

## *Electronic Supporting Information*

### **Utilization of DMSO as a solvent-cum-reactant: Synthesis of fused 2-aryl-4-methylquinolines**

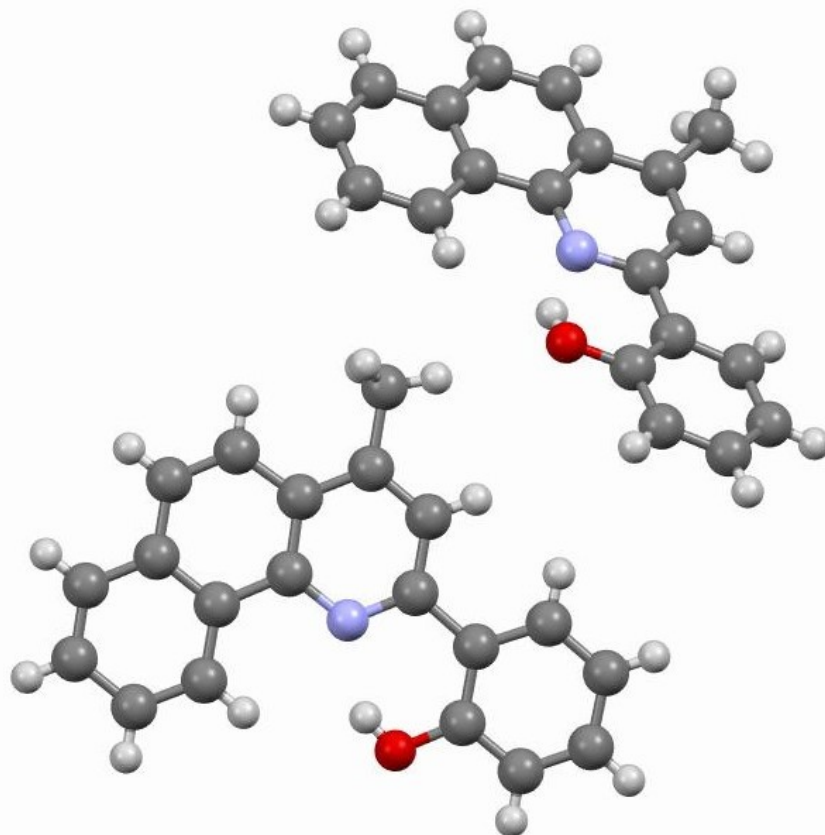
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## General information and methods

All chemicals were obtained from commercial sources and were used without further purifications. Reactions were monitored via TLC, prepared using silica gel for TLC with binder and fluorescence indicator GF254. The chromatography separation was carried out using 60–120 mesh-sized silica gel. Melting points were determined on a melting point apparatus and are uncorrected.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on 400, 500, and 600 MHz and 100, 125, and 150 MHz NMR spectrometers. Chemical shifts ( $\delta$  scale) are reported in parts per million (ppm). TMS was used as an internal reference; The  $^1\text{H}$  and  $^{13}\text{C}$  spectra are referenced for  $\text{CDCl}_3$  at 7.26 and 77.16 ppm respectively.  $^1\text{H}$  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. Complete crystallographic data of **3g** (CCDC no. 2291148) for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk).



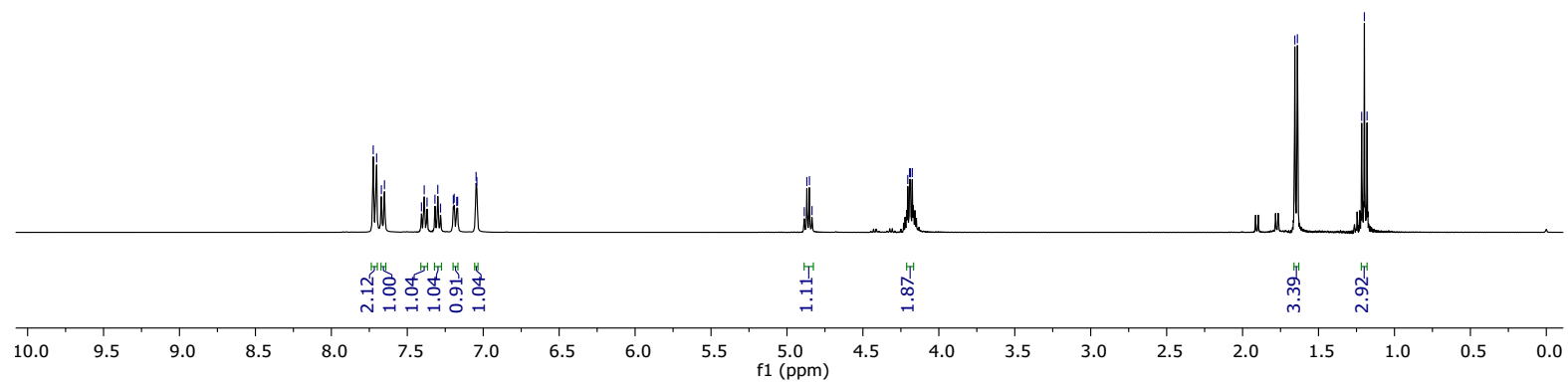
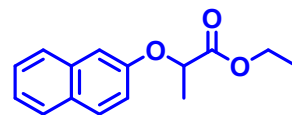
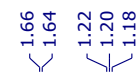
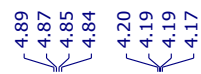
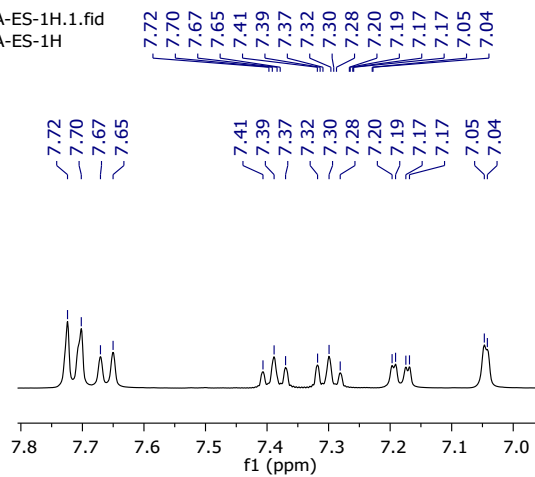
**Figure S1.** ORTEP diagrams of compound **3g**

**Table S1.** Crystal data and structure refinement for compound **3g**

<b>Entry</b>	<b>Identification code</b>	<b>Compound 3g</b>
01	Empirical formula	C <sub>20</sub> H <sub>15</sub> NO
02	Formula weight	285.3
03	Temperature	297 K
04	Wavelength	0.71073
05	Radiation type	MoK $\alpha$
06	Radiation system	Fine-focus sealed tube
07	Crystal system	Monoclinic
08	Space group	P 21/n
09	Cell length	a=16.9016 (15) b=8.6430 (8) c=21.0199 (8)
10	Cell angle	$\alpha$ =90 $\beta$ =108.891 (3) $\gamma$ =90
11	Cell volume	2905.2 (5)
12	Density	1.305
13	Completeness to theta	99.4
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F <sup>2</sup>
16	Index ranges	-10 $\leq$ h $\leq$ 10, -24 $\leq$ k $\leq$ 24, -13 $\leq$ l $\leq$ 13
17	Reflection number	3415
18	Theta (max)	25.02
19	Theta (min)	2.57
20	Cell formula units Z	4
21	CCDC no	2291148

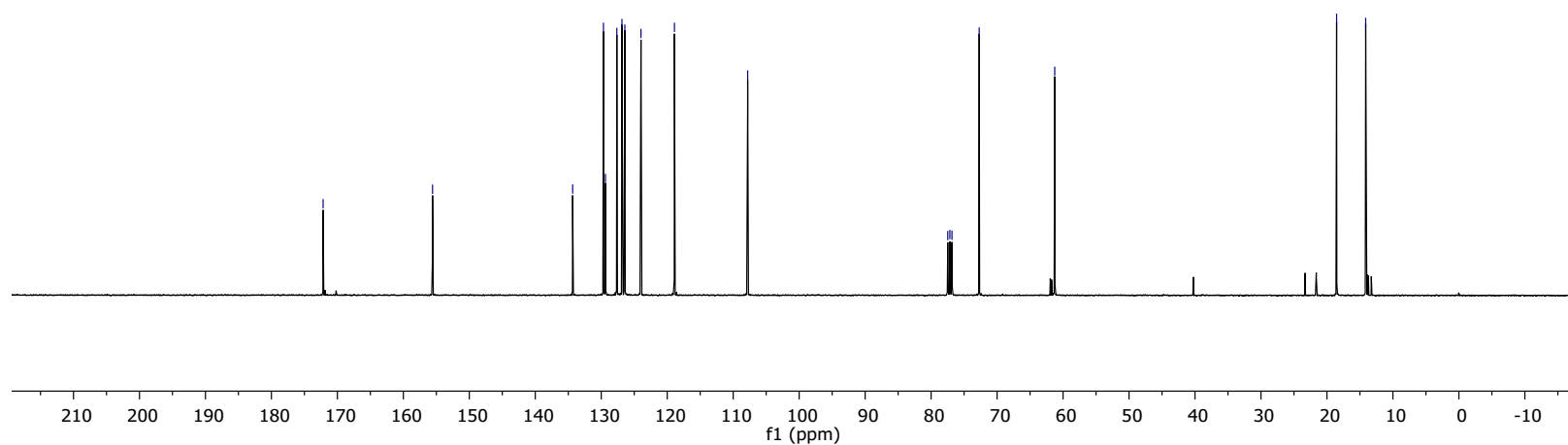
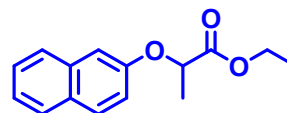
# <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 1bc

ATK-K-2NA-ES-1H.1.fid  
ATK-K-2NA-ES-1H



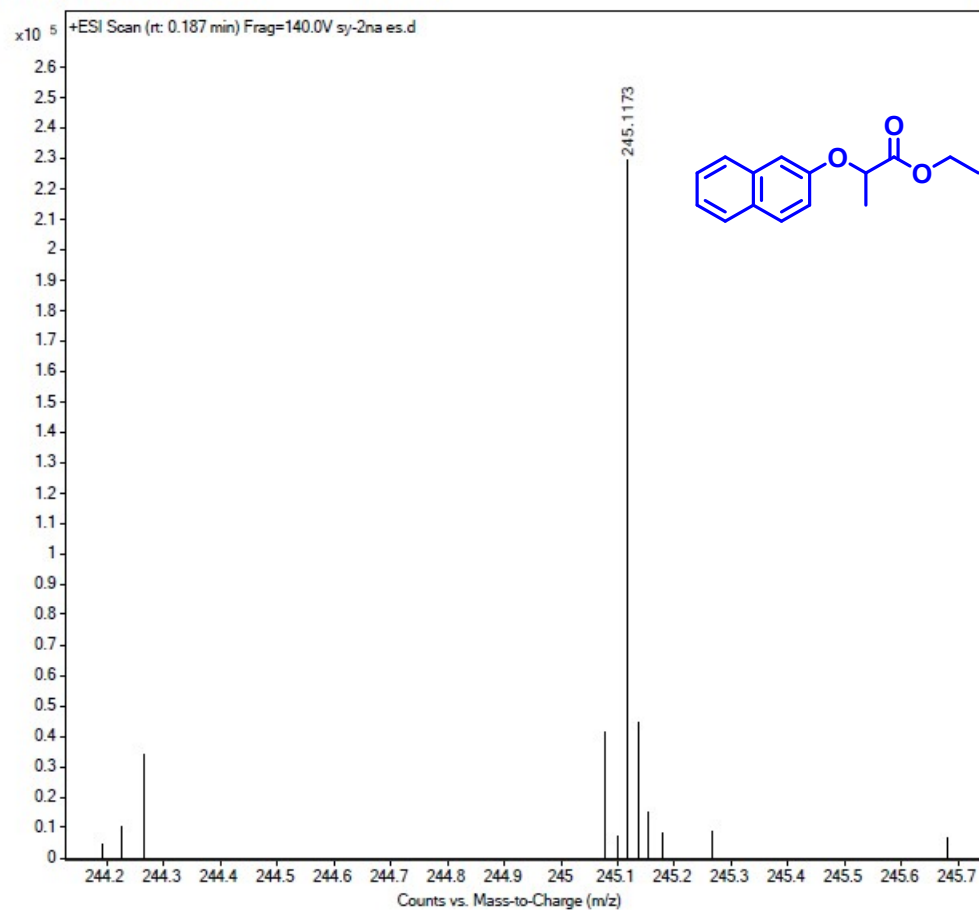
**$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) Spectrum of compound 1bc**

ATK-K-2NA-ES-13C.3.fid  
ATK-K-2NA-ES-13C



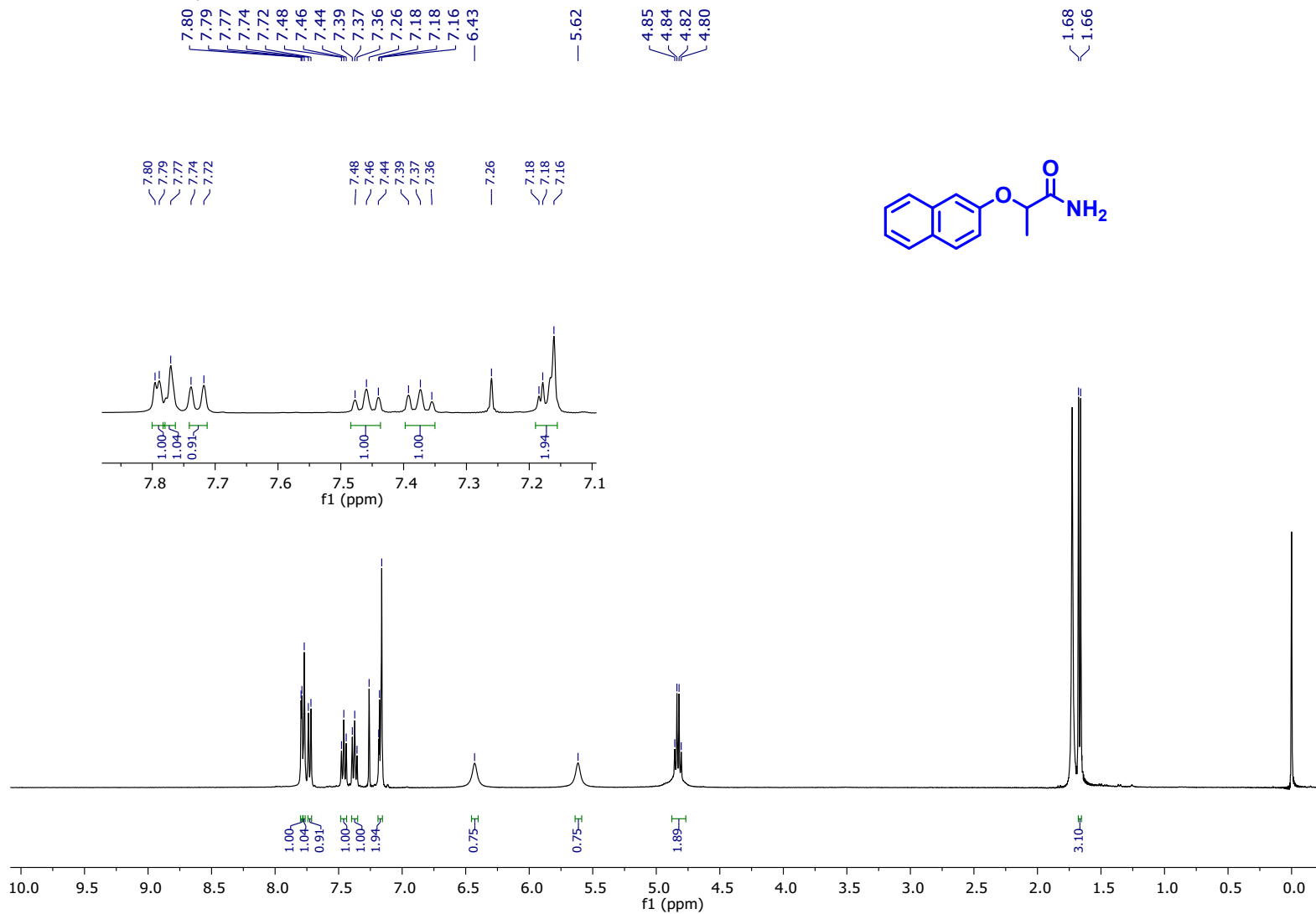
## HRMS spectrum of compound 1bc

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SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample	IRM Calibration Status	Success	Data Filename	sy-2na es.d
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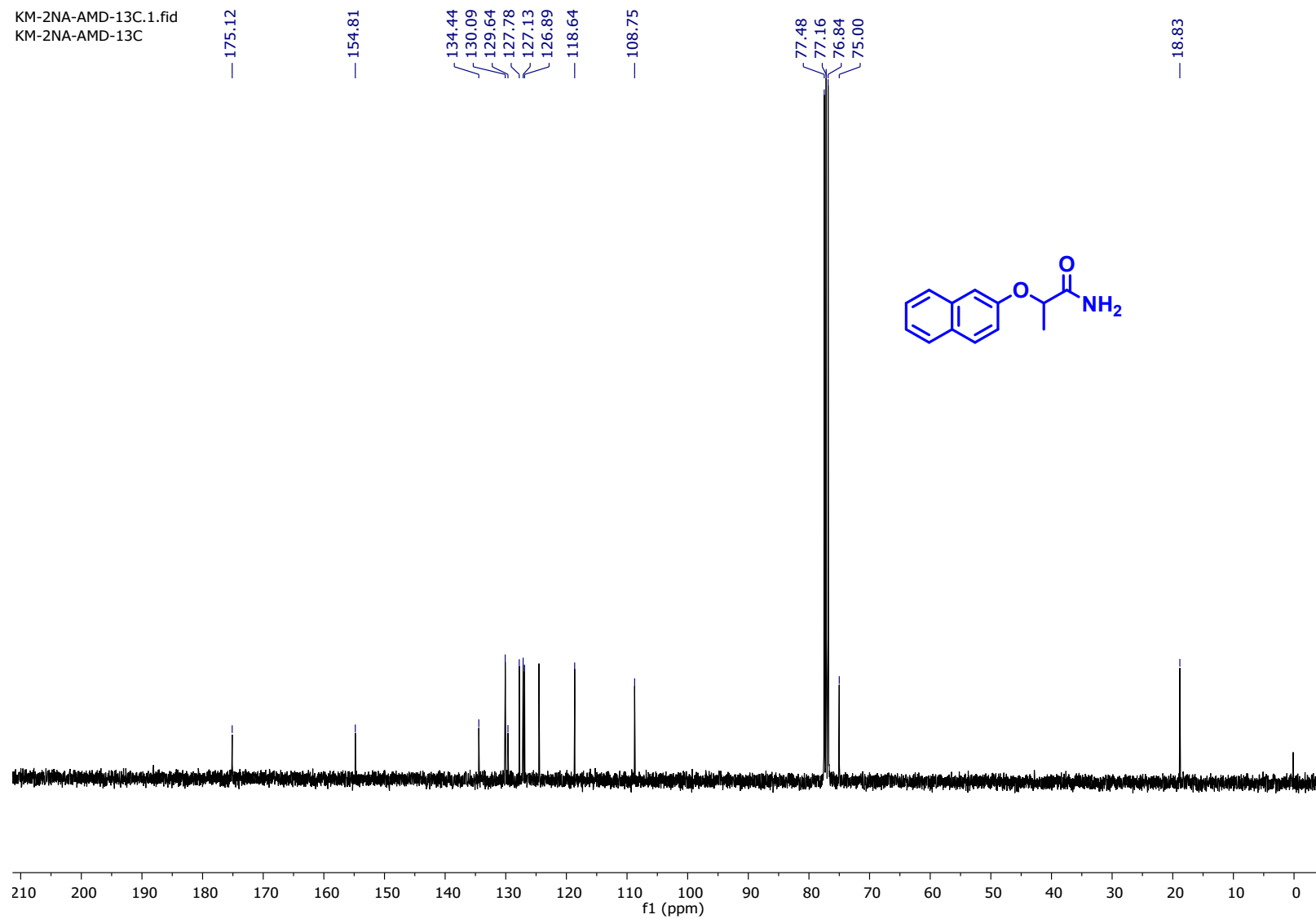
# <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) Spectrum of compound 1bd

ATK-KM-2NA-AMD-1H.1.fid — ATK-KM-2NA-AMD-1H



$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) Spectrum of compound 1bd

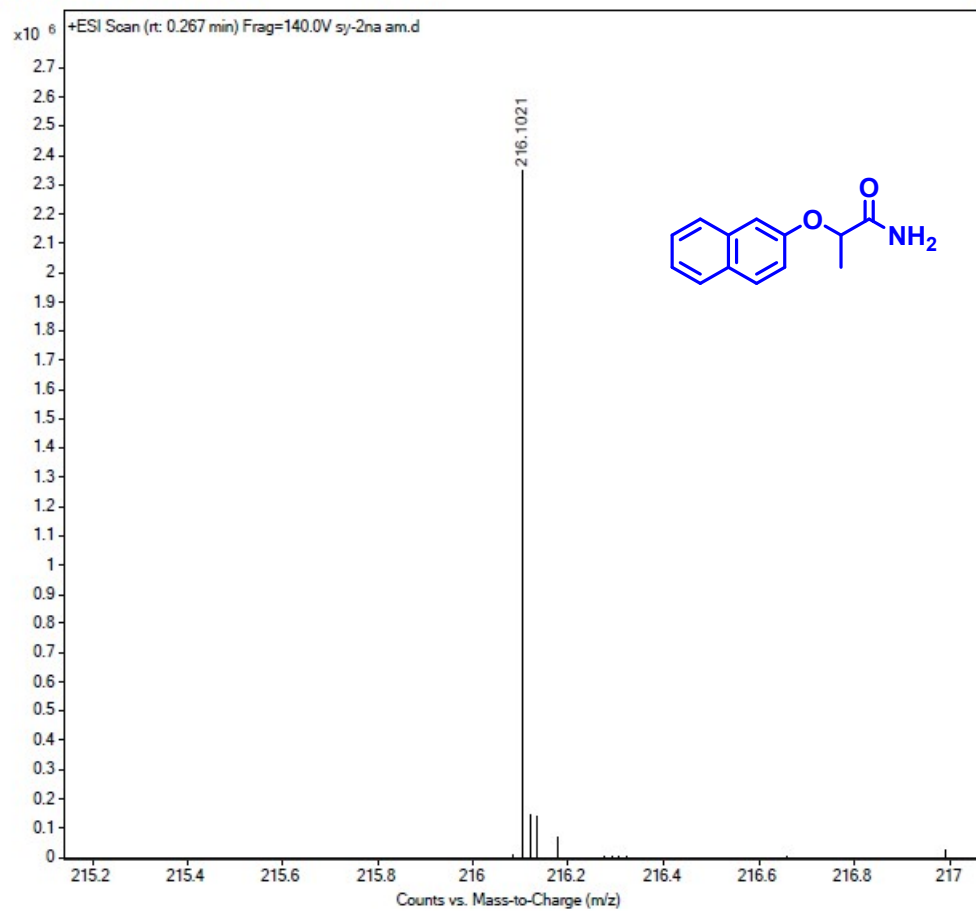
KM-2NA-AMD-13C.1.fid  
KM-2NA-AMD-13C





## HRMS spectrum of compound 1bd

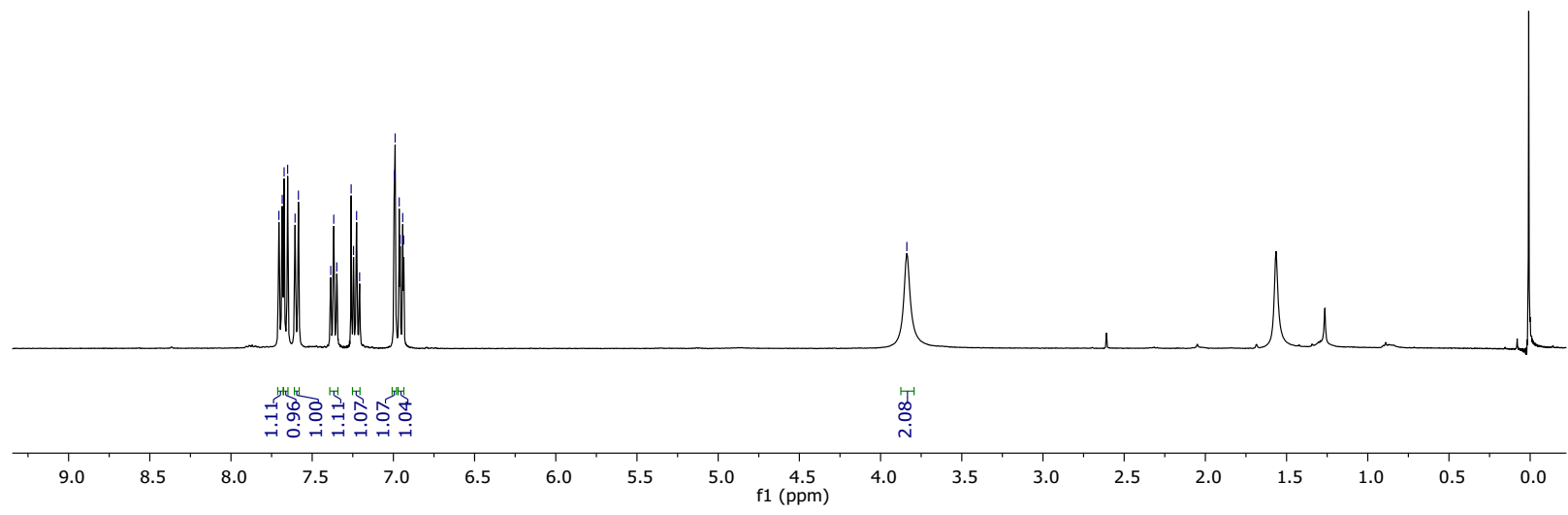
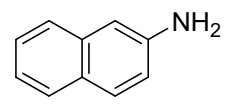
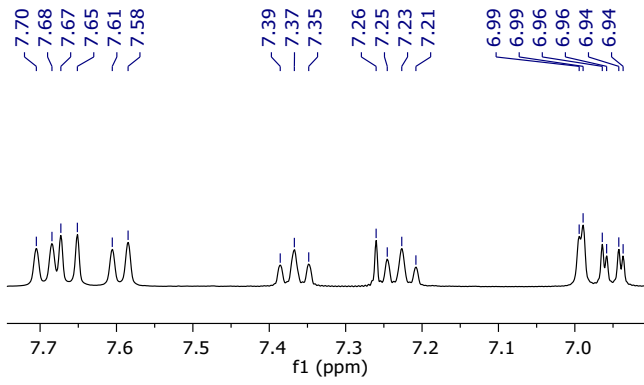
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SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample	IRM Calibration Status	Success	Data Filename	sy-2na am.d
DIRECT MASS_POSITIVE_100_1500.m	Comment		Acquired Time	13-Sep-23 09:



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) Spectrum of compound 1b**

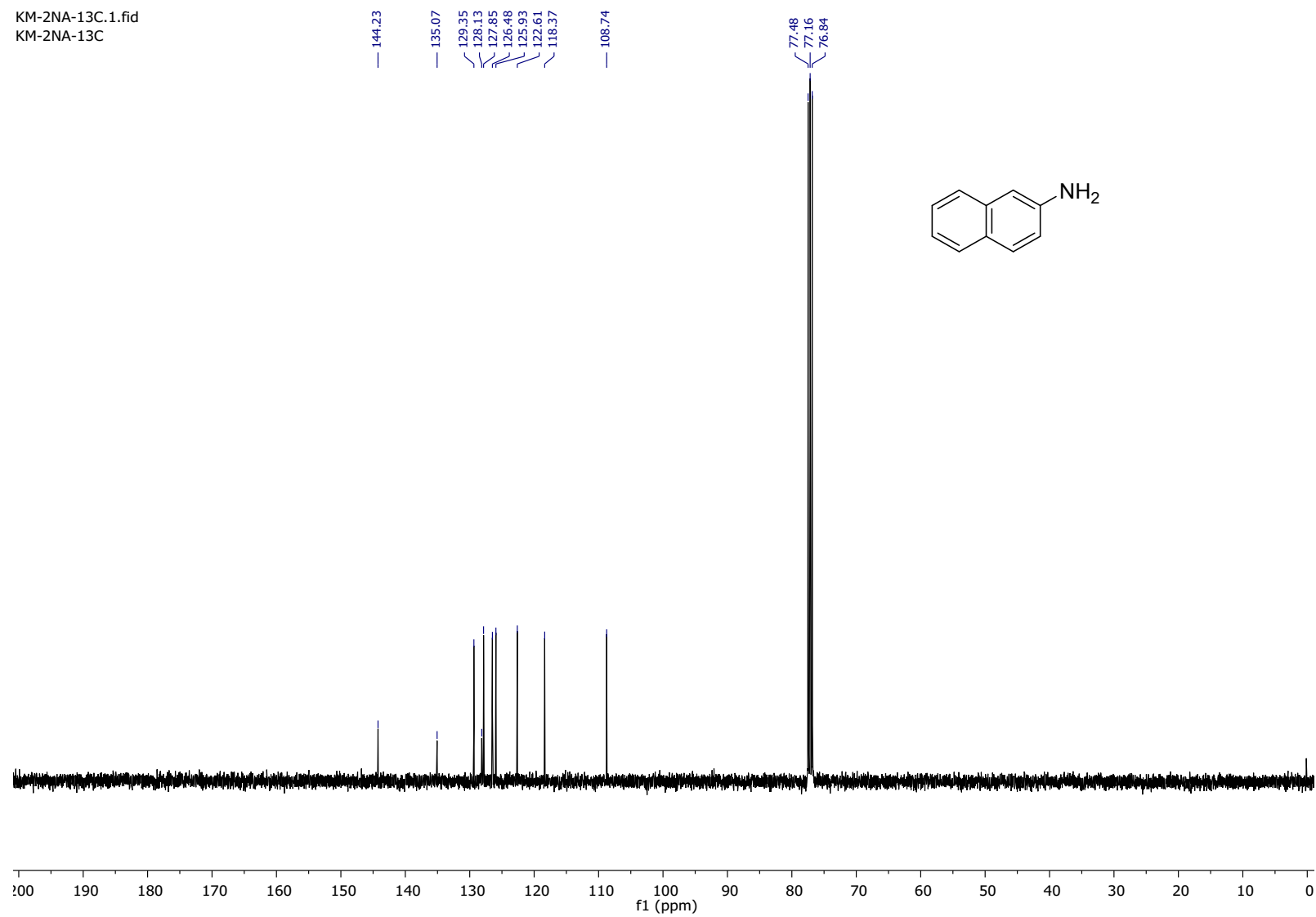
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ATK-KM-2NA-  
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7.6845  
7.6728  
7.6512  
7.6055  
7.5848  
7.3856  
7.3672  
7.3484  
7.2601  
7.2455  
7.2266  
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6.9584  
6.9425  
6.9368

3.8382



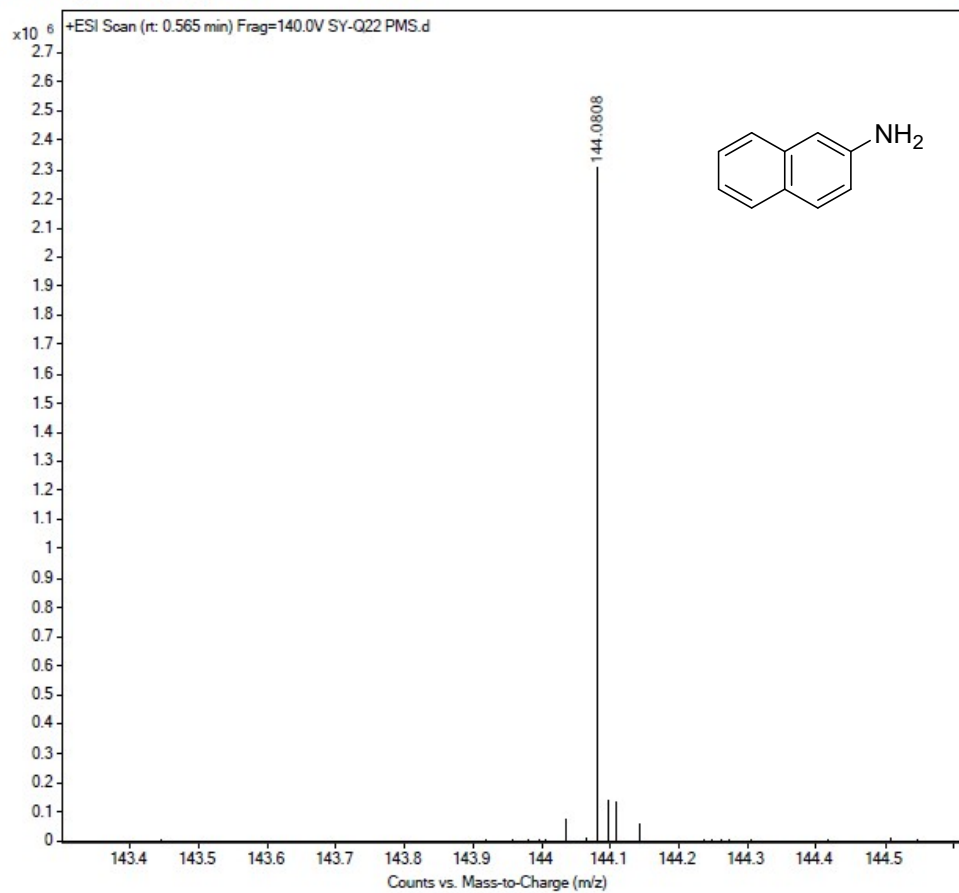
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) Spectrum of compound 1b

KM-2NA-13C.1.fid  
KM-2NA-13C



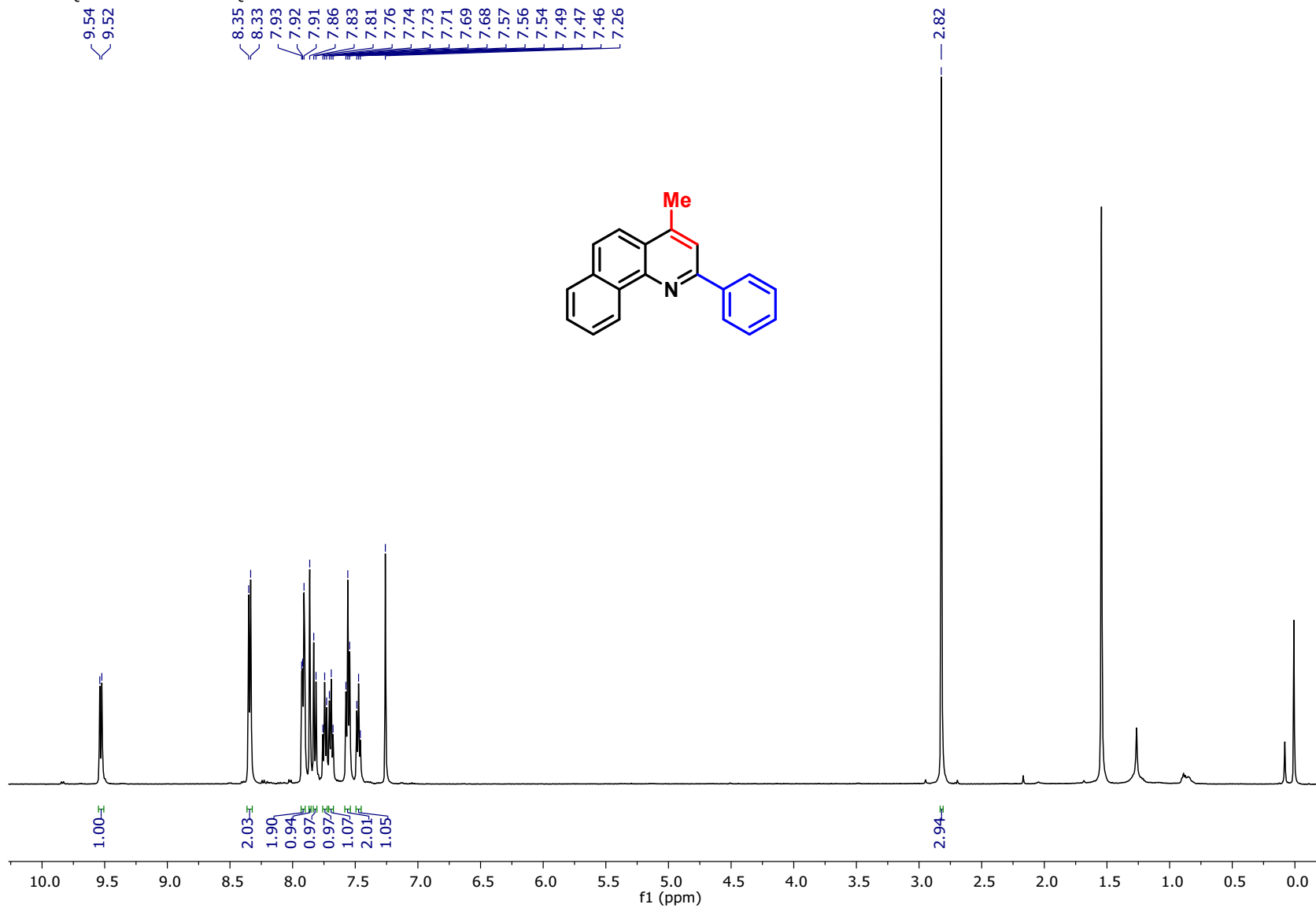
## HRMS spectrum of compound 1b

SY-Q22 PMS	Position	P1-A1	Instrument Name	QTOF
SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample	IRM Calibration Status	Success	Data Filename	SY-Q22 PMS.d
DIRECT MASS_POSITIVE_100_1500.m	Comment		Acquired Time	04-Sep-23 09:2



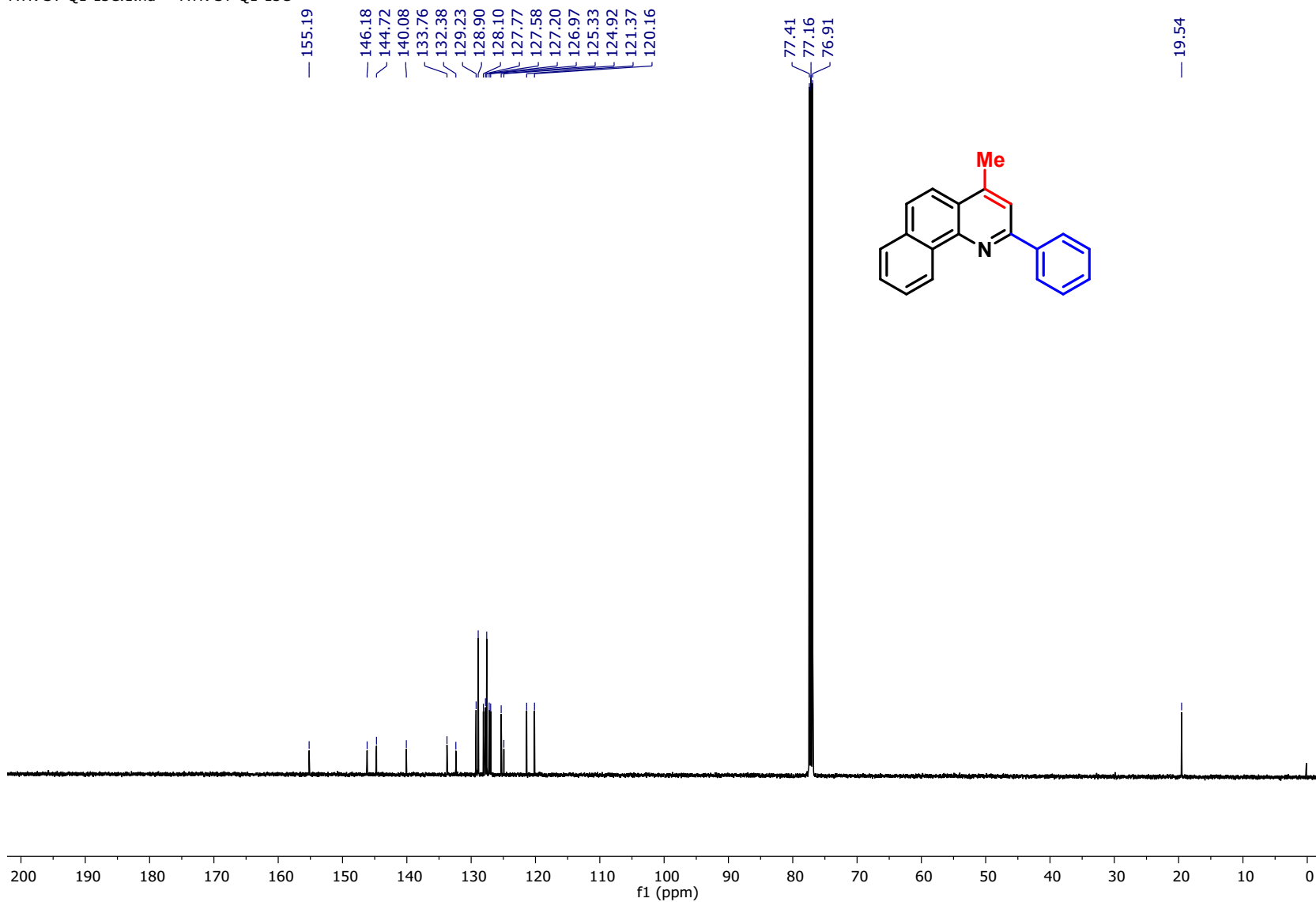
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3a**

ATK-SY-Q1-1H.3.fid — ATK-SY-Q1-1H



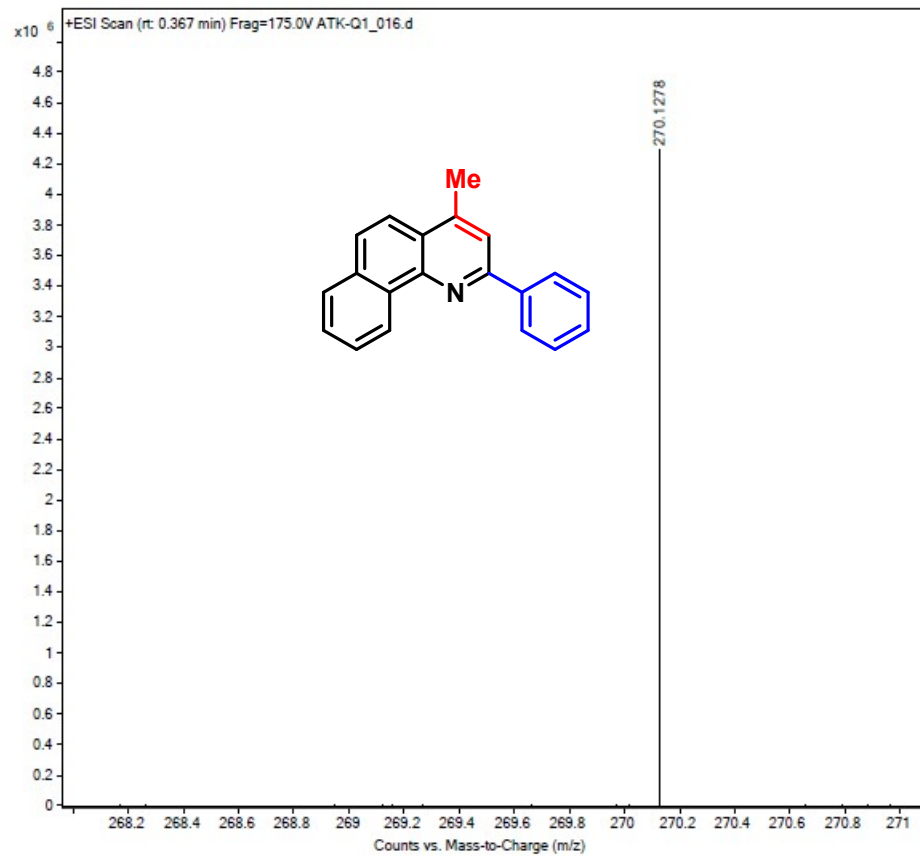
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3a

