Electronic Supporting Information

Title: A Short and Elegant Synthetic Approach for 9-Substituted Tetrahydro Coumestan Derivatives and Synthesis of Some Naturally Occurring Coumestan Derivatives

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Experimental

General Information and Methods

Melting points were determined on a melting point apparatus and were uncorrected. ^{1}H NMR spectra were recorded on 400 MHz, 500 MHz and 600 MHz, respectively. Similarly, ^{13}C NMR spectra were recorded on 100 MHz, 125 MHz and 150 MHz NMR spectrometers. TMS was used as an internal standard; chemical shifts (δ scale) are reported in parts per million(ppm). ^{1}H NMR spectra are reported in the order of 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 singlet). 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. X-ray crystal structures were determined with a diffractometer. Complete crystallographic data of compounds **3e** (CCDC no. 2253174) and **3j** (CCDC no. 2289245) 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).

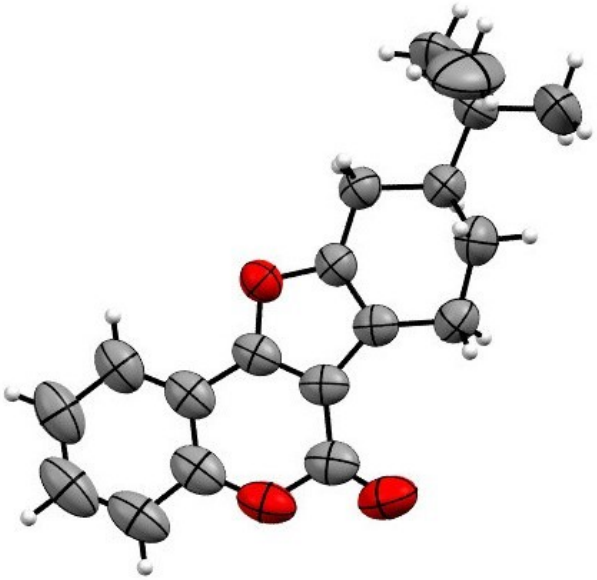

Figure S1. ORTEP Diagrams of compound **3e**

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

Entry	**Identification Code**	**Compound 3e**
01	Empirical formula	$C_{19}H_{20}O_3$
02	Formula weight	296.369
03	Temperature	298.00
04	Wavelength	0.71073
05	Radiation type	Mo Kα
06	Radiation system	Fine-focus sealed tube
07	Crystal system	orthorhombic
08	Space group	Pbca
09	Cell length	a=14.8561(10) b=7.4709(5) c=28.931(2)
10	Cell angle	α=90 β=90 γ=90
11	Cell volume	3211.0(4)
12	Density	1.226

13	Completeness to theta	99
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F2
16	Index ranges	$-17 \leq h \leq 17$, $-8 \leq k \leq 8$, $-34 \leq l \leq 34$
17	Reflection number	37896
18	2Θ range for data collection/°	5.48 to 49.98
19	Cell formula units Z	8
20	CCDC no	2253174

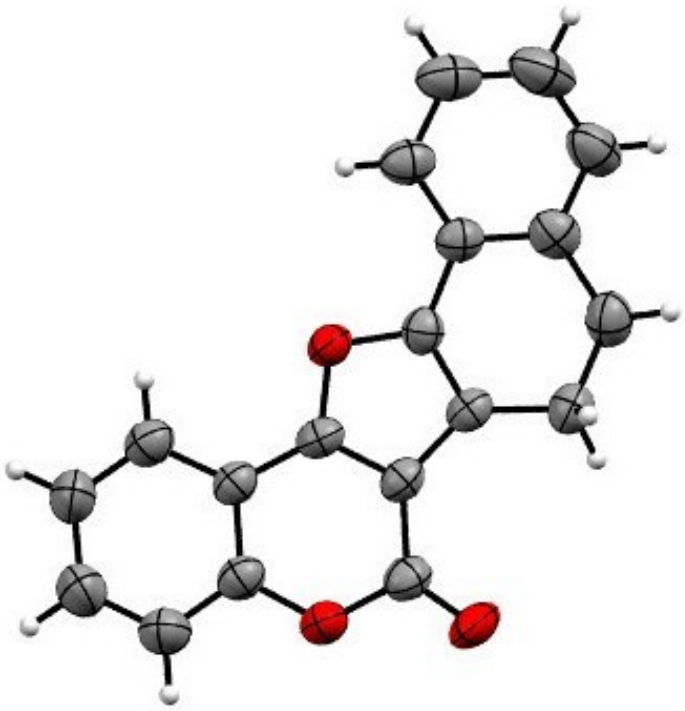

Figure S2. ORTEP Diagrams of compound **3j**

Table S2. Crystal data and structure refinement for compound **3j**

Entry	**Identification Code**	**Compound 3j**
01	Empirical formula	$C_{19}H_{12}O_3$

02	Formula weight	288.29
03	Temperature	288.29
04	Wavelength	0.71073
05	Radiation type	MoKα
06	Radiation system	Fine-focus sealed tube
07	Crystal system	orthorhombic
08	Space group	$P2_12_12_1$
09	Cell length	a=7.028(3) (10) b=13.206(4) c=13.206(4)
10	Cell angle	α=90 β=90 γ=90
11	Cell volume	1365.8(8)
12	Density	1.402
13	Completeness to theta	99
14	Absorption correction	multi-scan
15	Refinement method	Full-matrix least-squares on F2
16	Index ranges	$-8 \leq h \leq 8$, $-16 \leq k \leq 16$, $-18 \leq l \leq 18$
17	Reflection number	28563
18	2Θ range for data collection/°	4.144 to 52.91
19	Cell formula units Z	4
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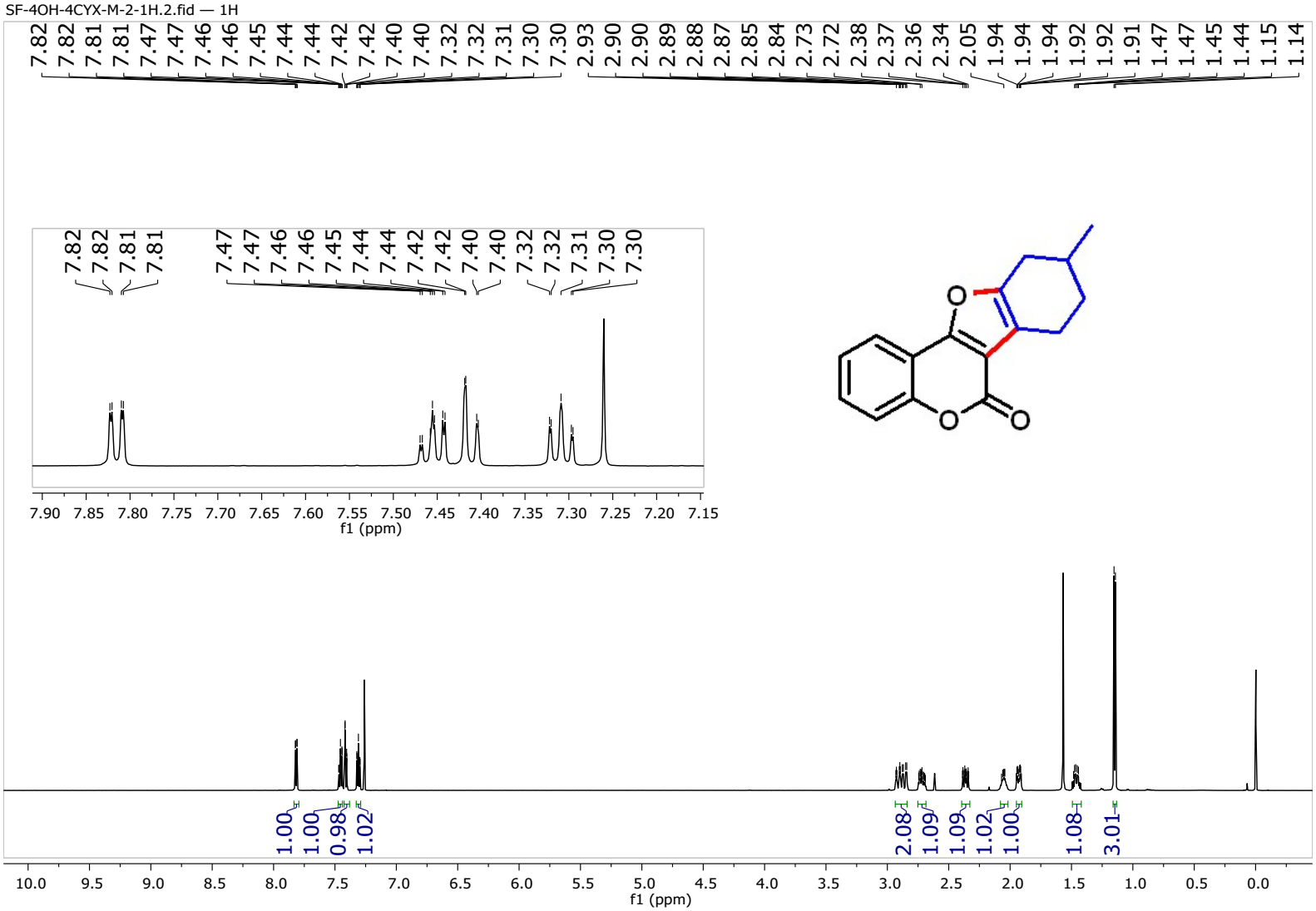
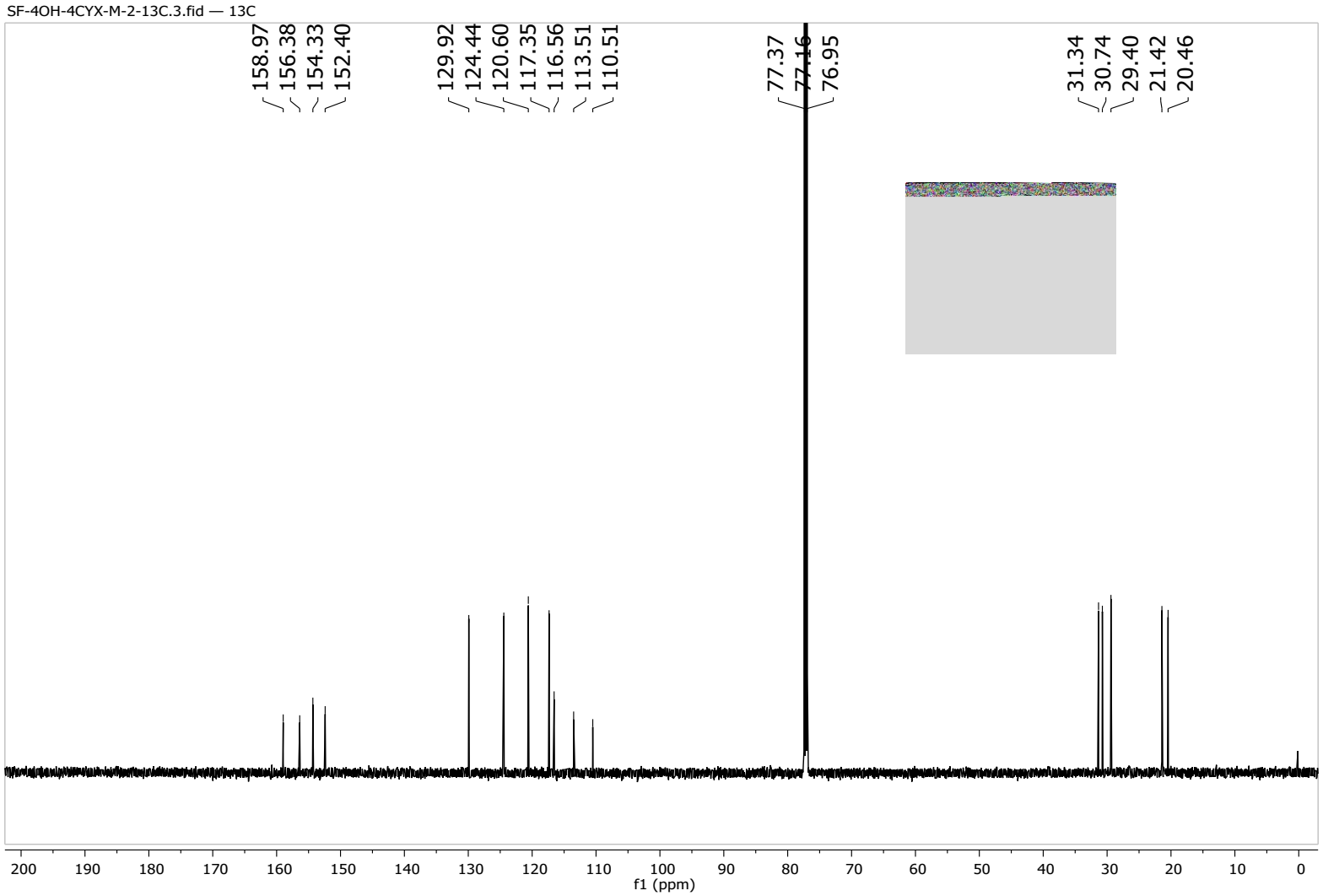
^{1}H NMR Spectrum of 9-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3a)

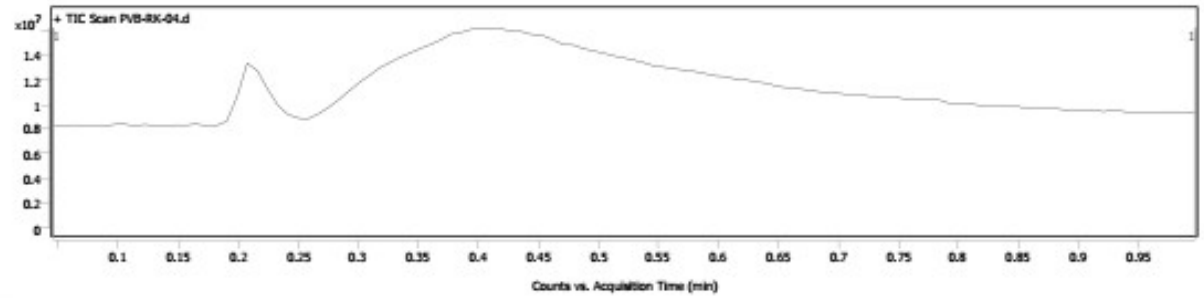


^{13}C NMR Spectrum of 9-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3a)



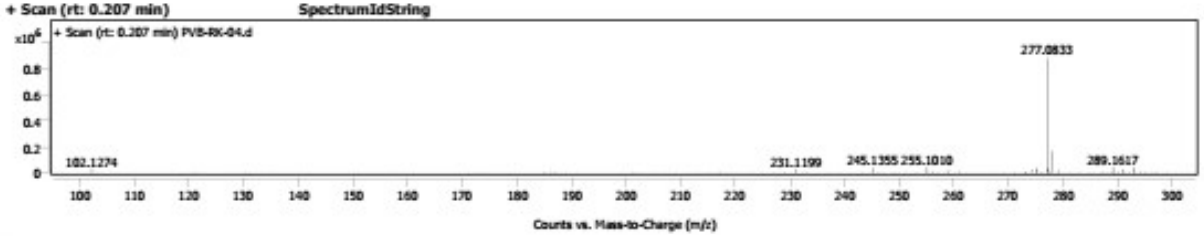
HRMS Spectrum of 9-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3a)

Sample Chromatograms



Peak Spec

+ Scan (rt: 0.207 min) **SpectrumIdString**



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255.1010		43489	4.94					
259.1511		14227	1.62					
261.1304		11149	1.27					
274.2736		20313	2.31					
275.0674		20662	2.35					
275.1458		34340	3.90					
277.0833	1	879741	100.00					
277.1205		34947	3.97					
277.1694		20706	2.35					
278.0863	1	165935	18.86					
279.0889	1	16825	1.91					
289.1617		42841	4.87					
291.0623		8811	1.00					
291.0984		23111	2.63					
293.0569		14094	1.60					
293.0779		41673	4.74					

MassHunter Qual 10.0
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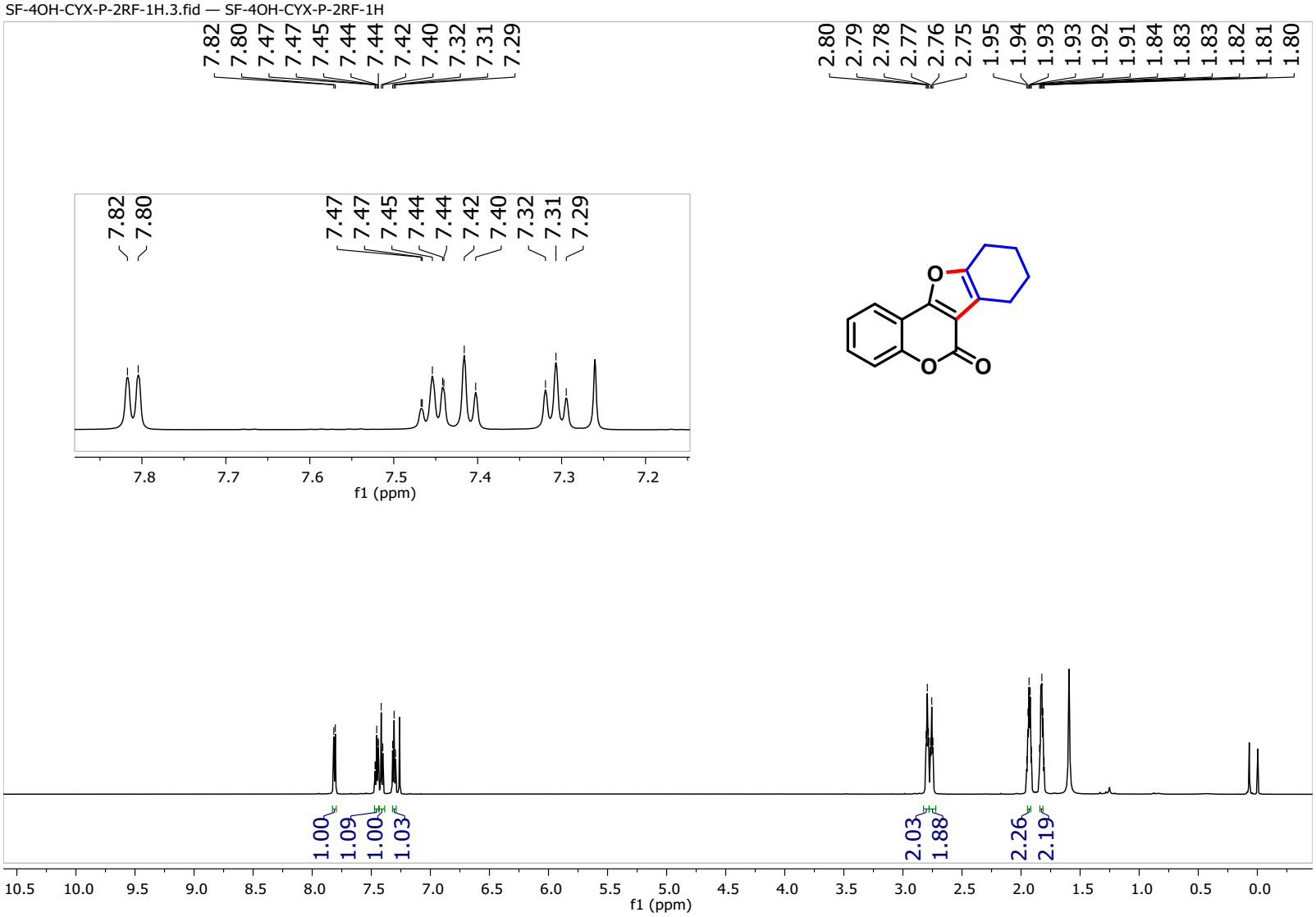
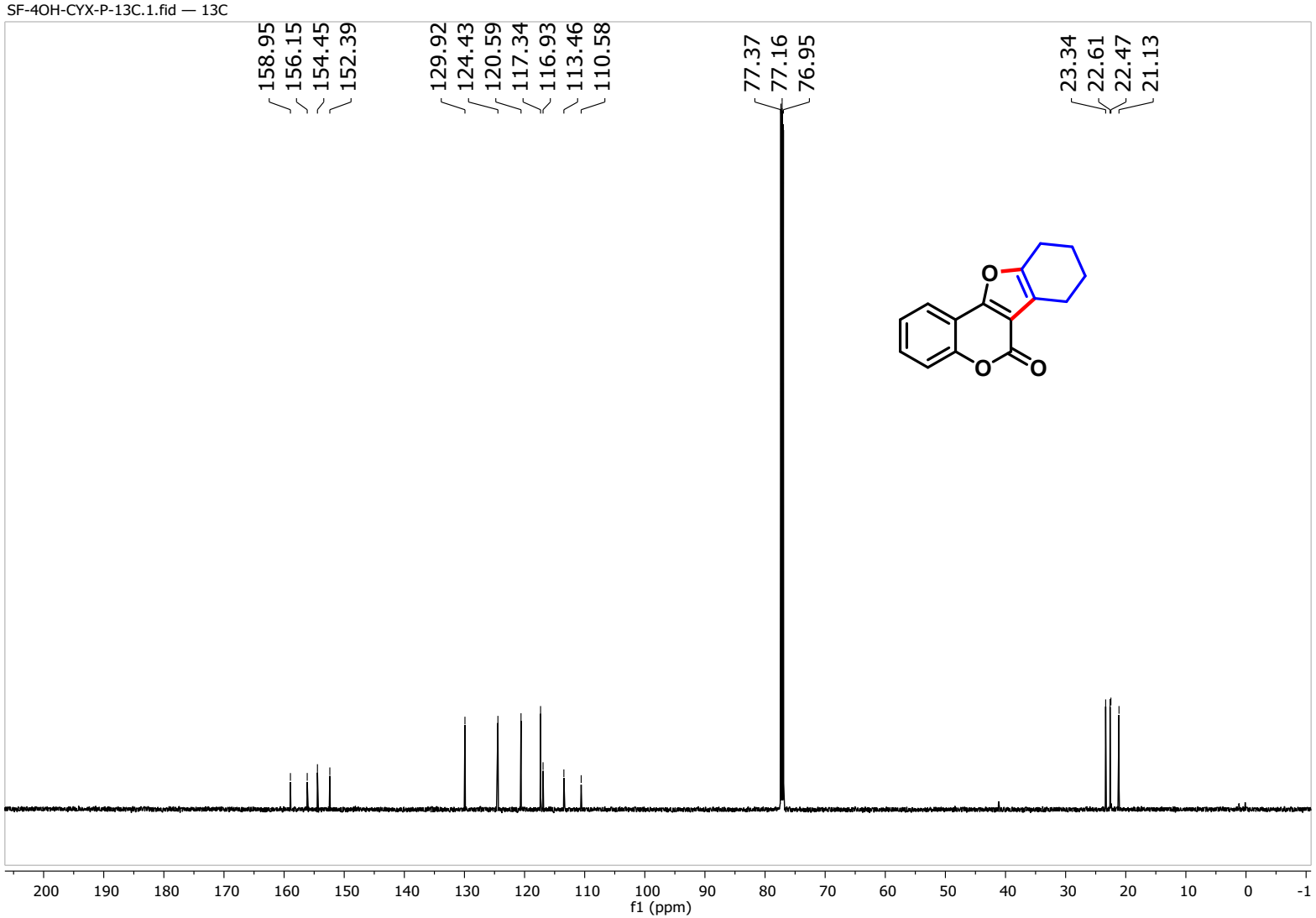
^{1}H NMR Spectrum of 7,8,9,10-Tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3b)



^{13}C NMR Spectrum of 7,8,9,10-Tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3b)



HRMS Spectrum of 7,8,9,10-Tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3b)

Sample Name		**Position**	P1-B1	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF6C20.d
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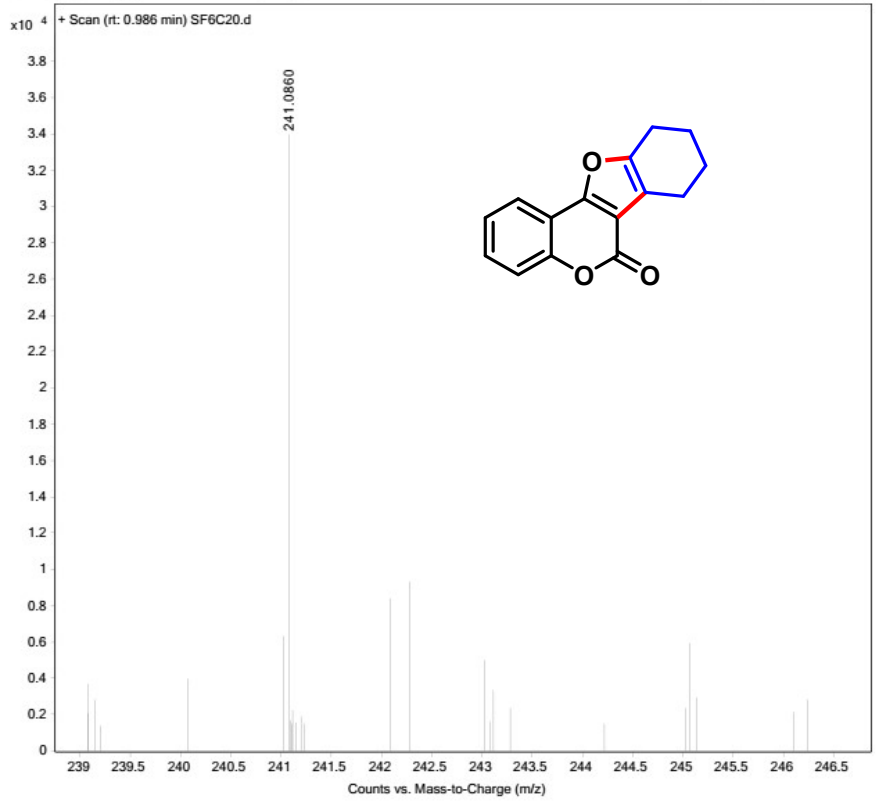
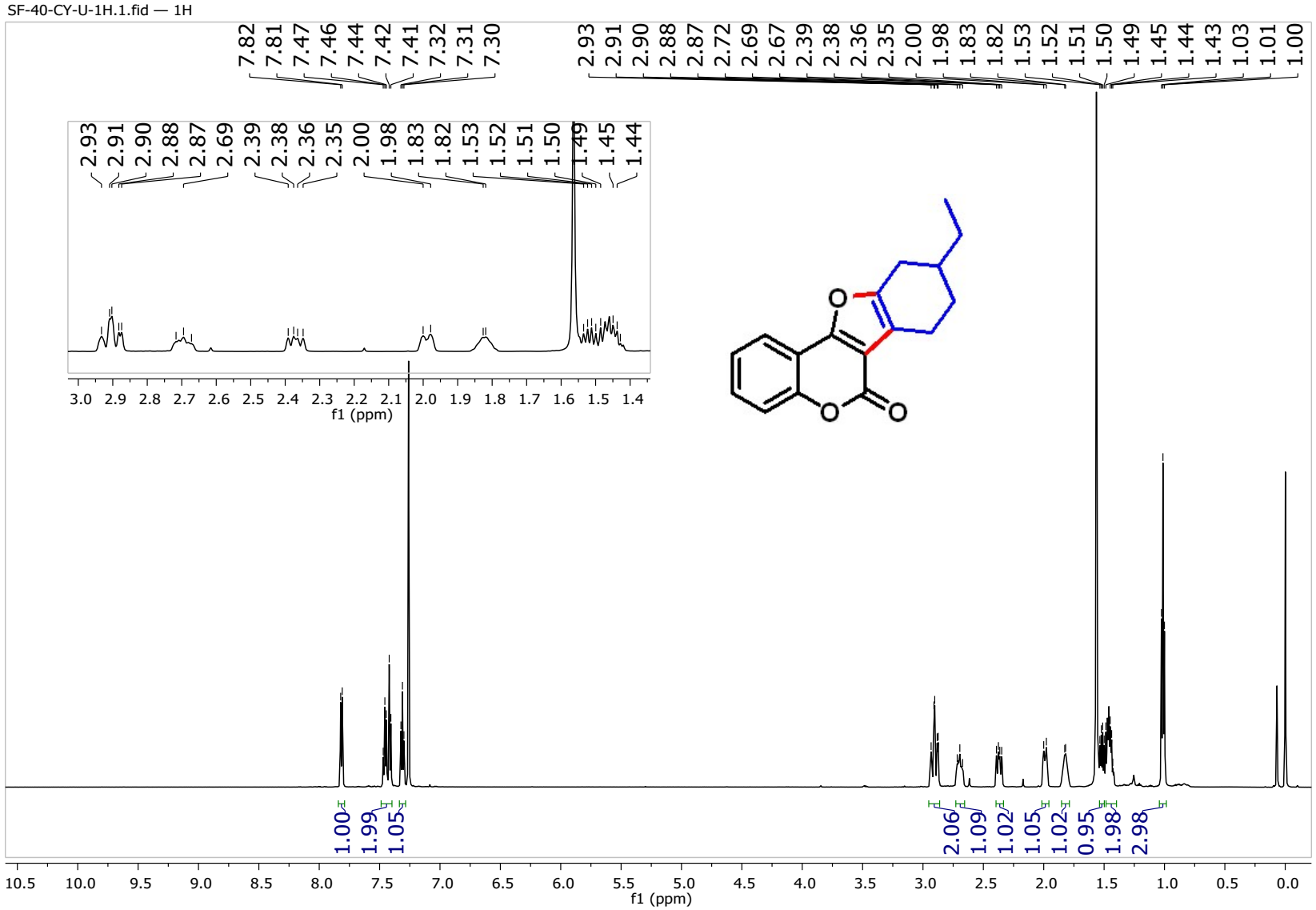
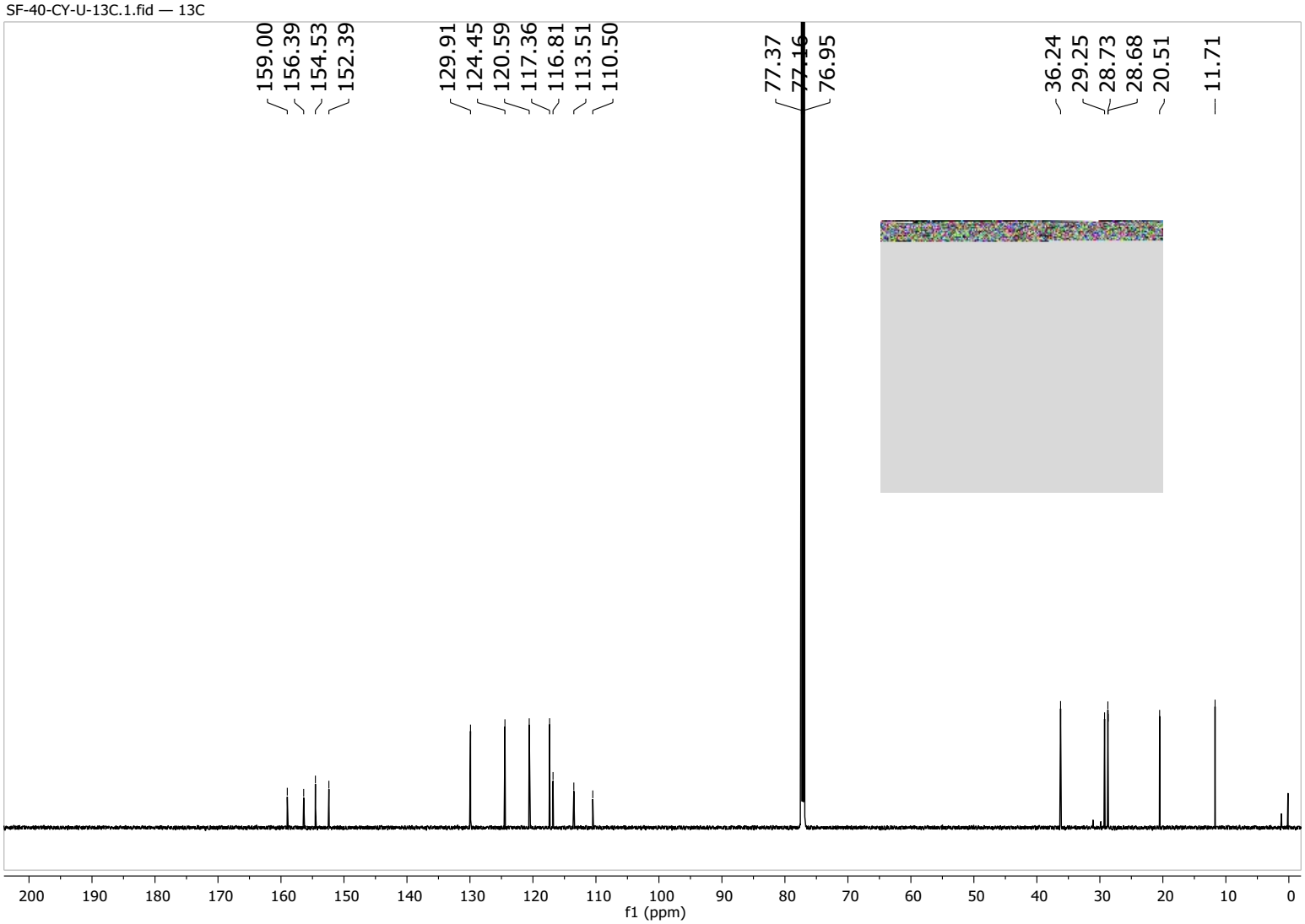


^{1}H NMR Spectrum of 9-Ethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3c)



^{13}C NMR Spectrum of 9-Ethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3c)



HRMS Spectrum of 9-Ethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3c)

Sample Information

Name	PVB-RK-03	**Data File Path**	D:\15-03-2023\PVB-RK-03.d
Sample ID		**Acq. Time (Local)**	15-03-2023 10:09:22 (UTC+05:30)
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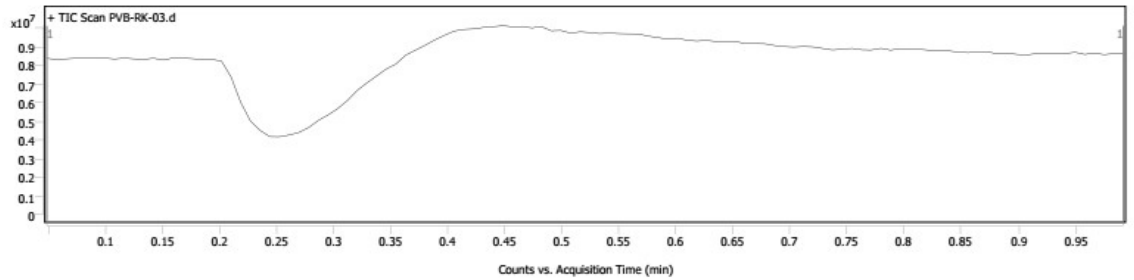
Inj. Vol. (ul)	1	**IRM Status**	Success
Position	P2-A9	**Method Path (DA)**	
Plate Pos.		**Target Source Path**	
Operator		**Result Summary**	

Sample Chromatograms



Peak Spec

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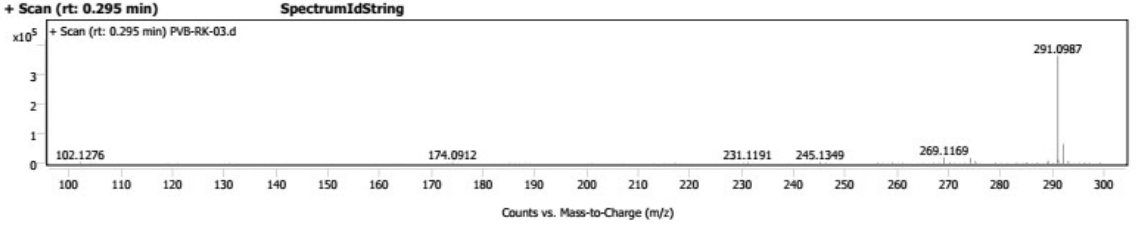

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275.1457		7365	2.01					
289.1614		9331	2.55					
291.0987	1	366450	100.00					
291.1359		12573	3.43					
292.1021	1	65941	17.99					
293.1044	1	7729	2.11					

MassHunter Qual 10.0
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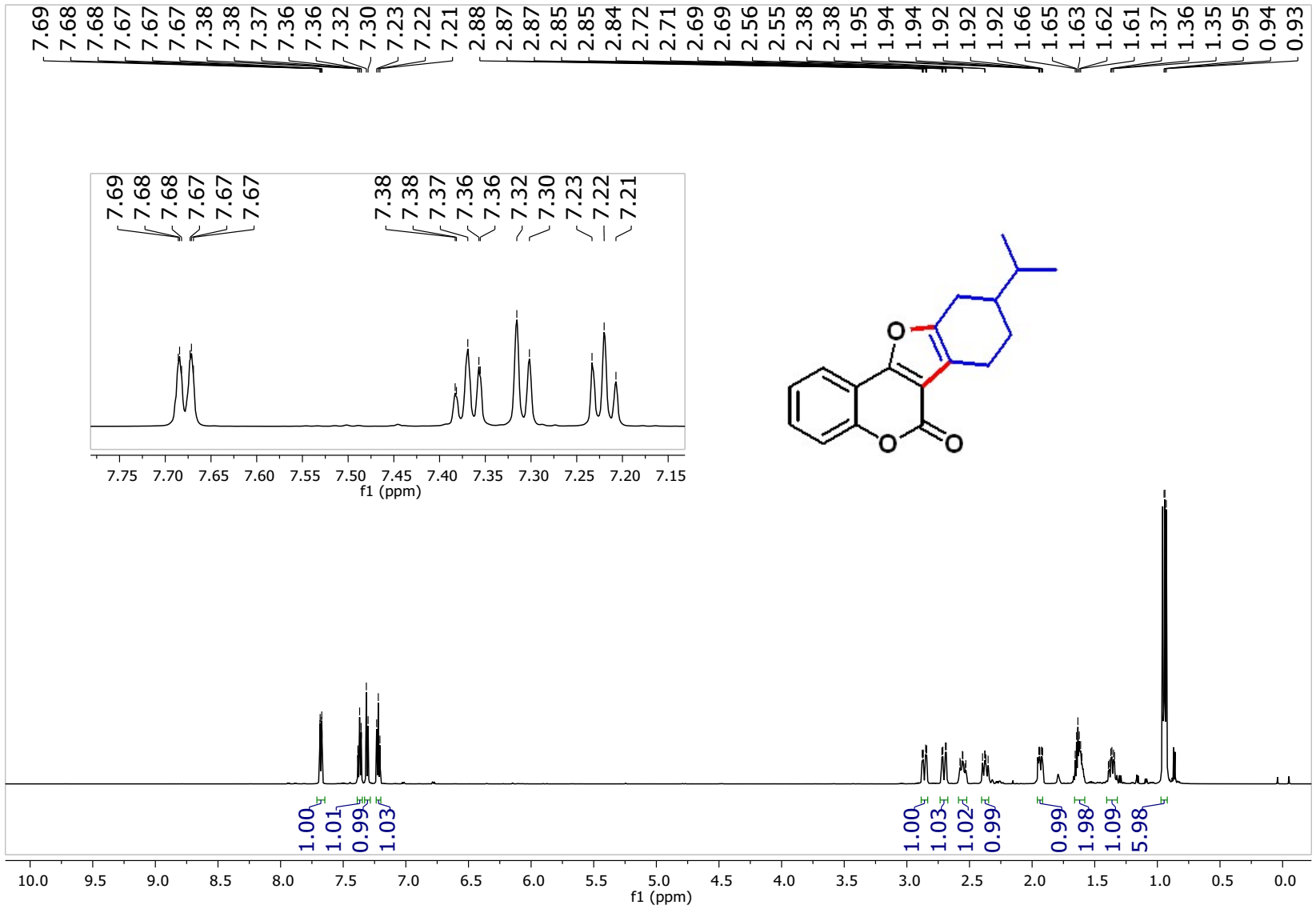
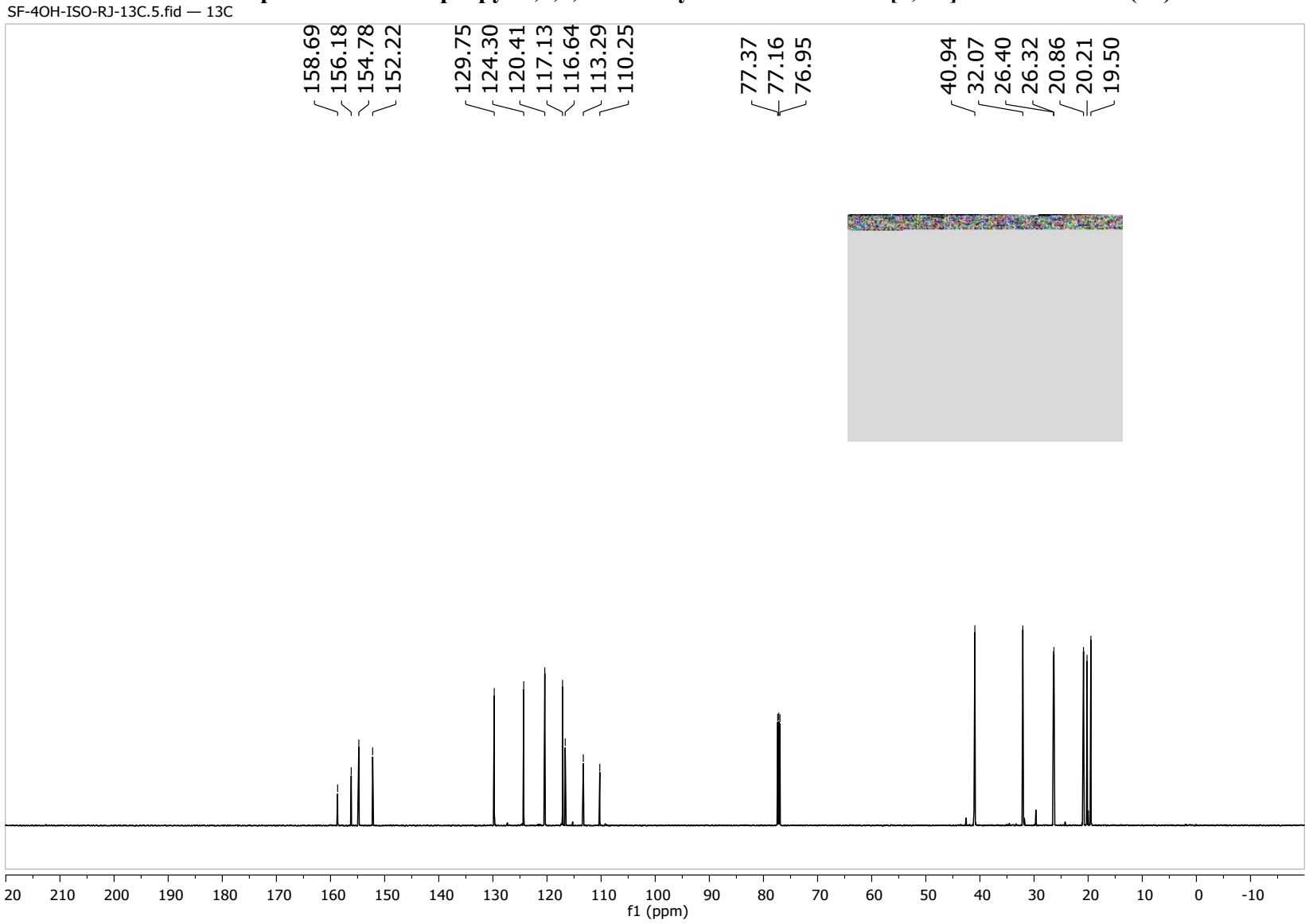
[1]HNMR Spectrum of 9-Isopropyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3d)



^{13}C NMR Spectrum of 9-Isopropyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3d)



HRMS Spectrum of 9-Isopropyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3d)

Counts vs. Acquisition Time (min)

Peak Spec

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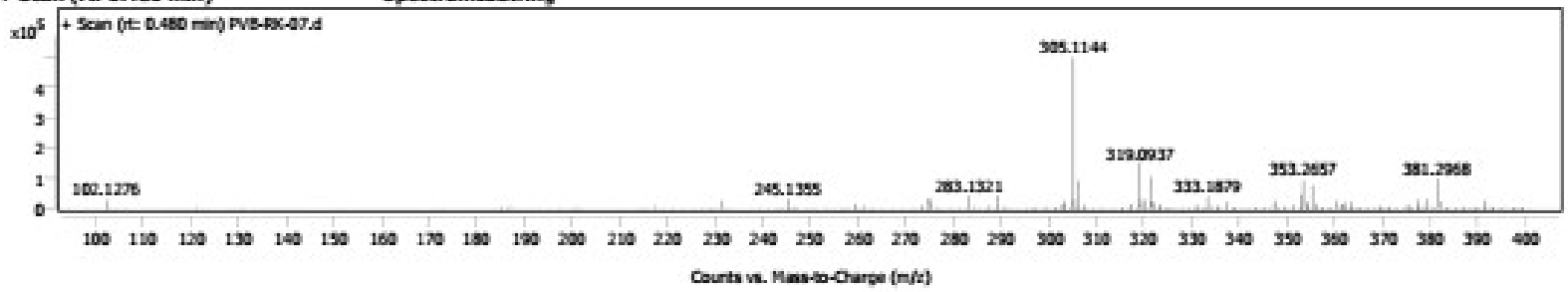

SpectrumIdString

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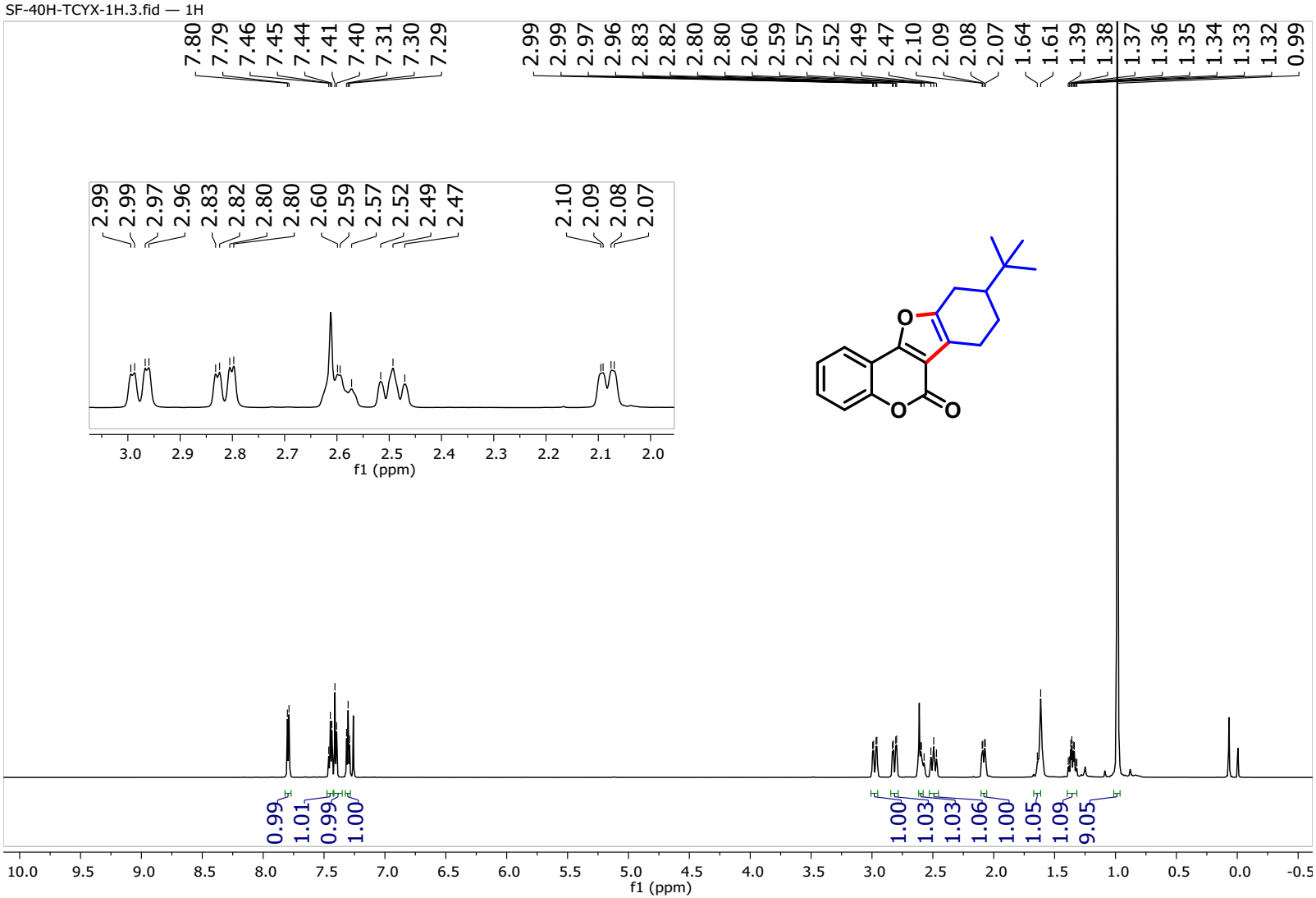
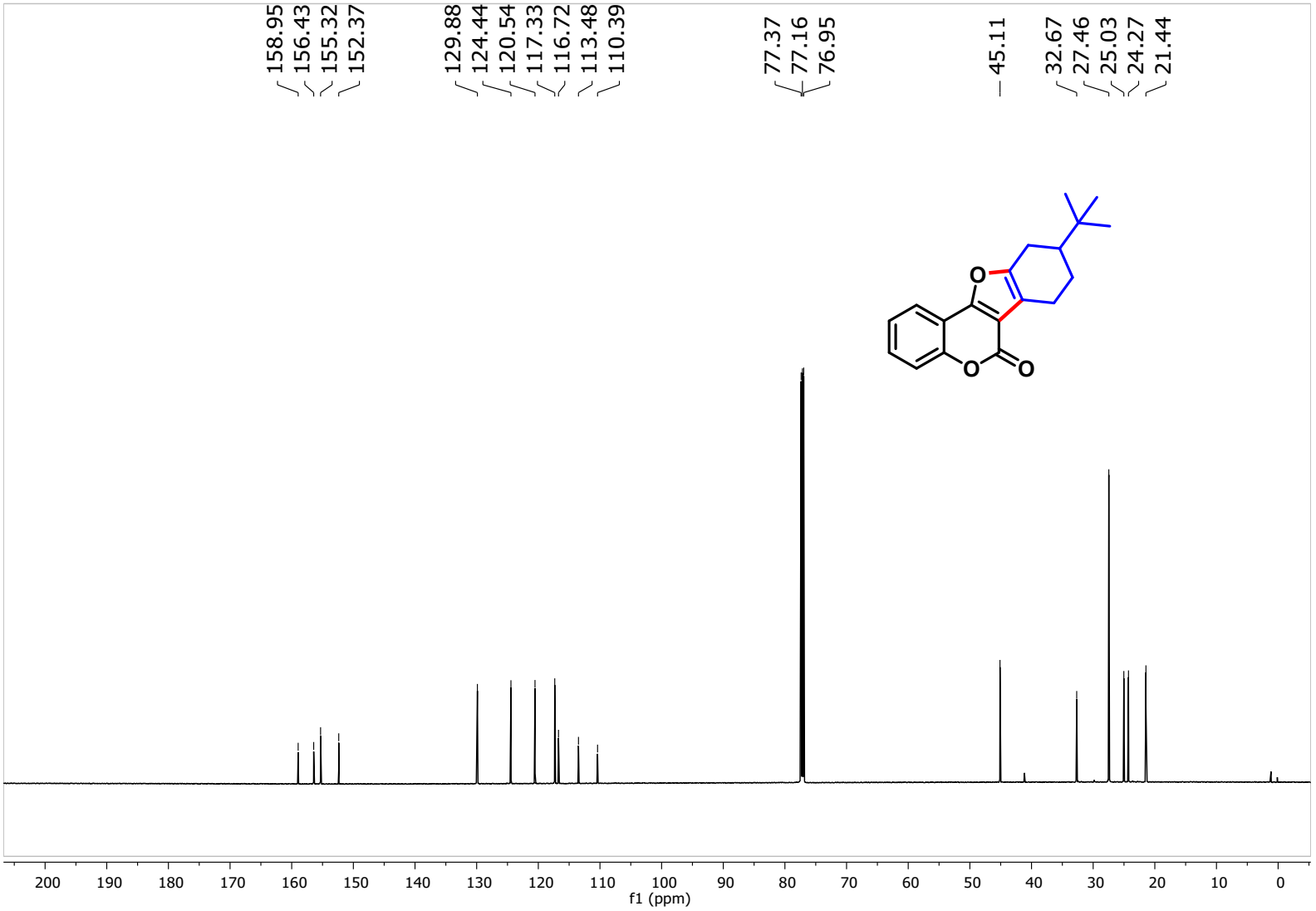
275.1461		29188	5.89					
283.1321		41484	8.38					
289.1615		41471	8.37					
305.1144	1	495311	100.00					
305.1541		27992	5.65					
306.1178	1	91964	18.57					
319.0937	1	150306	30.37					
319.1722		28654	5.79					
320.0972	1	26442	5.34					
321.1060		104409	21.08					
333.1879		38855	7.85					
353.1354		45087	9.10					
353.2657		93311	18.84					
355.1146		74092	14.96					
377.2138		28675	5.39					
379.1508		29087	5.87					
381.2968		98036	19.80					

MassHunter Qual 10.0
(End of Report)

^{1}H NMR Spectrum of 9-(*tert*-Butyl)-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3e)



^{13}C NMR Spectrum of 9-(*tert*-Butyl)-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3e)



HRMS Spectrum of 9-(*tert*-Butyl)-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3e)

