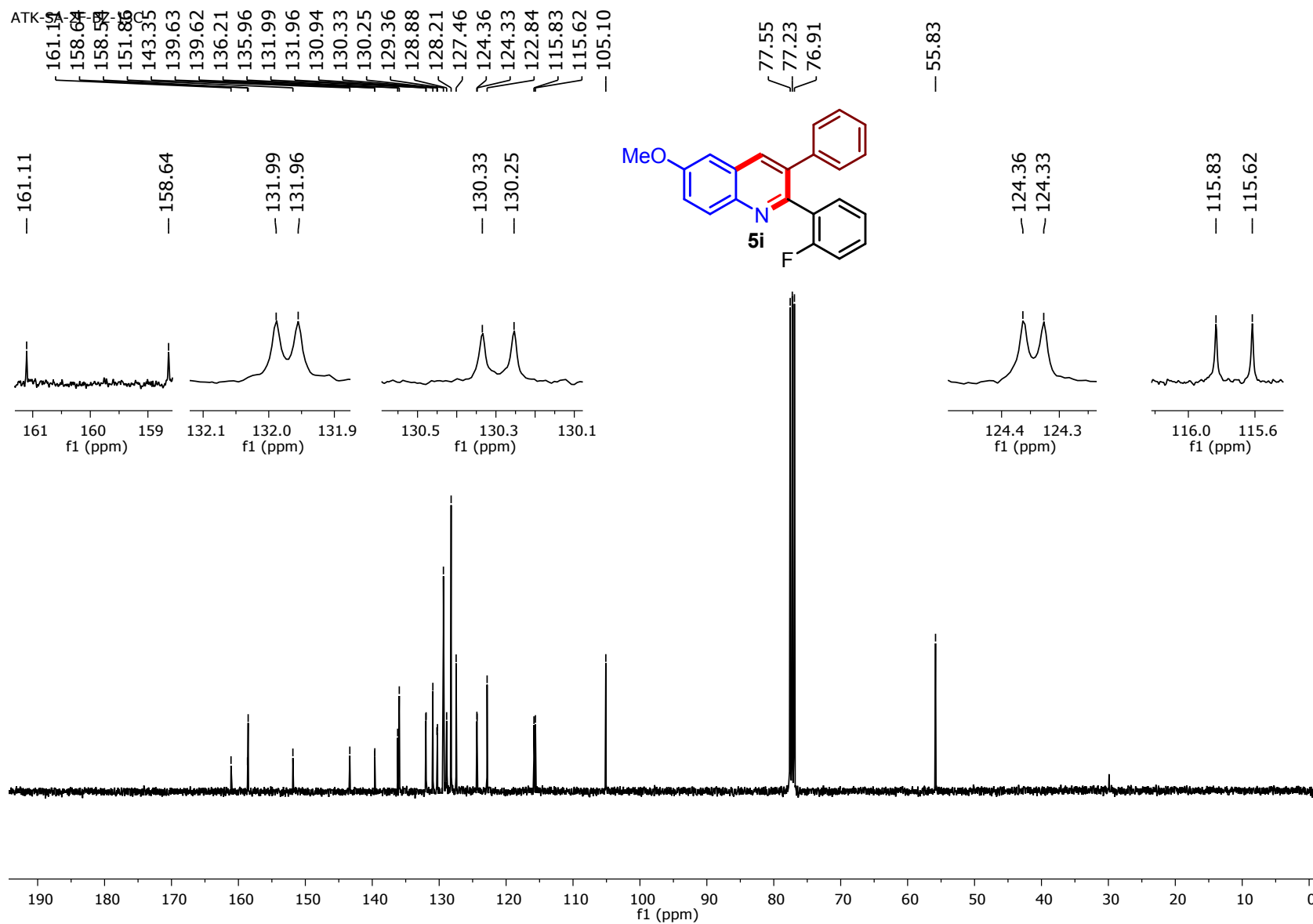
Sample Name	SAMPLE 22	Position	P1-D5	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	ATK-SA-3BR-B2.d	ACQ Method	ESI ALS 100-600.m	Comment		Acquired Time	10/29/2019 5:14:43 PM