ATK-SY-Q1-13C.1.fid — ATK-SY-Q1-13C



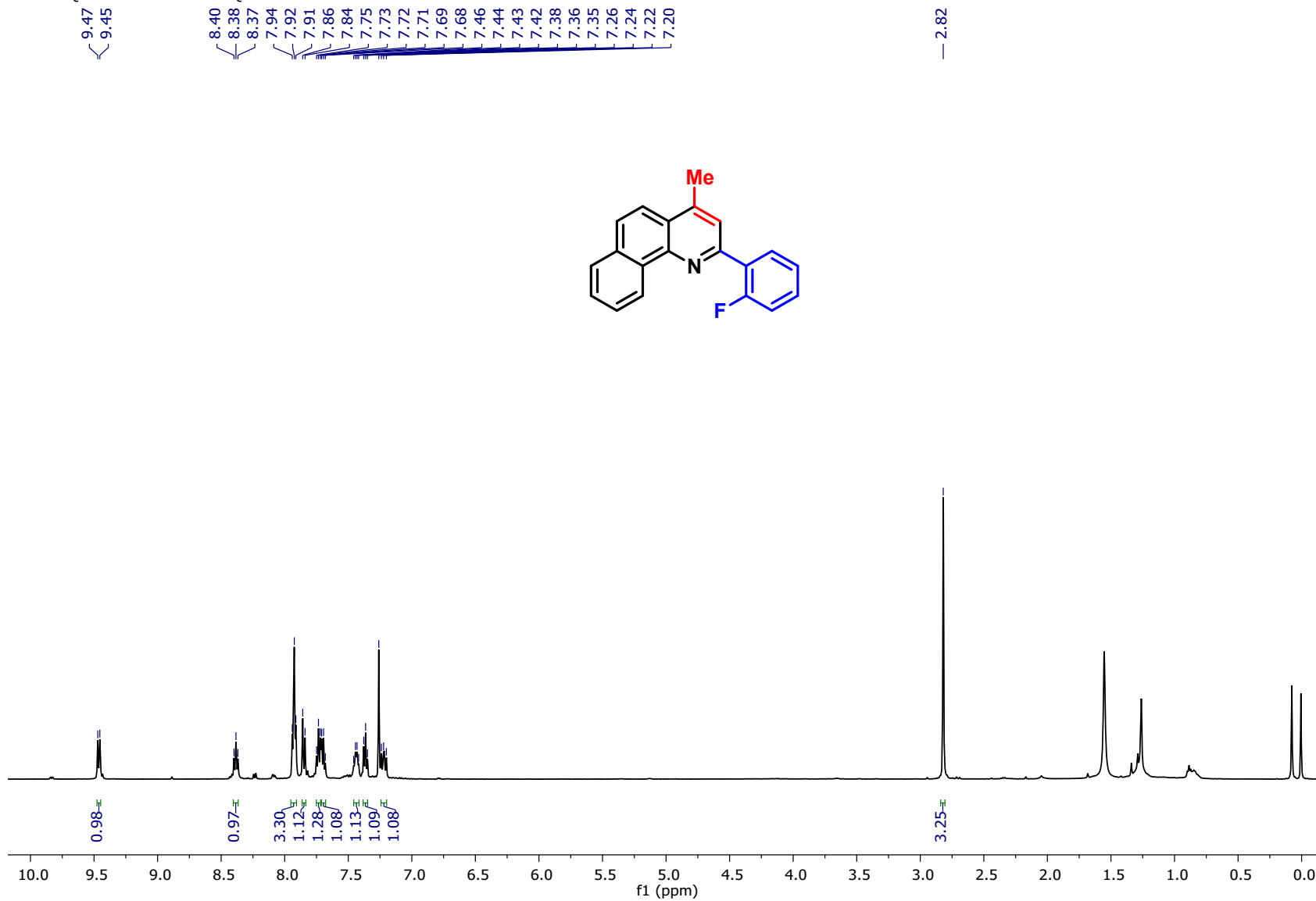
## HRMS spectrum of compound 3a

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User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK-Q1_016.d
ACQ Method	FULL_SCAN-POSITIVE.m	Comment		Acquired Time	27-Nov-22 08:36:18 PM (UTC+05:30)



**$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3b**

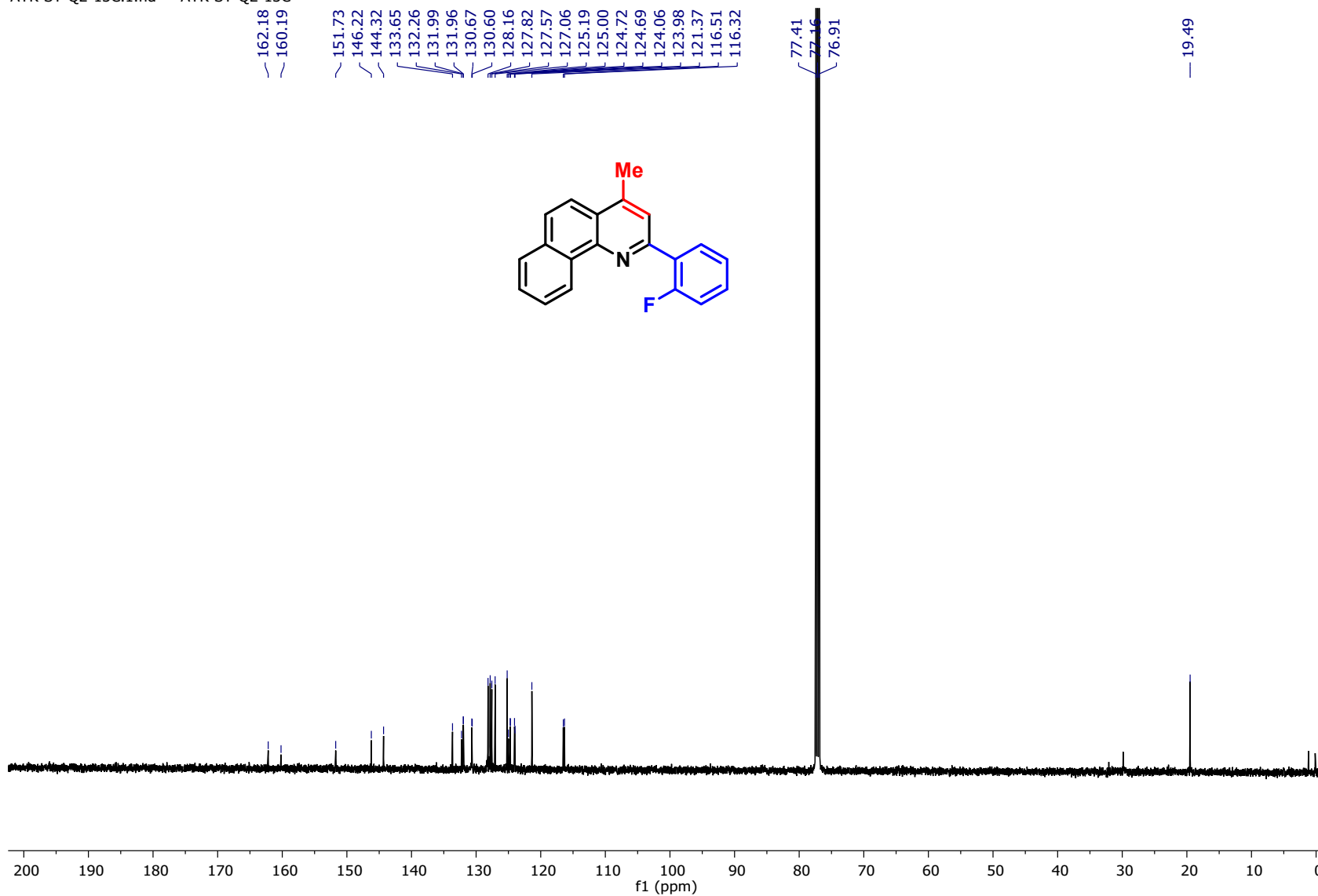
ATK-SY-Q2-1H.1.fid — ATK-SY-Q2-1H





**$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3b**

ATK-SY-Q2-13C.1.fid — ATK-SY-Q2-13C



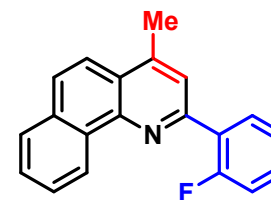
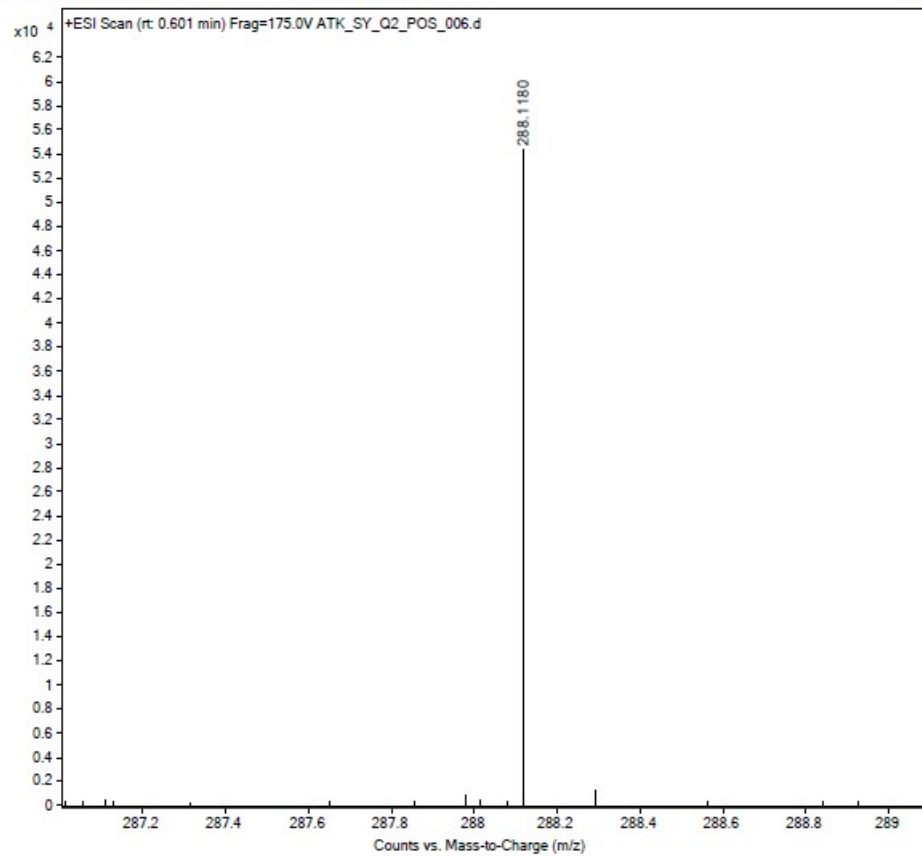
## HRMS spectrum of compound 3b

Sample Name  
User Name  
Sample Type  
ACQ Method

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Sample  
FULL\_SCAN-POSITIVE.m

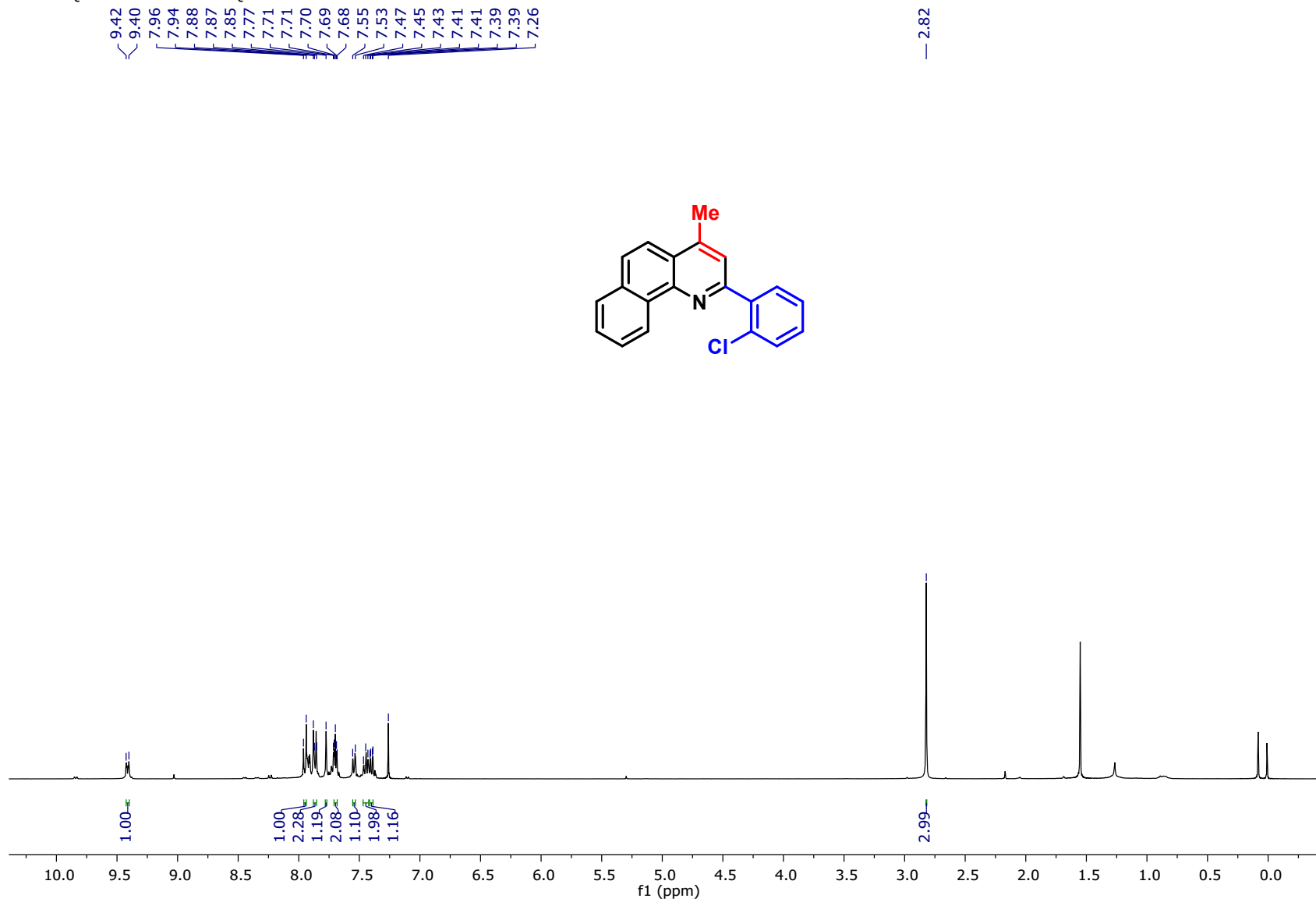
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Inj Vol 10  
IRM Calibration Status Success  
Comment

Instrument Name Instrument 1  
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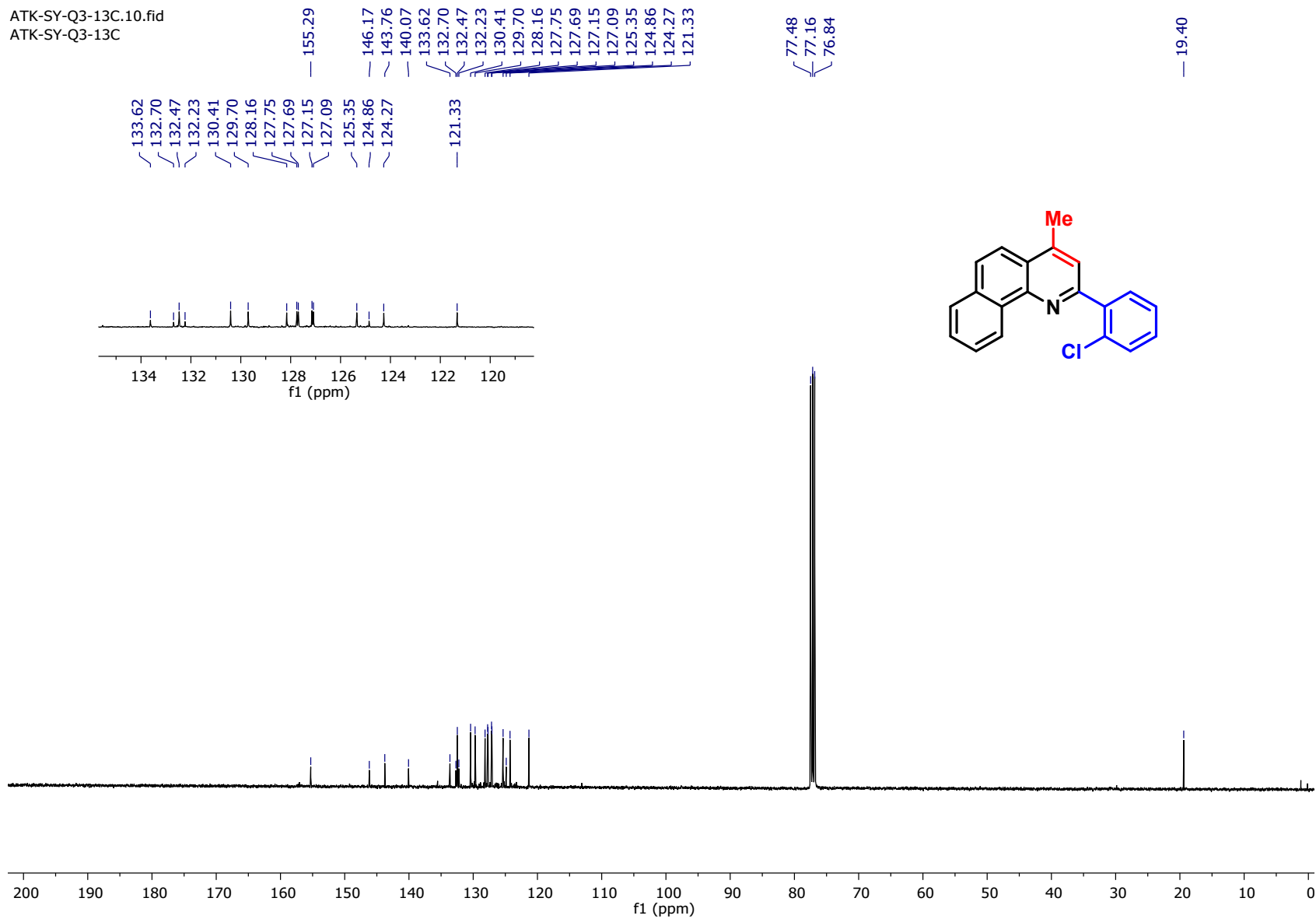
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3c**

ATK-SY-Q3-1H.1.fid — ATK-SY-Q3-1H



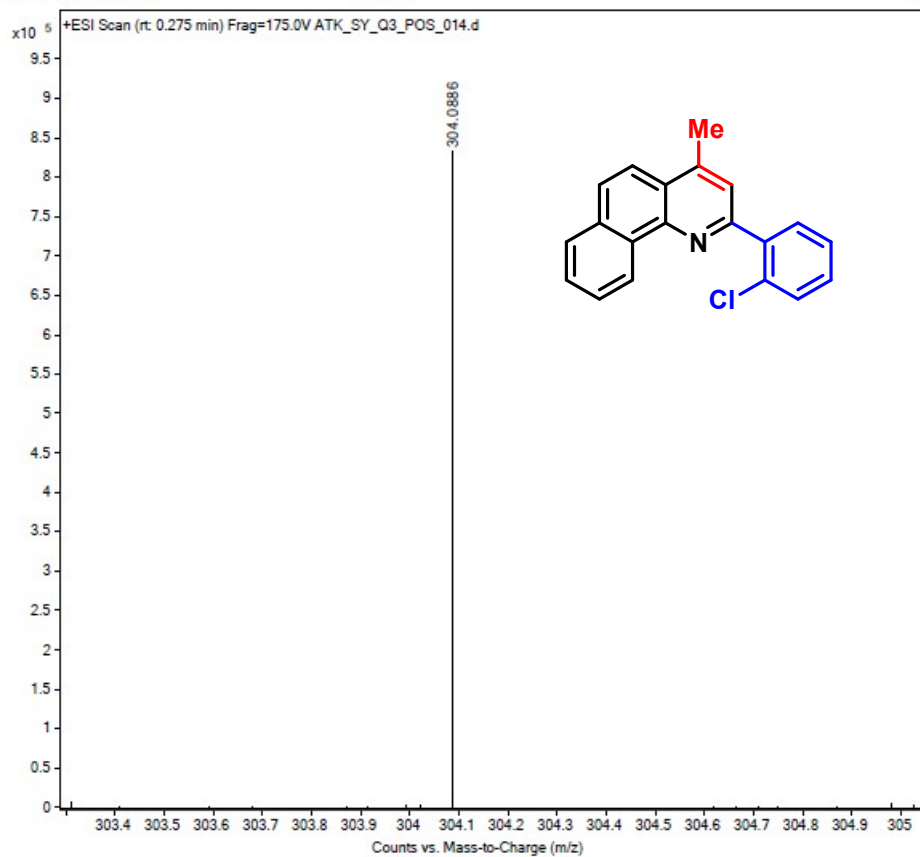
$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3c**

ATK-SY-Q3-13C.10.fid  
ATK-SY-Q3-13C



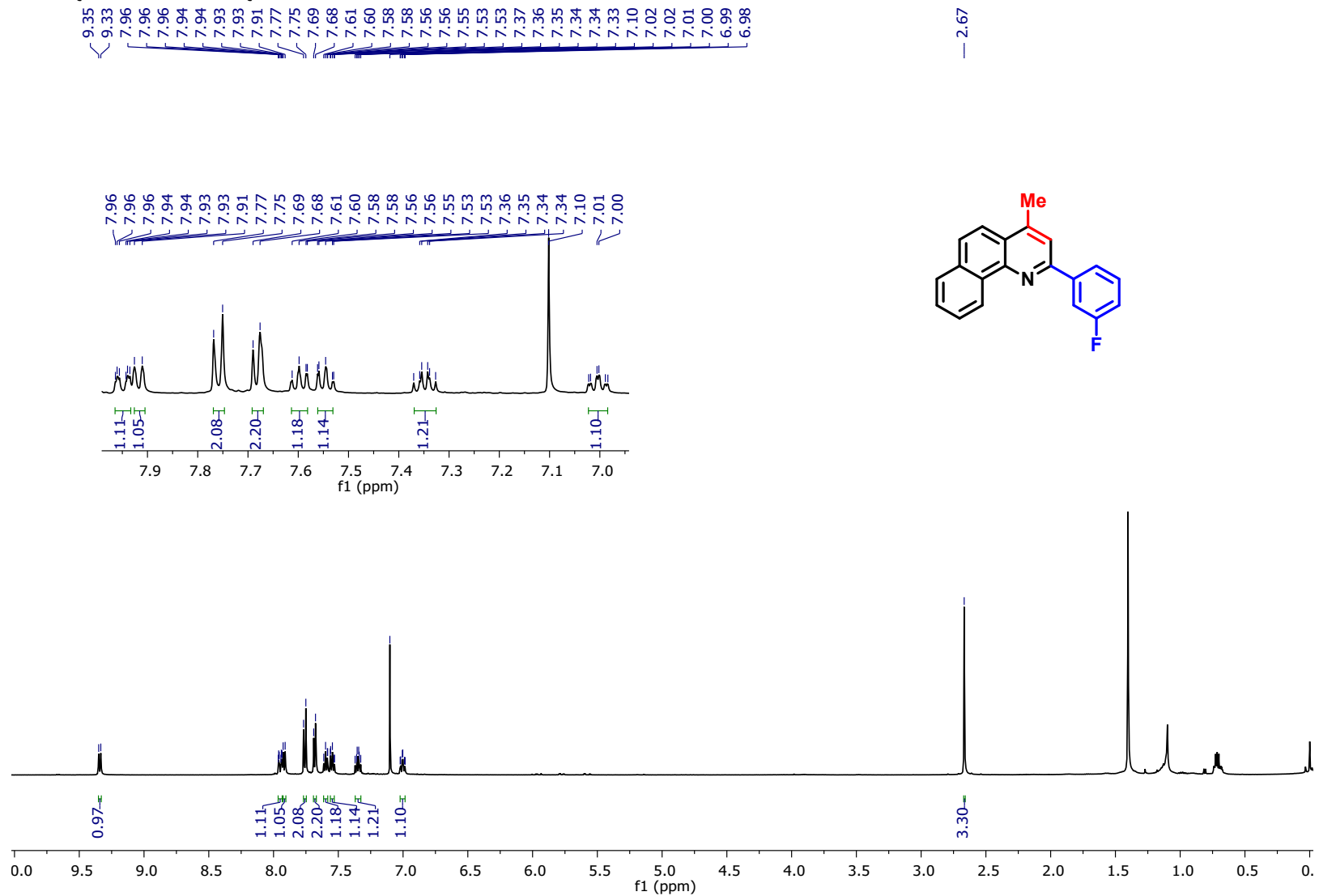
## HRMS spectrum of compound 3c

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User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q3_POS_014.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:24:00 PM (UTC+05:30)



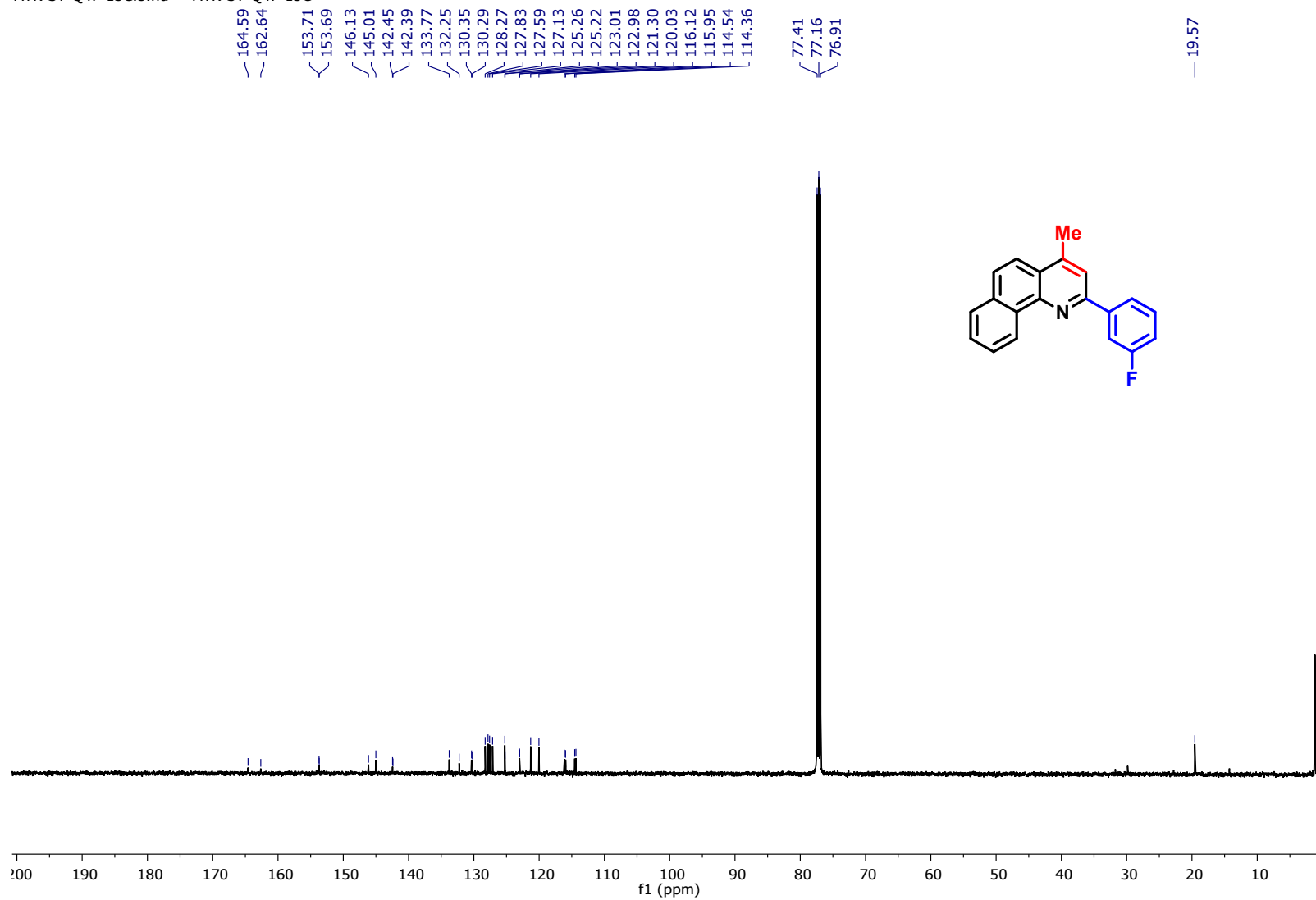
# <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3d

ATK-SY-Q47-1H.1.fid — ATK-SY-Q47-1H



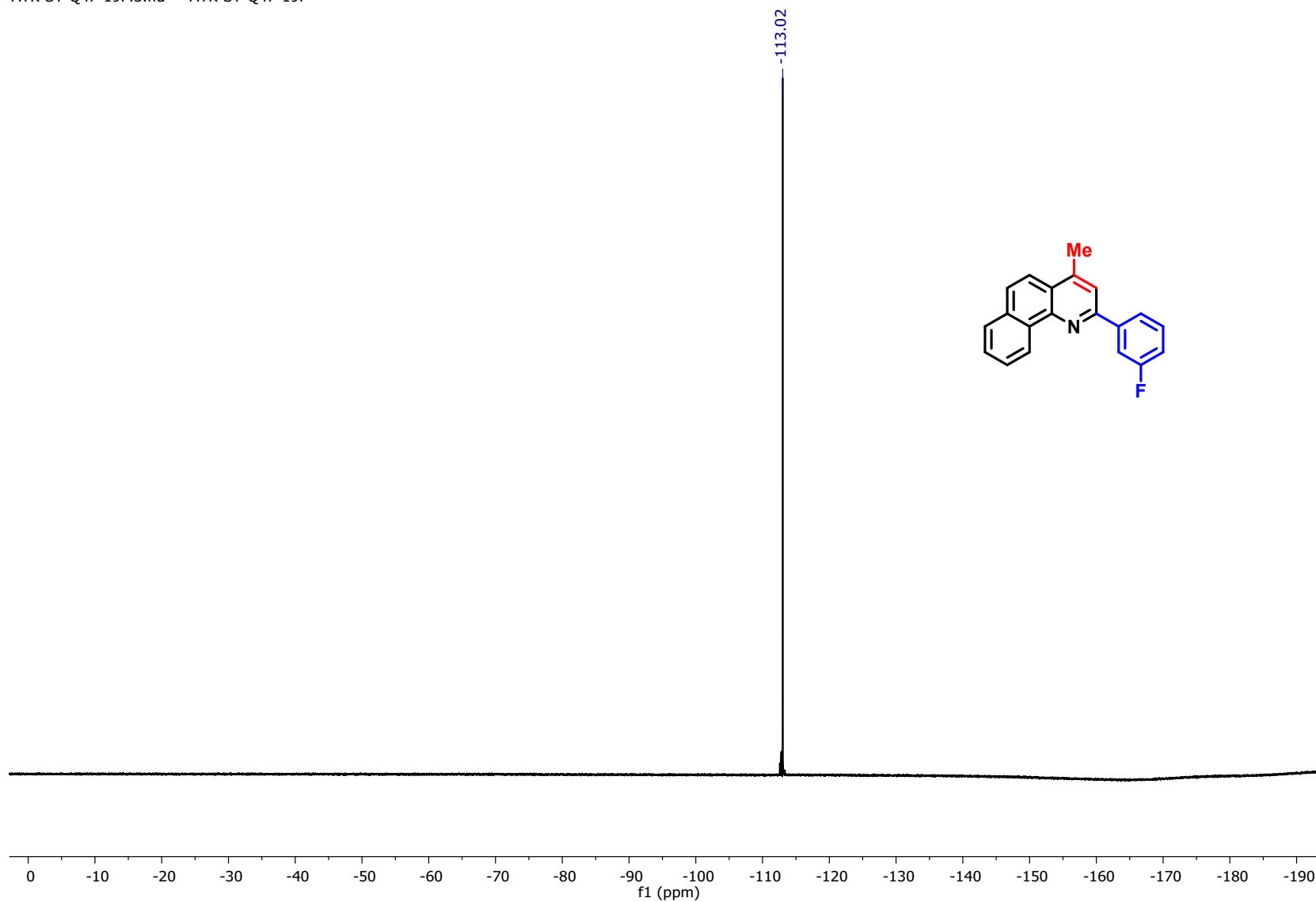
**$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3d**

ATK-SY-Q47-13C.5.fid — ATK-SY-Q47-13C



**$^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3d**

ATK-SY-Q47-19F.3.fid — ATK-SY-Q47-19F



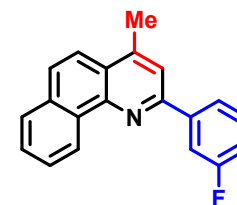
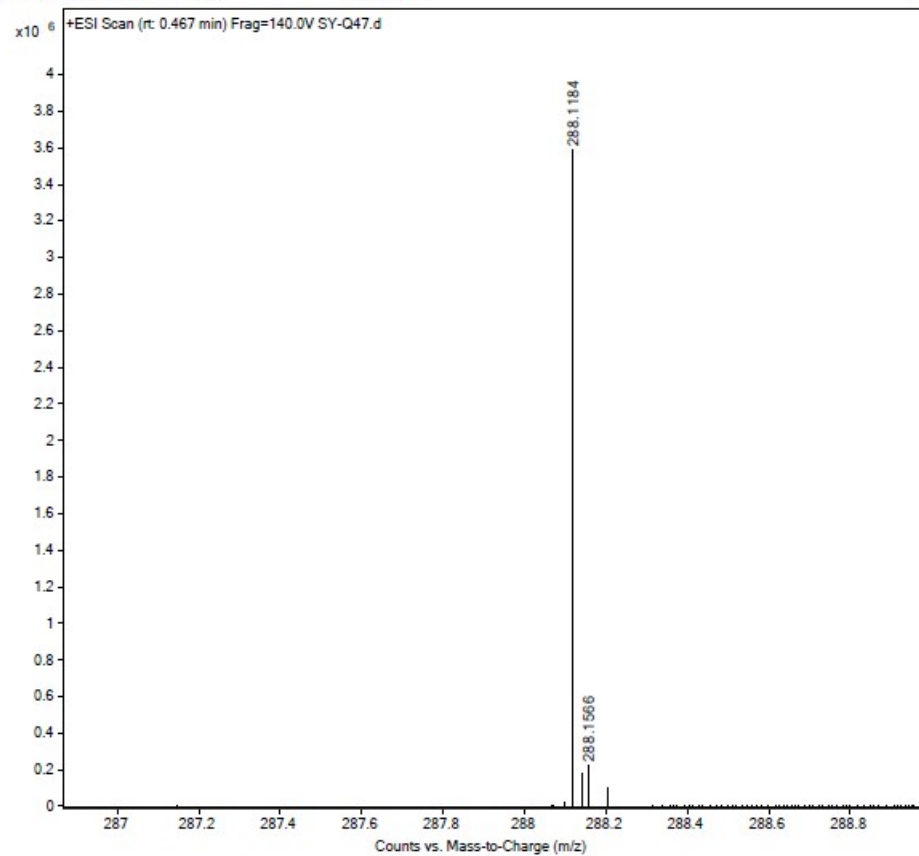


## HRMS spectrum of compound 3d

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User Name  
Sample Type  
ACQ Method

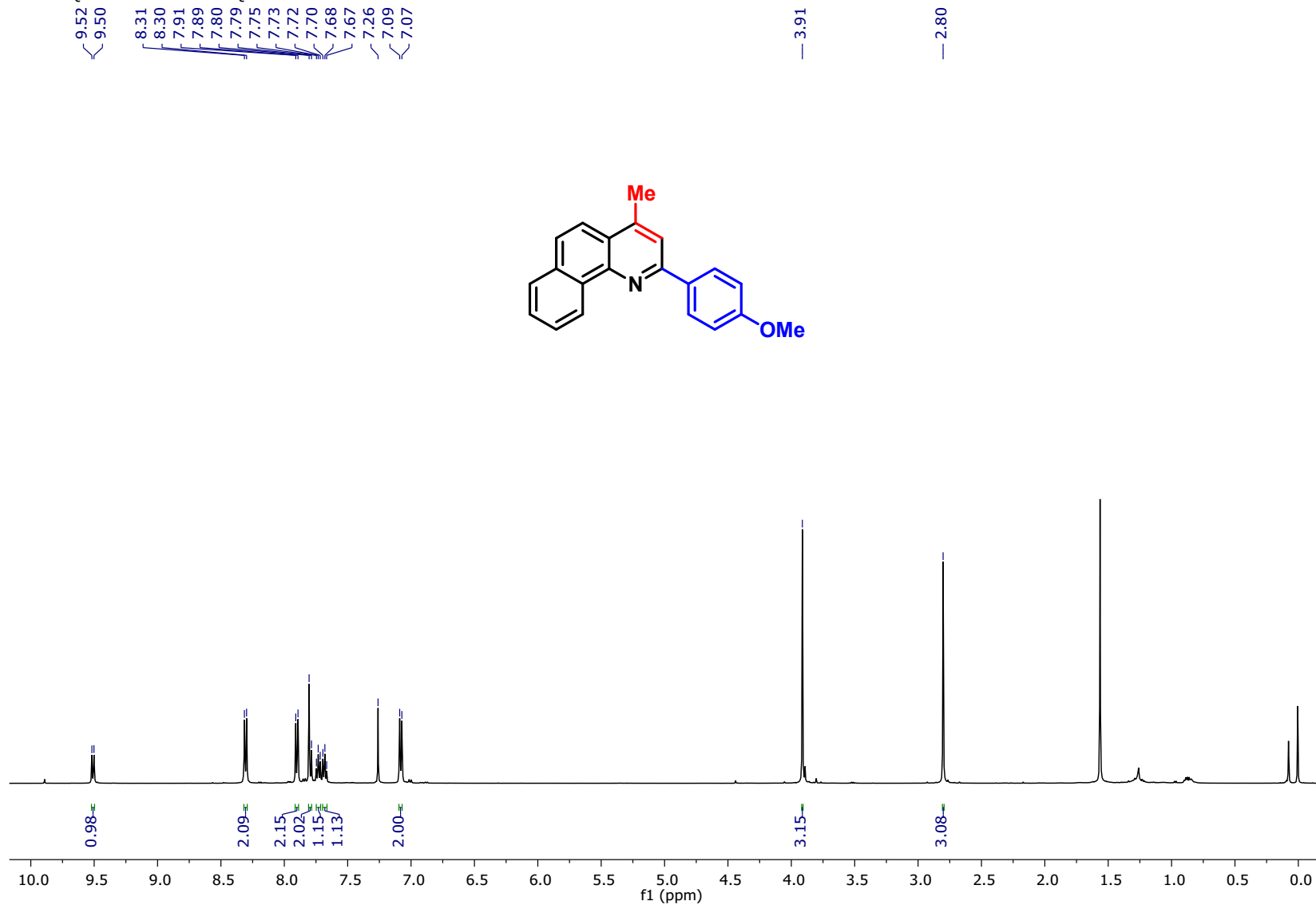
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Sample  
DIRECT MASS\_POSITIVE\_01\_1.m  
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Inj Vol  
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Comment  
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Success

Instrument Name  
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13-Jul-23 11:47:31 AM (UTC+05:30)



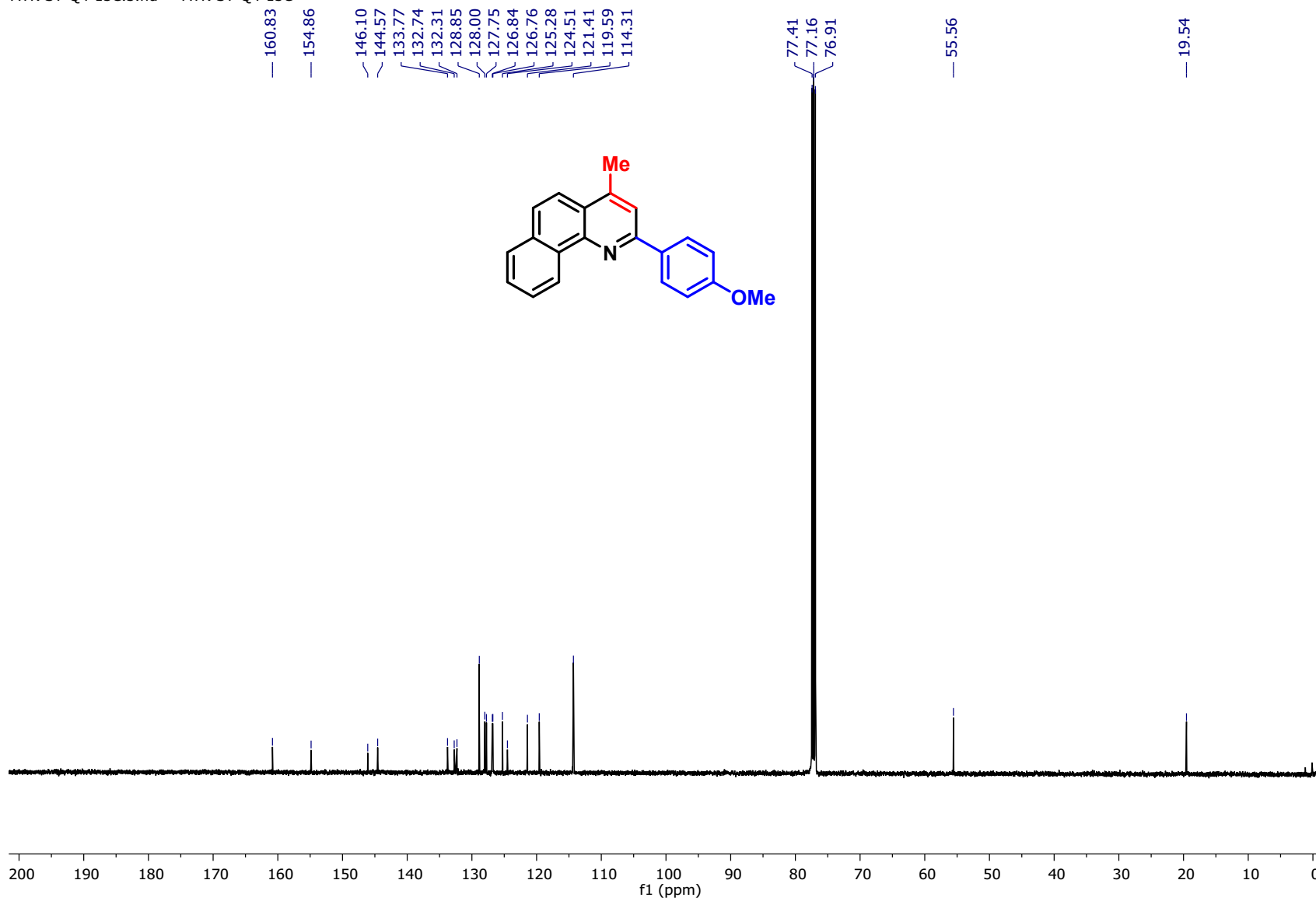
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3e

