

## *Supporting Information*

# Radical-Induced Cascade Annulation/Hydrocarbonylation for Construction of 2-Aryl-4*H*-chromen-4-ones

Xinwei He \*, Keke Xu, Yanan Liu, Demao Wang, Qiang Tang, Wenjie Hui, Haoyu Chen  
and Yongjia Shang

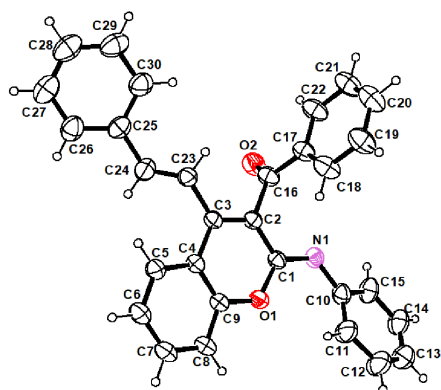
Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui  
Laboratory of Molecule-Based Materials (State Key Laboratory Cultivation  
Base), College of Chemistry and Materials Science, Anhui Normal University,  
Wuhu 241000, China

\* Correspondence: xinweihe@mail.ahnu.edu.cn

### Table of contents

1. X-ray crystallographic data of compound <b>2bo</b> -----	S2
2. NMR spectra for all compounds-----	S3
3. GC-MS spectra for mechanistic investigations-----	S56

## 1. X-ray crystallographic data of compound **2bo**



The purified compound **2bo** is dissolved in a mixed solvent of ethyl acetate and petroleum ether, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal was obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCD APEX-2 diffractometer (graphite-monochromated Mo  $K\alpha$  radiation,  $\lambda=0.71073$  nm) at 296(2) K.

**Figure S1.** ORTEP drawing of compound **2bo** (30% probability for the thermal ellipsoid).

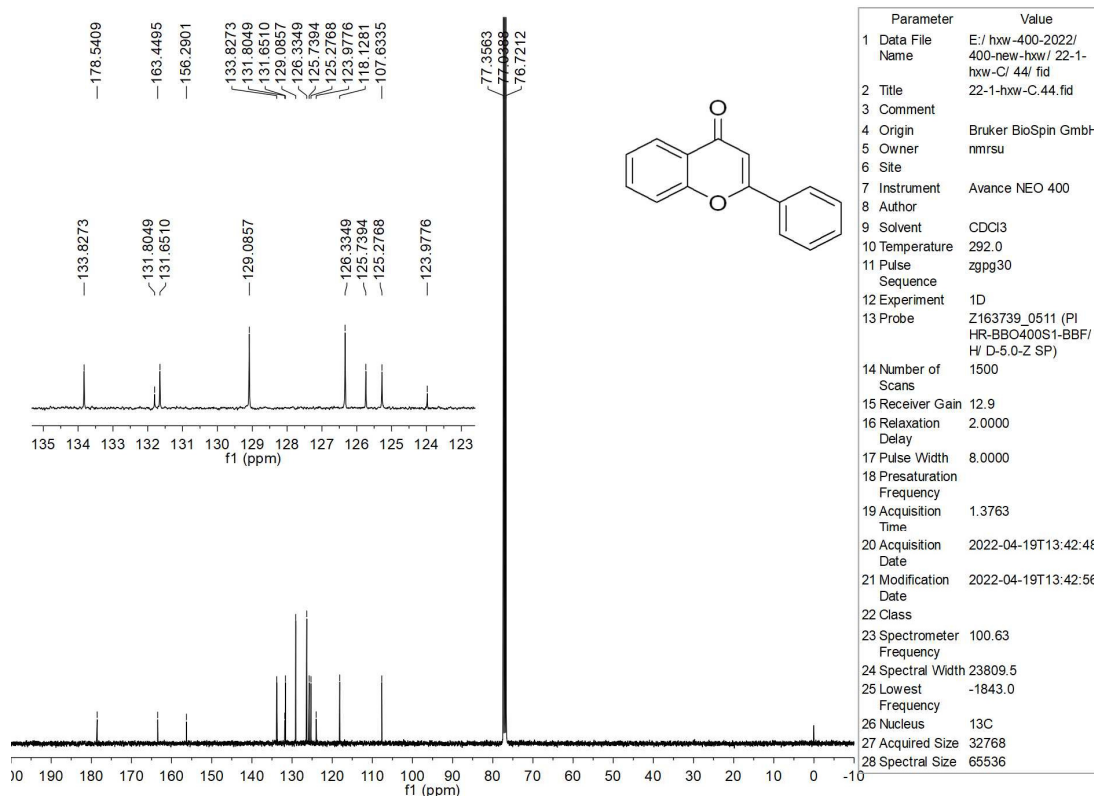
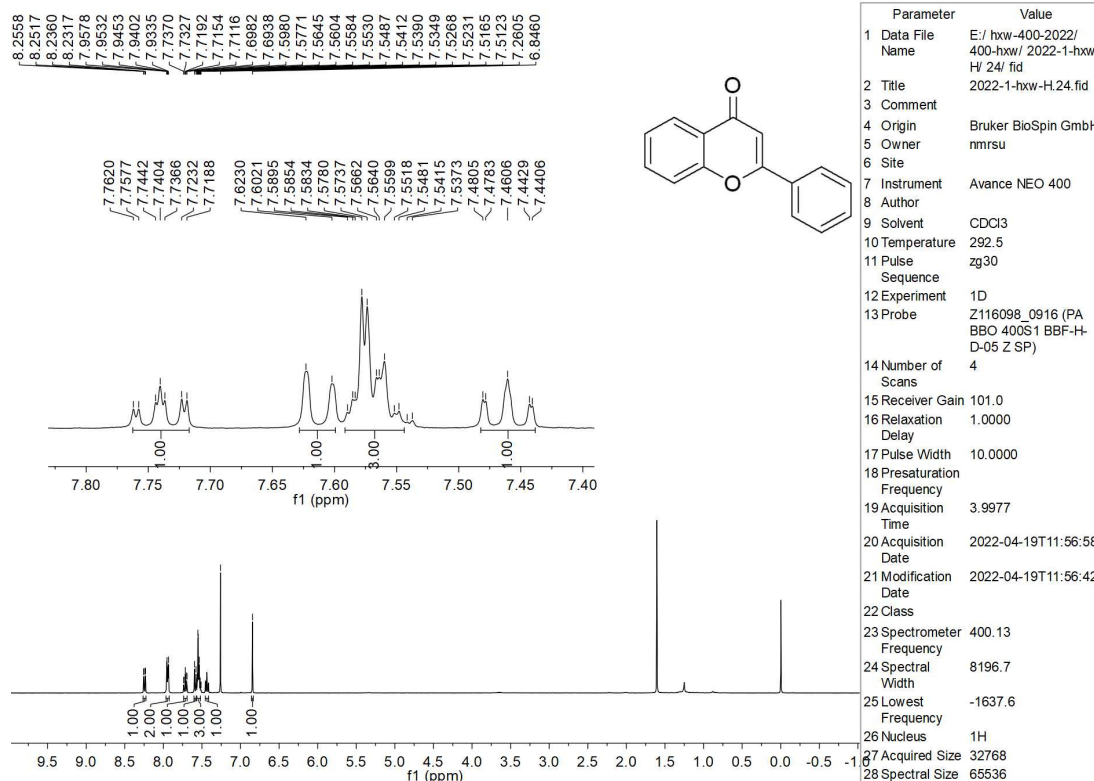
**Table S1.** Crystal data and structure refinement for compound **2bo**.

CCDC number	2195370
Identification code	210920b_0m_a
Empirical formula	C <sub>25</sub> H <sub>22</sub> O <sub>2</sub>
Formula weight	354.42
Temperature	293.15 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 <sub>1</sub> /c
Unit cell dimensions	a = 10.684(3) Å $\alpha = 90^\circ$ . b = 9.951(2) Å $\beta = 93.881(3)^\circ$ . c = 18.236(4) Å $\gamma = 90^\circ$ .
Volume	1934.3(8) Å <sup>3</sup>
Z	4
Density (calculated)	1.217 g/cm <sup>3</sup>
Absorption coefficient	0.076 mm <sup>-1</sup>
F(000)	752.0
Crystal size	0.21 × 0.2 × 0.19 mm <sup>3</sup>
2 $\theta$ range for data collection	3.82 to 55.092°
Index ranges	-13 ≤ h ≤ 13, -12 ≤ k ≤ 12, -23 ≤ l ≤ 23
Reflections collected	21949
Independent reflections	4407 [R(int) = 0.0427, R(sigma) = 0.0413]
Data / restraints / parameters	4407 / 0 / 246
Goodness-of-fit on F <sup>2</sup>	1.049
Final R indices [I > 2sigma(I)]	R1 = 0.0507, wR2 = 0.1302
Final R indices (all data)	R1 = 0.0946, wR2 = 0.1521
Largest diff. peak and hole	0.20 and -0.17 eÅ <sup>-3</sup>

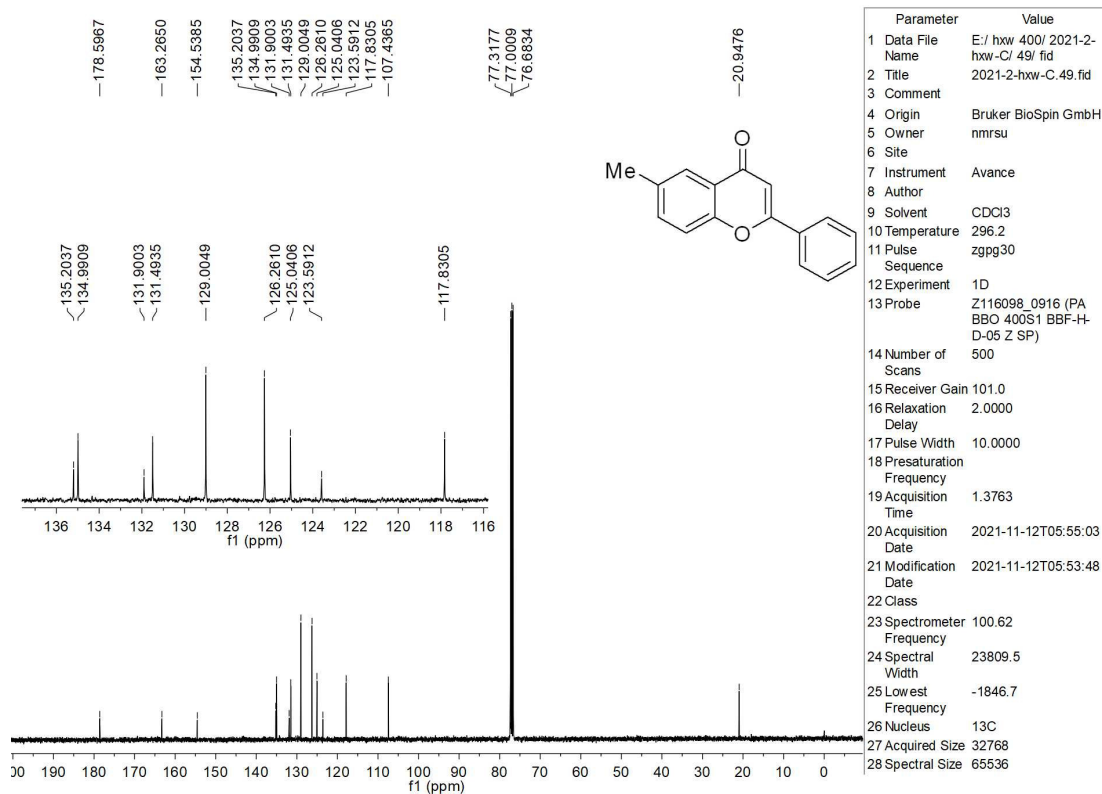
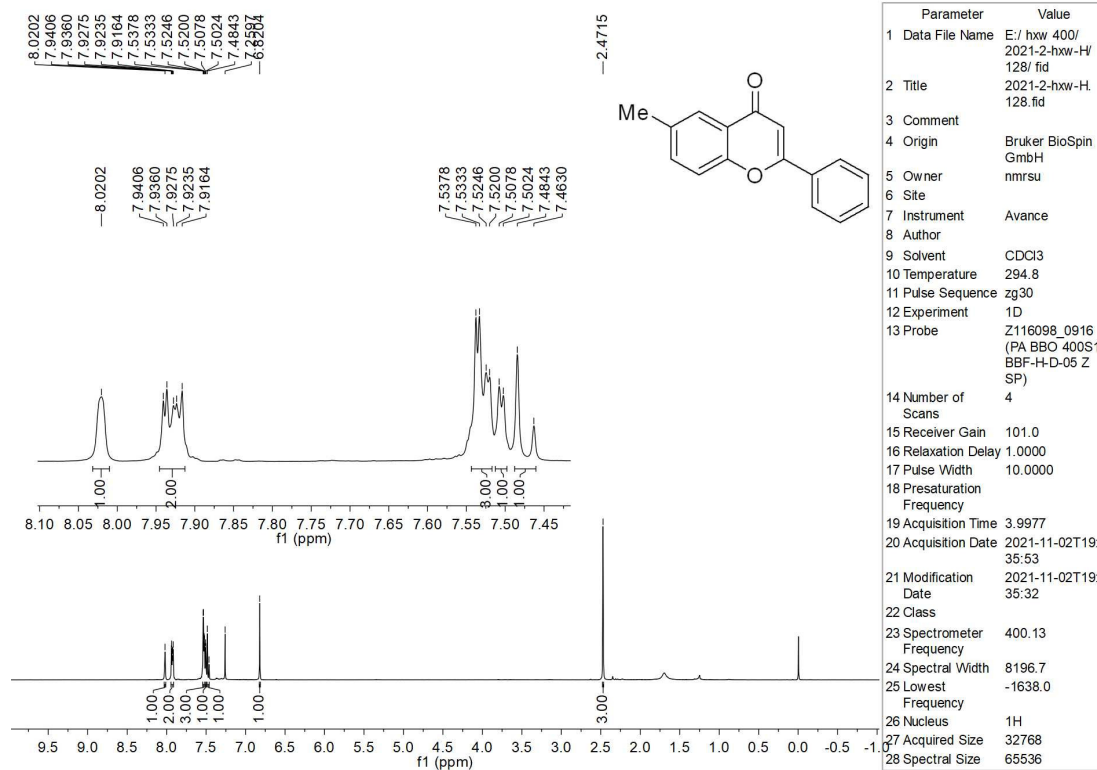


## 2. NMR spectra for all compounds

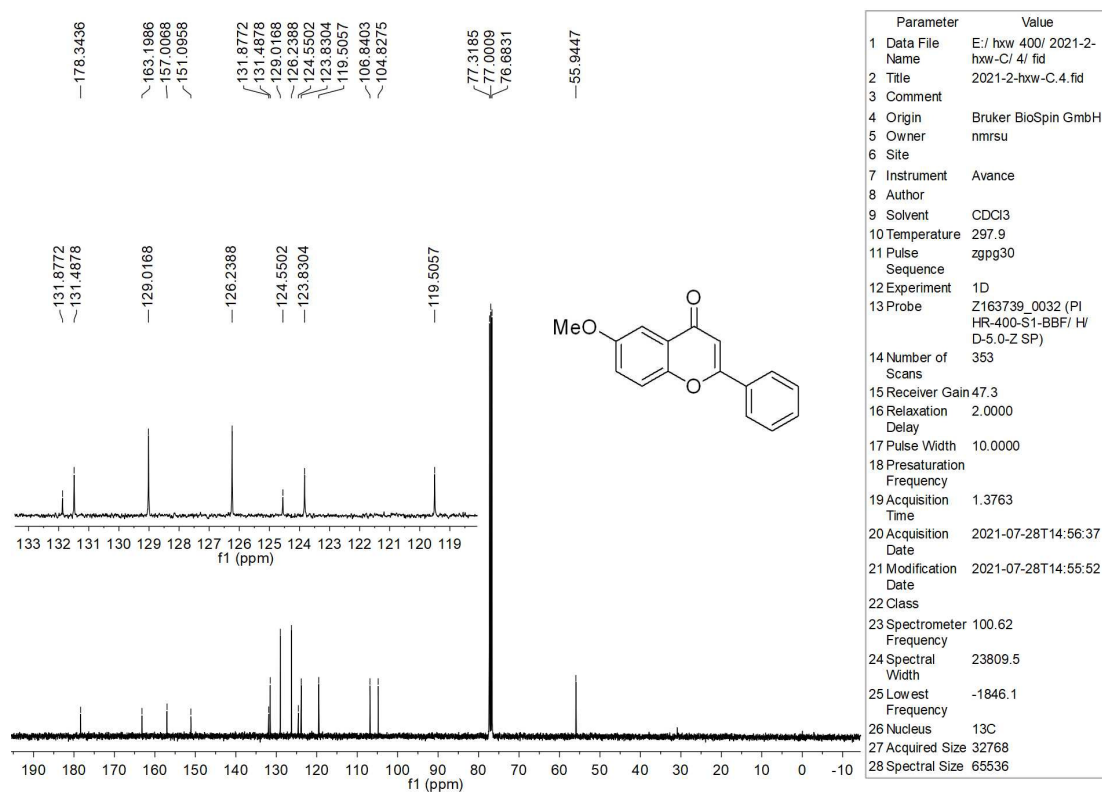
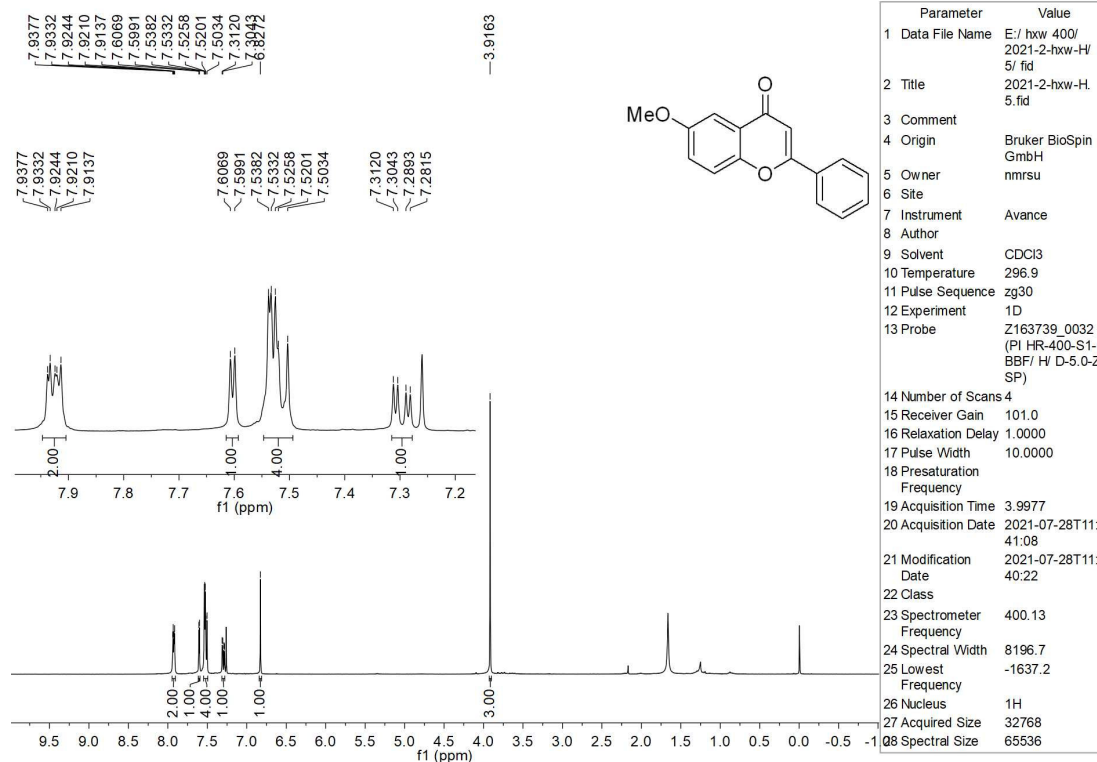
### 2-Phenyl-4H-chromen-4-one (2aa)



# 6-Methyl-2-phenyl-4H-chromen-4-one (2ba)



# 6-Methoxy-2-phenyl-4H-chromen-4-one (2ca)



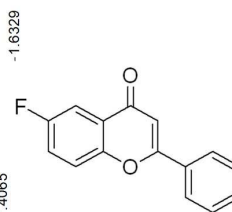
The figure displays two  $^1\text{H}$  NMR spectra of compound **1**. The top spectrum, recorded in  $\text{CDCl}_3$ , shows a complex multiplet between 7.3 and 8.4 ppm. The bottom spectrum, recorded in  $\text{DMSO}-d_6$ , shows a similar pattern with additional peaks at lower chemical shifts. Both spectra include integration values and a reference peak at 0 ppm.

**Top Spectrum ( $\text{CDCl}_3$ ):**

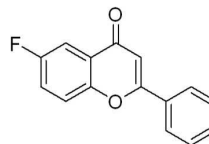
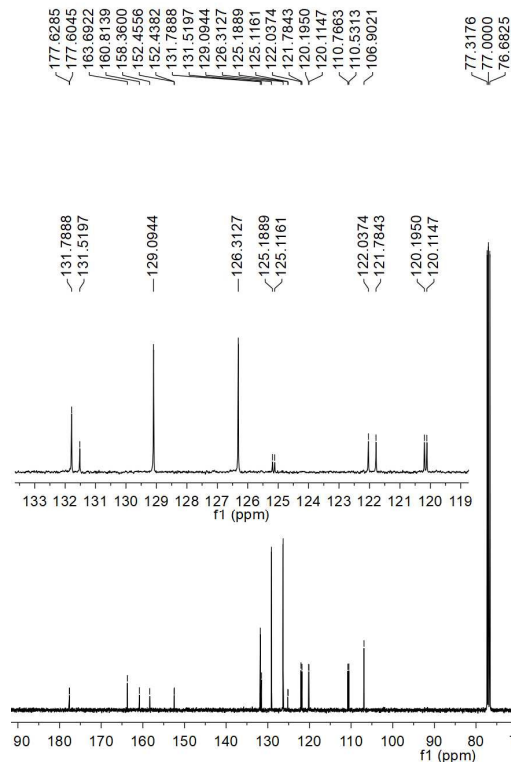
- Chemical shift range: 7.3 to 8.4 ppm.
- Integration values: 2.00, 1.00, 4.00, 1.00.
- Peak list (ppm): 7.9384, 7.9345, 7.9309, 7.9244, 7.9197, 7.9144, 7.8865, 7.8806, 7.8681, 7.8604, 7.8090, 7.5976, 7.5852, 7.5748, 7.5700, 7.5662, 7.5536, 7.5357, 7.5269, 7.5223, 7.5138, 7.4562, 7.4484, 7.4371, 7.4334, 7.4294, 7.4257, 7.4143, 7.4065, 7.2617, 6.8258, -1.6329.

**Bottom Spectrum ( $\text{DMSO}-d_6$ ):**

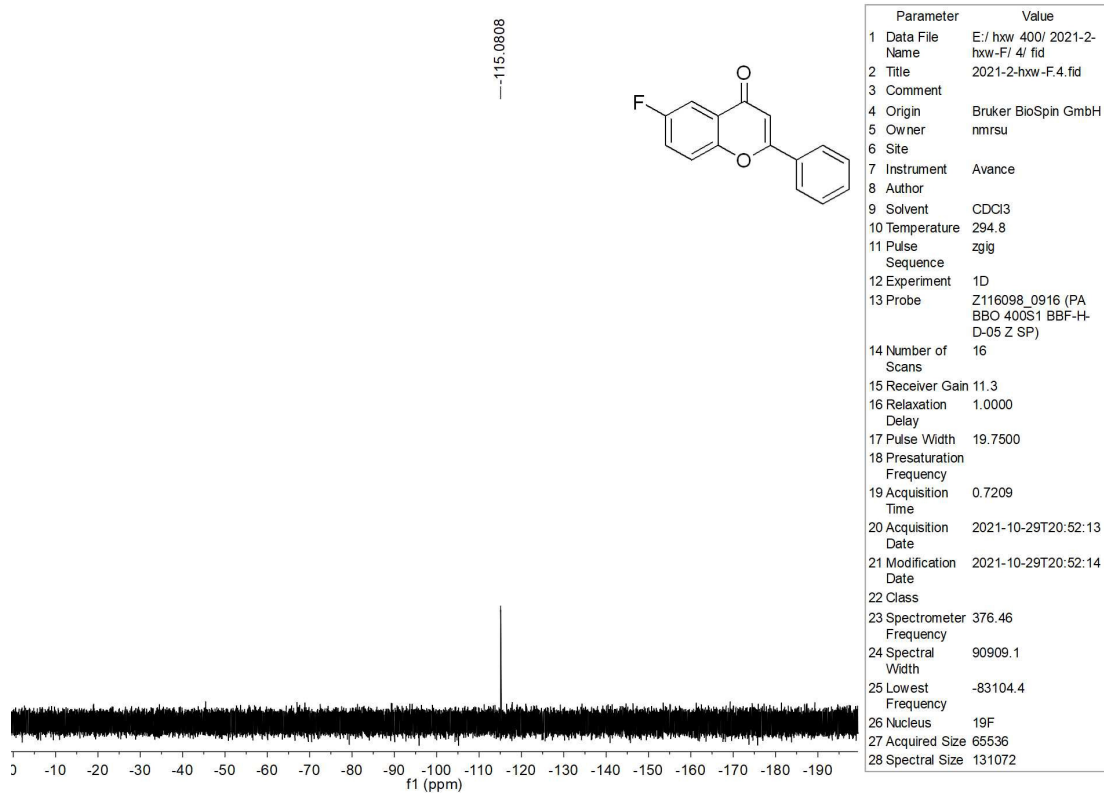
- Chemical shift range: 7.4 to 8.4 ppm.
- Integration values: 2.00, 1.00, 1.00, 1.00, 1.00.
- Peak list (ppm): 7.9384, 7.9345, 7.9309, 7.9244, 7.9197, 7.9144, 7.8865, 7.8808, 7.8681, 7.8604, 7.8090, 7.5976, 7.5852, 7.5748, 7.5700, 7.5662, 7.5536, 7.5357, 7.5269, 7.5223, 7.5138, 7.4562, 7.4484, 7.4371, 7.4334, 7.4294, 7.4257, 7.4143, 7.4065, 7.2617, 6.8258, -1.6329.



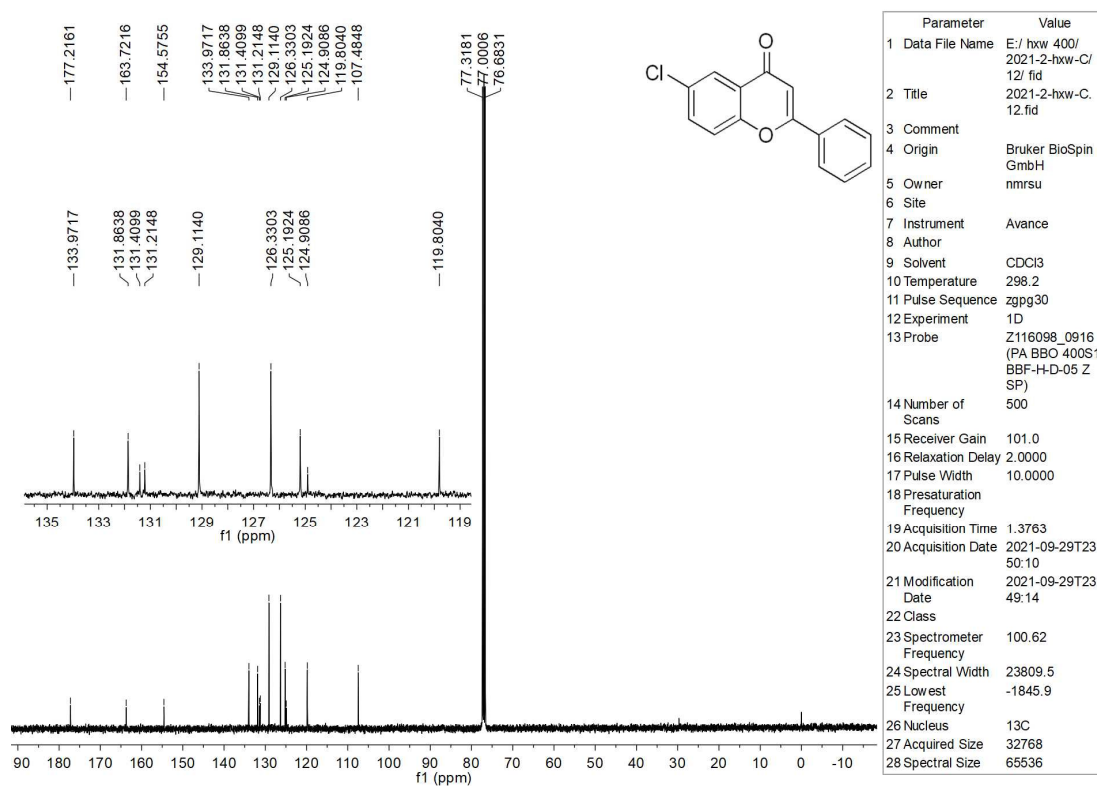
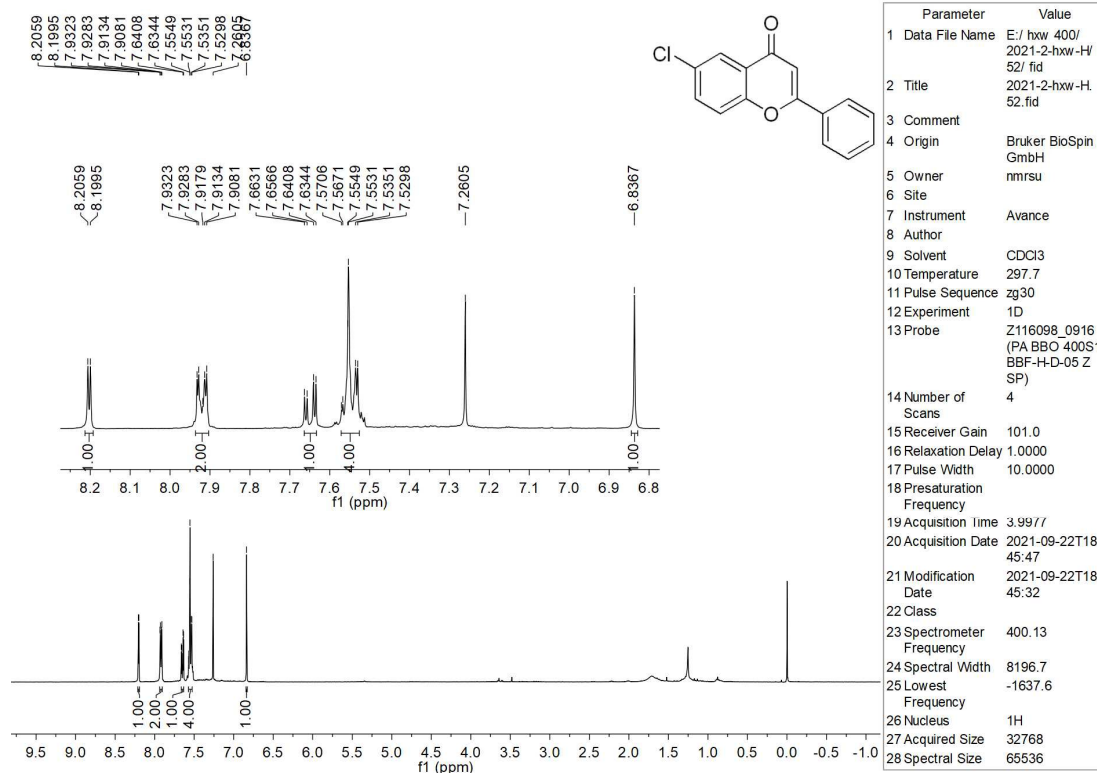
	Parameter	Value
1	Data File Name	E:/ hwx 400/ 2021-2-
2	Title	hwx-H/ 117/ fid
3	Comment	2021-2-hwx-H.117.fid
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	294.7
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	Z116098_0916 (PA BBO 400S1 BBF-H- D-05 Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Presaturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2021-10-29T20:30:4
21	Modification Date	2021-10-29T20:30:4
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1637.2
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ hwx 400/ 2021-2-hwx-C/ 46/ fid
2	Title	2021-2-hwx-C- 46.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsl
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.3
11	Pulse Sequence	zgpg30
12	Experiment	1d
13	Probe	Z116098_0916 (PA BBO 400S BBO-H-D-05 Z SP)
14	Number of Scans	800
15	Receiver Gain	101.0
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Pretsaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2021-11-12T04: 17.25
21	Modification Date	2021-11-12T04: 16.10
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	23809.5
25	Lowest Frequency	-1846.6
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

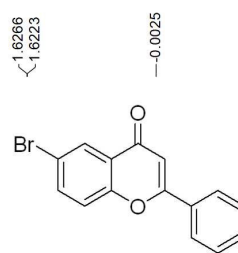
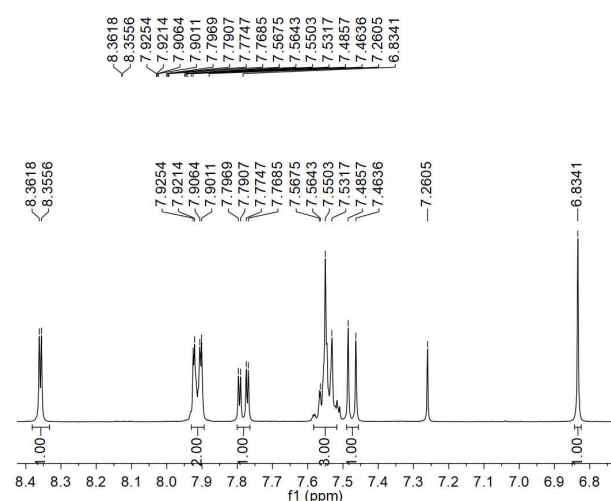


