

Electronic Supplementary Information

Synthesis of arene-functionalized fused heterocyclic scaffolds *via* a regioselective cascade 1,4-conjugate addition/5-*exo-dig* annulation strategy

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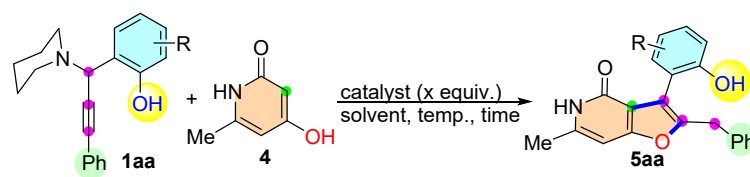
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Table S1. Optimization of the reaction conditions.^a

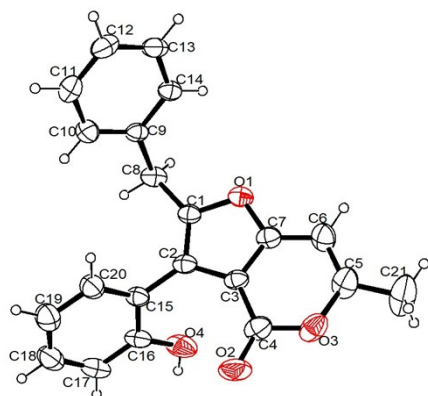


entry	catalyst (x equiv.)	solvent	time (h)	temp. (°C)	yield(%) ^b
1	FeCl ₃ (0.2)	MeCN	4	80	0
2	AlCl ₃ (0.2)	MeCN	4	80	0
3	ZnCl ₂ (0.2)	MeCN	4	80	0
4	Cu(OTf) ₂ (0.2)	MeCN	4	80	0
5	Zn(OTf) ₂ (0.2)	MeCN	4	80	0
6	DMAP (1.0)	MeCN	4	80	11
7	DBU (1.0)	MeCN	4	80	8
8	DABCO (1.0)	MeCN	4	80	32
9	Cs ₂ CO ₃ (1.0)	MeCN	4	80	30
10	NaHCO ₃ (1.0)	MeCN	4	80	35
11	TMG (1.0)	MeCN	4	80	43
12	TMG (1.0)	MeCN	8	80	46
13	TMG (1.0)	MeCN	10	80	47
14	TMG (1.0)	MeCN	12	80	48
15	TMG (1.0)	MeCN	20	80	45
16	TMG (1.0)	MeCN	32	80	46
17	TMG (0.5)	MeCN	12	80	40
18	TMG (1.5)	MeCN	12	80	53
19	TMG (2.0)	MeCN	12	80	45
20	TMG (3.0)	MeCN	12	80	41
21	TMG (1.5)	MeCN	12	90	60
22	TMG (1.5)	DCE	12	90	12
23	TMG (1.5)	THF	12	90	n.r.
24	TMG (1.5)	EtOAc	12	90	n.r.
25	TMG (1.5)	DMSO	12	90	n.r.
26 ^c	TMG (1.5)	MeCN	12	90	55
27 ^d	TMG (1.5)	MeCN	12	90	64
28 ^e	TMG (1.5)	MeCN	12	90	59

^aReaction conditions: propargylamine **1aa** (0.1 mmol), 4-hydroxy-6-methylpyridin-2(1H)-one **4** (0.1 mmol), and catalyst (20 mol%) in solvent (2 mL) under air atmosphere. ^bIsolated yields. ^cThe amount of **1aa** was 2.0 equivalences.

^dThe amount of **1aa** was 3.0 equivalences. ^eThe amount of **1aa** was 4.0 equivalences.

2. X-ray crystallographic data of compound **3aa**



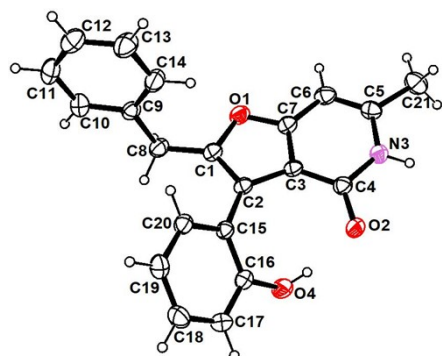
The purified compound **3aa** is dissolved in a mixed solvent of dichloromethane and *n*-hexane, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCD APEX-2 diffractometer (graphite-monochromated Mo *K* α radiation, $\lambda=0.71073$ nm) at 300 K.

Figure S1. ORTEP drawing of compound **3aa** (30% probability for the thermal ellipsoid).

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

CCDC number	2295482
Identification code	220330a_0m_a
Empirical formula	C ₂₁ H ₁₆ O ₄
Formula weight	332.34
Temperature	300.00 K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	$a = 8.460(7)$ Å $\alpha = 79.660(10)^\circ$ $b = 11.802(9)$ Å $\beta = 83.815(11)^\circ$ $c = 17.491(14)$ Å $\gamma = 89.445(11)^\circ$
Volume	1708(2) Å ³
Z	4
ρ_{calc}	1.292 g/cm ³
μ	0.089 mm ⁻¹
F(000)	696.0
Crystal size	0.21 × 0.2 × 0.19 mm ³
2 θ range for data collection	2.38 to 55.034°.
Index ranges	-10 ≤ <i>h</i> ≤ 10, -15 ≤ <i>k</i> ≤ 15, -22 ≤ <i>l</i> ≤ 22
Reflections collected	19706
Independent reflections	7626 [<i>R</i> _{int} = 0.0428, <i>R</i> _{sigma} = 0.0646]
Data / restraints / parameters	7626 / 0 / 455
Goodness-of-fit on <i>F</i> ²	0.995
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0545, <i>wR</i> ₂ = 0.1180
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.1211, <i>wR</i> ₂ = 0.1415
Largest diff. peak/hole	0.13 and -0.20 e.Å ⁻³

3. X-ray crystallographic data of compound **5aa**



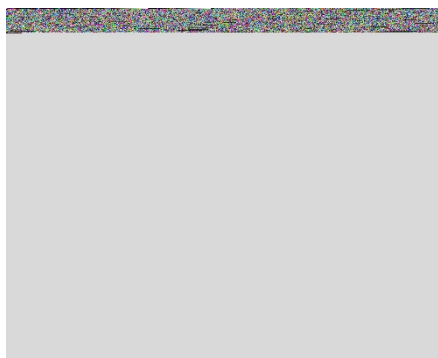
The purified compound **5aa** is dissolved in a mixed solvent of dichloromethane and *n*-hexane, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCD C APEX-2 diffractometer (graphite- monochromated Mo *K* α radiation, $\lambda=0.71073$ nm) at 300 K.

Figure S1. ORTEP drawing of compound **5aa** (30% probability for the thermal ellipsoid).

Table S1. Crystal data and structure refinement for compound **5aa**.

CCDC number	2295483
Identification code	20221017i
Empirical formula	C ₂₁ H ₁₇ NO ₃
Formula weight	331.36
Temperature	300.00 K
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	$a = 6.9547(6)$ Å $\alpha = 90^\circ$. $b = 19.975(2)$ Å $\beta = 90.477(4)^\circ$. $c = 12.2707(14)$ Å $\gamma = 90^\circ$.
Volume	1704.6(3) Å ³
Z	4
ρ_{calc}	1.291 g/cm ³
μ	0.087 mm ⁻¹
F(000)	696.0
Crystal size	0.29 × 0.26 × 0.23 mm ³
2 θ range for data collection	5.26 to 54.952°.
Index ranges	-9 ≤ <i>h</i> ≤ 8, -25 ≤ <i>k</i> ≤ 25, -15 ≤ <i>l</i> ≤ 15
Reflections collected	30892
Independent reflections	3885 [<i>R</i> _{int} = 0.1407, <i>R</i> _{sigma} = 0.0746]
Data / restraints / parameters	3885 / 0 / 229
Goodness-of-fit on <i>F</i> ²	1.022
Final <i>R</i> indexes [<i>I</i> ≥ 2σ (<i>I</i>)]	<i>R</i> ₁ = 0.0549, <i>wR</i> ₂ = 0.1119
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.1343, <i>wR</i> ₂ = 0.1430
Largest diff. peak/hole	0.27 and -0.21 e.Å ⁻³

4. X-ray crystallographic data of compound **10aa**



The purified compound **10aa** is dissolved in a mixed solvent of dichloromethane and *n*-hexane, and placed in a dark cabinet to slowly evaporate. After several days, a colourless bulk crystal is obtained. The X-ray crystal-structure determinations were obtained on a Bruker Smart CCD APEX-2 diffractometer (graphite-monochromated Mo *K* α radiation, $\lambda=0.71073$ nm) at 300 K.

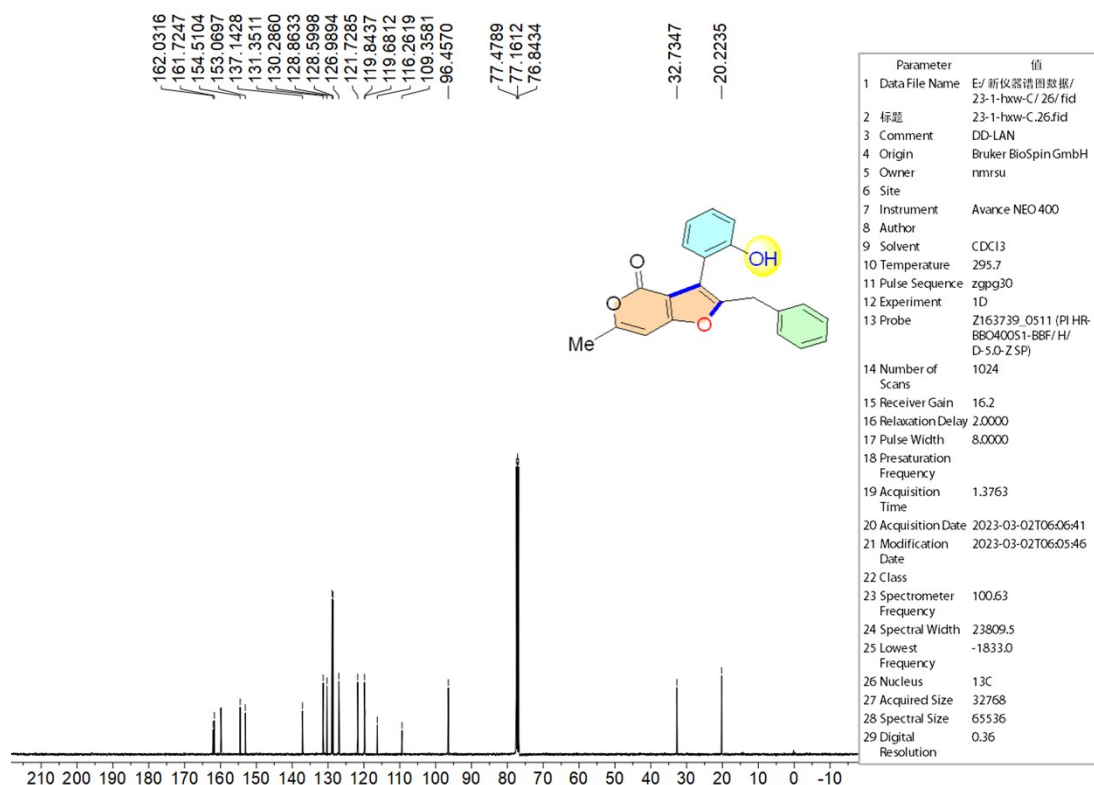
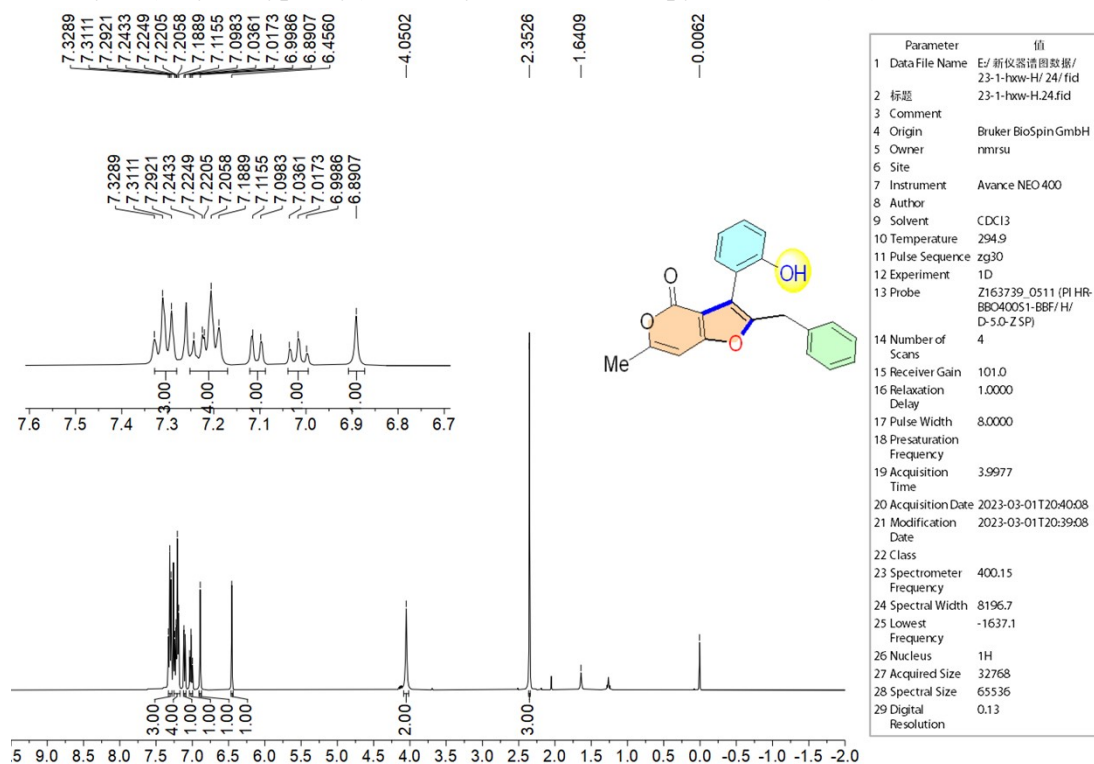
Figure S1. ORTEP drawing of compound **10aa** (30% probability for the thermal ellipsoid).

Table S1. Crystal data and structure refinement for compound **10aa**.

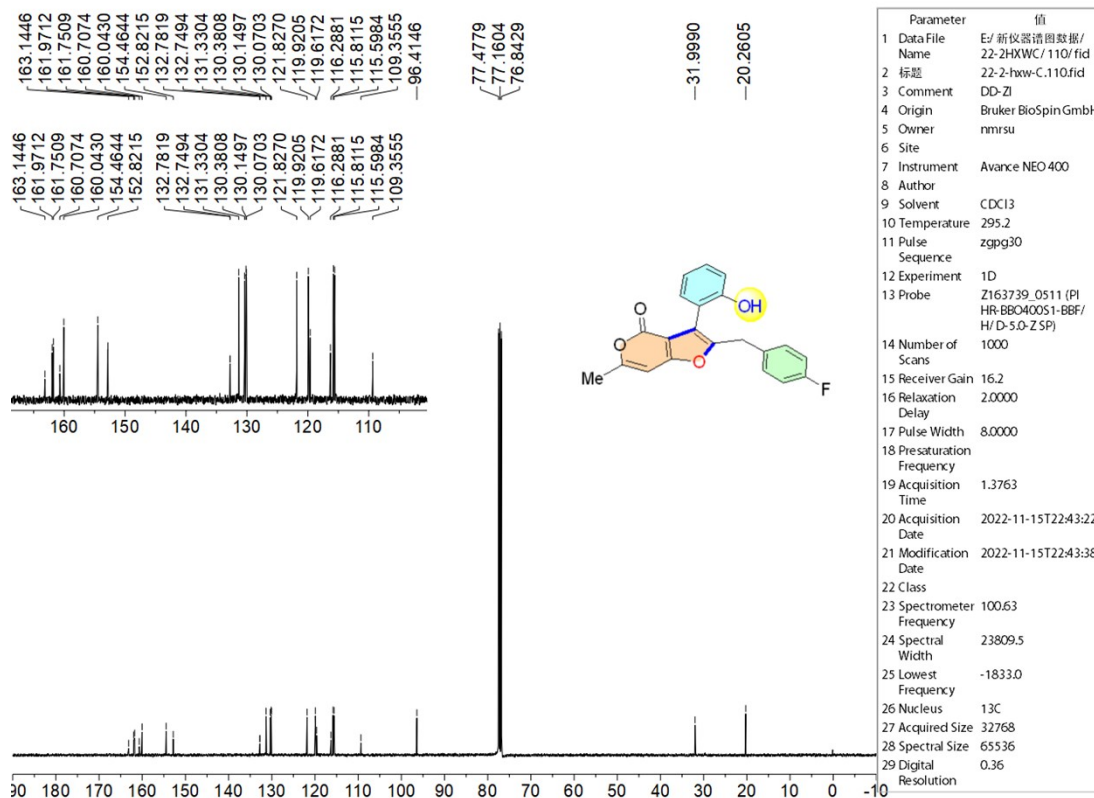
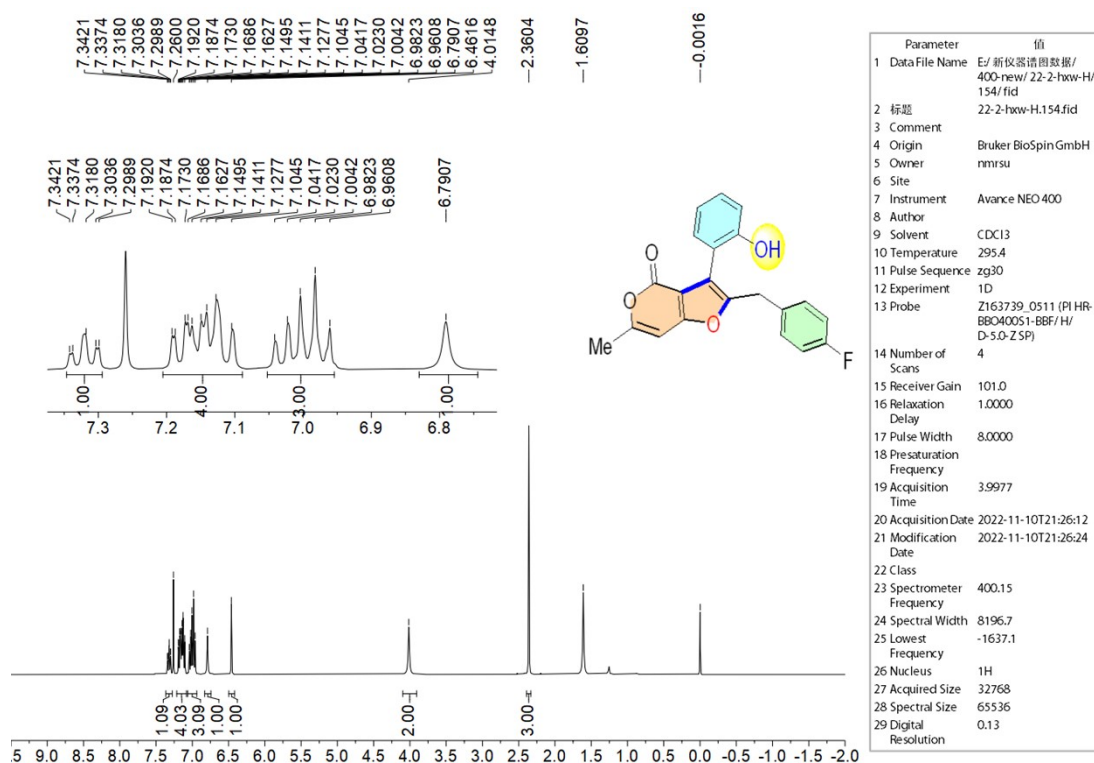
CCDC number	2295484
Identification code	230523c_sq
Empirical formula	C ₂₁ H ₁₇ NO ₃
Formula weight	331.36
Temperature	300.00 K
Wavelength	0.71073 Å
Crystal system	tetragonal
Space group	I4 ₁ /a
Unit cell dimensions	a = 23.118(12) Å $\alpha = 90^\circ$. b = 23.118(12) Å $\beta = 90^\circ$. c = 14.243(9) Å $\gamma = 90^\circ$.
Volume	7612(9) Å ³
Z	16
ρ_{calc}	1.157 g/cm ³
μ	0.078 mm ⁻¹
F(000)	2784.0
Crystal size	0.09 × 0.08 × 0.07 mm ³
2 θ range for data collection	3.358 to 49.5°.
Index ranges	-27 ≤ h ≤ 27, -27 ≤ k ≤ 25, -16 ≤ l ≤ 16
Reflections collected	26587
Independent reflections	3248 [R _{int} = 0.1790, R _{sigma} = 0.0923]
Data / restraints / parameters	3248 / 320 / 267
Goodness-of-fit on F ²	1.014
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0862, wR ₂ = 0.1958
Final R indexes [all data]	R ₁ = 0.2022, wR ₂ = 0.2671
Largest diff. peak/hole	0.14 and -0.18 e.Å ⁻³

