Electronic Supporting Information

Regioselective synthetic approach for key precursors of 6-aryl-benzo[*c*]phenanthridin-10-ol derivatives: A useful compound for selective chromogenic recognition of fluoride†

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General Information and Methods

Melting points were determined on a melting point apparatus and are uncorrected. ^1H and ^{13}C NMR spectra were recorded on 400, 500, and 600 MHz and 100, 125, and 150 MHz NMR spectrometers. TMS was used as an 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 bs (broad). IR spectra were recorded on an IR spectrophotometer. HRMS spectra were recorded using ESI and APCI (TOF) mode. The crystal structure was determined using a single crystal XRD diffractometer.

The anionic salts were procured from Sigma Aldrich and were used as obtained. The solvents were of analytical grade and were used without further purification. The UV-Vis spectroscopic studies were carried out in CARY 60 UV-Vis spectrophotometer in the wavelength range of 200-800 nm.

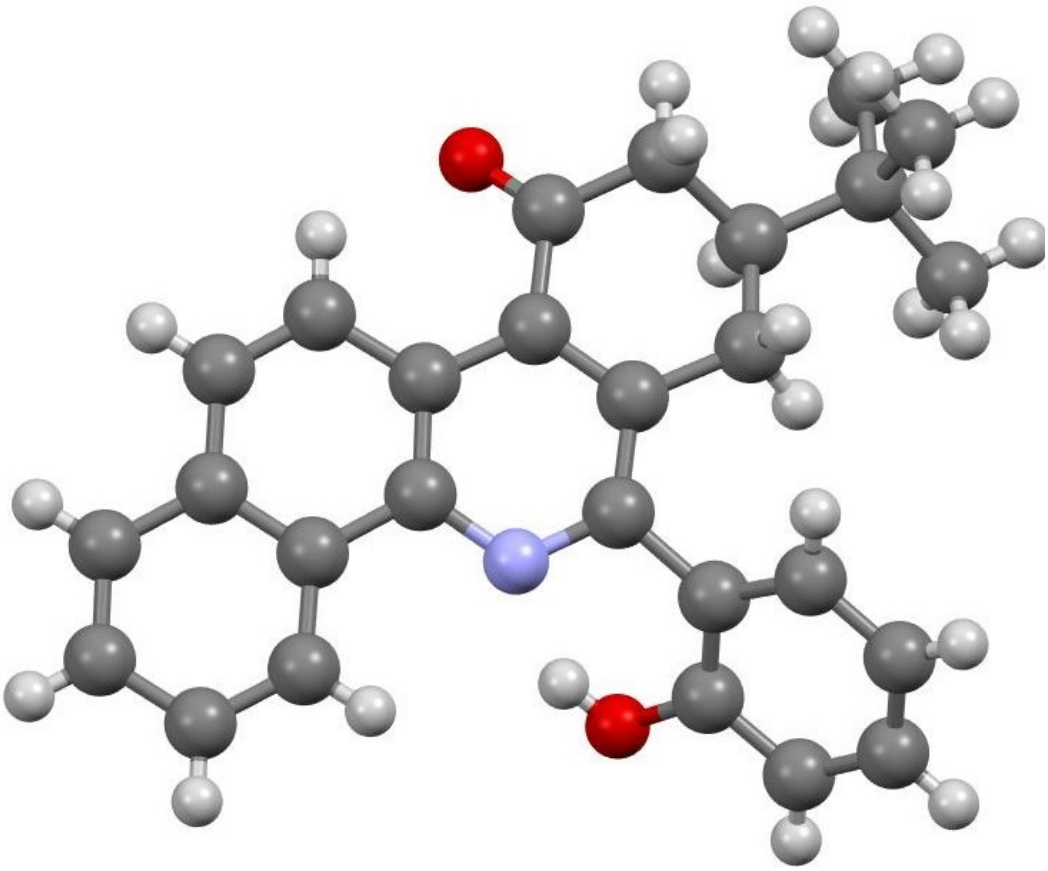


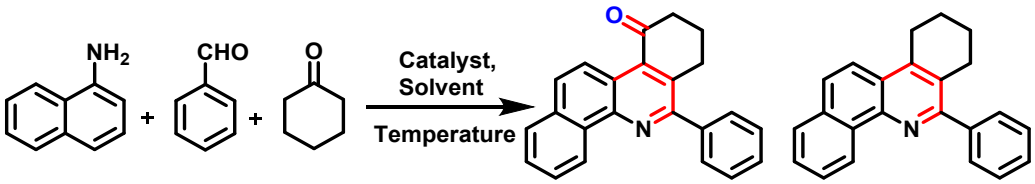
Figure S1. ORTEP Diagrams of compound **4t**.

Table S1. Crystal data and structure refinement for compound **4t**.

Entry	Identification Code	Compound 4t
01	Empirical formula	$C_{27}H_{25}NO_2$
02	Formula weight	395.48
03	Temperature	296 K
04	Wavelength	0.71073
05	Radiation type	Mo K\a
06	Radiation system	Fine-focus sealed tube
07	Crystal system	Monoclinic
08	Space group	P 21/c
09	Cell length	a 16.672(6) b 11.449(4) c 11.109(4)
10	Cell angle	α 90 β94.864(10) γ 90
11	Cell volume	2112.7(12)

12	Density	1.243
13	Completeness to theta	99.7
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F2
16	Index ranges	-19<=h<=19, -13<=k<=13, -13<=l<=13
17	Reflection number	3640
18	Theta range	24.829
19	Cell formula units Z	4
20	CCDC no	2060048

Table S2. Optimization of Reaction Conditions.[a,b]

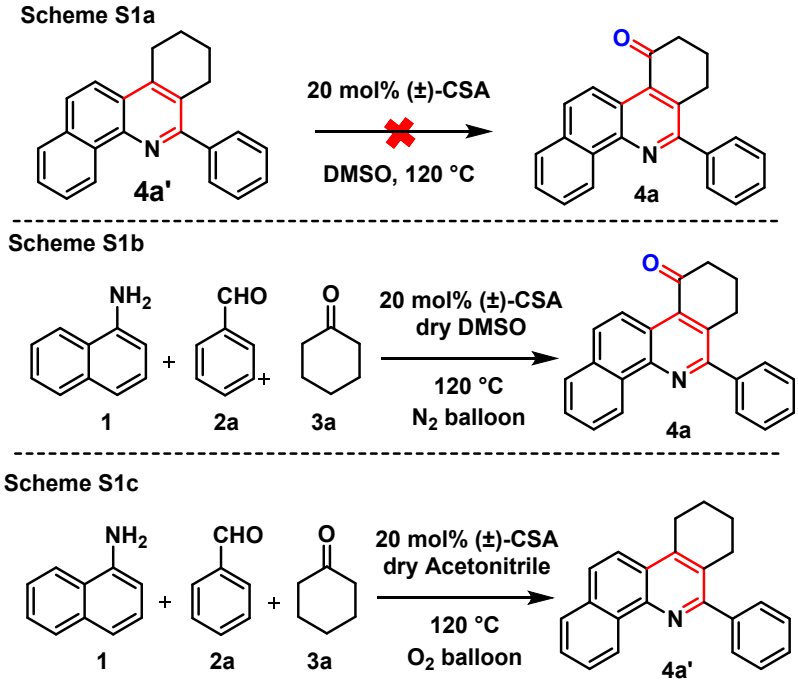


1 2a 3a 4a 4a'

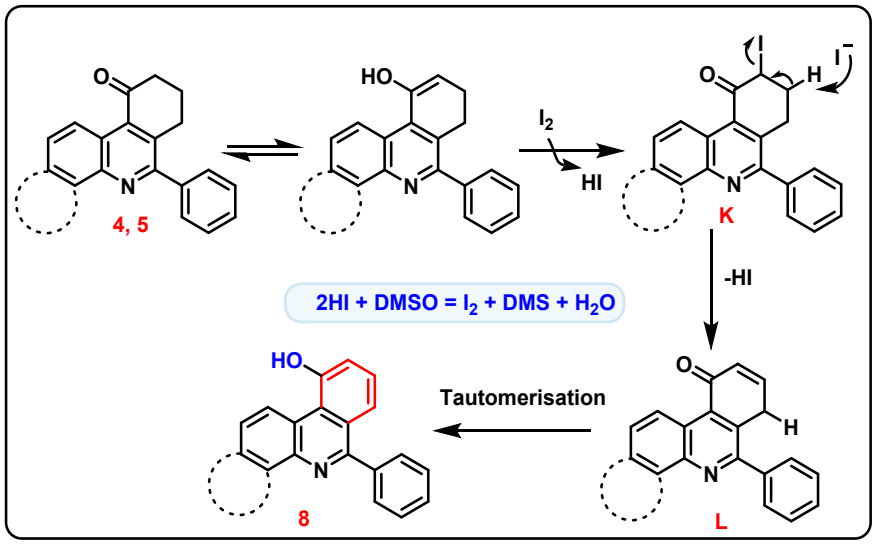
Entry	Catalyst	Mol%	Solvent	Temperature	Time (h)	%Yield[b] (4a)	%Yield[b] (4a')
1.	(±)-CSA	10	DMSO	80 °C	15	-	20
2.	(±)-CSA	10	DMSO	100 °C	10	25	10
3.	(±)-CSA	10	DMSO	120 °C	7	45	05
4.	**(±)-CSA**	**20**	**DMSO**	**120 °C**	**2.5**	**65**	**01**
5.	(±)-CSA	30	DMSO	120 °C	2.5	66	01
6.	(±)-CSA	20	DMSO	130 °C	2.5	65	01
7.	*p*-TSA	20	DMSO	120 °C	12	50	-
8.	TFA	20	DMSO	120 °C	24	12	-
9.	TfOH	20	DMSO	120 °C	24	20	-
10.	Acetic acid	20	DMSO	120 °C	12	-	-
11.	L-Proline	20	DMSO	120 °C	12	-	-
12.	(±)-CSA	20	H_2O	100 °C	24	-	-
13.	(±)-CSA	20	DMF	120 °C	8	40	-

[a]All reactions were carried out with 1-naphthylamine **1** (0.143 g, 1 mmol), benzaldehyde **2a** (0.106 g, 1 mmol), and cyclohexanone **3a** (0.098 g, 1 mmol) in 1 mL of solvent at different temperatures mentioned above. [b]Yield of the isolated product.

Control Experiment

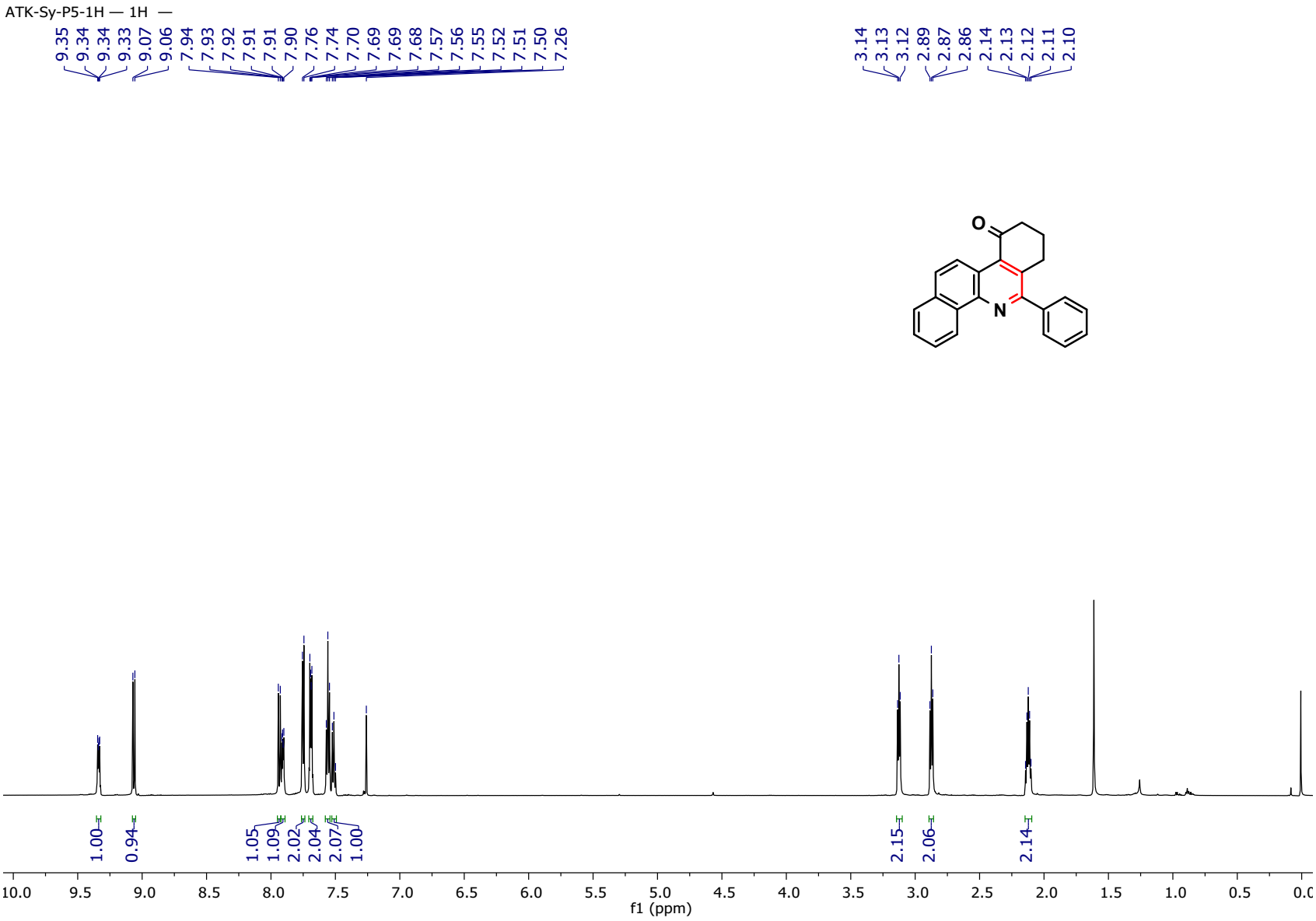


Scheme S1. Control experiment to establish reaction mechanism for the formation of **4** or **6**.

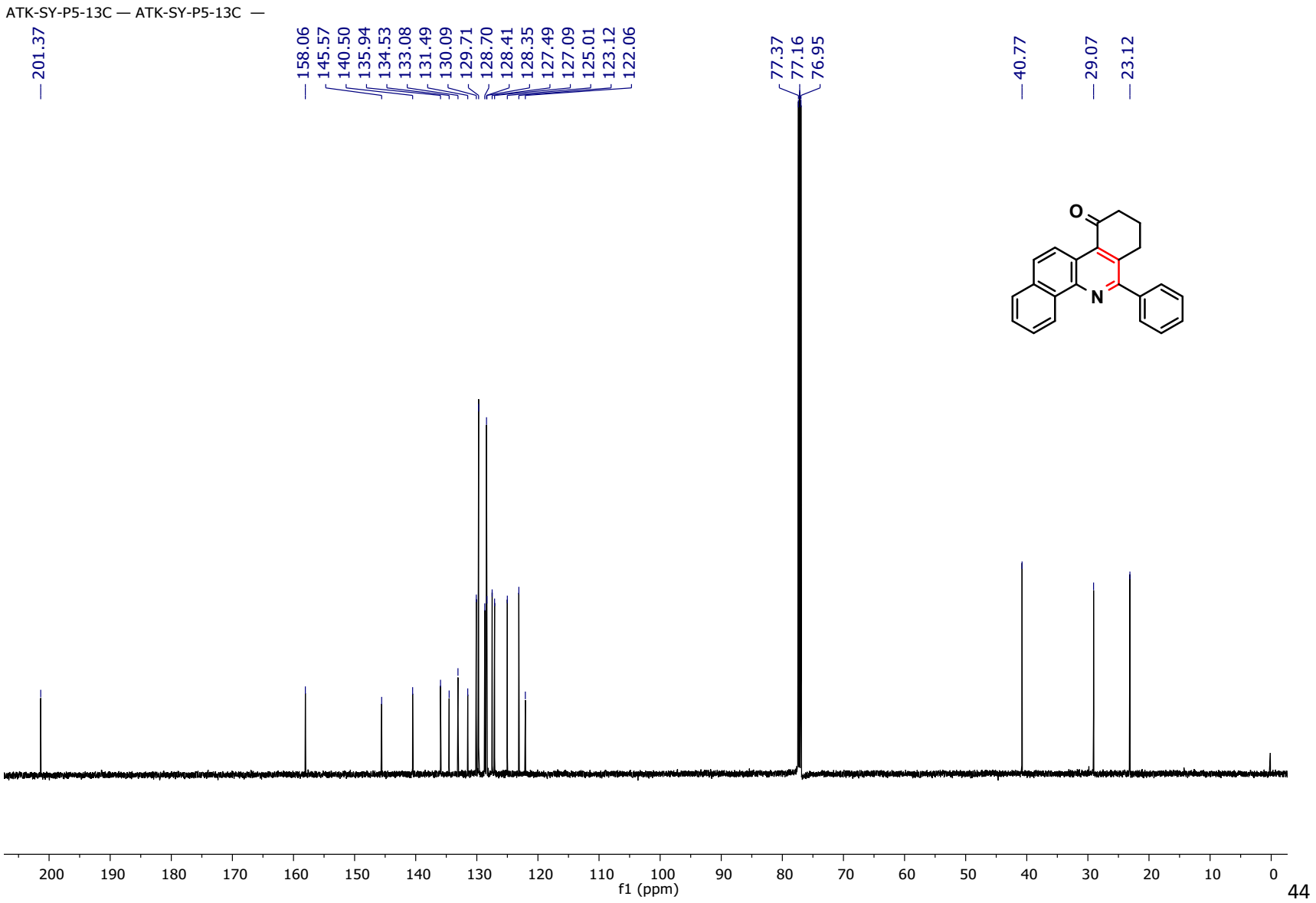


Scheme S2. A plausible mechanism for the synthesis of 6-arylbenzo[*c*]phenanthridin-10-ol & 6-arylphenanthridin-10-ol derivatives.

^{1}H NMR Spectrum of Compound 4a

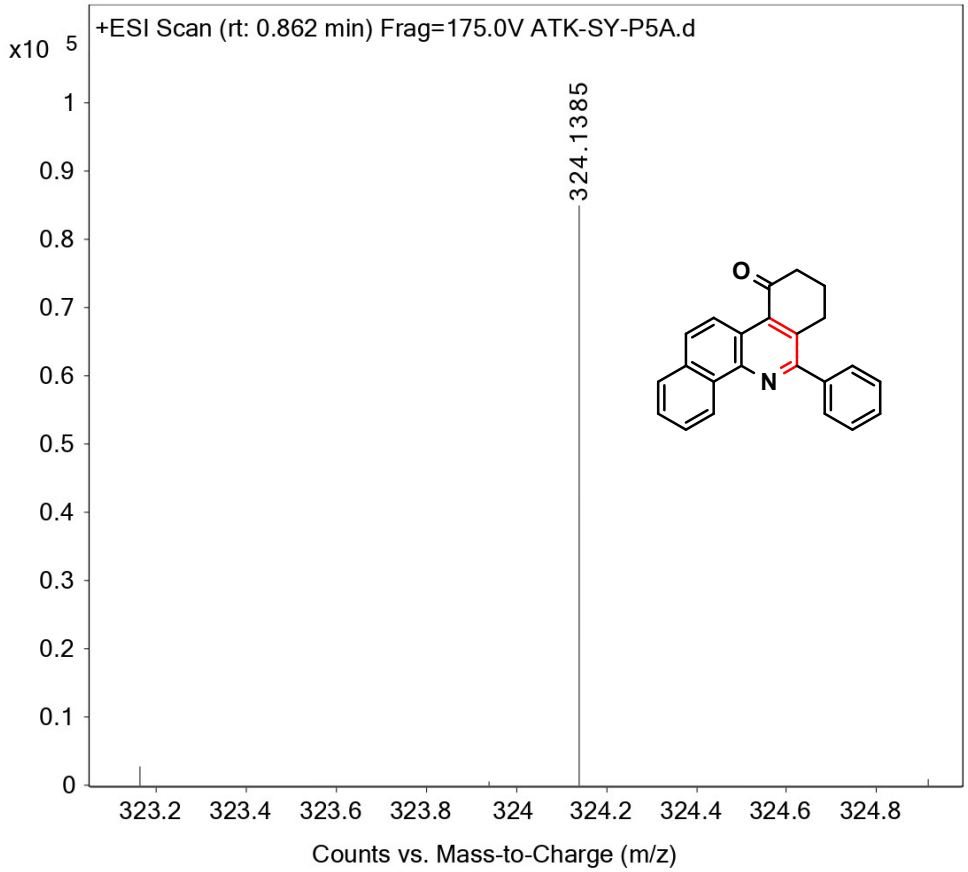


^{13}C NMR Spectrum of Compound 4a

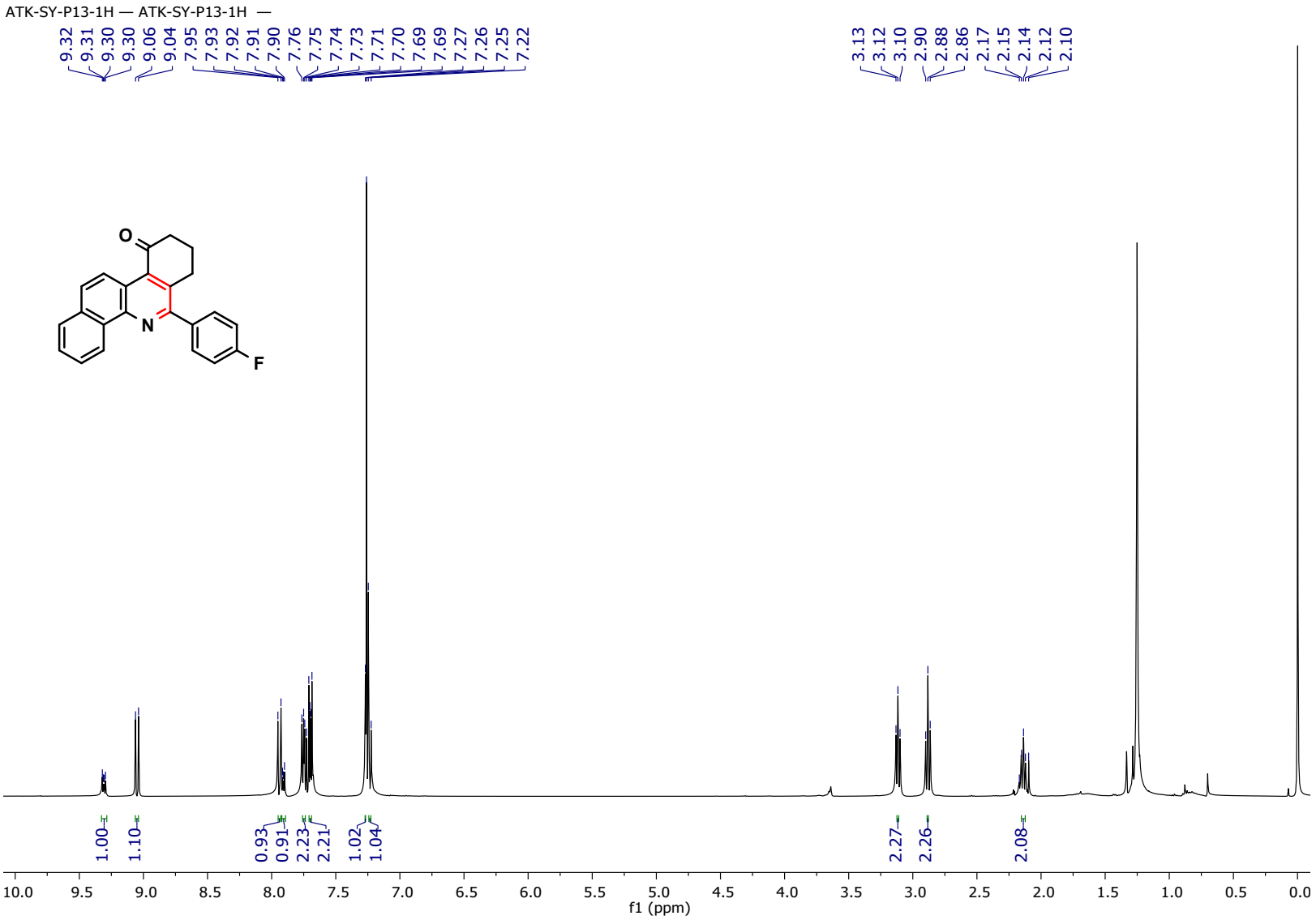


HRMS Spectrum of compound 4a

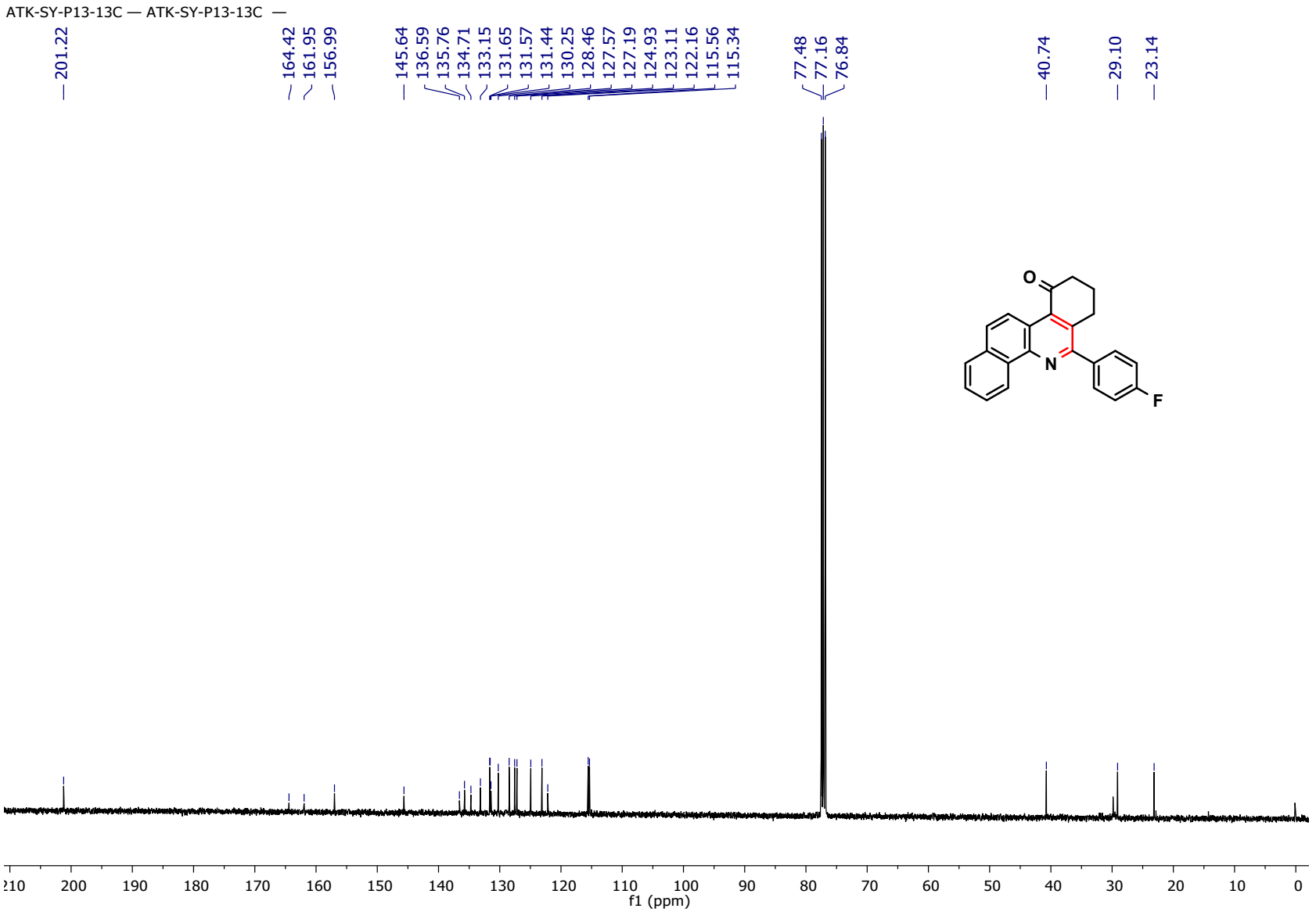
Sample Name	SAMPLE 26	**Position**	P2-C6	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P5A.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	28-12-2020 21:57:45 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4b

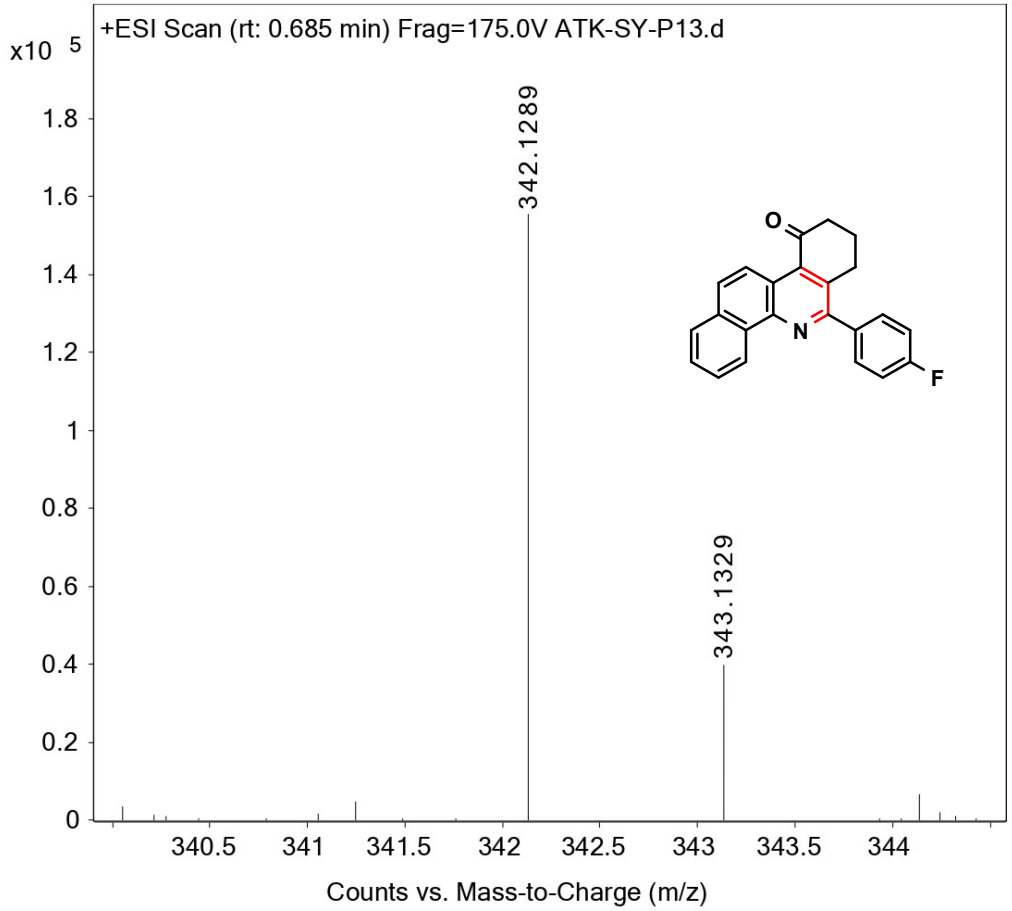


^{13}C NMR Spectrum of Compound 4b

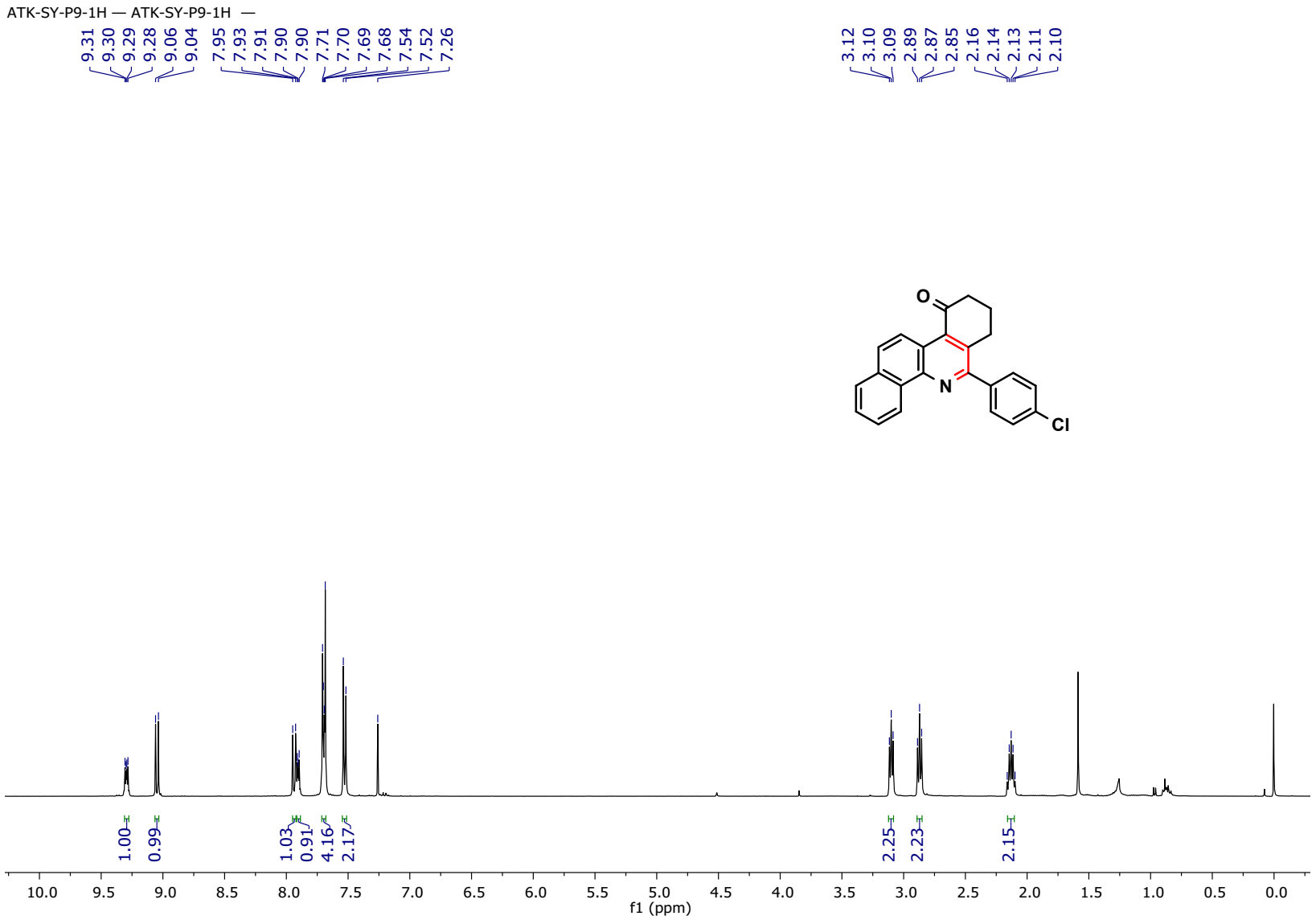


HRMS Spectrum of Compound 4b

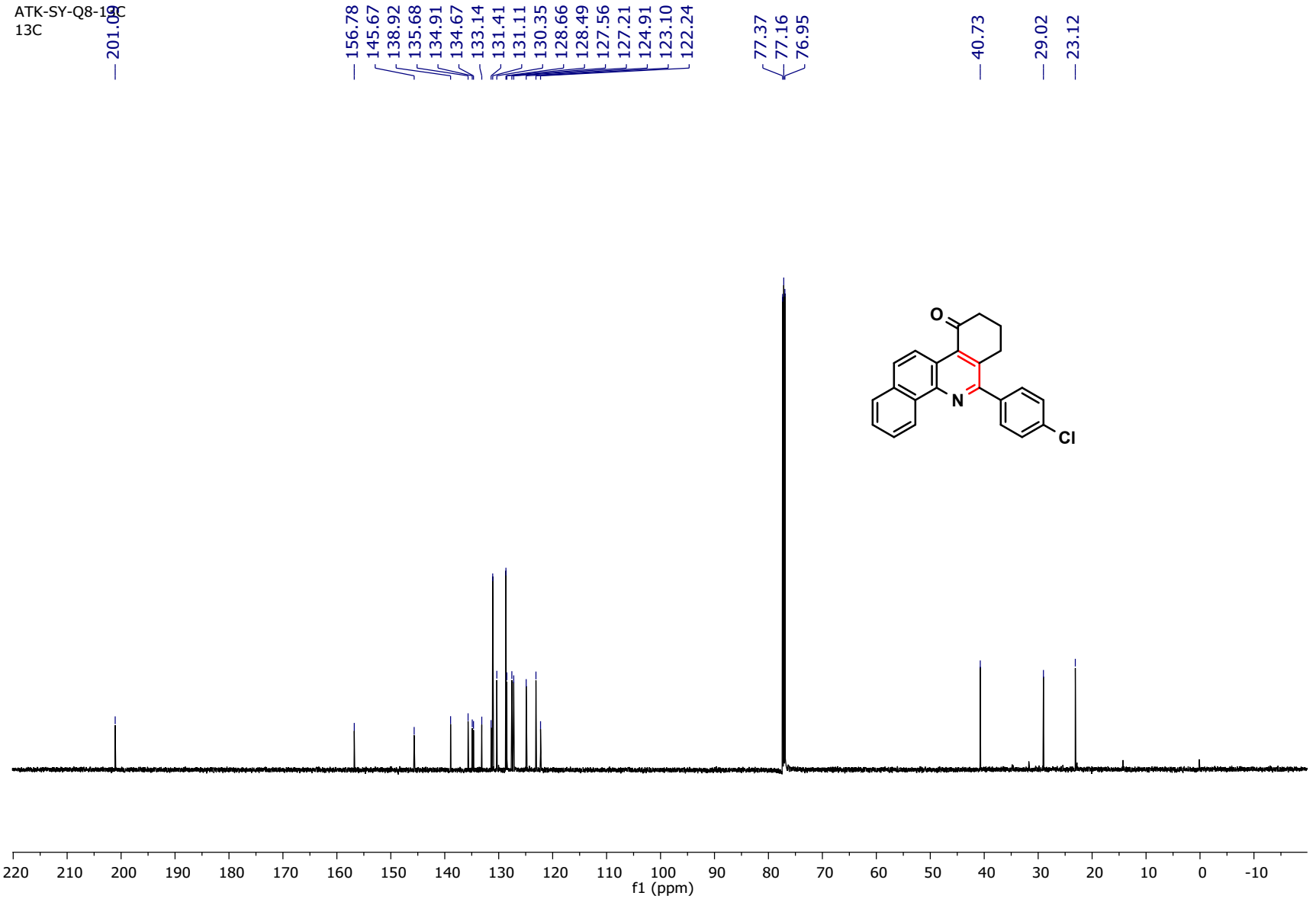
Sample Name	SAMPLE	**Position**	P1-A10	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P13.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	29-01-2021 18:04:12 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4c

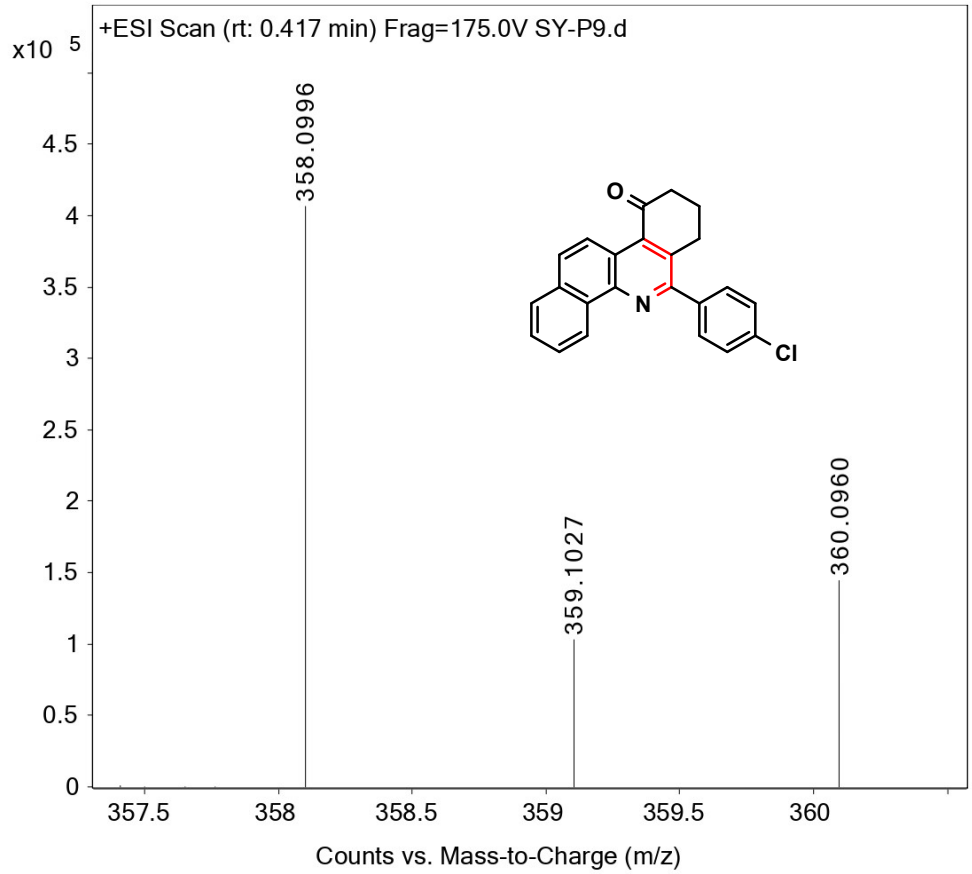


^{13}C NMR Spectrum of Compound 4c

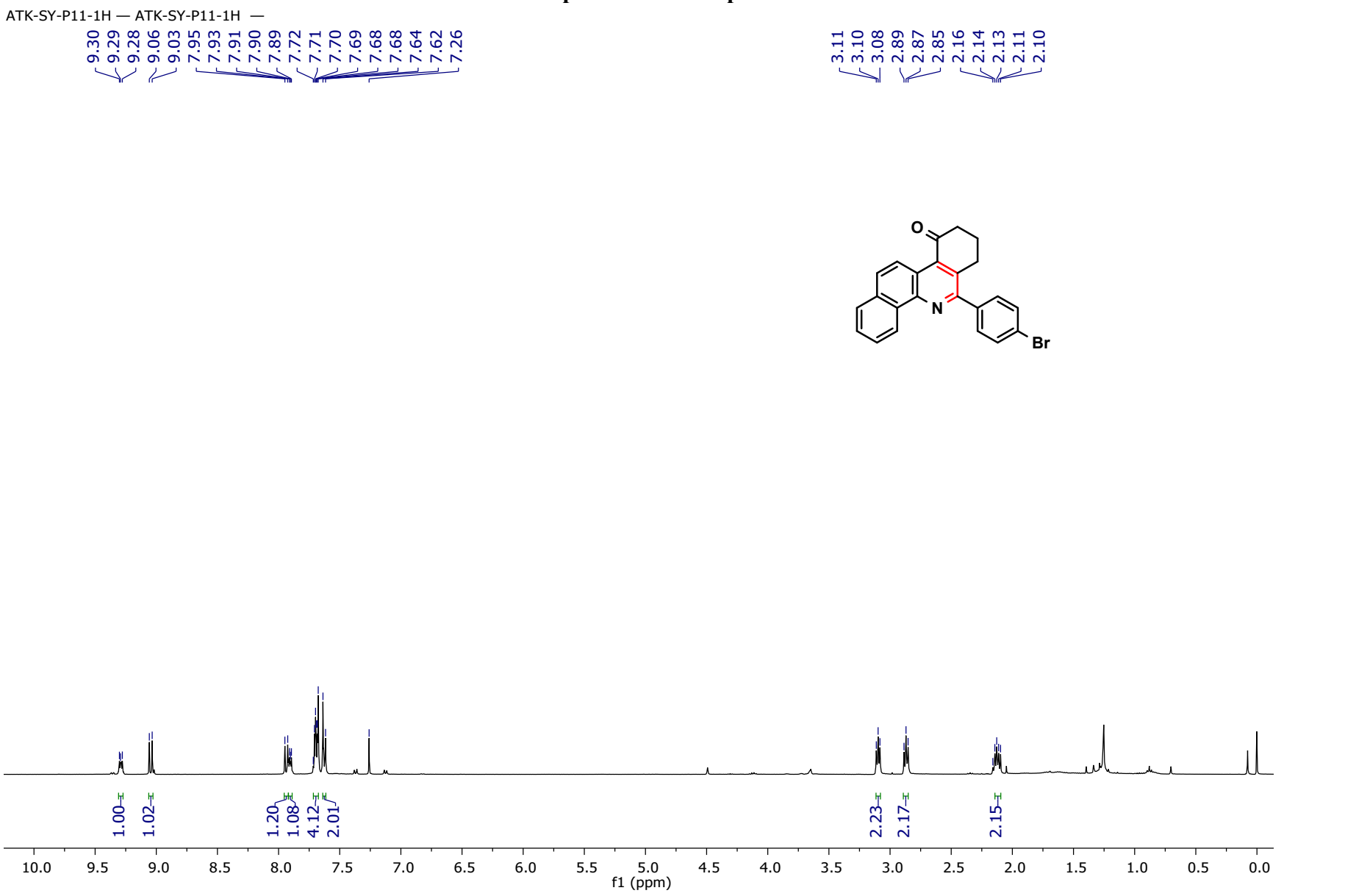


HRMS Spectrum of Compound 4c

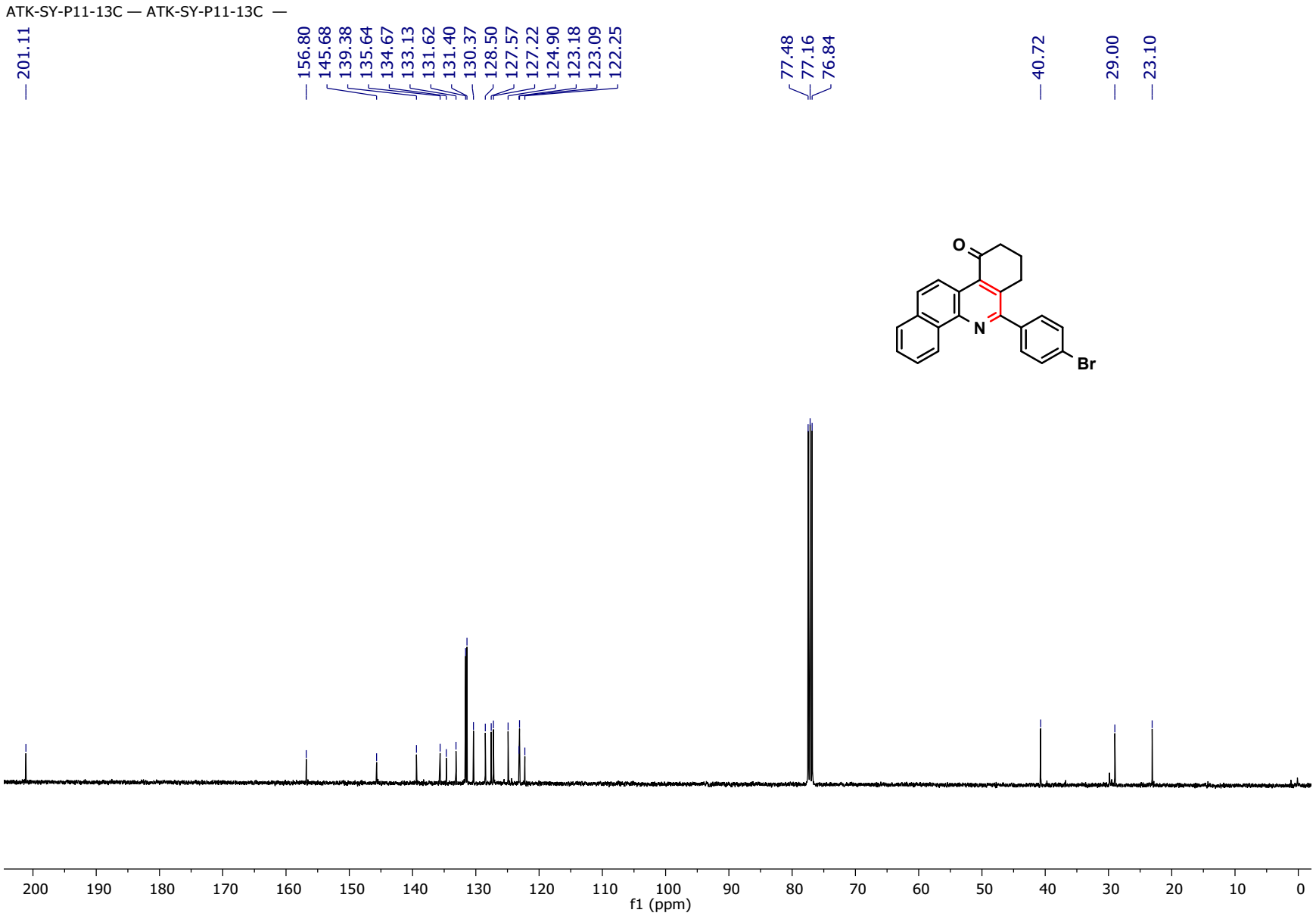
Sample Name	SY-P9	**Position**	P2-B7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P9.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	29-12-2020 20:29:31 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4d

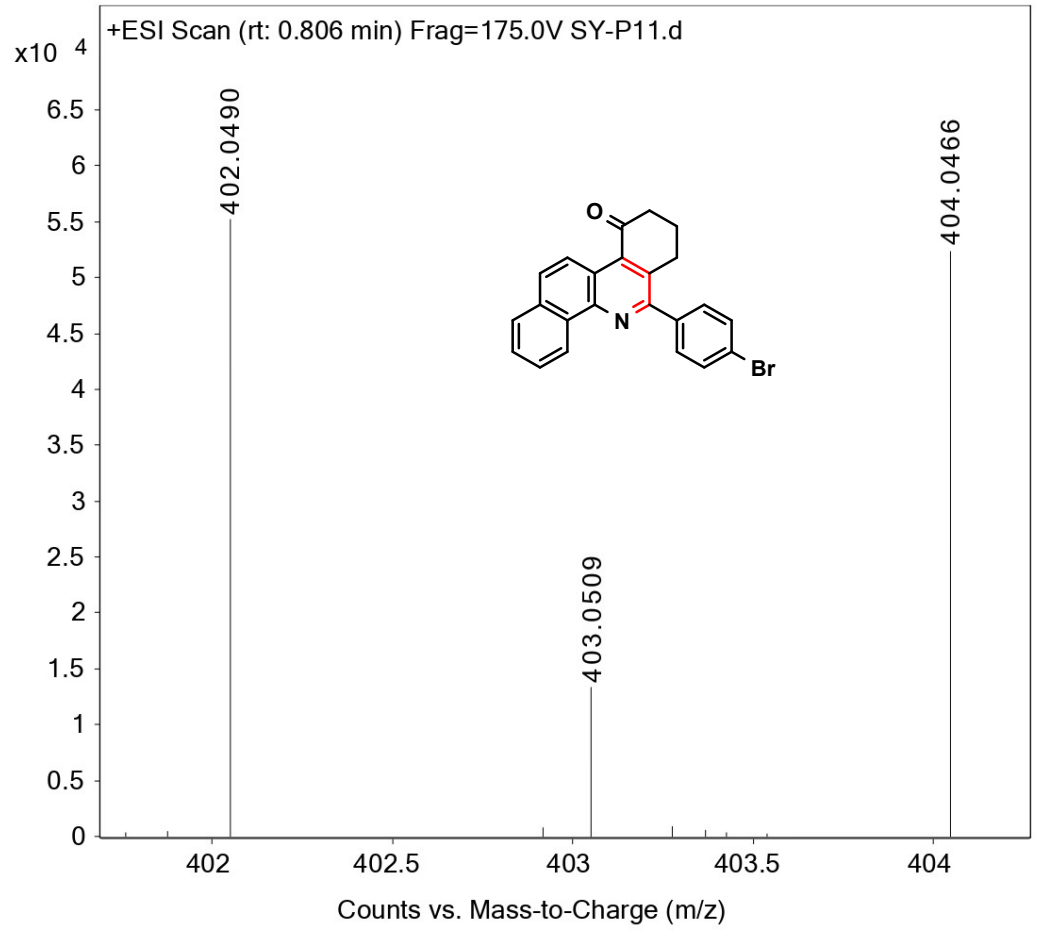


^{13}C NMR Spectrum of Compound 4d

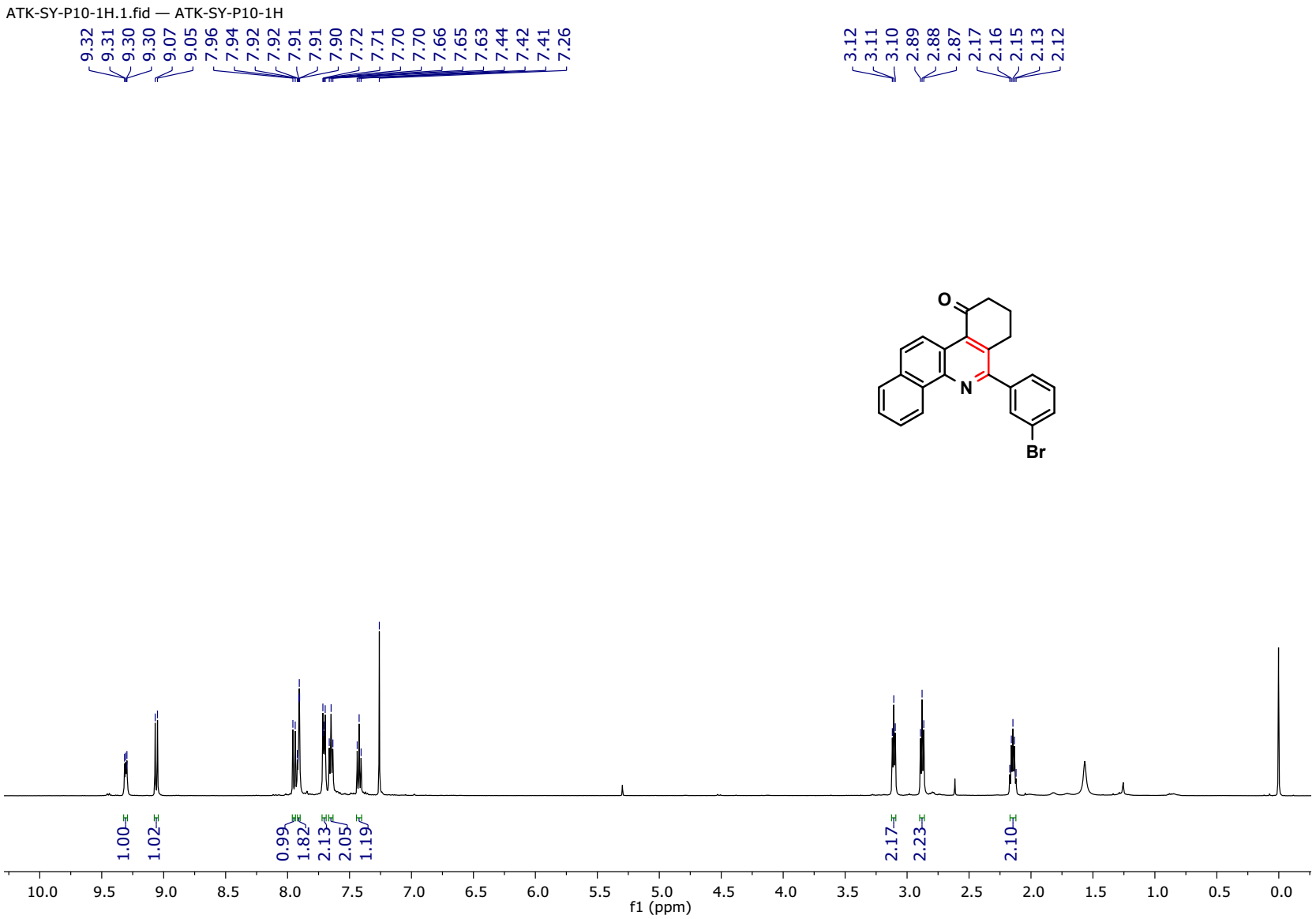


HRMS Spectrum of Compound 4d

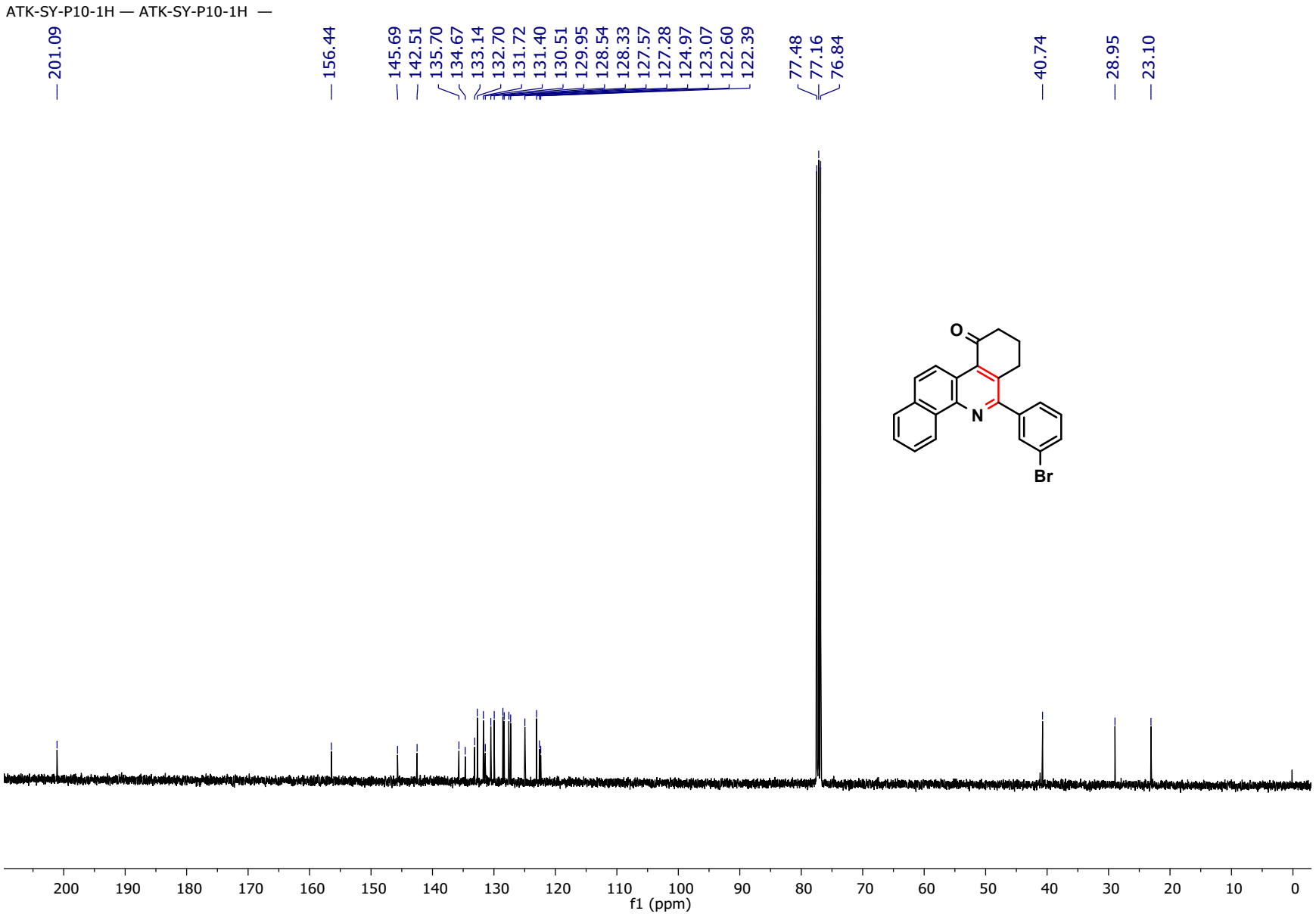
Sample Name	SY-P11	**Position**	P2-B9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P11.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	29-12-2020 20:50:40 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4e

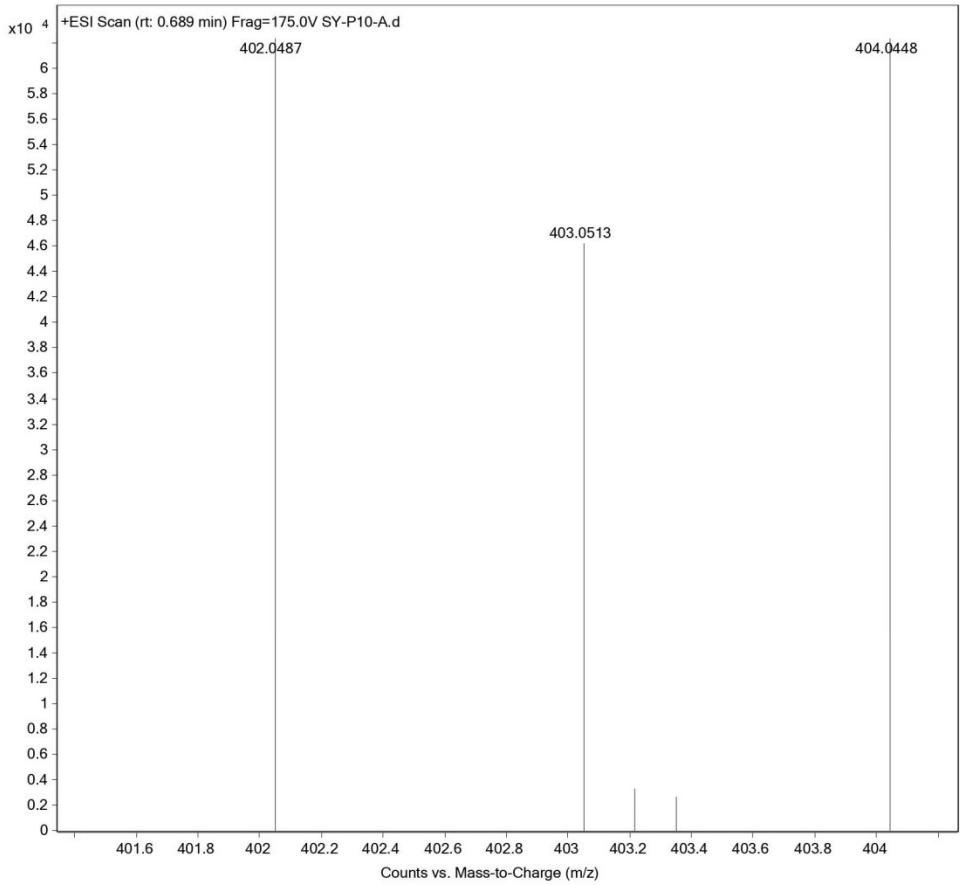


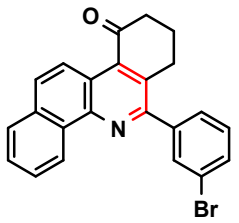
^{13}C NMR Spectrum of Compound 4e



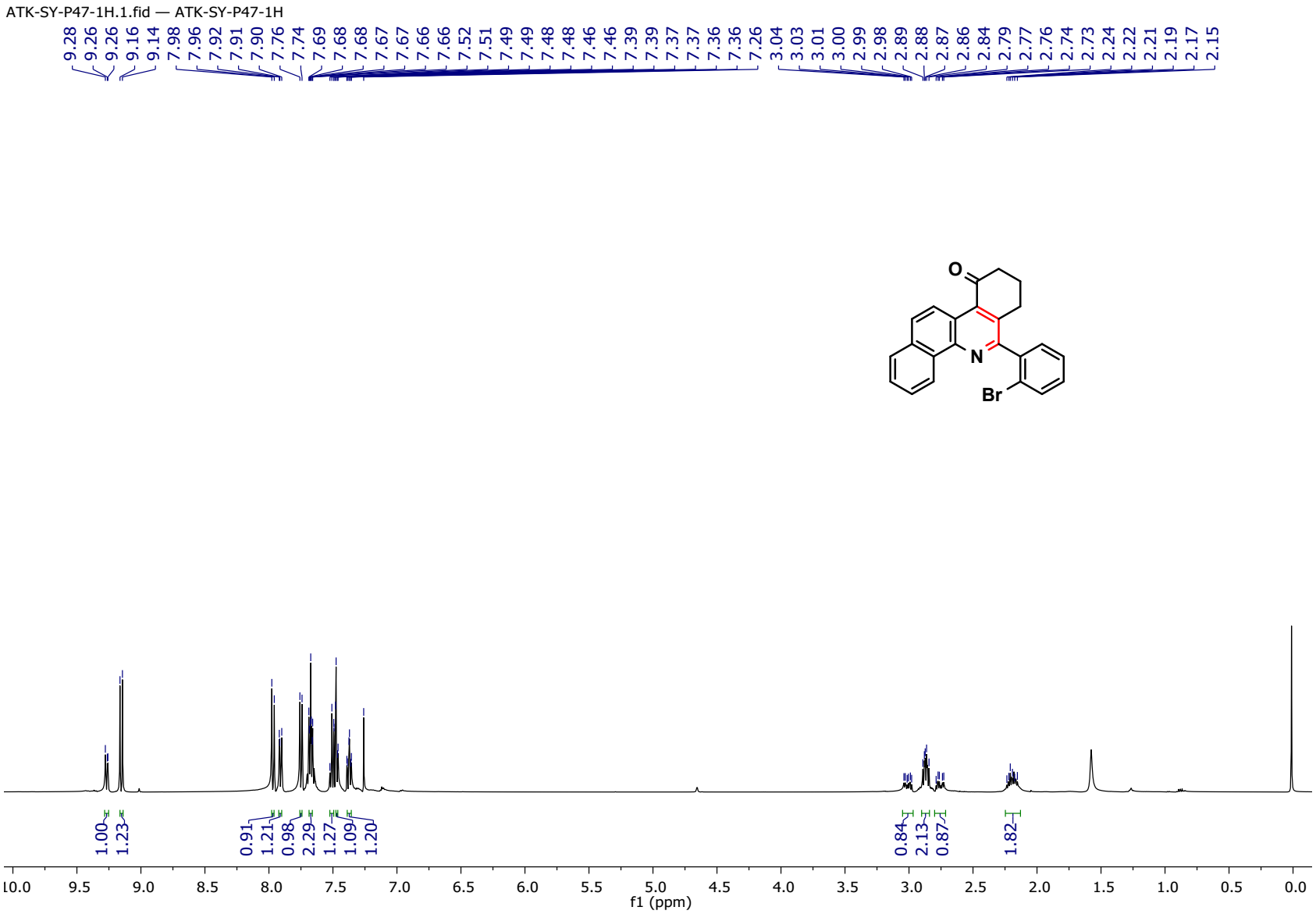
HRMS Spectrum of Compound 4e

Sample Name	SAMPLE 15	**Position**	P2-B6	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P10-A.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	31-Mar-21 08:15:54 PM (UTC+05:30)