¹HNMR spectrum of compound: 5i

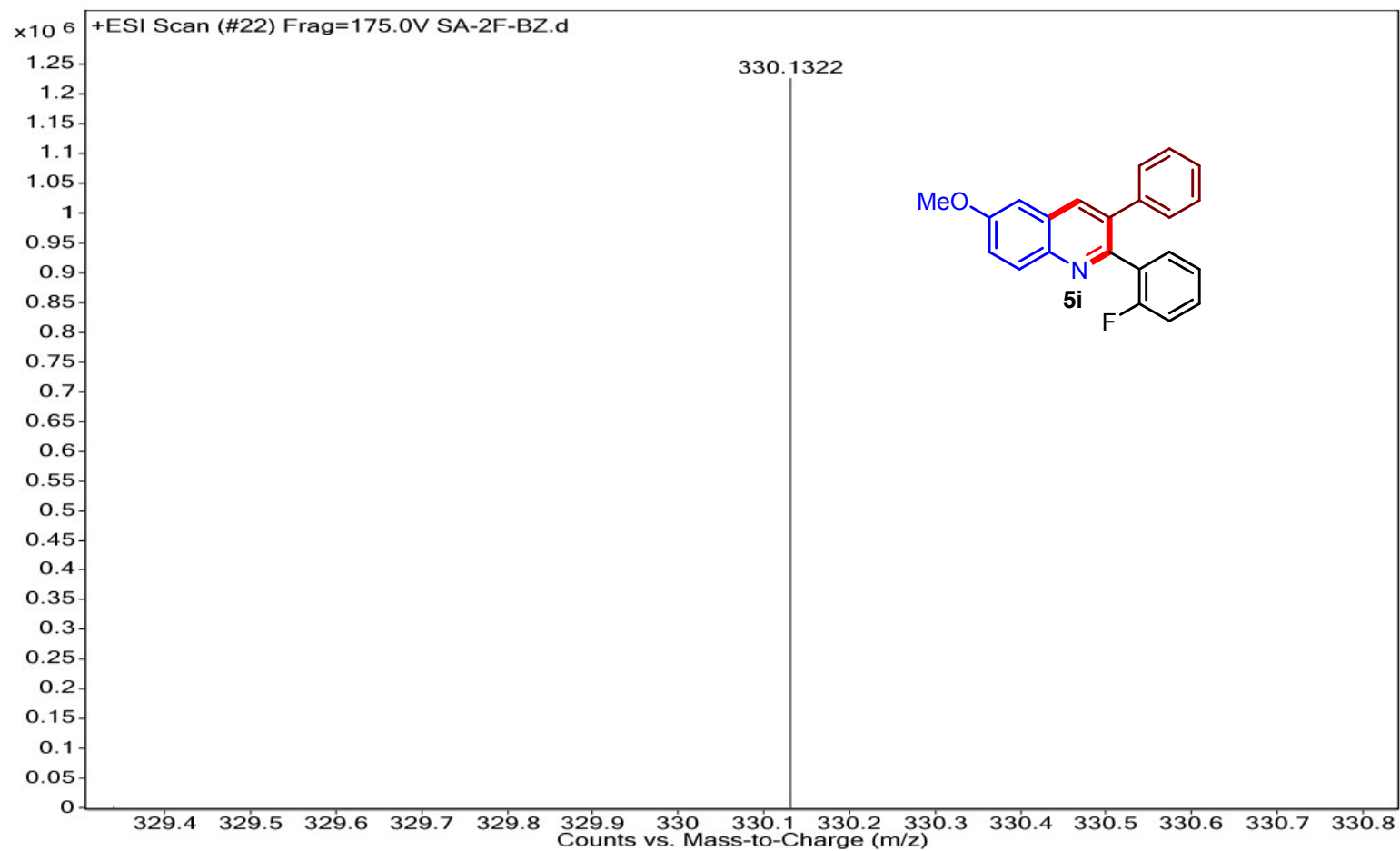


¹³CNMR spectrum of compound: **5i**

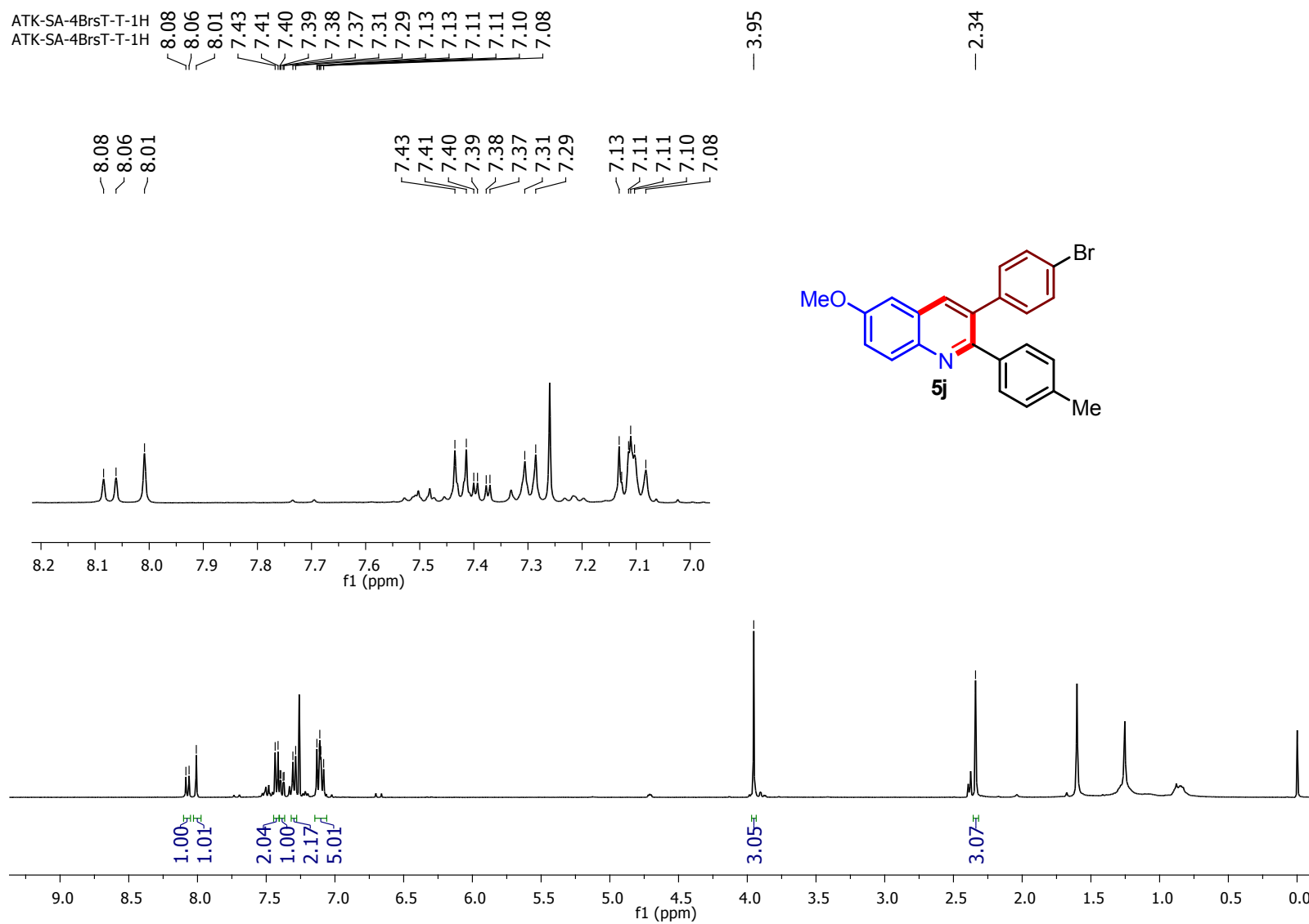


HRMS spectrum of compound: 5i