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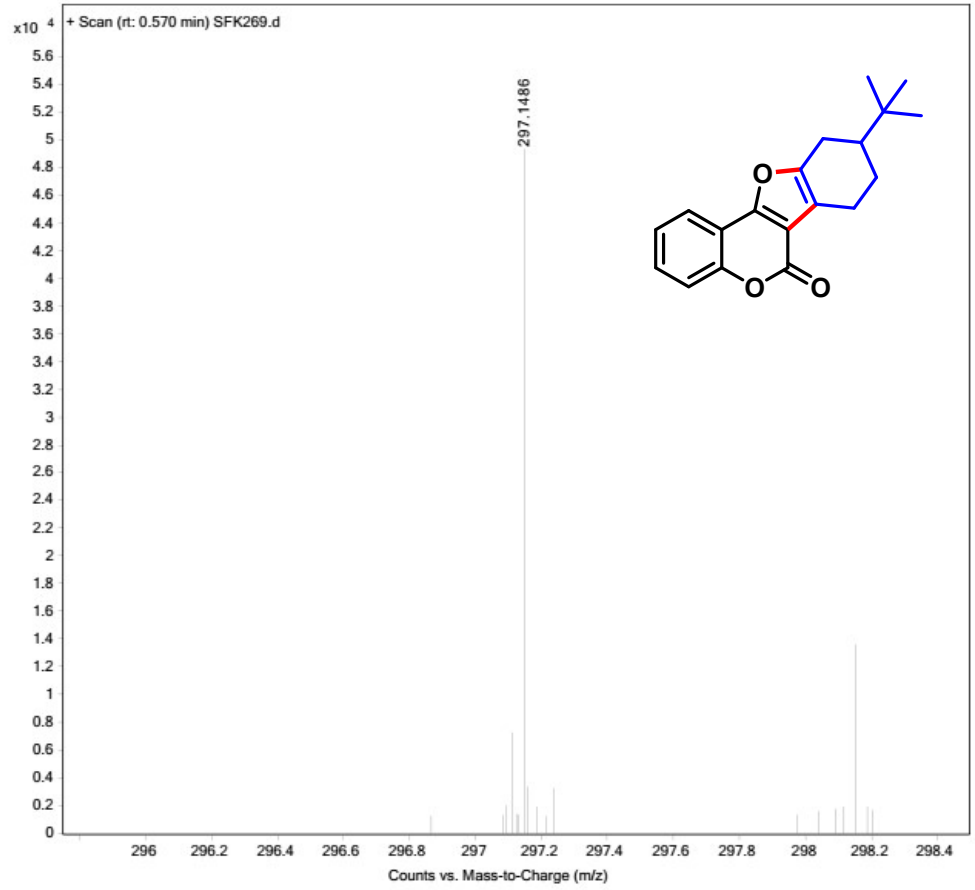
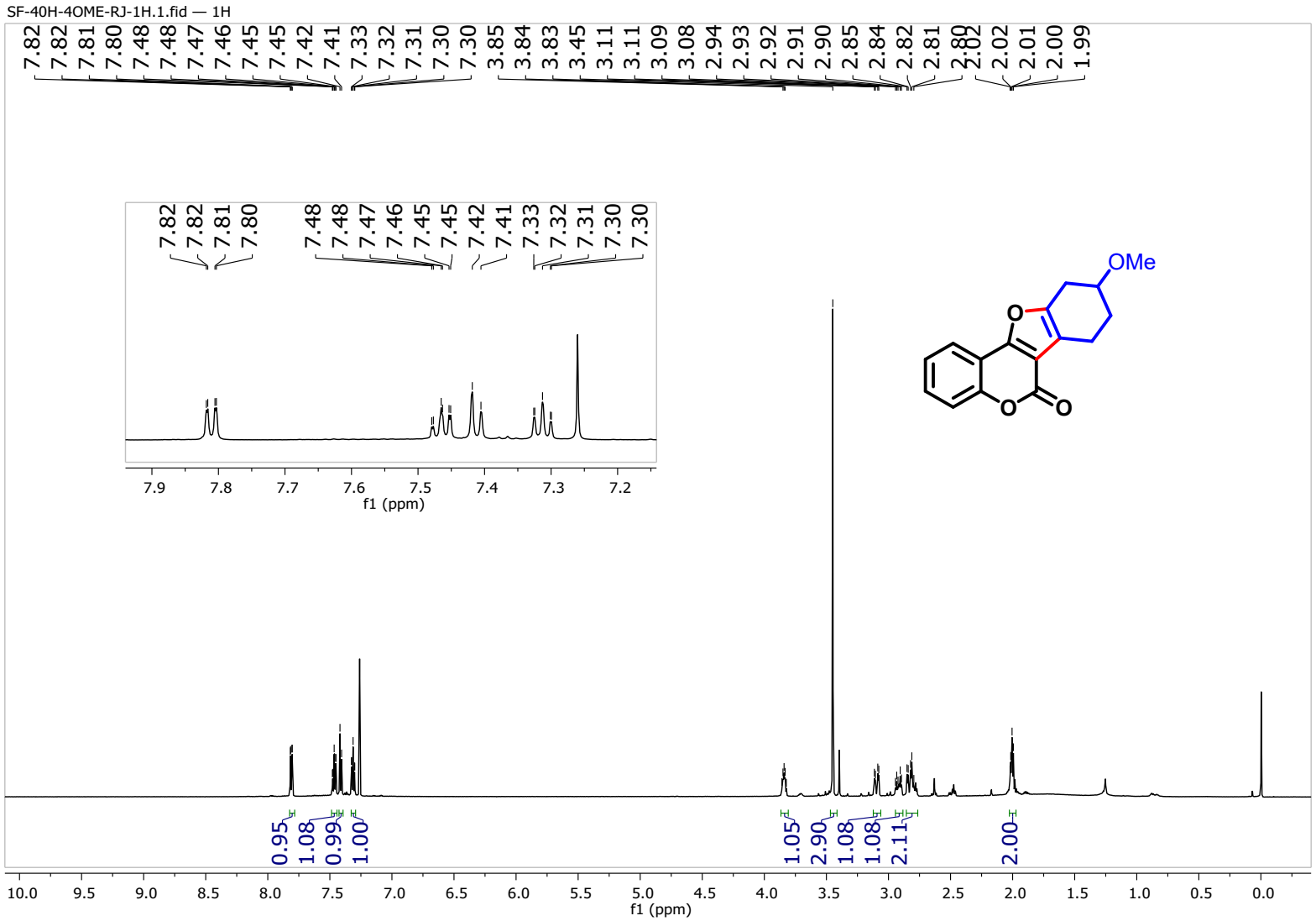
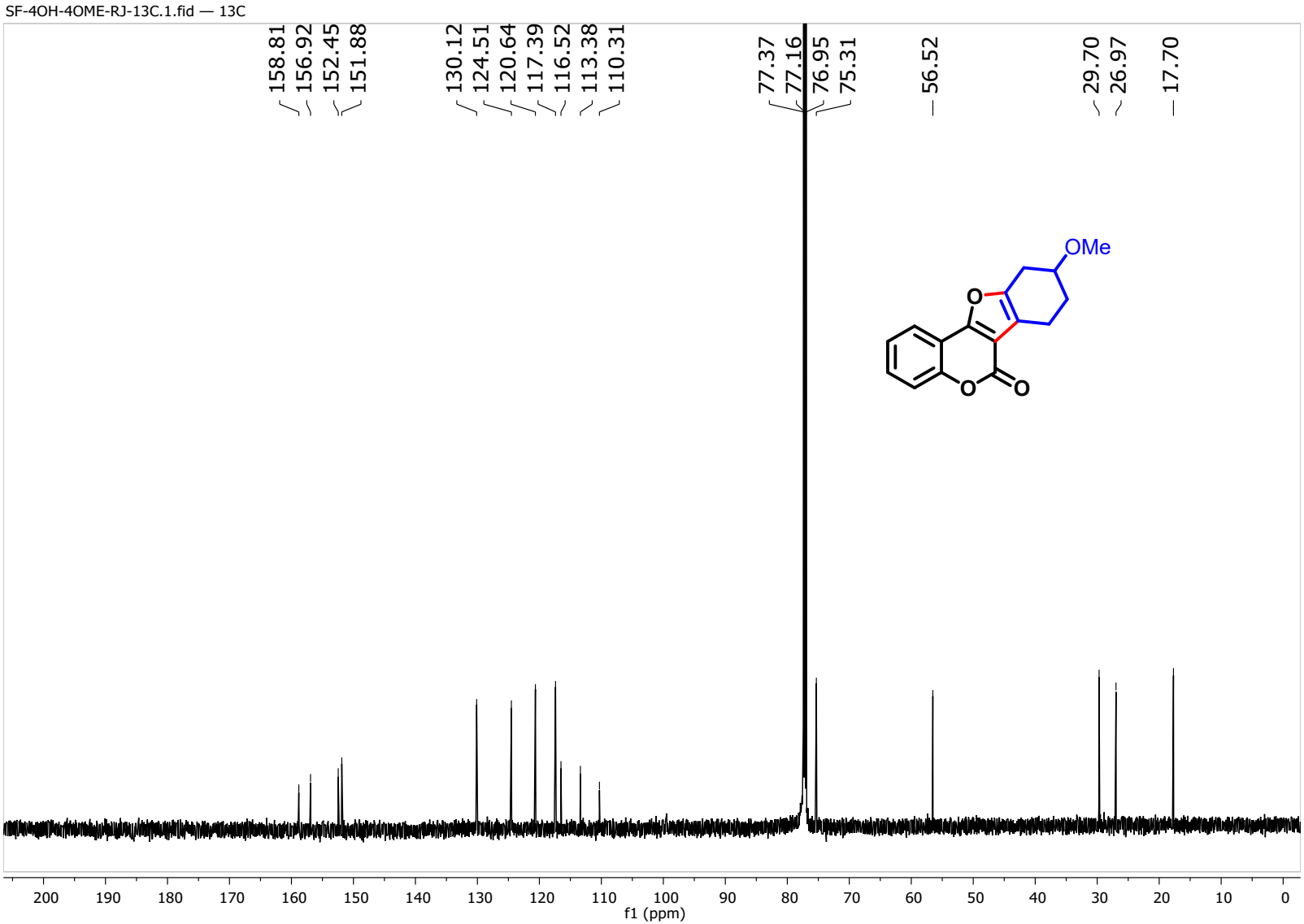


^{1}H NMR Spectrum of 9-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3f)



^{13}C NMR Spectrum of 9-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3f)



HRMS Spectrum of 9-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3f)

Sample Name	Sample20	**Position**	P1-B8	**Instrument Name**	QTOF
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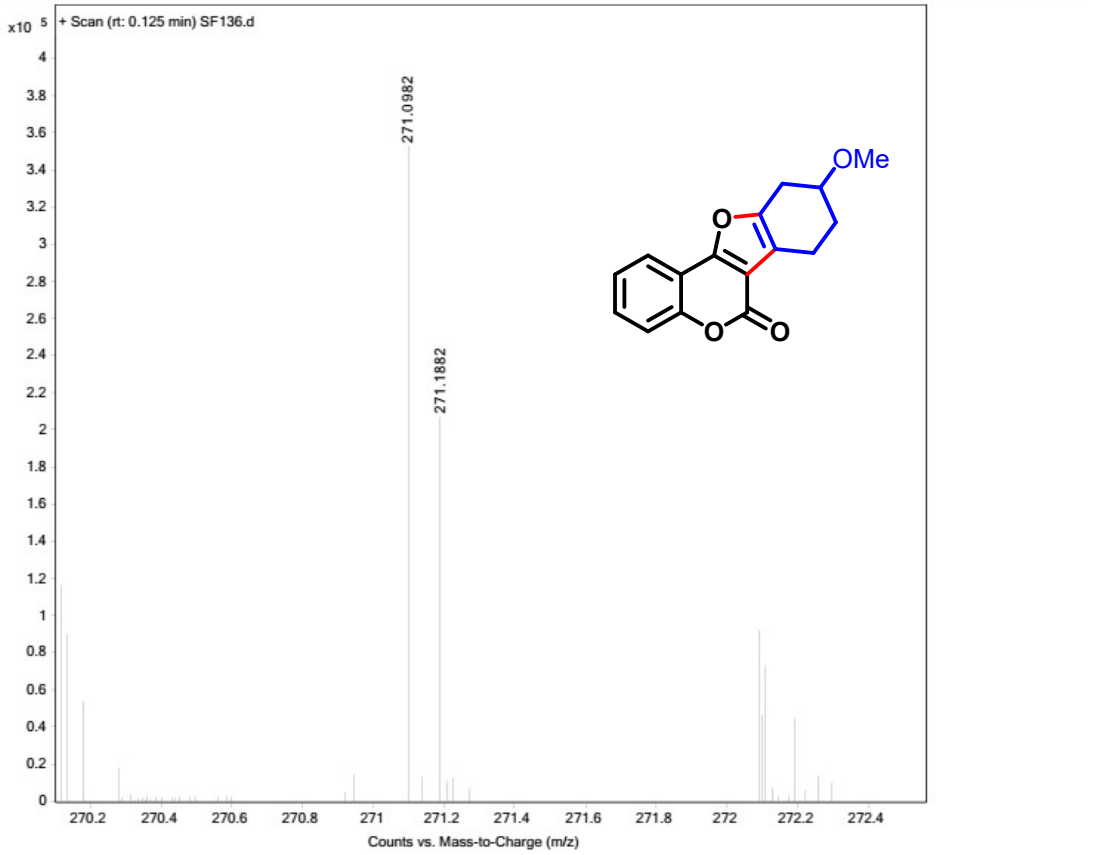
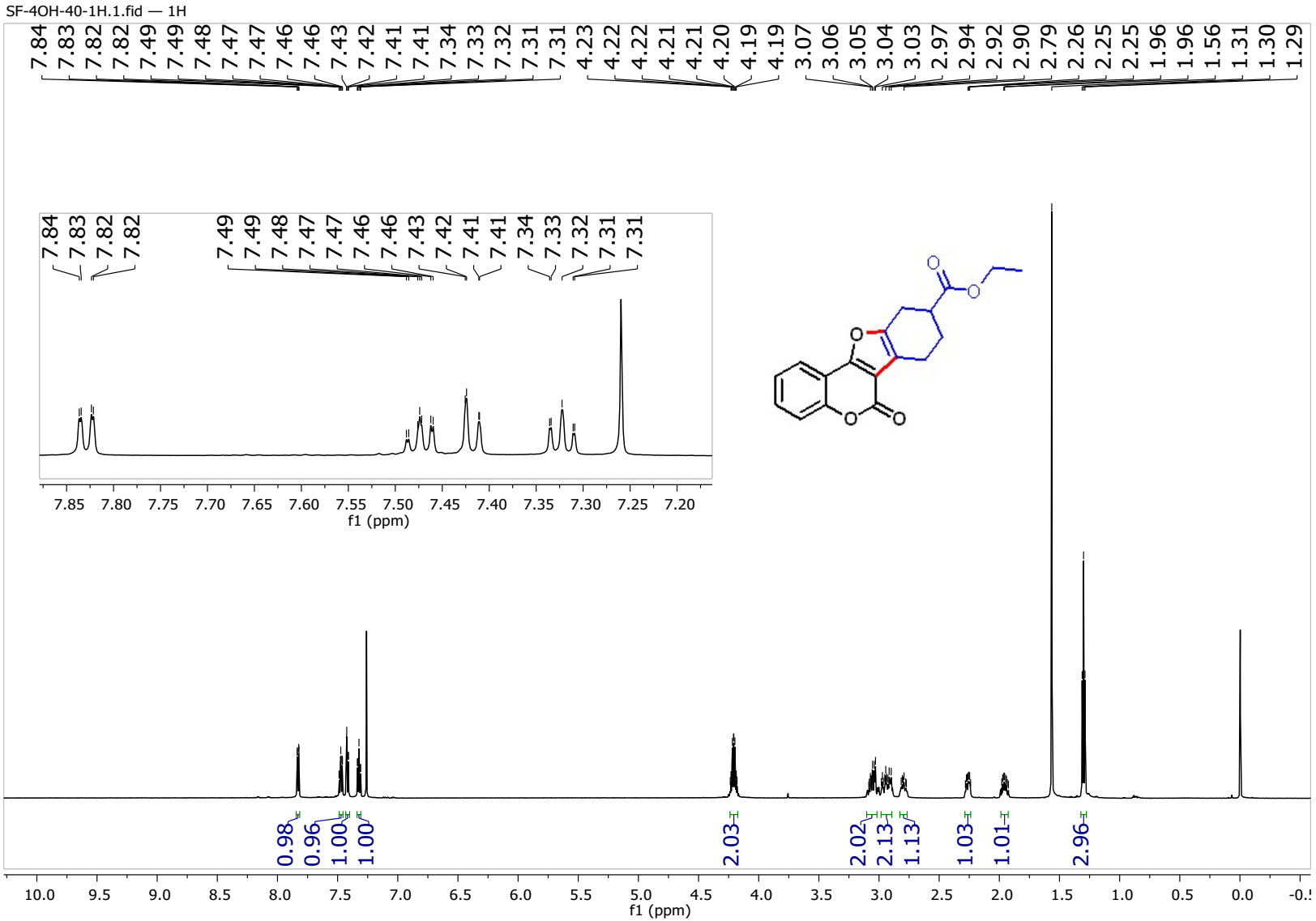
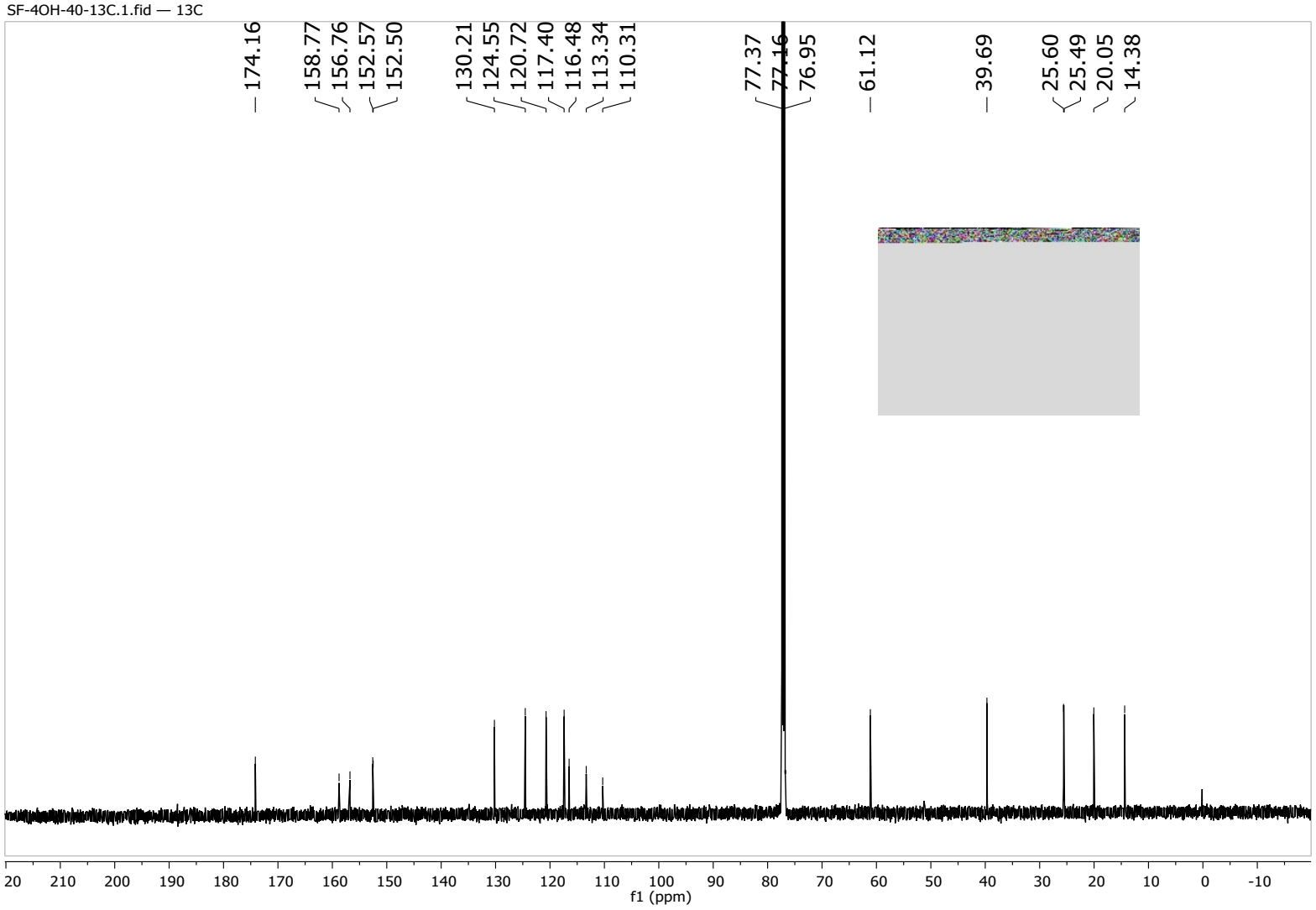


^{1}H NMR Spectrum of Ethyl 6-oxo-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromene-9-carboxylate (3g)



^{13}C NMR Spectrum of Ethyl 6-oxo-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromene-9-carboxylate (3g)



HRMS Spectrum of Ethyl 6-oxo-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromene-9-carboxylate (3g)

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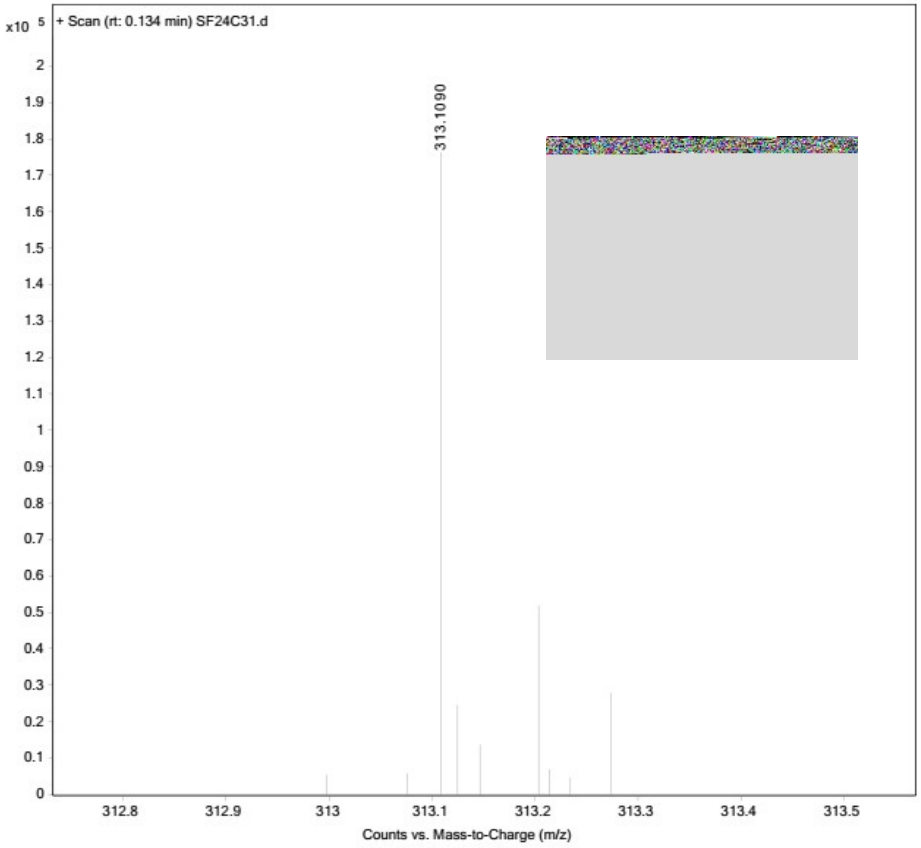
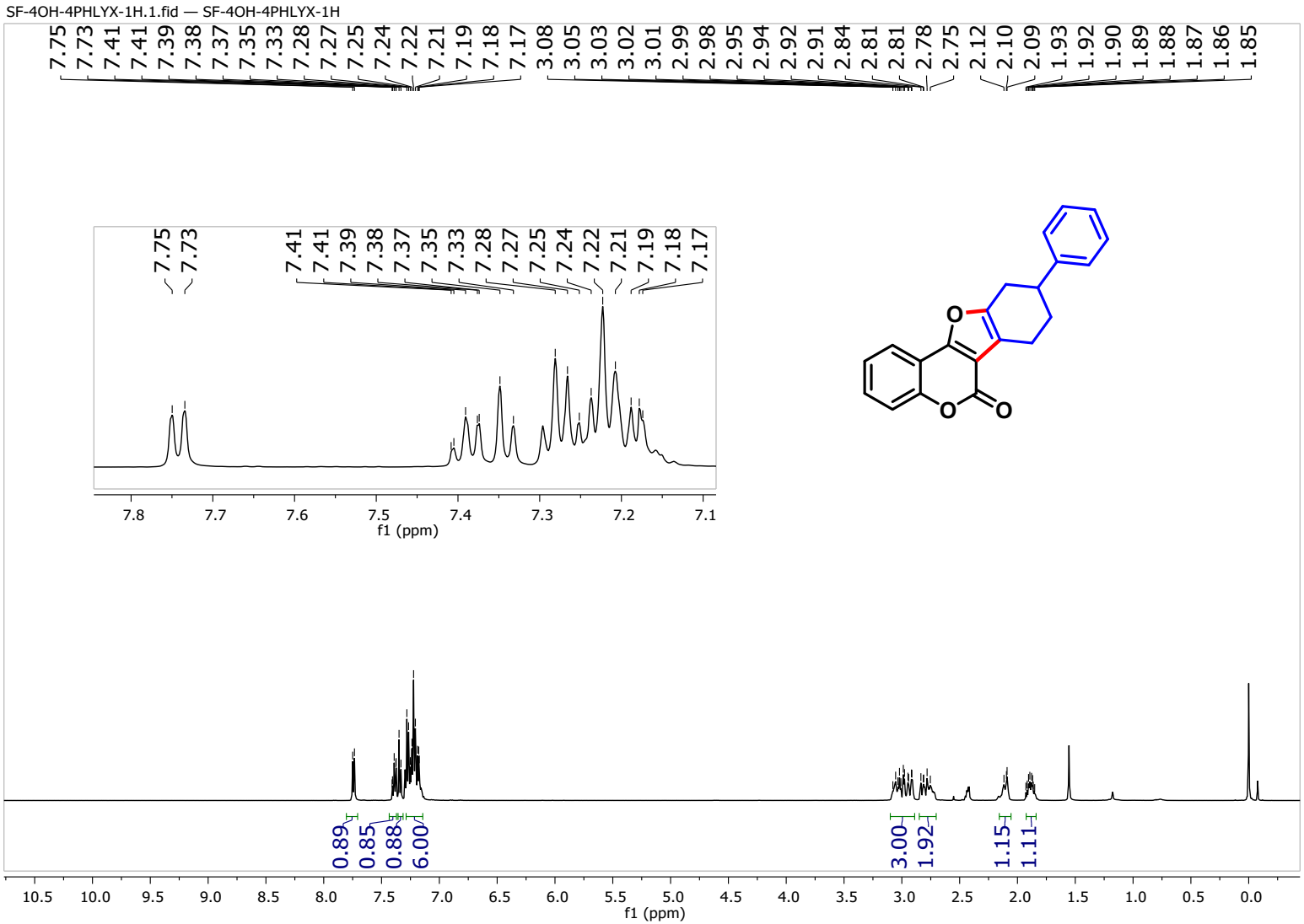
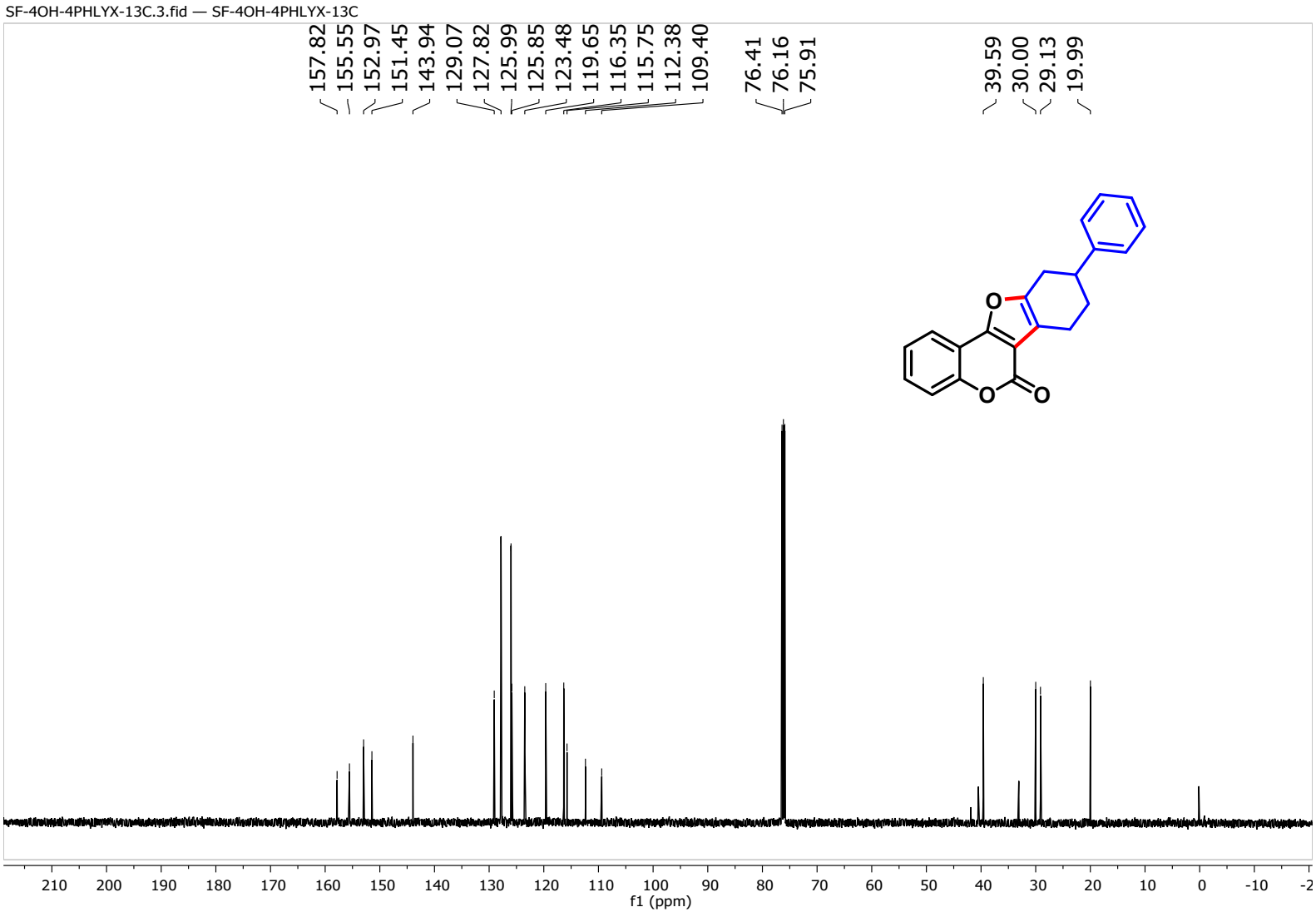


^{1}H NMR Spectrum of 9-Phenyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3h)



^{13}C NMR Spectrum of 9-Phenyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3h)



HRMS Spectrum of 9-Phenyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3h)

Sample Name	Sample9	**Position**	P1-A9	**Instrument Name**	QTOF
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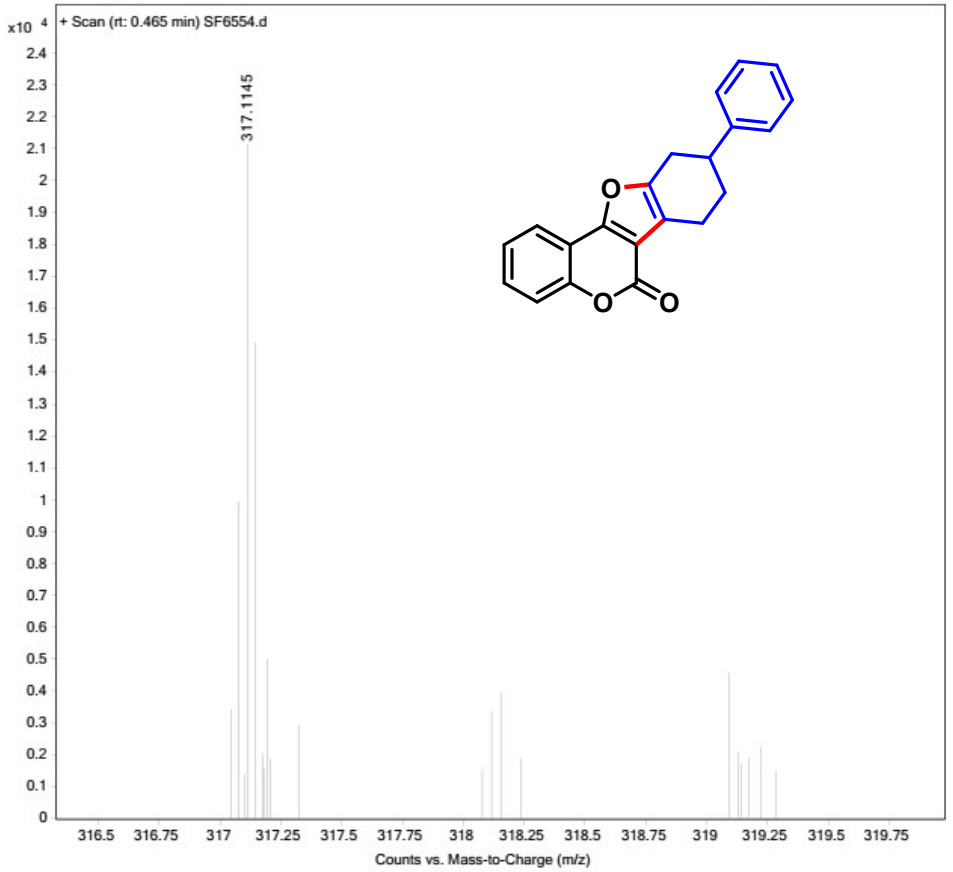
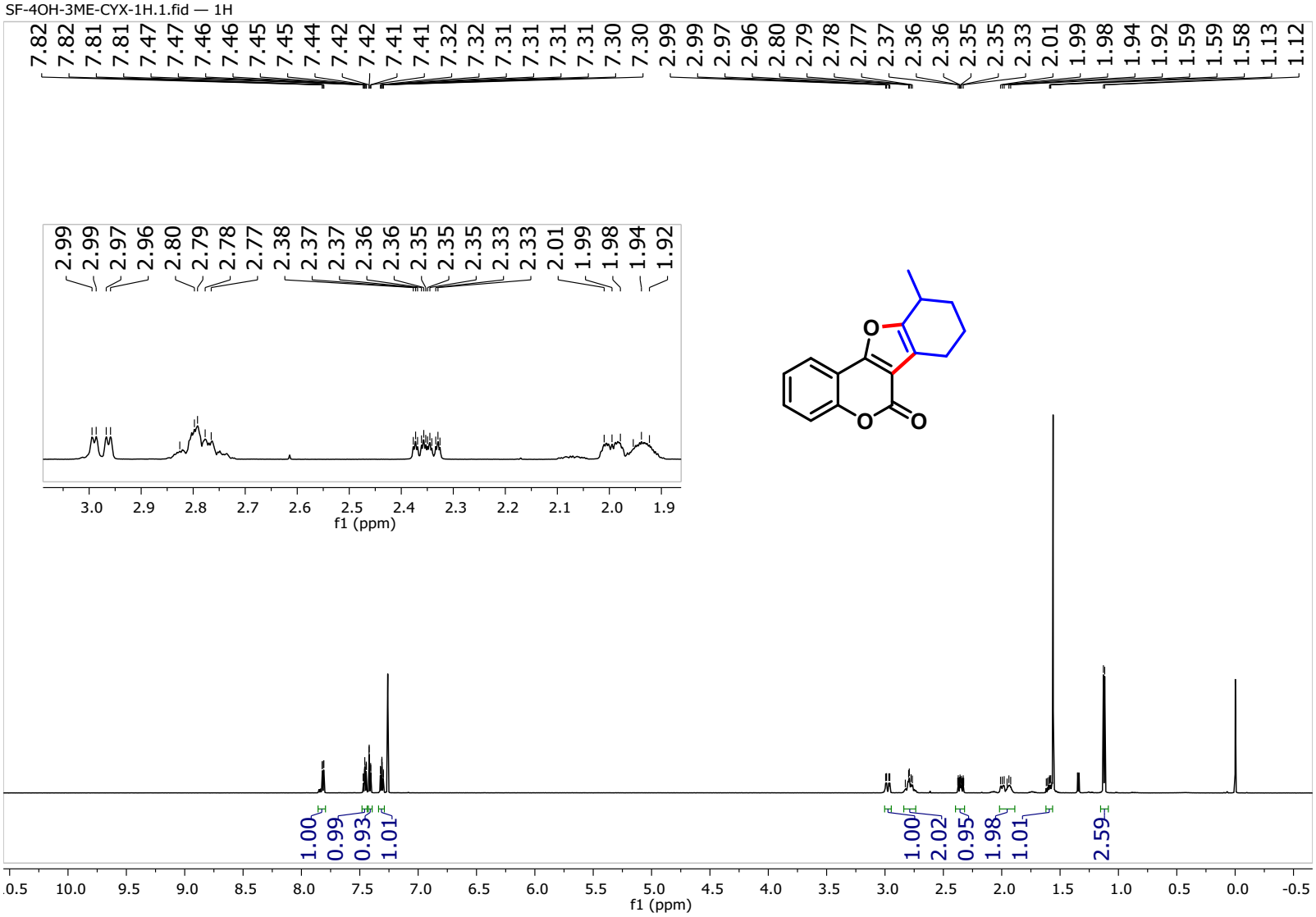
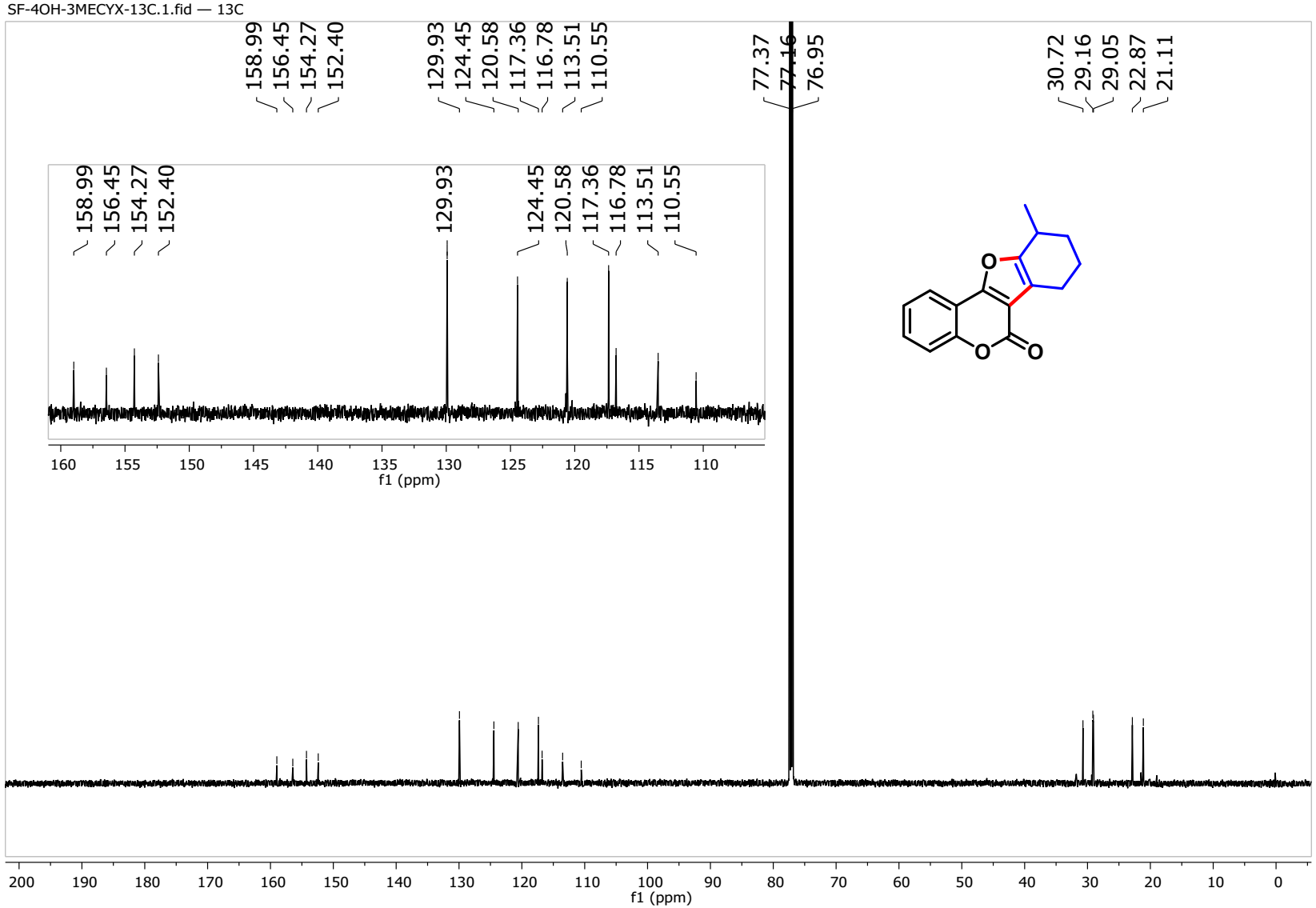


^{1}H NMR Spectrum of 10-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3i)

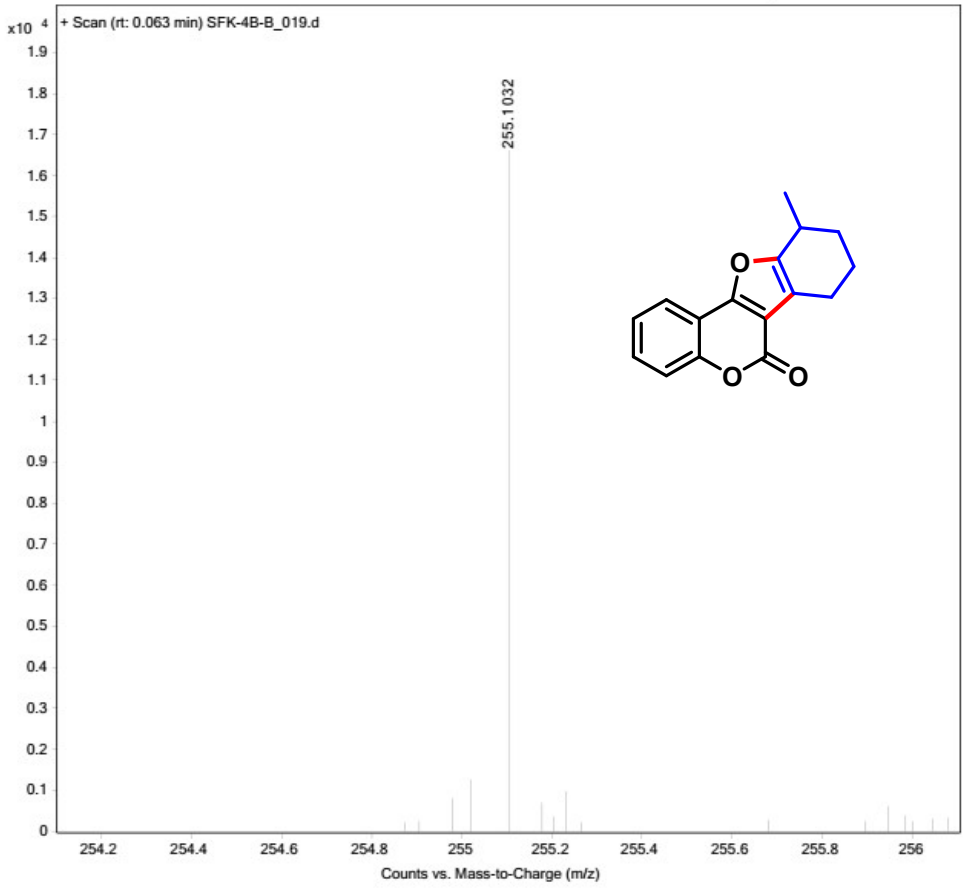


^{13}C NMR Spectrum of 10-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3i)

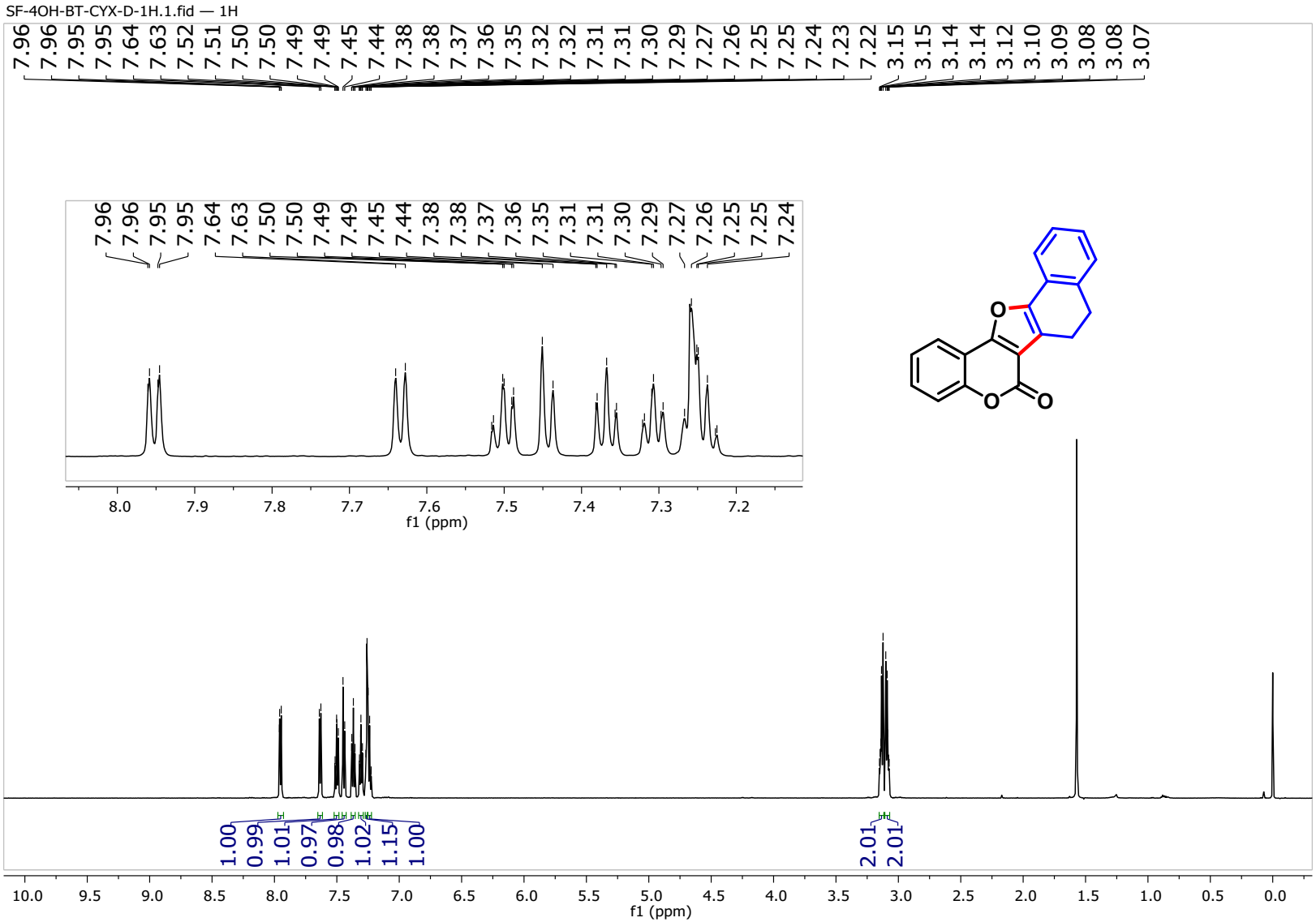


HRMS Spectrum of 10-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (3i)

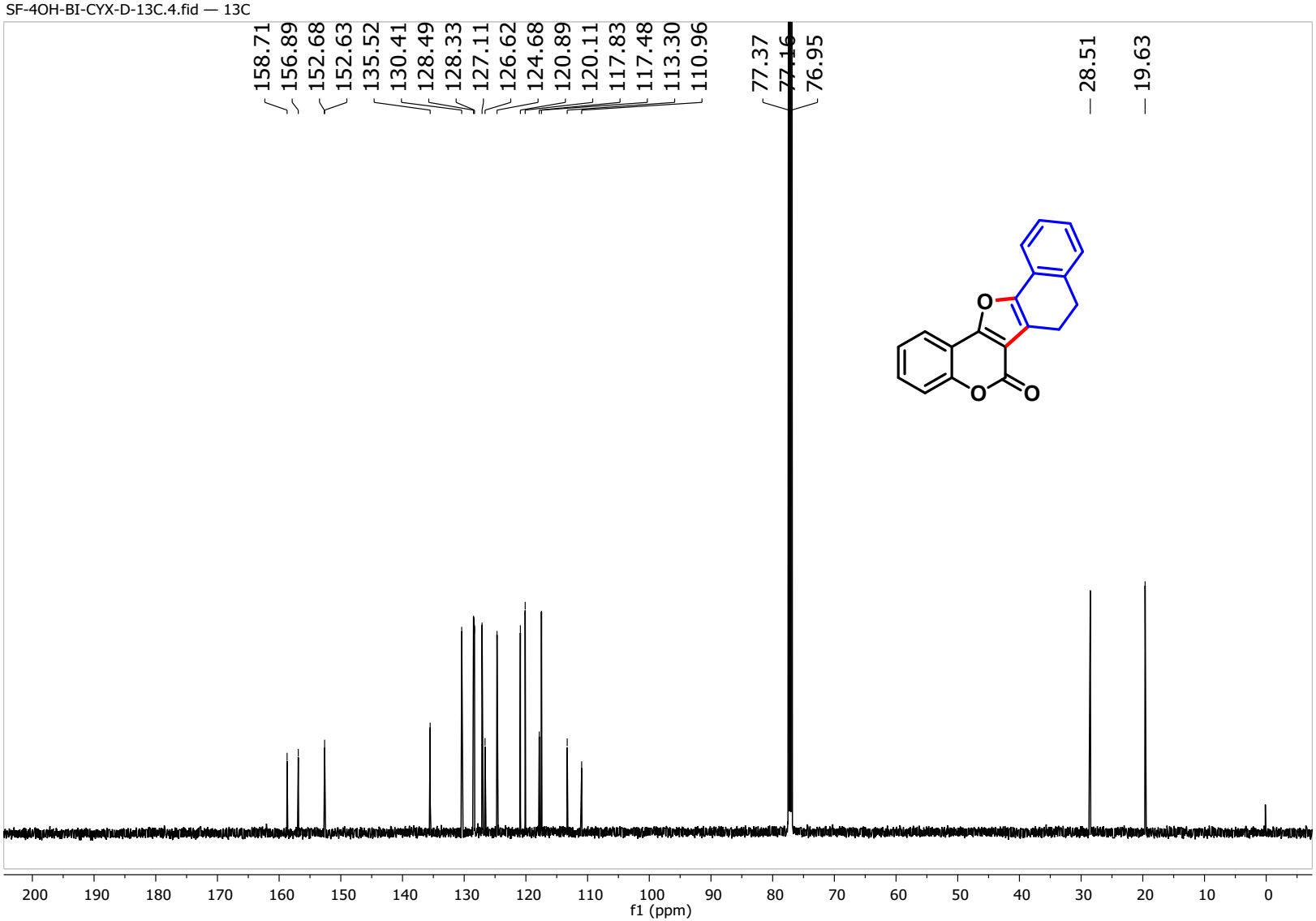
Sample Name	SFK-4B-B	**Position**	P2-D6	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFK-4B-B_019.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	16-12-2022 18:28:48 (UTC+05:30)



^{1}H NMR Spectrum of 7,8-Dihydro-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one (3j)

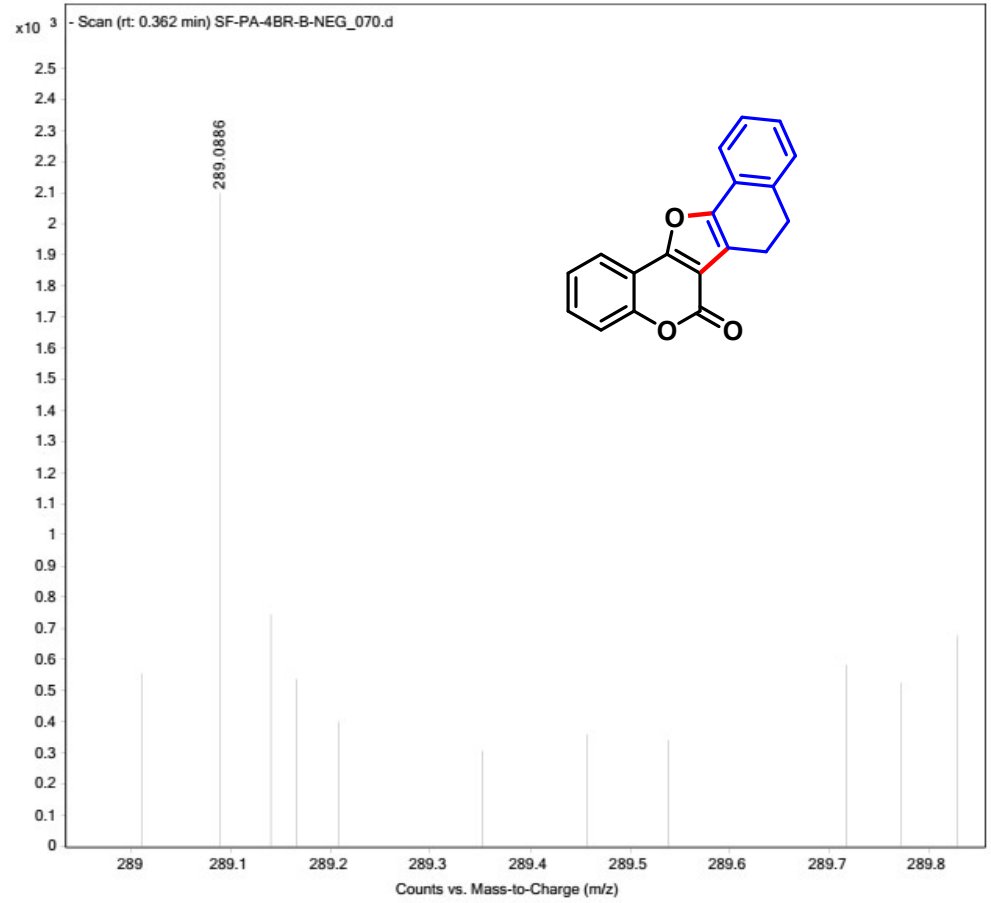


^{13}C NMR Spectrum of 7,8-Dihydro-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one (3j)

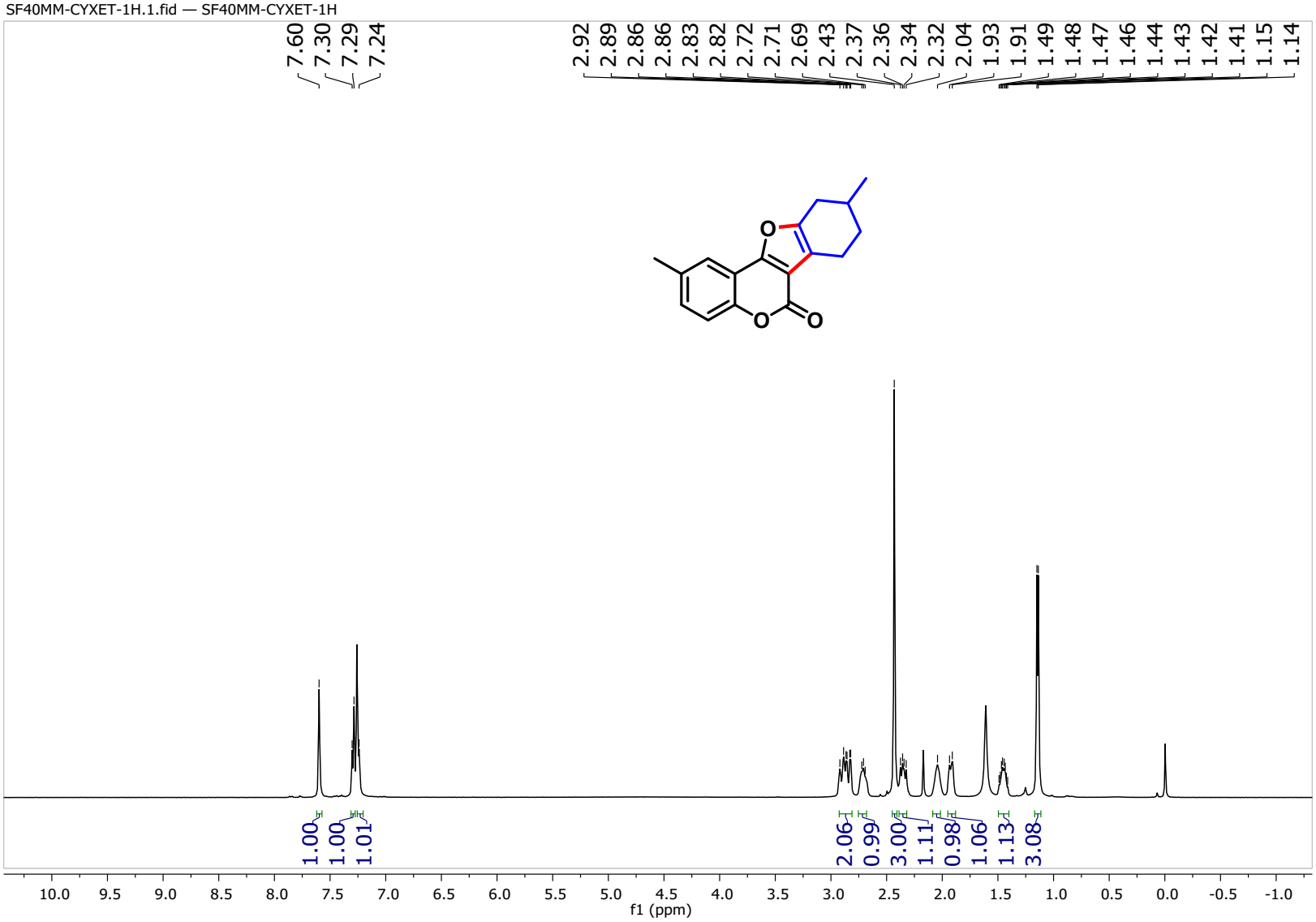


HRMS Spectrum of 7,8-Dihydro-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one (3j)