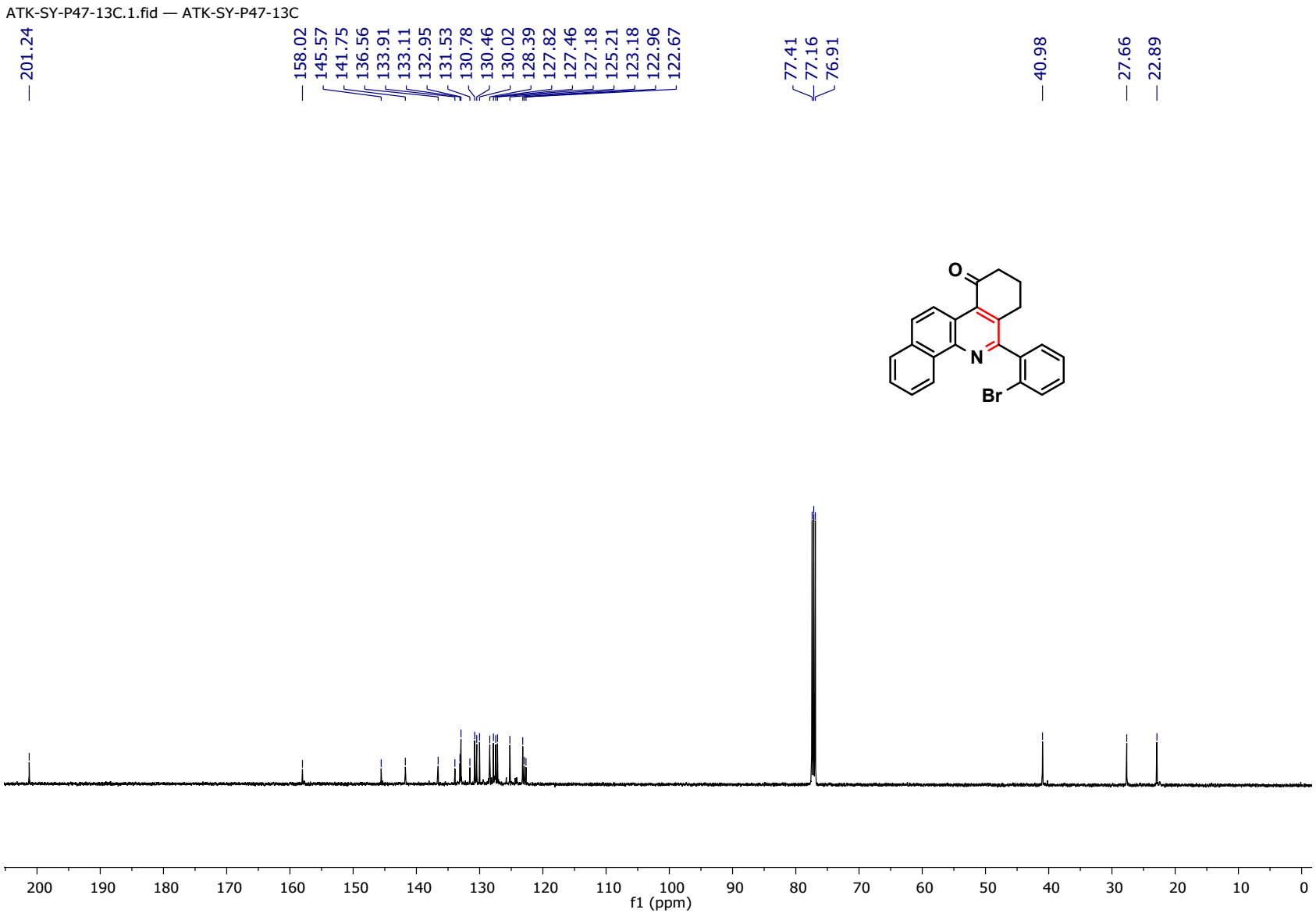




^{1}H NMR Spectrum of Compound 4f

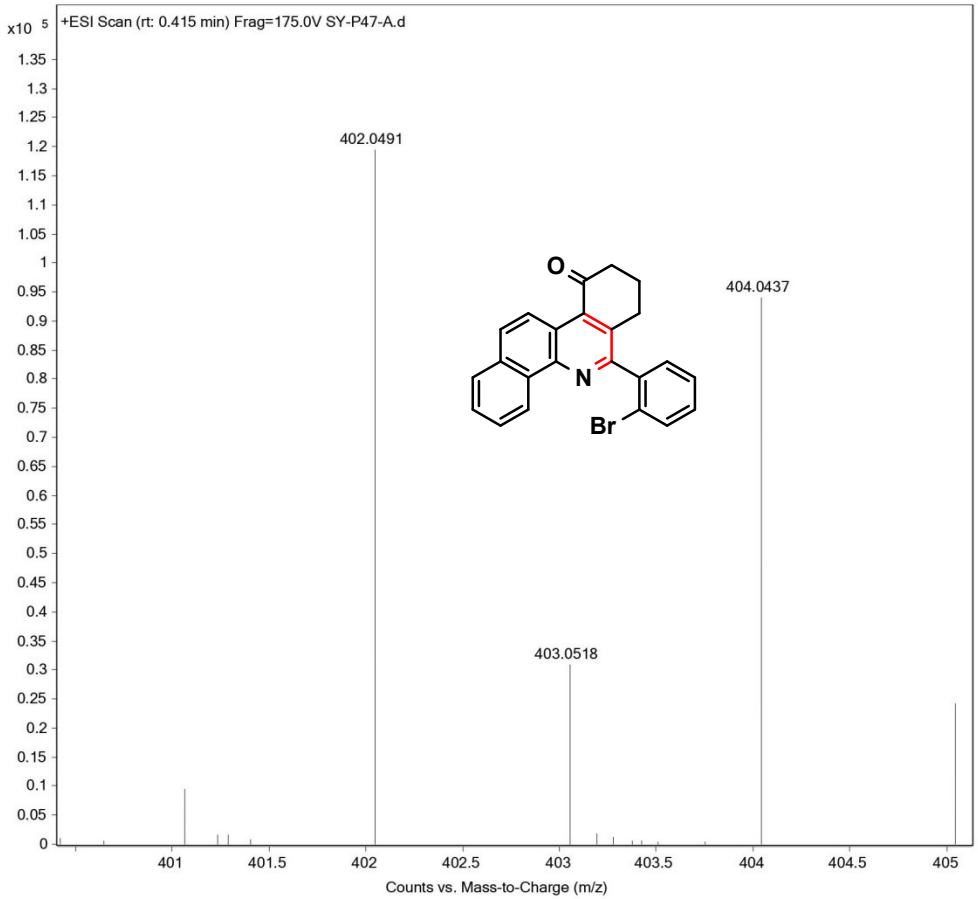


^{13}C NMR Spectrum of Compound 4f

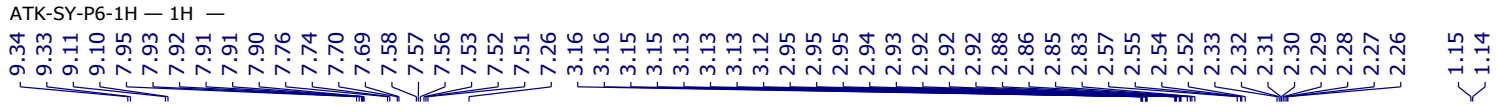


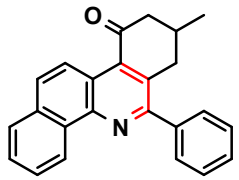
HRMS Spectrum of Compound 4f

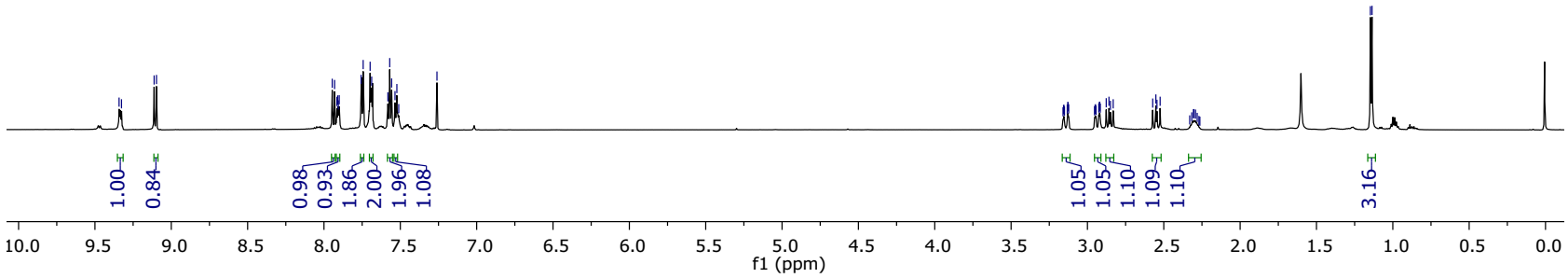
Sample Name	WASH	**Position**	P2-A6	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P47-A.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	31-Aug-21 06:07:41 PM (UTC+05:30)



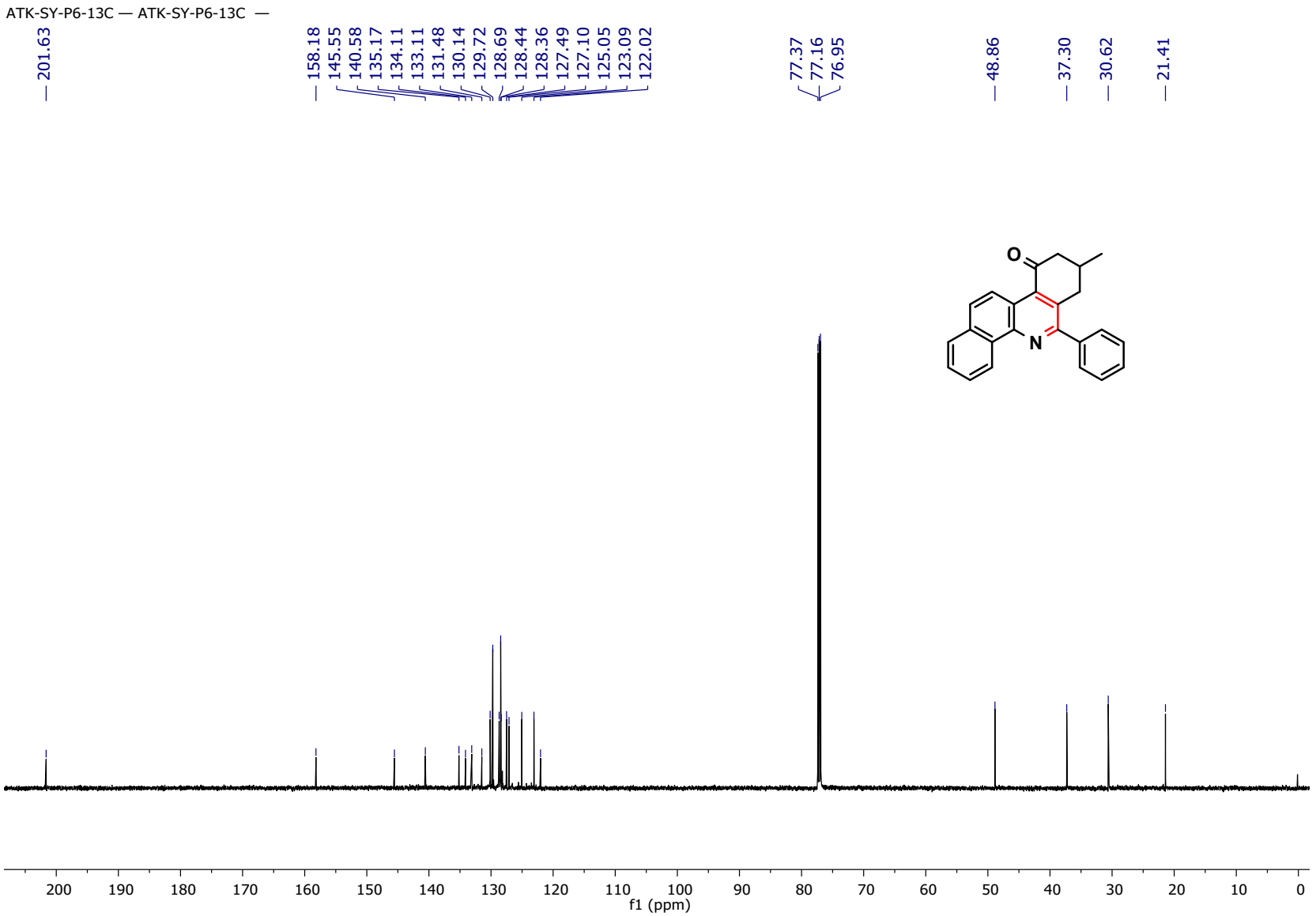
^{1}H NMR Spectrum of Compound 4g





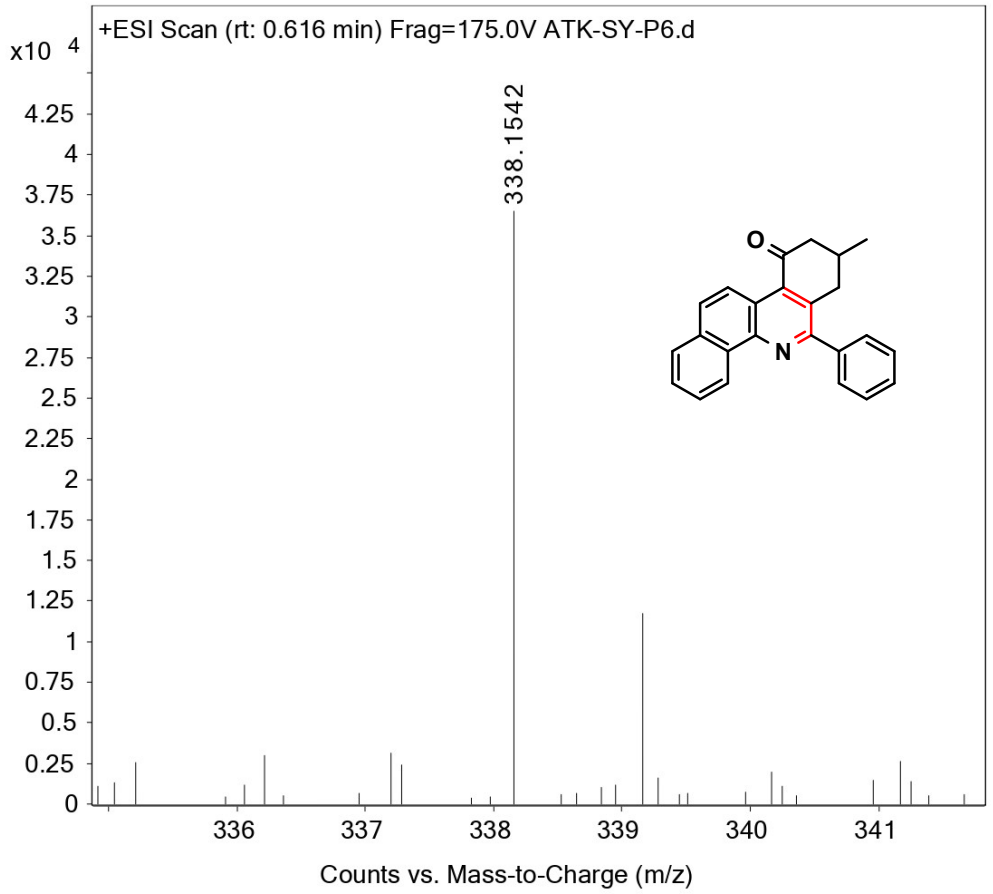


^{13}C NMR Spectrum of Compound 4g

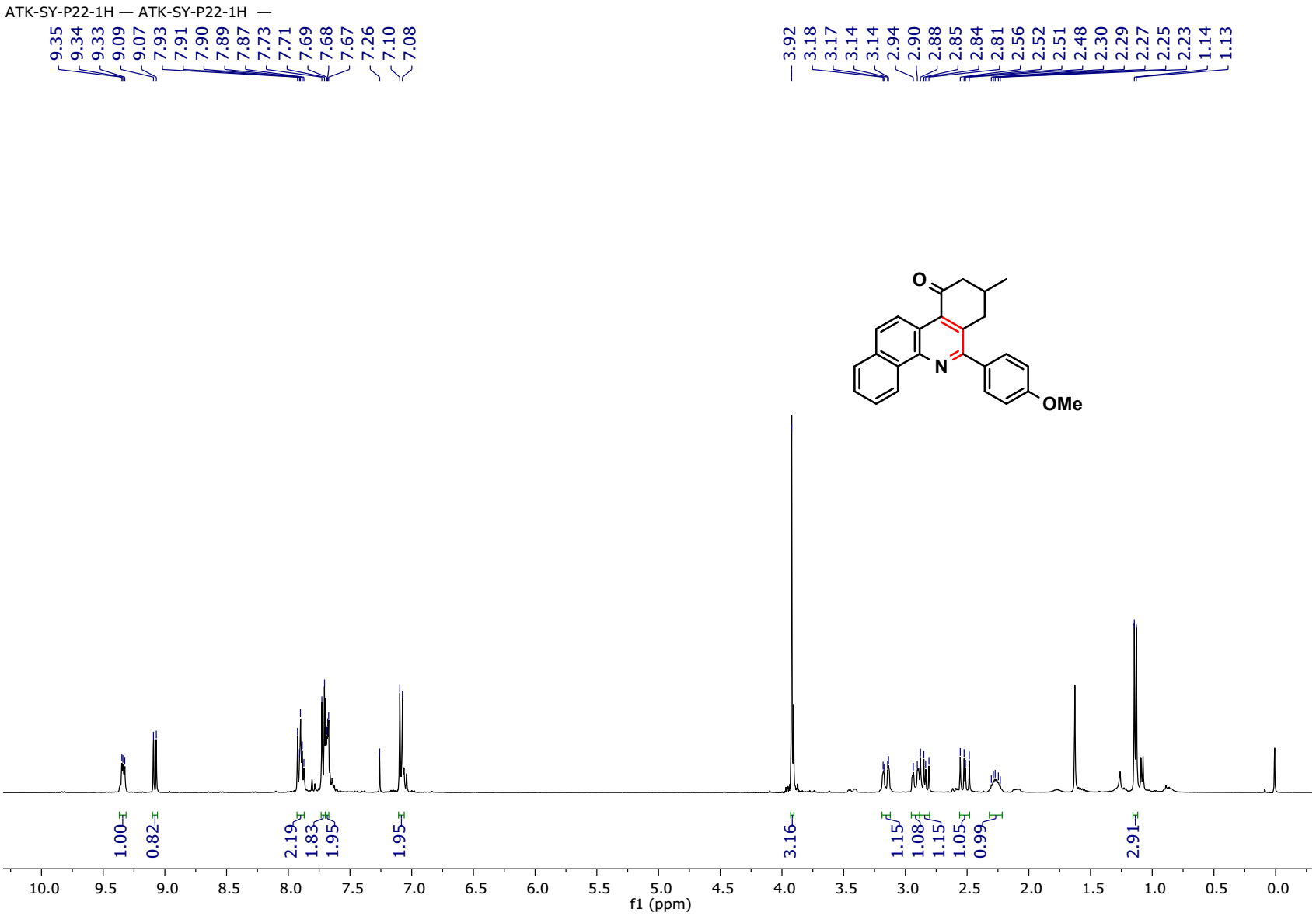


HRMS Spectrum of Compound 4g

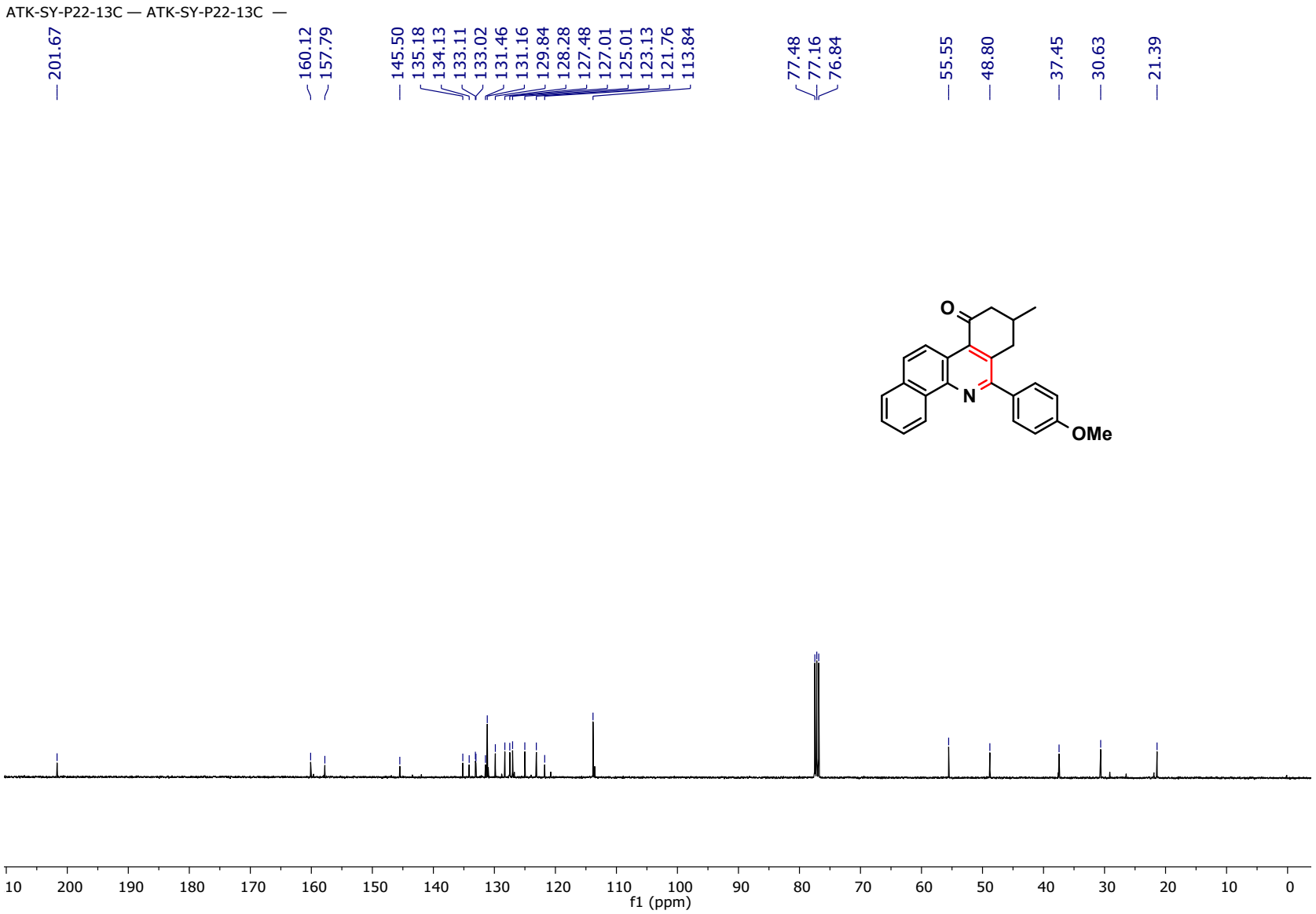
Sample Name	ATK-SY-P6	**Position**	P2-A4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P6.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	15-12-2020 16:44:55 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4h

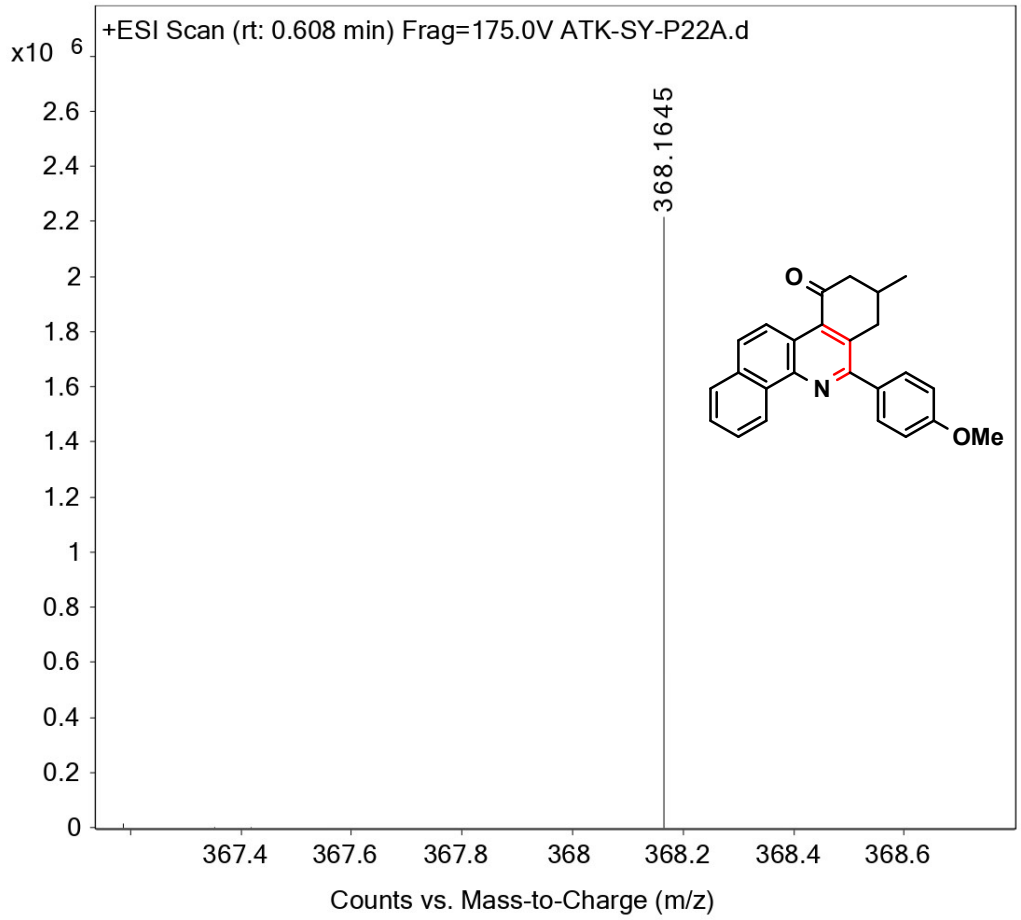


^{13}C NMR Spectrum of Compound 4h

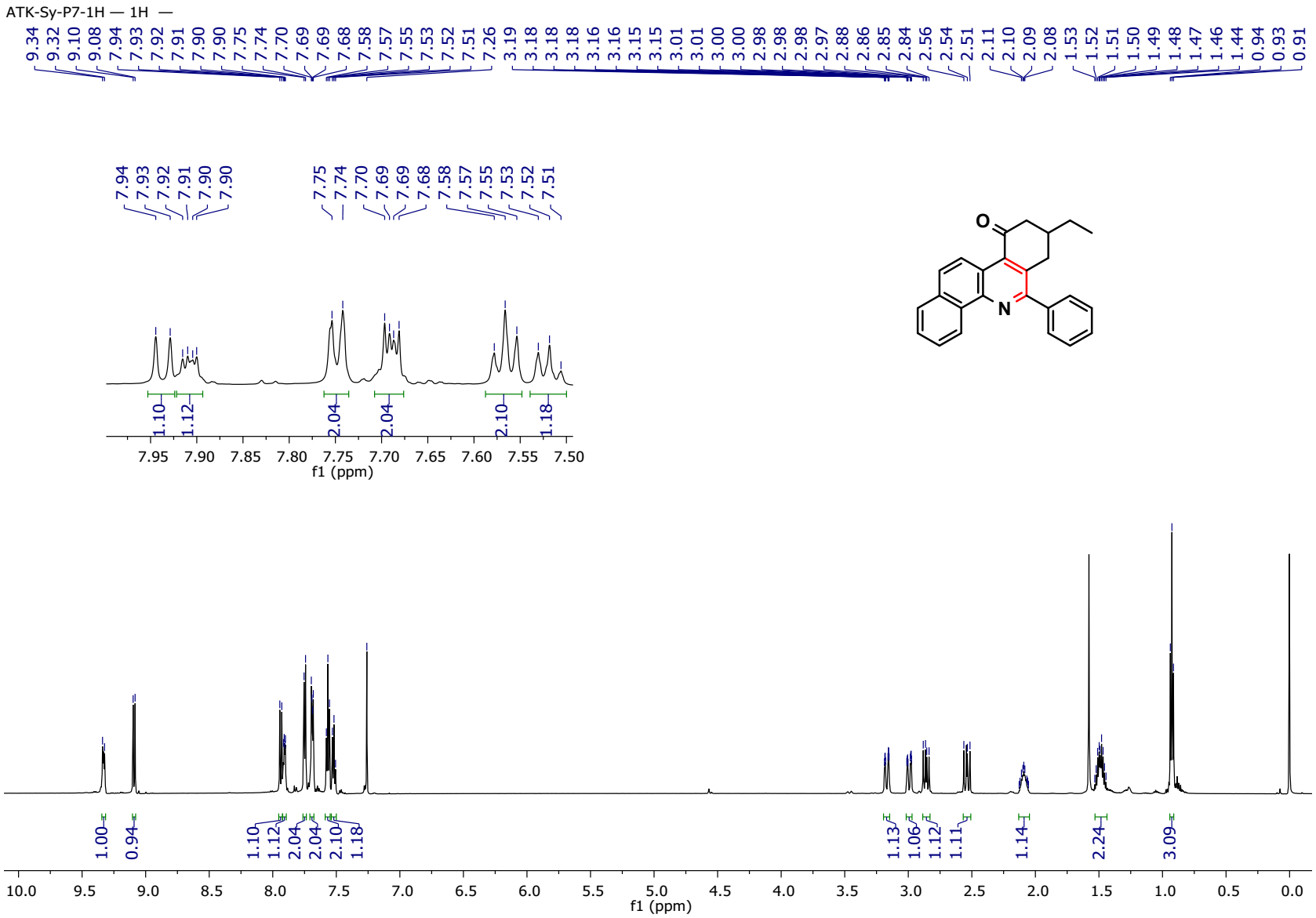


HRMS Spectrum of compound 4h

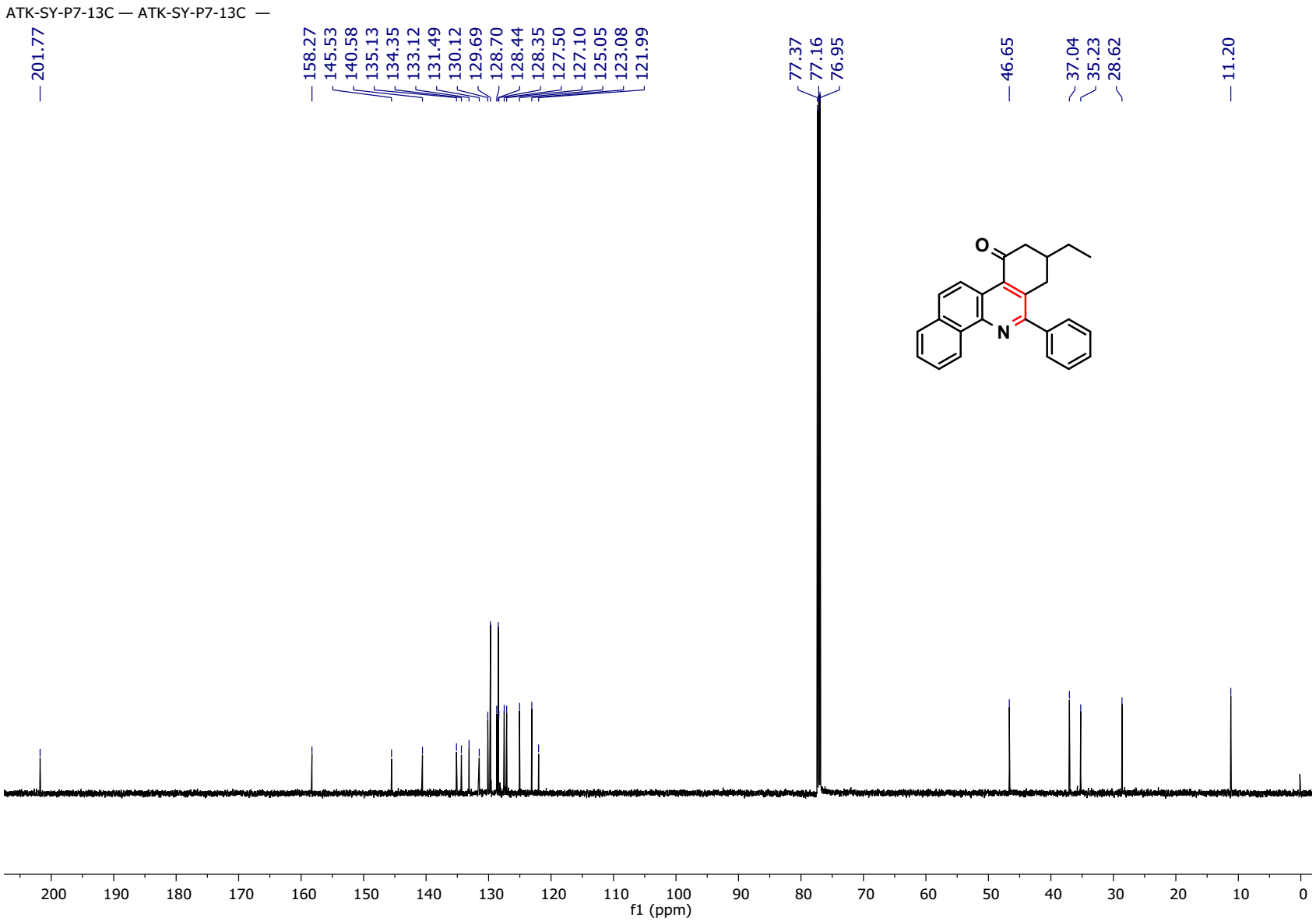
Sample Name	SAMPLE 17	**Position**	P2-B8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P22A.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	27-01-2021 23:03:54 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4i

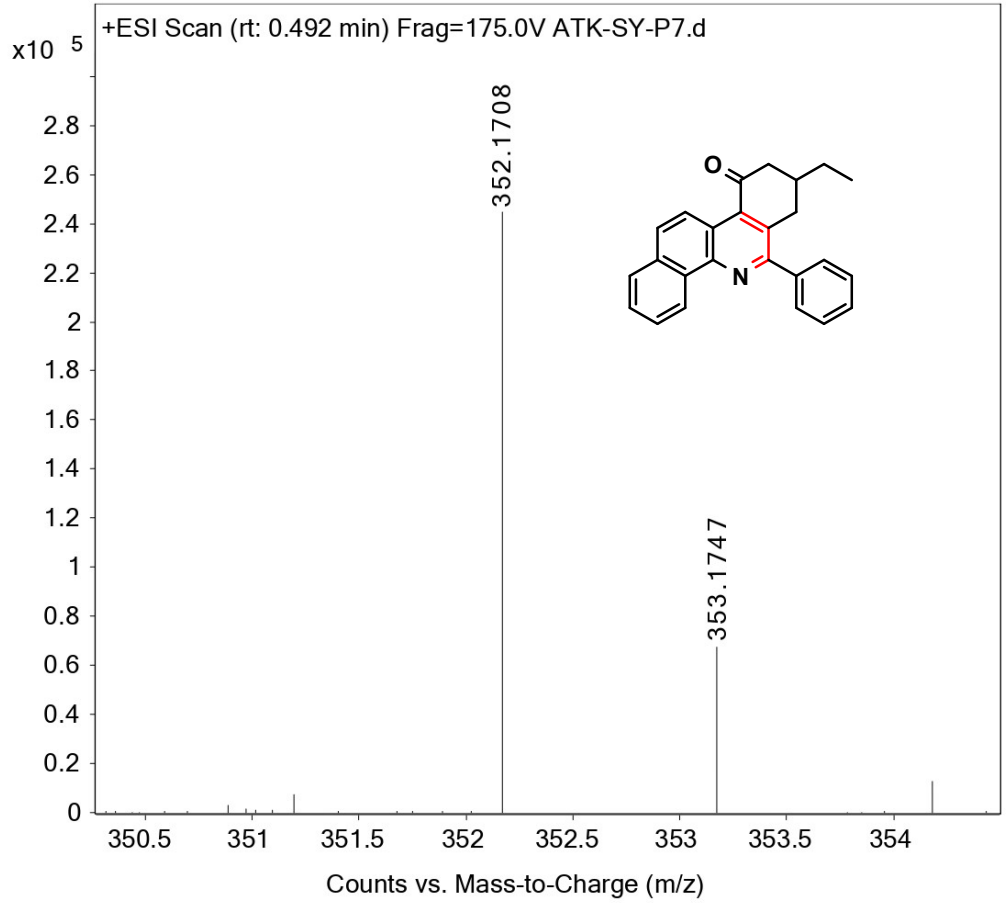


^{13}C NMR Spectrum of Compound 4i

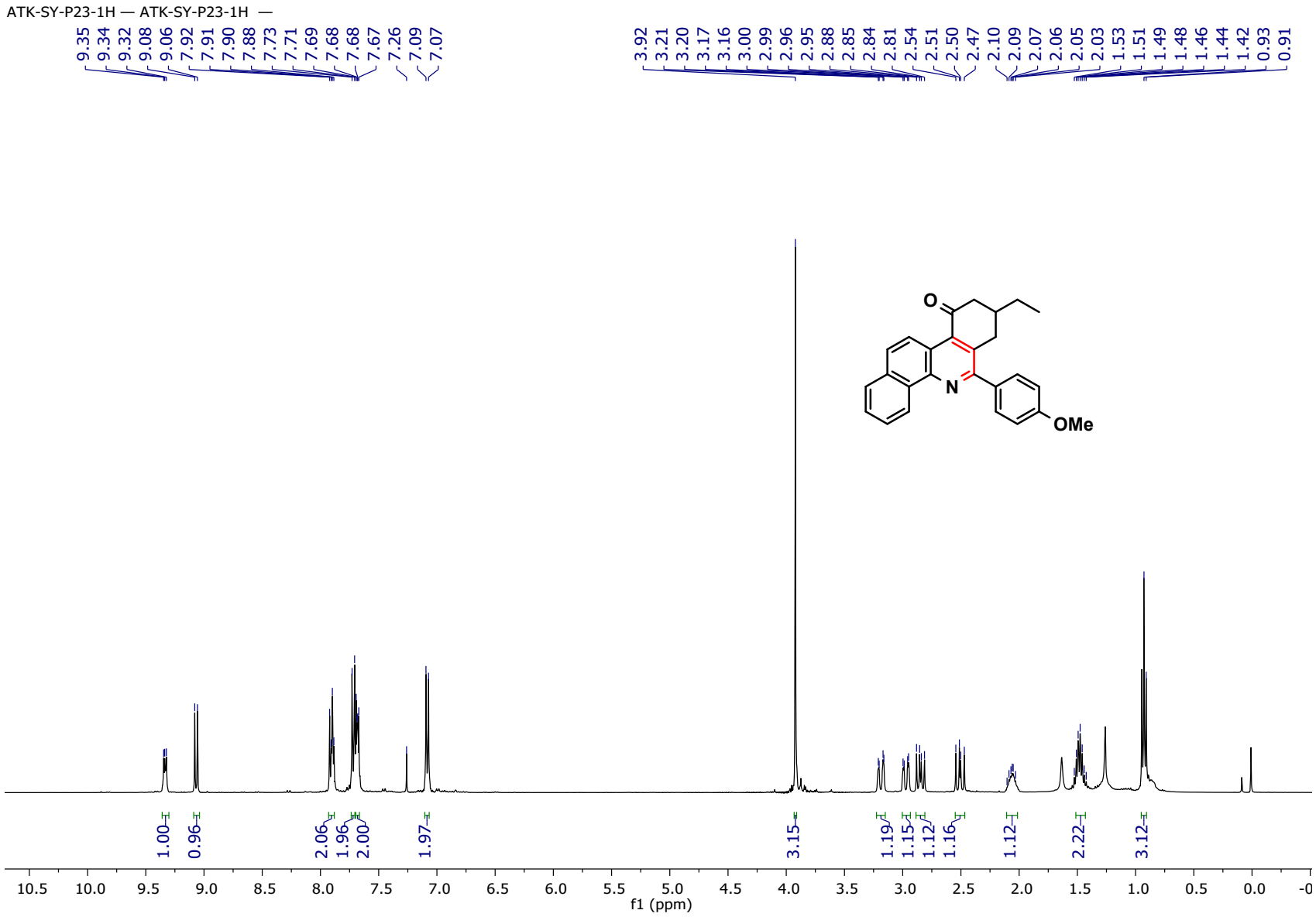


HRMS Spectrum of Compound 4i

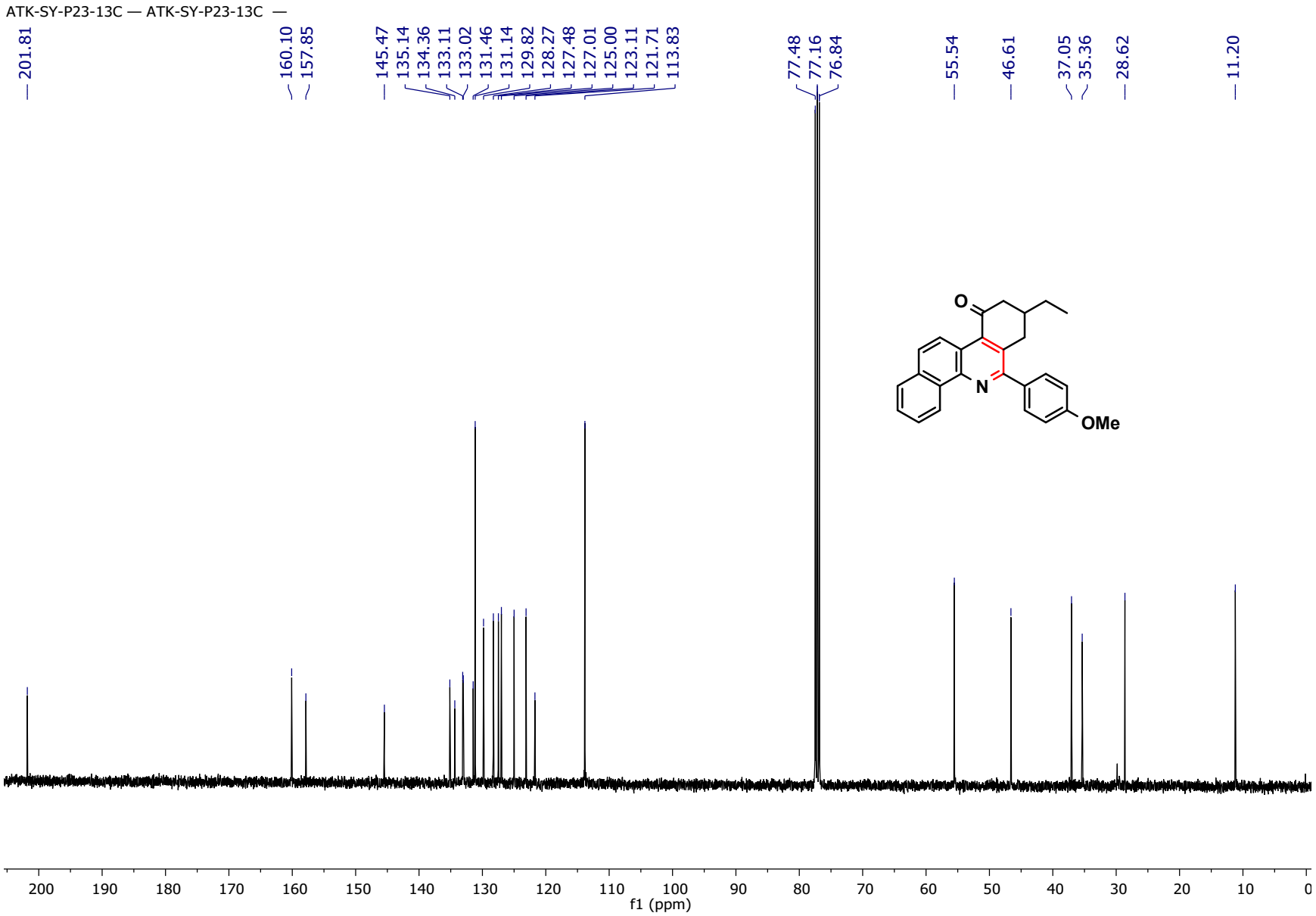
Sample Name	ATK-SY-P7	**Position**	P2-A5	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P7.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	15-12-2020 16:54:33 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4j

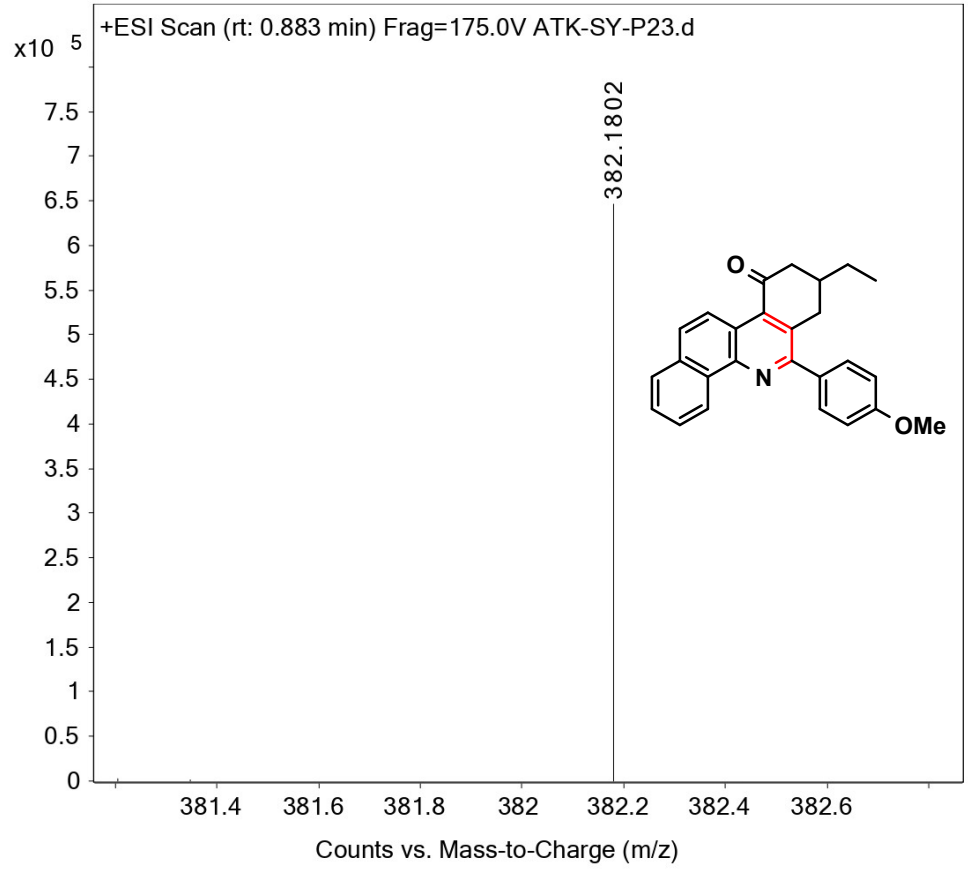


^{13}C NMR Spectrum of Compound 4j

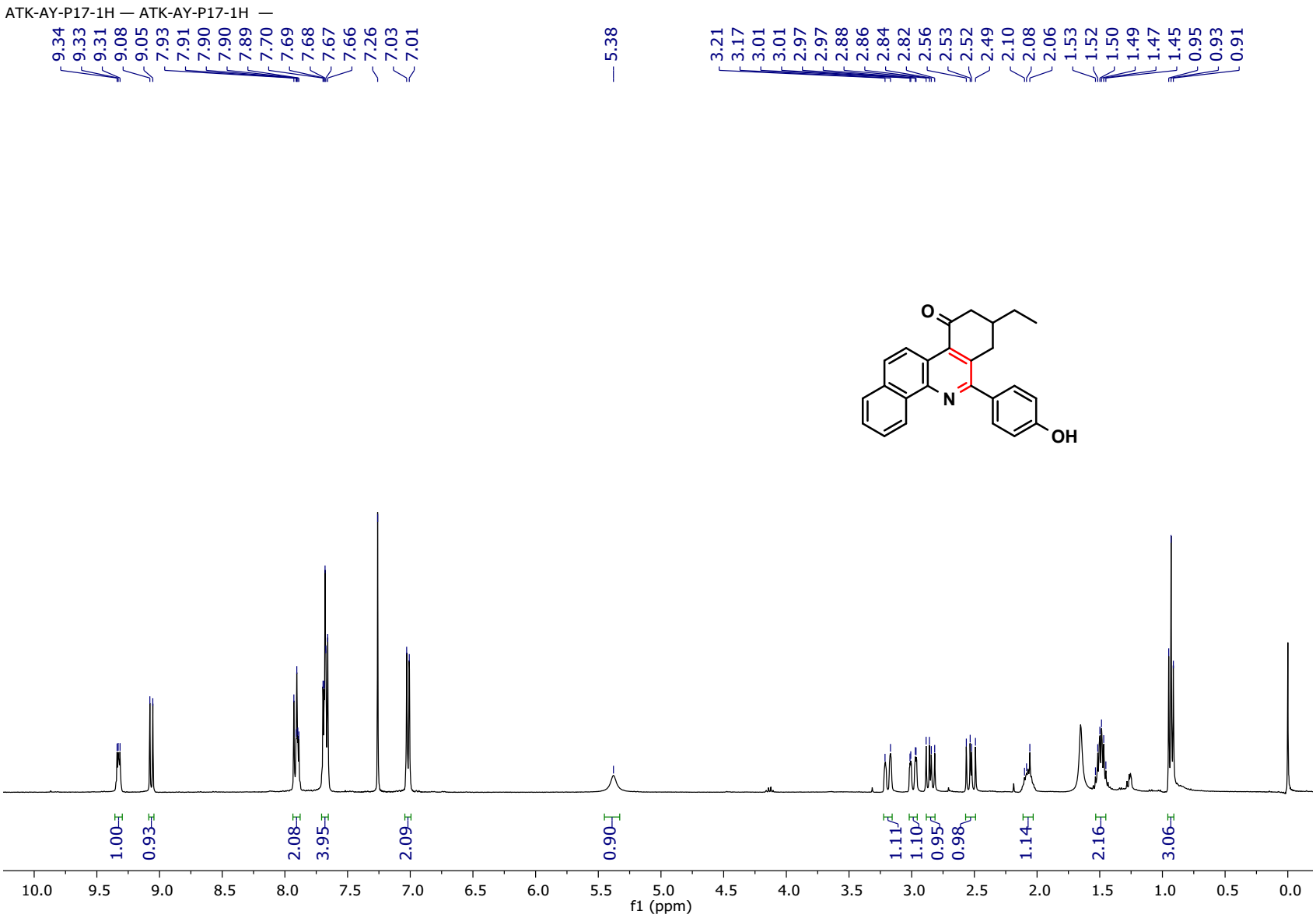


HRMS Spectrum of compound 4j

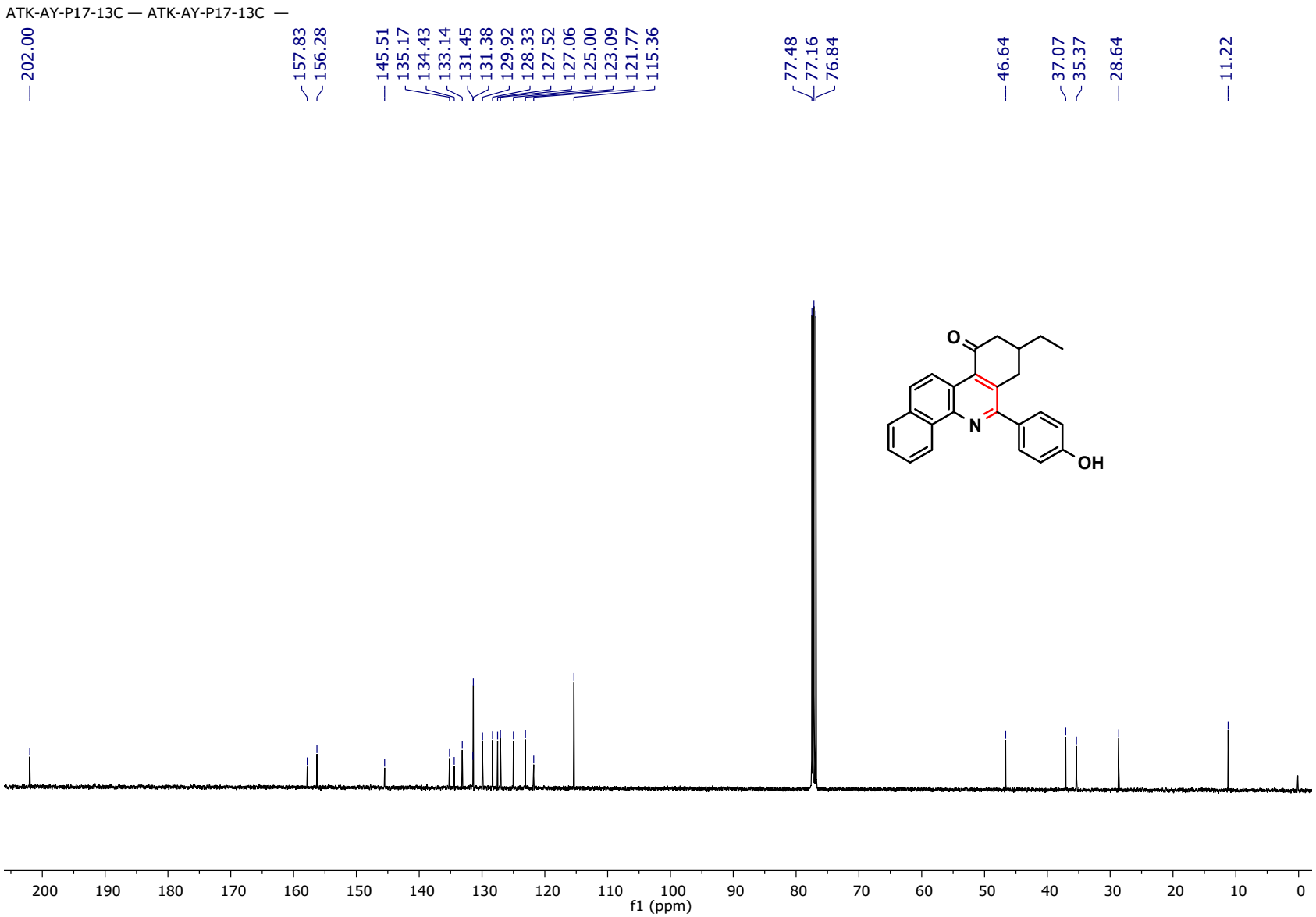
Sample Name	SAMPLE	**Position**	P2-B9	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P23.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	23-01-2021 09:47:04 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4k

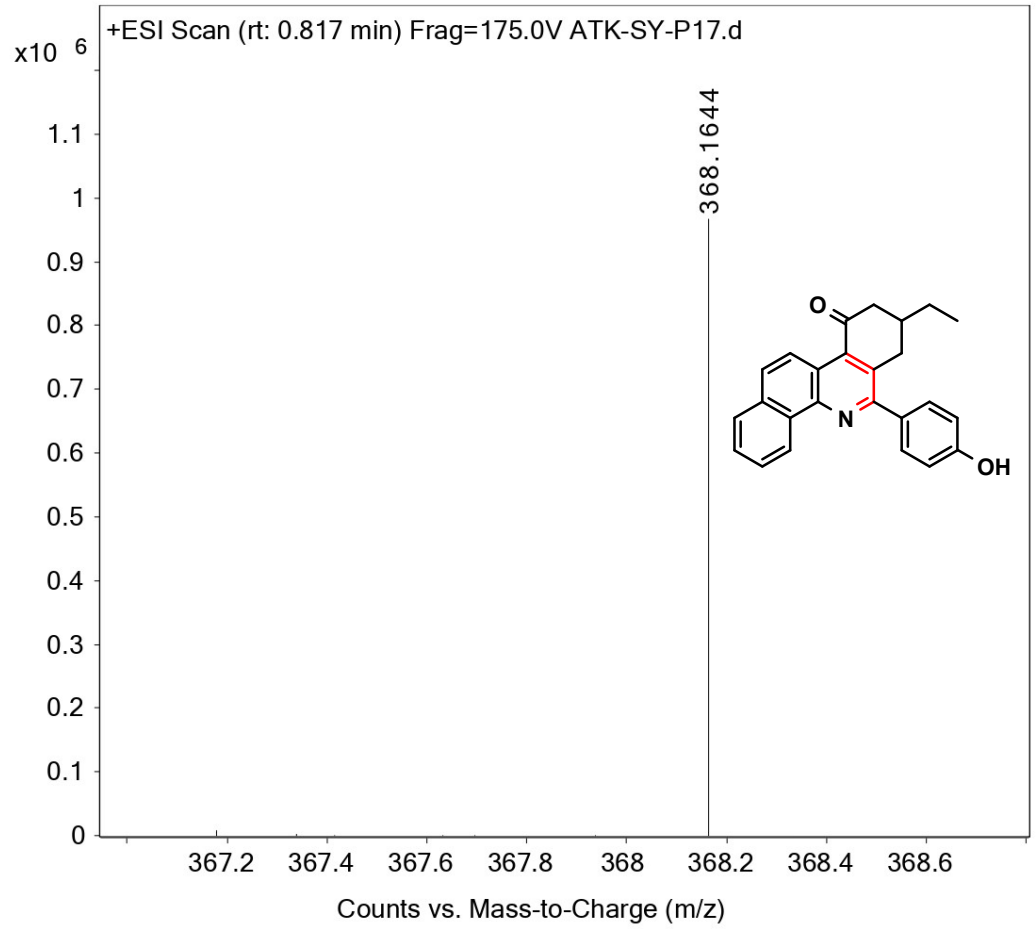


^{13}C NMR Spectrum of Compound 4k

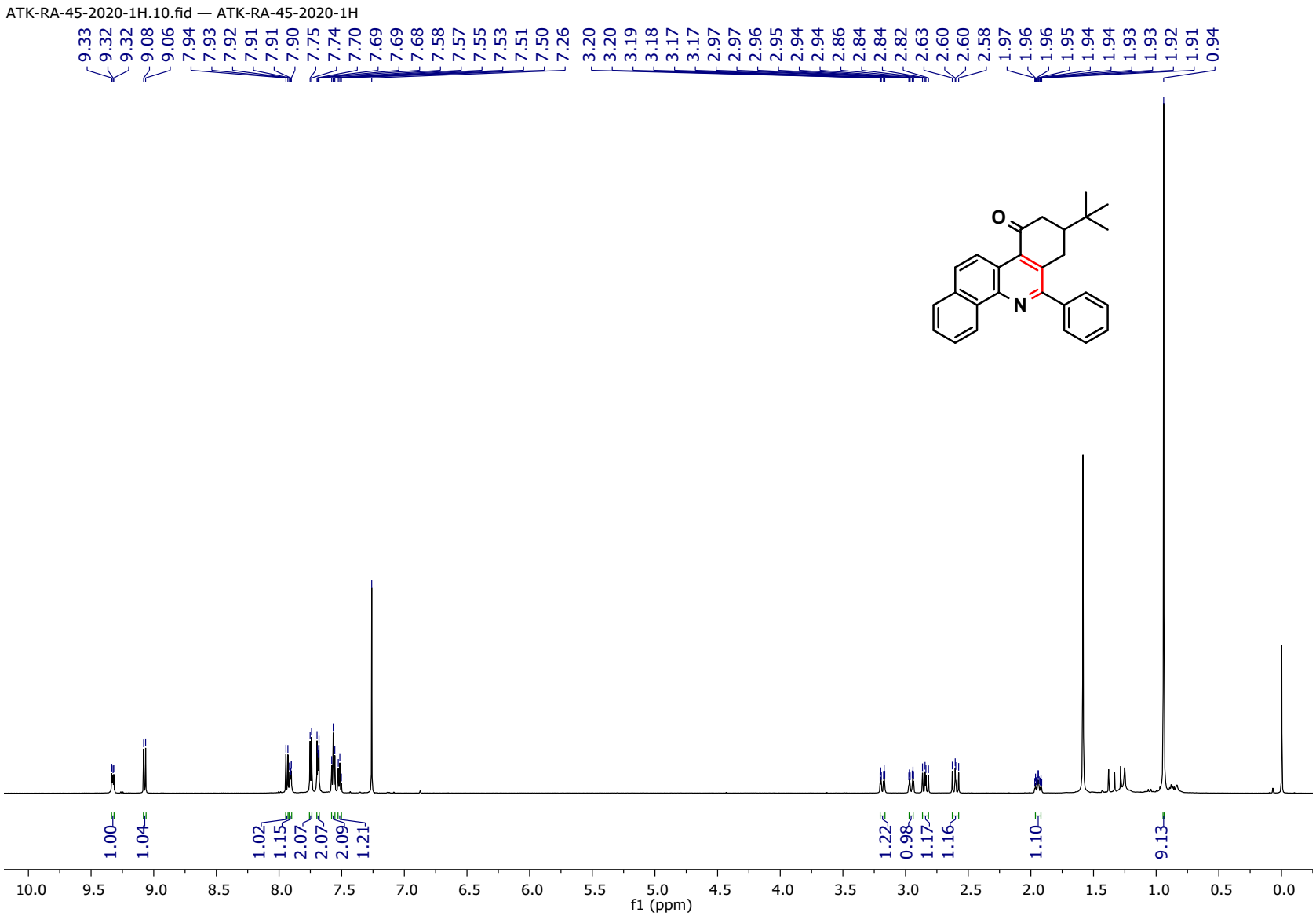


HRMS Spectrum of Compound 4k

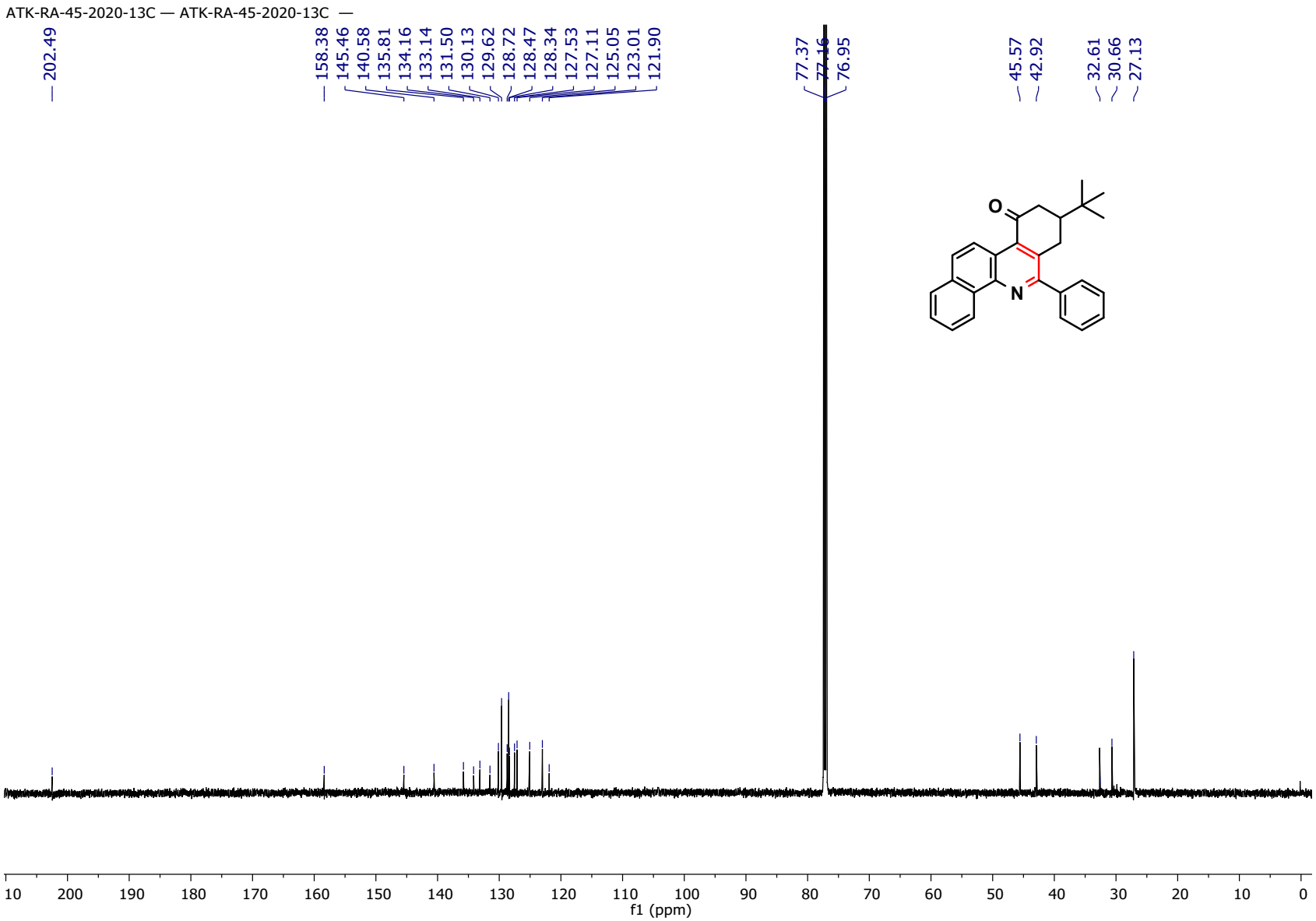
Sample Name	SAMPLE	**Position**	P2-B7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P17.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	23-01-2021 09:25:14 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4l