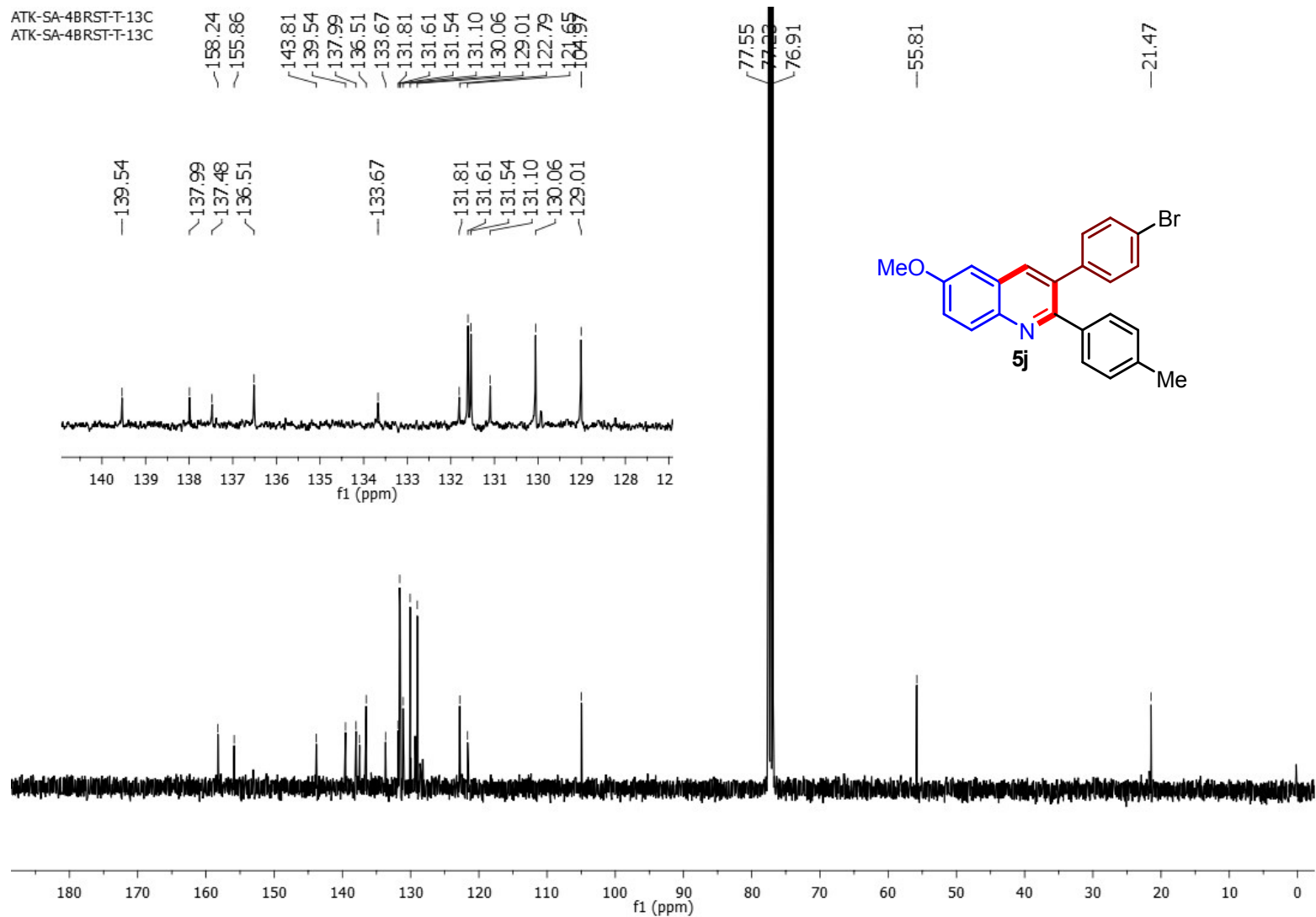
Sample Name	SAMPLE	Position	P1-F3	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-2F-BZ.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/6/2020 6:08:12 PM