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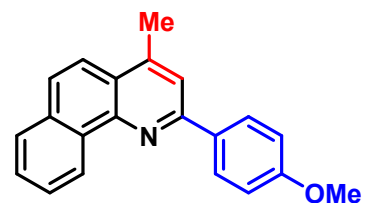
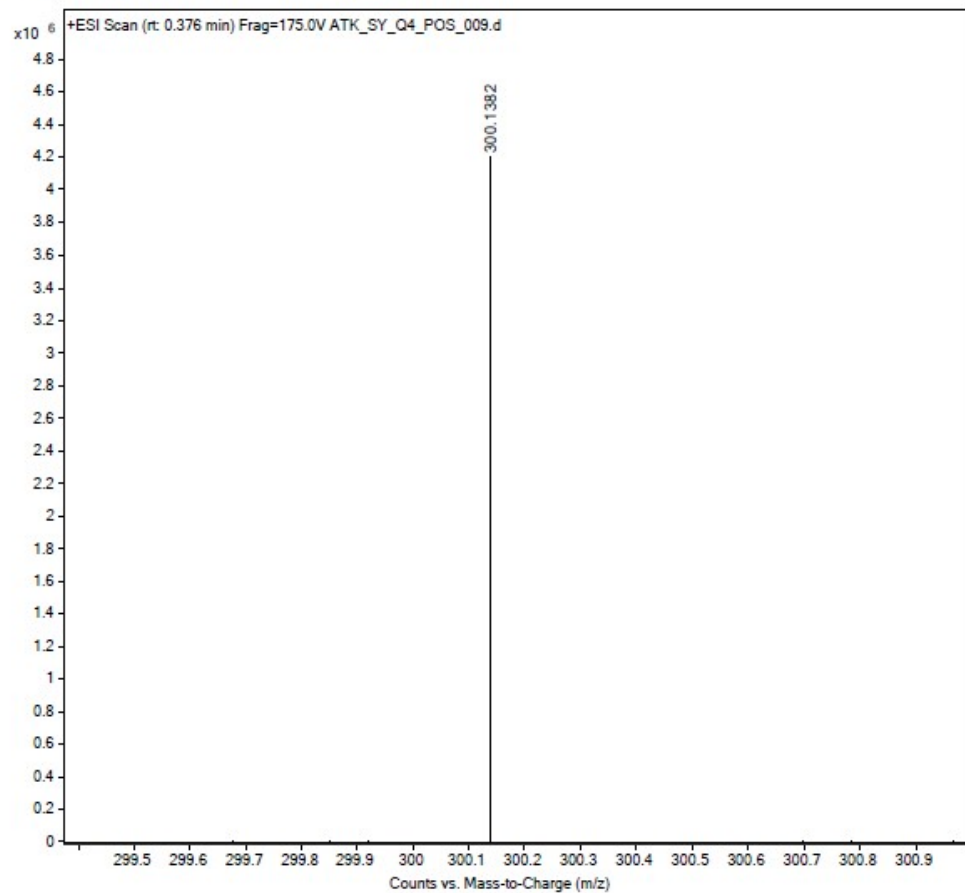
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3e

ATK-SY-Q4-13C.3.fid — ATK-SY-Q4-13C



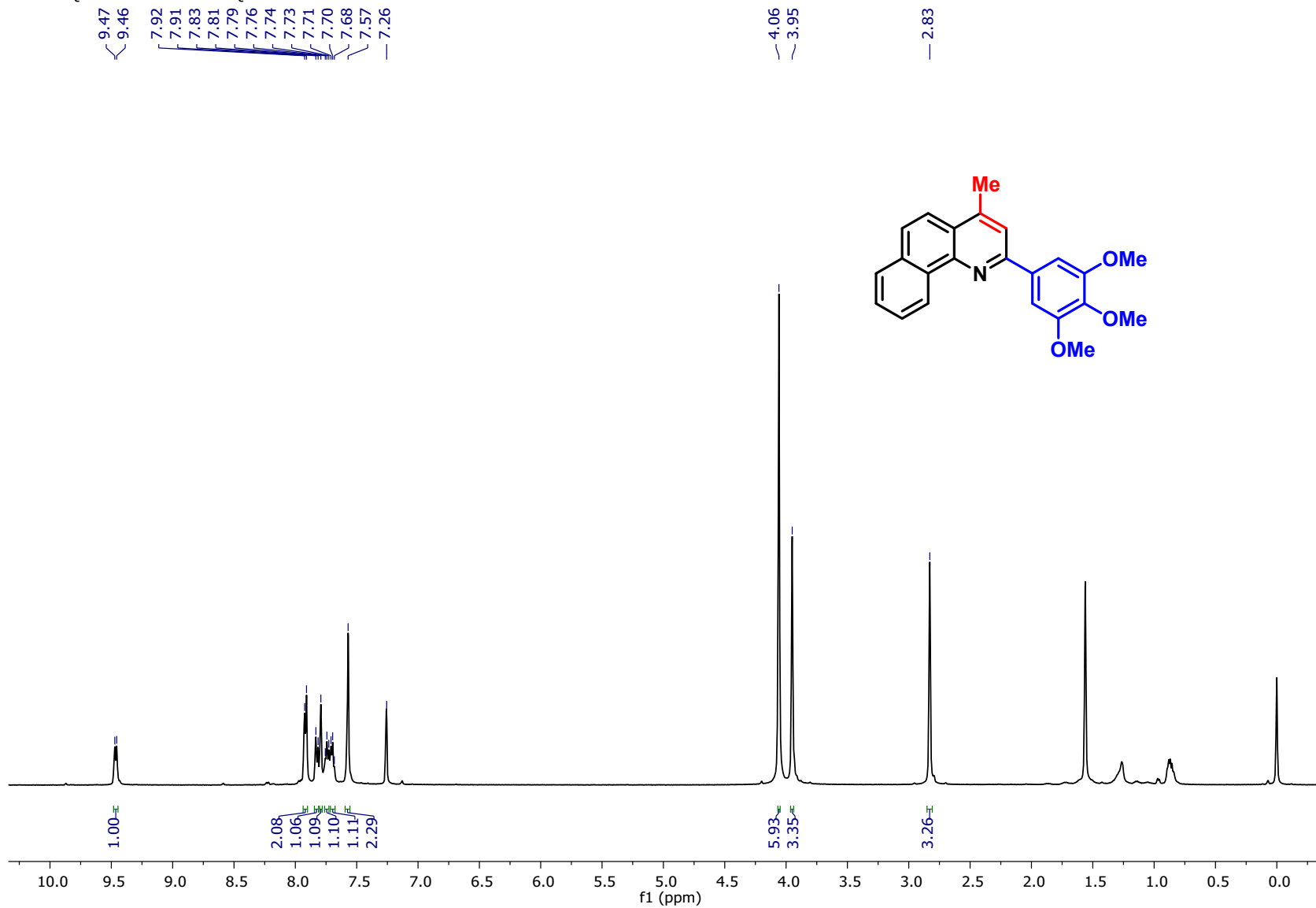
## HRMS spectrum of compound 3e

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User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q4_POS_009.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:16:05 PM (UTC+05:30)



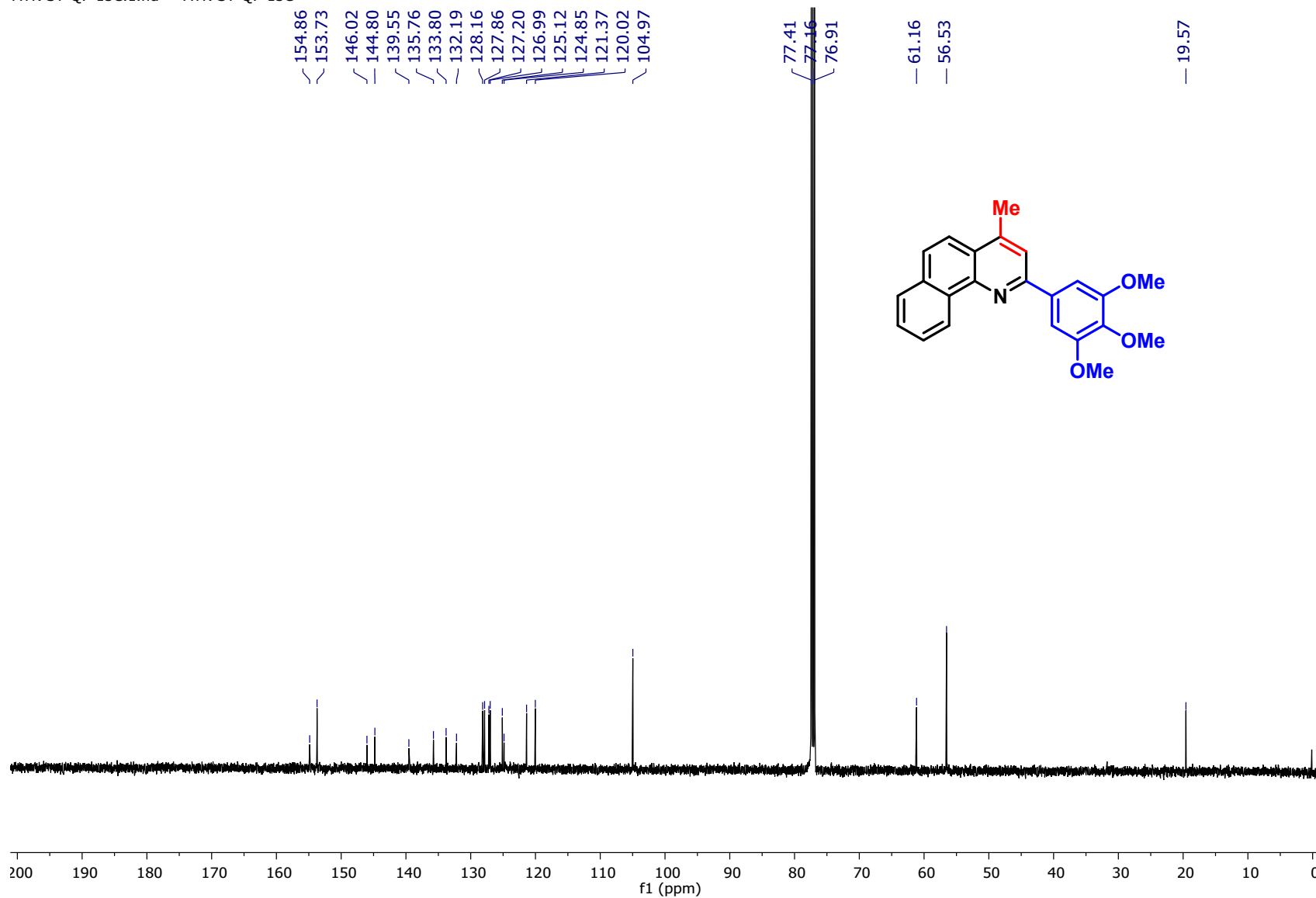
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3f**

ATK-SY-Q7-1H.3.fid — ATK-SY-Q7-1H



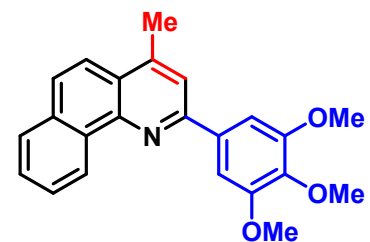
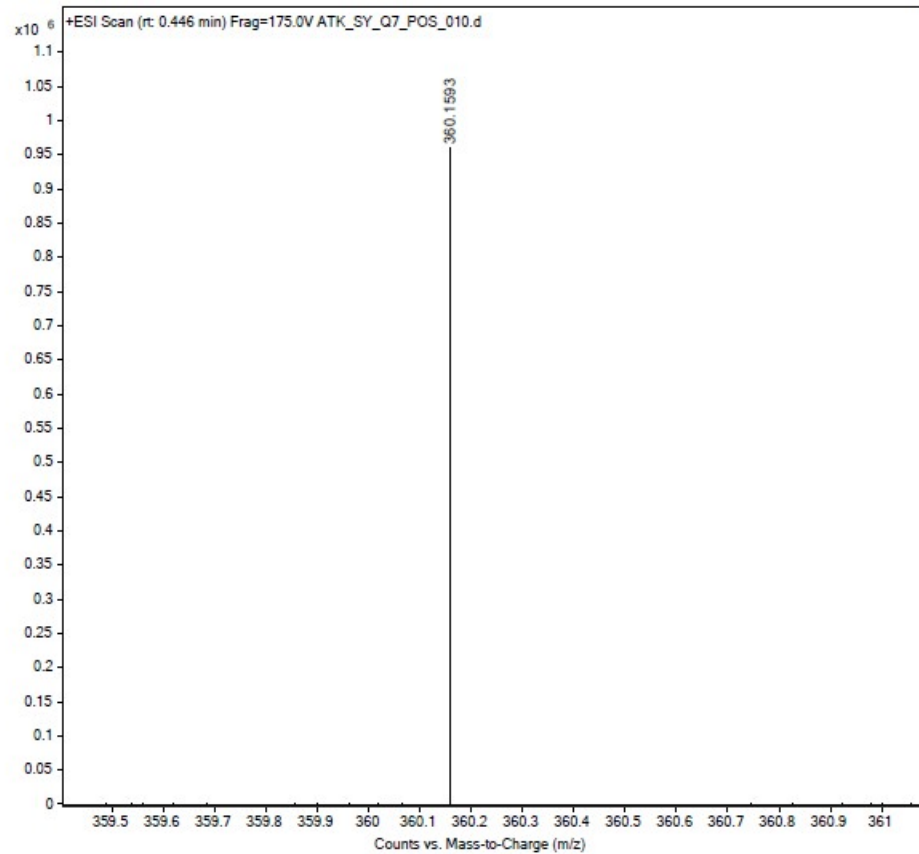
**$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3f**

ATK-SY-Q7-13C.1.fid — ATK-SY-Q7-13C



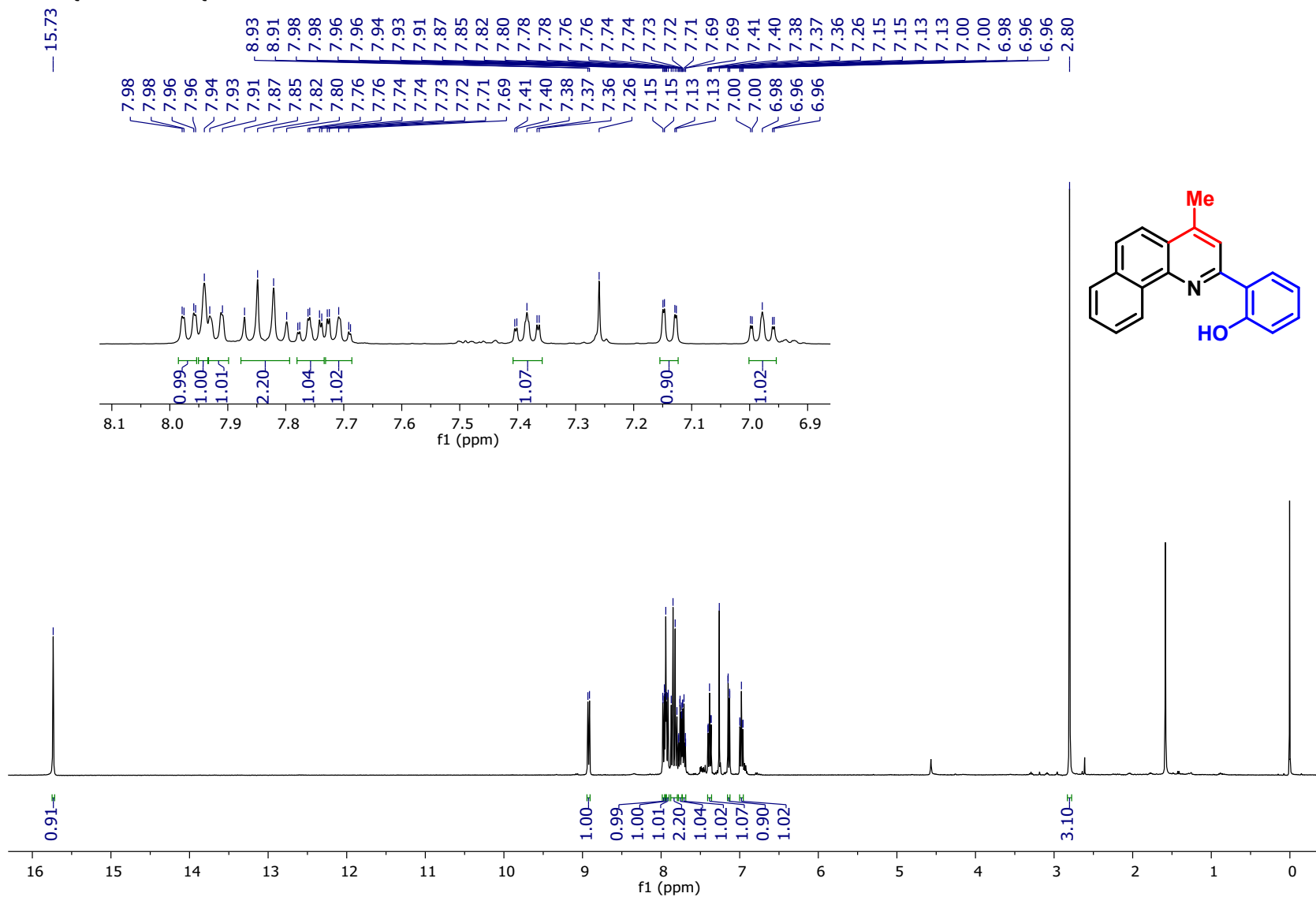
## HRMS spectrum of compound 3f

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User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q7_POS_010.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:17:39 PM (UTC+05:30)



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3g**

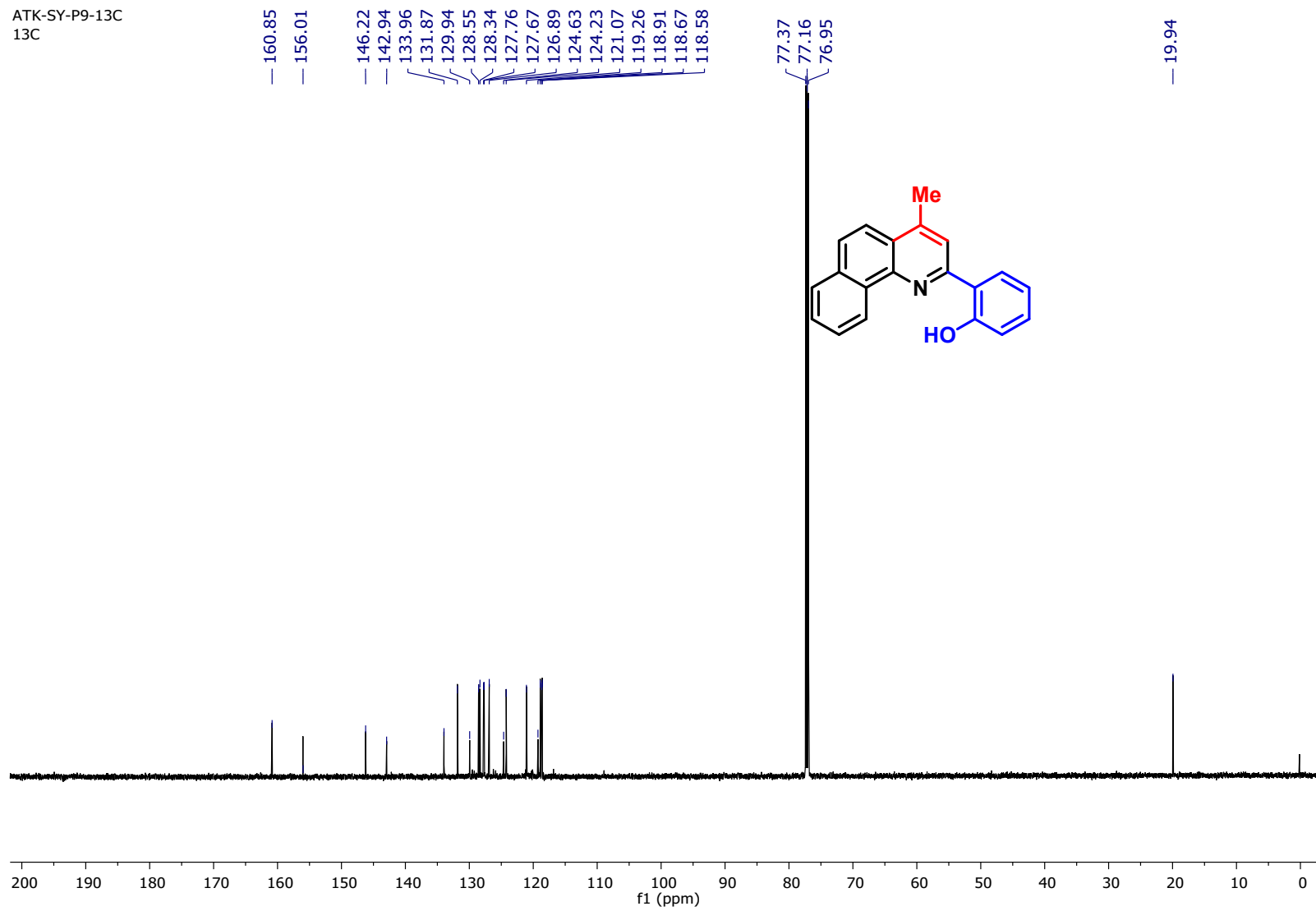
ATK-SY-Q8-1H — ATK-SY-Q8-1H —





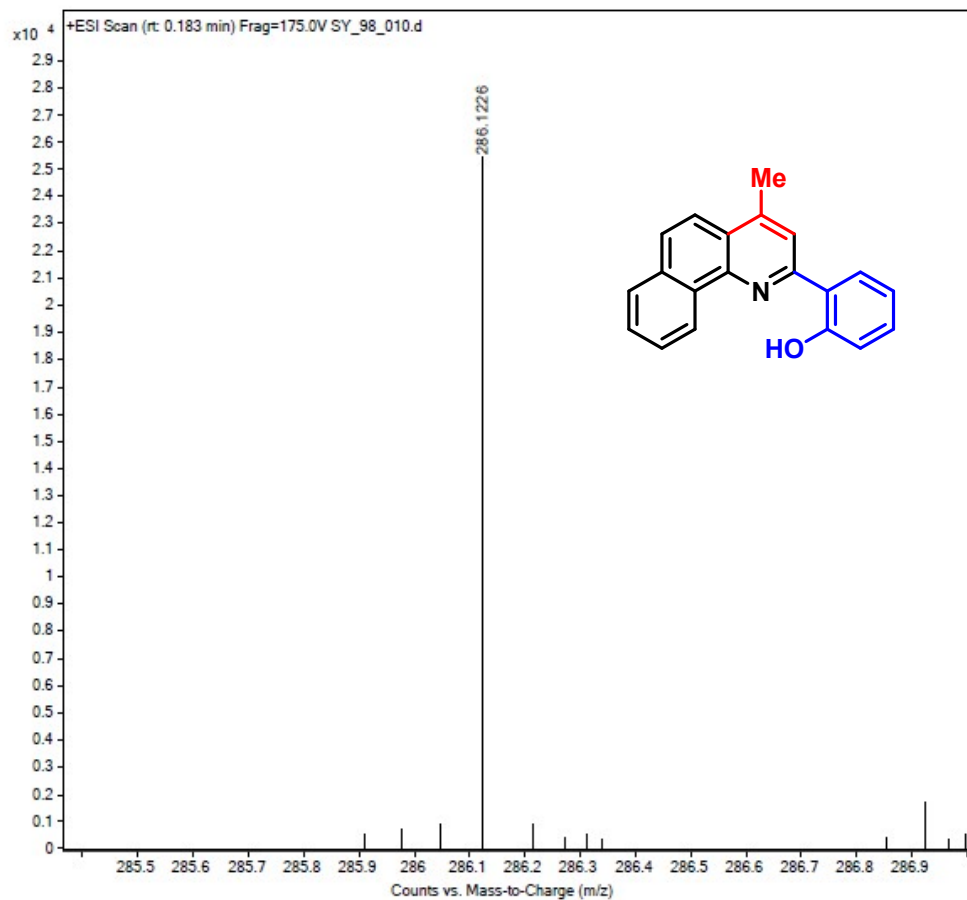
$^{13}\text{C}\{^1\text{H}\}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3g

ATK-SY-P9-13C  
13C



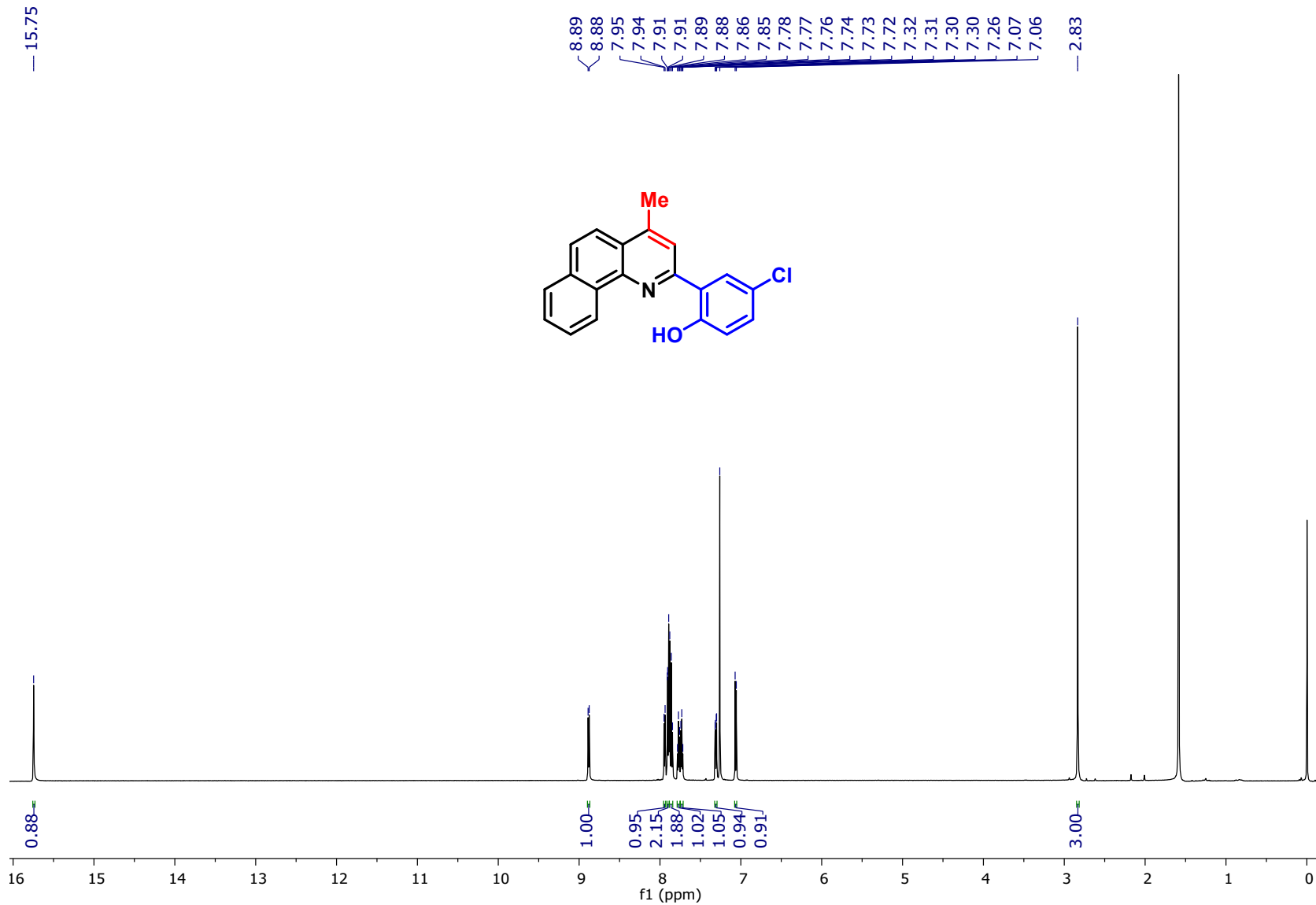
## HRMS spectrum of compound 3g

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User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SY_98_010.d
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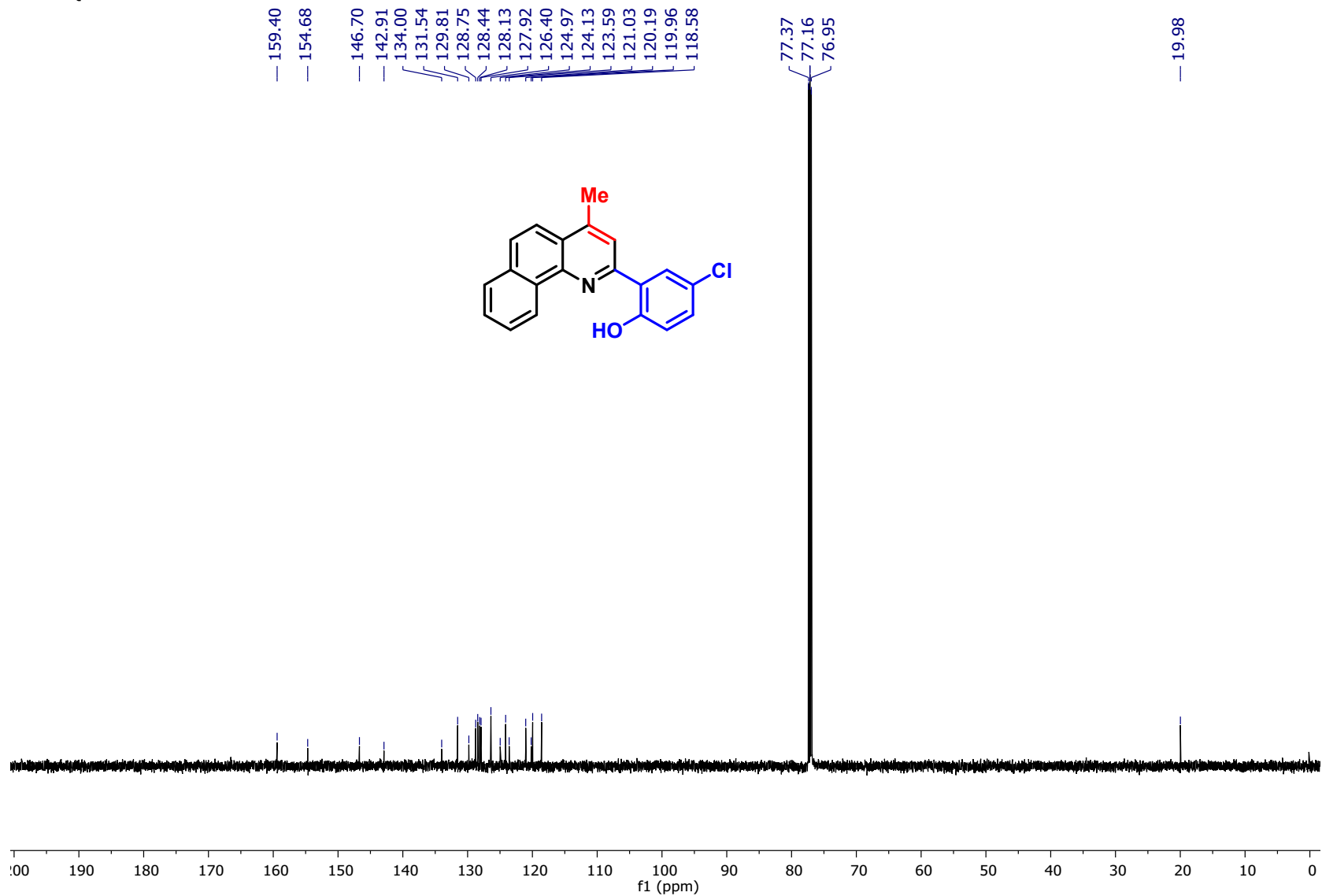
**<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 3h**

ATK-SY-Q10-1H — 1H —



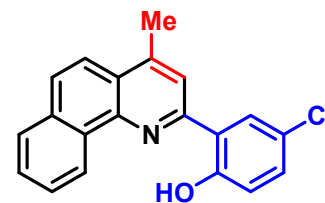
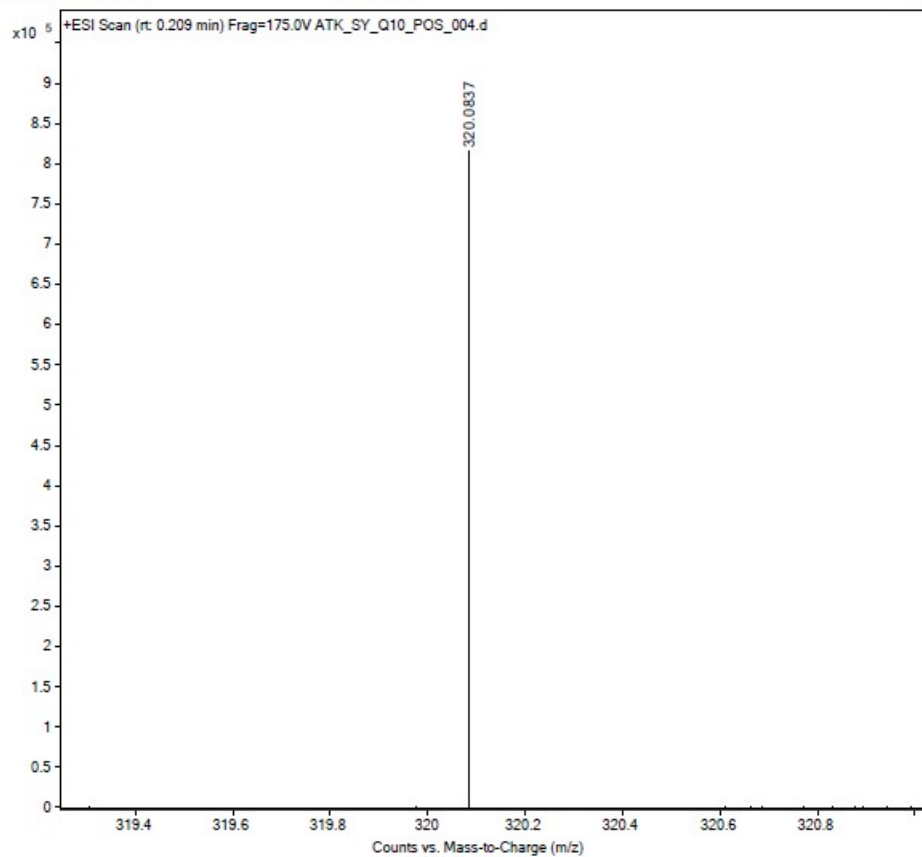
$^{13}\text{C}\{^1\text{H}\}$  (150 MHz,  $\text{CDCl}_3$ ) NMR spectrum of compound 3h

ATK-SY-Q10-13C — 13C —



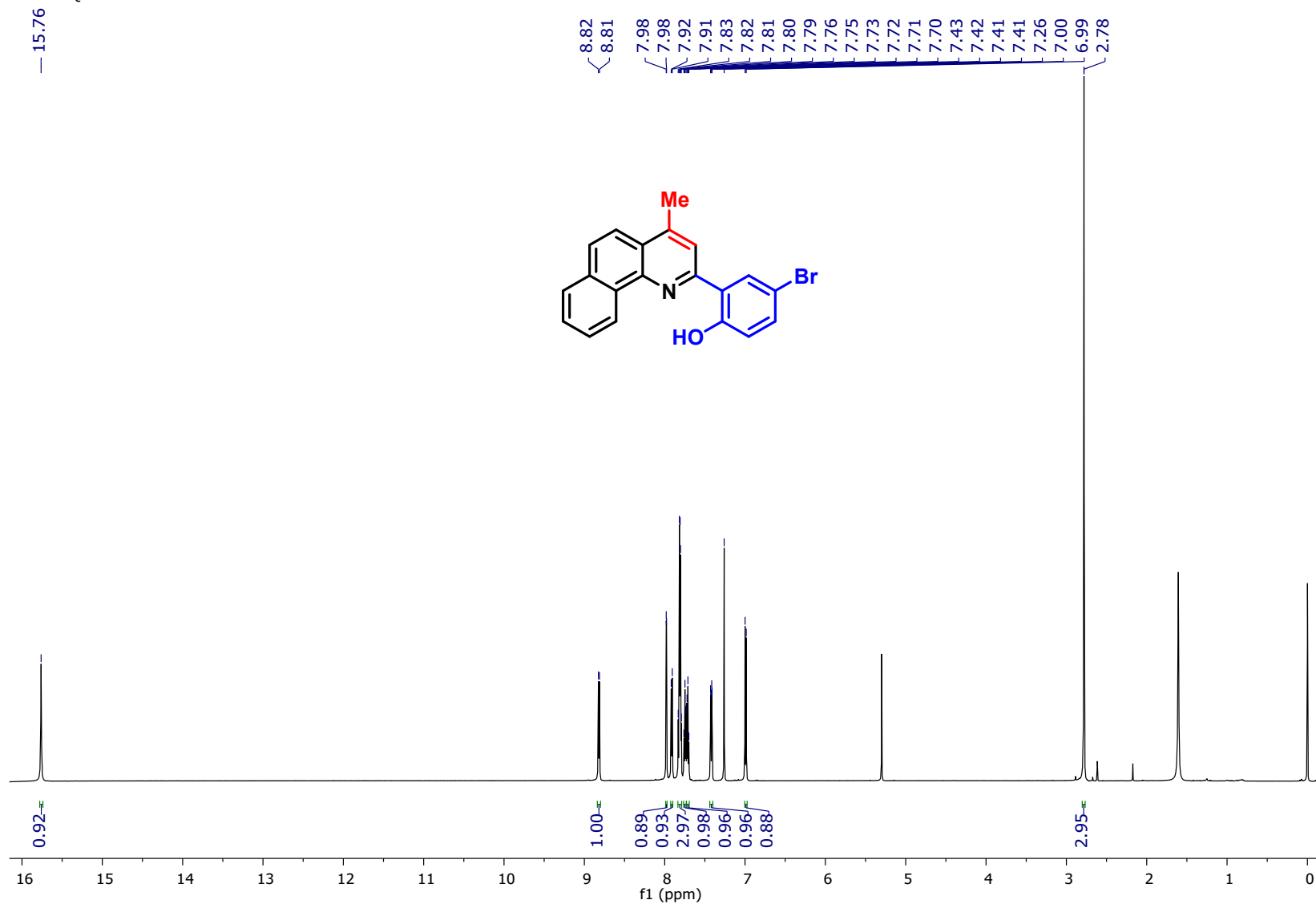
## HRMS spectrum of compound 3h

Sample Name	ATK_SY_Q10_POS	Position	P1-C9	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q10_POS_004.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:06:49 PM (UTC+05:30)



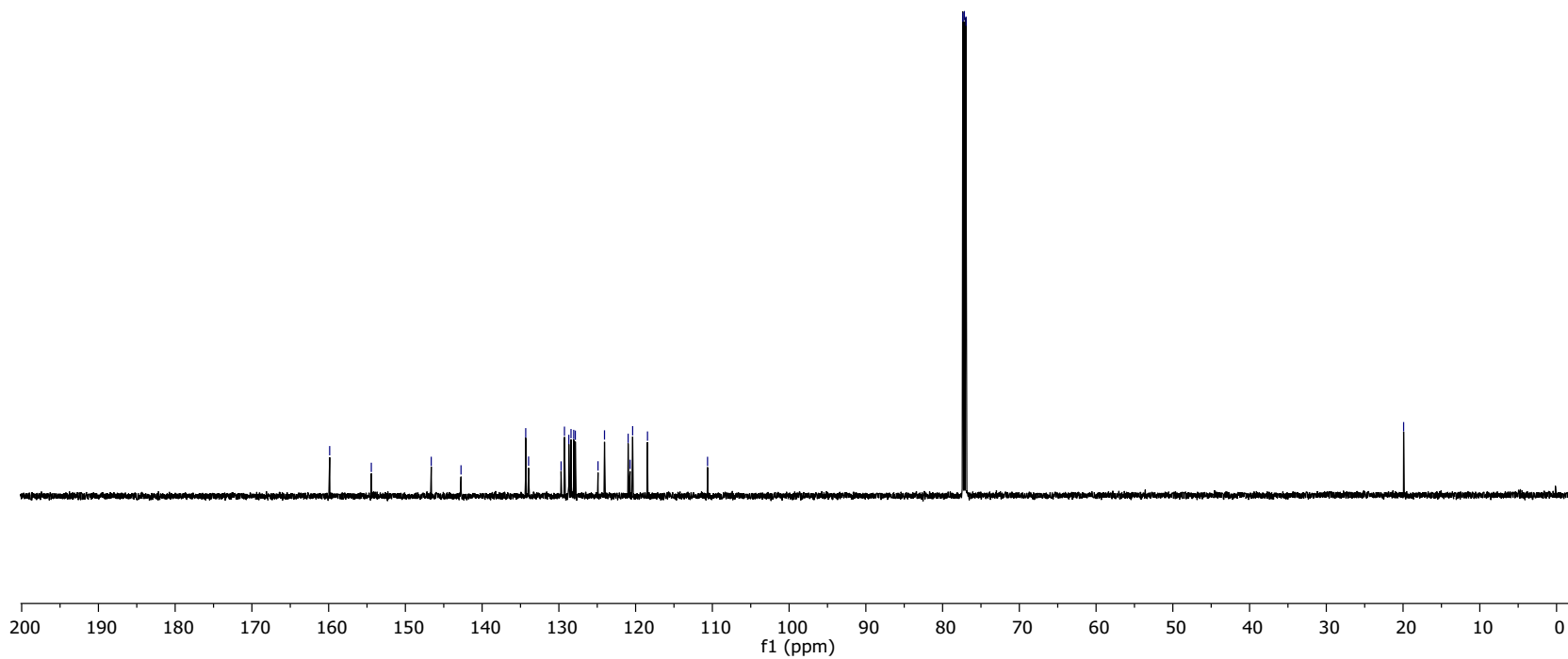
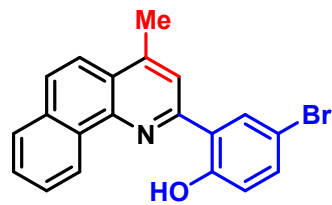
**<sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of compound 3i**