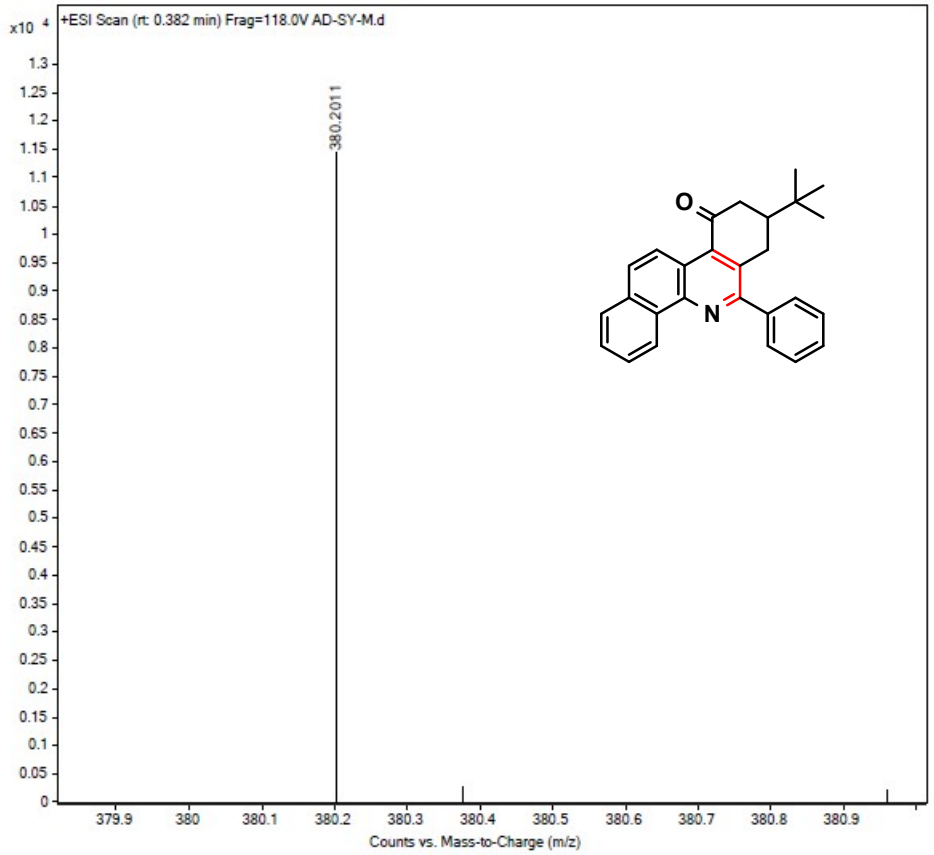


^{13}C NMR Spectrum of Compound 4l

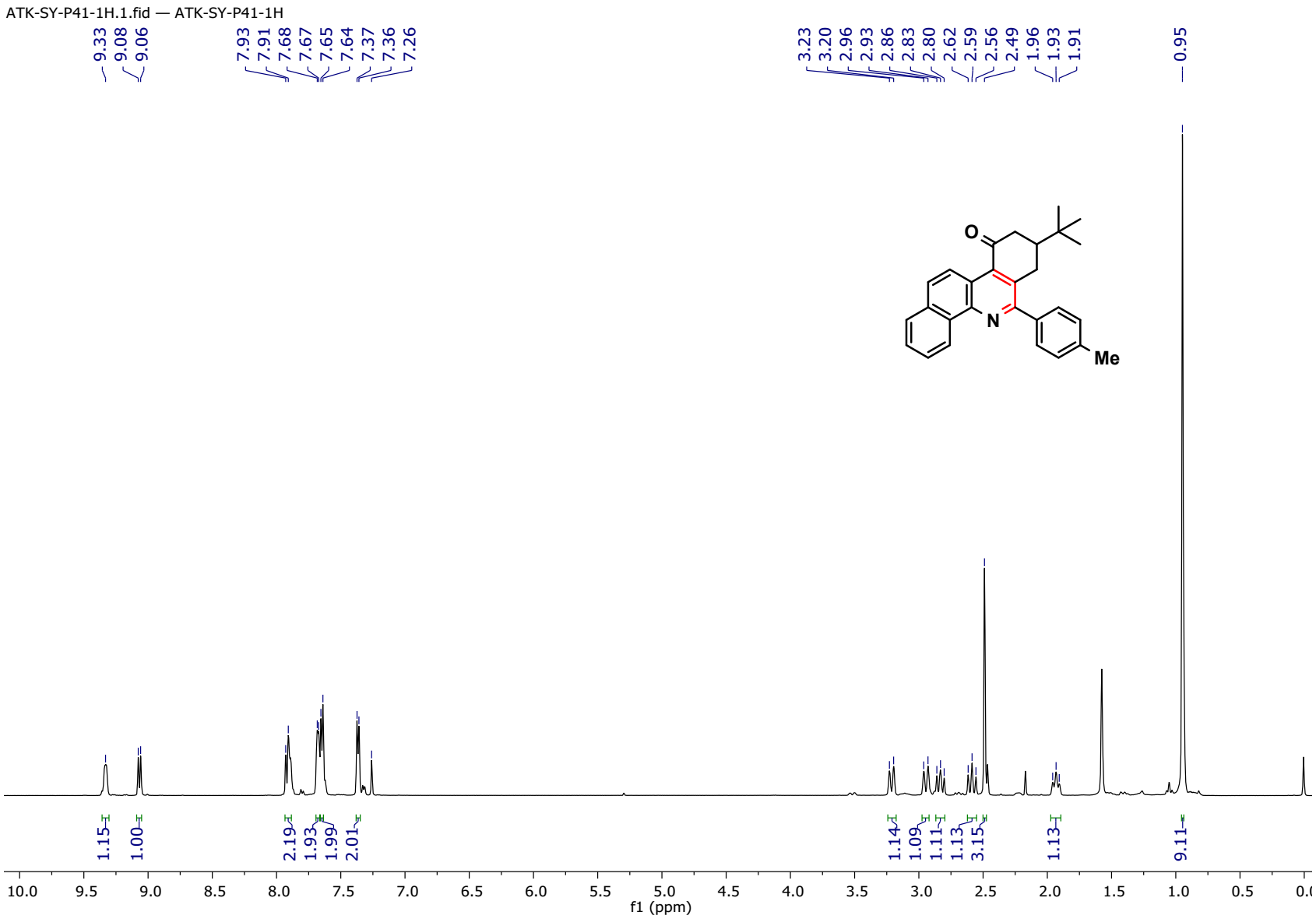


HRMS Spectrum of Compound 4l

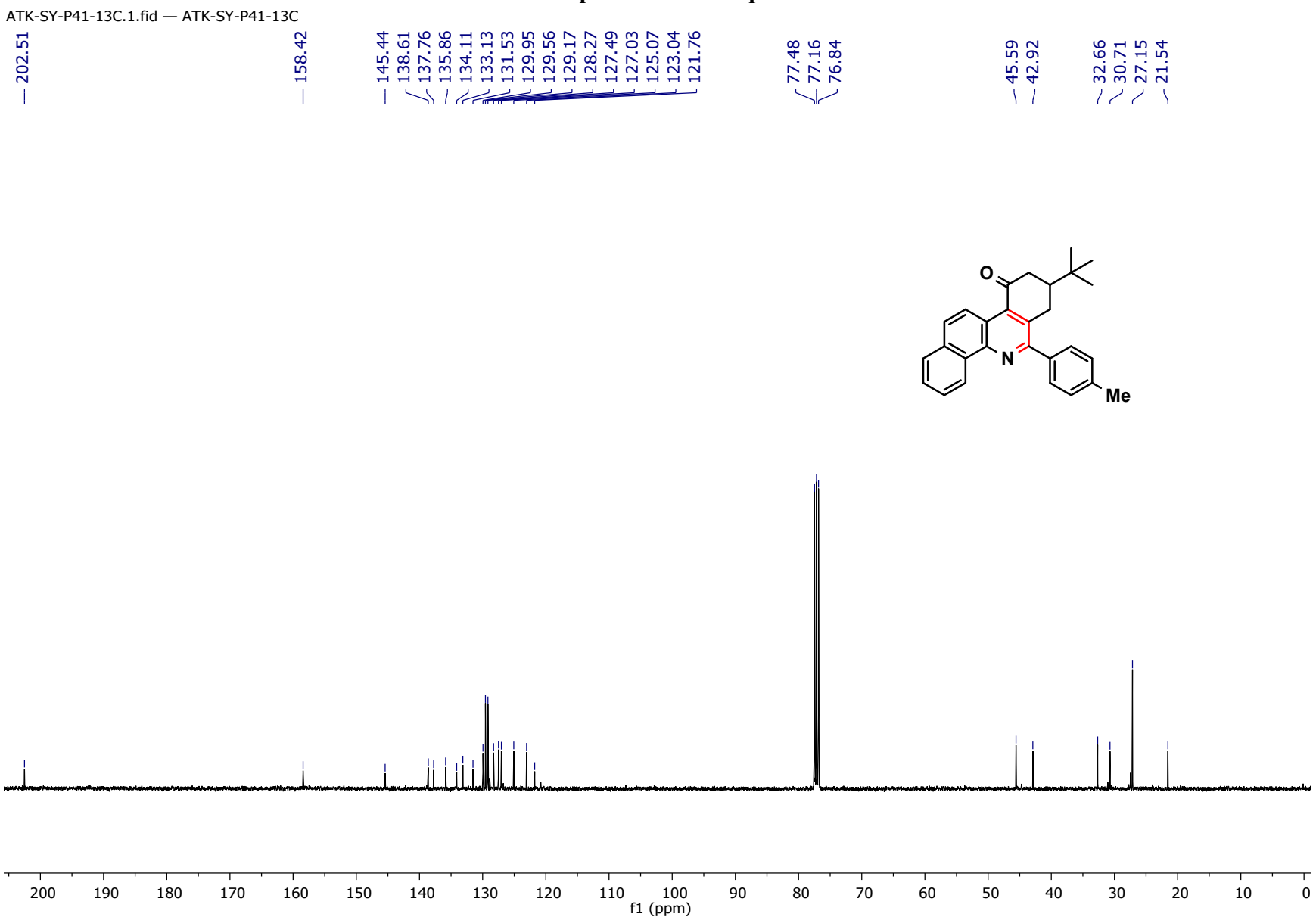
Sample Name	AD-SY-M	**Position**	Vial 25	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	0.1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Some Ions Missed	**Data Filename**	AD-SY-M.d
ACQ Method	Direct Mass-2017.m	**Comment**		**Acquired Time**	28-Mar-22 09:14:42 PM (UTC+05:30)



^{1}H NMR Spectrum of Compound 4m

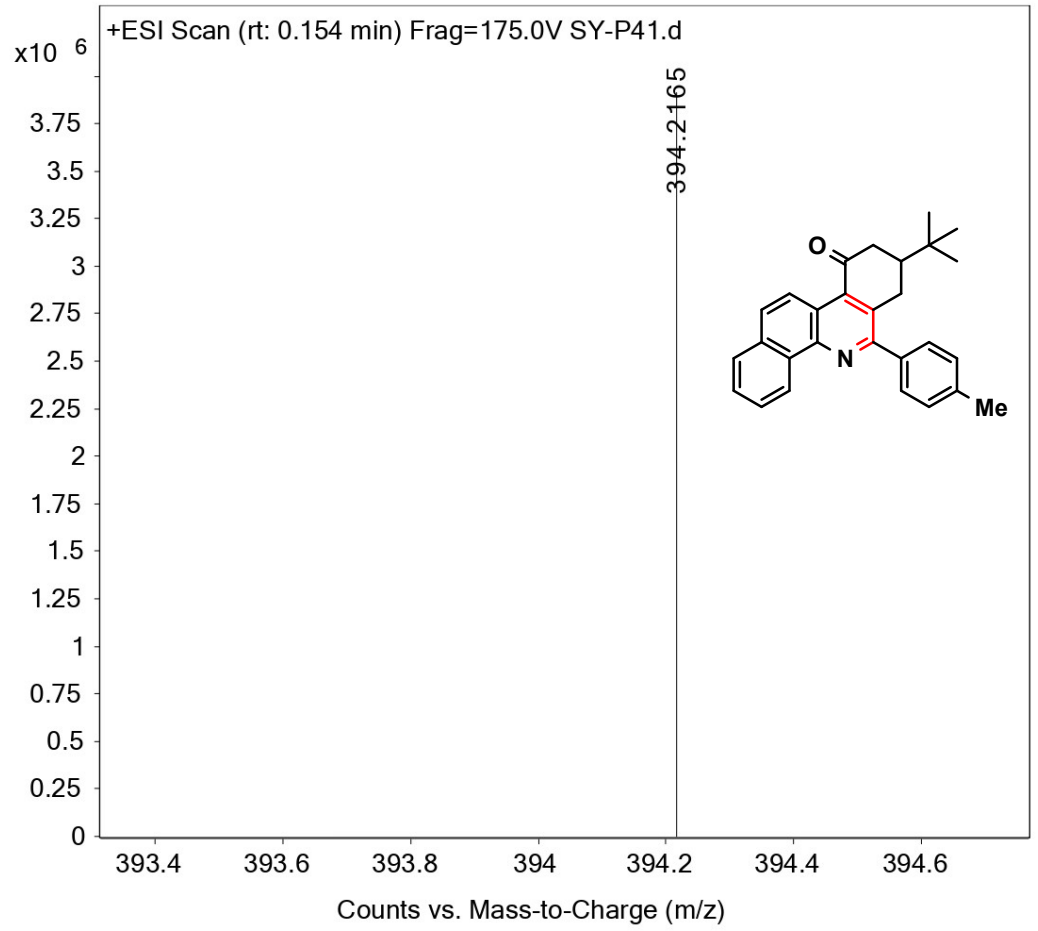


^{13}C NMR Spectrum of Compound 4m

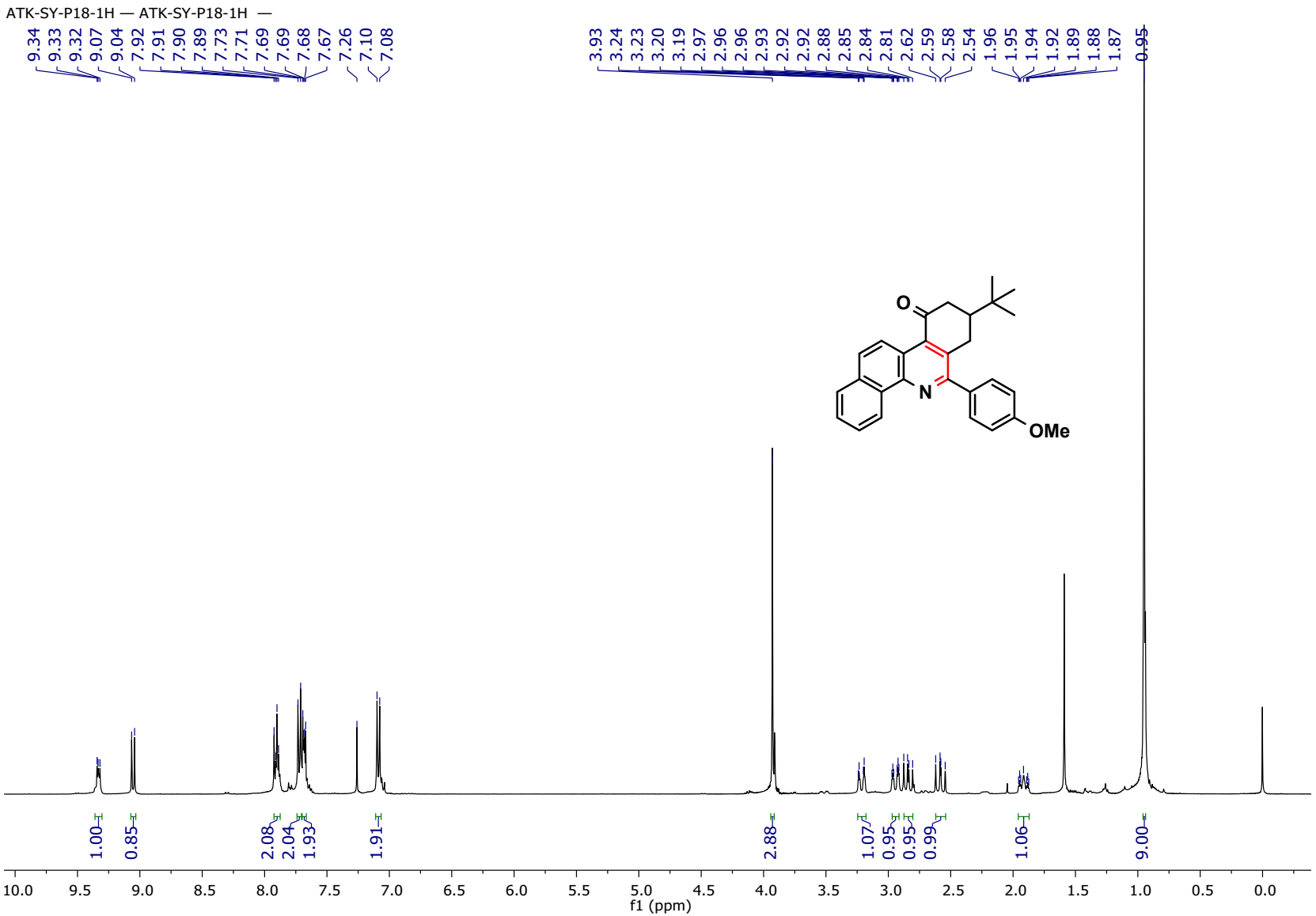


HRMS Spectrum of compound 4m

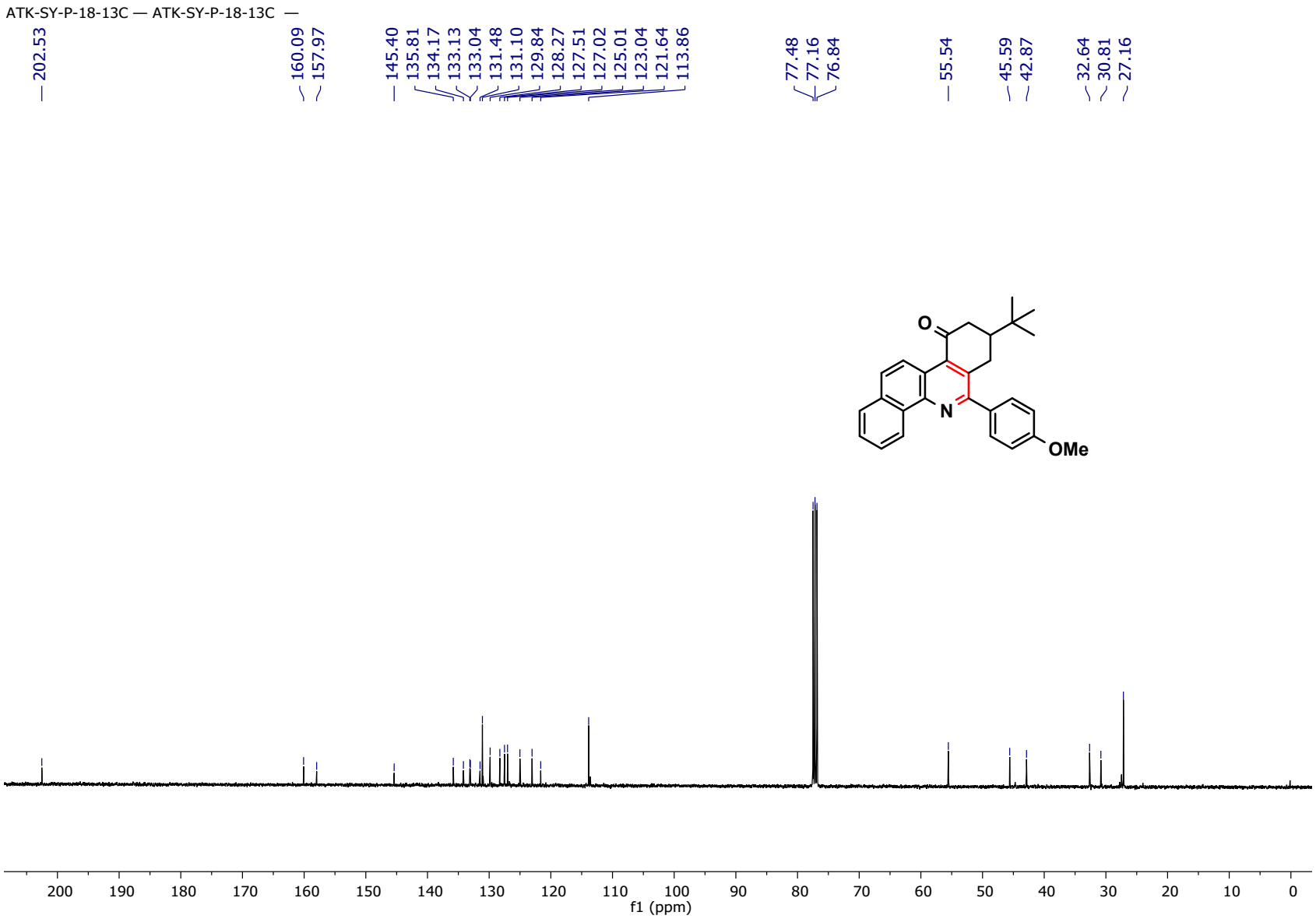
Sample Name	SAMPLE	**Position**	P1-E3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P41.d
ACQ Method	ESI ALS 200-1000.m	**Comment**		**Acquired Time**	27-02-2021 02:59:31 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4n

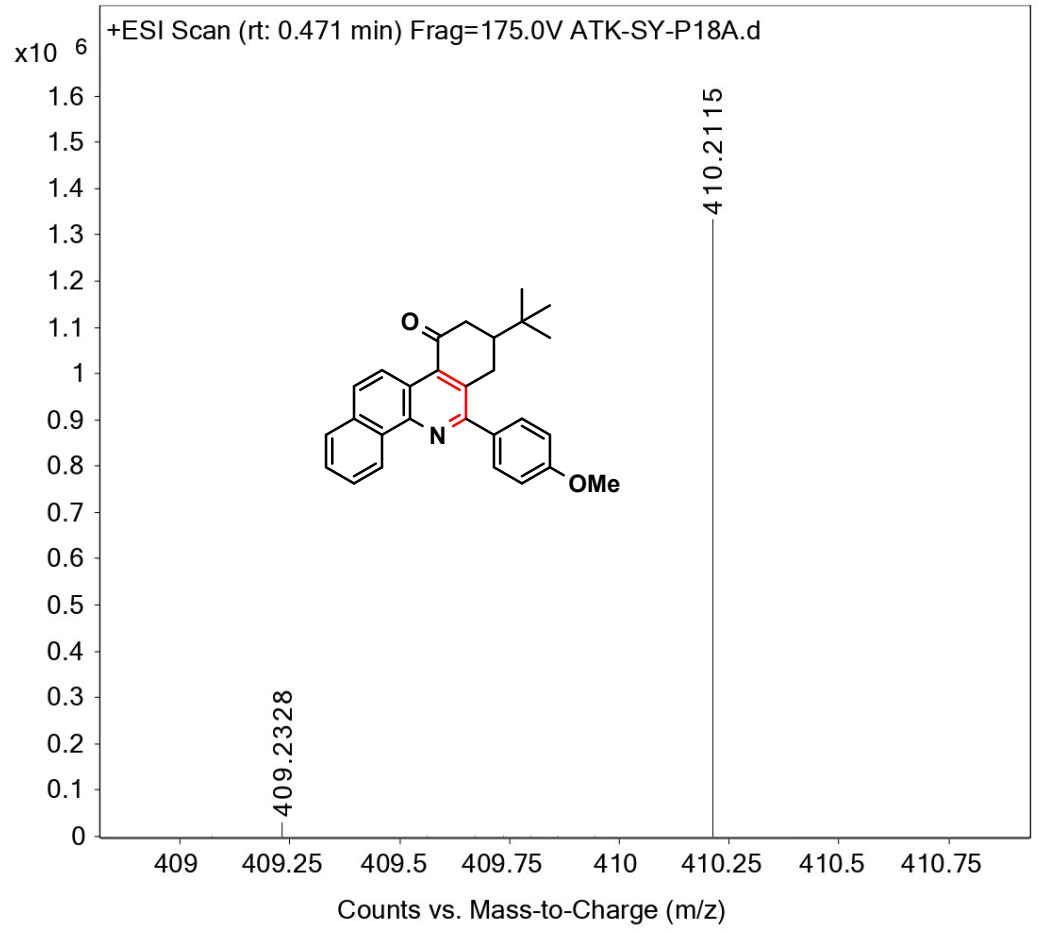


^{13}C NMR Spectrum of Compound 4n

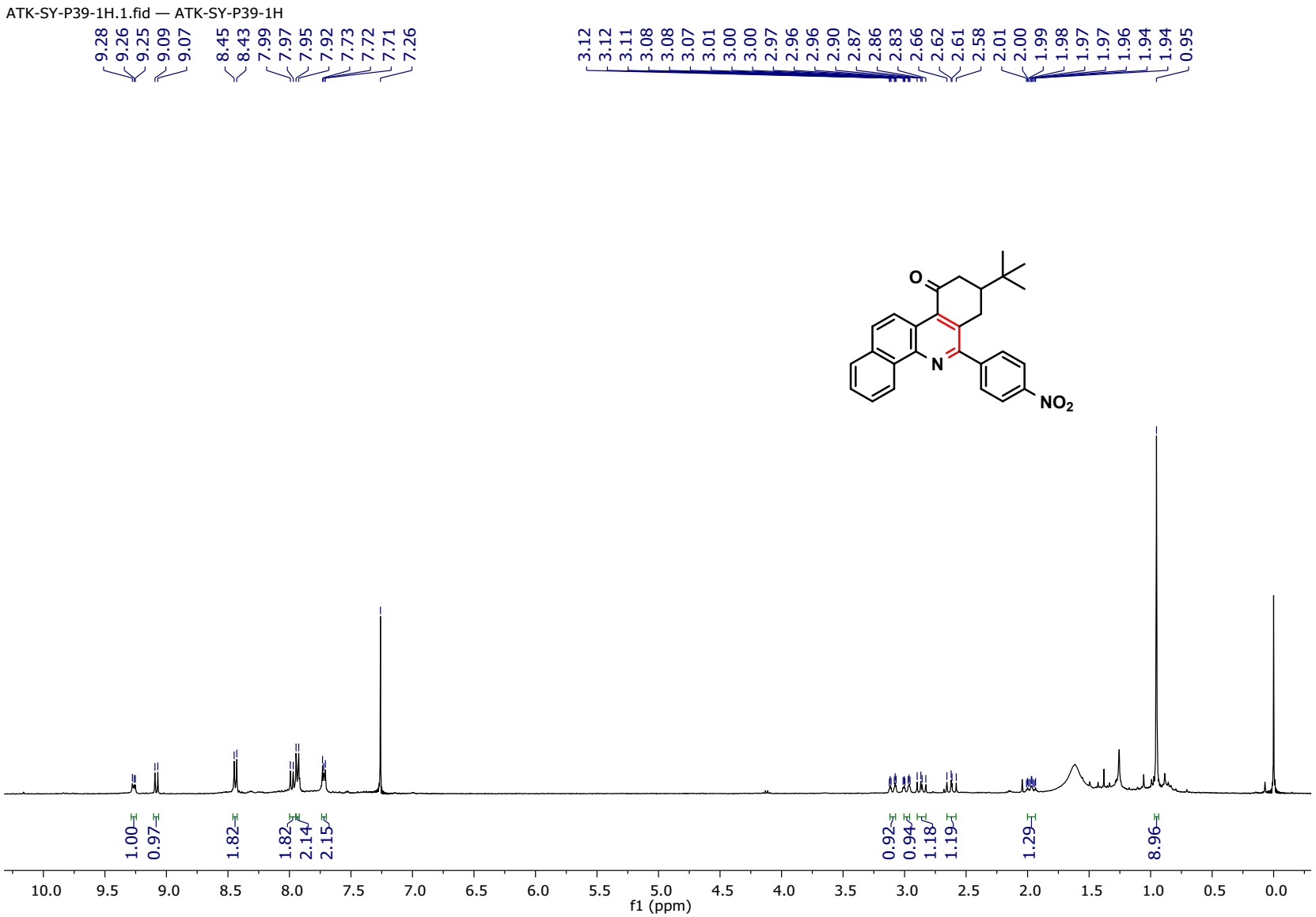


HRMS Spectrum of compound 4n

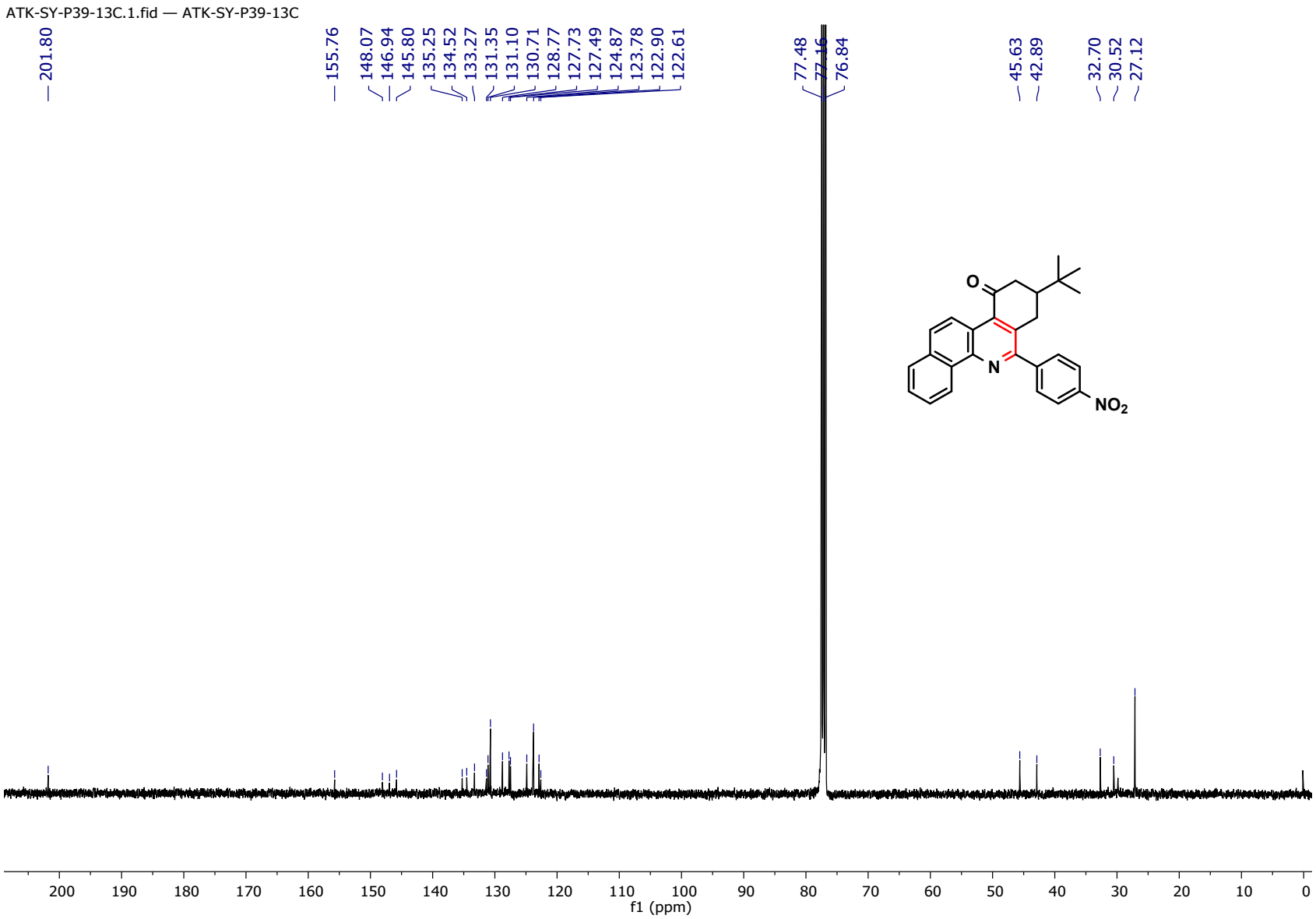
Sample Name	SAMPLE 16	**Position**	P2-B7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P18A.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	27-01-2021 22:52:01 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4o

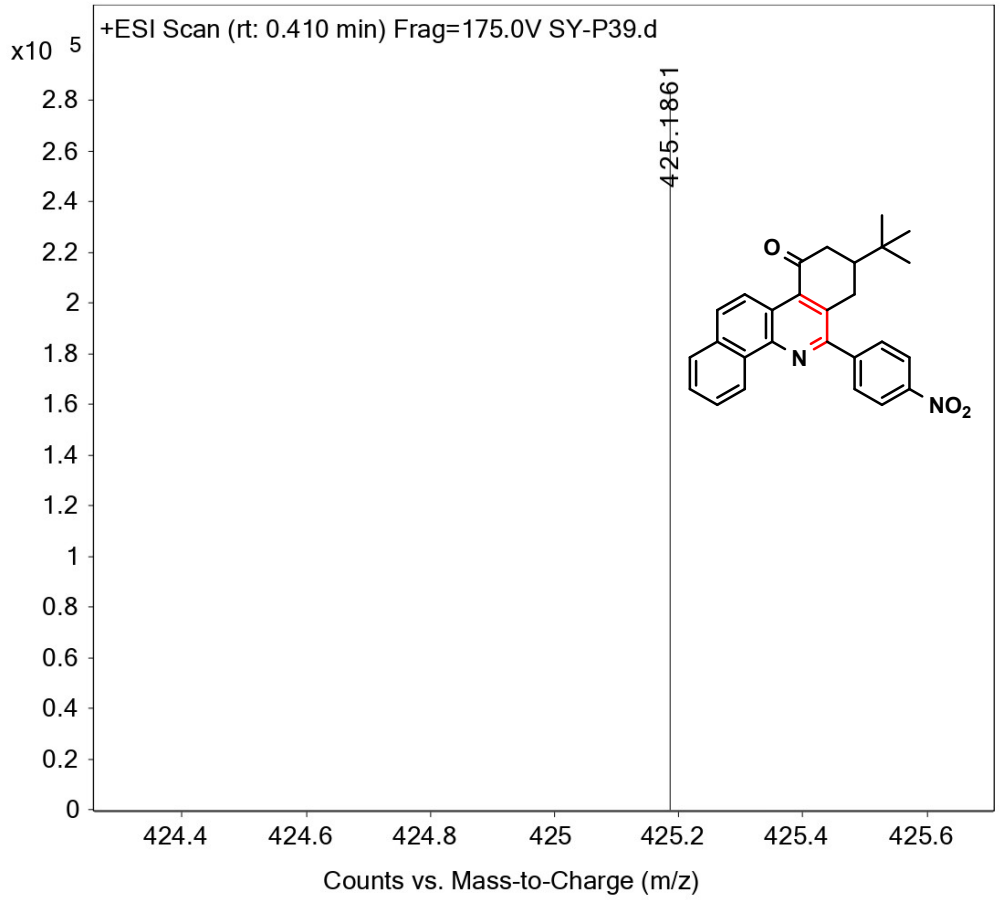


^{13}C NMR Spectrum of Compound 4o

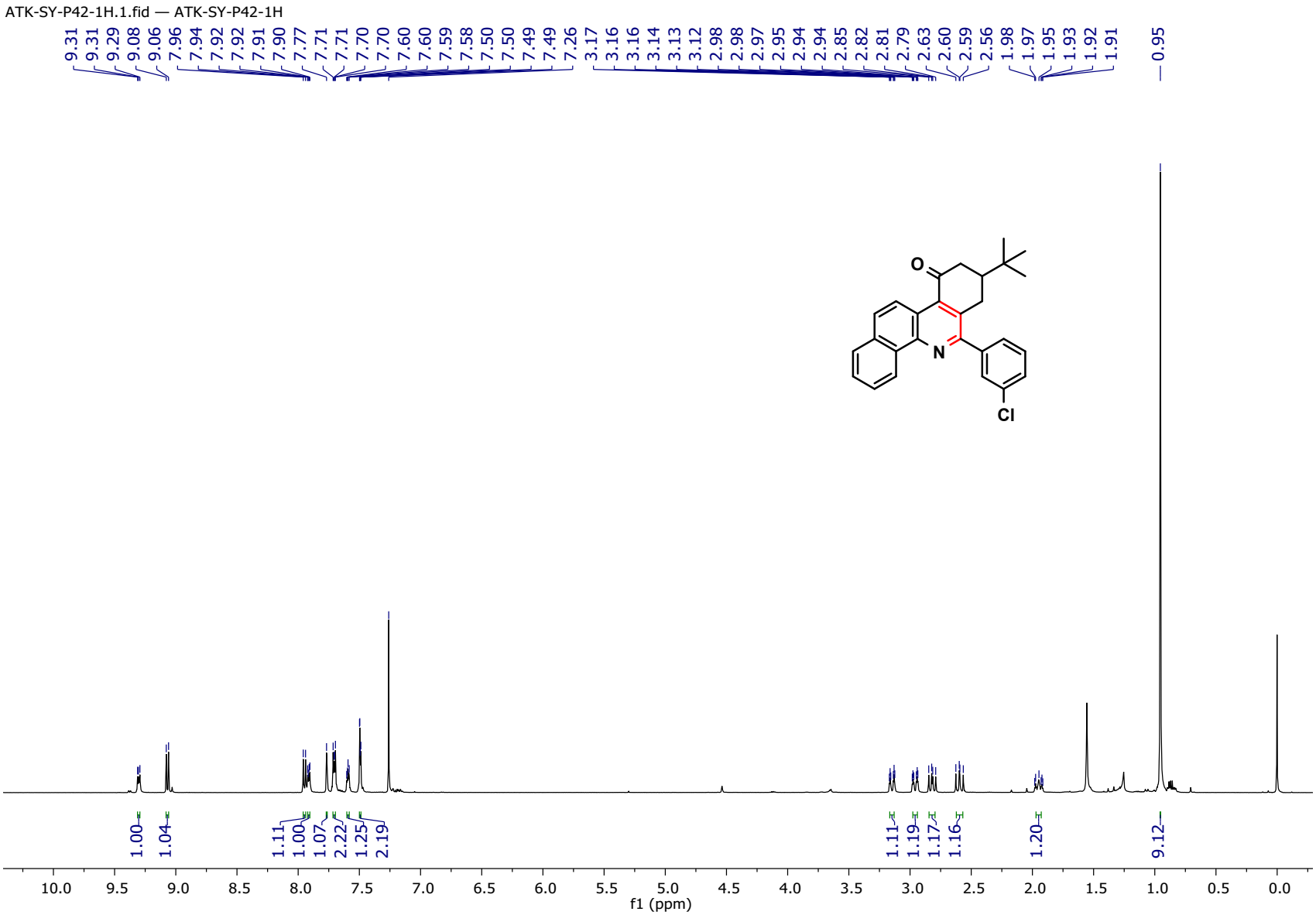


HRMS Spectrum of Compound 4o

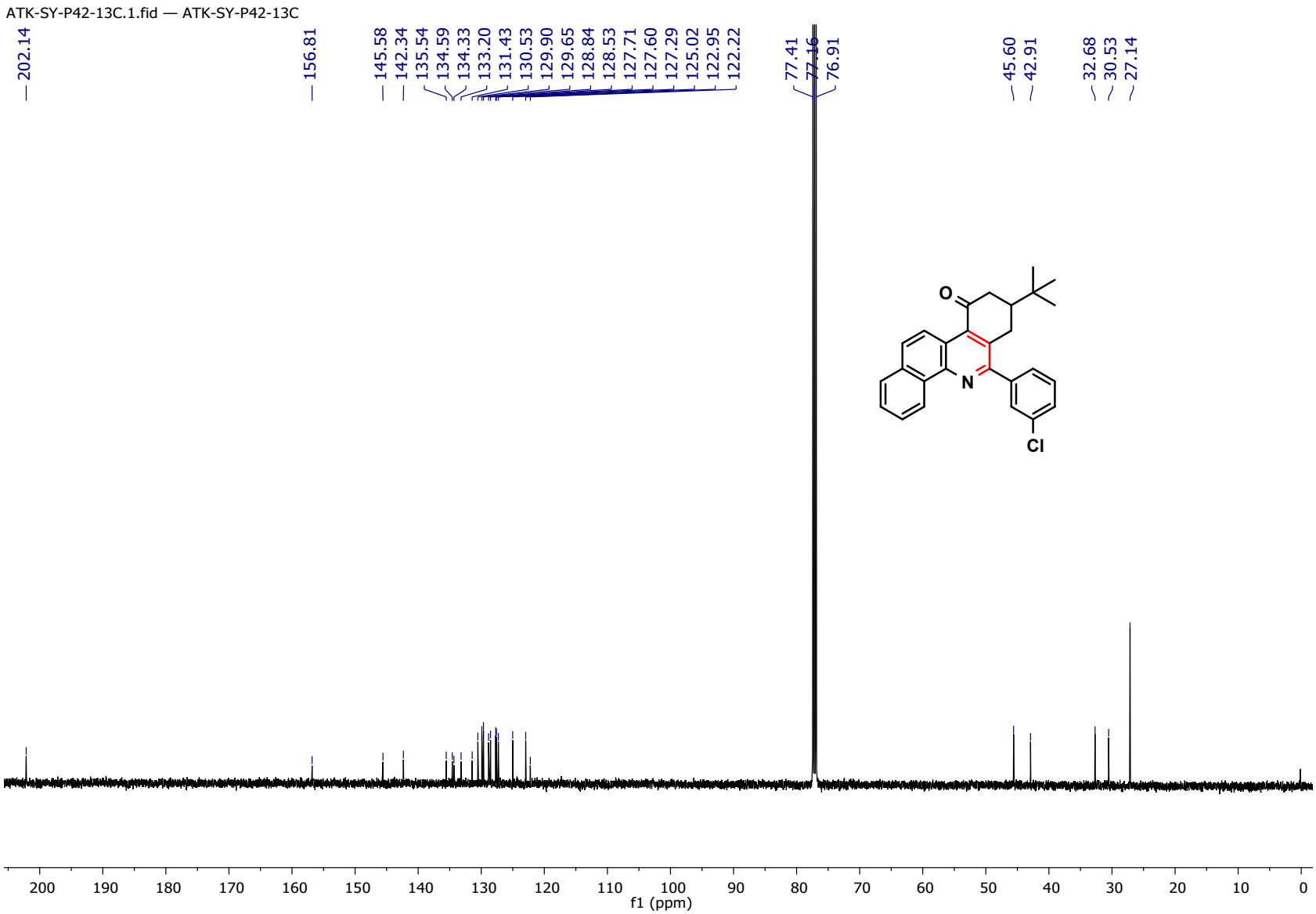
Sample Name	SAMPLE 19	**Position**	P2-B4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P39.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	22-02-2021 18:53:44 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4p

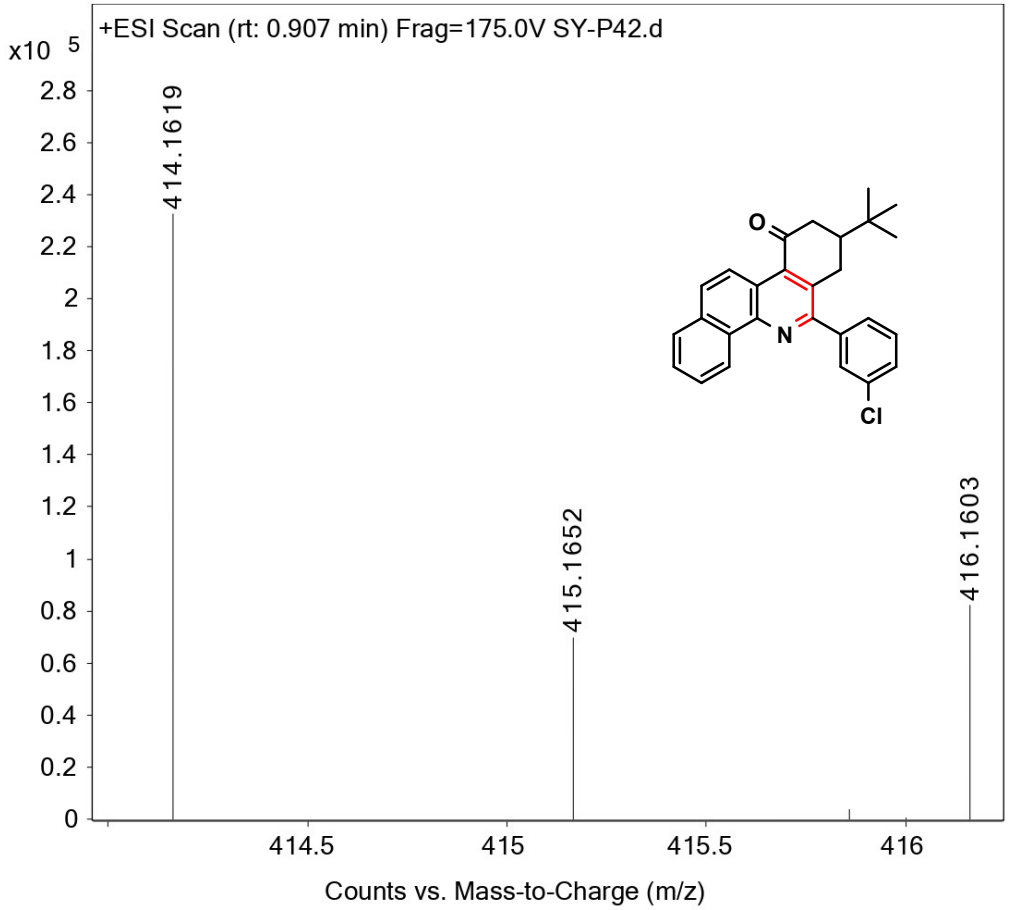


^{13}C NMR Spectrum of Compound 4p

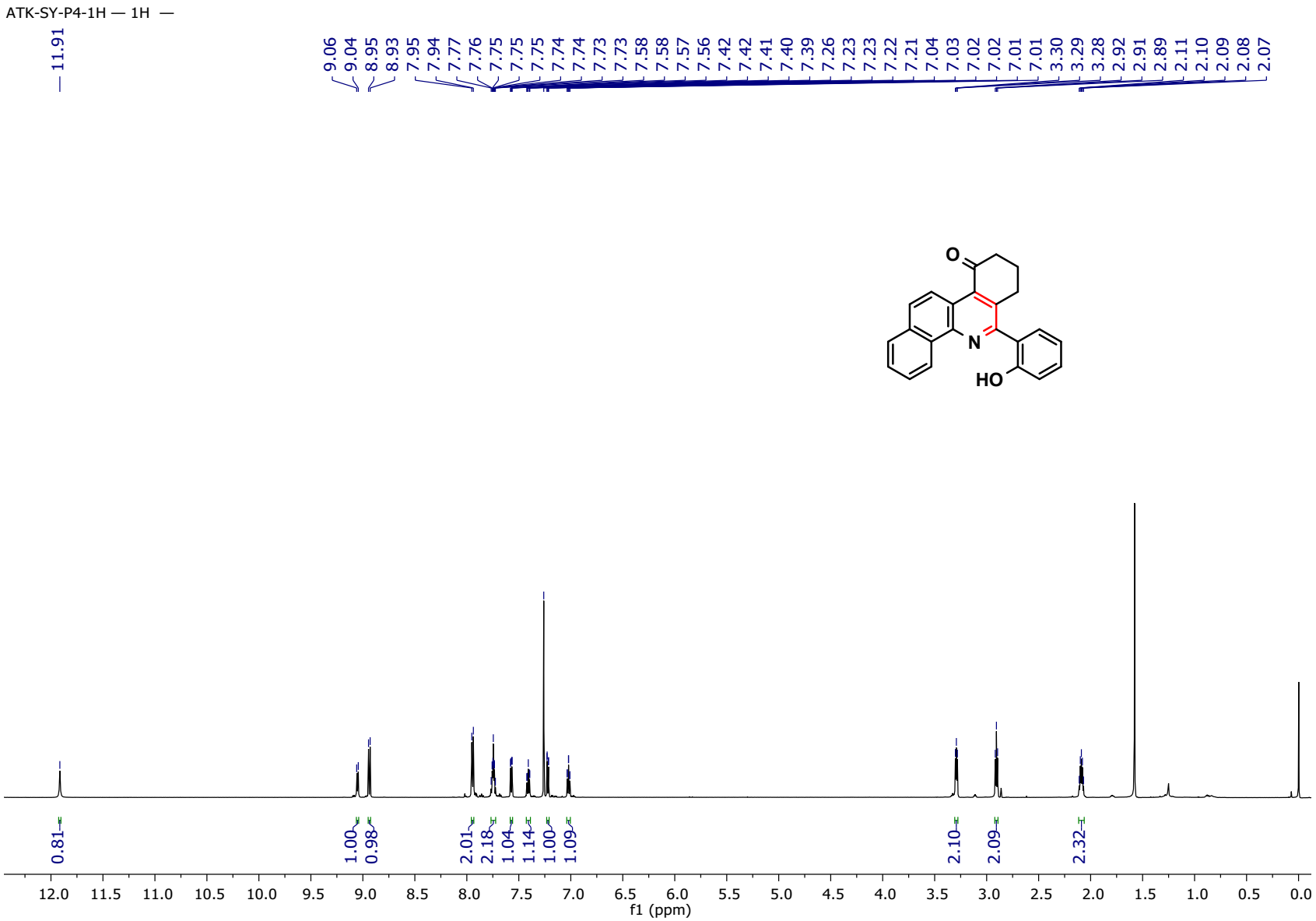


HRMS Spectrum of Compound 4p

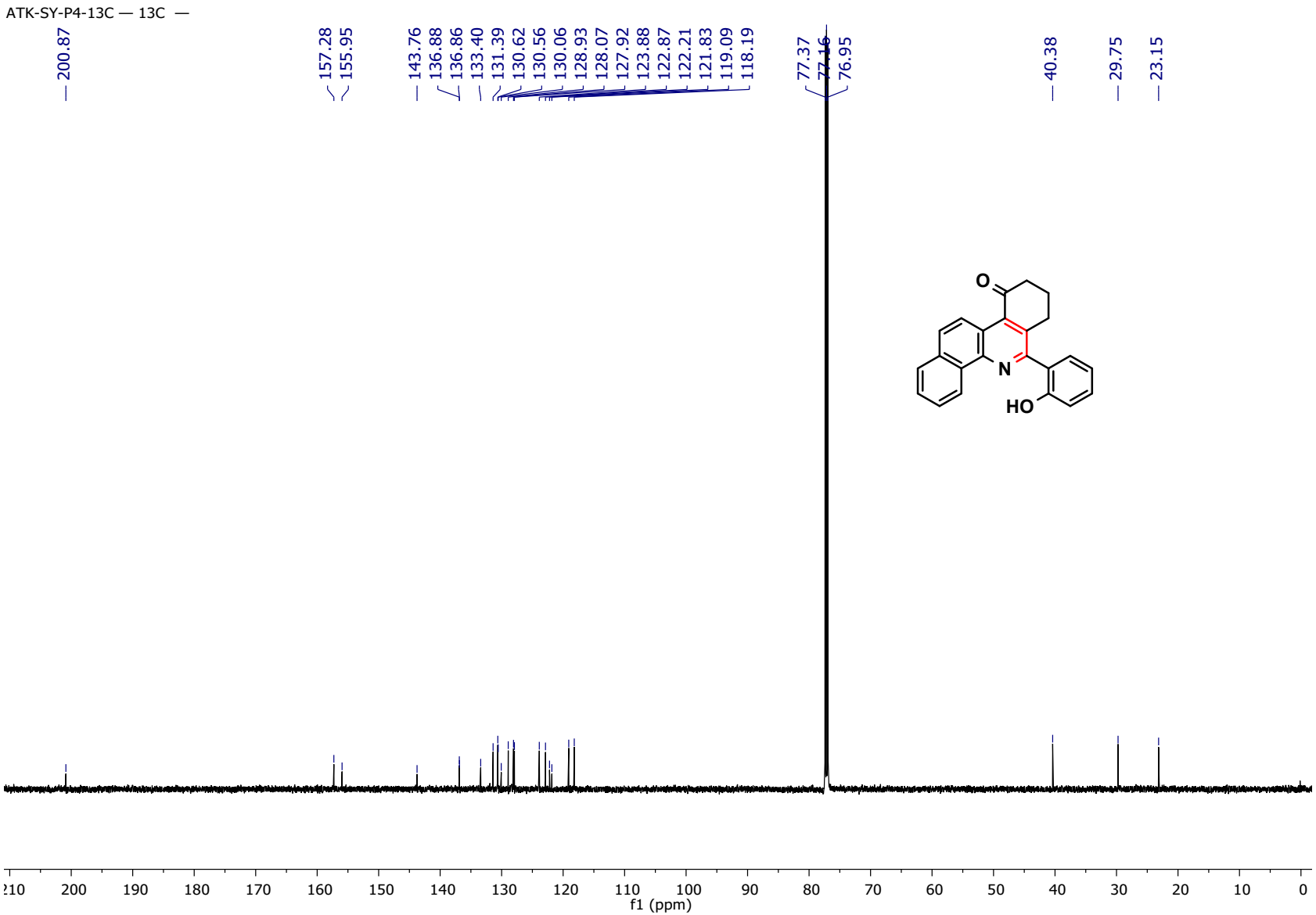
Sample Name	SAMPLE 18	**Position**	P2-B3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P42.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	22-02-2021 18:42:54 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4q

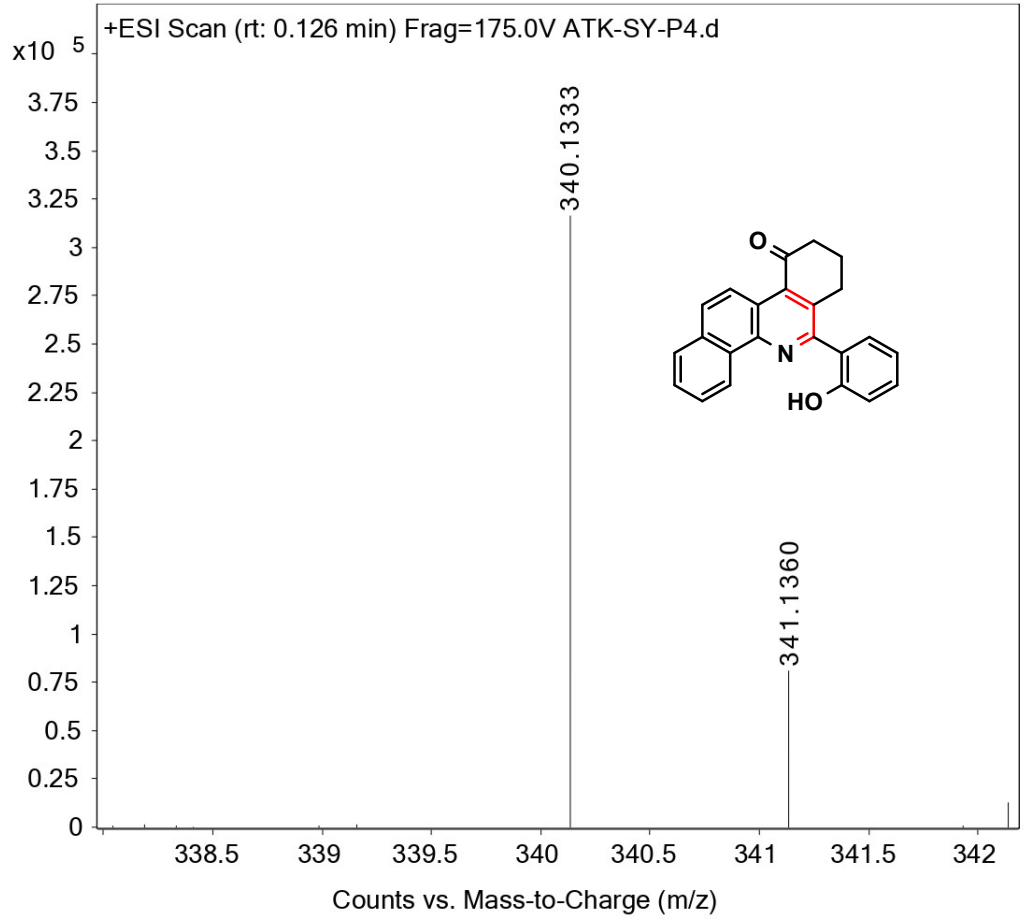


^{13}C NMR Spectrum of Compound 4q

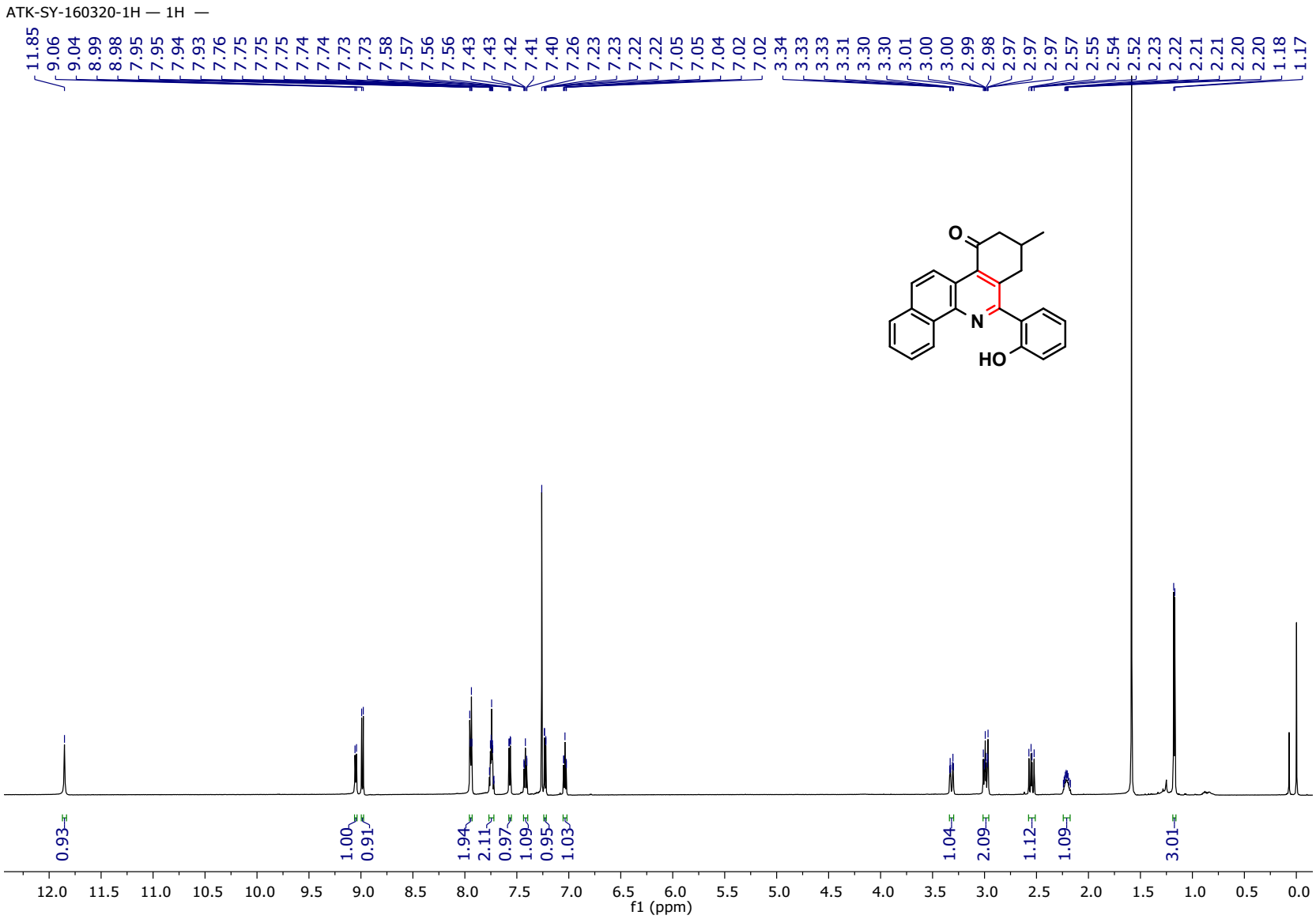


HRMS Spectrum of Compound 4q

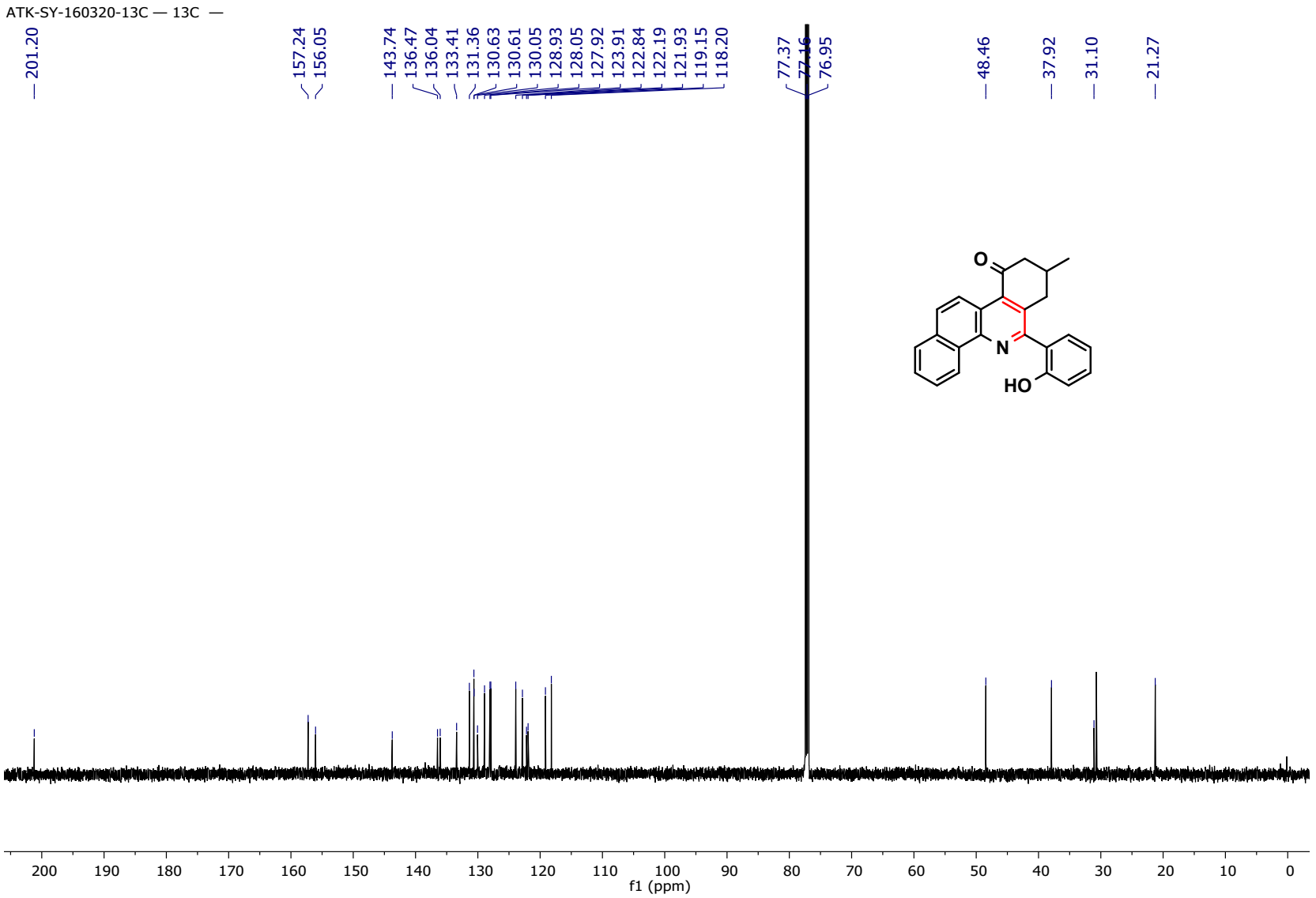
Sample Name	SAMPLE 19	**Position**	P2-B10	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-P4.d
ACQ Method	ESI ALS 100-500.m	**Comment**		**Acquired Time**	14-12-2020 16:40:14 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4r