¹HNMR spectrum of compound: 5j

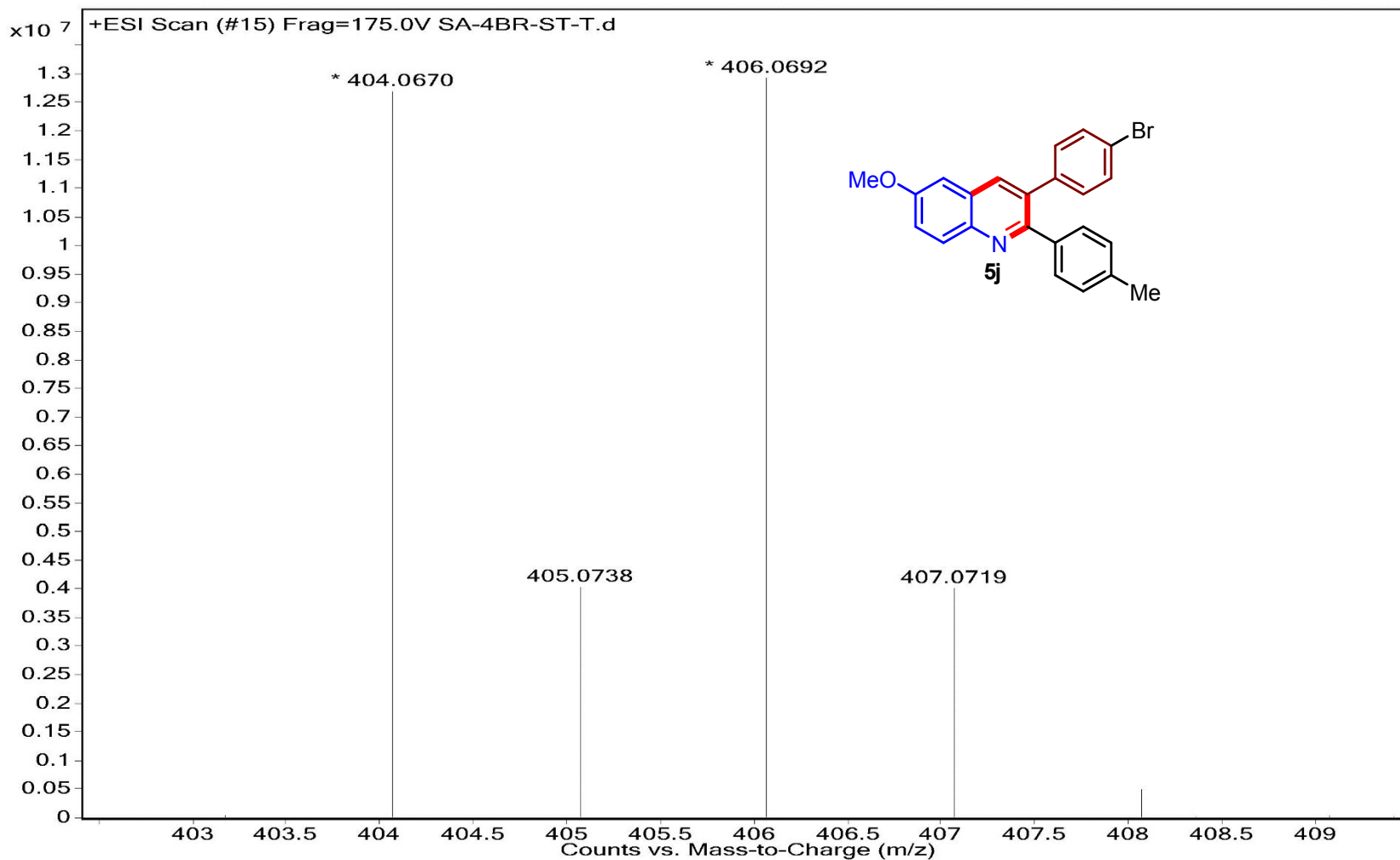


^{13}C NMR spectrum of compound: 5j



HRMS spectrum of compound: 5j

Sample Name	SAMPLE	Position	P1-F5	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-4BR-ST-T.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/6/2020 6:13:49 PM