ATK-SY-Q12-1H — 1H —



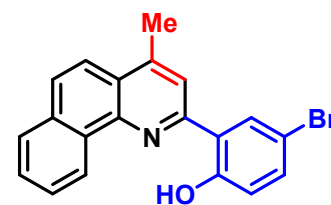
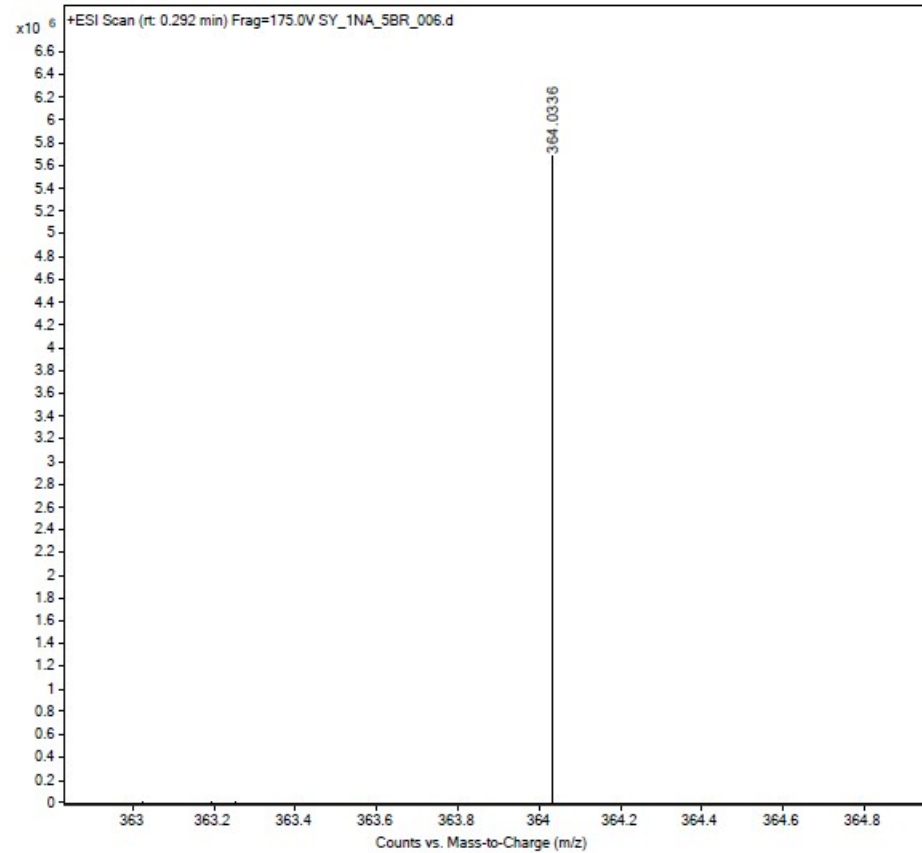
**$^{13}\text{C}\{^1\text{H}\}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3i**

ATK-SY-Q12-13C  
13C



## HRMS spectrum of compound 3i

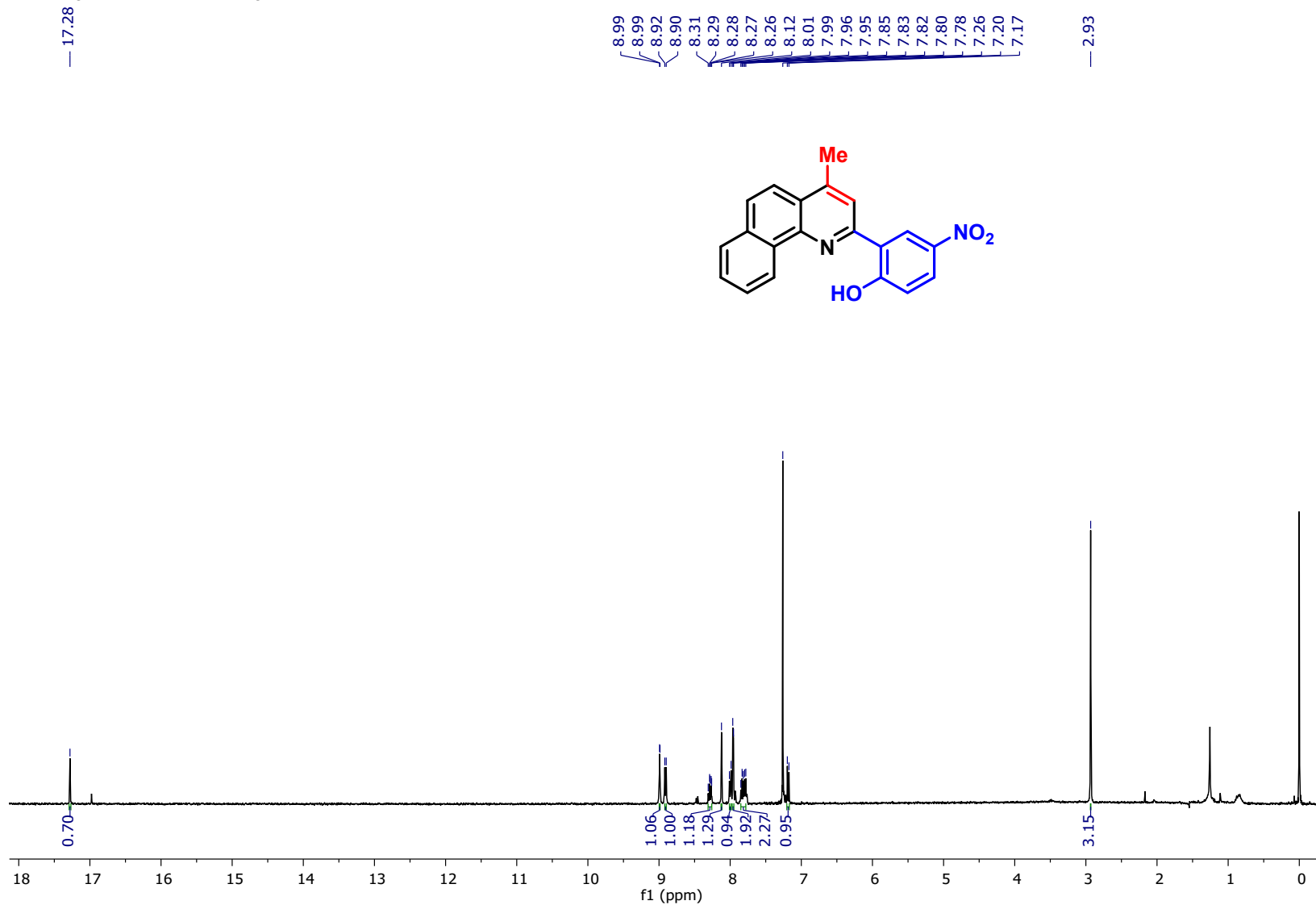
Sample Name	SY_1NA_5BR	Position	P1-A6	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SY_1NA_5BR_006.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Aug-22 12:17:11 AM (UTC+05:30)





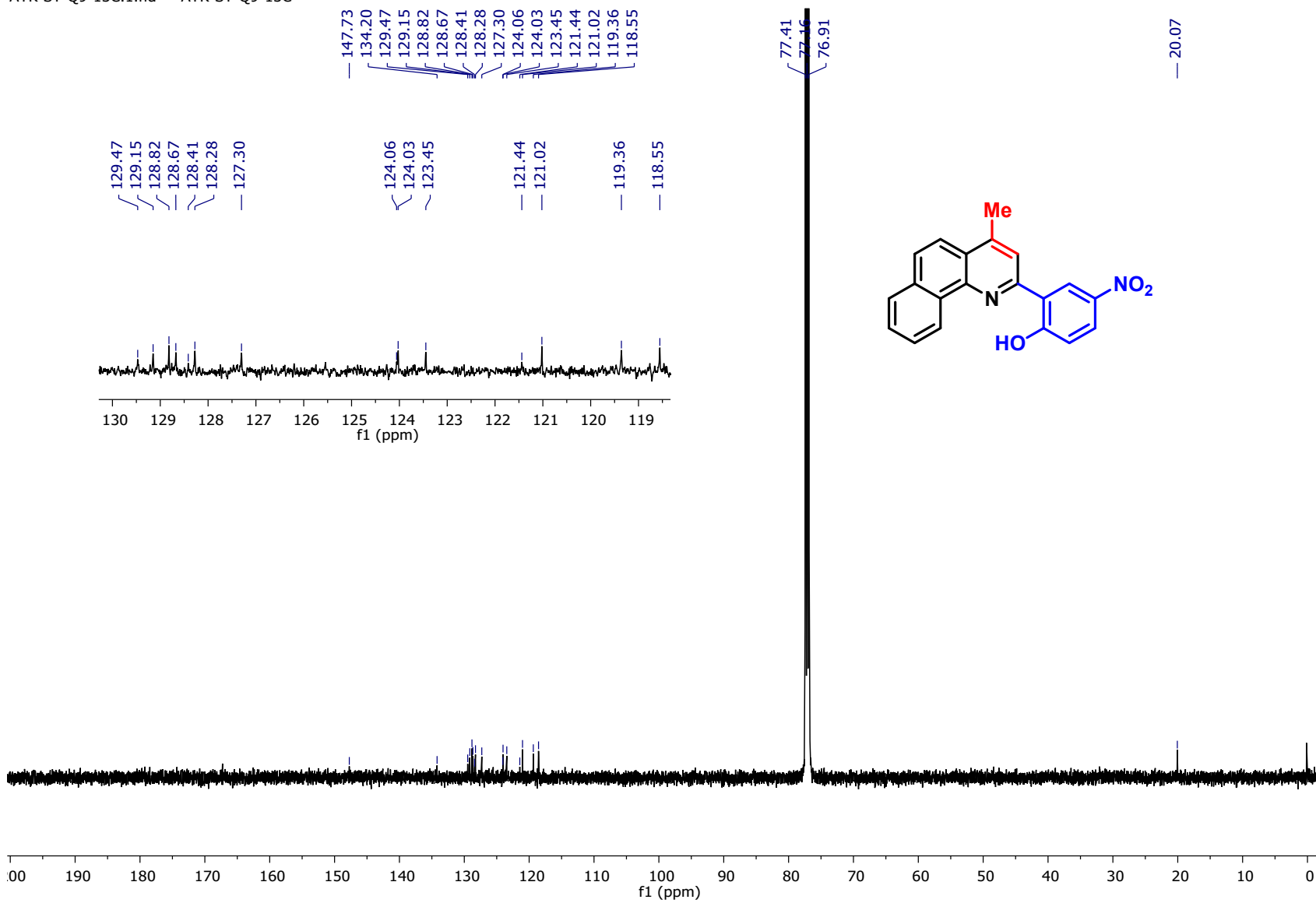
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3j**

ATK-SY-Q9-A-1H.3.fid — ATK-SY-Q9-A-1H



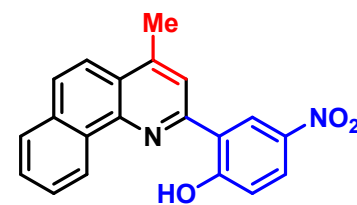
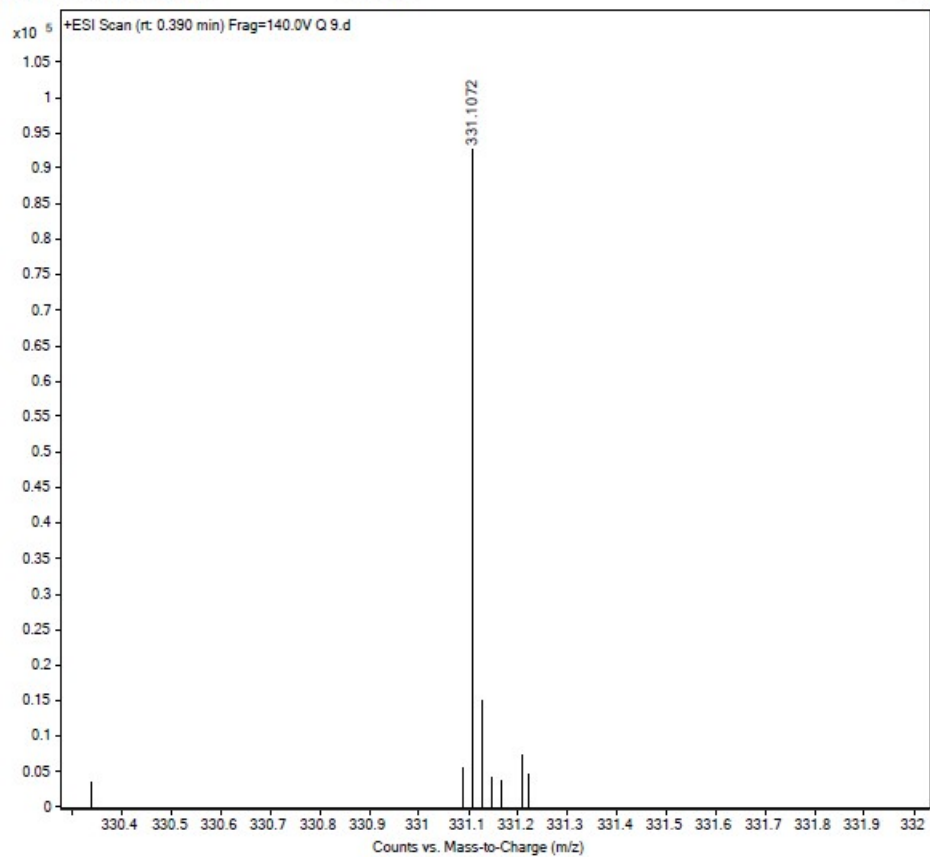
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3j

ATK-SY-Q9-13C.1.fid — ATK-SY-Q9-13C



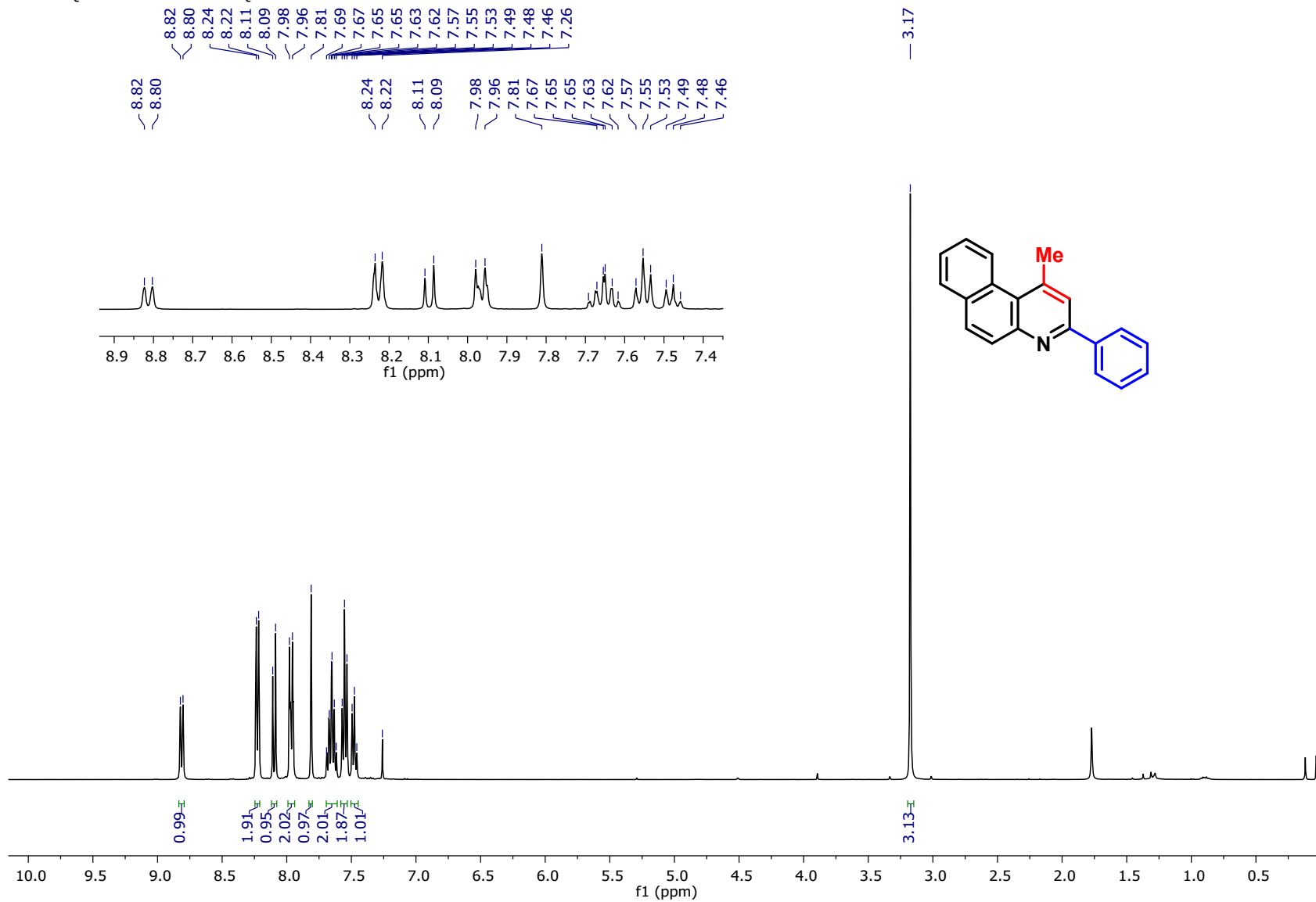
## HRMS spectrum of compound 3j

Sample Name	Sample44	Position	P1-D10	Instrument Name	QTOF
User Name	SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	Q 9.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	Comment		Acquired Time	22-May-23 11:37:31 AM (UTC+05:30)



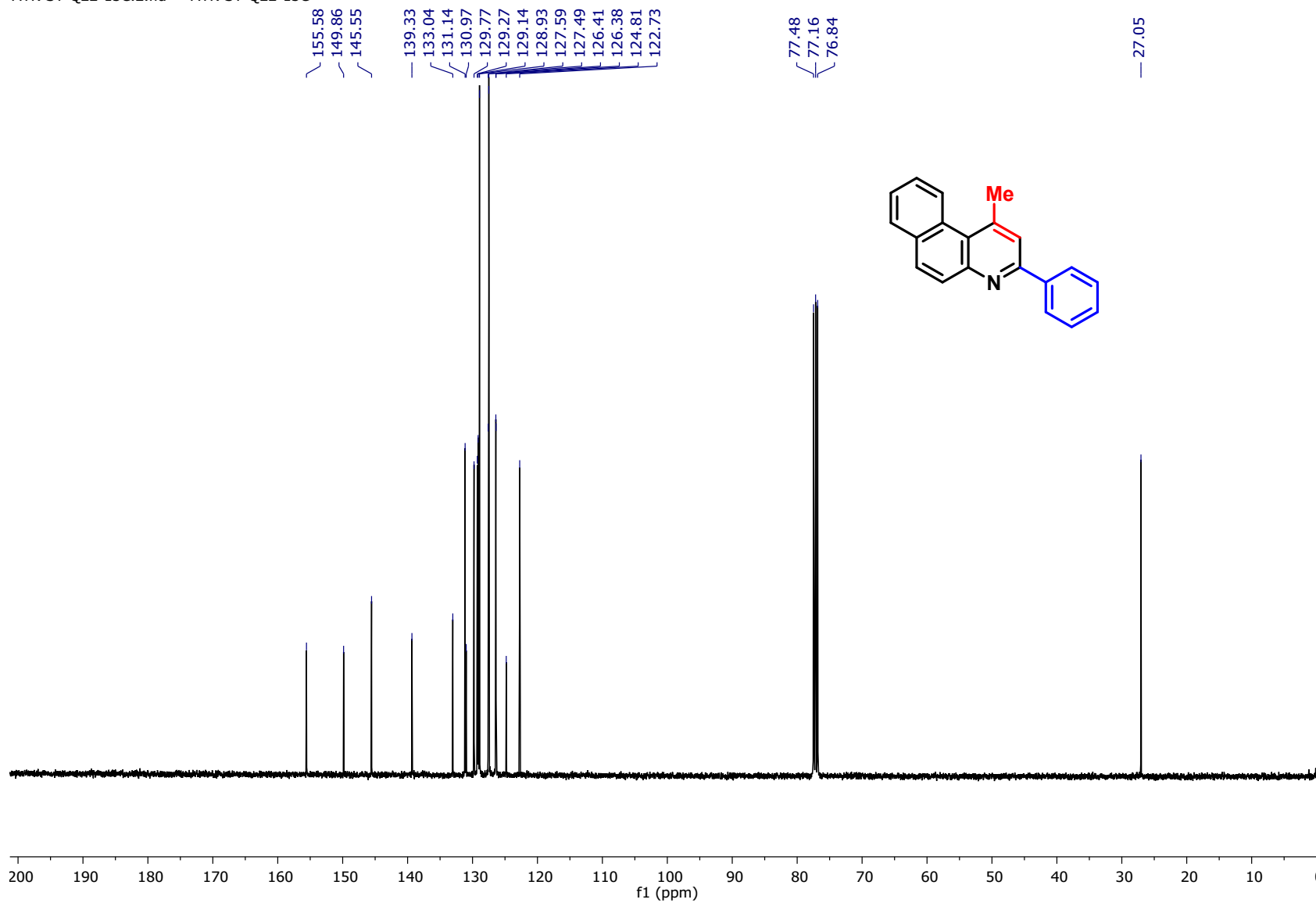
# <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3k

ATK-SY-Q22-1H.1.fid — ATK-SY-Q22-1H



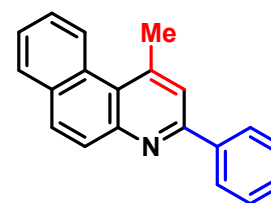
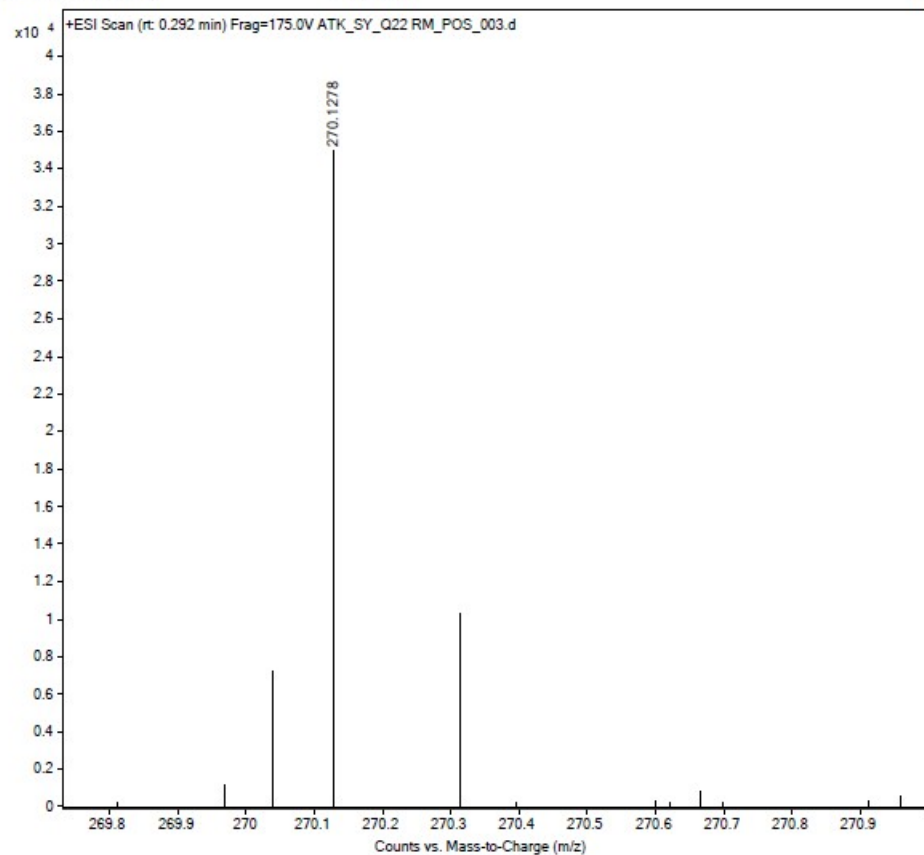
**$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3k**

ATK-SY-Q22-13C.2.fid — ATK-SY-Q22-13C



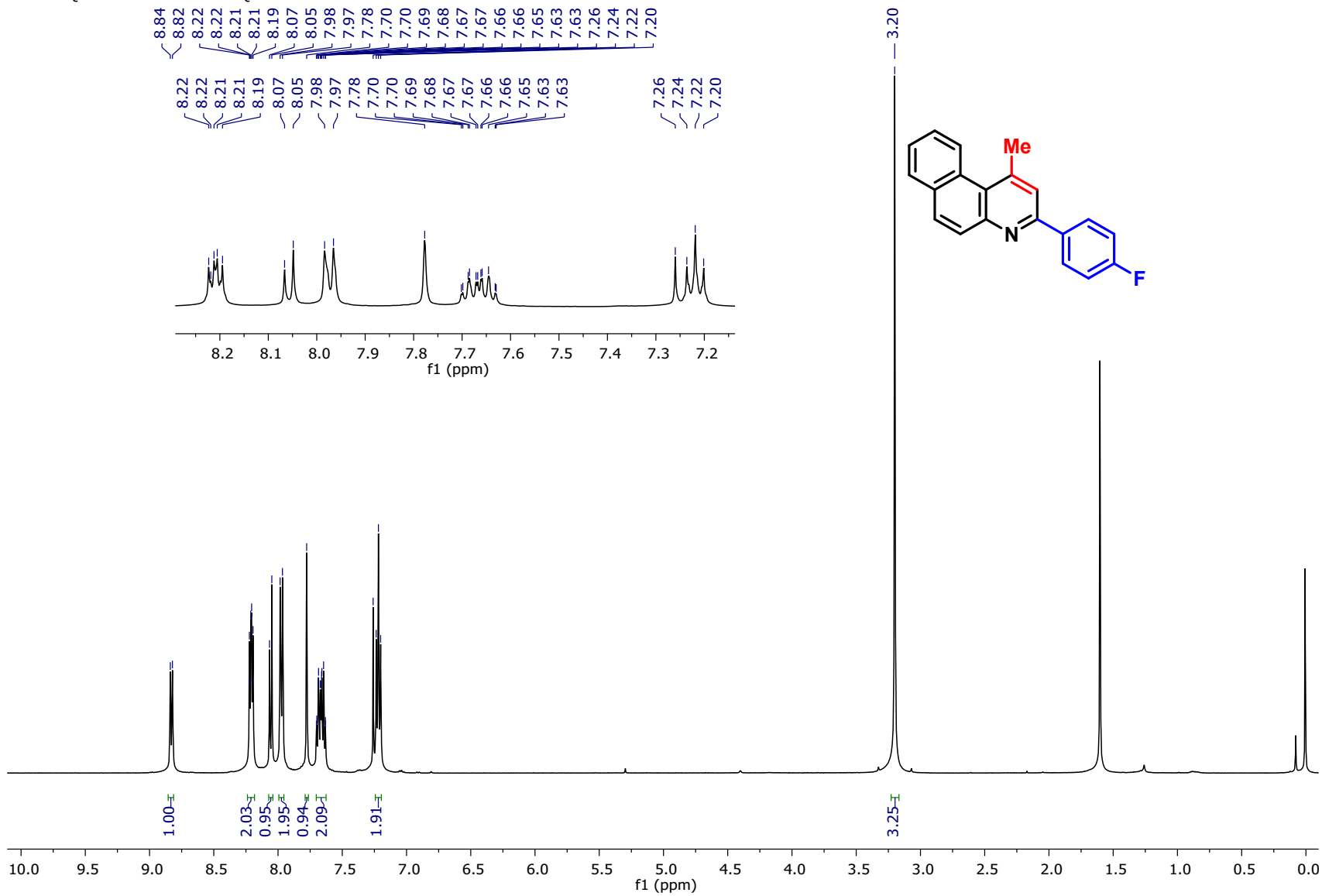
## HRMS spectrum of compound 3k

Sample Name	ATK_SY_Q22 RM_POS	Position	P1-C8	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q22 RM_POS_003.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:05:15 PM (UTC+05:30)



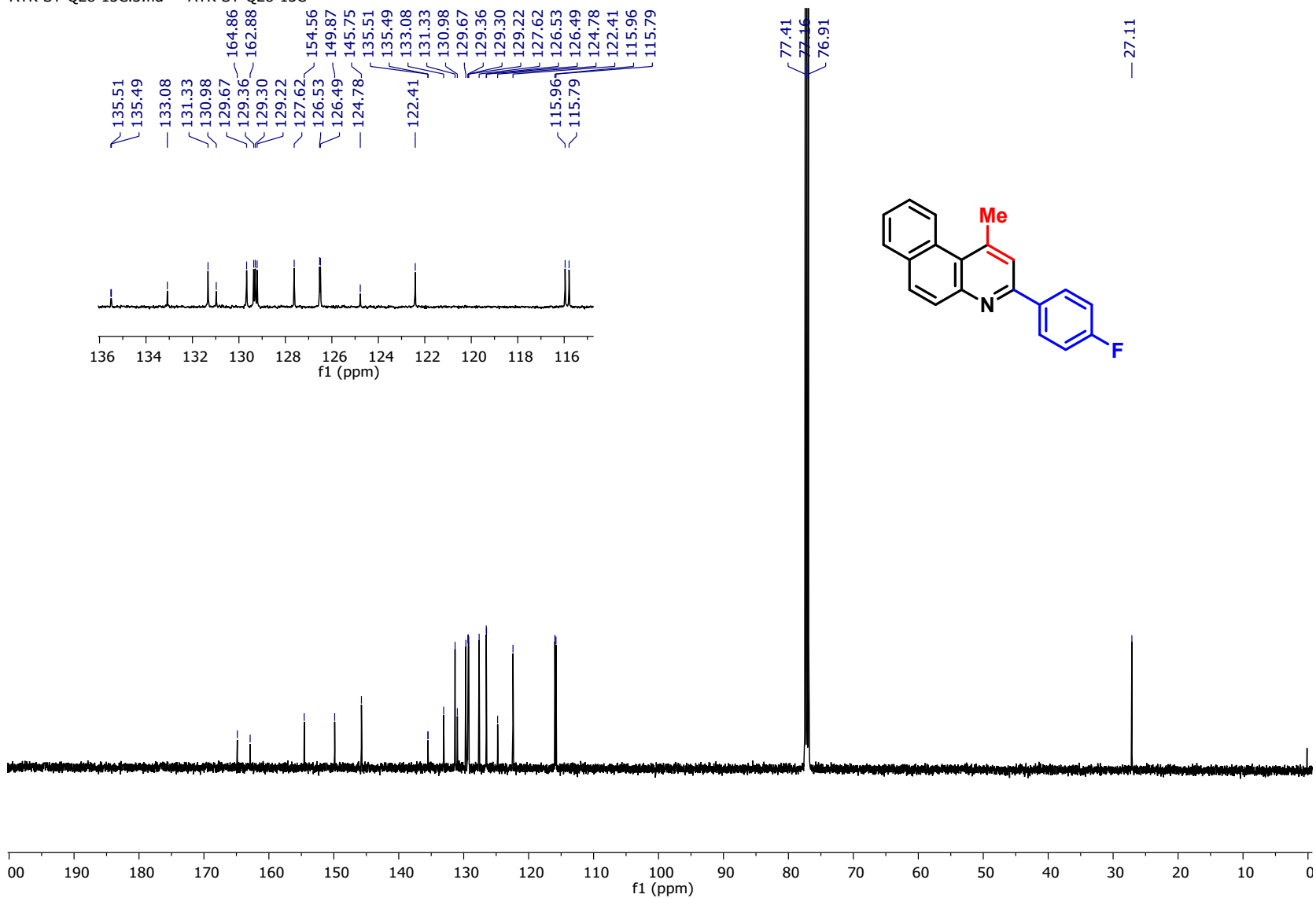
# <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3l

ATK-SY-Q28-1H.1.fid — ATK-SY-Q28-1H



$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3l

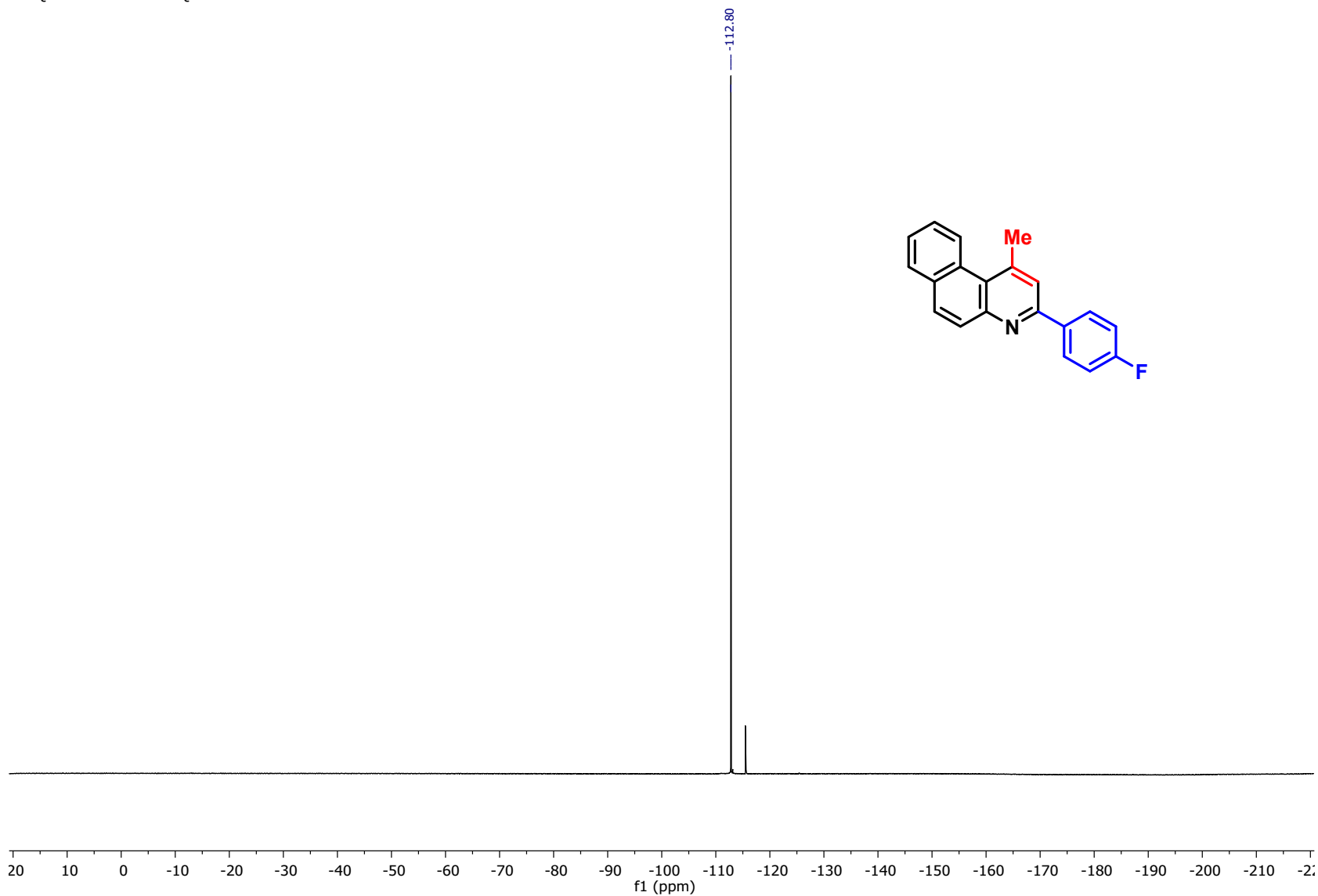
ATK-SY-Q28-13C.3.fid — ATK-SY-Q28-13C





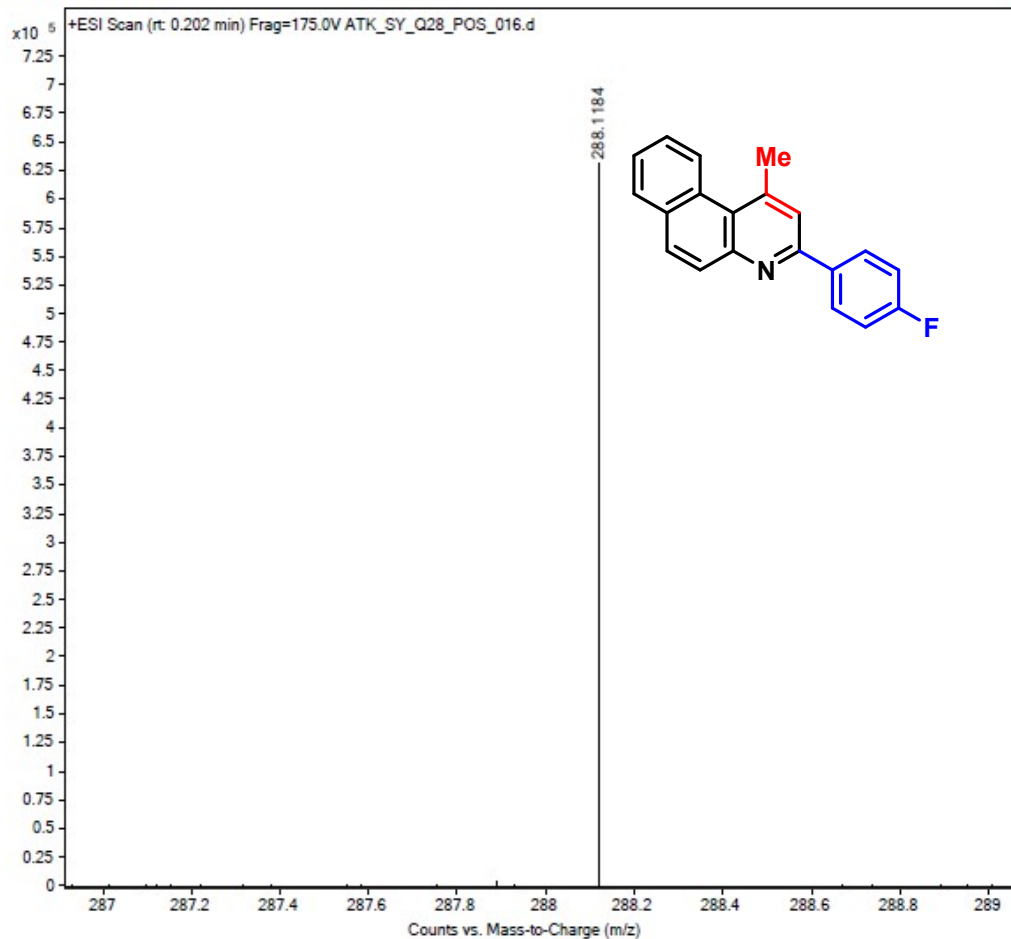
**<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) spectrum of compound 31**

SY-Q28-19F.1.fid — SY-Q28-19F



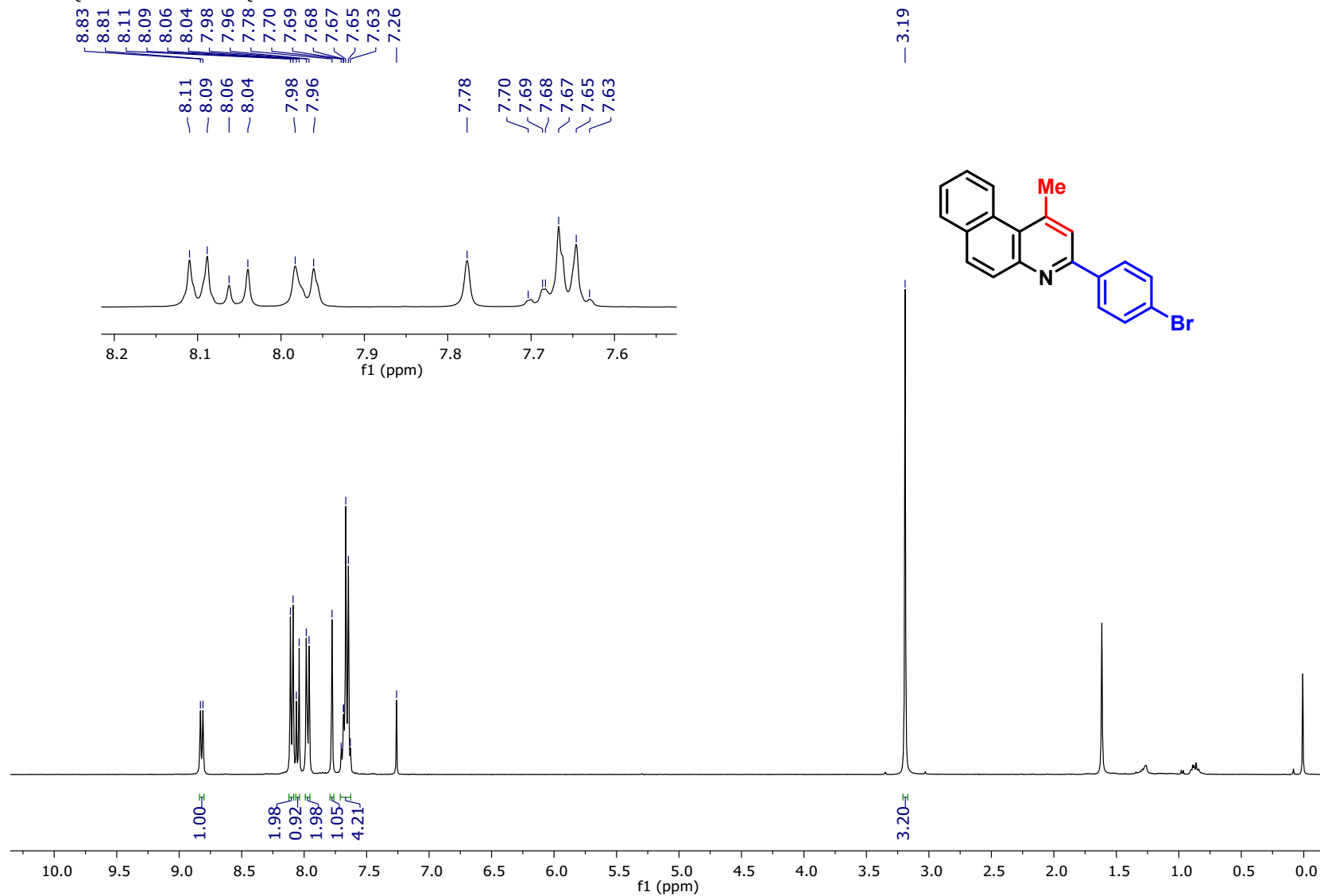
## HRMS spectrum of compound 3l

Sample Name	ATK_SY_Q28_POS	Position	P1-E2	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q28_POS_016.d
ACQ Method	FULL_SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:27:12 PM (UTC+05:30)