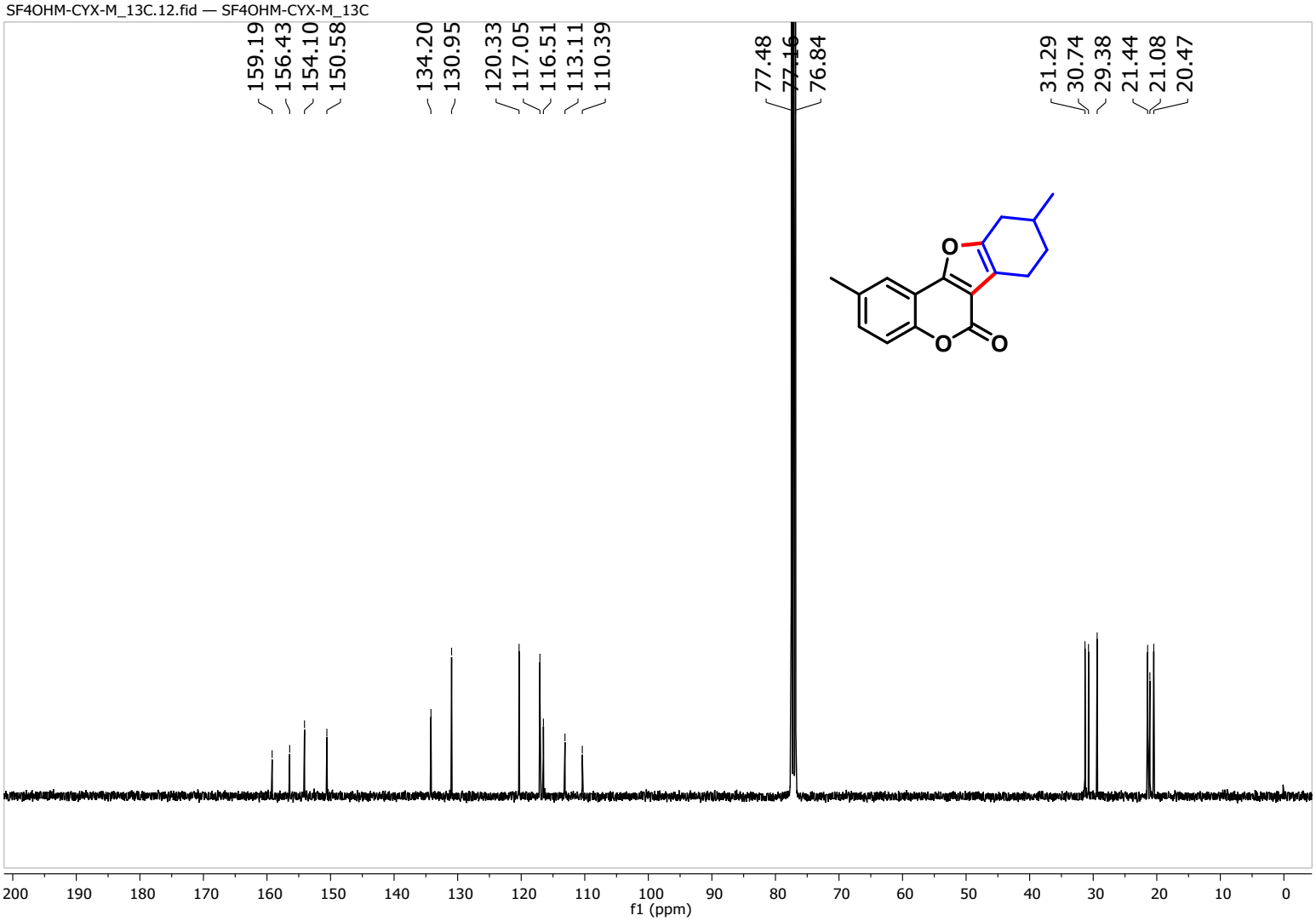
Sample Name	SF-PA-4BR-B-NEG	**Position**	P1-E5	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-PA-4BR-B-NEG_070.d
ACQ Method	FULL SCAN-NEG.m	**Comment**		**Acquired Time**	27-01-2023 20:03:19 (UTC+05:30)



^{1}H NMR Spectrum of 2,9-Dimethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4a)

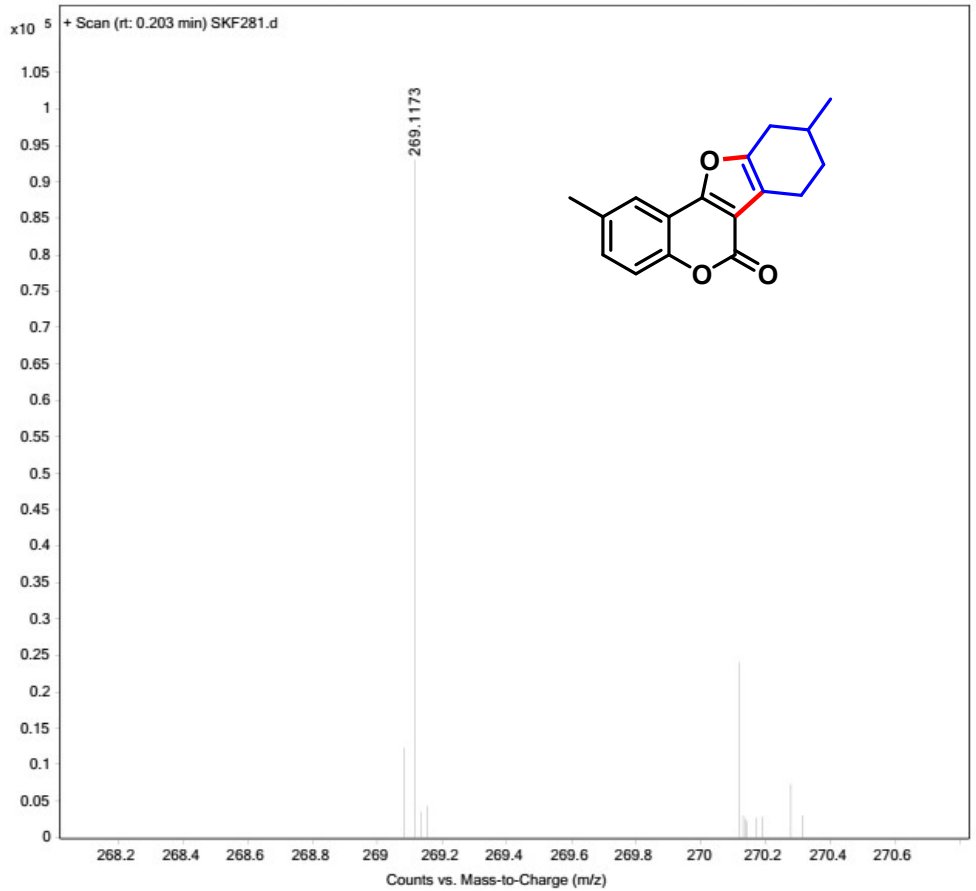


^{13}C NMR Spectrum of 2,9-Dimethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4a)

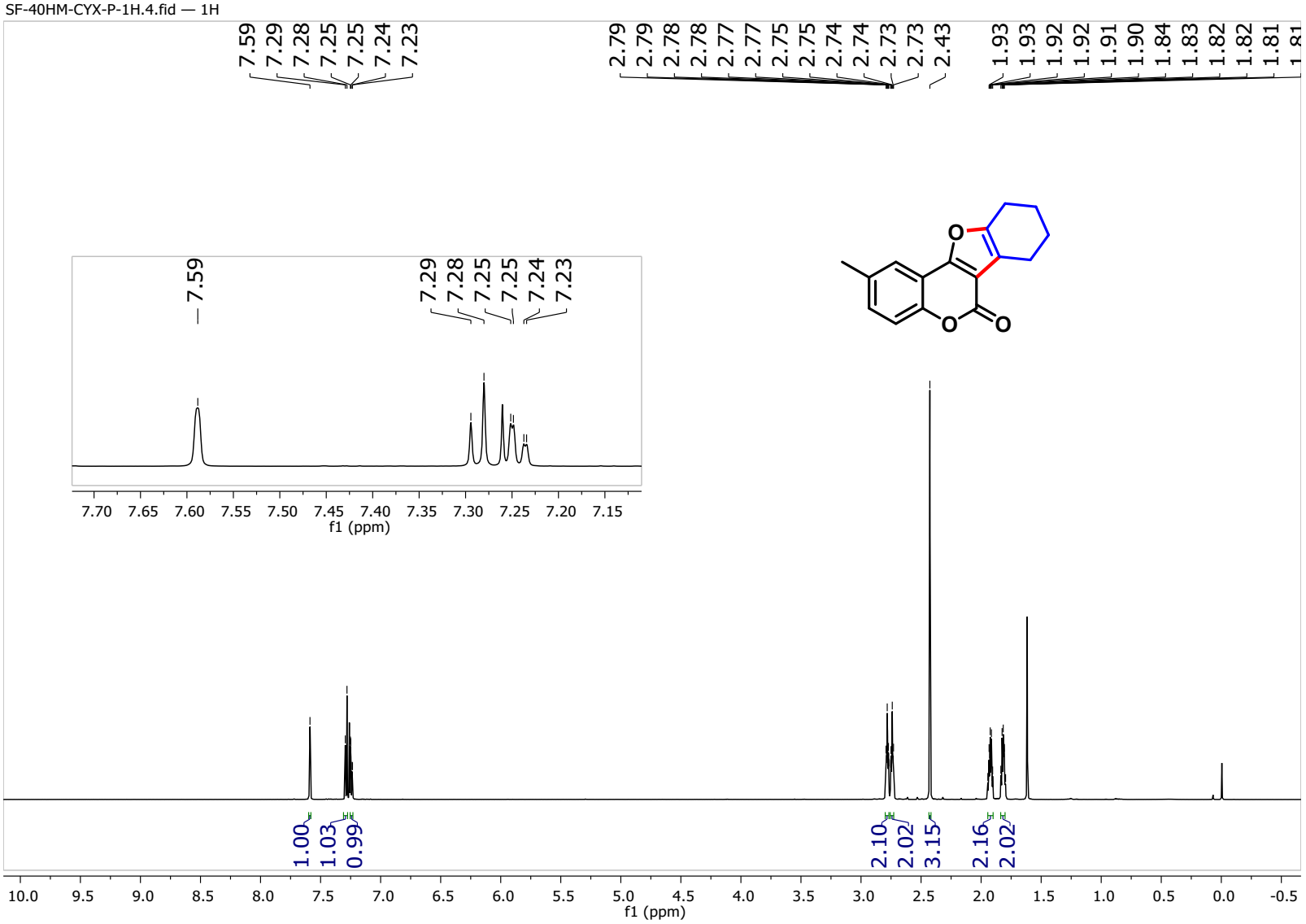


HRMS Spectrum of 2,9-Dimethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4a)

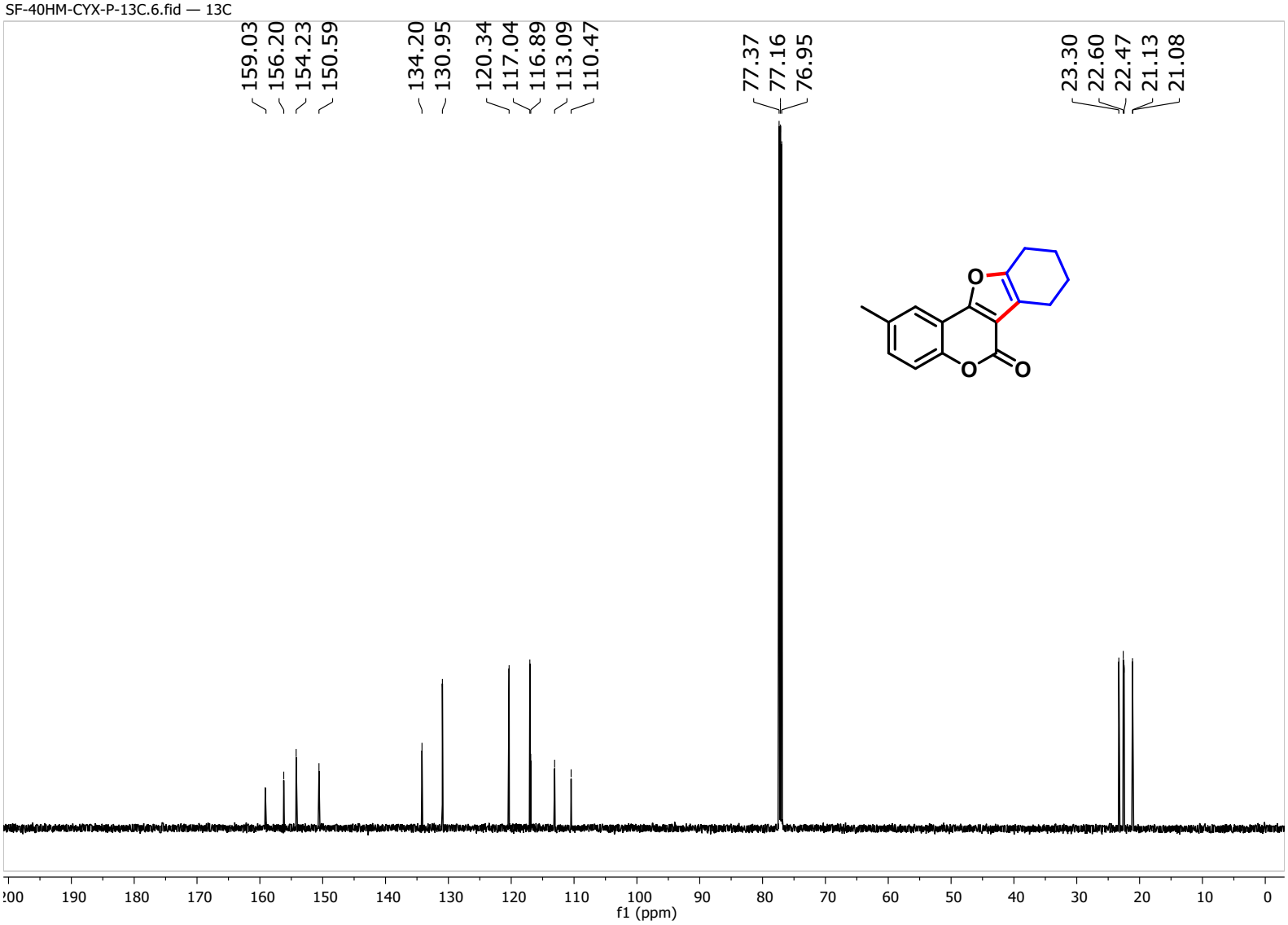
Sample Name	Sample23	**Position**	P1-C1	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SKF281.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	30-06-2023 10:41:59 (UTC+05:30)



^{1}H NMR Spectrum of 2-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4b)

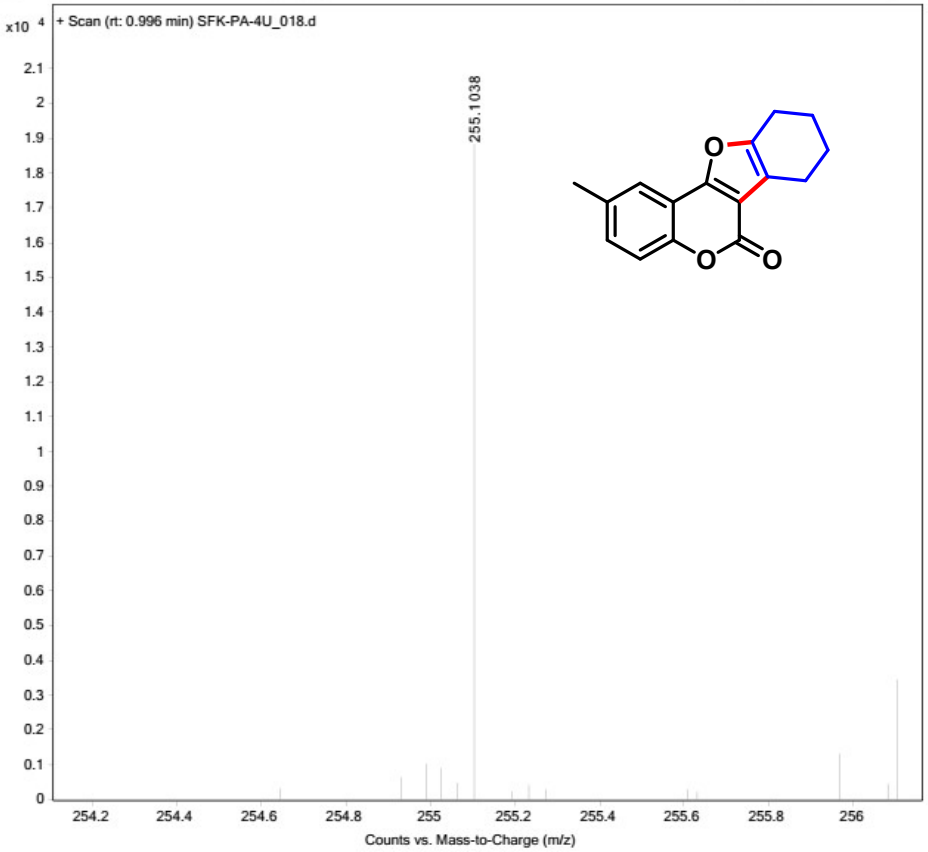


^{13}C NMR Spectrum of 2-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4b)

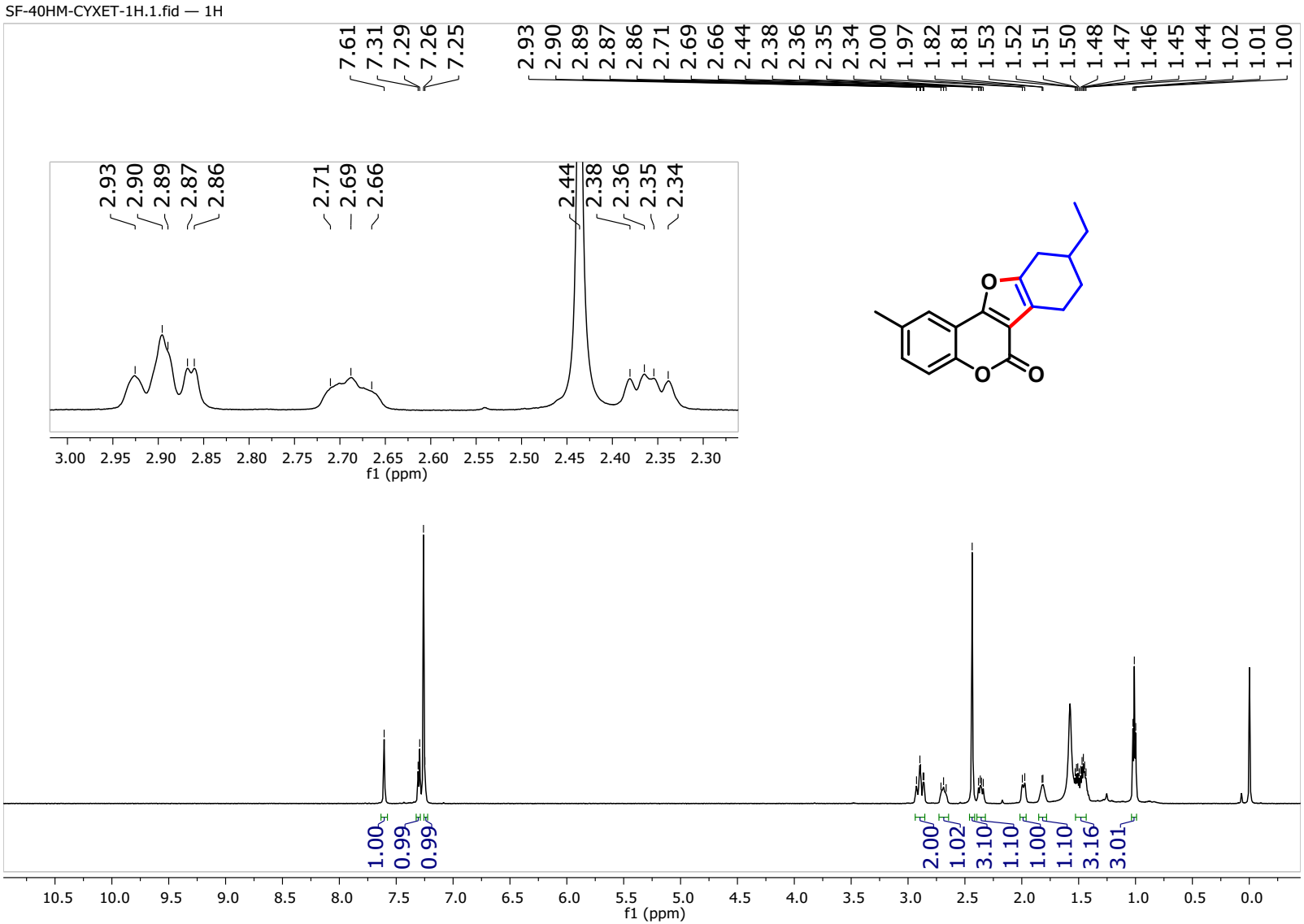


HRMS Spectrum of 2-Methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4b)

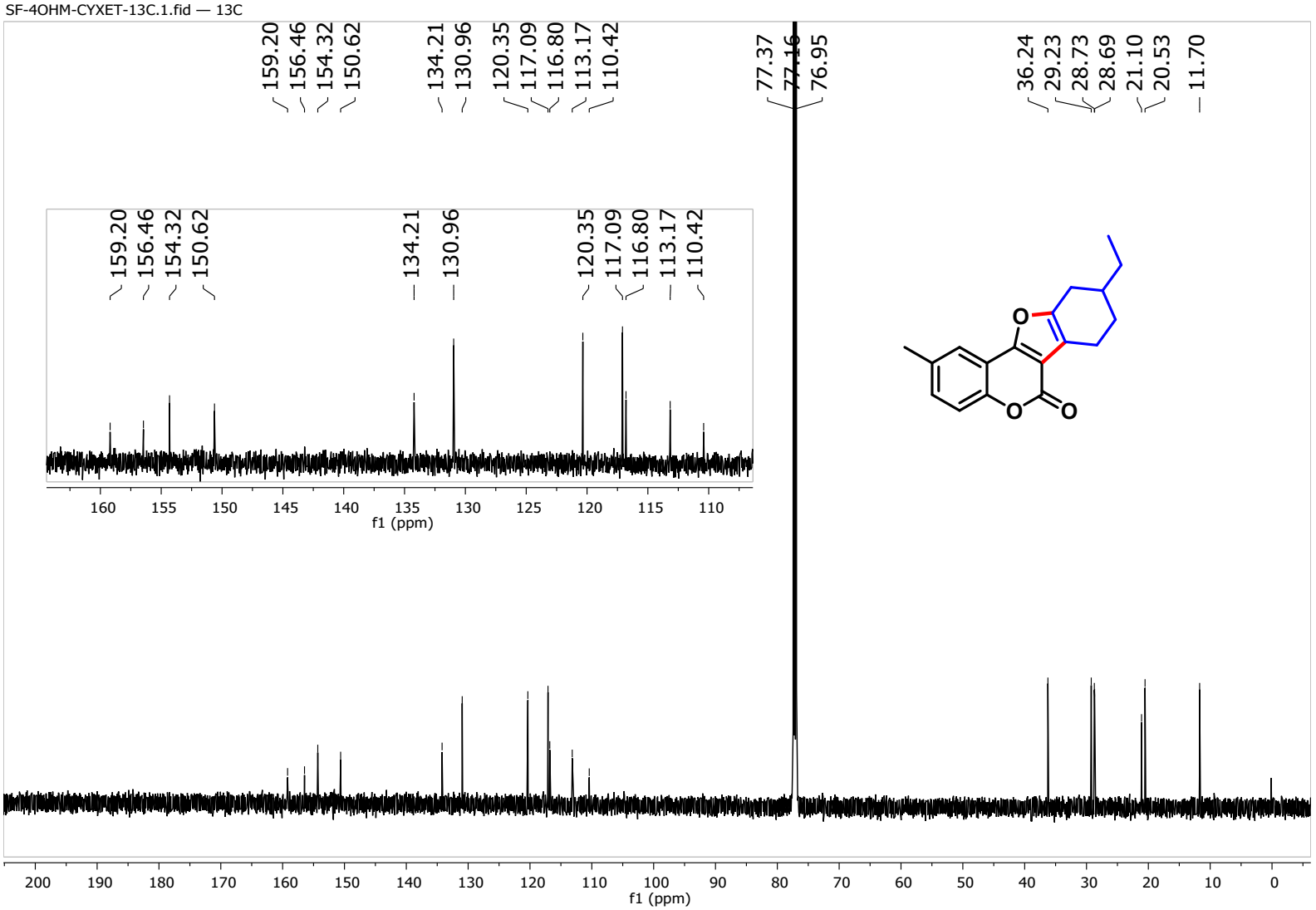
Sample Name	SFK-PA-4U	**Position**	P2-D5	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFK-PA-4U_018.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	16-12-2022 18:27:12 (UTC+05:30)



^{1}H NMR Spectrum of 9-Ethyl-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4c)

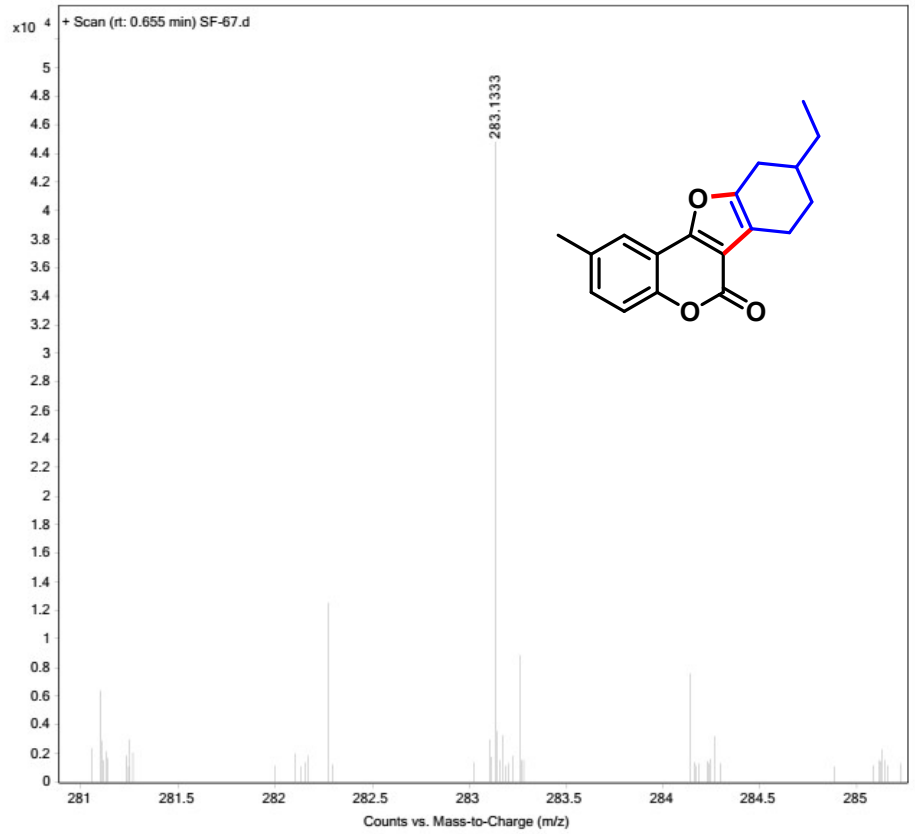


^{13}C NMR Spectrum of 9-Ethyl-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4c)

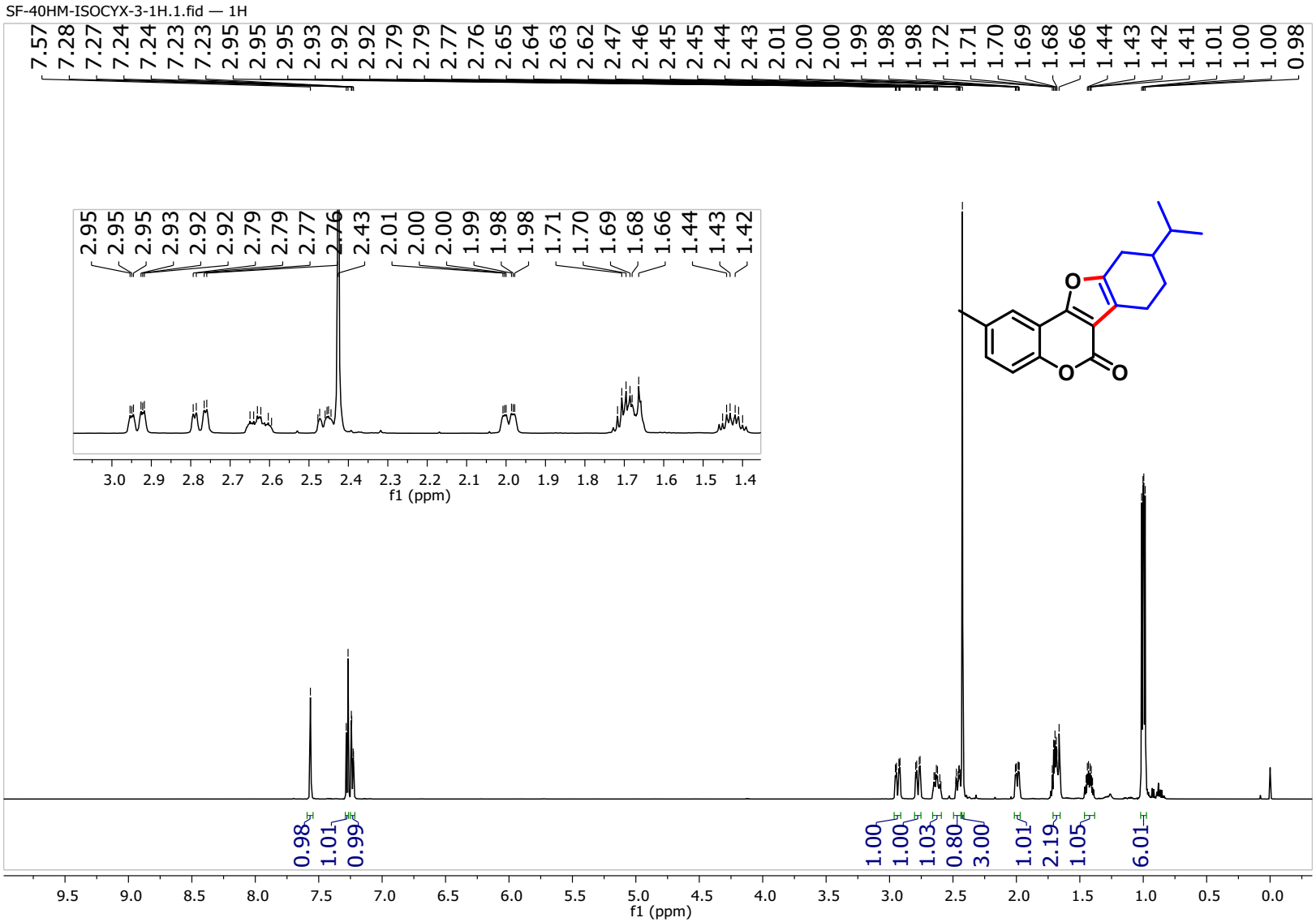


HRMS Spectrum of 9-Ethyl-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4c)

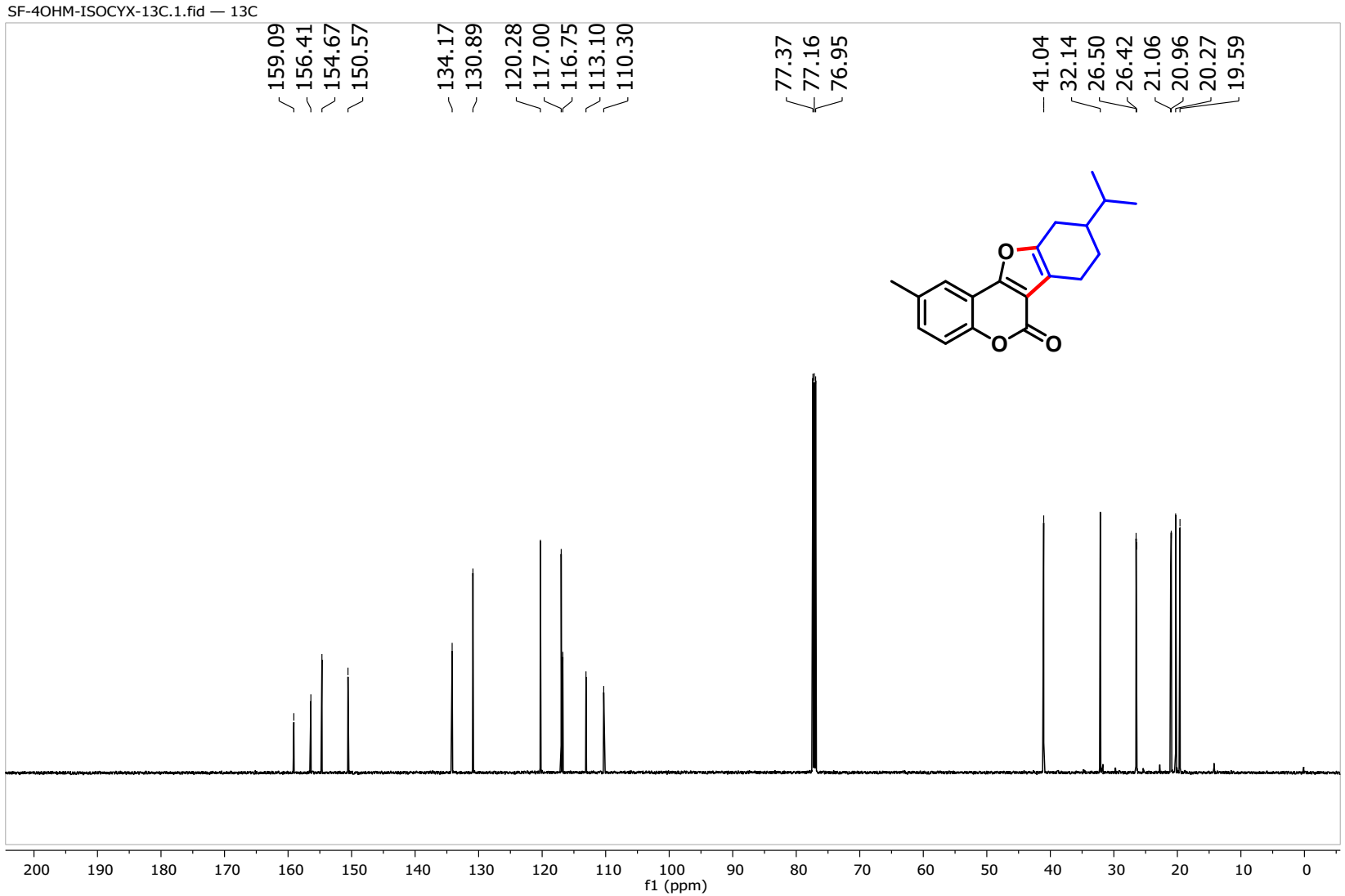
Sample Name	Sample28	**Position**	P1-C6	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-67.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	05-06-2023 18:18:06 (UTC+05:30)



^{1}H NMR Spectrum of 9-Isopropyl-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4d)

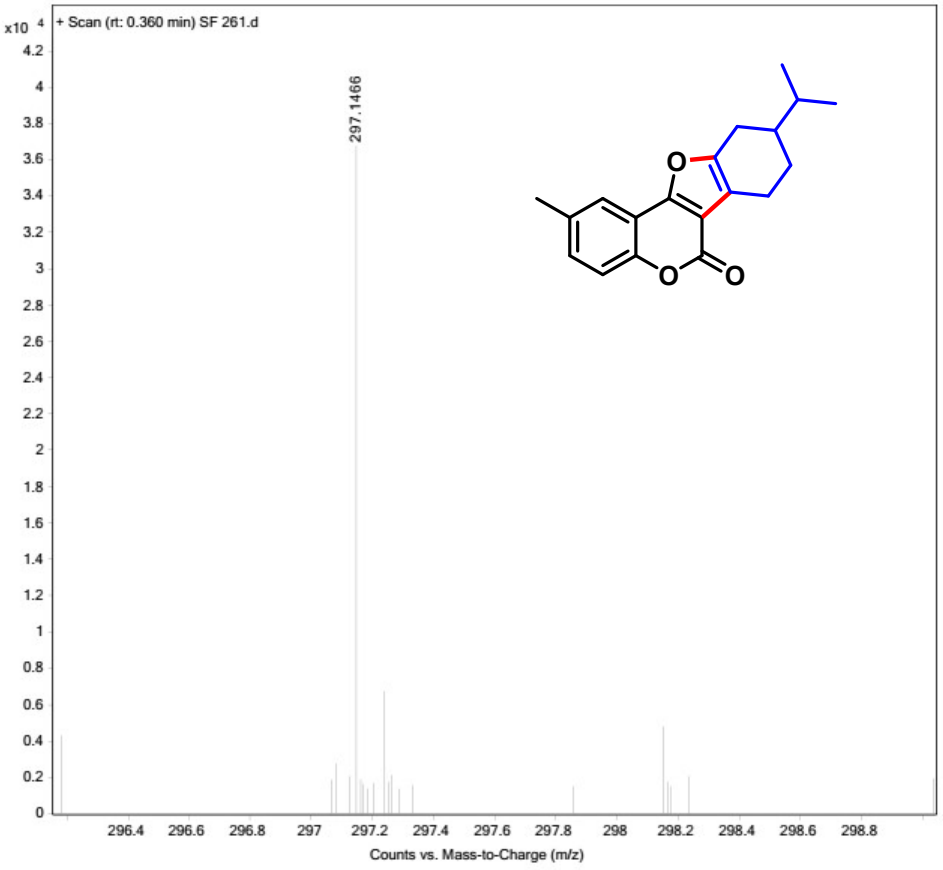


^{13}C NMR Spectrum of 9-Isopropyl-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4d)

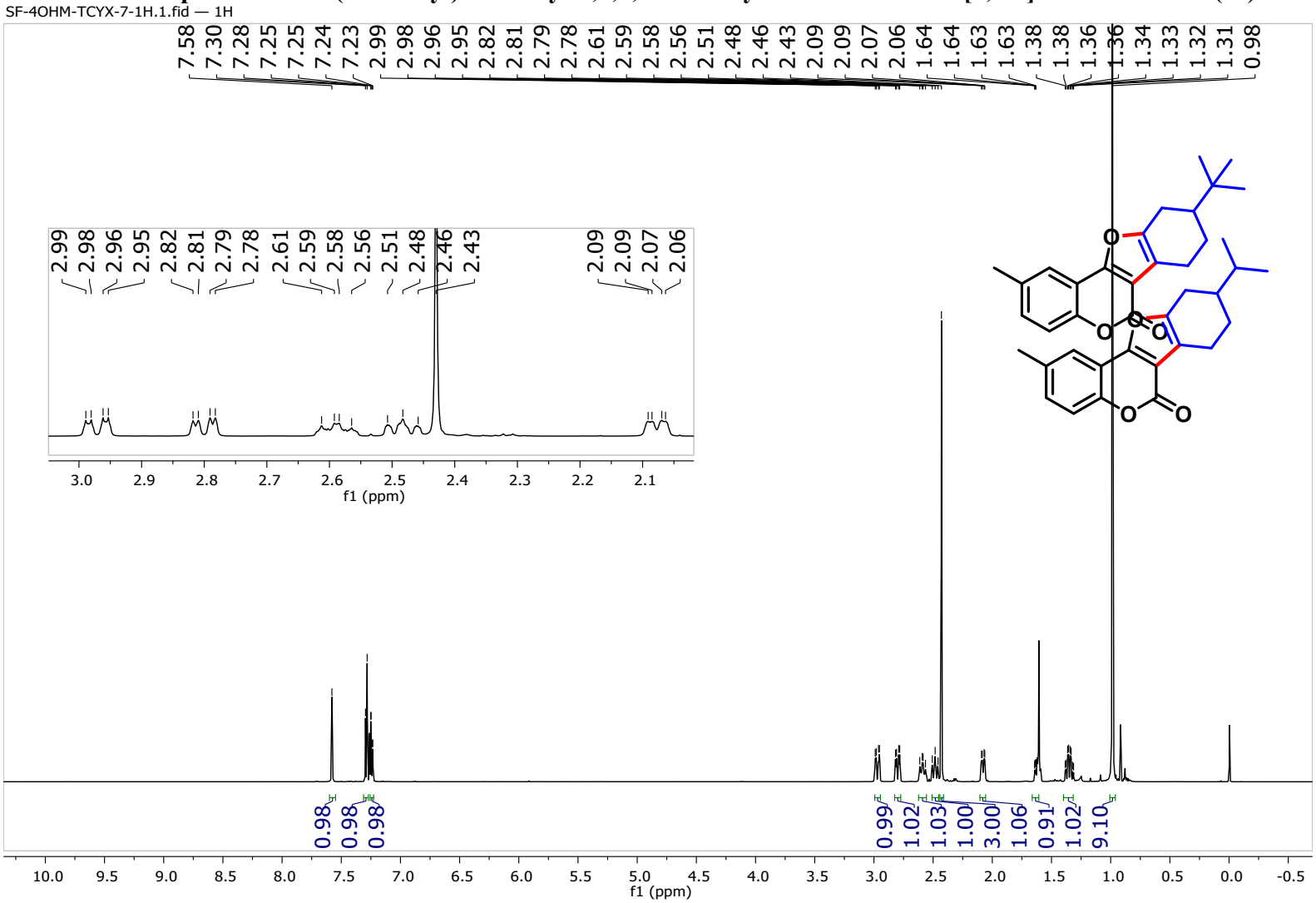


HRMS Spectrum of 9-Isopropyl-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4d)

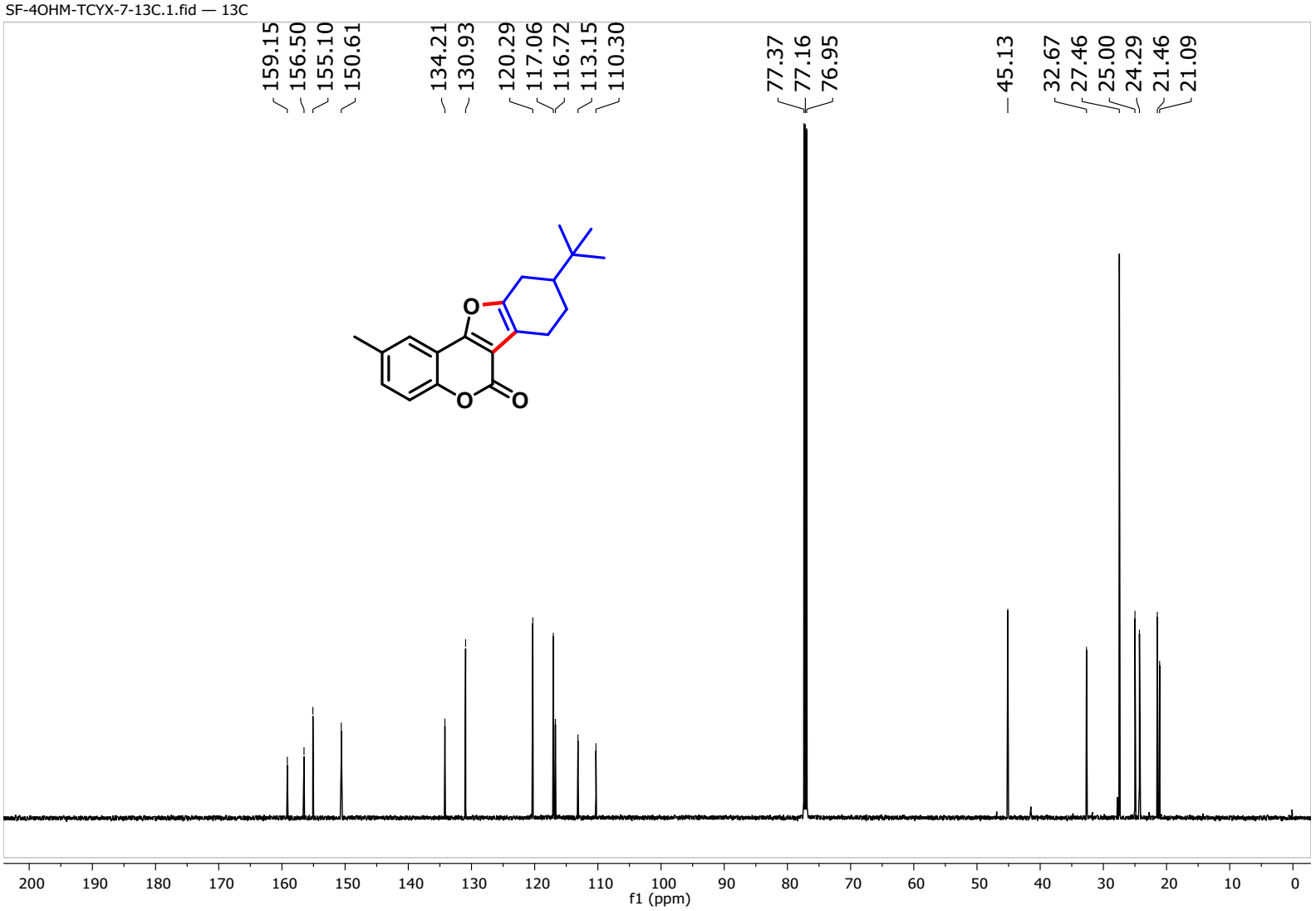
Sample Name	Sample22	**Position**	P1-B11	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF 261.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	19-06-2023 10:48:56 (UTC+05:30)



^{1}H NMR Spectrum of 9-(*tert*-Butyl)-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4e)

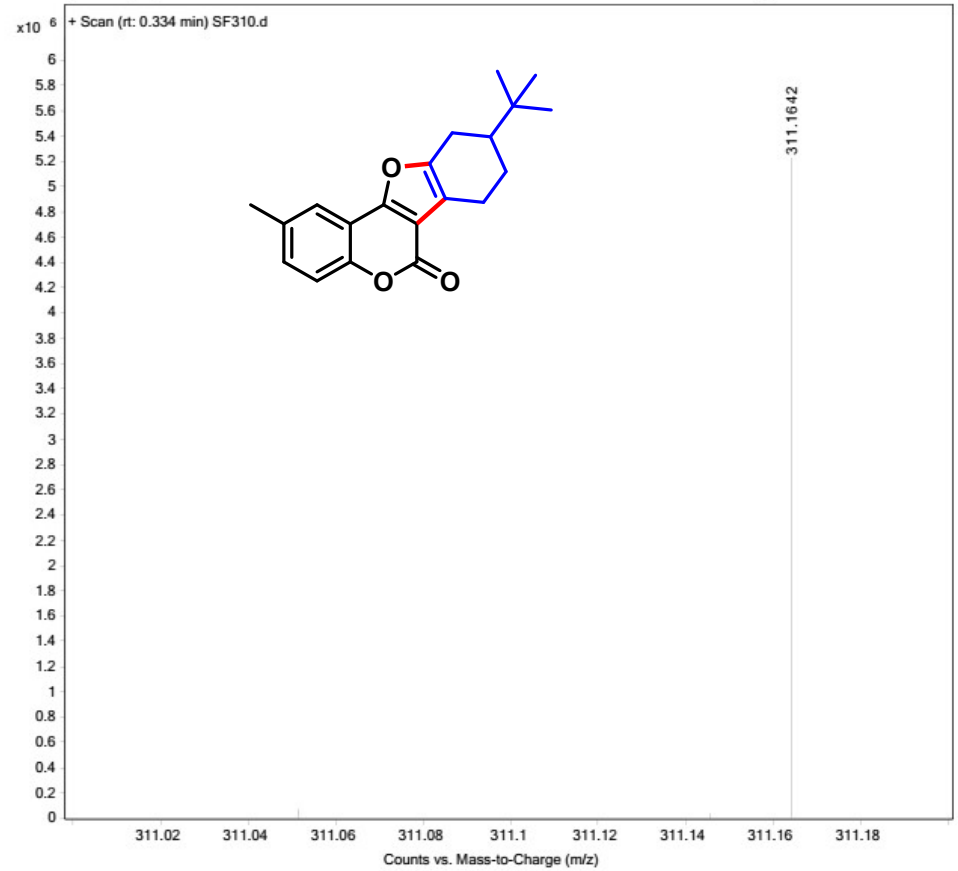


^{13}C NMR Spectrum of 9-(*tert*-Butyl)-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4e)

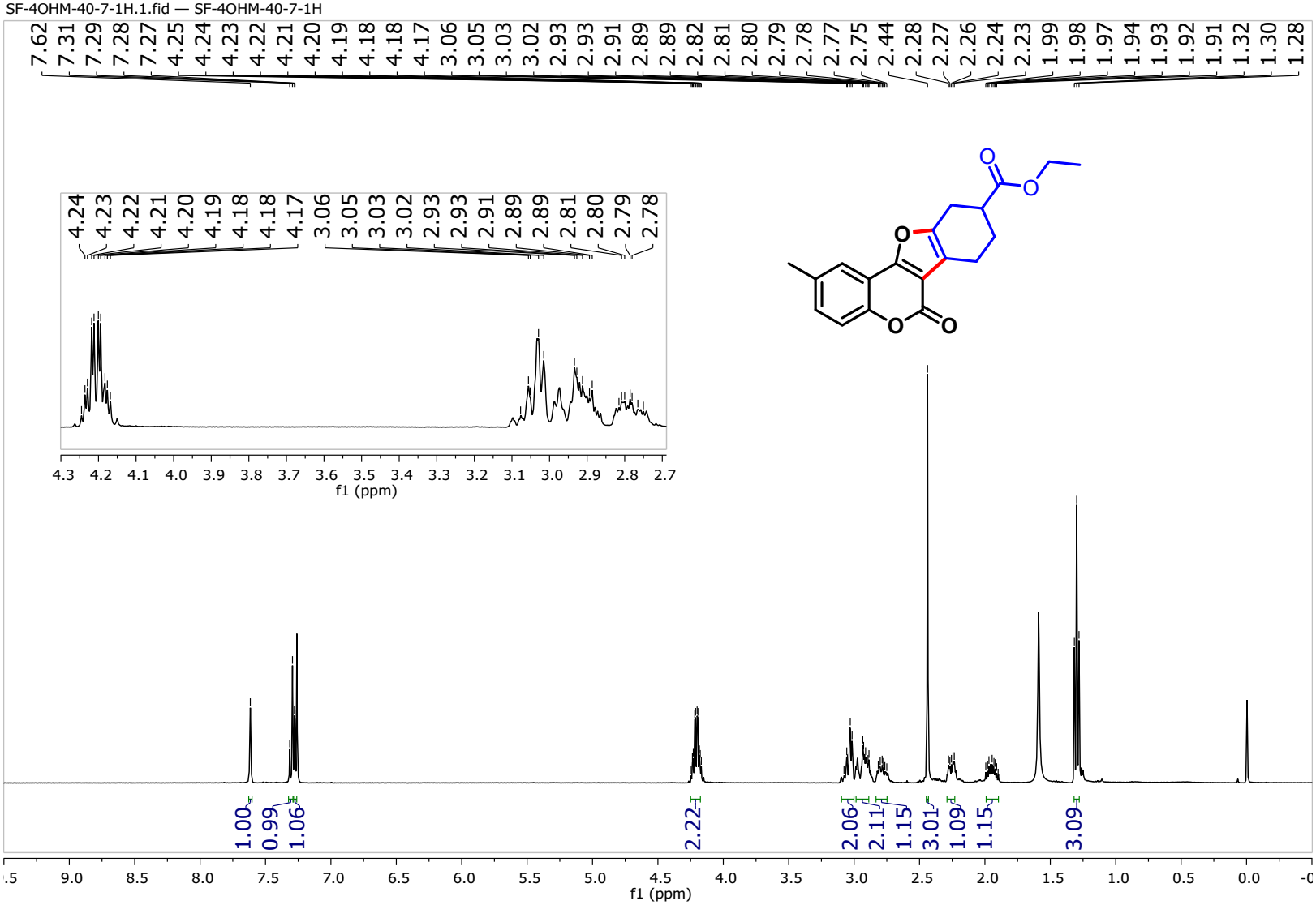


HRMS Spectrum of 9-(*tert*-Butyl)-2-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4e)

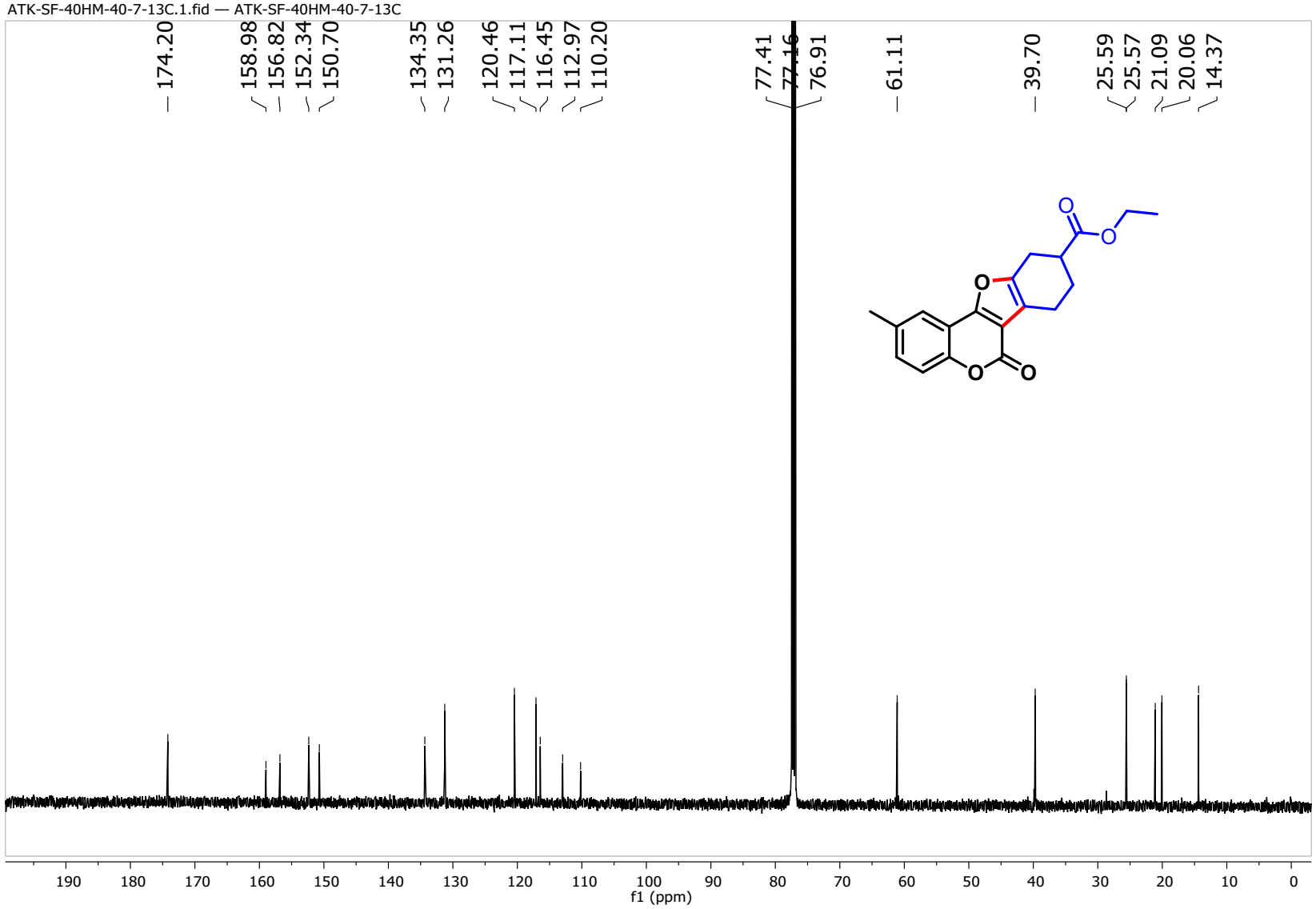
Sample Name	Sample58	**Position**	P1-A10	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF310.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	27-04-2023 15:26:09 (UTC+05:30)



^{1}H NMR Spectrum of Ethyl 2-methyl-6-oxo-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromene-9-carboxylate (4f)

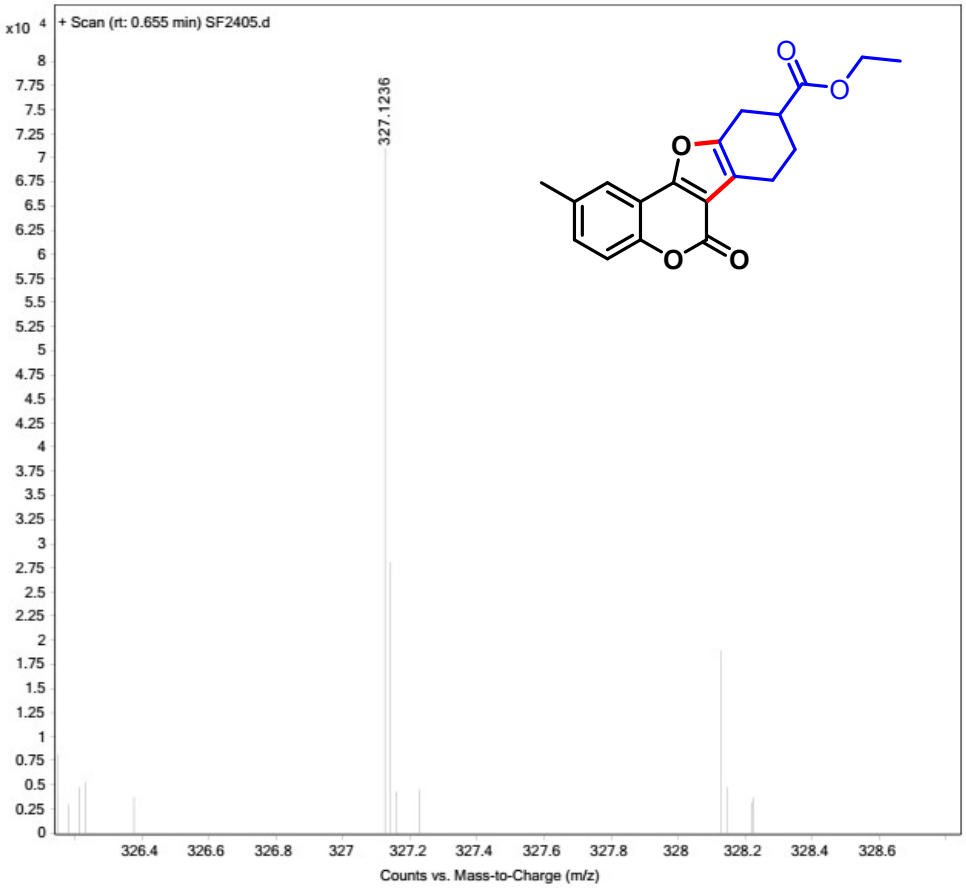


^{13}C NMR Spectrum of Ethyl 2-methyl-6-oxo-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromene-9-carboxylate (4f)