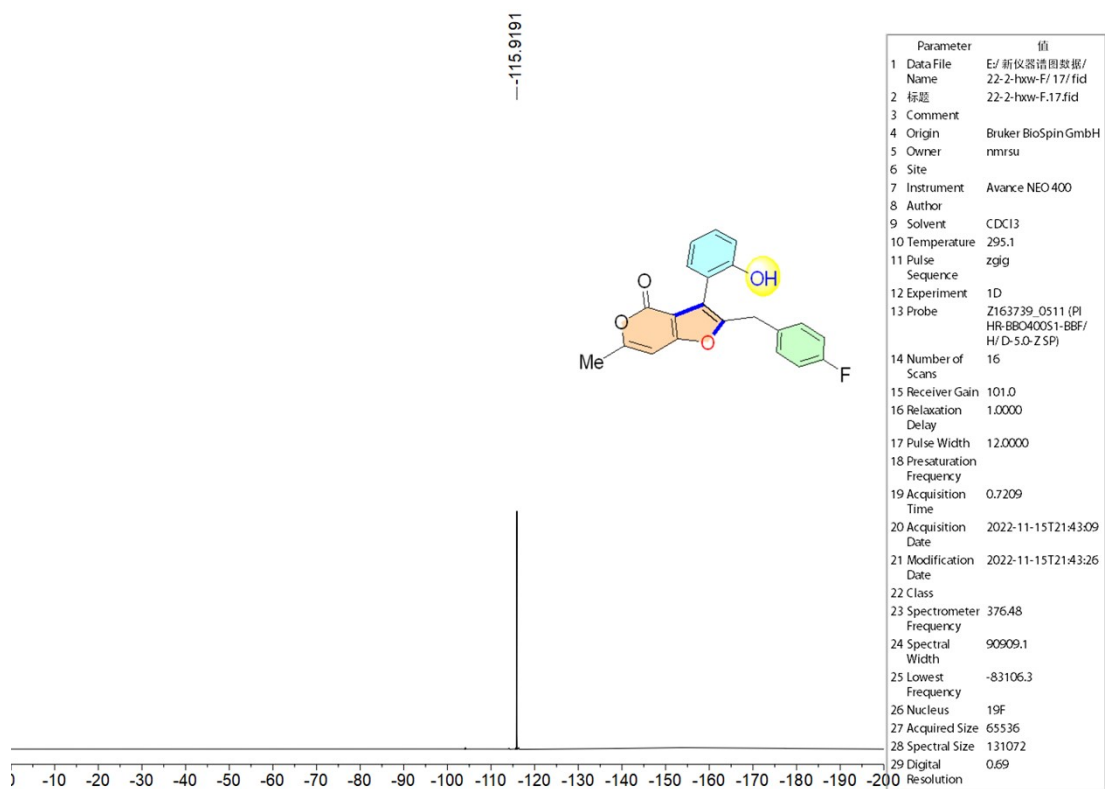
5. ^1H , ^{13}C and/or ^{19}F NMR spectra for all compounds

2-Benzyl-3-(2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3aa)

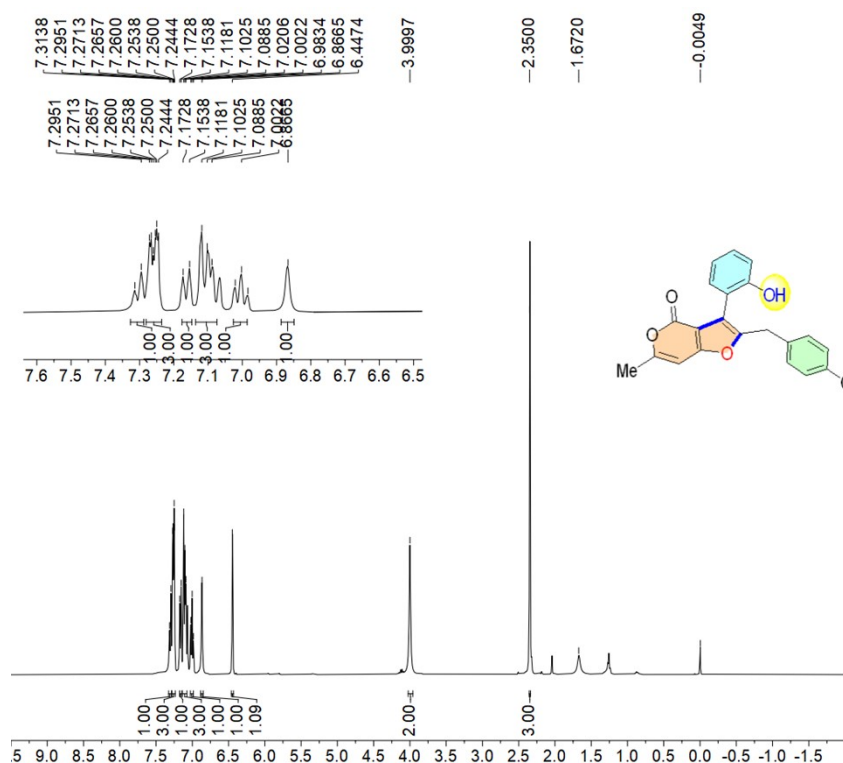


2-(4-Fluorobenzyl)-3-(2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3ab)

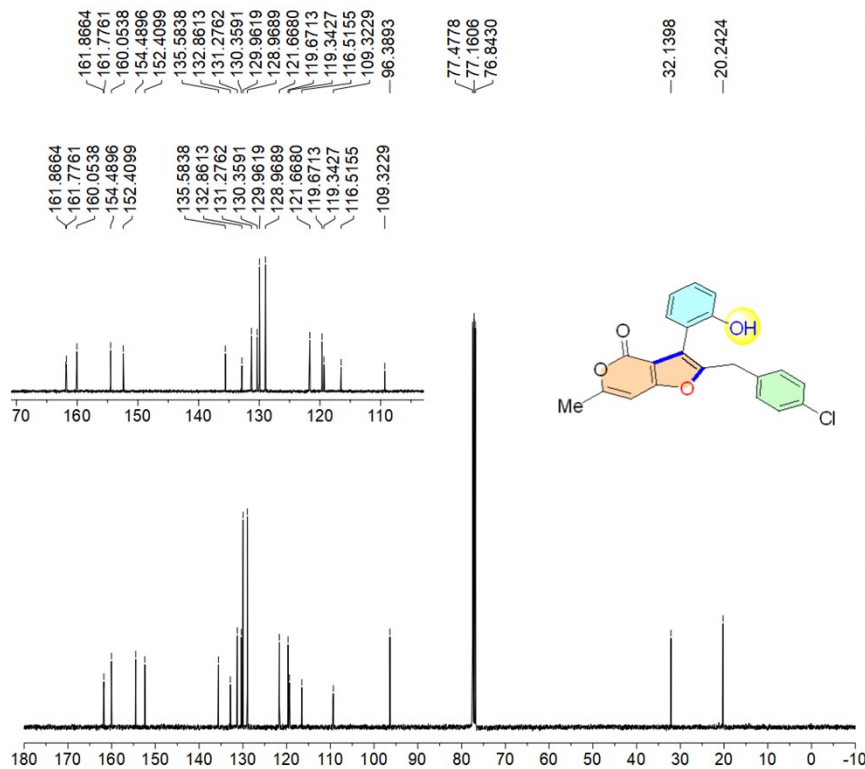




2-(4-Chlorobenzyl)-3-(2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3ac)



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4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.2
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	2022-10-17T20:23:20
21 Modification Date	2022-10-17T20:23:30
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



Parameter	值
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7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.8
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	350
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-10-19T05:00:34
21 Modification Date	2022-10-19T05:00:38
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

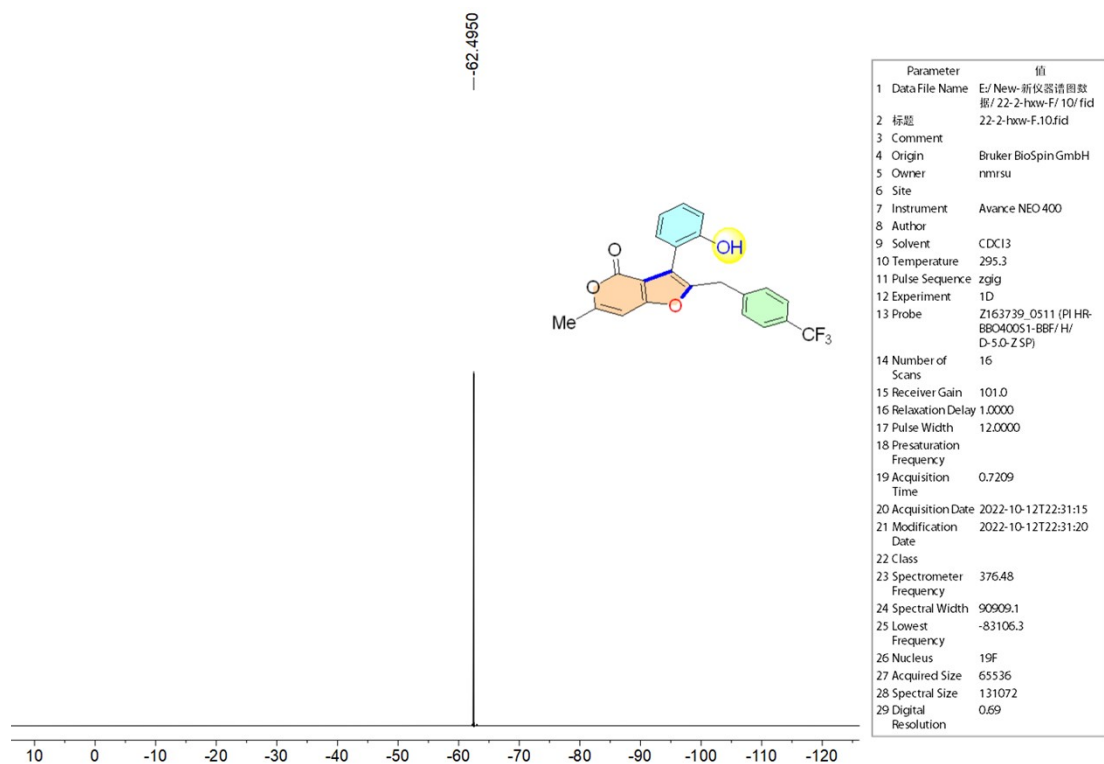
Chemical structure of 22-2-hw-H.163 is shown, with a yellow circle highlighting the phenolic OH group.

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4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
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10 Temperature	295.1
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
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21 Modification Date	2022-11-15T20:50:54
22 Class	
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25 Lowest Frequency	-1637.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

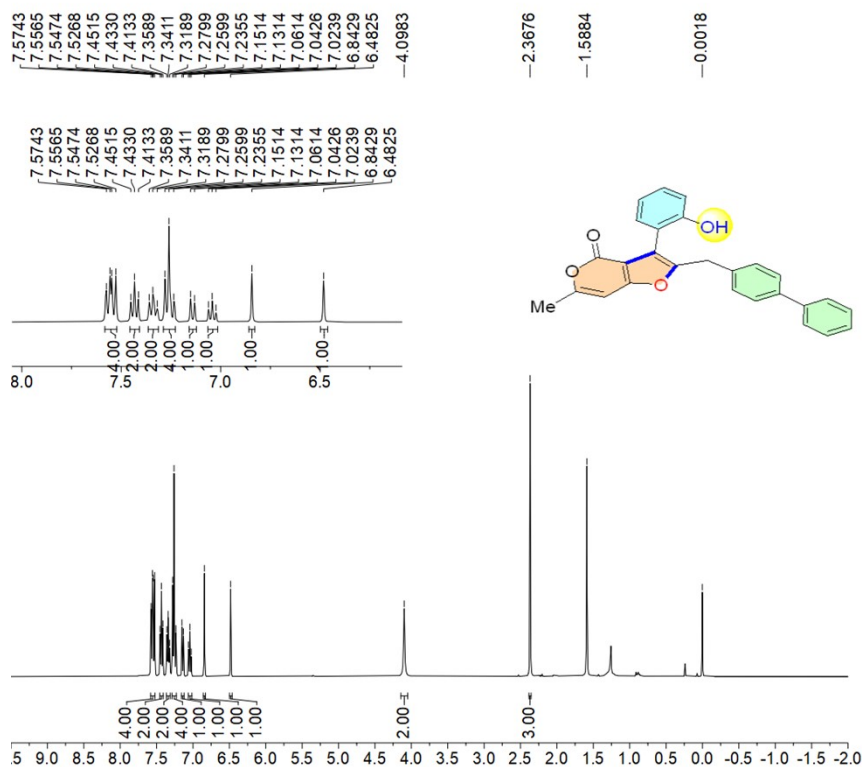


Figure 1 displays the ^1H NMR spectrum of compound 22-2-hw in CDCl_3 . The spectrum shows peaks from 0 to 10 ppm. Aromatic and heterocyclic protons appear between 6.5 and 8.0 ppm, while aliphatic protons are between 3.5 and 4.5 ppm. Integration values are shown below the peaks. The chemical structure of 22-2-hw is shown, highlighting the phenol and 4-(4-chlorophenyl)-2-methyl-1,2,4-oxadiazol-5-yl groups.