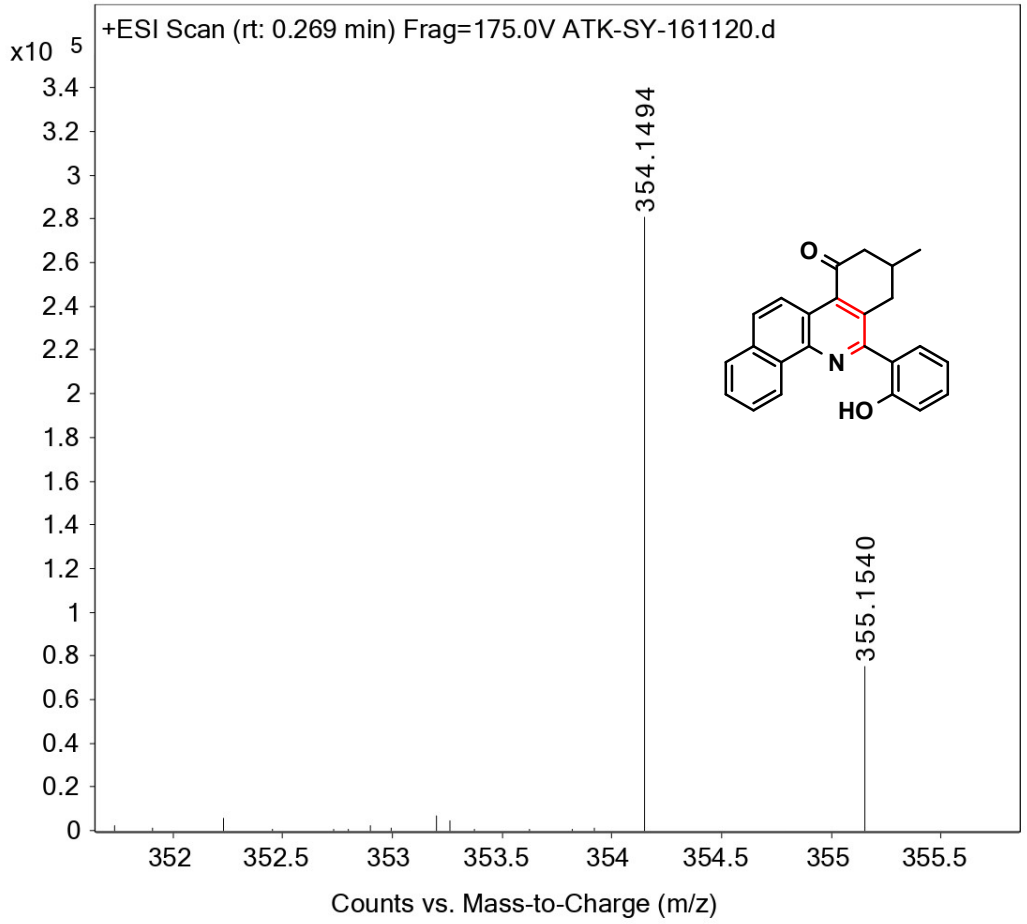


^{13}C NMR Spectrum of Compound 4r

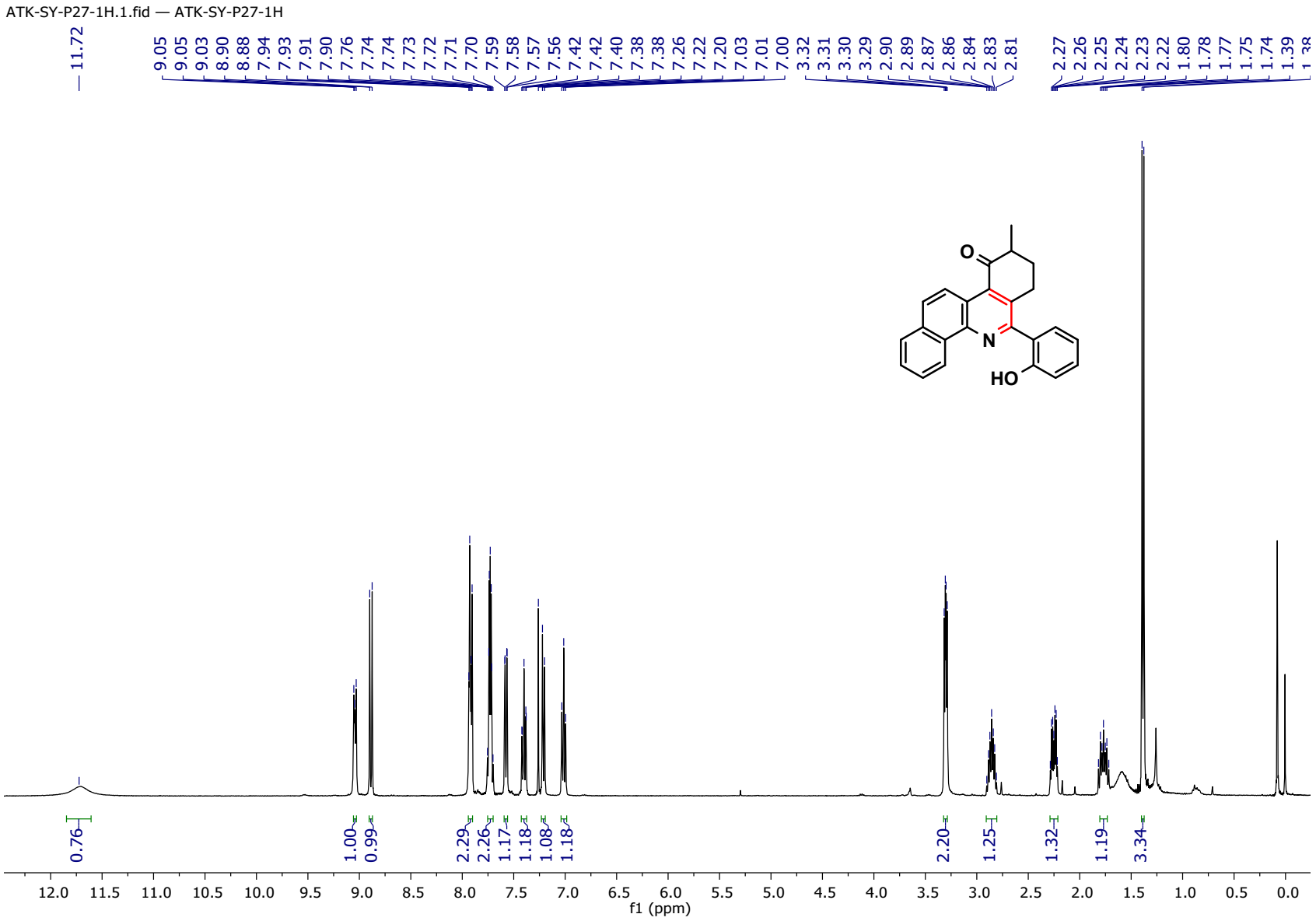


HRMS Spectrum of Compound 4r

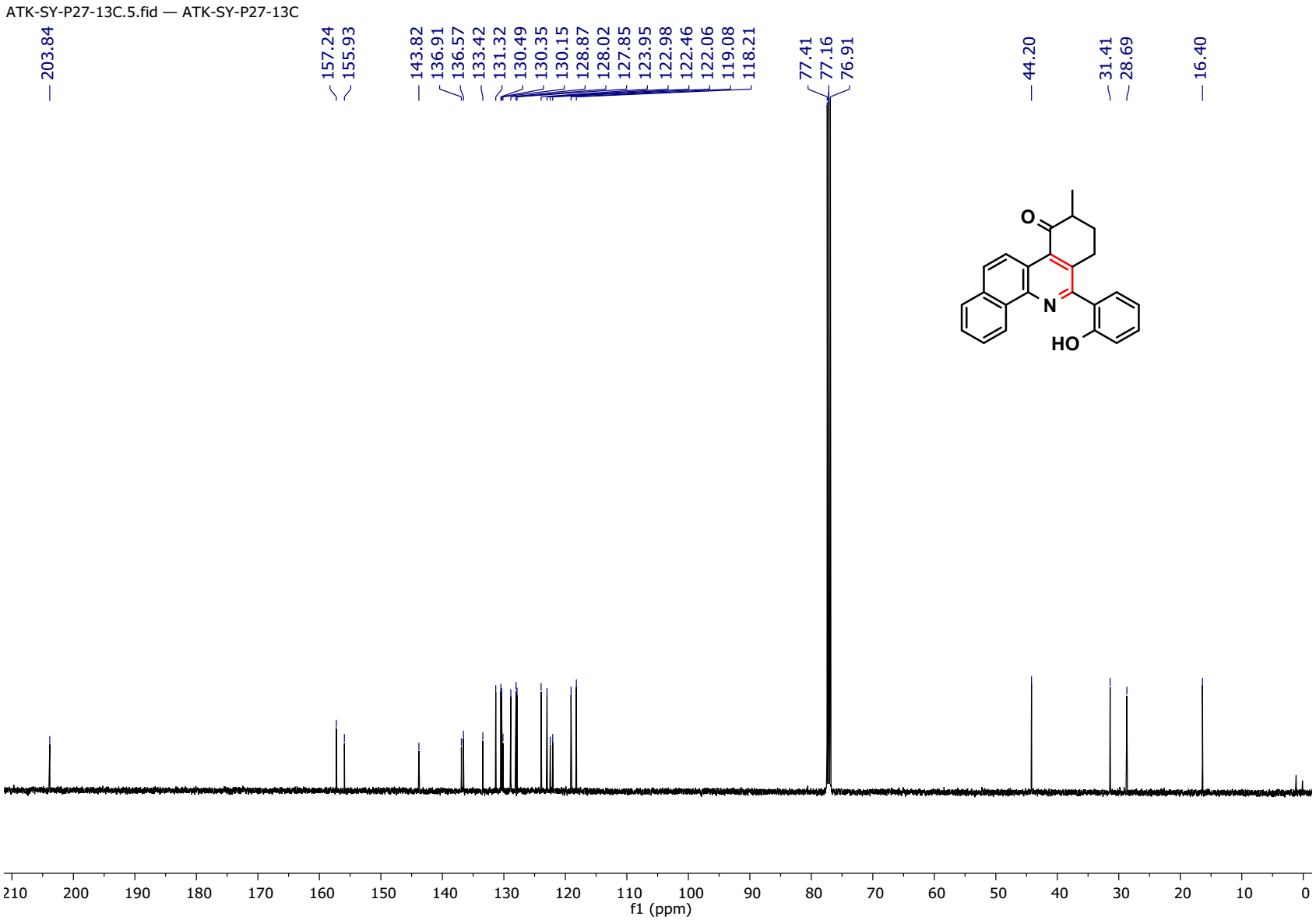
Sample Name	161120	**Position**	P1-C3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-161120.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	03-12-2020 12:23:48 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4s

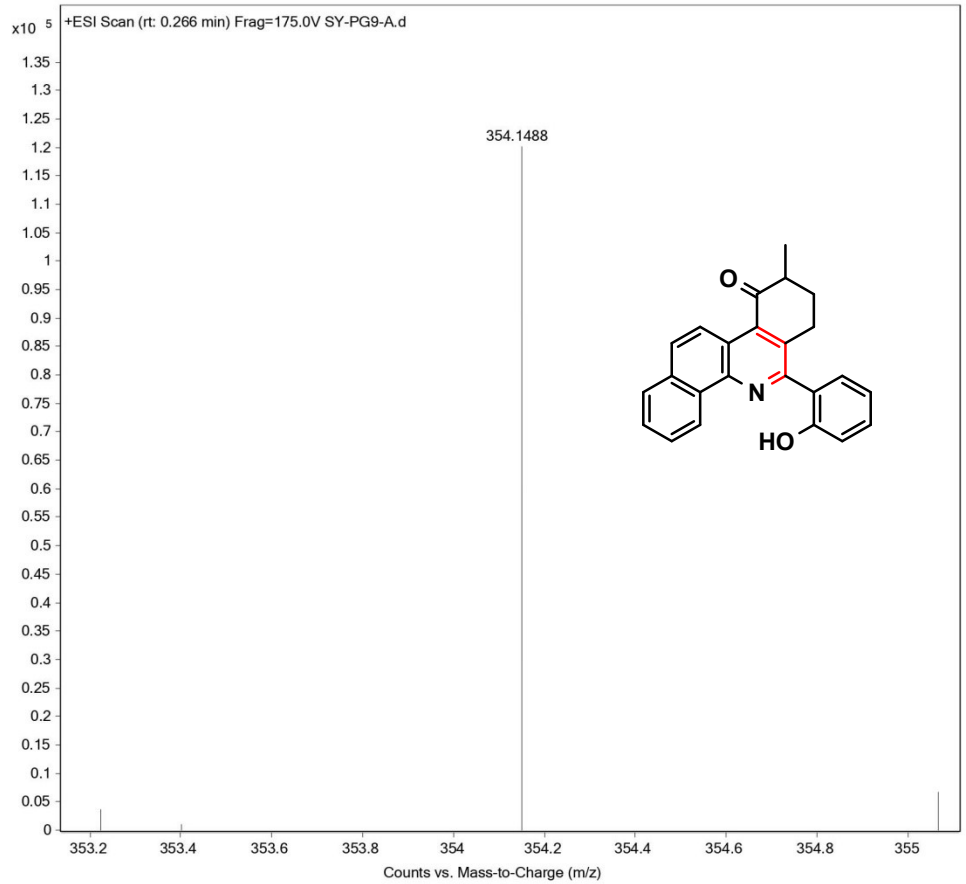


^{13}C NMR Spectrum of Compound 4s

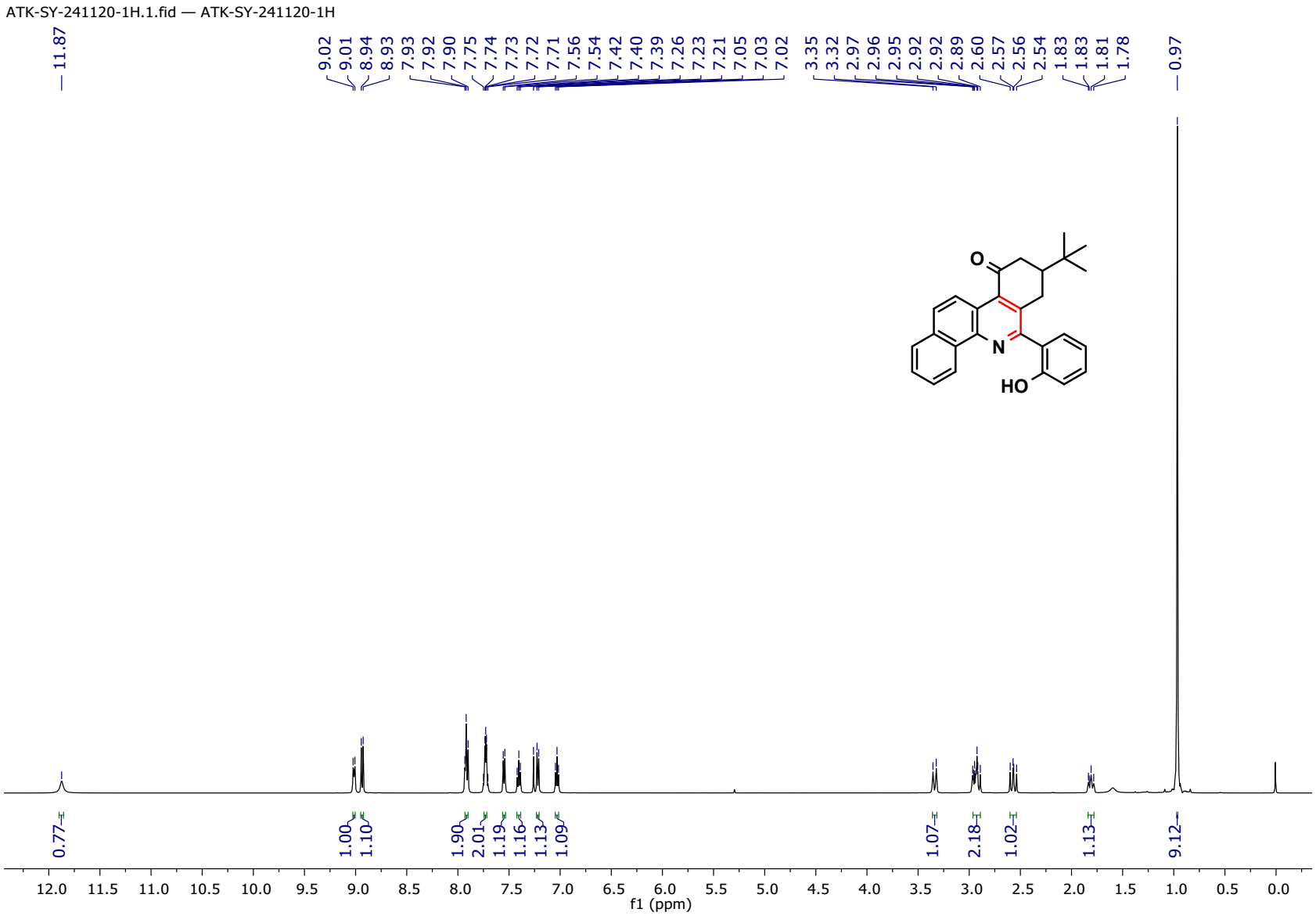


HRMS Spectrum of Compound 4s

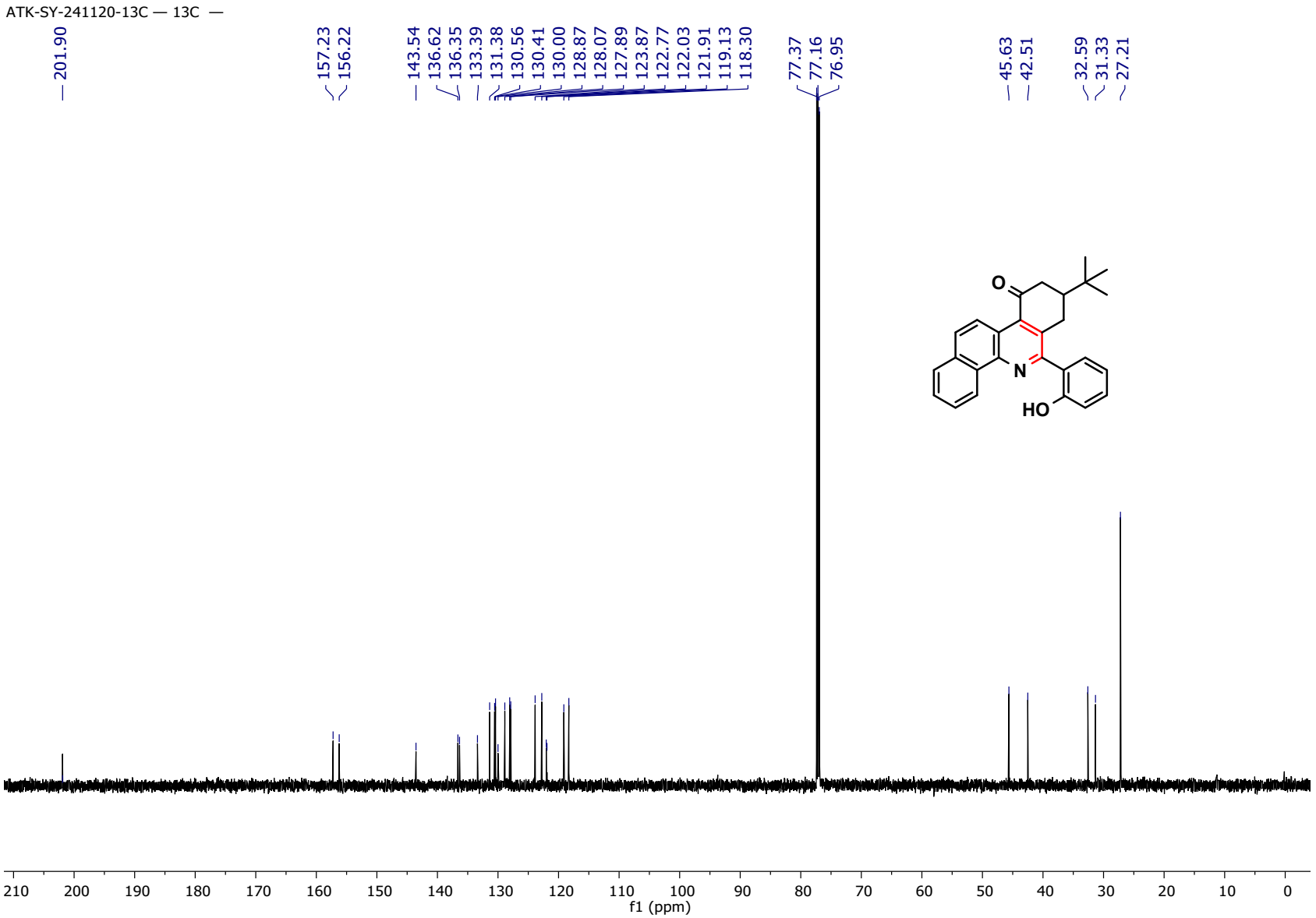
Sample Name	WASH	**Position**	P2-A4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-PG9-A.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	31-Aug-21 05:53:06 PM (UTC+05:30)



^{1}H NMR Spectrum of Compound 4t

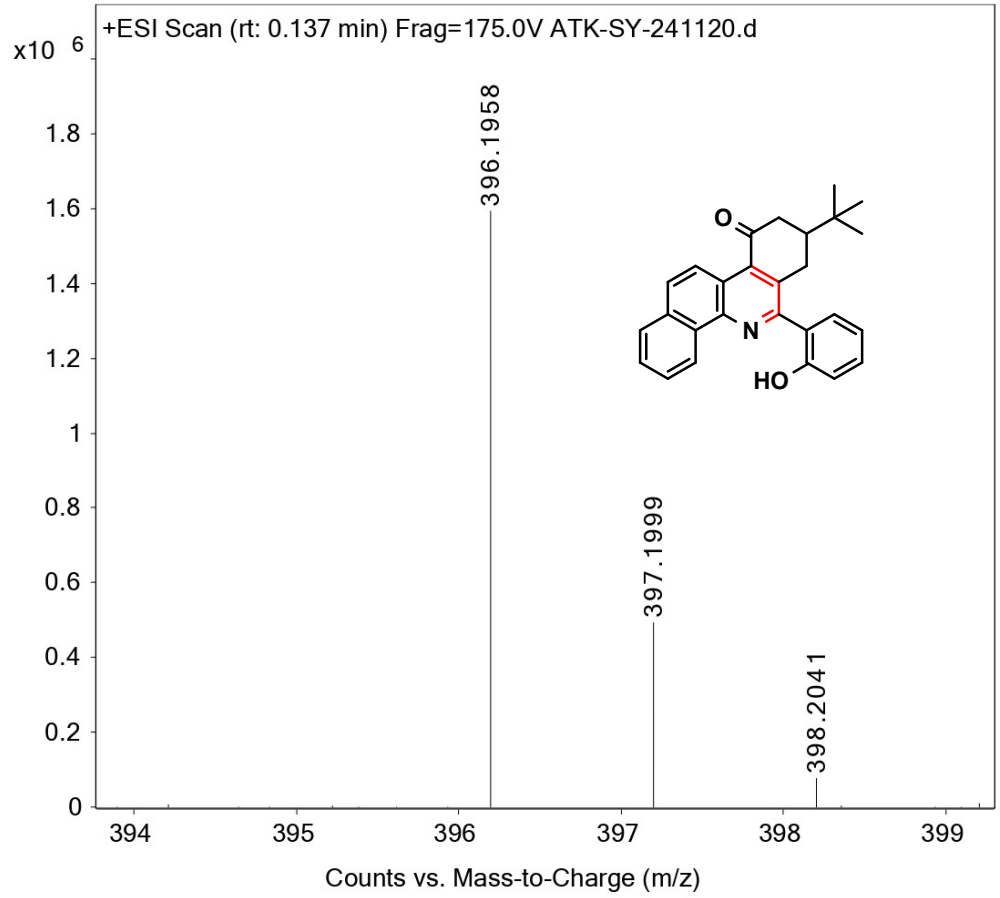


^{13}C NMR Spectrum of Compound 4t

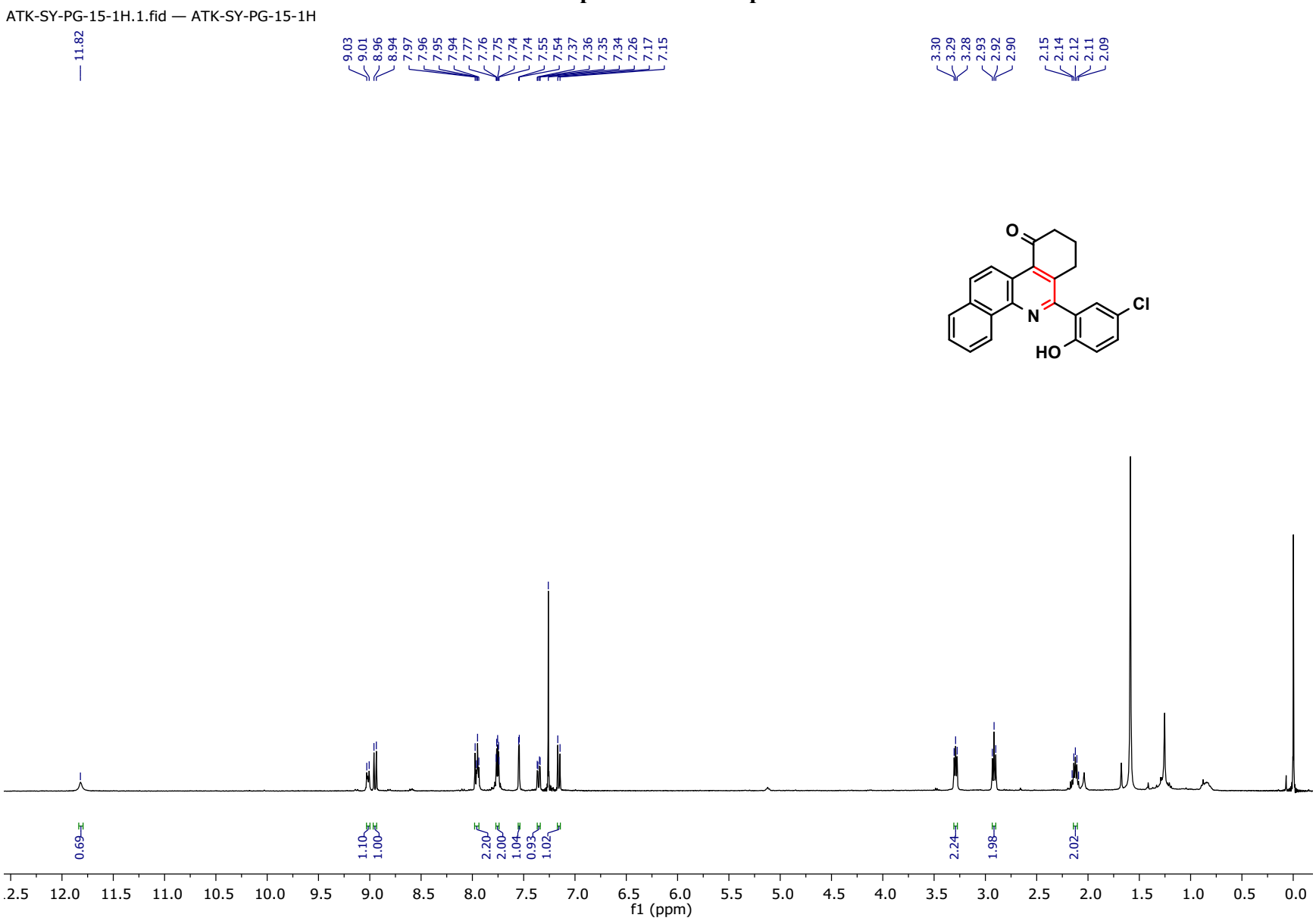


HRMS Spectrum of Compound 4t

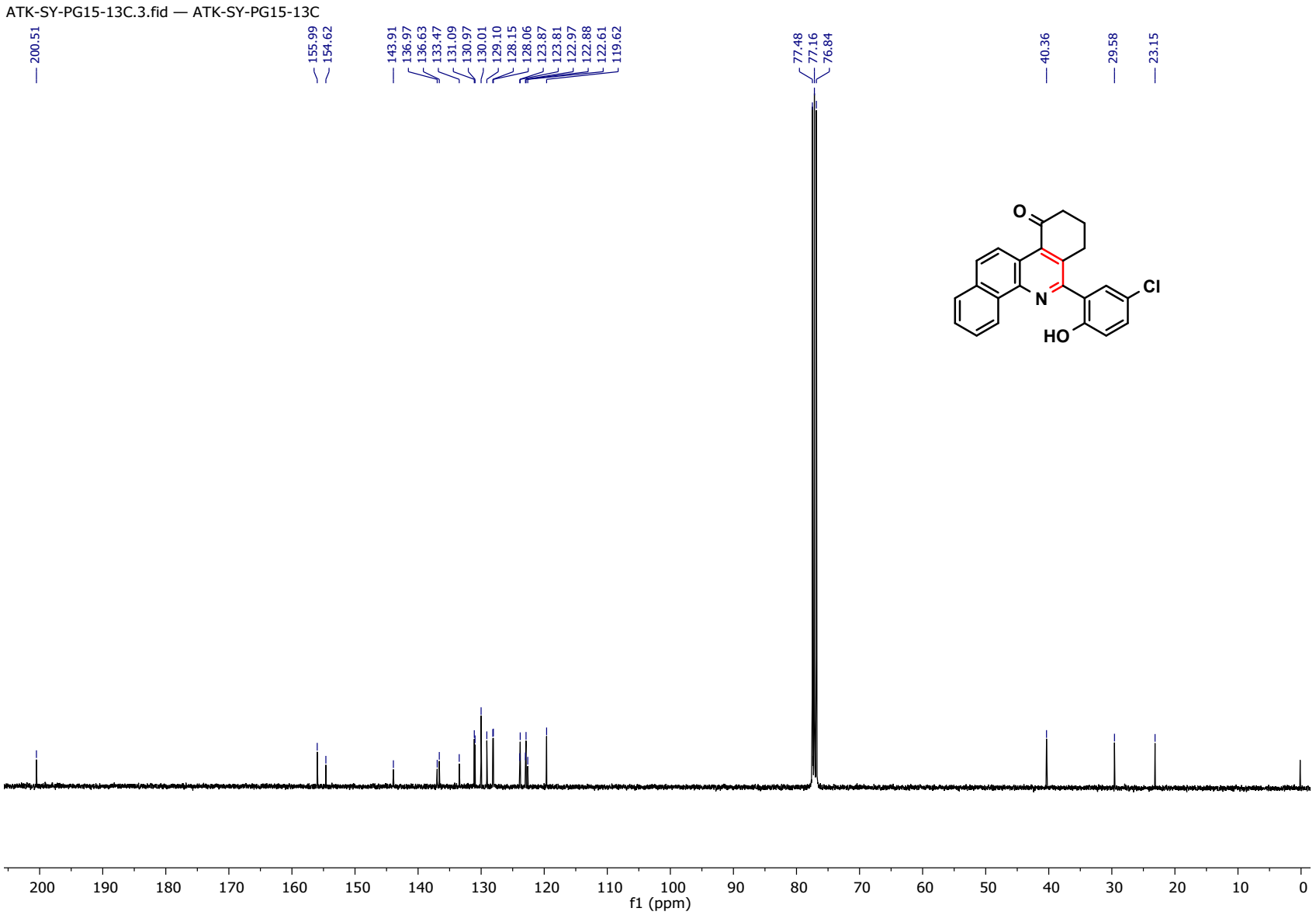
Sample Name	ATK-SY-261120	**Position**	P1-C2	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-241120.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	03-12-2020 12:19:52 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4u

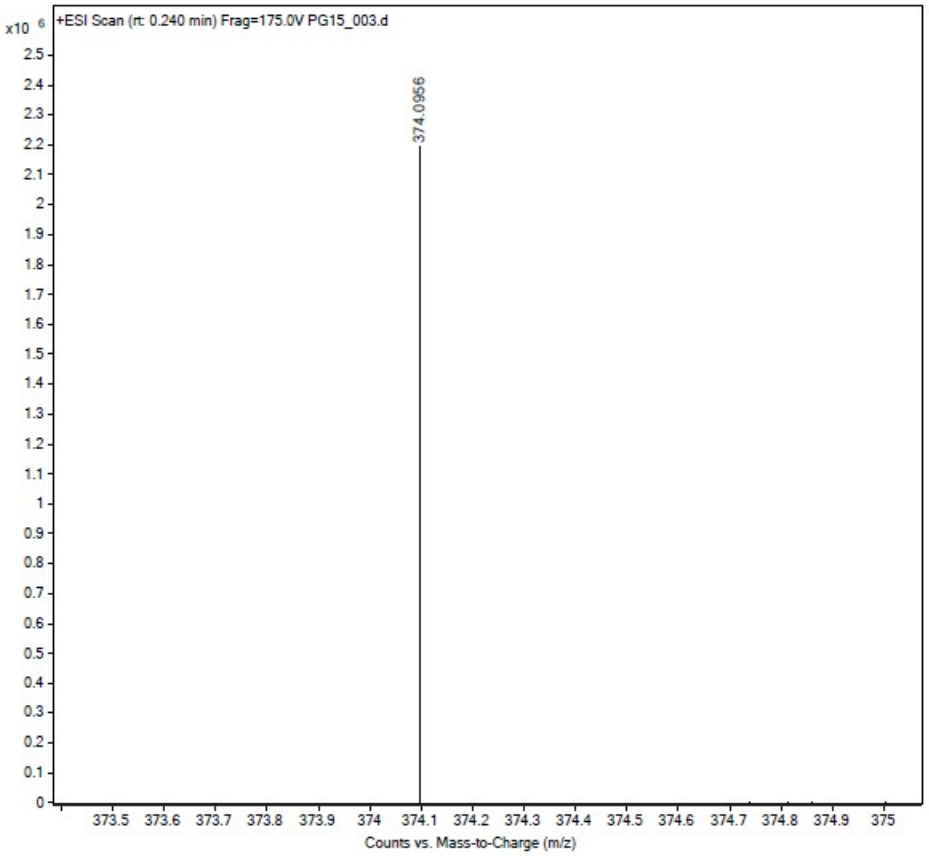


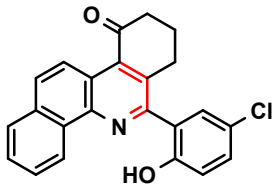
^{13}C NMR Spectrum of Compound 4u



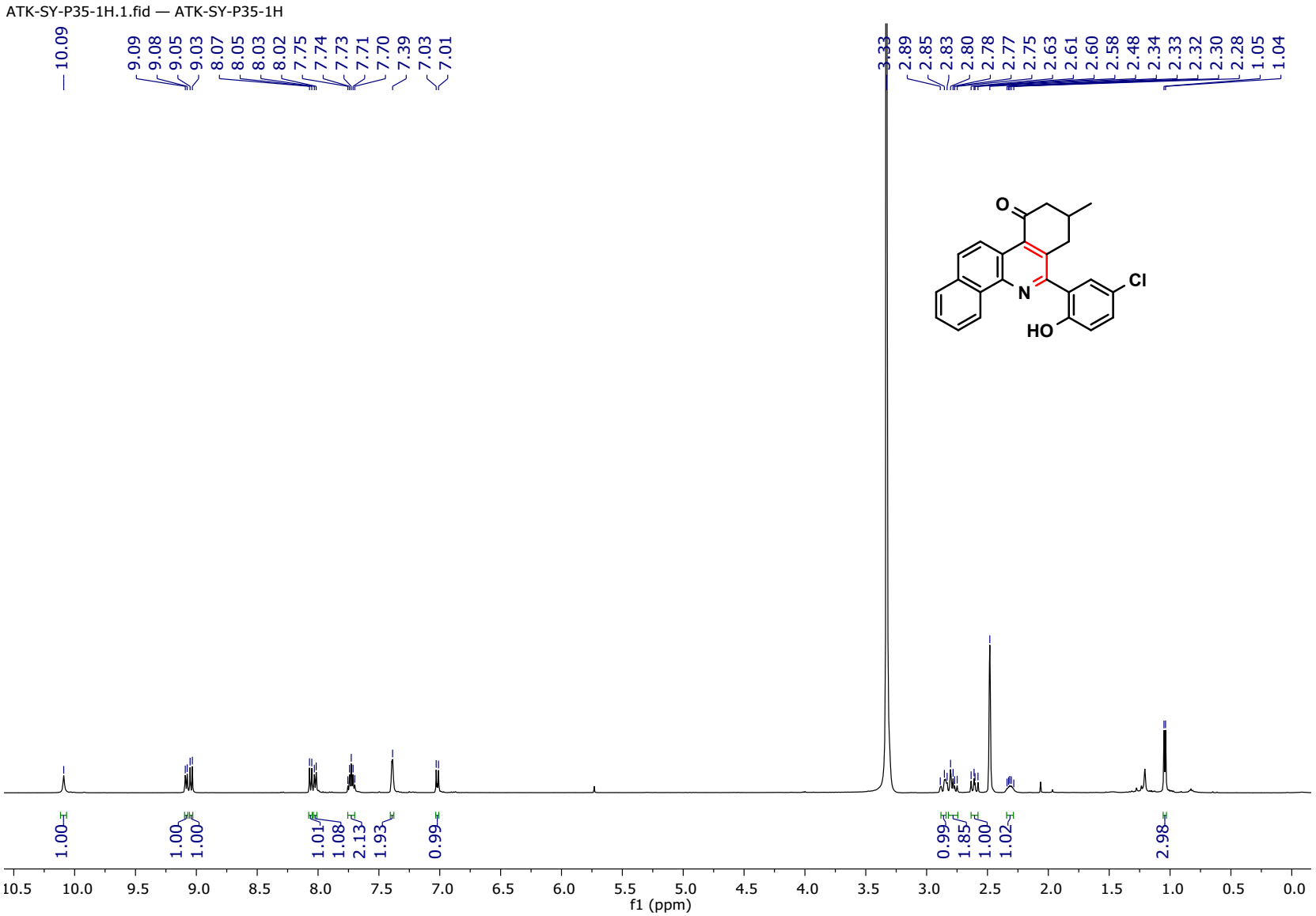
^{1}H NMR Spectrum of Compound 4u

Sample Name	PG15	**Position**	P1-A3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	PG15_003.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	18-Aug-22 12:14:03 PM (UTC+05:30)

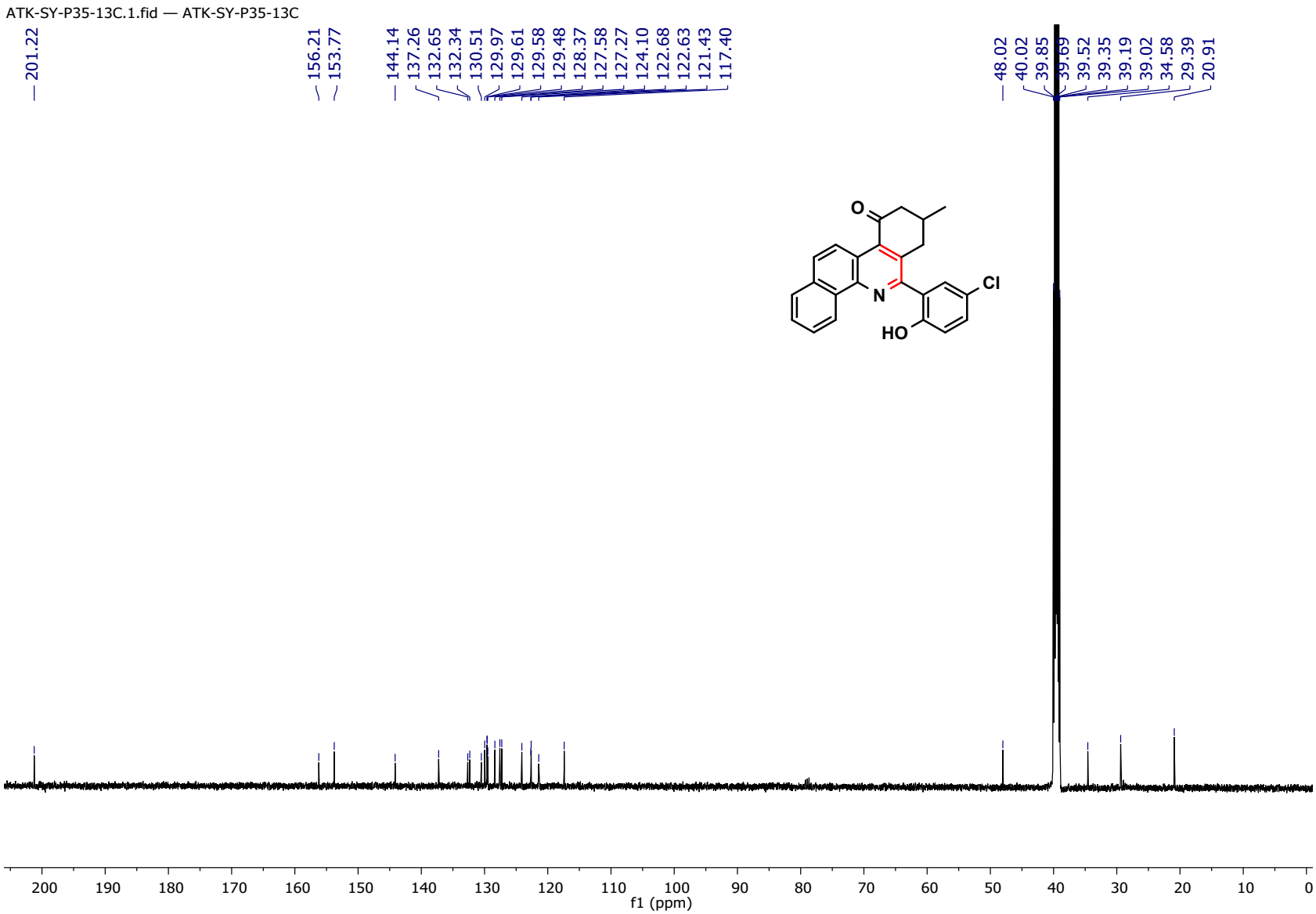




^{1}H NMR Spectrum of Compound 4v

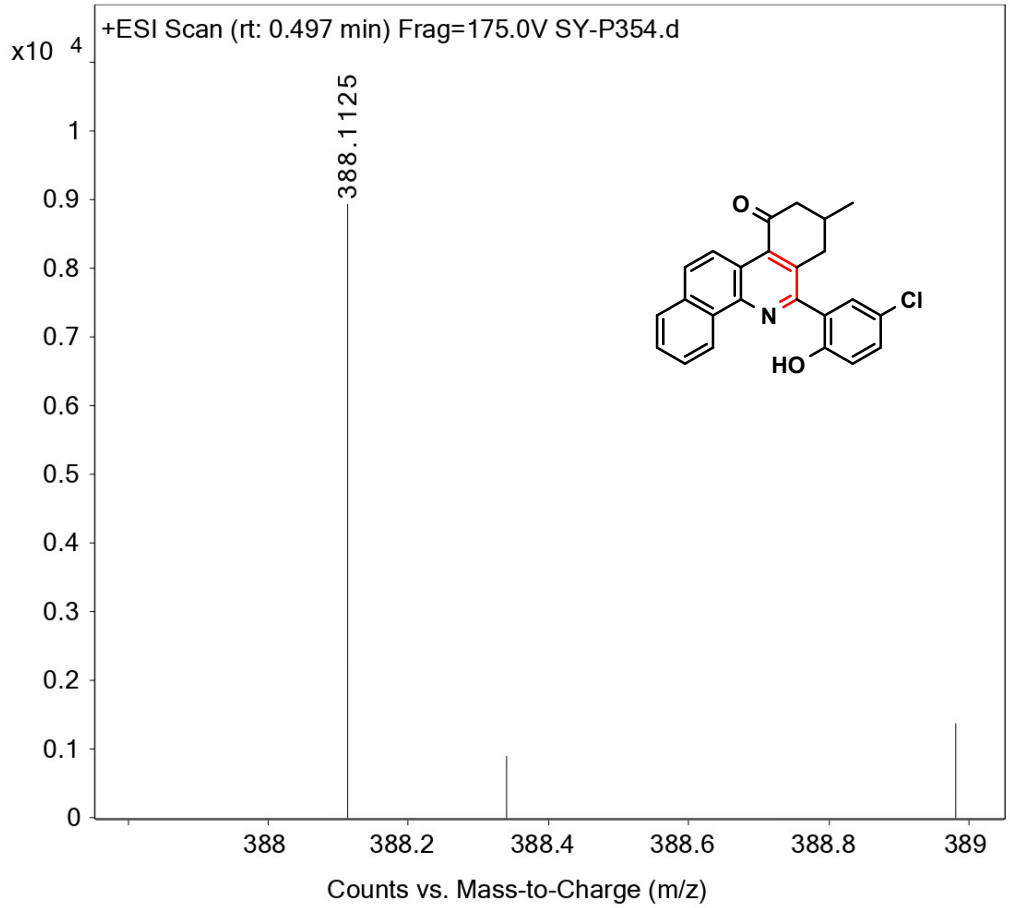


^{13}C NMR Spectrum of Compound 4v

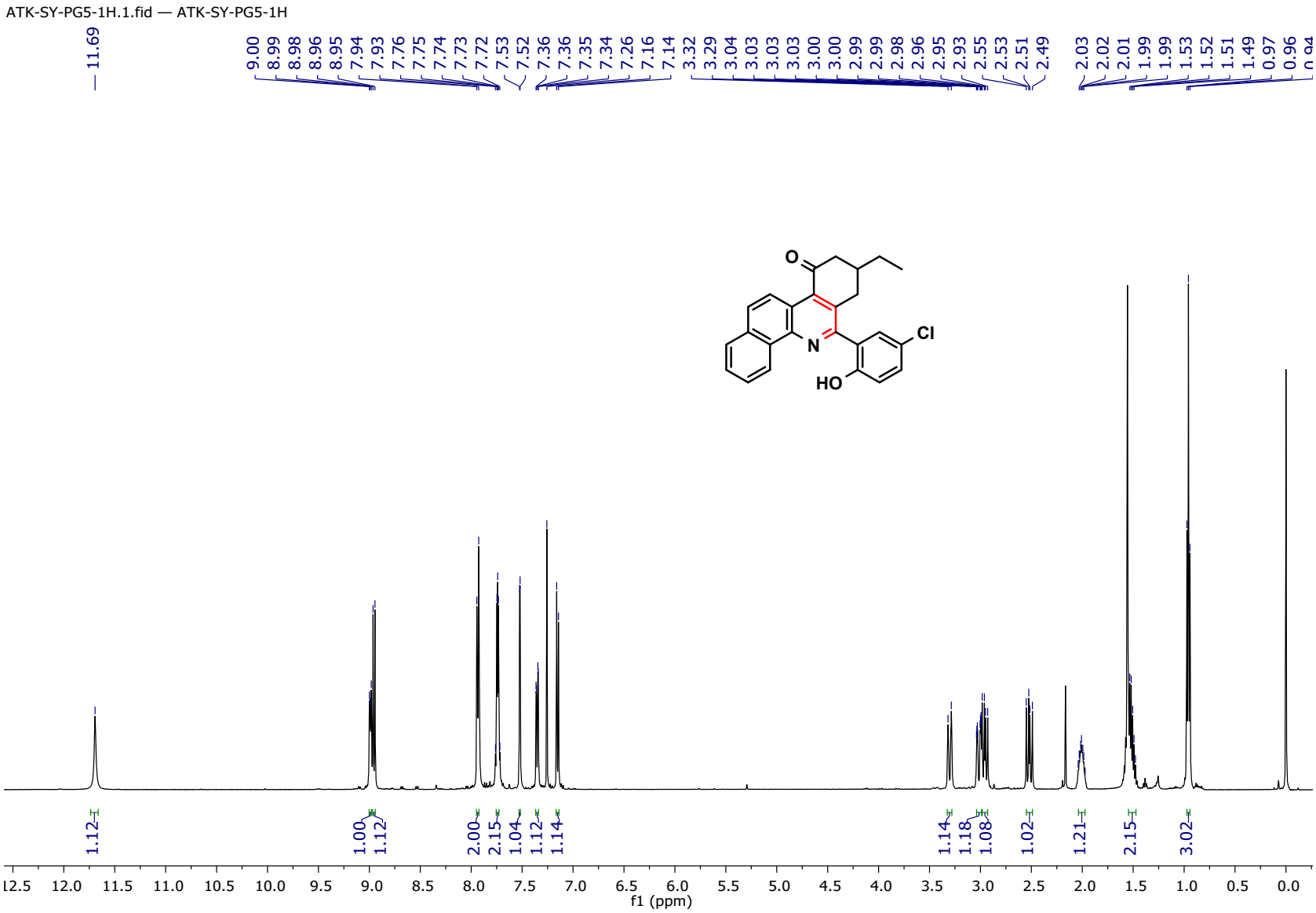


HRMS Spectrum of Compound 4v

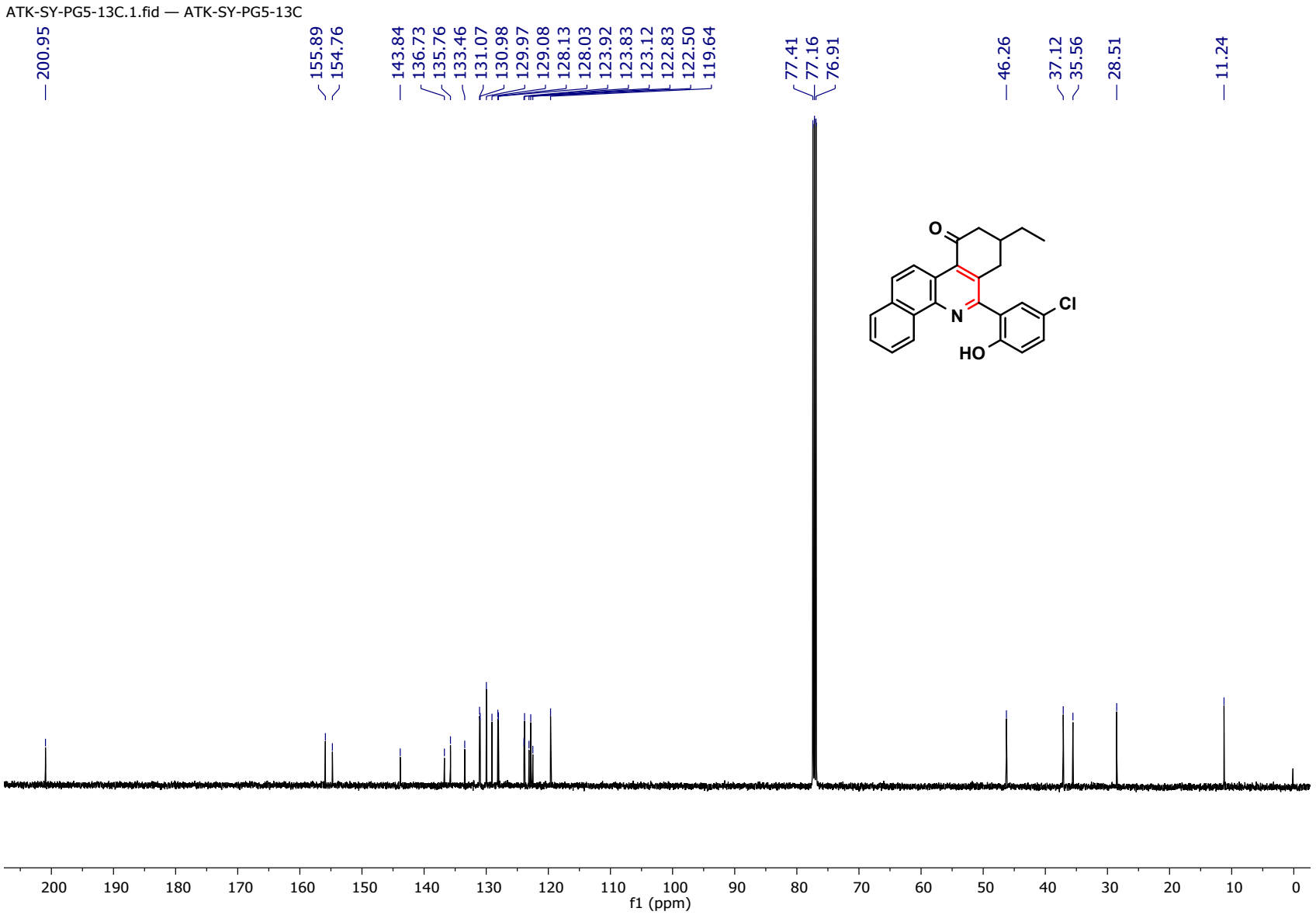
Sample Name	SAMPLE	**Position**	P1-C7	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P354.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	11-02-2021 12:52:03 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4w



^{13}C NMR Spectrum of Compound 4w



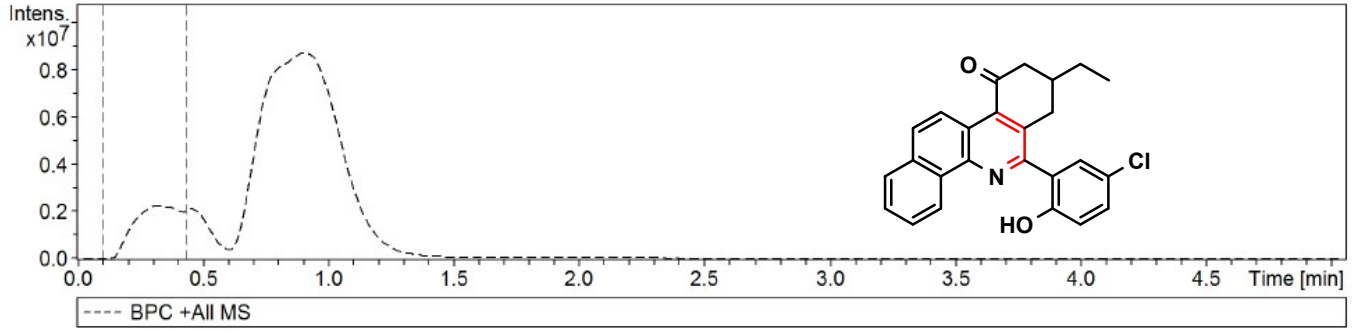
HRMS Spectrum of Compound 4w

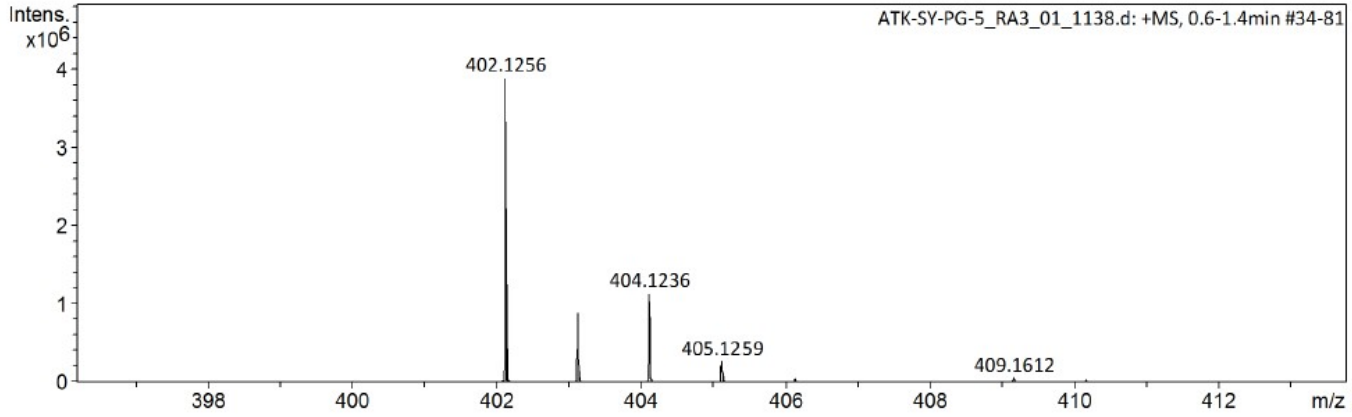
Analysis Info

Acquisition Date	11/2/2021 7:46:59 AM		
Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\30.10.2021\ATK-SY-PG-5_RA3_01_1138.d		
Method	low mass bruker.m	Operator	vidhi
Sample Name	ATK-SY-PG-5	Instrument	impact HD 1819696.00197
Comment			

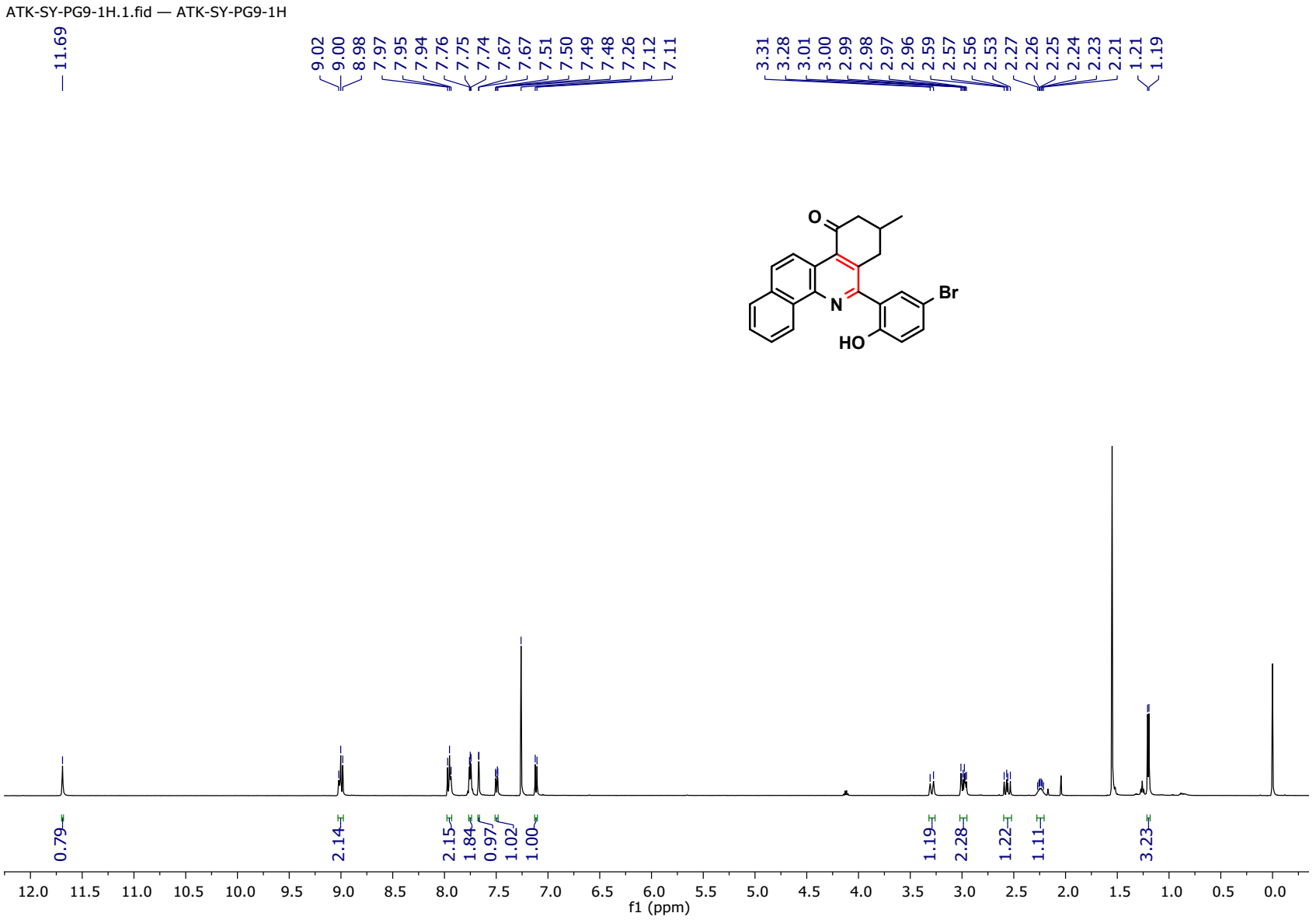
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