# 6-Chloro-2-phenyl-4H-chromen-4-one (2ea)

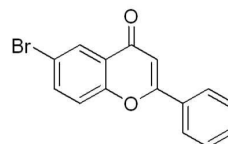
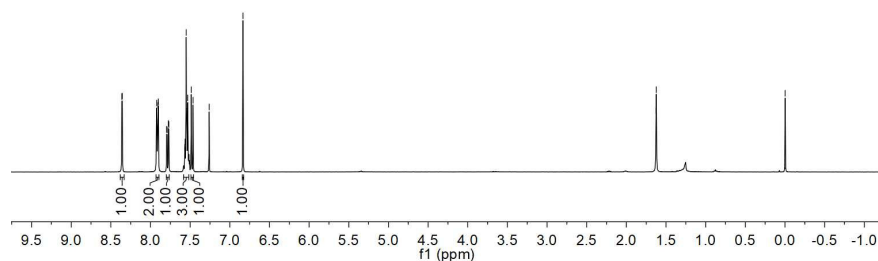




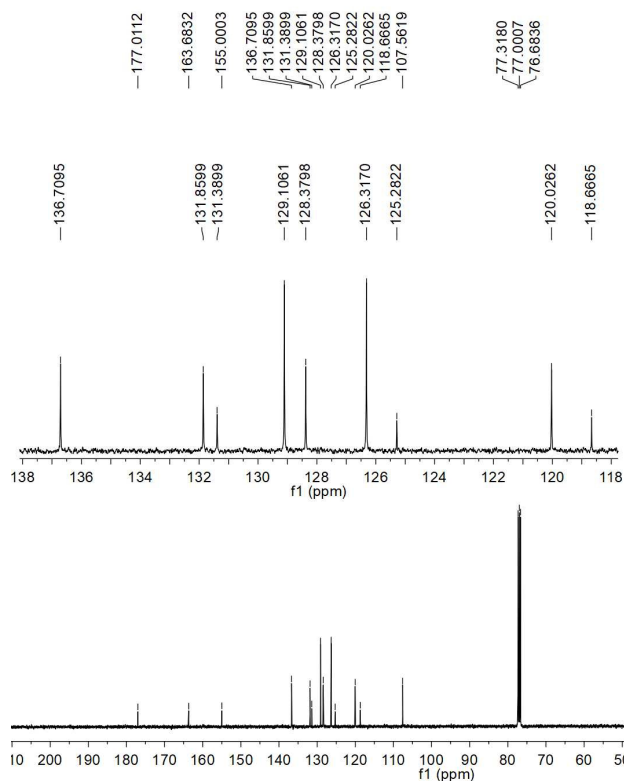
# 6-Bromo-2-phenyl-4*H*-chromen-4-one (2fa)



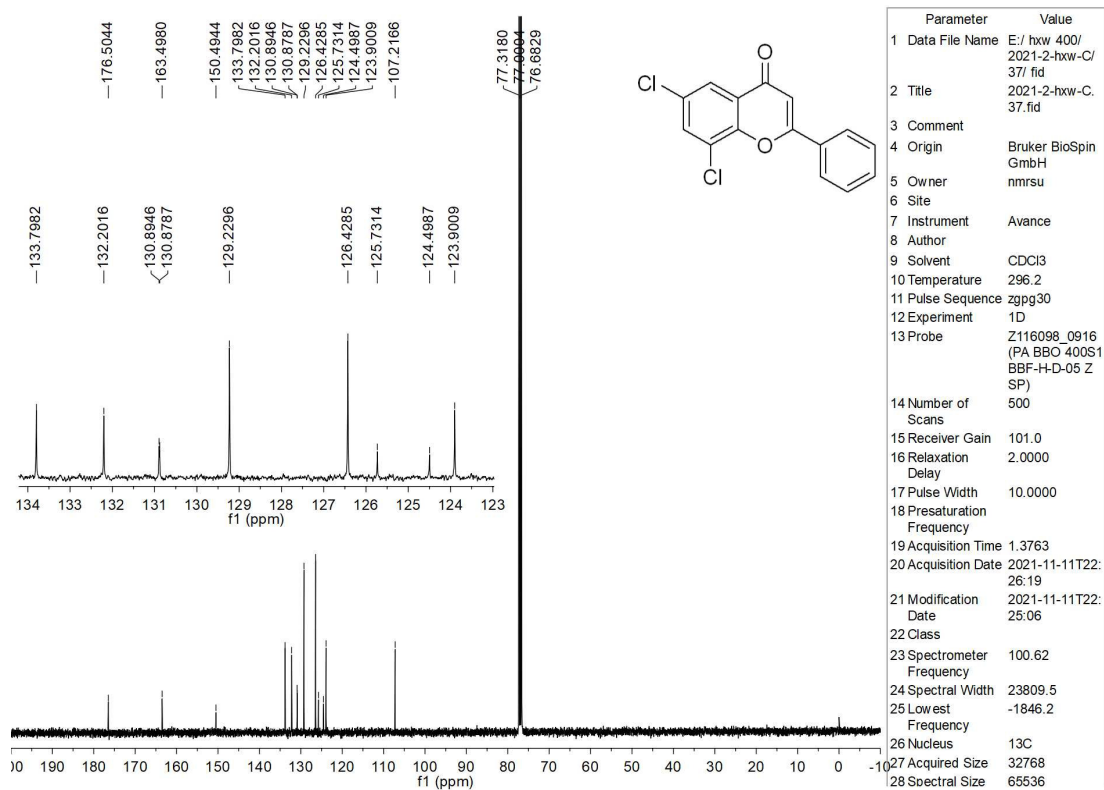
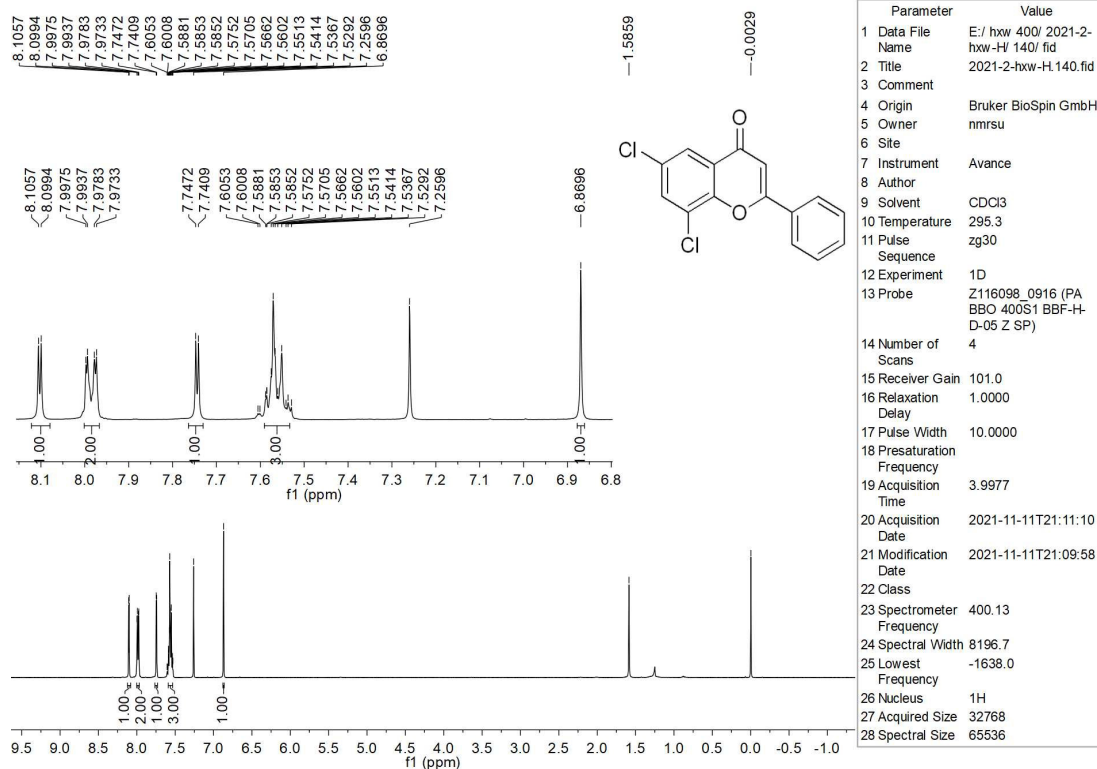
Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-H/ 101/ fid
2 Title	2021-2-hwx-H- 101.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	297.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-10-23T10:54:40
21 Modification Date	2021-10-23T10:53:58
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-C/ 36/ fid
2 Title	2021-2-hwx-C- 36.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	400
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2021-10-27T03:23:33
21 Modification Date	2021-10-27T03:22:28
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1846.4
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536

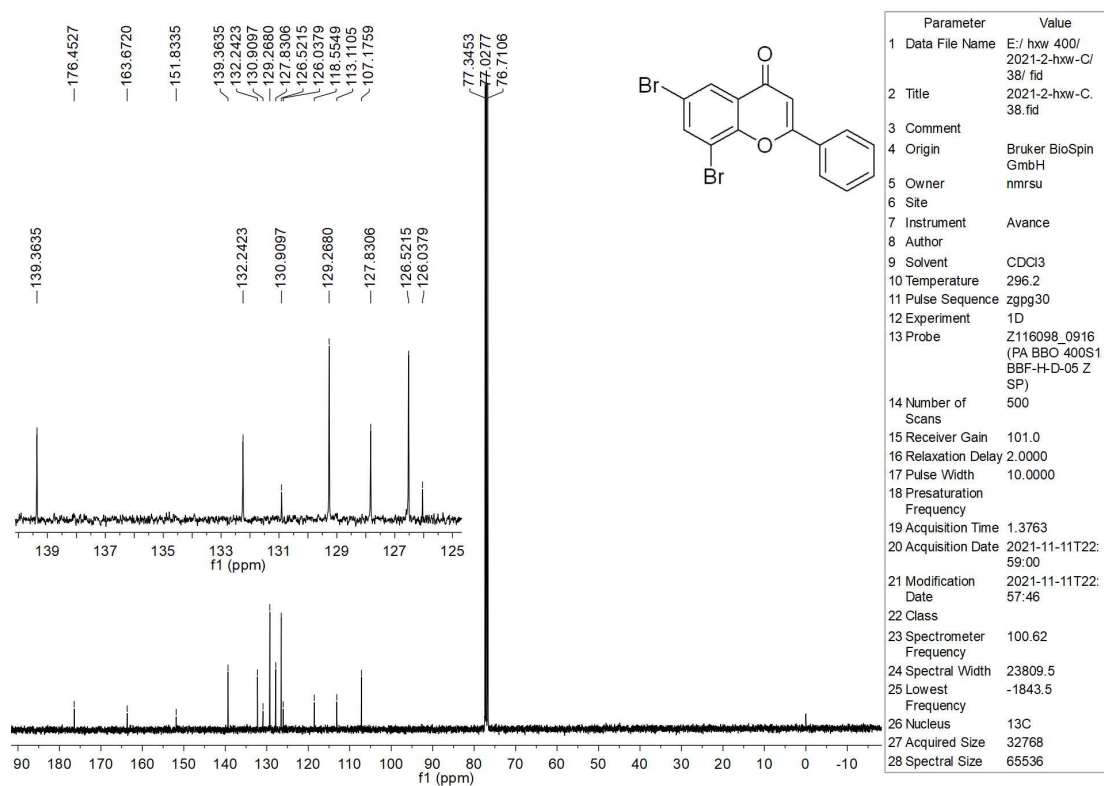
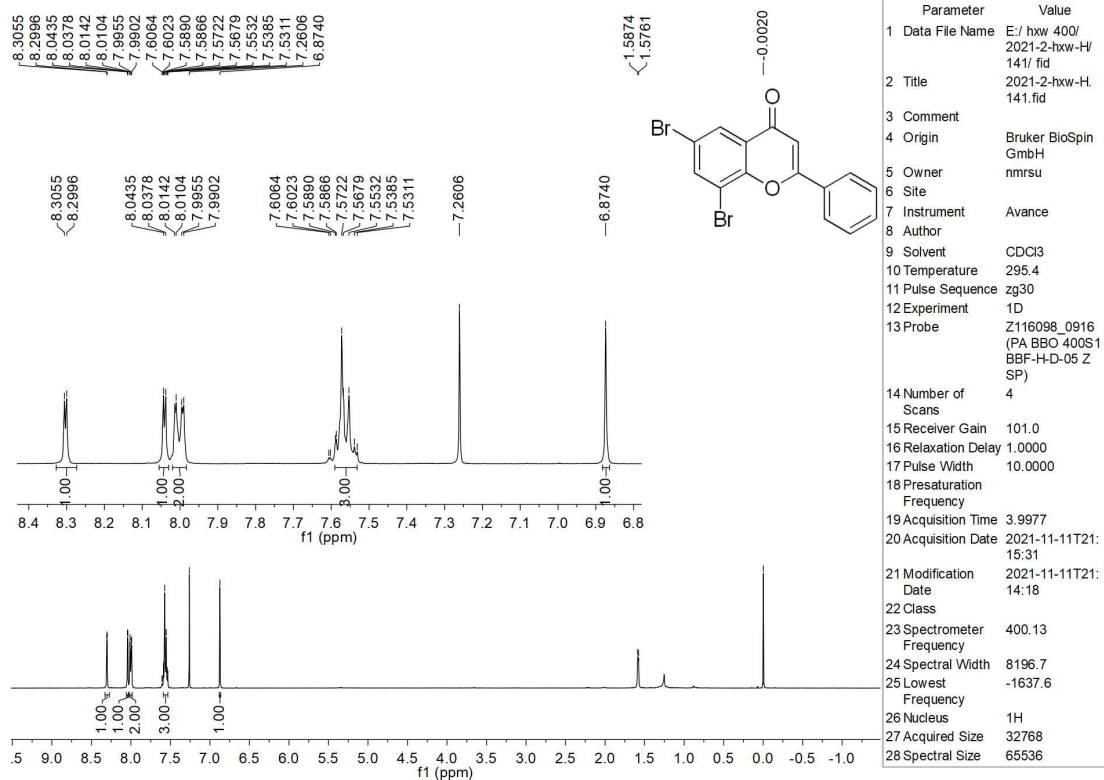


## 6,8-Dichloro-2-phenyl-4H-chromen-4-one (2ga)

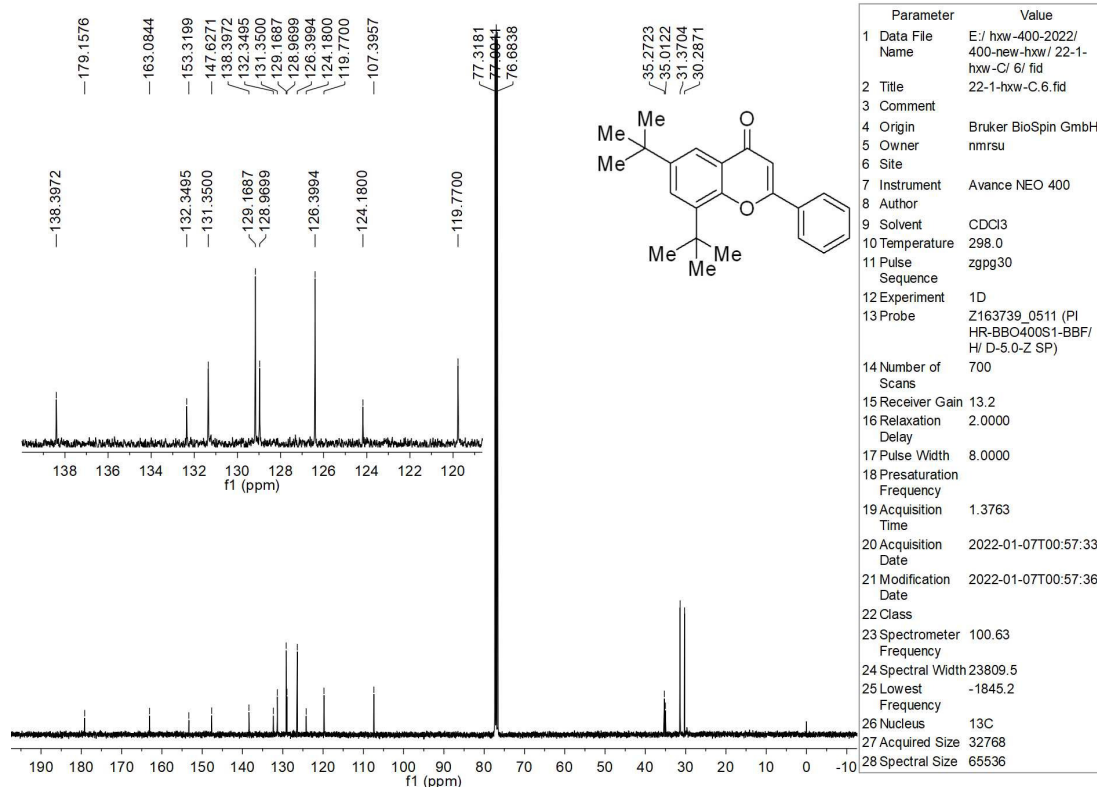
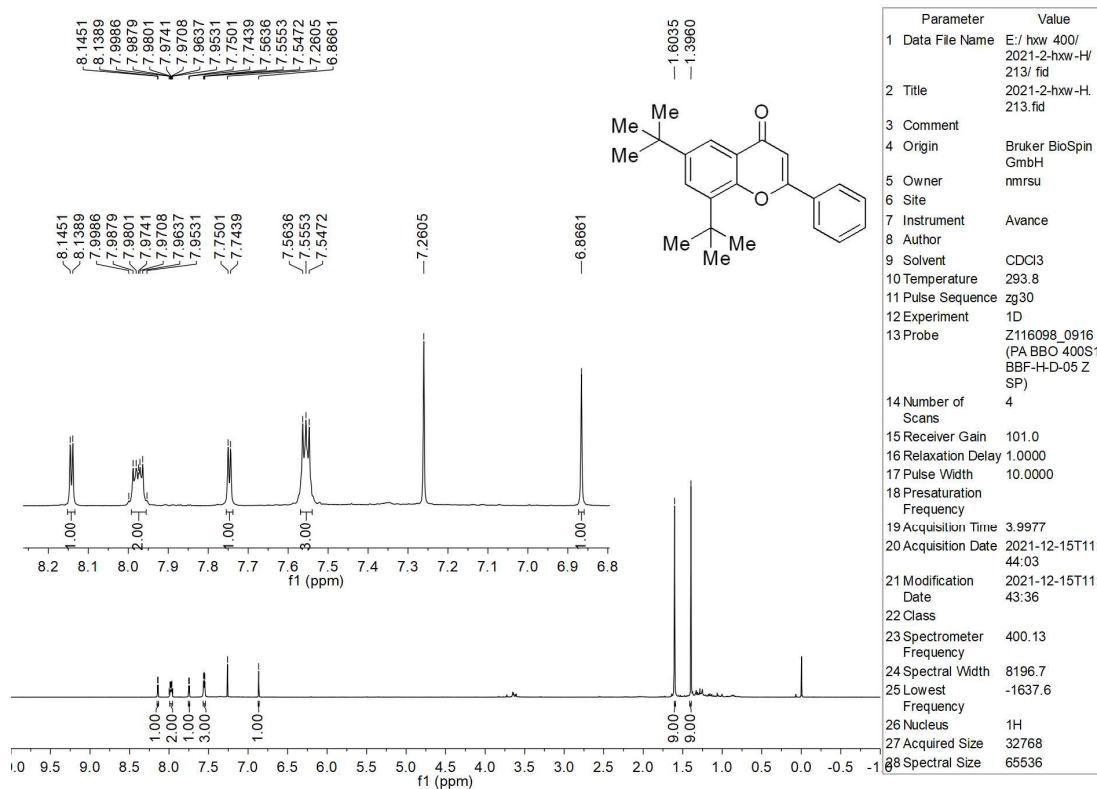




## 6,8-Dibromo-2-phenyl-4H-chromen-4-one (2ha)



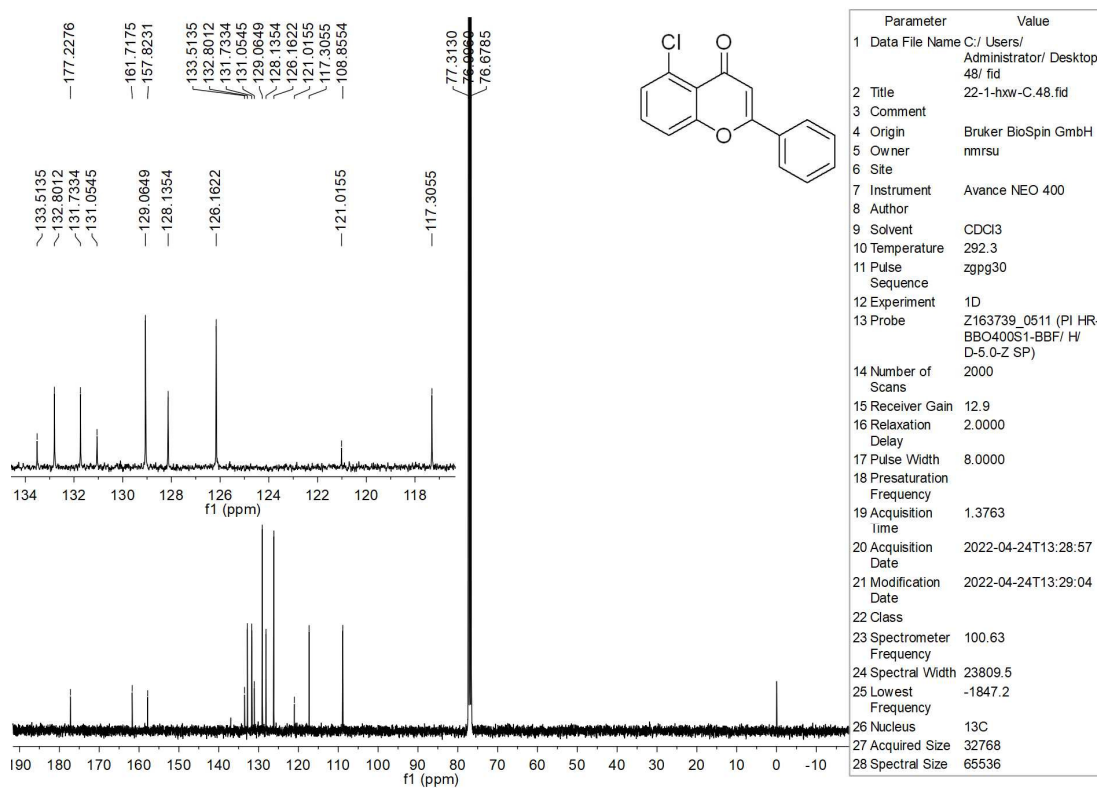
# 6,8-Di-*tert*-butyl-2-phenyl-4*H*-chromen-4-one(2ia)



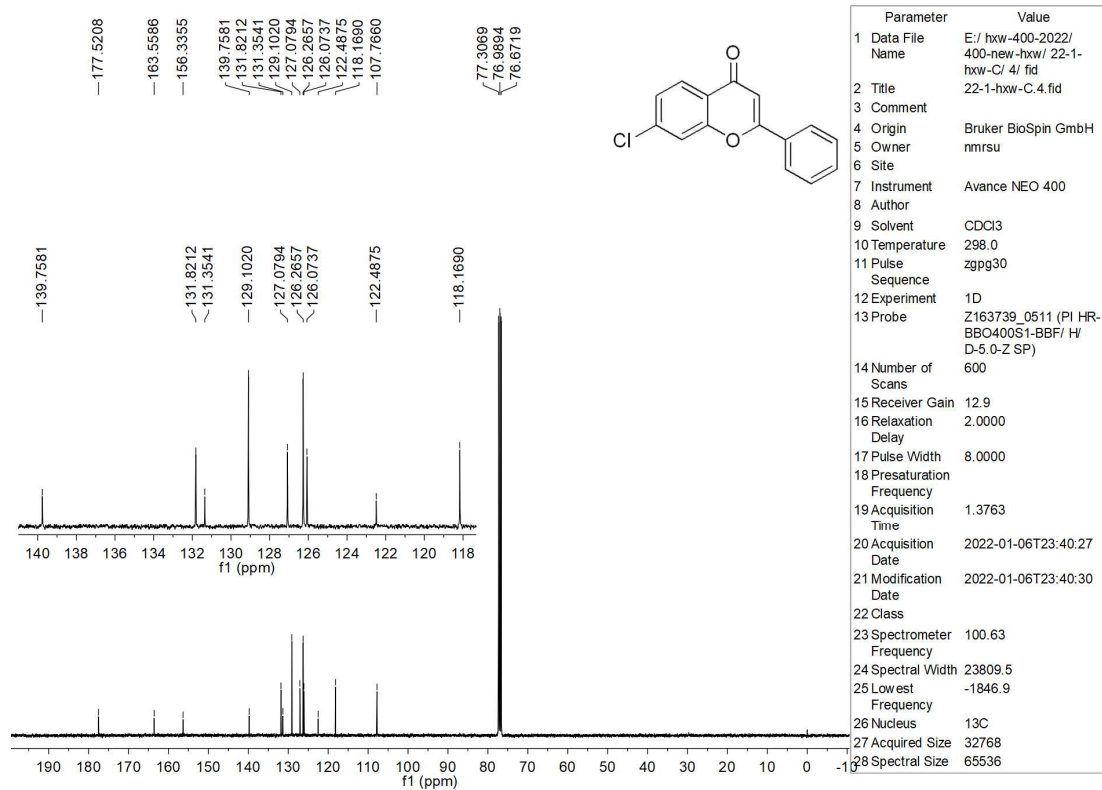
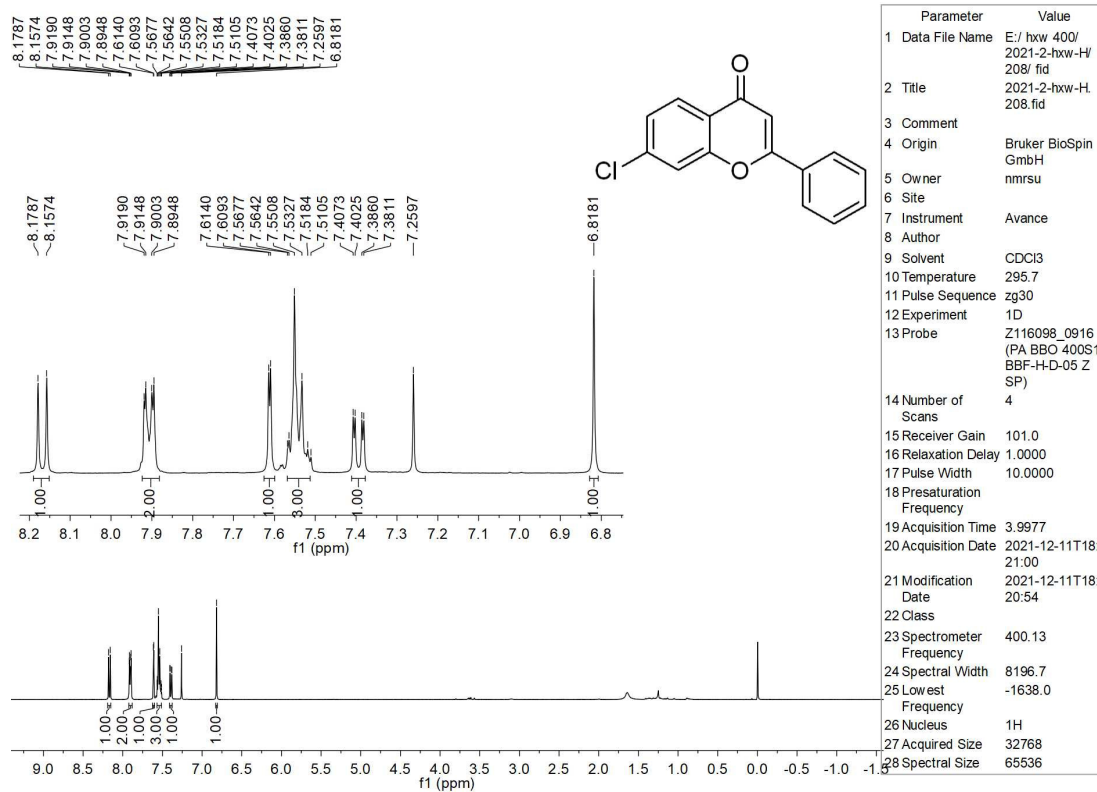
Chemical structure of 2-(4-chlorophenyl)-4-phenyl-2H-chromene is shown in the top right corner of the figure.