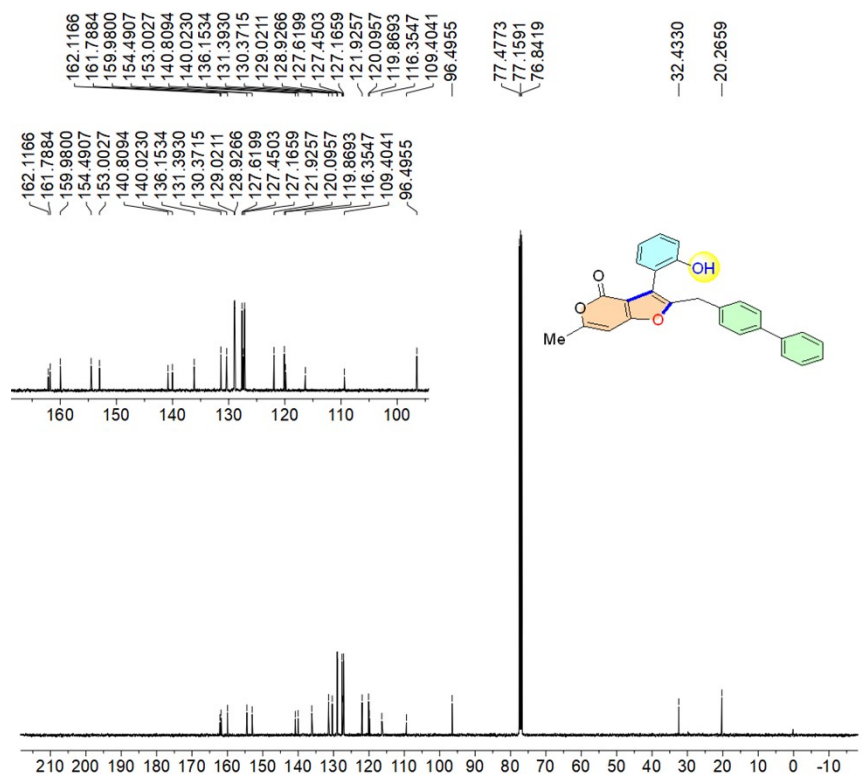




**2-([1,1'-Biphenyl]-4-ylmethyl)-3-(2-hydroxyphenyl)-6-methyl-4*H*-furo[3,2-*c*]pyran-4-one
(3af)**

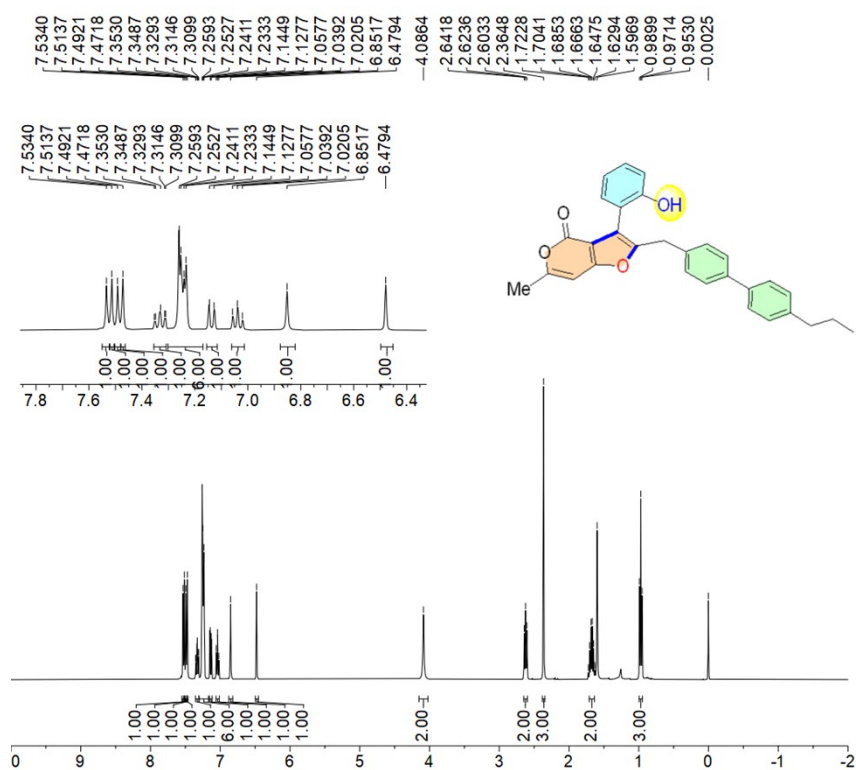


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5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2022-11-25T21:28:58
21 Modification Date	2022-11-25T21:29:00
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

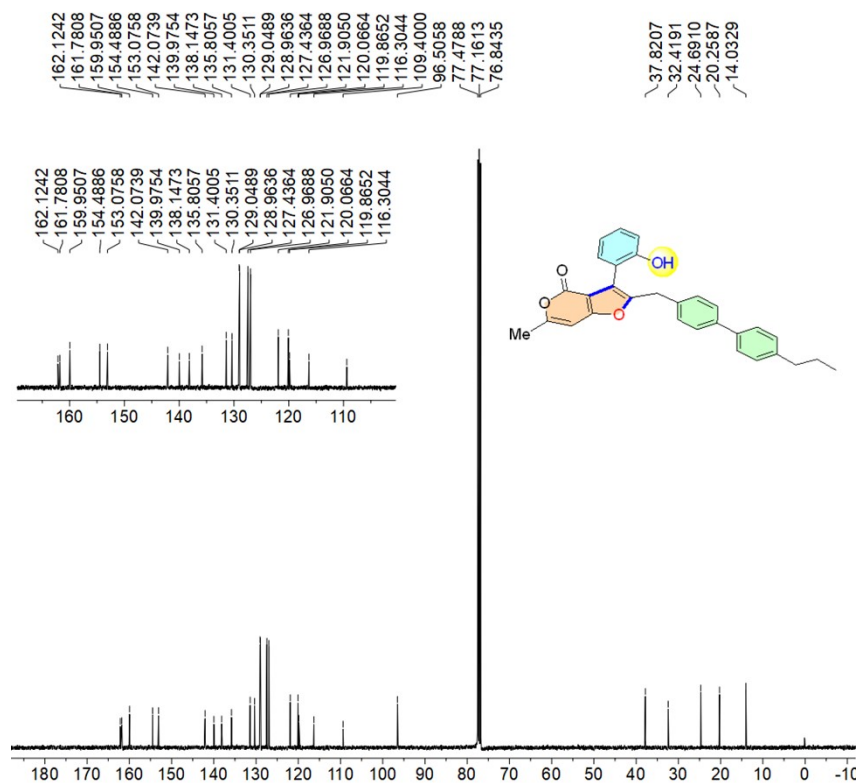


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8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	14.8
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
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20 Acquisition Date	2022-11-26T05:22:58
21 Modification Date	2022-11-26T05:23:00
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

3-(2-Hydroxyphenyl)-6-methyl-2-((4'-propyl-[1,1'-biphenyl]-4-yl)methyl)-4H-furo[3,2-c]pyran-4-one (3ag)

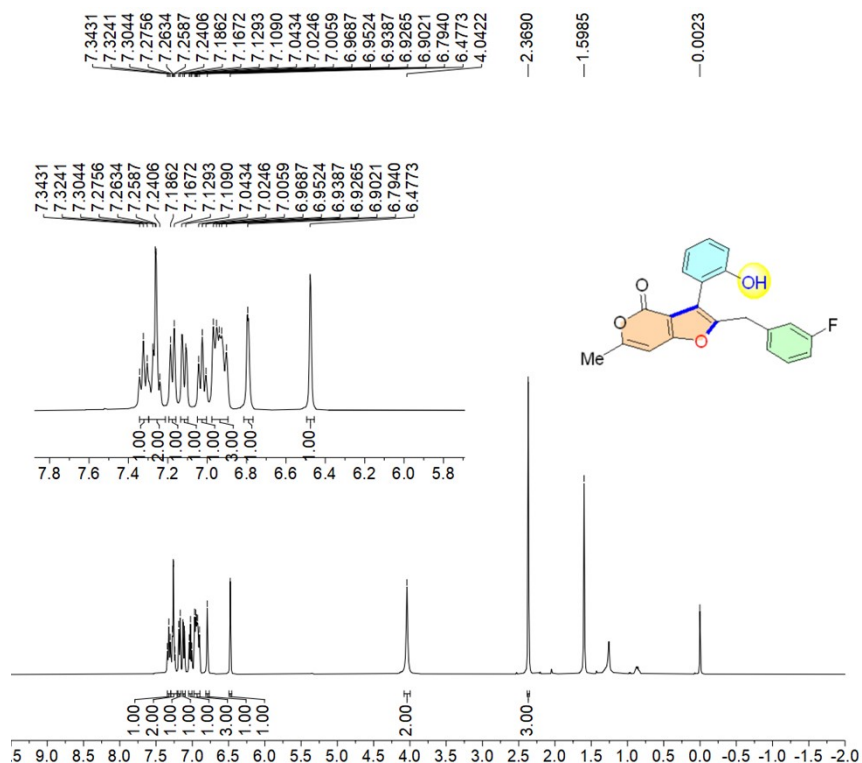


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7 Instrument	Avance NEO 400
8 Author	
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12 Experiment	1D
13 Probe	Z163739_0511 (PI HR- BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
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20 Acquisition Date	2022-11-15T21:00:53
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25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

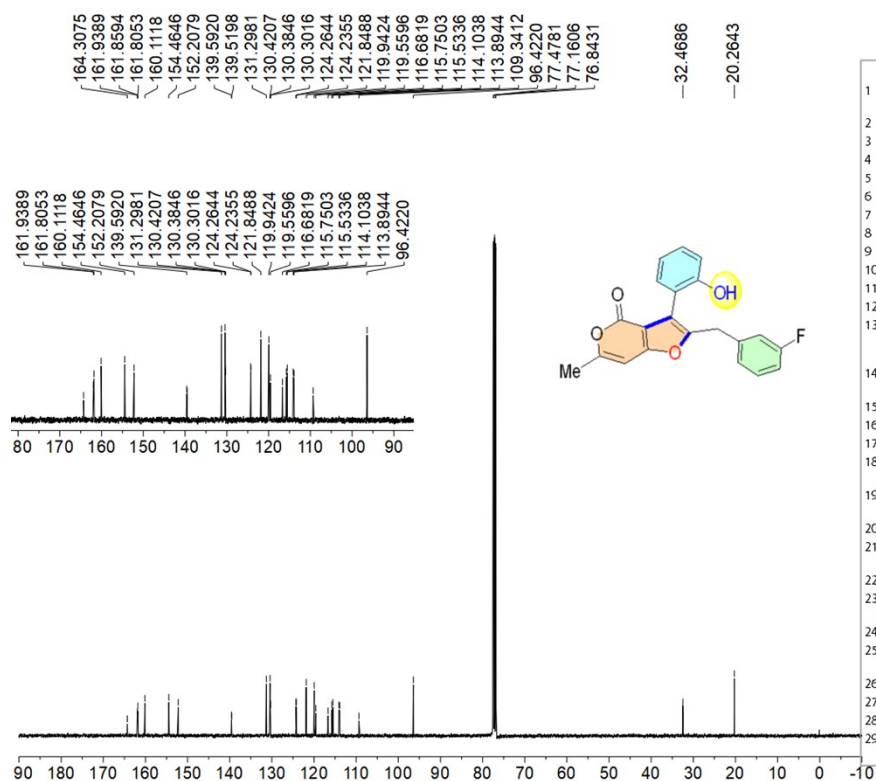


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8 Author	
9 Solvent	CDCl ₃
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12 Experiment	1D
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27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

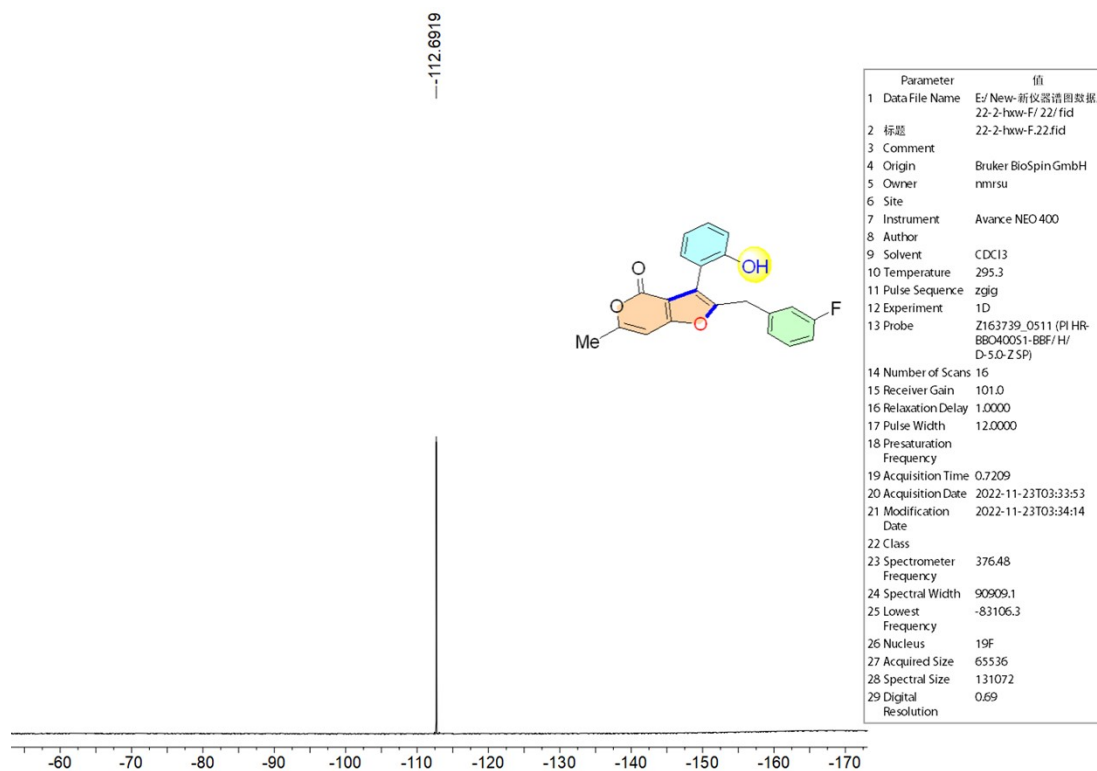
2-(3-Fluorobenzyl)-3-(2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3ah)



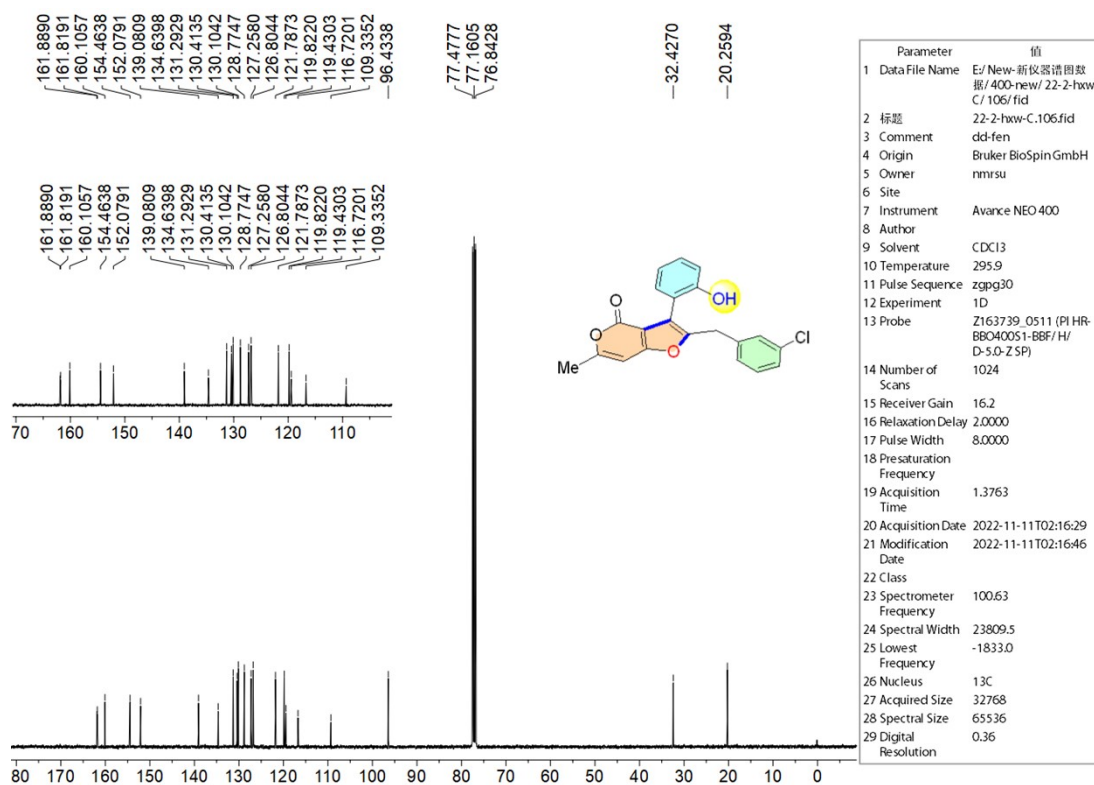
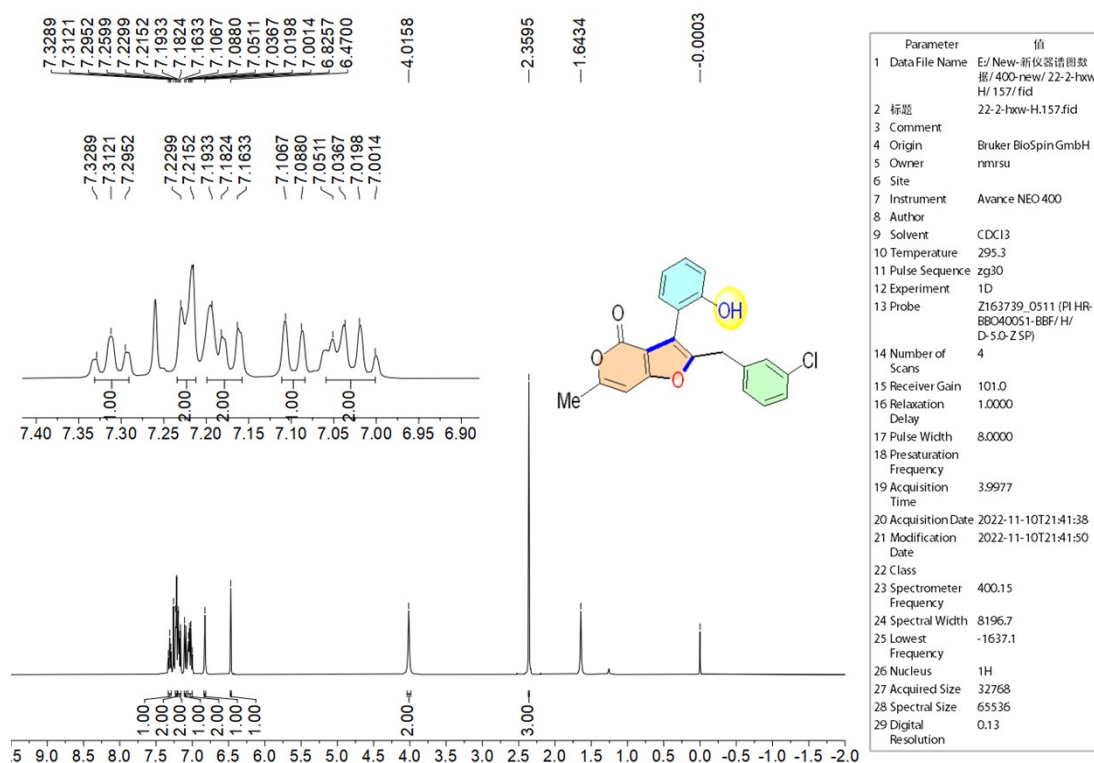
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8 Author	
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11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
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17 Pulse Width	8.0000
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24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