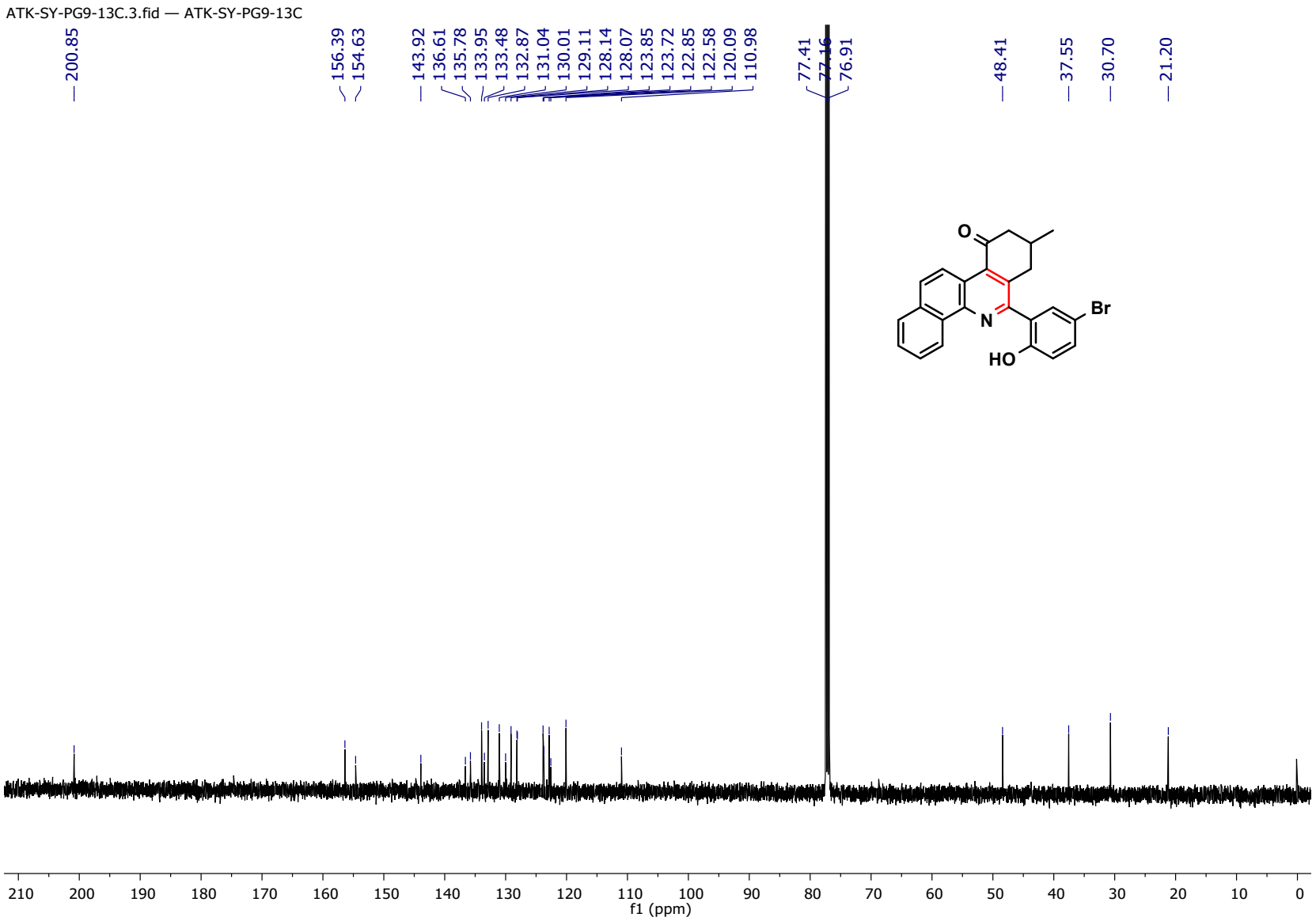




^{1}H NMR Spectrum of Compound 4x

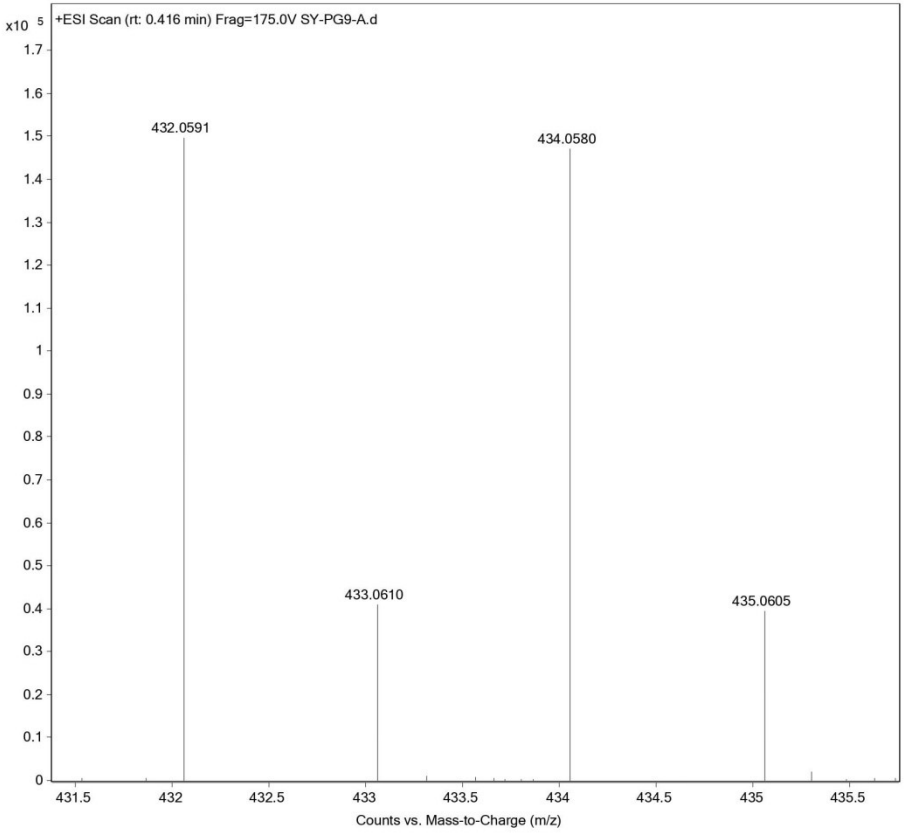


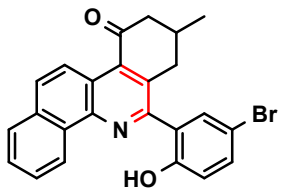
^{13}C NMR Spectrum of Compound 4x



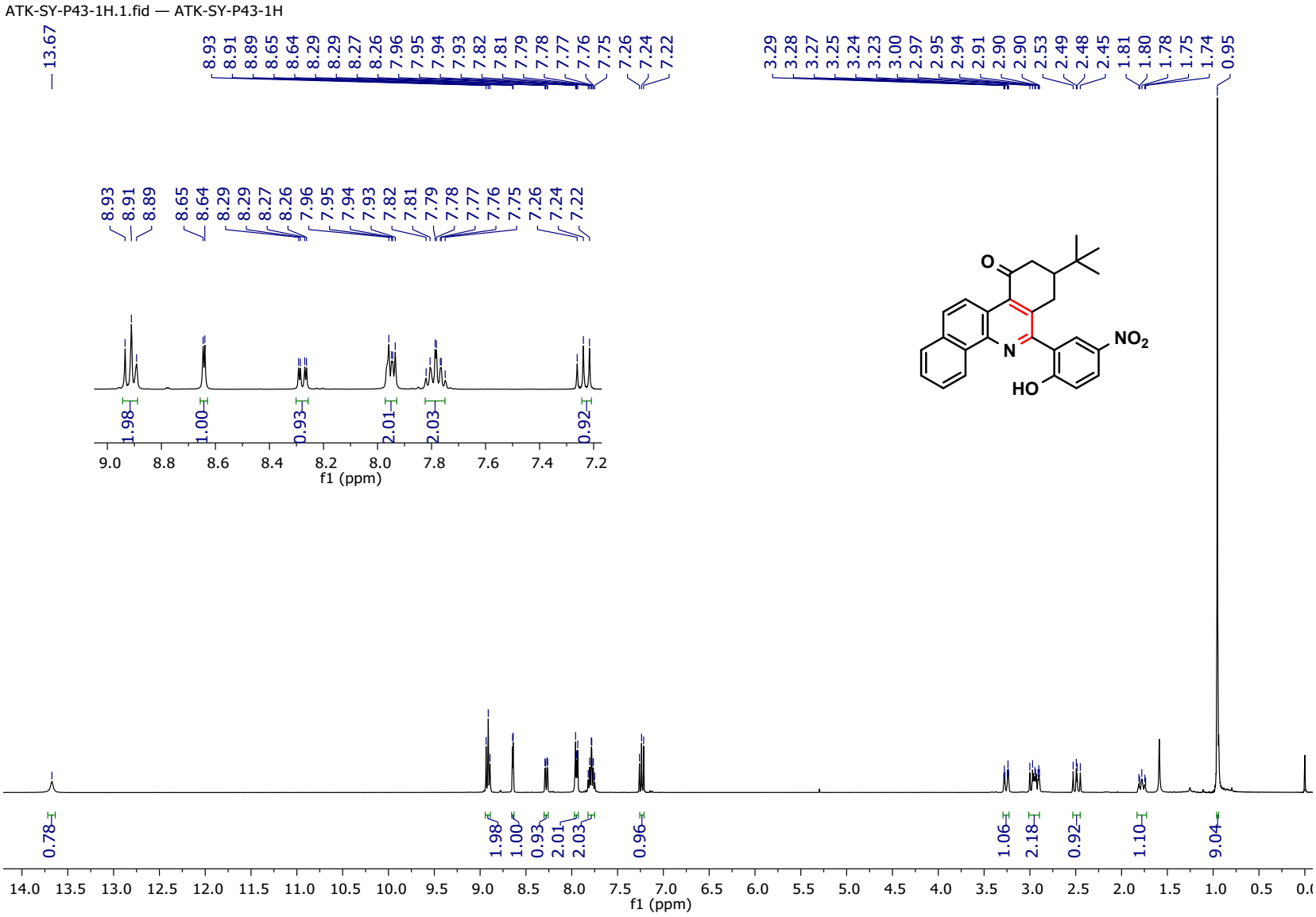
HRMS Spectrum of Compound 4x

Sample Name	WASH	**Position**	P2-A4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-PG9-A.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	31-Aug-21 05:53:06 PM (UTC+05:30)

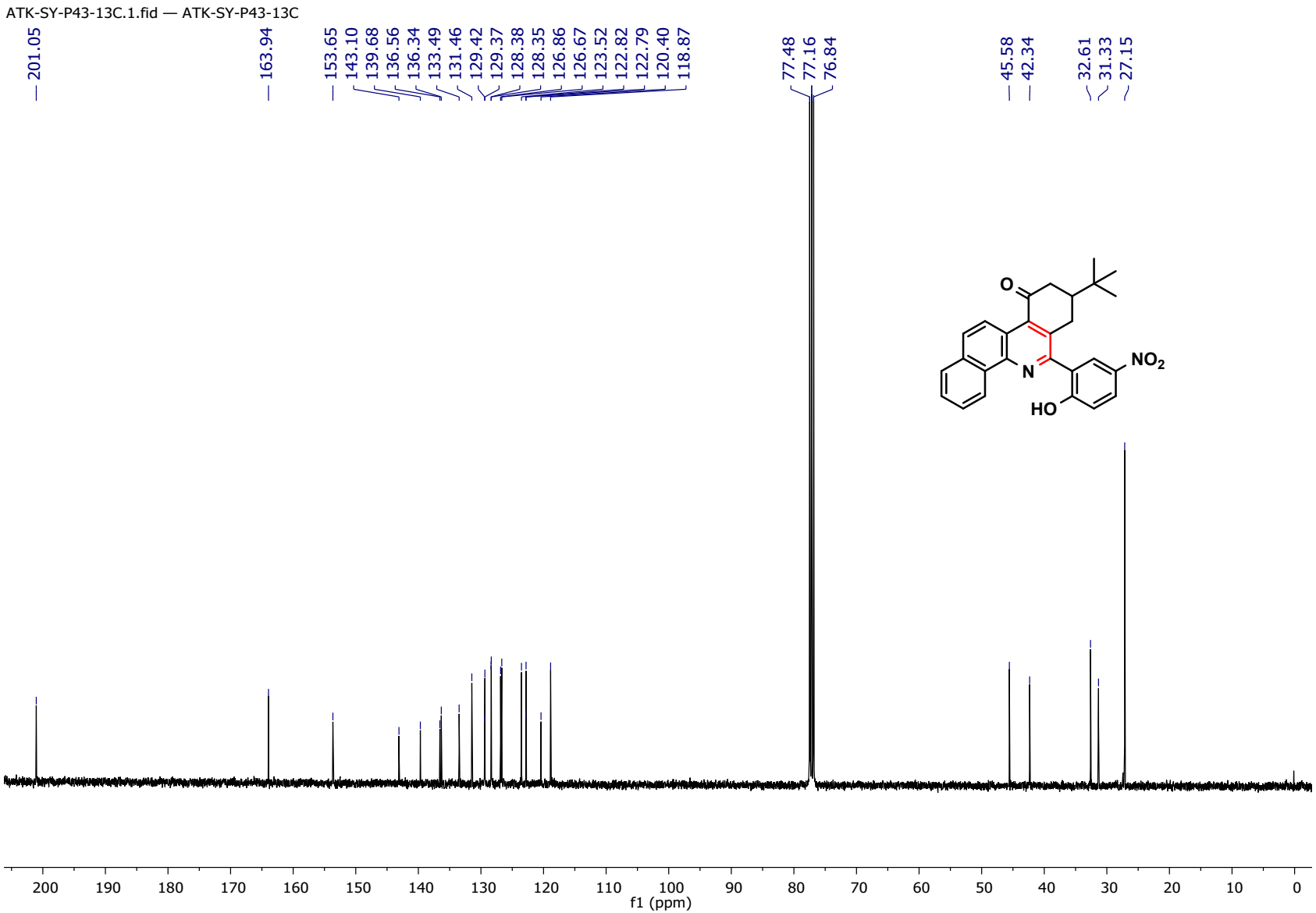




^{1}H NMR Spectrum of Compound 4y

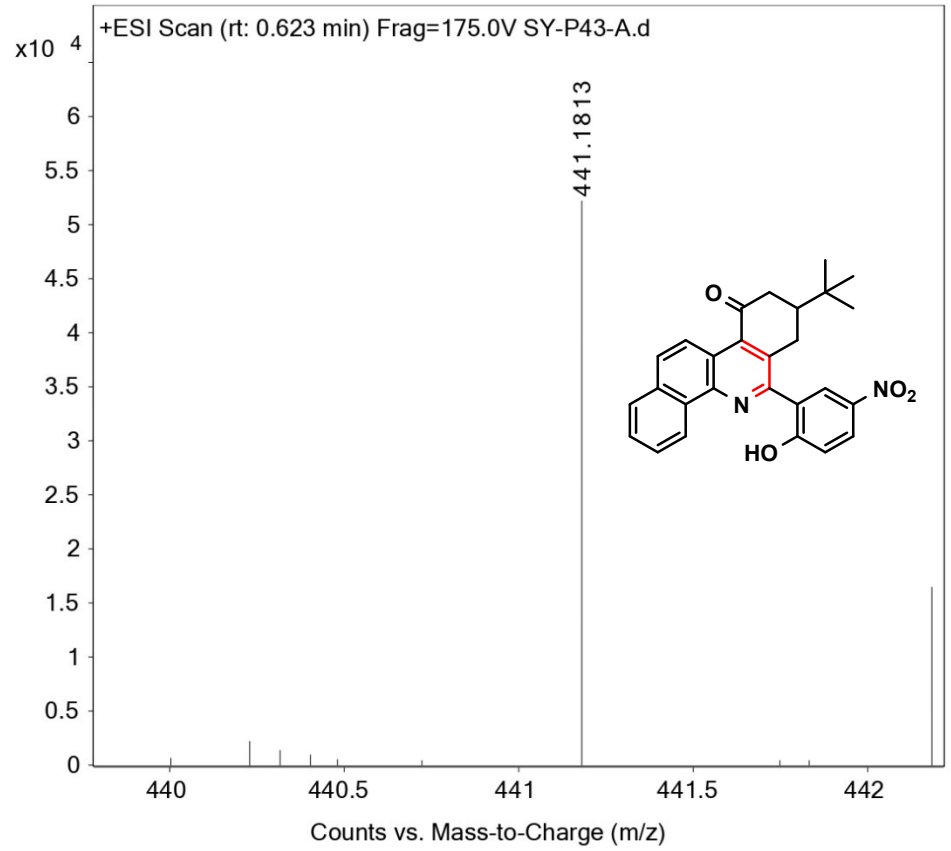


^{13}C NMR Spectrum of Compound 4y

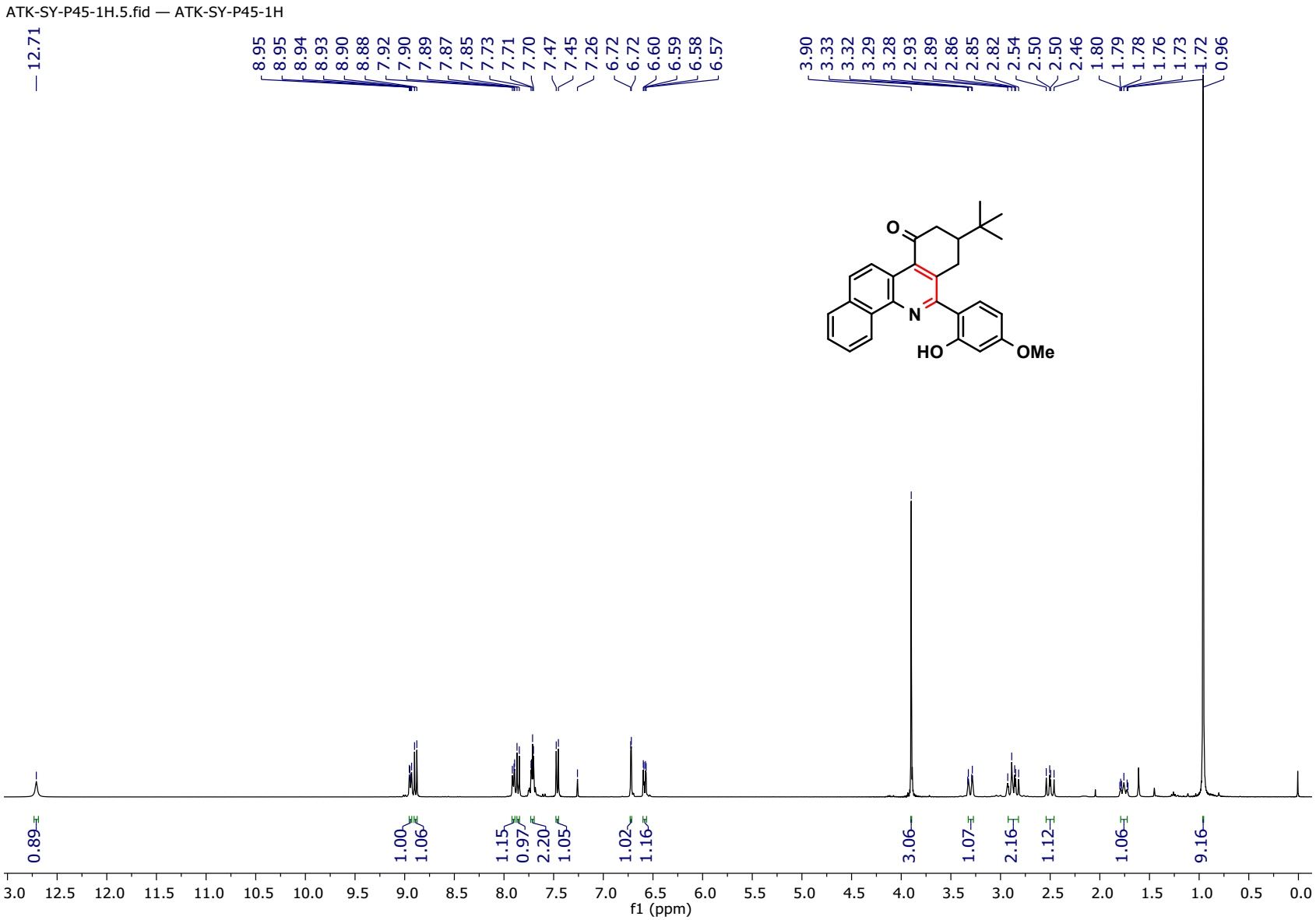


HRMS Spectrum of Compound 4y

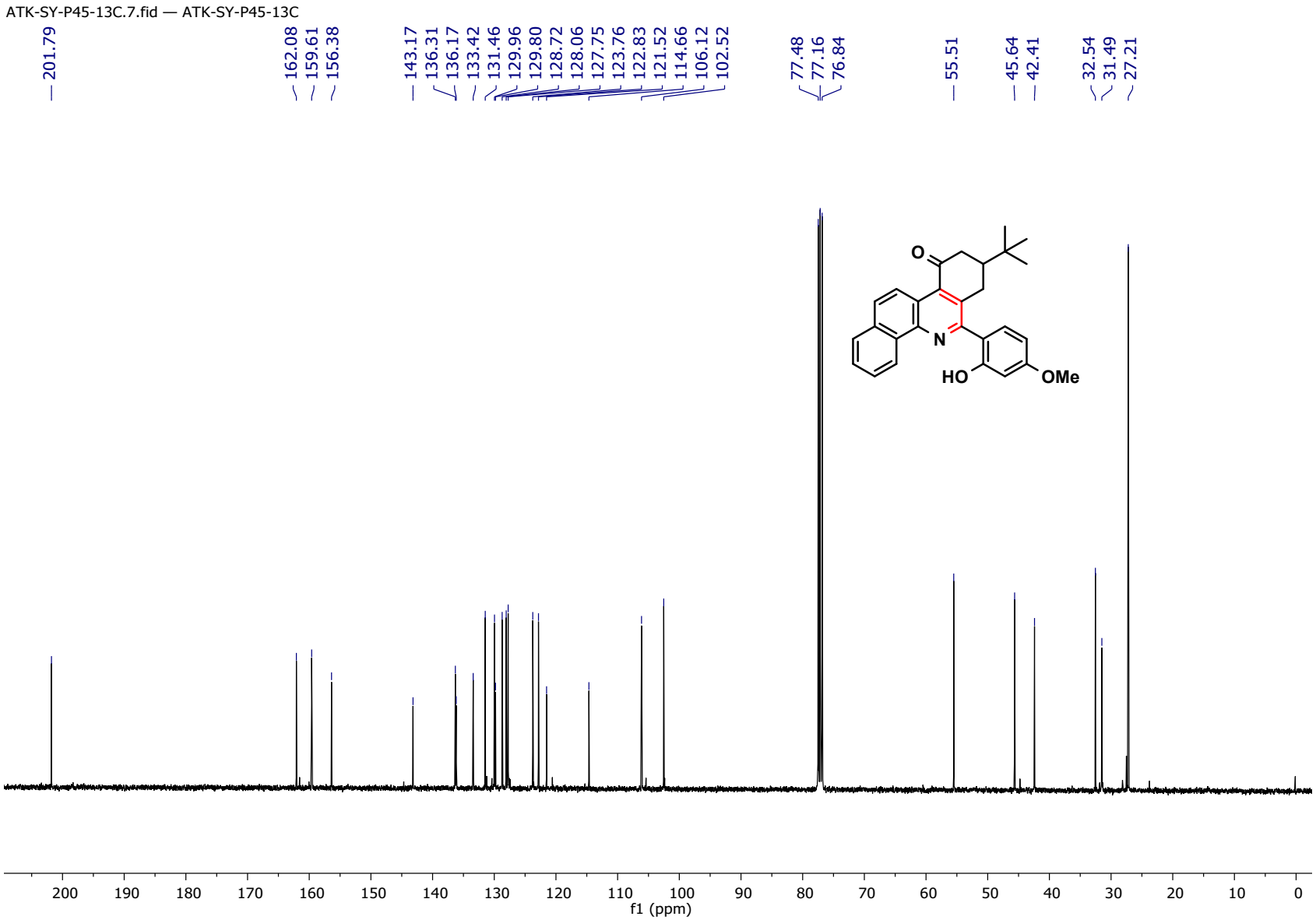
Sample Name	SAMPLE 17	**Position**	P2-B8	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P43-A.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	31-03-2021 20:34:37 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4z

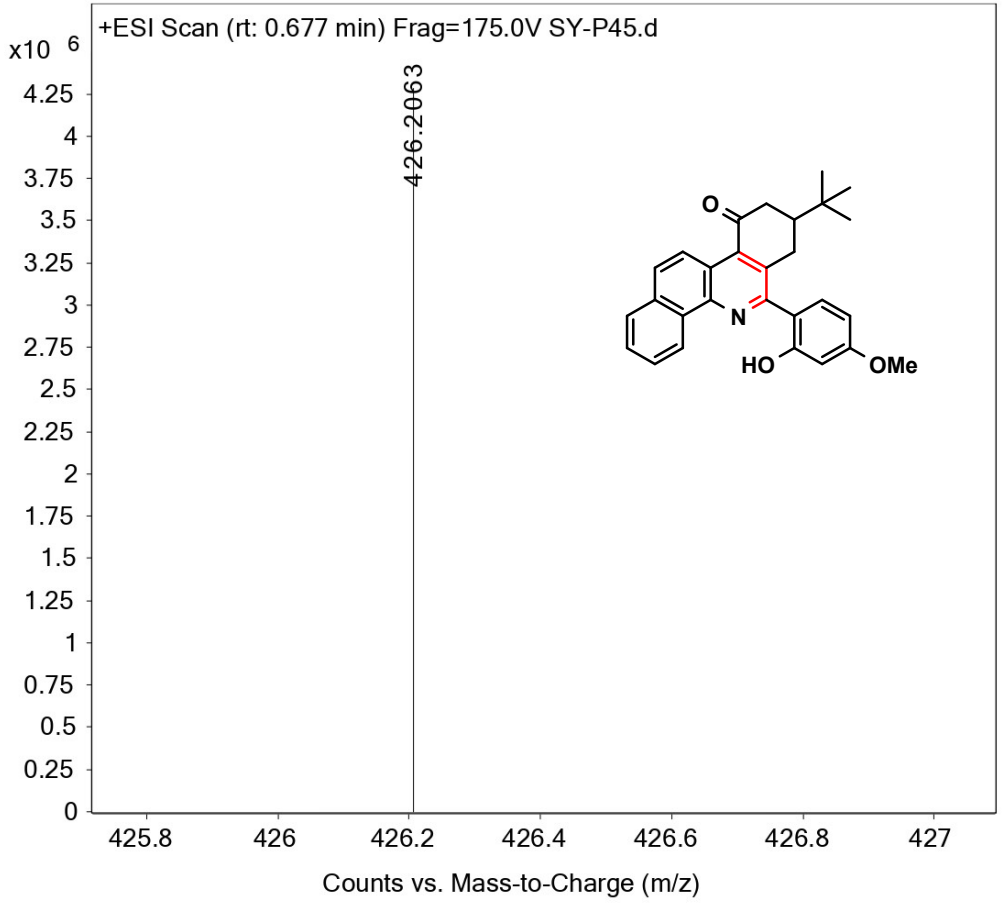


^{13}C NMR Spectrum of Compound 4z

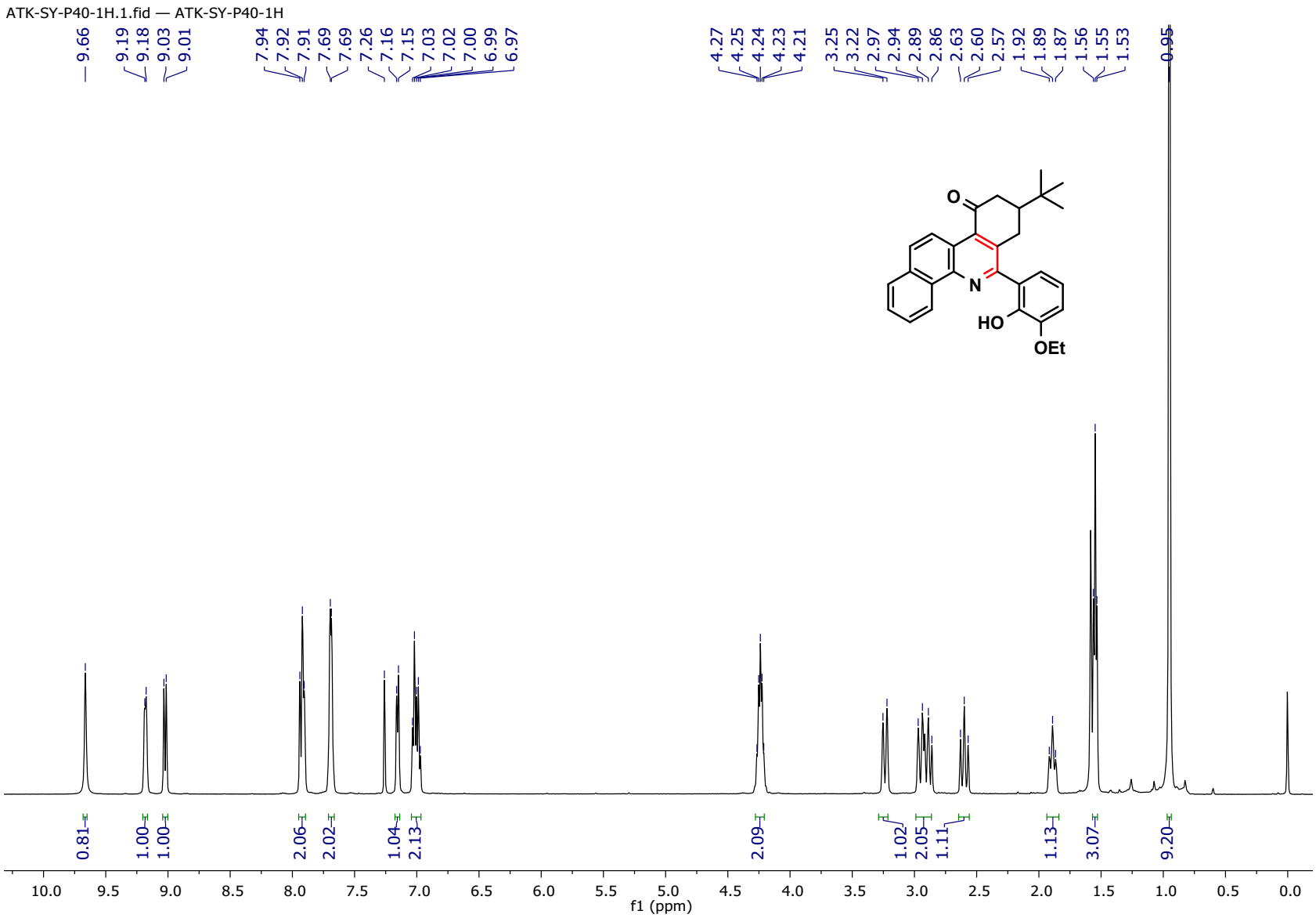


HRMS Spectrum of Compound 4z

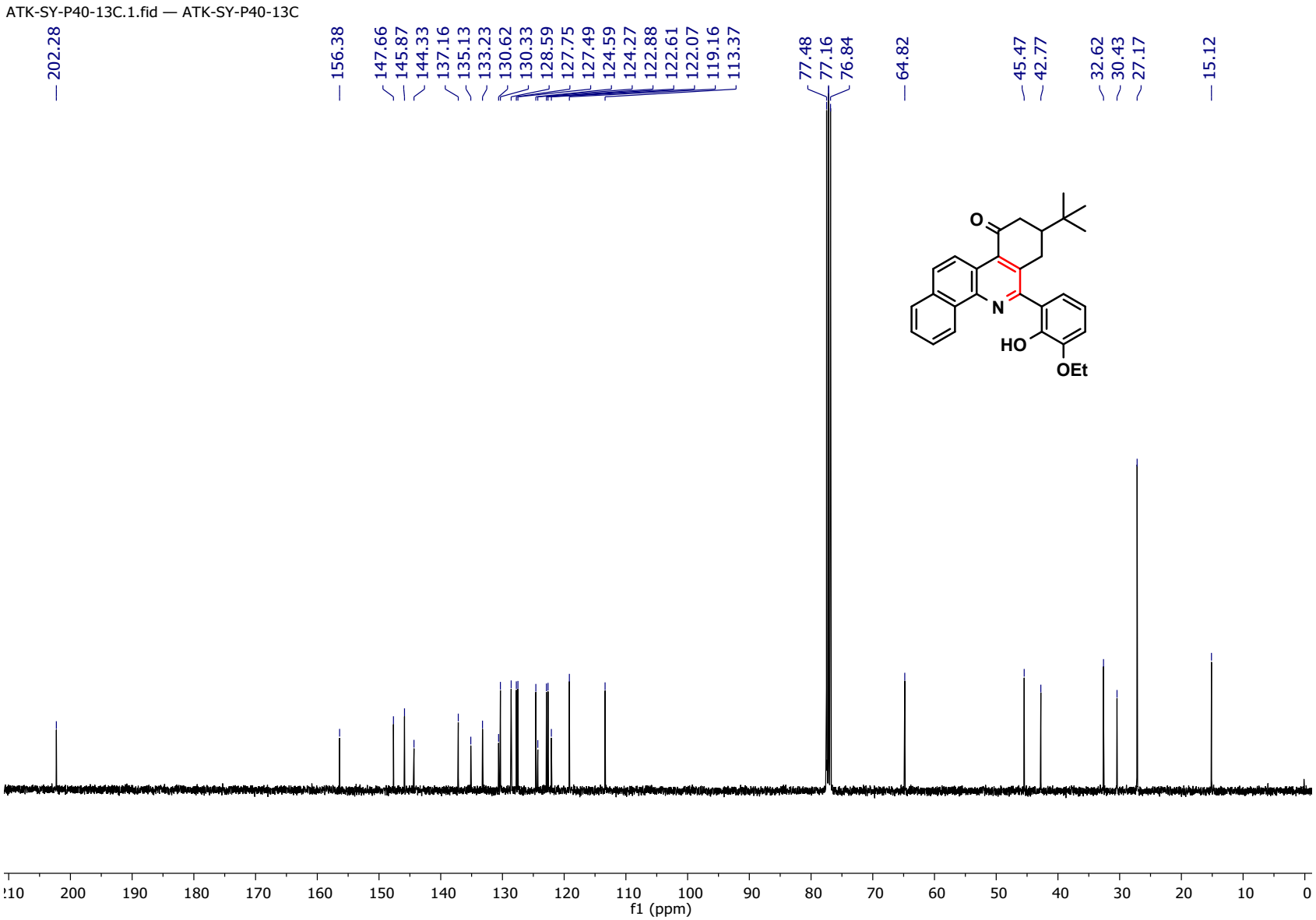
Sample Name	SAMPLE	**Position**	P1-D3	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P45.d
ACQ Method	ESI ALS 100-1000.m	**Comment**		**Acquired Time**	27-02-2021 00:52:43 (UTC+05:30)



^{1}H NMR Spectrum of Compound 4aa

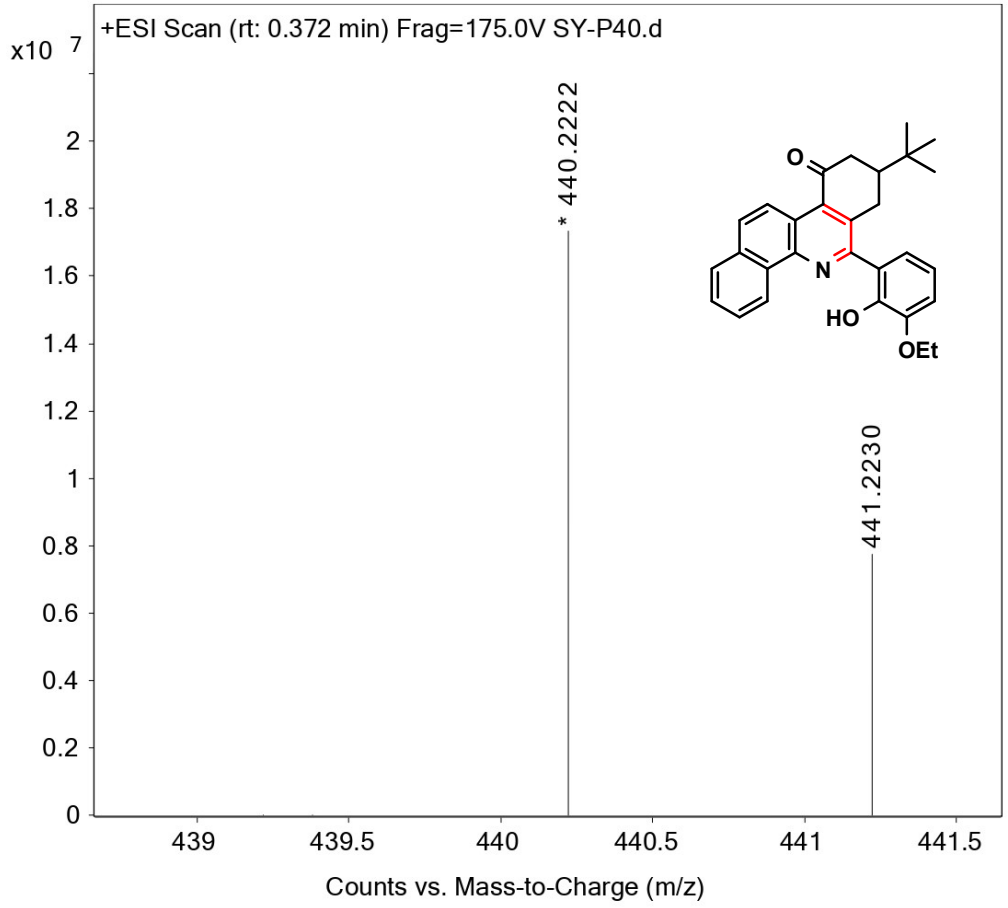


^{13}C NMR Spectrum of Compound 4aa

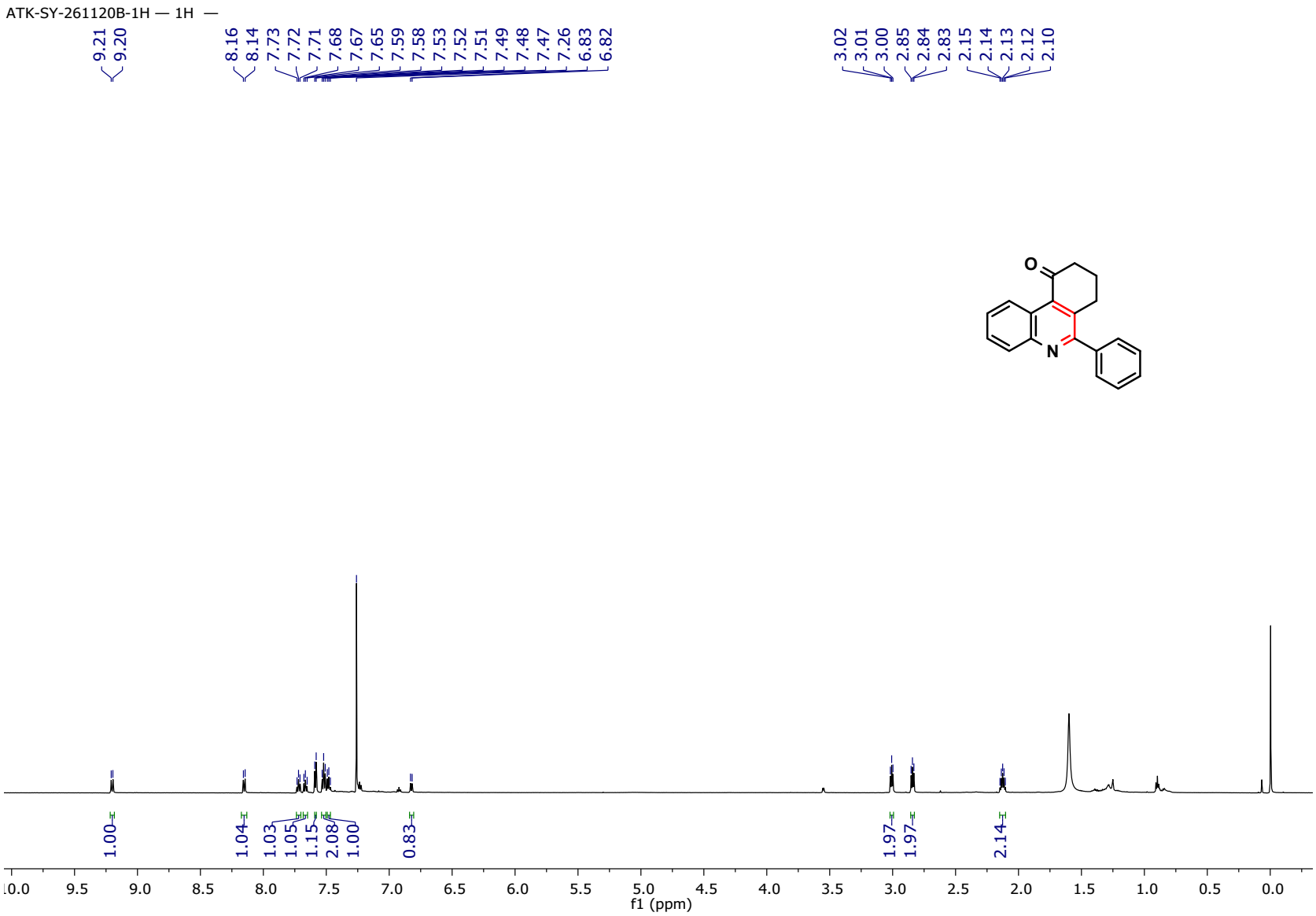


HRMS Spectrum of Compound 4aa

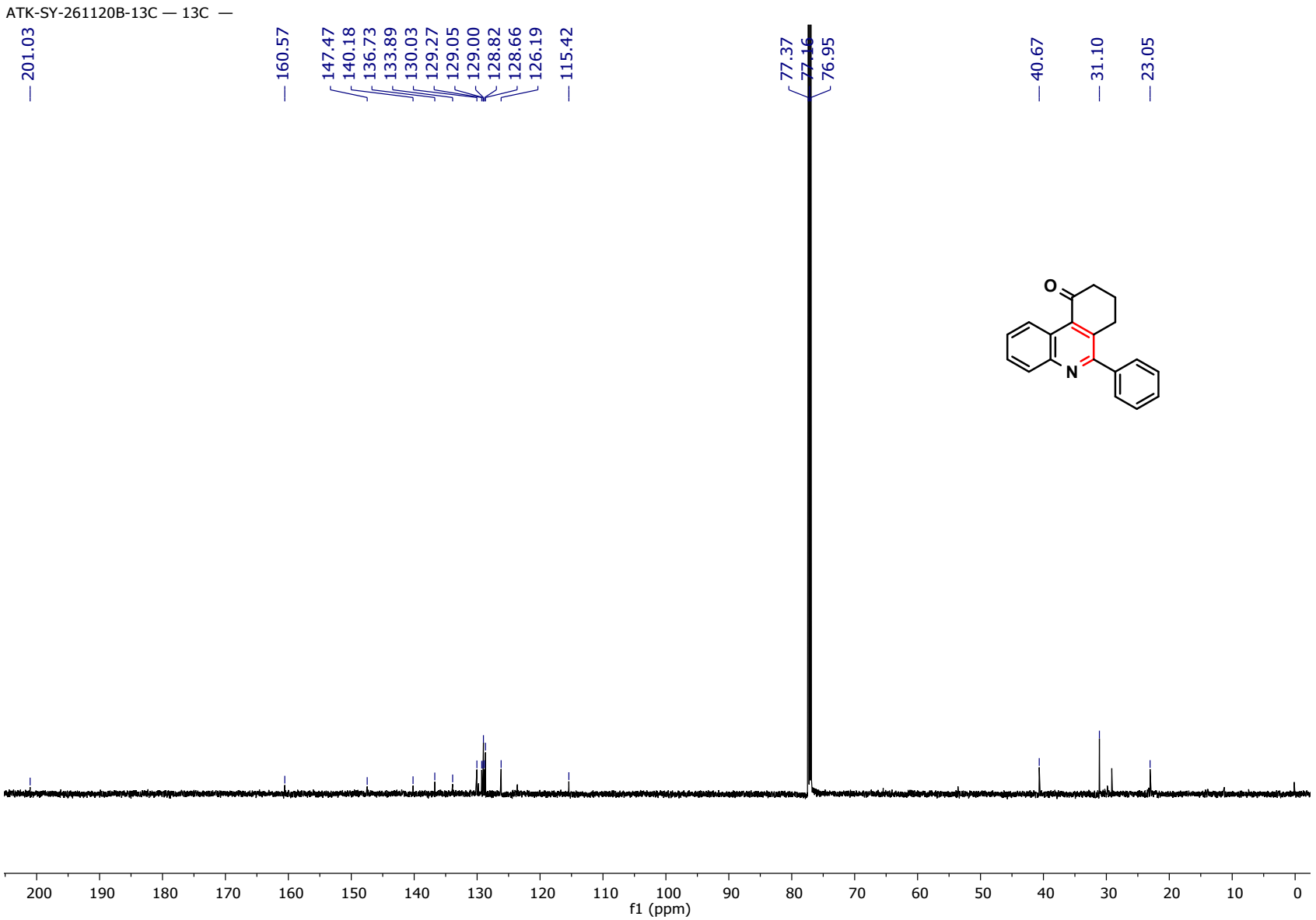
Sample Name	SAMPLE	**Position**	P1-E2	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P40.d
ACQ Method	ESI ALS 200-1000.m	**Comment**		**Acquired Time**	27-02-2021 02:45:59 (UTC+05:30)



^{1}H NMR Spectrum of Compound 6a

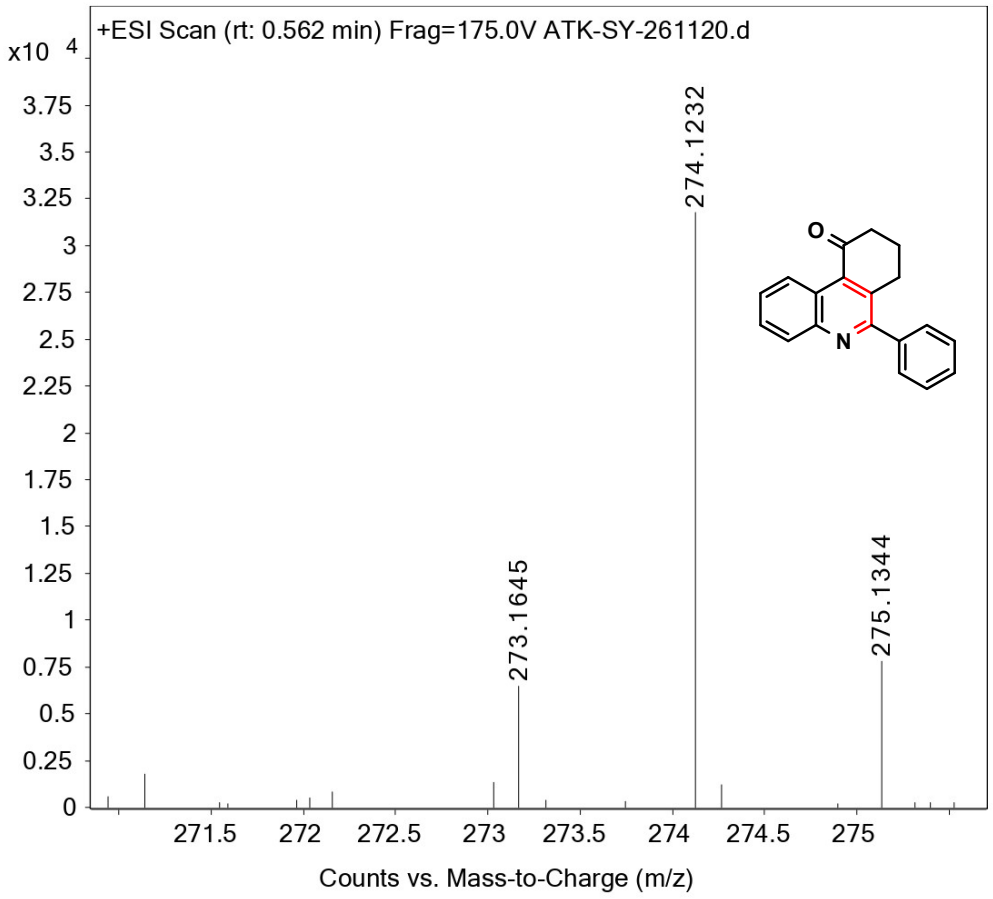


^{13}C NMR Spectrum of Compound 6a

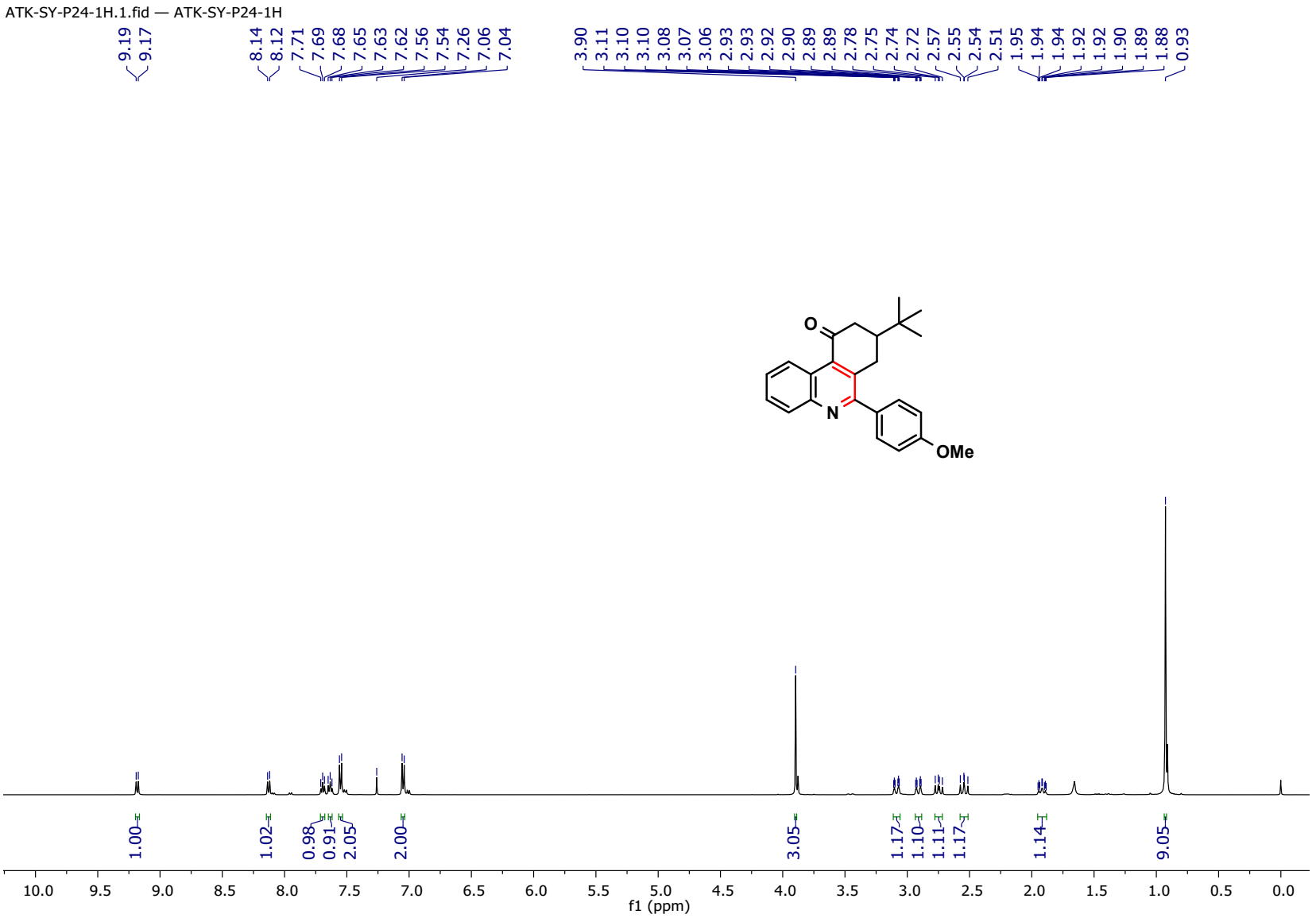


HRMS Spectrum of Compound 6a

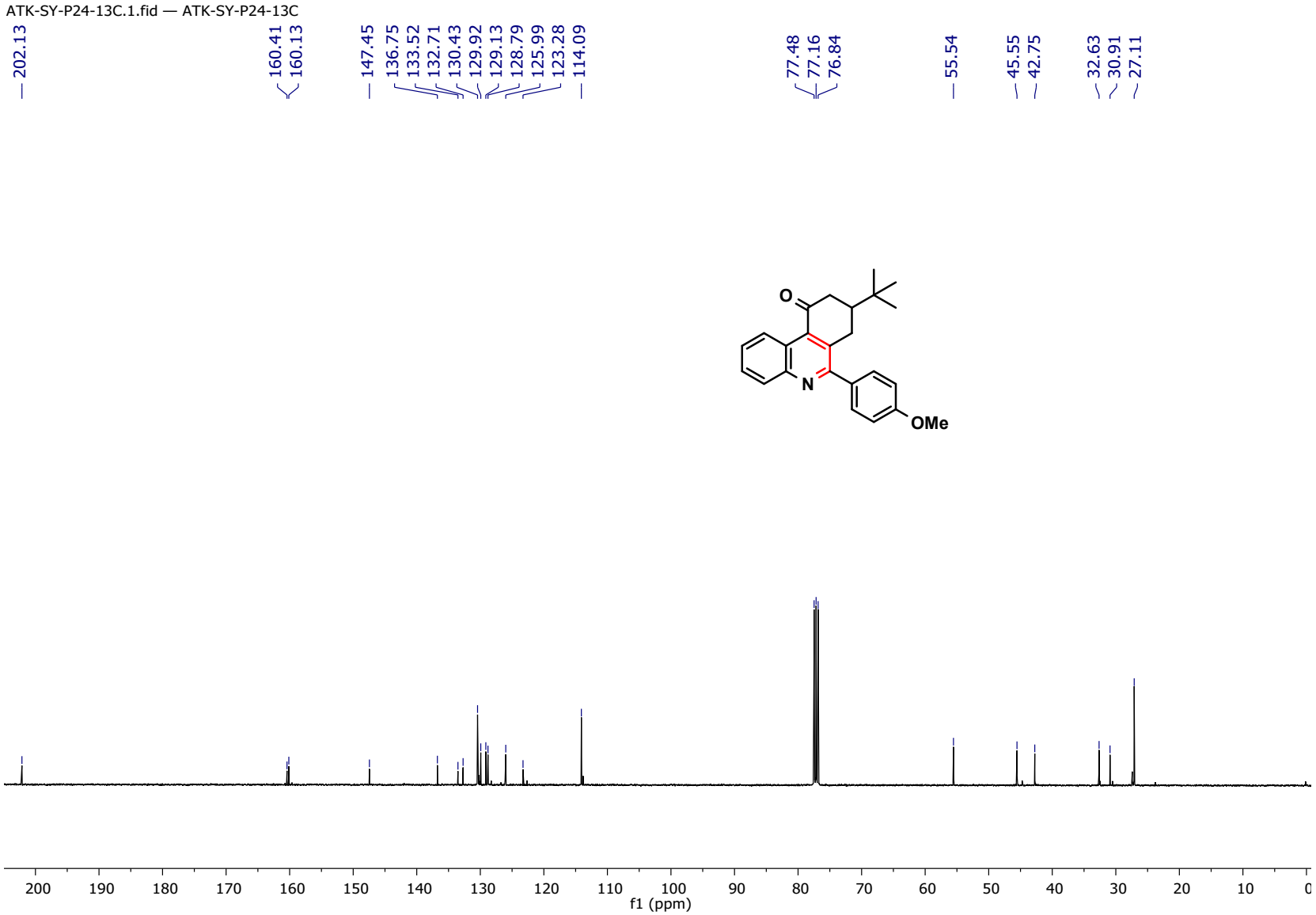
Sample Name	ATK-SY-261120	**Position**	P1-C1	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	ATK-SY-261120.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	03-12-2020 12:15:58 (UTC+05:30)



^{1}H NMR Spectrum of Compound 6b

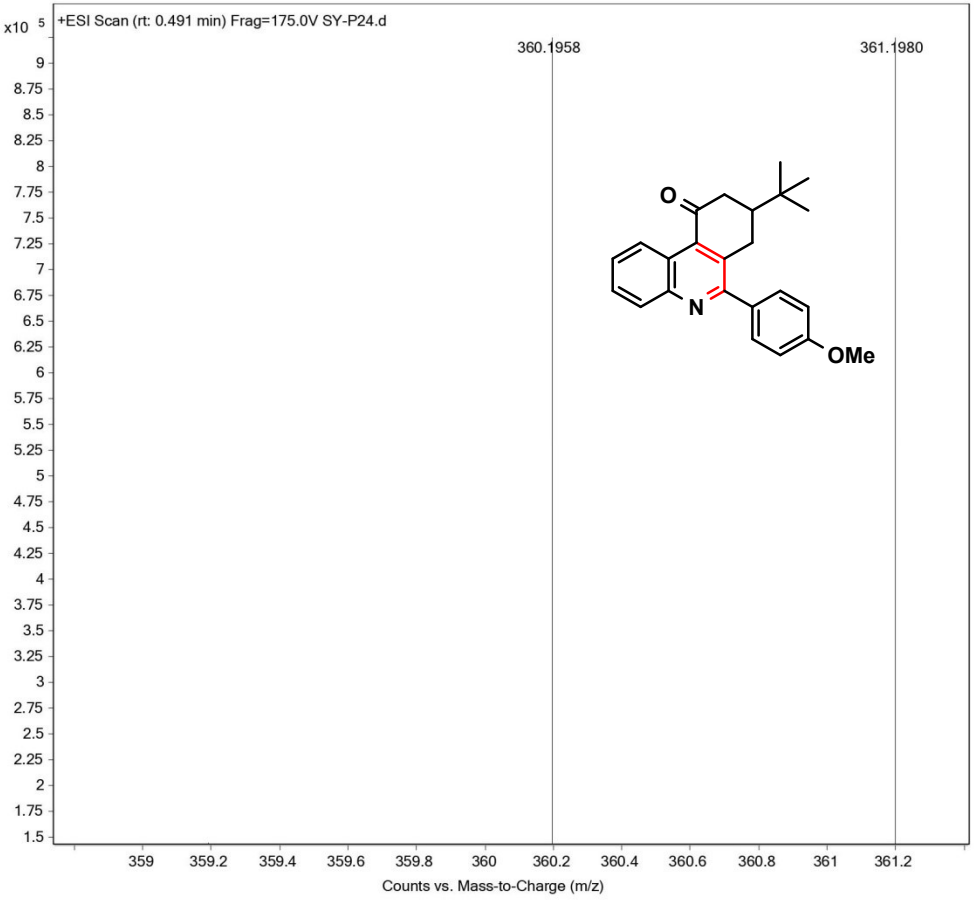


^{13}C NMR Spectrum of Compound 6b

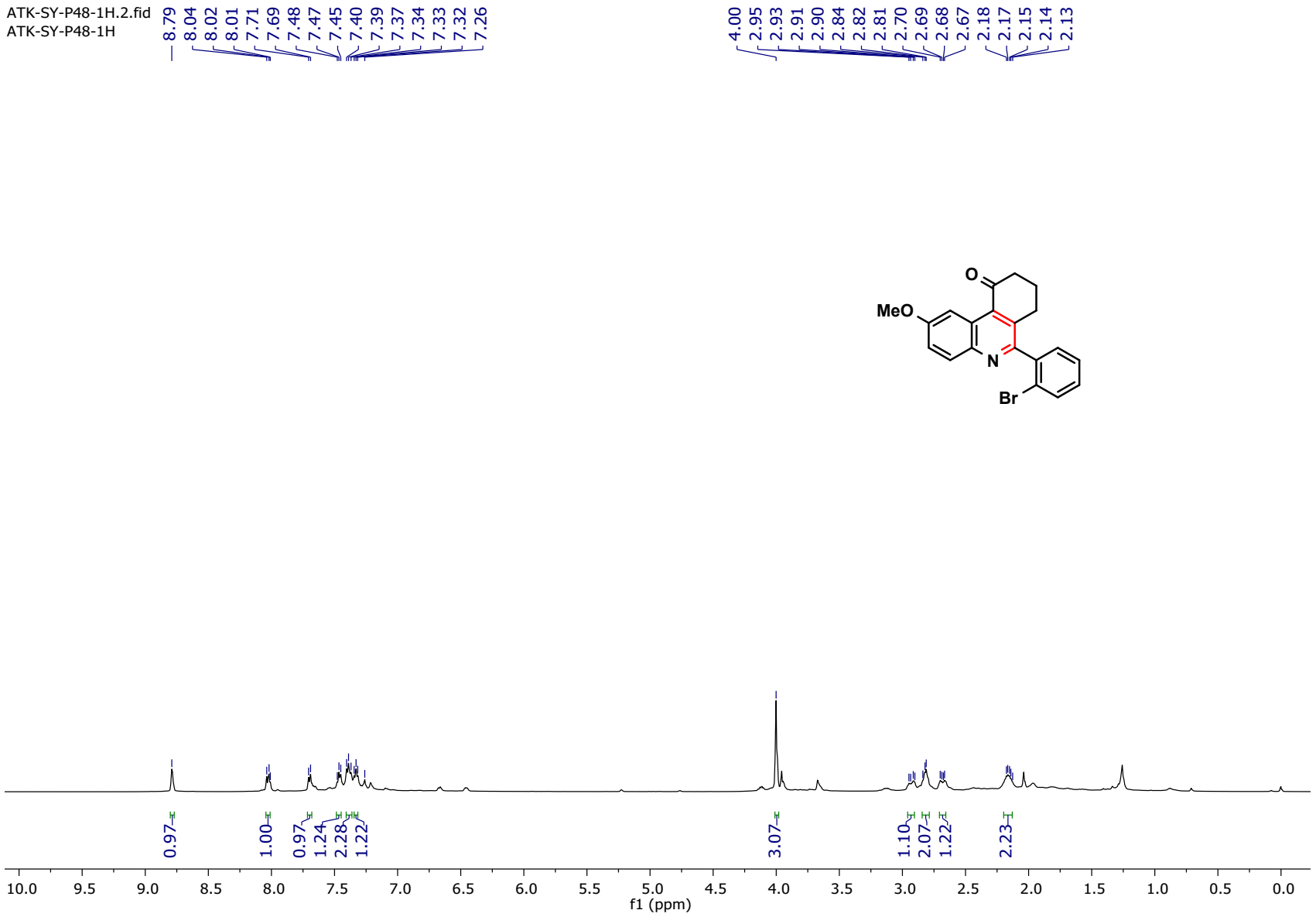


HRMS Spectrum of Compound 6b

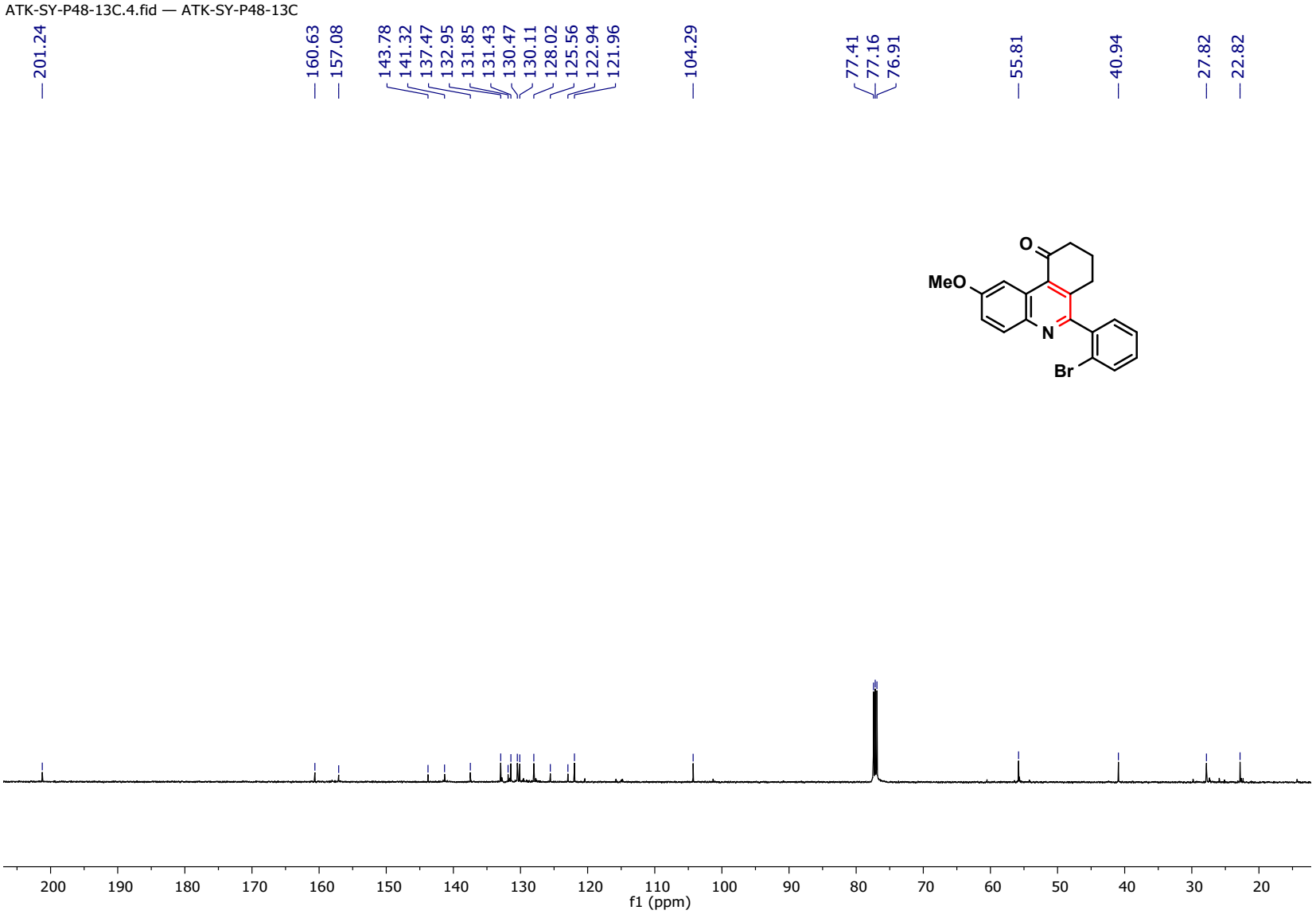
Sample Name	WASH	**Position**	P1-C11	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P24.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	26-Aug-21 03:30:53 PM (UTC+05:30)