¹HNMR spectrum of compound: 5k

ATK-SA-4Cl-ST-T-1H
ATK-SA-4Cl-ST-T-1H

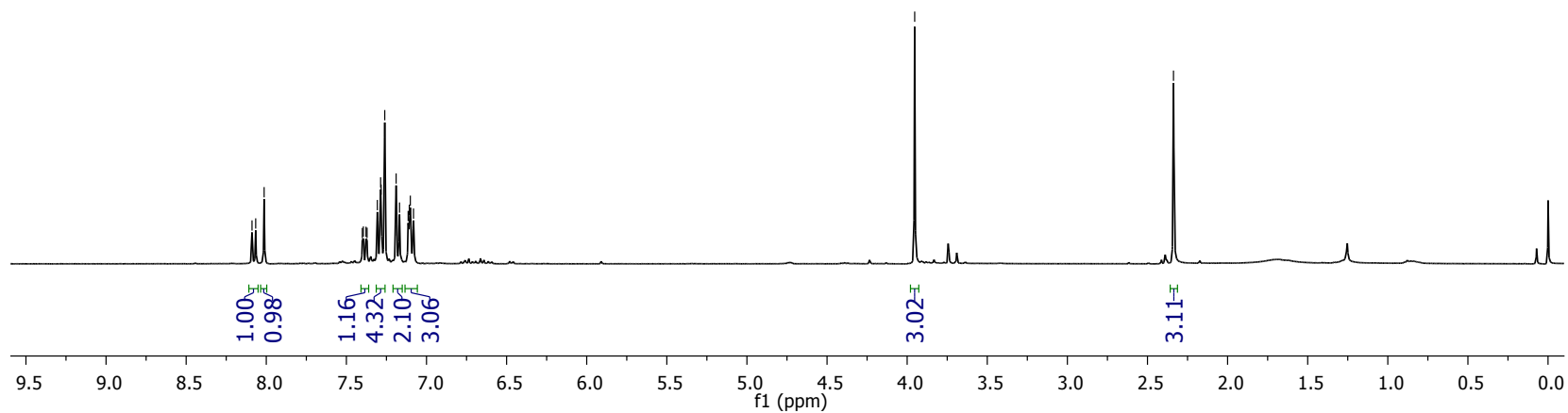
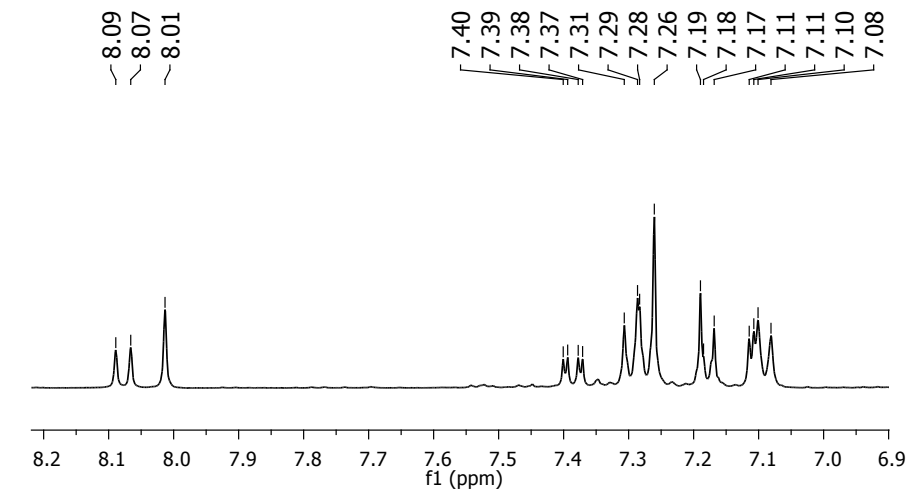
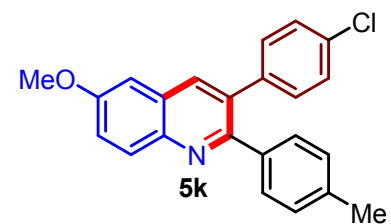
8.09
8.07
8.01
7.40
7.39
7.38
7.37
7.31
7.29
7.28
7.26
7.19
7.18
7.17
7.11
7.11
7.10
7.08