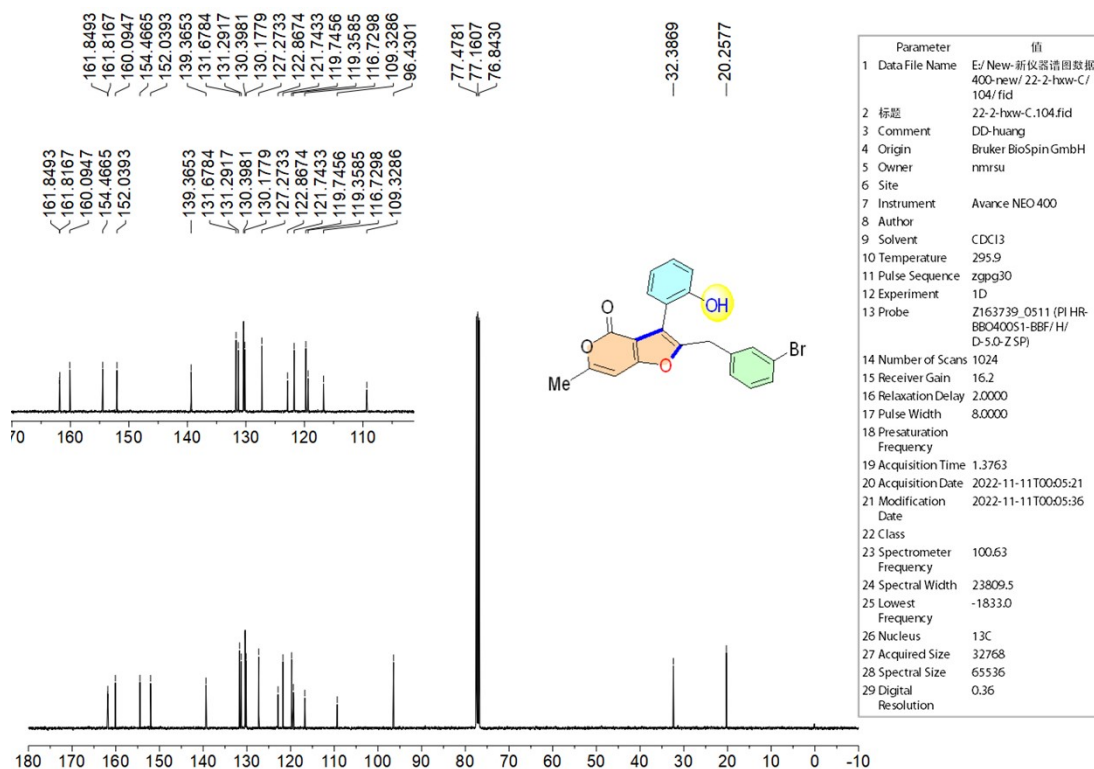
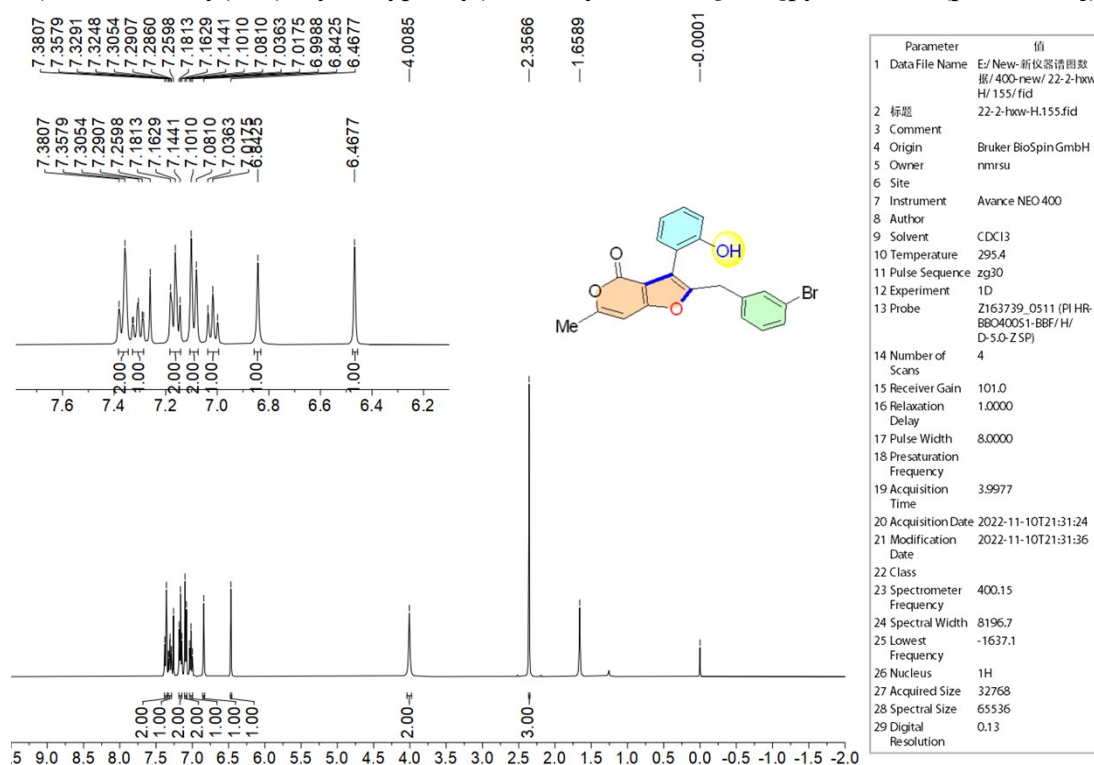
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2 标题	22-2-hxw-C.136.fid
3 Comment	DD-cheng1-F
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-11-25T22:38:03
21 Modification Date	2022-11-25T22:38:06
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36



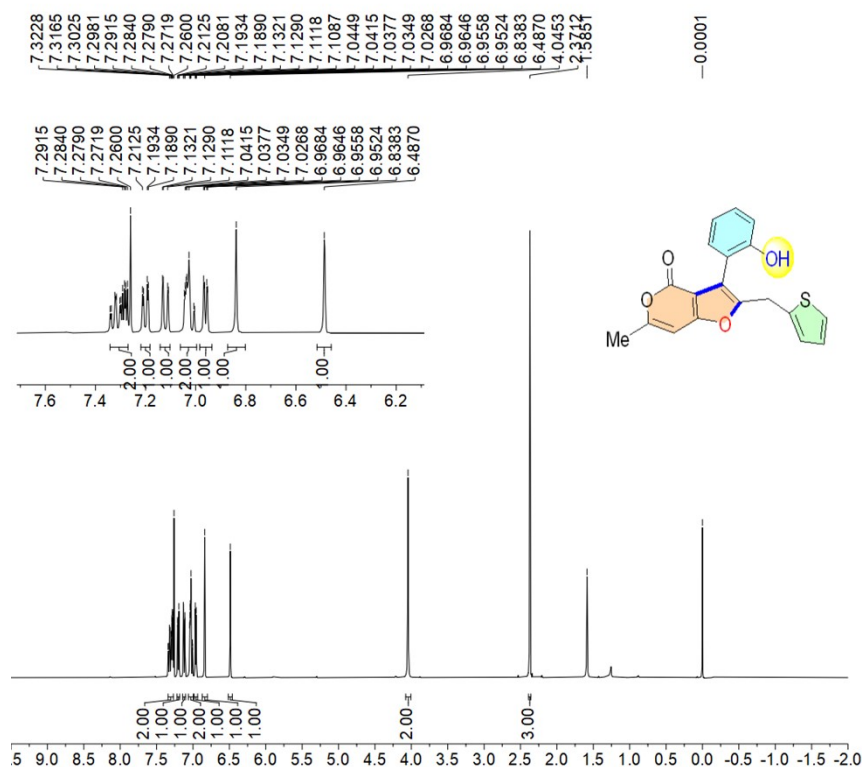
2-(3-Chlorobenzyl)-3-(2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3ai)



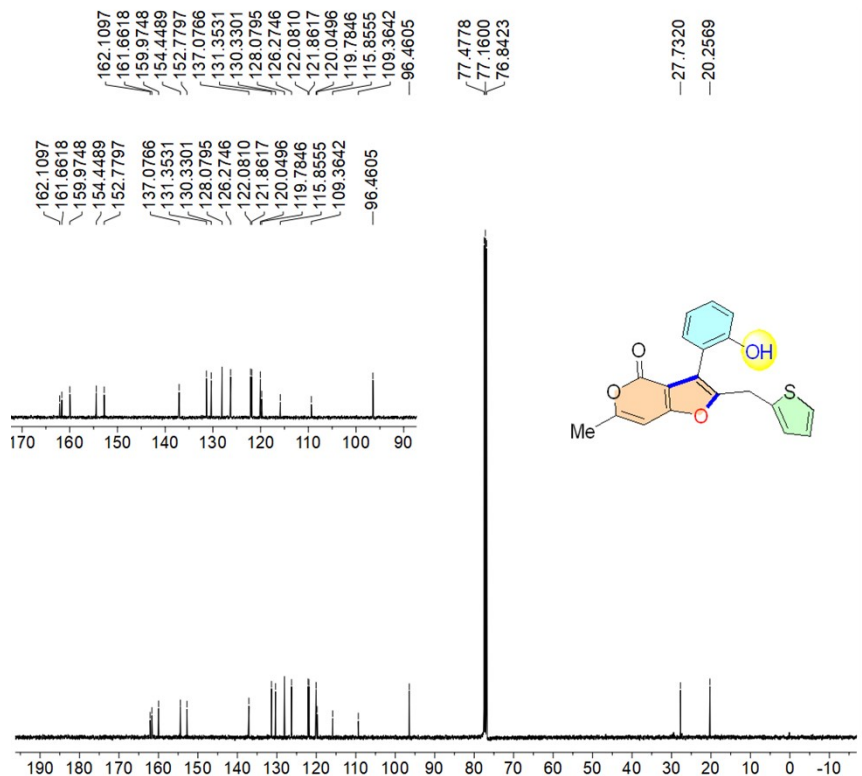
2-(3-Bromobenzyl)-3-(2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (product 3aj)



3-(2-Hydroxyphenyl)-6-methyl-2-(thiophen-2-ylmethyl)-4H-furo[3,2-c]pyran-4-one (3ak)

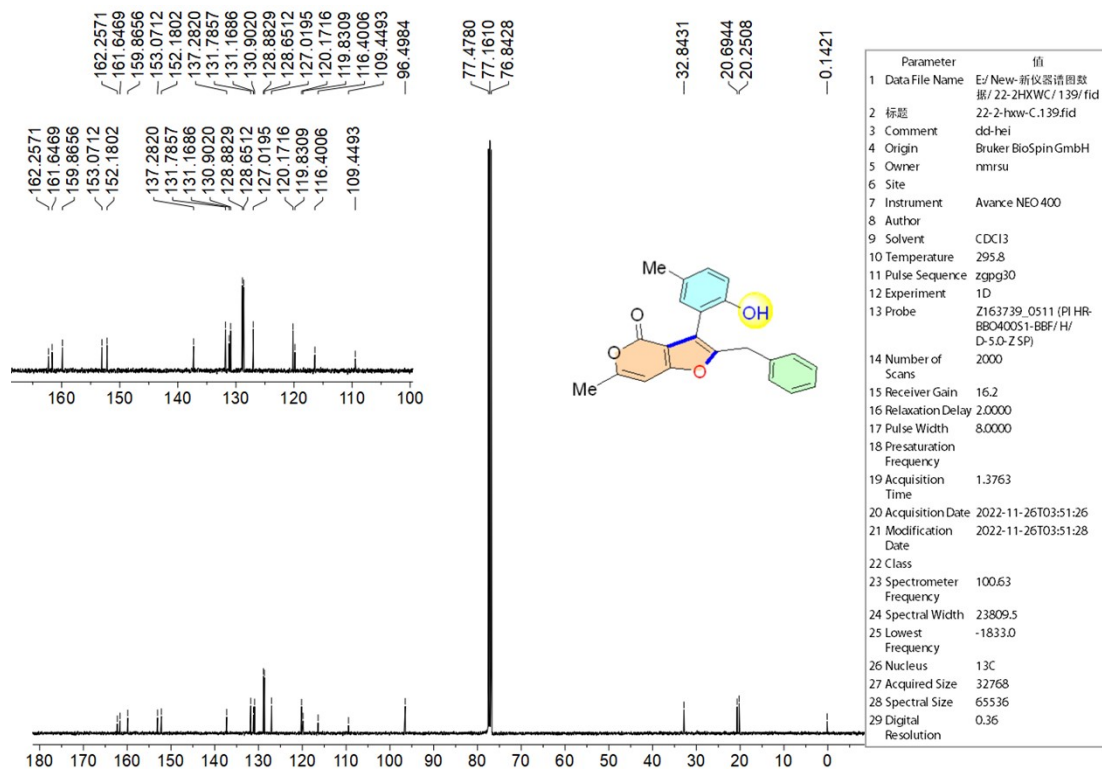
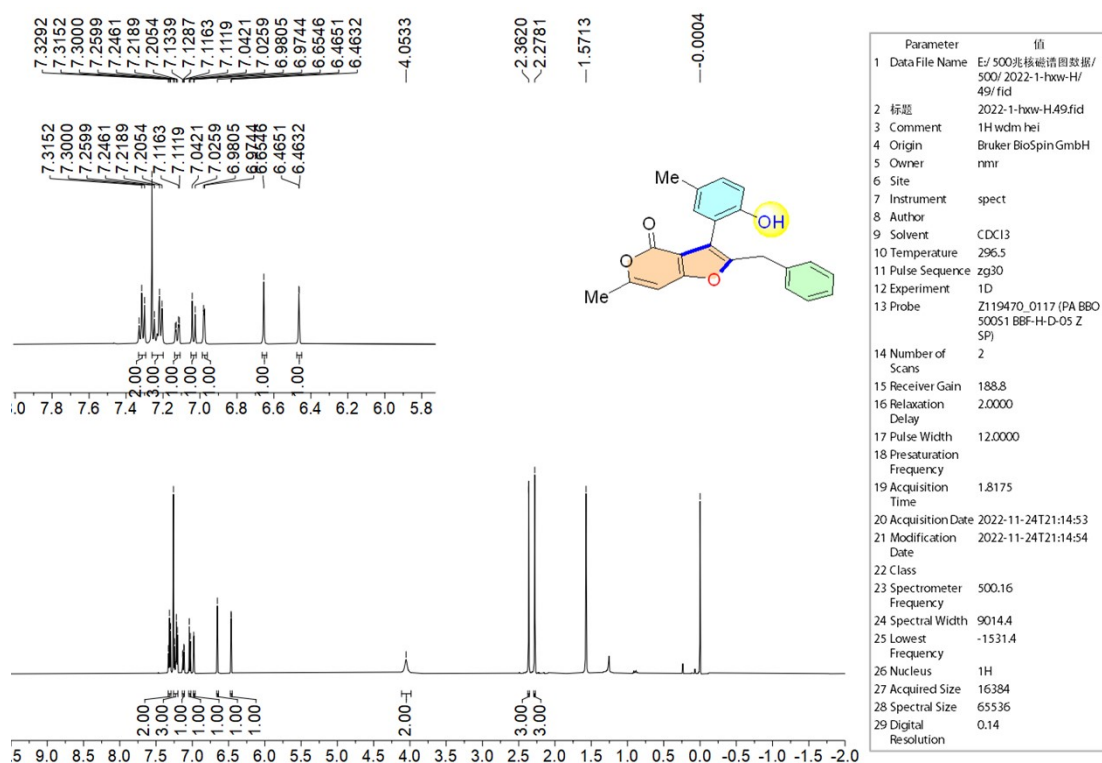


Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 400-new/ 22-2-hw-H/ 48/ fid
2 标题	22-2-hw-H.48.fid
3 Comment	
4 Origin	Brker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ 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	2022-10-11T21:42:53
21 Modification Date	2022-10-11T21:42:56
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