The <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) shows the following peaks (ppm) and integration values:

Peak (ppm)	Integration
7.9288, 7.9216, 7.9176, 7.9133, 7.9111, 7.9077, 7.9029, 7.8975	2.00
7.5623, 7.5541, 7.5473, 7.5398, 7.5350, 7.5290, 7.5081, 7.5047, 7.4871, 7.4836, 7.4156, 7.4120, 7.3965, 7.3929, 7.2604	4.00
7.2604	1.00
6.7962	1.00



## 7-Chloro-2-phenyl-4H-chromen-4-one (2ka)



# **8-(*tert*-Butyl)-2-phenyl-4*H*-chromen-4-one(2la)**

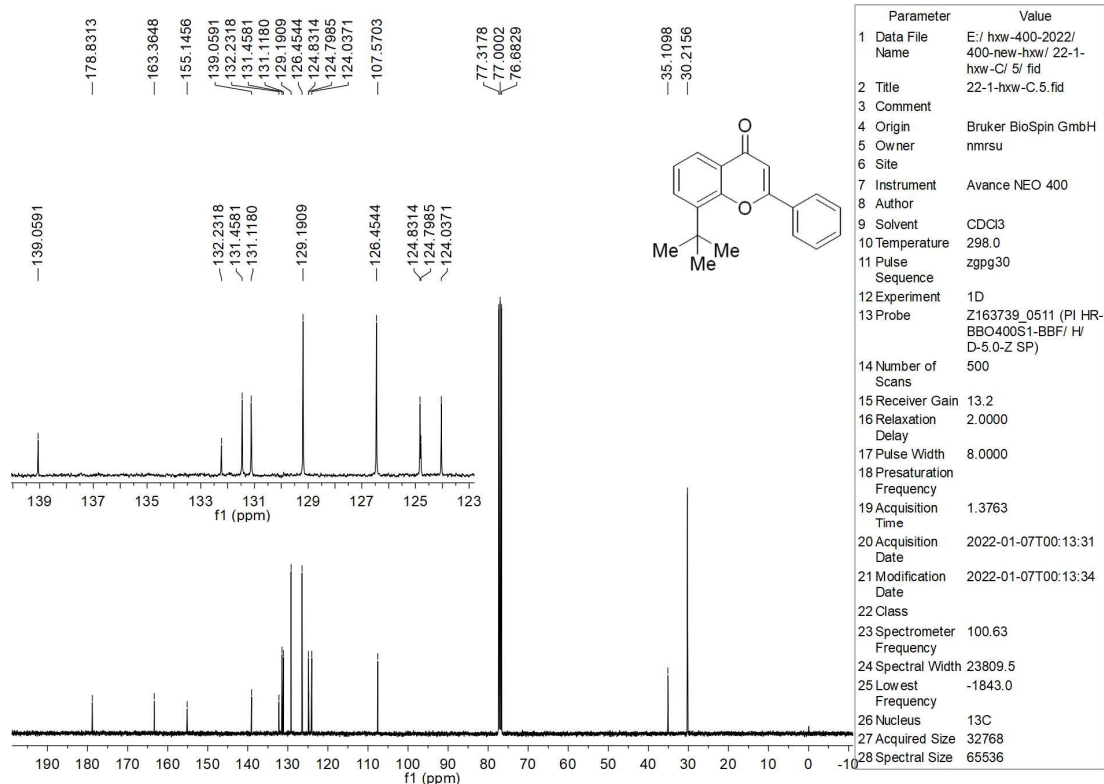
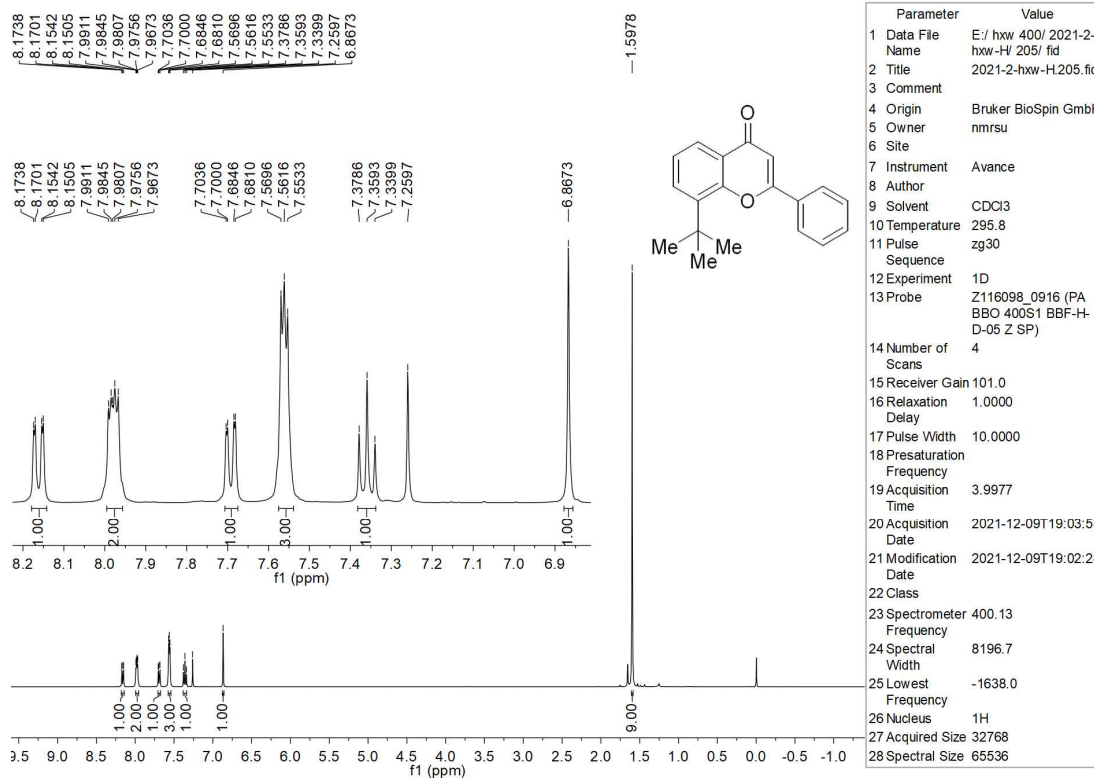
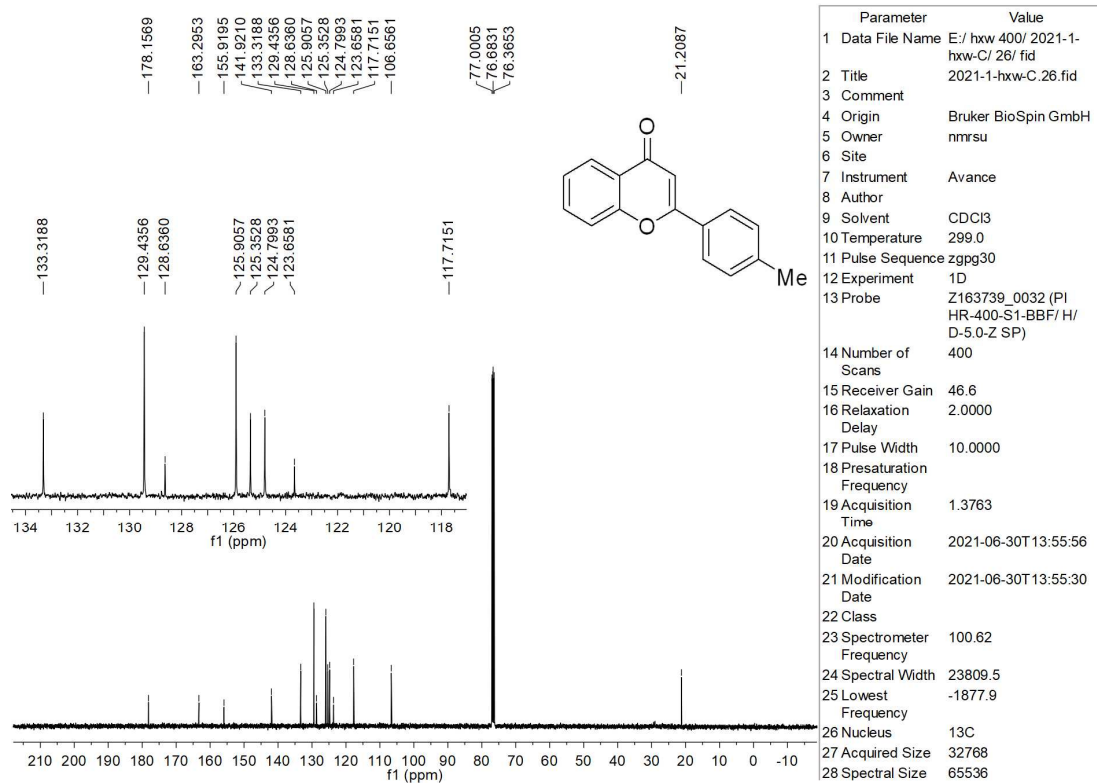


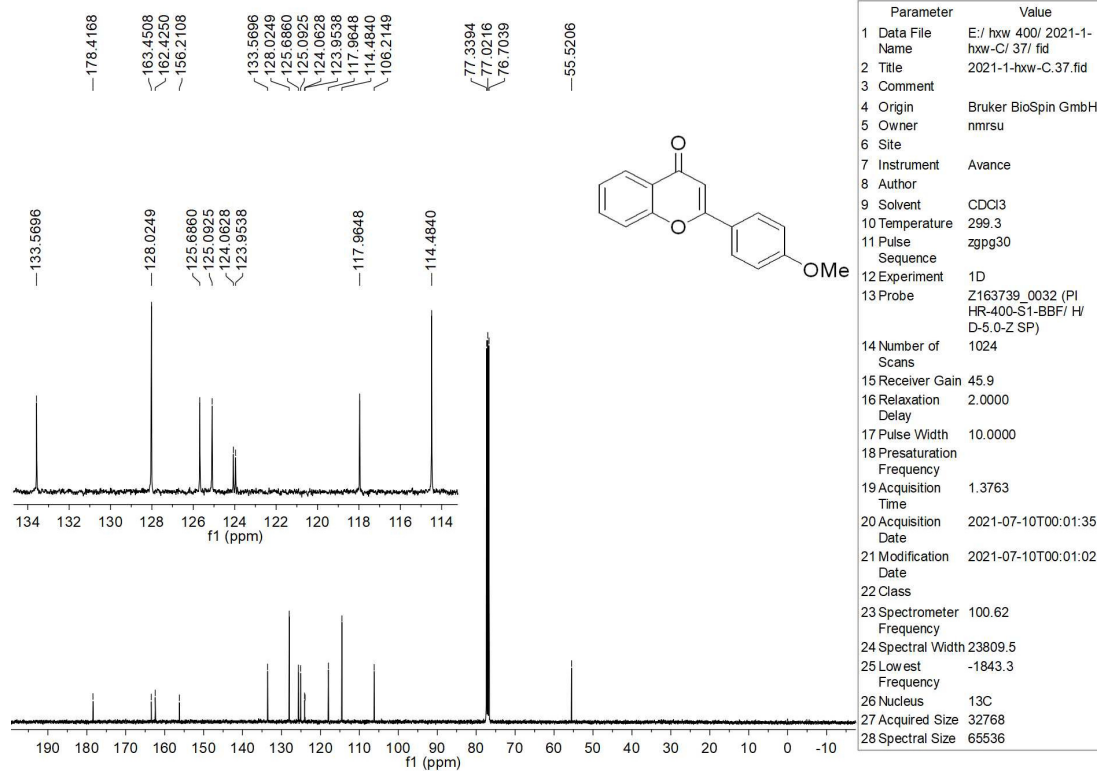
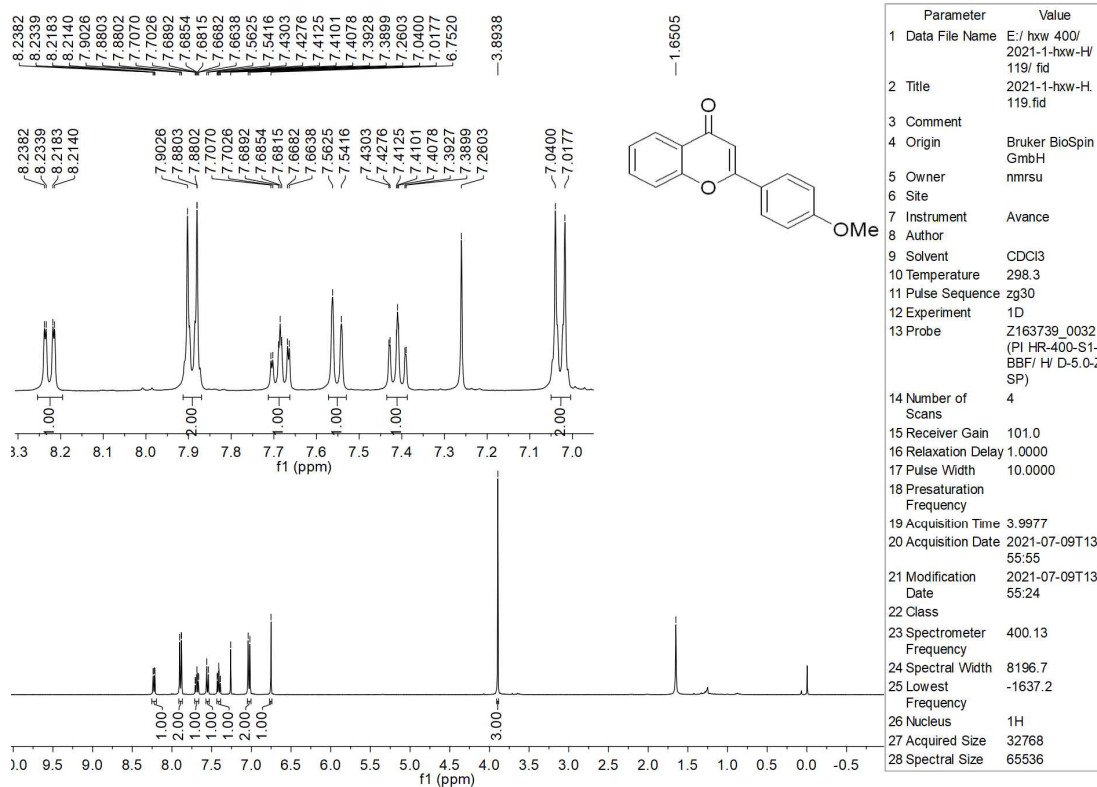


Figure 1 displays the  $^1\text{H}$  NMR spectra of compound **1**. The top spectrum shows the  $^1\text{H}$  NMR in  $\text{CDCl}_3$ , and the bottom spectrum shows the  $^1\text{H}$  NMR in  $\text{DMSO}-d_6$ . The chemical structure of **1** is shown as a benzofuran derivative with a 4-methylphenyl group. The table on the right lists the acquisition parameters.

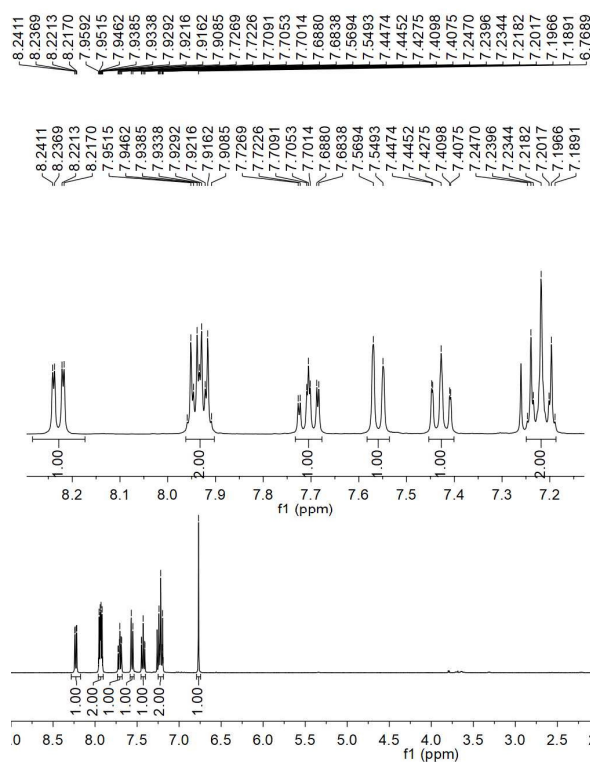
Parameter	Value
1 Data File Name	E:/ hww 400/ 2021-1-hxw-HV 98/ fid
2 Title	2021-1-hxw-H. 98.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	$\text{CDCl}_3$
10 Temperature	298.3
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF) H $^1$ D-5.0-2-SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-06-30T12:11:44
21 Modification Date	2021-06-30T12:11:18
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	$^1\text{H}$
27 Acquired Size	32768
28 Spectral Size	65536



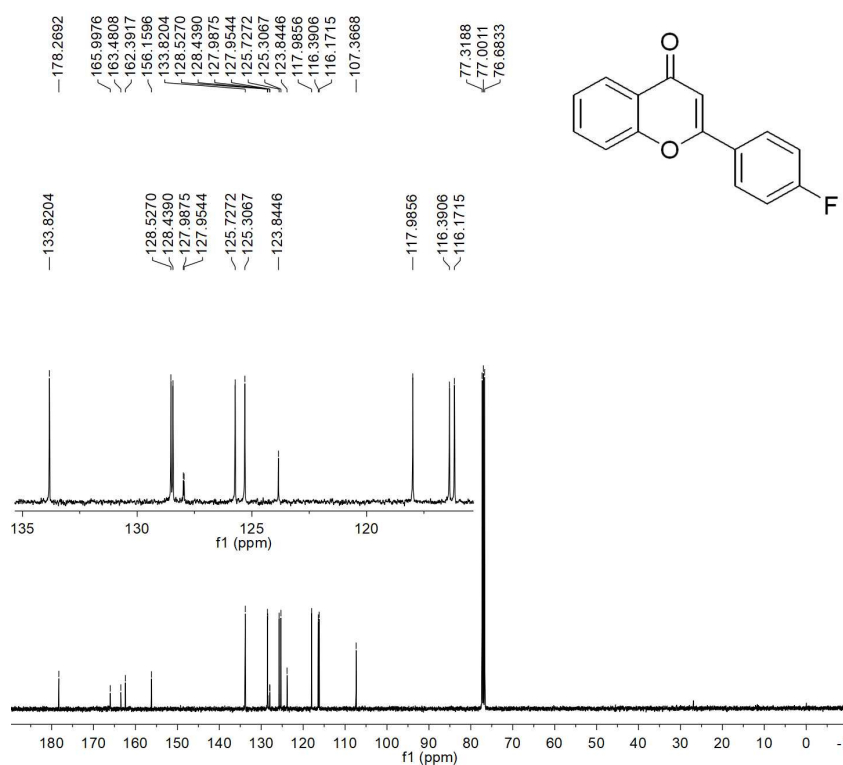
## 2-(4-Methoxyphenyl)-4H-chromen-4-one (2ac)



## 2-(4-Fluorophenyl)-4H-chromen-4-one (2ad)

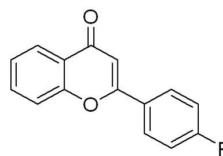
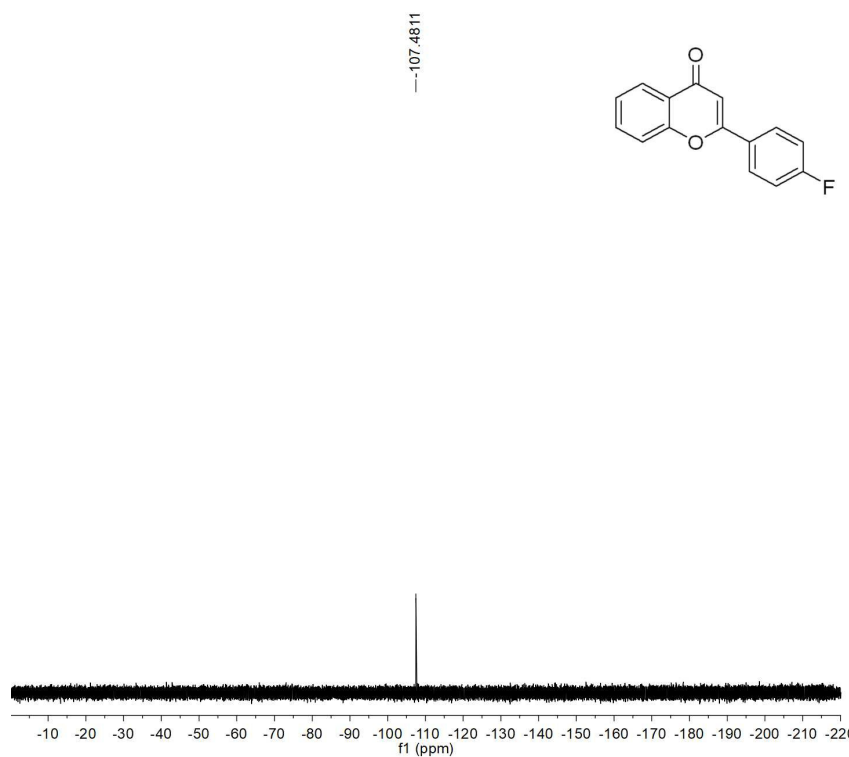


Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-H/ 100/ fid
2 Title	2021-2-hwx-H.100.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	297.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-10-23T10:50:57
21 Modification Date	2021-10-23T10:50:14
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	<sup>1</sup> H
27 Acquired Size	32768
28 Spectral Size	65536



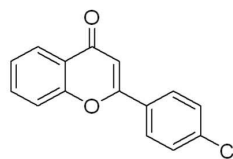
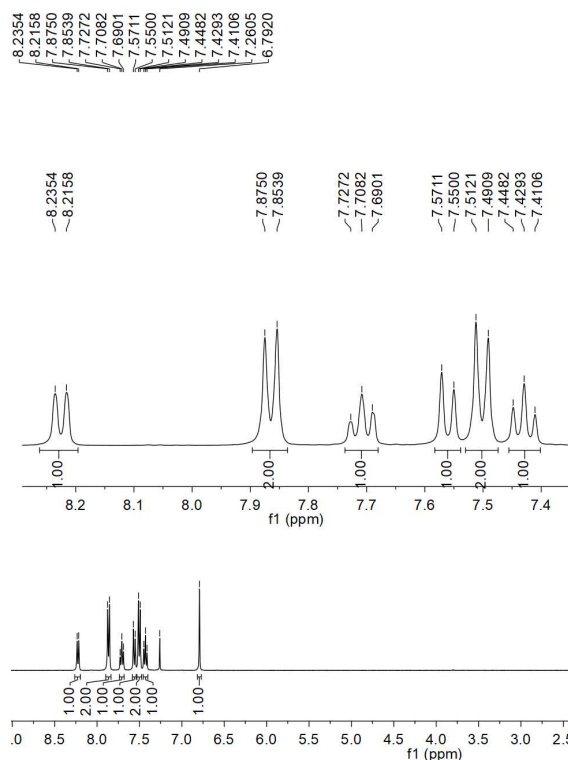
Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-C/ 33/ fid
2 Title	2021-2-hwx-C.33.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	298.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	400
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2021-10-27T01:55:08
21 Modification Date	2021-10-27T01:54:04
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1846.8
26 Nucleus	<sup>13</sup> C
27 Acquired Size	32768
28 Spectral Size	65536



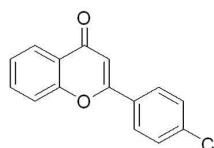
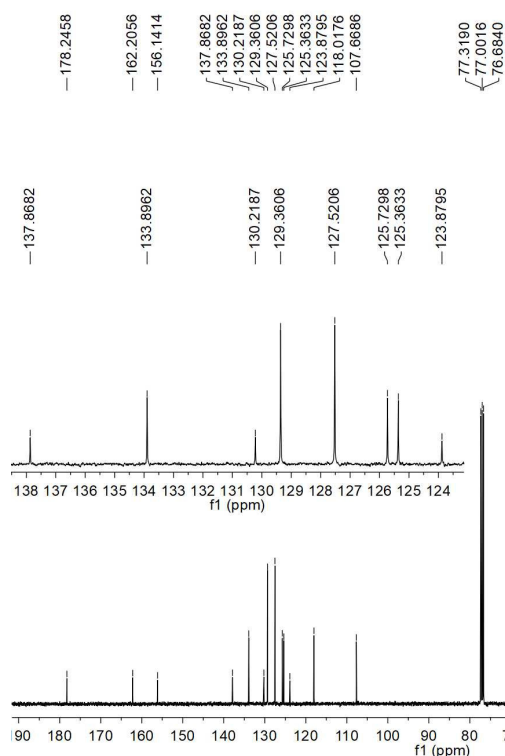


Parameter	Value
1 Data File Name	E:/ hww 400/ 2021-2-hww-F/ 3/ fid
2 Title	2021-2-hww-F.3.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	298.4
11 Pulse Sequence	zgig
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	16
15 Receiver Gain	13.1
16 Relaxation Delay	1.0000
17 Pulse Width	19.7500
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2021-10-27T01:30:39
21 Modification Date	2021-10-27T01:29:36
22 Class	
23 Spectrometer Frequency	376.46
24 Spectral Width	90909.1
25 Lowest Frequency	-83104.4
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	131072

## 2-(4-Chlorophenyl)-4H-chromen-4-one (2ae)

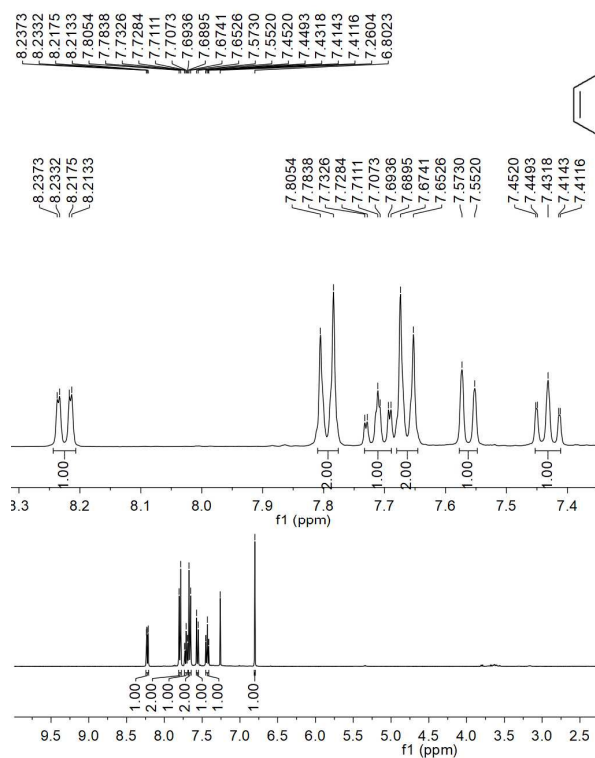


Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-H-69.fid
2 Title	2021-2-hwx-H-69.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	297.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-10-11T19:03:46
21 Modification Date	2021-10-11T19:01:42
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	<sup>1</sup> H
27 Acquired Size	32768
28 Spectral Size	65536

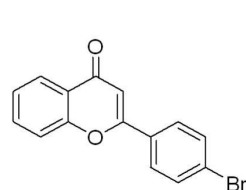
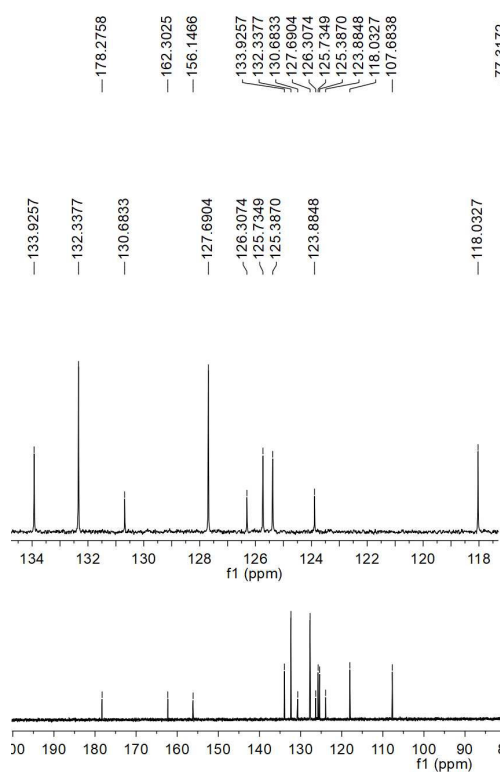


Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-C/ 19.fid
2 Title	2021-2-hwx-C-19.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	400
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2021-10-11T22:49:58
21 Modification Date	2021-10-11T22:47:54
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1847.1
26 Nucleus	<sup>13</sup> C
27 Acquired Size	32768
28 Spectral Size	65536

## 2-(4-Bromophenyl)-4H-chromen-4-one (2af)



Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-H/ 27/ fid
2 Title	2021-2-hwx-H.27.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	297.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-08-21T11:18:06
21 Modification Date	2021-08-21T11:17:34
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	<sup>1</sup> H
27 Acquired Size	32768
28 Spectral Size	65536



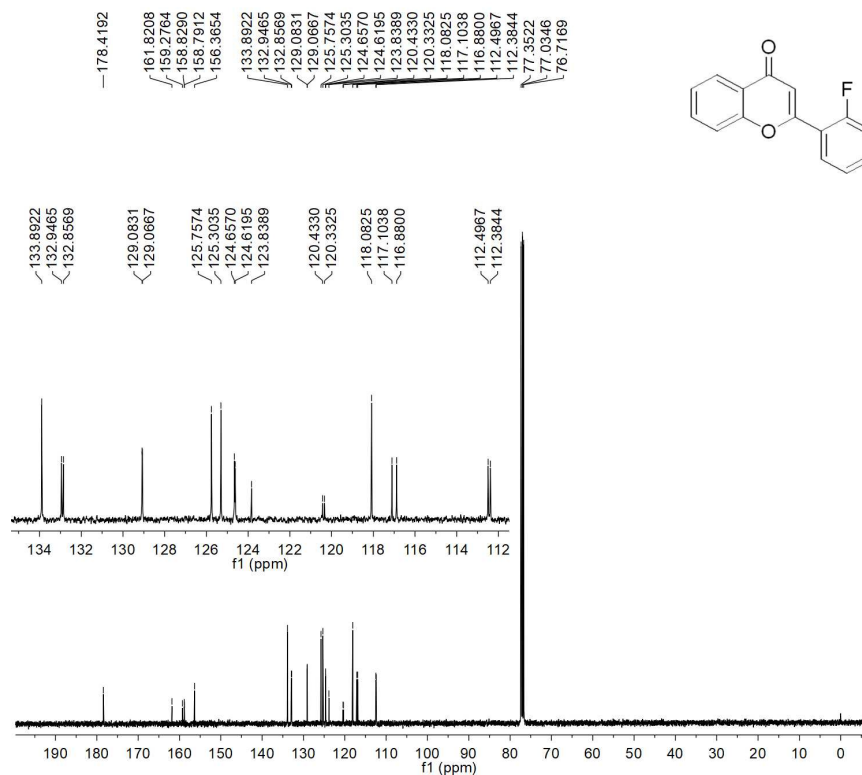
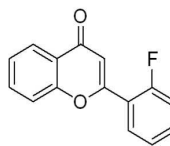
Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-C/ 7/ fid
2 Title	2021-2-hwx-C.7.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	297.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	500
15 Receiver Gain	49.5
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2021-08-21T11:59:01
21 Modification Date	2021-08-21T11:58:28
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1846.7
26 Nucleus	<sup>13</sup> C
27 Acquired Size	32768
28 Spectral Size	65536

**<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of 2-(2-fluorophenyl)-2H-chromene.**

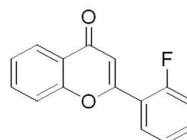
**Chemical structure:** O=C1C(=C(C2=CC=CC=C2F)OC3=CC=CC=C13)C4=CC=CC=C4

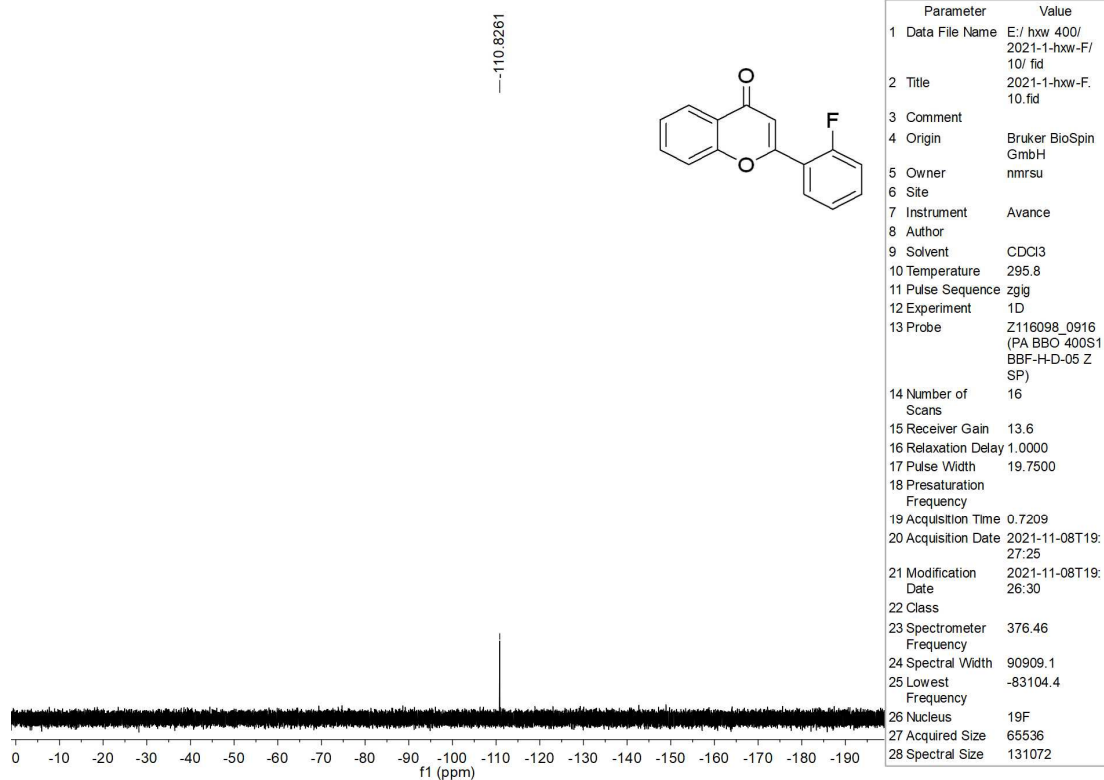
**Peak list (ppm):** 8.2512, 8.2470, 8.2434, 8.2314, 8.2270, 8.2270, 7.9578, 7.9533, 7.9385, 7.9341, 7.9194, 7.9148, 7.7117, 7.7078, 7.7039, 7.6905, 7.7117, 7.7078, 7.7039, 7.6905, 7.5886, 7.5392, 7.5267, 7.5067, 7.4526, 7.4326, 7.4149, 7.4126, 7.3472, 7.3447, 7.3277, 7.3259, 7.3090, 7.3065, 7.2802, 7.2376, 7.2352, 7.2298, 7.2275, 7.2090, 7.2067, 2.472, 2.468, 2.464, 2.460, 2.456, 2.452, 2.448, 2.444, 2.440, 2.436, 2.432, 2.428, 2.424, 2.420, 2.416, 2.412, 2.408, 2.404, 2.400, 2.396, 2.392, 2.388, 2.384, 2.380, 2.376, 2.372, 2.368, 2.364, 2.360, 2.356, 2.352, 2.348, 2.344, 2.340, 2.336, 2.332, 2.328, 2.324, 2.320, 2.316, 2.312, 2.308, 2.304, 2.300, 2.296, 2.292, 2.288, 2.284, 2.280, 2.276, 2.272, 2.268, 2.264, 2.260, 2.256, 2.252, 2.248, 2.244, 2.240, 2.236, 2.232, 2.228, 2.224, 2.220, 2.216, 2.212, 2.208, 2.204, 2.200, 2.196, 2.192, 2.188, 2.184, 2.180, 2.176, 2.172, 2.168, 2.164, 2.160, 2.156, 2.152, 2.148, 2.144, 2.140, 2.136, 2.132, 2.128, 2.124, 2.120, 2.116, 2.112, 2.108, 2.104, 2.100, 2.096, 2.092, 2.088, 2.084, 2.080, 2.076, 2.072, 2.068, 2.064, 2.060, 2.056, 2.052, 2.048, 2.044, 2.040, 2.036, 2.032, 2.028, 2.024, 2.020, 2.016, 2.012, 2.008, 2.004, 2.000, 1.996, 1.992, 1.988, 1.984, 1.980, 1.976, 1.972, 1.968, 1.964, 1.960, 1.956, 1.952, 1.948, 1.944, 1.940, 1.936, 1.932, 1.928, 1.924, 1.920, 1.916, 1.912, 1.908, 1.904, 1.900, 1.896, 1.892, 1.888, 1.884, 1.880, 1.876, 1.872, 1.868, 1.864, 1.860, 1.856, 1.852, 1.848, 1.844, 1.840, 1.836, 1.832, 1.828, 1.824, 1.820, 1.816, 1.812, 1.808, 1.804, 1.800, 1.796, 1.792, 1.788, 1.784, 1.780, 1.776, 1.772, 1.768, 1.764, 1.760, 1.756, 1.752, 1.748, 1.744, 1.740, 1.736, 1.732, 1.728, 1.724, 1.720, 1.716, 1.712, 1.708, 1.704, 1.700, 1.696, 1.692, 1.688, 1.684, 1.680, 1.676, 1.672, 1.668, 1.664, 1.660, 1.656, 1.652, 1.648, 1.644, 1.640, 1.636, 1.632, 1.628, 1.624, 1.620, 1.616, 1.612, 1.608, 1.604, 1.600, 1.596, 1.592, 1.588, 1.584, 1.580, 1.576, 1.572, 1.568, 1.564, 1.560, 1.556, 1.552, 1.548, 1.544, 1.540, 1.536, 1.532, 1.528, 1.524, 1.520, 1.516, 1.512, 1.508, 1.504, 1.500, 1.496, 1.492, 1.488, 1.484, 1.480, 1.476, 1.472, 1.468, 1.464, 1.460, 1.456, 1.452, 1.448, 1.444, 1.440, 1.436, 1.432, 1.428, 1.424, 1.420, 1.416, 1.412, 1.408, 1.404, 1.400, 1.396, 1.392, 1.388, 1.384, 1.380, 1.376, 1.372, 1.368, 1.364, 1.360, 1.356, 1.352, 1.348, 1.344, 1.340, 1.336, 1.332, 1.328, 1.324, 1.320, 1.316, 1.312, 1.308, 1.304, 1.300, 1.296, 1.292, 1.288, 1.284, 1.280, 1.276, 1.272, 1.268, 1.264, 1.260, 1.256, 1.252, 1.248, 1.244, 1.240, 1.236, 1.232, 1.228, 1.224, 1.220, 1.216, 1.212, 1.208, 1.204, 1.200, 1.196, 1.192, 1.188, 1.184, 1.180, 1.176, 1.172, 1.168, 1.164, 1.160, 1.156, 1.152, 1.148, 1.144, 1.140, 1.136, 1.132, 1.128, 1.124, 1.120, 1.116, 1.112, 1.108, 1.104, 1.100, 1.096, 1.092, 1.088, 1.084, 1.080, 1.076, 1.072, 1.068, 1.064, 1.060, 1.056, 1.052, 1.048, 1.044, 1.040, 1.036, 1.032, 1.028, 1.024, 1.020, 1.016, 1.012, 1.008, 1.004, 1.000, 0.996, 0.992, 0.988, 0.984, 0.980, 0.976, 0.972, 0.968, 0.964, 0.960, 0.956, 0.952, 0.948, 0.944, 0.940, 0.936, 0.932, 0.928, 0.924, 0.920, 0.916, 0.912, 0.908, 0.904, 0.900, 0.896, 0.892, 0.888, 0.884, 0.880, 0.876, 0.872, 0.868, 0.864, 0.860, 0.856, 0.852, 0.848, 0.844, 0.840, 0.836, 0.832, 0.828, 0.824, 0.820, 0.816, 0.812, 0.808, 0.804, 0.800, 0.796, 0.792, 0.788, 0.784, 0.780, 0.776, 0.772, 0.768, 0.764, 0.760, 0.756, 0.752, 0.748, 0.744, 0.740, 0.736, 0.732, 0.728, 0.724, 0.720, 0.716, 0.712, 0.708, 0.704, 0.700, 0.696, 0.692, 0.688, 0.684, 0.680, 0.676, 0.672, 0.668, 0.664, 0.660, 0.656, 0.652, 0.648, 0.644, 0.640, 0.636, 0.632, 0.628, 0.624, 0.620, 0.616, 0.612, 0.608, 0.604, 0.600, 0.596, 0.592, 0.588, 0.584, 0.580, 0.576, 0.572, 0.568, 0.564, 0.560, 0.556, 0.552, 0.548, 0.544, 0.540, 0.536, 0.532, 0.528, 0.524, 0.520, 0.516, 0.512, 0.508, 0.504, 0.500, 0.496, 0.492, 0.488, 0.484, 0.480, 0.476, 0.472, 0.468, 0.464, 0.460, 0.456, 0.452, 0.448, 0.444

Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-11-hwx-H/ 144.fid
2 Title	2021-1-hwx-H 144.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	295.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H- D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-11-08T19:24:11
21 Modification Date	2021-11-08T19:23:22
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ hwx 400/ 2021-2-hwx-C/ 47/ fid
2	Title	2021-2-hwx-C. 47.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.2
11	Pulse Sequence	zgpg30
12	Experiment	1d
13	Probe	Z116098_0916 (PA BBO 400S BBF-H-D-05 Z SP)
14	Number of Scans	500
15	Receiver Gain	101.0
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Presetration Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2021-11-12T04: 50:12
21	Modification Date	2021-11-12T04: 48:58
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	23809.5
25	Lowest Frequency	-1843.5
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536



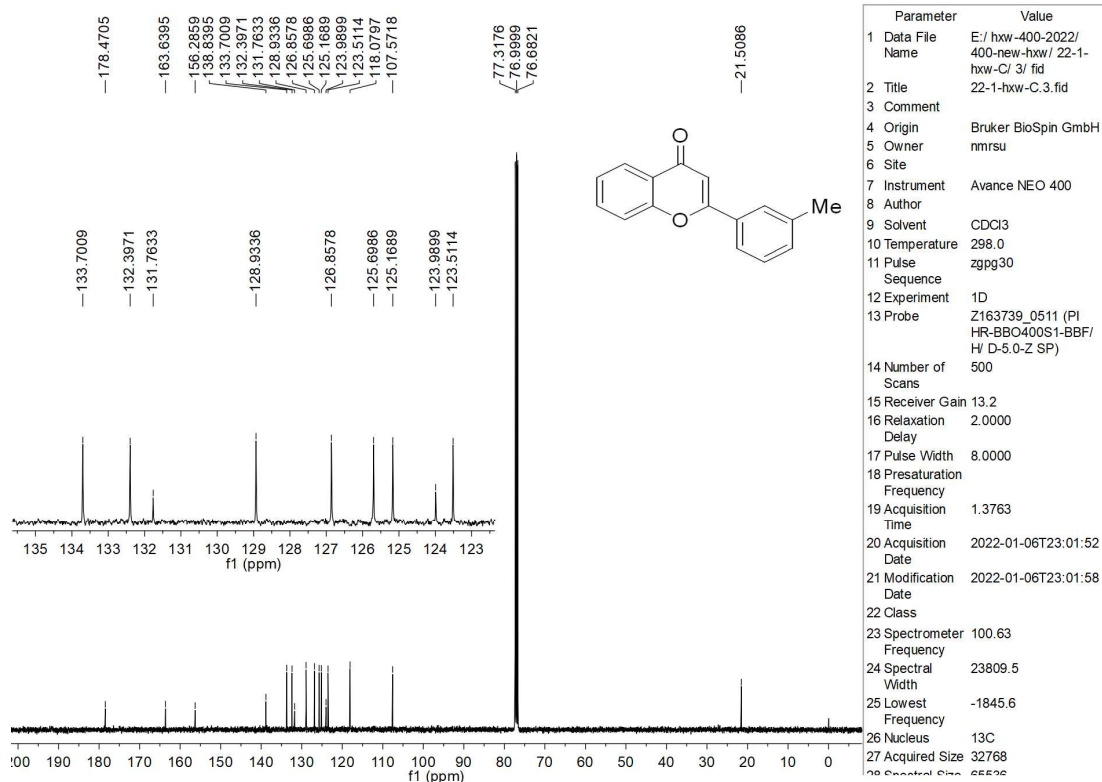


Chemical structure: Clc1cccc(c1)-c2cc3ccccc3oc2=O

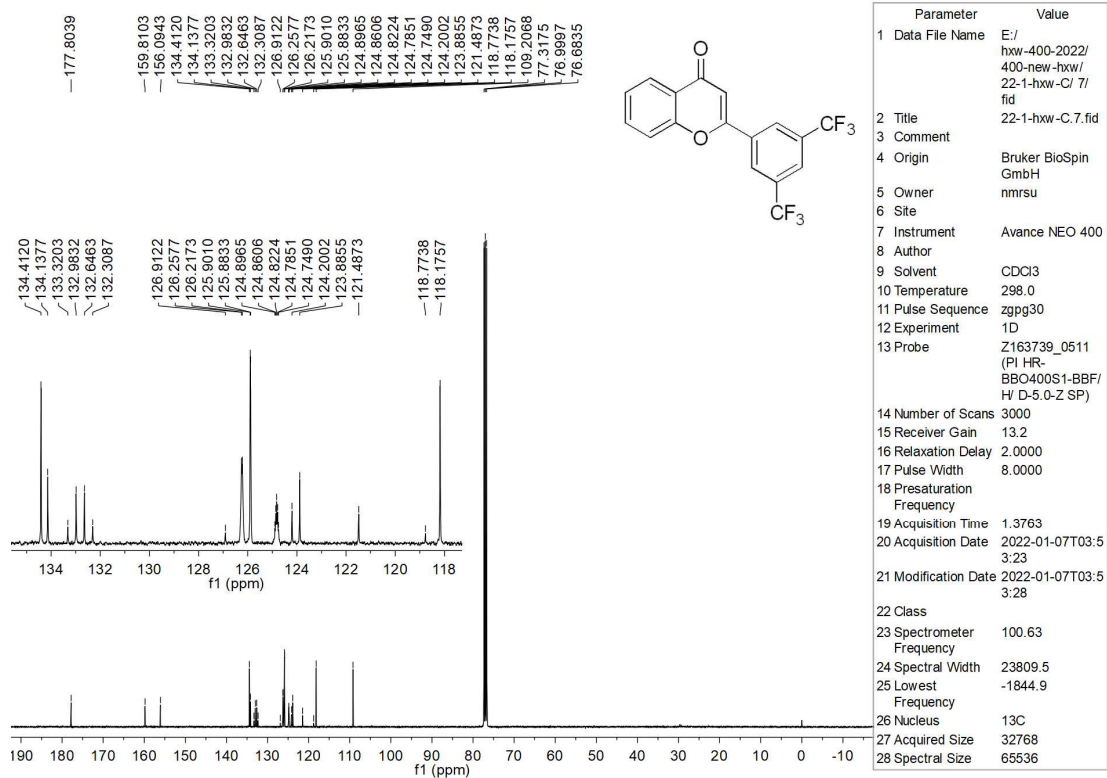
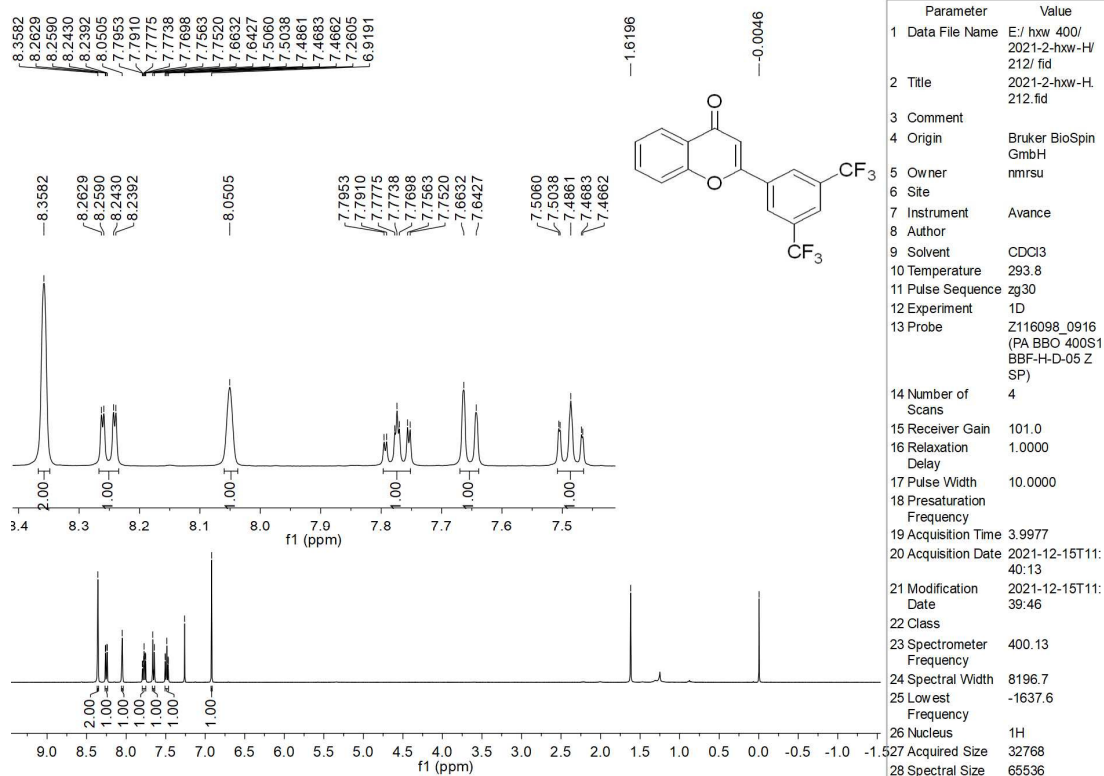
Parameter	Value
1 Data File Name	E:/ hsw 400/ 2021-2-hsw-H/ 130/ fid
2 Title	2021-2-hsw-H- 130.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.00000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-11-02T19: 43:44
21 Modification Date	2021-11-02T19: 43:22
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1638.0
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



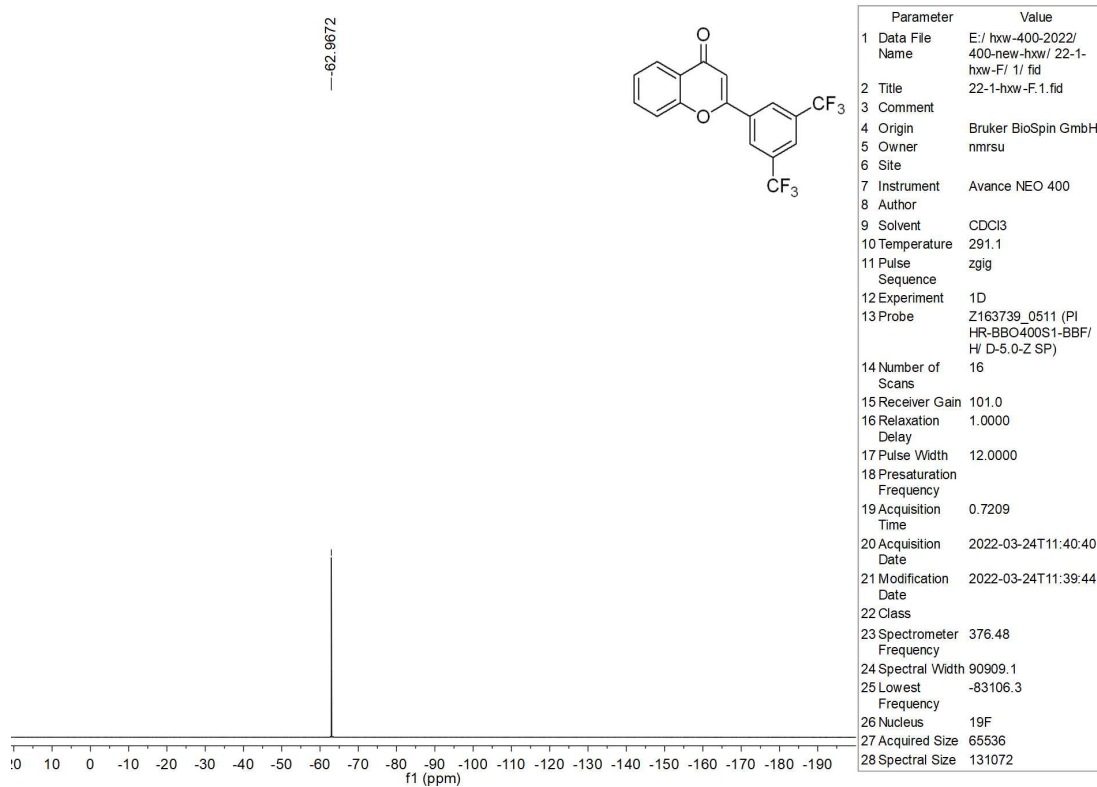


[illegible]

## 2-(3,5-Bis(trifluoromethyl)phenyl)-4H-chromen-4-one (2aj)





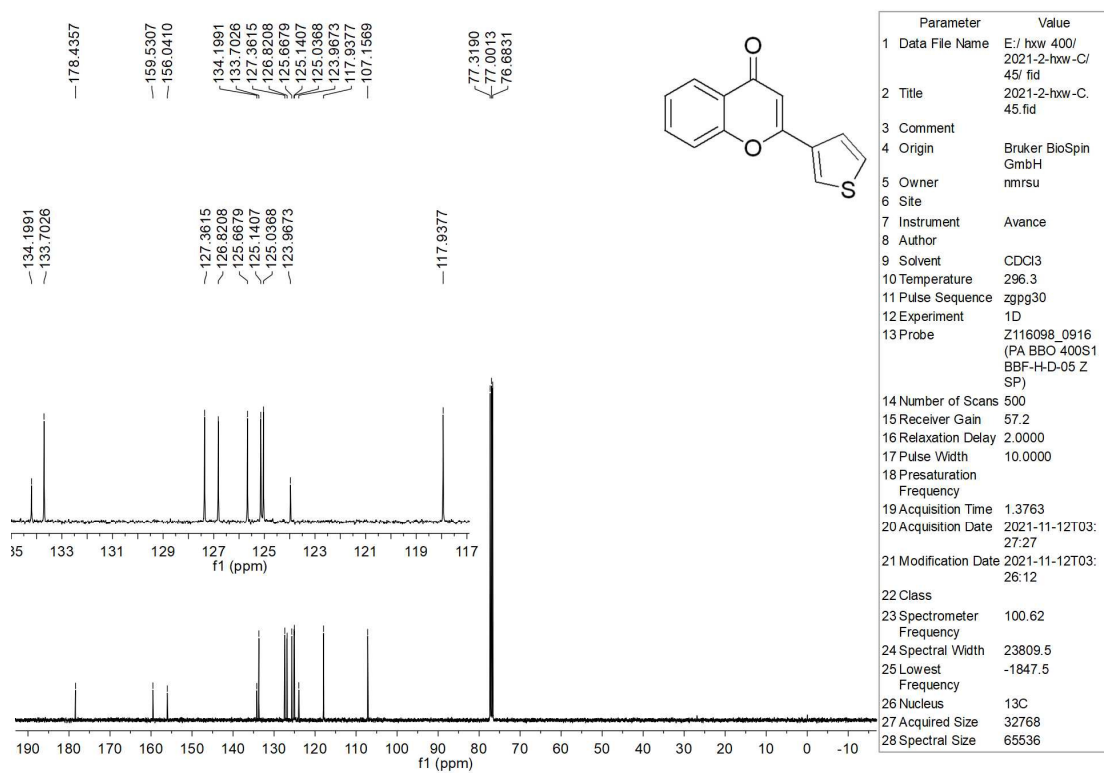


Chemical structure of 2-(thiophen-2-yl)-2H-chromene:

c1ccc2c(c1)oc3ccccc3c2-c4ccsc4

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of compound 1. The x-axis represents the chemical shift in ppm (f1), ranging from 0.0 to 10.0. The spectrum shows several multiplets in the aromatic region (6.8-8.3 ppm) and a singlet in the aliphatic region (7.4 ppm). Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
8.2280, 8.2236, 8.2083, 8.2039	1.00
8.0360, 8.0327, 8.0253	1.00
7.7094, 7.7050, 7.6916, 7.6878, 7.6839, 7.6704, 7.6661, 7.5413, 7.5206	1.00
7.5079, 7.5045, 7.4950, 7.4916, 7.4873, 7.4598, 7.4545, 7.4470, 7.4302, 7.4275, 7.4100, 7.3925, 7.3898, 7.3860	1.00
7.4000	1.00



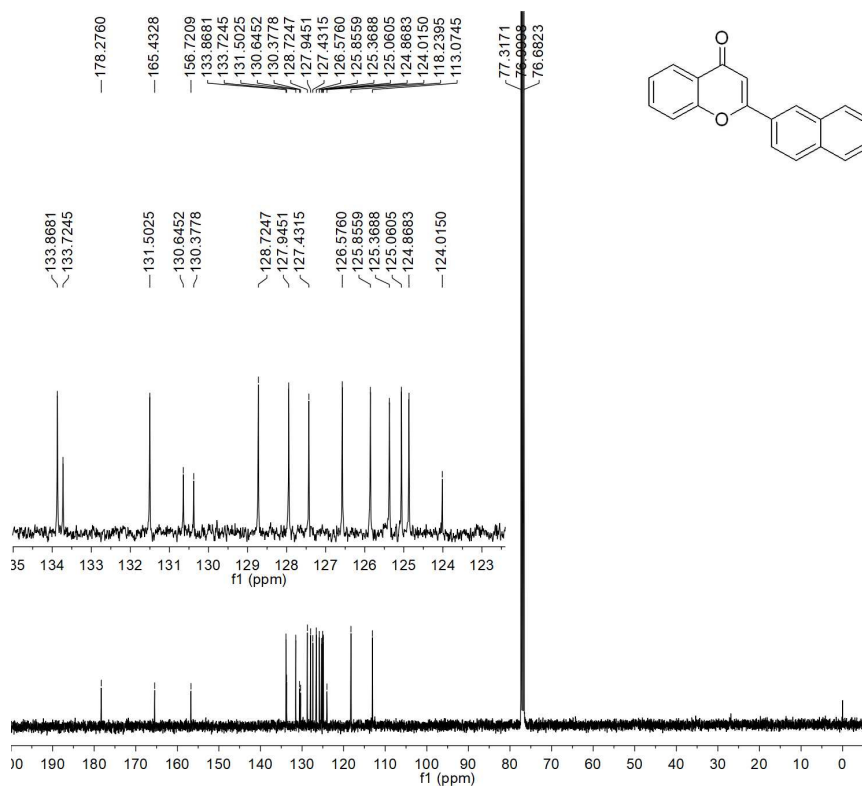
The figure displays two <sup>1</sup>H NMR spectra of compound 1 in CDCl<sub>3</sub>. The top spectrum shows the full range from 0 to 9 ppm, with peaks labeled with their chemical shifts. The bottom spectrum is a zoomed-in view of the aromatic region from 7.4 to 9.5 ppm. The chemical structure of compound 1 is shown as an inset. The x-axis is labeled 'f1 (ppm)'.

Chemical structure of compound 1: O=C1C(=O)c2ccccc2O1-c3ccc4ccccc4c3

<sup>1</sup>H NMR peaks (ppm):

- 8.3307, 8.3264, 8.3264, 8.3107, 8.3065, 8.1558, 8.1506, 8.1485, 8.1453, 8.1396, 8.1313, 8.1226, 8.0482, 8.0276, 7.9717, 7.9635, 7.9477, 7.7897, 7.7865, 7.7719, 7.7687, 7.7335, 7.7297, 7.7259, 7.7125, 7.7081, 7.6122, 7.6122, 7.6042, 7.6021, 7.5943, 7.5871, 7.5854, 7.5794, 7.5768, 7.5726, 7.5702, 7.5557, 7.5535, 7.5008, 7.4986, 7.4808, 7.4631, 7.4609, 7.2596, 6.9986, 1.5984, 1.5933, -0.0019.

	Parameter	Value
1	Data File Name	E:/ hwx 400/ 2021-2-hwx-H 112/ fid
2	Title	2021-2-hwx-H 112. fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	294.9
11	Pulse Sequence	zg30
12	Experiment	1D
13	Probe	1216098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14	Number of Scans	4
15	Receiver Gain	101.0
16	Relaxation Delay	1.0000
17	Pulse Width	10.0000
18	Preset Saturation Frequency	
19	Acquisition Time	3.9977
20	Acquisition Date	2021-10-28T19:18:10
21	Modification Date	2021-10-28T19:16:56
22	Class	
23	Spectrometer Frequency	400.13
24	Spectral Width	8196.7
25	Lowest Frequency	-1638.0
26	Nucleus	1H
27	Acquired Size	32768
28	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/hww 400/ 2021-2-hxw-C/ 41.fid
2	Title	2021-2-hxw-C. 41.fid
3	Comment	
4	Origin	Bruker BioSph GmbH
5	Owner	nmrsl
6	Site	
7	Instrument	Avance
8	Author	
9	Solvent	CDCl3
10	Temperature	296.4
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Probe	Z161098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14	Number of Scans	800
15	Receiver Gain	101.0
16	Relaxation Delay	2.0000
17	Pulse Width	10.0000
18	Prestaturation Frequency	
19	Acquisition Time	1.3763
20	Acquisition Date	2021-11-12T01: 42:41
21	Modification Date	2021-11-12T01: 41:28
22	Class	
23	Spectrometer Frequency	100.62
24	Spectral Width	23809.5
25	Lowest Frequency	-1846.2
26	Nucleus	13C
27	Acquired Size	32768
28	Spectral Size	65536

Chemical structure of 2-(benzo[c][1,2,5]oxadiazol-2-yl)naphthalene is shown in the top right corner.

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) of 2-(benzo[c][1,2,5]oxadiazol-2-yl)naphthalene. The spectrum displays aromatic signals in the range of 7.5 to 8.5 ppm. Integration values are provided below the peaks.

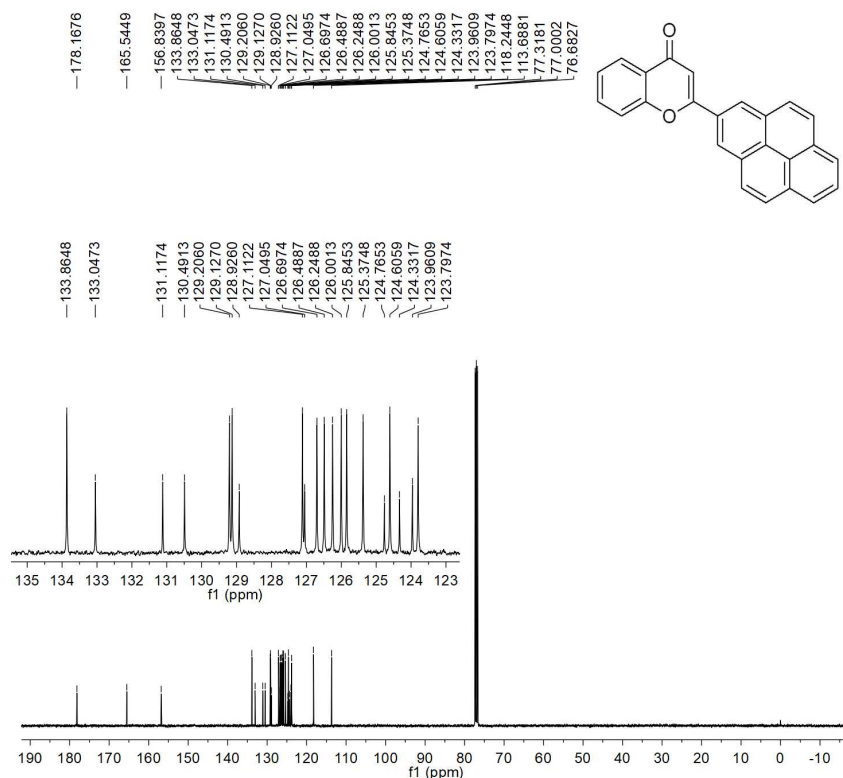
Chemical shift (ppm) labels (from left to right):

- 8.4389, 8.4157, 8.3631, 8.3433, 8.2713, 8.2619, 8.2463, 8.1889, 8.1784, 8.1689, 8.1553, 8.1158, 8.0919, 8.0711, 8.0521, 7.7645, 7.7451, 7.7258, 7.6088, 7.5879, 7.5155, 7.4964, 7.4778, 7.2604, 7.2570, 6.8477

Integration values (from left to right):

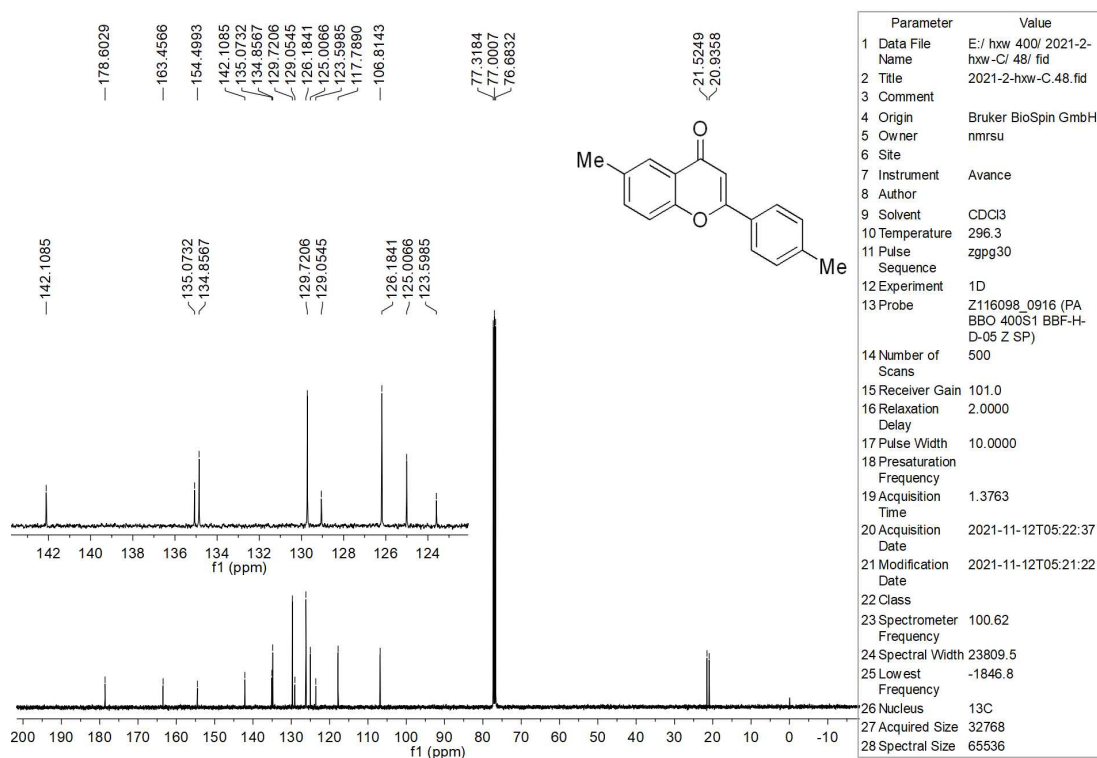
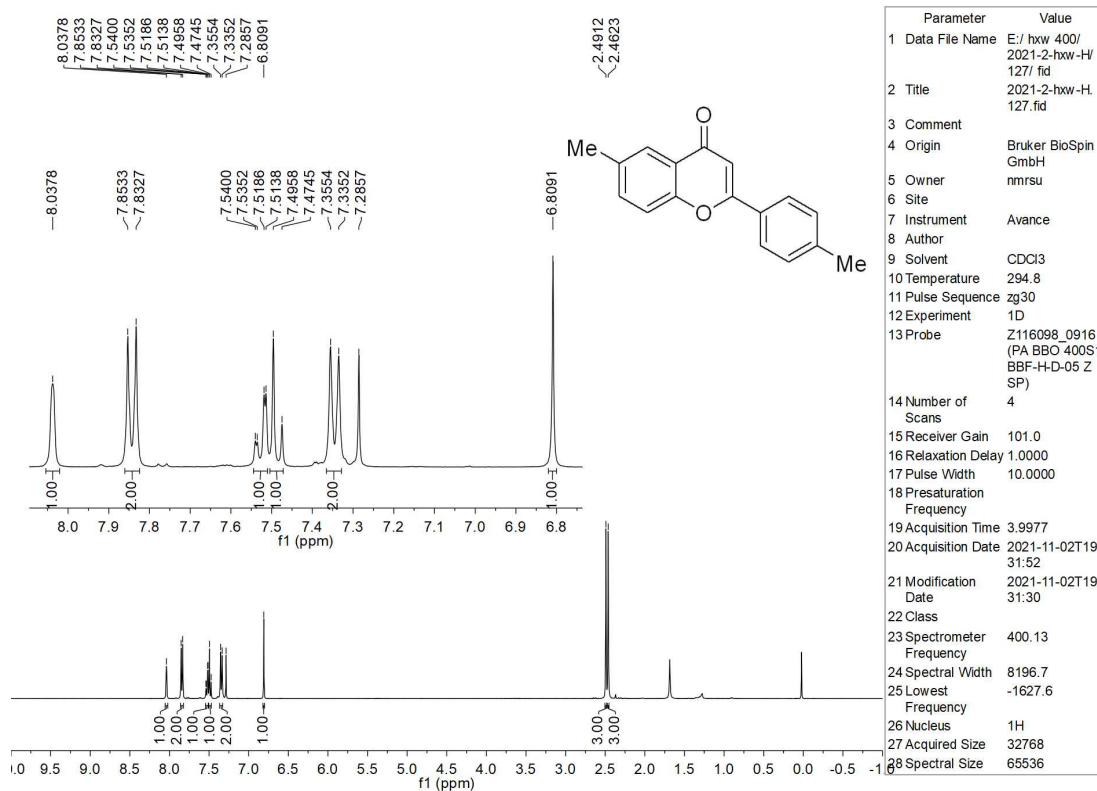
- 1.00, 1.00, 2.00, 1.00, 1.00, 1.00, 1.00, 1.00, 4.00, 2.00, 2.00, 1.00, 4.00, 1.00, 1.00, 1.00

Parameter	Value
1 Data File Name	E:/ hwx-400-2022/ 400-new-hwx/ 22-1- hwx-H' 41/ fid
2 Title	22-1-hwx-H.41.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	290.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H' D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-03-22T19:20:20
21 Modification Date	2022-03-22T19:19:24
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1638.2
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536