3.95

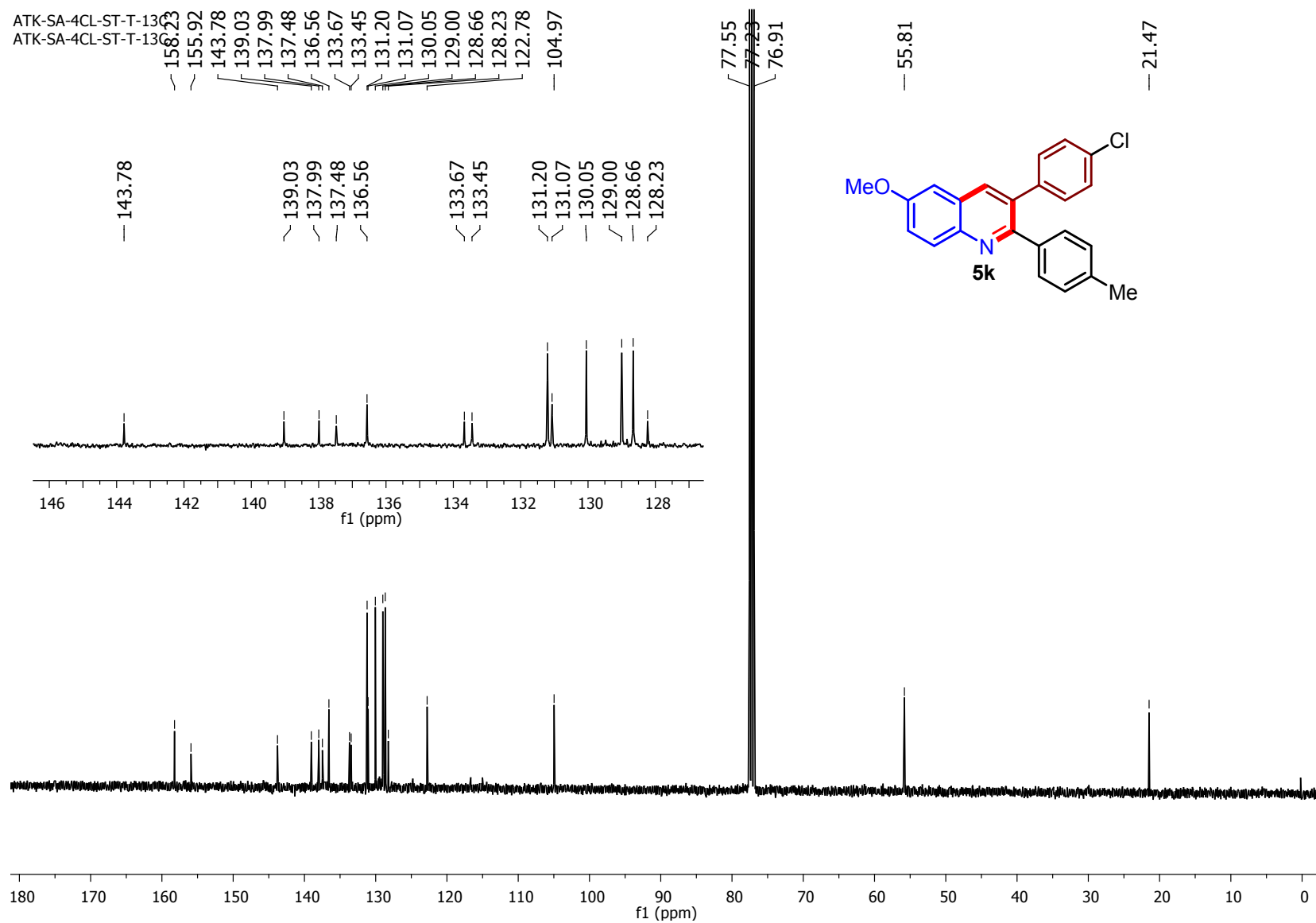
2.34

8.09
8.07
8.01

7.40
7.39
7.38
7.37
7.31
7.29
7.28
7.26
7.19
7.18
7.17
7.11
7.11
7.10
7.08

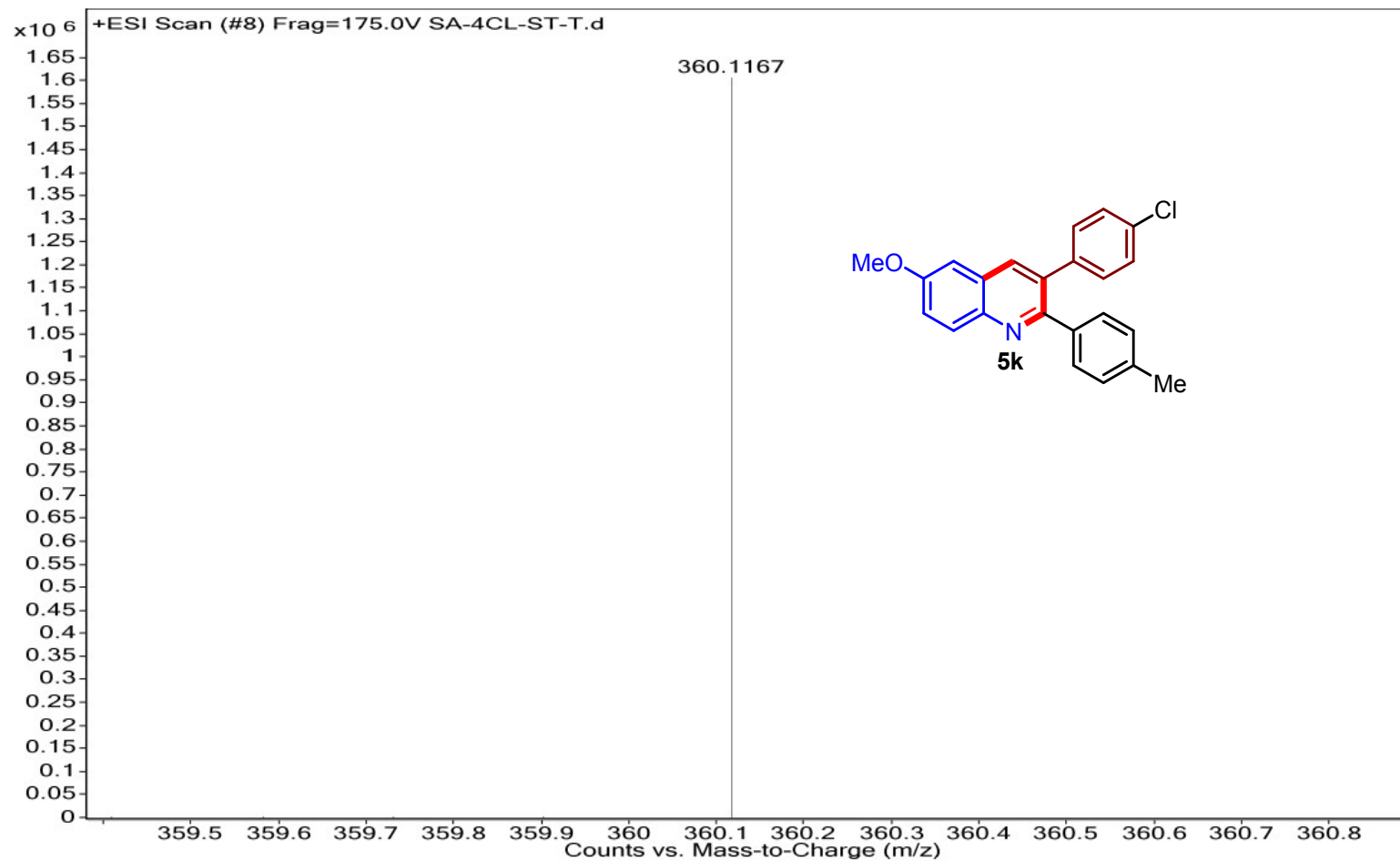


¹³CNMR spectrum of compound: 5k

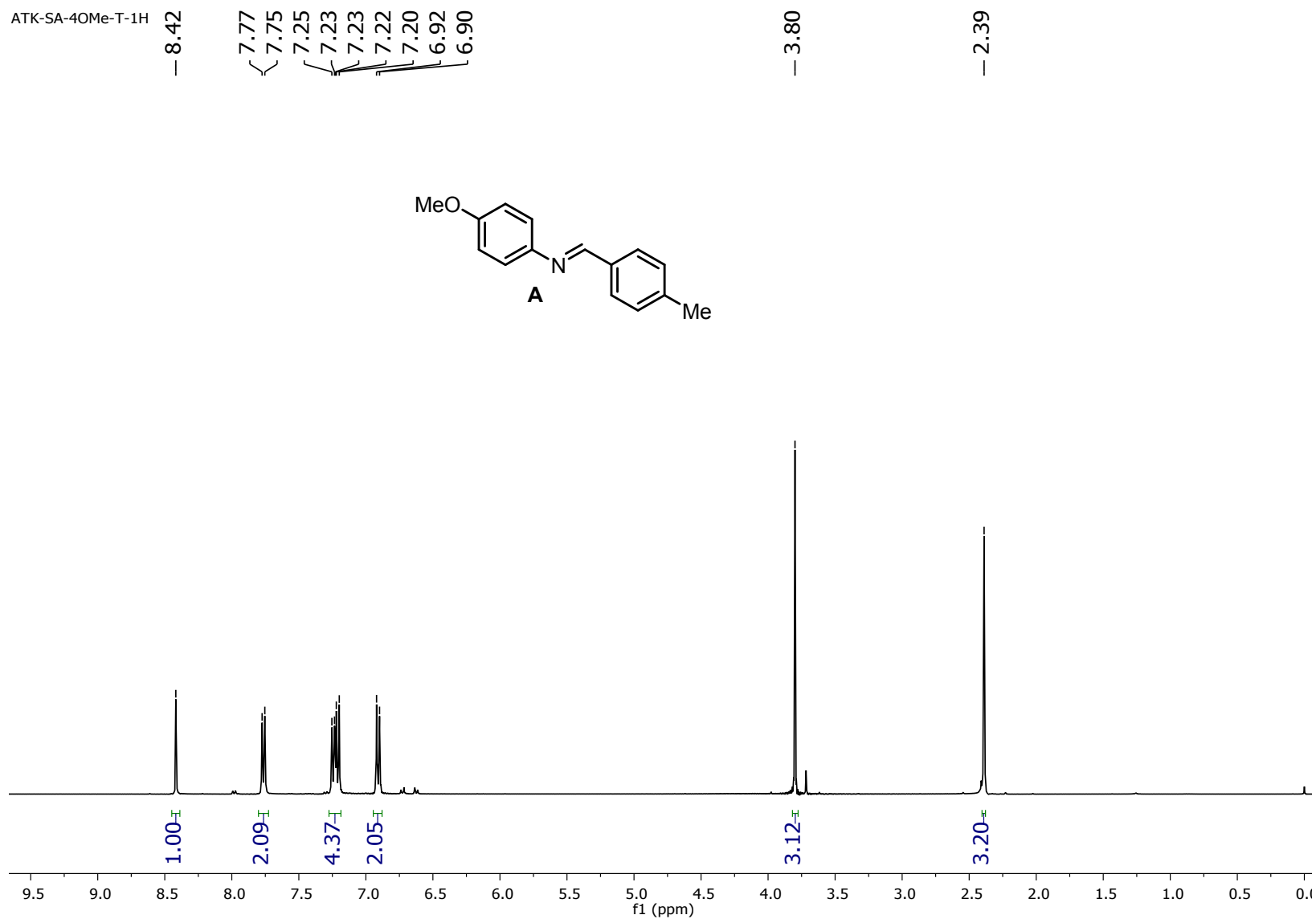


HRMS spectrum of compound: 5k