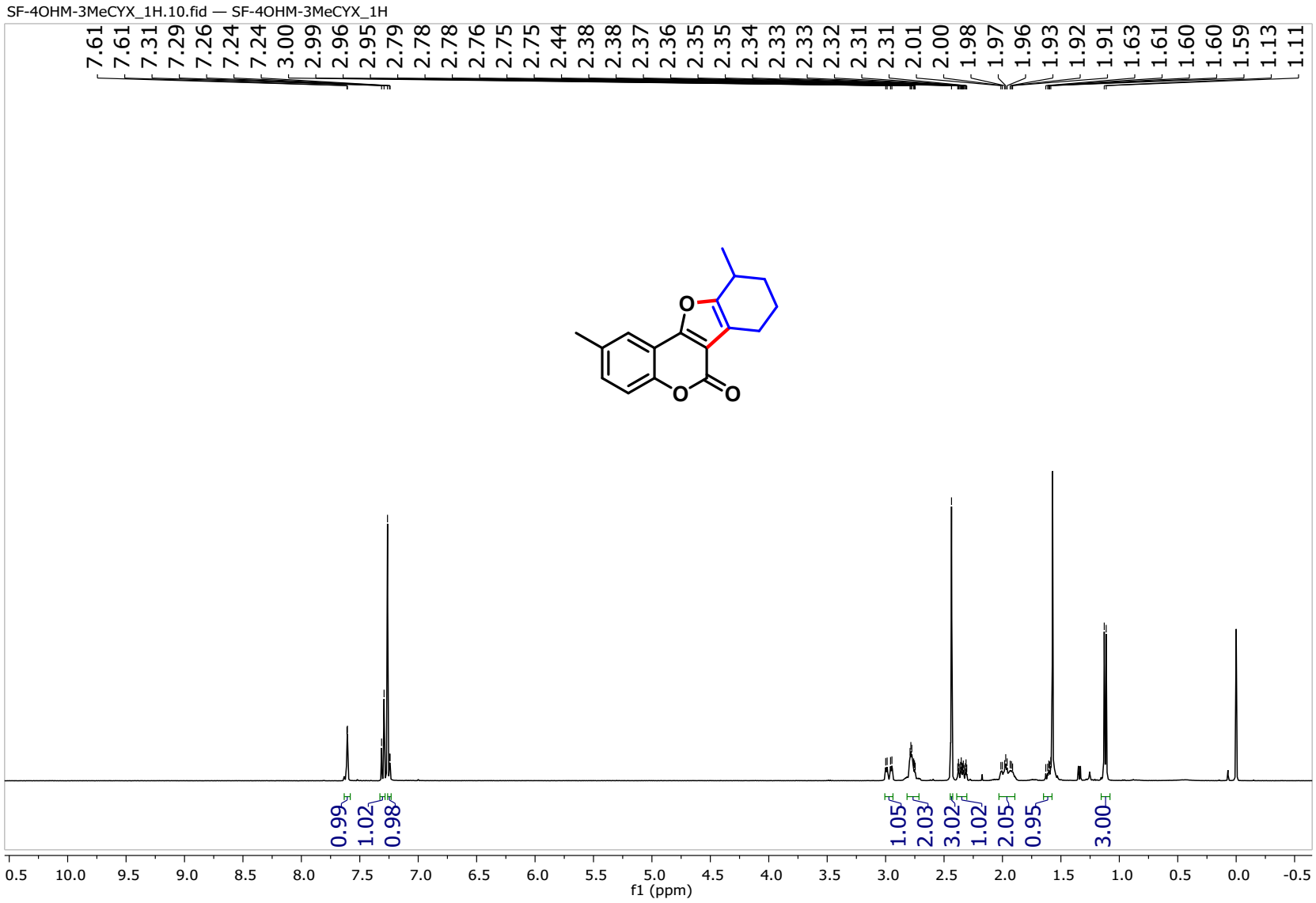


HRMS Spectrum of Ethyl 2-methyl-6-oxo-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromene-9-carboxylate (4f)

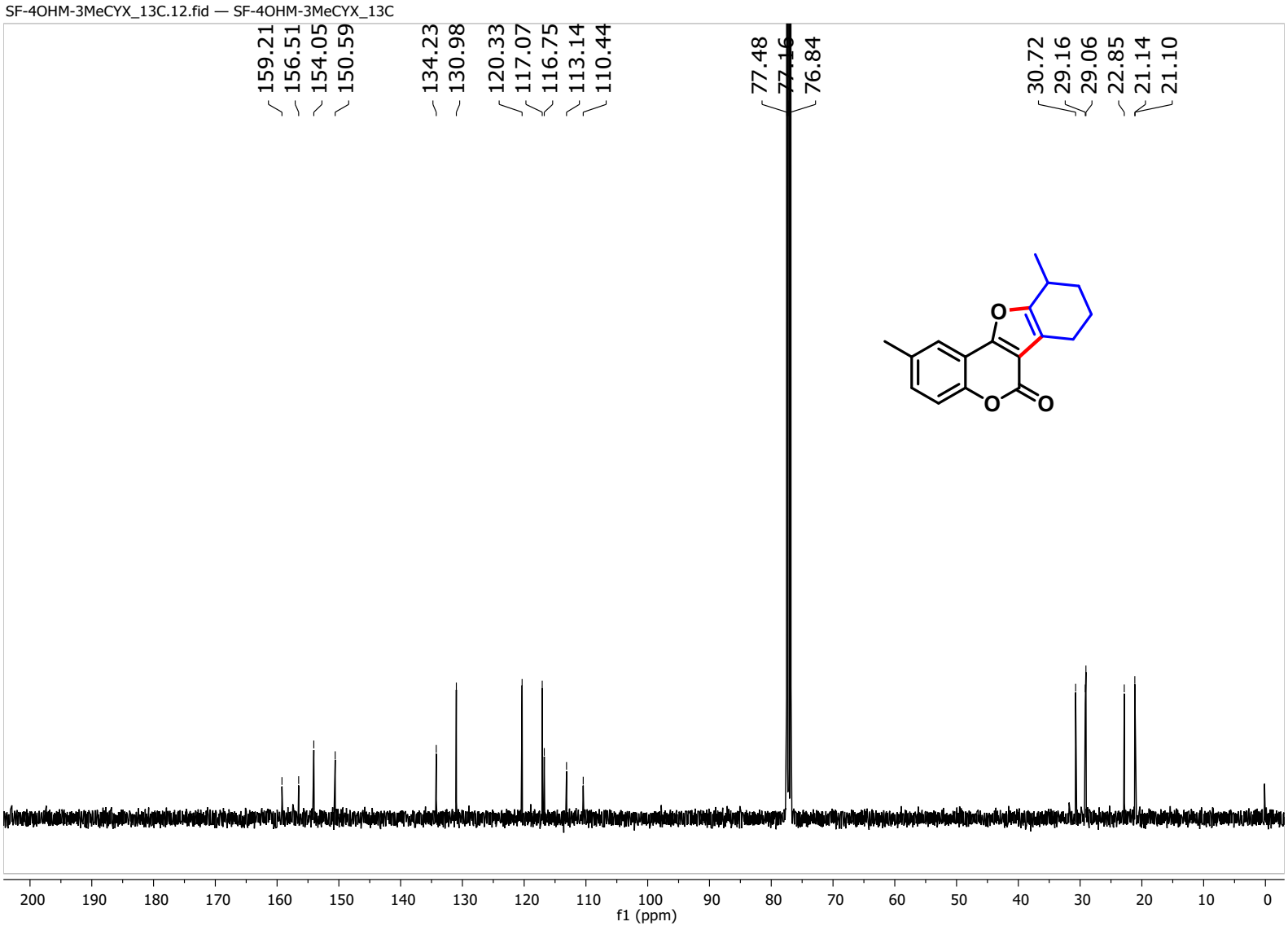
Sample Name	Sample1	**Position**	P1-A1	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF2405.d
ACQ Method	DIRECT MASS_POSITIVE_01.m	**Comment**		**Acquired Time**	17-04-2023 11:47:08 (UTC+05:30)



^{1}H NMR Spectrum of 2,10-Dimethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4g)

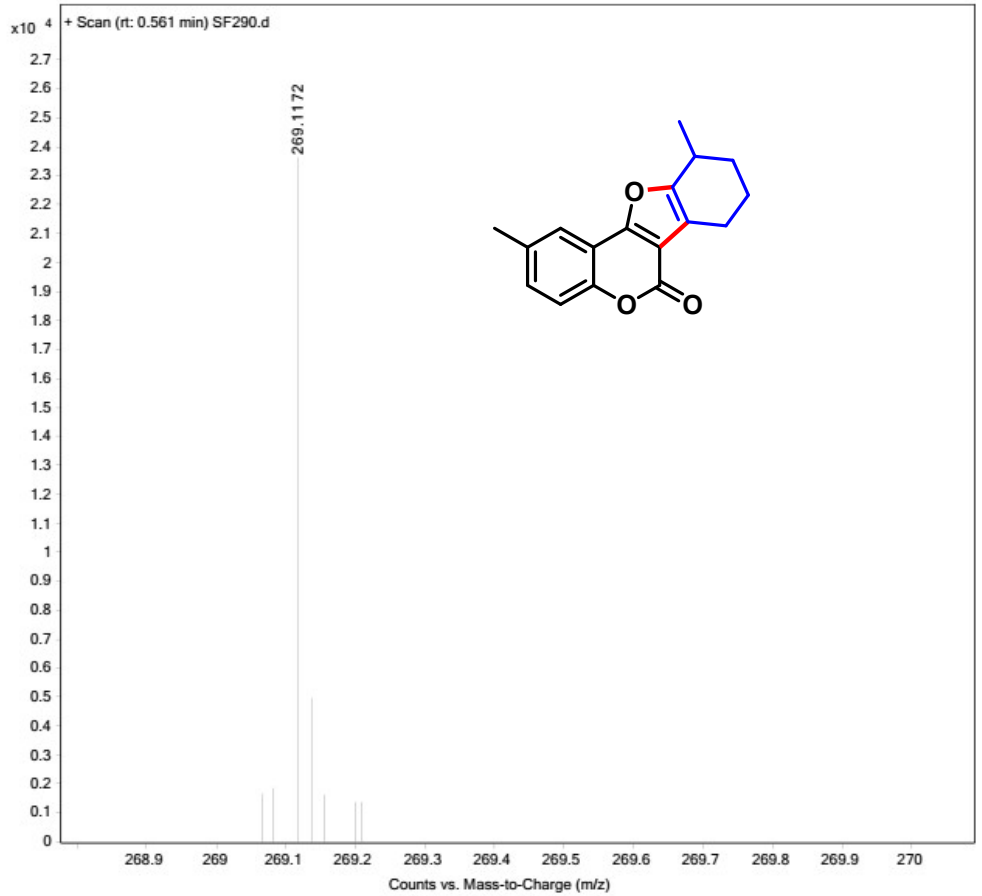


^{13}C NMR Spectrum of 2,10-Dimethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4g)

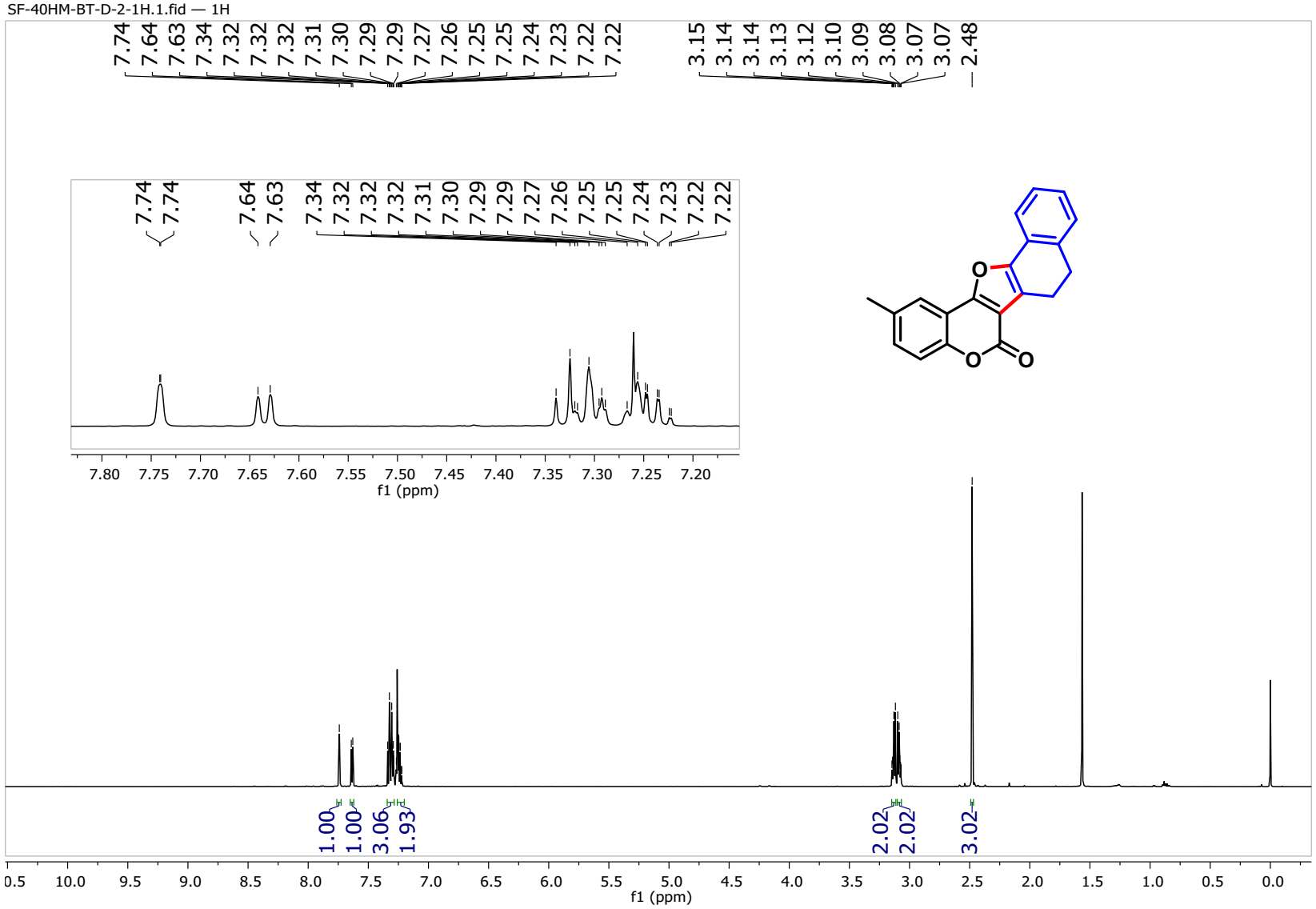


HRMS Spectrum of 2,10-Dimethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (4g)

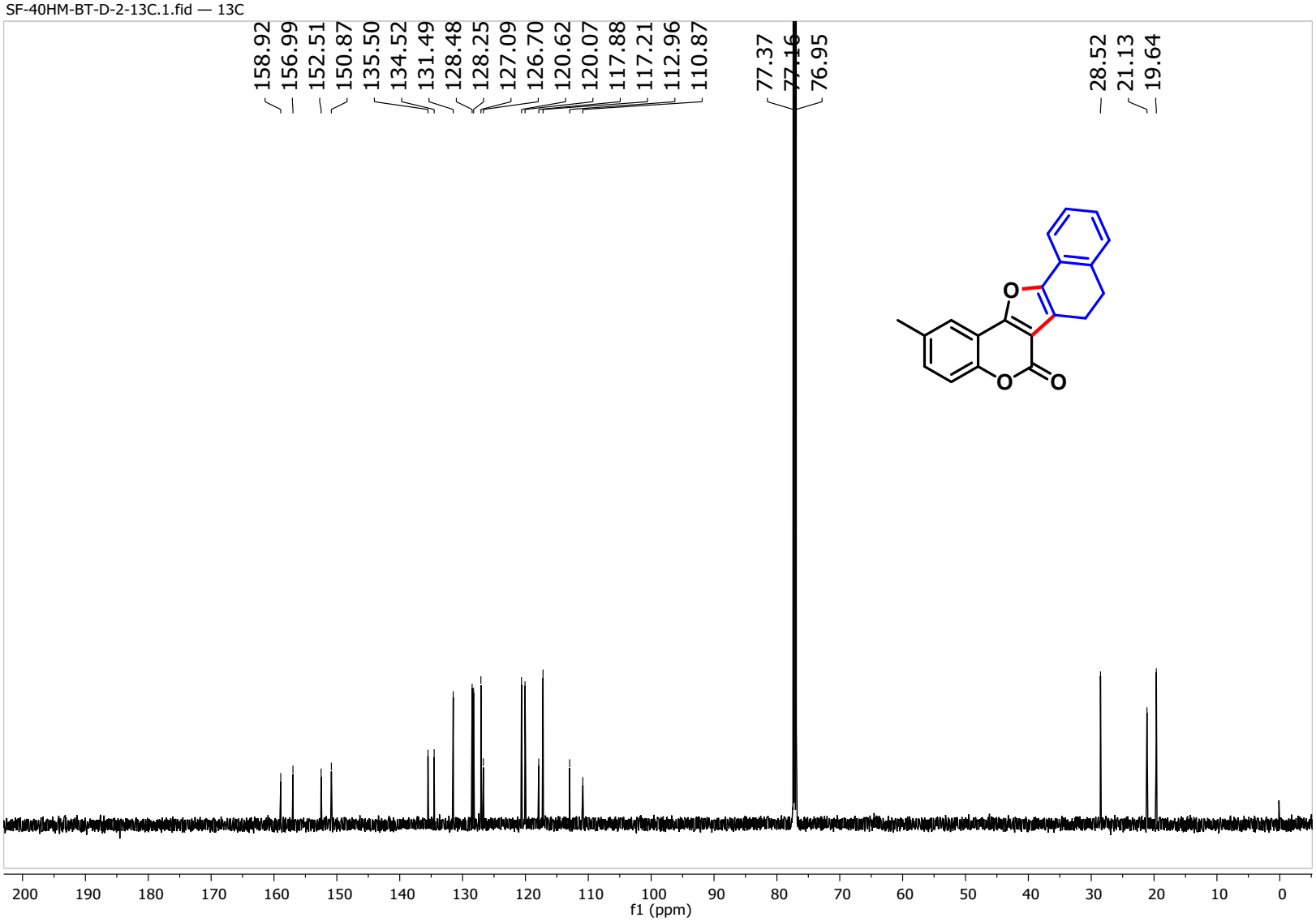
Sample Name	Sample22	**Position**	P1-B6	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF290.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	30-06-2023 15:26:27 (UTC+05:30)



^{1}H NMR Spectrum of 2-Methyl-7,8-dihydro-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one(4h)

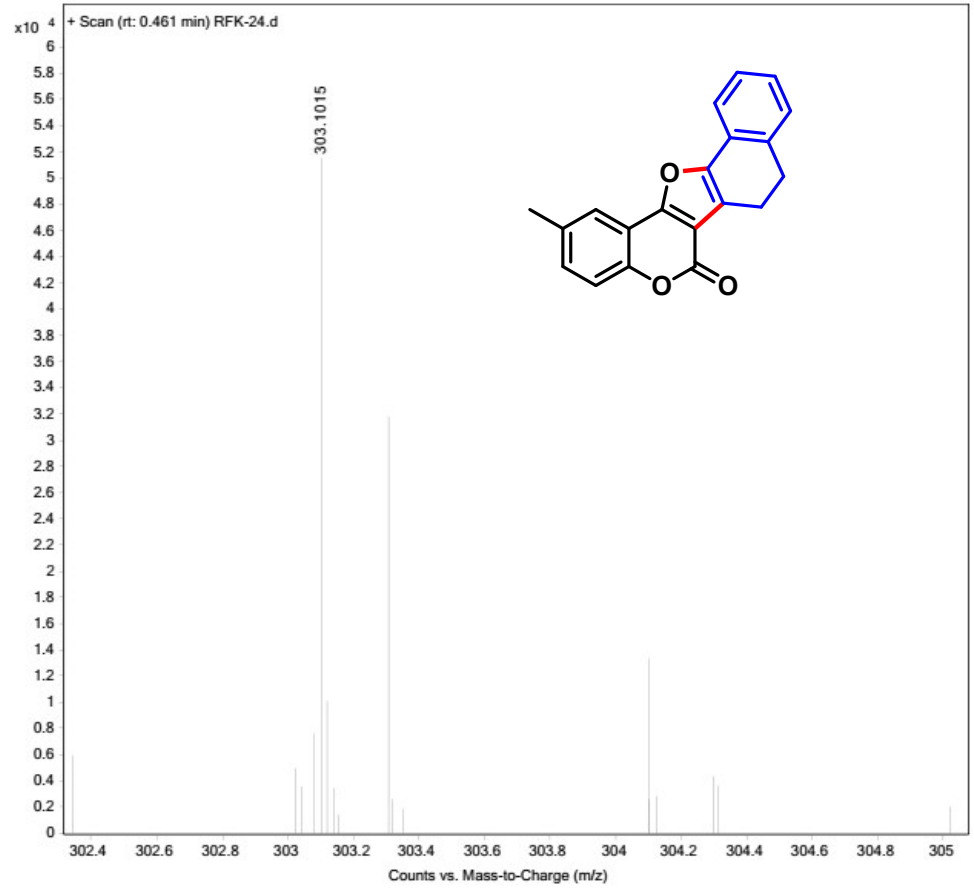


^{13}C NMR Spectrum of 2-Methyl-7,8-dihydro-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one(4h)

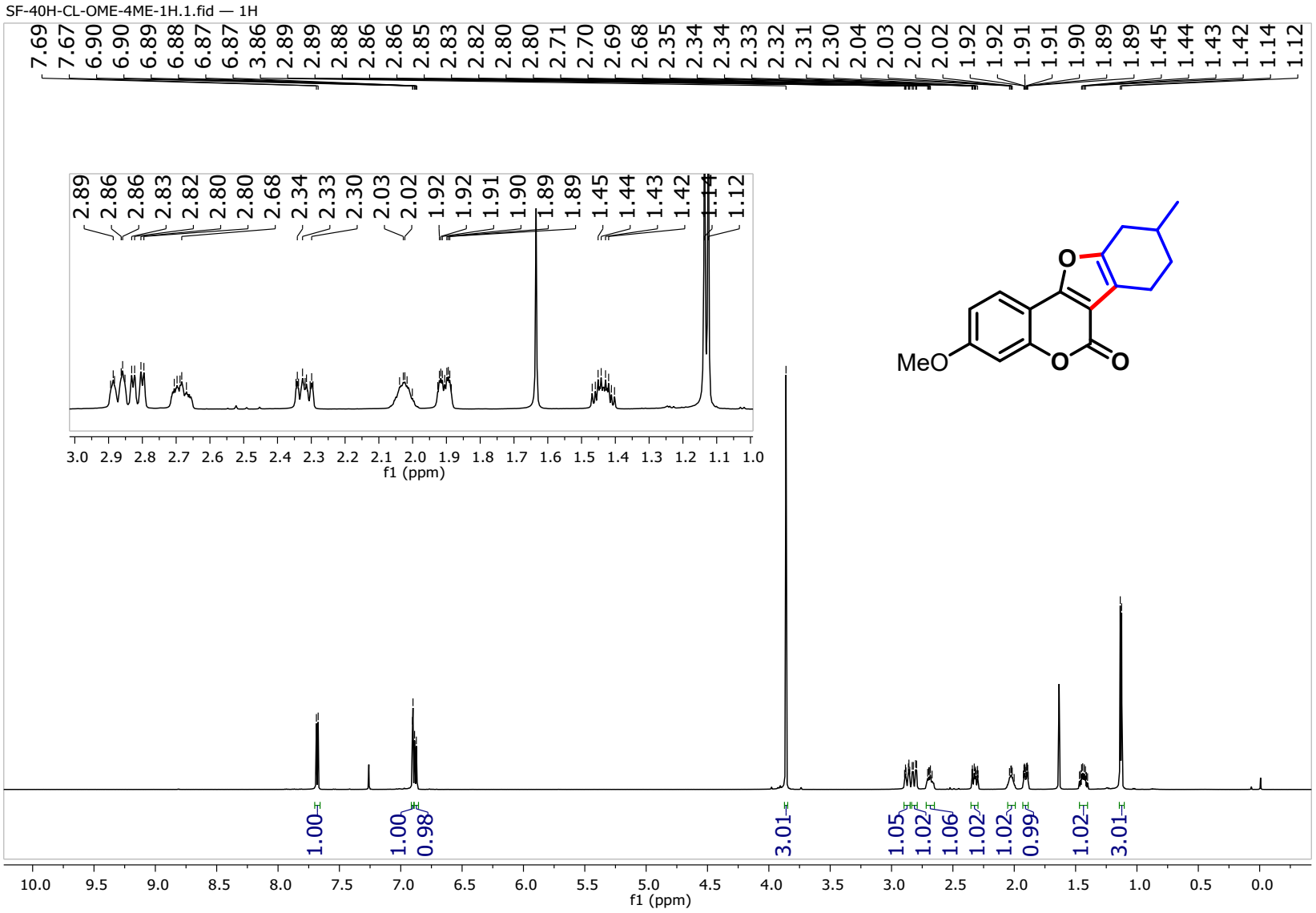


HRMS Spectrum of 2-Methyl-7,8-dihydro-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one(4h)

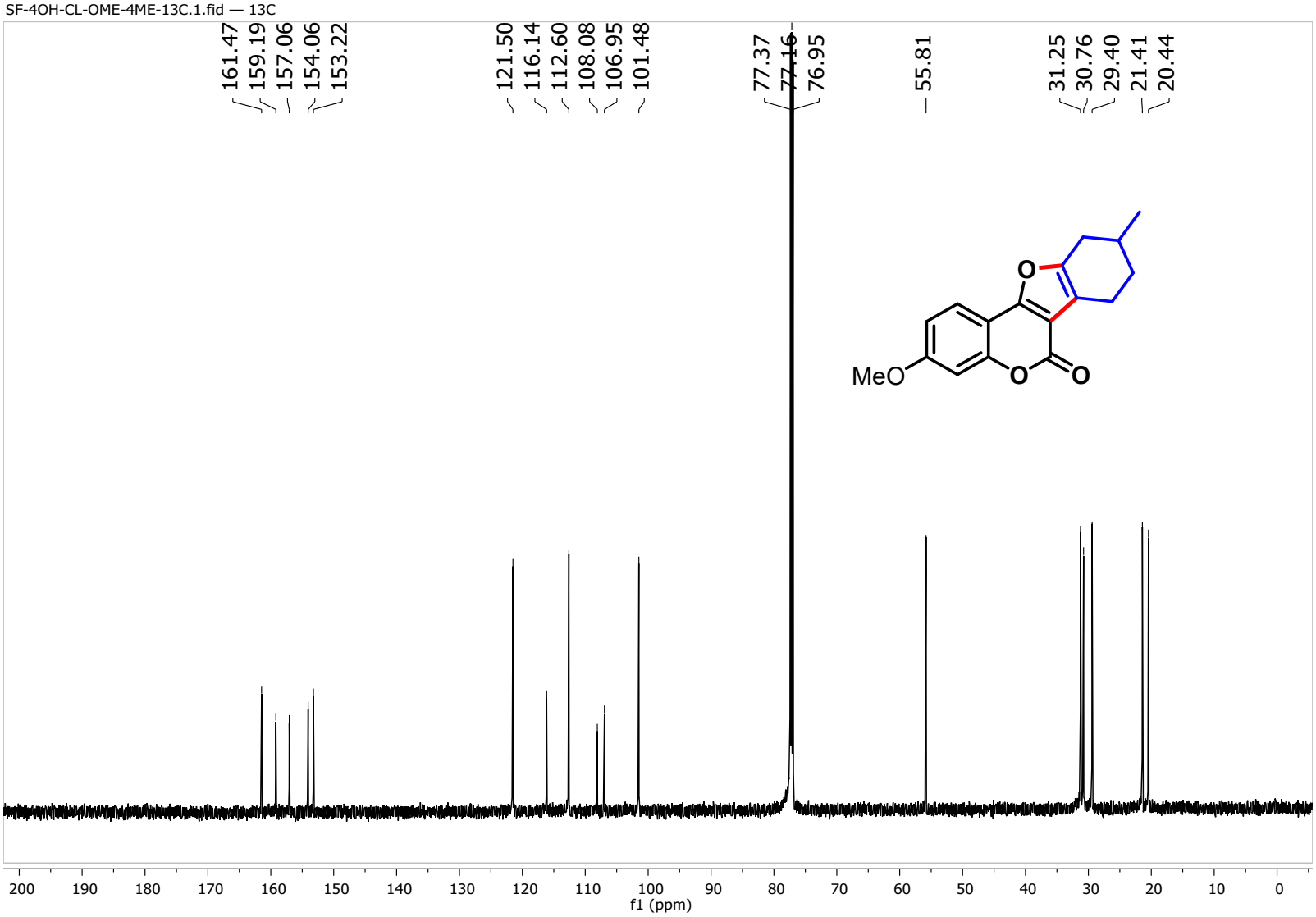
Sample Name	Sample40	**Position**	P1-D6	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	RFK-24.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	31-07-2023 11:01:10 (UTC+05:30)



^{1}H NMR Spectrum of 3-Methoxy-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5a)

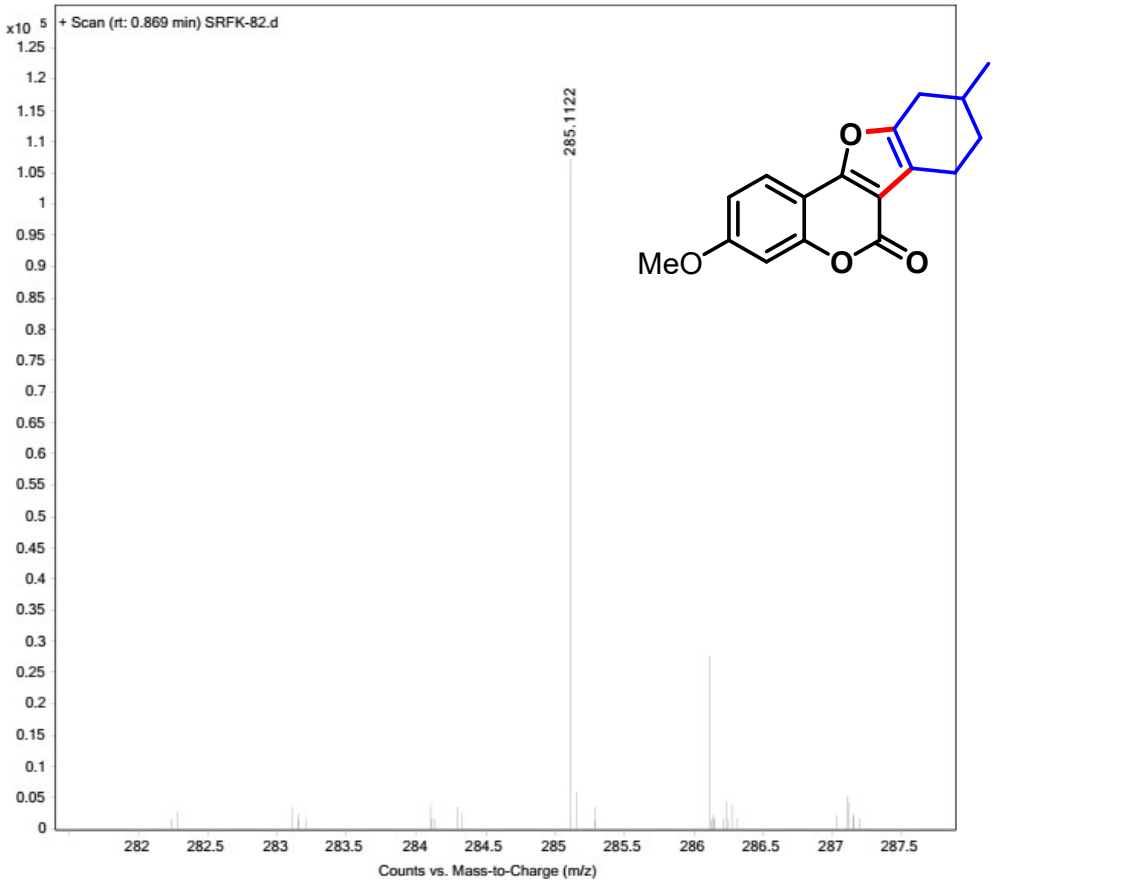


^{13}C NMR Spectrum of 3-Methoxy-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5a)

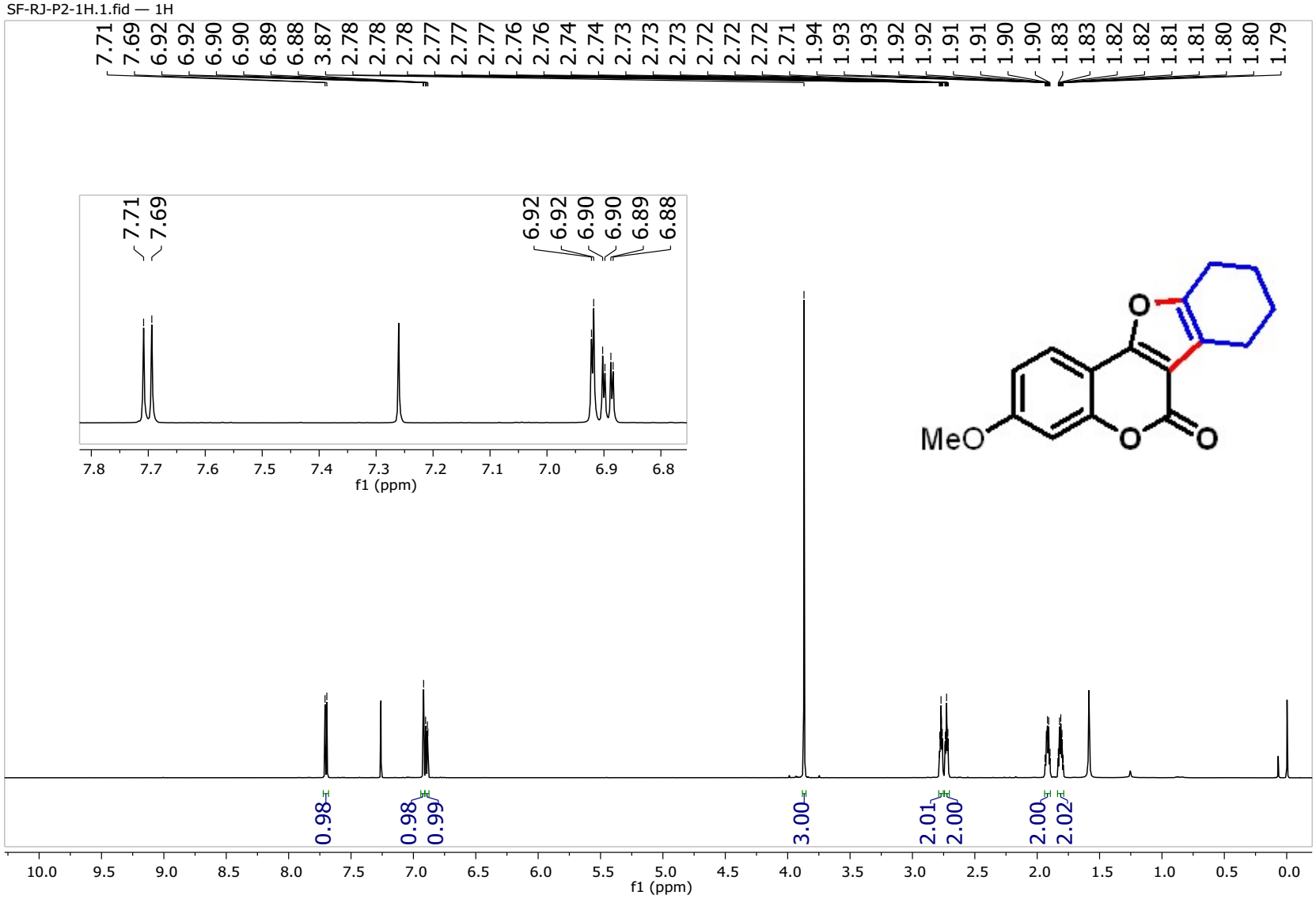


HRMS Spectrum of 3-Methoxy-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5a)

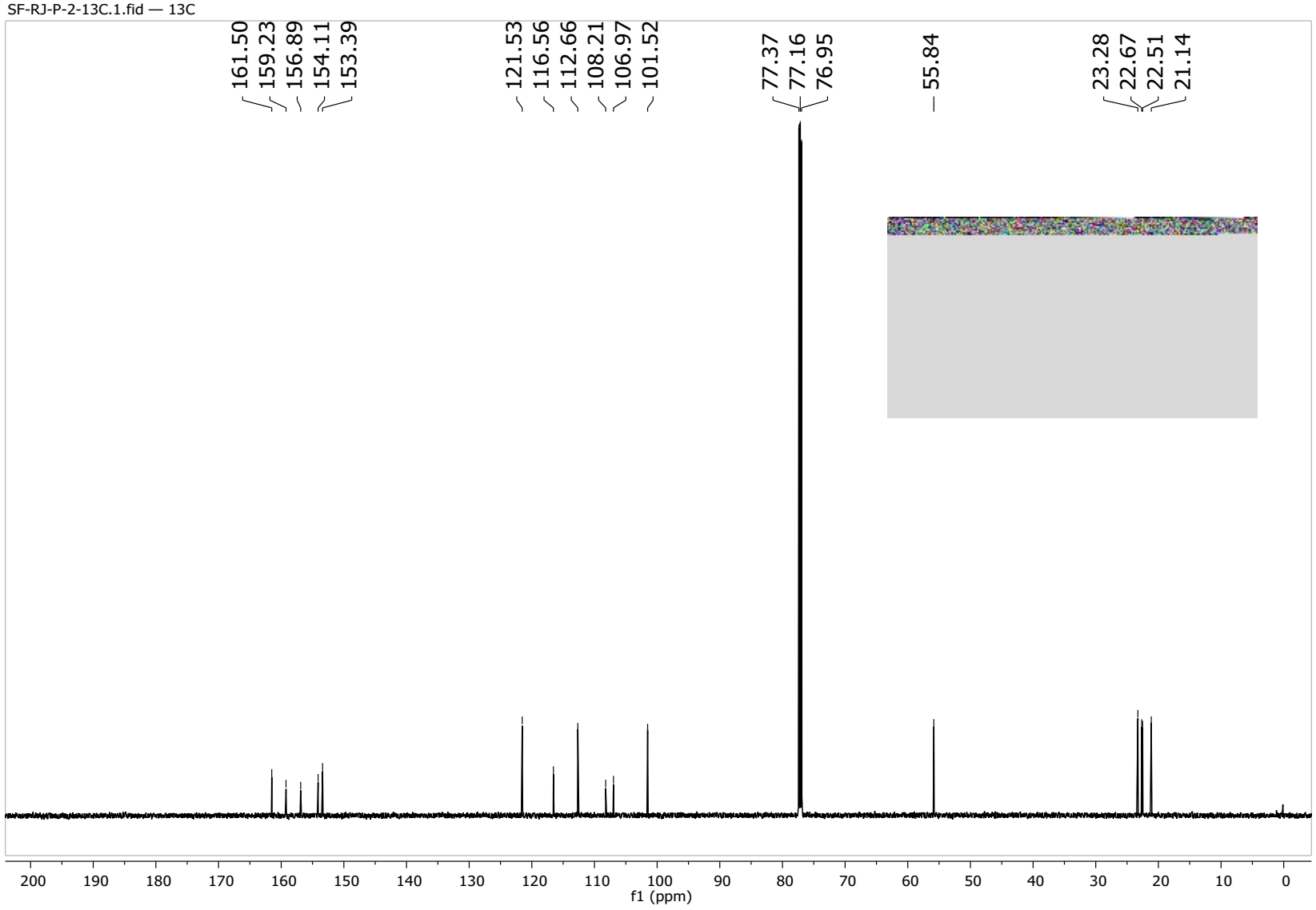
Sample Name	Sample3	**Position**	P1-A2	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SRFK-82.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	14-08-2023 09:55:44 (UTC+05:30)



^{1}H NMR Spectrum of 3-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5b)

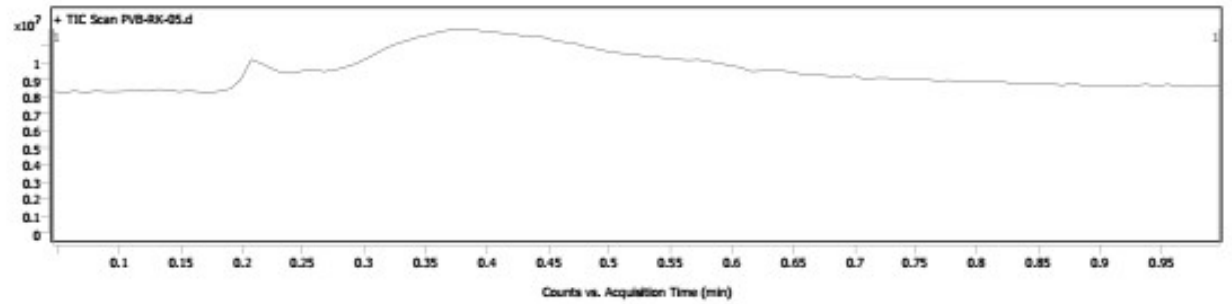


^{13}C NMR Spectrum of 3-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5b)



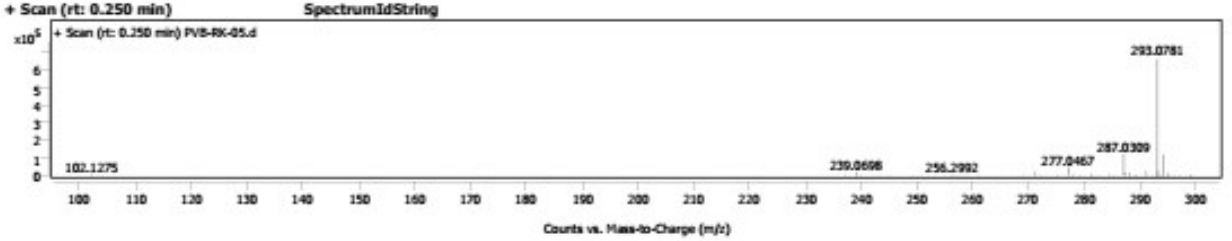
HRMS Spectrum of 3-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5b)

Sample Chromatograms



Peak Spec

+ Scan (rt: 0.250 min) **SpectrumIdString**

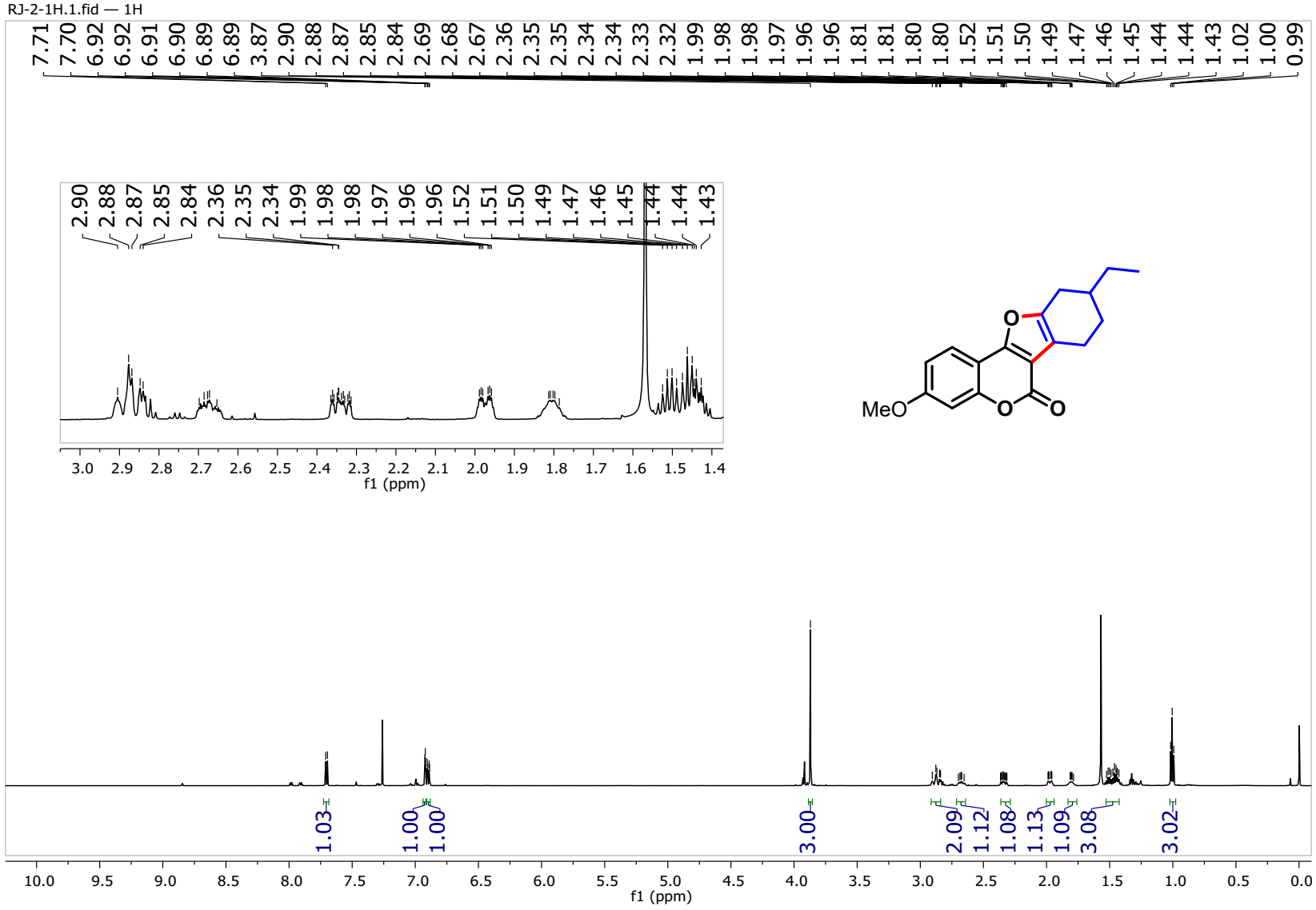


SpectrumIdString

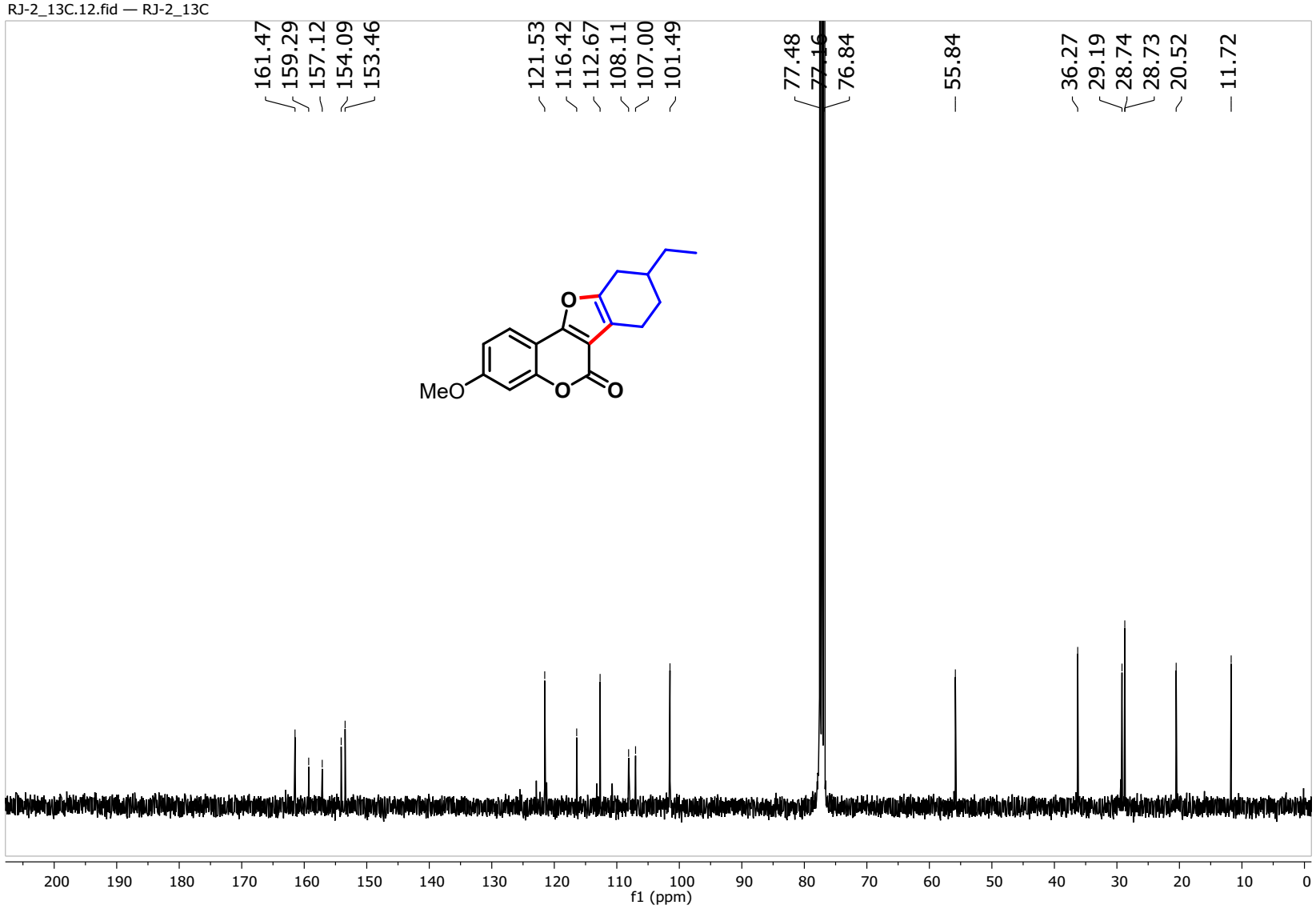
m/z	Z	Abund	Abund %	m/z (Calc)	Diff (ppm)	Ion Species	Formula	Ion Type
102.1275		8538	1.29					
239.0698		17285	2.61					
256.2992		8720	1.32					
271.0956		21581	3.26					
277.0467	1	46998	7.10					
278.0499	1	8494	1.28					
281.0777		9422	1.42					
284.3305		9269	1.40					
287.0309	1	120123	18.15					
287.1460		16620	2.51					
288.0344	1	16225	2.45					
291.0620		25251	3.82					
293.0781	1	661683	100.00					
293.1160		24884	3.76					
294.0811	1	119104	18.00					
295.0836	1	13857	2.09					

MassHunter Qual 10.0
(End of Report)

^{1}H NMR Spectrum of 9-Ethyl-3-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5c)

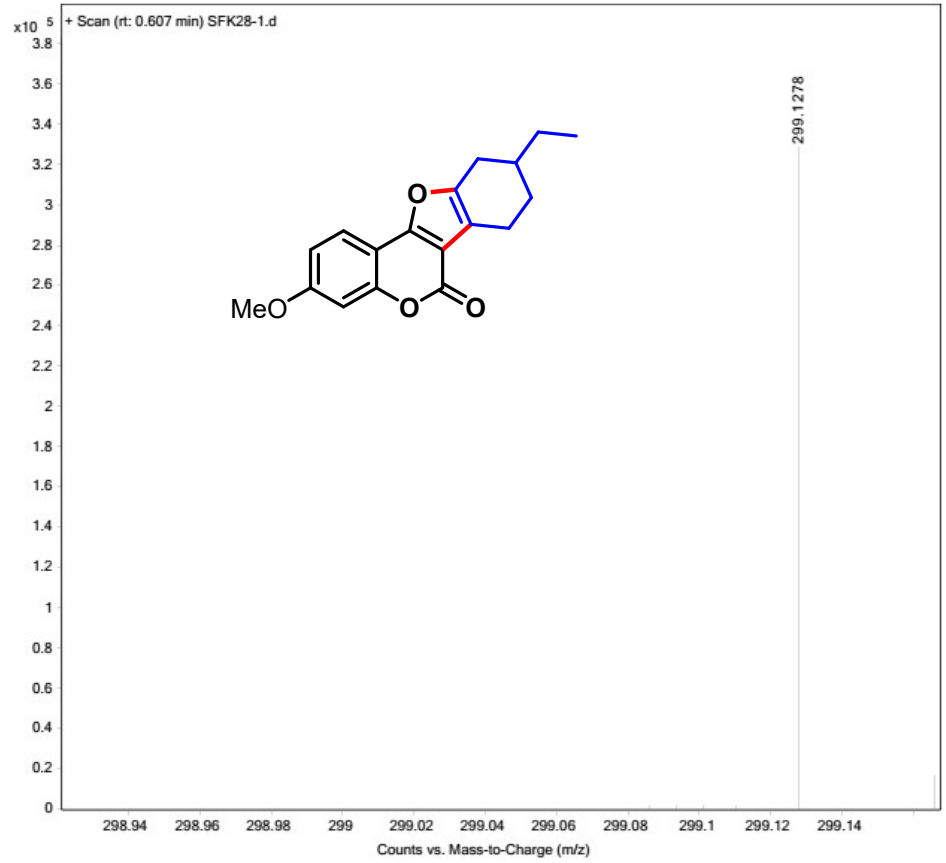


^{13}C NMR Spectrum of 9-Ethyl-3-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5c)

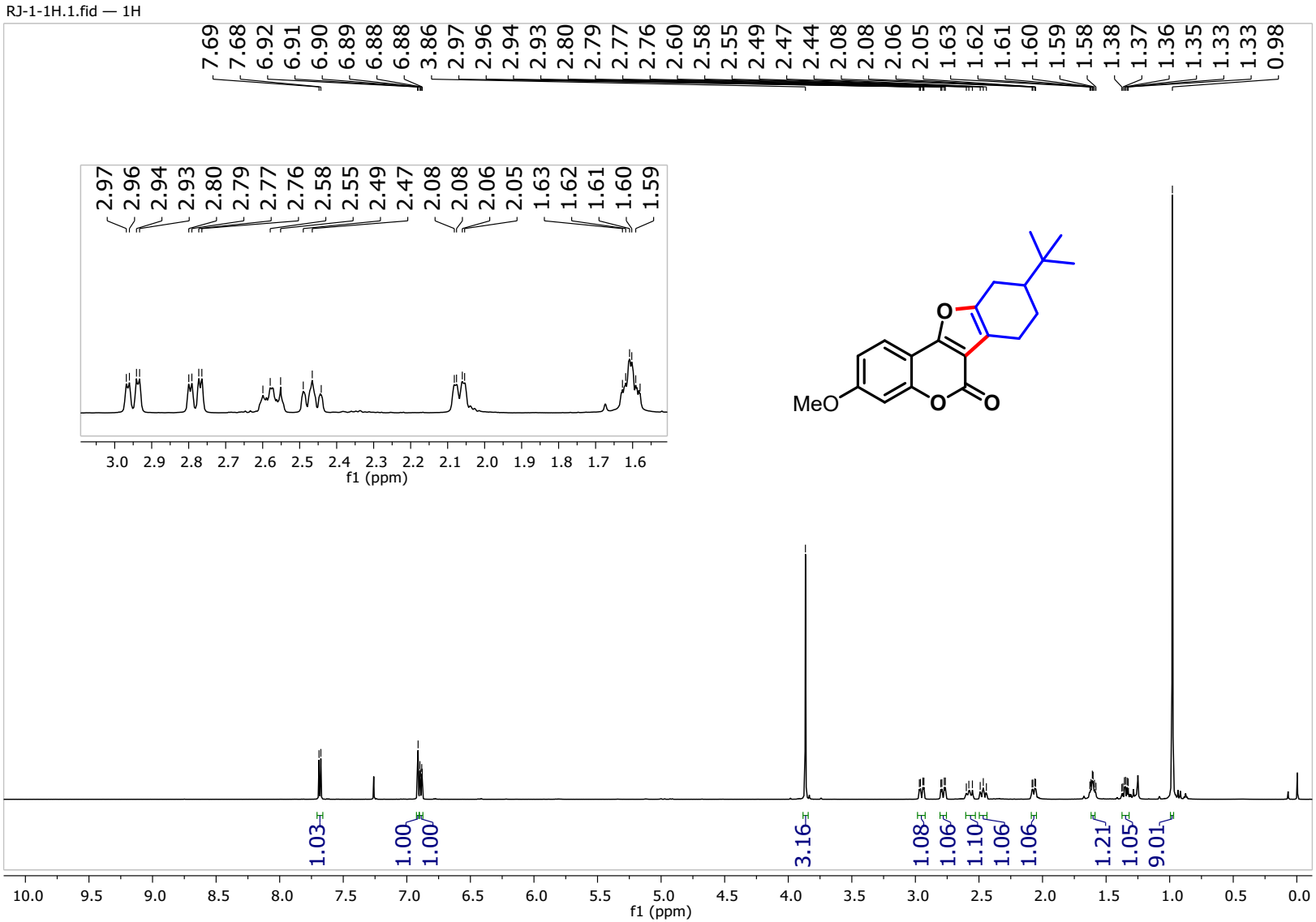


HRMS Spectrum of 9-Ethyl-3-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5c)