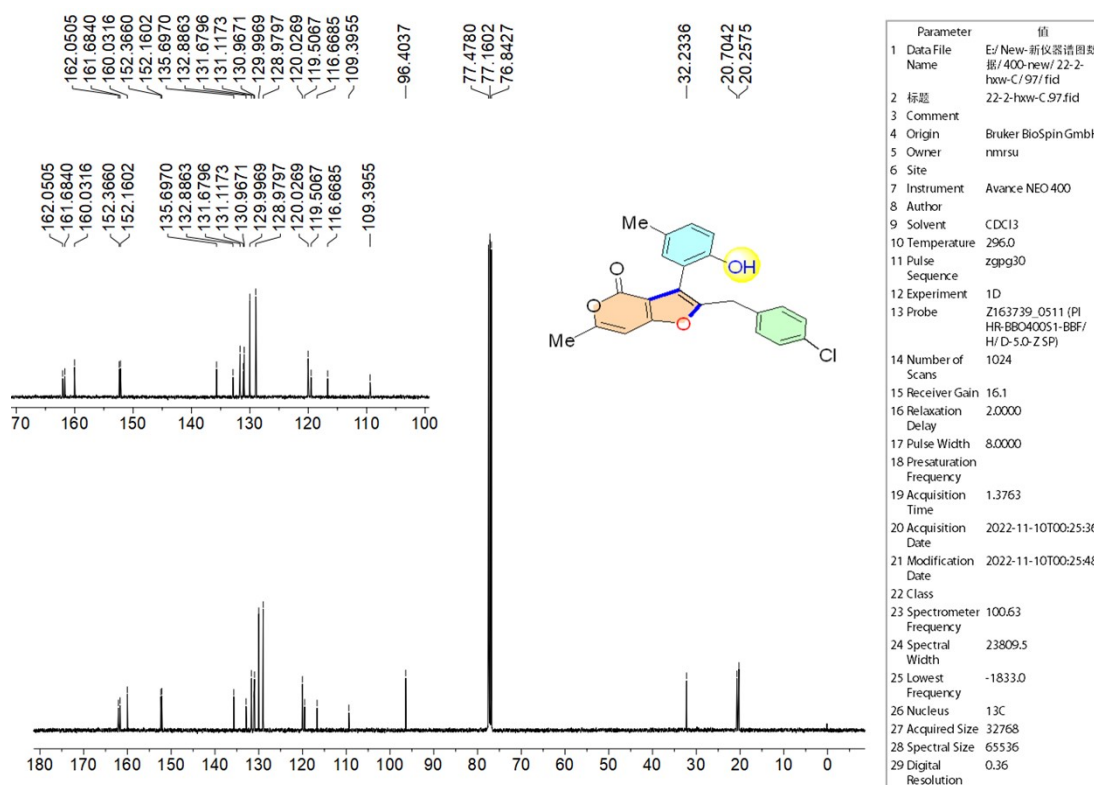
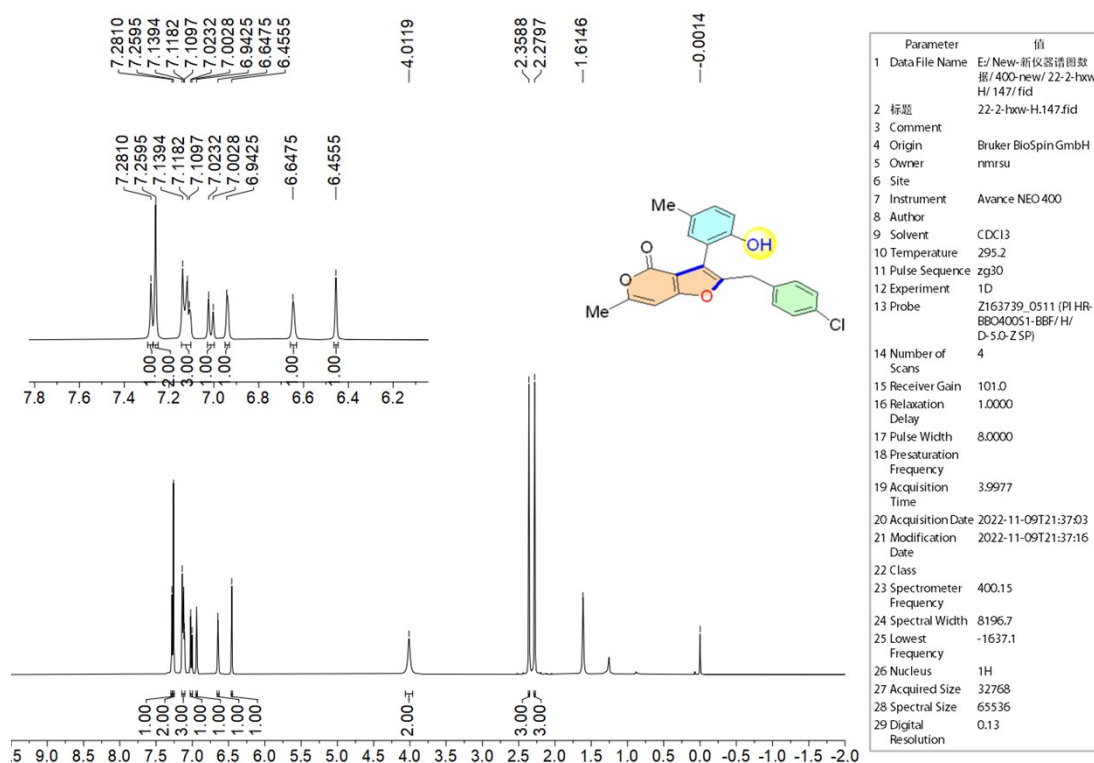


Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 400-new/ 22-2-hw-C/ 32/ fid
2 标题	22-2-hw-C.32.fid
3 Comment	
4 Origin	Brker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	512
15 Receiver Gain	14.6
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-10-12T22:25:49
21 Modification Date	2022-10-12T22:25:54
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

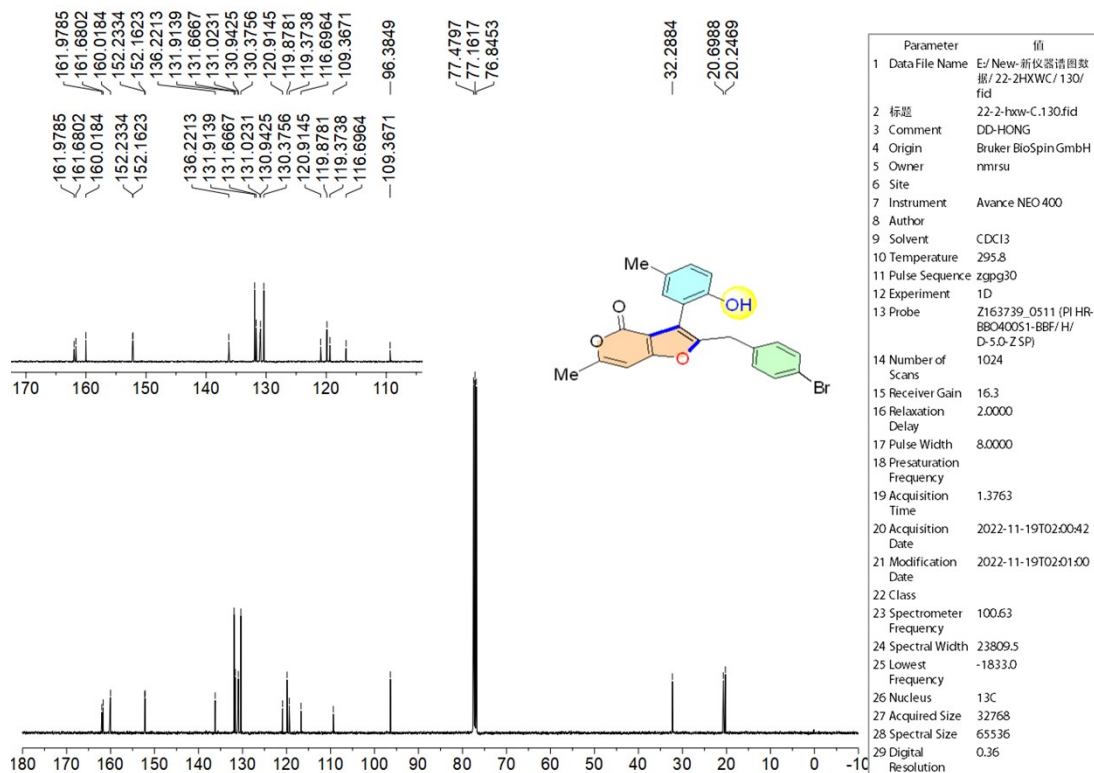
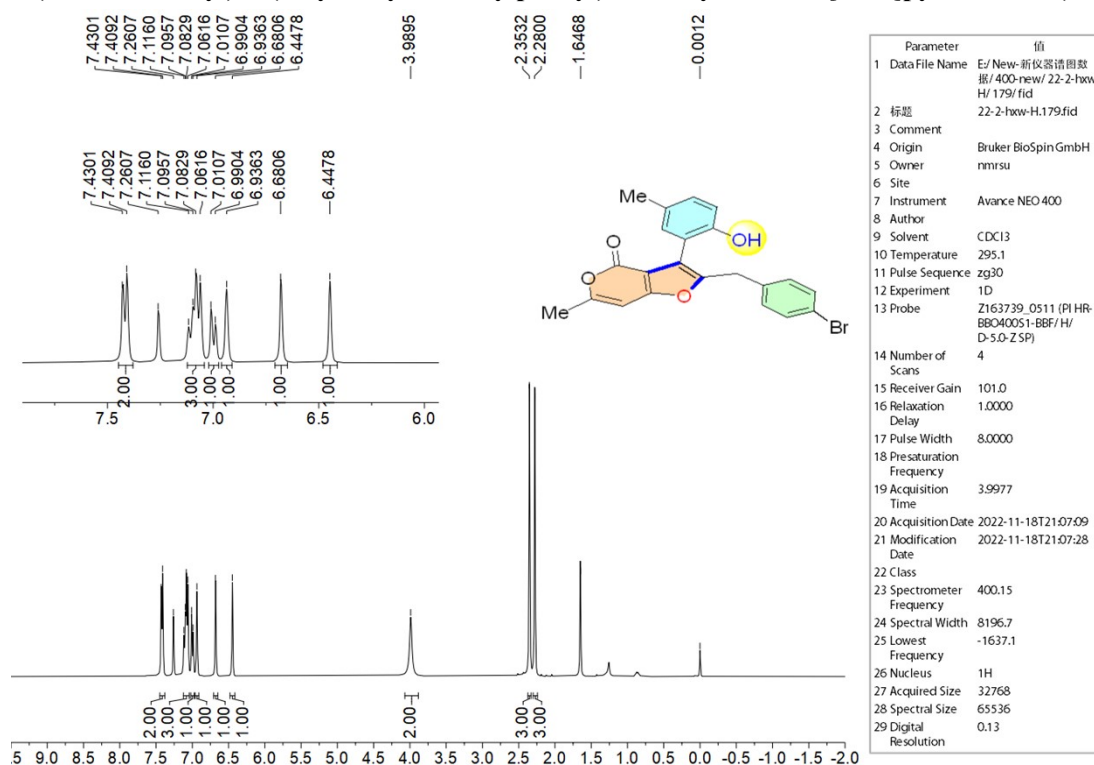
2-Benzyl-3-(2-hydroxy-5-methylphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3ba)



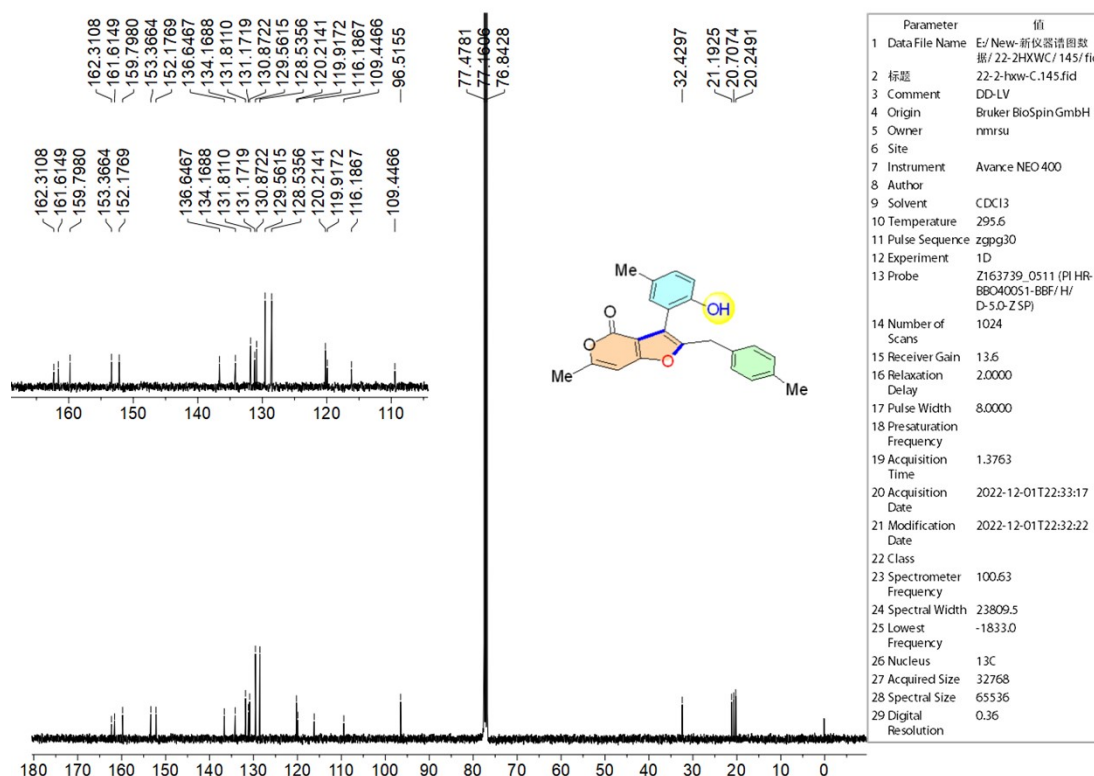
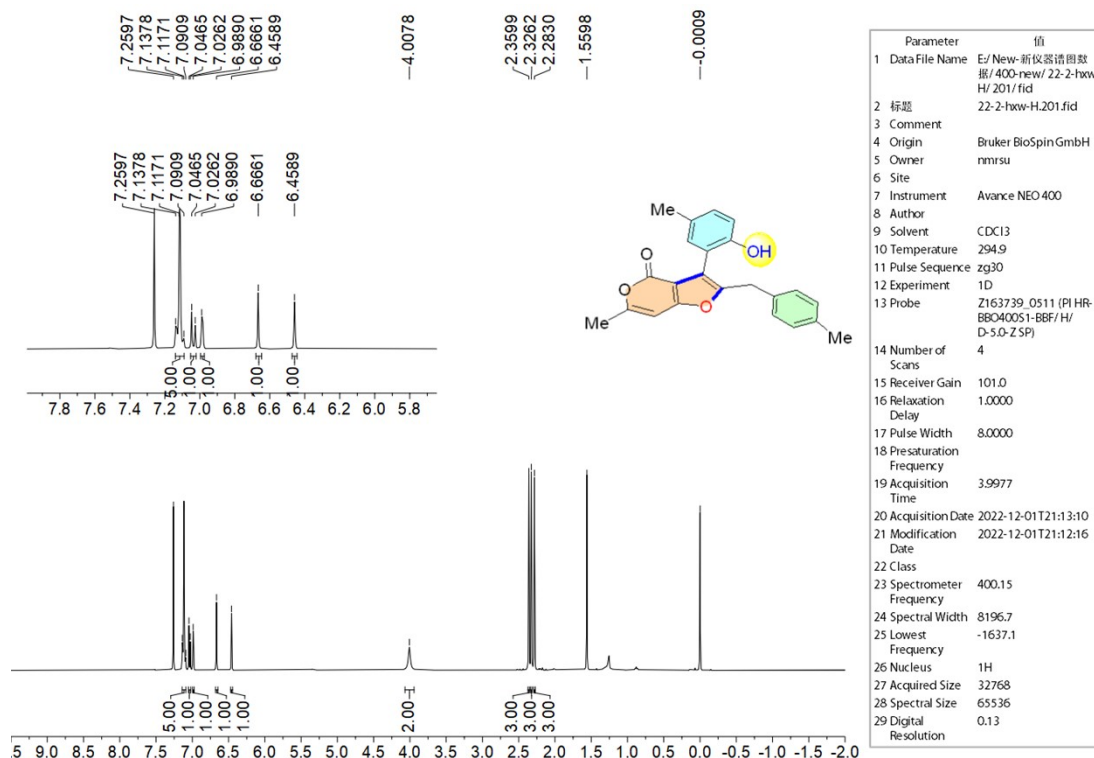
2-(4-Chlorobenzyl)-3-(2-hydroxy-5-methylphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3bc)



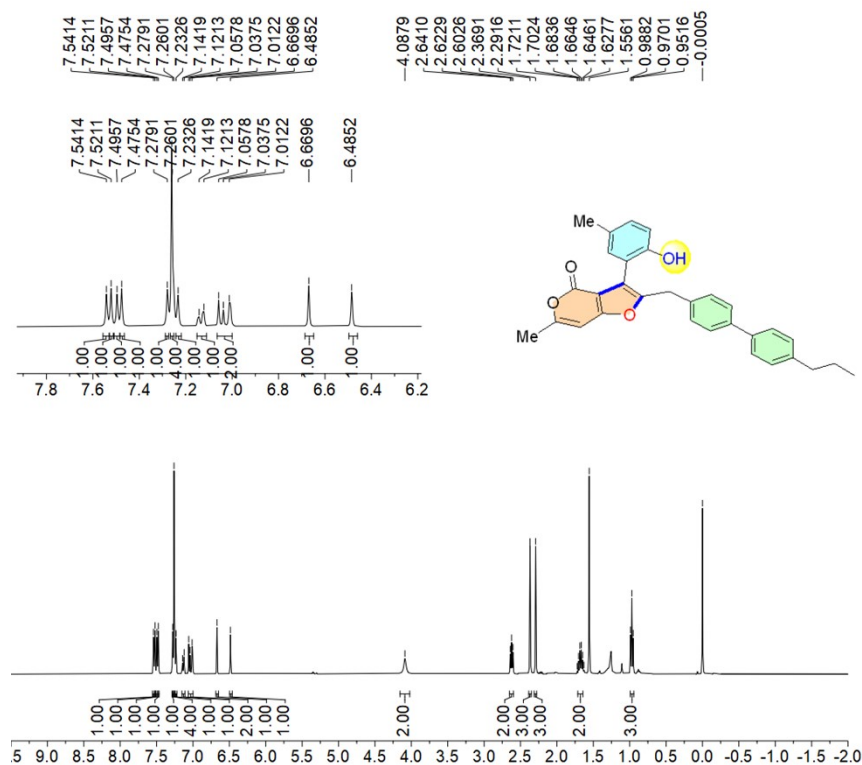
2-(4-Bromobenzyl)-3-(2-hydroxy-5-methylphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3bd)