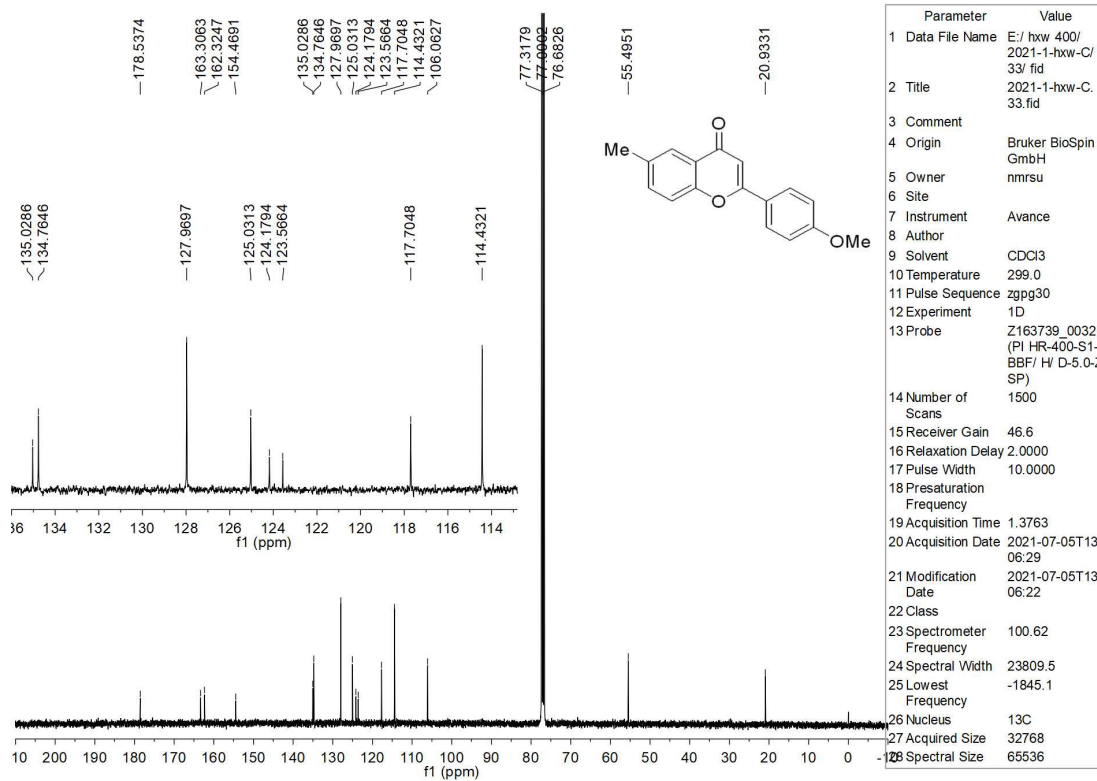
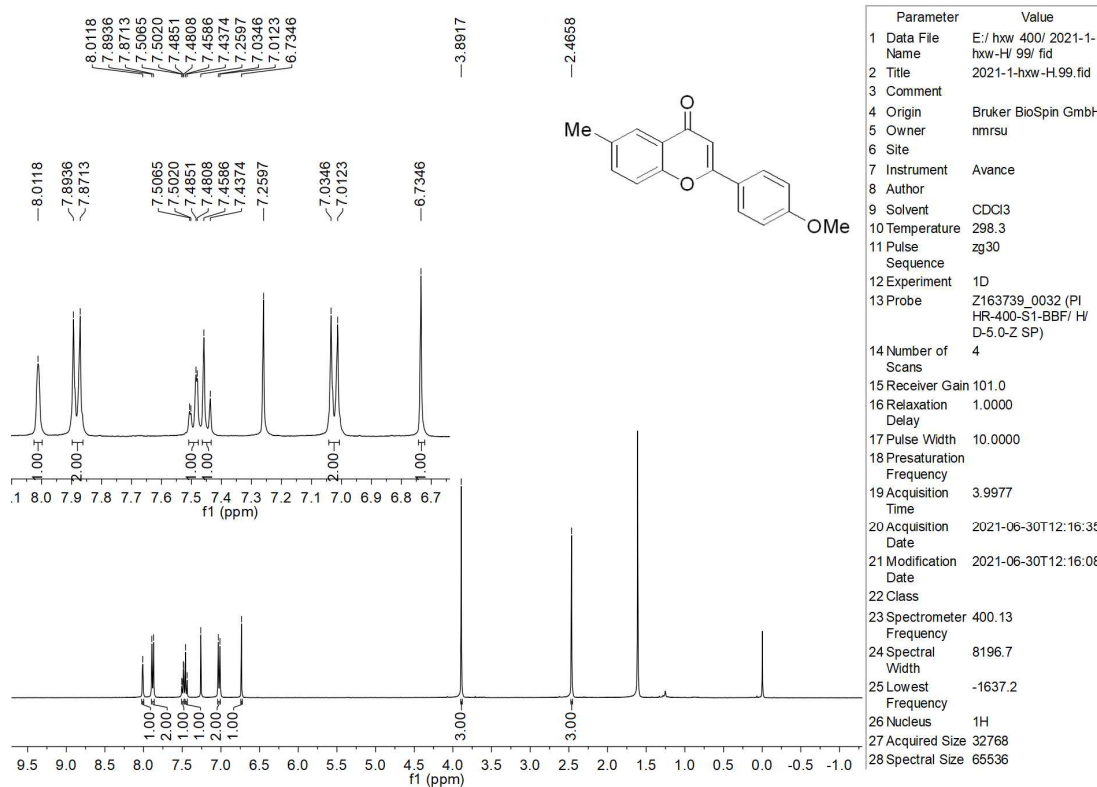
Parameter	Value
1 Data File Name	E:/ hwx-400-2022/ 400- new-hwx/ 22-1-hwx-C/ 27/ fid
2 Title	22-1-hwx-C.27.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	291.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	D163739_0511 (PI HR- BB0400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	600
15 Receiver Gain	13.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-03-23T11:47:16
21 Modification Date	2022-03-23T11:46:20
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1849.8
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536

# 6-Methyl-2-(*p*-tolyl)-4*H*-chromen-4-one (2bb)

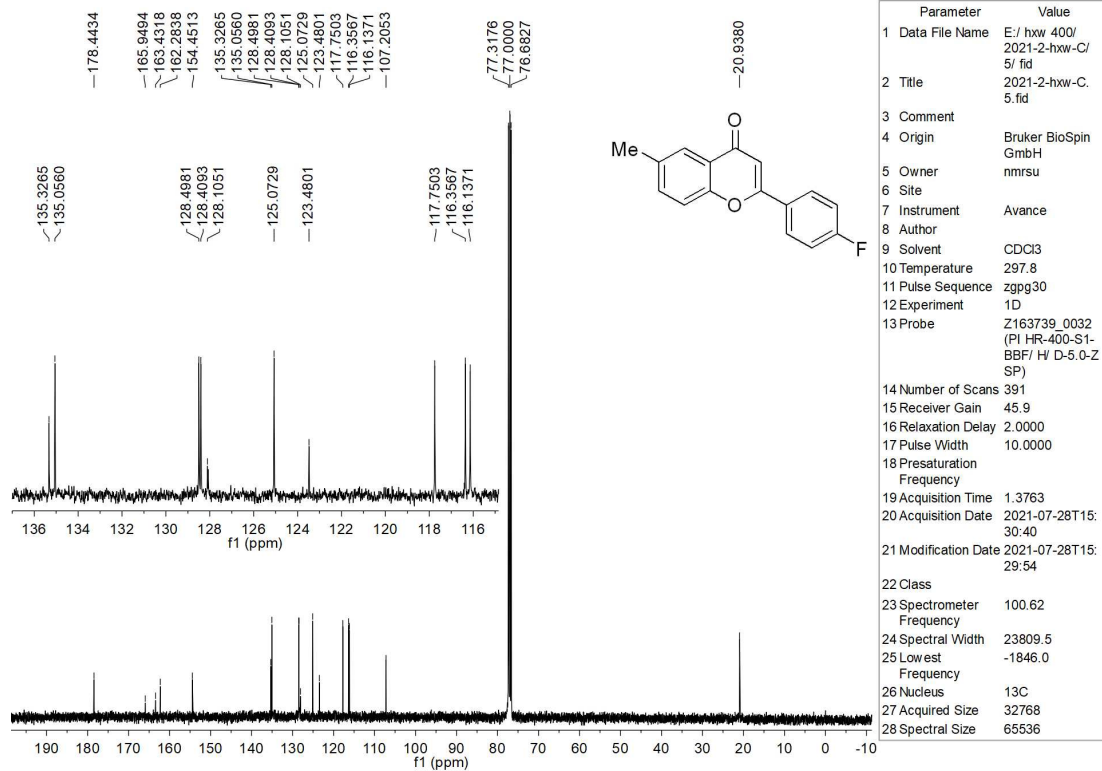
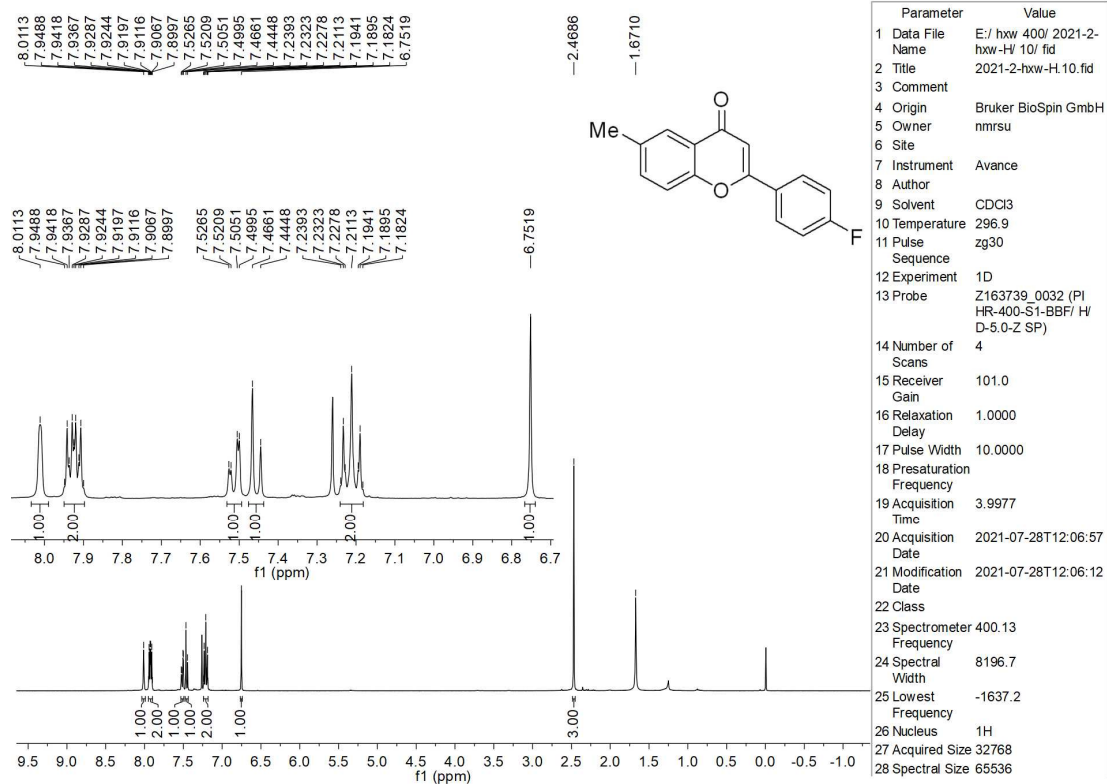


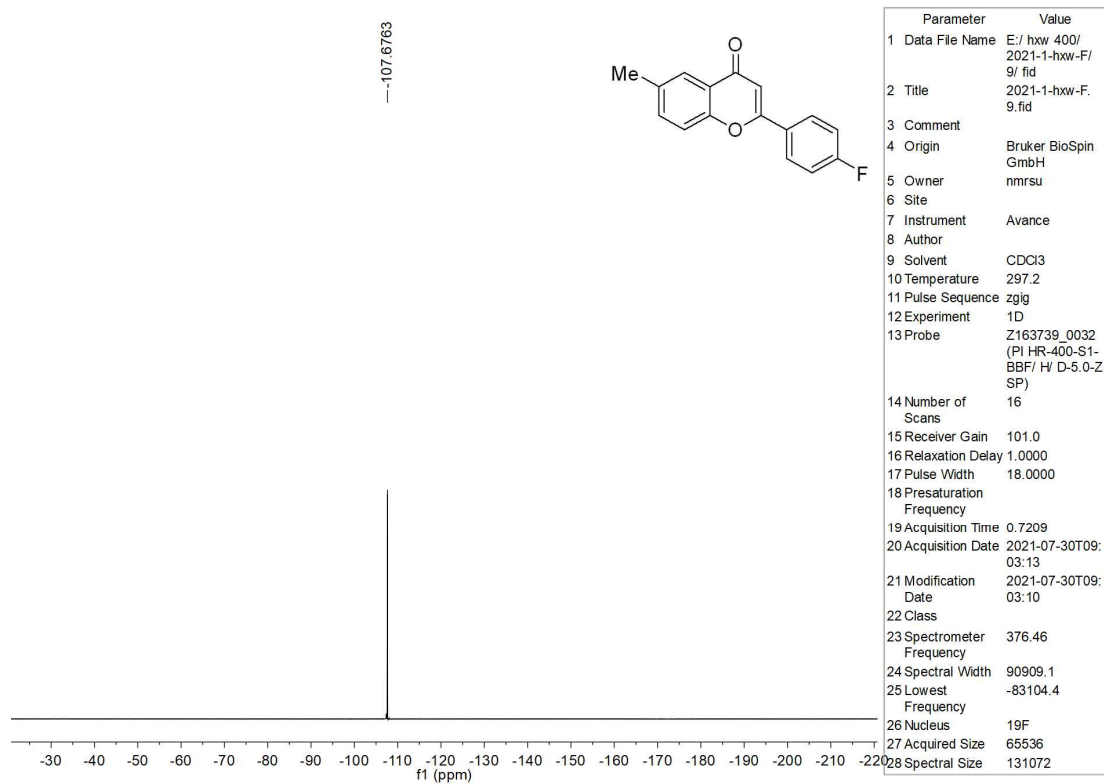


## 2-(4-Methoxyphenyl)-6-methyl-4H-chromen-4-one (2bc)



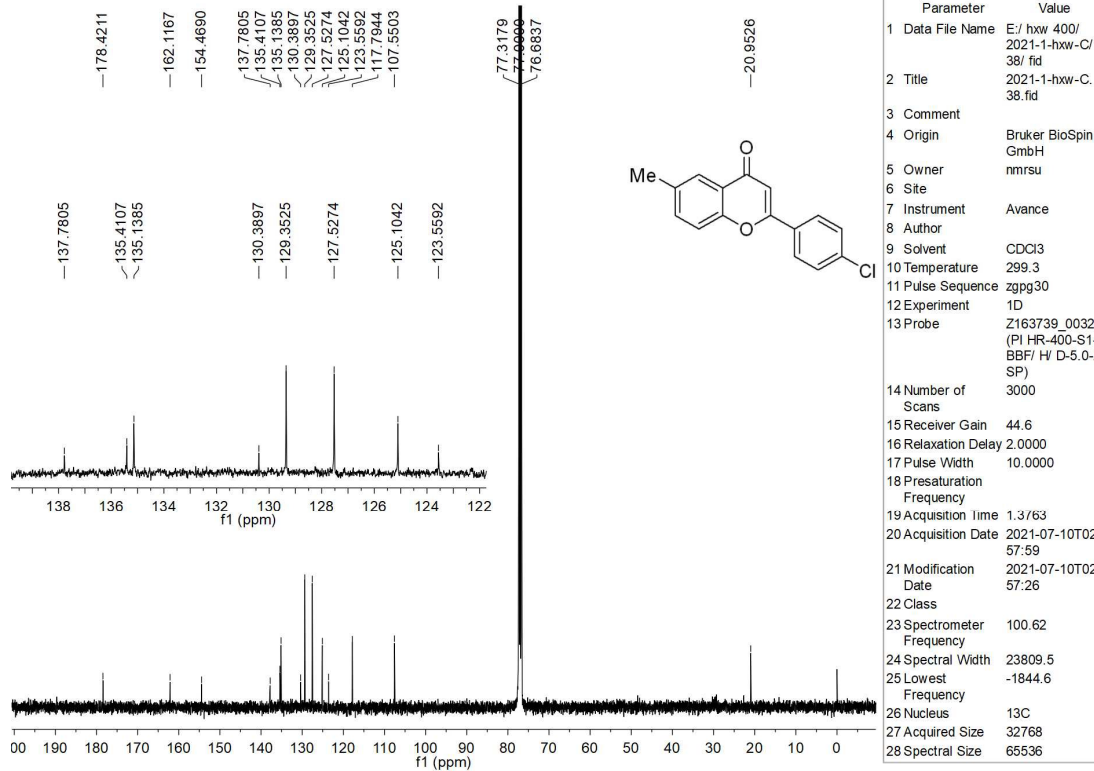
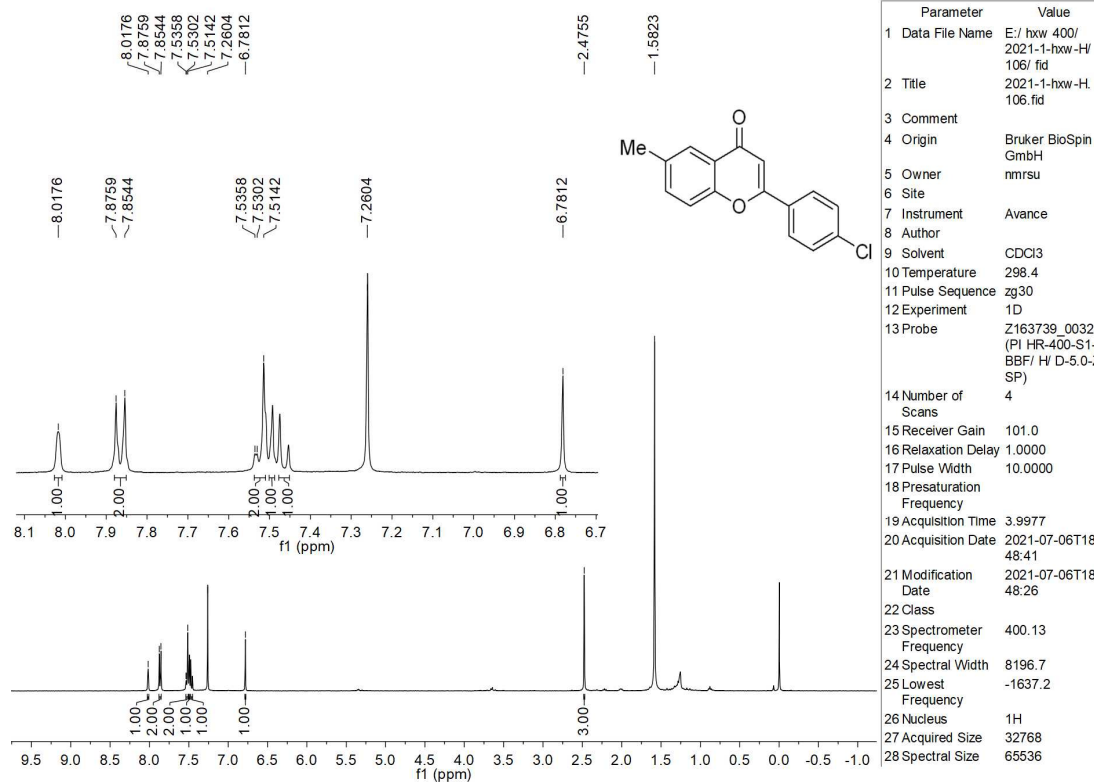
## 2-(4-Fluorophenyl)-6-methyl-4H-chromen-4-one (2bd)



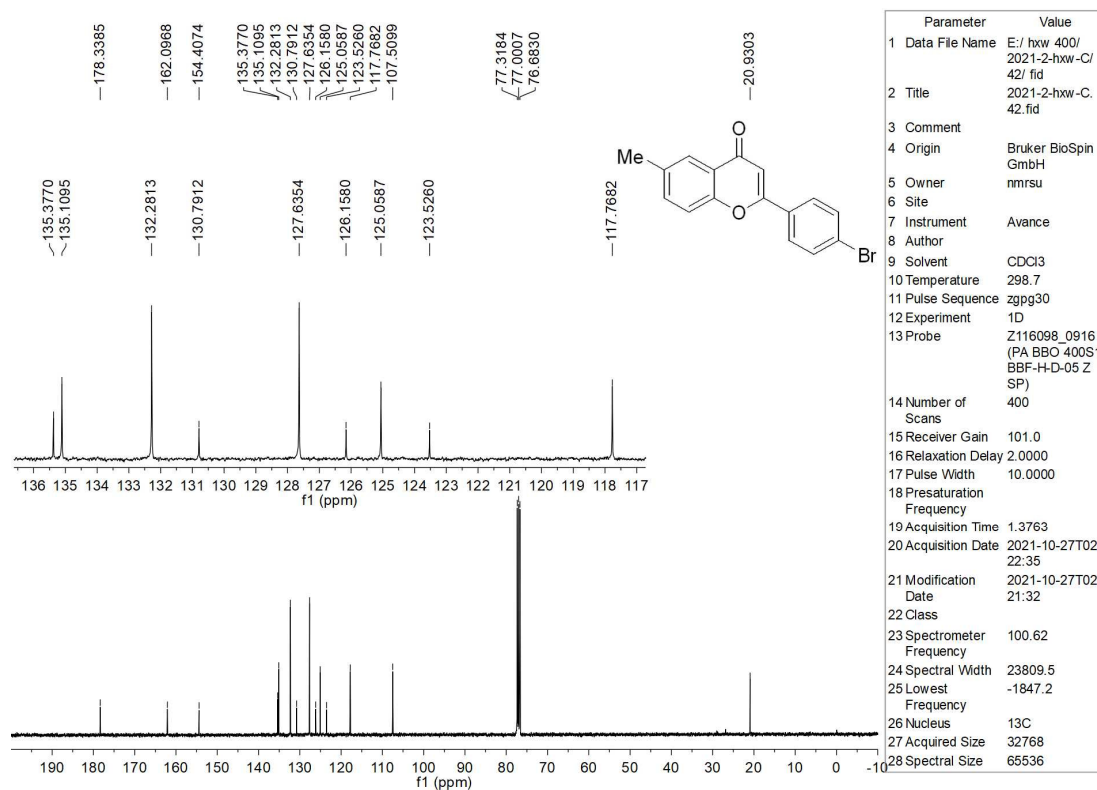
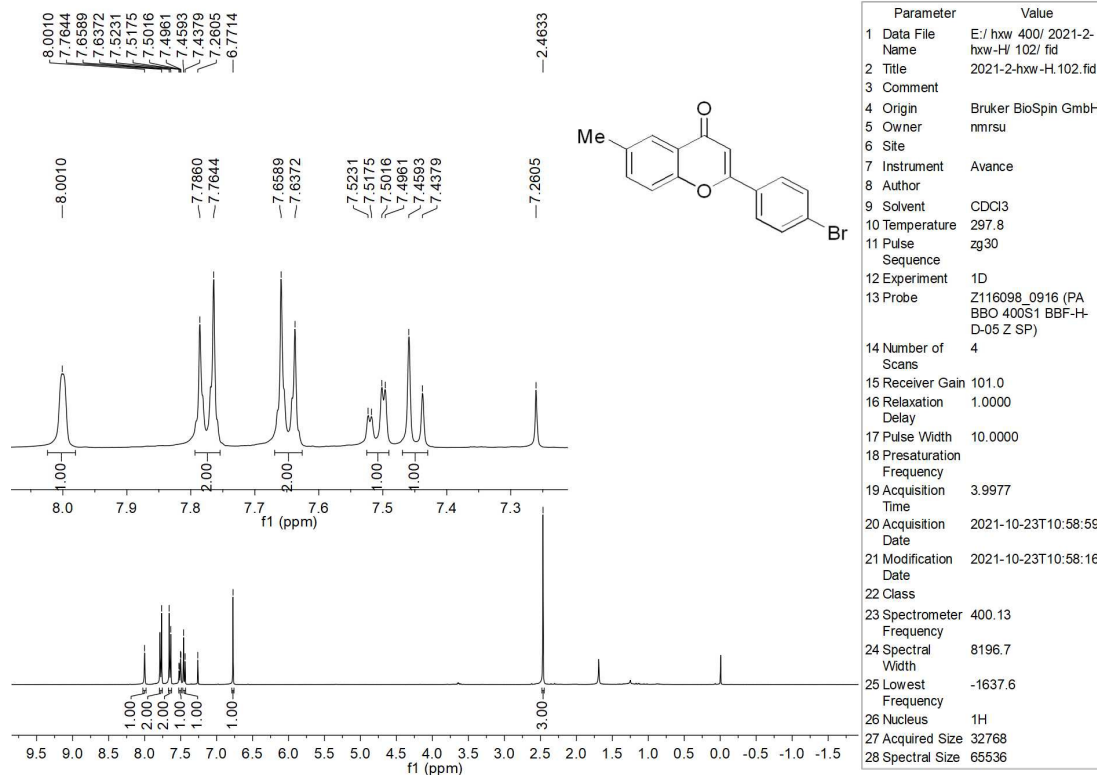




## 2-(4-Chlorophenyl)-6-methyl-4H-chromen-4-one (2be)



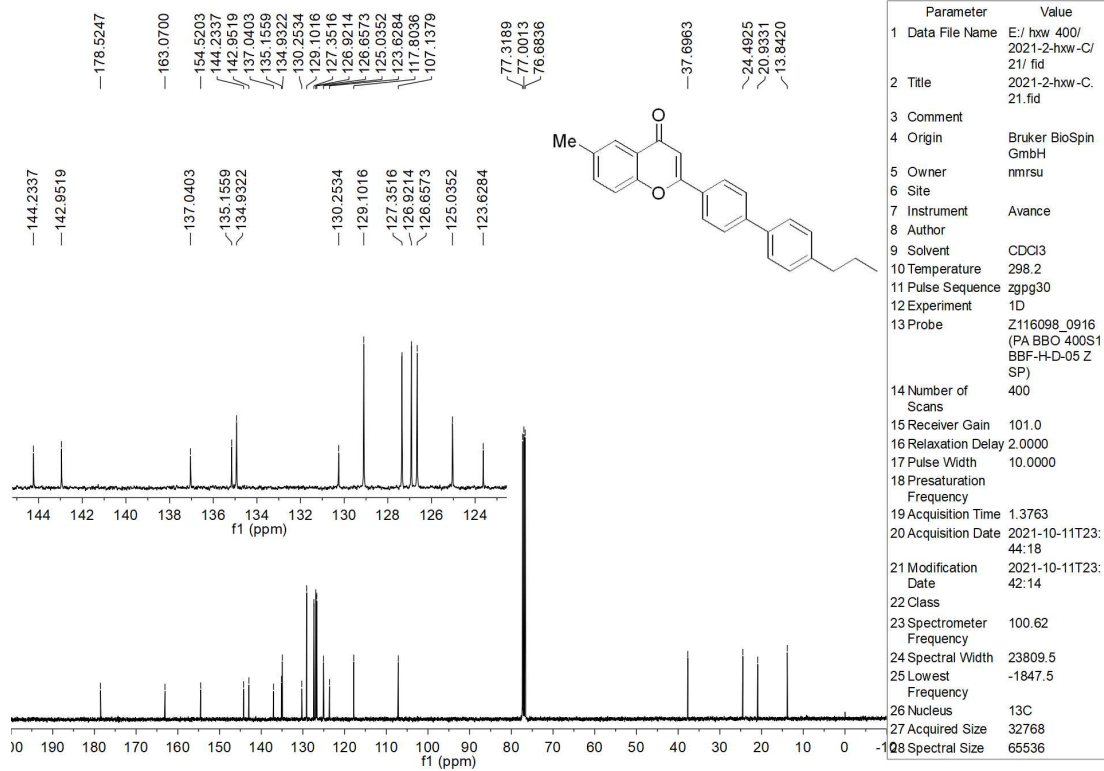
## 2-(4-Bromophenyl)-6-methyl-4H-chromen-4-one (2bf)



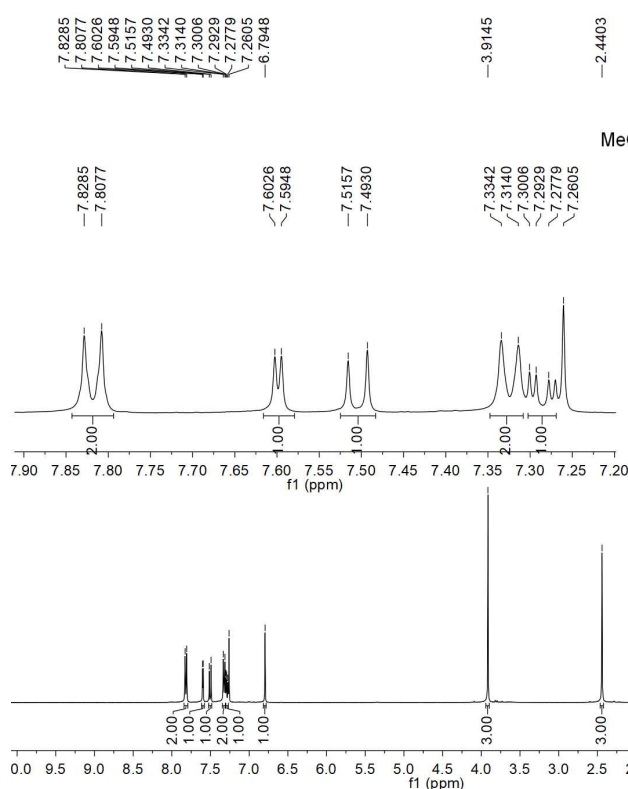
Chemical structure of compound 10: CC1=CC=C(C=C1C2=CC=CC=C2C3=CC(=C(C=C3)OC(=O)C4=CC=CC=C4C)C)C

<sup>1</sup>H NMR (CDCl<sub>3</sub>) peaks (ppm): 8.0248, 7.9886, 7.9676, 7.7424, 7.7212, 7.5818, 7.5614, 7.5275, 7.5062, 7.5009, 7.4907, 7.4695, 7.3045, 7.2841, 7.2844.

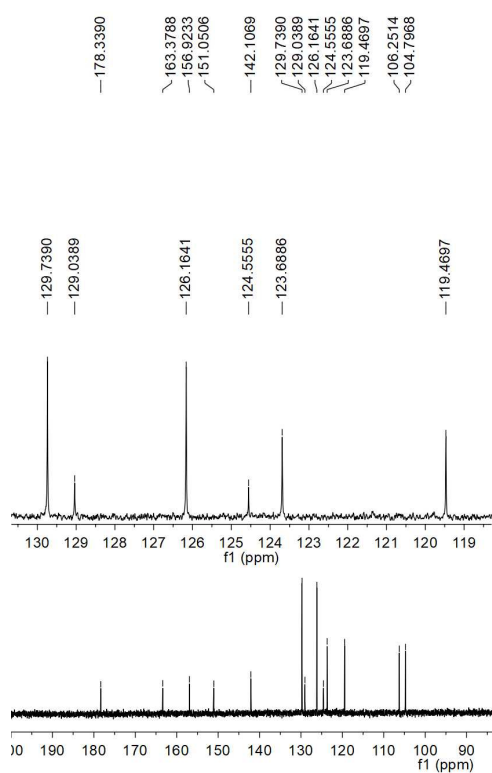
<sup>13</sup>C NMR (CDCl<sub>3</sub>) peaks (ppm): 267.04, 2.6516, 2.6322, 2.4713, 1.7237, 1.7049, 1.6859, 1.6673, 1.0039, 0.9856, 0.9672.