Sample Name	SAMPLE	Position	P1-F1	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-4CL-ST-T.d	ACQ Method	ESI ALS 100-500.m	Comment		Acquired Time	2/6/2020 5:58:31 PM



¹H NMR spectrum of intermediate: A



¹³C NMR spectrum of intermediate: A

ATK-SA-4OMe-T

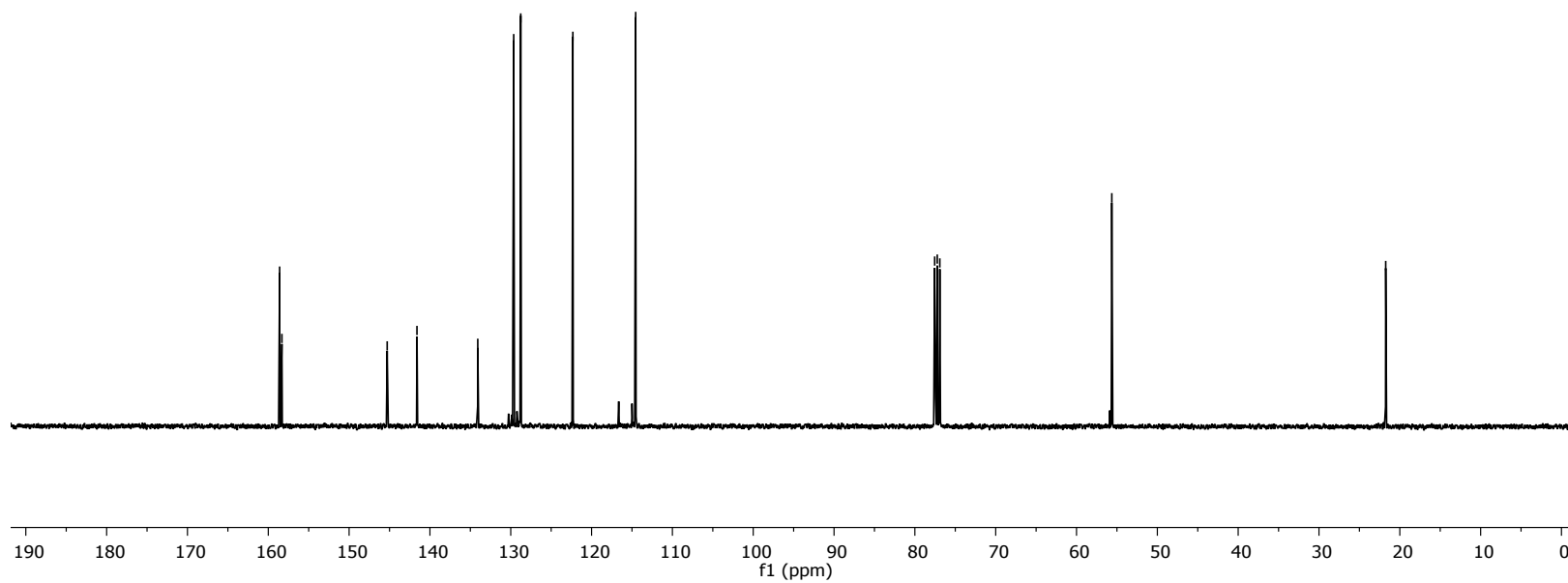
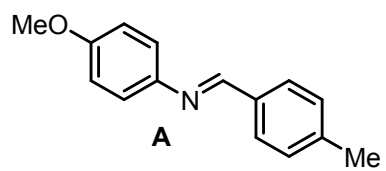
158.59
158.31