^{1}H NMR Spectrum of Compound 6c

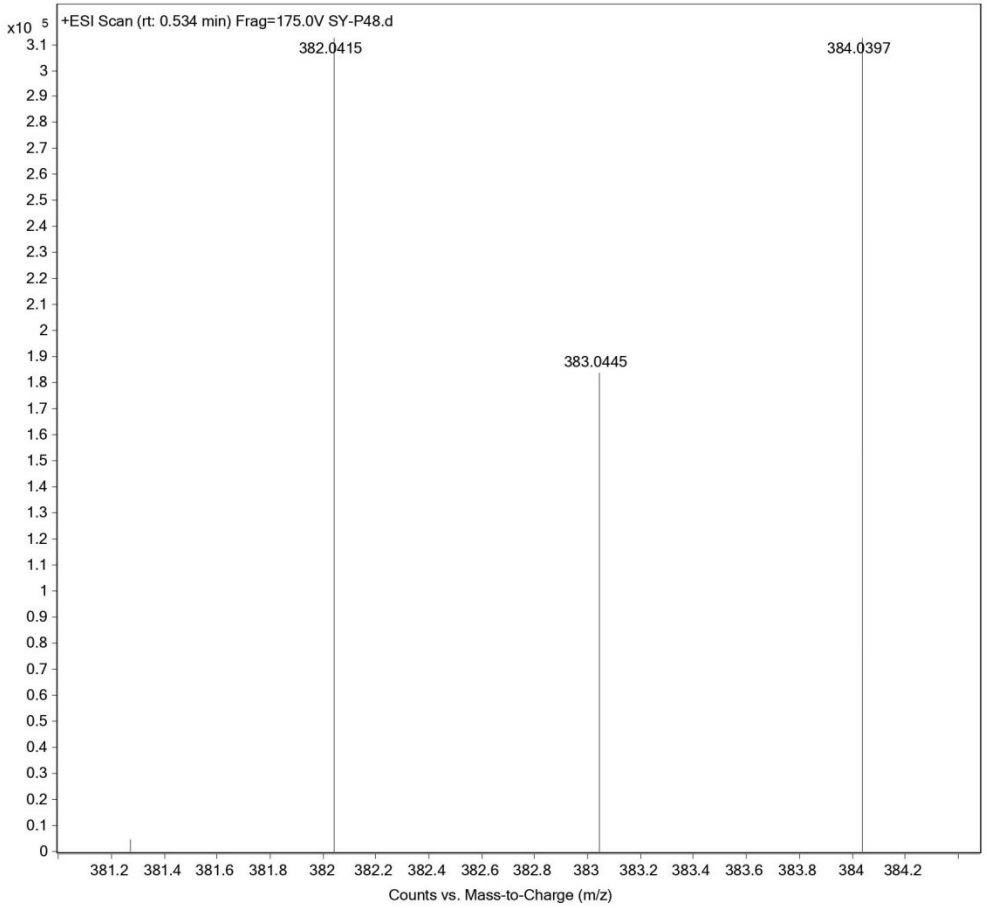


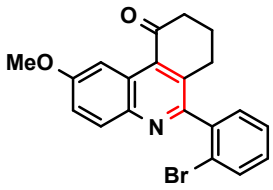
^{13}C NMR Spectrum of Compound 6c



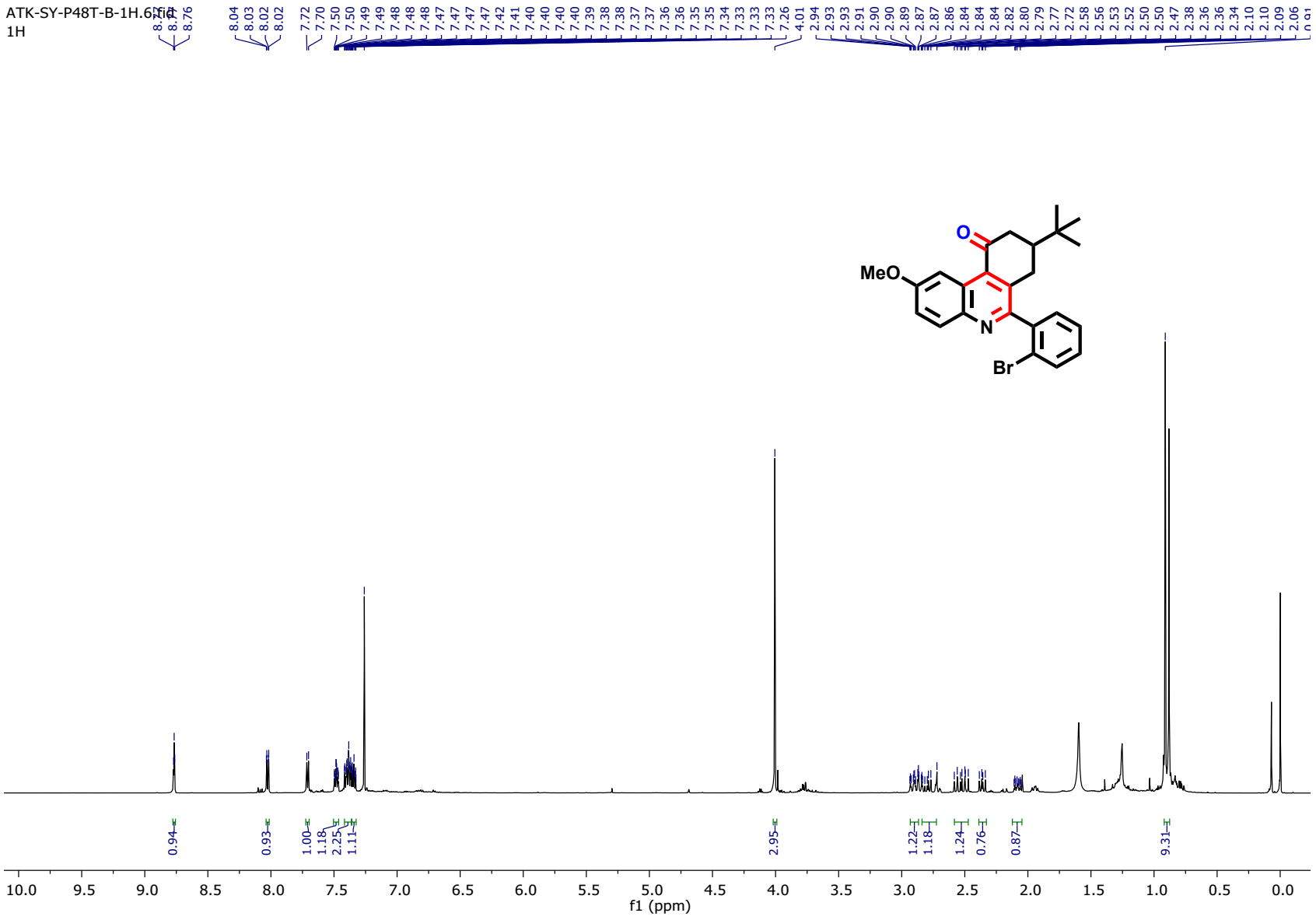
HRMS Spectrum of Compound 6c

Sample Name	WASH	**Position**	P1-C4	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	20	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SY-P48.d
ACQ Method	ESI ALS 100-600.m	**Comment**		**Acquired Time**	26-Aug-21 02:13:44 PM (UTC+05:30)

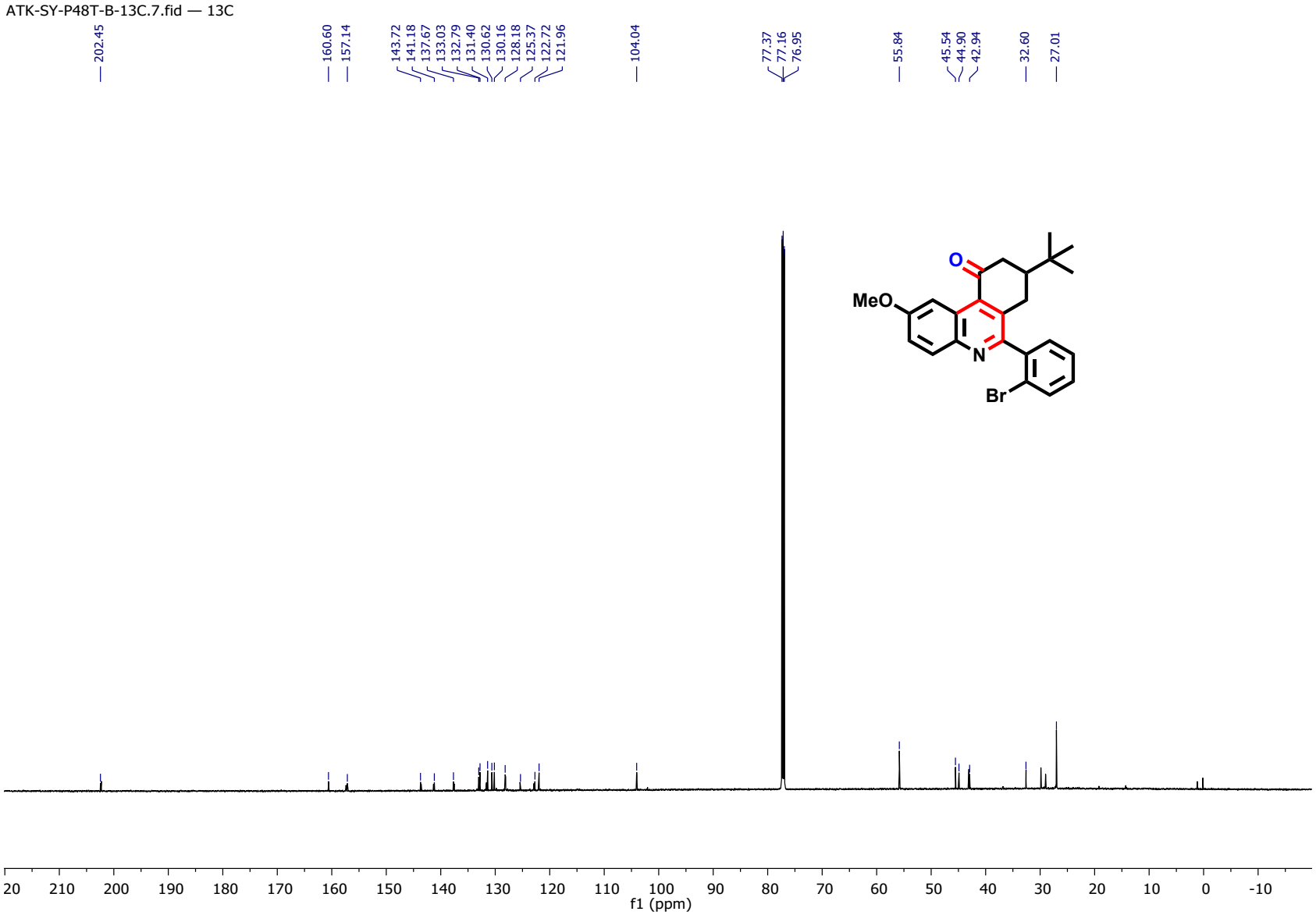




^{1}H NMR Spectrum of Compound 6d



^{13}C NMR Spectrum of Compound 6d



HRMS Spectrum of Compound 6d

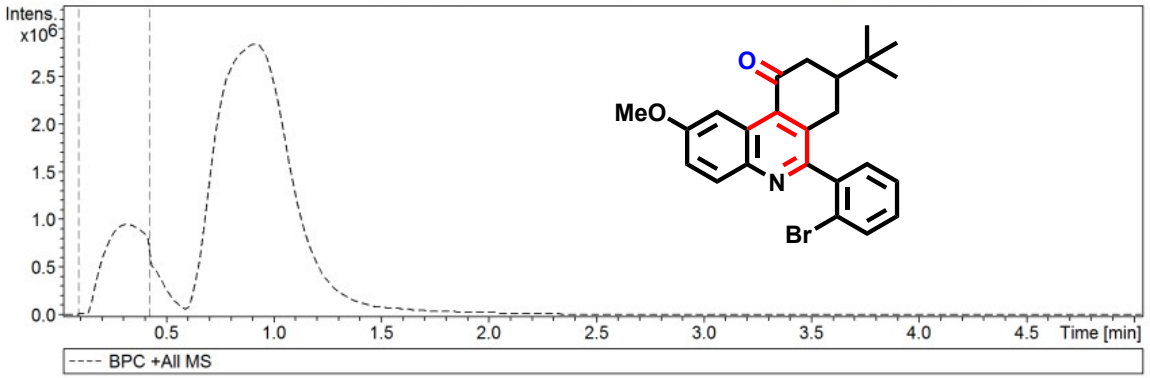
Display Report

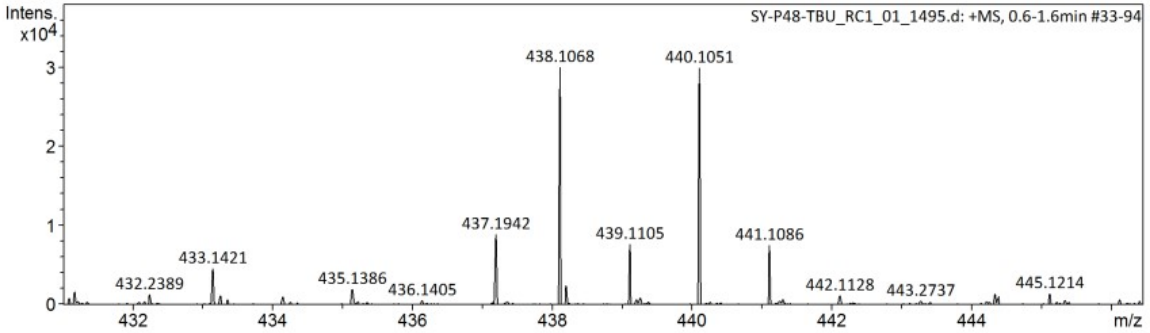
Analysis Info

Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\PRABHAS\SY-P48-TBU_RC1_01_1495.d	Acquisition Date	1/27/2022 1:33:50 PM
Method	low mass bruker.m	Operator	vidhi
Sample Name	SY-P48-TBU	Instrument	impact HD 1819696.00197
Comment			

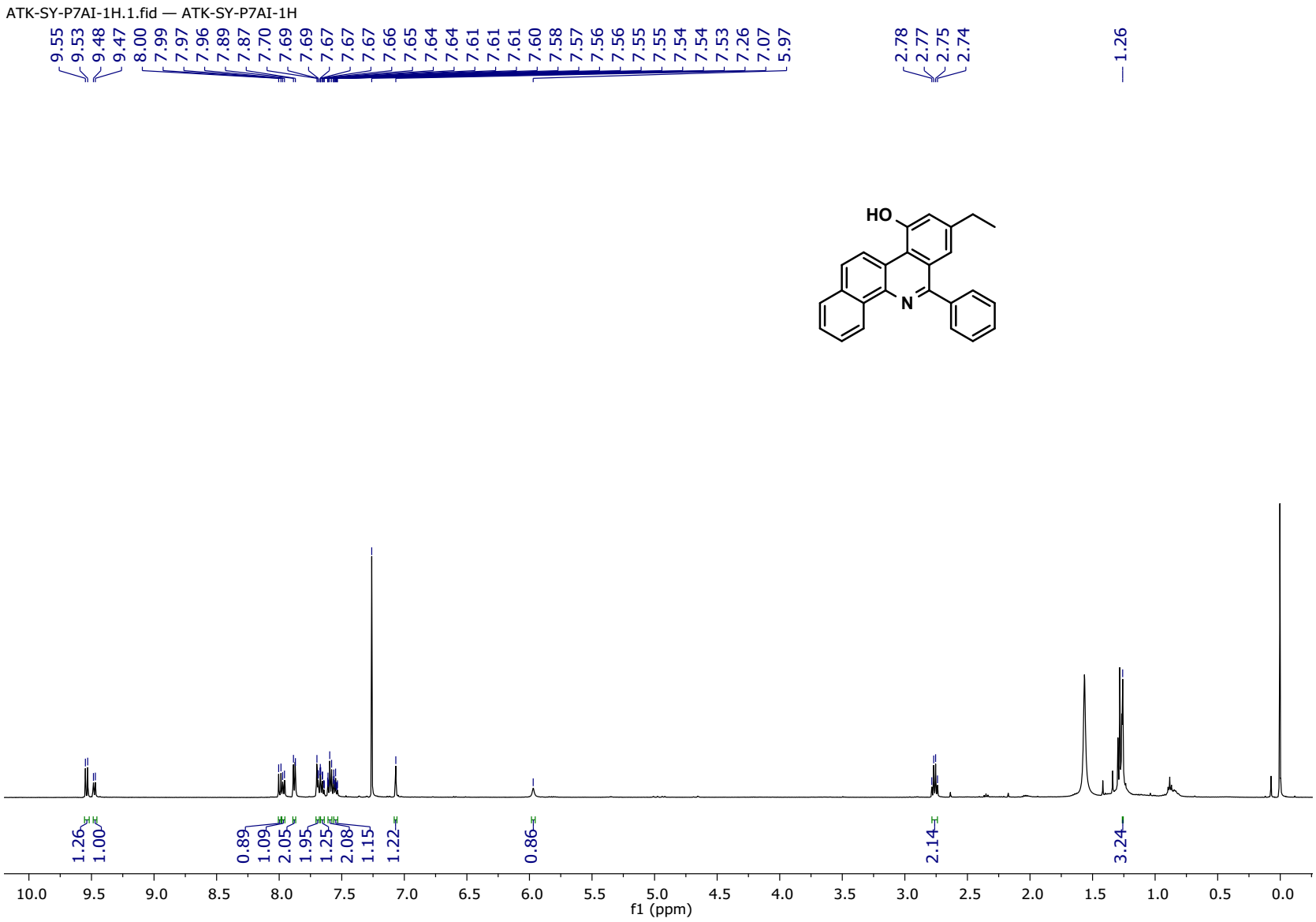
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

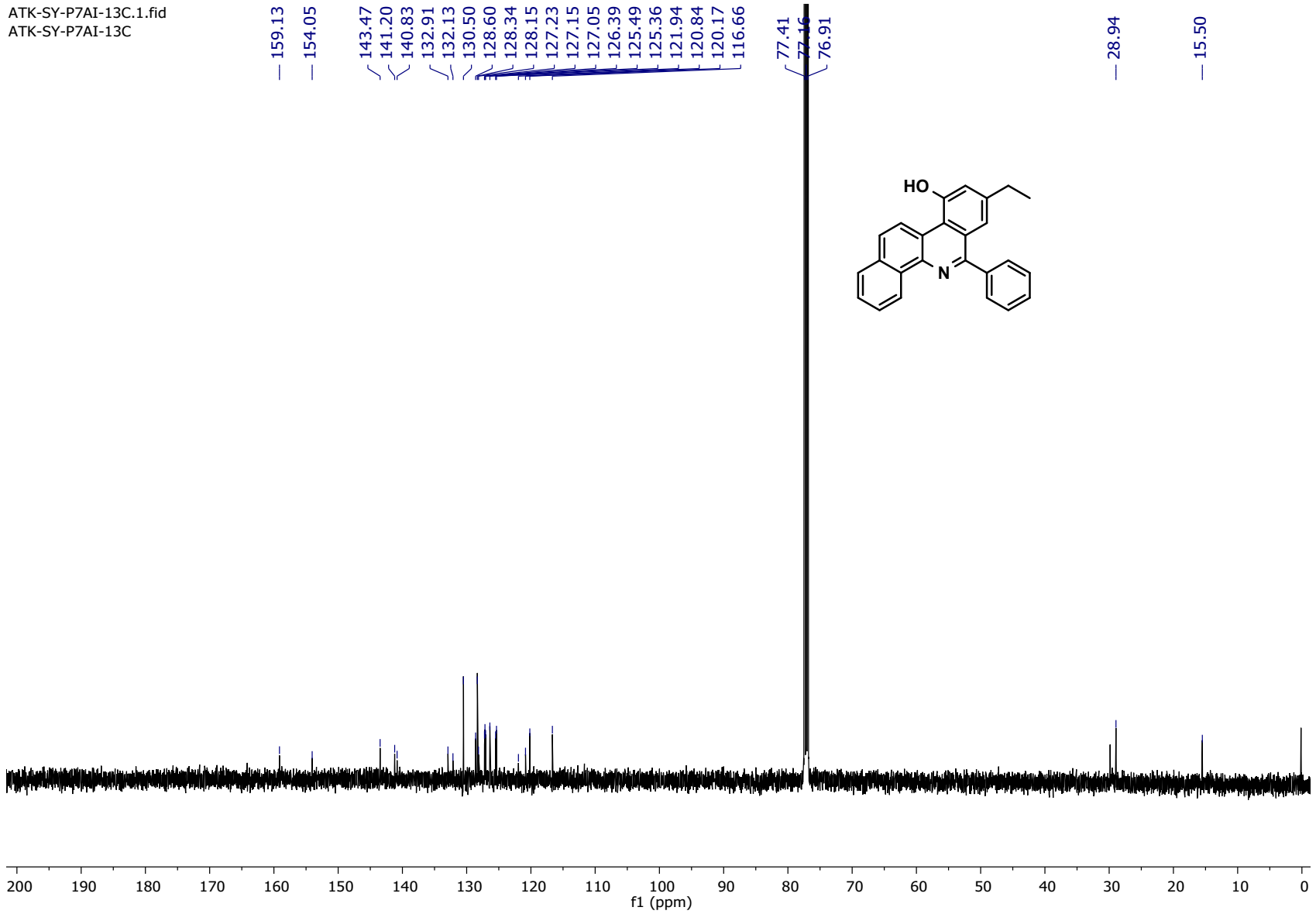




^{1}H NMR Spectrum of Compound 7i



^{13}C NMR Spectrum of Compound 7i



HRMS Spectrum of Compound 7i

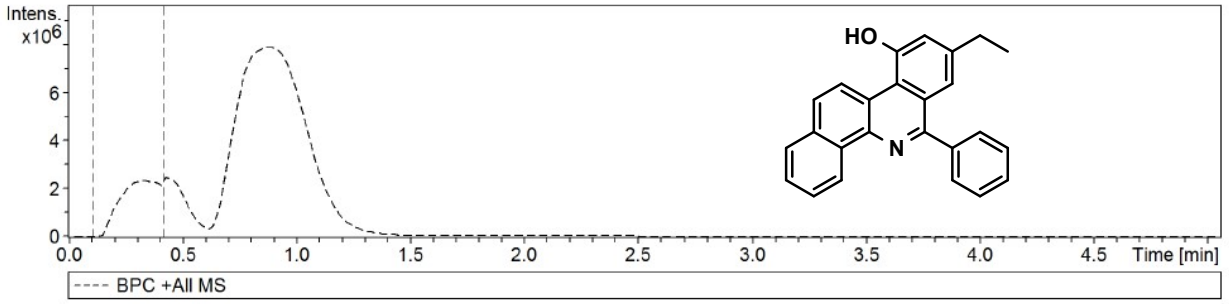
Display Report

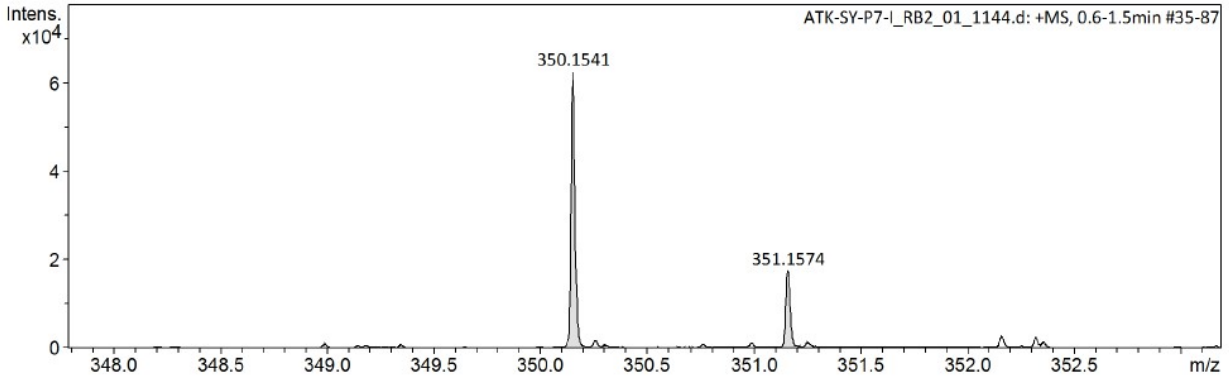
Analysis Info

Acquisition Date	11/2/2021 8:26:03 AM		
Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\30.10.2021\ATK-SY-P7-I_RB2_01_1144.d		
Method	low mass bruker.m	Operator	vidhi
Sample Name	ATK-SY-P7-I	Instrument	impact HD 1819696.00197
Comment			

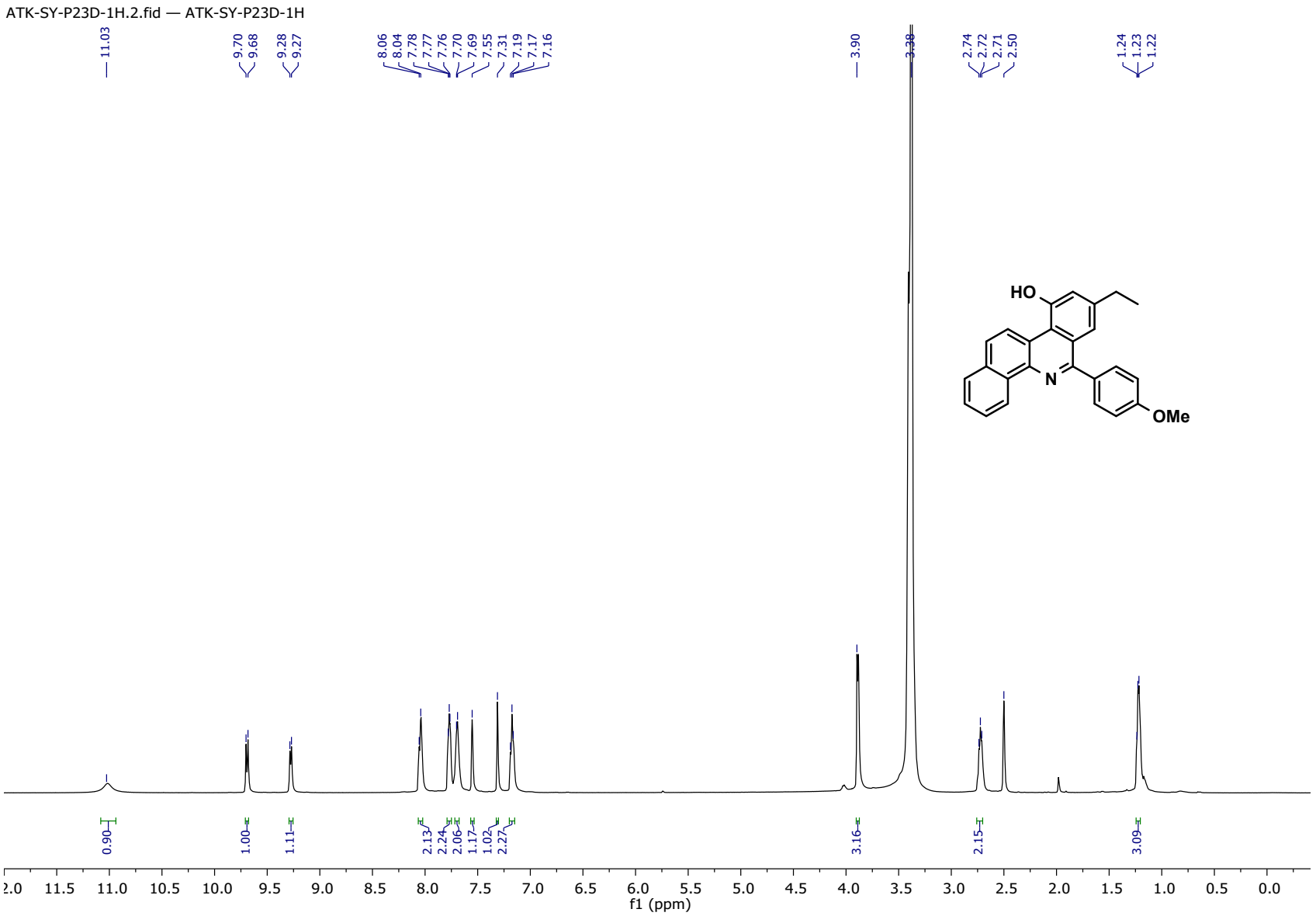
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

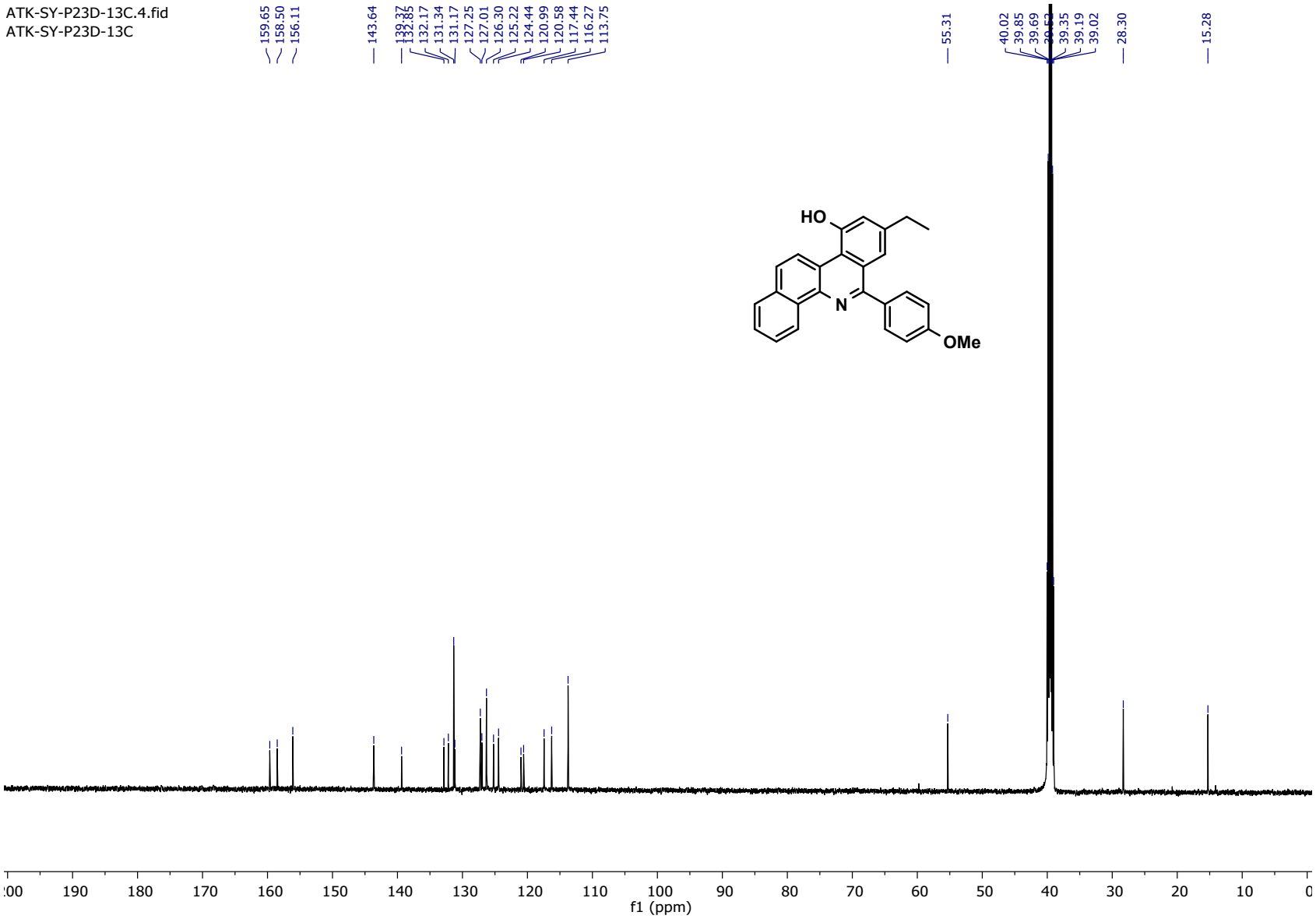




^{1}H NMR Spectrum of Compound 7j



^{13}C NMR Spectrum of Compound 7j



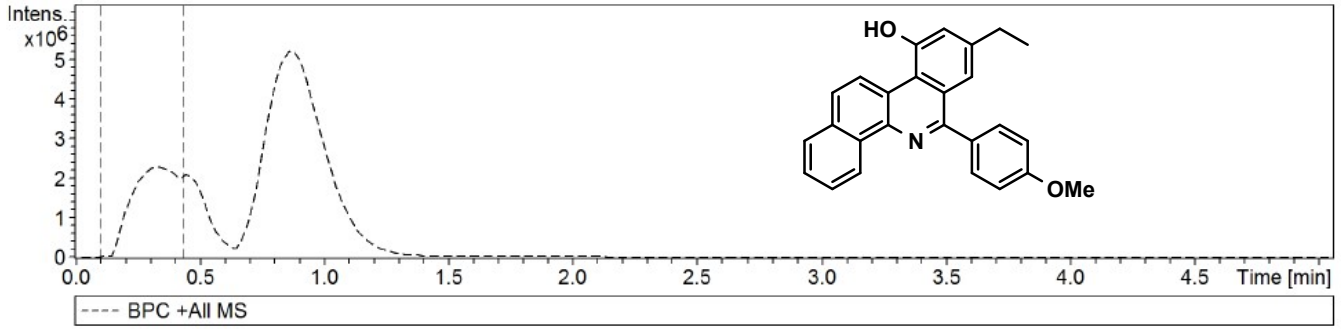
HRMS Spectrum of Compound 7j

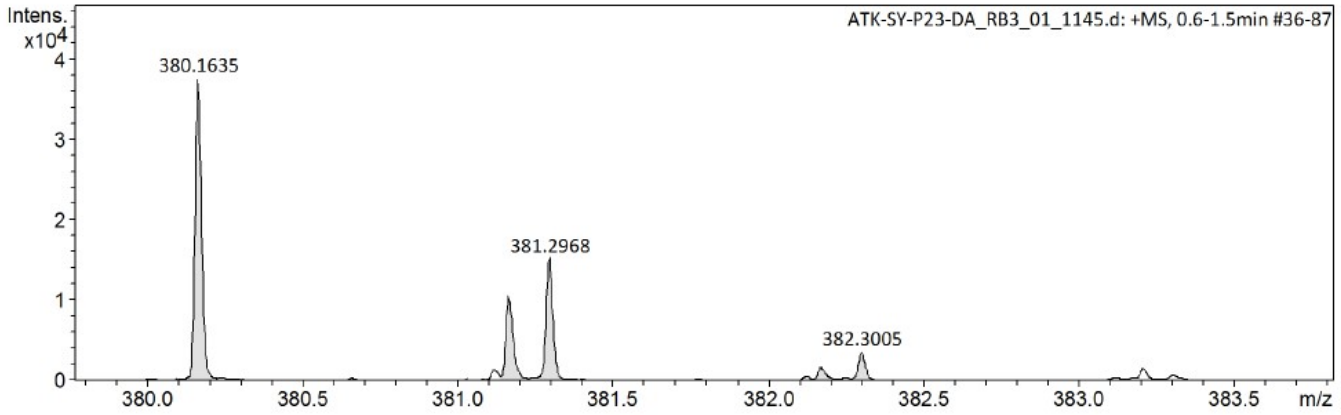
Analysis Info

Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\30.10.2021\ATK-SY-P23-DA_RB3_01_1145.d	Acquisition Date	11/2/2021 8:32:41 AM
Method	low mass bruker.m	Operator	vidhi
Sample Name	ATK-SY-P23-DA	Instrument	impact HD 1819696.00197
Comment			

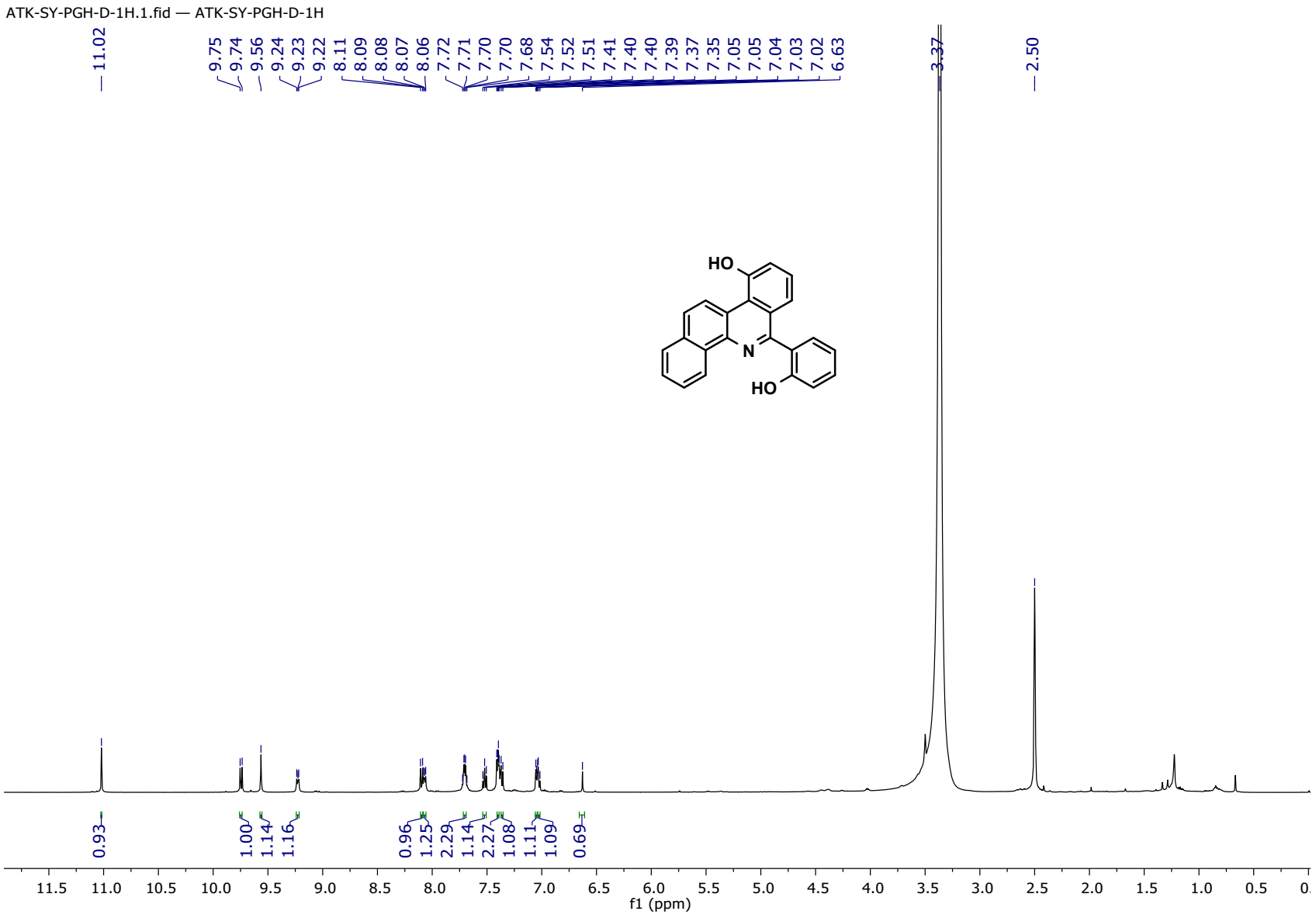
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

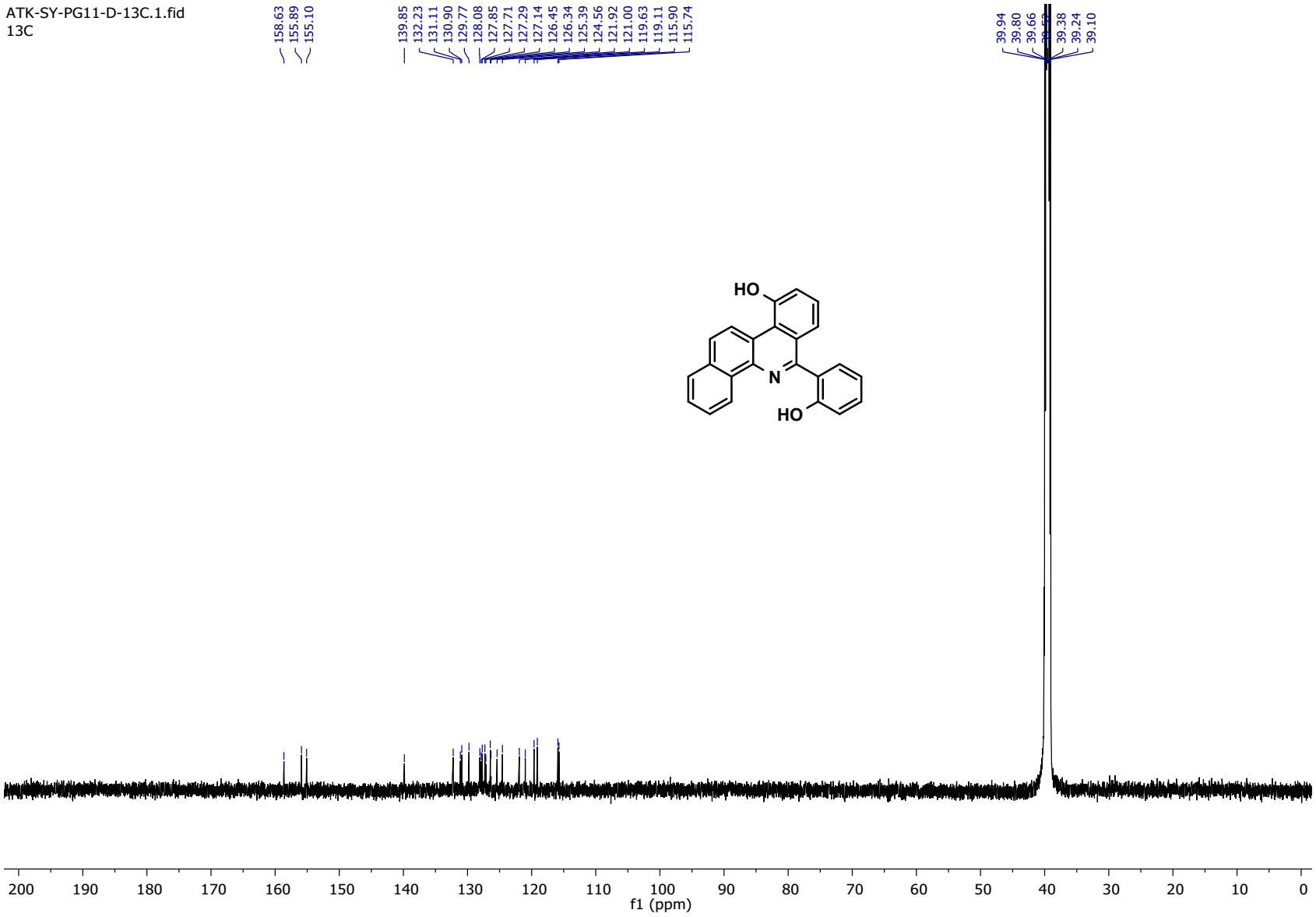




^{1}H NMR Spectrum of Compound 7q



^{13}C NMR Spectrum of Compound 7q



HRMS Spectrum of Compound 7q

Display Report

Analysis Info

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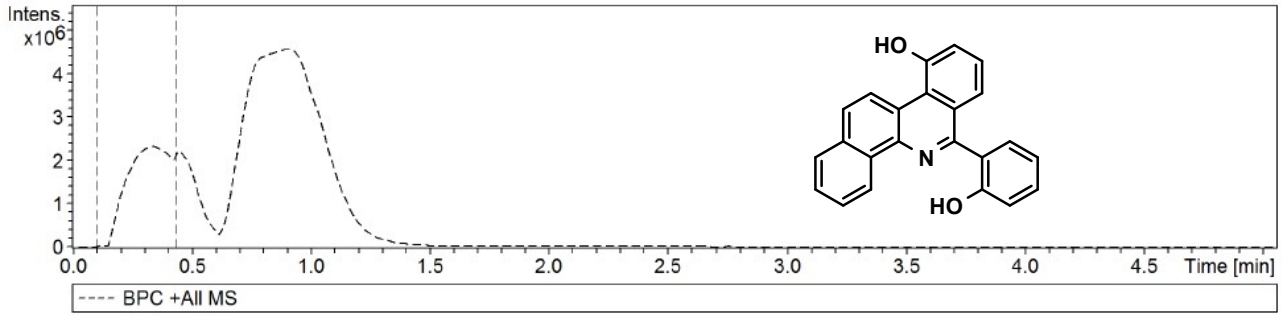
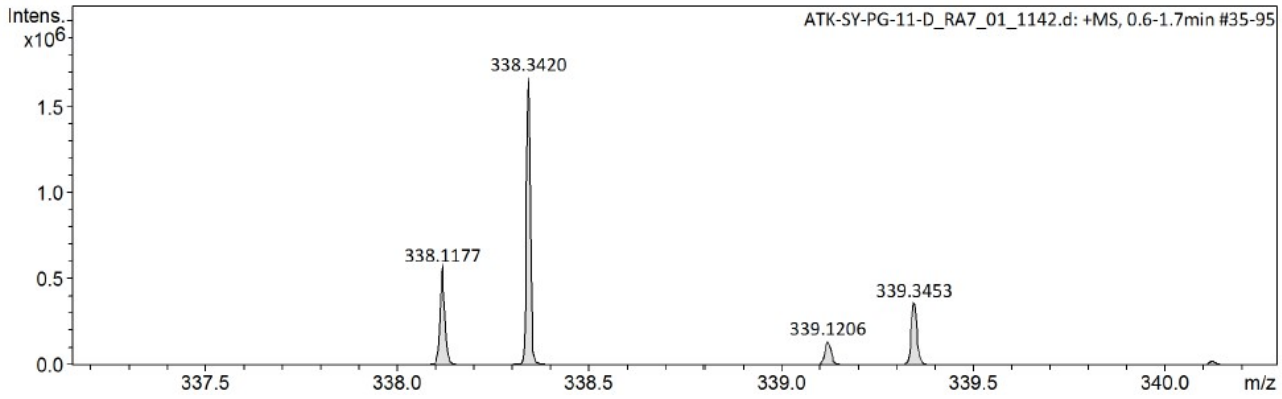
Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\30.10.2021\ATK-SY-PG-11-D_RA7_01_1142.d		
Method	low mass bruker.m	Operator	vidhi
Sample Name	ATK-SY-PG-11-D	Instrument	impact HD 1819696.00197
Comment			

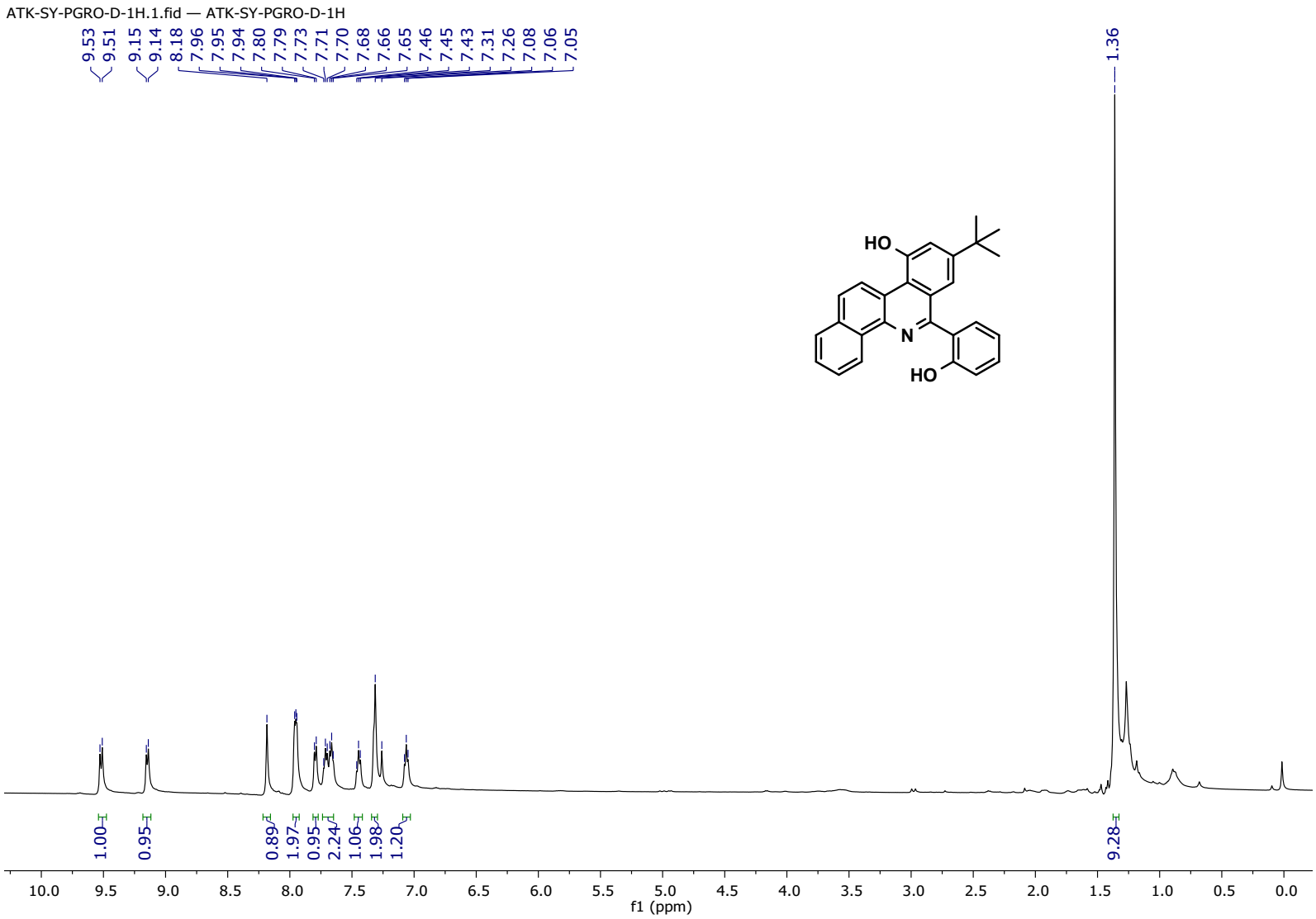
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C





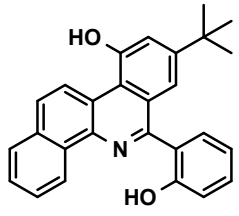
^{1}H NMR Spectrum of Compound 7t

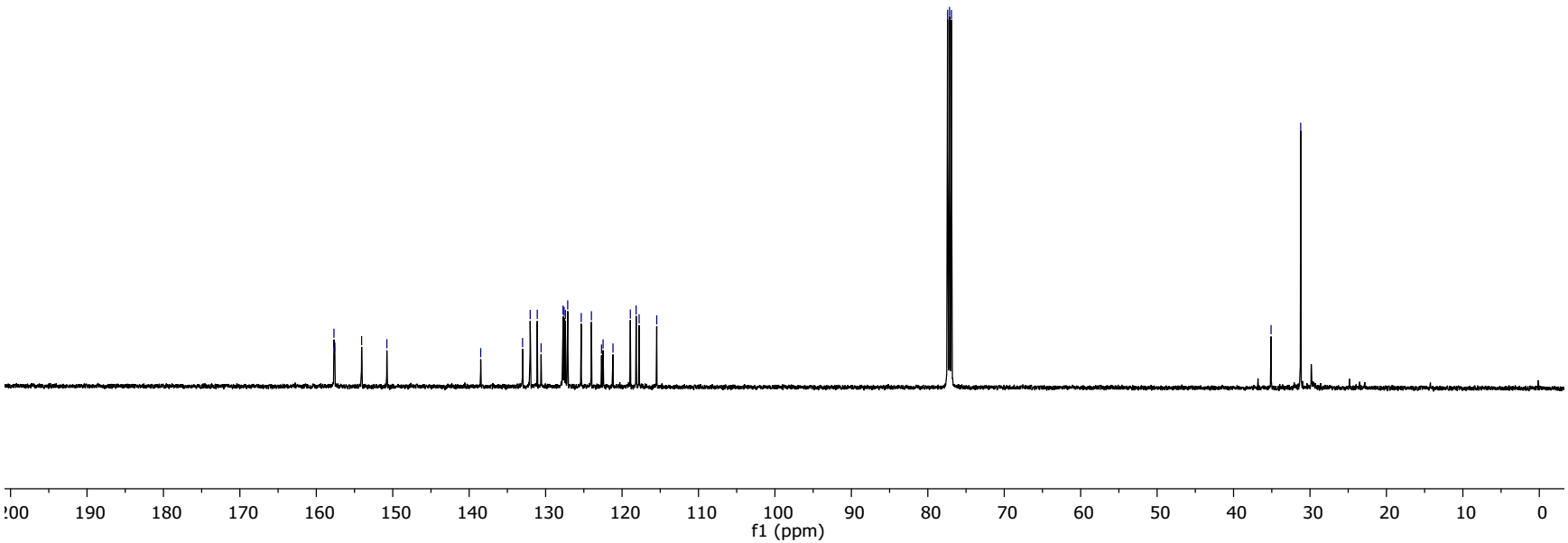


^{13}C NMR Spectrum of Compound 7t

ATK-SY-PGRO-D-13C.3.fid
ATK-SY-PGRO-D-13C

157.69, 157.57, 154.07, 150.77, 138.49, 133.01, 132.02, 131.09, 130.59, 127.72, 127.58, 127.42, 127.11, 125.34, 124.01, 122.69, 122.48, 121.19, 118.92, 118.16, 117.77, 115.46, 77.41, 77.16, 76.91, 35.09, 31.22





HRMS Spectrum of Compound 7t

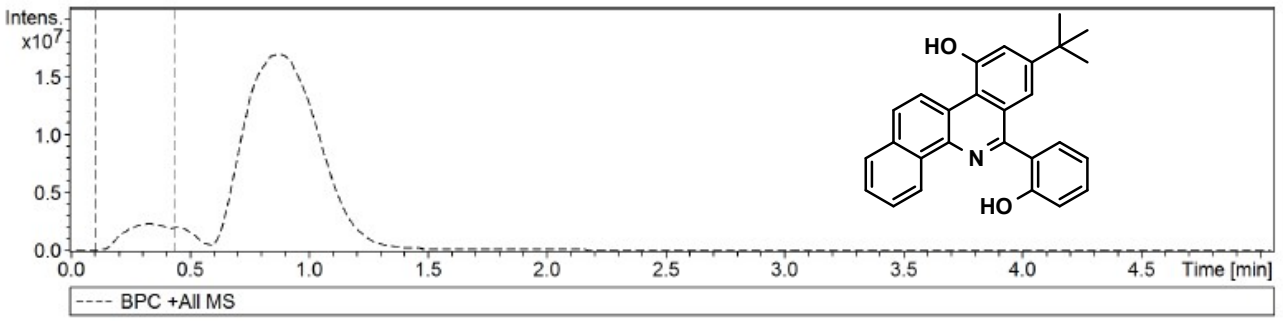
Display Report

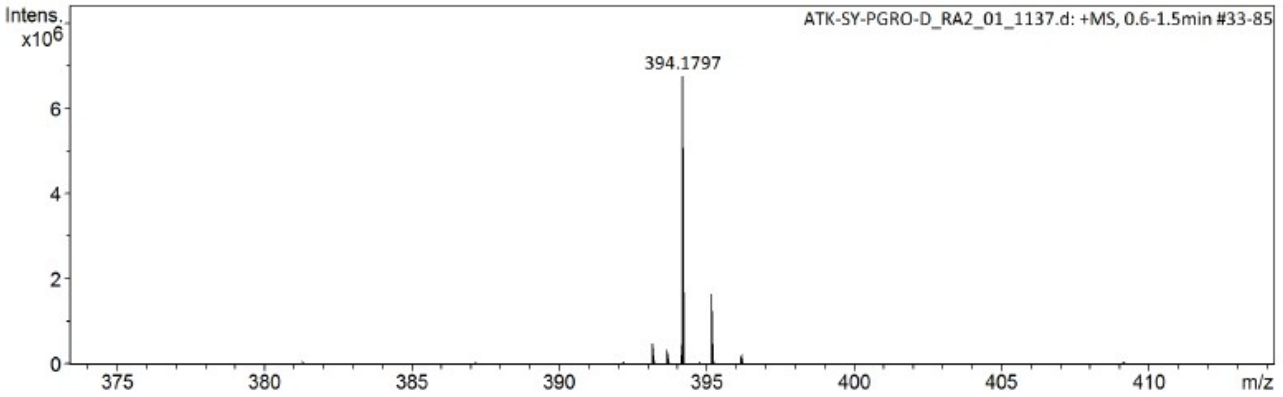
Analysis Info

Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\30.10.2021\ATK-SY-PGRO-D_RA2_01_1137.d	Acquisition Date	11/2/2021 7:40:26 AM
Method	low mass bruker.m	Operator	vidhi
Sample Name	ATK-SY-PGRO-D	Instrument	impact HD 1819696.00197
Comment			

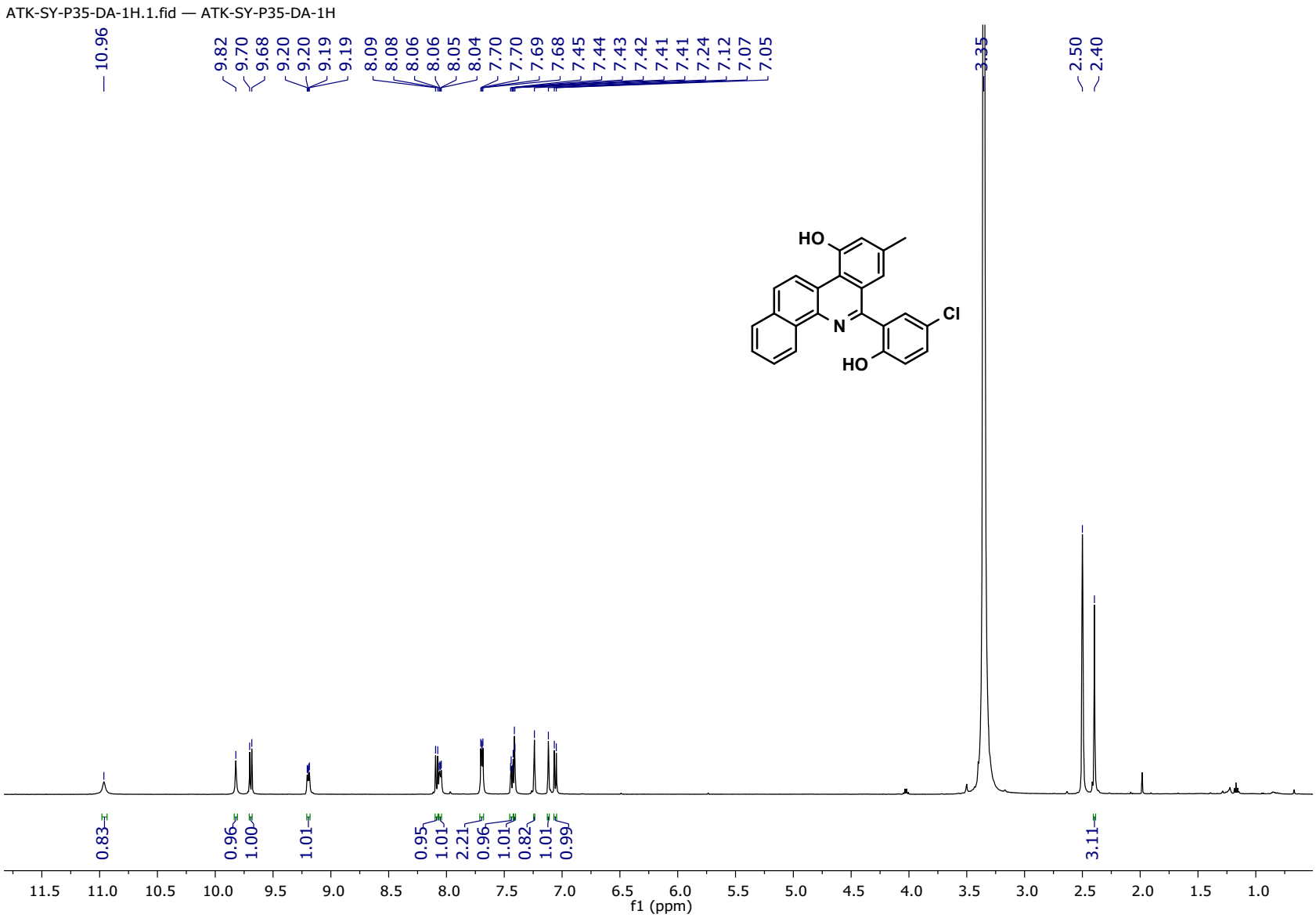
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