# **6-Methoxy-2-(*p*-tolyl)-4*H*-chromen-4-one (2cb)**

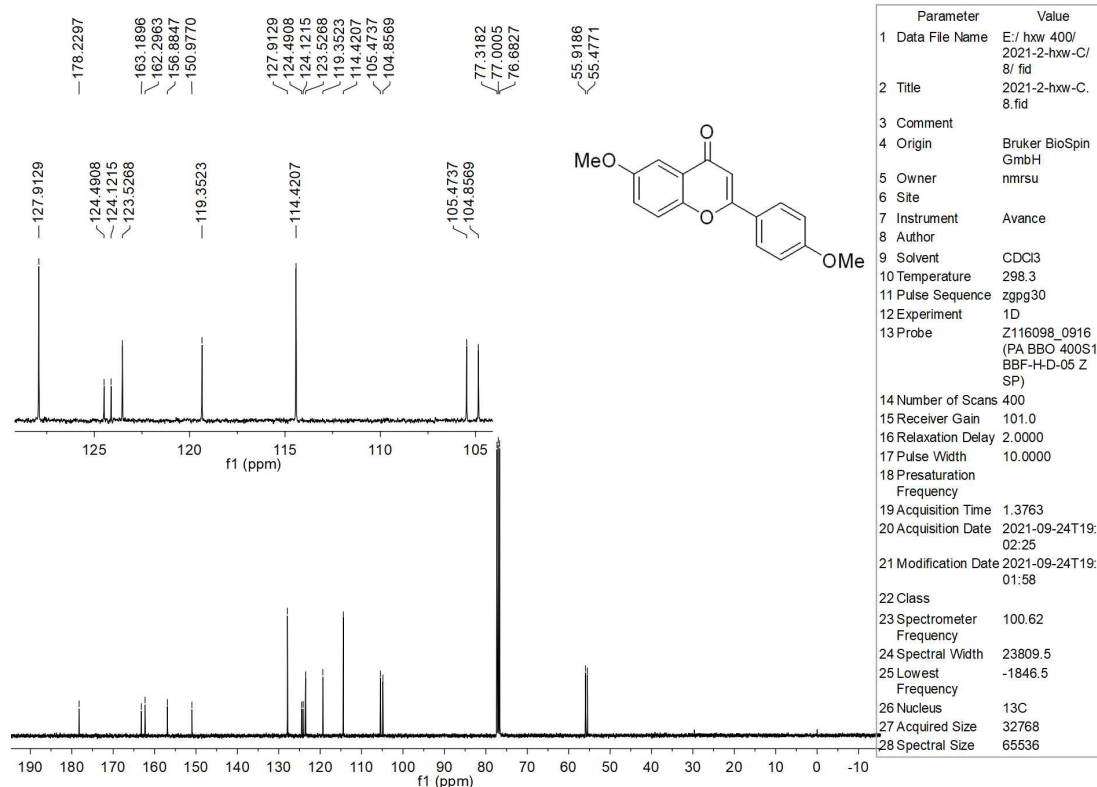
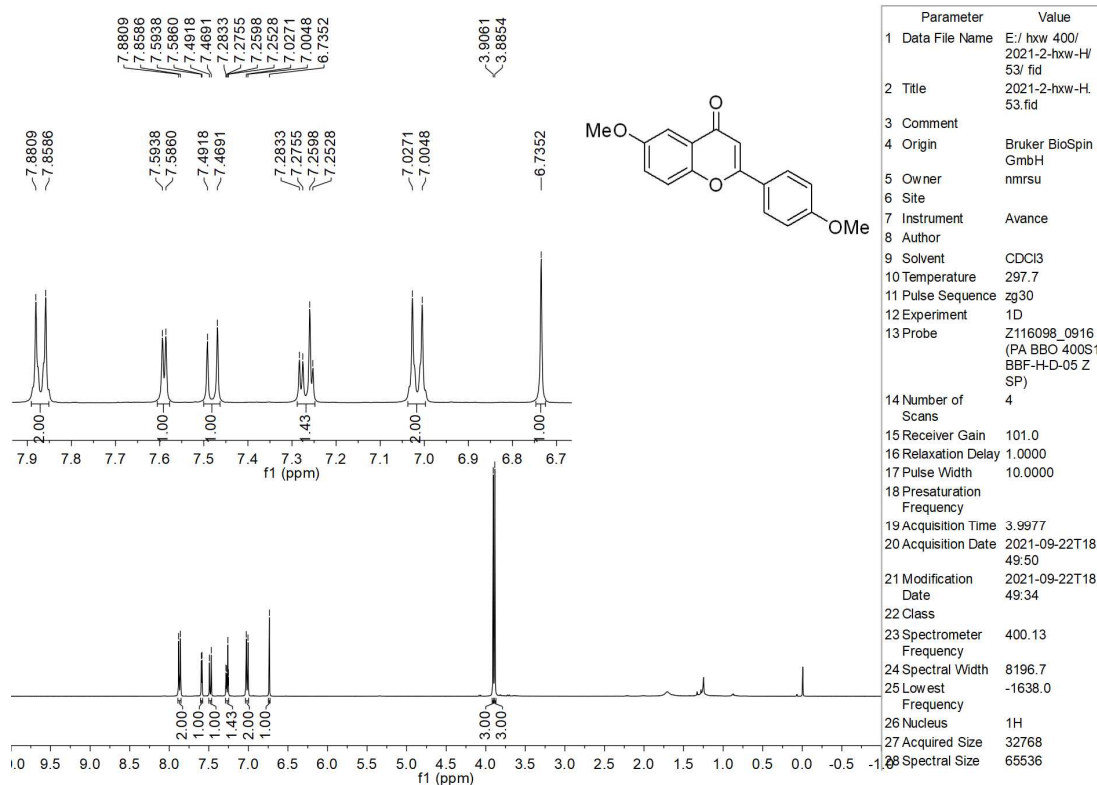


Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-H/ 142/ fid
2 Title	2021-2-hwx-H-142.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	295.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-11-11T21:19:47
21 Modification Date	2021-11-11T21:18:34
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	<sup>1</sup> H
27 Acquired Size	32768
28 Spectral Size	65536



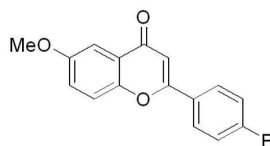
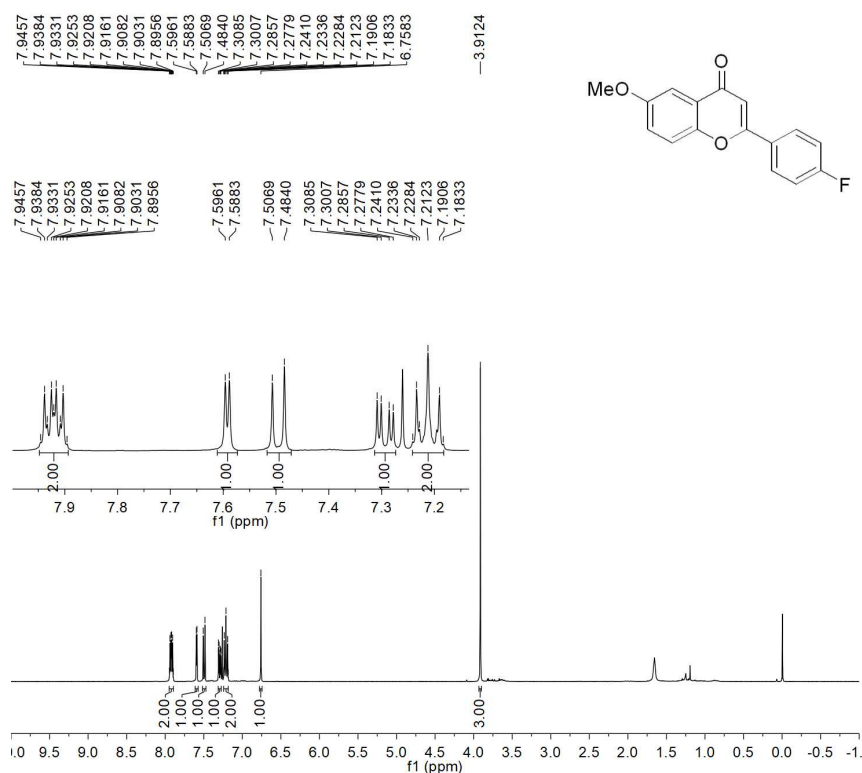
Parameter	Value
1 Data File Name	E:/ hwx 400/ 2021-2-hwx-C/ 39/ fid
2 Title	2021-2-hwx-C-39.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	296.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	800
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2021-11-11T23:49:49
21 Modification Date	2021-11-11T23:48:36
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1846.5
26 Nucleus	<sup>13</sup> C
27 Acquired Size	32768
28 Spectral Size	65536

# 6-Methoxy-2-(4-methoxyphenyl)-4H-chromen-4-one (2cc)

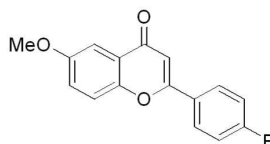
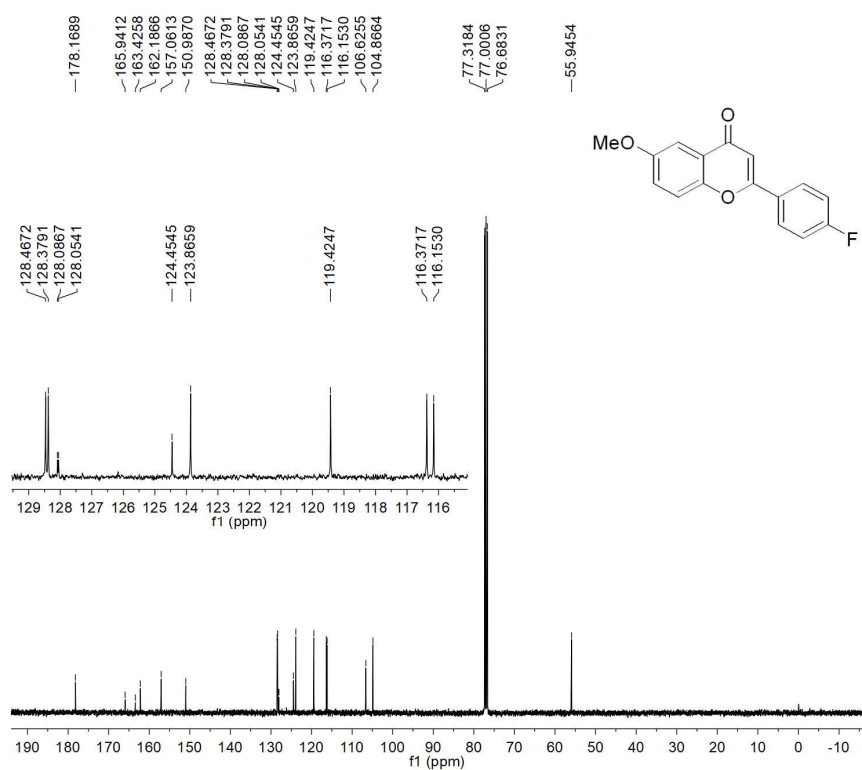




## 2-(4-Fluorophenyl)-6-methoxy-4H-chromen-4-one (2cd)

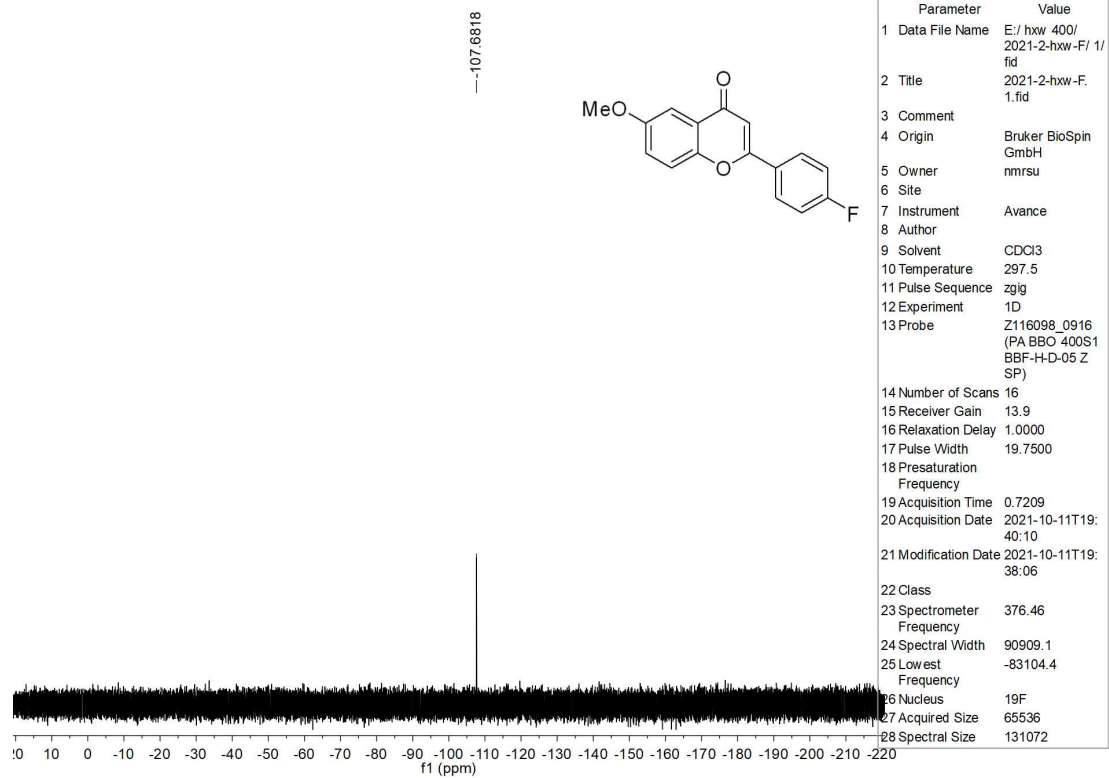


Parameter	Value
1 Data File	E:/ hwx 400/ 2021-2-hwx-H 74/ fid
2 Title	2021-2-hwx-H.74.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	297.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2021-10-11T19:07:40
21 Modification Date	2021-10-11T19:05:38
22 Class	
23 Spectrometer	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	<sup>1</sup> H
27 Acquired Size	32768
28 Spectral Size	65536

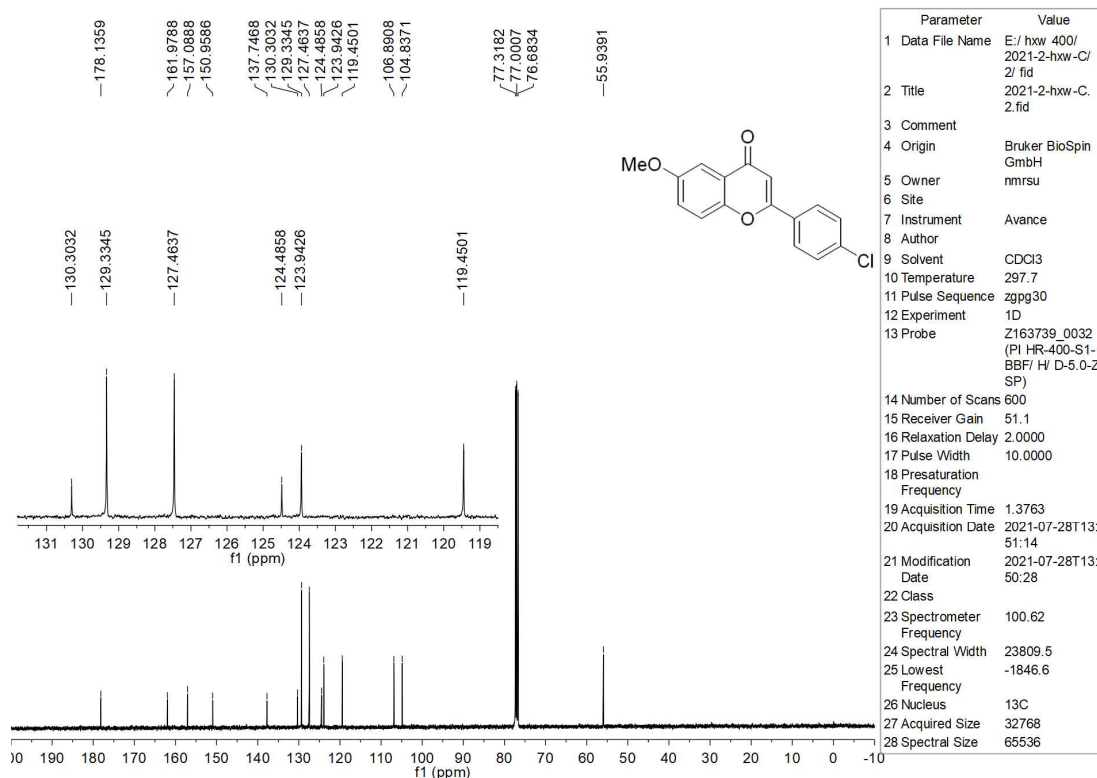
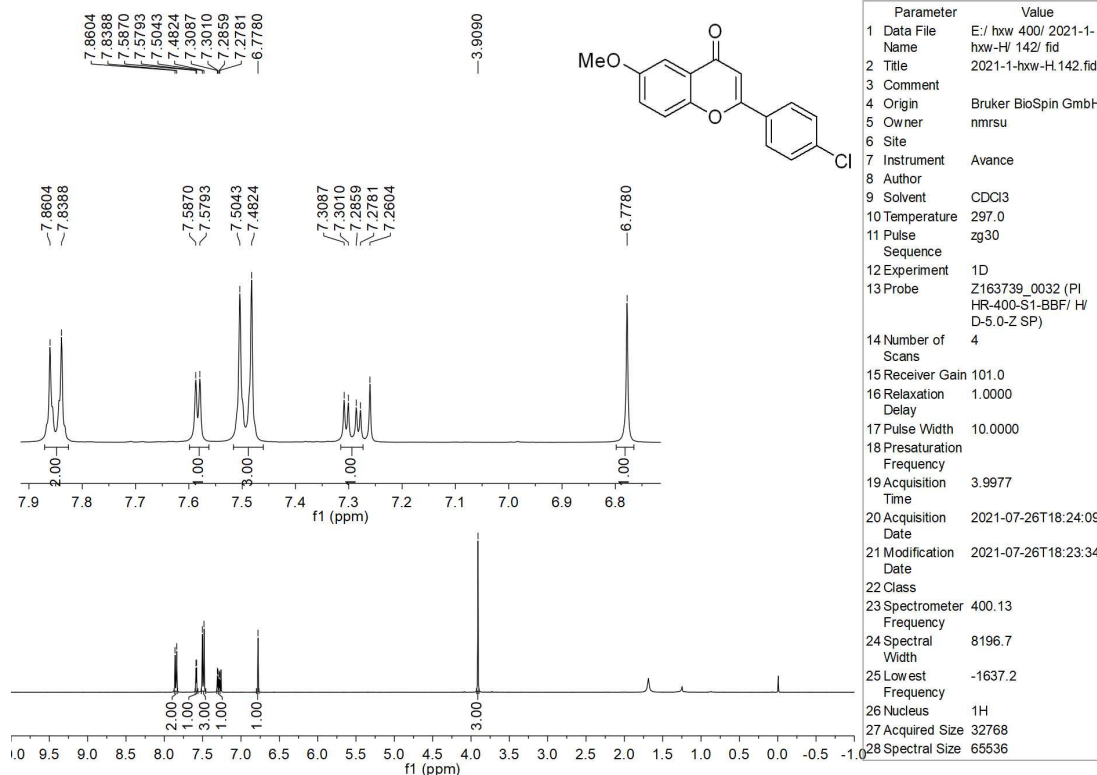


Parameter	Value
1 Data File	E:/ hwx 400/ 2021-2-hwx-C/ 20/ fid
2 Title	2021-2-hwx-C.20.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance
8 Author	
9 Solvent	CDCl <sub>3</sub>
10 Temperature	298.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H-D-05 Z SP)
14 Number of Scans	400
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2021-10-11T23:17:06
21 Modification Date	2021-10-11T23:15:02
22 Class	
23 Spectrometer	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1846.1
26 Nucleus	<sup>13</sup> C
27 Acquired Size	32768
28 Spectral Size	65536

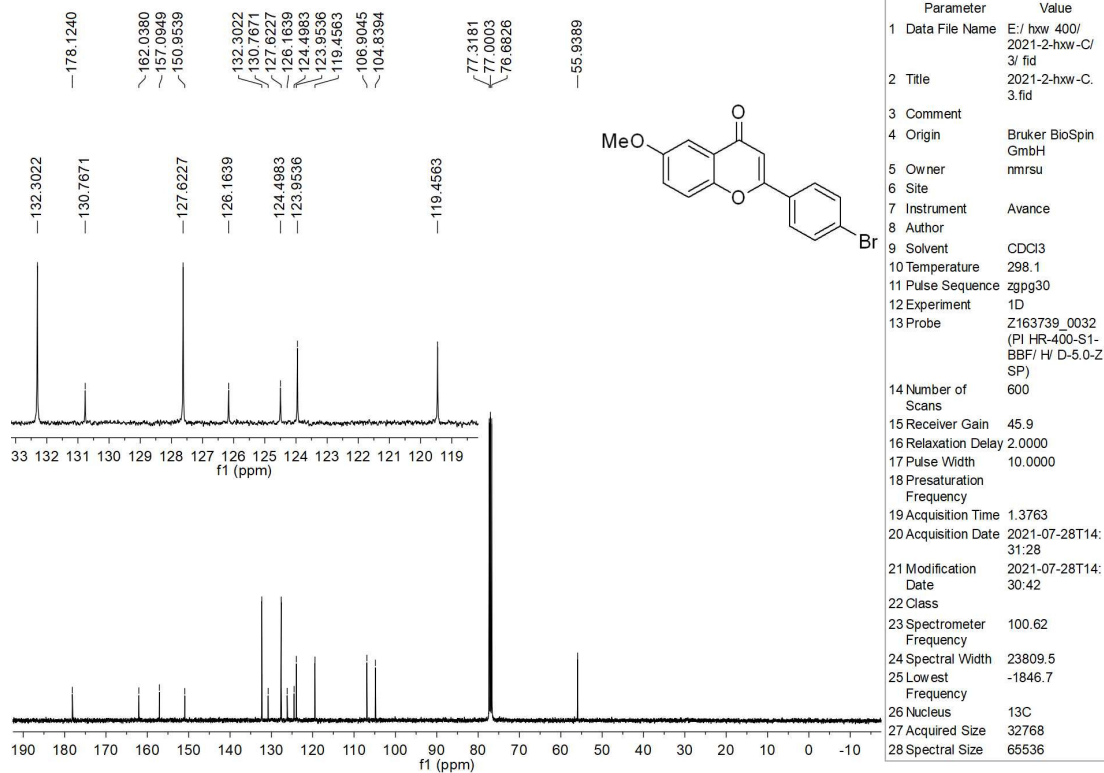
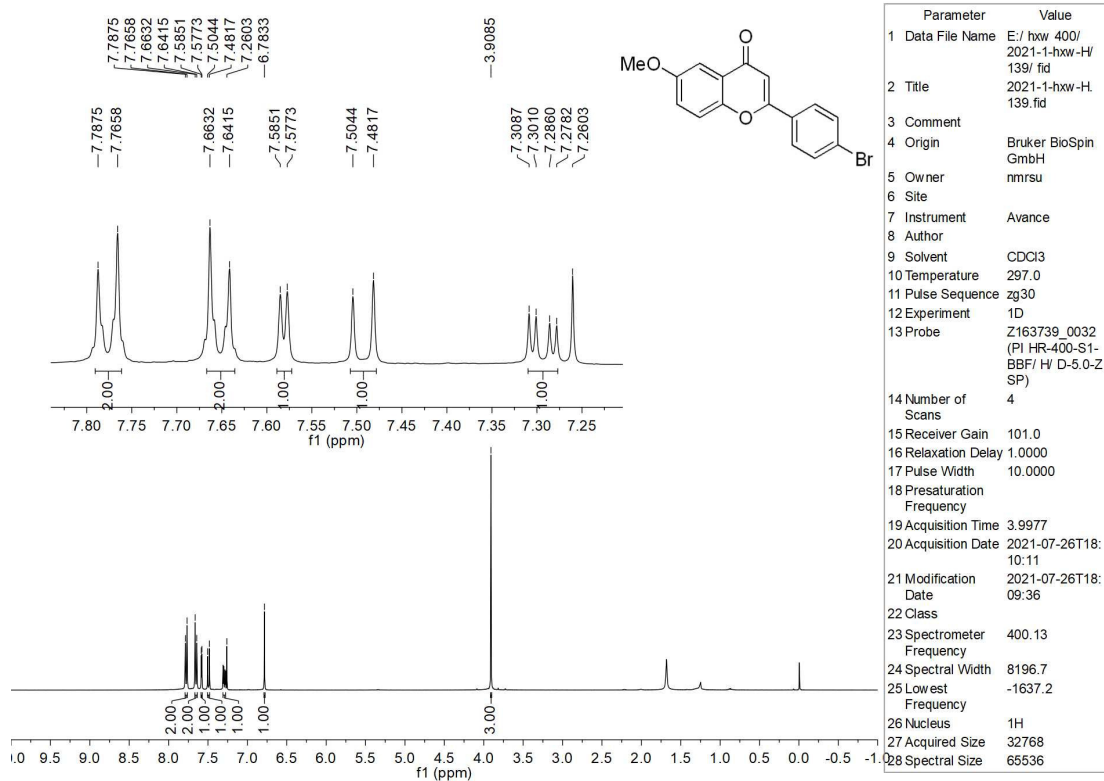




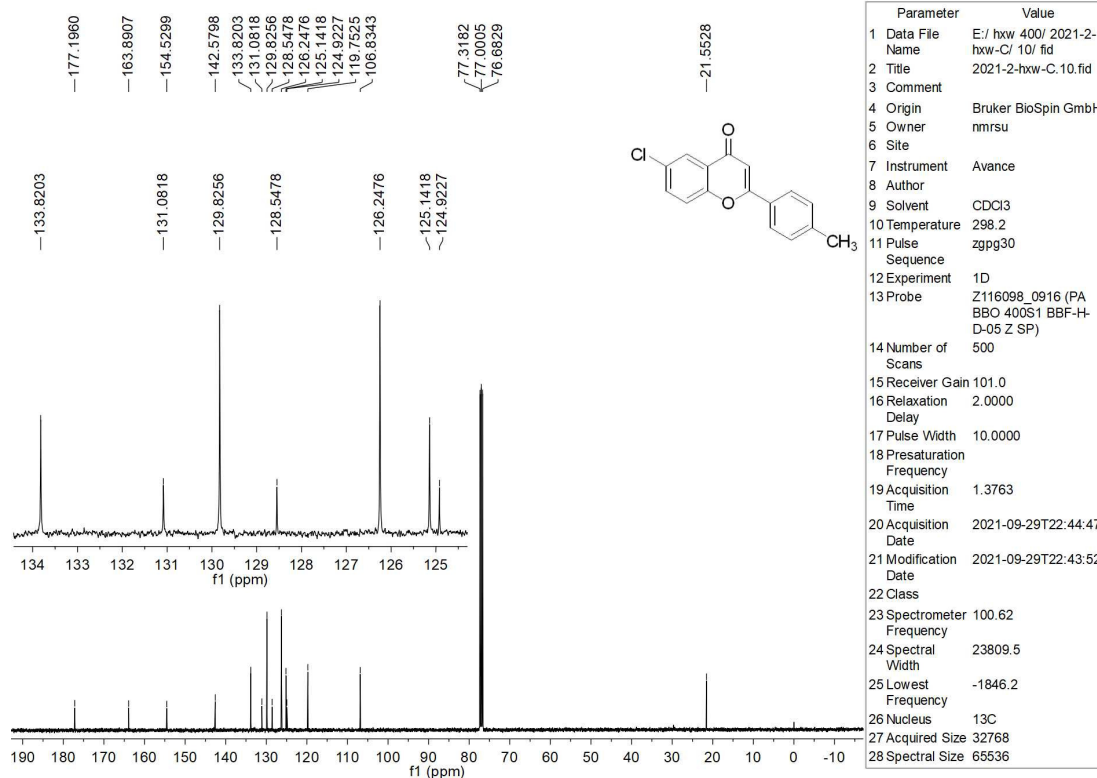
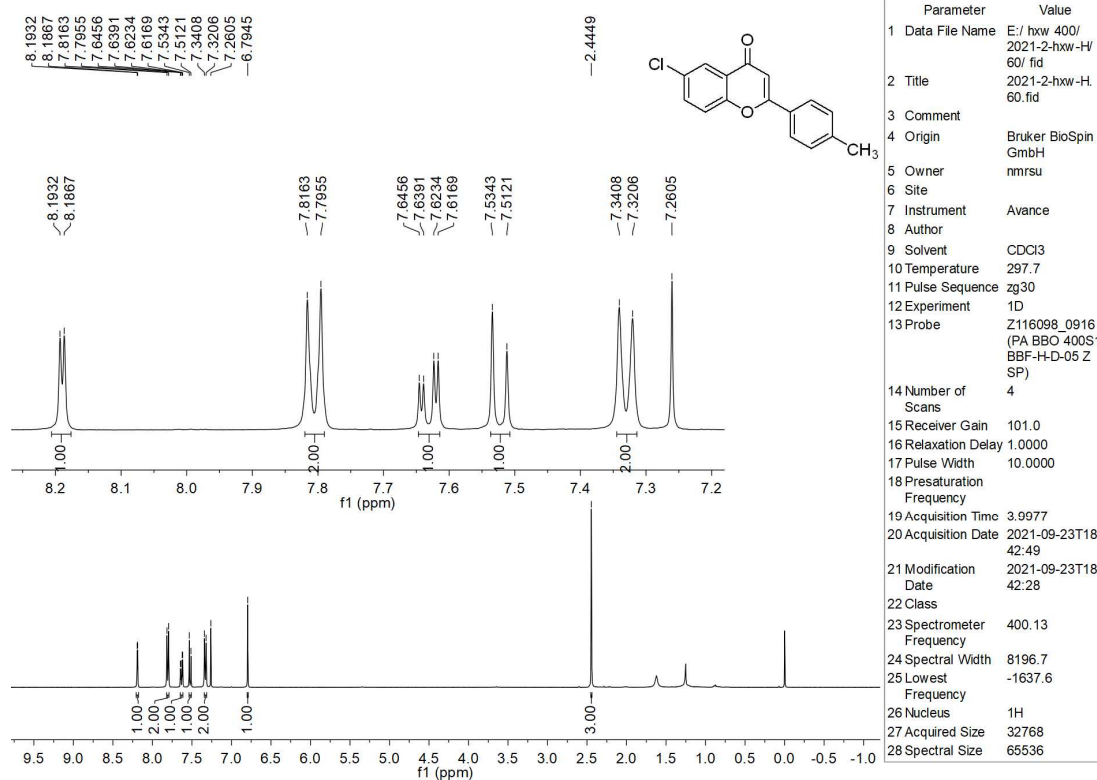
## 2-(4-Chlorophenyl)-6-methoxy-4H-chromen-4-one (2ce)



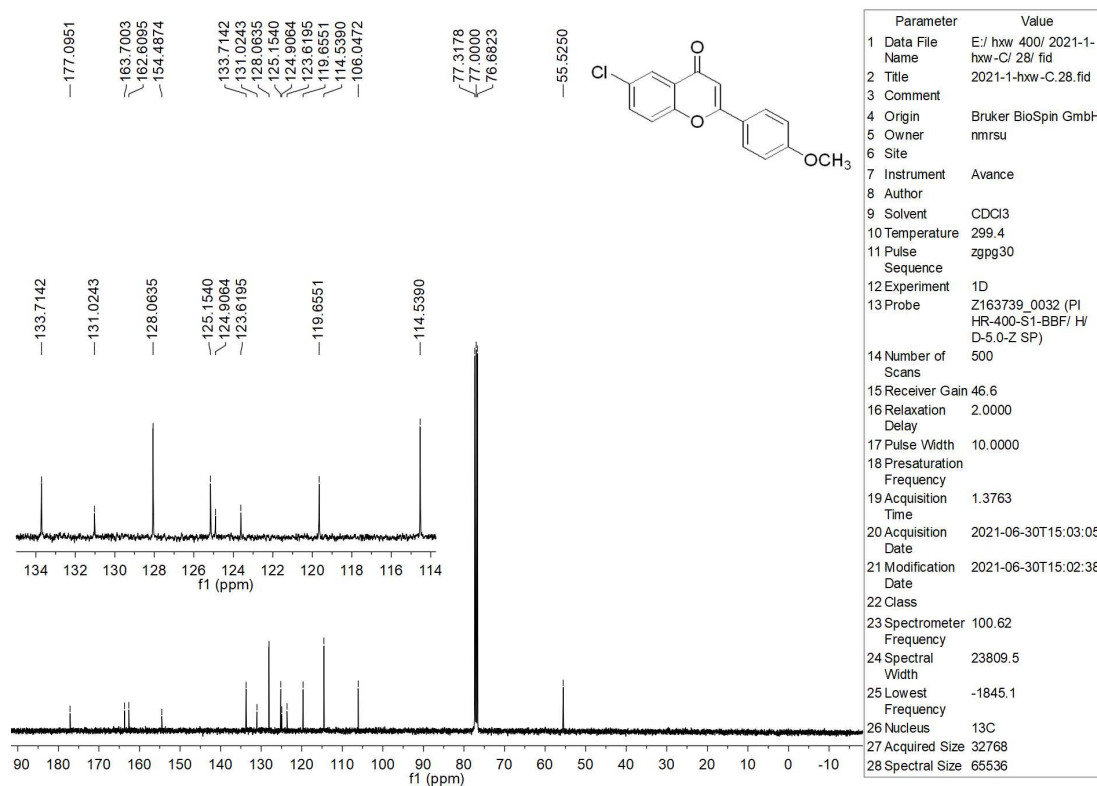
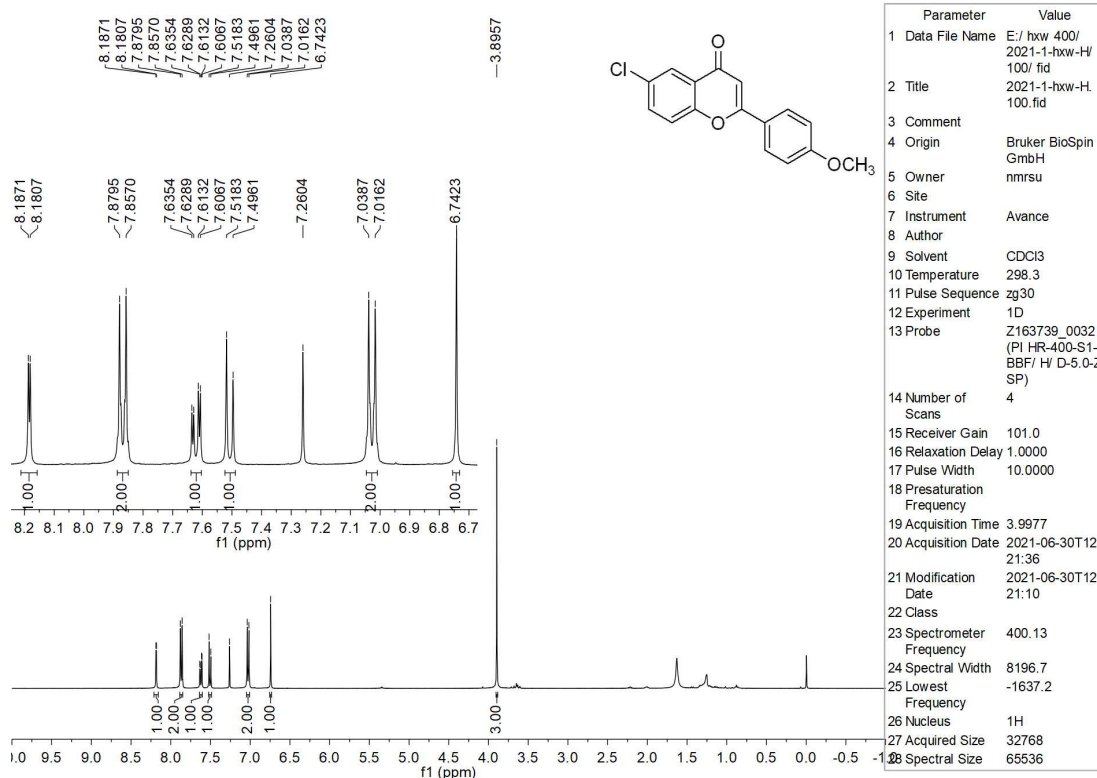
## 2-(4-Bromophenyl)-6-methoxy-4H-chromen-4-one (2cf)