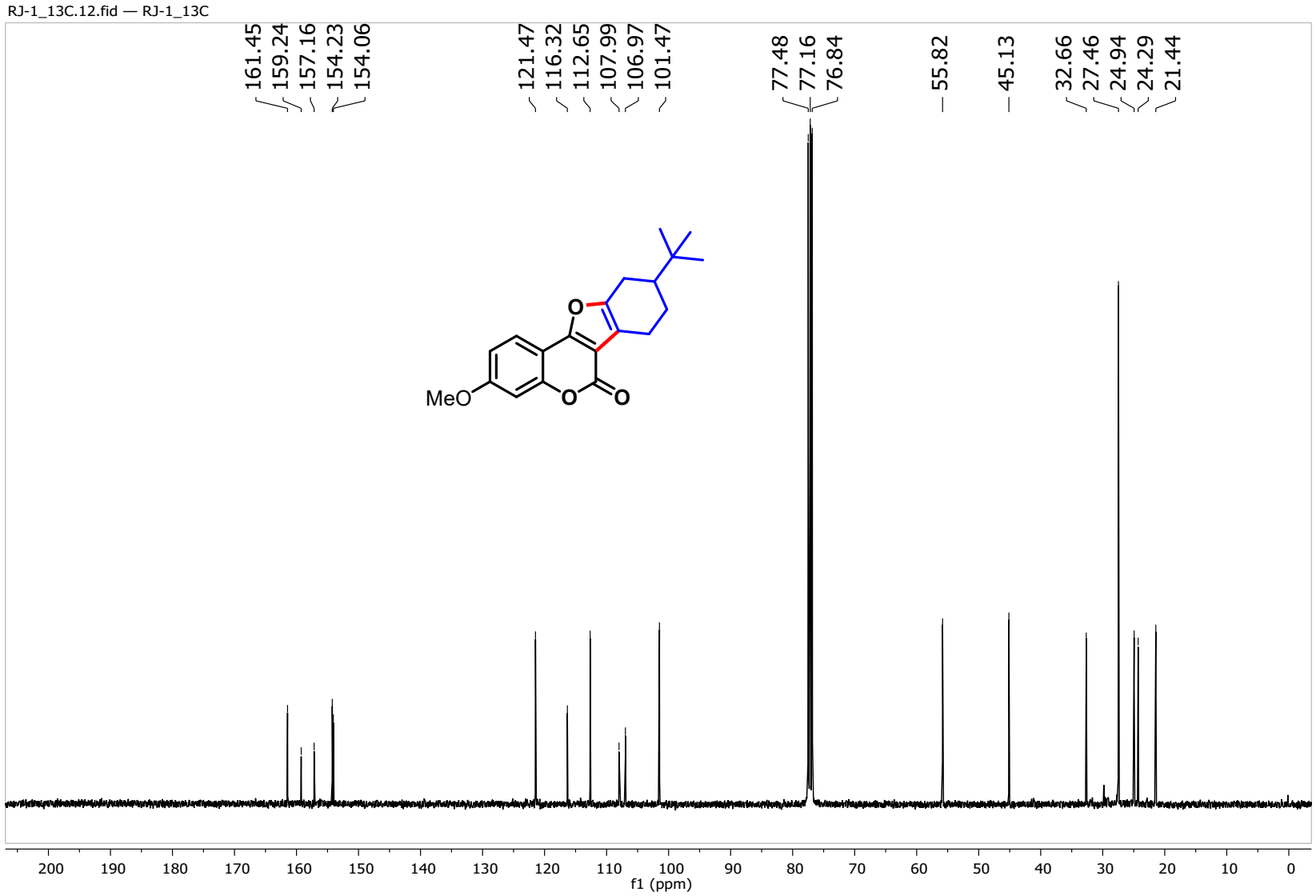
Sample Name		**Position**	P1-A5	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFK28-1.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	03-10-2023 15:11:42 (UTC+05:30)



^{1}H NMR Spectrum of 9-(*tert*-butyl)-3-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5d)

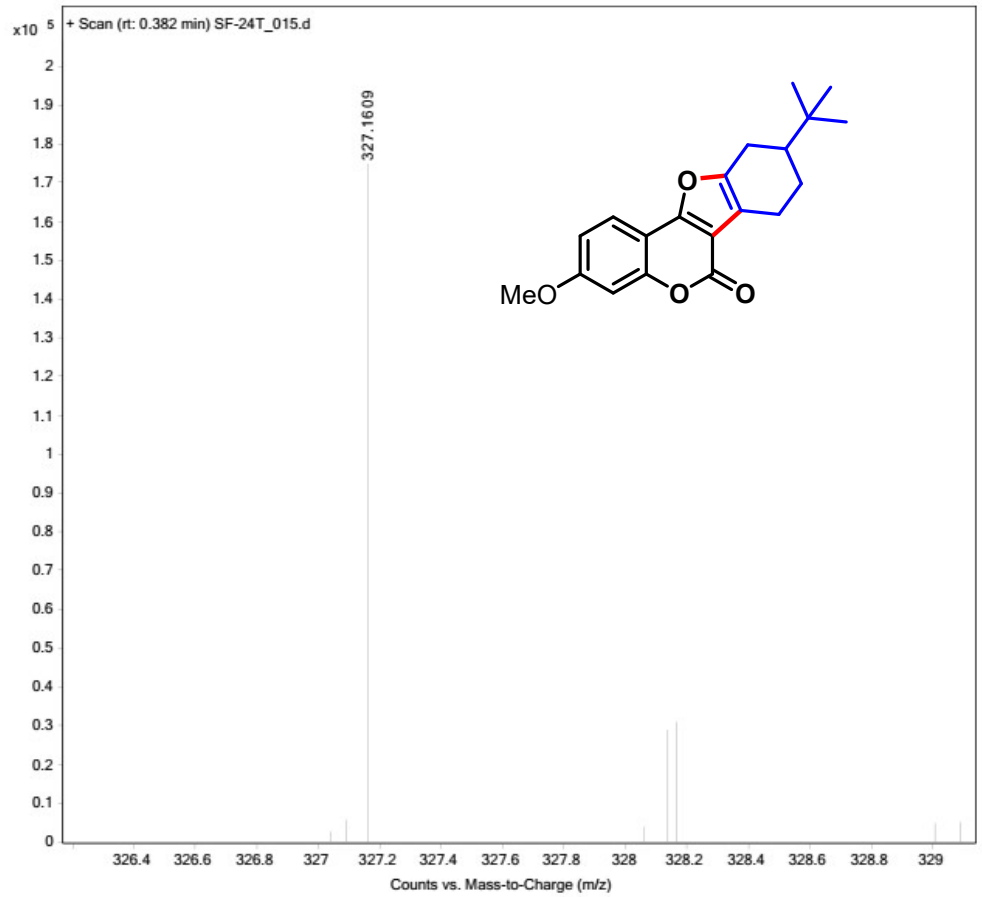


^{13}C NMR Spectrum of 9-(*tert*-butyl)-3-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5d)

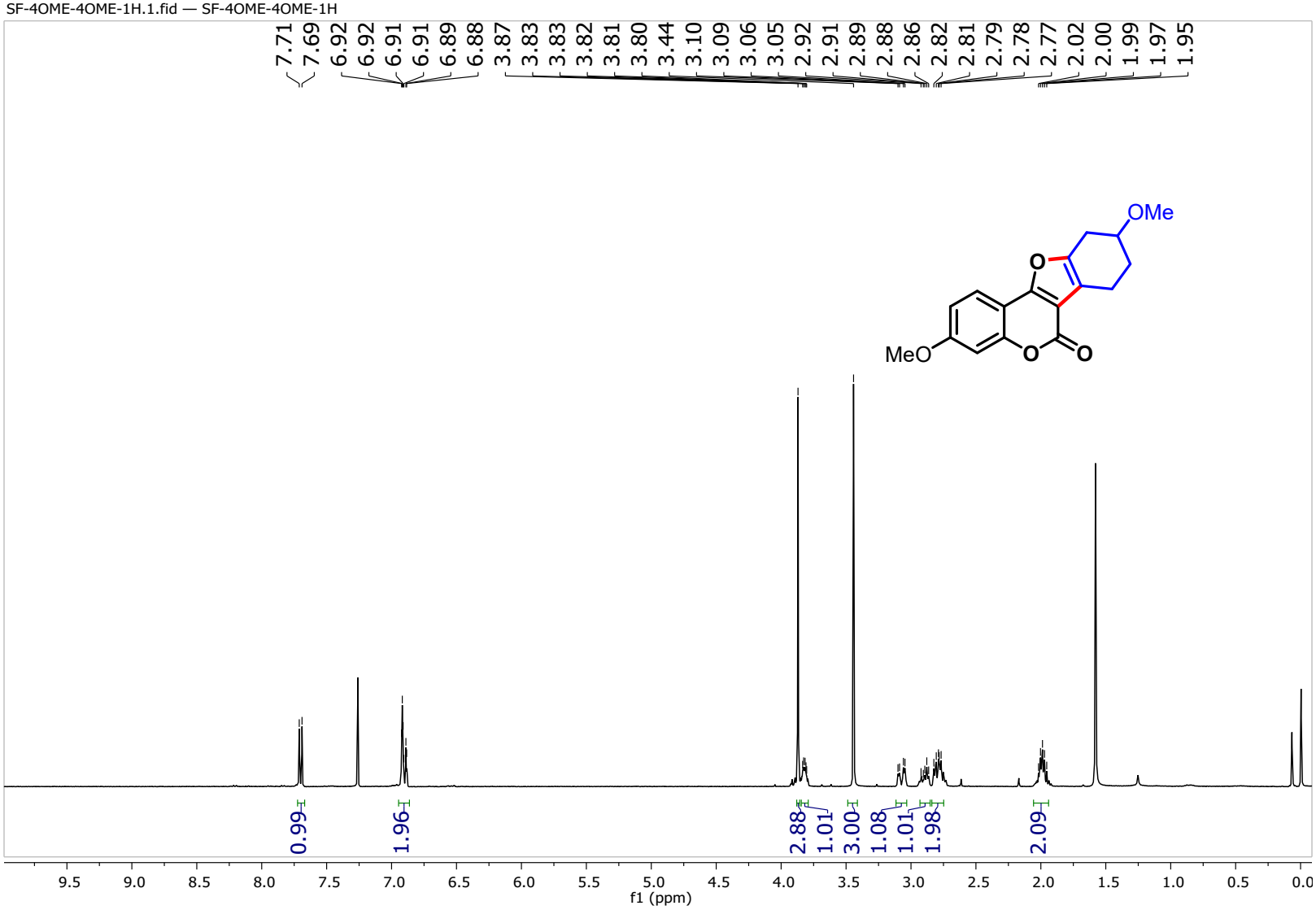


HRMS Spectrum of 9-(*tert*-butyl)-3-Methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5d)

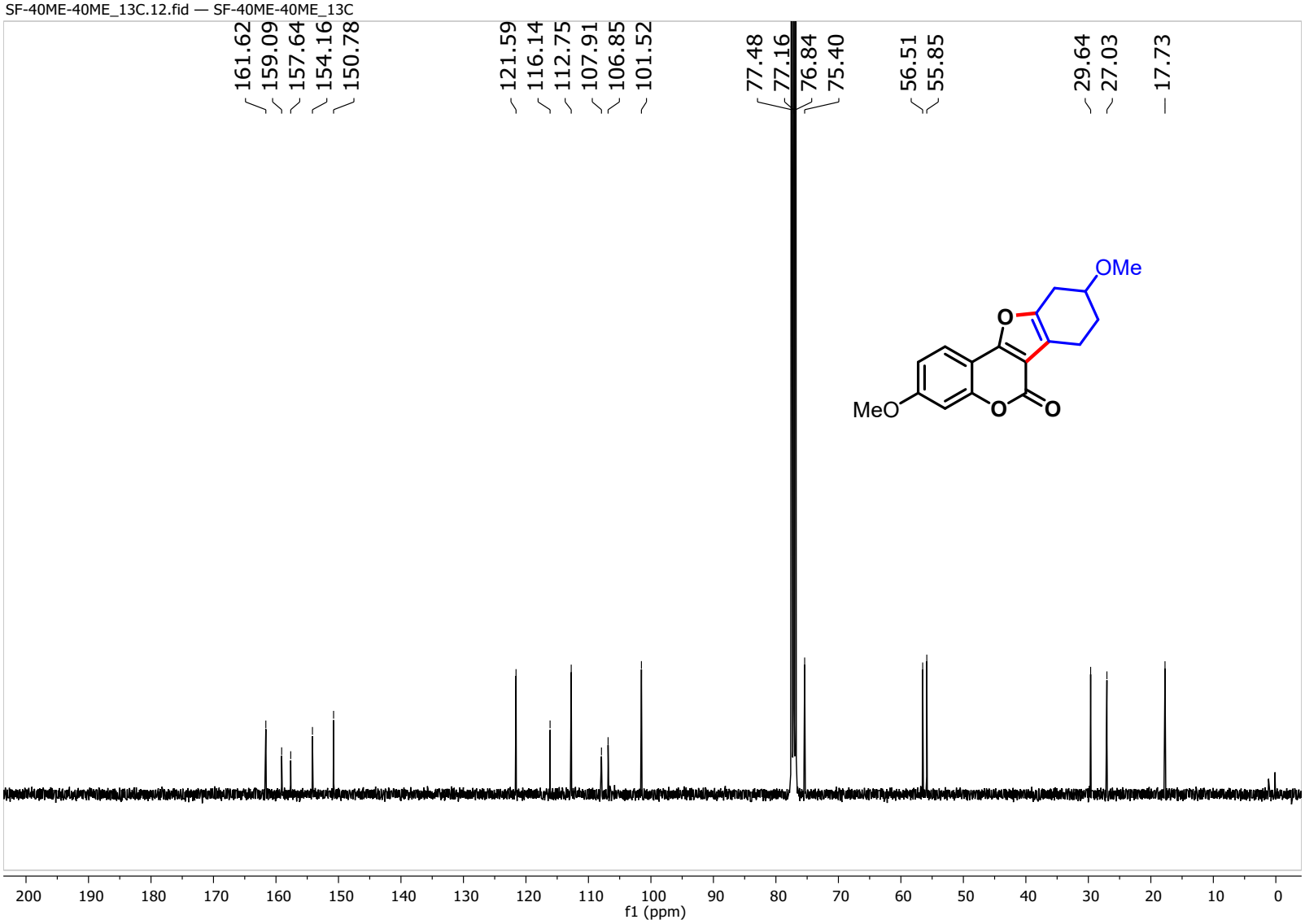
Sample Name	SF-24T	**Position**	P2-D2	**Instrument Name**	Instrument 1
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-24T_015.d
ACQ Method	FULL SCAN-POSITIVE.m	**Comment**		**Acquired Time**	16-12-2022 18:22:27 (UTC+05:30)



^{1}H NMR Spectrum of 3,9-Dimethoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5e)

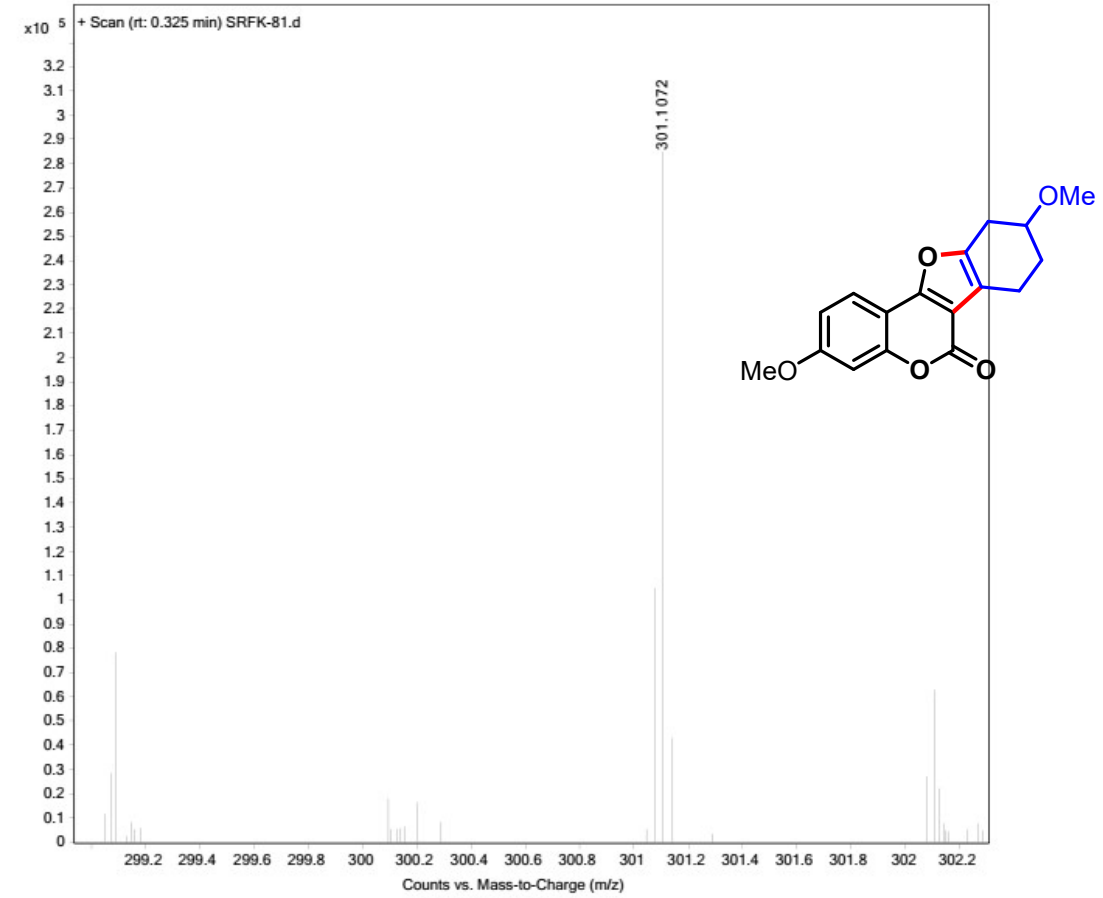


^{13}C NMR Spectrum of 3,9-Dimethoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5e)

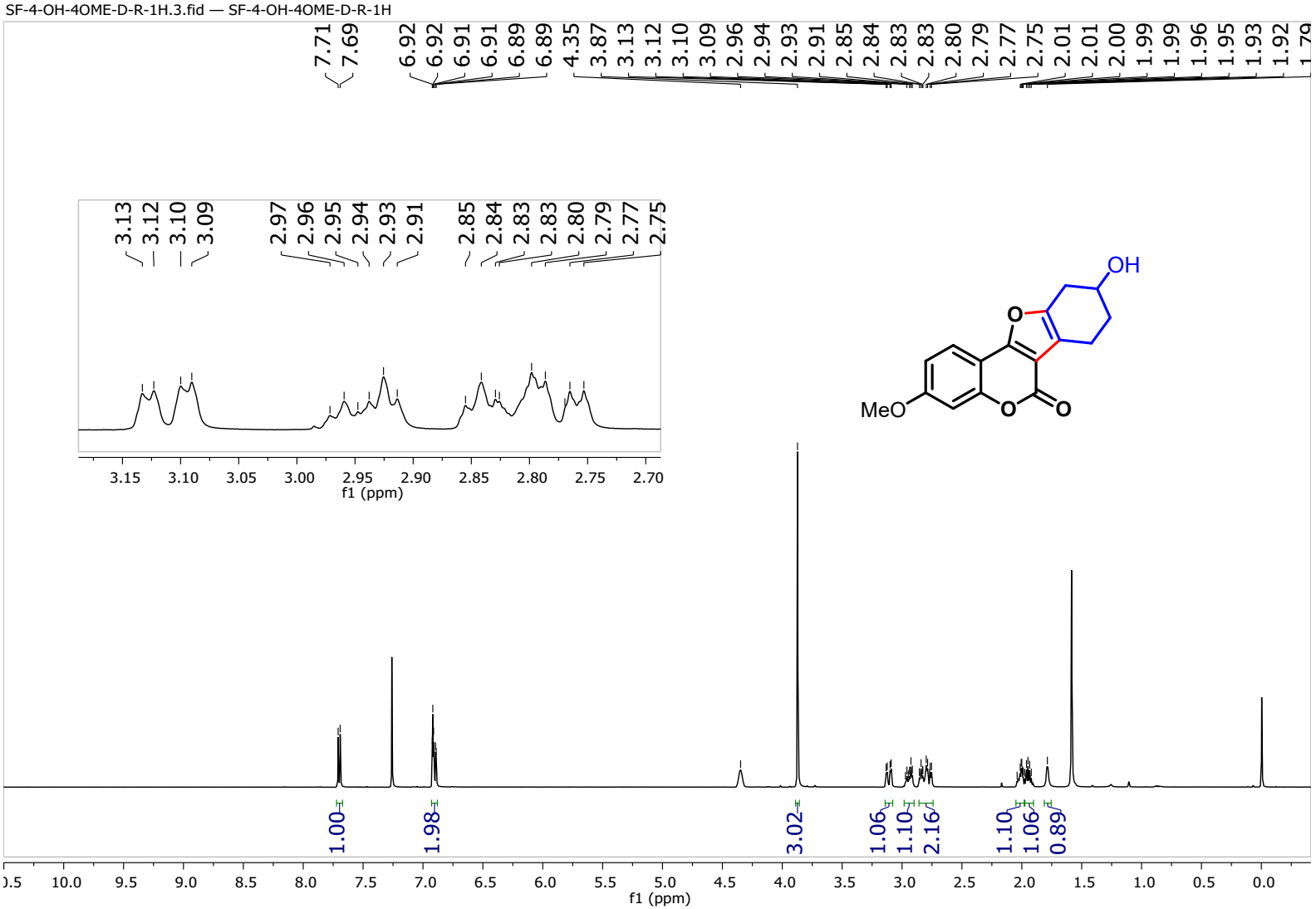


HRMS Spectrum of 3,9-Dimethoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5e)

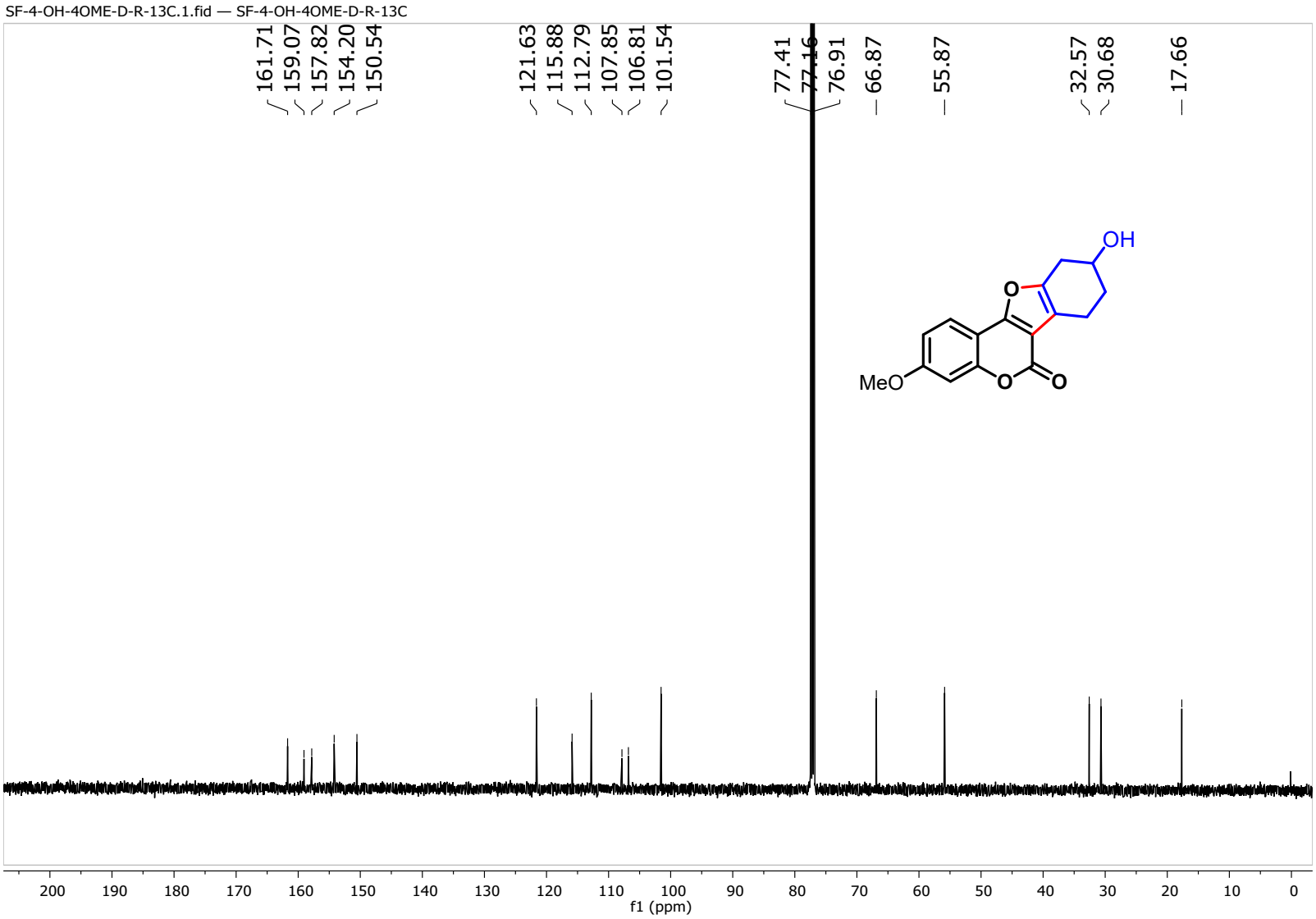
Sample Name	Sample2	**Position**	P1-A1	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SRFK-81.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	14-08-2023 09:53:54 (UTC+05:30)



^{1}H NMR Spectrum of 9-Hydroxy-3-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5f)

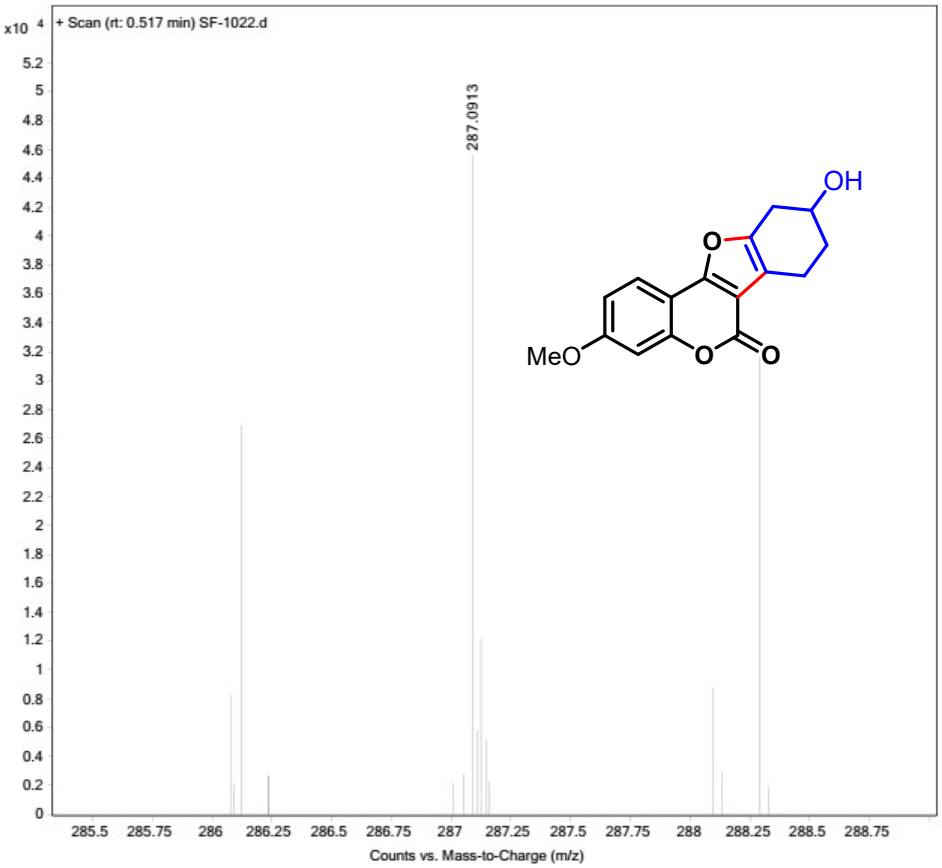


^{13}C NMR Spectrum of 9-Hydroxy-3-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5f)

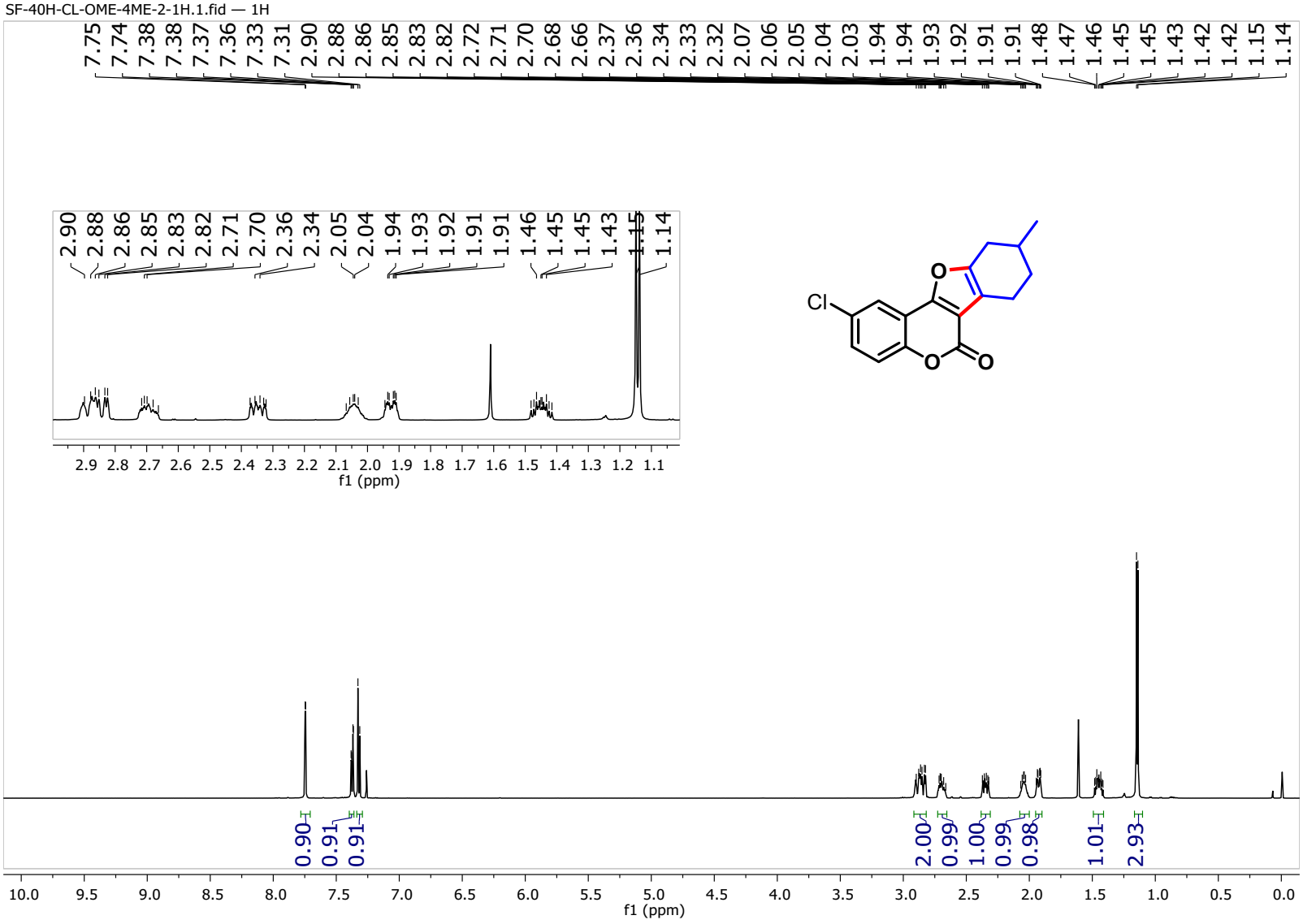


HRMS Spectrum of 9-Hydroxy-3-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (5f)

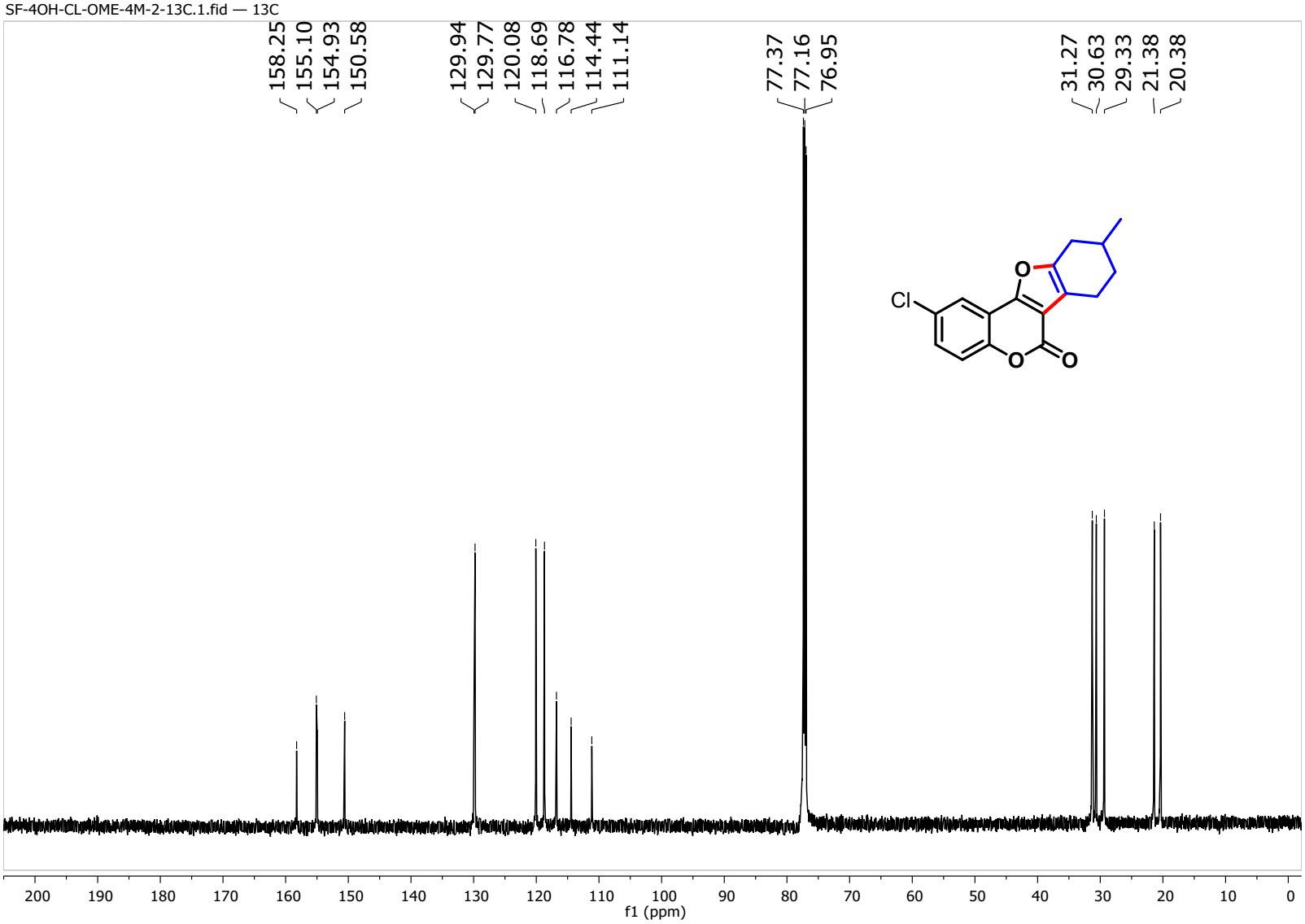
Sample Name	Sample15	**Position**	P1-B3	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-1022.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	28-08-2023 15:29:08 (UTC+05:30)



^{1}H NMR Spectrum of 2-Chloro-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6a)

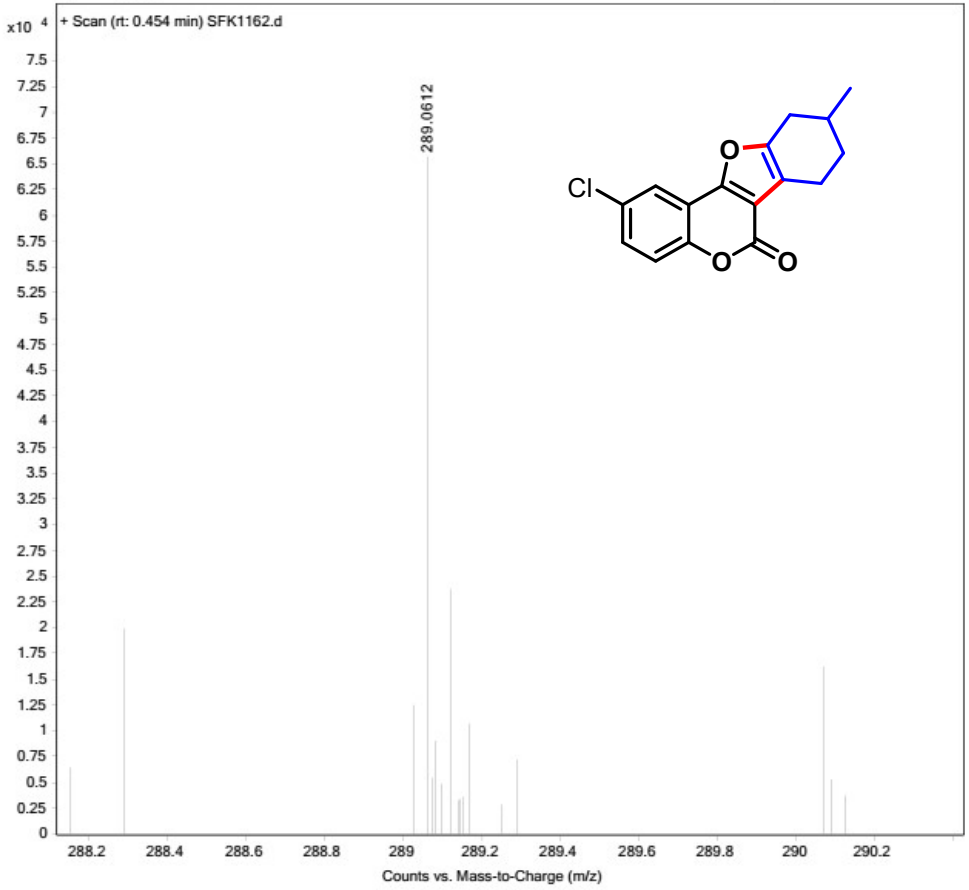


^{13}C NMR Spectrum of 2-Chloro-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6a)

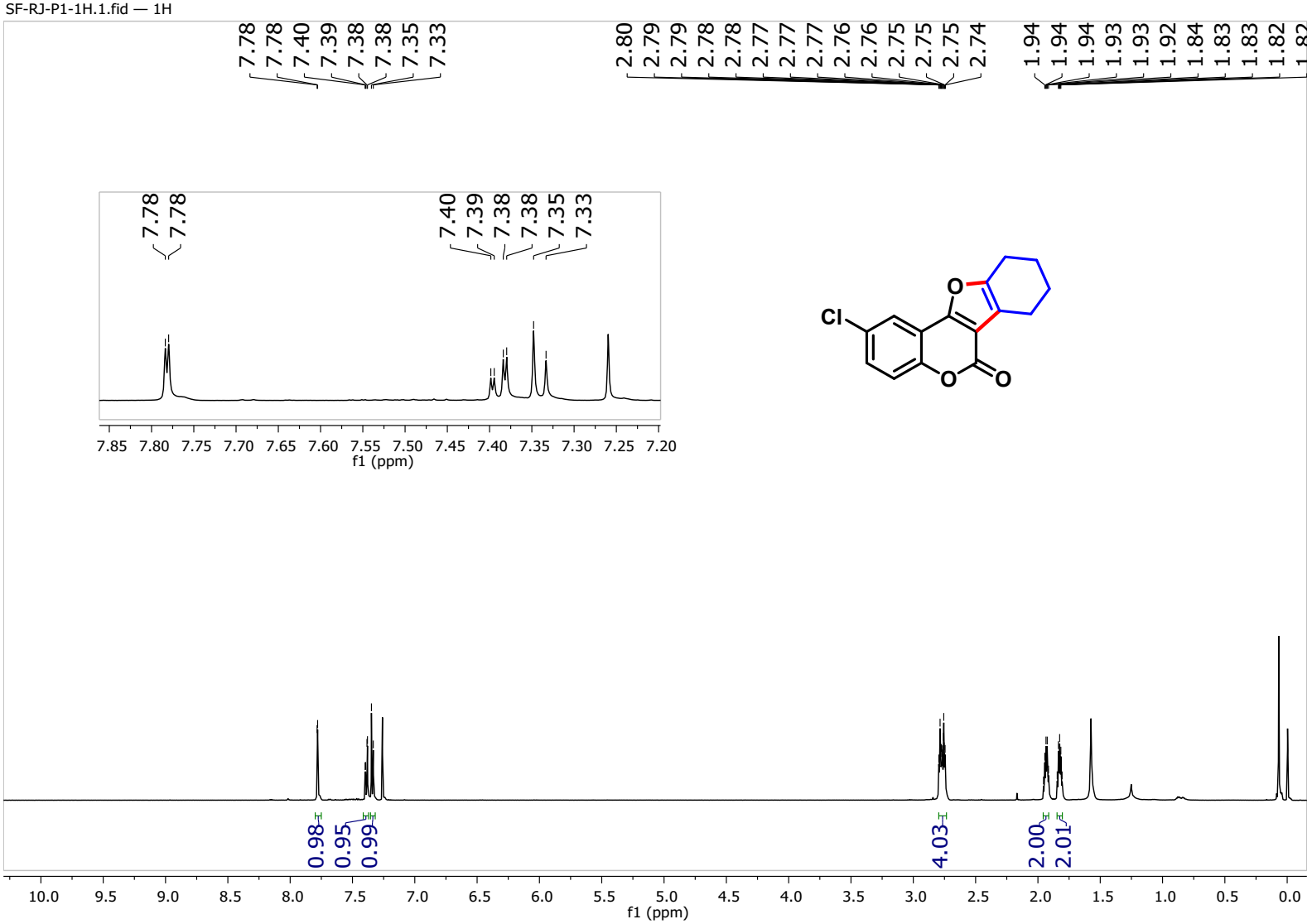


HRMS Spectrum of 2-Chloro-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6a)

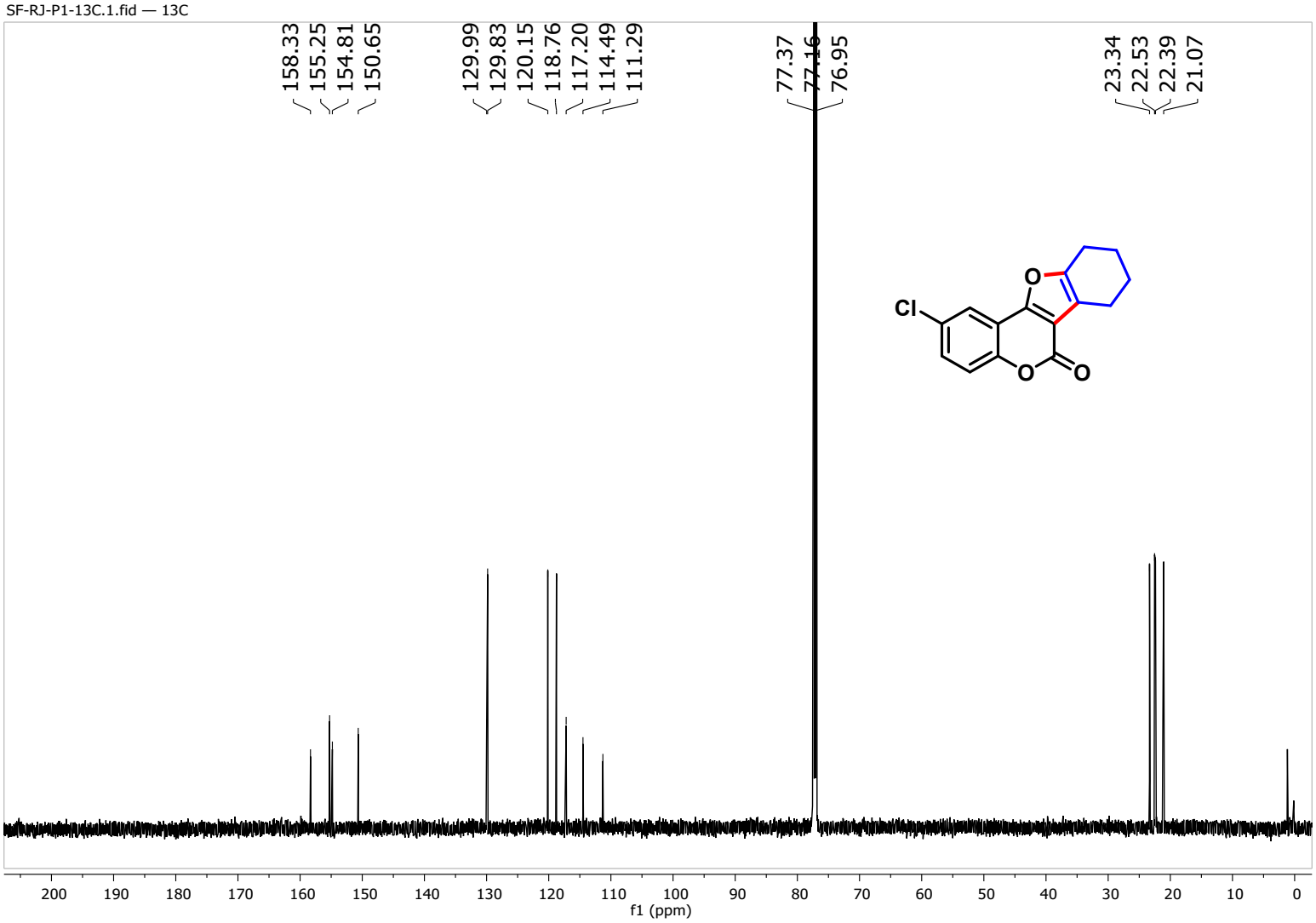
Sample Name	Sample12	**Position**	P1-A10	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFK1162.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	01-09-2023 17:20:30 (UTC+05:30)



^{1}H NMR Spectrum of 2-Chloro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6b)

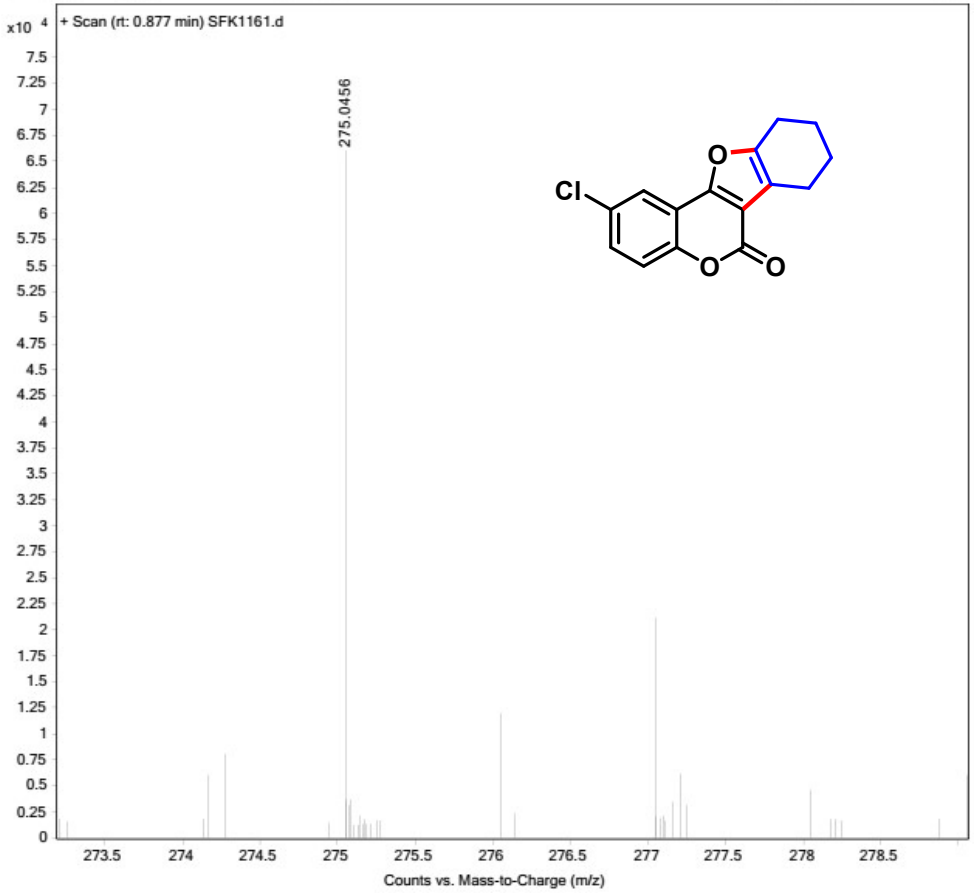


^{13}C NMR Spectrum of 2-Chloro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6b)

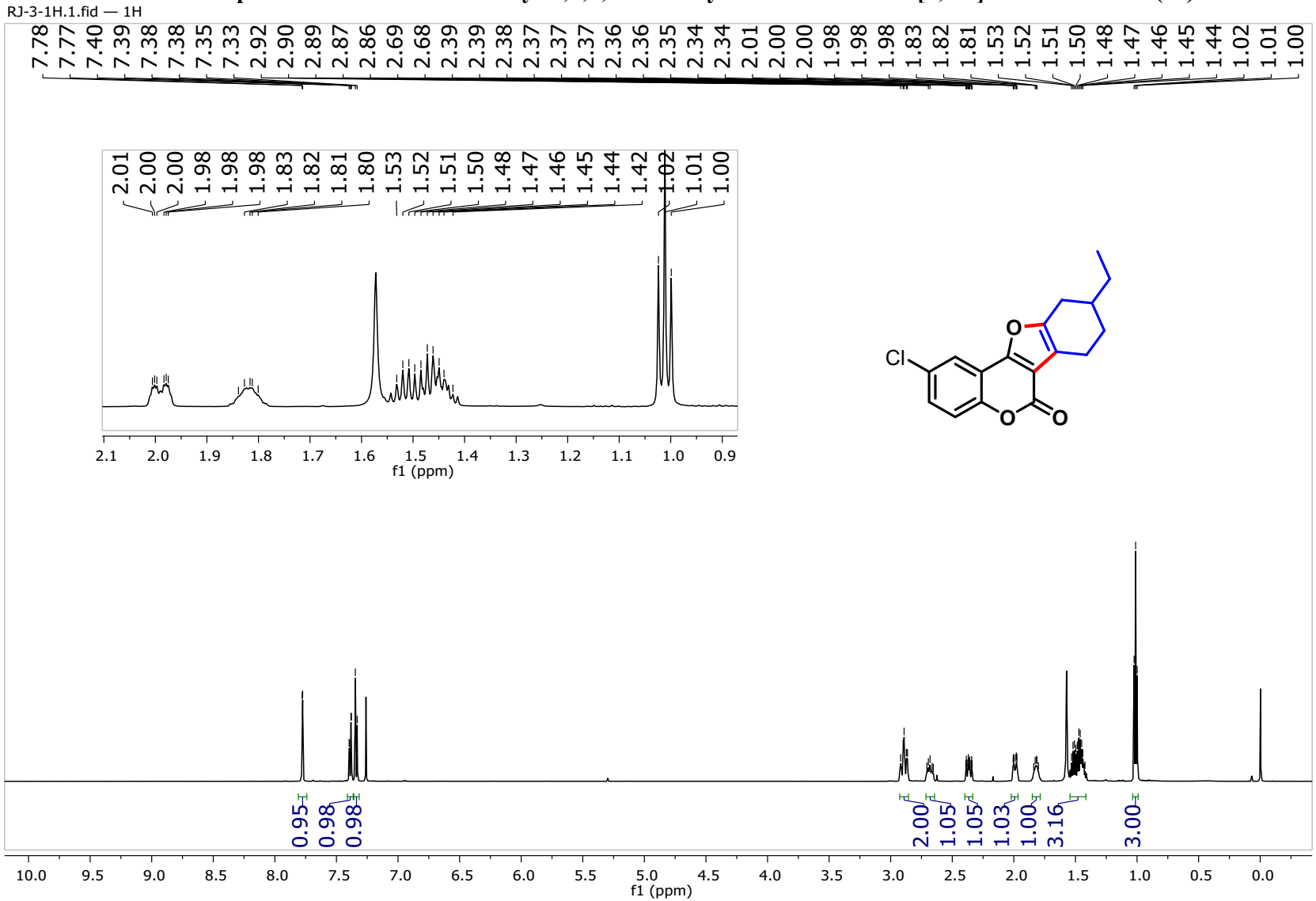


HRMS Spectrum of 2-Chloro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6b)