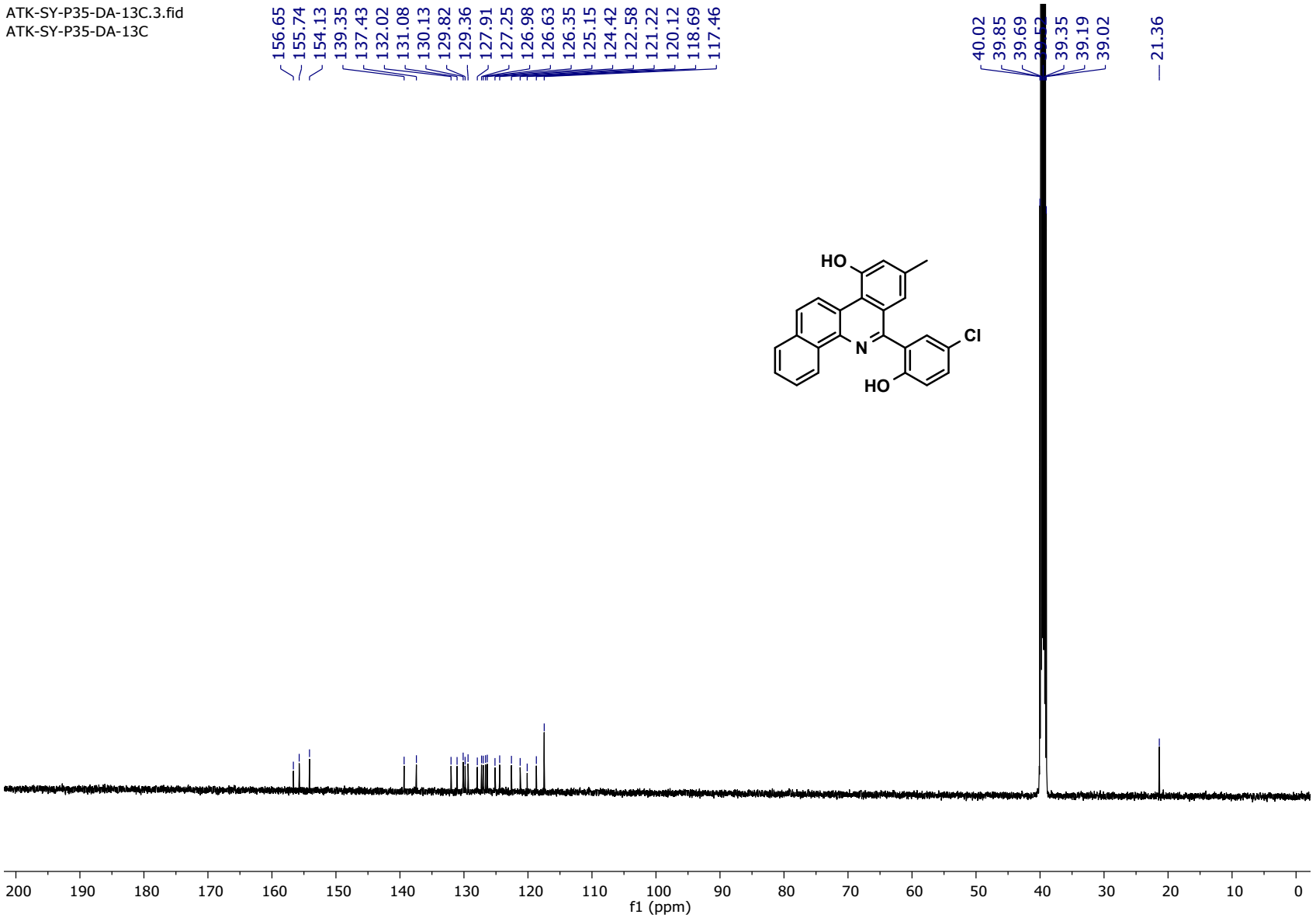




^{1}H NMR Spectrum of Compound 7v



^{13}C NMR Spectrum of Compound 7v



HRMS Spectrum of Compound 7v

Display Report

Analysis Info

Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\30.10.2021\ATK-SY-P35-DA_RA6_01_1141.d	Acquisition Date	11/2/2021 8:06:33 AM
Method	low mass bruker.m	Operator	vidhi
Sample Name	ATK-SY-P35-DA	Instrument	impact HD 1819696.00197
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
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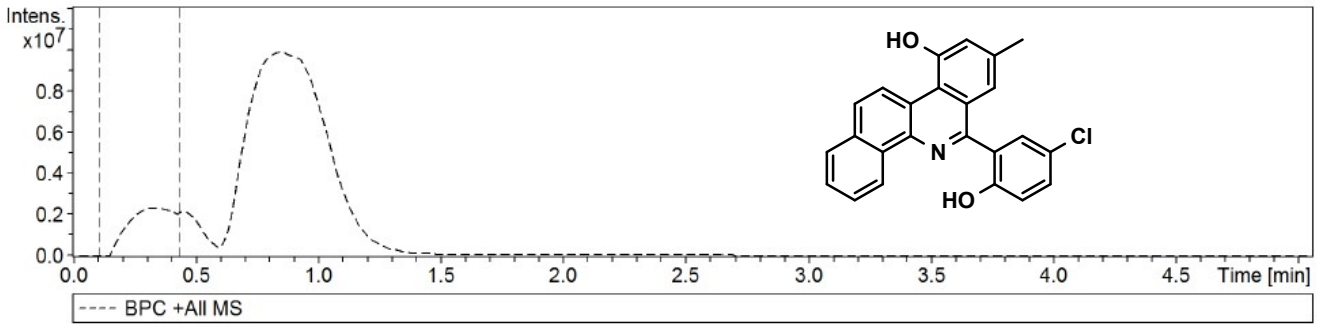
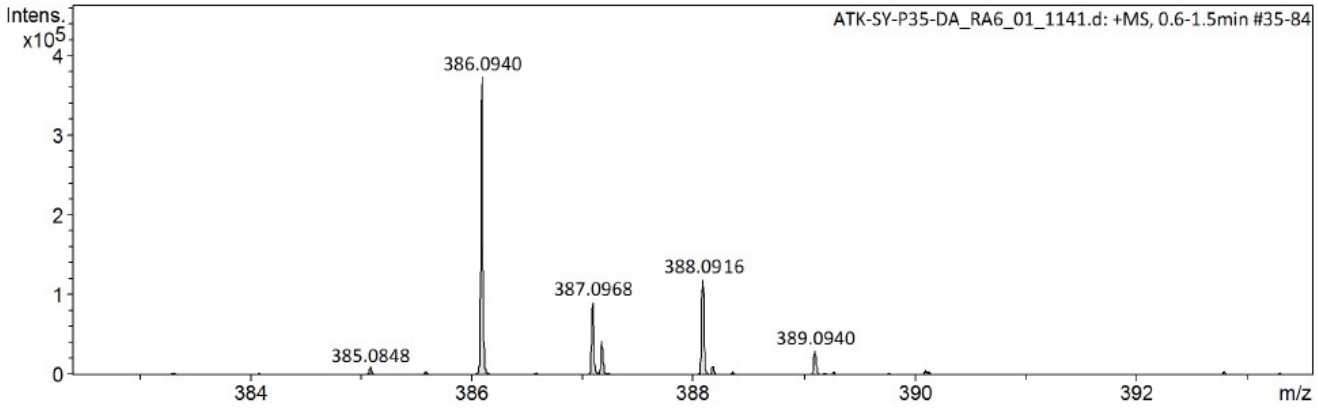
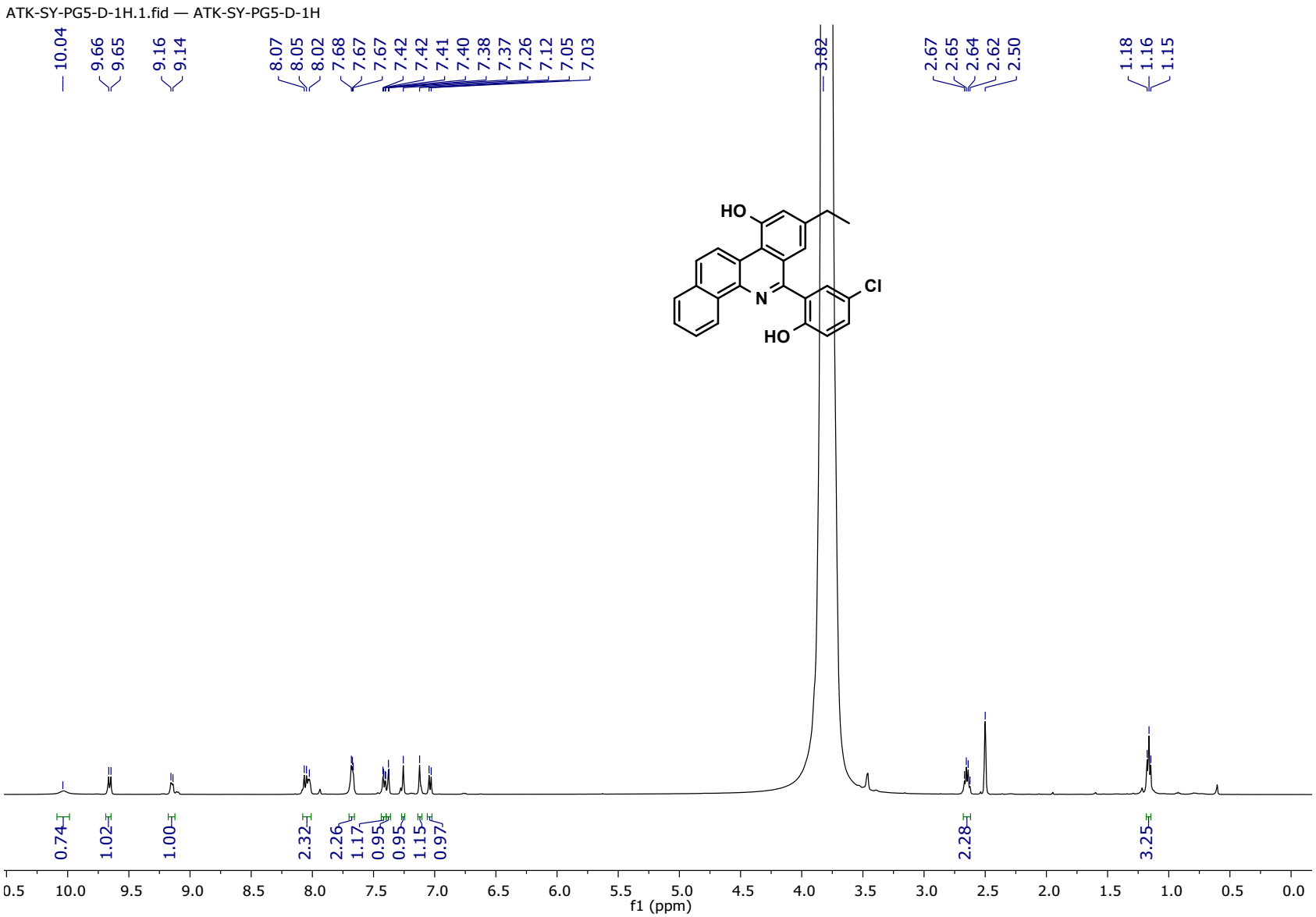
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

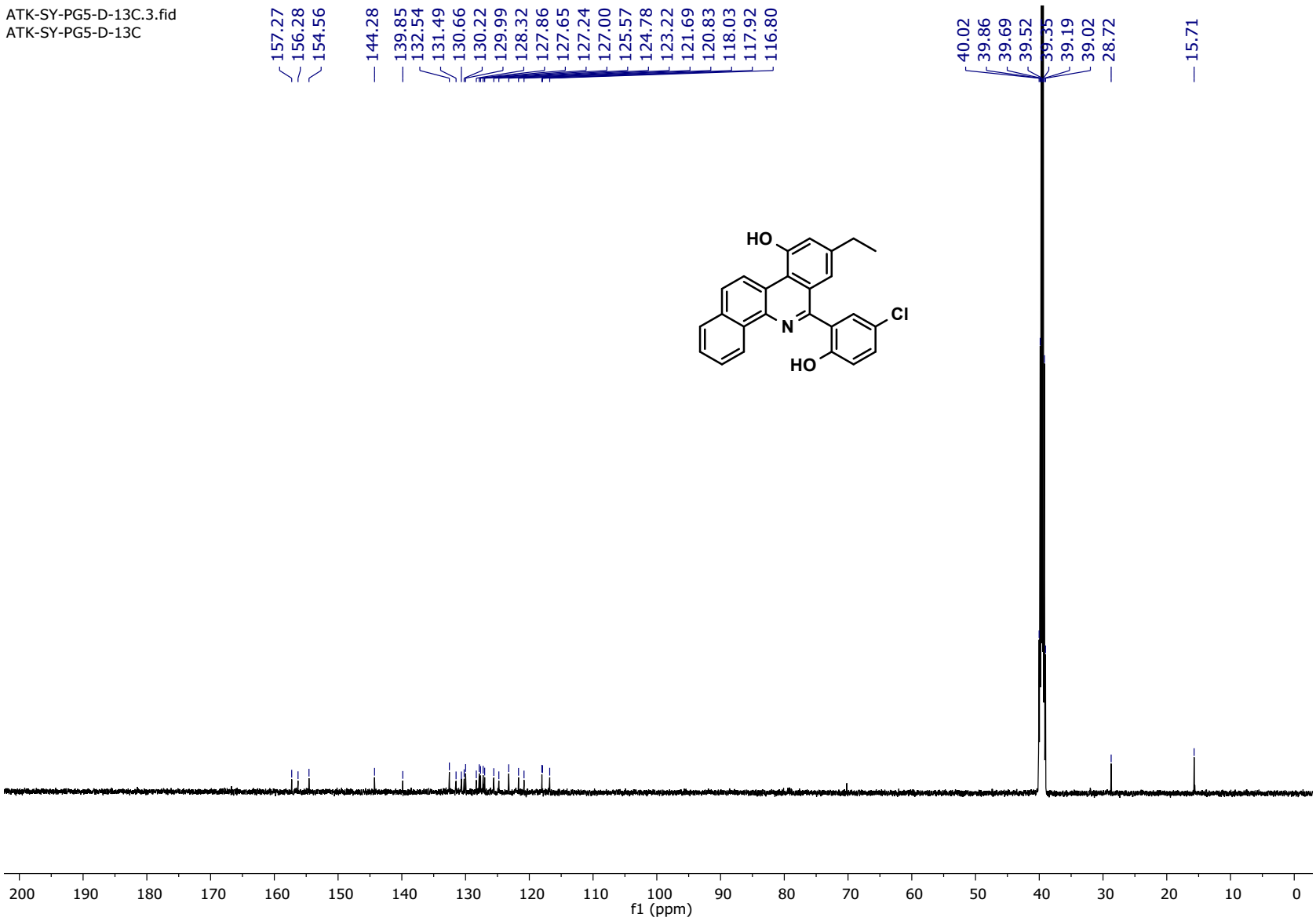




^{1}H NMR Spectrum of Compound 7w



^{13}C NMR Spectrum of Compound 7w



HRMS Spectrum of Compound 7w

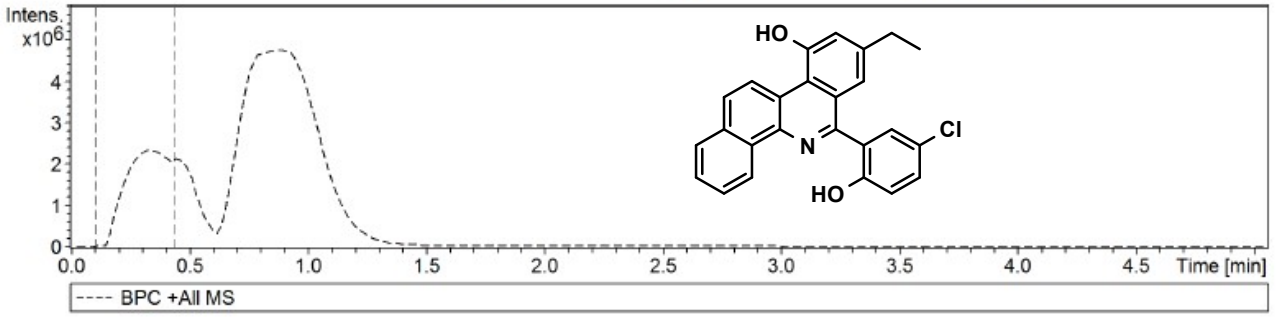
Display Report

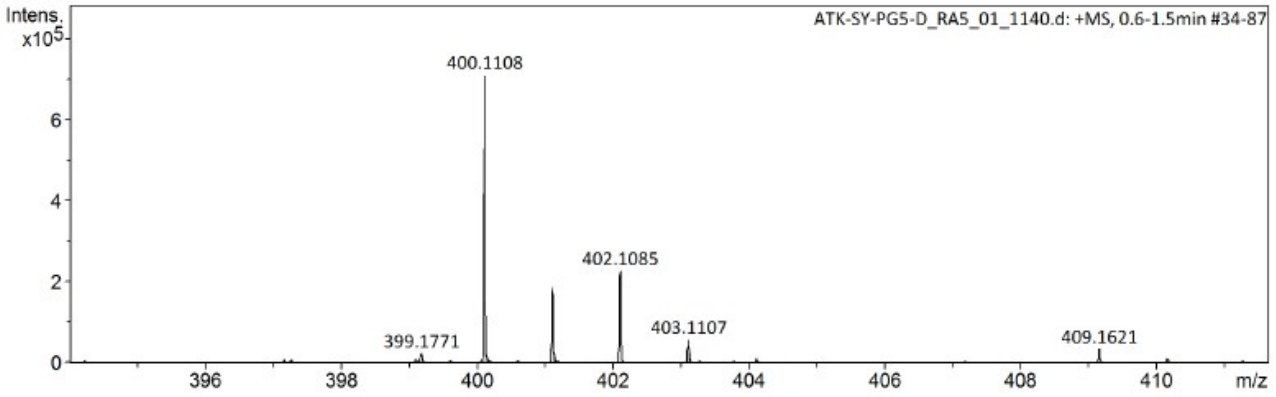
Analysis Info

Analysis Name	D:\Data\user data\HPLC\DR LOKMAN\30.10.2021\ATK-SY-PG5-D_RA5_01_1140.d	Acquisition Date	11/2/2021 8:00:04 AM
Method	low mass bruker.m	Operator	vidhi
Sample Name	ATK-SY-PG5-D	Instrument	impact HD 1819696.00197
Comment			

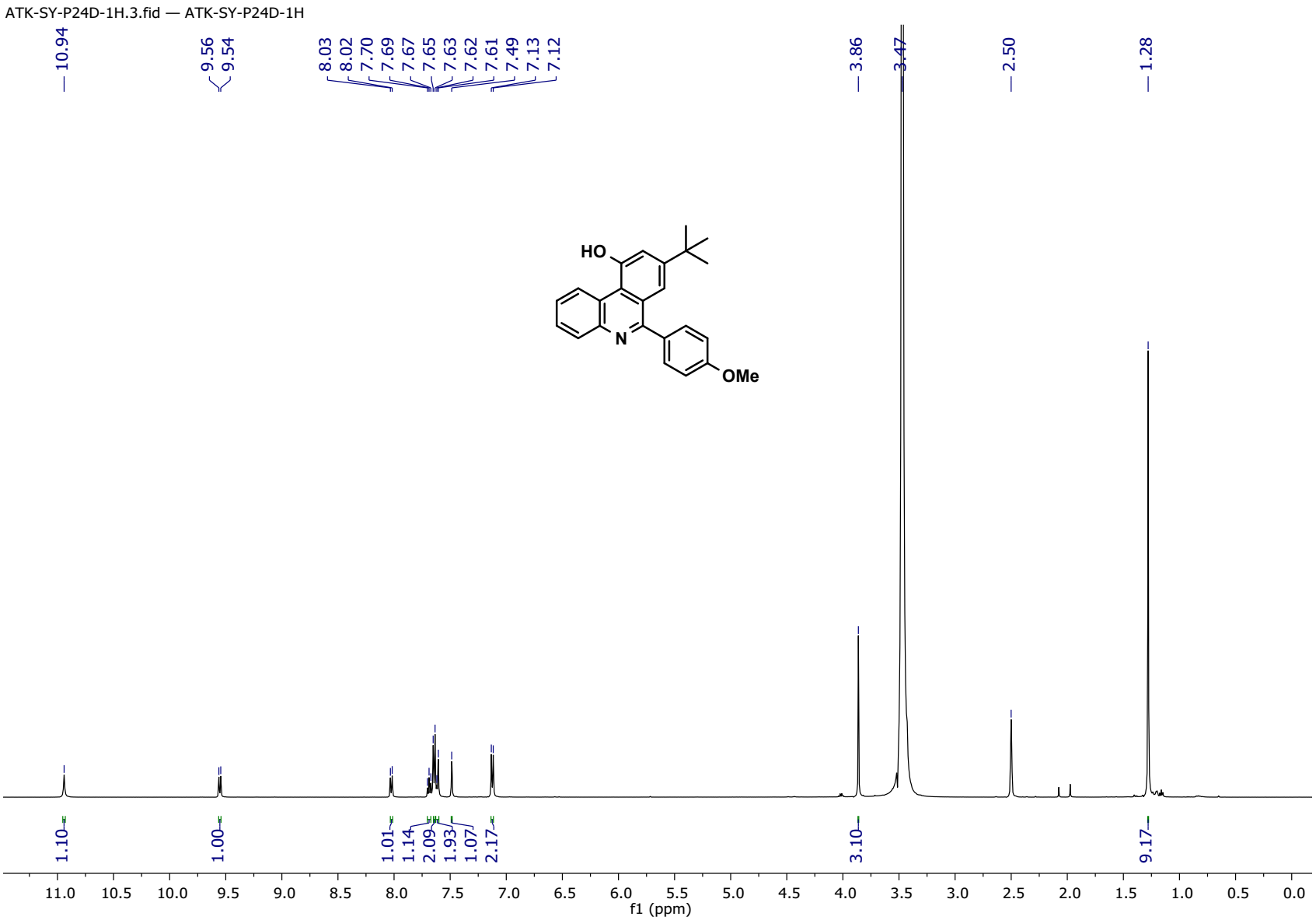
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.8 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C

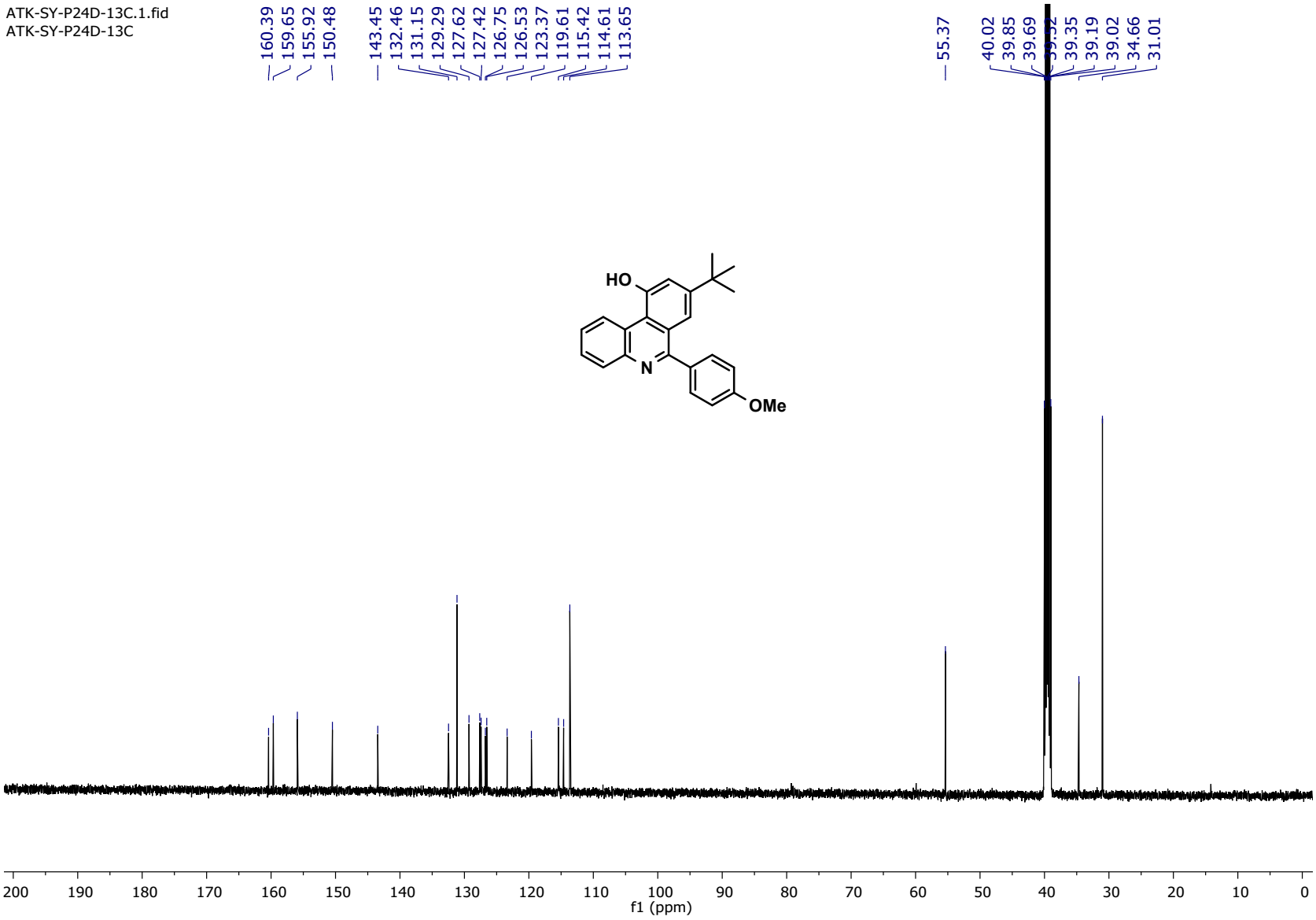




^{1}H NMR Spectrum of Compound 8b

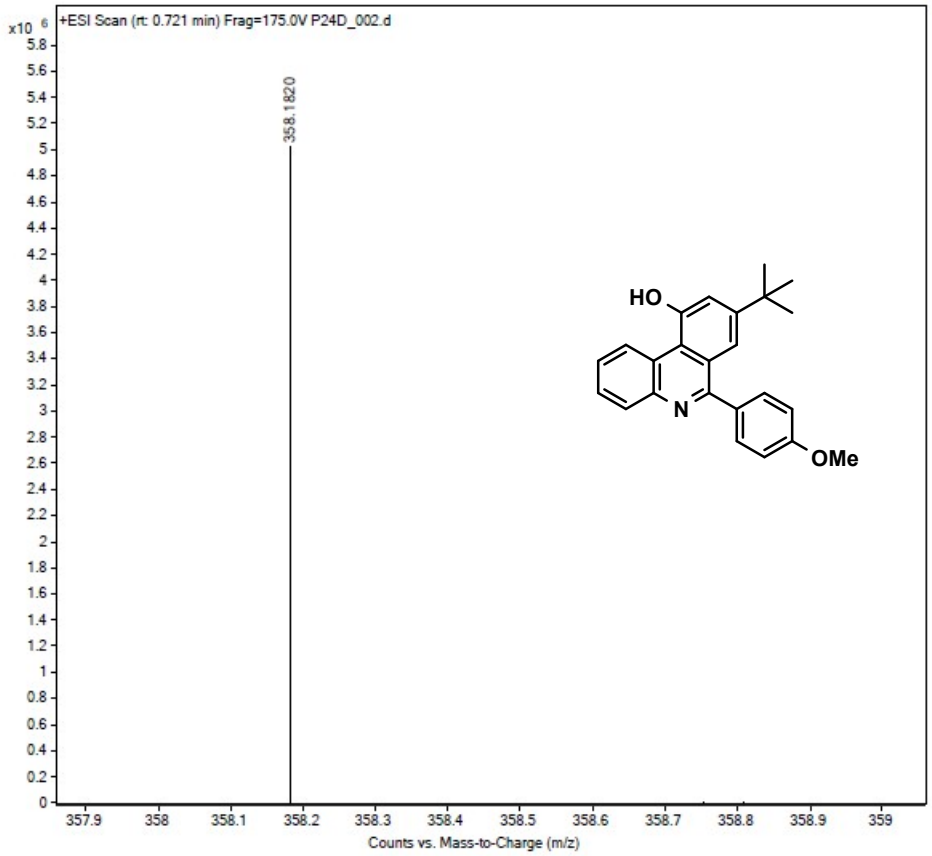


^{13}C NMR Spectrum of Compound 8b

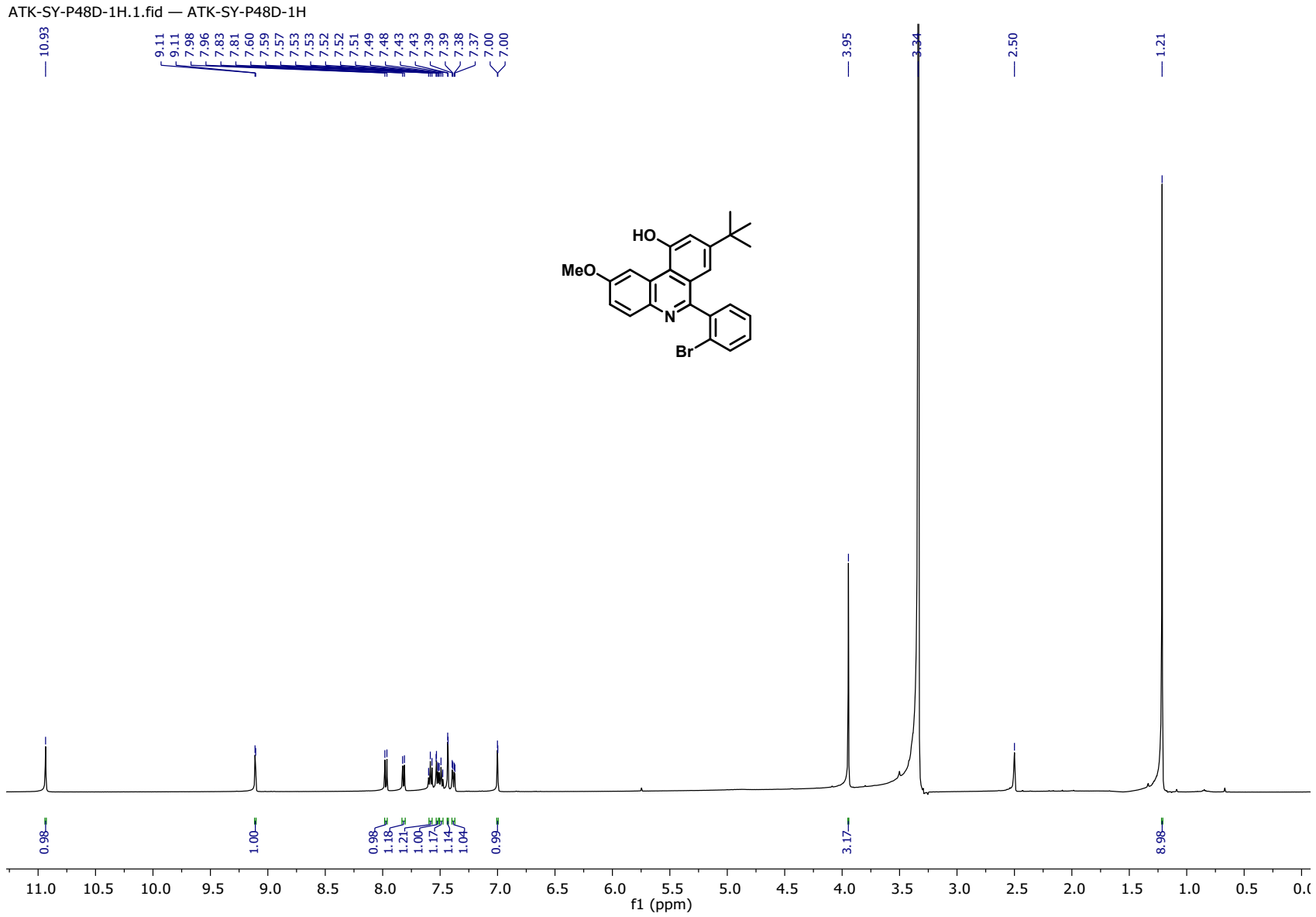


HRMS Spectrum of Compound 8b

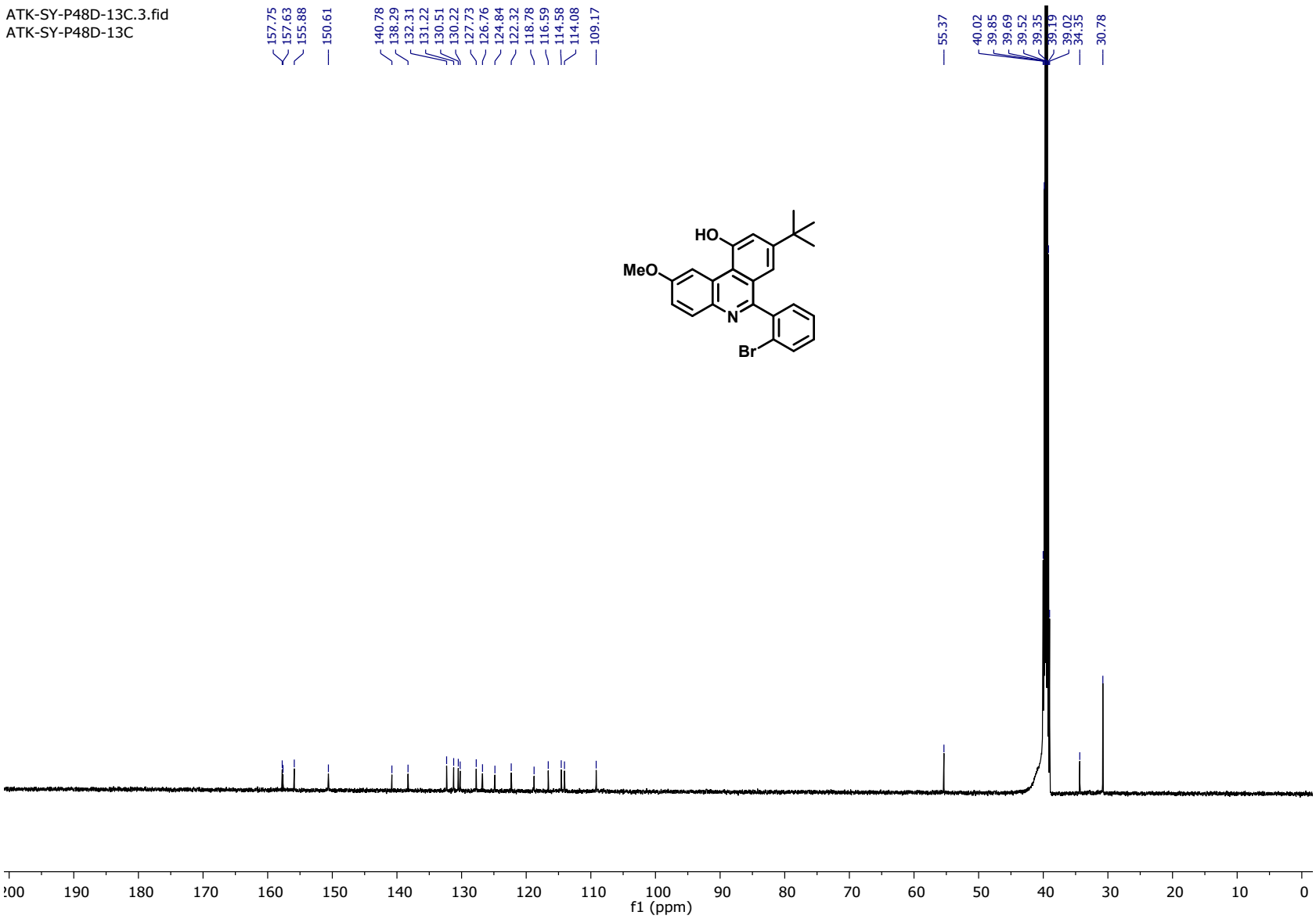
Sample Name	P24D	**Position**	P1-A2	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	P24D_002.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	18-Aug-22 12:12:14 PM (UTC+05:30)



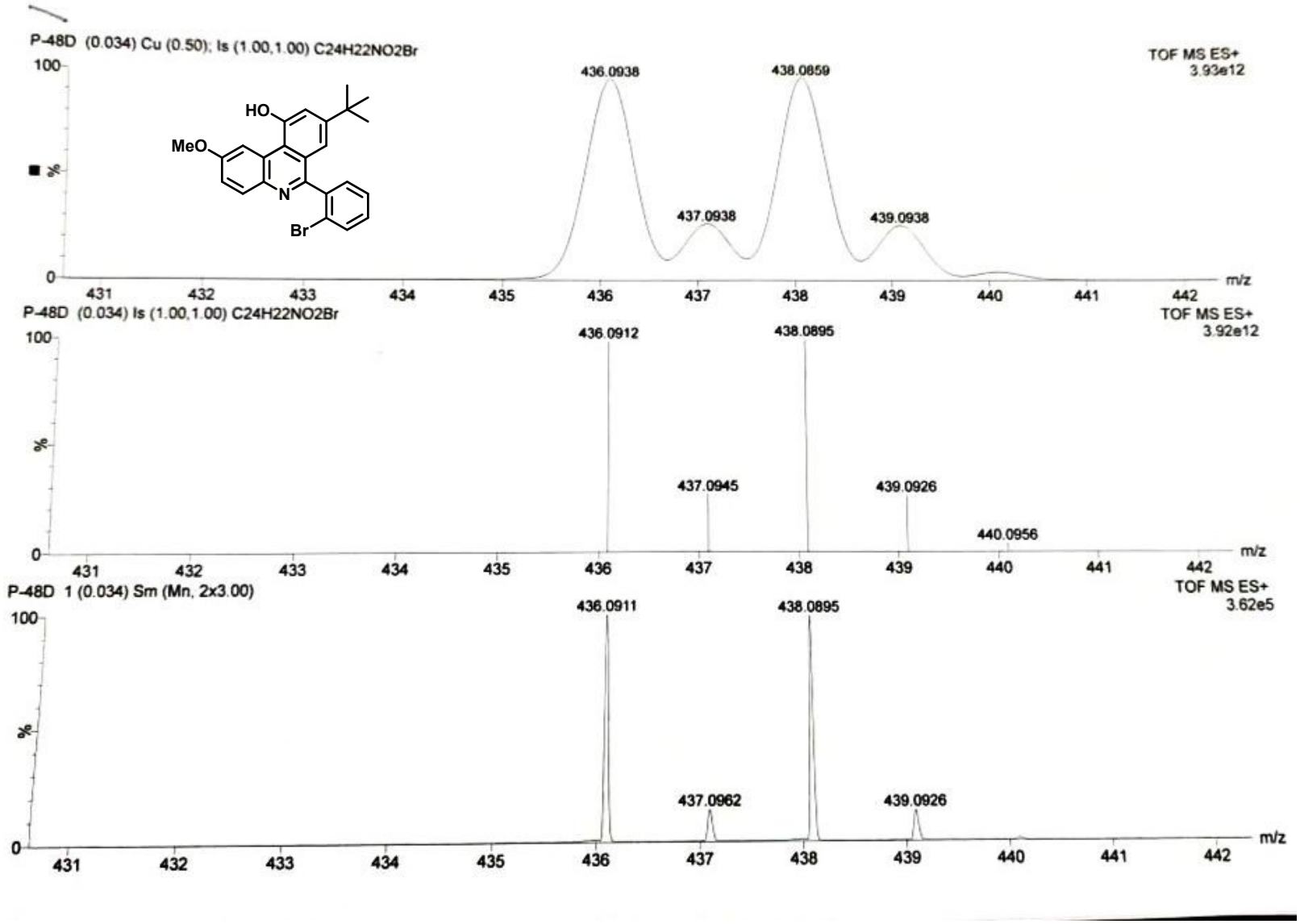
^{1}H NMR Spectrum of Compound 8d



^{13}C NMR Spectrum of Compound 8d



HRMS Spectrum of Compound 8d

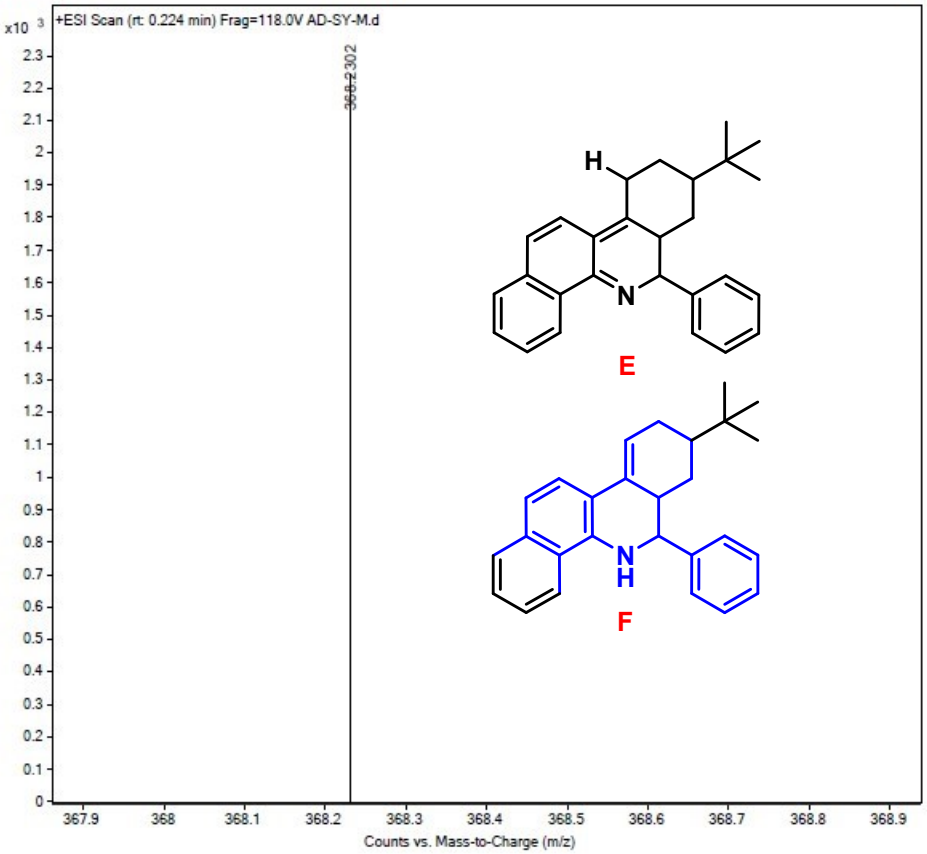


Detection of intermediates in HRMS

2-naphthylamine (1 mmol), benzaldehyde (1 mmol), and 4-*tert*butylcyclohexanone (1 mmol), 20 mol% CSA (46 mg) were taken in a r.b and dissolved in 1 mL DMSO. The reaction mixture was stirred at 120 ^{o}C temperature in a preheated oil-bath. After 2 h, reaction was stopped and a very little amount of it was subjected to ESI-MS mass experiment, and the intermediates **E, F, H** and **K** were detected by HRMS values. The spectra and observed m/z values for the intermediates are given below.

HRMS Spectrum of Intermediate E or F of compound 4l

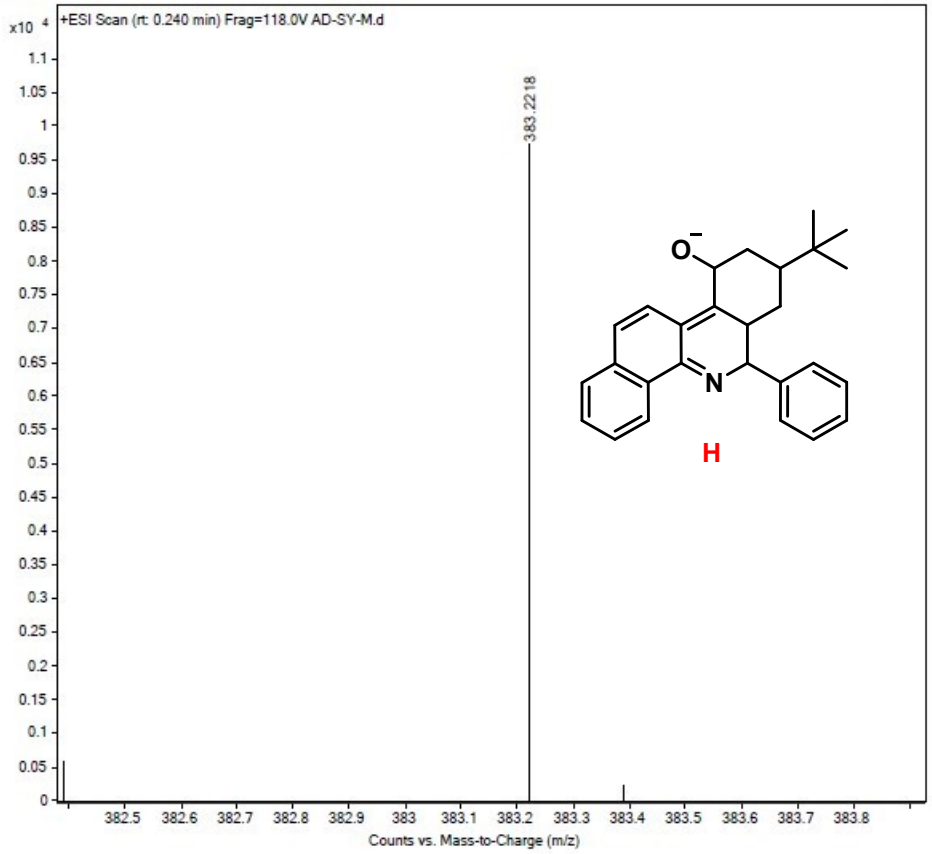
Sample Name	AD-SY-M	**Position**	Vial 25	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	0.1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Some Ions Missed	**Data Filename**	AD-SY-M.d
ACQ Method	Direct Mass-2017.m	**Comment**		**Acquired Time**	28-Mar-22 09:14:42 PM (UTC+05:30)



HRMS (ESI) Calcd for $C_{27}H_{30}N$ 368.2373 ($M + H^+$); Found 368.2302

HRMS Spectrum of Intermediate H of compound 4l

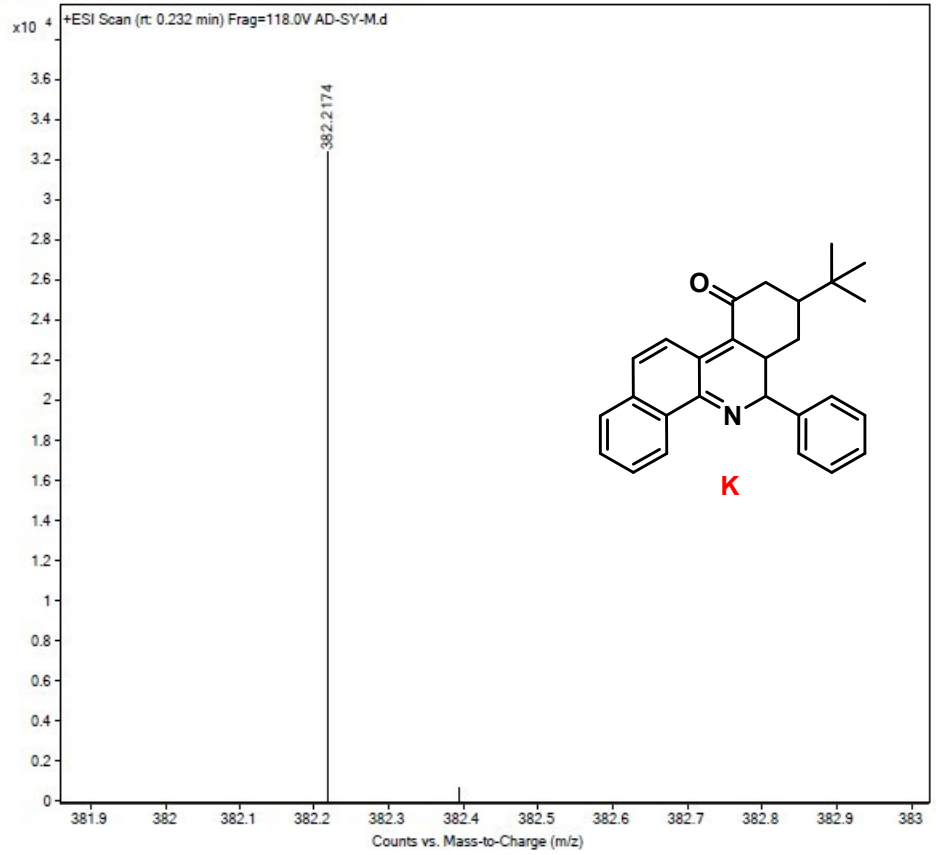
Sample Name	AD-SY-M	**Position**	Vial 25	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	0.1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Some Ions Missed	**Data Filename**	AD-SY-M.d
ACQ Method	Direct Mass-2017.m	**Comment**		**Acquired Time**	28-Mar-22 09:14:42 PM (UTC+05:30)



HRMS (ESI) Calcd for $C_{27}H_{29}NO$ 383.2249 ($M + H^+$); Found 383.2218

HRMS Spectrum of Intermediate K of compound 4l

Sample Name	AD-SY-M	**Position**	Vial 25	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	0.1	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Some Ions Missed	**Data Filename**	AD-SY-M.d
ACQ Method	Direct Mass-2017.m	**Comment**		**Acquired Time**	28-Mar-22 09:14:42 PM (UTC+05:30)



HRMS (ESI) Calcd for $C_{27}H_{28}NO$ 382.2166 ($M + H^+$); Found 382.2174

Stock solutions preparation

The stock solutions of the chemosensors (**4s**, **4x** and **4u**) were prepared in DMSO at 10^{-3} M and the solutions were diluted as per experimental requirements. The anionic salts (with tetrabutylammonium counterion), like F^-, HSO_4^-, PO_4^{3-}, OAc^-, Cl^-, Br^-, I^-, CN^-, CO_3^{2-}, ClO_4^-, NO_3^-, N_3^-*etc*. were prepared in 10^{-2} M in DMSO/H_2O (v/v 7/3) and were similarly diluted as per requirement.

Table S3. Optical data of **4s**, **4x**, and **4u** in different organic solvents.

Solvents	λ_{Em} /nm		
	4s	**4x**	**4u**
Hexane	430	434	440
Dichloromethane (DCM)	435	434	448
Methanol (MeOH)	448	438	460
Acetonitrile (MeCN)	437	438	447
Dimethyl sulfoxide (DMSO)	442	450	454

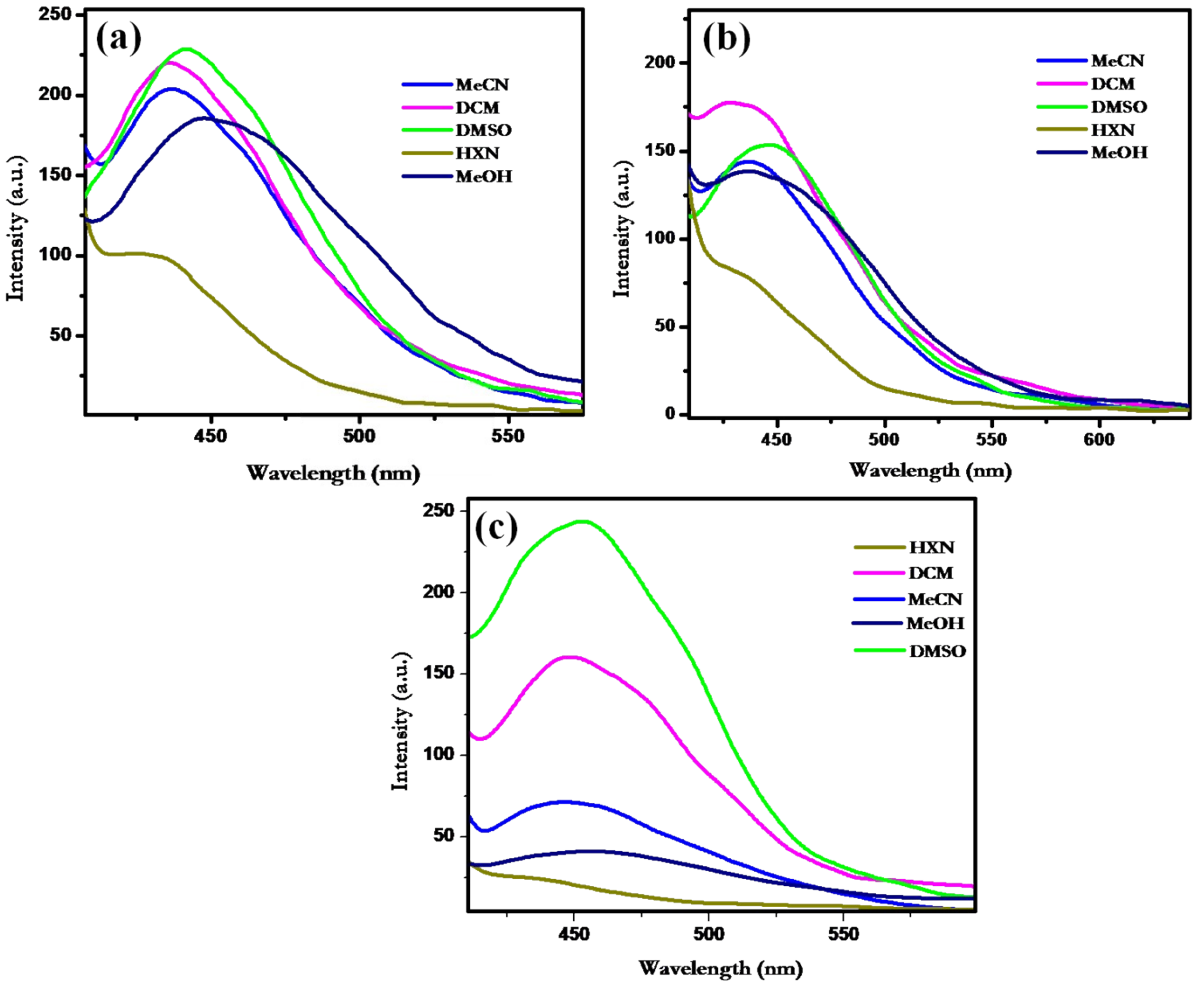


Figure S2. Emission spectral changes of **(a) 4s, (b) 4x** and **(c) 4u** in different organic solvents.

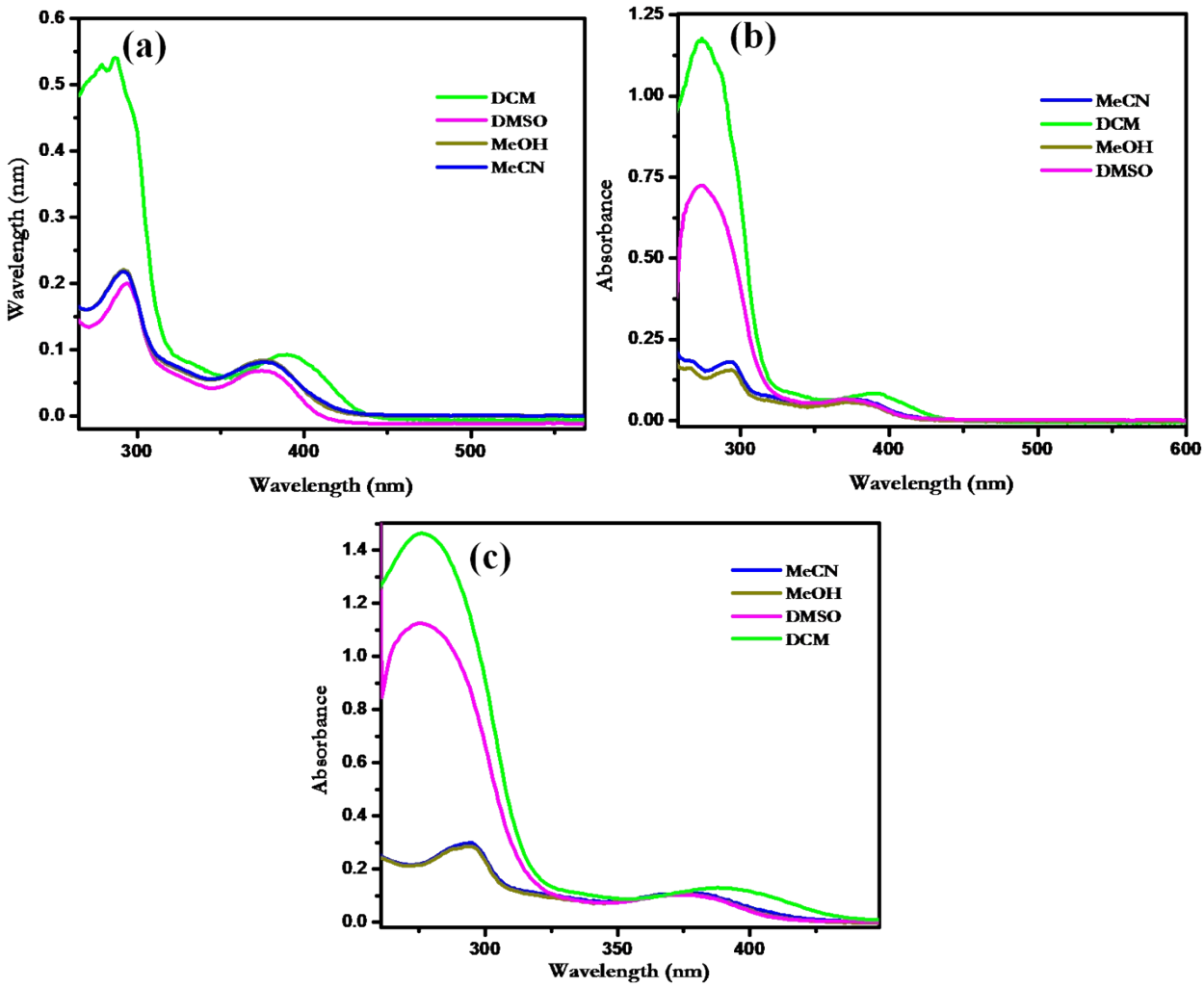
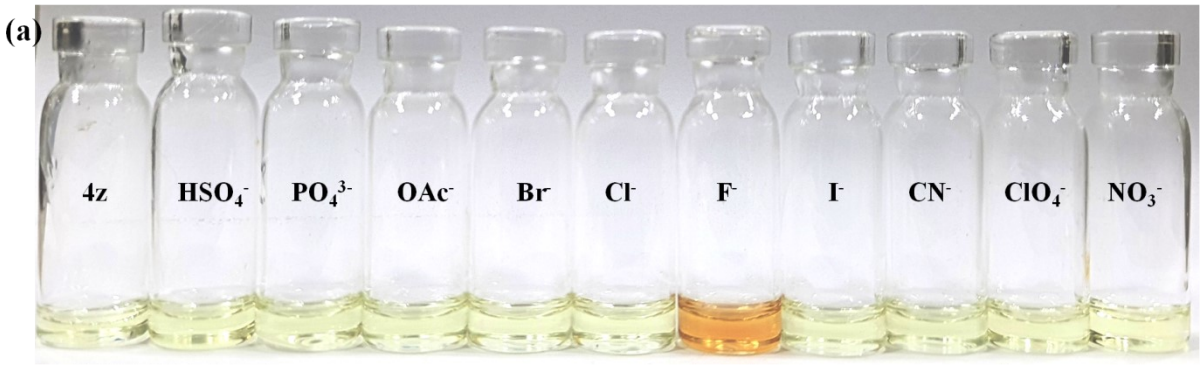


Figure S3. UV-Vis absorption spectral changes of **(a) 4s, (b) 4x** and **(c) 4u** in different organic solvents.



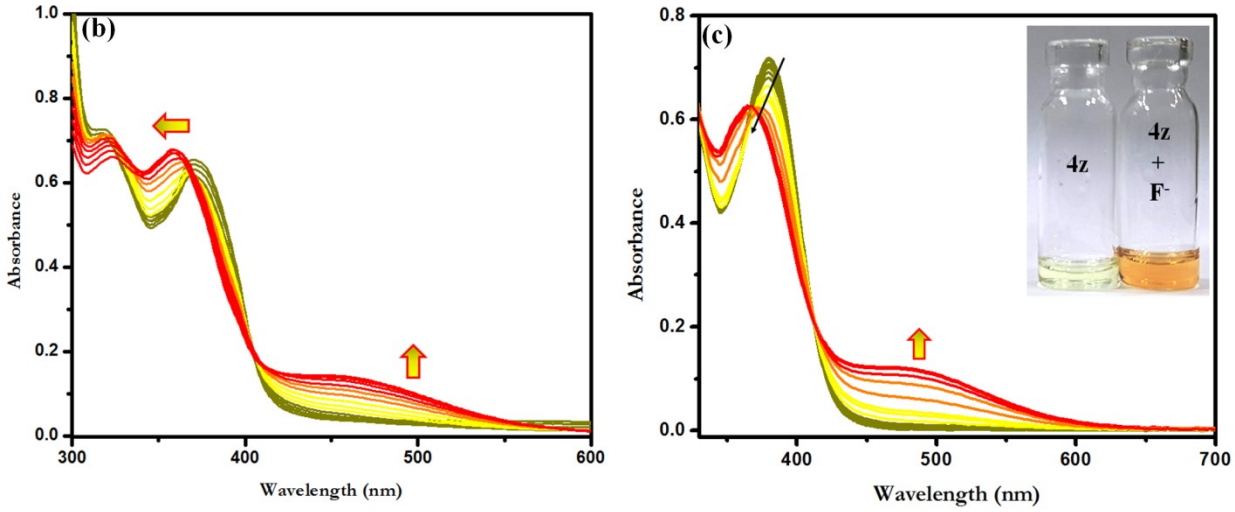
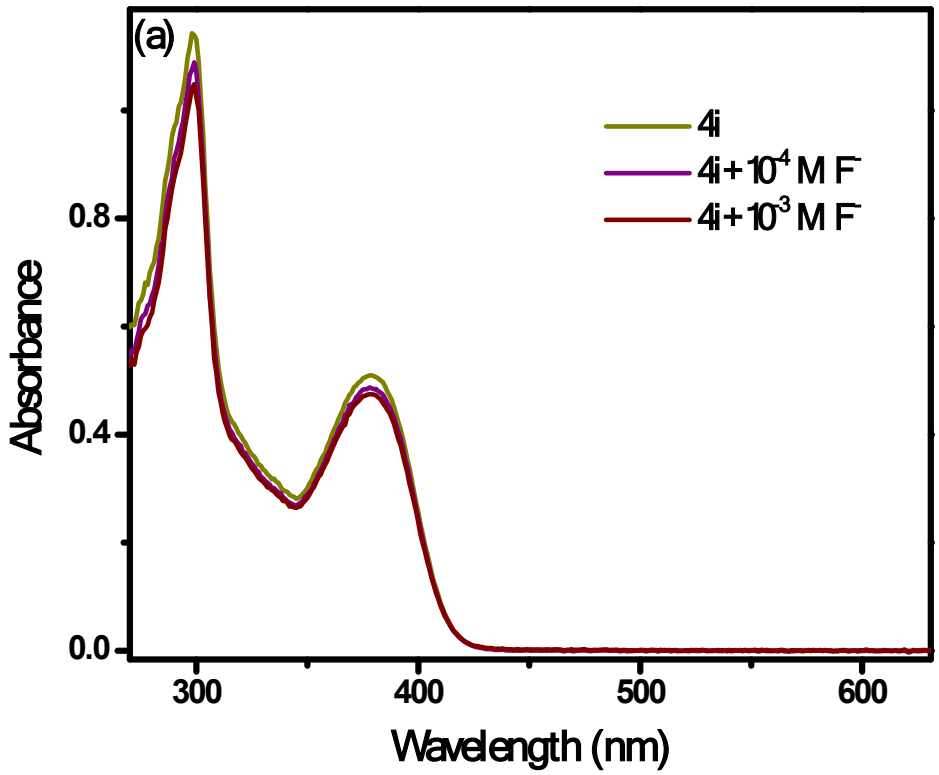


Figure S4. (a) Selectivity of **4z** in presence of diverse anions; UV-Vis titration of **(b) 4x** and **(c) 4z** (100 μM in DMSO) in presence of 60 μL and 100 μL F^- in 0.5 mM DMSO/H_2O (v/v 7/3) respectively.