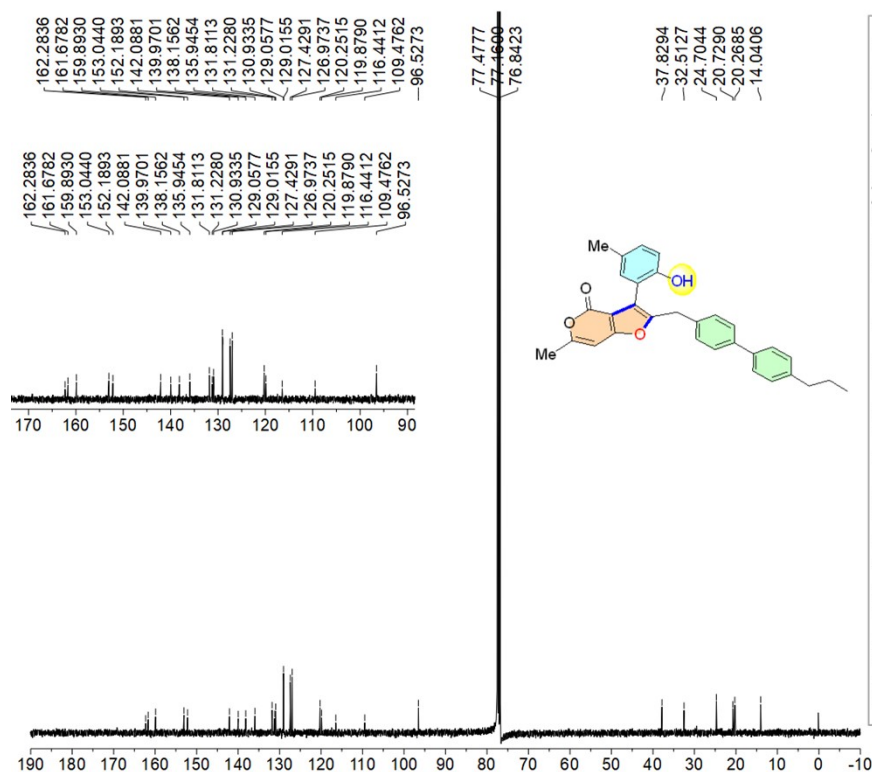
**3-(2-Hydroxy-5-methylphenyl)-6-methyl-2-(4-methylbenzyl)-4H-furo[3,2-c]pyran-4-one
(product 3bl)**



3-(2-Hydroxy-5-methylphenyl)-6-methyl-2-((4'-propyl-[1,1'-biphenyl]-4-yl)methyl)-4H-furo[3,2-c]pyran-4-one (3bg)

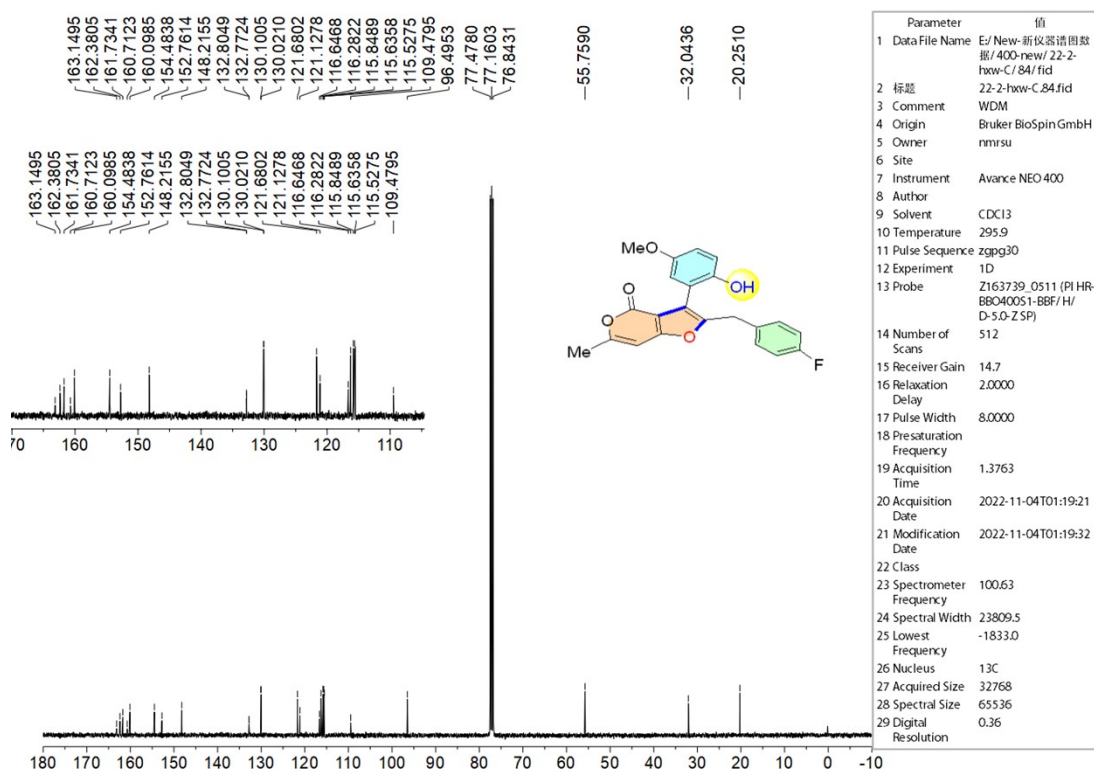
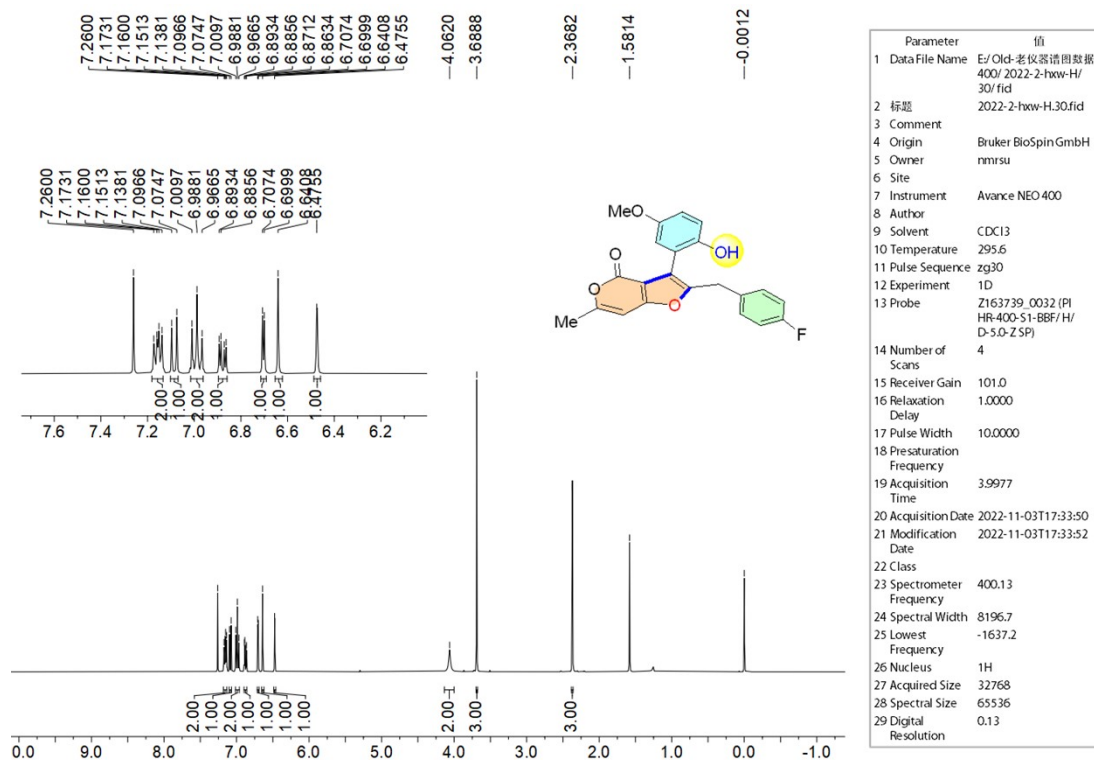


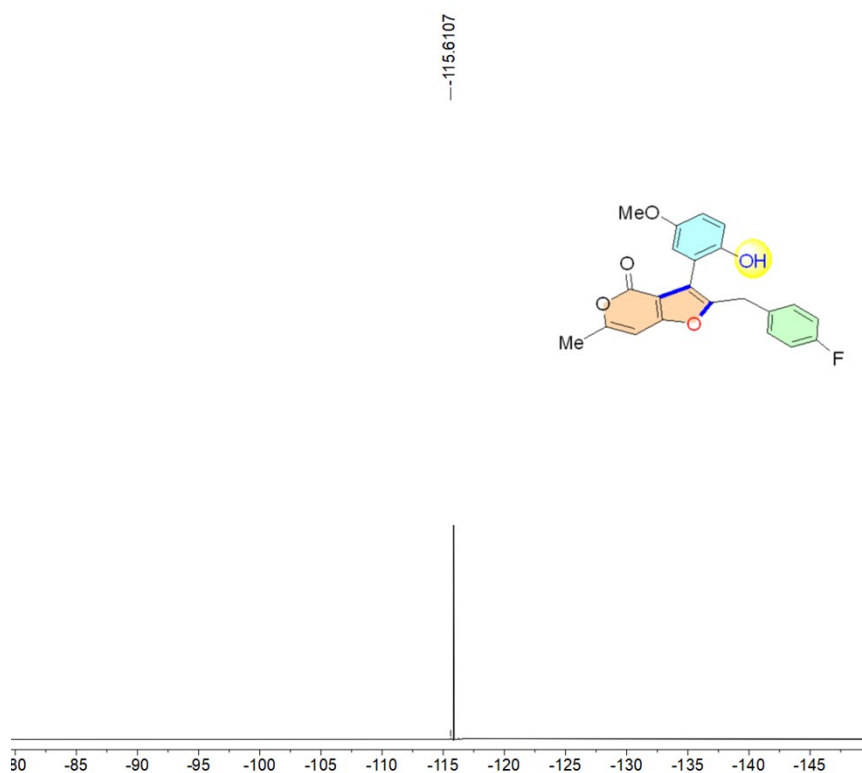
Parameter	值
1 Data File Name	E:/New-前仪器谱图数据/2024-new/22-2-hxw-H/204/fid
2 标题	22-2-hxw-H.204.fid
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI 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	2022-12-01T21:28:23
21 Modification Date	2022-12-01T21:27:28
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



Parameter	值
1 Data File Name	E:/New-前仪器谱图数据/22-2-hxw-C/148/fid
2 标题	22-2-hxw-C.148.fid
3 Comment	DD-lan
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.6
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	1600
15 Receiver Gain	16.8
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-12-02T08:14:26
21 Modification Date	2022-12-02T08:13:32
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

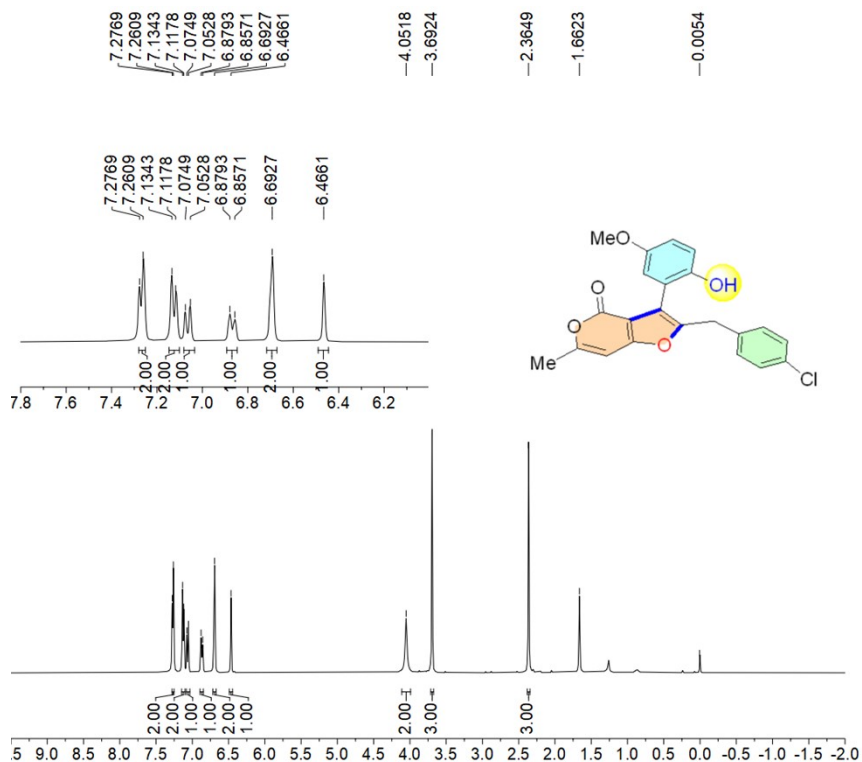
**2-(4-Fluorobenzyl)-3-(2-hydroxy-5-methoxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one
(3cb)**



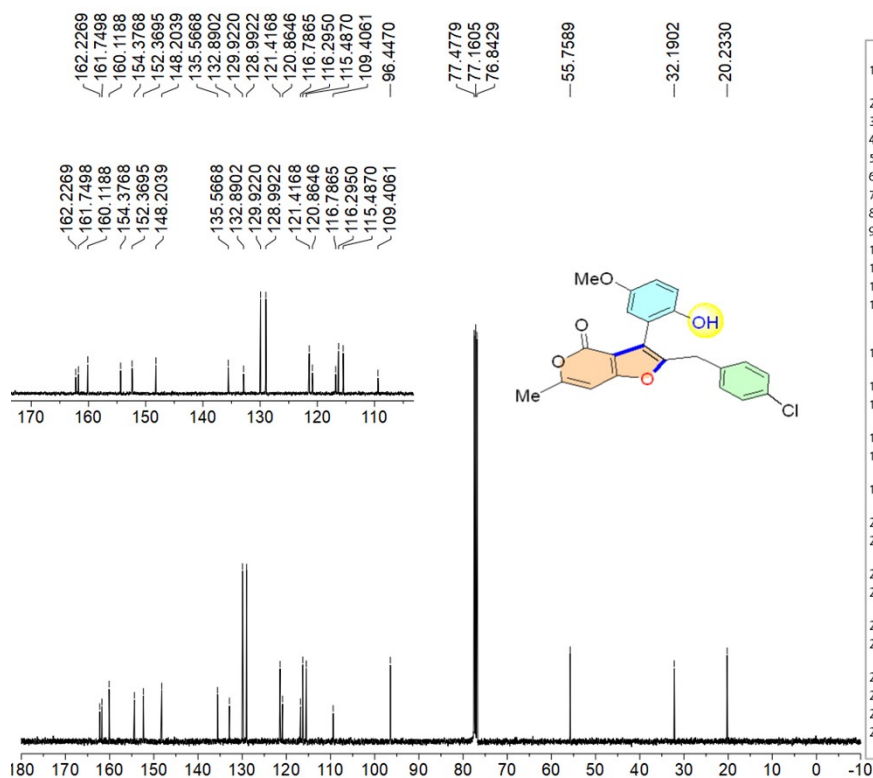


Parameter	值
1 Data File Name	E:/Old-老仪器谱图数据/400/2022-2-hww-F/32/fid
2 标题	2022-2-hww-F.32.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.7
11 Pulse Sequence	zgpg
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	18.0000
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2022-11-03T17:36:39
21 Modification Date	2022-11-03T17:36:42
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
29 Digital Resolution	0.69

2-(4-Chlorobenzyl)-3-(2-hydroxy-5-methoxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one
(3cc)

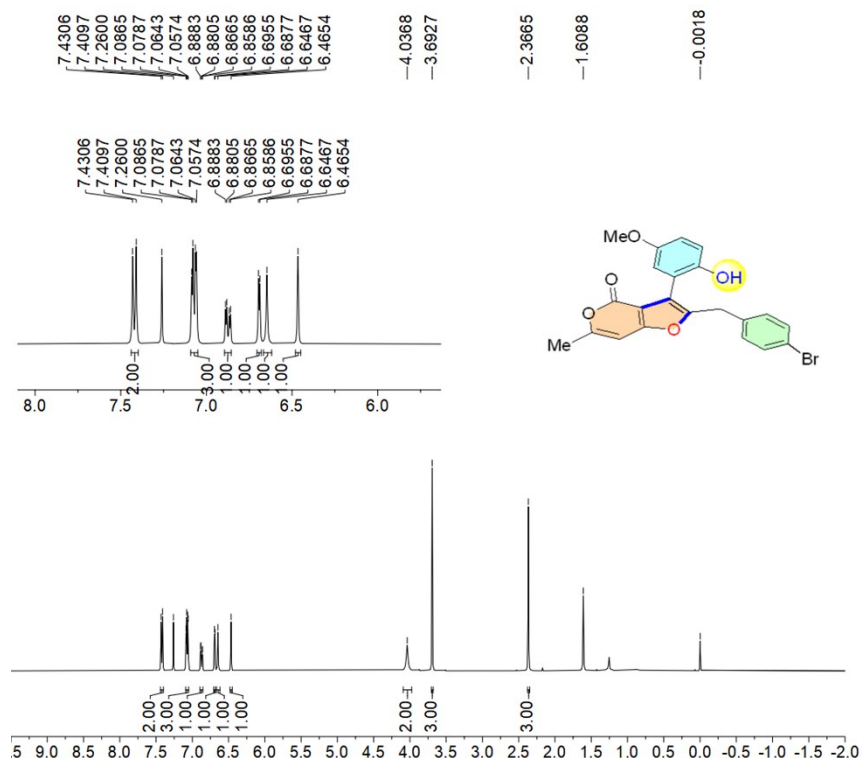


Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 400-new/ 22-2-hxw-H/ 178/ fid
2 标题	22-2-hxw-H.178.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI 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	2022-11-18T21:01:12
21 Modification Date	2022-11-18T21:01:30
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