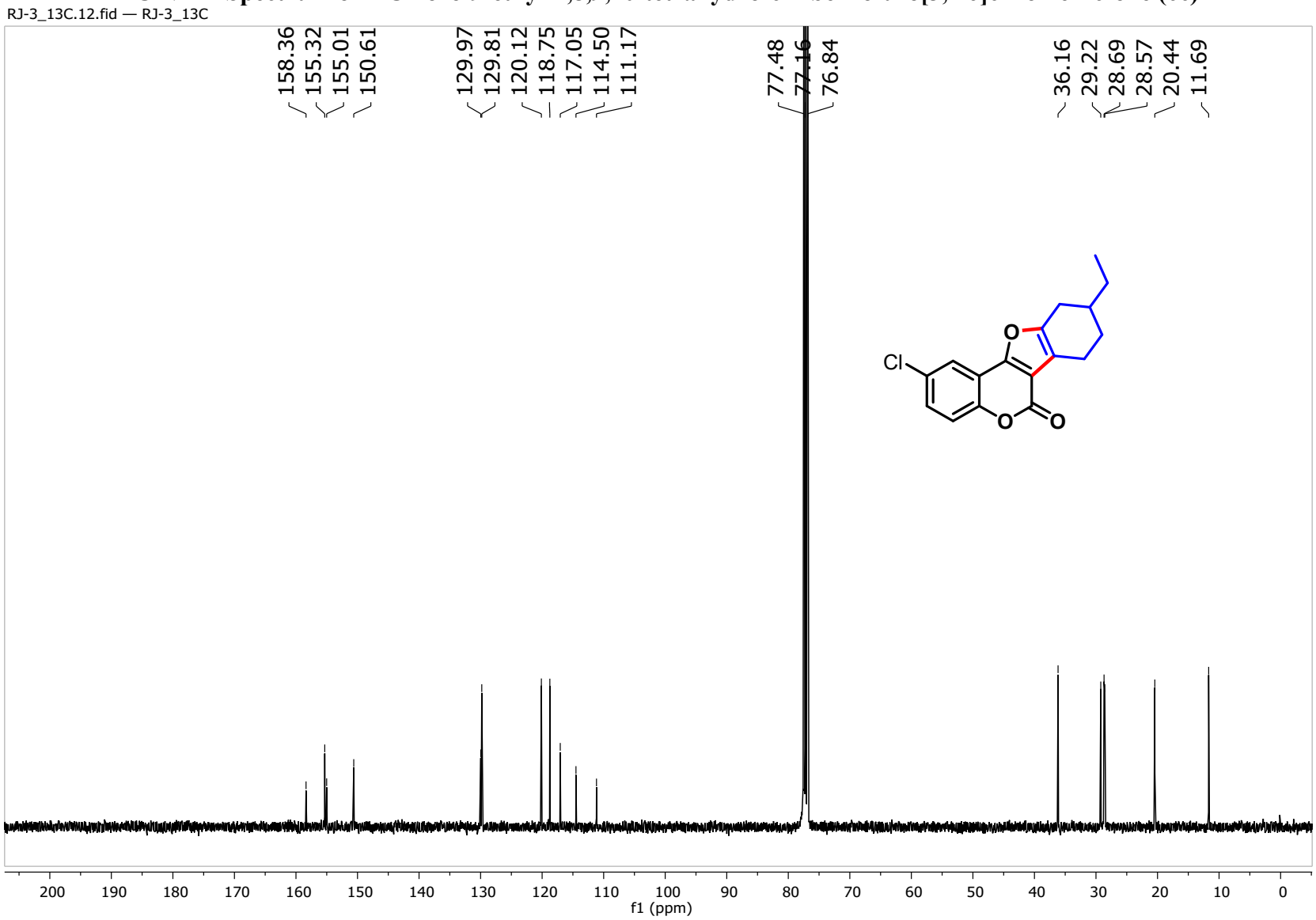
Sample Name	Sample11	**Position**	P1-A9	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFK1161.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	01-09-2023 17:18:40 (UTC+05:30)



^{1}H NMR Spectrum of 2-Chloro-9-ethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6c)

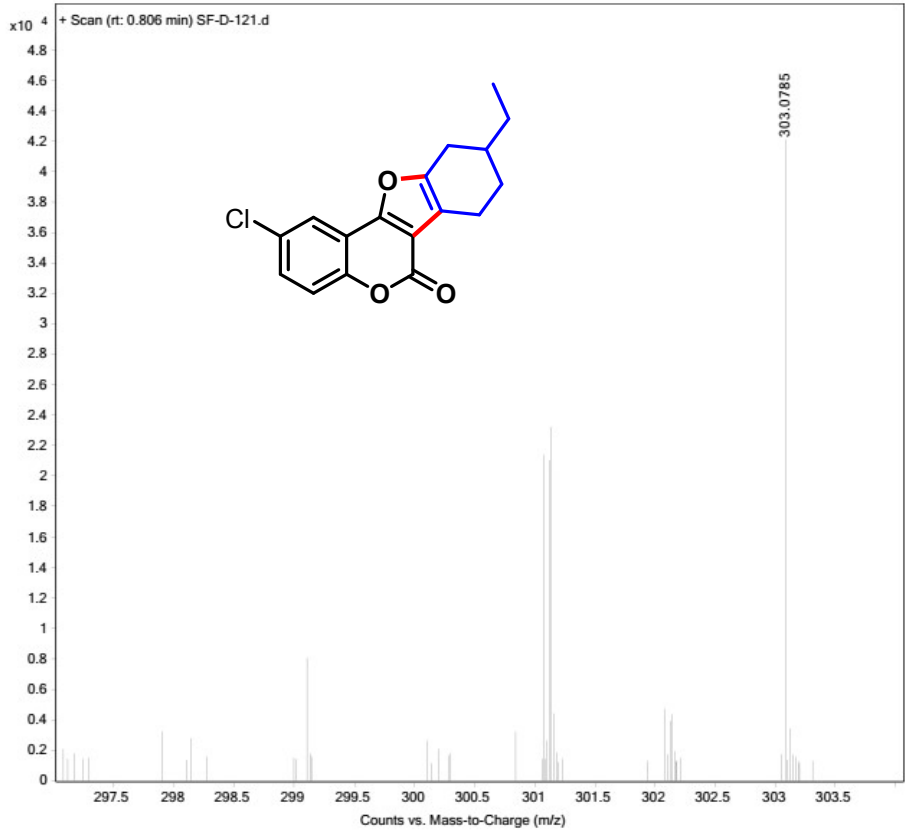


^{13}C NMR Spectrum of 2-Chloro-9-ethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6c)

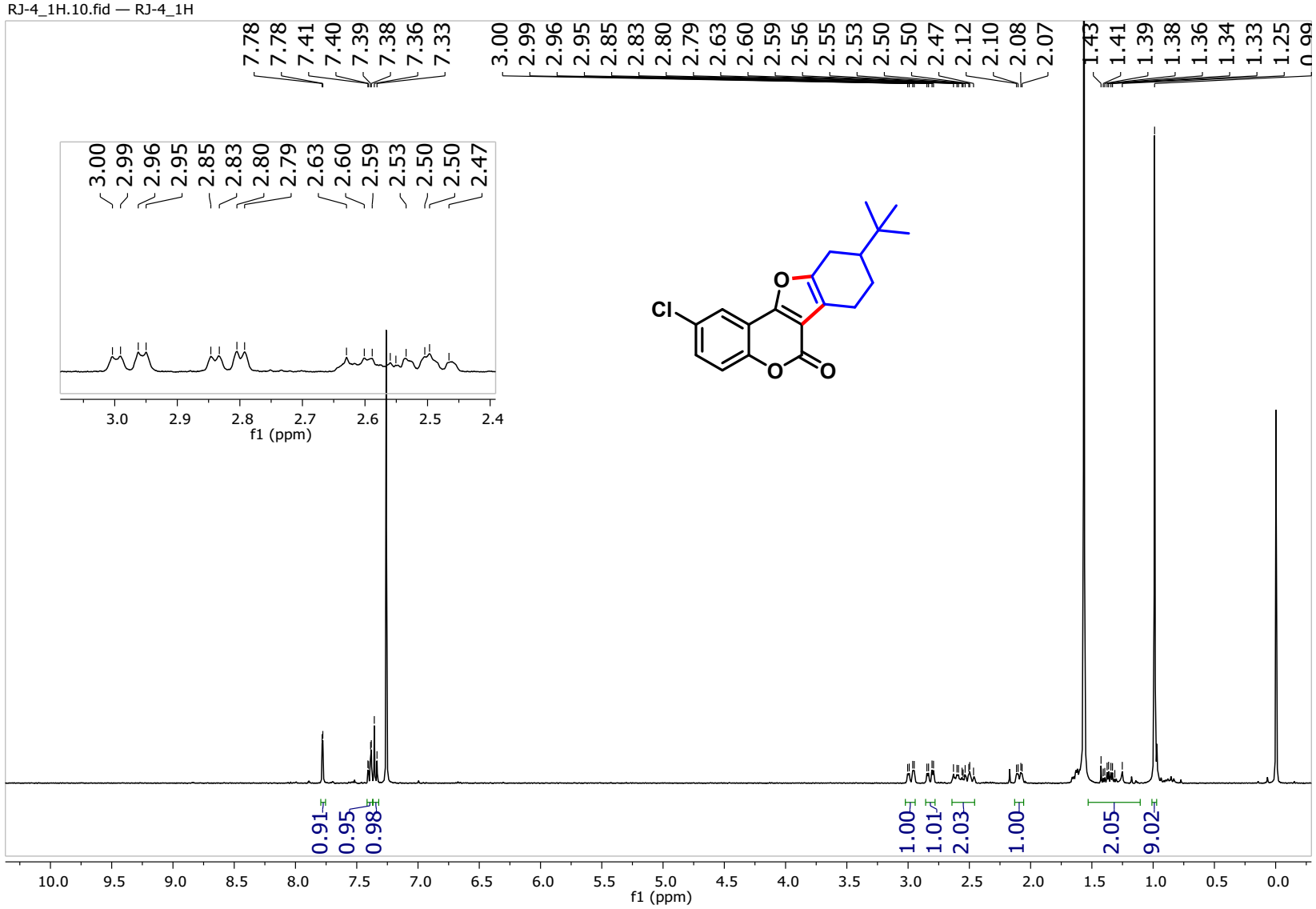


HRMS Spectrum of 2-Chloro-9-ethyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6c)

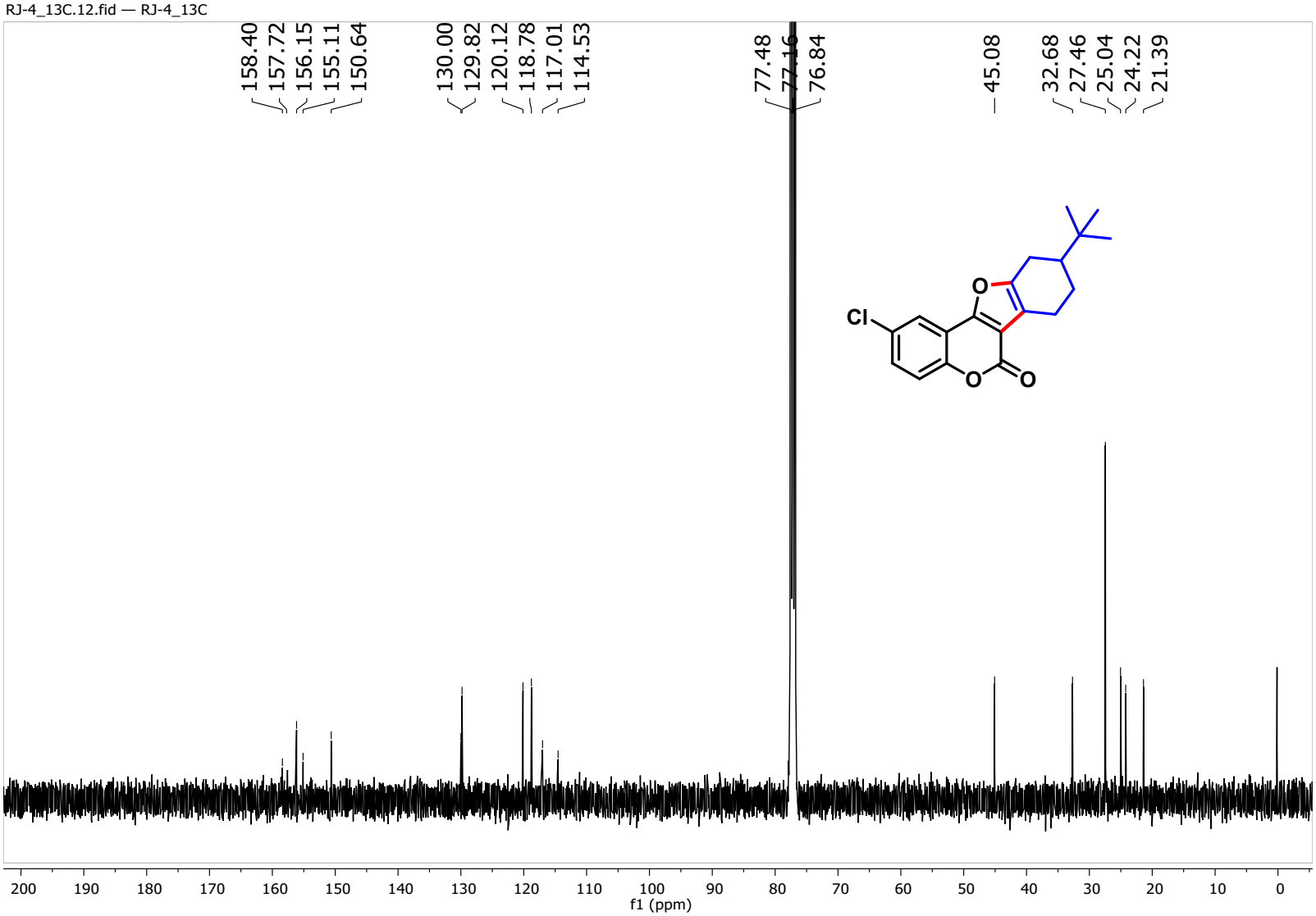
Sample Name		**Position**	P1-B2	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-D-121.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	26-09-2023 16:10:55 (UTC+05:30)



^{1}H NMR Spectrum of 9-(*tert*-Butyl)-2-chloro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6d)

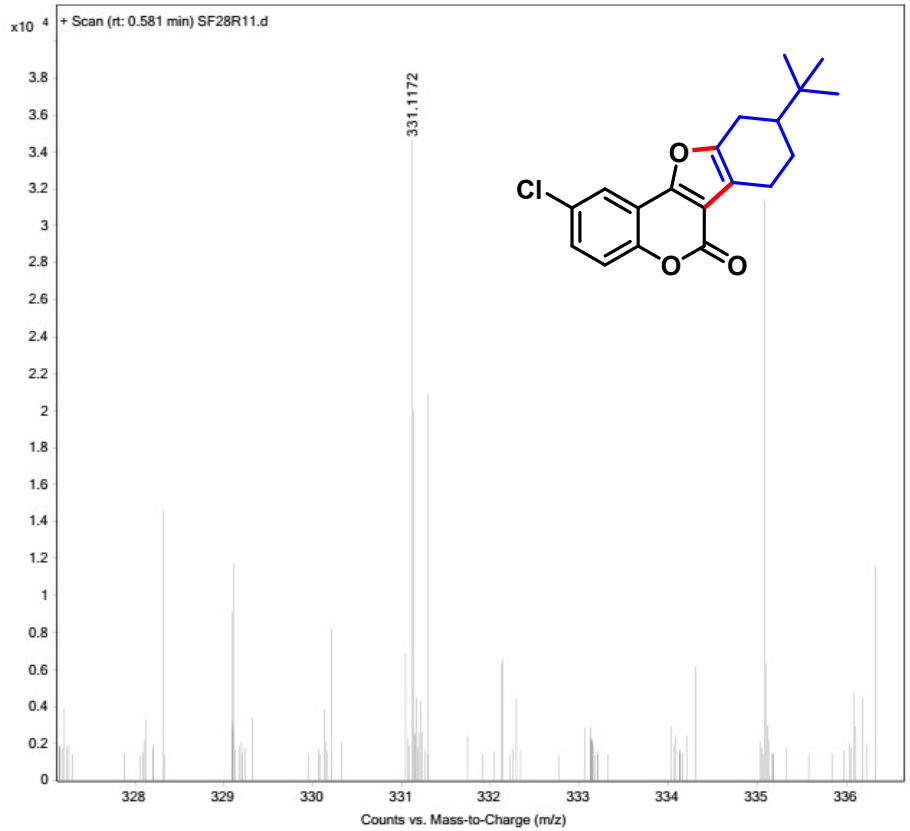


^{13}C NMR Spectrum of 9-(*tert*-Butyl)-2-chloro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6d)

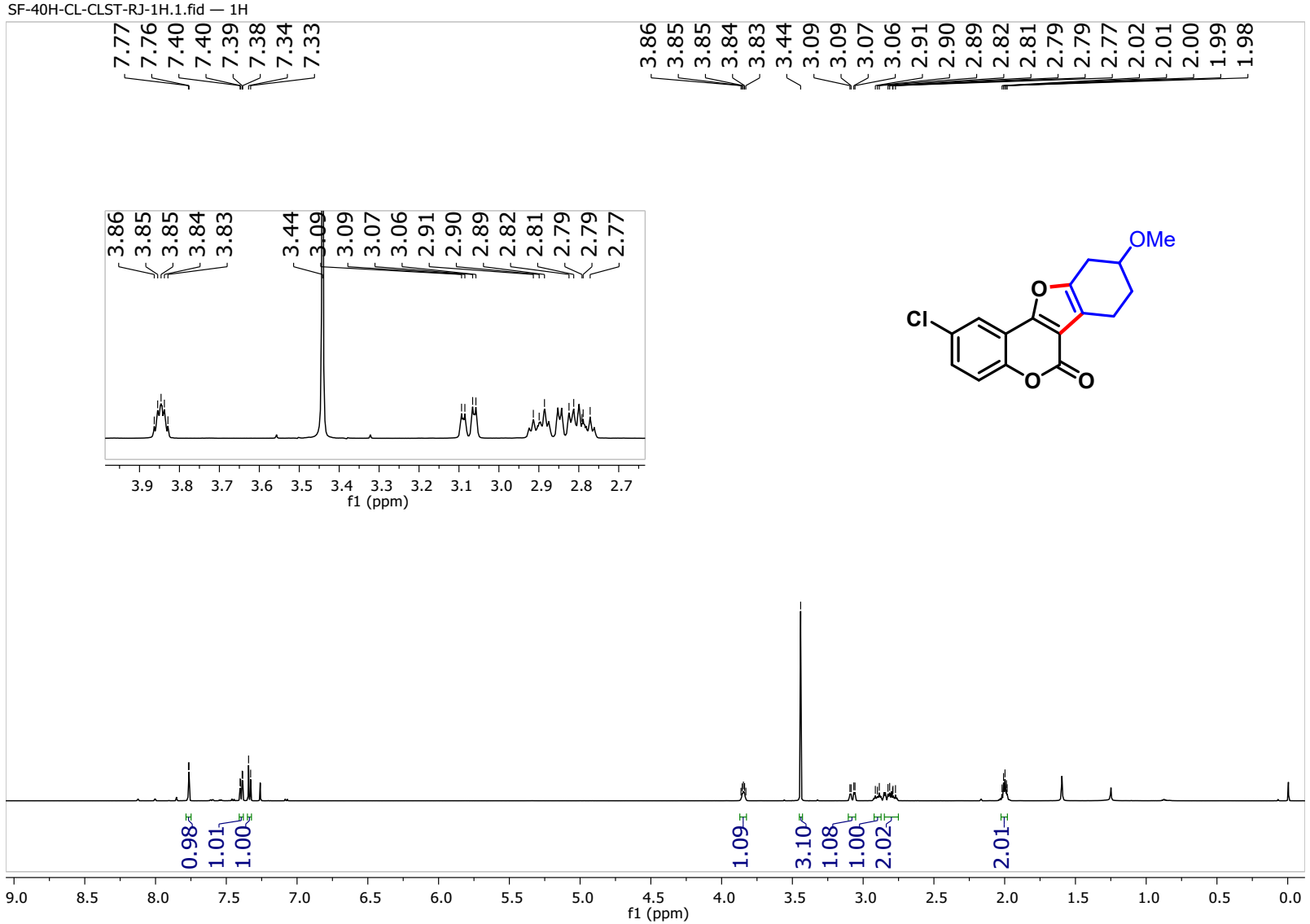


HRMS Spectrum of 9-(*tert*-Butyl)-2-chloro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6d)

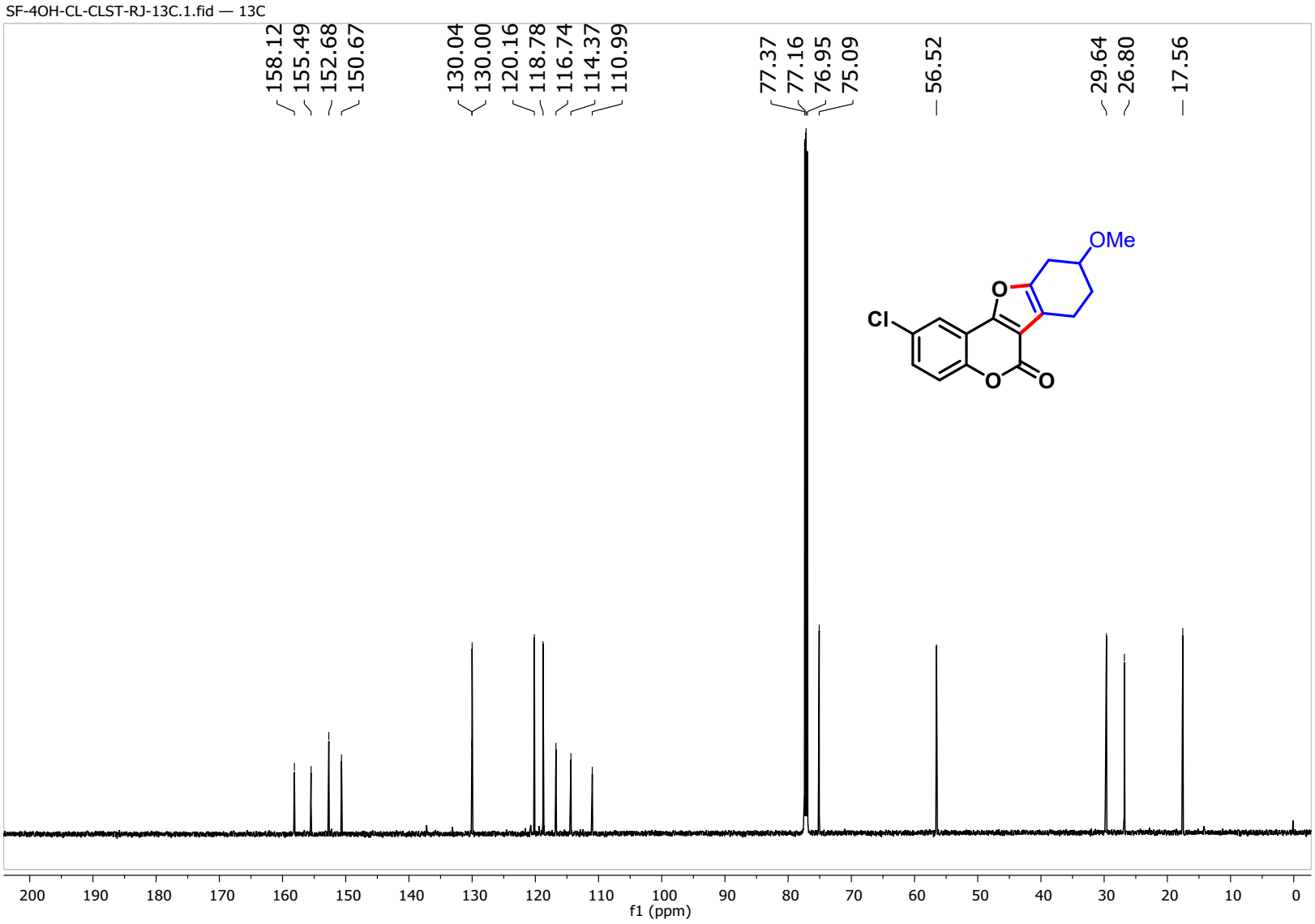
Sample Name	Sample8	**Position**	P1-A8	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF28R11.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	13-10-2023 10:10:28 (UTC+05:30)



^{1}H NMR Spectrum of 2-Chloro-9-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6e)

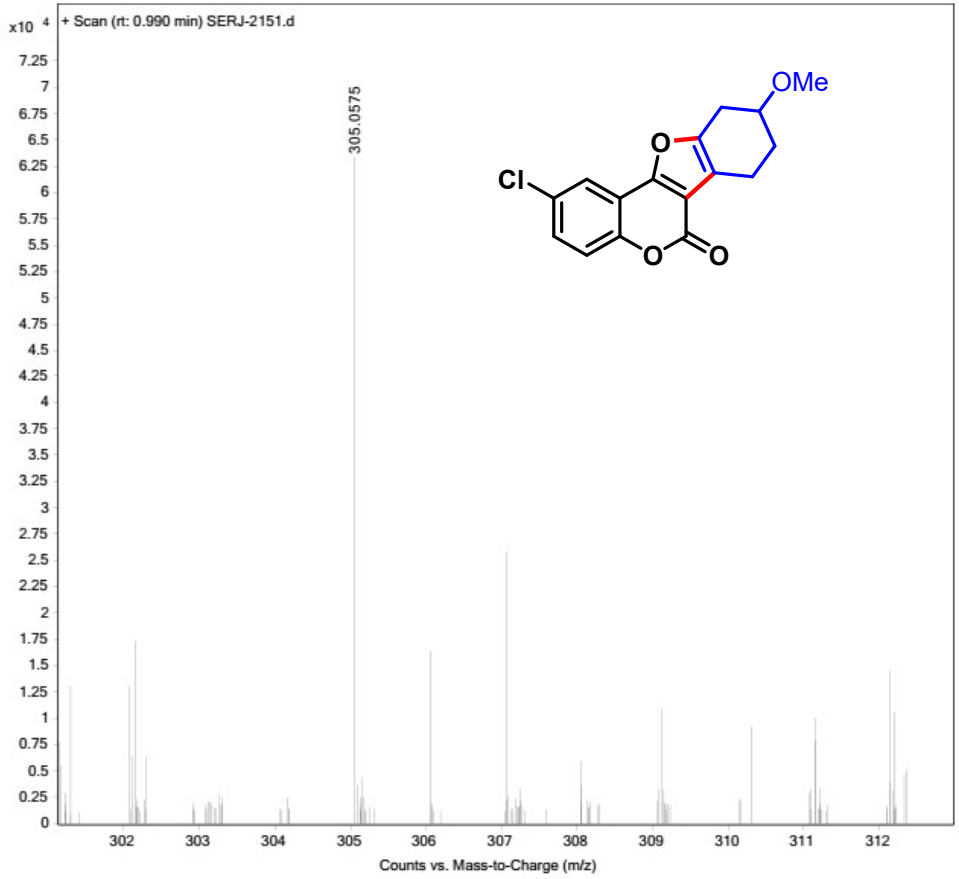


^{13}C NMR Spectrum of 2-Chloro-9-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6e)

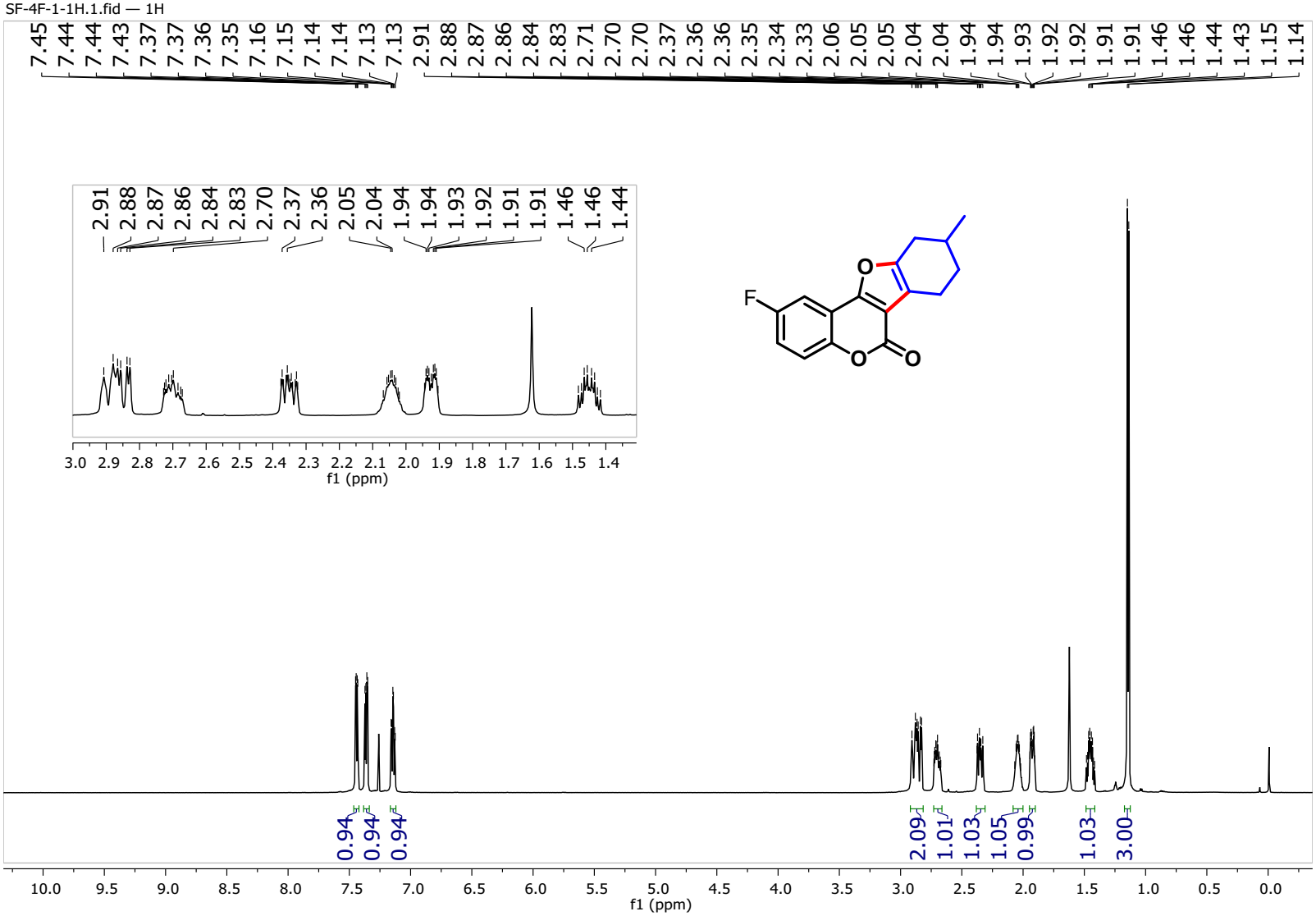


HRMS Spectrum of 2-Chloro-9-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (6e)

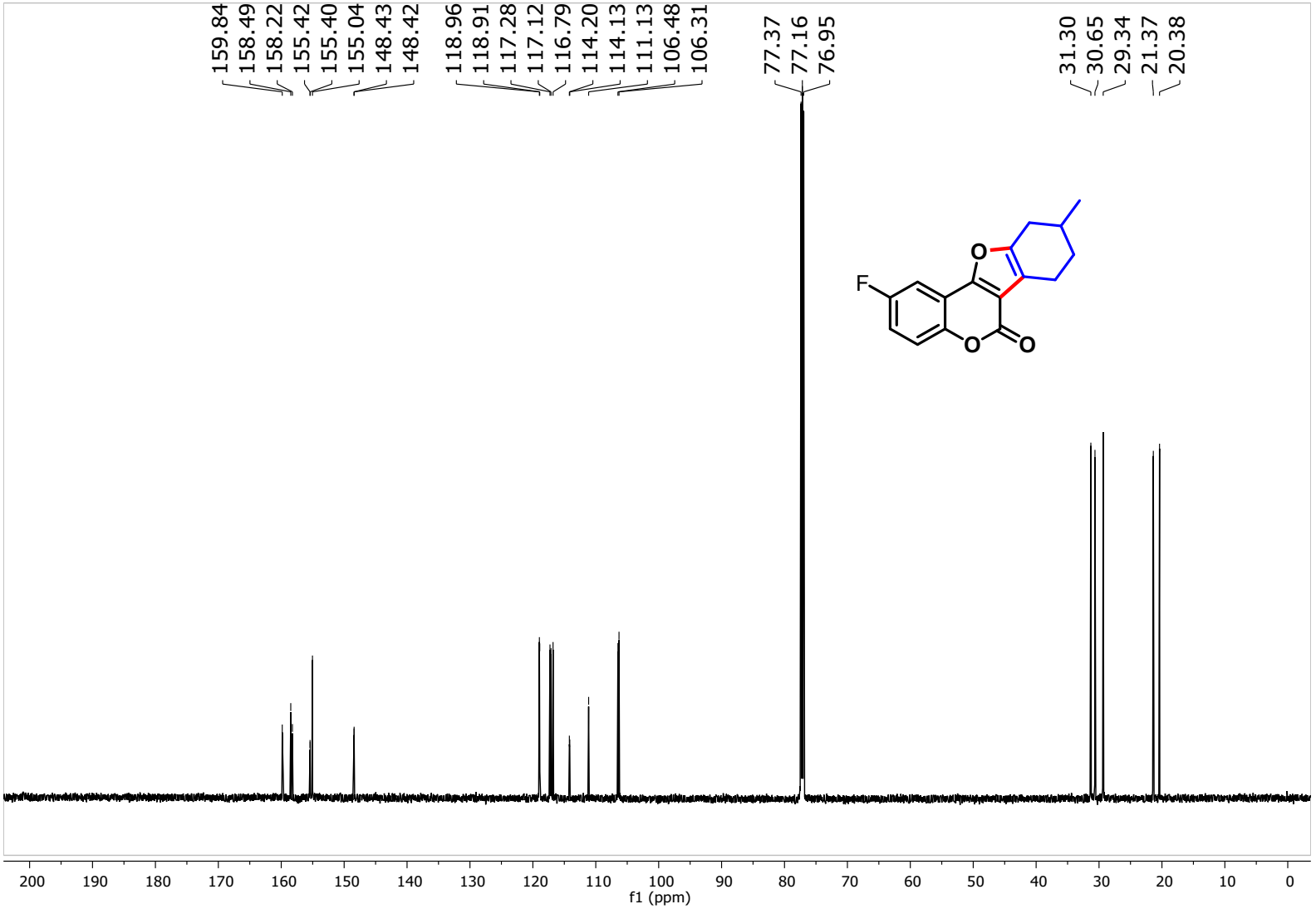
Sample Name	Sample18	**Position**	P1-B7	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SERJ-2151.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	26-10-2023 11:04:12 (UTC+05:30)



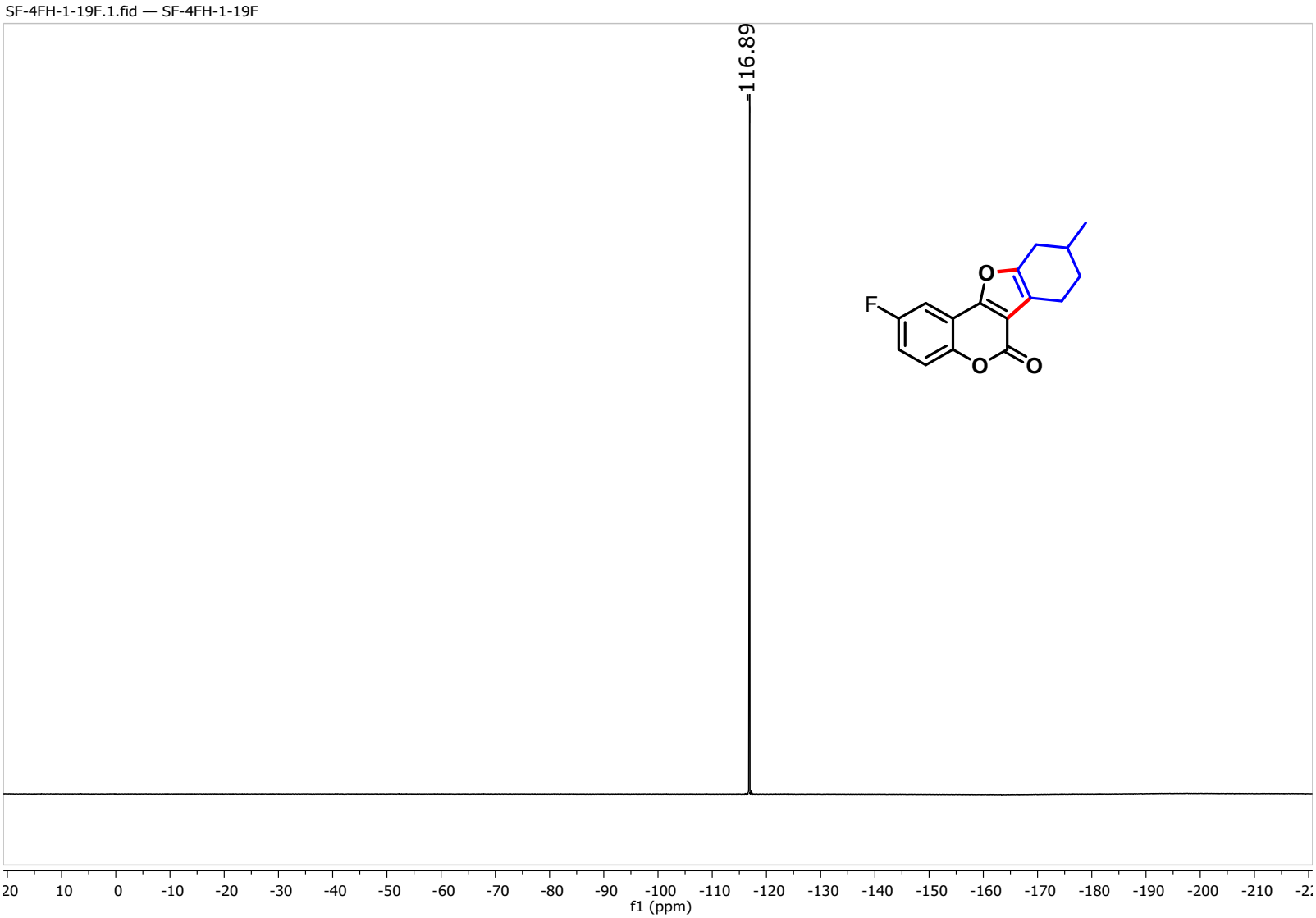
^{1}H NMR Spectrum of 2-Fluoro-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7a)



^{13}C NMR Spectrum of 2-Fluoro-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7a)

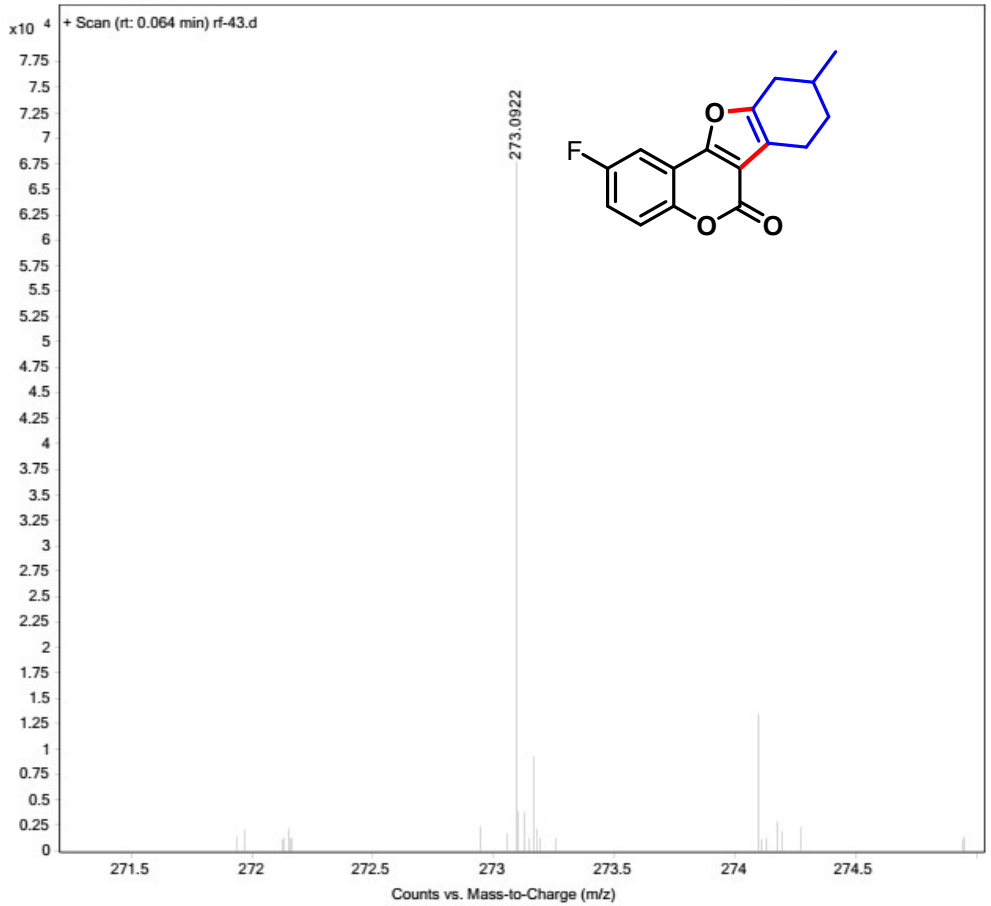


^{19}F NMR Spectrum of 2-Fluoro-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7a)

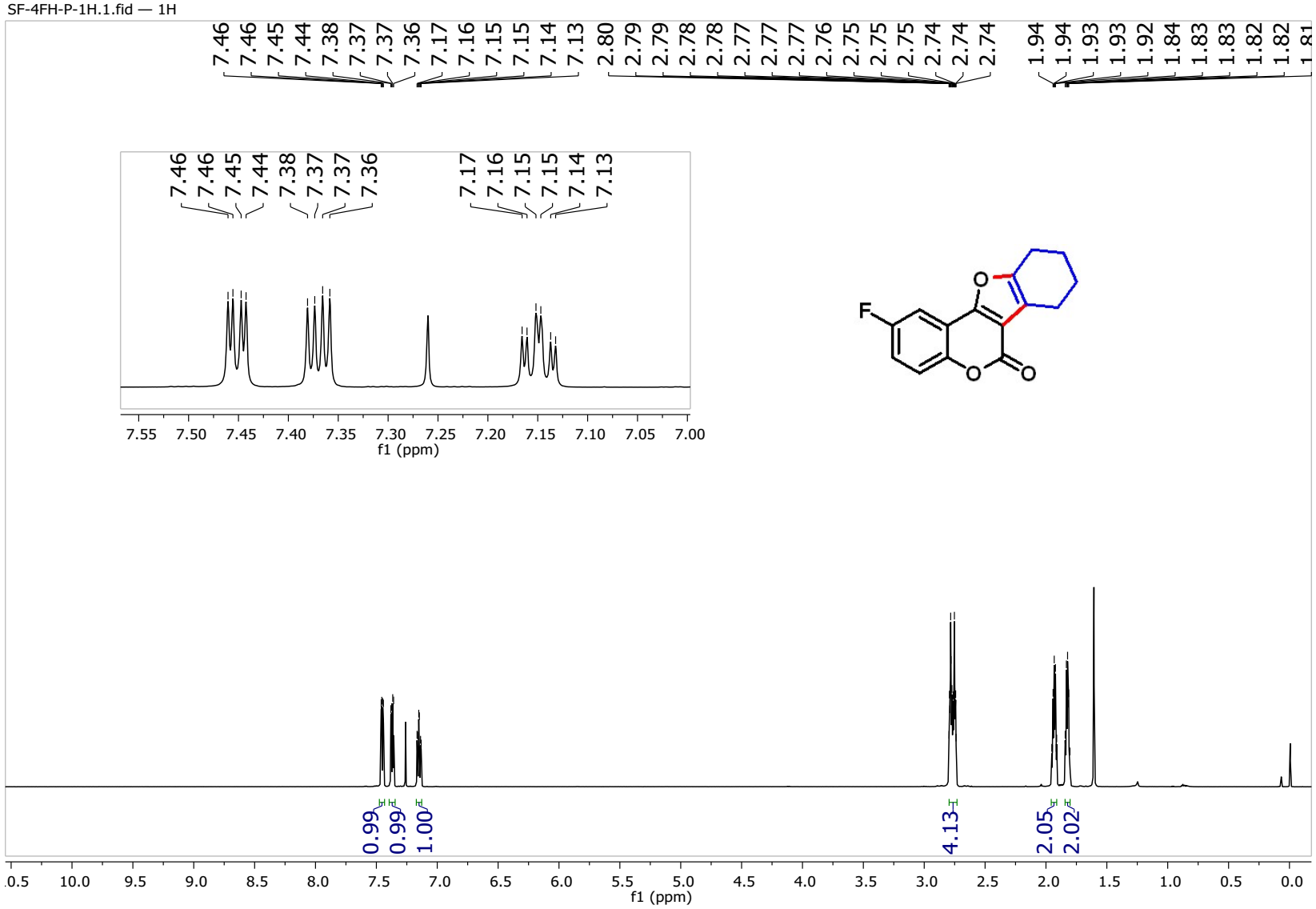


HRMS Spectrum of 2-Fluoro-9-methyl-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7a)

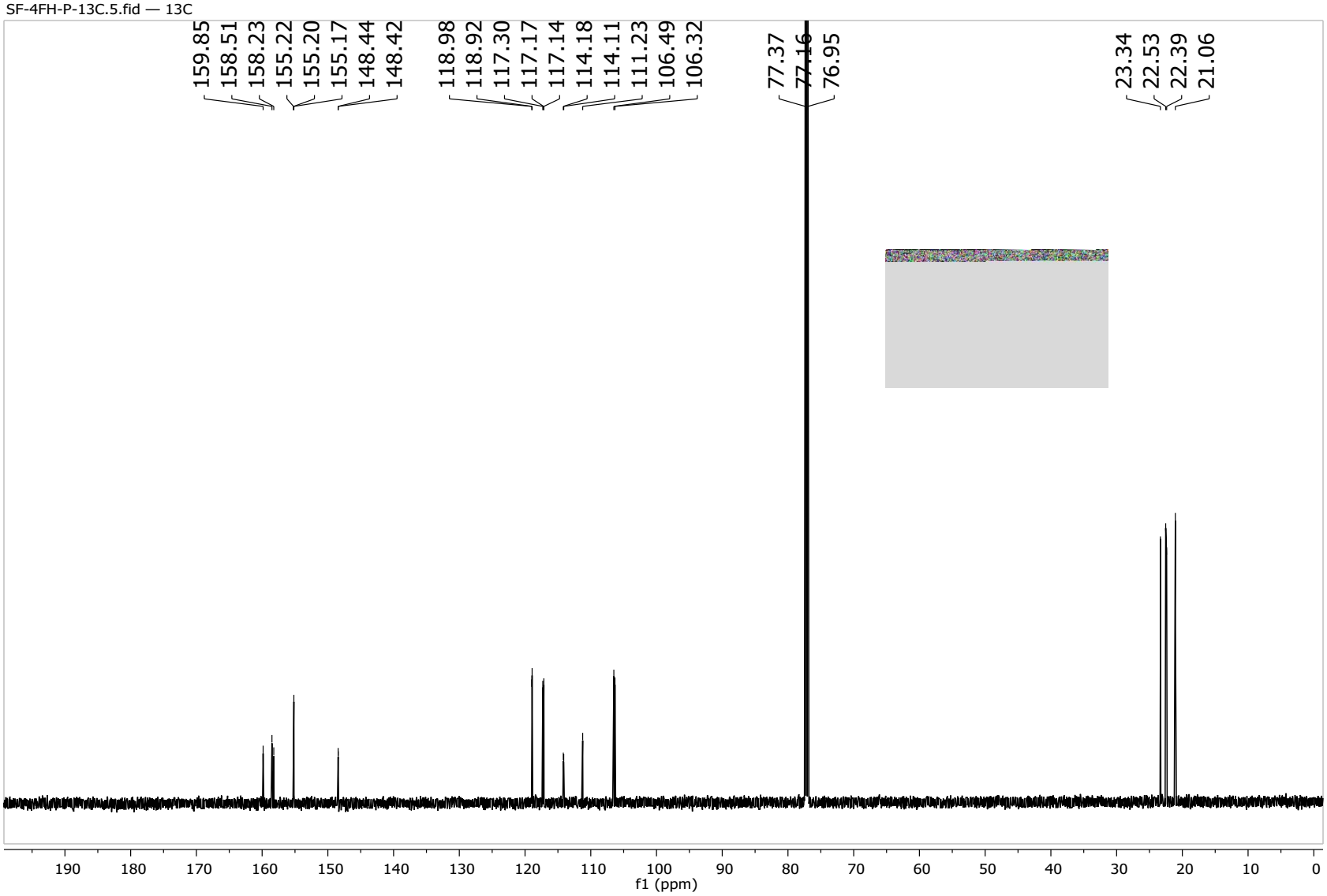
Sample Name	Sample8	**Position**	P1-A8	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	rf-43.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	07-08-2023 14:41:34 (UTC+05:30)



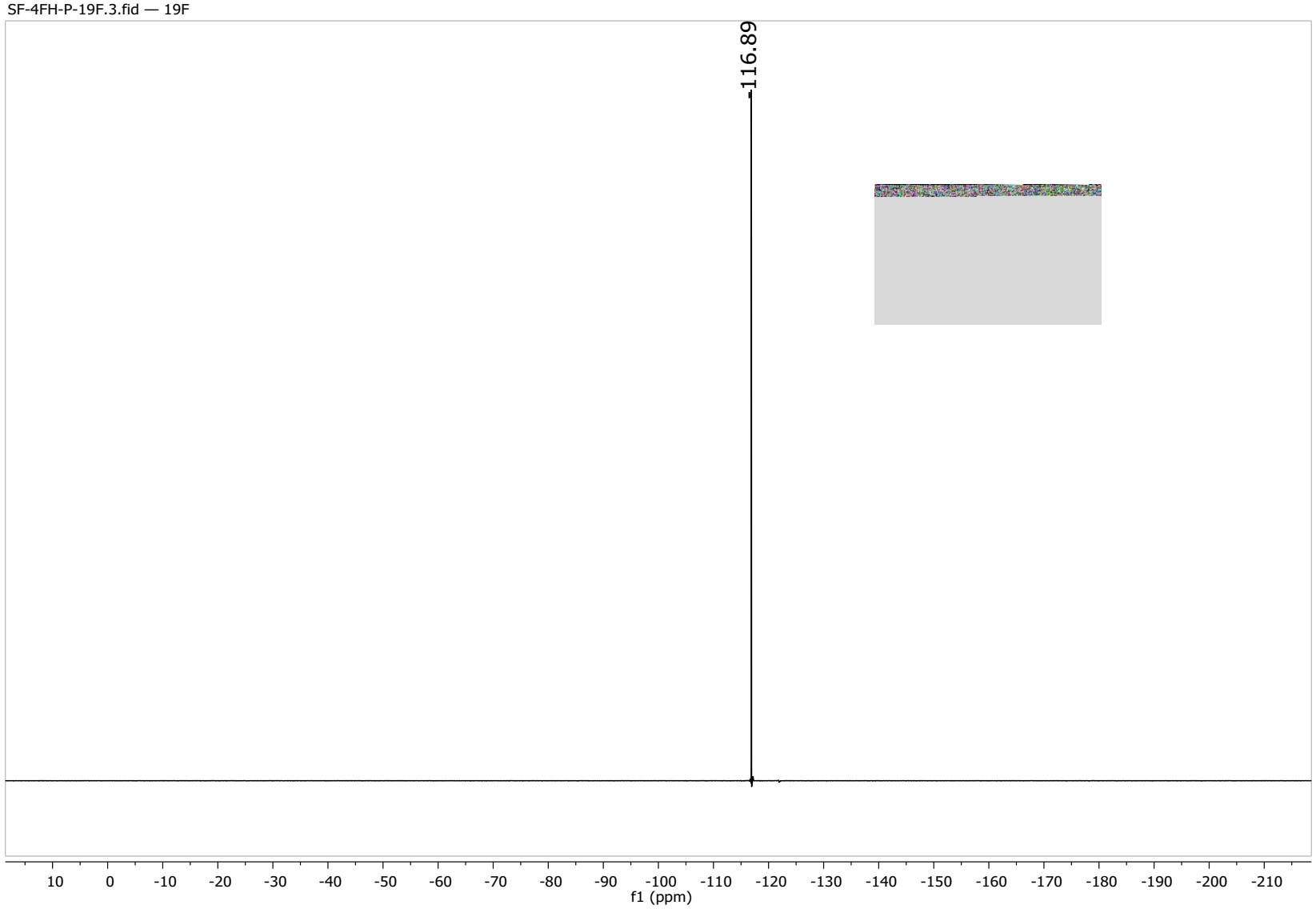
^{1}H NMR Spectrum of 2-Fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7b)



^{13}C NMR Spectrum of 2-Fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7b)

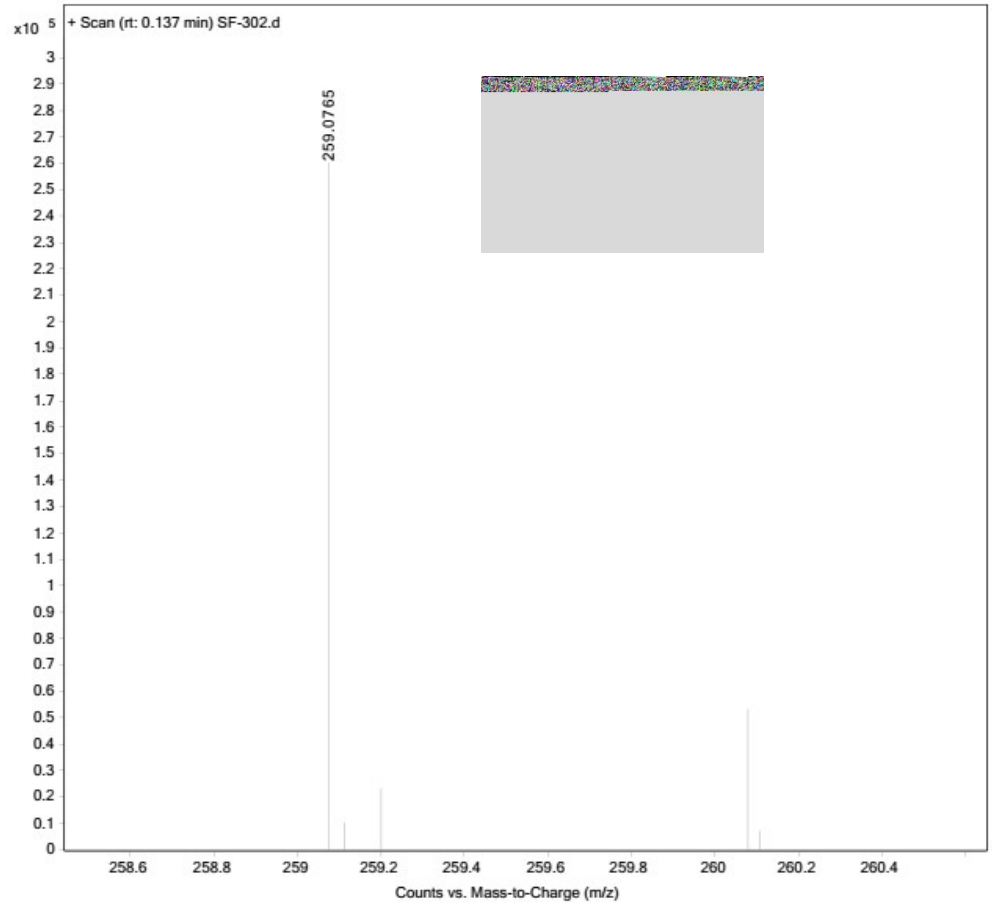


^{19}F NMR Spectrum of 2-Fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7b)

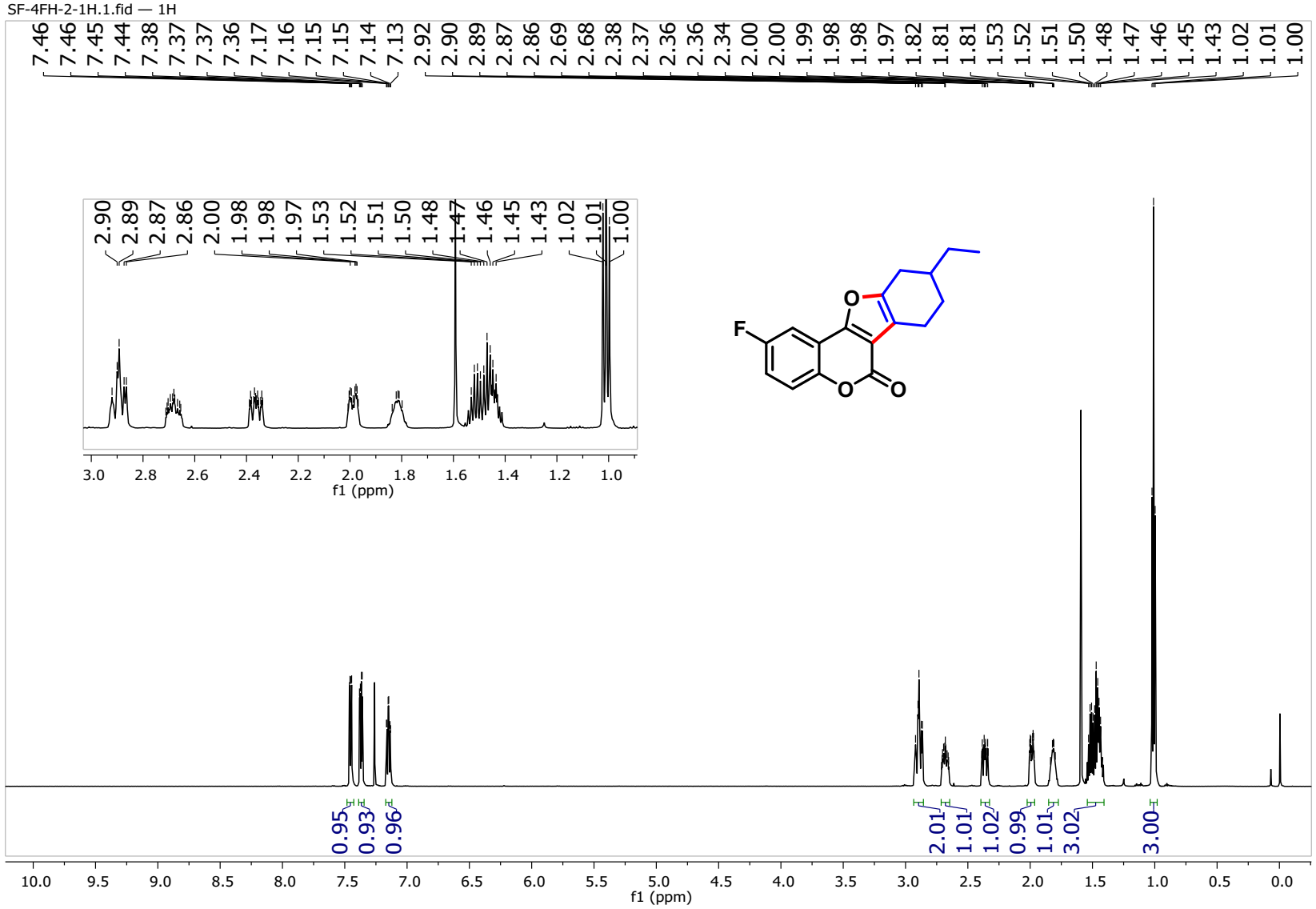


HRMS Spectrum of 2-Fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7b)