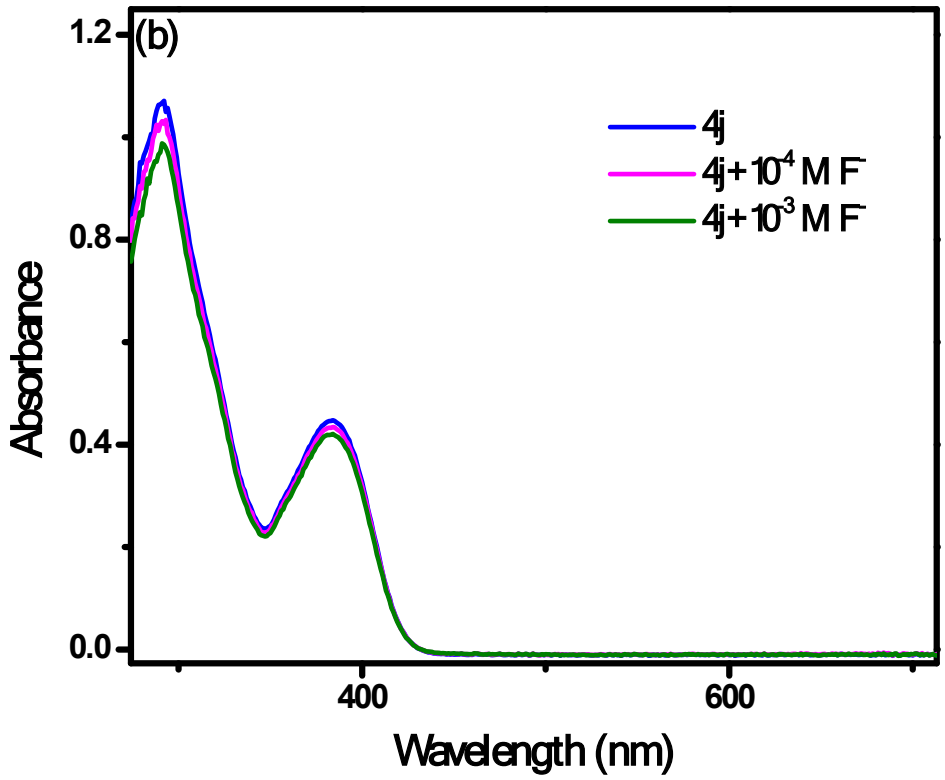
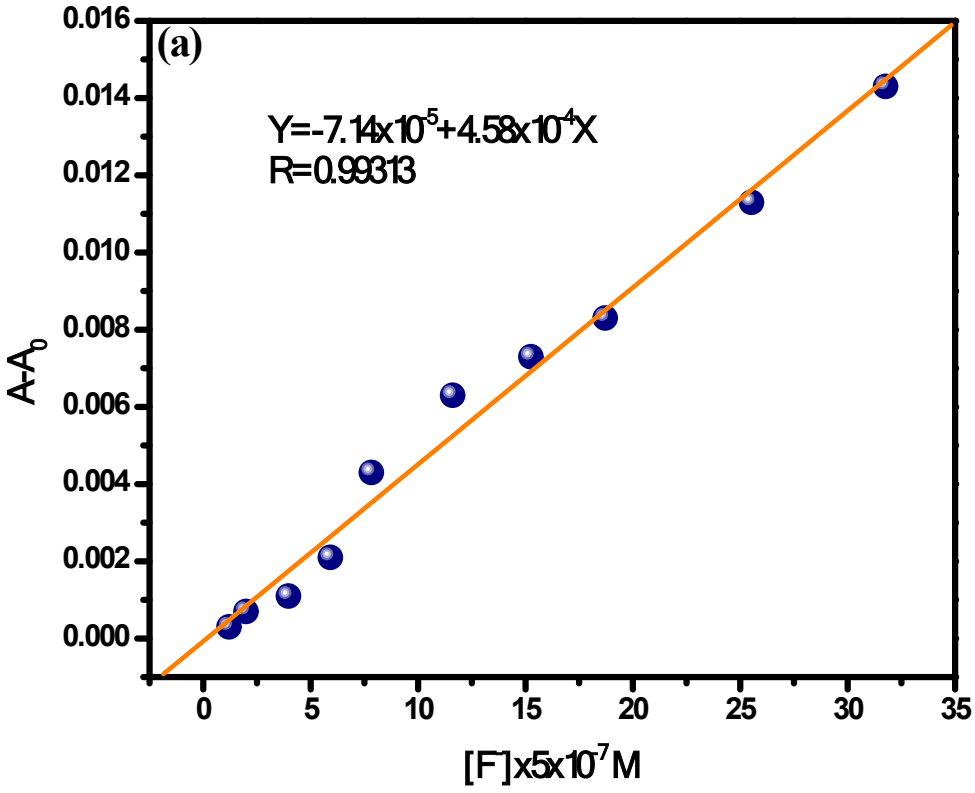
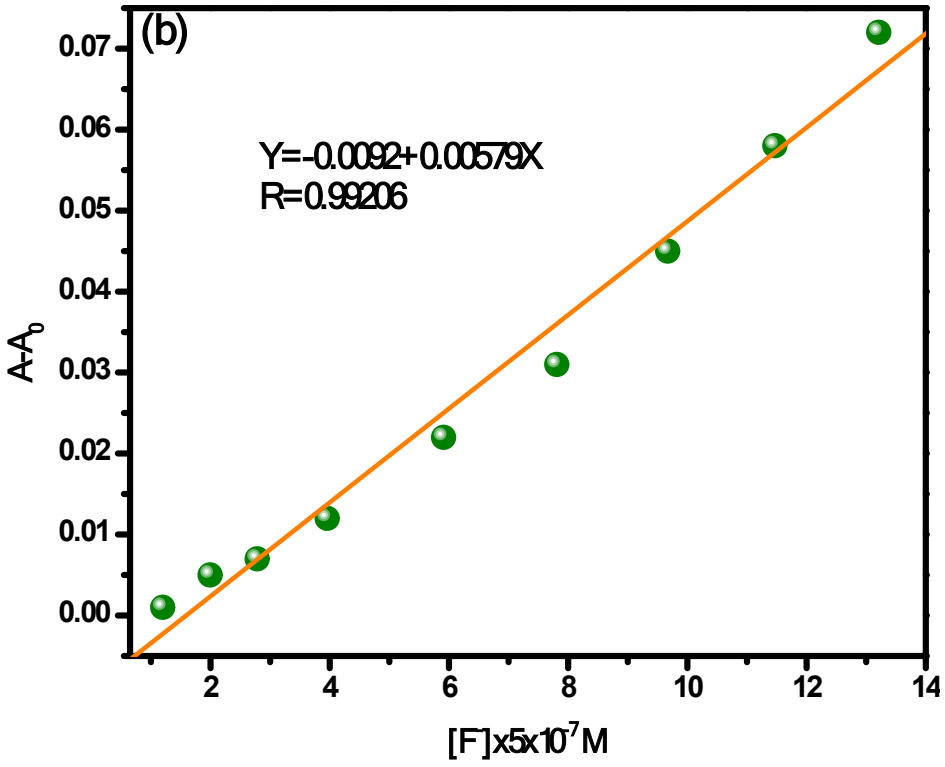
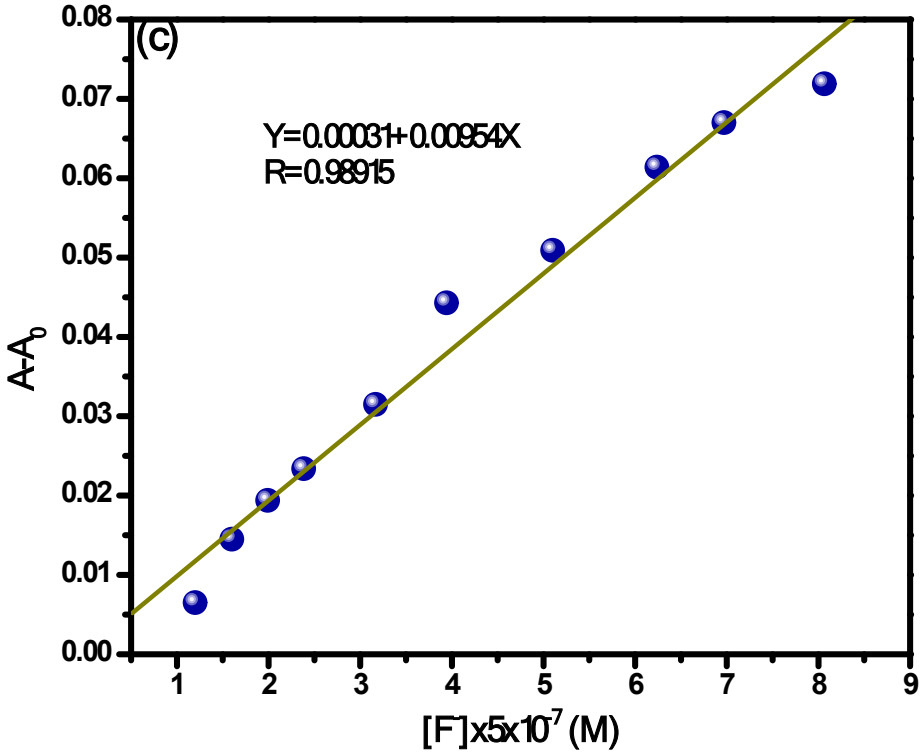


Figure S5. UV-Vis spectral data of **(a) 4i** (100 μM in DMSO) (b) **4j** (100 μM in DMSO) in presence of F^- in DMSO/H_2O (v/v 7/3).




(b)
Y=-0.0092+0.00579X
R=0.99206
A-A0
[F]x5x10-7 M


(c)
Y=0.00031+0.00954X
R=0.98915
A-A0
[F]x5x10-7 (M)

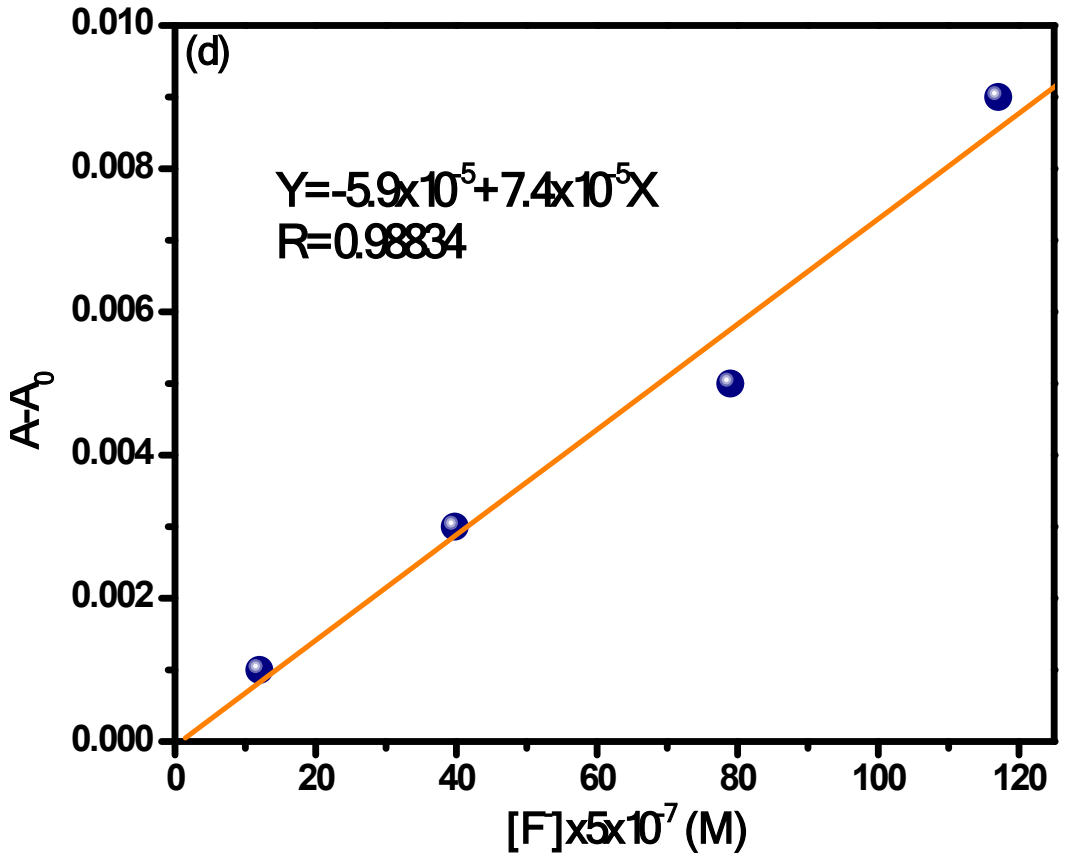


Figure S6. Calculation of LOD of **(a) 4s, (b) 4x, (c) 4u** and **(d) 4z** towards F^-.

Table S4. Comparative literature survey of the recently reported F^- specific chemosensors

Sl. No.	Sensing materials	LOD	Response time	Solid state sensing	Application in molecular electronics	*Ref.*
1.	Porphyrin-based receptor	10 µM	-	NO	NO	S1
2.	Bispyrenyl thioureas-polyethylene glycol (PEG)conjugatesbased receptor	2.43 µM	-	NO	NO	S2
3.	Schiff base chemosensor	0.12µM	-	NO	YES	S3
4.	Triphenylphosphoniumsalt based receptor	0.2 ppm	-	NO	NO	S4
5.	Nickel-POCOP Pincer Receptors	5.66 µM	-	NO	NO	S5
6.	Copper(II)bis(terpyridine) complex	5.07 µM	-	NO	NO	S6
7.	Carbon dotsbased receptor	1.26 µM	-	NO	NO	S7
8.	CdTe quantum dots	0.285 µM	15 min	YES	NO	S8

	based receptor					
9.	2,3-dipyrrol-2′-yl-quinoxaline based receptor	0.15 ppm	-	NO	NO	S9
10.	**6-aryl-8,9-dihydrobenzo[c]phenanthridine-10(7H)-ones based receptor**	**4s: 2.5 µM (0.65 ppm), 4x: 1.3 µM (0.34 ppm) and 4u: 2.3 µM (0.6 ppm) 4z: 6.9 µM (2.2 ppm)**	**~18 s**	**YES**	**YES**	**Present work**

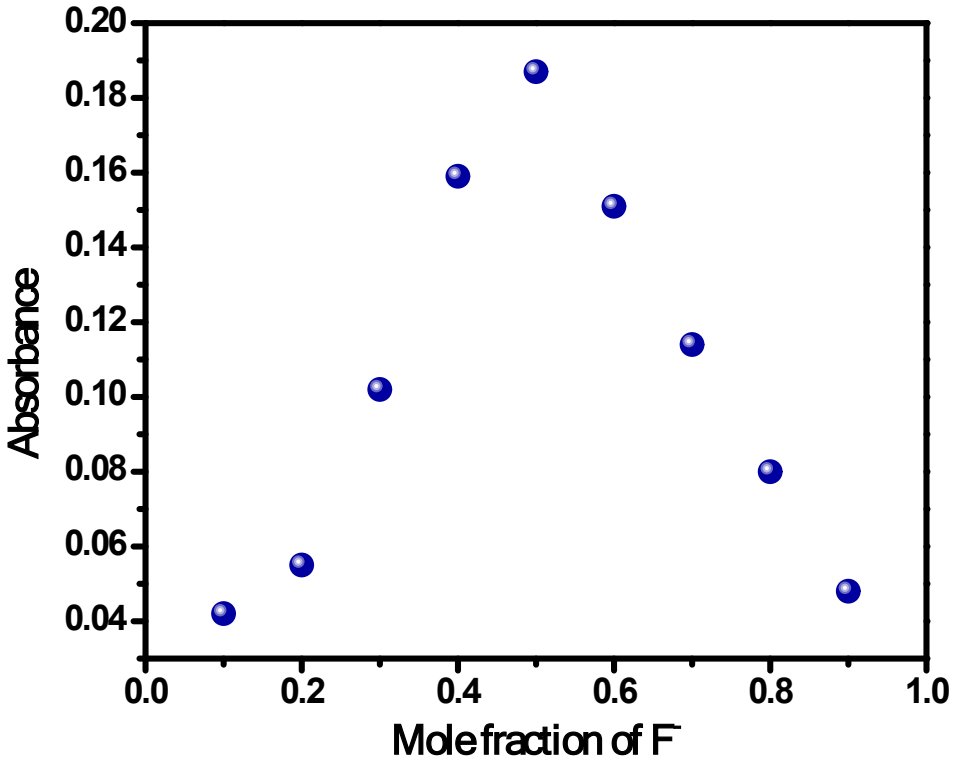
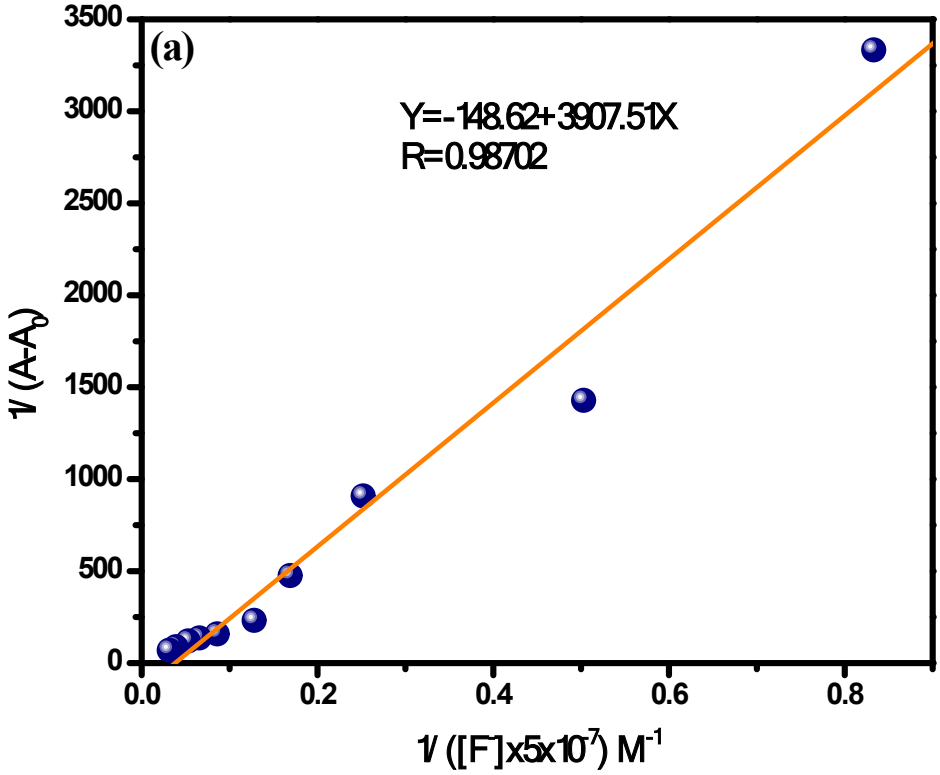
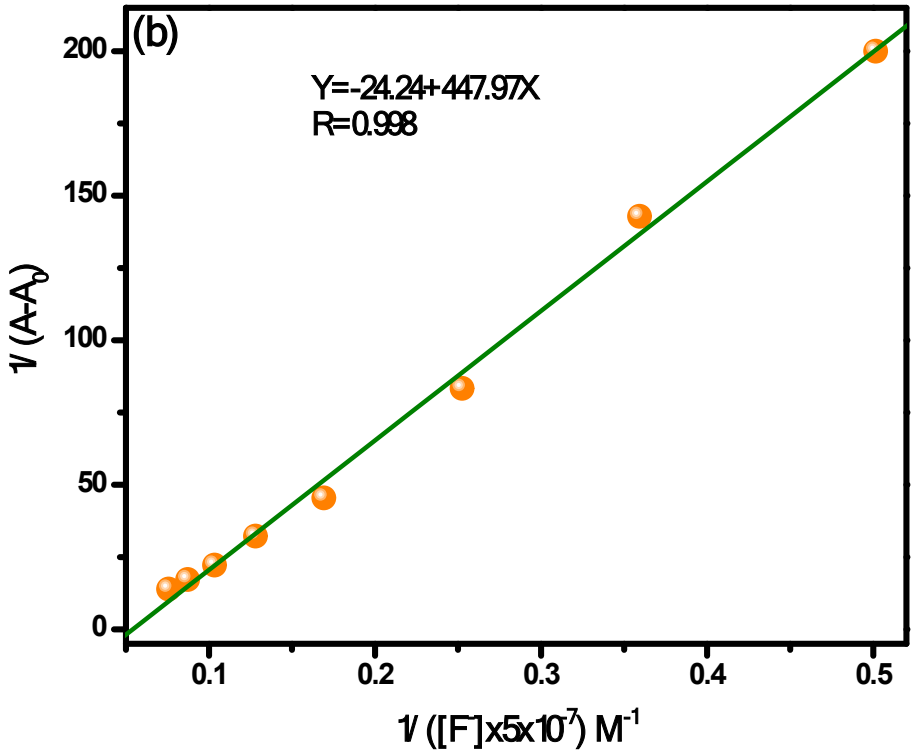


Figure S7. Job's plot of **4s** with F^- for the stoichiometry determination monitoring the change of absorbance at 460 nm.


(a)
Y=-148.62+3907.51X
R=0.98702
1/ (A-A0)
1/ ([F-]x5x10-7) M-1
3500
3000
2500
2000
1500
1000
500
0
0.0
0.2
0.4
0.6
0.8


(b)
Y=-24.24+447.97X
R=0.998
1/ (A-A0)
1/ ([F-]x5x10-7) M-1
200
150
100
50
0
0.1
0.2
0.3
0.4
0.5

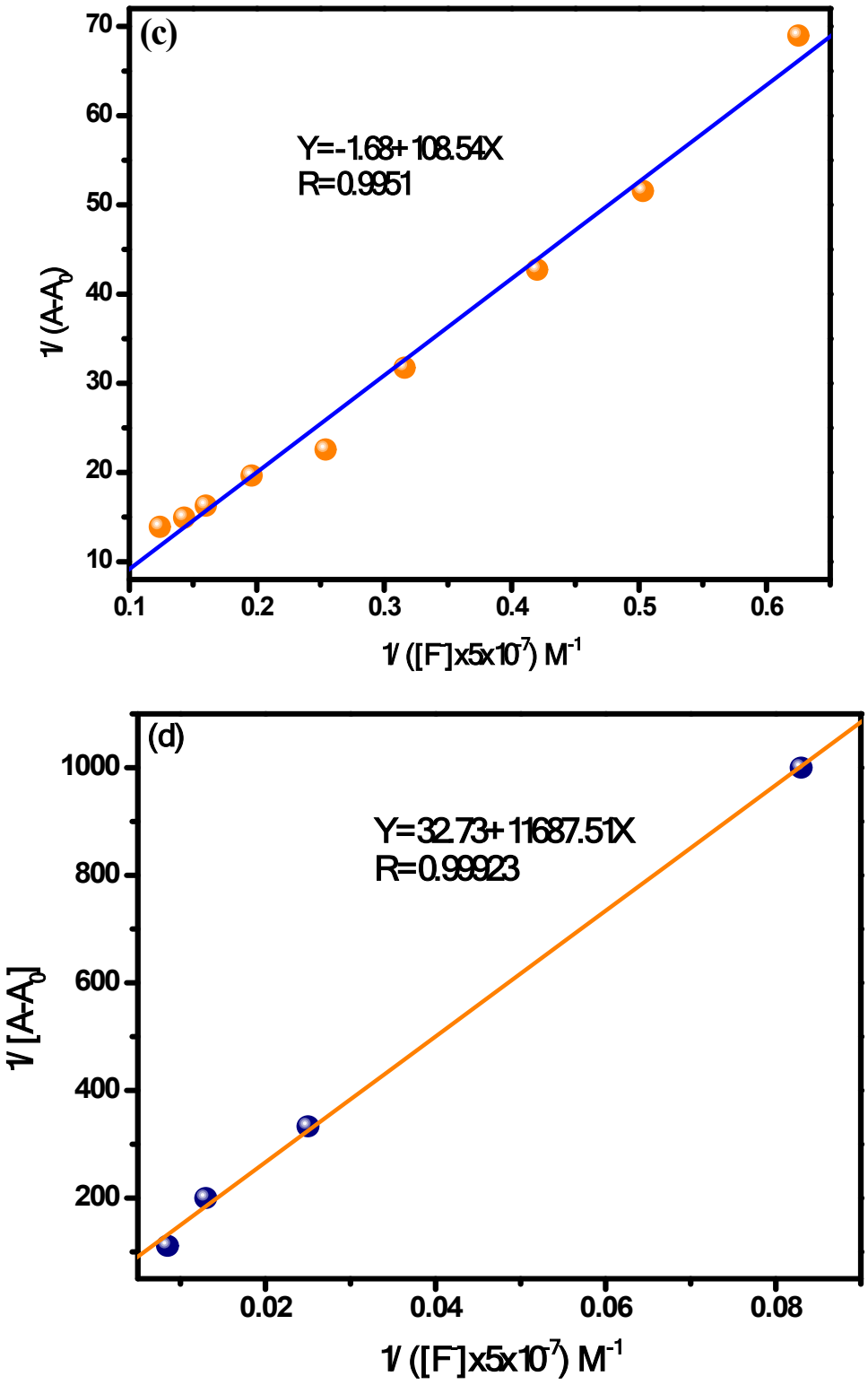
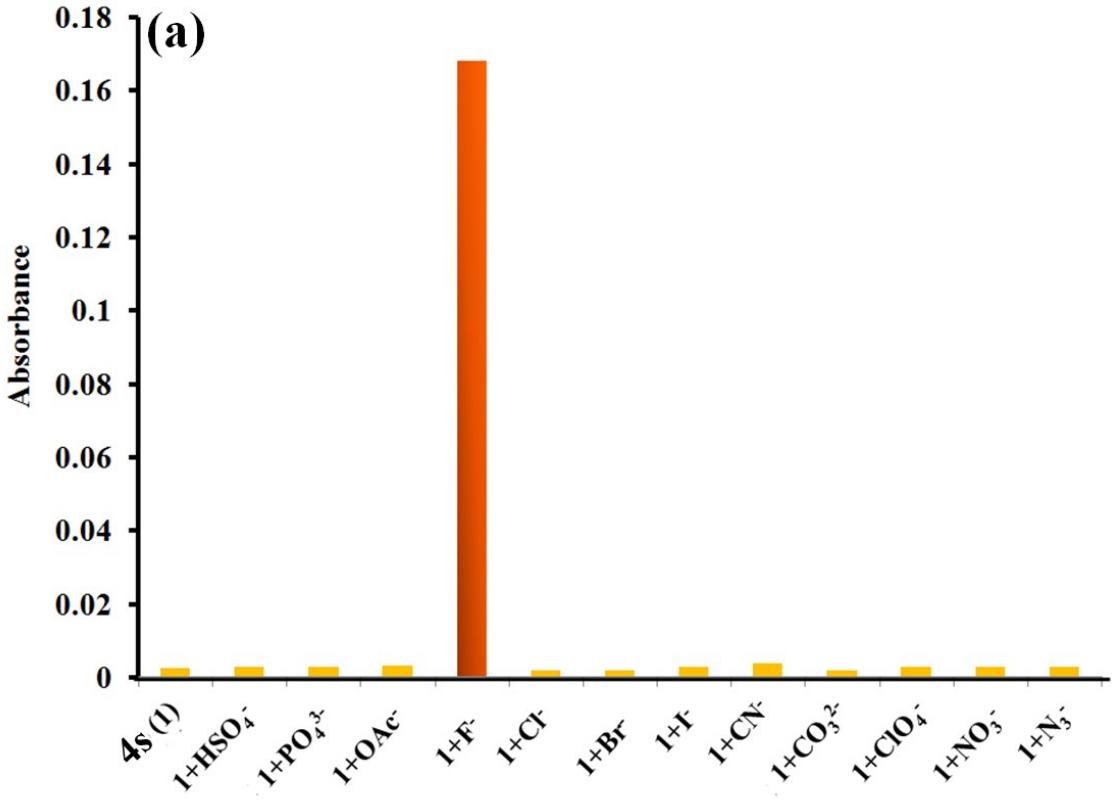
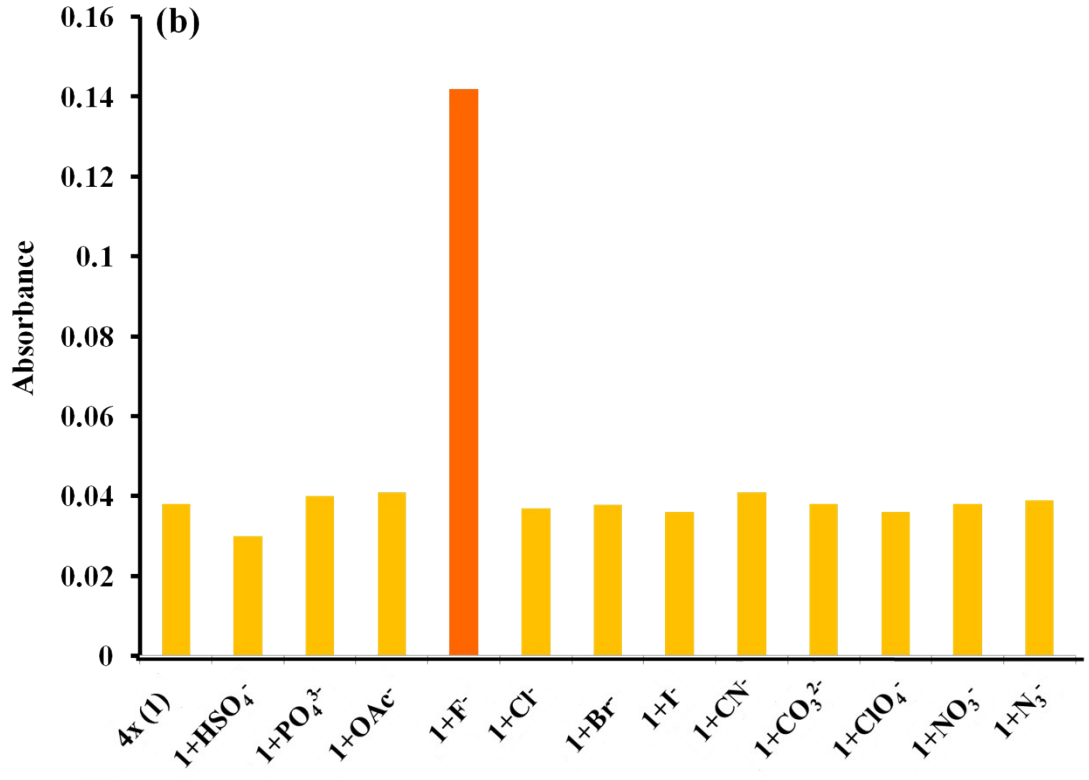


Figure S8. B–H plot of **(a) 4s**, **(b) 4x**, **(c) 4u** and **(d) 4z** for the association constant determination towards F^-.


(a)
Absorbance
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
4s (1)
1+HSO4-
1+PO4 3-
1+OAc-
1+F-
1+Cl-
1+Br-
1+I-
1+CN-
1+CO3 2-
1+ClO4-
1+NO3-
1+N3-


(b)
Absorbance
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
4x (1)
1+HSO4-
1+PO4 3-
1+OAc-
1+F-
1+Cl-
1+Br-
1+I-
1+CN-
1+CO3 2-
1+ClO4-
1+NO3-
1+N3-

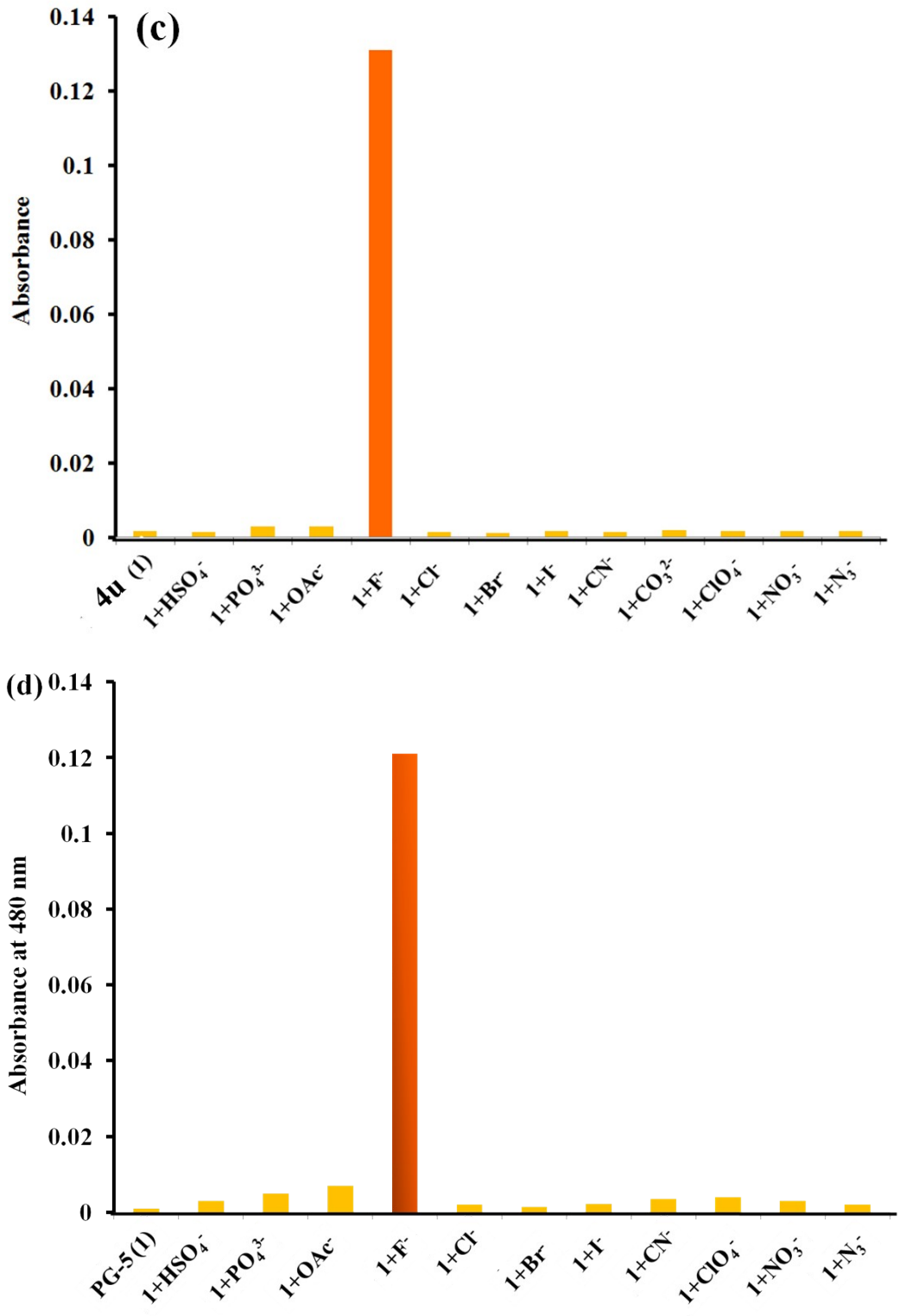
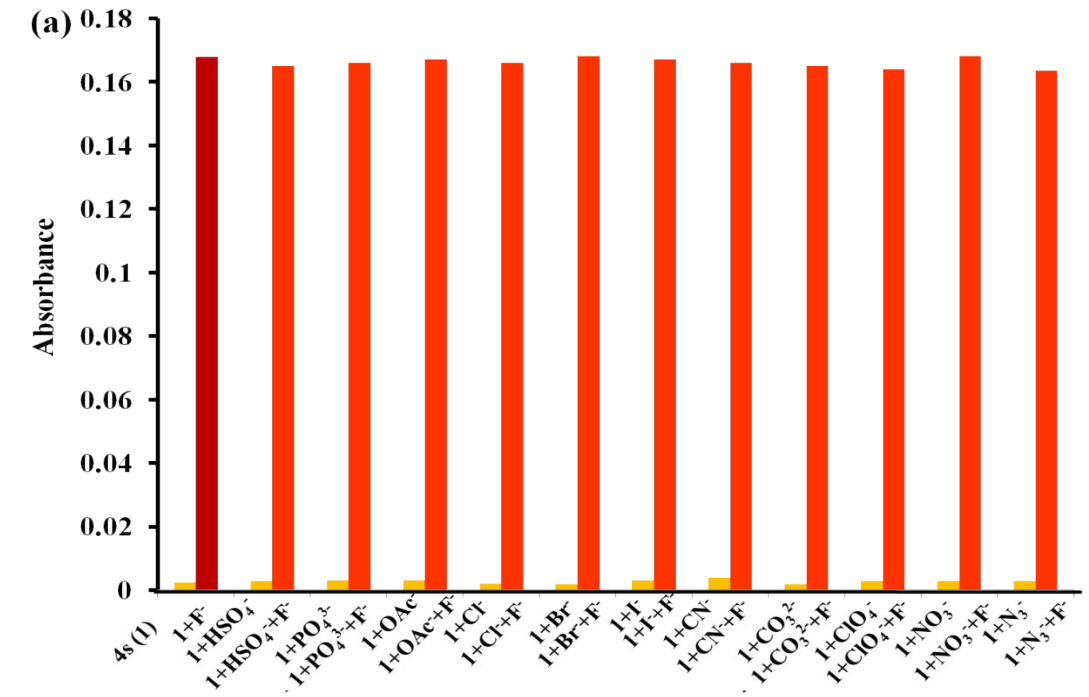
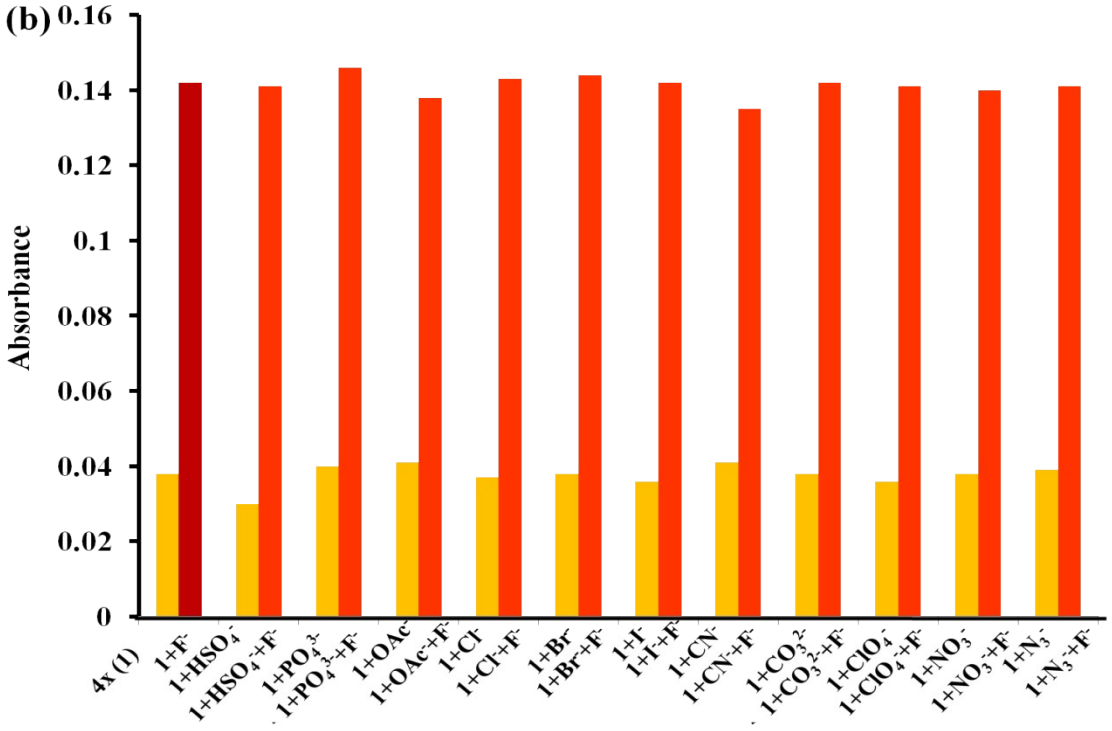


Figure S9. UV-Vis spectral response of **(a) 4s**, **(b) 4x** and **(c) 4u** (100 μM) in presence of different anions in 0.5 mM DMSO/H_2O (v/v 7/3) at 460 nm and (d) UV-Vis spectral response of **4z** (100 μM) in presence of different anions in 0.5 mM DMSO/H_2O (v/v 7/3).


(a)
Absorbance
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
4s (1)
1+F-
1+HSO4-
1+HSO4-+F-
1+PO43-
1+PO43-+F-
1+OAc-
1+OAc-+F-
1+Cl-
1+Cl-+F-
1+Br-
1+Br-+F-
1+I-
1+I-+F-
1+CN-
1+CN-+F-
1+CO32-
1+CO32-+F-
1+ClO4-
1+ClO4-+F-
1+NO3-
1+NO3-+F-
1+N3-
1+N3-+F-


(b)
Absorbance
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
4x (1)
1+F-
1+HSO4-
1+HSO4-+F-
1+PO43-
1+PO43-+F-
1+OAc-
1+OAc-+F-
1+Cl-
1+Cl-+F-
1+Br-
1+Br-+F-
1+I-
1+I-+F-
1+CN-
1+CN-+F-
1+CO32-
1+CO32-+F-
1+ClO4-
1+ClO4-+F-
1+NO3-
1+NO3-+F-
1+N3-
1+N3-+F-

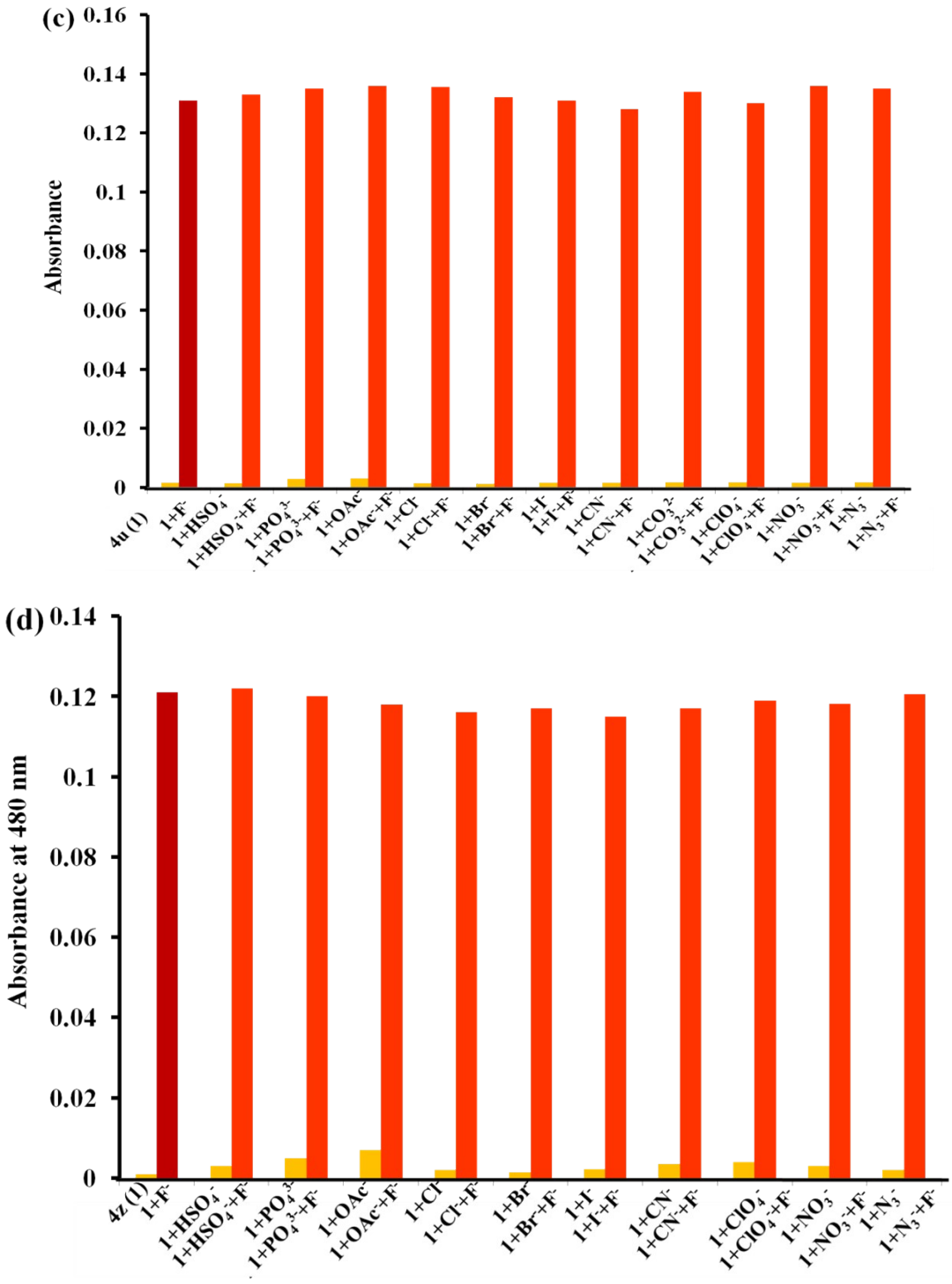


Figure S10. UV-Vis spectral response of **(a)4s**, **(b) 4x** and **(c) 4u** (100 μM) towards F^- in the co-existence of different anions in 0.5 mM DMSO/H_2O (v/v 7/3) at 460 nm and **(d)** UV-Vis spectral response of **4z** (100 μM) towards F^- in the co-existence of different anions in 0.5 mM DMSO/H_2O (v/v 7/3).

Response time study of the chemosensors towards fluoride sensing

Response time of any sensing event is another important thing to be considered for real time applications. Therefore, to check the reaction kinetics of the chemosensors, 50 µL 0.5 mM F^- in DMSO/H_2O (v/v 7/3) was taken in **4s** (100 µM, DMSO) and the absorption spectral changes were recorded as a function of time. From **Figure S11**, ESI, it has been observed that the absorbance at 460 nm reached maximum within ~18 s and then remained almost constant. The photostability of the chemosensor was also confirmed by the almost constant absorbance values of the bare chemosensor at 460 nm. Thus, this kinetic study revealed that the interaction of the chemosensors with F^- rapidly reached the equilibrium condition, which indicates the real time applicability of the chemosensors for quantitative detection of F^- without any sample pretreatment.

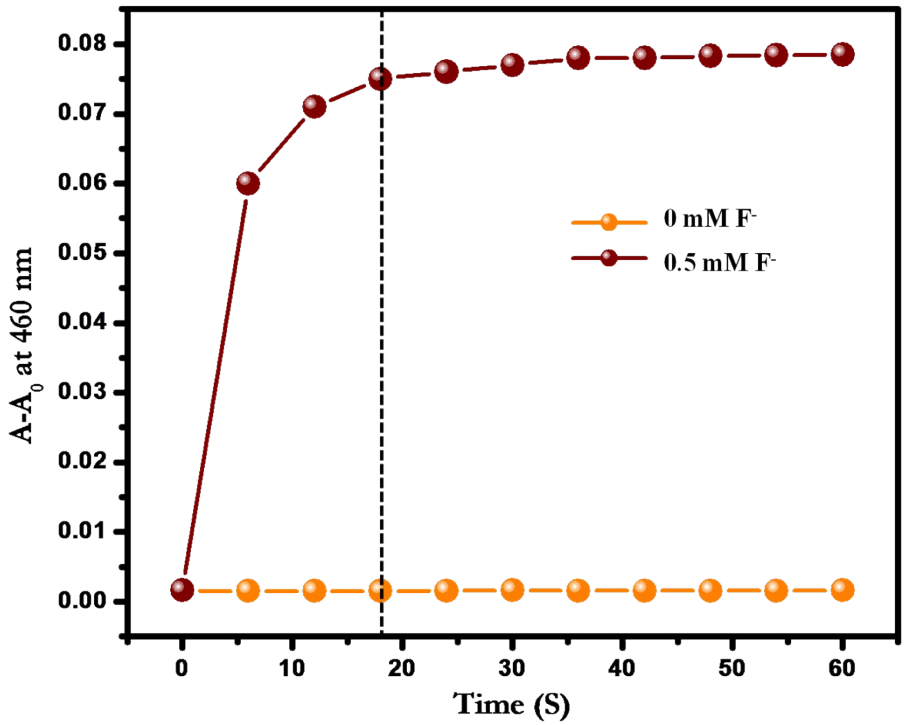


Figure S11. UV-Vis spectral response of **4s** (100 µM, DMSO) towards F^- (0.5 mM in DMSO/H_2O (v/v 7/3)) as a function of exposure time.

Table S5. Cartesian coordinates ofgeometry optimized structure of **4s**.

Atoms	Cartesian coordinates		
1 n	9.54997186921020	-17.57924663153041	-20.15730795284442
2 c	9.28942672426034	-18.05768499321611	-17.65961568286206

3 c	9.33539266771600	-20.69158236723568	-16.87034758276627
4 c	9.16391590834480	-21.27564797345726	-14.24404673184330
5 c	8.90065006836767	-19.24870975367521	-12.46586123330883
6 c	8.78199258427475	-16.77873135666376	-13.21267667566615
7 c	8.96342031677341	-16.07817557723723	-15.83684510564680
8 c	8.87310961811985	-13.53161216669644	-16.76436554333382
9 c	9.09789423538214	-13.15982732791385	-19.43888951433157
10 c	9.42265670397734	-15.26264555914701	-21.12177736304065
11 c	9.50937452144650	-22.71068032830836	-18.62422647948858
12 c	9.56207601810067	-25.20047768367432	-17.80786434086882
13 c	9.43598025882467	-25.77040570277283	-15.20352487531487
14 c	9.23087075155267	-23.83318184854578	-13.45262910518412
15 c	8.57017863976910	-11.28340908915006	-14.99015026581731
16 c	9.04841651799151	-10.56929297866518	-20.06911031490018
17 h	8.77185458047885	-19.71498931722476	-10.45480375371329
18 h	8.55530597492697	-15.29484719699943	-11.81458748107387
19 h	9.56149489917596	-22.30769796789949	-20.64469913051578
20 h	9.69044098626594	-26.73019624988554	-19.19291642114805
21 h	9.48284120756206	-27.73963960804390	-14.57432377711186
22 h	9.10746690300088	-24.25583117487626	-11.43187046376825
23 c	8.97524889158499	-12.80426771138479	-25.21168741154283
24 c	9.27994302502813	-12.56013168629363	-27.81224049192355
25 c	10.32710437600287	-14.56790439398477	-29.19638935757900
26 c	9.68721100282903	-15.01776924408622	-23.89448136265208
27 c	10.68563936641889	-17.06729346906724	-25.35227767161351

28 c	11.01825106770361	-16.79224186881771	-27.97687538068037
29 o	11.36450501124589	-19.27289349428588	-24.29929916796454
30 h	8.11828259844832	-11.24024404210402	-24.17166355060946
31 h	8.69114958671990	-10.82232517483034	-28.76259878027936
32 h	10.58335463683730	-14.39956880611170	-31.24221208404002
33 h	11.81388055470164	-18.38899486077599	-29.01983437031287
34 c	8.52317833480767	-8.63931233980823	-16.02278717972553
35 c	8.77745820484510	-8.73362090933310	-18.59679665159326
36 o	8.35191768534723	-11.51084107351546	-12.67587502808771
37 c	8.22115548702270	-6.45410239282567	-14.27372410363494
38 h	10.83546766677597	-19.16144820994414	-22.46584913471898
39 h	9.77854588232125	-6.41118307937204	-12.88026939243045
40 h	6.45309744381431	-6.63606896655139	-13.17449921204908
41 h	8.19423582789242	-4.65747920694014	-15.32129830950963

Table S6. Cartesian coordinates of geometry optimized structure of **4s** with F^-.

Atoms	**Cartesian coordinates**		
1 n	9.20556179385480	-17.14880388706549	-20.94335612232867
2 c	8.95217302253863	-17.93933110548009	-18.53723771970571
3 c	8.86716495123301	-20.66485405247724	-18.15445529363961
4 c	8.46214547109820	-21.64521026210130	-15.67979338070157
5 c	8.18812114553340	-19.90372625578453	-13.61650102860803
6 c	8.33601575700649	-17.34458447595005	-13.95301026258689
7 c	8.74040297273815	-16.25369395806720	-16.41648252510095
8 c	8.96206746899418	-13.60282700847361	-16.92340070158949
9 c	9.33873388922465	-12.87711302251704	-19.50710793026495

10 c	9.37594311674667	-14.71848450672537	-21.49964112511438
11 c	9.20320236838760	-22.35803244931850	-20.20324545345162
12 c	9.10717848406941	-24.94875493856735	-19.79813336118674
13 c	8.67235884465835	-25.92833442260473	-17.35240314926936
14 c	8.35949174305594	-24.29780091060280	-15.32313038511262
15 c	8.86238895298701	-11.63334017909509	-14.83994322330012
16 c	9.67938644107856	-10.23901567712718	-19.76172494515347
17 c	8.18274852437679	-11.88349650874032	-25.09609723987009
18 c	8.23668461324557	-11.16432457927201	-27.63250354683531
19 c	9.73029337127760	-12.56729062908296	-29.32410613930026
20 c	9.56214969815797	-13.97676050549546	-24.18508209525388
21 c	11.13551927749314	-15.41605515619471	-25.89420642895341
22 c	11.13015662596727	-14.62450618934668	-28.47612727086571
23 o	12.55467718669803	-17.27270982958936	-25.15125129645504
24 c	9.24403911330336	-8.88864825190915	-15.46172693976677
25 c	9.58889628972812	-8.63692703248570	-18.01398466090863
26 o	8.47188351796145	-12.16409208974162	-12.59448846731553
27 c	9.15748425336868	-6.96057031327545	-13.40772760767202
28 h	7.86919381915059	-20.66754336274222	-11.71995238647079
29 h	8.14305287607263	-16.08318148623071	-12.34442118558183
30 h	9.57269889533749	-21.59833758690790	-22.08966995462085
31 h	9.37982489564314	-26.24308503747599	-21.38914580789428
32 h	8.59427342463954	-27.97453102198926	-17.05803395344750
33 h	8.03756705924285	-25.04241540123622	-13.41982807976976
34 h	6.96373820201045	-10.84202360396820	-23.78875598447607

35 h	7.11105604685271	-9.55926753406784	-28.29050073014938
36 h	9.79250011162040	-12.04727037478495	-31.32857676844558
37 h	12.31178108040053	-15.71060482256741	-29.78388137214916
38 h	11.59791739696074	-19.57868924255146	-25.64216184189746
39 h	10.49785961797164	-7.44939023365241	-11.88243623617550
40 h	7.25989608298807	-6.90765124666465	-12.52957822694275
41 h	9.61054152275377	-5.06695104908931	-14.14086779077245
42 f	10.78436462409794	-21.32841182139233	-26.04676981339317
43 n	7.05234671875387	-19.51848401972508	-43.37772147347339
44 c	9.18611674065189	-18.08370507244376	-42.17070719706069
45 c	5.55939587962654	-17.76946433801409	-45.04494234575699
46 c	8.10503208623228	-21.64562941532696	-44.93826495805211
47 c	5.35911525353117	-20.57501767715429	-41.35623984581529
48 h	4.60426678230814	-19.00131887036587	-40.23028680877241
49 h	6.47361871624539	-21.84920125249823	-40.15267831625147
50 h	3.80886246137845	-21.61727178165421	-42.26407405672620
51 h	6.52662518659619	-22.67704979224590	-45.80947166471496
52 h	9.18985700862308	-22.90870131451110	-43.69661082820348
53 h	9.33912718911639	-20.84751662829169	-46.40598626758224
54 h	4.80241064414744	-16.22456375969206	-43.88116644777080
55 h	4.00684976667954	-18.84125401826328	-45.91399117627599
56 h	6.81895864980422	-17.01221301961979	-46.51260965033367
57 h	8.39052657782681	-16.53452994563551	-41.03896619516538
58 h	10.40856756115213	-17.32365025110674	-43.66814105670360
59 h	10.26012248357353	-19.38282473677058	-40.95710800013284

Table S7. Cartesian coordinates of geometry optimized structure of **4u**.

Atoms	Cartesian coordinates		
1 n	9.50514077574996	-17.71026161083915	-20.15880765209527
2 c	9.26673214274833	-18.16643999582583	-17.66335681823626
3 c	9.32430484271339	-20.77777487937581	-16.80756545820717
4 c	9.14823986200343	-21.28727265329839	-14.16528923693049
5 c	8.88664658339323	-19.21887165728603	-12.42852109476822
6 c	8.77267592947308	-16.76640134731154	-13.22907276262716
7 c	8.95359379437365	-16.15230547744866	-15.87001525745779
8 c	8.94114462946756	-13.64160799453724	-16.83495617512133
9 c	9.35316312060773	-13.24640234274523	-19.45772637291772
10 c	9.49649656898450	-15.38398168436257	-21.11227700630490
11 c	9.51949196825556	-22.83583965442007	-18.50854002573579
12 c	9.58185085510031	-25.30317817006786	-17.62636816200699
13 c	9.44266392238427	-25.80343691241326	-15.00905681941178
14 c	9.22127659844125	-23.82299717789465	-13.30860688027910
15 c	8.36660354344161	-11.35808014145610	-15.15076990620835
16 c	9.92840403941629	-10.69360442186672	-20.21302210825731
17 c	8.91398405088381	-12.81607780236532	-25.05104053265600
18 c	9.25859330923524	-12.45713289155387	-27.63377666176486
19 c	10.33015045321022	-14.36872995165950	-29.11941489463890
20 c	9.66929056904764	-15.08478195267093	-23.86667342448514
21 c	10.66610467722264	-17.06755127134316	-25.40449993445436
22 c	11.01827410971460	-16.65078999363763	-28.00293305829262
23 o	11.32355645076255	-19.31688405273319	-24.44048321640758

24 c	9.27911199275764	-9.03106152460894	-16.41431136872085
25 c	8.86186396532310	-8.89817330394806	-18.81829658881705
26 o	7.27940919923954	-11.46388875109551	-13.13370366596336
27 cl	8.27218817570254	-9.62335463920540	-29.04443933740578
28 h	8.76655796305379	-19.64278501908112	-10.40814411932220
29 h	8.54319269203319	-15.24740567871056	-11.86318057948403
30 h	9.58264291352867	-22.48060846922560	-20.53838253295420
31 h	9.72985035989340	-26.86852031877643	-18.96866499615755
32 h	9.49340860106103	-27.75518879975629	-14.32836428945970
33 h	9.09359613007204	-24.19513653282809	-11.27851013627145
34 h	7.93261580638009	-11.35283749961070	-23.97189097258454
35 h	10.58578442393215	-14.08521892154133	-31.14880864209191
36 h	11.82688092634155	-18.17498621849714	-29.13844875729322
37 h	10.79680642201717	-19.30383486986685	-22.61662674271322

Table S8. Cartesian coordinates of geometry optimized structure of **4u** with F^-.

Atoms	**Cartesian coordinates**		
1 n	9.79971094883987	-16.98321194009421	-21.35010908386724
2 c	9.72335286891313	-17.81436849076757	-18.95561401067922
3 c	10.17826255770352	-20.49724455251539	-18.53426172420323
4 c	10.08042370707435	-21.47496149636885	-16.02672028817478
5 c	9.55569894181544	-19.78179653963569	-13.96722735538765
6 c	9.14784209544847	-17.25803883305629	-14.33946176679810
7 c	9.21924463612863	-16.18057231468538	-16.83652955317933
8 c	8.90205831963991	-13.56921997078083	-17.37469511621308
9 c	9.21985497848518	-12.73395623831172	-19.90819181695180

10 c	9.53697407471434	-14.55392460870856	-21.89696126839192
11 c	10.71982388254394	-22.14319761717299	-20.57334937824578
12 c	11.14615623563657	-24.69383480144542	-20.12611096261826
13 c	11.04237054713577	-25.67438609996525	-17.64583358379883
14 c	10.51740441809945	-24.08608160878563	-15.62652574213236
15 c	8.09899318121890	-11.66396469896762	-15.35949110237626
16 c	9.41913481600069	-10.04535615730453	-20.32626201470023
17 c	7.91697847090549	-11.66137933746545	-25.20635762053628
18 c	7.90595260071654	-10.67790816464985	-27.64637184161505
19 c	9.49370902498020	-11.71417617200815	-29.49695439314468
20 c	9.50595898812453	-13.70406699179031	-24.53812674397828
21 c	11.15994650112150	-14.83256567479152	-26.41142538213953
22 c	11.06422831747024	-13.72620766445861	-28.87599510417434
23 o	12.71911276041537	-16.63836481297540	-25.91759716214321
24 c	8.67060554001281	-9.04446419815253	-16.22195658730081
25 c	8.20599716910588	-8.68121725376866	-18.59095403848652
26 o	7.07864866461547	-12.21352519115939	-13.37608139306402
27 cl	5.84259122841971	-8.18146393857111	-28.42655760208380
28 h	9.49504517009810	-20.55645586044789	-12.05001160565459
29 h	8.75263219335792	-16.03202052528846	-12.73615887822904
30 h	10.79899574111725	-21.37764141741652	-22.49158909671217
31 h	11.56700807483875	-25.95467219713086	-21.71139775212912
32 h	11.37834007207762	-27.68878097534003	-17.31716671061928
33 h	10.43832554954262	-24.83260475327166	-13.69895460256208
34 h	6.54898125426558	-10.93207962055395	-23.83815641296725

35 h	9.47206676509300	-10.94670148706505	-31.41682842603243
36 h	12.32855432645488	-14.53947153776186	-30.29696332918883
37 h	11.85998090578140	-19.07894422379897	-26.20708018158905
38 f	11.20629296598200	-20.88276895652986	-26.50714421388057
39 n	15.17242429356049	-15.20460937368791	-38.09342055919366
40 c	15.48405044279240	-13.86122631376034	-35.61156108989780
41 c	15.02689199669863	-13.29491727195365	-40.19196983647819
42 c	17.39574040340679	-16.92036112795960	-38.52502384674649
43 c	12.78496775830361	-16.74316942660015	-38.04468322173987
44 h	12.58040981104549	-17.71490591650063	-39.86879594256348
45 h	11.17513820477071	-15.46817928389999	-37.73164058246183
46 h	12.91771137454724	-18.13239437627046	-36.50626416633516
47 h	17.47959229017735	-18.30352320178946	-36.97771175134688
48 h	17.14293515054953	-17.89063002171477	-40.34385447768022
49 h	19.12598613777755	-15.77184614313537	-38.55697045596778
50 h	14.79951992937985	-14.30301443738166	-41.99363777595072
51 h	16.78293505130516	-12.18598520618451	-40.20530424478367
52 h	13.39599438588674	-12.05444632867643	-39.85170665768003
53 h	13.85265727466974	-12.60747390921755	-35.32315473995585
54 h	17.23385710338471	-12.74389762075911	-35.66884709438902
55 h	15.59233617276048	-15.27794079136166	-34.09600008098064

Reversibility of the sensory probes and proposition of logic circuitry

As discussed in the main text, initially in absence of any input (*i.e*, both IN 1 and IN 2 are 0) the chemosensor, **4u** was pale yellow colored and the absorbance of **4u** at 460 nm is below the threshold value, which will keep OUT 1 in *OFF* state. However, in presence of F^- (*i.e* IN 1 is 1),

the color of the chemosensor changed to orange, which led to the generation of new peak at 460 nm. Therefore OUT 1 will be in the *ON* state. The presence of H^+ (*i.e* IN 2 is 1) in **4u** could not induce any subtle variation in the spectral behaviour. So, OUT 1 would be remained in *OFF* state. The sequential addition of F^- and H^+, the inherent spectral behaviour of **4u** was reverted back. Thus, the absorbance at 460 nm would be again below the threshold value, which led the OUT Y1 to stay in *OFF* state. The corresponding spectral outcomes have been shown in **Figure 4b, c** which is useful for INHIBIT logic circuit formulation.

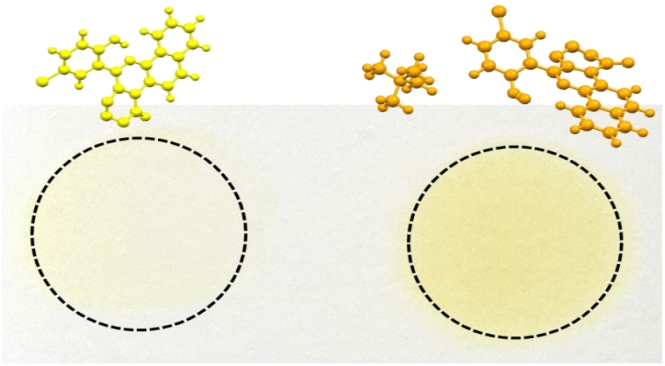


Figure S12. Naked eye solid state chromogenic recognition of F^- by**4u** (left: only **4u**, right: **4u** in presence of F^-).

References

S1. V. V. Kumar, D.Ramadevi, V. M.Ankathi, T. K. Pradhan, K. Basavaiah, *Microchem. J*.**2020**, *157*, 105028.

S2. D. Thongkum,T. Tuntulani, *Tetrahedron***2011**, *67*, 8102–8109.

S3. S. P. Mahanta, R.Das, S. P. Bharati, A. Borborah, P. J. Sarma, B. Das, S. Choudhury, G. Chakraborty, *New J. Chem*.**2018**,*42*, 3758–3764.

S4. Madhuprasad, D. R. Trivedi, *ChemPlusChem***2014**, *79*, 1001–1008.

S5. D. Morales-Morales, A. Dorazco-Gonzalez, M. A. Garcia, J. J. Guerra-Garcia, M. K. Salomón-Flores, I. J. Bazany-Rodríguez, D. Martínez-Otero, *Dalton Trans*. **2017**, *46*, 4950–4959.

S6. A. K. Purohit, S. K.Padhan, J. R. Mohanty, P. K. Kar, *Photochem. Photobiol. Sci*.**2018**, *17*, 815–821.

S7. S.Kainth,N. Goel,S.Basu,B.Maity, *New J. Chem*. **2022**,*46*, 686–694.

S8. X. Yu, L. Yang, T. Zhao, R. Zhang, L. Yang, C. Jiang, J. Zhao, B. Liu,Z. Zhang,*RSC Adv.***2017**,*7*, 53379–53384.

S9. S. P. Mahanta, R. Das, P. J. Sarma, A. Borborah, S. P. Bharati,*New J. Chem.***2019**, *43*, 3447–3453.