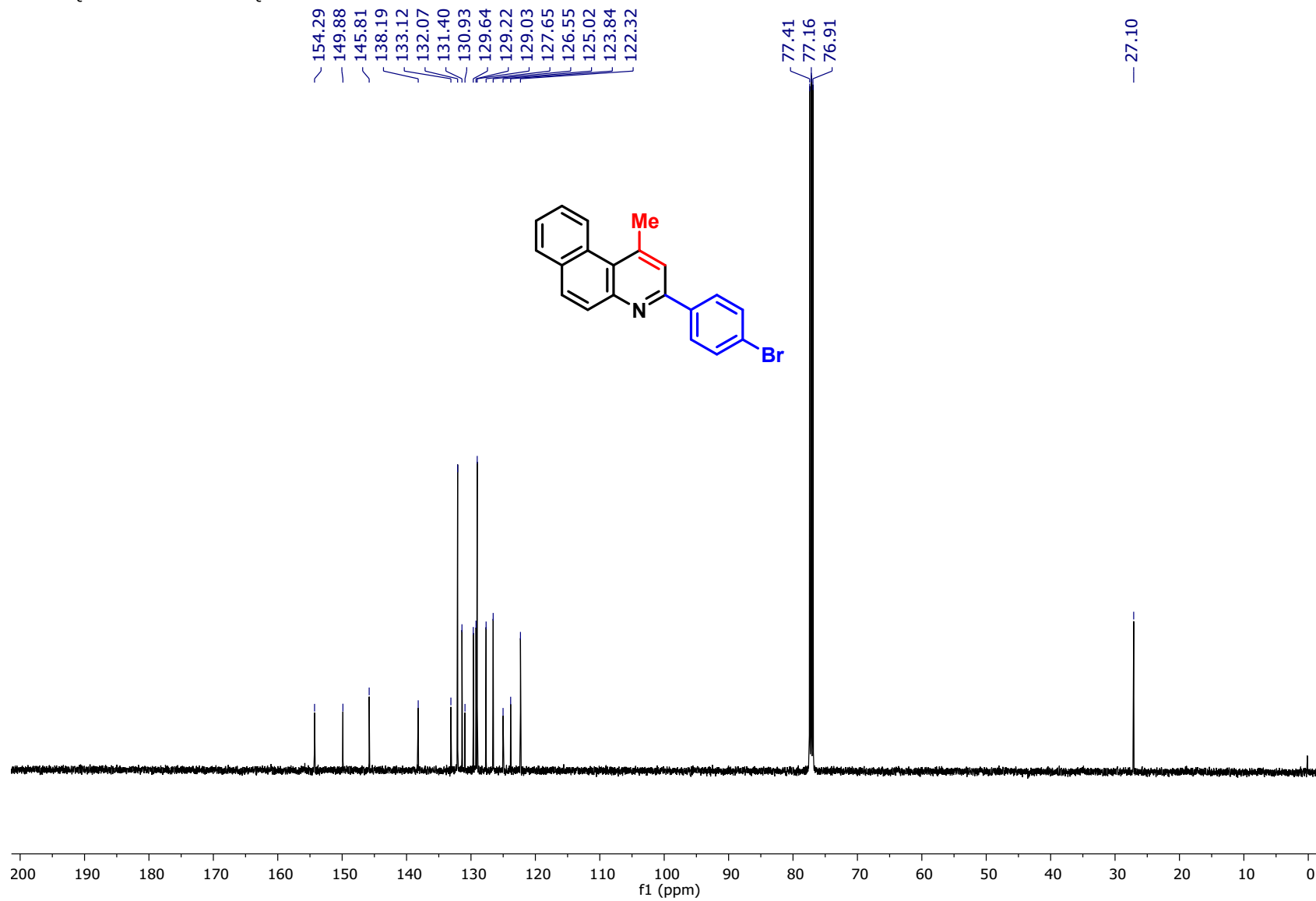
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3m**

ATK-SY-Q26-1H.1.fid — ATK-SY-Q26-1H



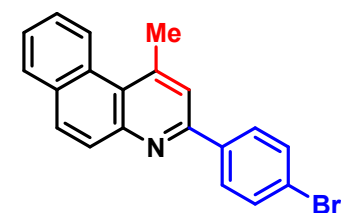
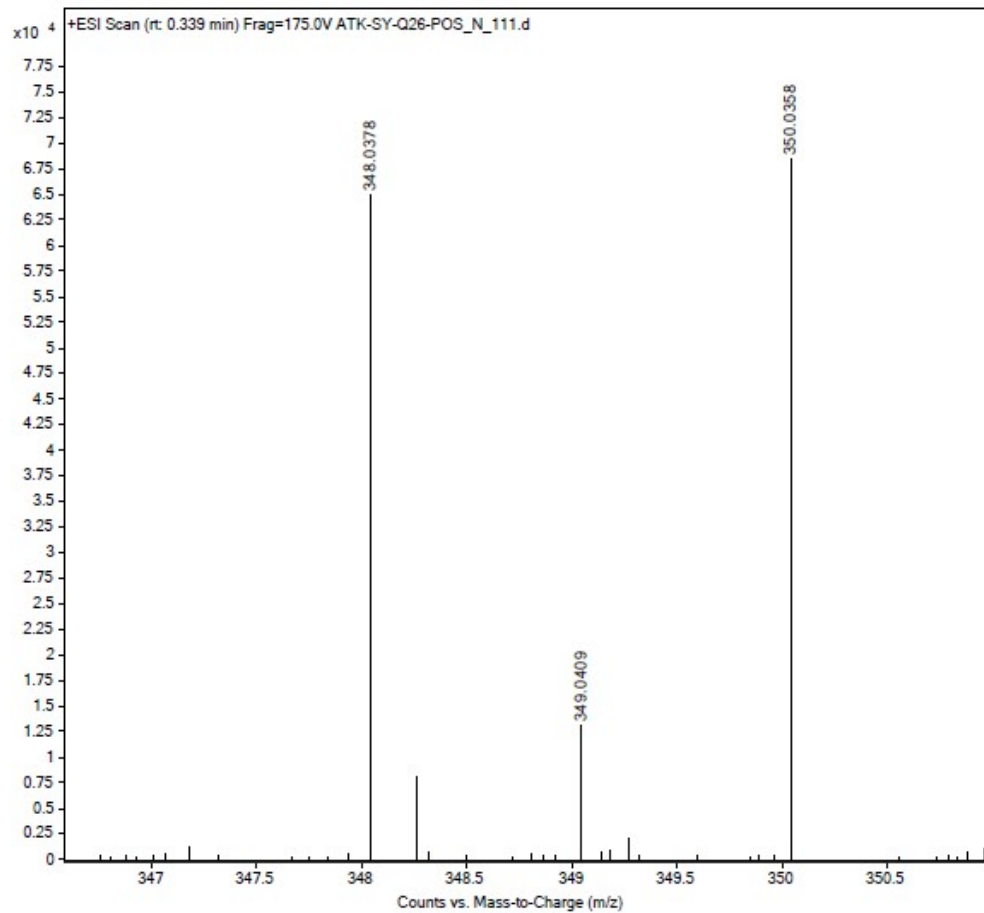
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3m

ATK-SY-Q26-13C.1.fid — ATK-SY-Q26-13C



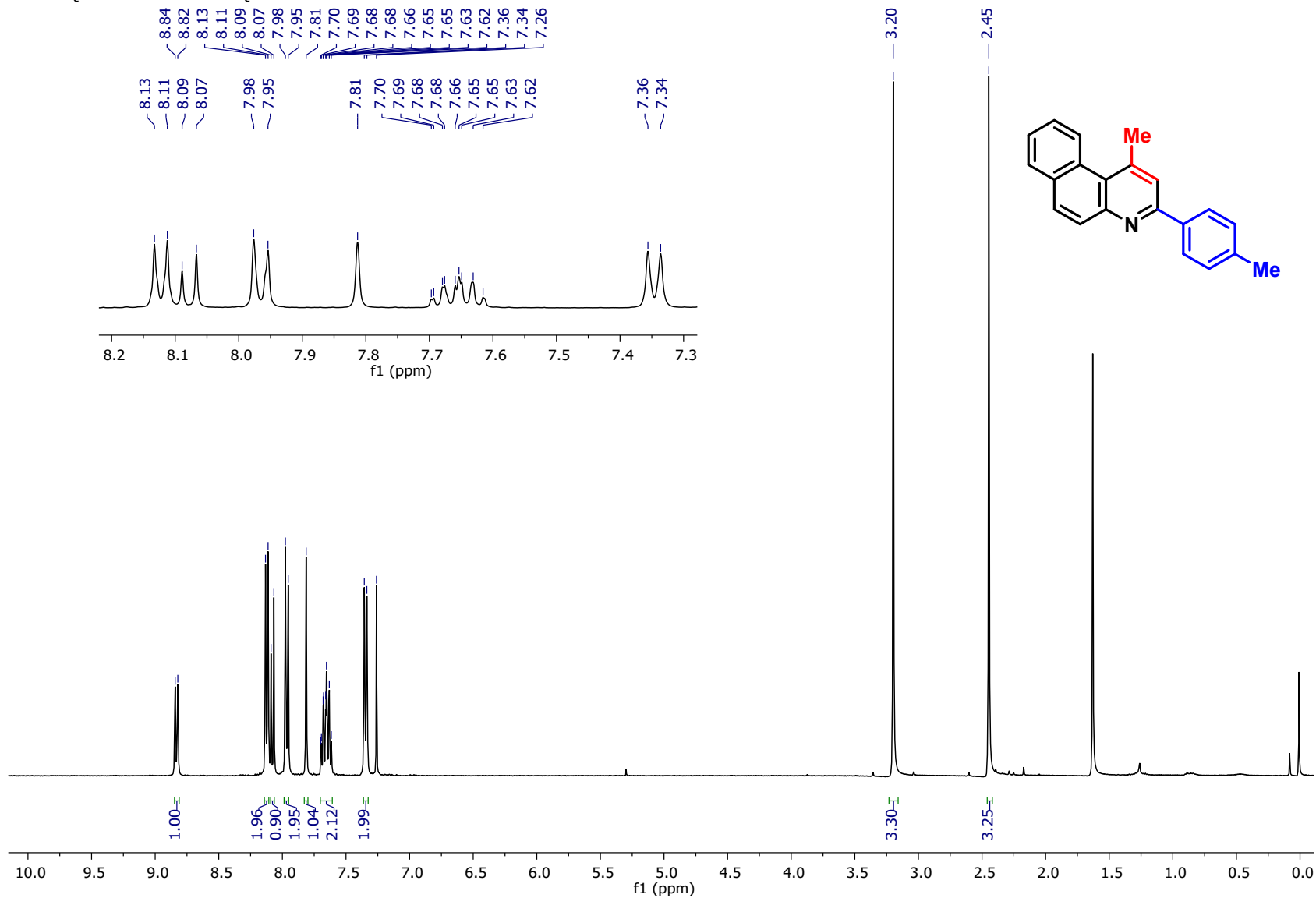
## HRMS spectrum of compound 3m

Sample Name	ATK-SY-Q26-POS_N	Position	P2-B1	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK-SY-Q26-POS_N_111.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	27-Jan-23 10:03:30 PM (UTC+05:30)



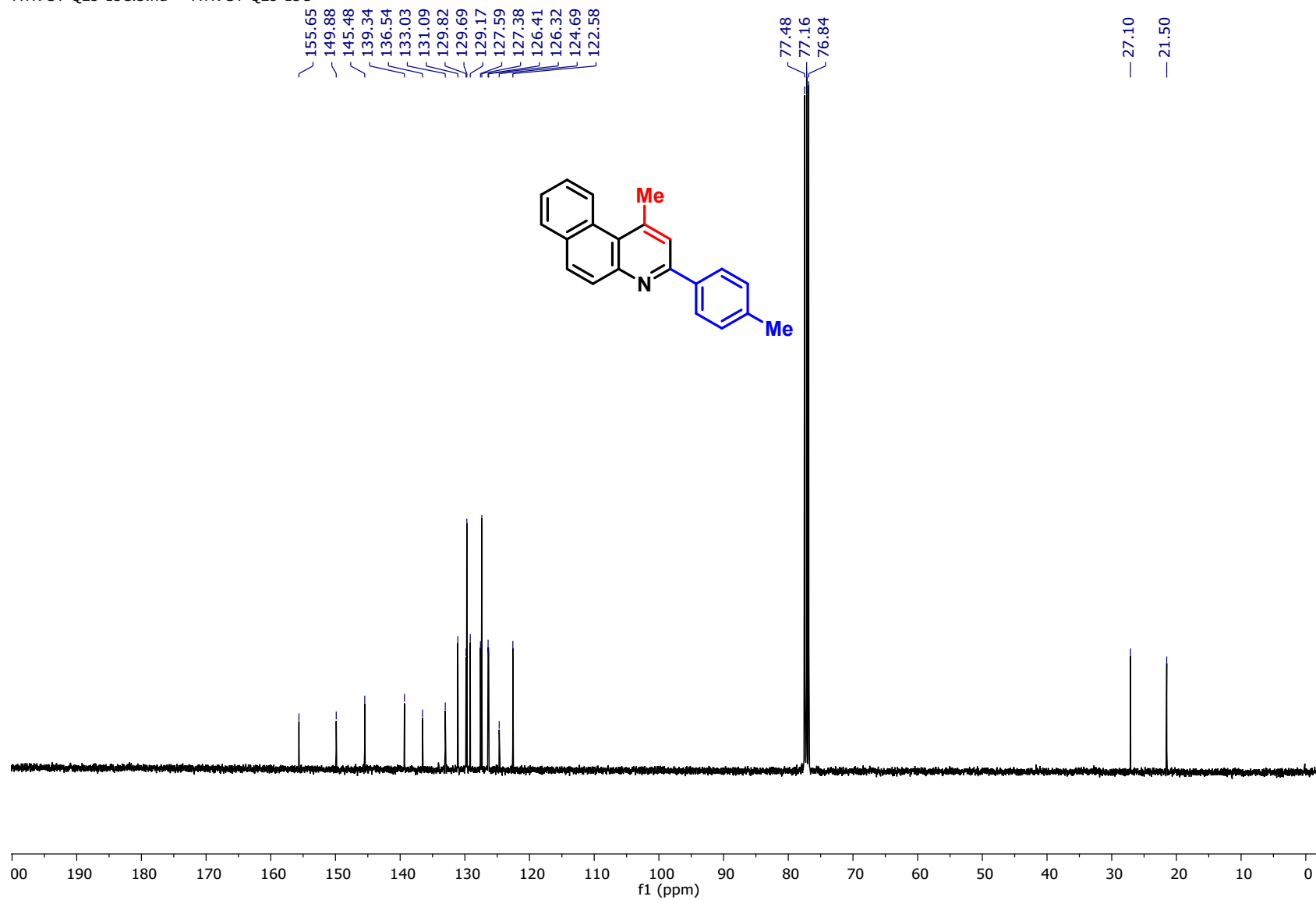
# <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3n

ATK-SY-Q25-1H.1.fid — ATK-SY-Q25-1H



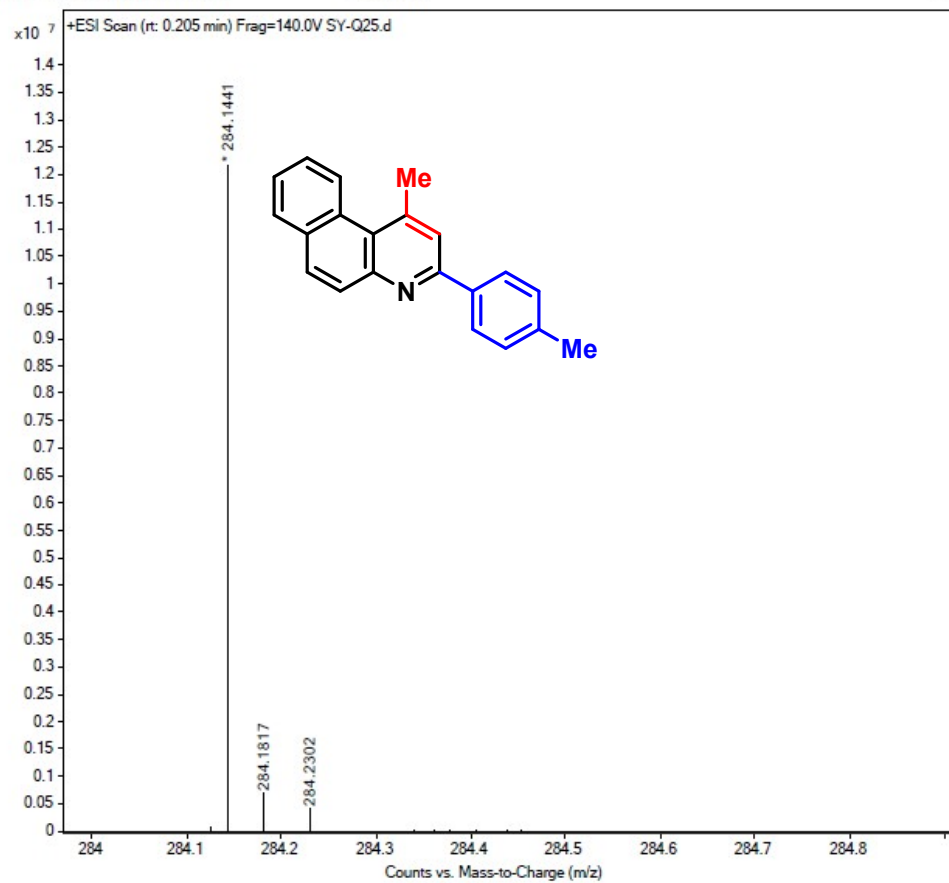
**$^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3n**

ATK-SY-Q25-13C.3.fid — ATK-SY-Q25-13C



## HRMS spectrum of compound 3n

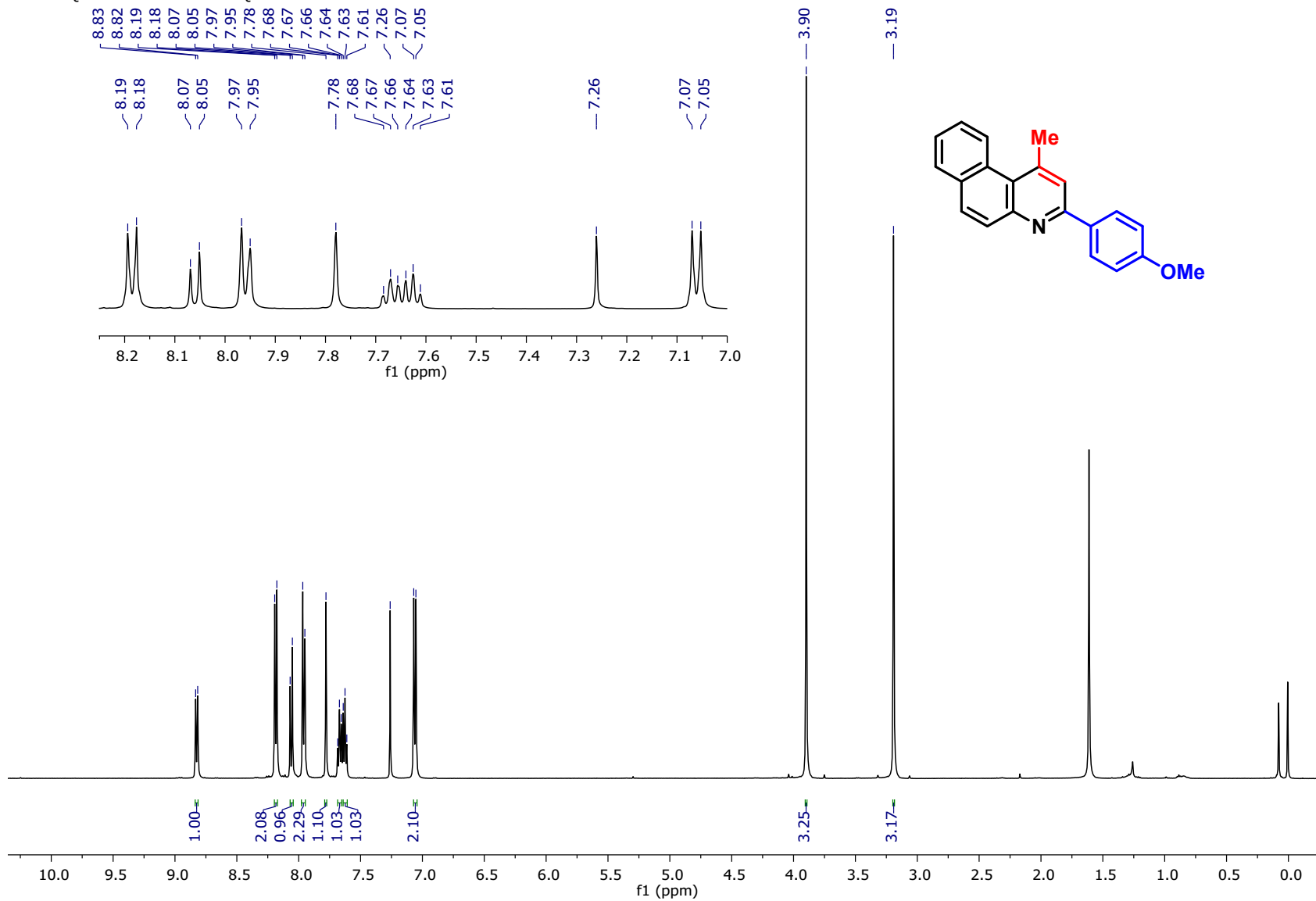
<b>Sample Name</b>	Sample12	<b>Position</b>	P1-A11	<b>Instrument Name</b>	QTOF
<b>User Name</b>	SYSTEM (SYSTEM)	<b>Inj Vol</b>	5	<b>InjPosition</b>	
<b>Sample Type</b>	Sample	<b>IRM Calibration Status</b>	Success	<b>Data Filename</b>	SY-Q25.d
<b>ACQ Method</b>	DIRECT MASS_POSITIVE_01_1.m	<b>Comment</b>		<b>Acquired Time</b>	27-Jul-23 10:31:08 AM (UTC+05:30)





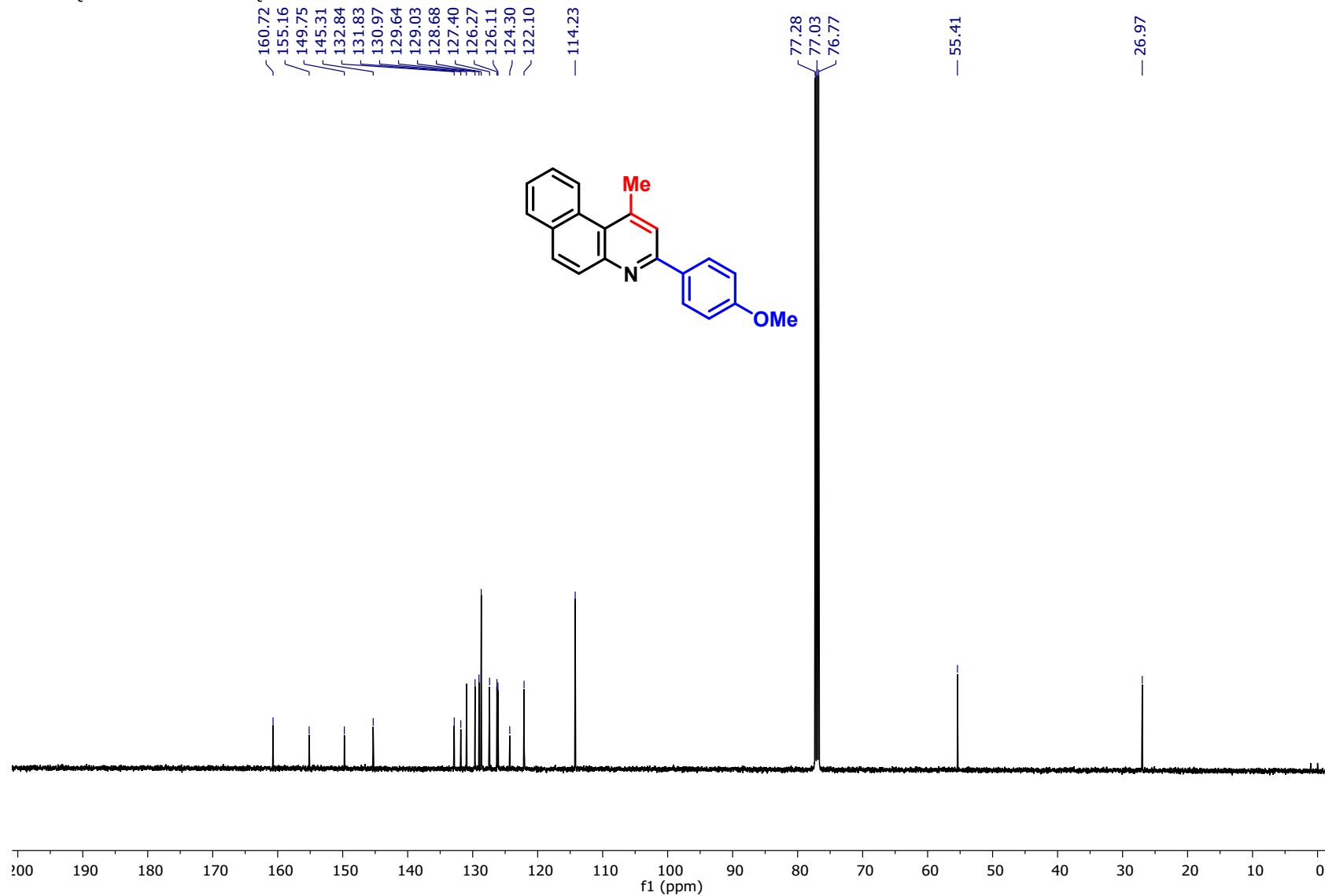
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3o**

ATK-SY-Q18-1H.1.fid — ATK-SY-Q18-1H



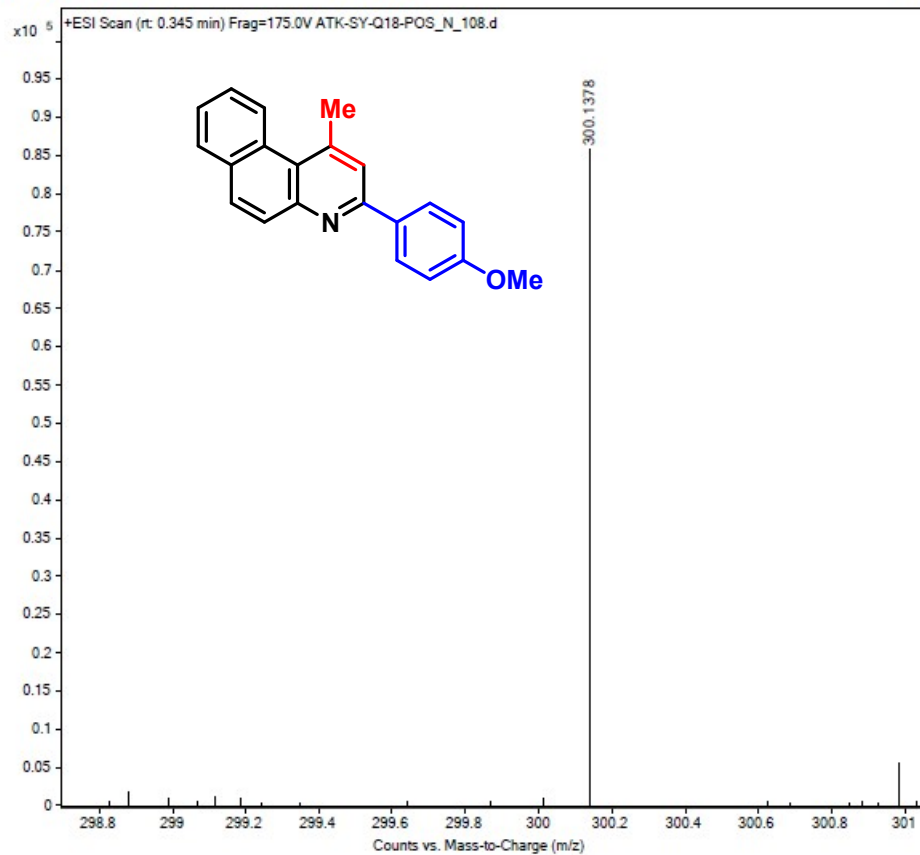
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3o

ATK-SY-Q18-13C.3.fid — ATK-SY-Q18-13C



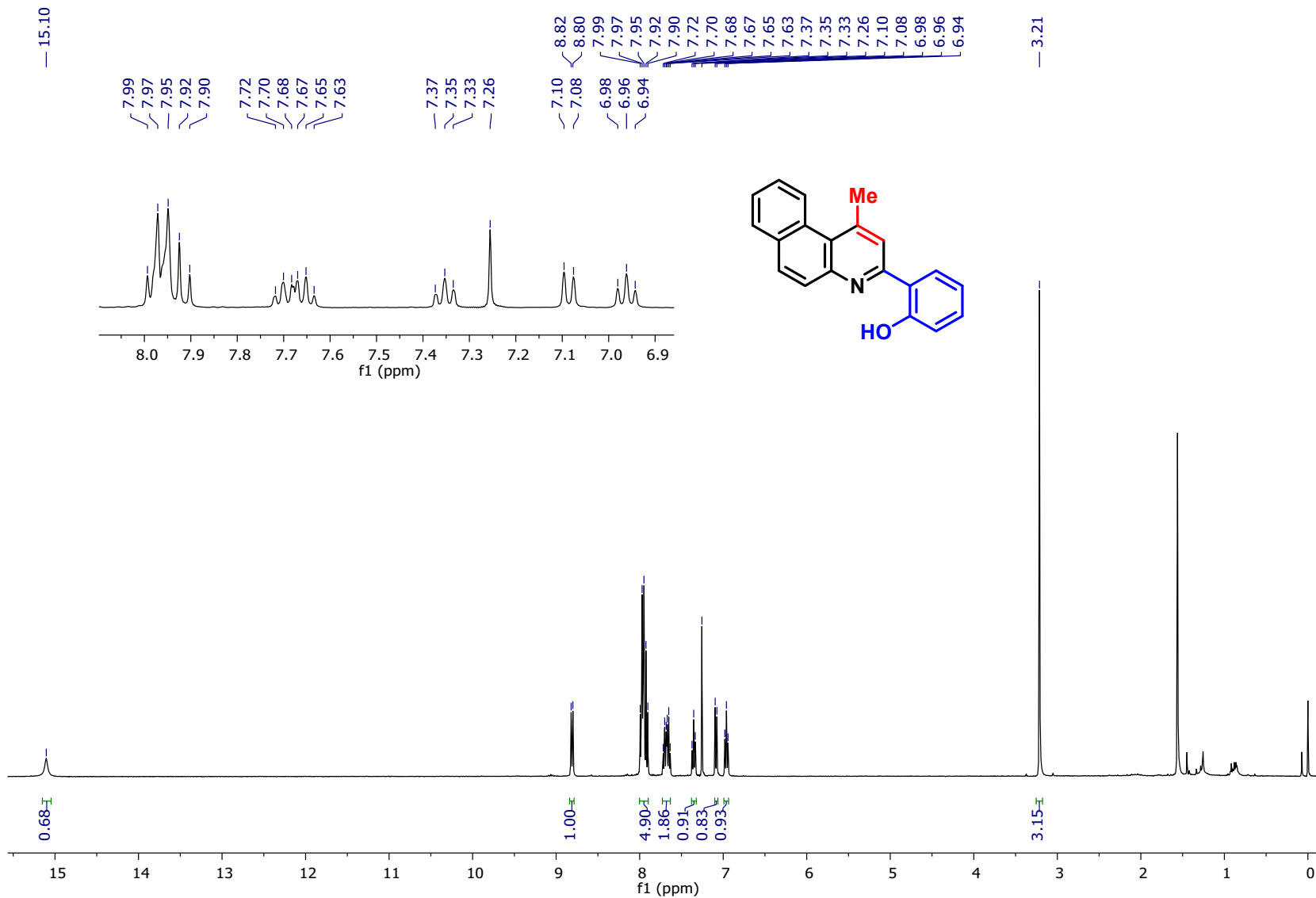
## HRMS spectrum of compound 3o

Sample Name	ATK-SY-Q18-POS_N	Position	P1-F9	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK-SY-Q18-POS_N_108.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	27-Jan-23 09:58:41 PM (UTC+05:30)



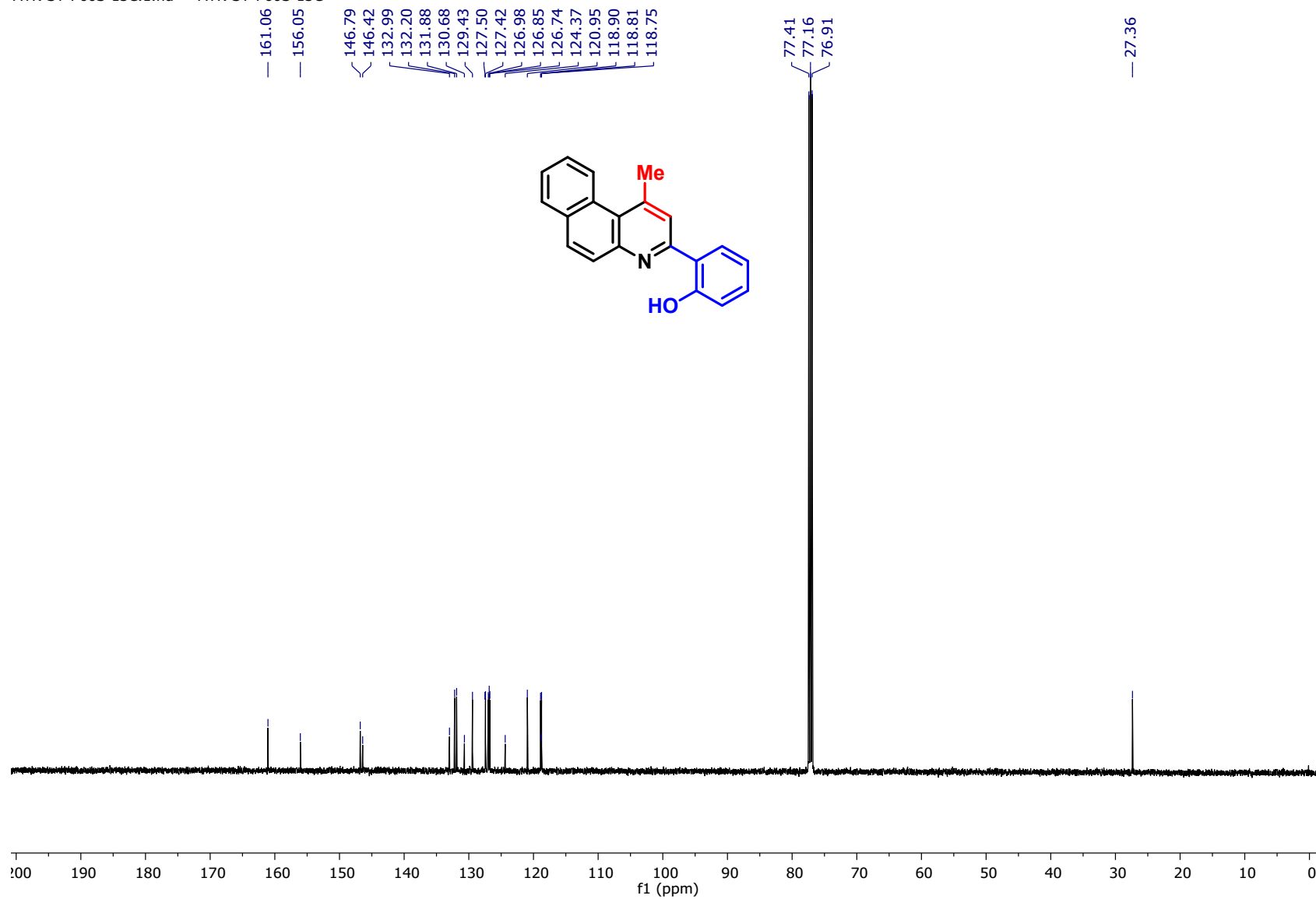
# <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3p

ATK-SY-P60S-1H.1.fid — ATK-SY-P60S-1H

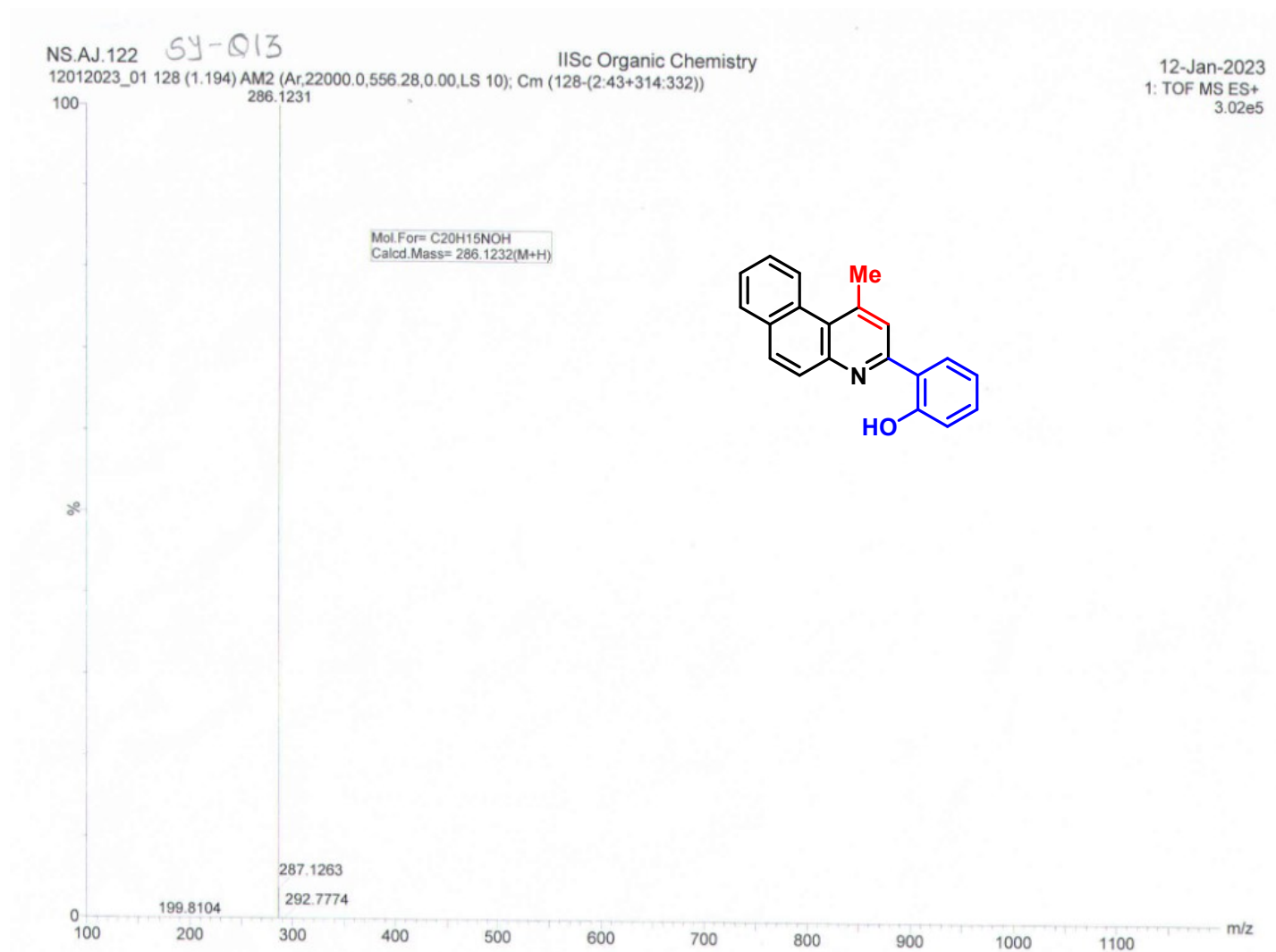


$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3p

ATK-SY-P60S-13C.1.fid — ATK-SY-P60S-13C

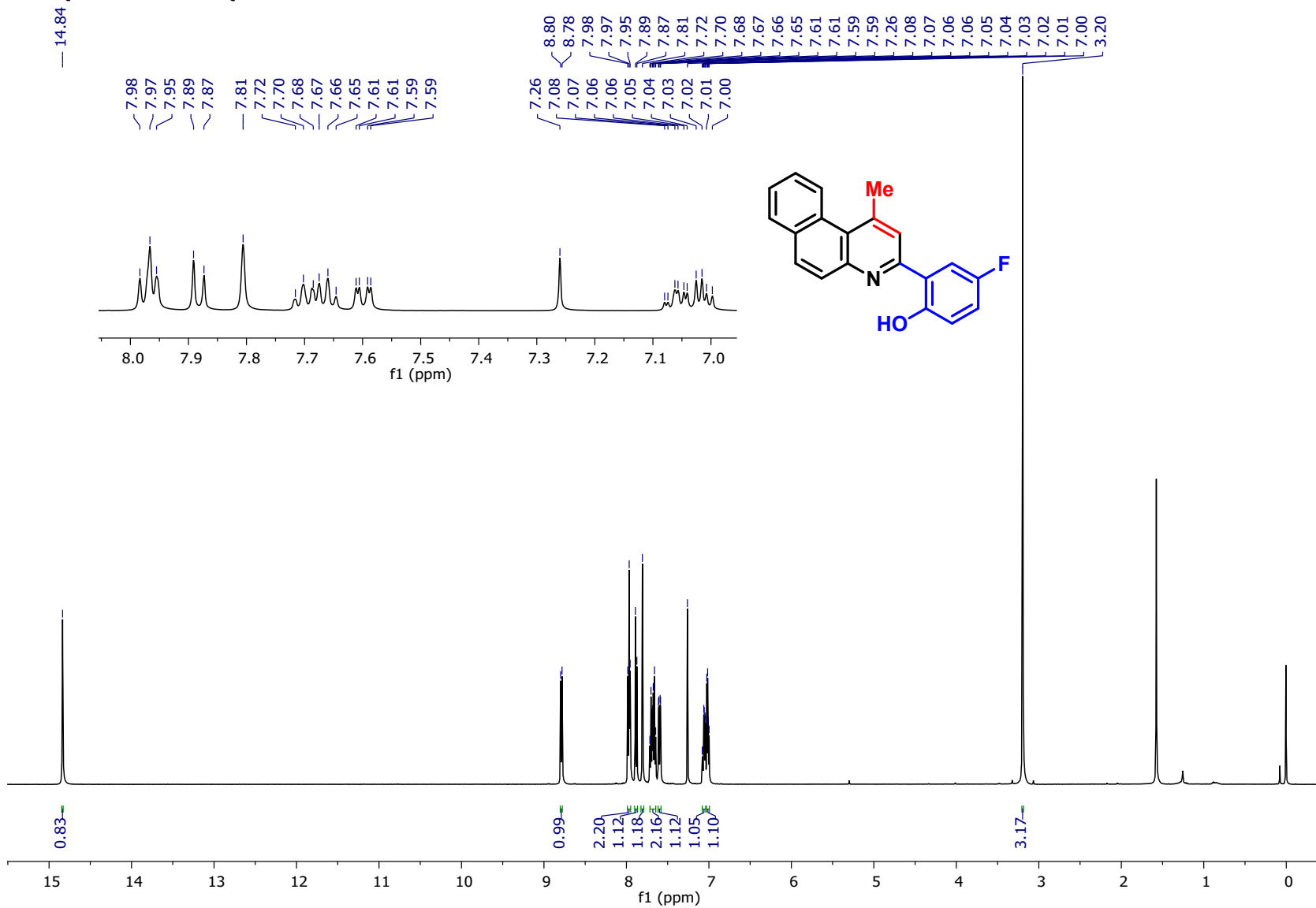


# HRMS spectrum of compound 3p



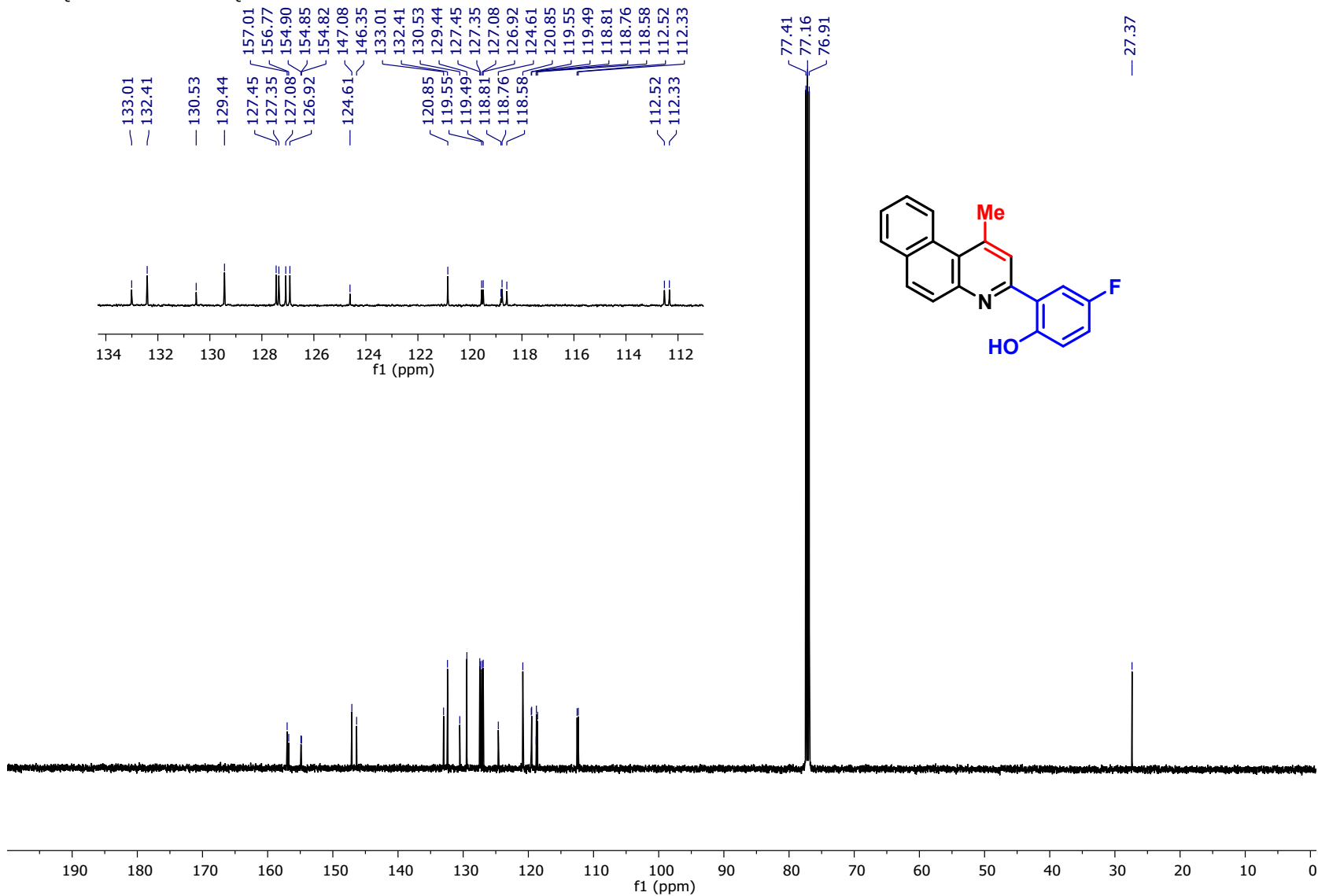
# <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3q