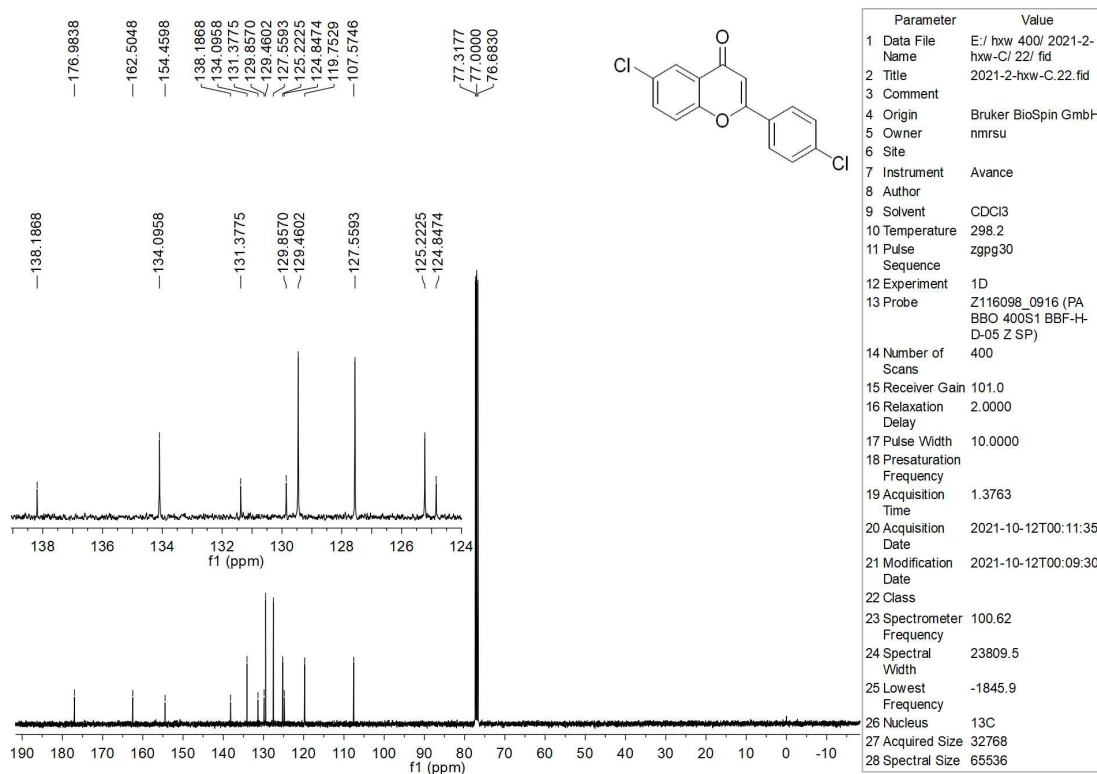
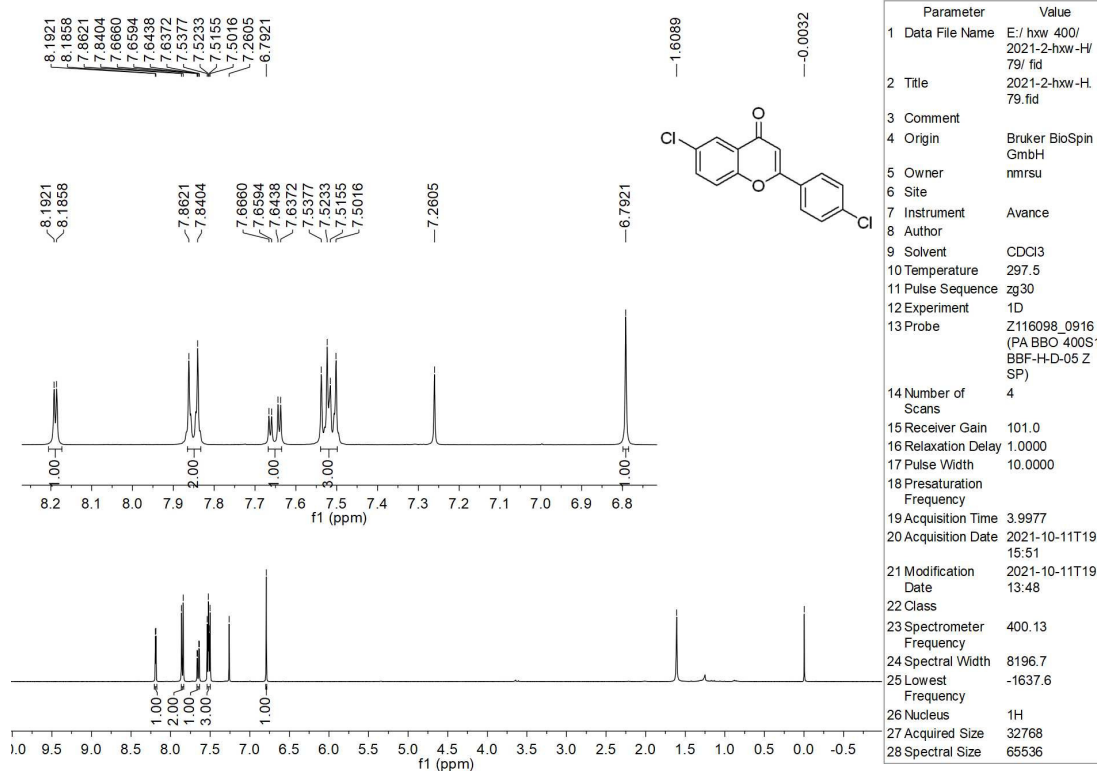
# 6-Chloro-2-(*p*-tolyl)-4*H*-chromen-4-one (2db)



# 6-Chloro-2-(4-methoxyphenyl)-4H-chromen-4-one (2dc)

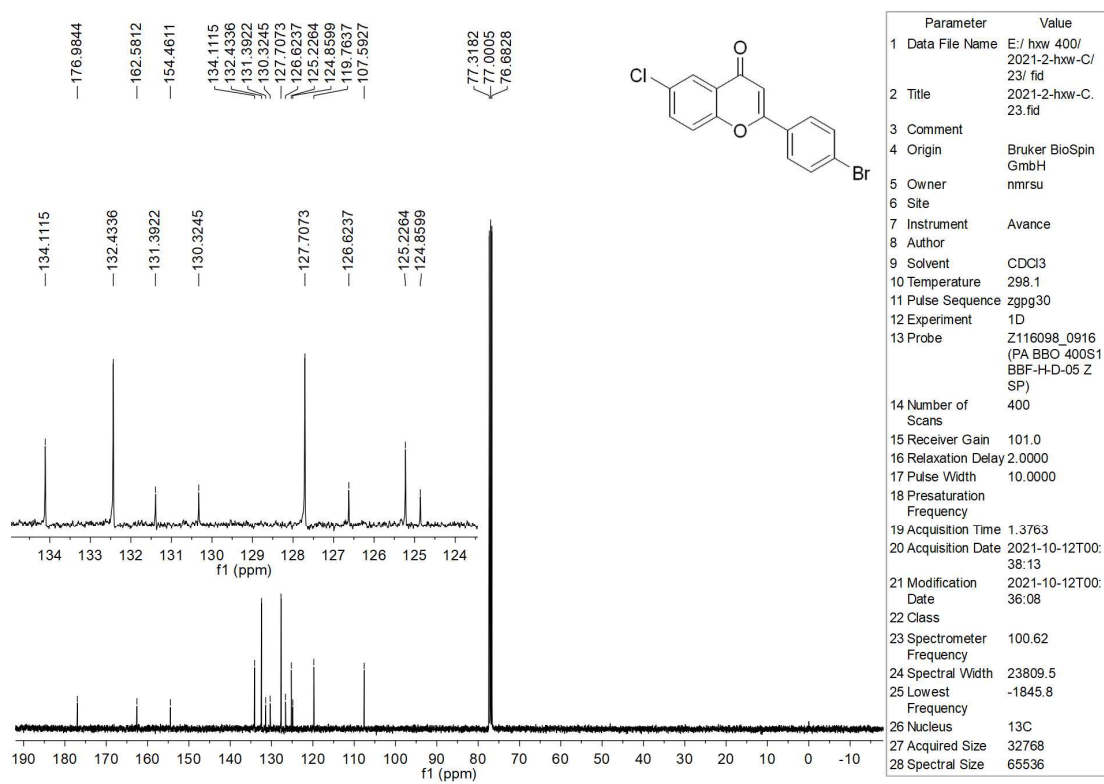
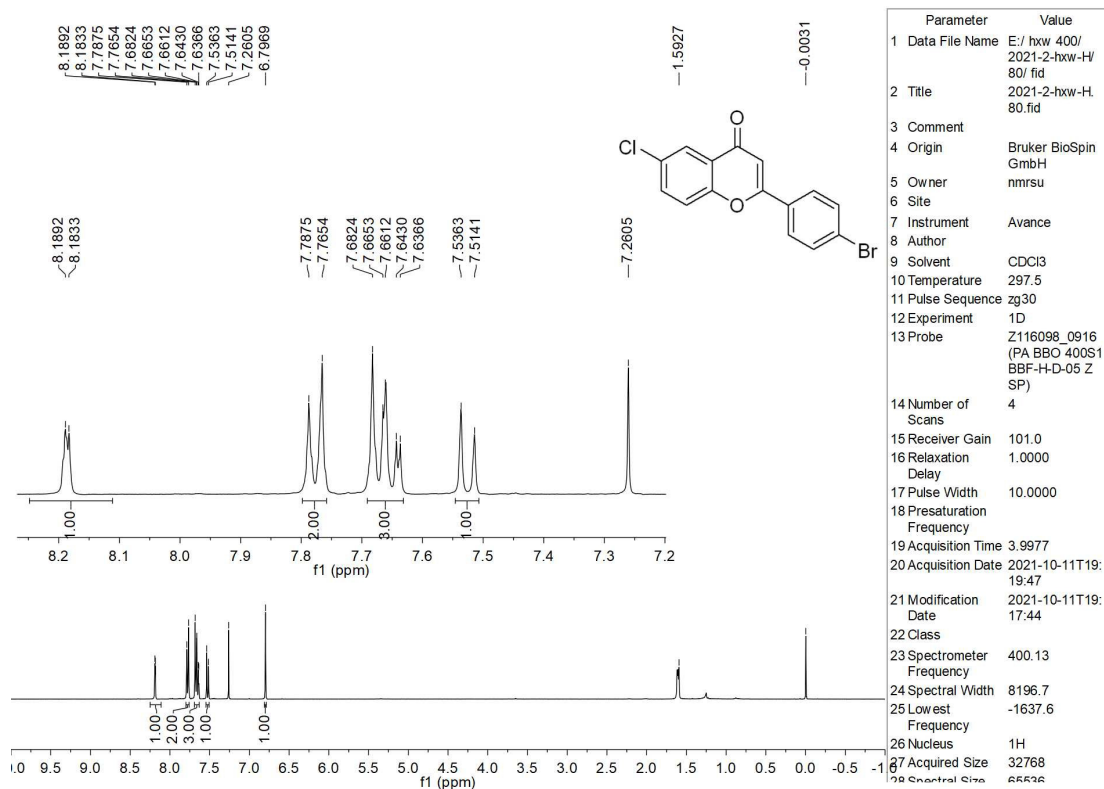


# 6-Chloro-2-(4-chlorophenyl)-4H-chromen-4-one (2de)

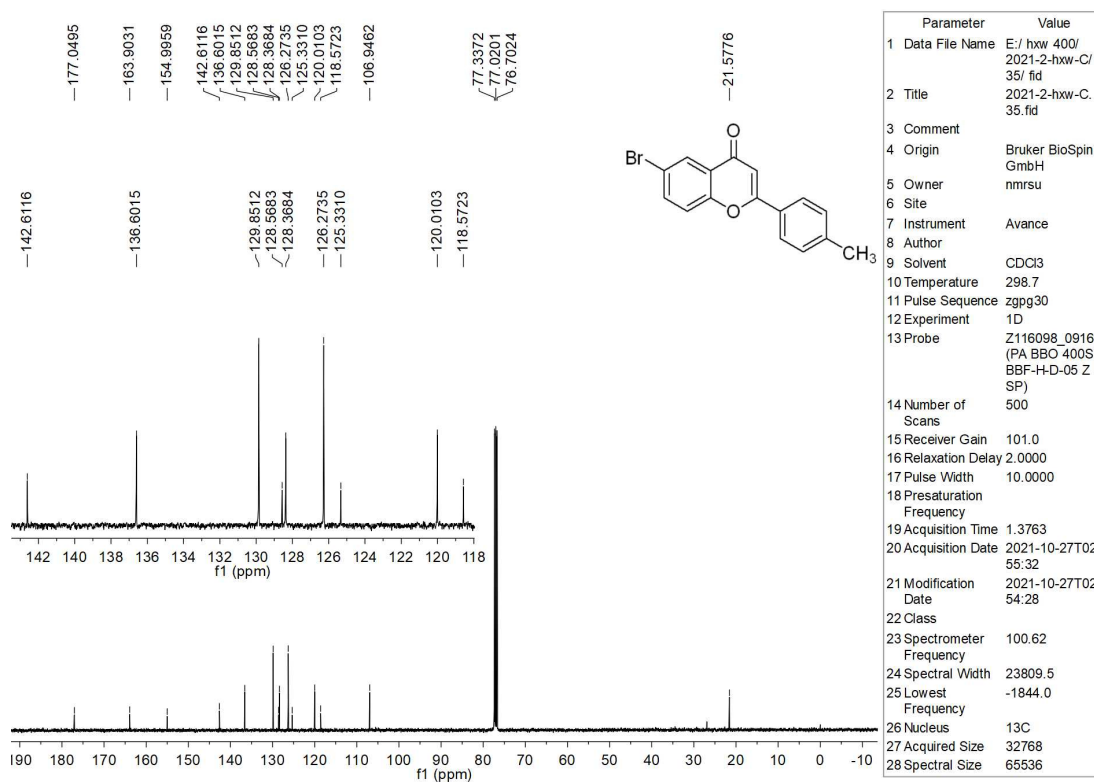
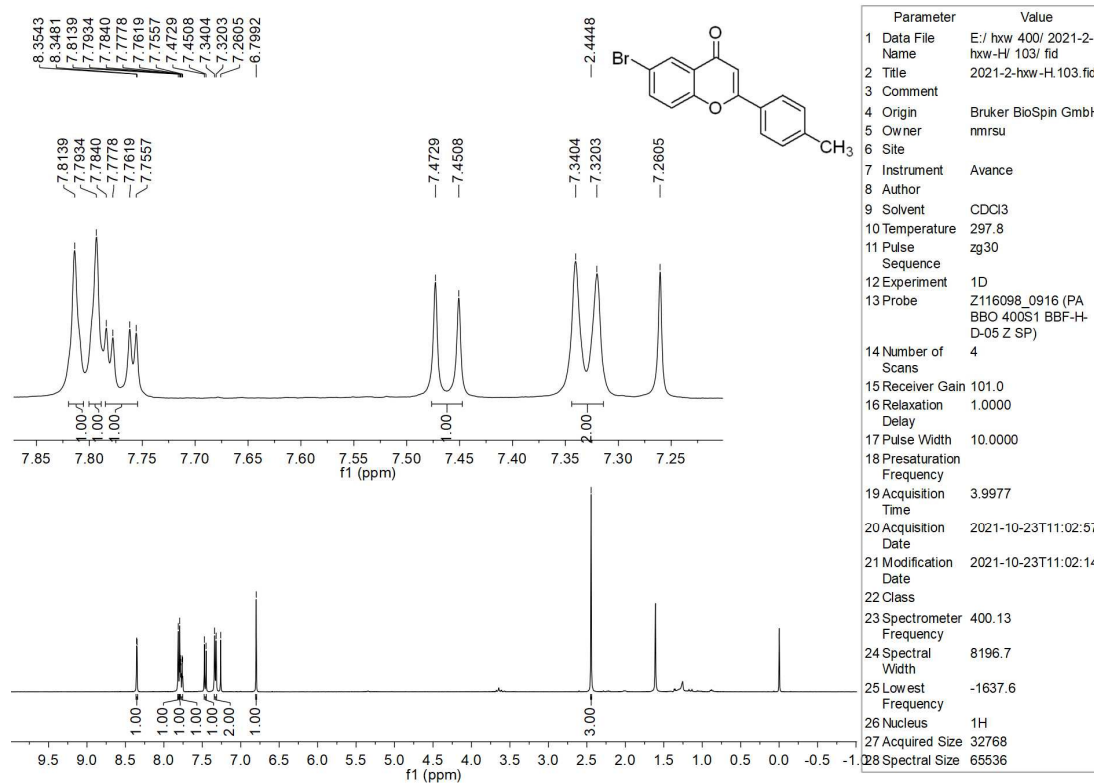




## 2-(4-Bromophenyl)-6-chloro-4H-chromen-4-one (2df)



# 6-Bromo-2-(*p*-tolyl)-4*H*-chromen-4-one (2eb)



Chemical structure of 6-bromo-2-(4-methoxyphenyl)chromone (39):

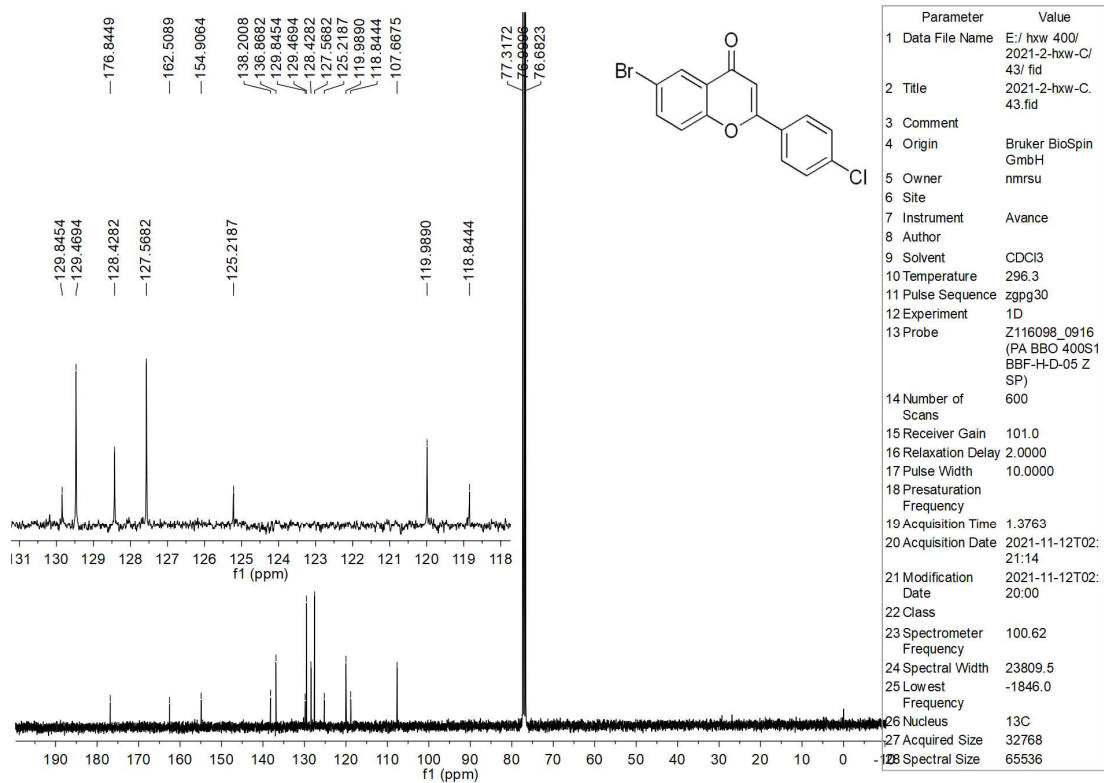
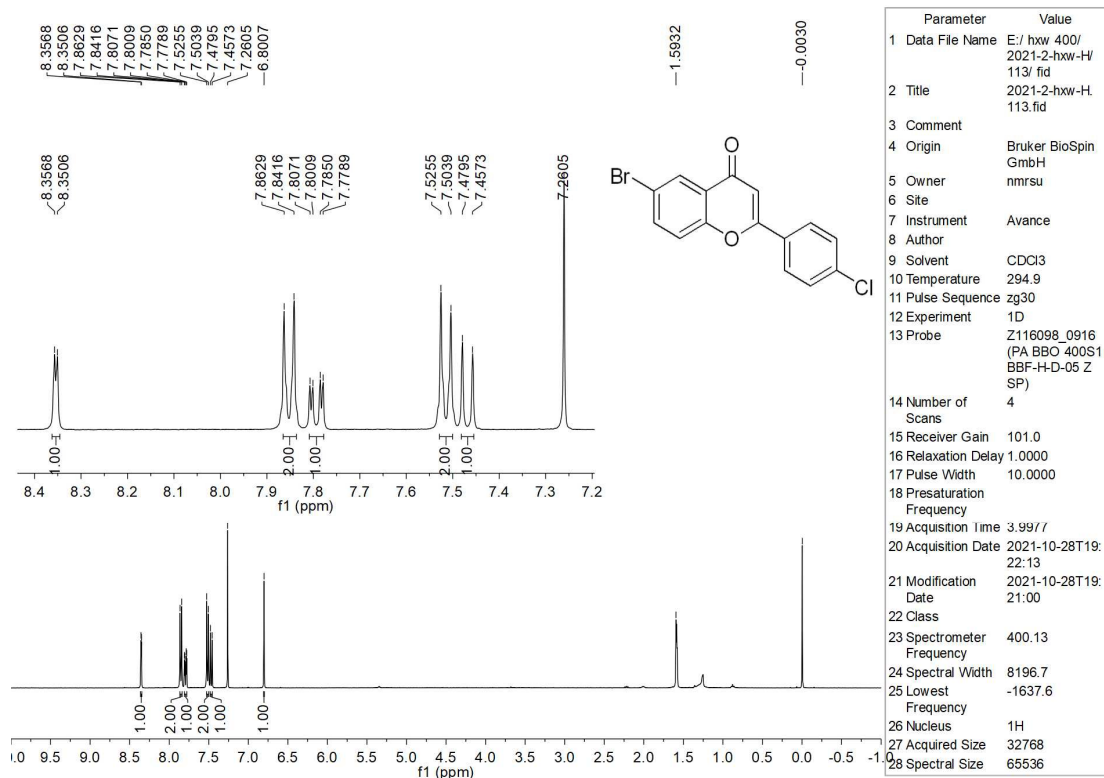
COc1ccc(cc1)/C=C2/C(=O)c3cc(Br)ccc3O2

<sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>) showing peaks and integration values:

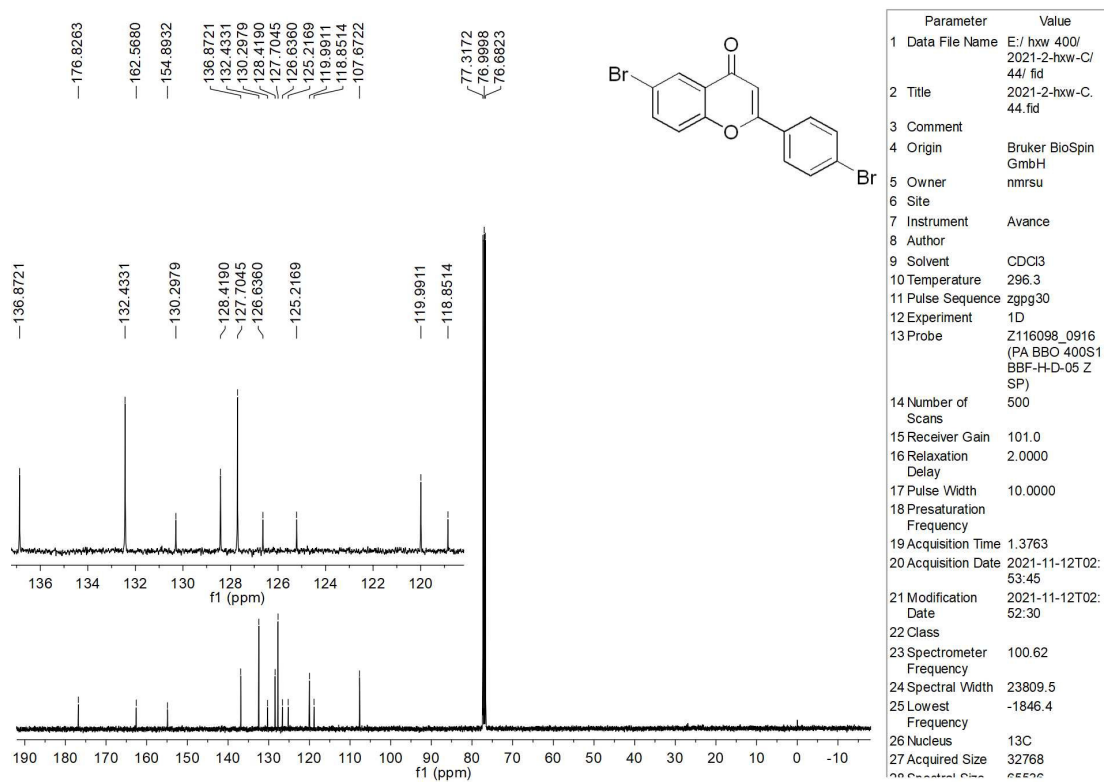
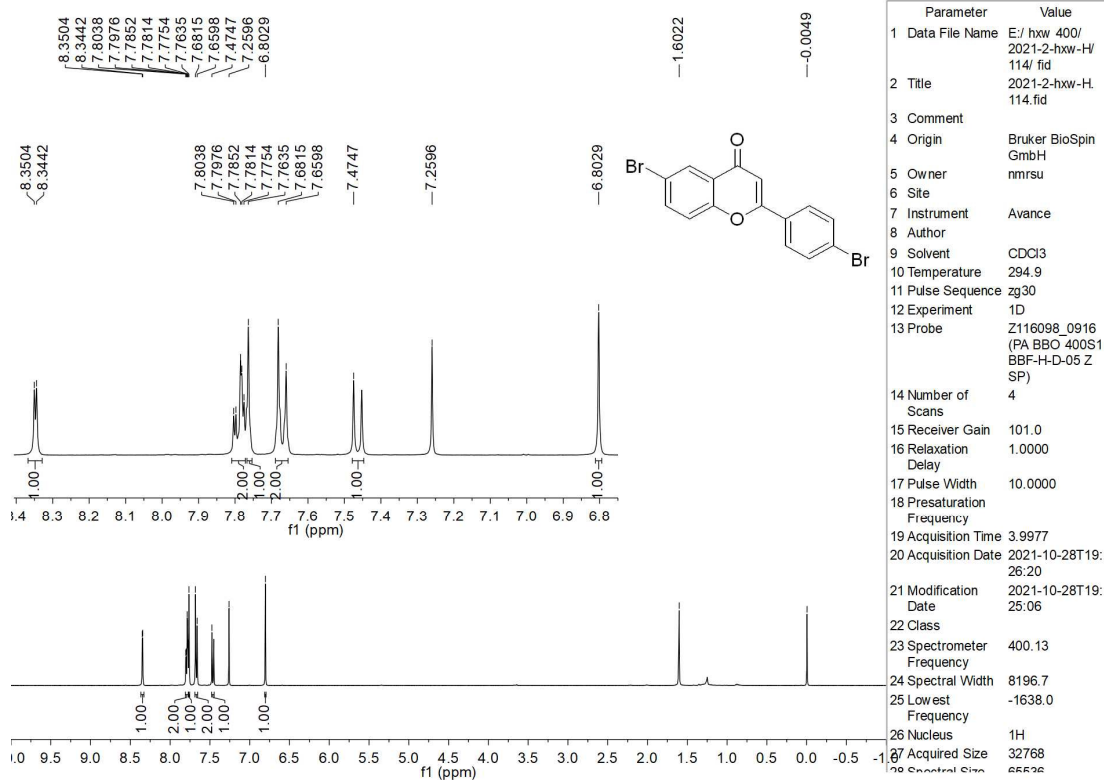
Chemical Shift (ppm)	Integration
8.3446, 8.3384	2.00
7.8814, 7.8741, 7.8691, 7.8568, 7.8517, 7.8446	1.00
7.7714, 7.7652, 7.7483, 7.7431	1.00
7.4543, 7.4322	1.00
7.2603	1.00
7.0426, 7.0354, 7.0304, 7.0180, 7.0130, 7.0058	2.00
3.937	3.00



# **6-Bromo-2-(4-chlorophenyl)-4H-chromen-4-one (2ee)**

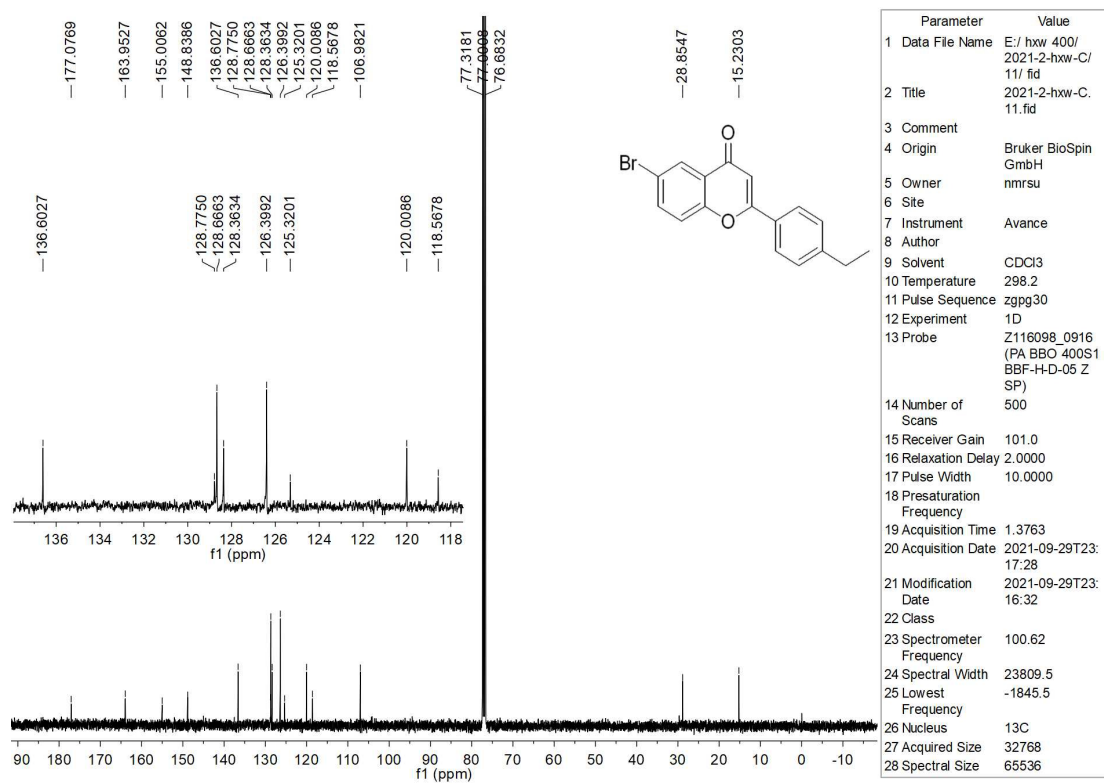
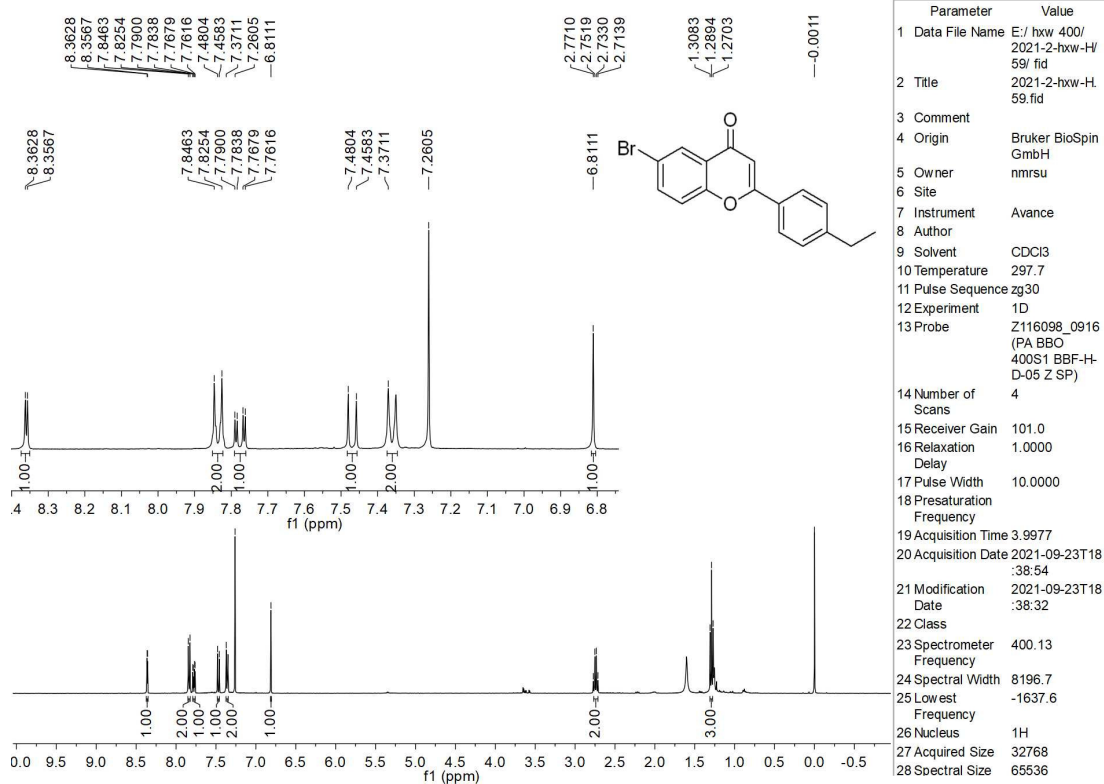