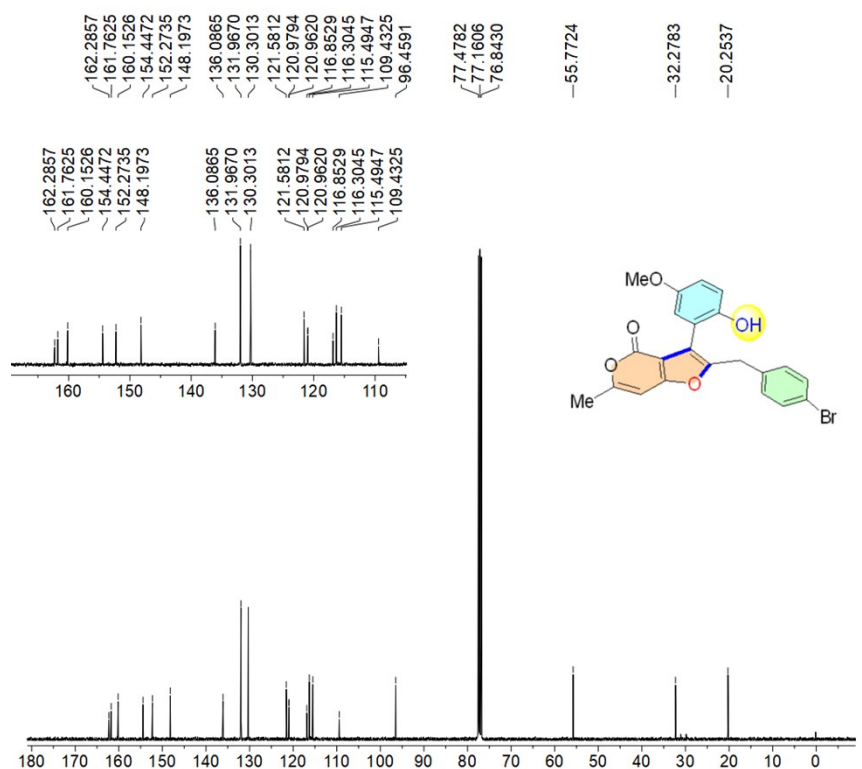


Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 22-2-HXWC/ 129/ fid
2 标题	22-2-hxw-C.129.fid
3 Comment	DD-BAL
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	256
15 Receiver Gain	11.5
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-11-18T21:51:41
21 Modification Date	2022-11-18T21:52:00
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

2-(4-Bromobenzyl)-3-(2-hydroxy-5-methoxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one
(3cd)

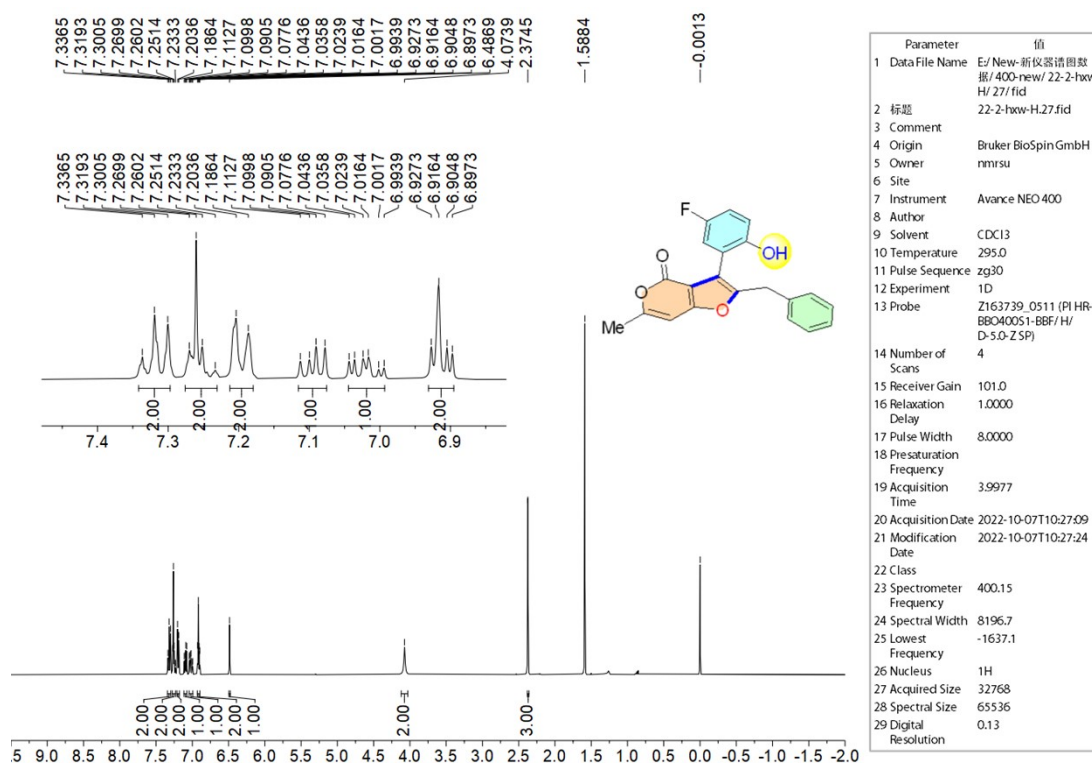


Parameter	值
1 Data File Name	E:/New-新仪器谱图数据/400-new/22-2-hxw-H/175/fid
2 标题	22-2-hxw-H.175.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z 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	2022-11-17T20:57:49
21 Modification Date	2022-11-17T20:58:06
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

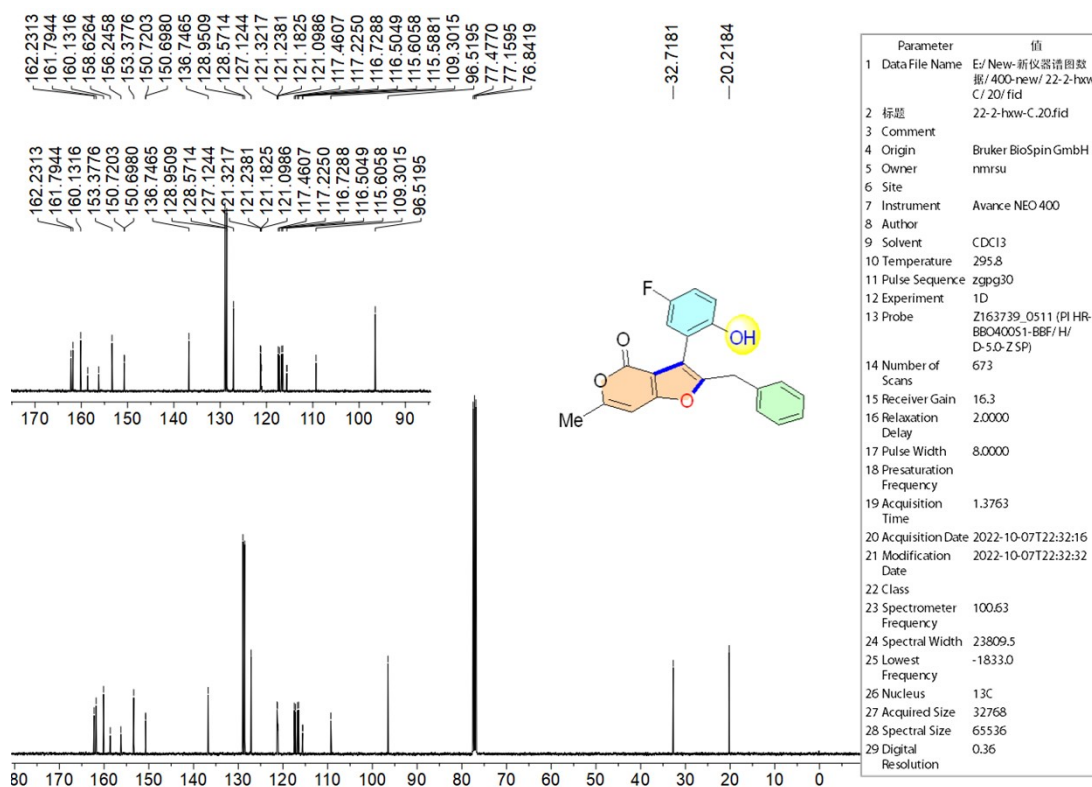


Parameter	值
1 Data File Name	E:/New-新仪器谱图数据/22-2-HXWC/127/fid
2 标题	22-2-hxw-C.127.fid
3 Comment	DD-LV
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	14.8
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-11-18T05:37:52
21 Modification Date	2022-11-18T05:38:10
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

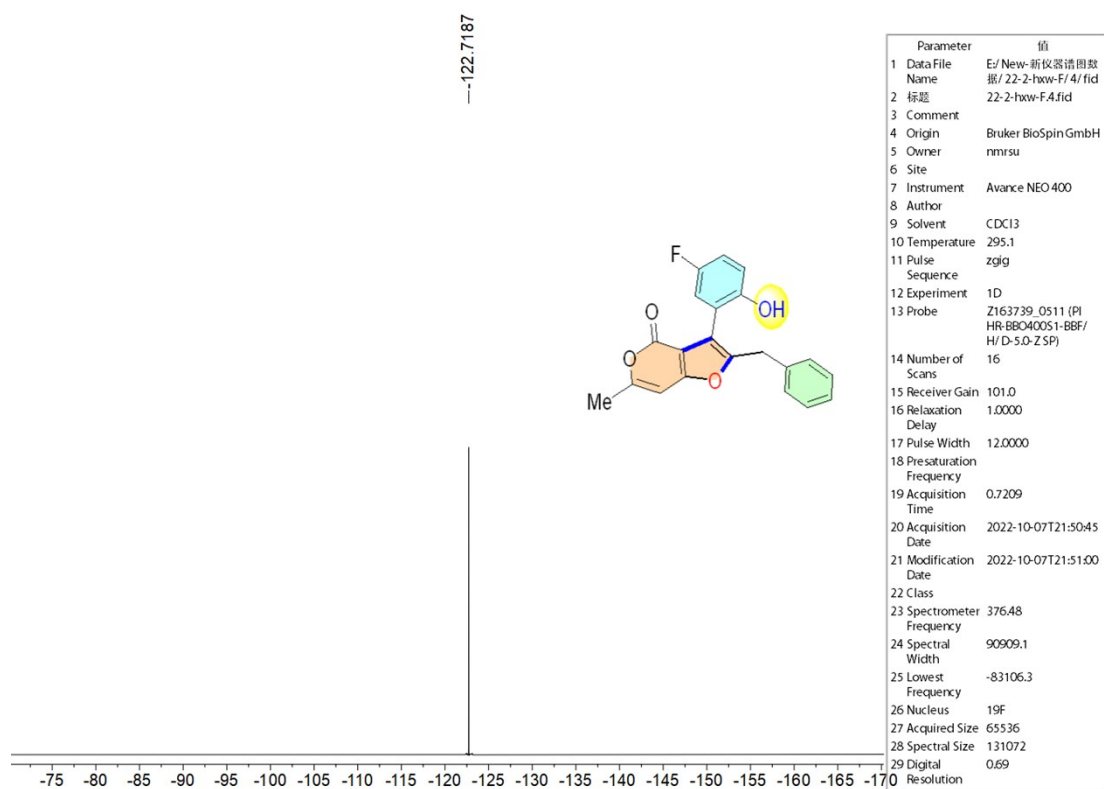
2-Benzyl-3-(5-fluoro-2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (product 3da)



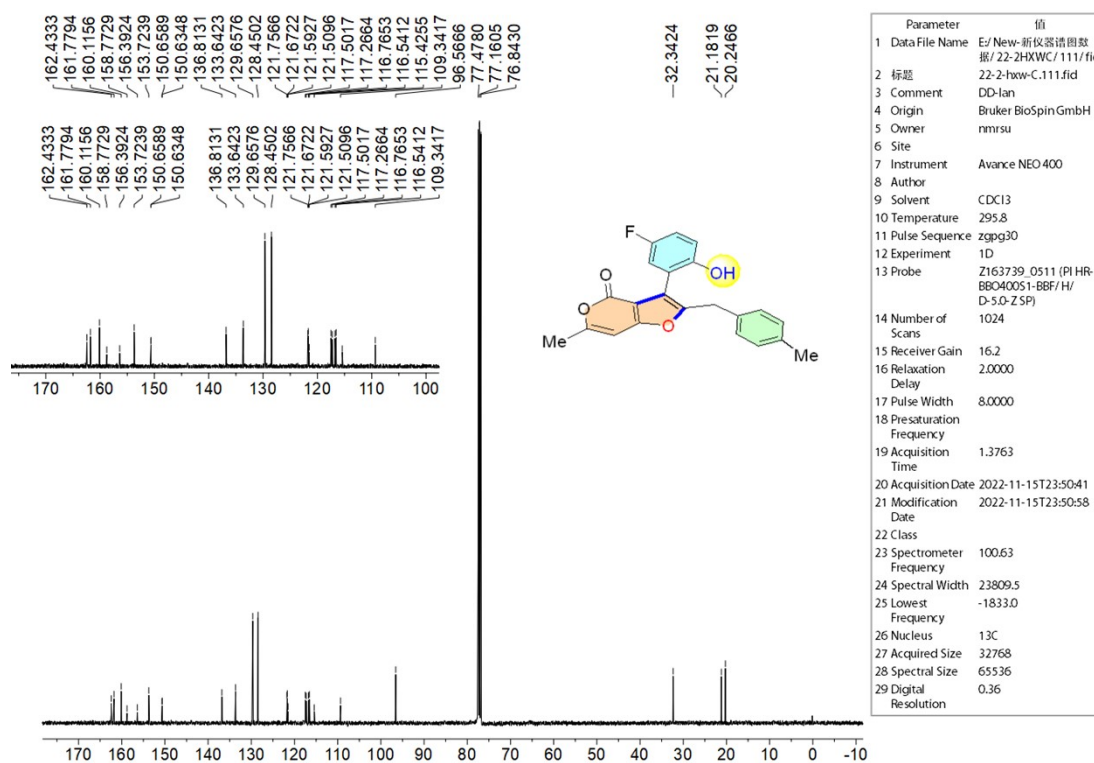
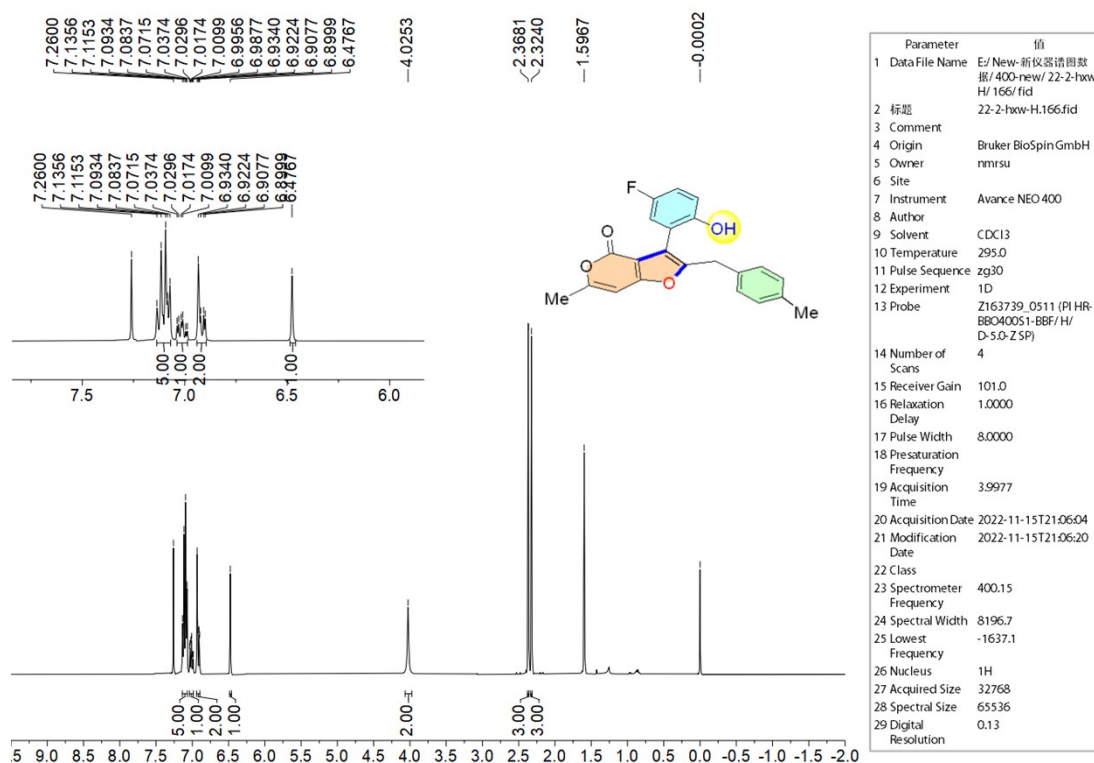
Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 400-new/ 22-2-hxw-H/ 277.fid
2 标题	22-2-hxw-H.27.fid
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI 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	2022-10-07T10:27:09
21 Modification Date	2022-10-07T10:27:24
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