AD-SY-Q27-1H.1.fid — AD-SY-Q27-1H



$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3q

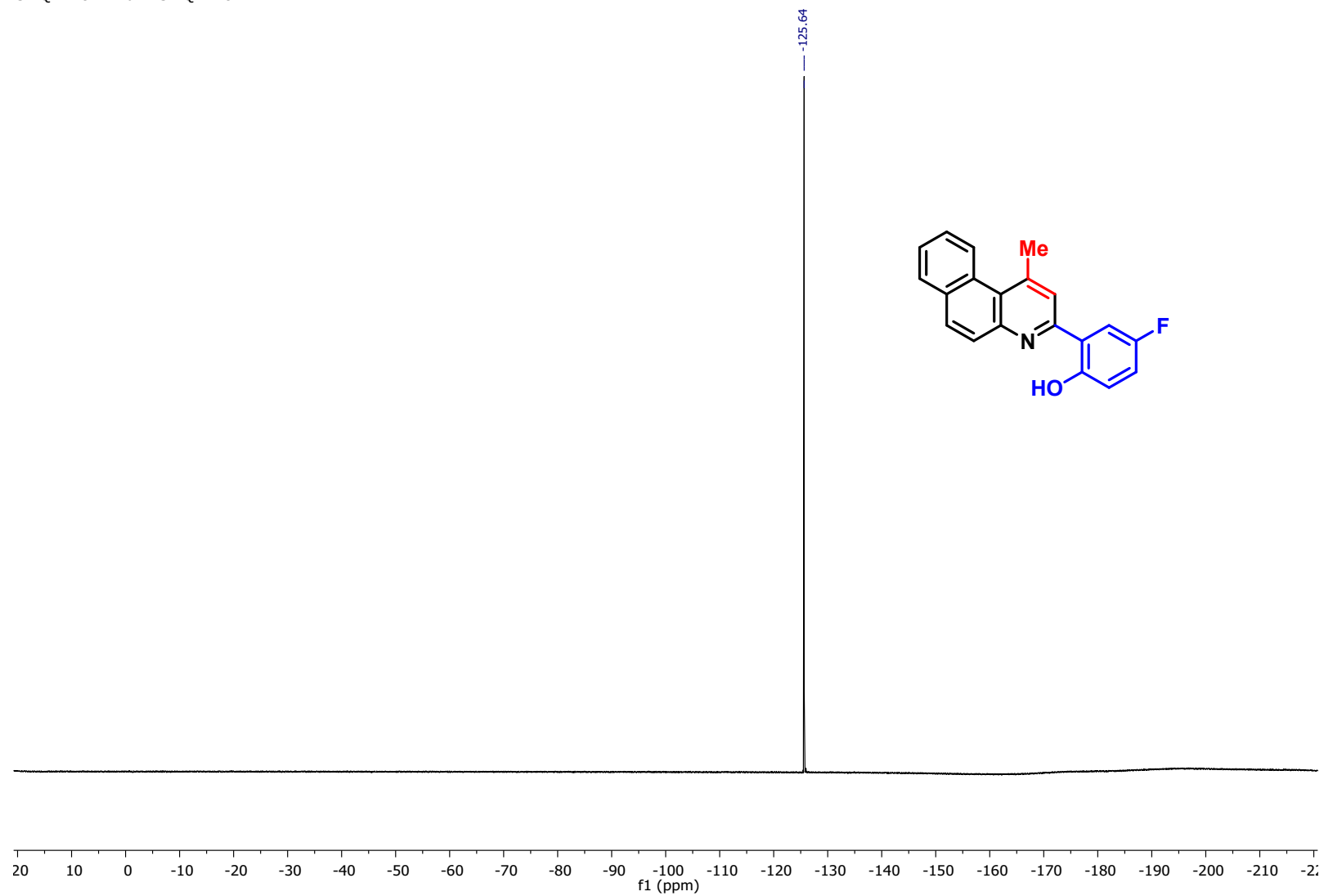
AD-SY-Q27-13C.3.fid — AD-SY-Q27-13C





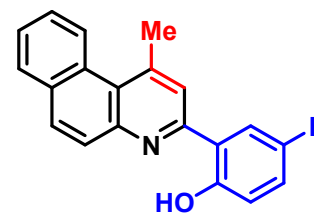
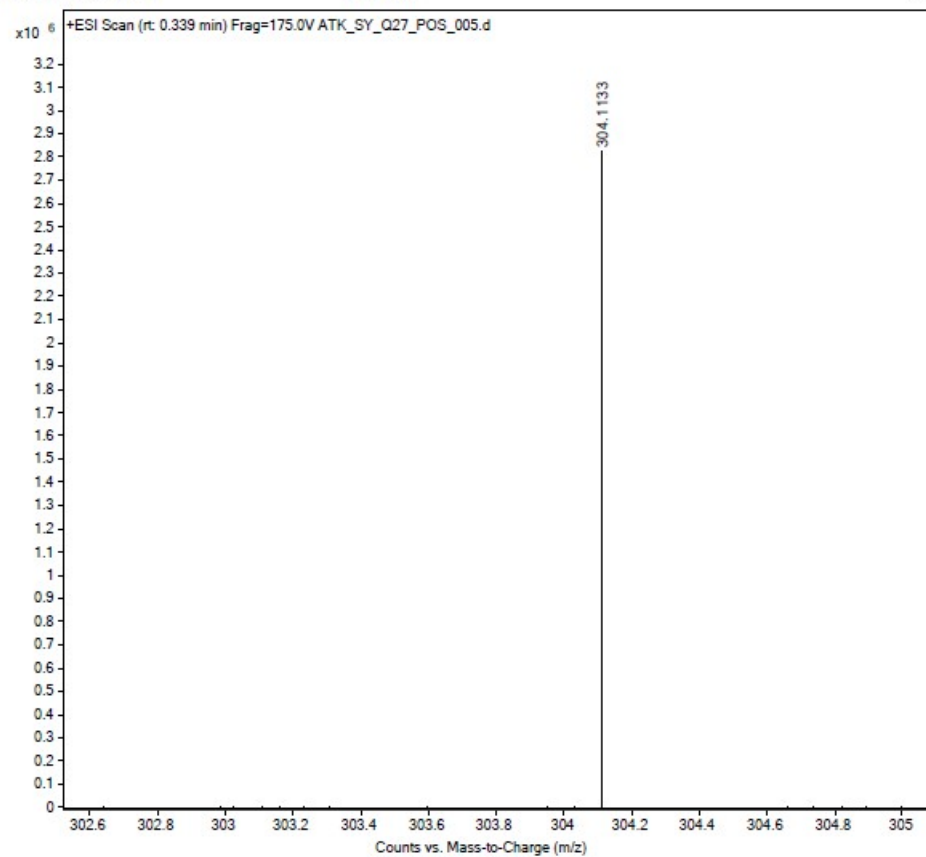
**<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) spectrum of compound 3q**

SY-Q27-19F.1.fid — SY-Q27-19F



## HRMS spectrum of compound 3q

Sample Name	ATK_SY_Q27_POS	Position	P1-D1	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q27_POS_005.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:09:23 PM (UTC+05:30)

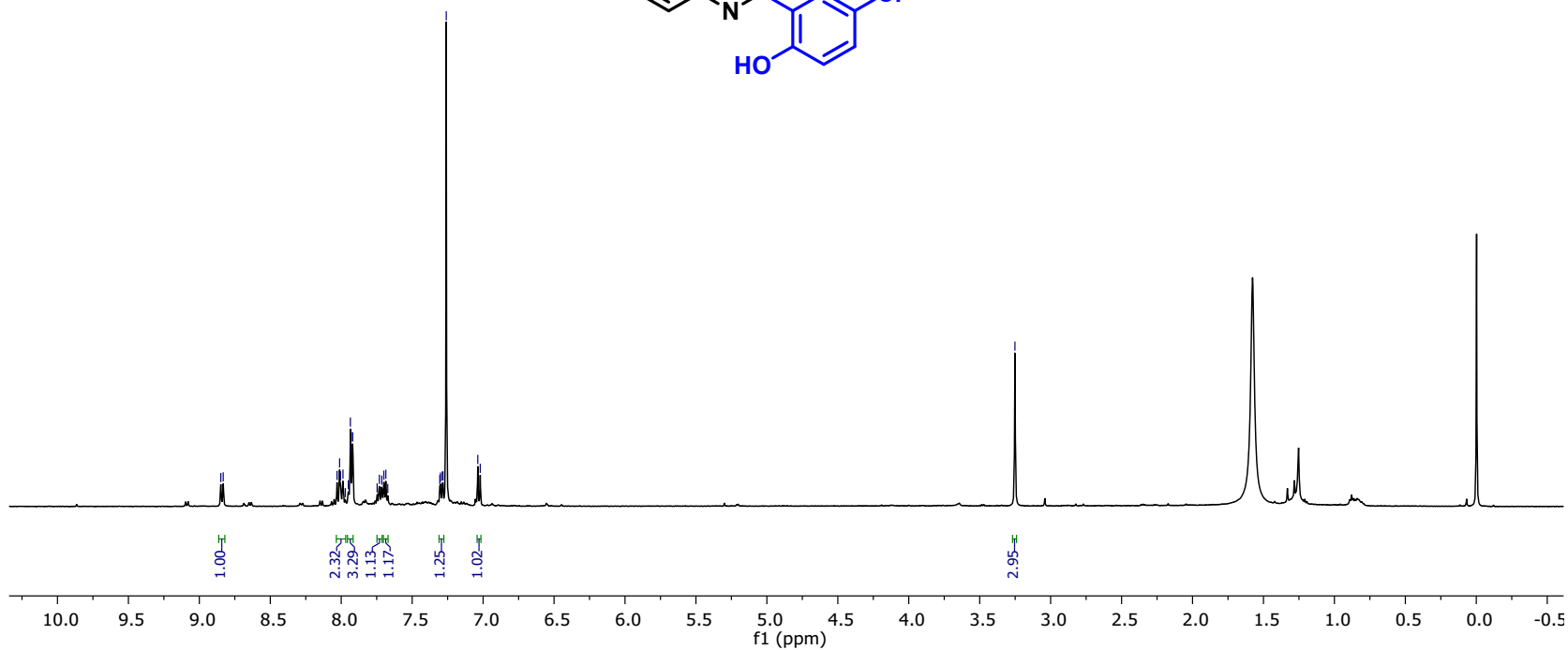
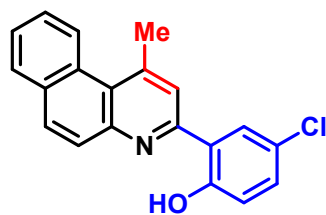


**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3r**

ATK-SY-Q20-1H.1.fid — ATK-SY-Q20-1H

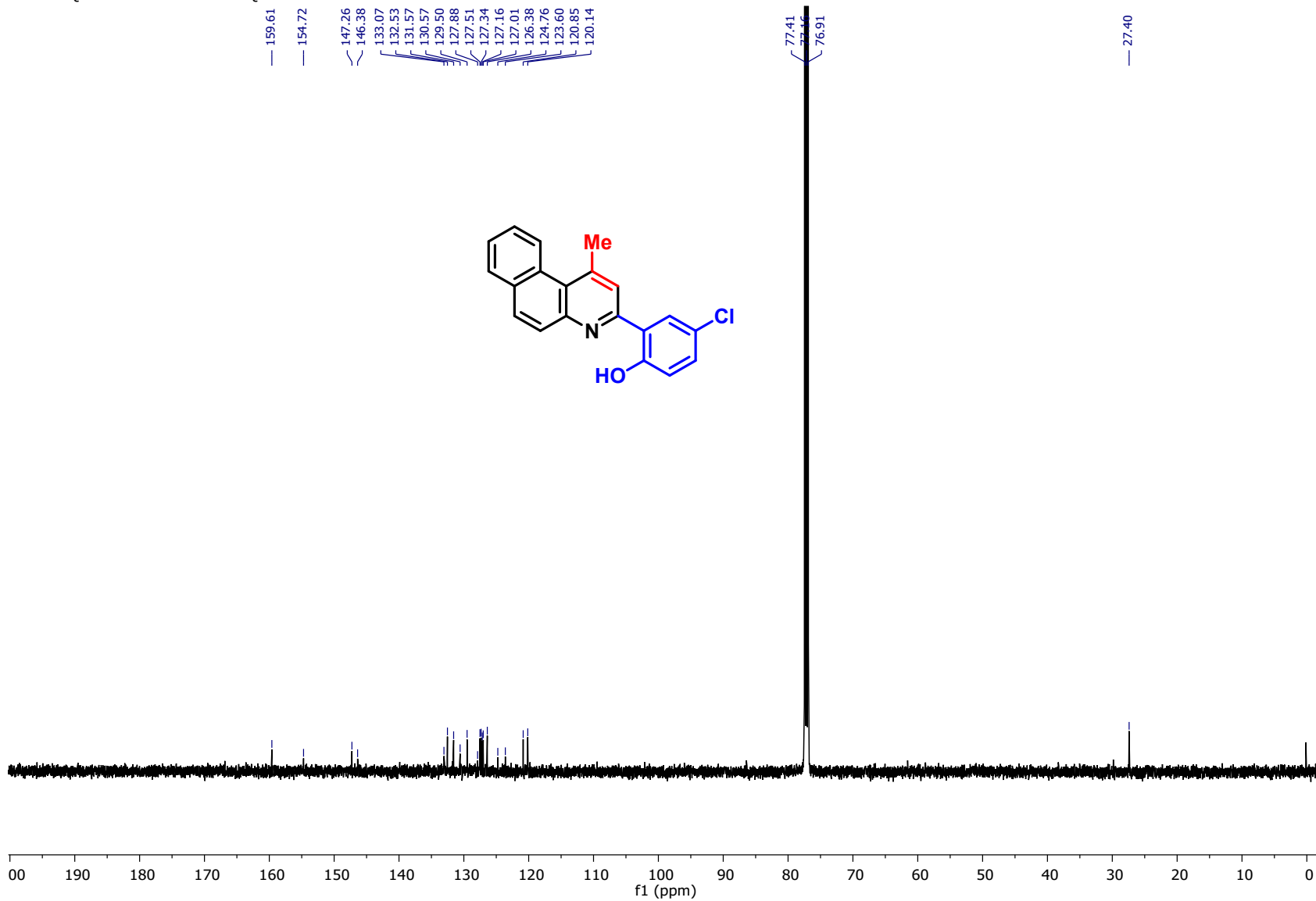
8.85  
8.83  
8.03  
8.01  
8.01  
7.99  
7.97  
7.95  
7.94  
7.93  
7.92  
7.75  
7.73  
7.71  
7.70  
7.69  
7.67  
7.31  
7.30  
7.29  
7.28  
7.26  
7.04  
7.02

— 3.25



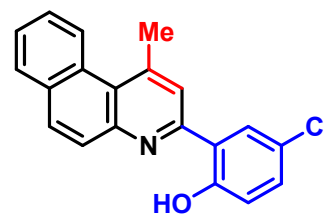
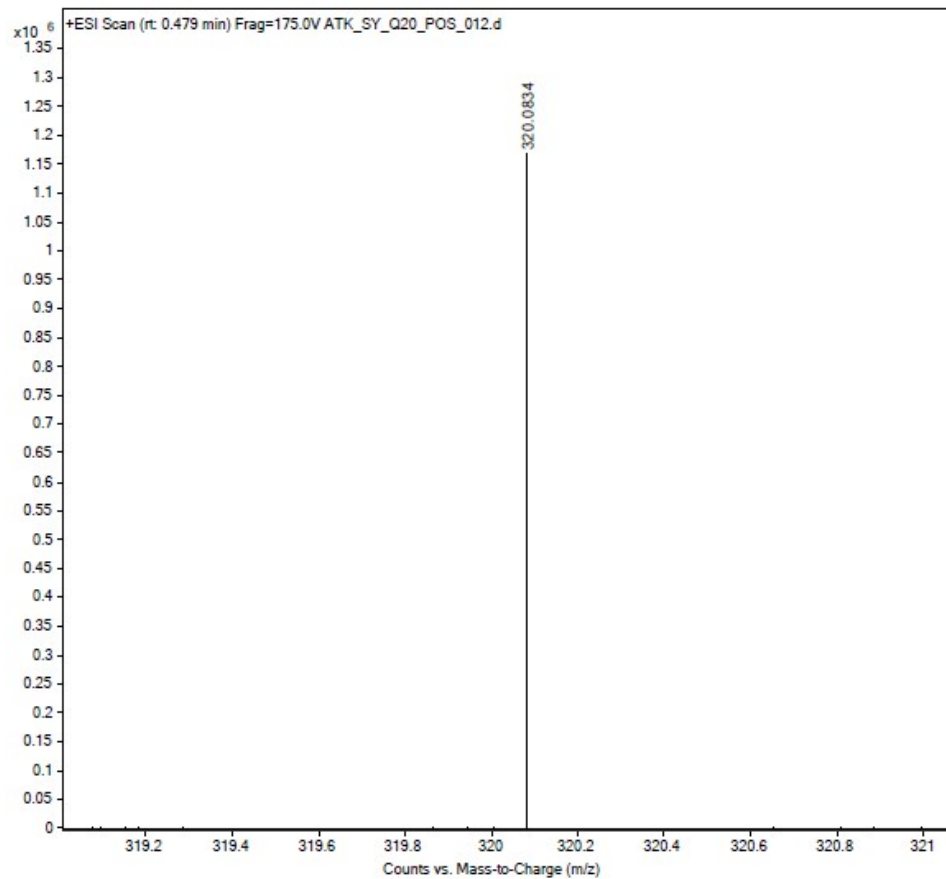
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3r

ATK-SY-Q20-13C.1.fid — ATK-SY-Q20-13C



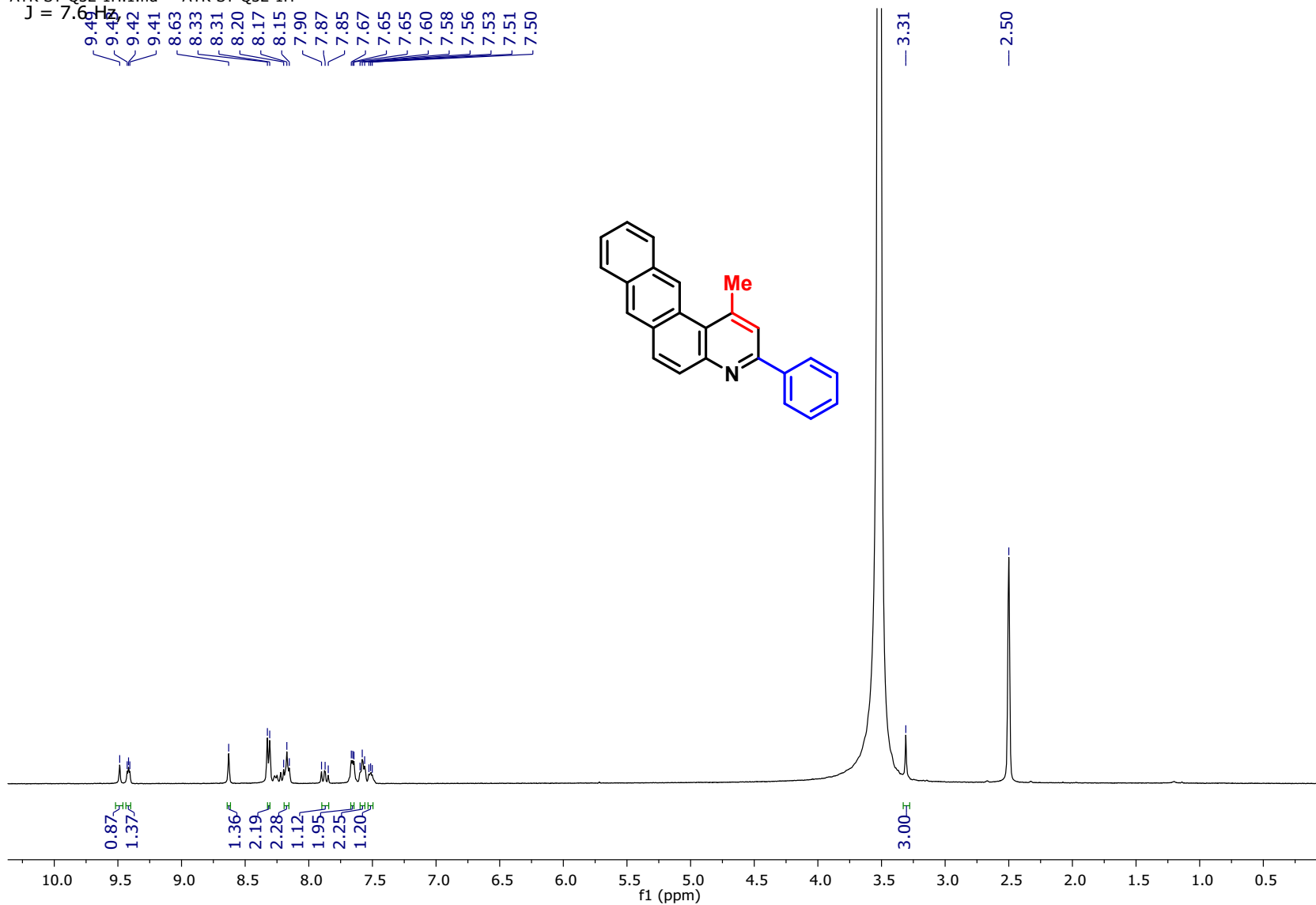
## HRMS spectrum of compound 3r

Sample Name	ATK_SY_Q20_POS	Position	P1-D7	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q20_POS_012.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:20:49 PM (UTC+05:30)



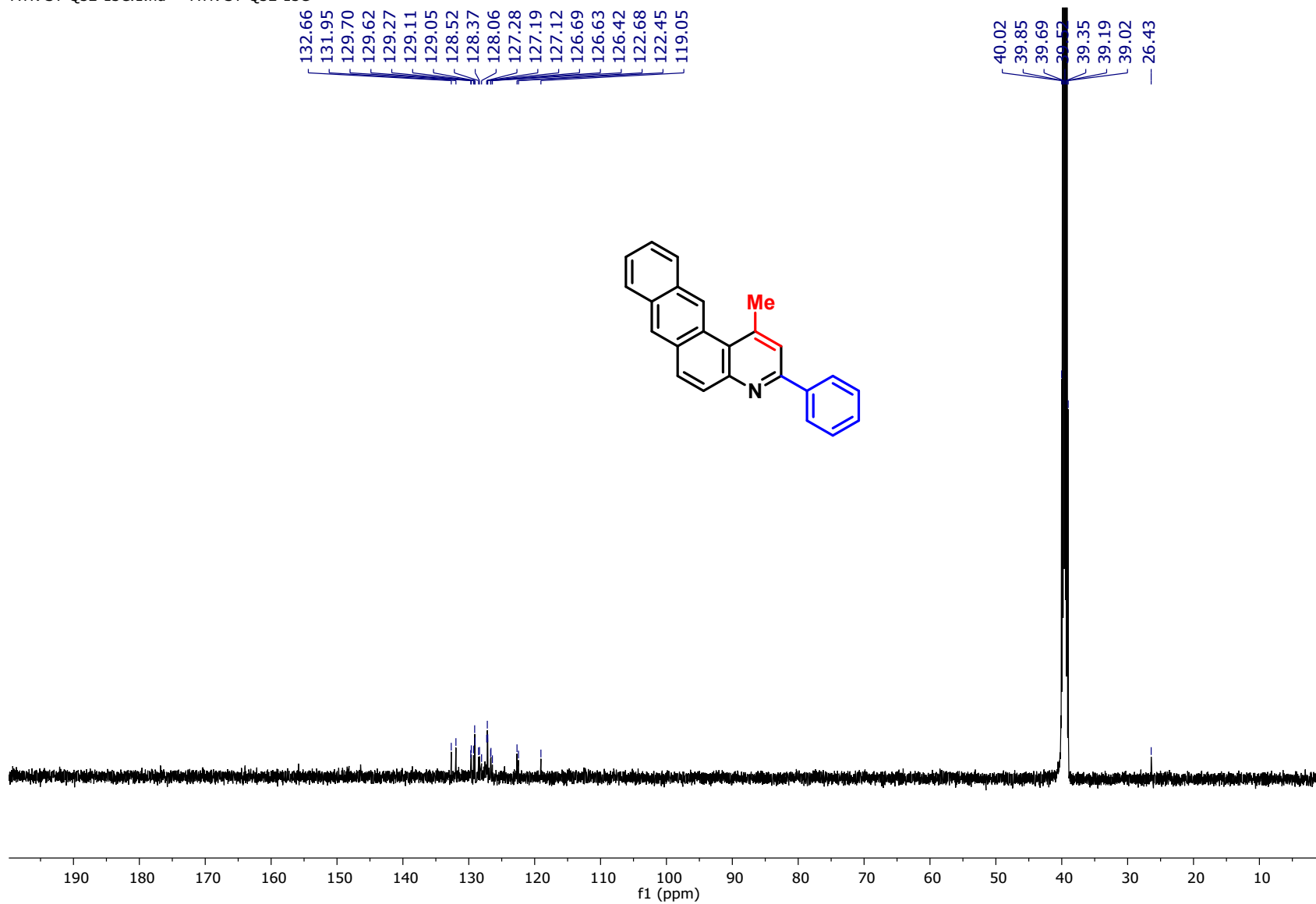
**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 3s**

ATK-SY-Q32-1H.1.fid — ATK-SY-Q32-1H



$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound 3s

ATK-SY-Q32-13C.1.fid — ATK-SY-Q32-13C



## HRMS spectrum of compound 3s

Sample Name  
User Name  
Sample Type  
ACQ Method

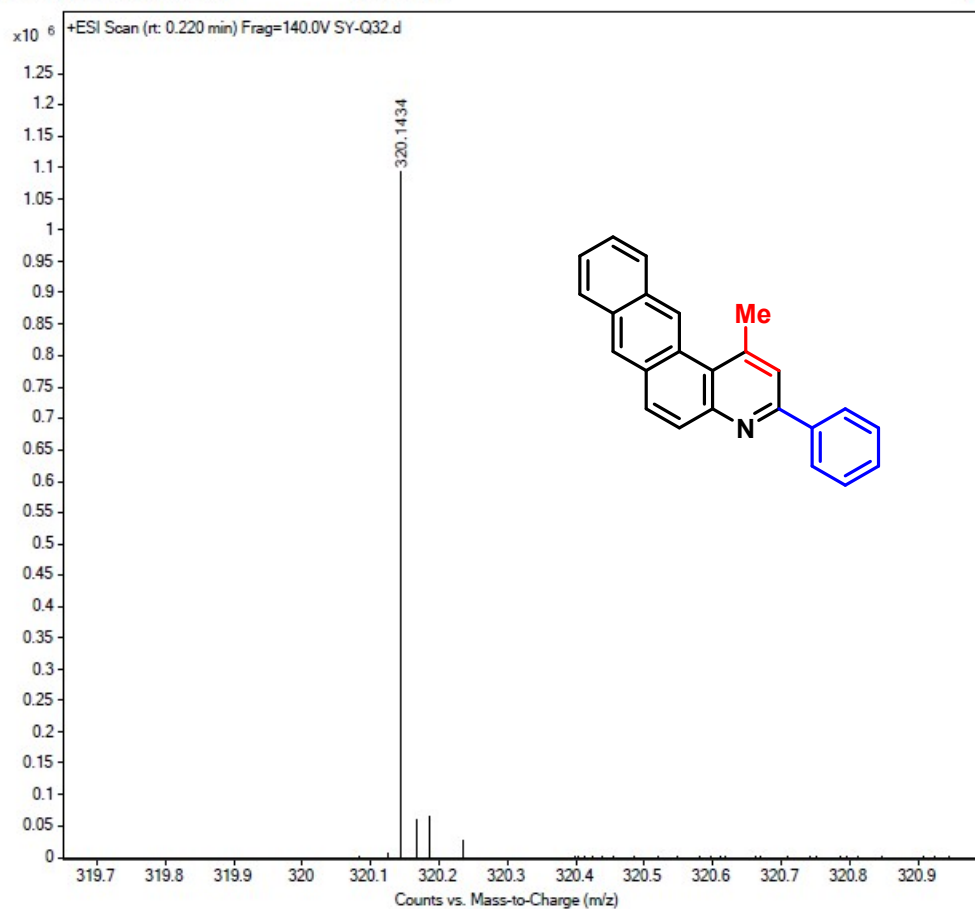
Sample13  
SYSTEM (SYSTEM)  
Sample  
DIRECT MASS\_POSITIVE\_01\_1.m

Position  
Inj Vol  
IRM Calibration Status  
Comment

P1-B1  
5  
Success

Instrument Name  
InjPosition  
Data Filename  
Acquired Time

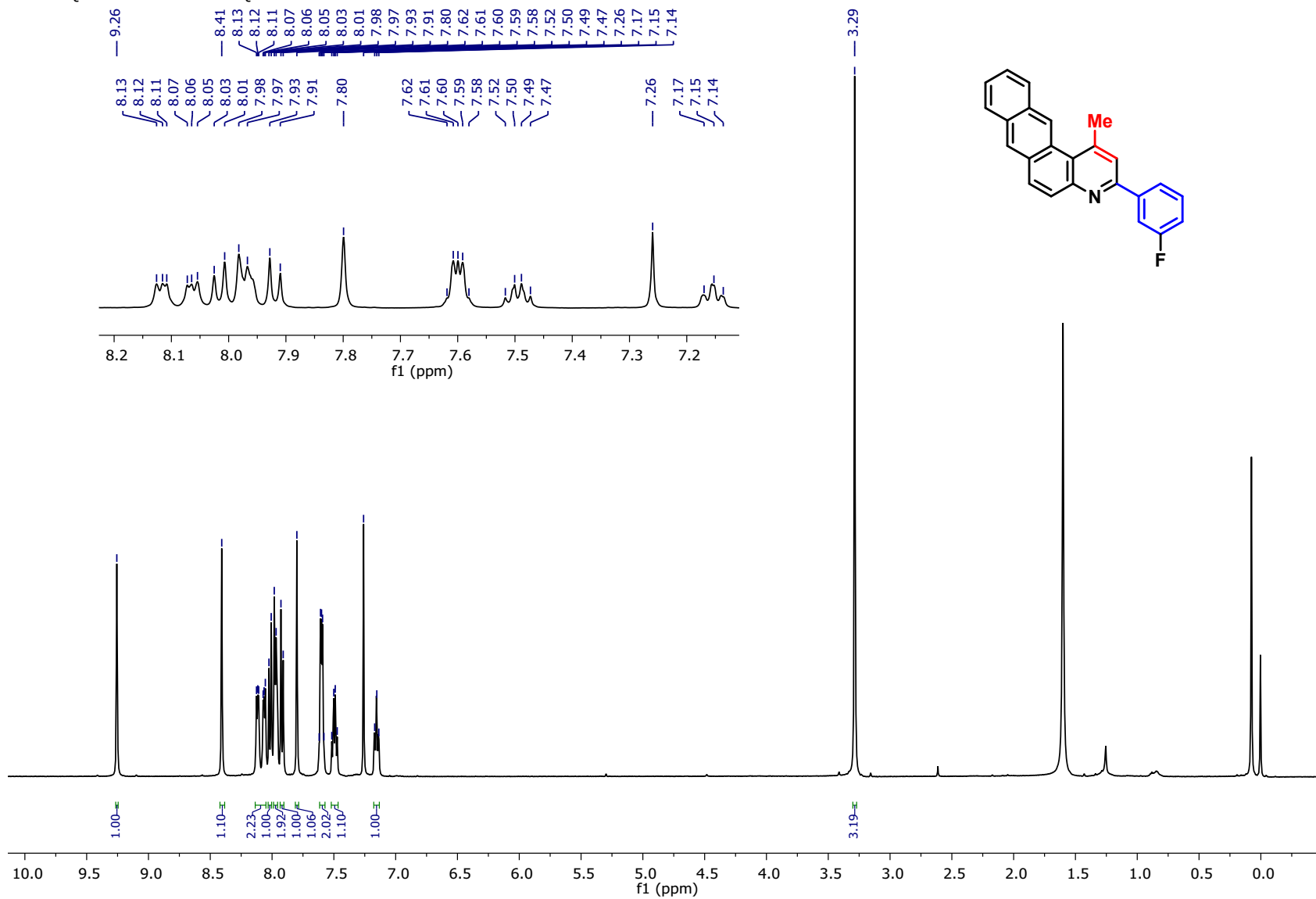
QTOF  
5Y-Q32.d  
27-Jul-23 10:36:30 AM (UTC+05:30)





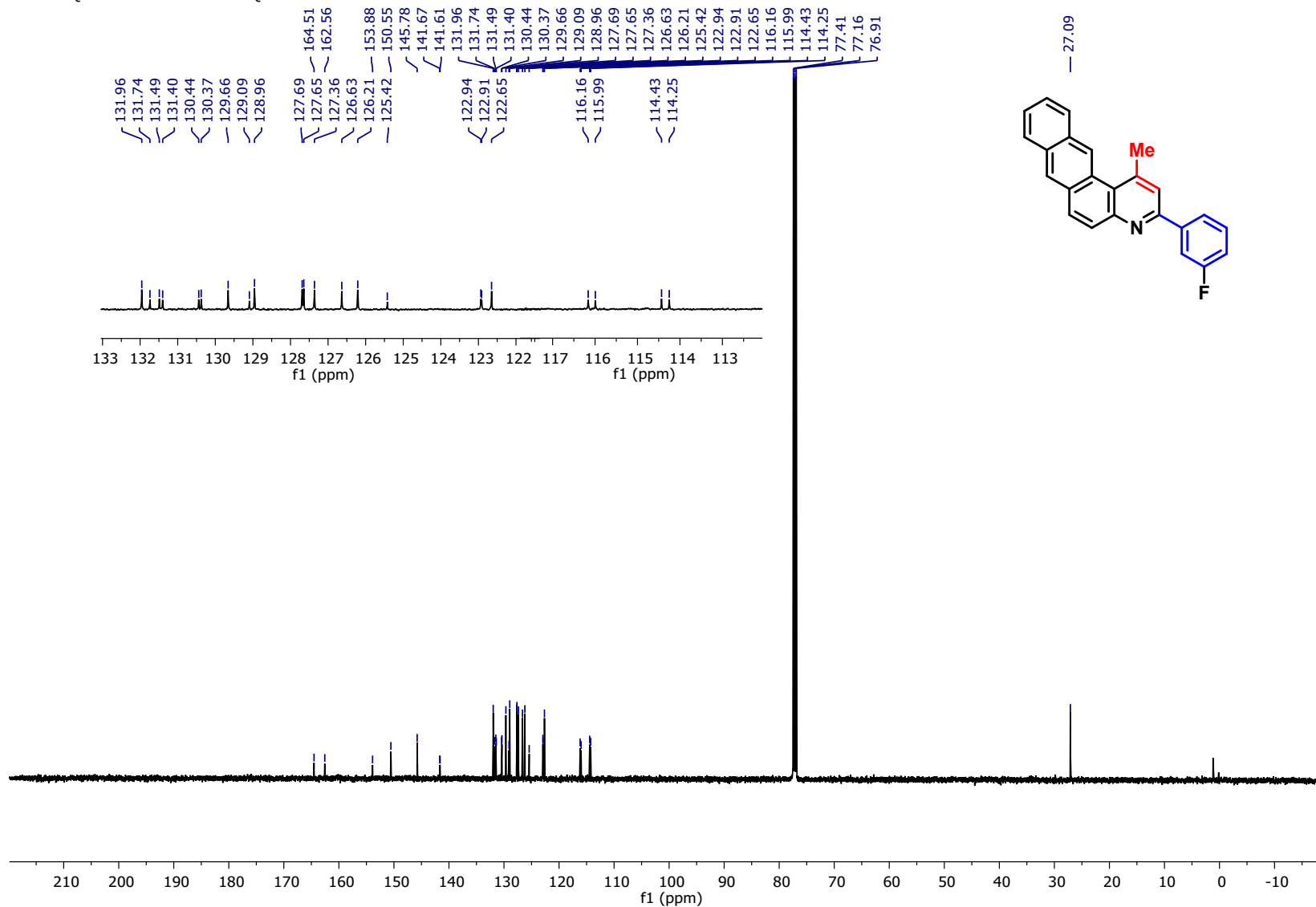
# <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3t

ATK-SY-Q42-1H.3.fid — ATK-SY-Q42-1H



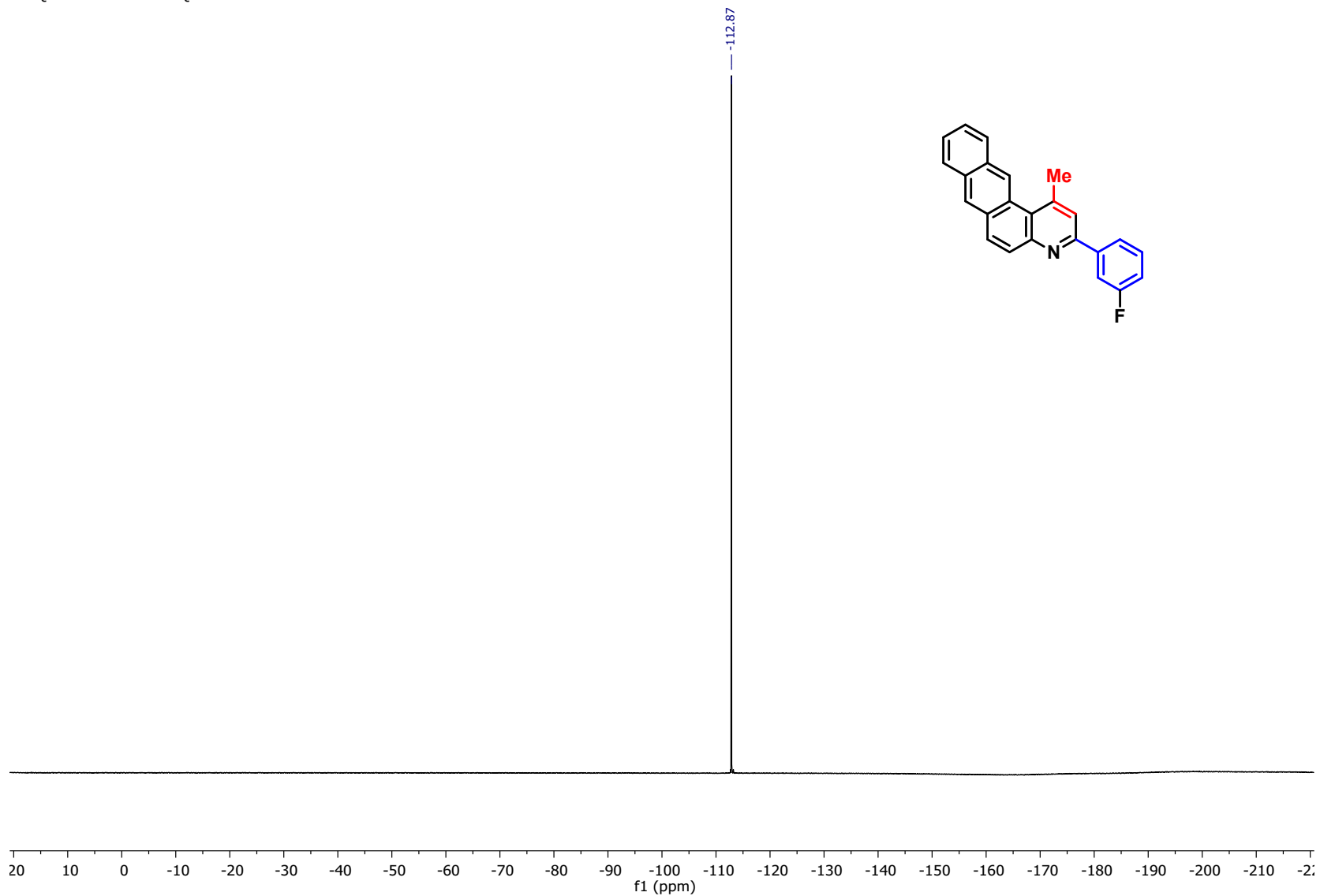
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3t