# 6-Bromo-2-(4-bromophenyl)-4H-chromen-4-one (2ef)



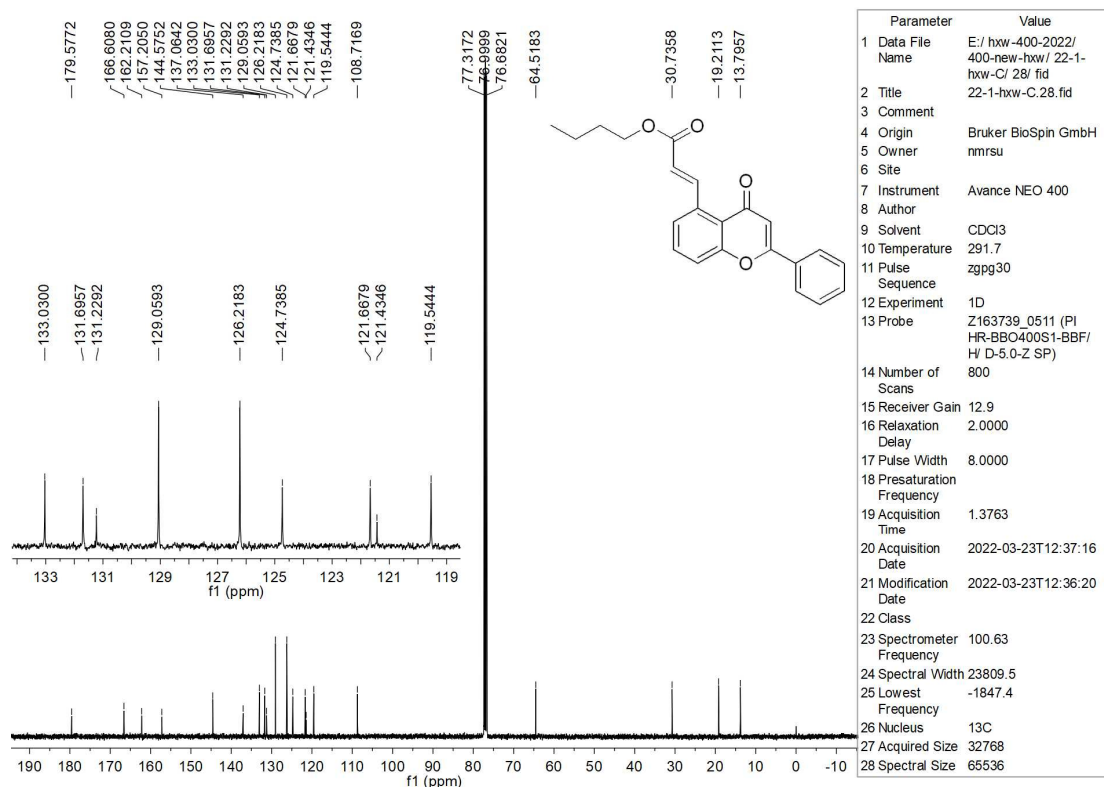
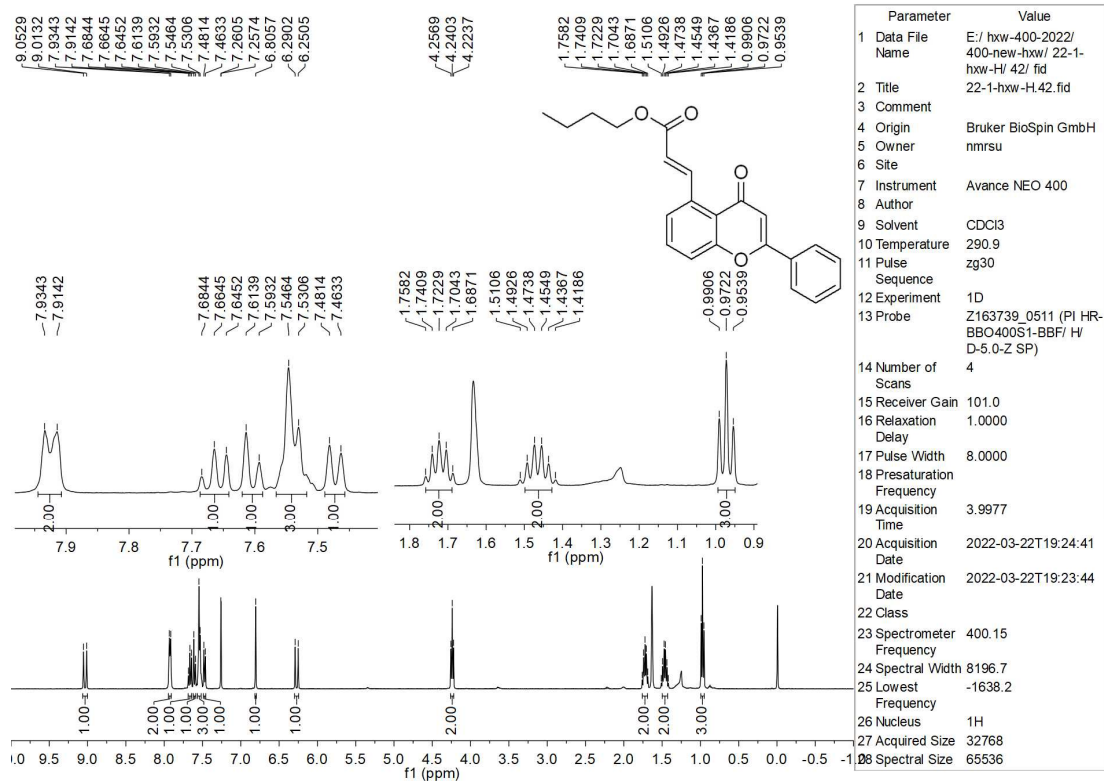


# 6-Bromo-2-(4-ethylphenyl)-4H-chromen-4-one (2en)

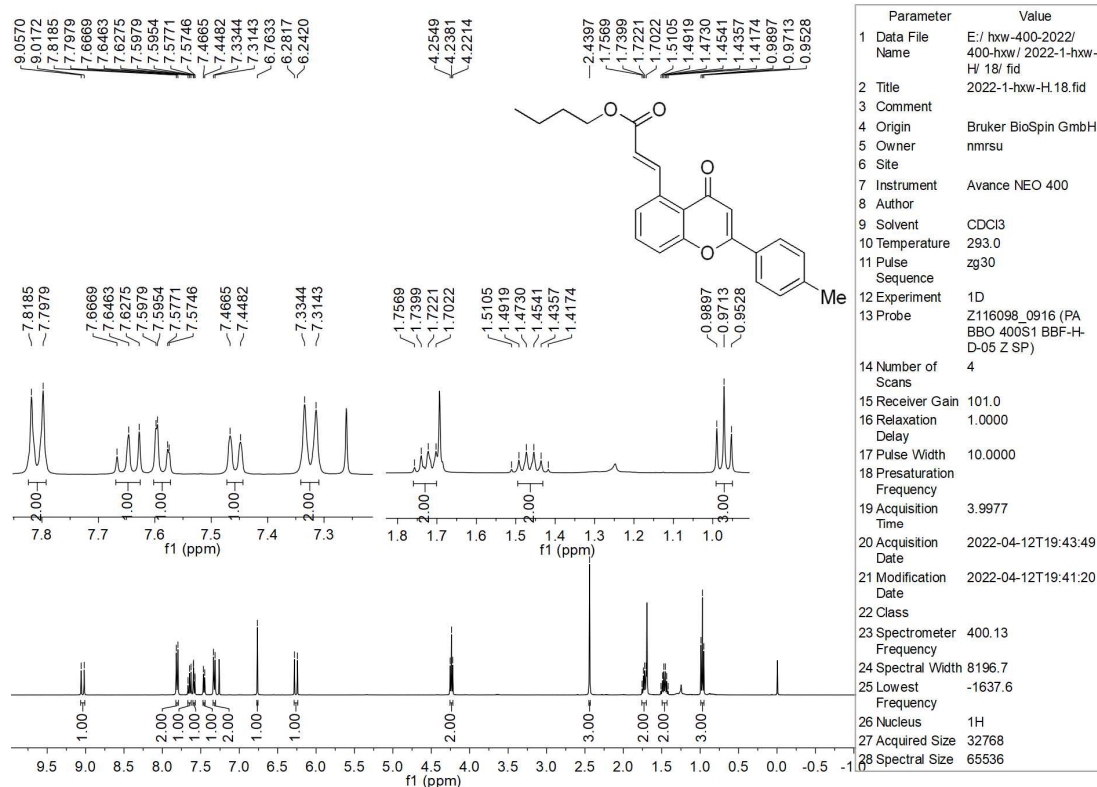




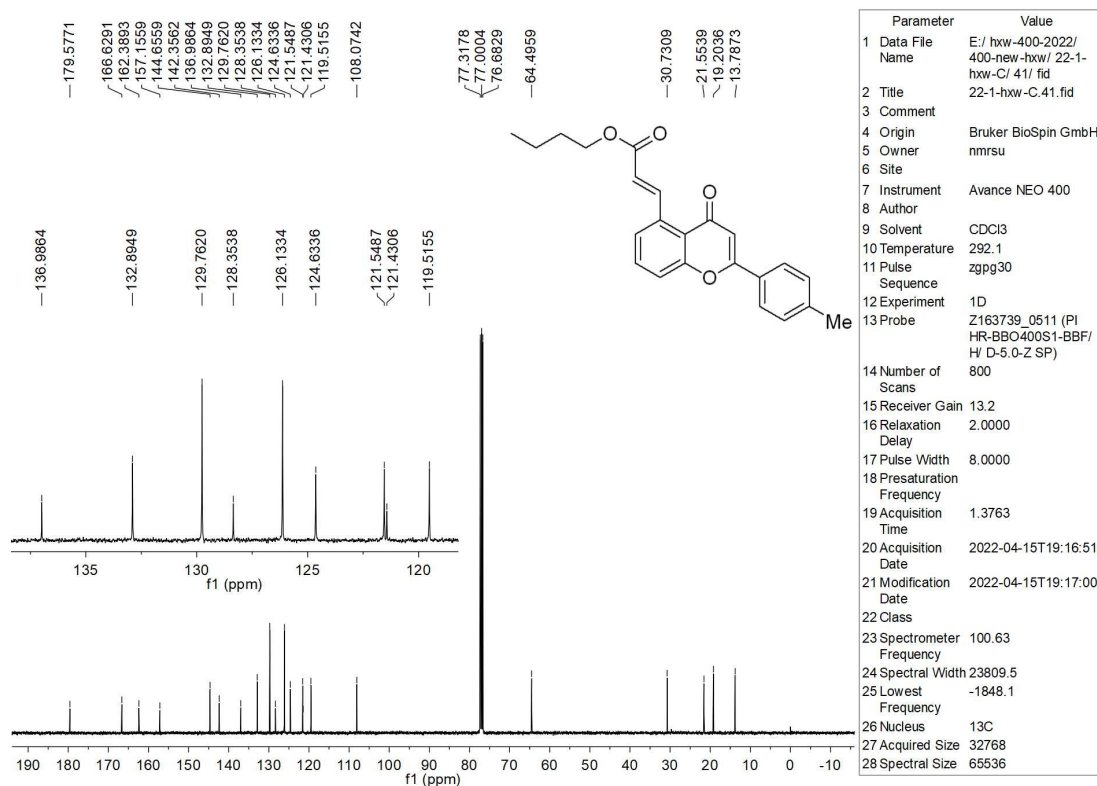
# Butyl (*E*)-3-(4-oxo-2-phenyl-4*H*-chromen-5-yl)acrylate (4aa)



# Butyl (*E*)-3-(4-oxo-2-(*p*-tolyl)-4*H*-chromen-5-yl)acrylate (4ab)

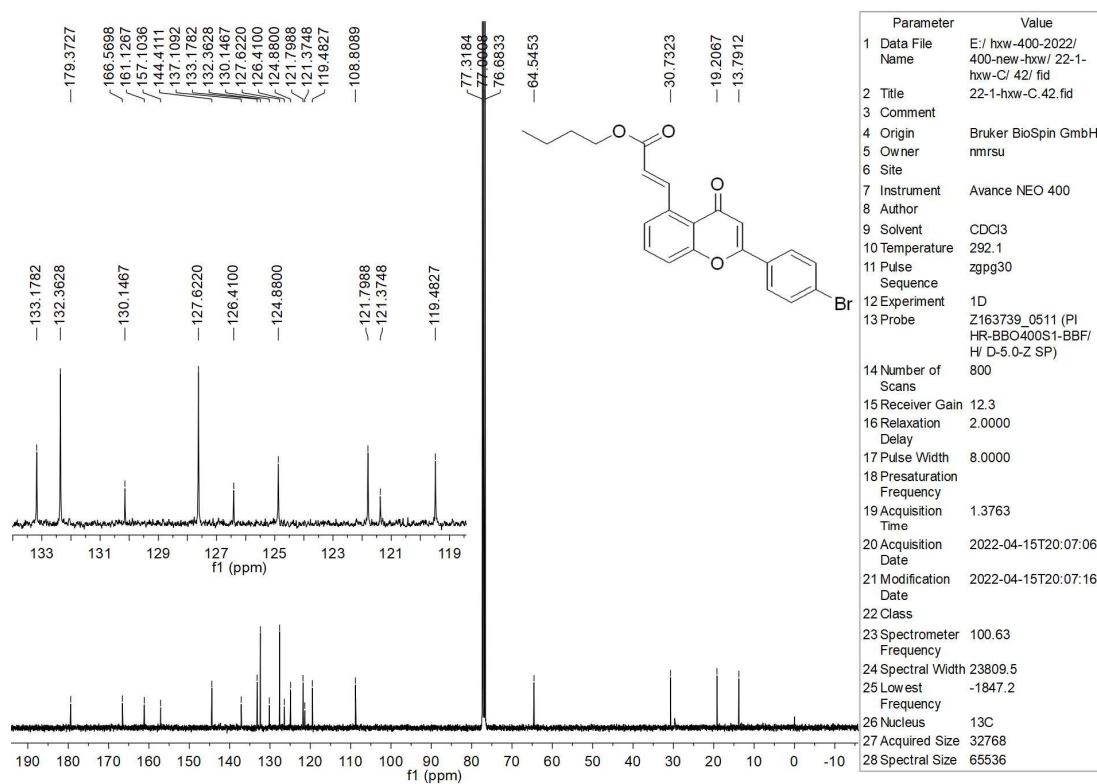
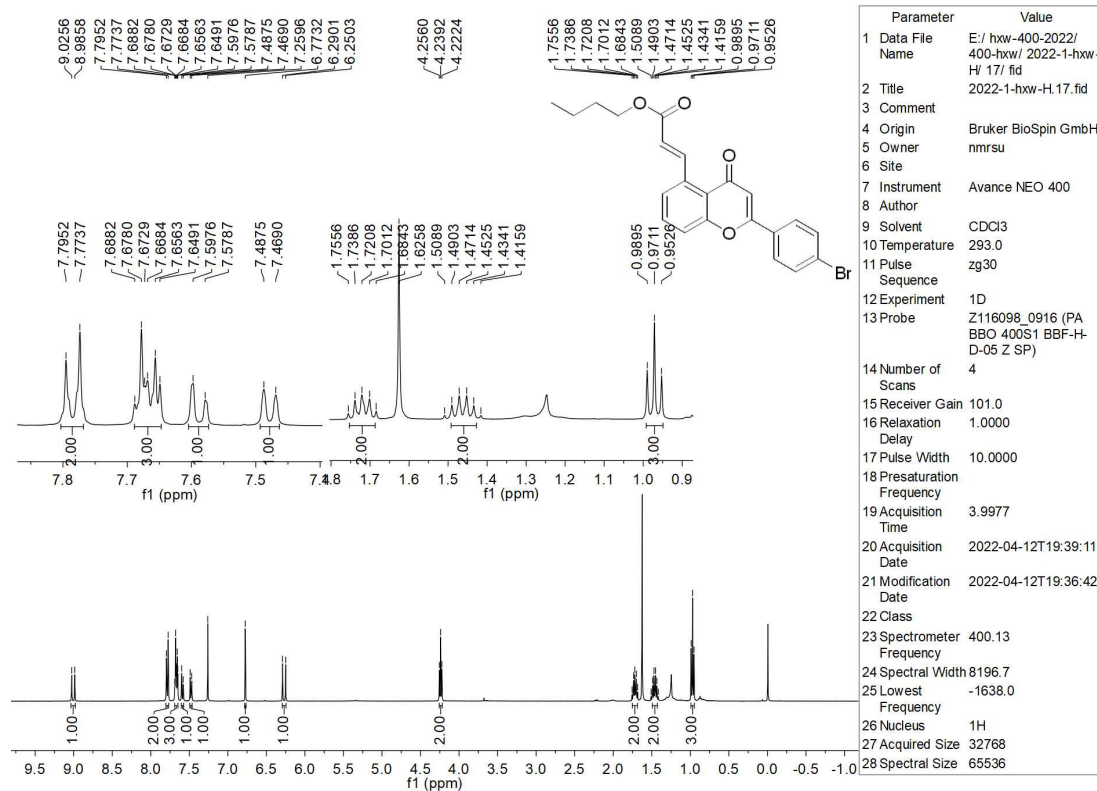


Parameter	Value
1 Data File Name	E:/ hwx-400-2022/ 400-hwx/ 2022-1-hwx-H/ 18/ fid
2 Title	2022-1-hwx-H.18.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	293.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z116098_0916 (PA BBO 400S1 BBF-H- D-05 Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-04-12T19:43:49
21 Modification Date	2022-04-12T19:41:20
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.6
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536

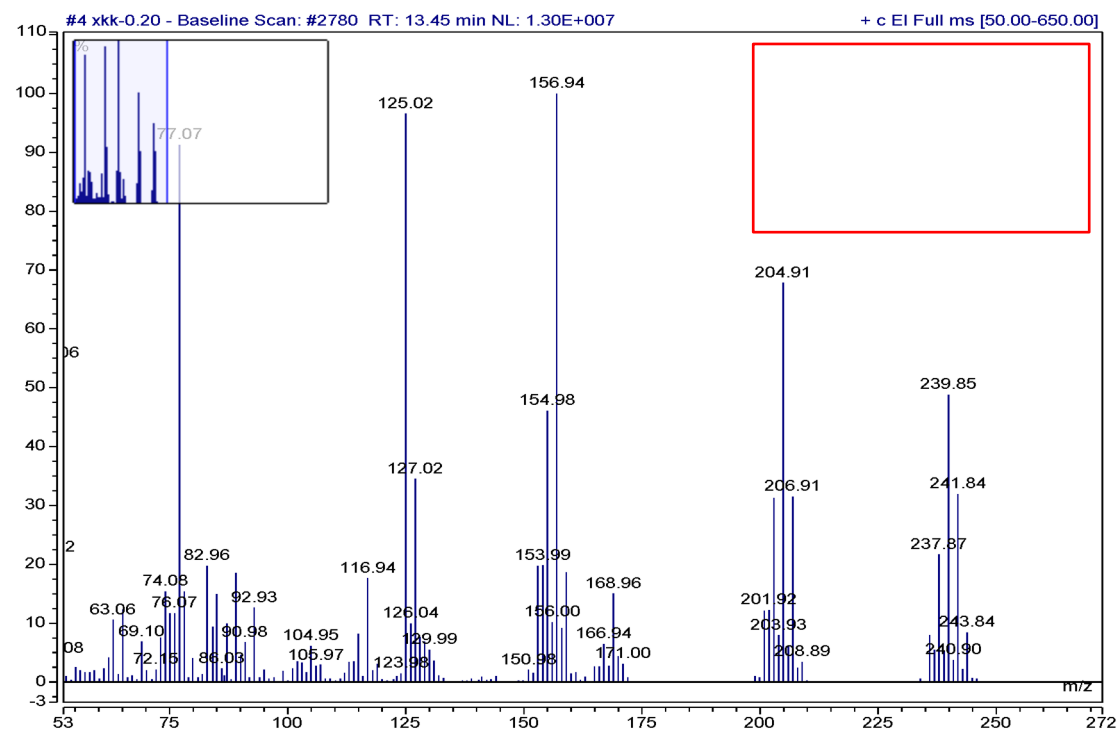
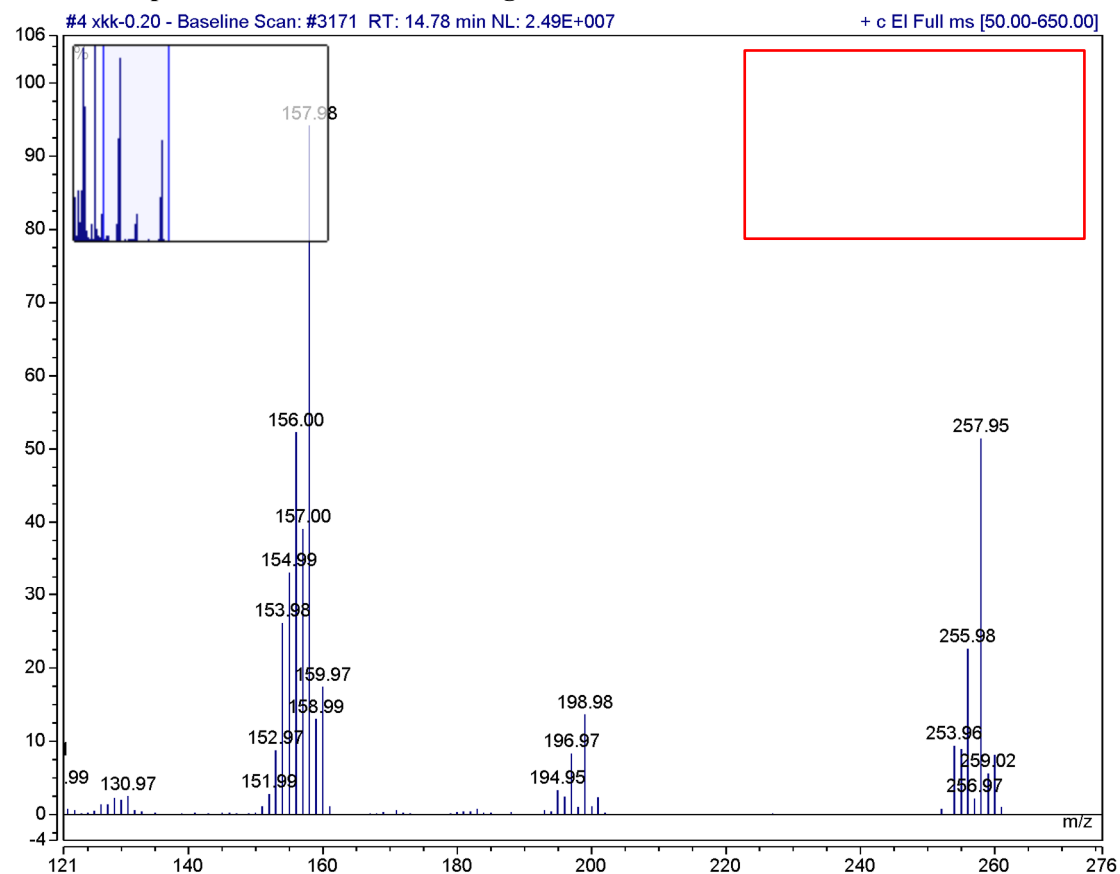


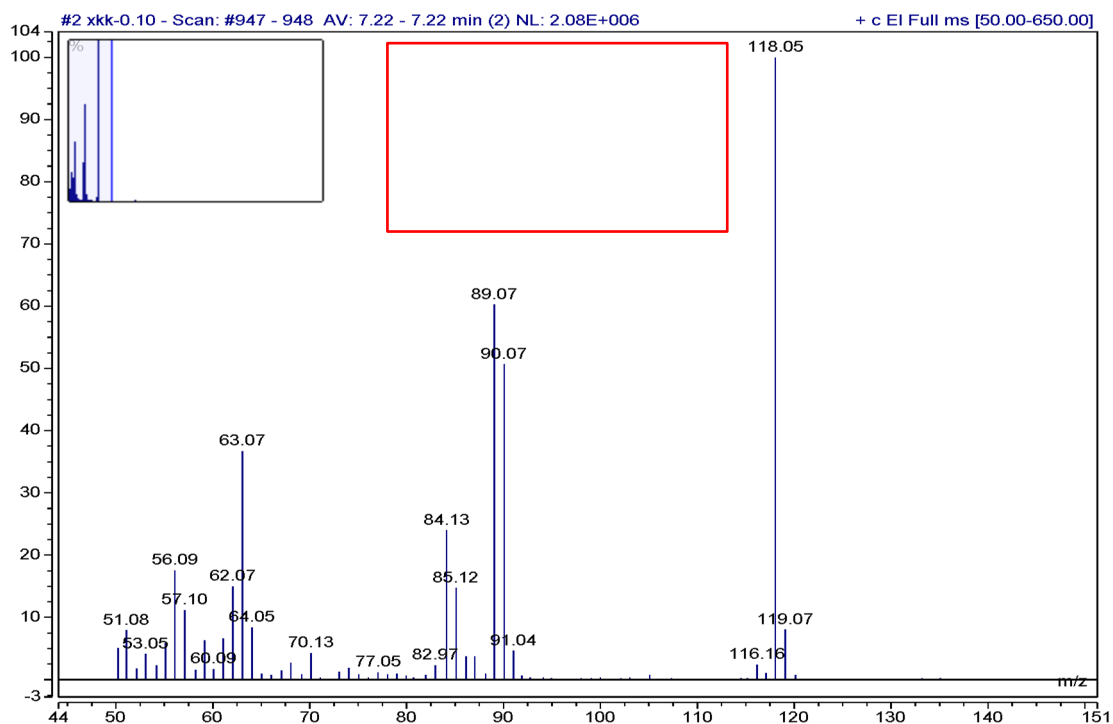
Parameter	Value
1 Data File Name	E:/ hwx-400-2022/ 400-new-hwx/ 22-1-hwx-C/ 41/ fid
2 Title	22-1-hwx-C.41.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	292.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	800
15 Receiver Gain	13.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-04-15T19:16:51
21 Modification Date	2022-04-15T19:17:00
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1848.1
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536

# Butyl (E)-3-(2-(4-bromophenyl)-4-oxo-4H-chromen-5-yl)acrylate (4af)

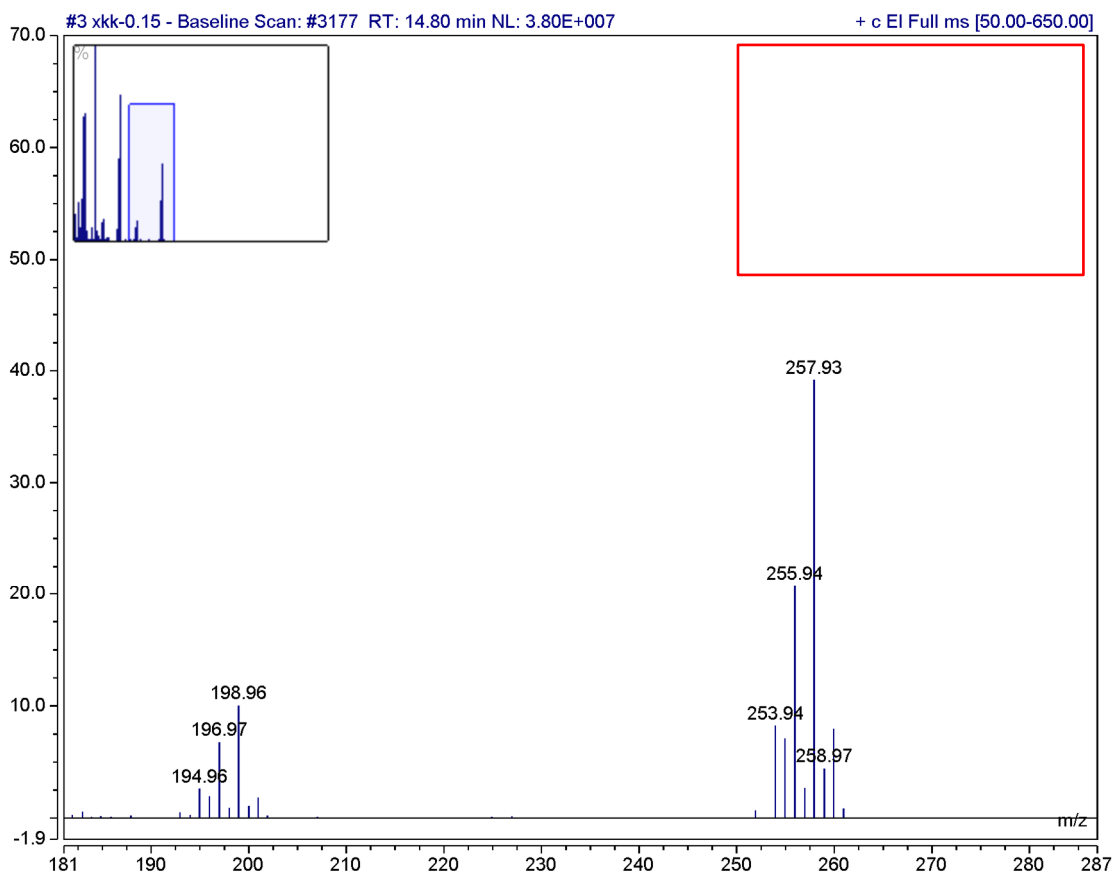


## 9. GC-MS spectra for mechanistic investigations

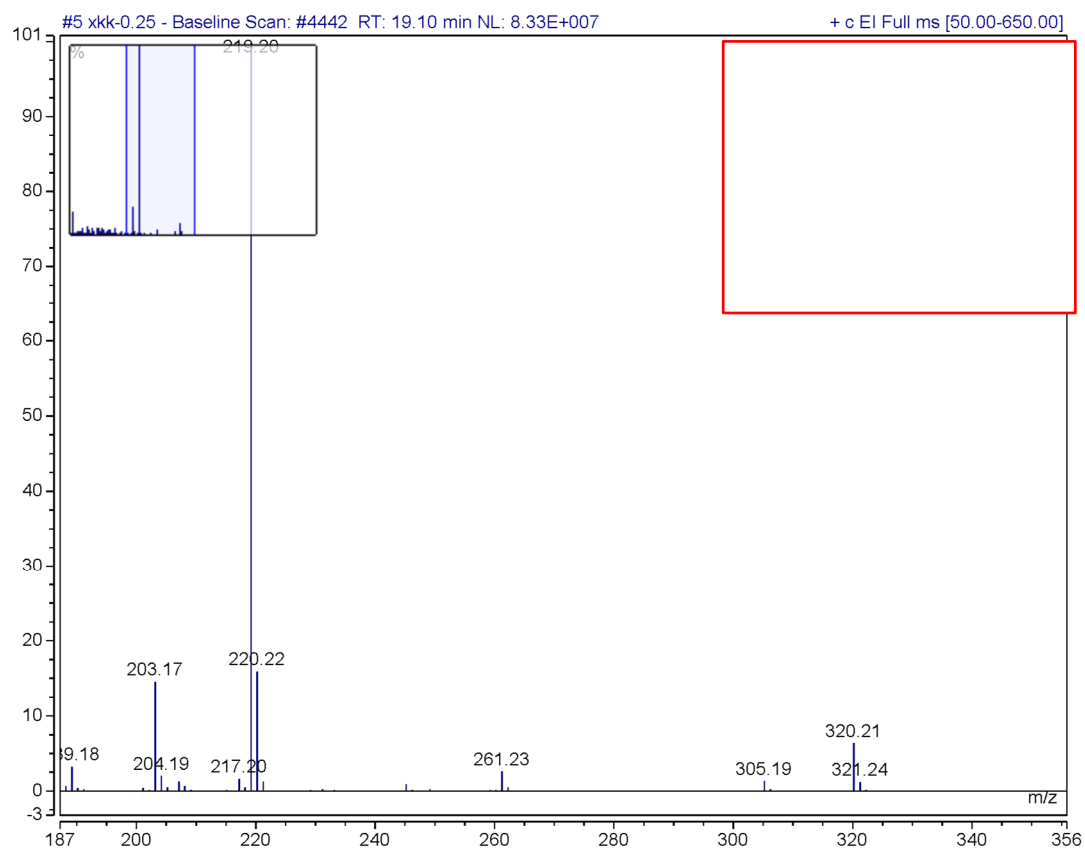




**Figure S4.** GC-MS spectra of methyl 2-hydroxy-2-methylpropanoate



**Figure S5.** GC-MS spectra of the control experiment in the presence of TEMPO.



**Figure S6.** GC-MS spectra of the control experiment in the presence of BHT.