145.29
141.60
134.08
129.63
128.76
122.32
114.54

77.55
77.23
76.91

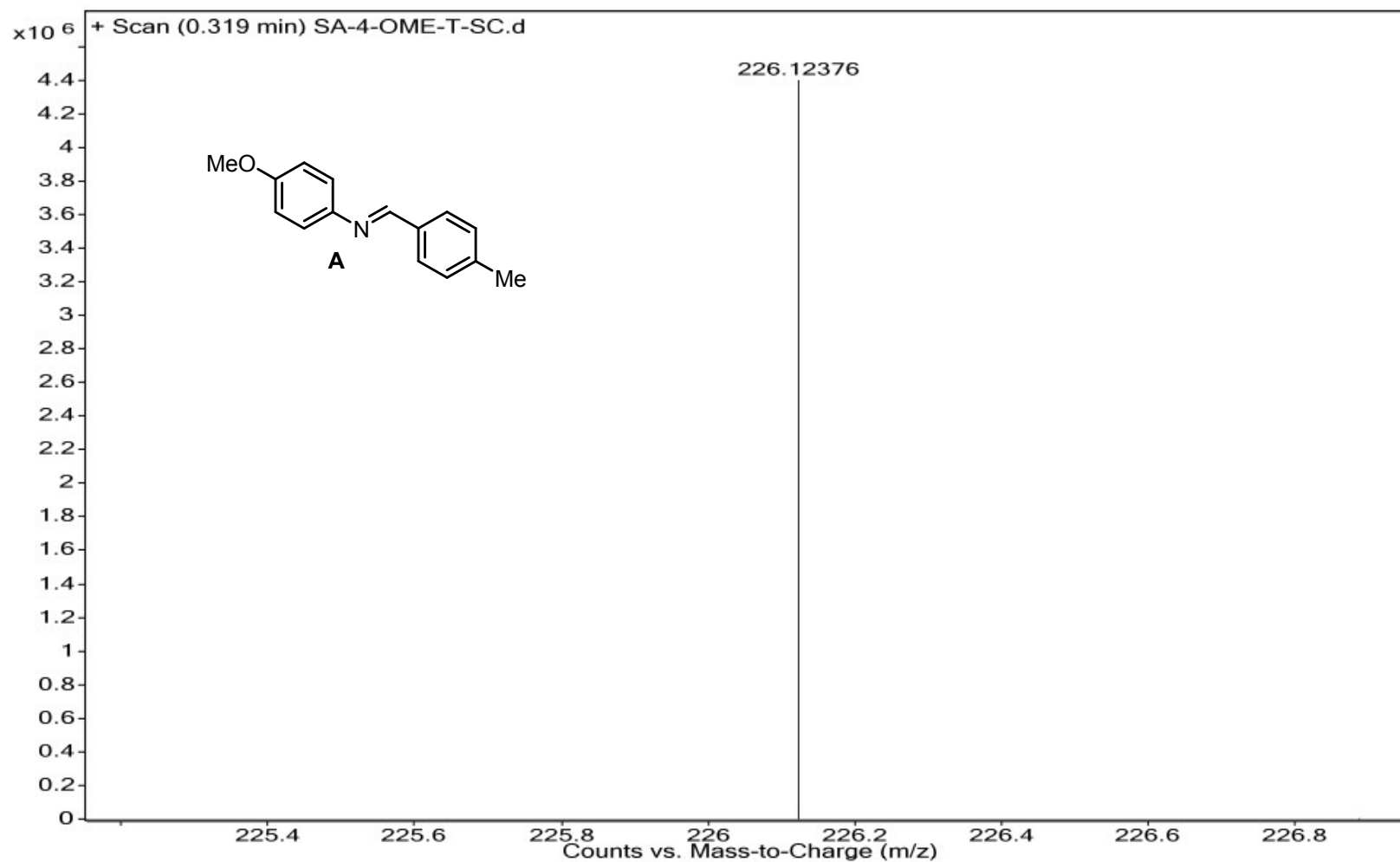
55.63

21.74



HRMS spectrum of intermediate: A

Sample Name	WASH	Position	P1-B8	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-4-OME-T-SC.d	ACQ Method	ESI ALS 100-1000.m	Comment		Acquired Time	3/1/2021 1:09:38 PM



HRMS spectrum of intermediate: C

Sample Name	SA-IMP-1	Position	P1-C9	Instrument Name	Instrument 1	User Name	
Inj Vol	20	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	SA-IMP-1.d	ACQ Method	ESI ALS 100-2000-NEG	Comment		Acquired Time	3/2/2021 6:26:37 PM