ATK-SY-Q42-13C.1.fid — ATK-SY-Q42-13C



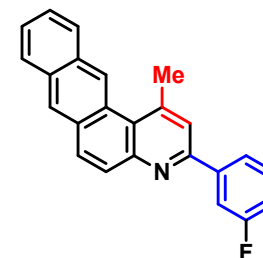
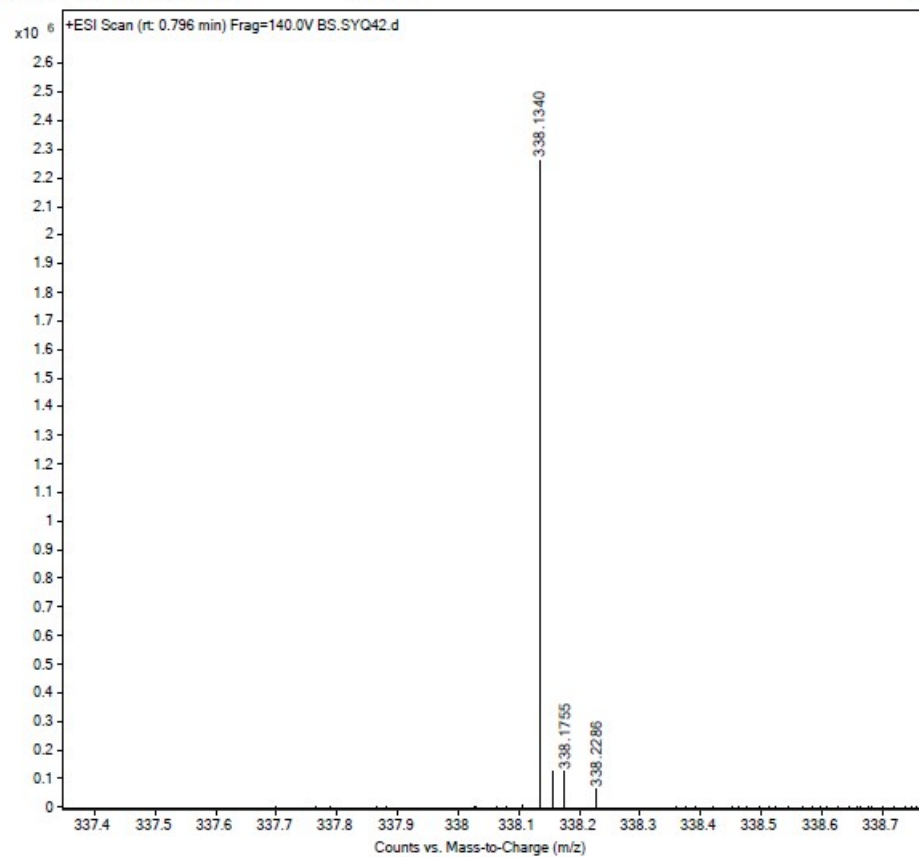
**$^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3t**

SY-Q42-19F.2.fid — SY-Q42-19F



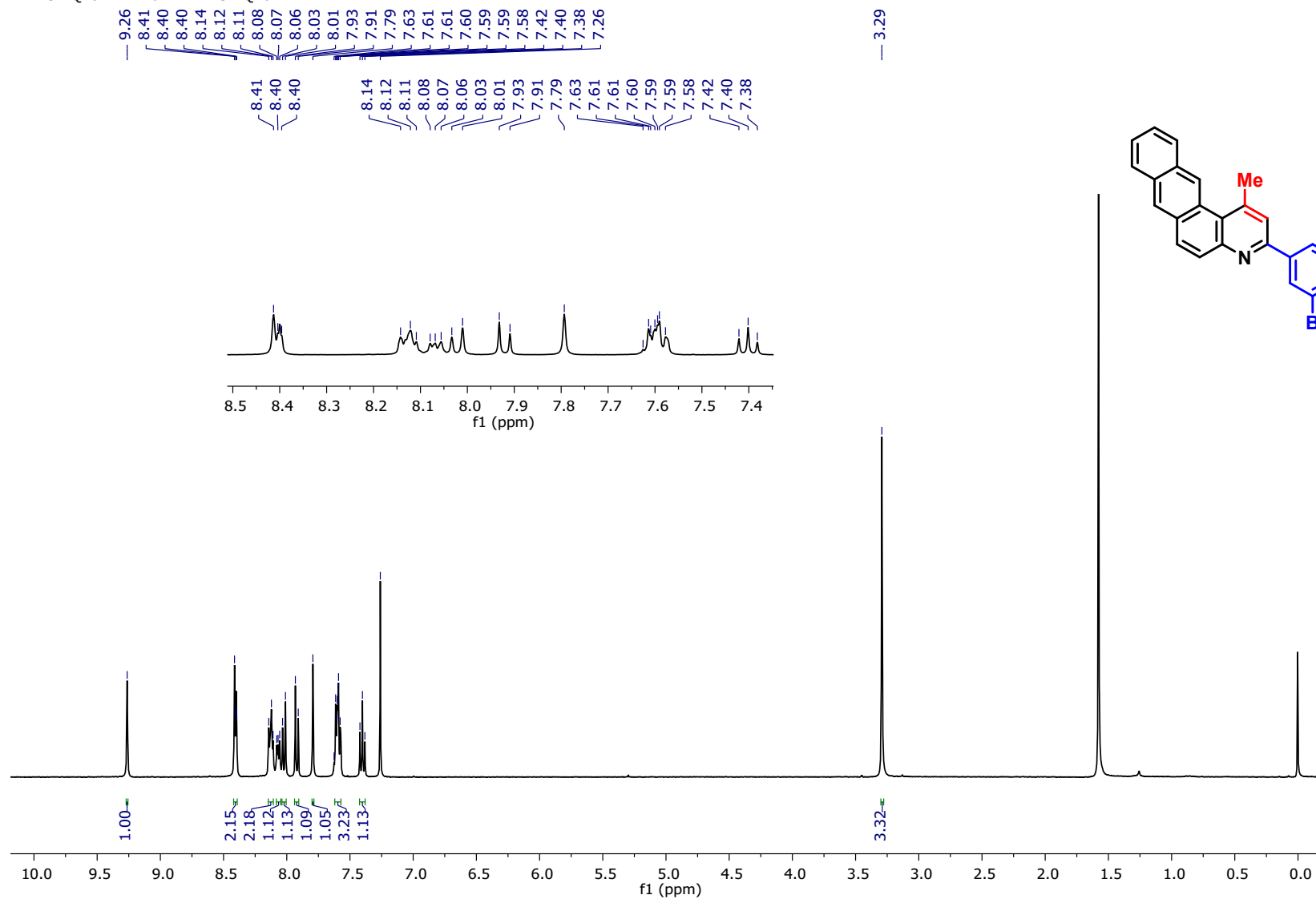
## HRMS spectrum of compound 3t

Sample Name	Sample25	Position	P1-C3	Instrument Name	QTOF
User Name	SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	BS.SYQ42.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	Comment		Acquired Time	16-Jun-23 10:38:22 AM (UTC+05:30)



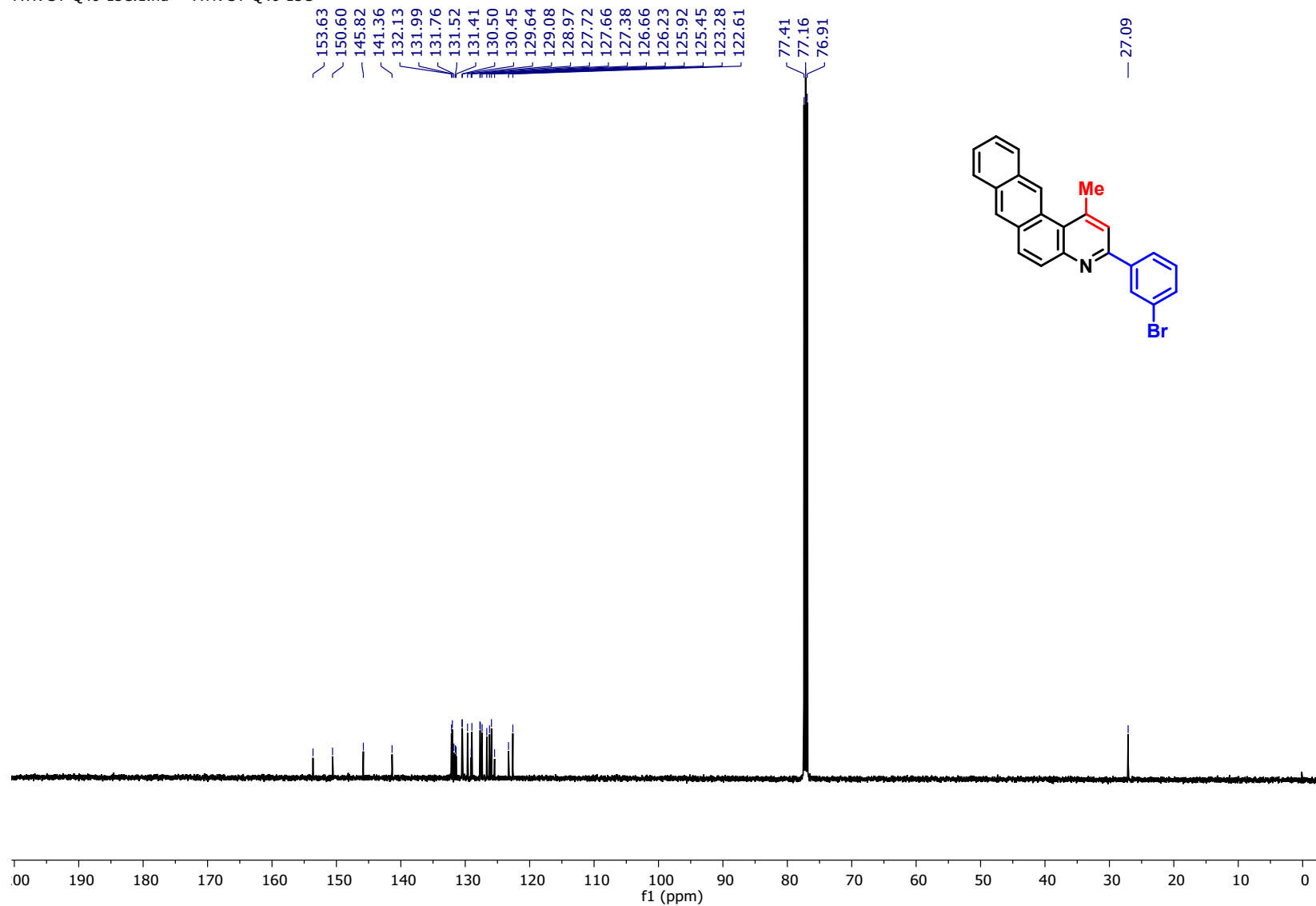
# <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 3u

ATK-SY-Q46-1H.1.fid — ATK-SY-Q46-1H



**$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3u**

ATK-SY-Q46-13C.1.fid — ATK-SY-Q46-13C

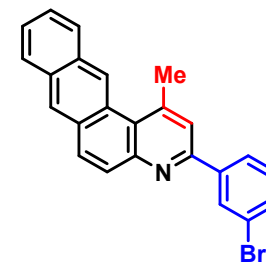
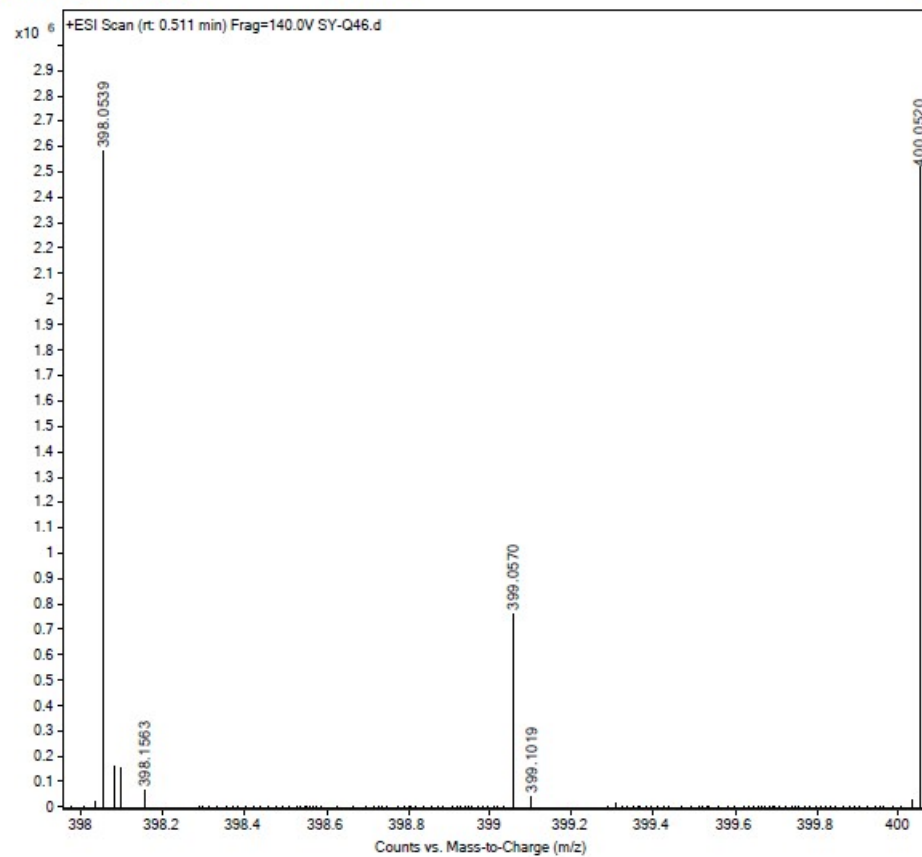


## HRMS spectrum of compound 3u

Sample Name  
User Name  
Sample Type  
ACQ Method

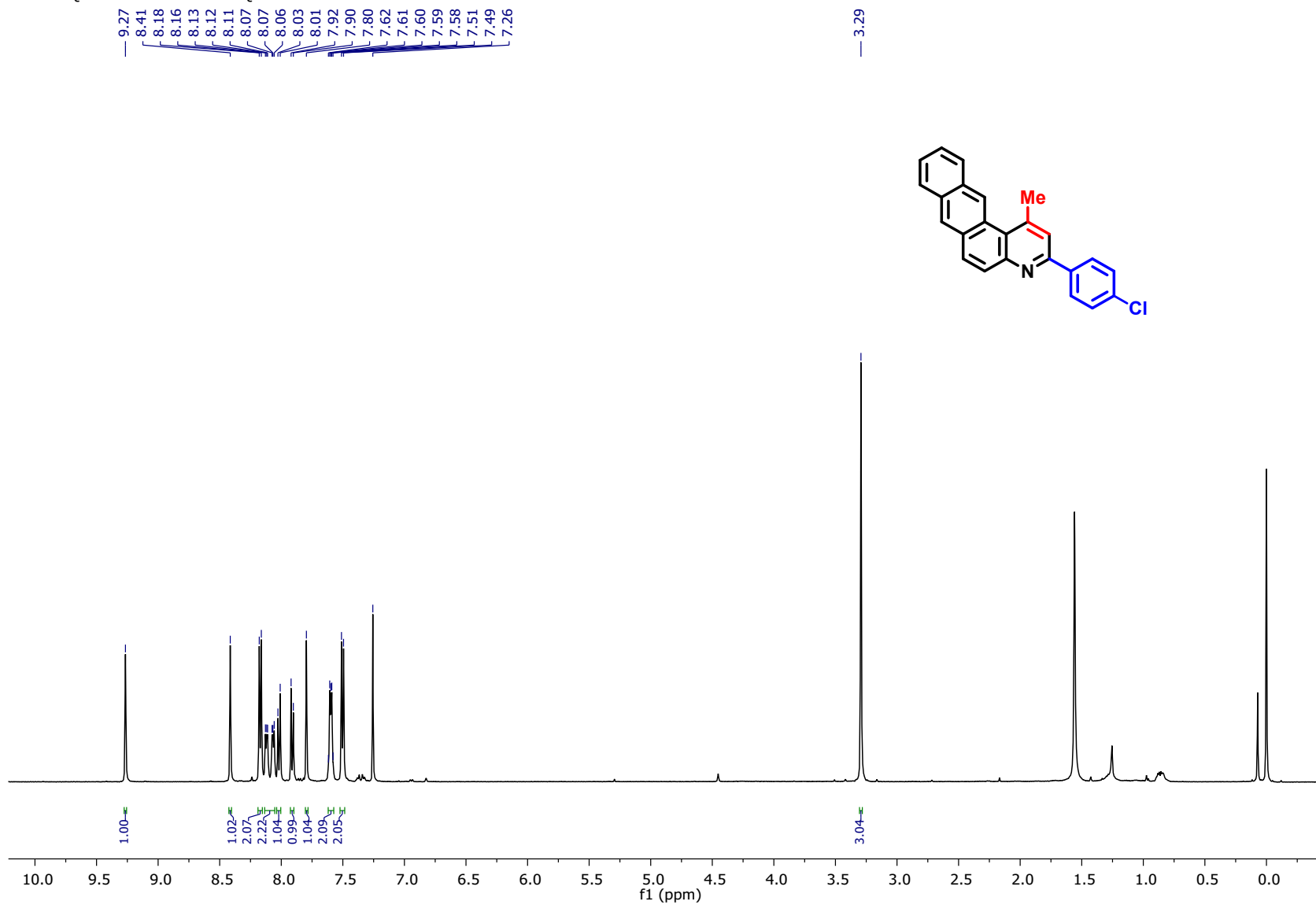
Sample22  
SYSTEM (SYSTEM)  
Sample  
DIRECT MASS\_POSITIVE\_01\_1.m  
Position  
Inj Vol  
IRM Calibration Status  
Comment  
P1-B11  
5  
Success

Instrument Name  
InjPosition  
Data Filename  
Acquired Time  
QTOF  
5  
SY-Q46.d  
13-Jul-23 11:4



**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3v**

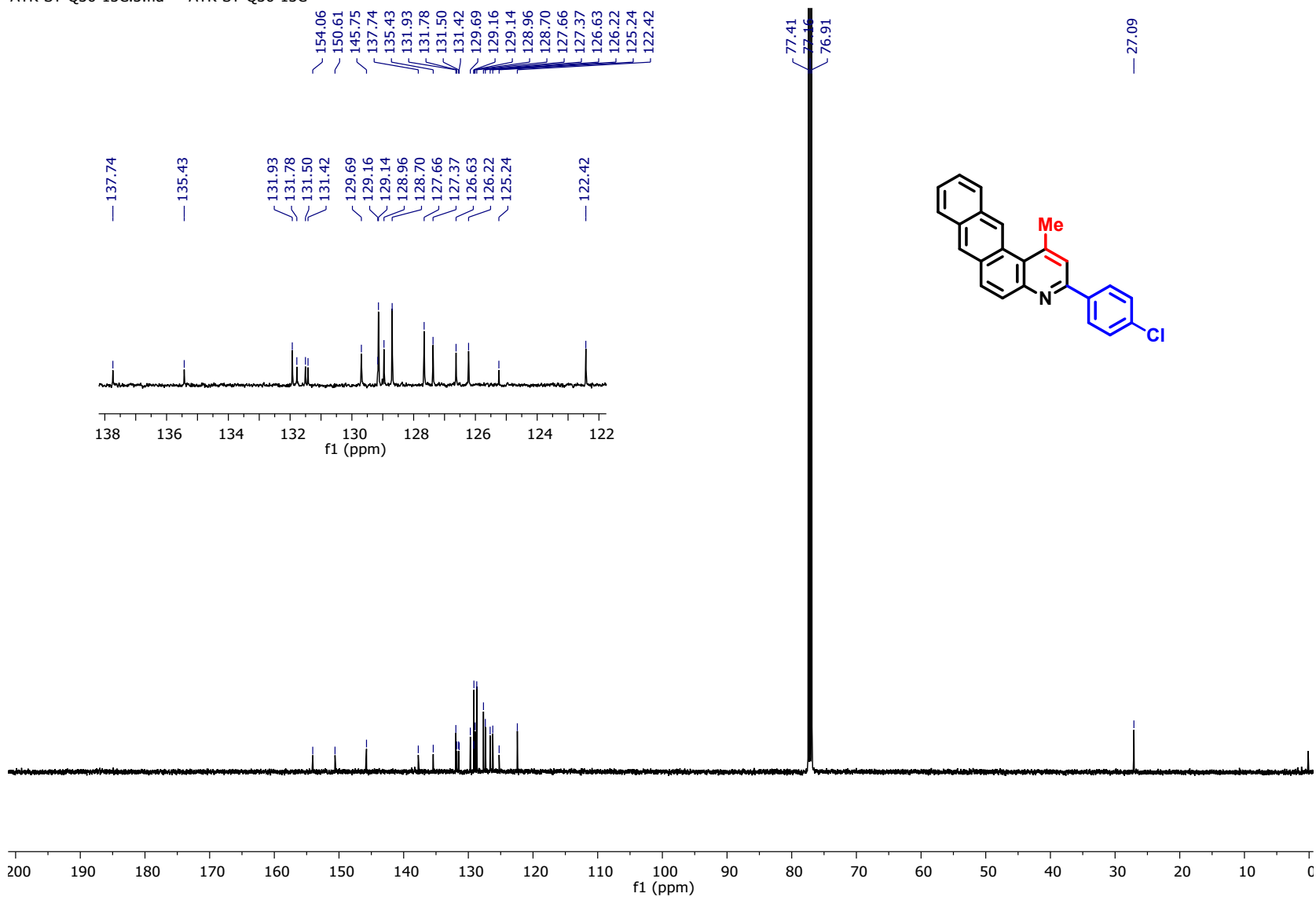
ATK-SY-Q36-1H.1.fid — ATK-SY-Q36-1H





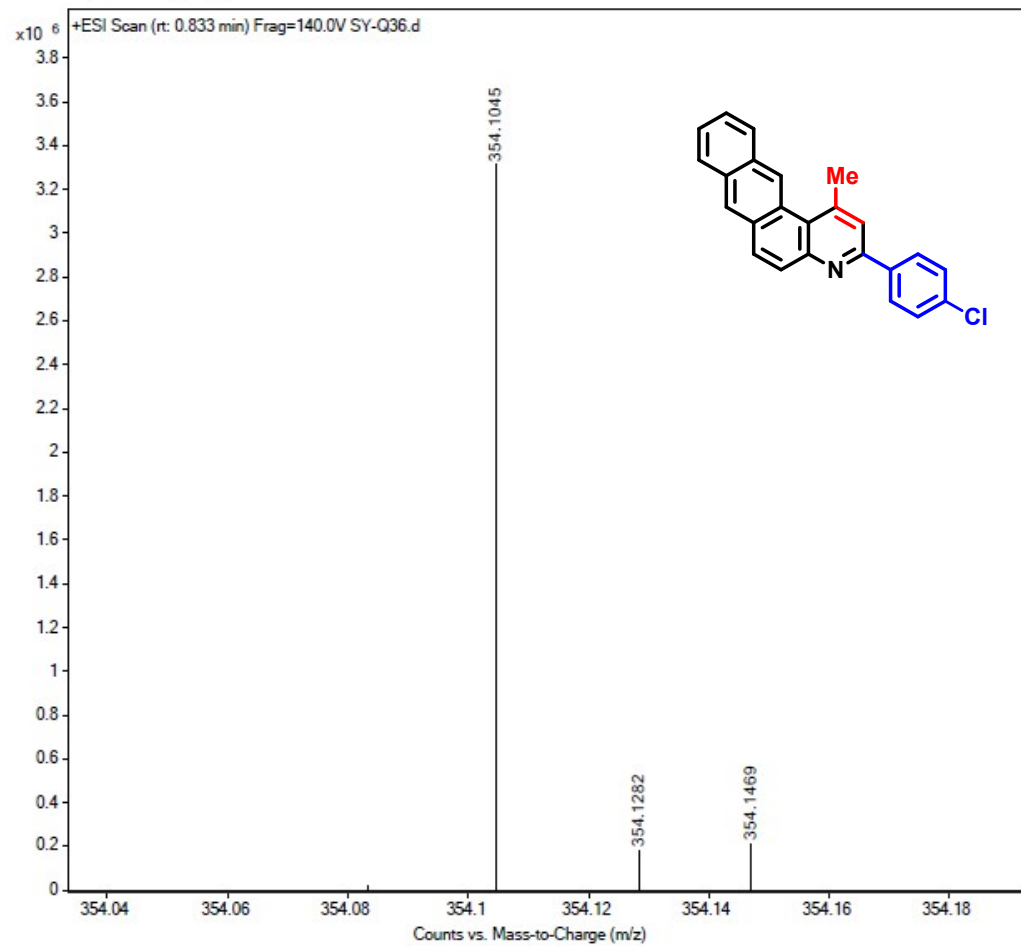
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3v

ATK-SY-Q36-13C.3.fid — ATK-SY-Q36-13C



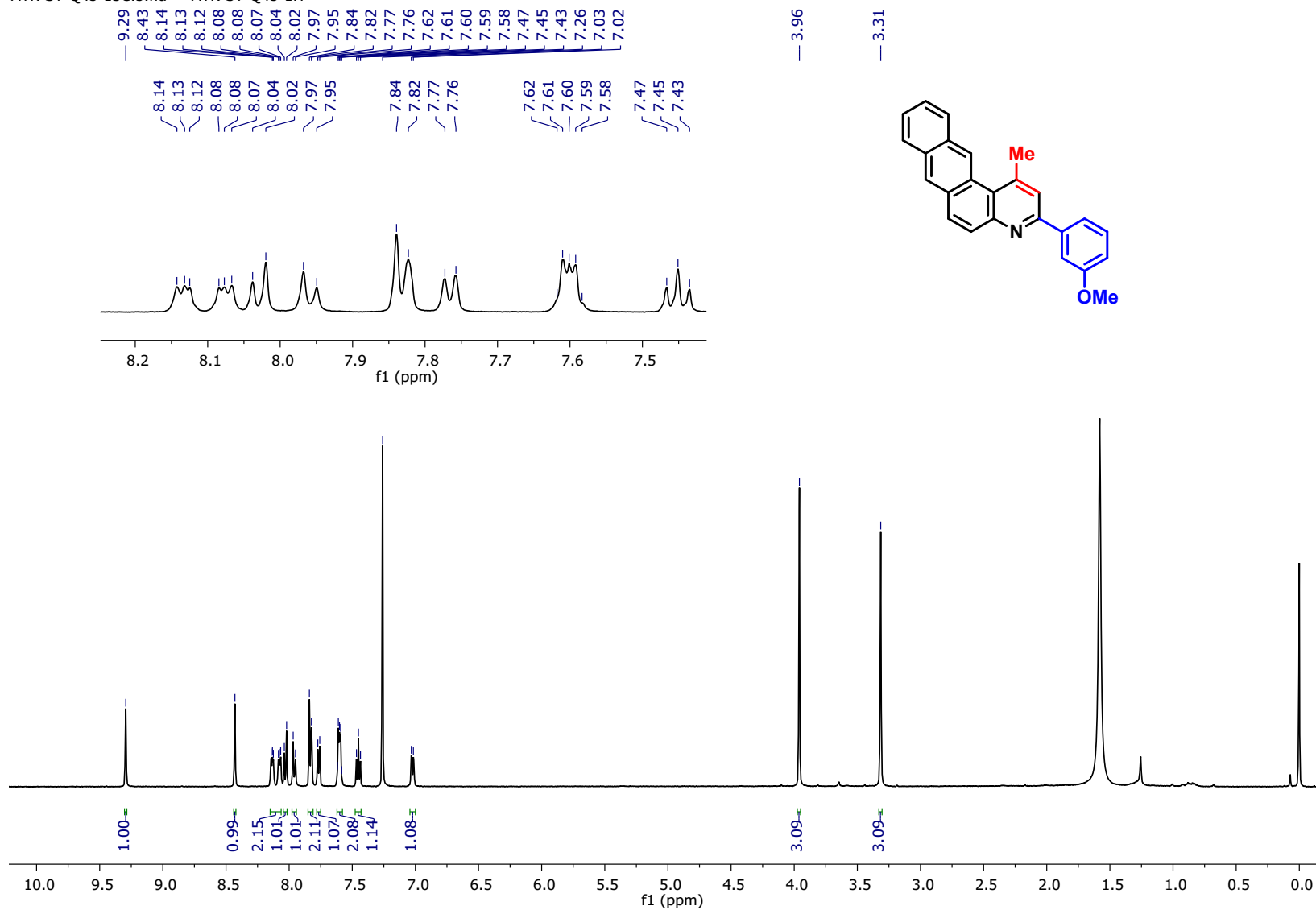
## HRMS spectrum of compound 3v

Sample14	Position	P1-B3	Instrument Name	QTOF
SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample	IRM Calibration Status	Success	Data Filename	SY-Q36.d
DIRECT MASS_POSITIVE_100_1500.m	Comment		Acquired Time	05-Sep-23 1



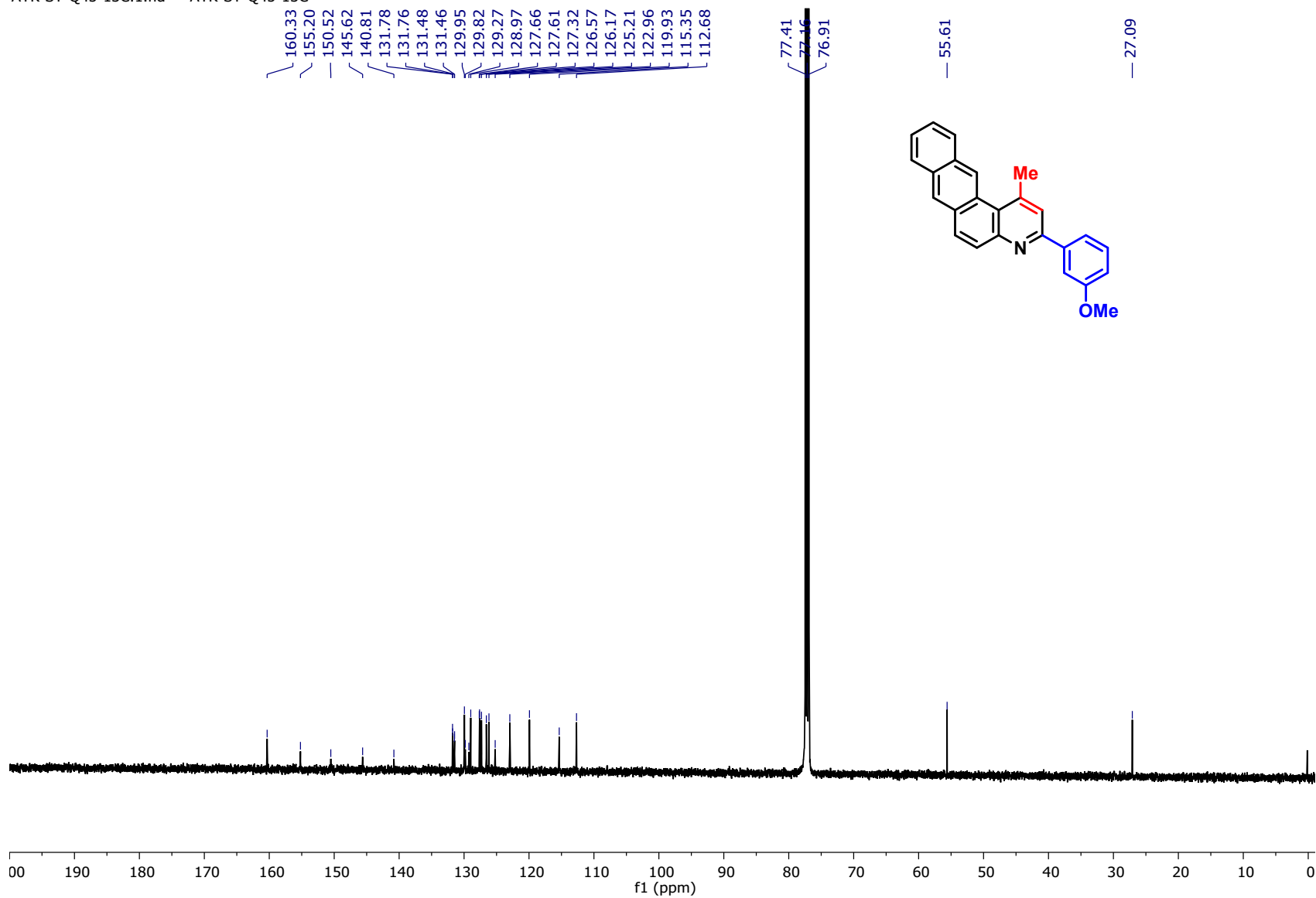
# <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 3w

ATK-SY-Q45-13C.5.fid — ATK-SY-Q45-1H



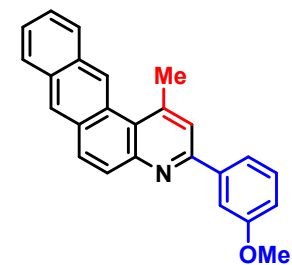
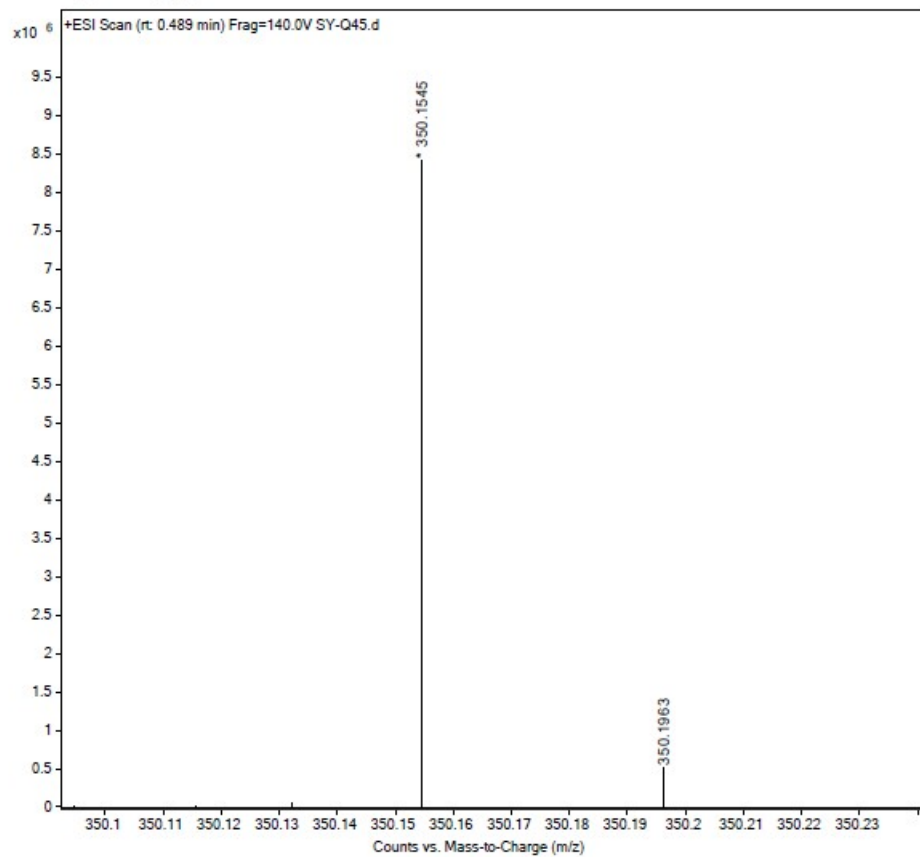
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 3w

ATK-SY-Q45-13C.1.fid — ATK-SY-Q45-13C



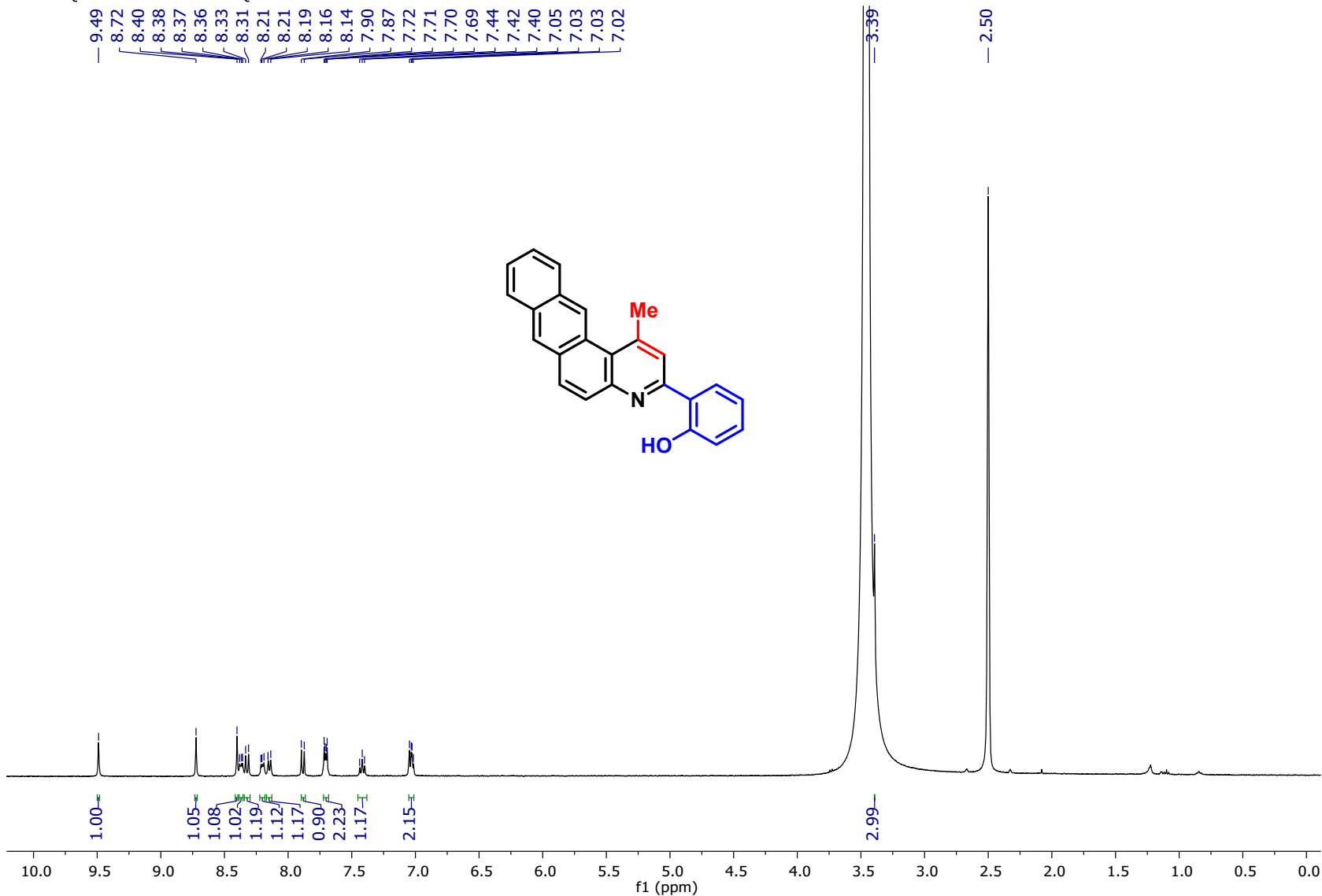
## HRMS spectrum of compound 3w

Sample Name	Sample24	Position	P1-C2	Instrument Name	QTOF
User Name	SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SY-Q45.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	Comment		Acquired Time	13-Jul-23 11:45:29 AM (UTC+05:30)



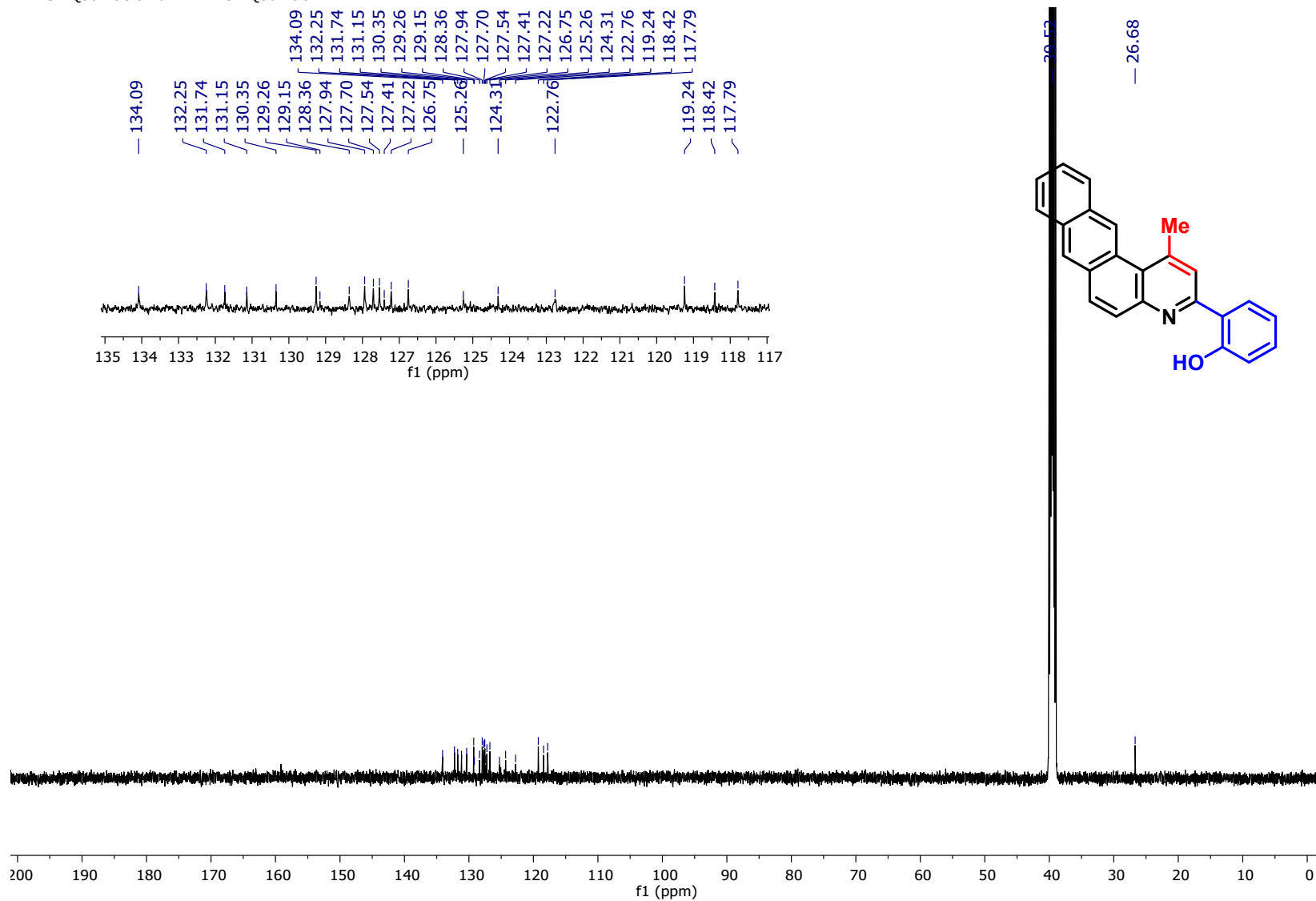
**<sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 3x**

ATK-SY-Q30-1H.1.fid — ATK-SY-Q30-1H



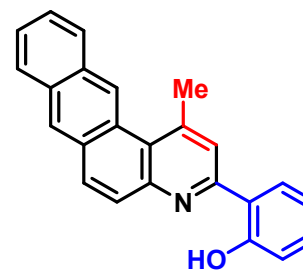
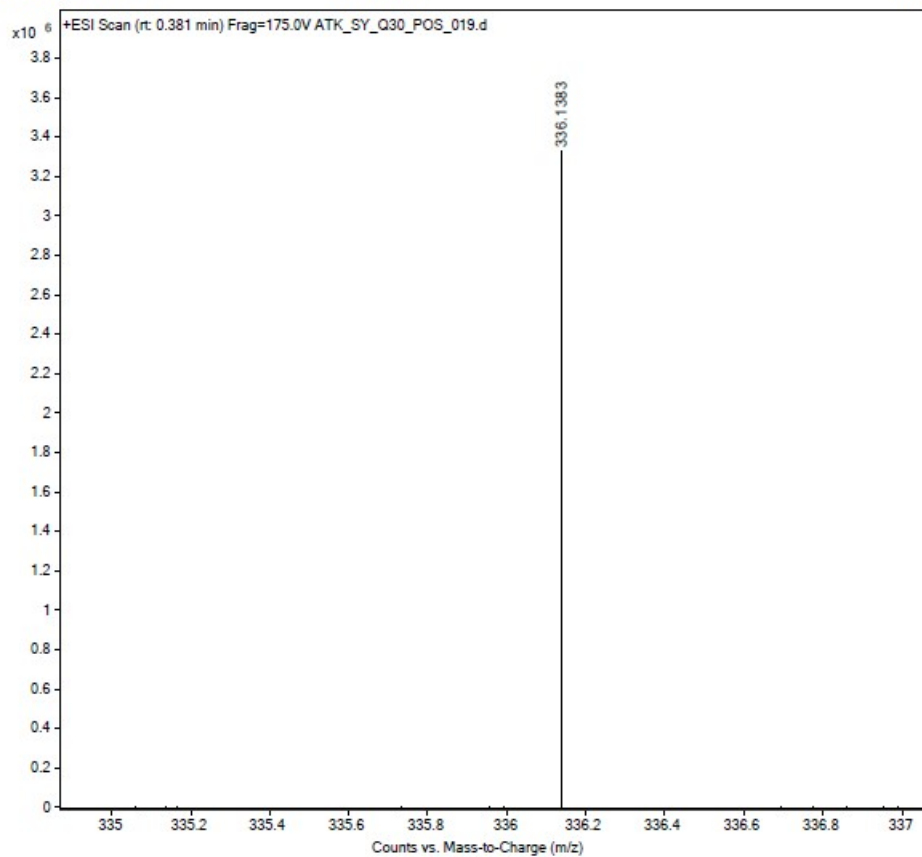
# $^{13}\text{C}\{^1\text{H}\}$ NMR (125 MHz, $\text{DMSO-}d_6$ ) spectrum of compound 3x