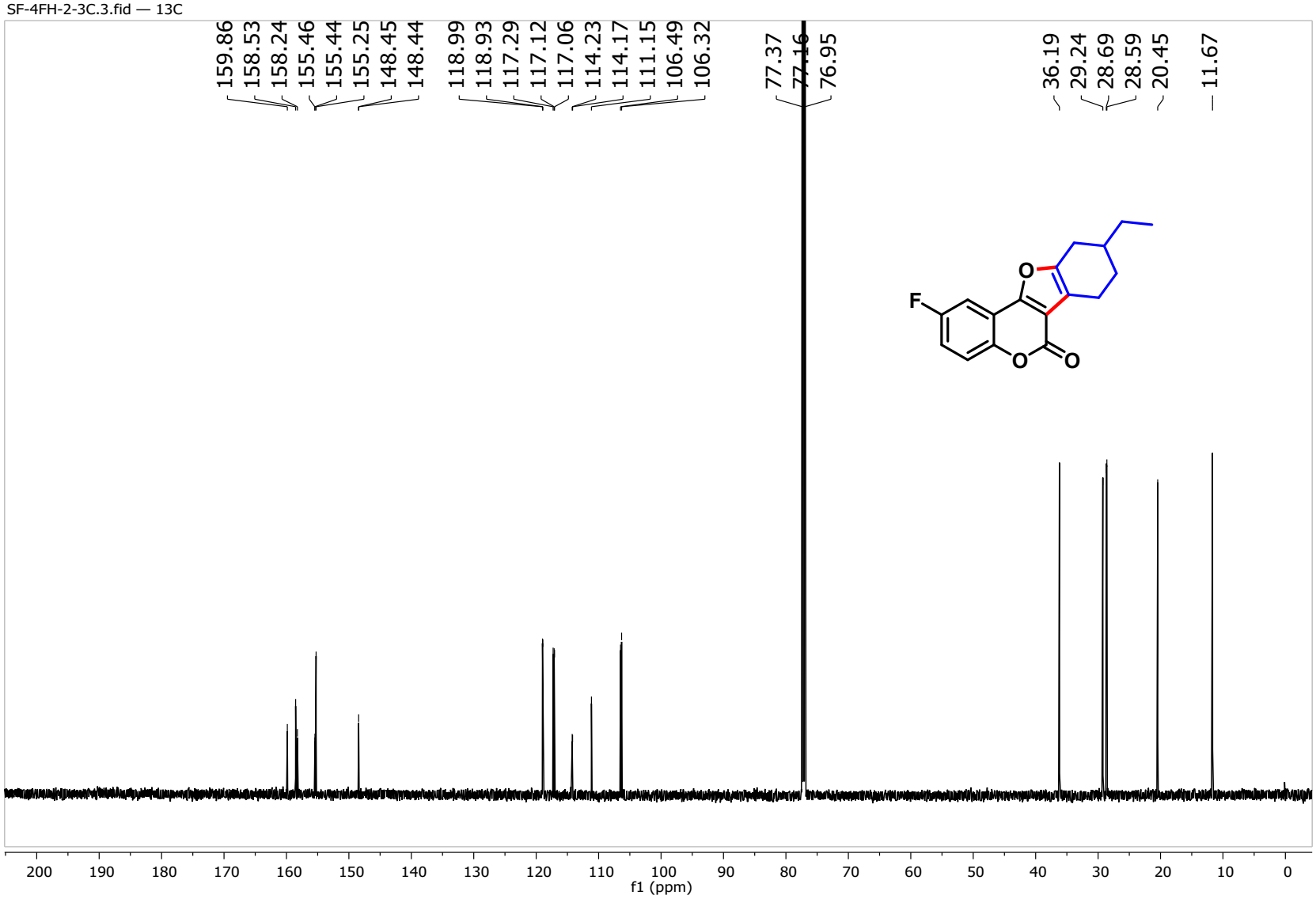
Sample Name	Sample47	**Position**	P1-E1	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-302.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	24-04-2023 15:23:24 (UTC+05:30)



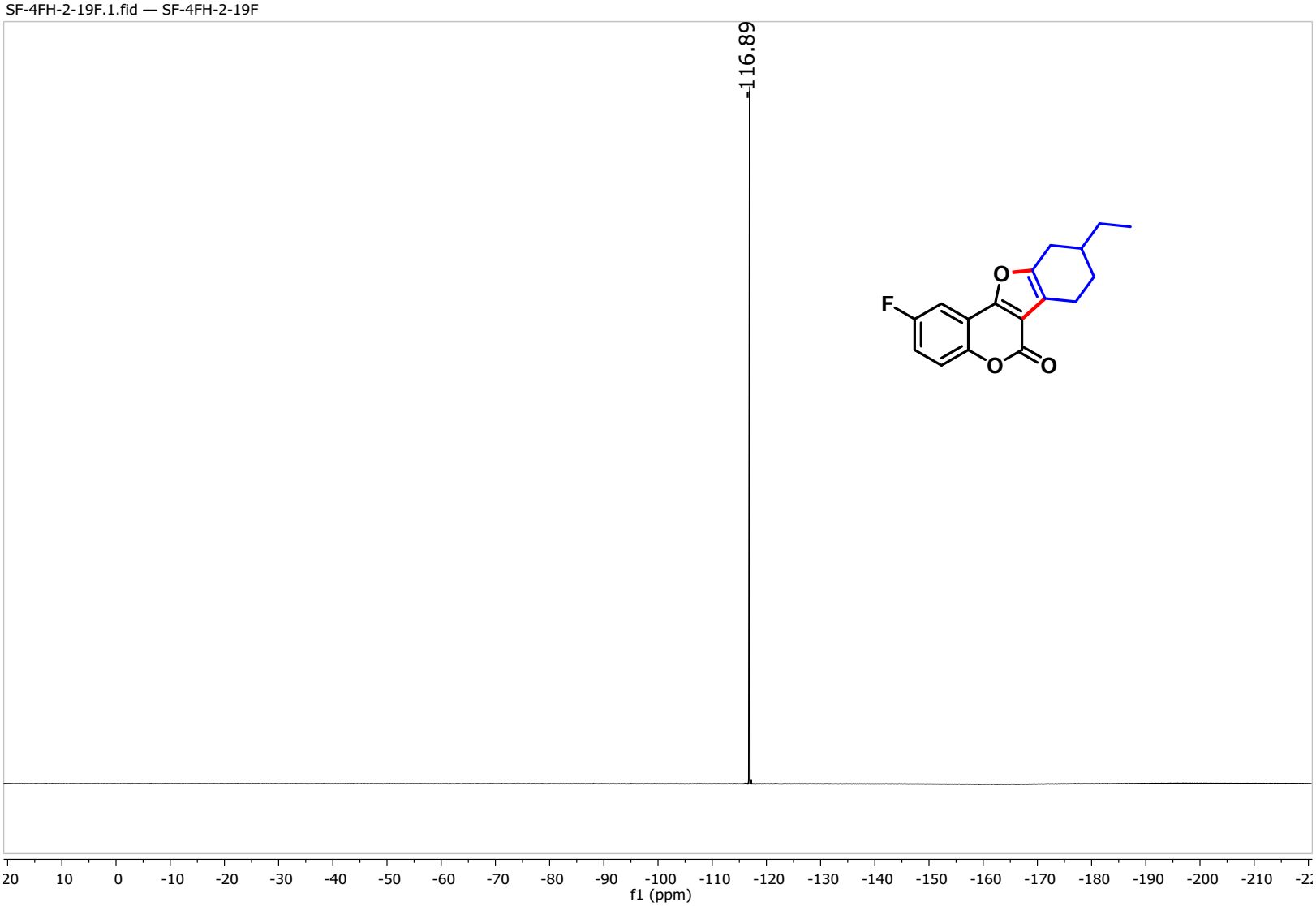
^{1}H NMR Spectrum of 9-Ethyl-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7c)



^{13}C NMR Spectrum of 9-Ethyl-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7c)

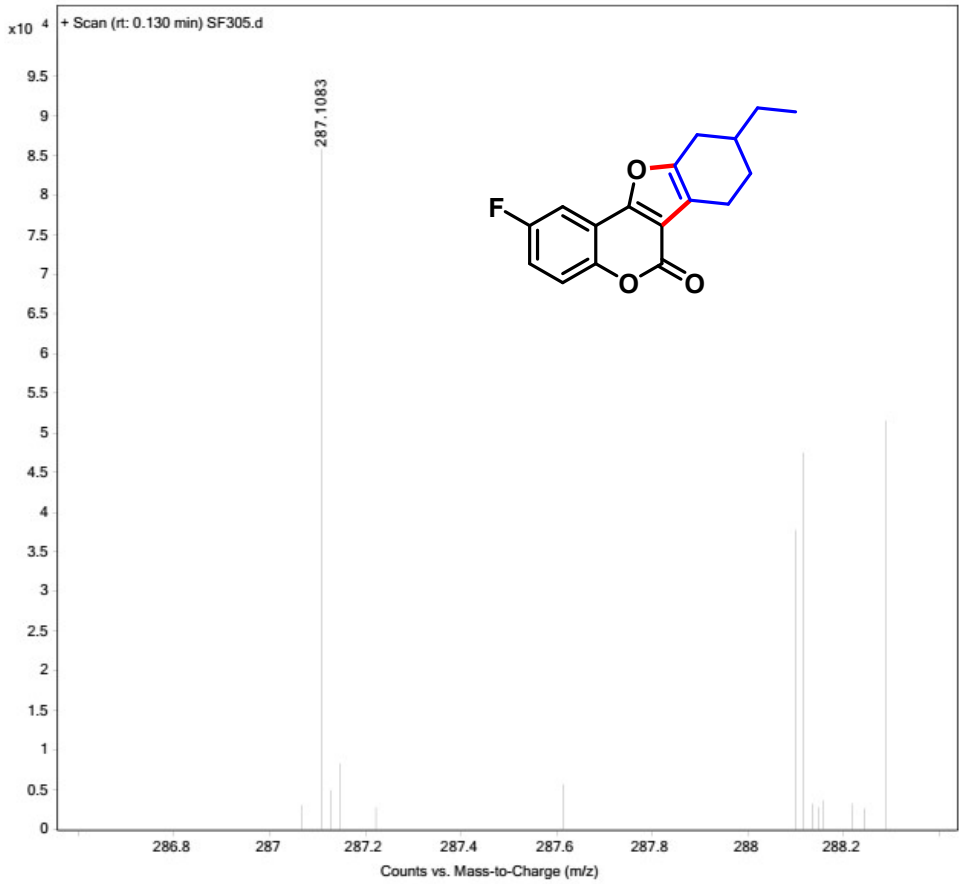


^{19}F NMR Spectrum of 9-Ethyl-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7c)

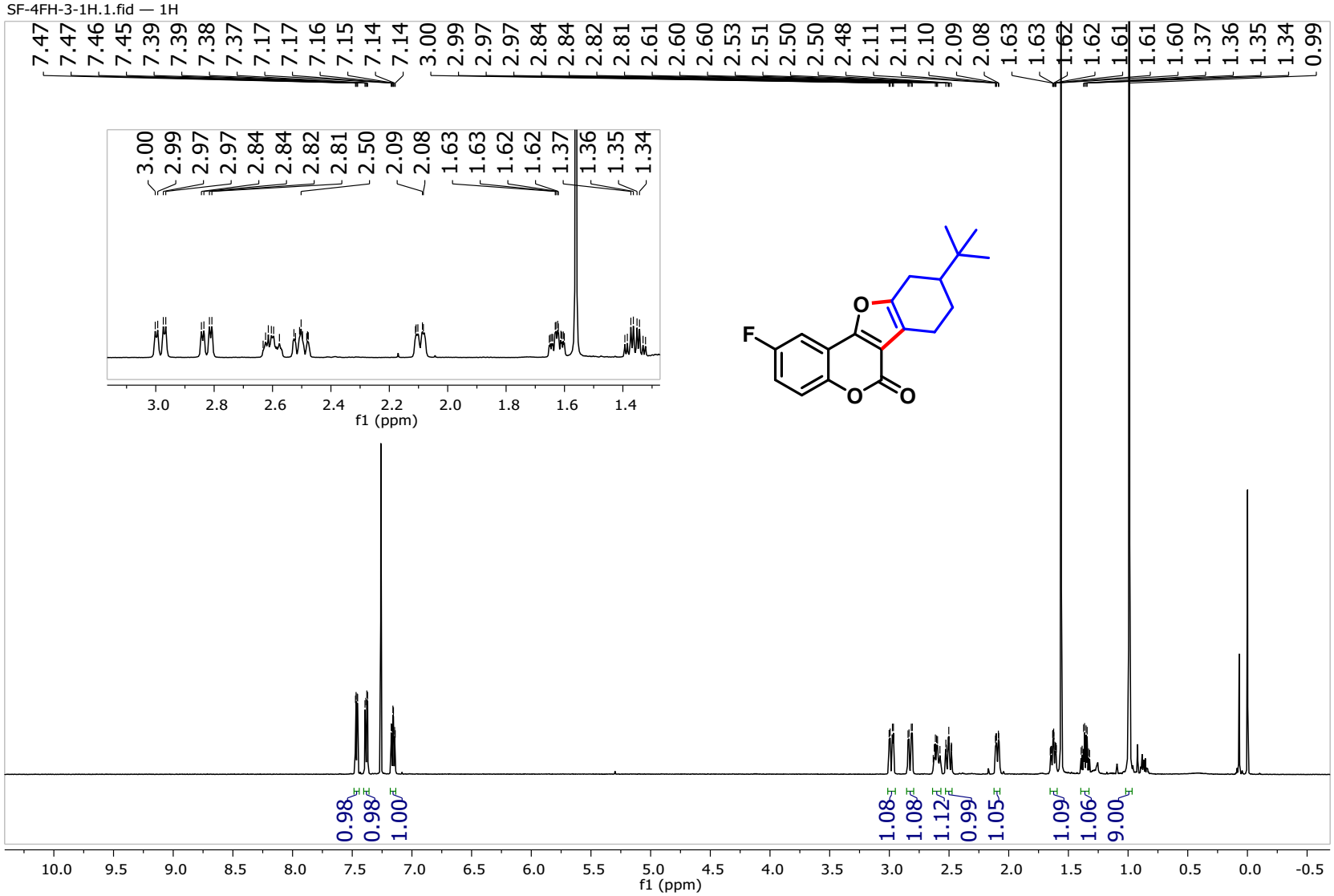


HRMS Spectrum of 9-Ethyl-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7c)

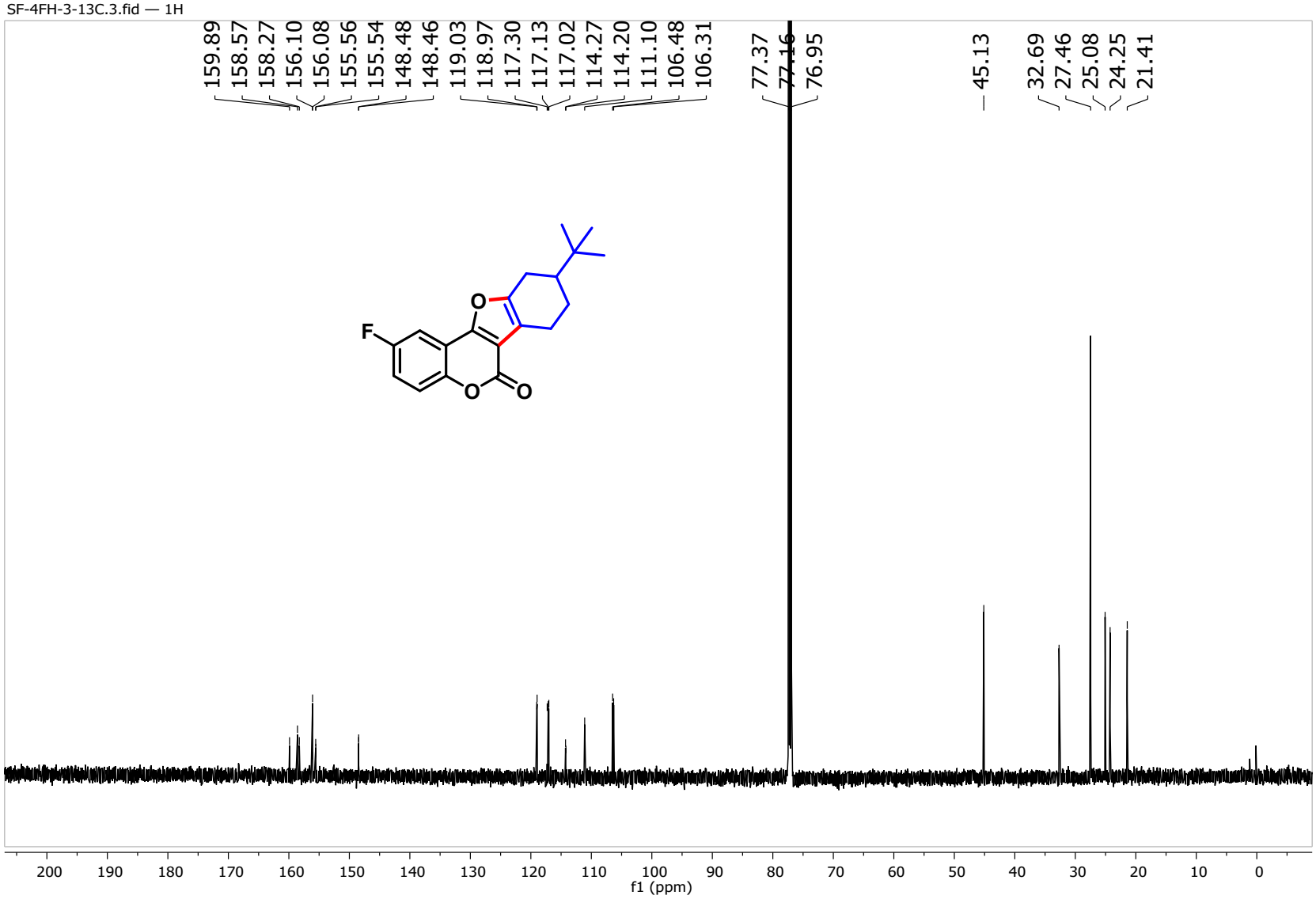
Sample Name	Sample3	**Position**	P1-A3	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF305.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	25-04-2023 15:40:32 (UTC+05:30)



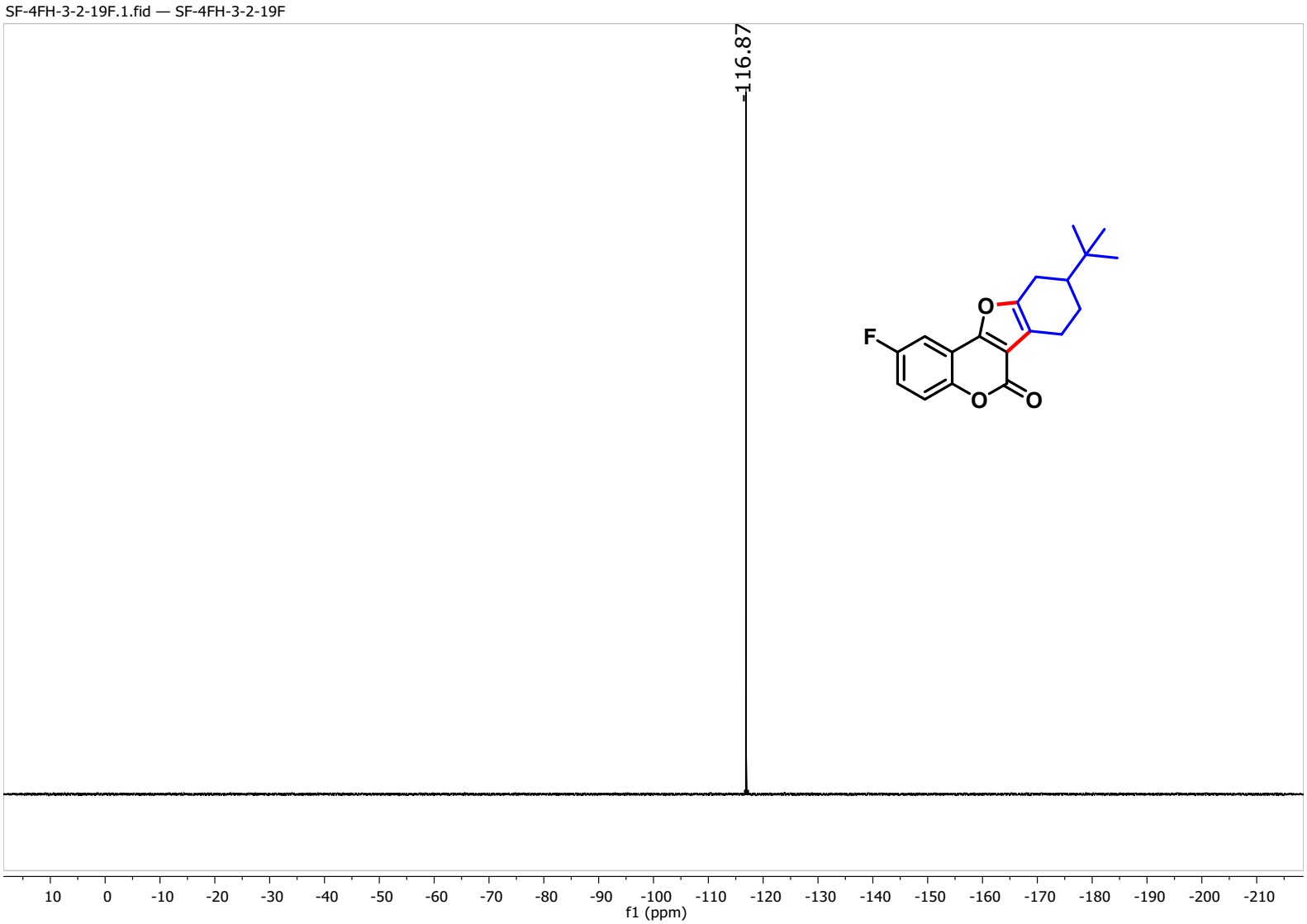
^{1}H NMR Spectrum of 9-(*tert*-Butyl)-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7d)



^{13}C NMR Spectrum of 9-(*tert*-Butyl)-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7d)

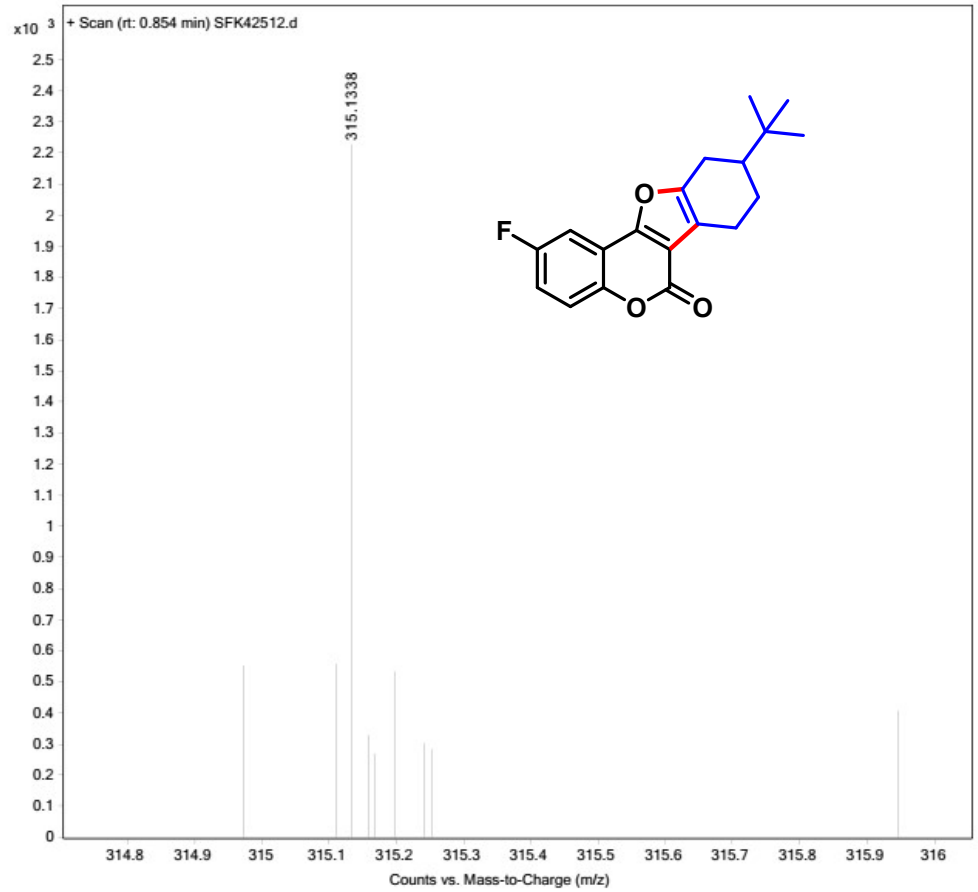


^{19}F NMR Spectrum of 9-(*tert*-Butyl)-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7d)

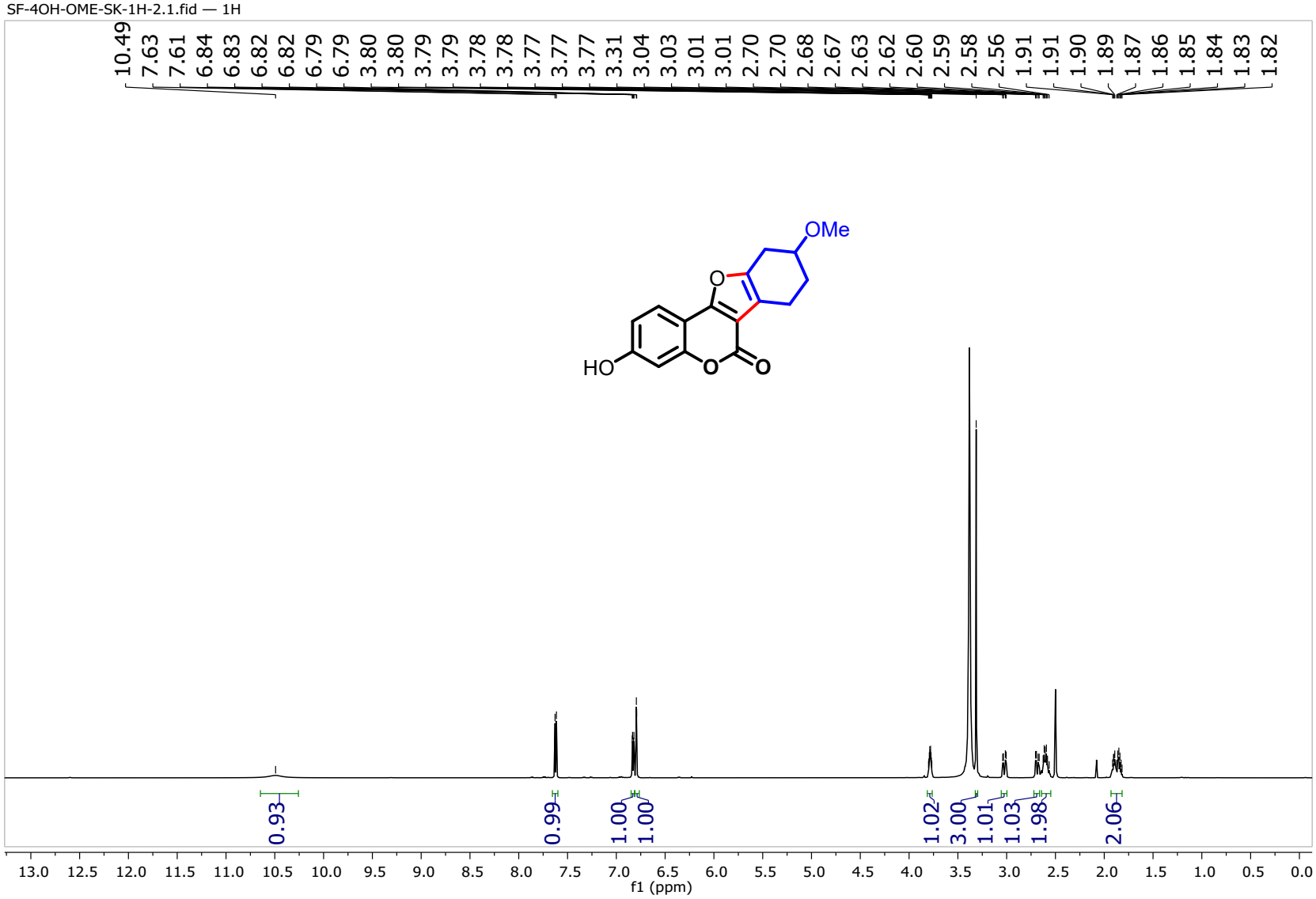


HRMS Spectrum of 9-(*tert*-Butyl)-2-fluoro-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (7d)

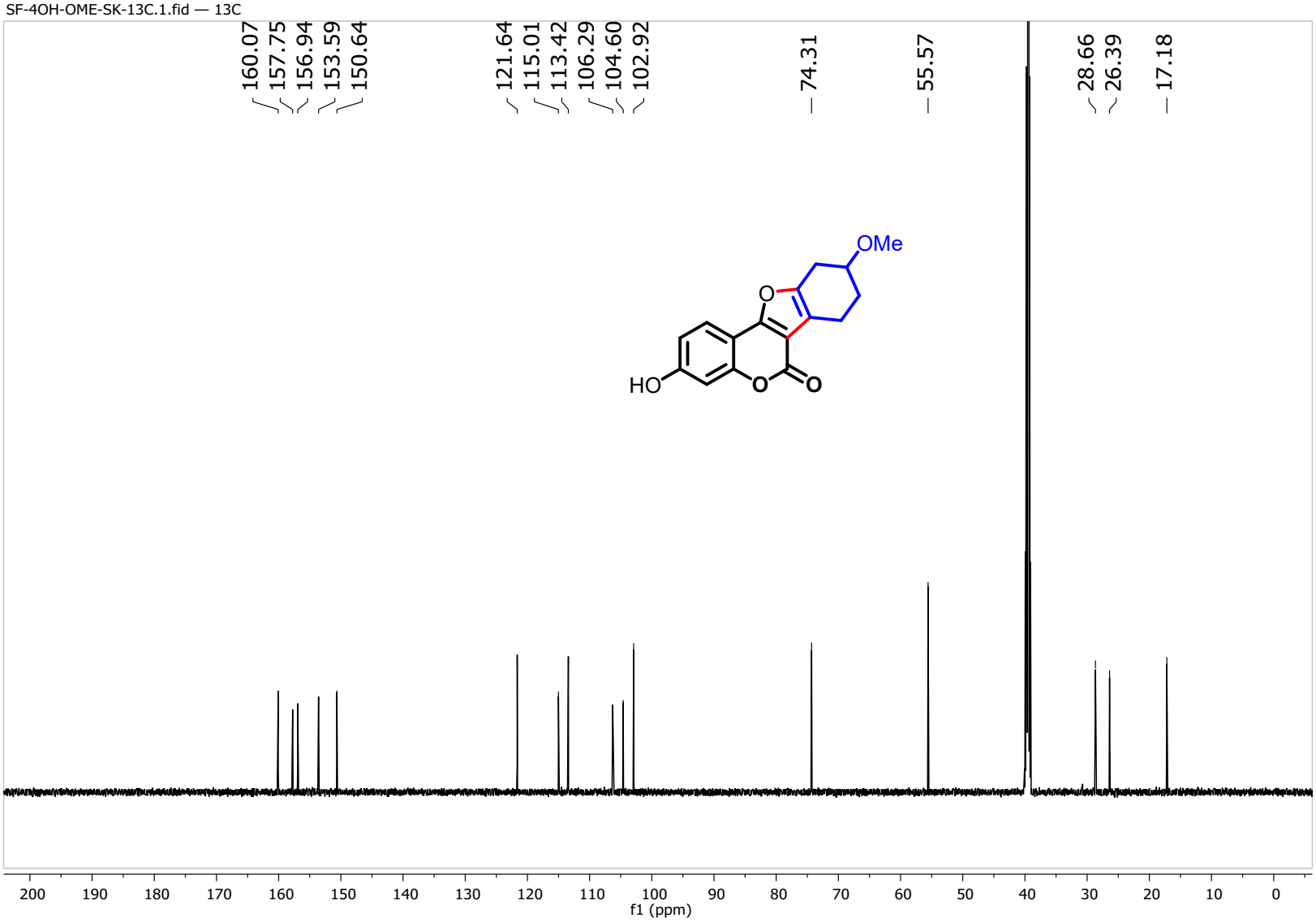
Sample Name		**Position**	P1-B10	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFK42512.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	05-12-2023 15:33:04 (UTC+05:30)



^{1}H NMR Spectrum of 3-Hydroxy-9-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (8a)

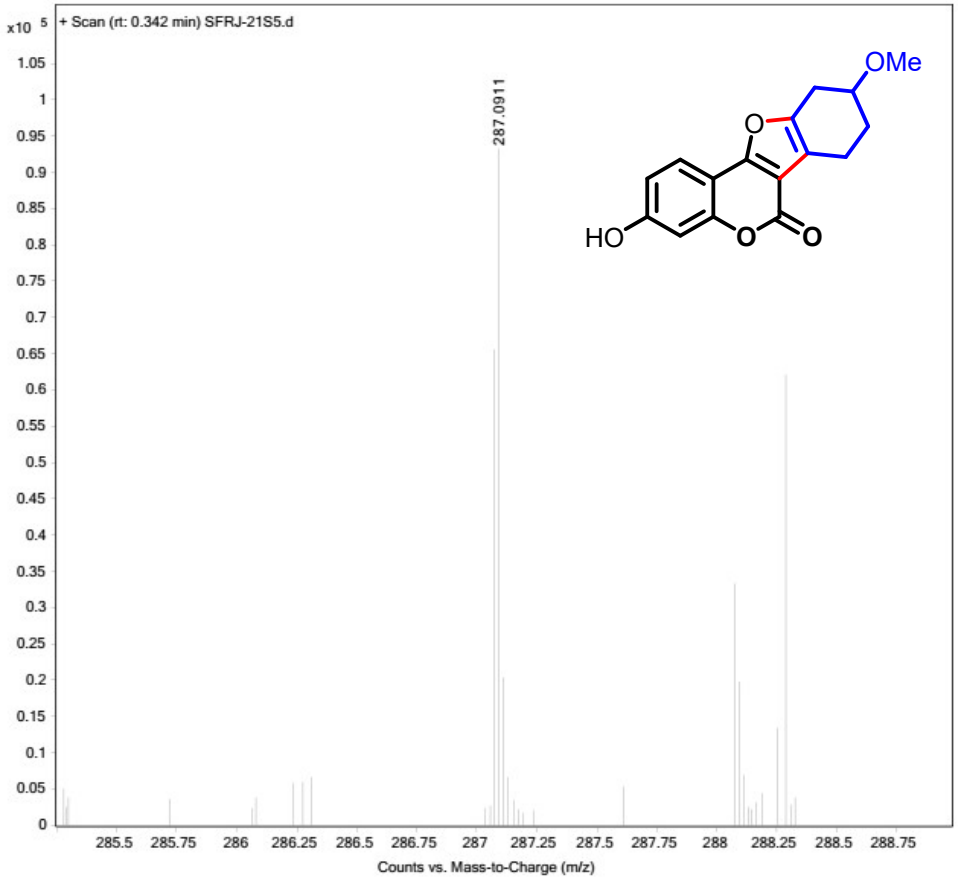


^{13}C NMR Spectrum of 3-Hydroxy-9-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (8a)

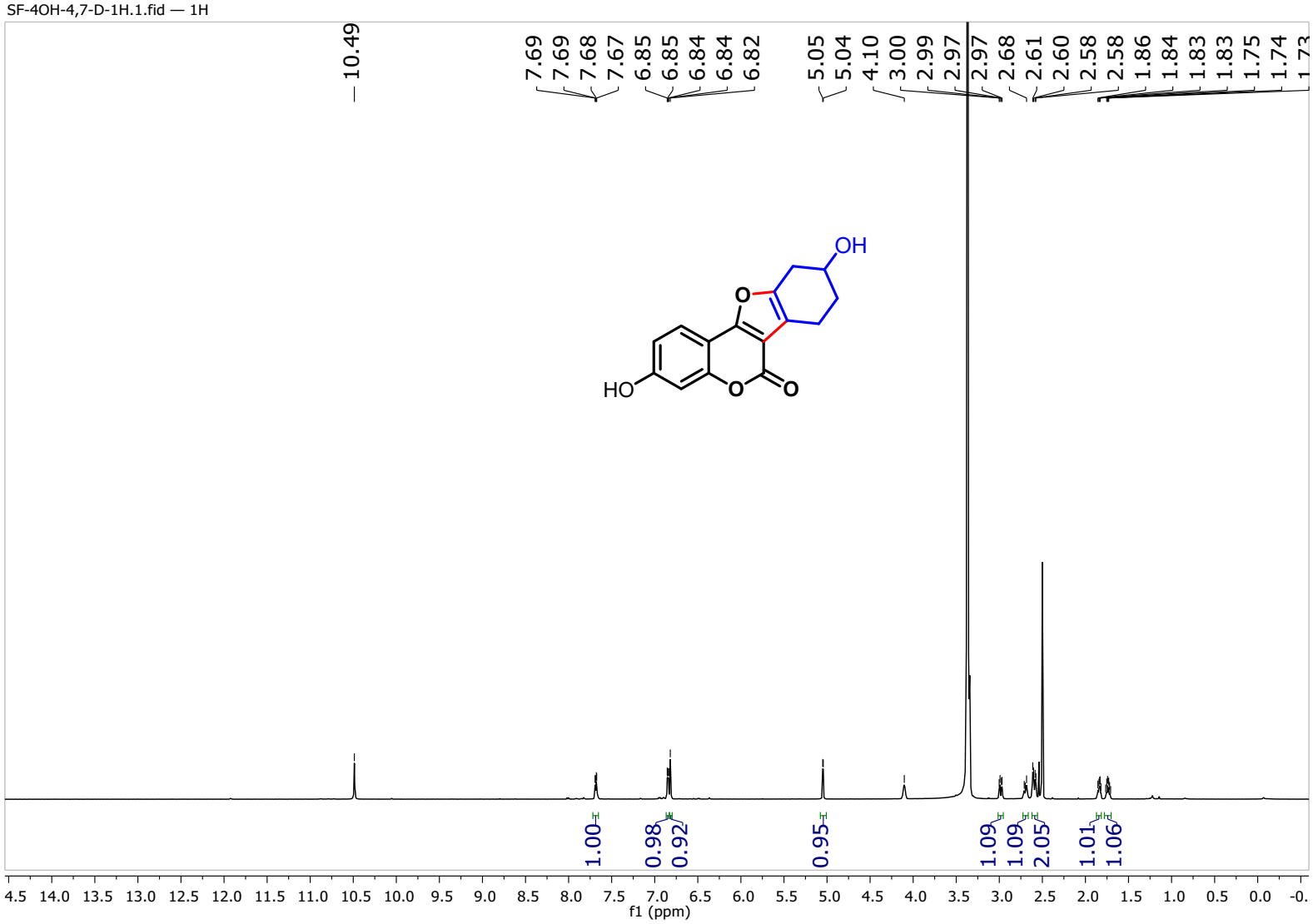


HRMS Spectrum of 3-Hydroxy-9-methoxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (8a)

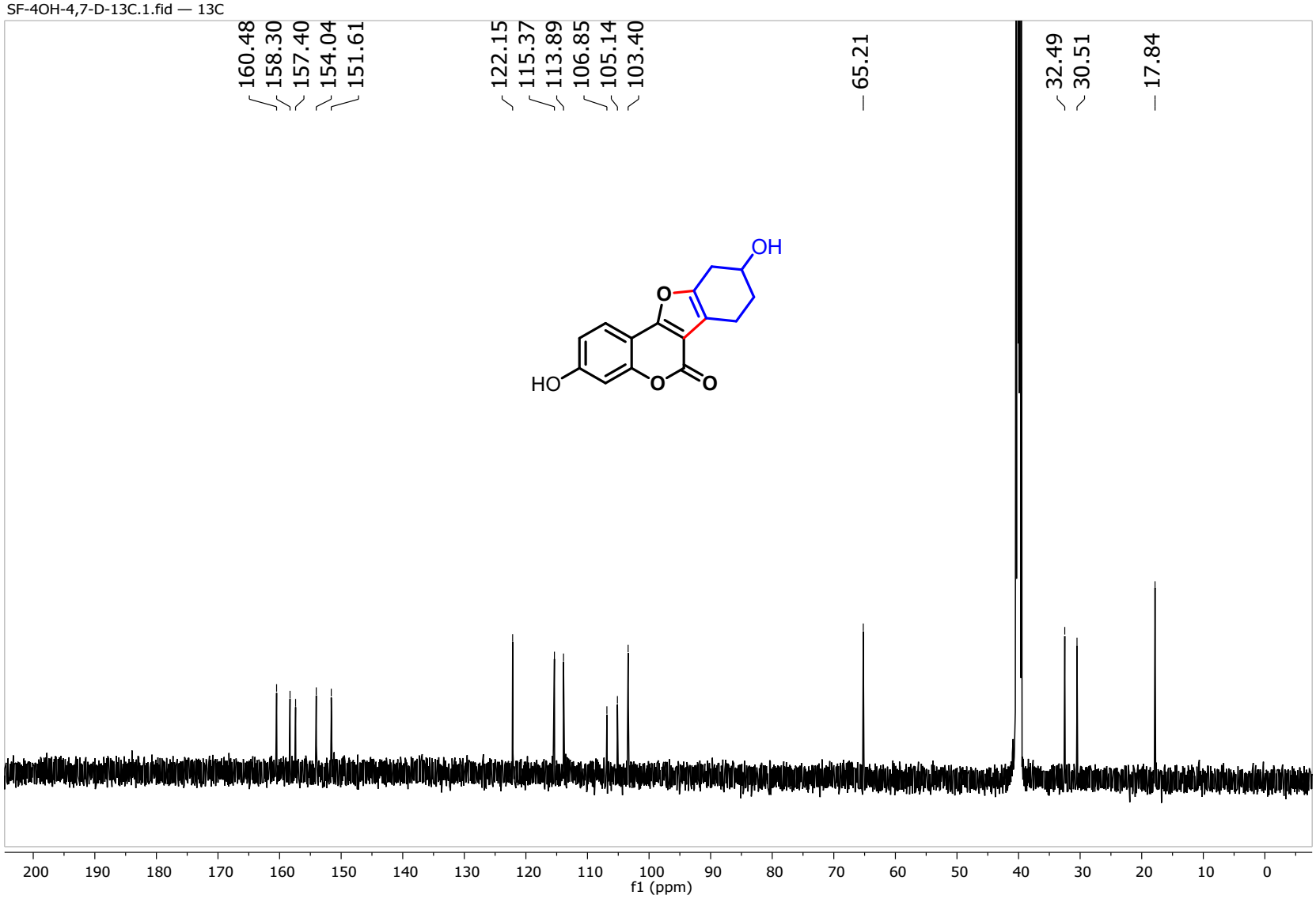
Sample Name	Sample19	**Position**	P1-B8	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFRJ-21S5.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	26-10-2023 11:07:45 (UTC+05:30)



^{1}H NMR Spectrum of 3,9-Dihydroxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (8b)

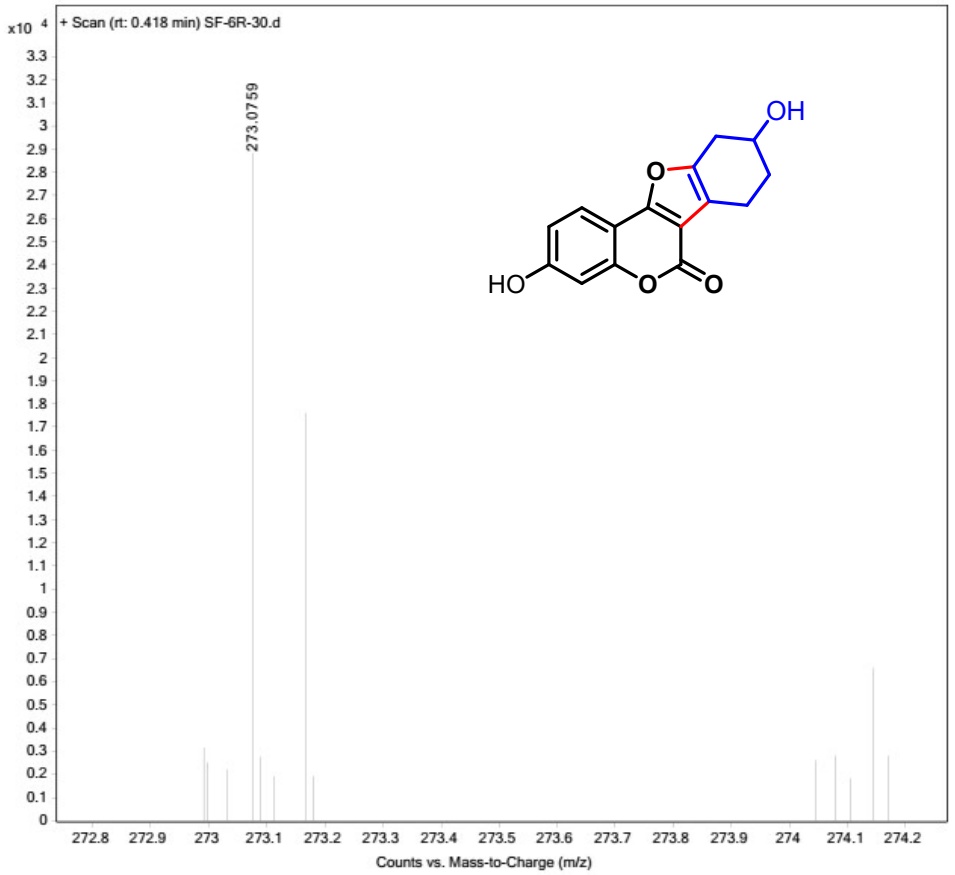


^{13}C NMR Spectrum of 3,9-Dihydroxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (8b)

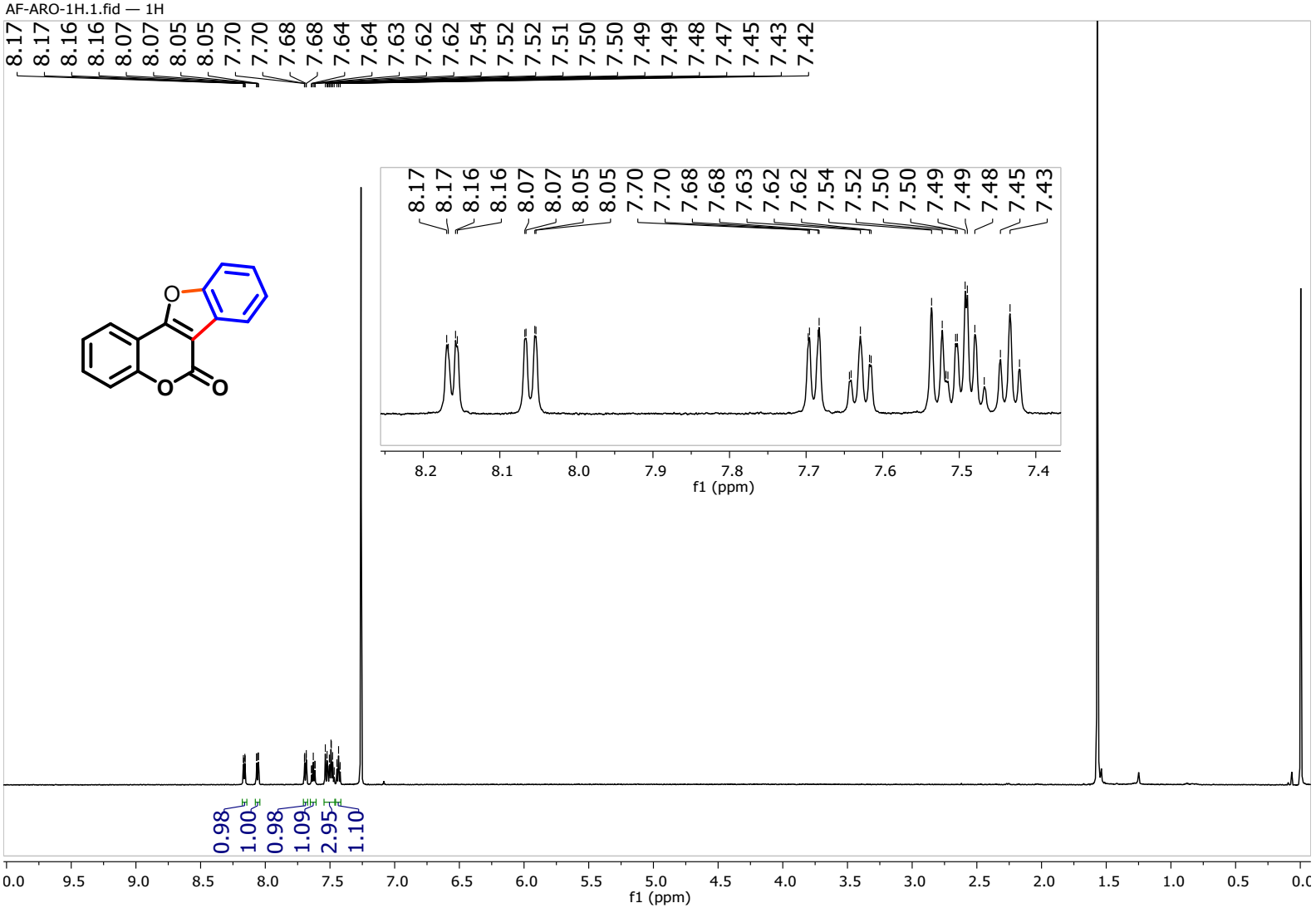


HRMS Spectrum of 3,9-Dihydroxy-7,8,9,10-tetrahydro-6*H*-benzofuro[3,2-*c*]chromen-6-one (8b)

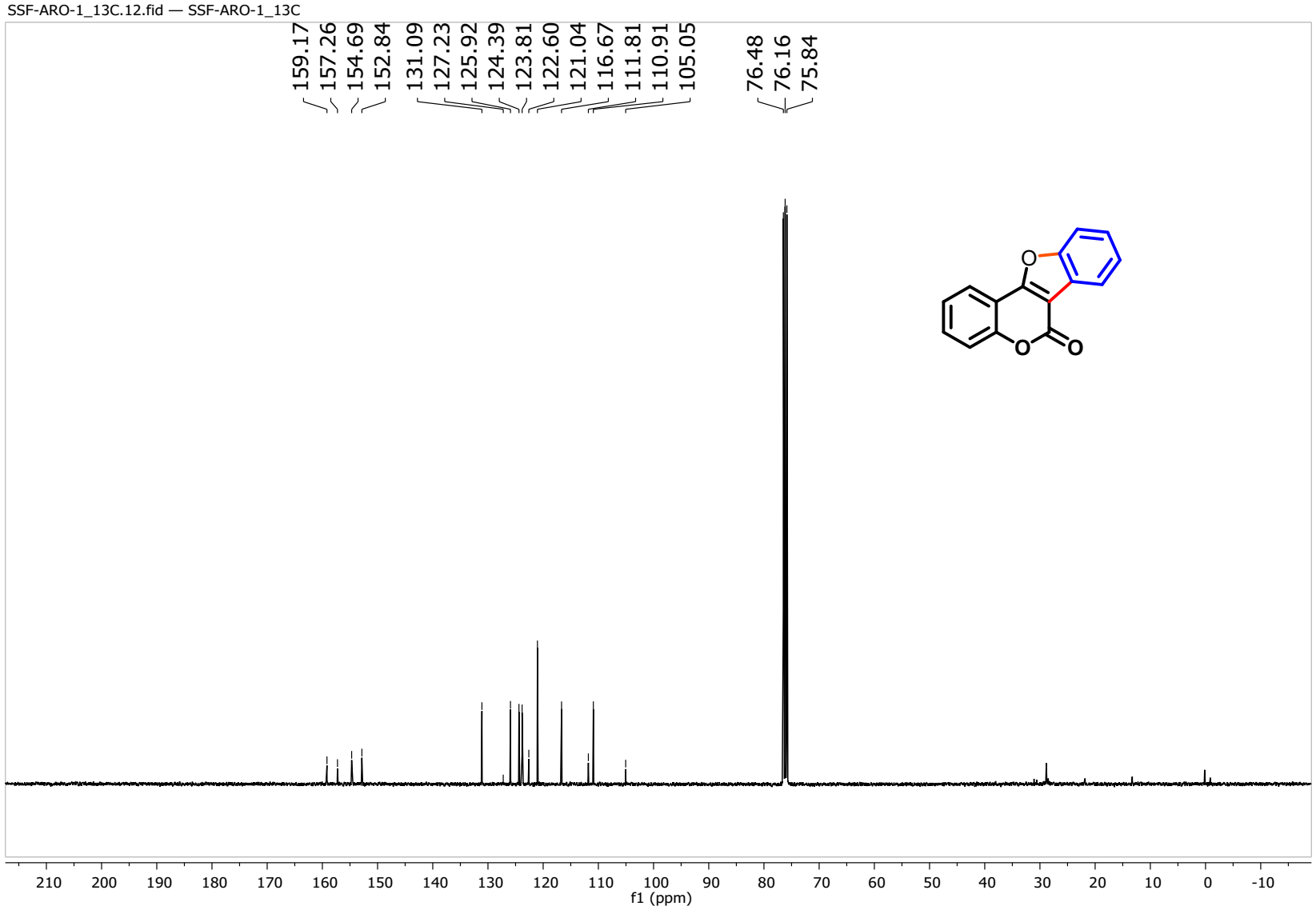
Sample Name	Sample7	**Position**	P1-A7	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-6R-30.d
ACQ Method	DIRECT MASS_POSITIVE_100_1500.m	**Comment**		**Acquired Time**	28-07-2023 10:31:08 (UTC+05:30)



^{1}H NMR Spectrum of 6*H*-benzofuro[3,2-*c*]chromen-6-one (9a)