ATK-SY-Q30-13C.3.fid — ATK-SY-Q30-13C



## HRMS spectrum of compound 3x

Sample Name	ATK_SY_Q30_POS	Position	P1-E5	Instrument Name	Instrument 1
User Name		Inj Vol	10	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q30_POS_019.d
ACQ Method	FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:31:58 PM (UTC+05:30)

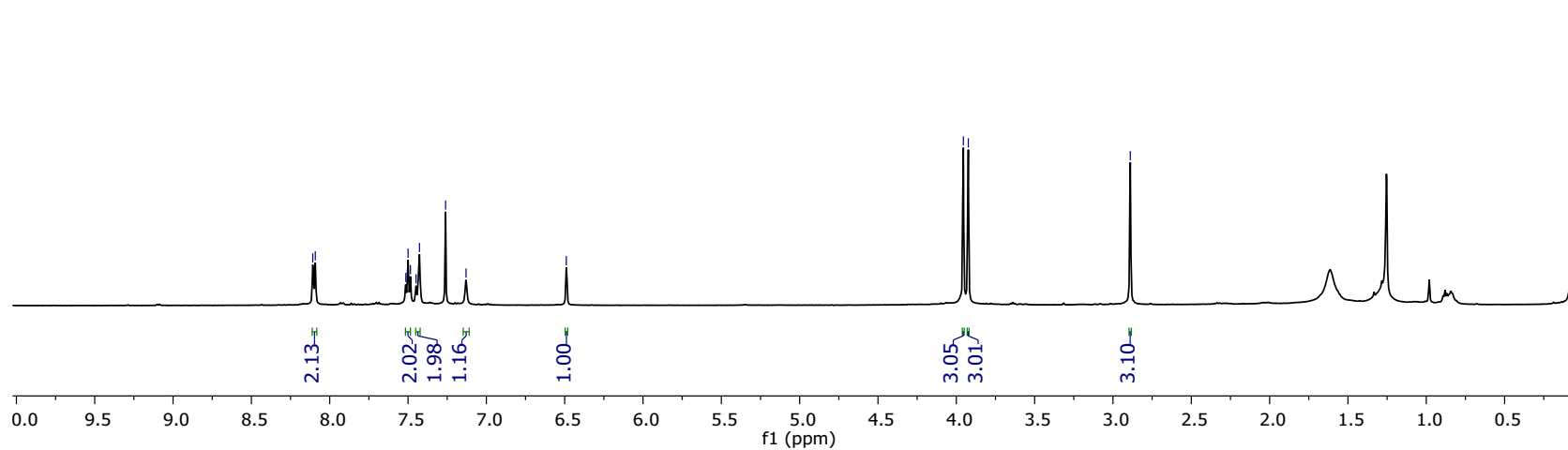
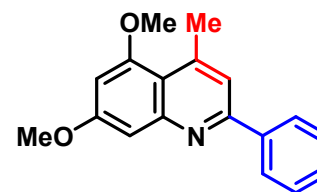




**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 4a**

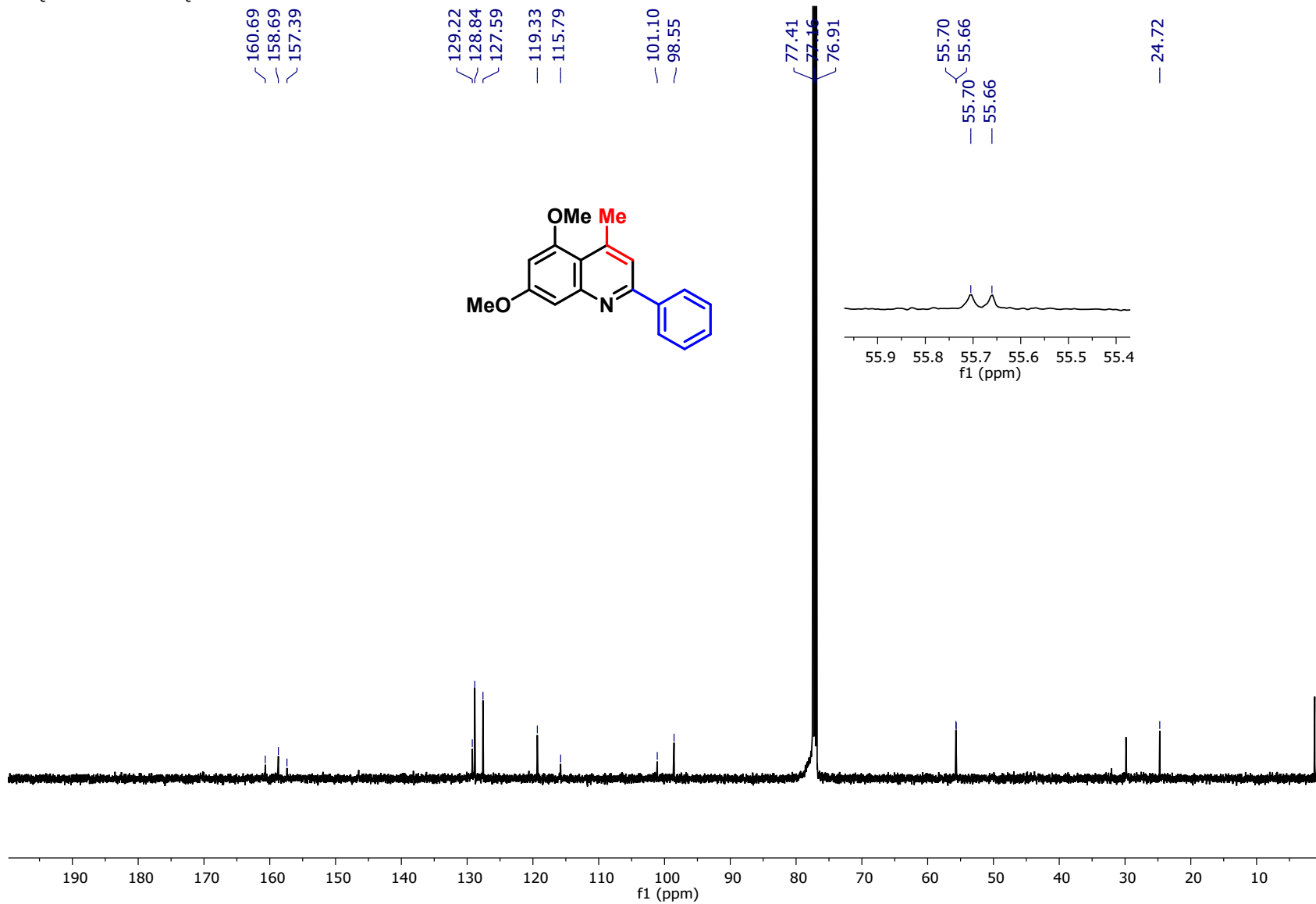
SY-Q39-1H.3.fid — SY-Q39-1H

8.11  
8.09  
7.51  
7.50  
7.48  
7.45  
7.43  
7.26  
7.13  
6.49  
3.96  
3.92  
2.89



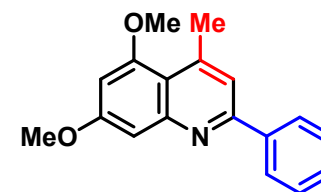
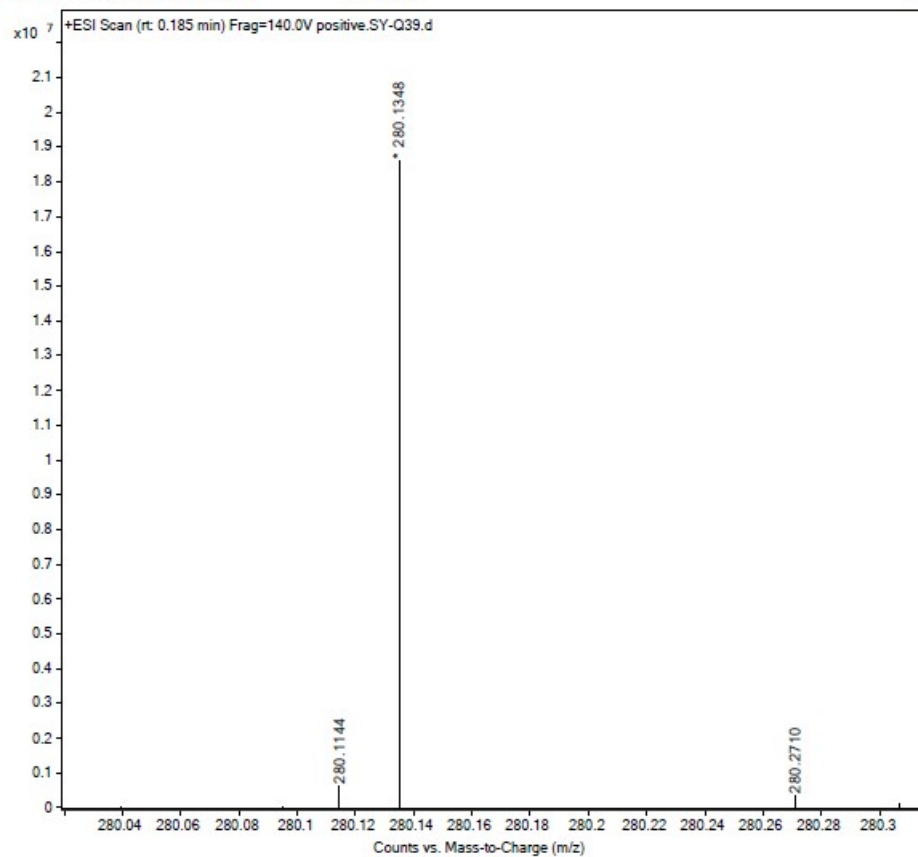
$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 4a

SY-Q39-13C.1.fid — SY-Q39-13C



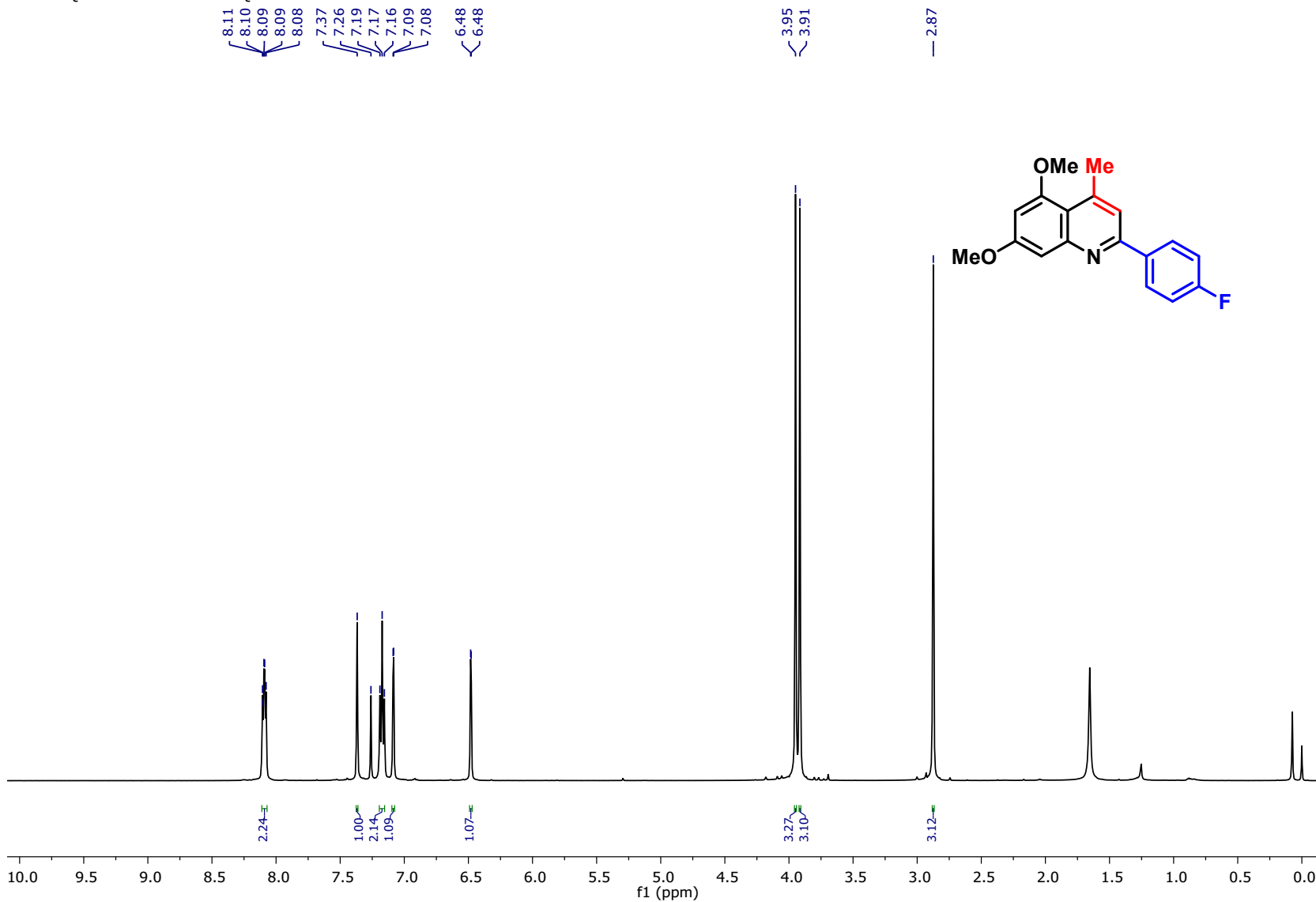
## HRMS spectrum of compound 4a

Sample Name	Sample35	Position	P1-C9	Instrument Name	QTOF
User Name	SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	positive.SY-Q39.d
ACQ Method	DIRECT MASS_POSITIVE_100_1000.m	Comment		Acquired Time	09-Jun-23 12:17:16 PM (UTC+05:30)



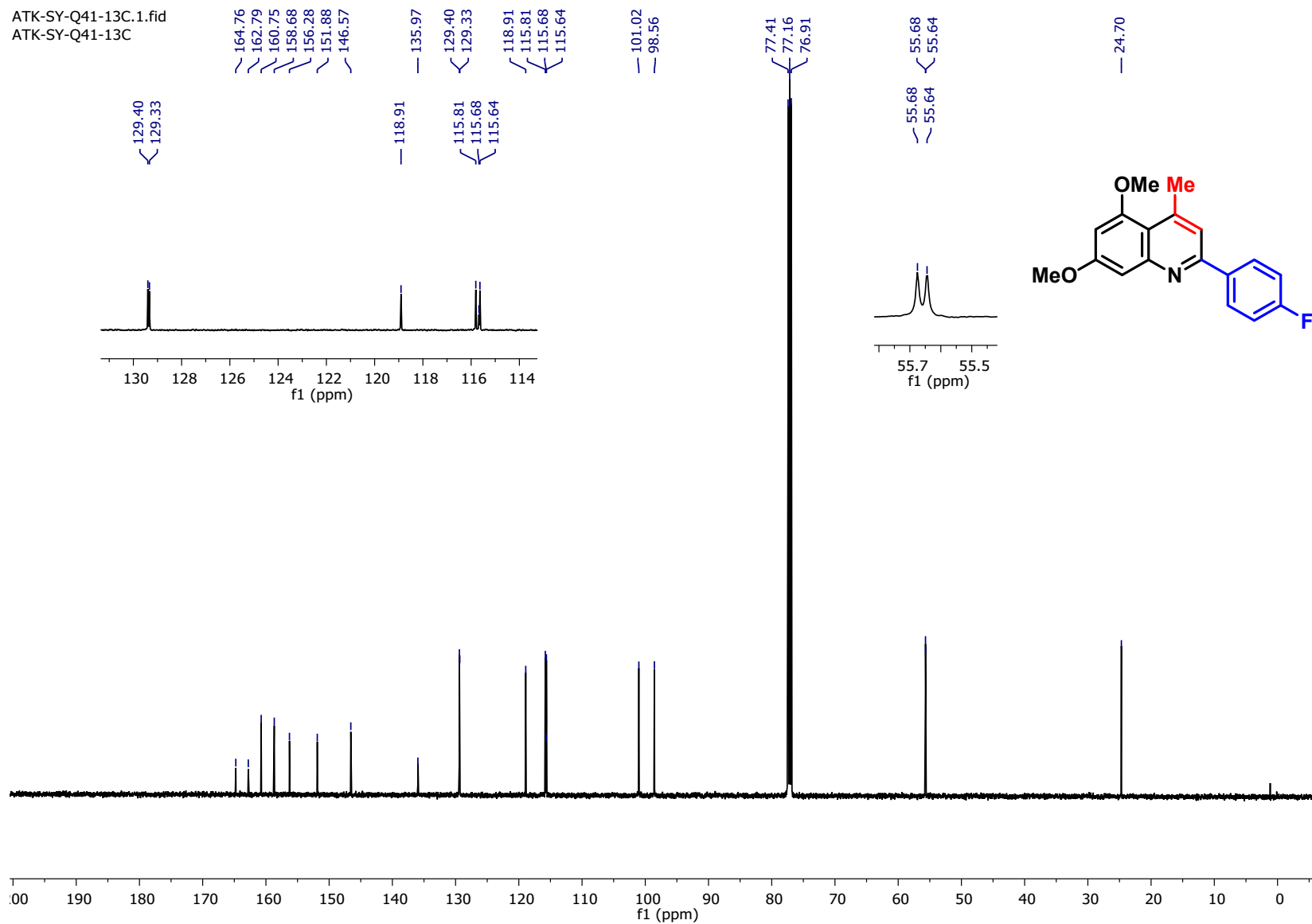
# <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 4b

ATK-SY-Q41-1H.3.fid — ATK-SY-Q41-1H



$^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound 4b

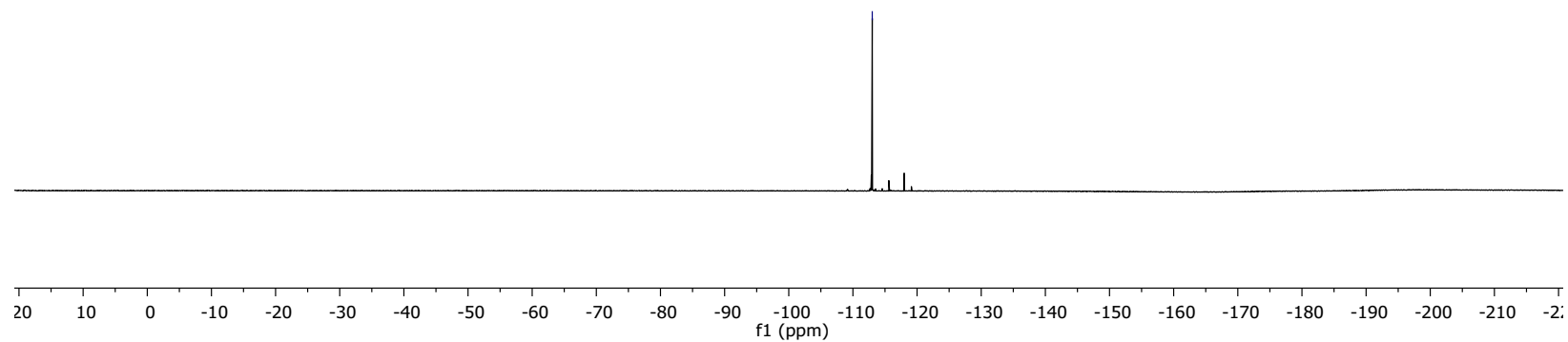
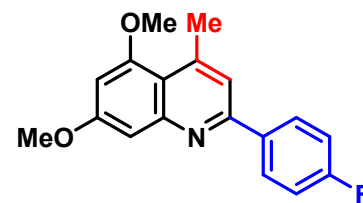
ATK-SY-Q41-13C.1.fid  
ATK-SY-Q41-13C



**<sup>19</sup>F NMR (471 MHz, CDCl<sub>3</sub>) spectrum of compound 4b**

SY-Q41-19F.1.fid — SY-Q41-19F

— -113.01

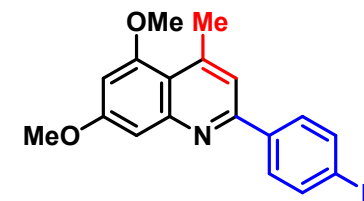
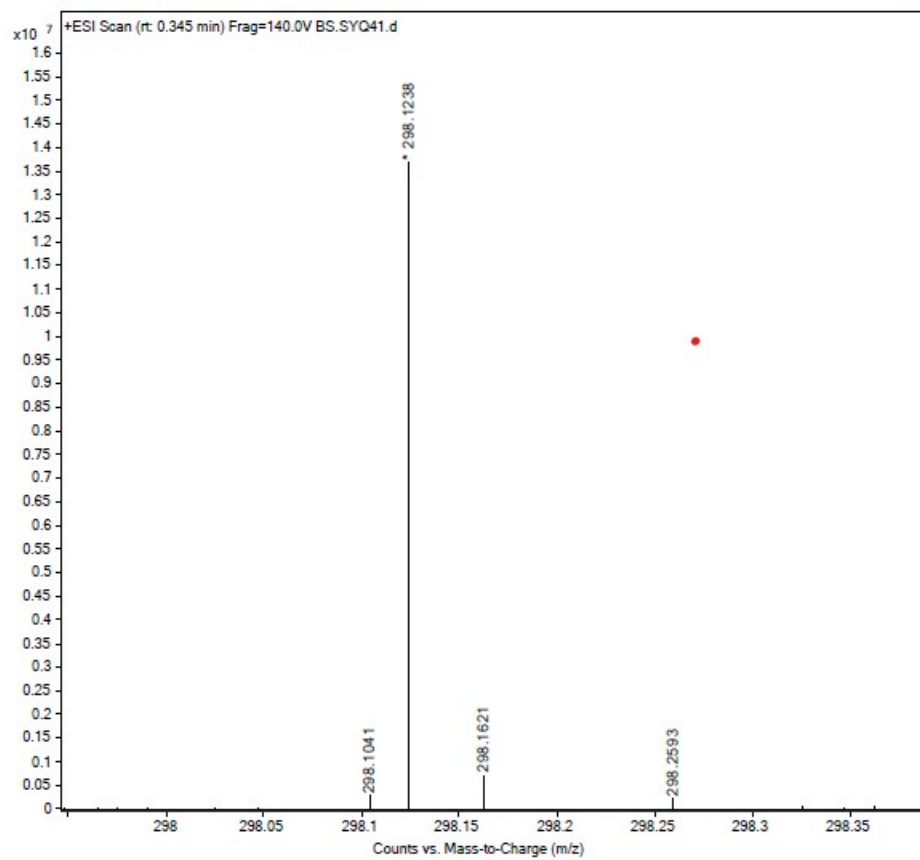


## HRMS spectrum of compound 4b

Sample Name  
User Name  
Sample Type  
ACQ Method

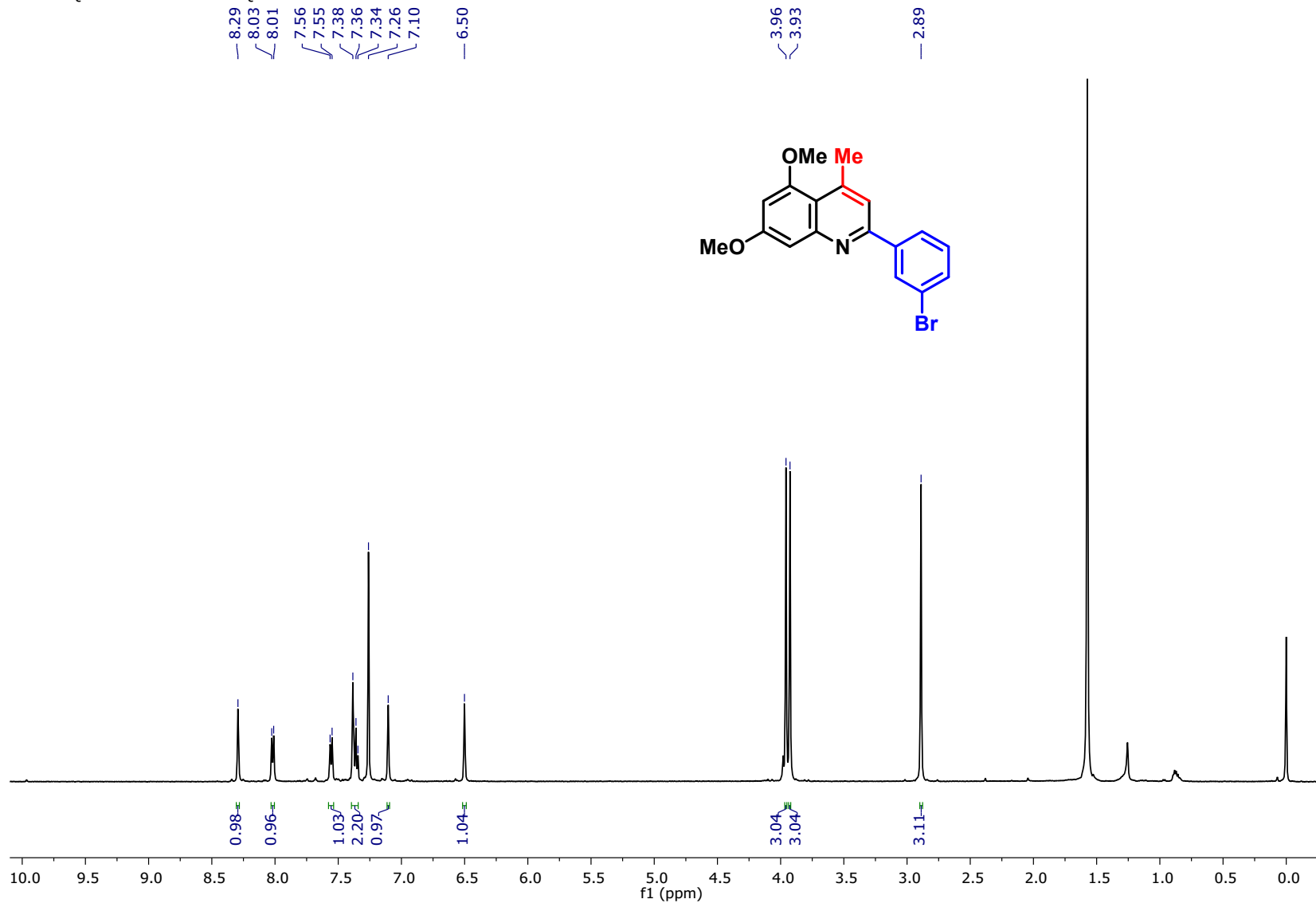
Sample24  
SYSTEM (SYSTEM)  
Sample  
DIRECT MASS\_POSITIVE\_100\_1500.m  
Position  
Inj Vol  
IRM Calibration Status  
Comment  
P1-C2  
5  
Success

Instrument Name  
InjPosition  
Data Filename  
Acquired Time  
QTOF  
BS.SYQ41.d  
16-Jun-23 10:36:34 AM (UTC+05:30)



**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) spectrum of compound 4c**

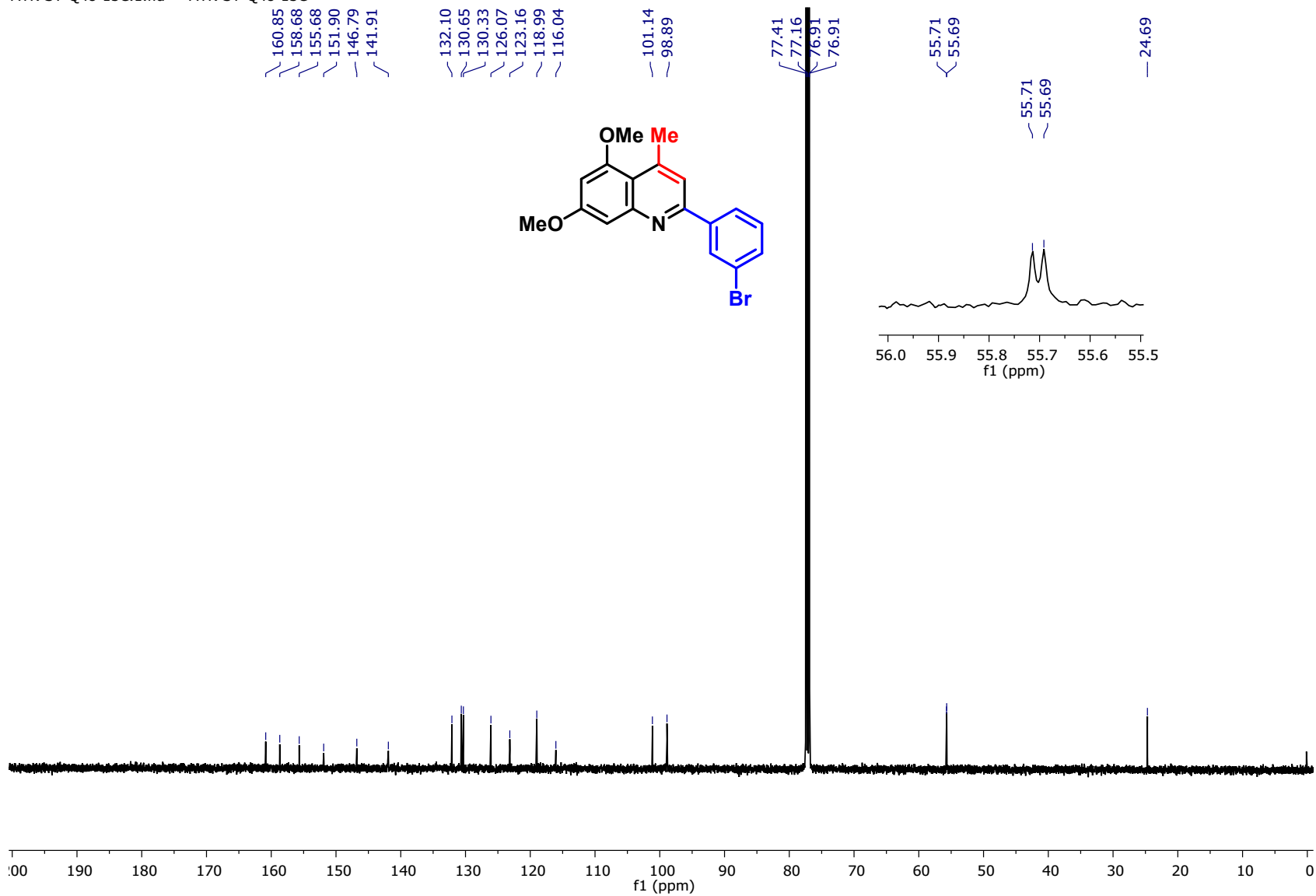
ATK-SY-Q48-1H.3.fid — ATK-SY-Q48-1H





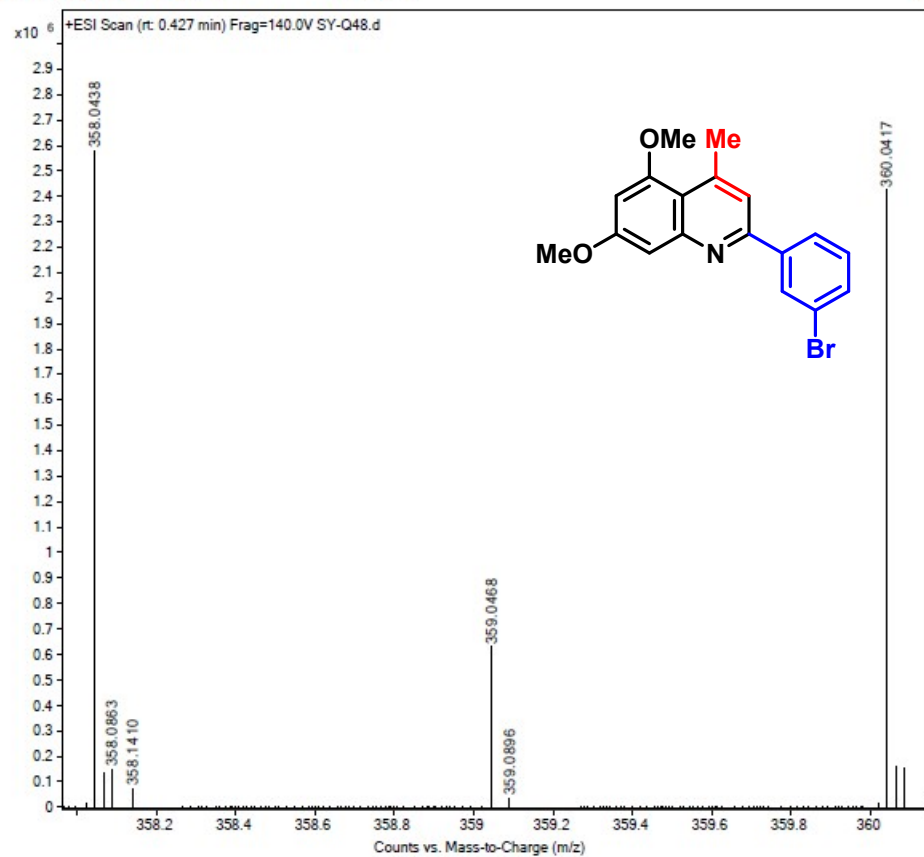
$^{13}\text{C}\{^1\text{H}\}$  (125 MHz,  $\text{CDCl}_3$ ) NMR spectrum of compound 4c

ATK-SY-Q48-13C.1.fid — ATK-SY-Q48-13C



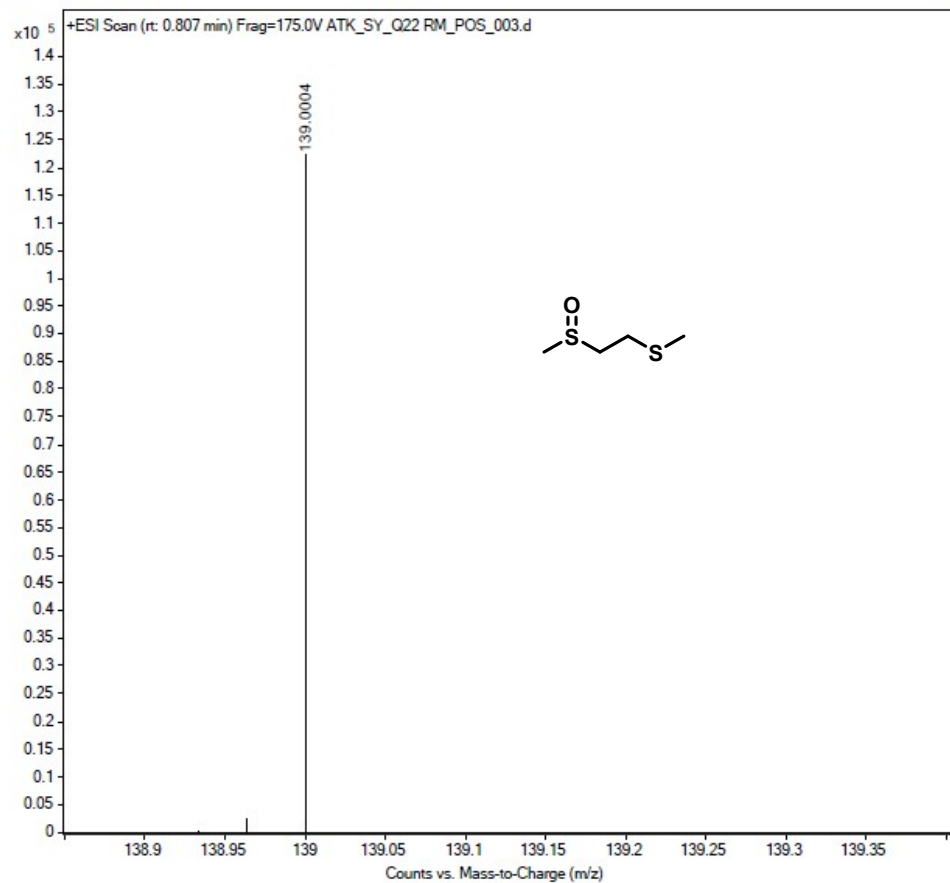
## HRMS spectrum of compound 4c

Sample Name	Sample23	Position	P1-C1	Instrument Name	QTOF
User Name	SYSTEM (SYSTEM)	Inj Vol	5	InjPosition	
Sample Type	Sample	IRM Calibration Status	Success	Data Filename	SY-Q48.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	Comment		Acquired Time	13-Jul-23 11:43:22 AM (UTC+05:30)



## HRMS spectrum of reaction intermediate B

ATK_SY_Q22_RM_POS	Position	P1-C8	Instrument Name	Instrun
	Inj Vol	10	InjPosition	
Sample	IRM Calibration Status	Success	Data Filename	ATK_S1
FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb



## HRMS spectrum of reaction intermediate D

ATK\_SY\_Q22 RM\_POS

Position P1-C8

Instrument Name

Instrument 1

Inj Vol 10

InjPosition

Sample

IRM Calibration Status Success

Data Filename

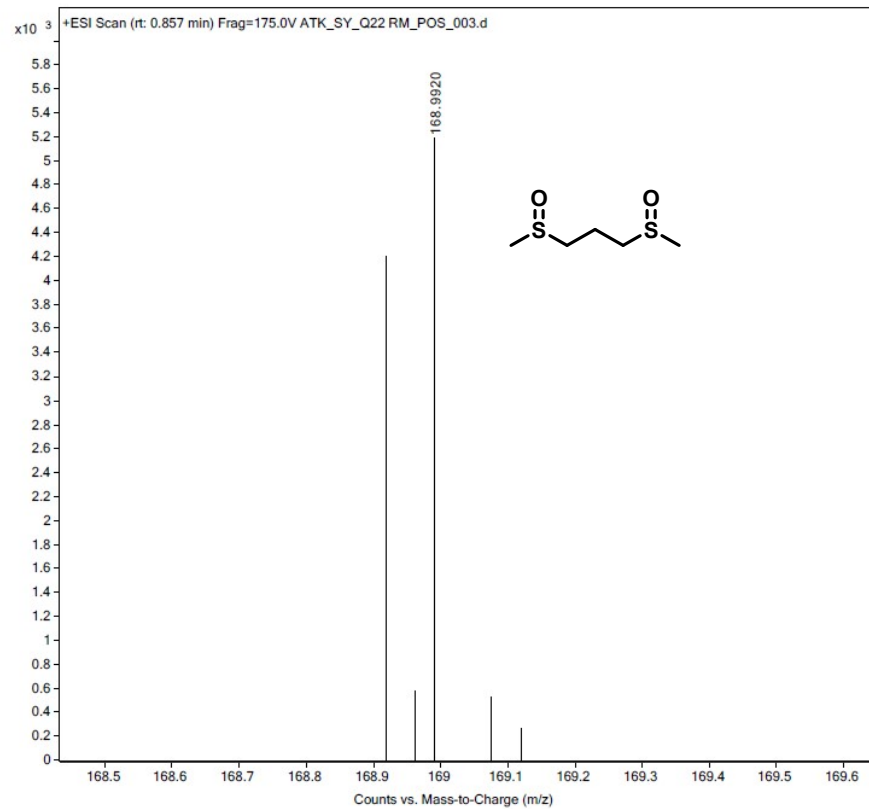
ATK\_SY\_Q22 RM\_

FULL SCAN-POSITIVE.m

Comment

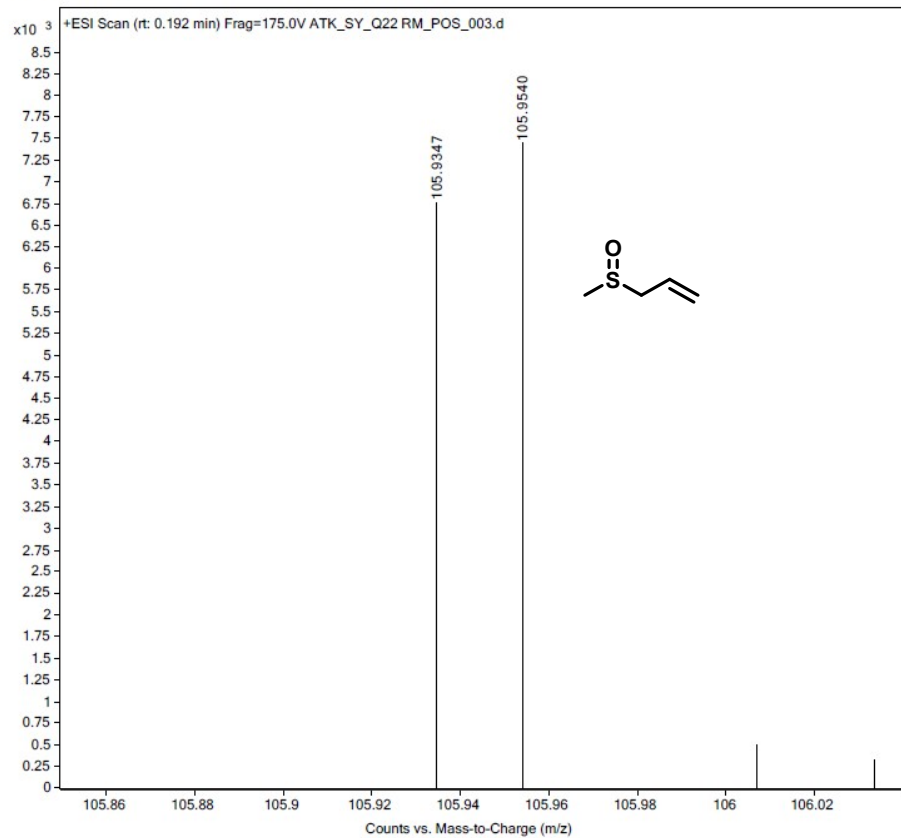
Acquired Time

28-Feb-23 05:05::



## HRMS spectrum of reaction intermediate H

ATK_SY_Q22_RM_POS	Position	P1-C8	Instrument Name	Instrument 1
	Inj Vol	10	InjPosition	
Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q22_RM
FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:05



## HRMS spectrum of intermediate L of compound 3k

ATK_SY_Q22 RM_POS	Position	P1-C8	Instrument Name	Instrument 1
	Inj Vol	10	InjPosition	
Sample	IRM Calibration Status	Success	Data Filename	ATK_SY_Q22 RM_Pos
FULL SCAN-POSITIVE.m	Comment		Acquired Time	28-Feb-23 05:05:15