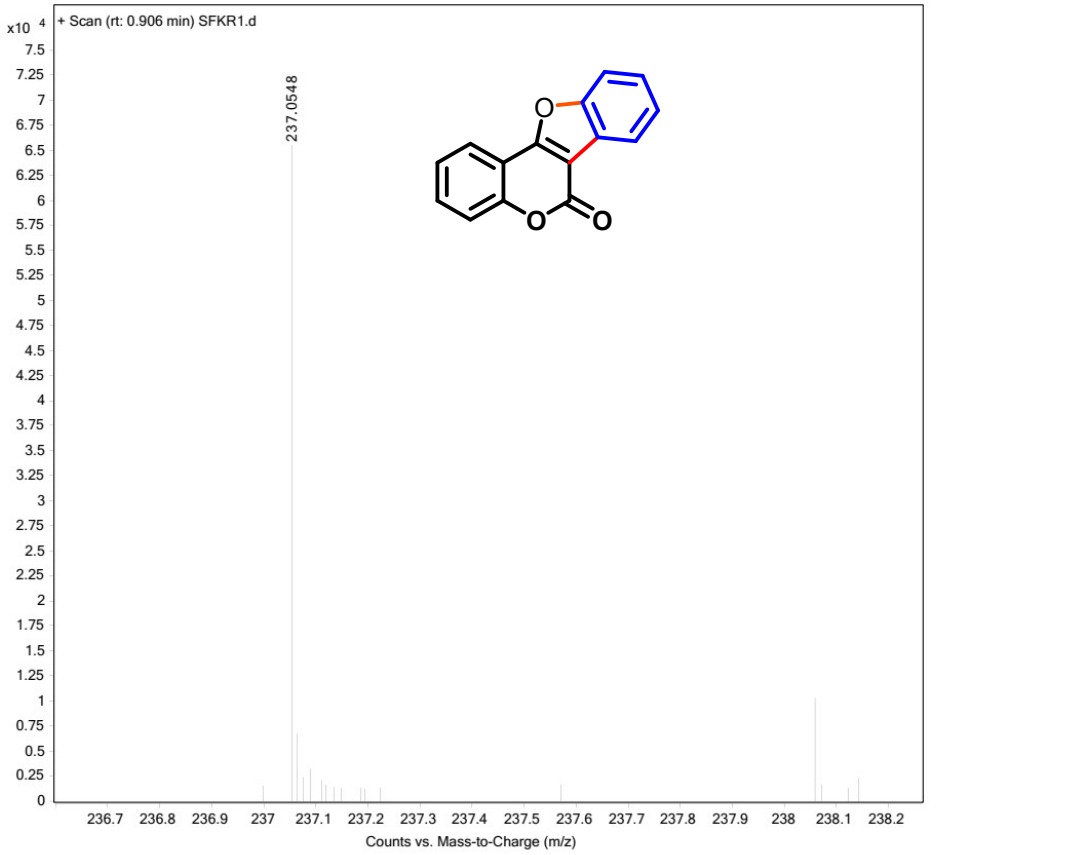


^{13}C NMR Spectrum of 6*H*-benzofuro[3,2-*c*]chromen-6-one (9a)

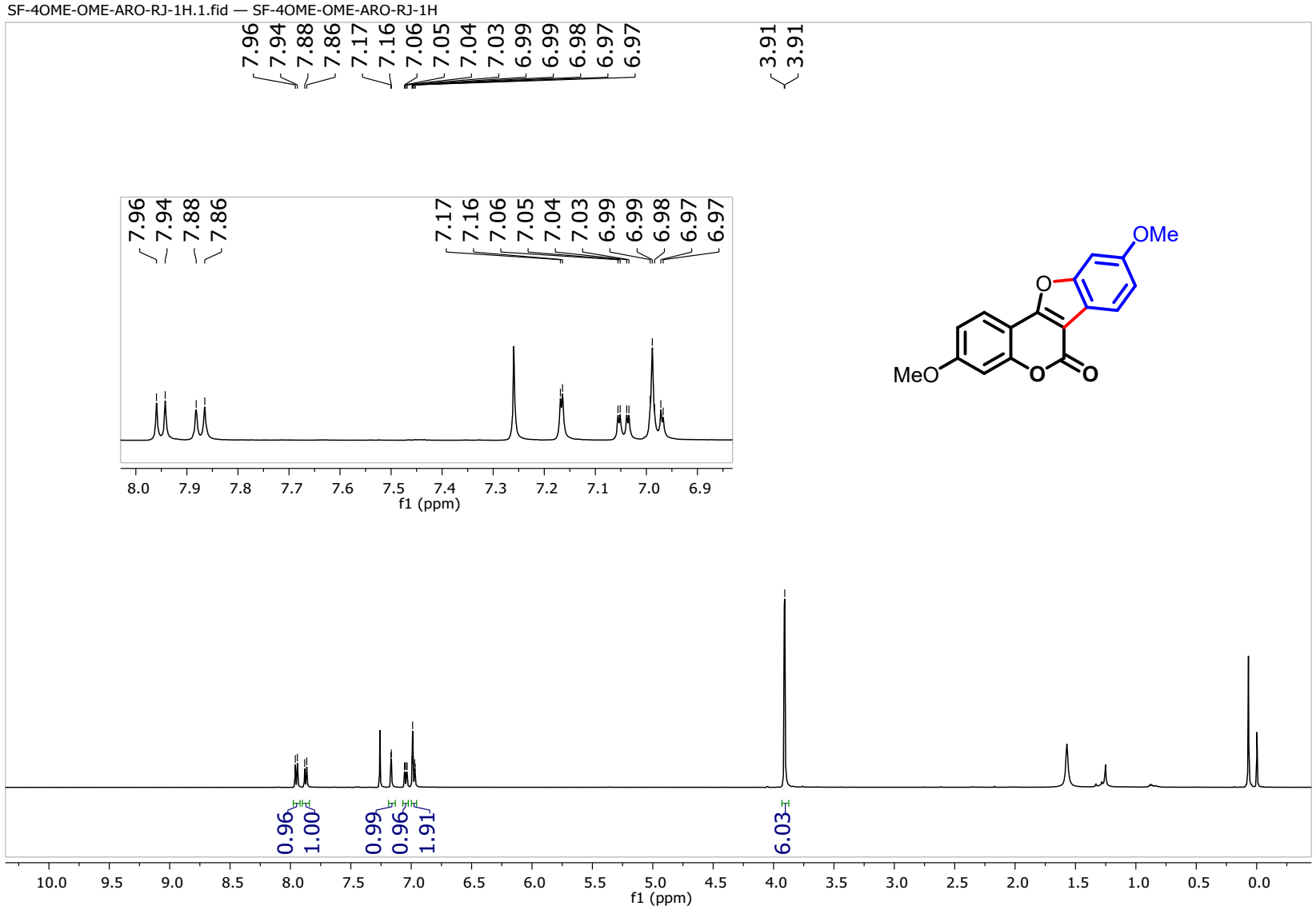


HRMS Spectrum of 6*H*-benzofuro[3,2-*c*]chromen-6-one (9a)

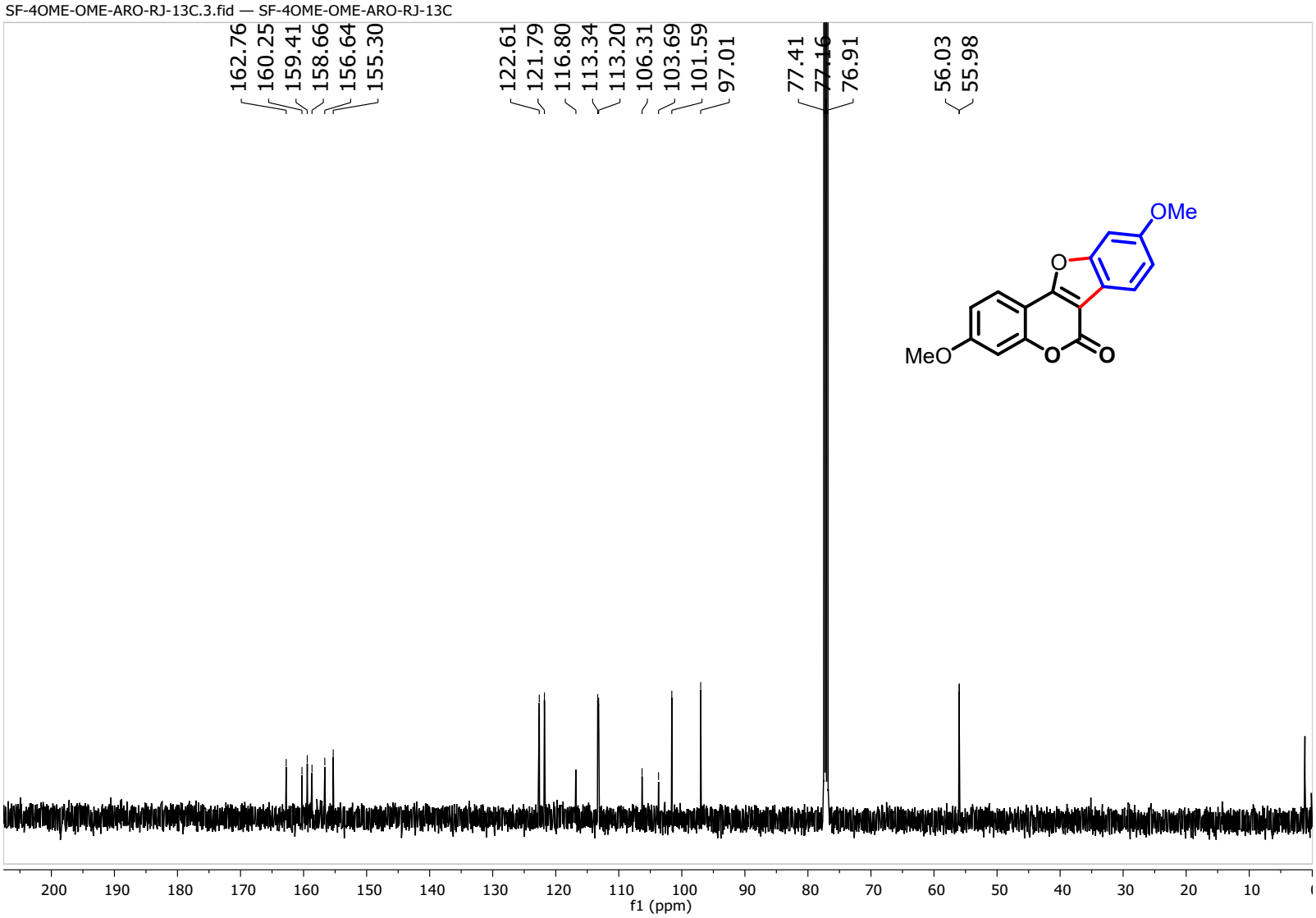
Sample Name		**Position**	P1-B6	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFKR1.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	12-09-2023 16:08:02 (UTC+05:30)



^{1}H NMR Spectrum of 3,9-Dimethoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9b)

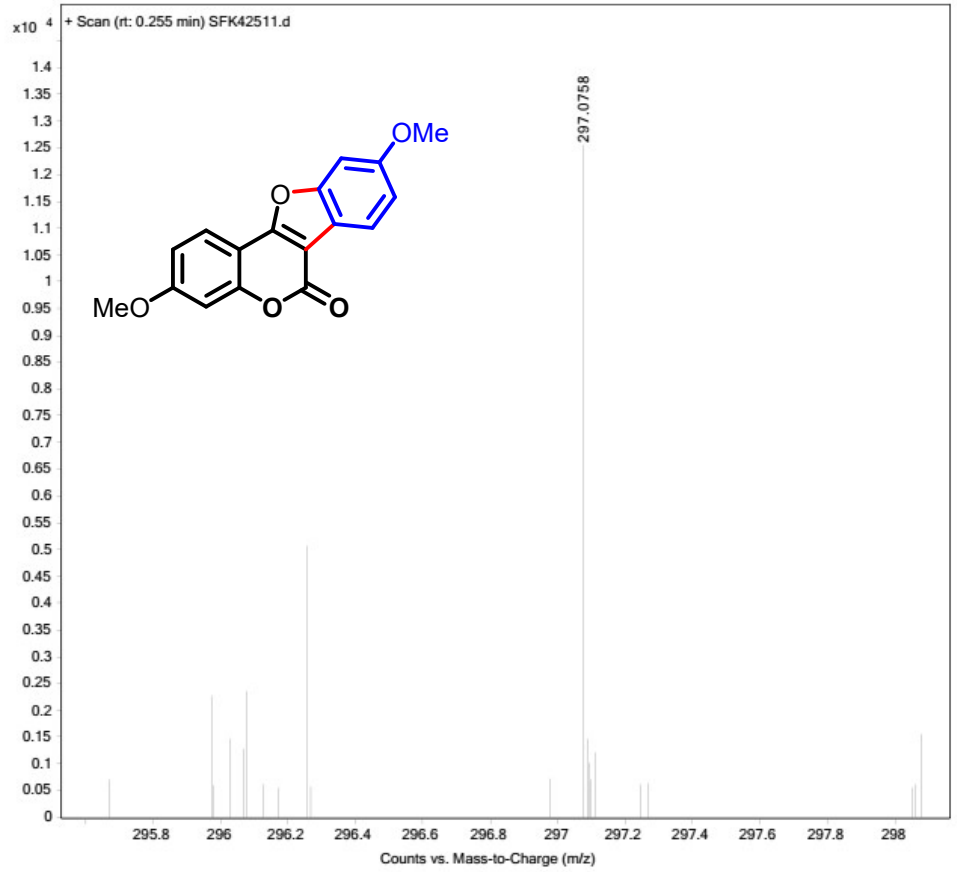


^{13}C NMR Spectrum of 3,9-Dimethoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9b)

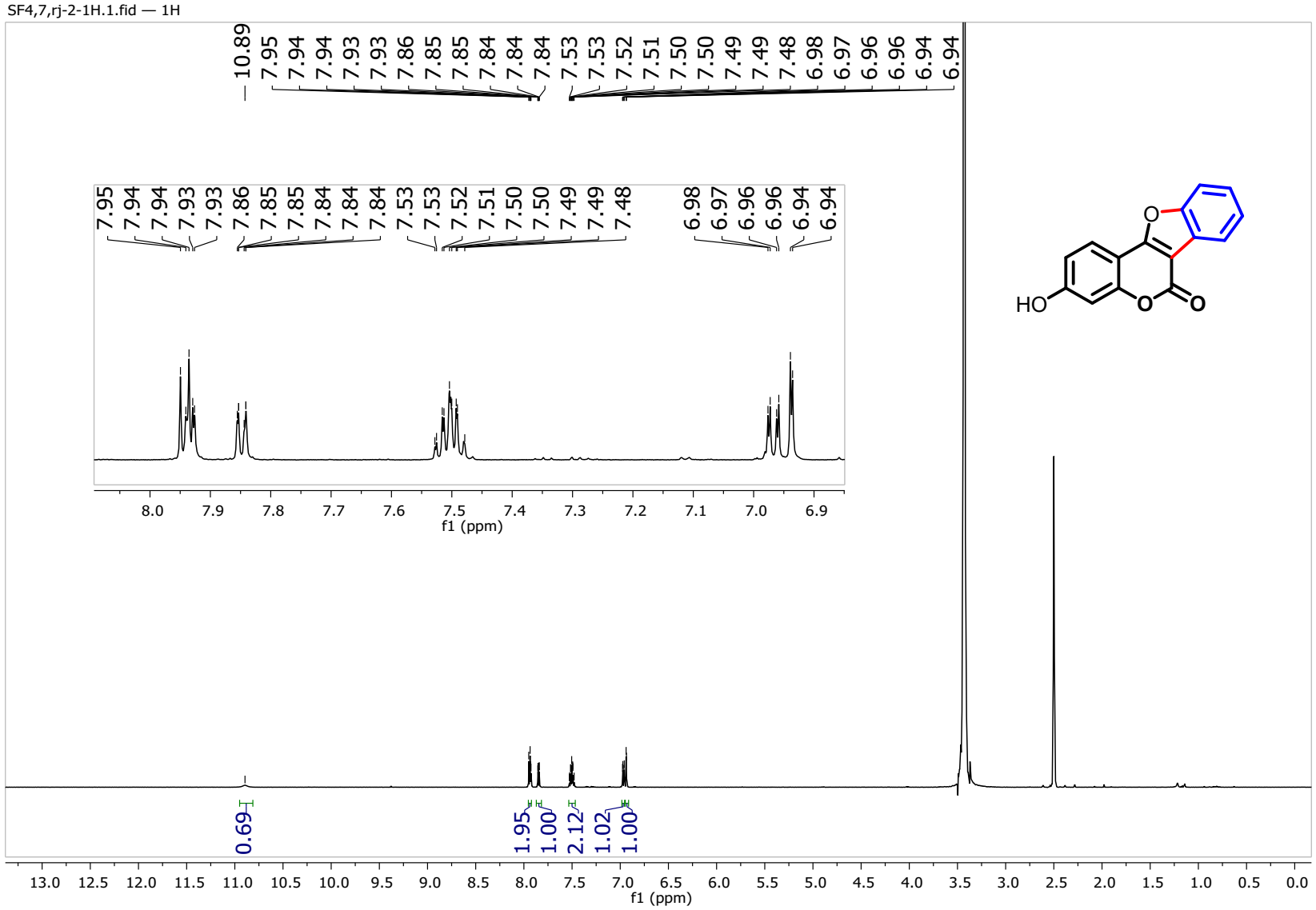


HRMS Spectrum of 3,9-Dimethoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9b)

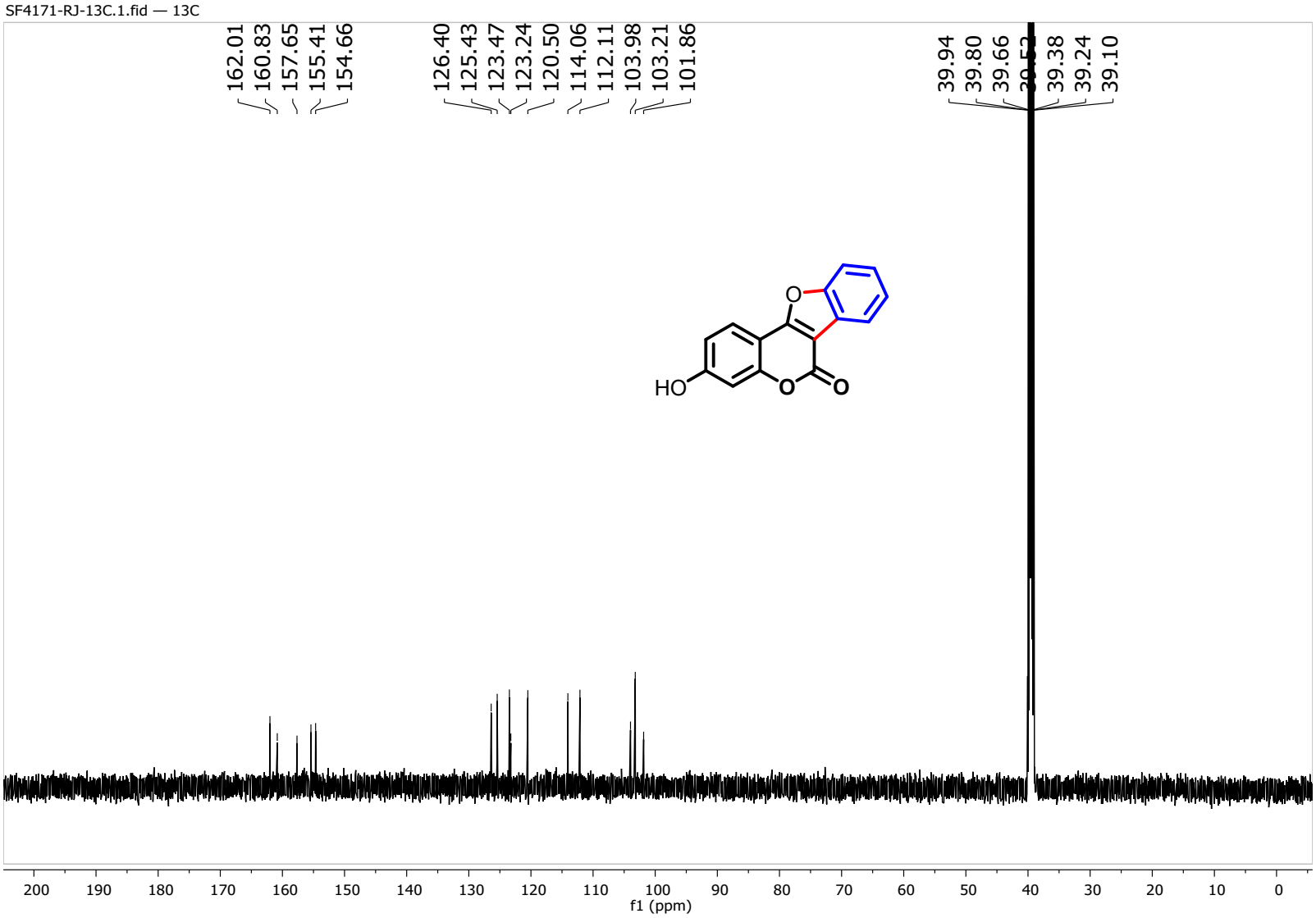
Sample Name		**Position**	P1-B11	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFK42511.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	05-12-2023 15:34:54 (UTC+05:30)



^{1}H NMR Spectrum of 3-Hydroxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9d)

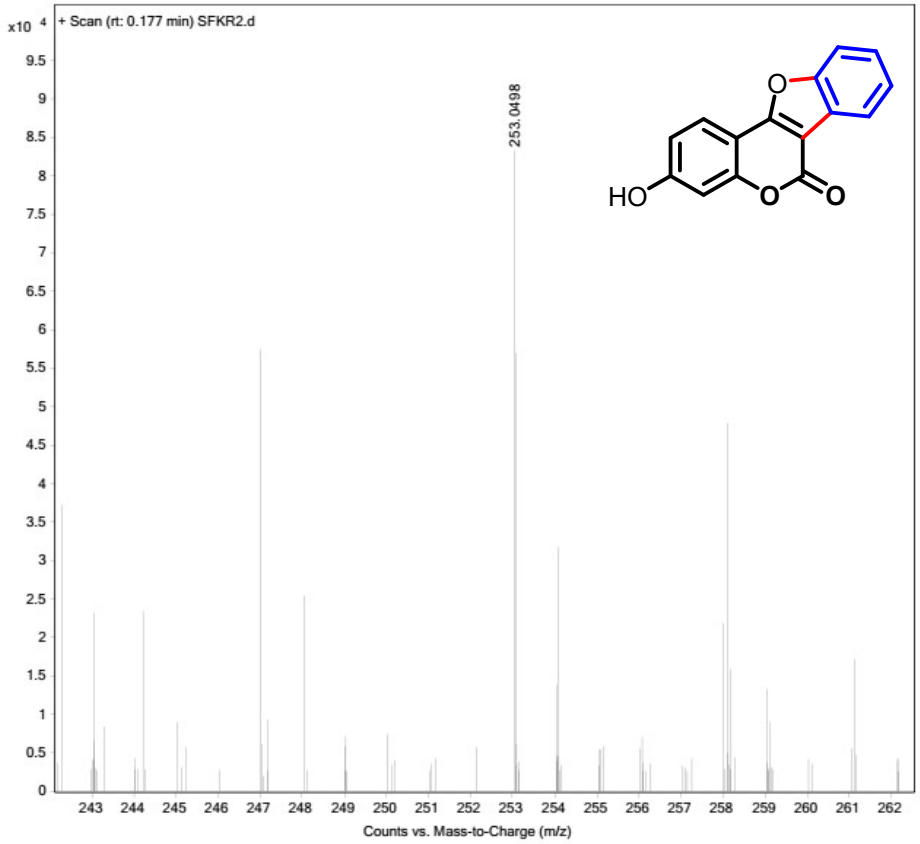


^{13}C NMR Spectrum of 3-Hydroxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9d)

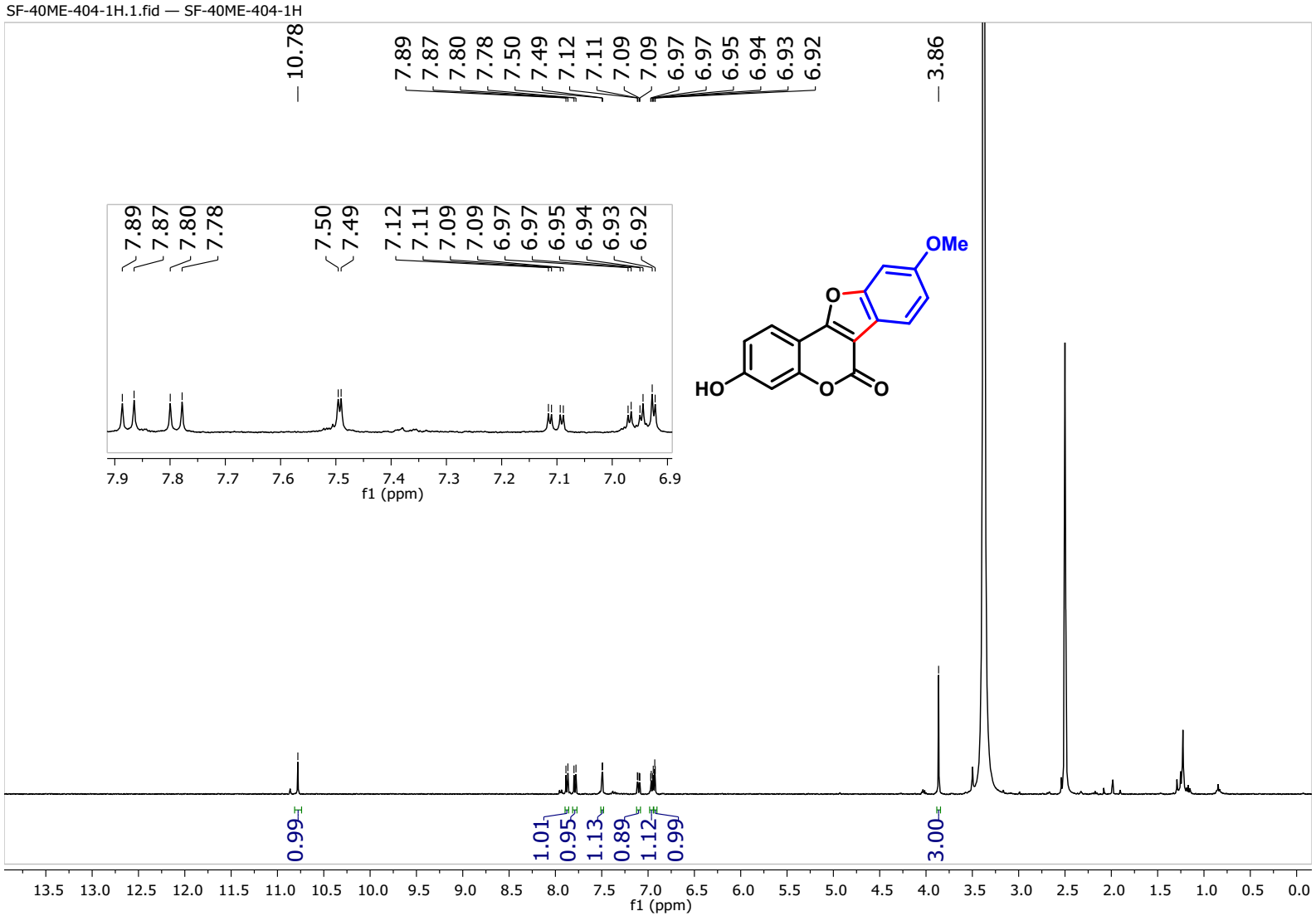


HRMS Spectrum of 3-Hydroxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9d)

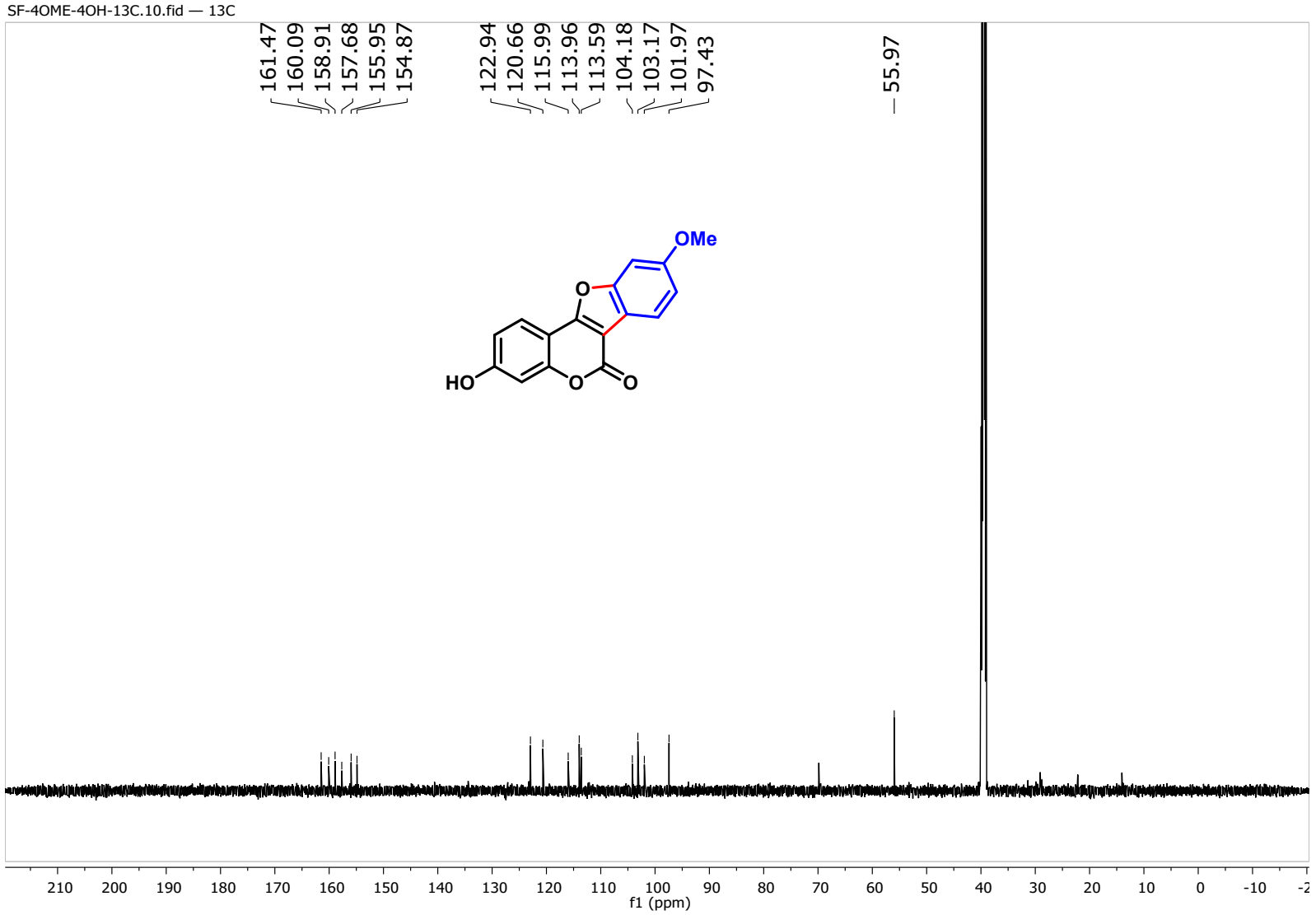
Sample Name		**Position**	P1-B7	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SFKR2.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	12-09-2023 16:09:50 (UTC+05:30)



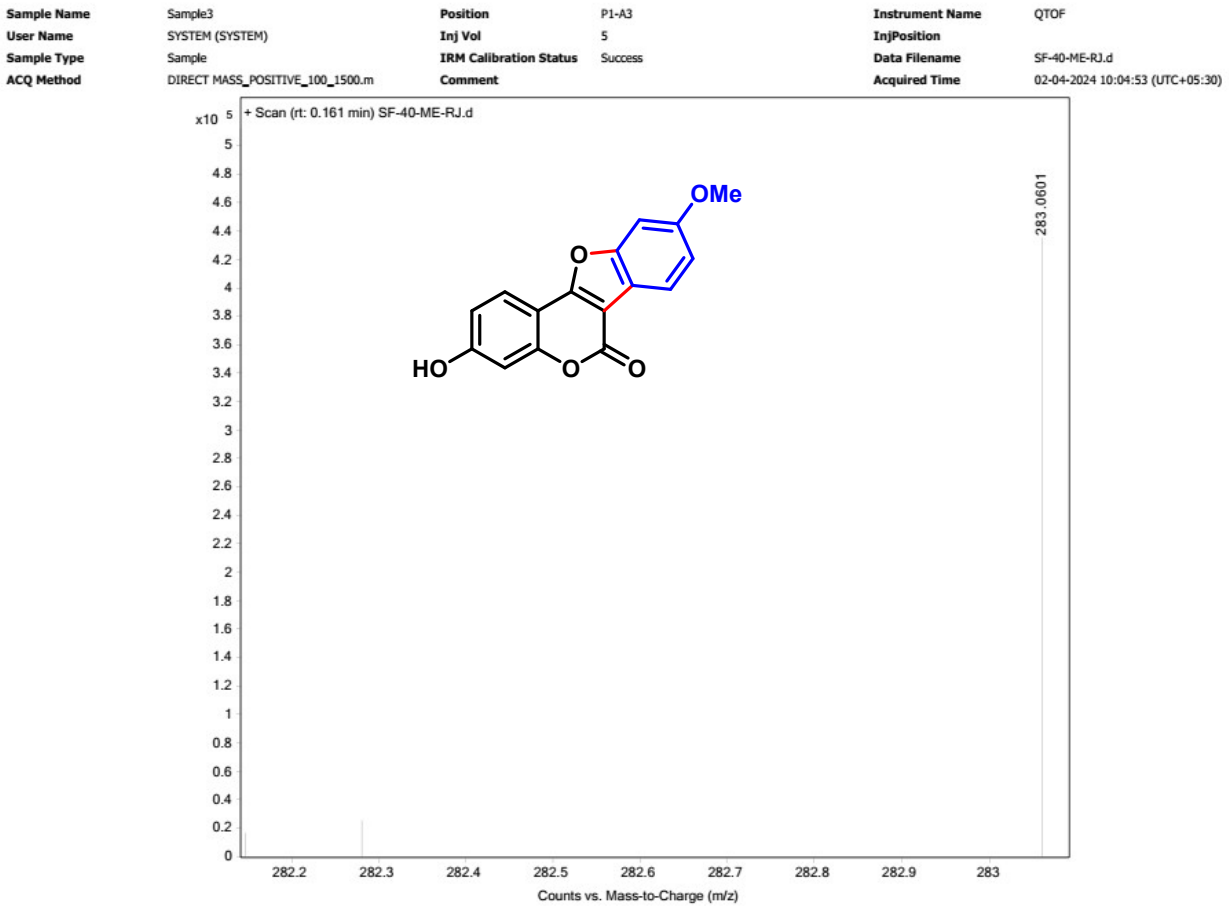
^{1}H NMR Spectrum of 3-Hydroxy-9-methoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9e)



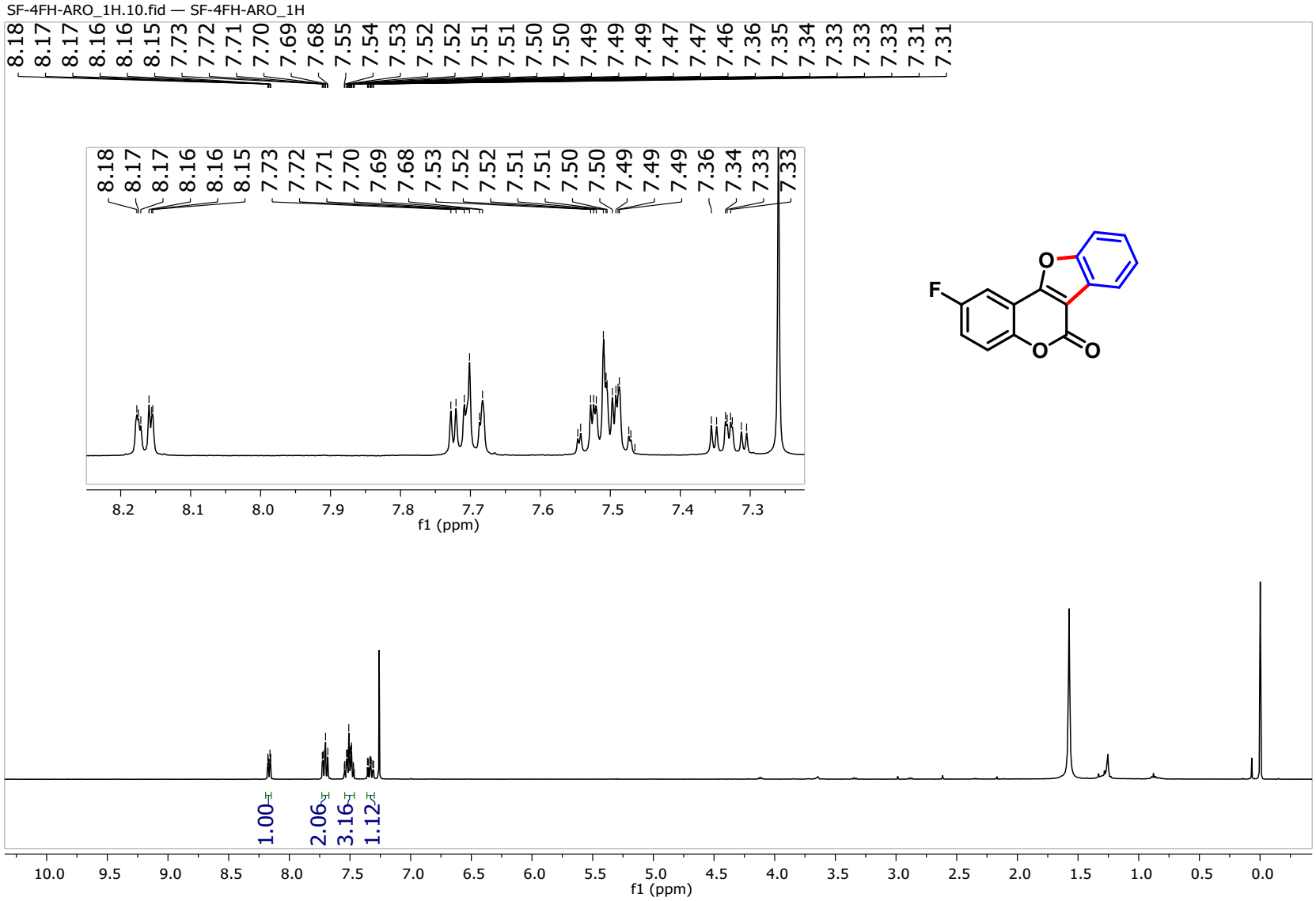
^{13}C NMR Spectrum of 3-Hydroxy-9-methoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9e)


SF-4OME-4OH-13C.10.fid — 13C
161.47
160.09
158.91
157.68
155.95
154.87
122.94
120.66
115.99
113.96
113.59
104.18
103.17
101.97
97.43
55.97
OMe
O
HO
O
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

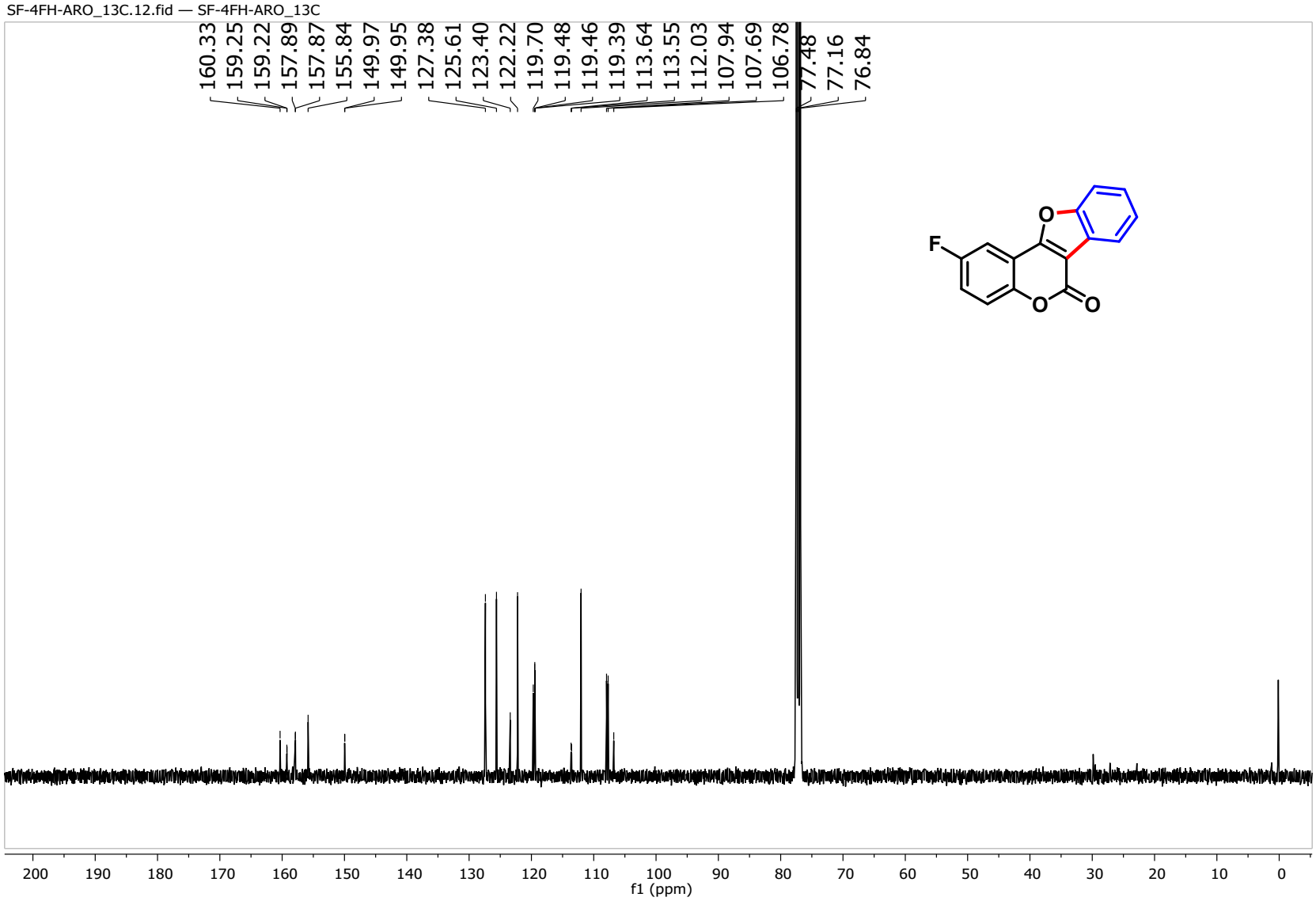
HRMS Spectrum of 3-Hydroxy-9-methoxy-6*H*-benzofuro[3,2-*c*]chromen-6-one (9e)



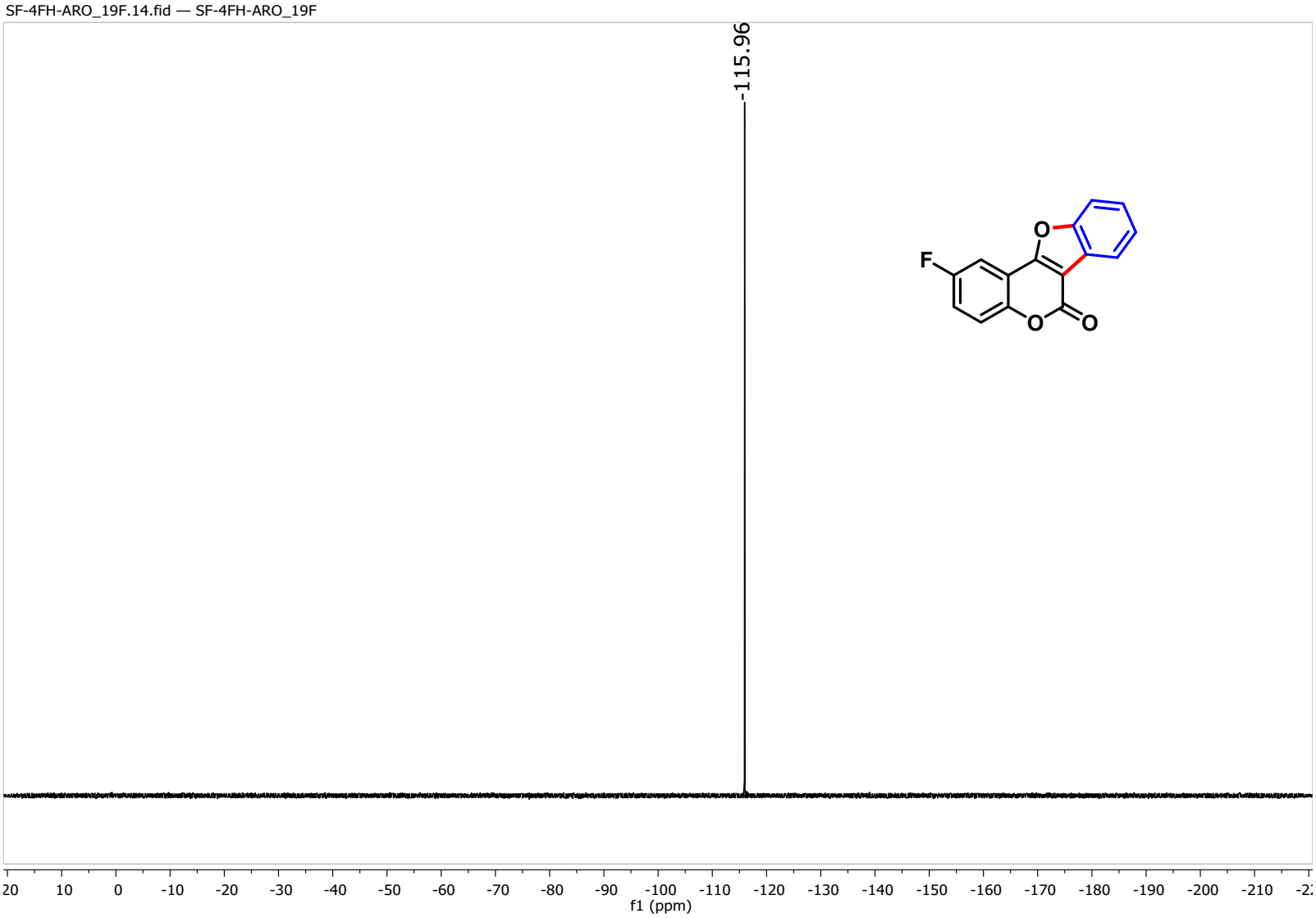
^{1}H NMR Spectrum of 2-Fluoro-6*H*-benzofuro[3,2-*c*]chromen-6-one (9f)



^{13}C NMR Spectrum of 2-Fluoro-6*H*-benzofuro[3,2-*c*]chromen-6-one (9f)

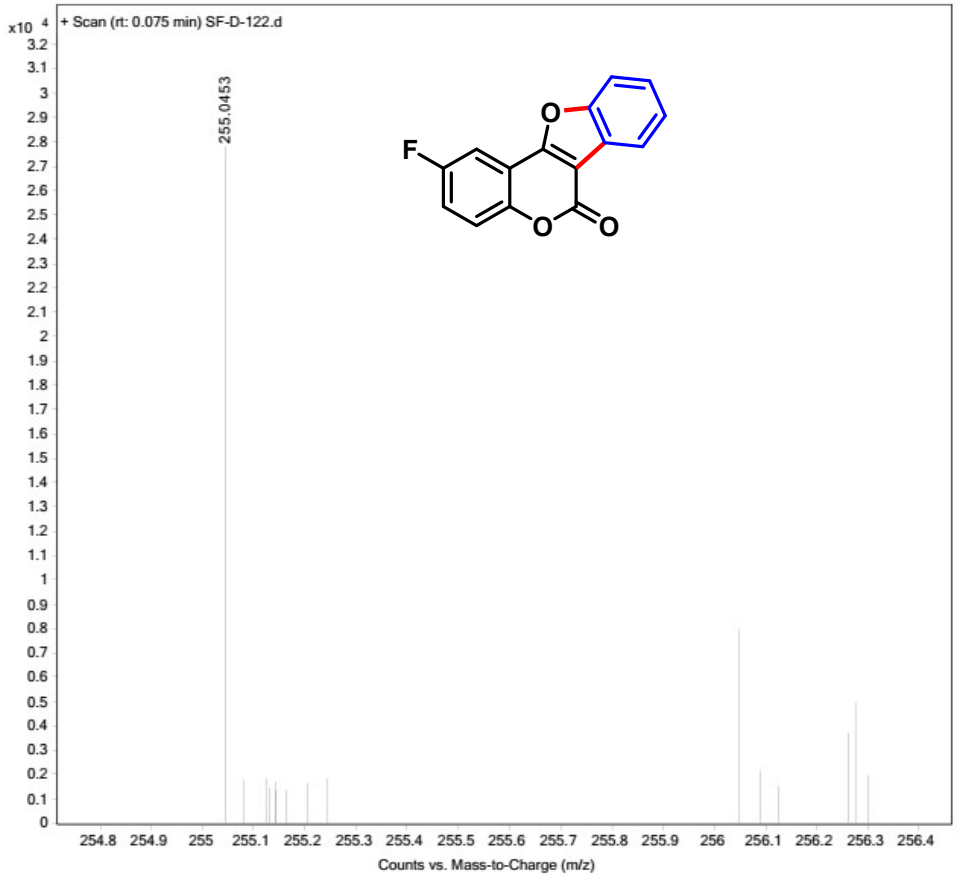


^{19}F NMR Spectrum of 2-Fluoro-6*H*-benzofuro[3,2-*c*]chromen-6-one (9f)

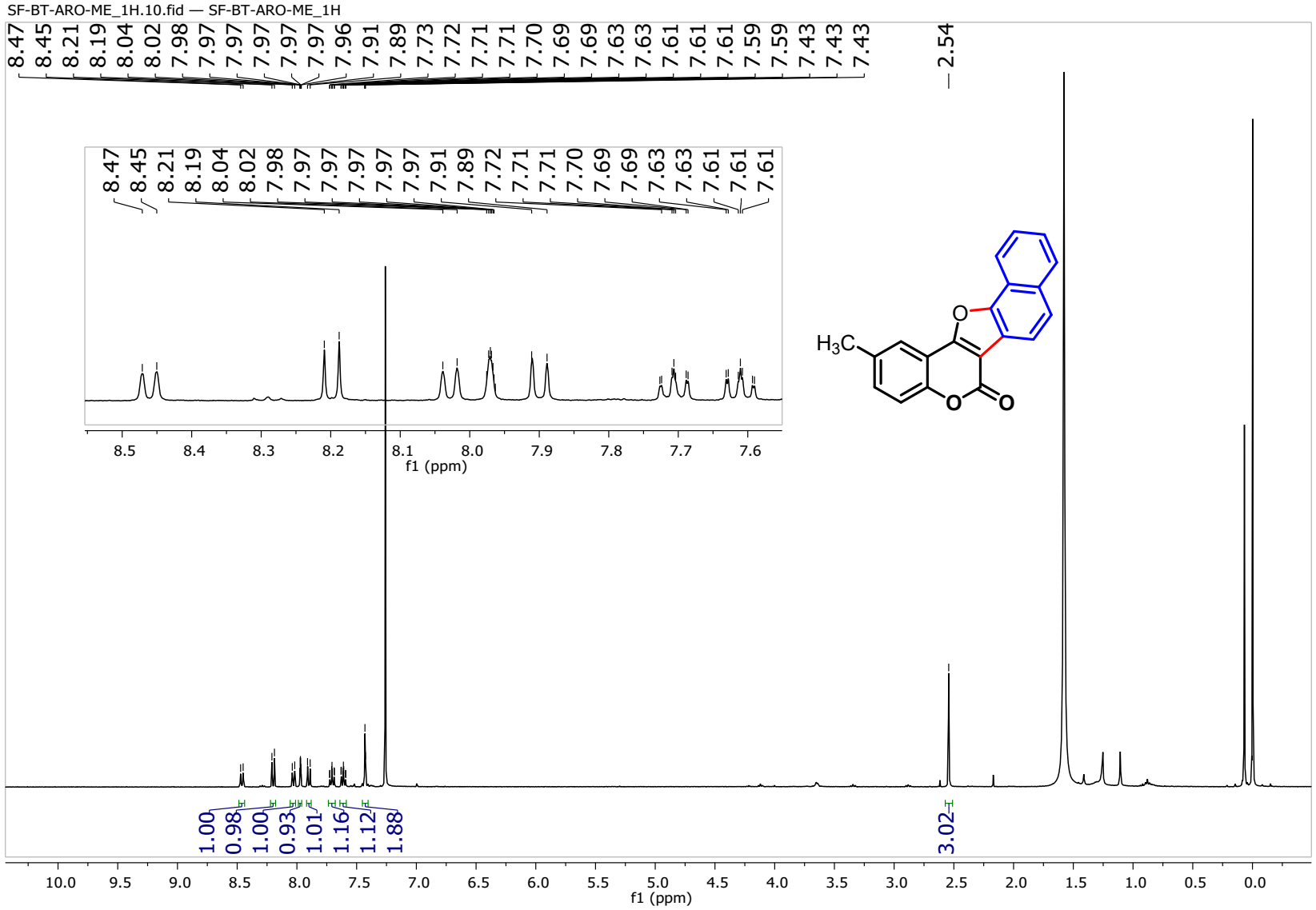


HRMS Spectrum of 2-Fluoro-6*H*-benzofuro[3,2-*c*]chromen-6-one (9f)

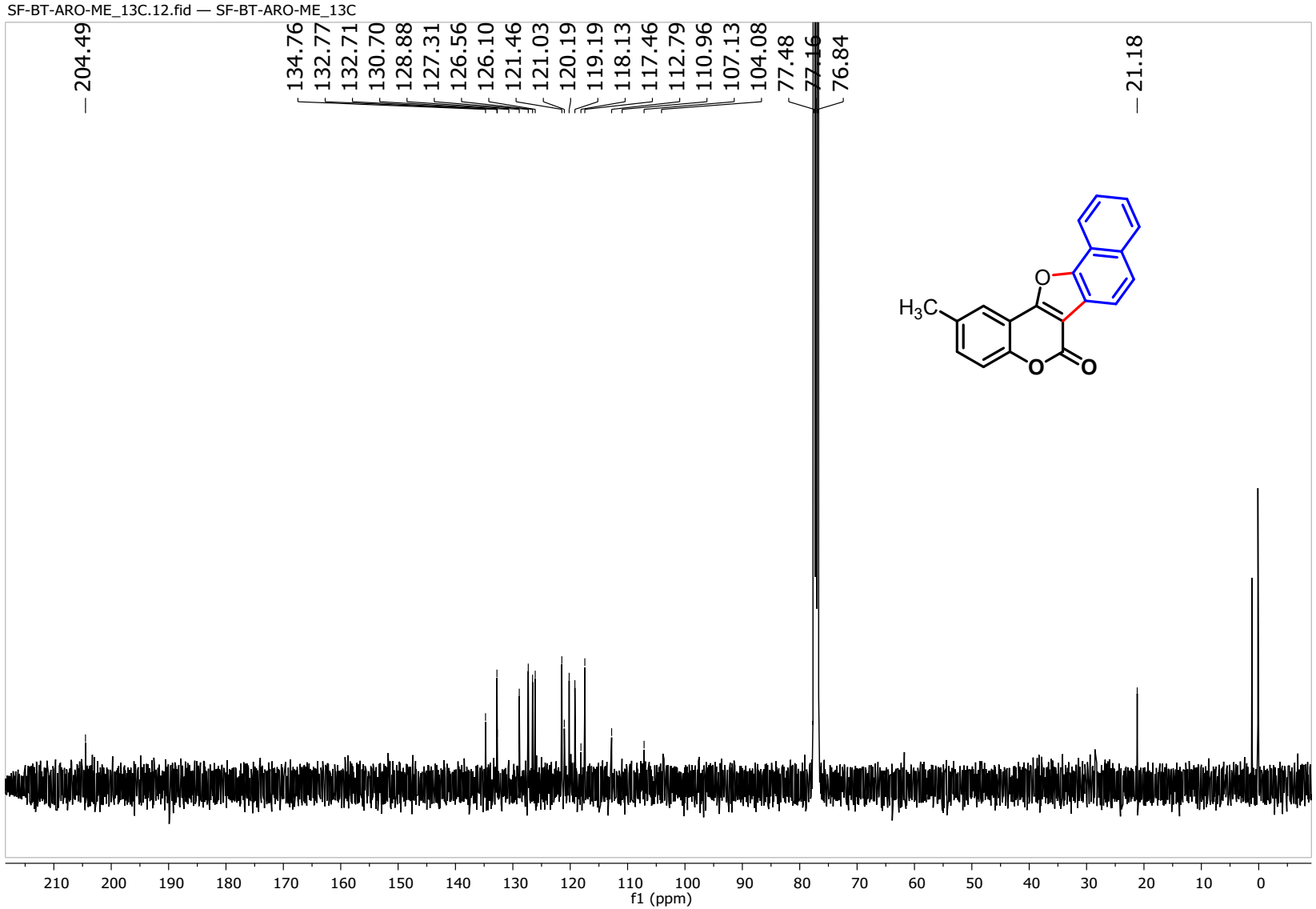
Sample Name		**Position**	P1-B3	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-D-122.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	26-09-2023 16:12:42 (UTC+05:30)



^{1}H NMR Spectrum of 2-Methyl-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one (9g)



^{13}C NMR Spectrum of 2-Methyl-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one (9g)



HRMS Spectrum of 2-Methyl-6*H*-naphtho[2',1':4,5]furo[3,2-*c*]chromen-6-one (9g)

Sample Name	Sample12	**Position**	P1-A11	**Instrument Name**	QTOF
User Name	SYSTEM (SYSTEM)	**Inj Vol**	5	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	SF-26-RJ-1.d
ACQ Method	DIRECT MASS_POSITIVE_01_1.m	**Comment**		**Acquired Time**	17-10-2023 10:31:50 (UTC+05:30)