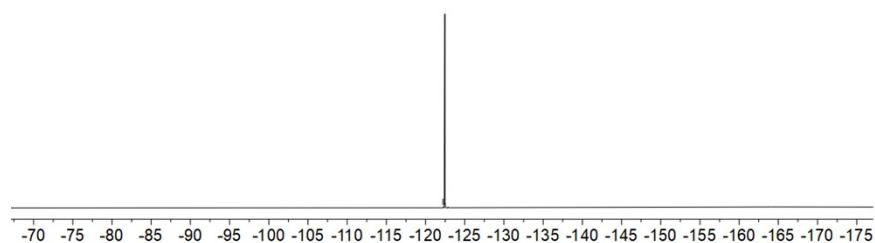


Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 400-new/ 22-2-hxw-C/ 201.fid
2 标题	22-2-hxw-C.201.fid
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	673
15 Receiver Gain	16.3
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-10-07T22:32:16
21 Modification Date	2022-10-07T22:32:32
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36



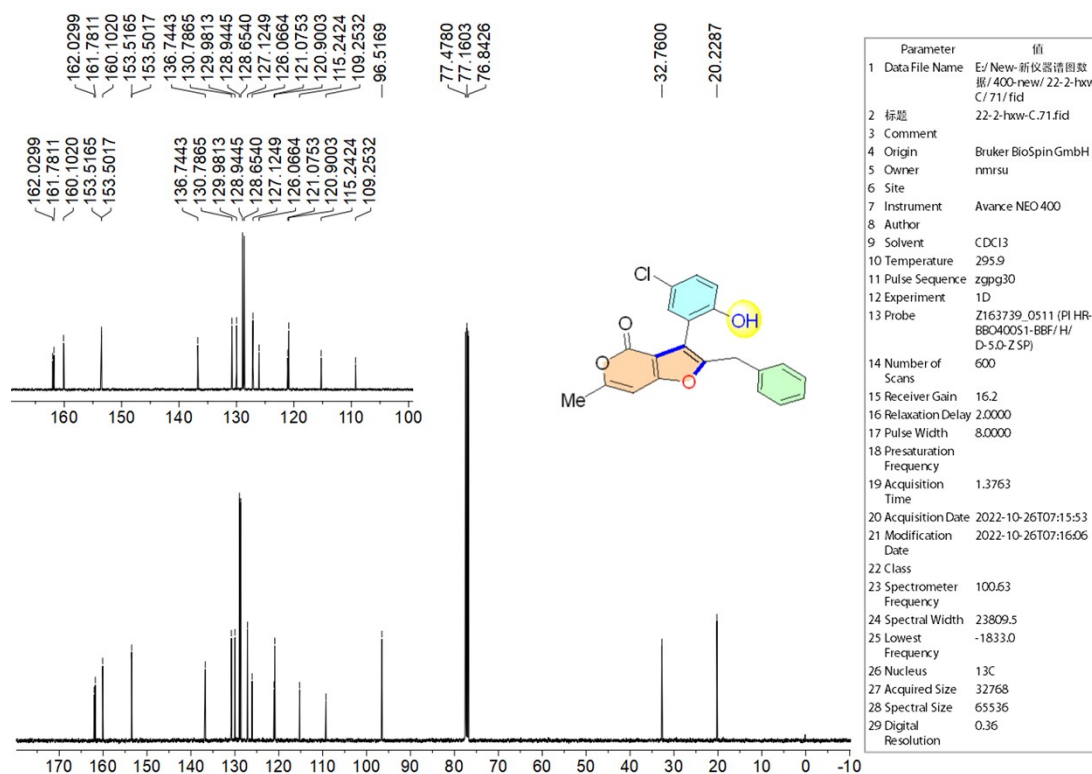
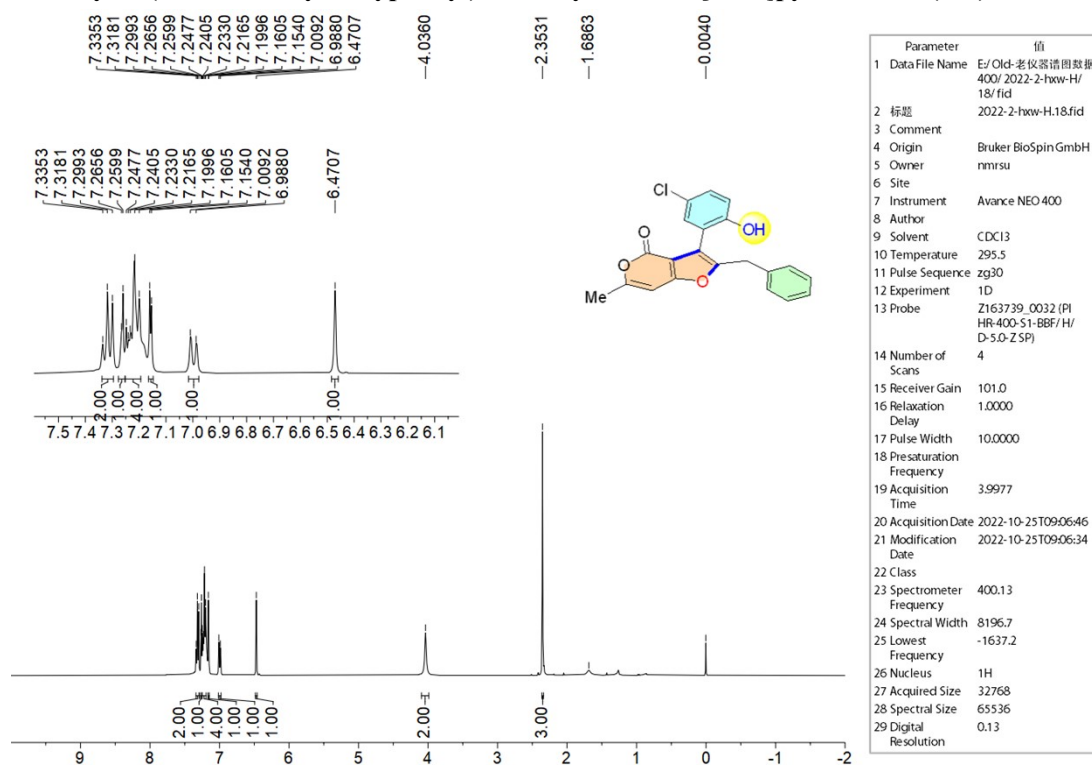
3-(5-Fluoro-2-hydroxyphenyl)-6-methyl-2-(4-methylbenzyl)-4H-furo[3,2-c]pyran-4-one (3dl)



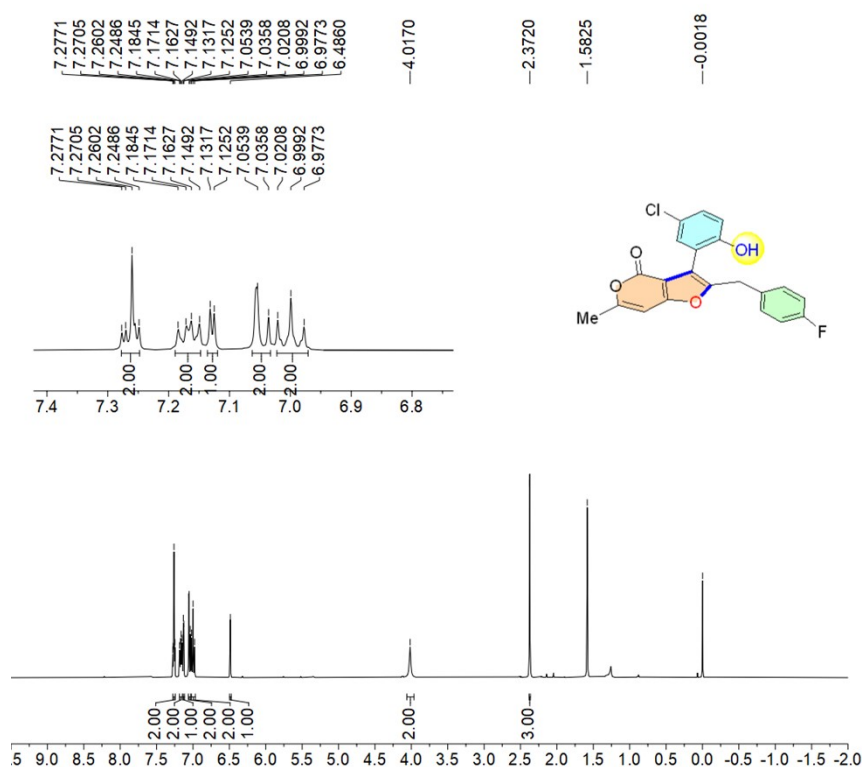


Parameter	值
1 Data File Name	E:/New-前仪器谱图数据/22-2-hw-F/18/fid
2 标题	22-2-hw-F-18.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.3
11 Pulse Sequence	zgig
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR- BB040051-BBF/ S/H D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.00000
17 Pulse Width	12.00000
18 Preacquisition Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2022-11-15T22:49:00
21 Modification Date	2022-11-15T22:49:16
22 Class	
23 Spectrometer Frequency	376.48
24 Spectral Width	90909.1
25 Lowest Frequency	-83106.3
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	131072
29 Digital Resolution	0.69

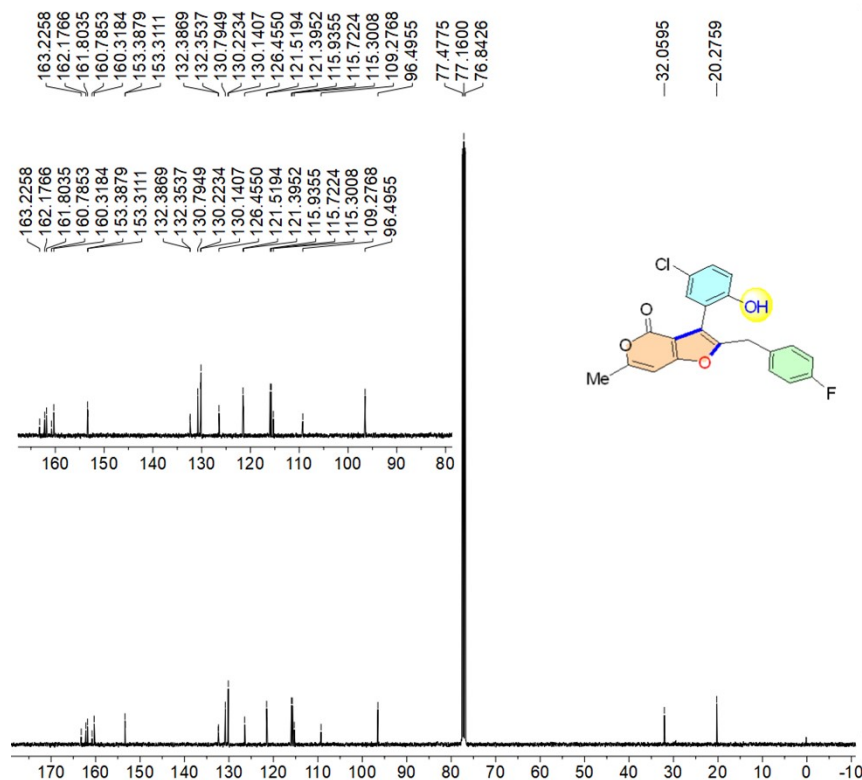
2-Benzyl-3-(5-chloro-2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3ea)



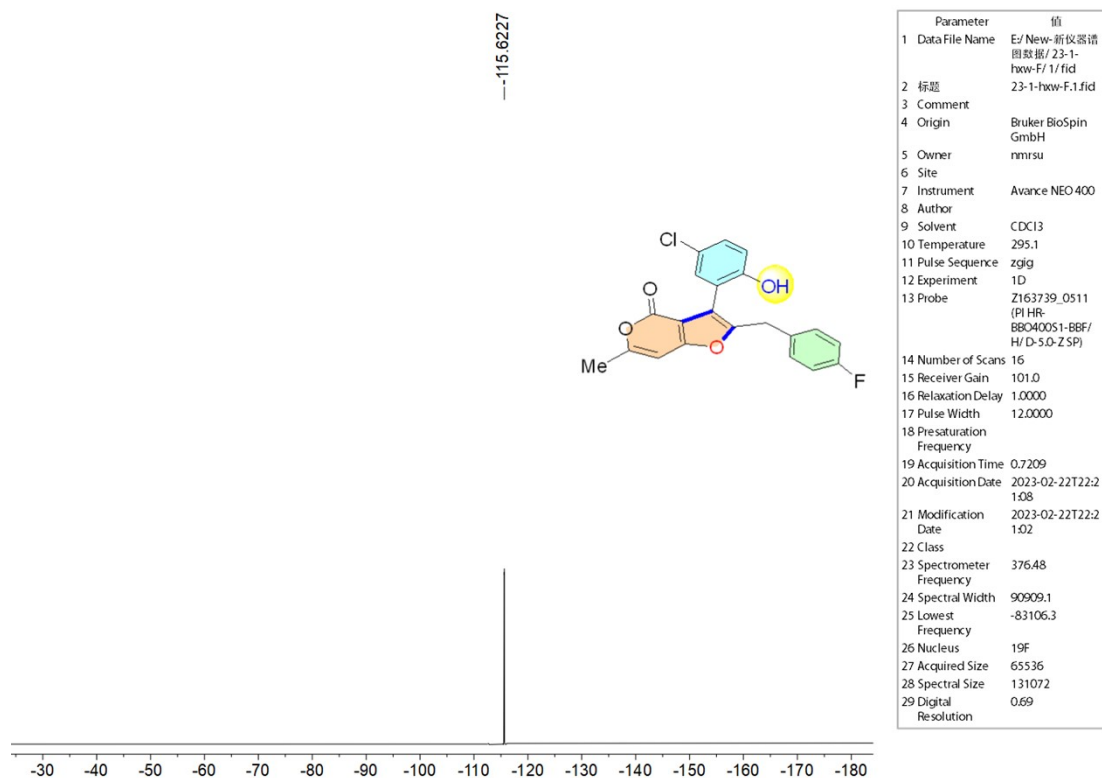
3-(5-chloro-2-hydroxyphenyl)-2-(4-fluorobenzyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3eb)



Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 23-1-hww-H/ 3/ fid
2 标题	23-1-hww-H.3.fid
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.1
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	2023-02-18T11:25:10
21 Modification Date	2023-02-18T11:25:00
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 23-1-hww-C/ 7/ fid
2 标题	23-1-hww-C.7.fid
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.7
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	1024
15 Receiver Gain	11.5
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-02-22T23:23:10
21 Modification Date	2023-02-22T23:23:10
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

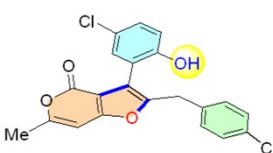


Chemical Structure of Compound 10:

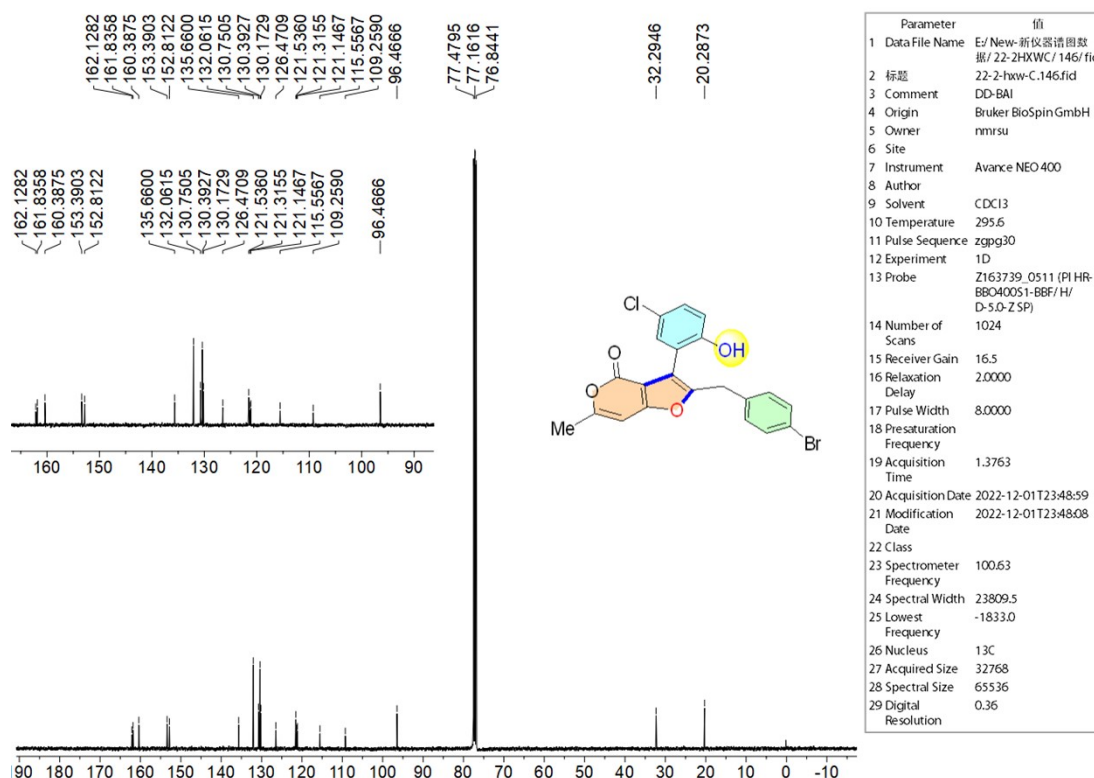
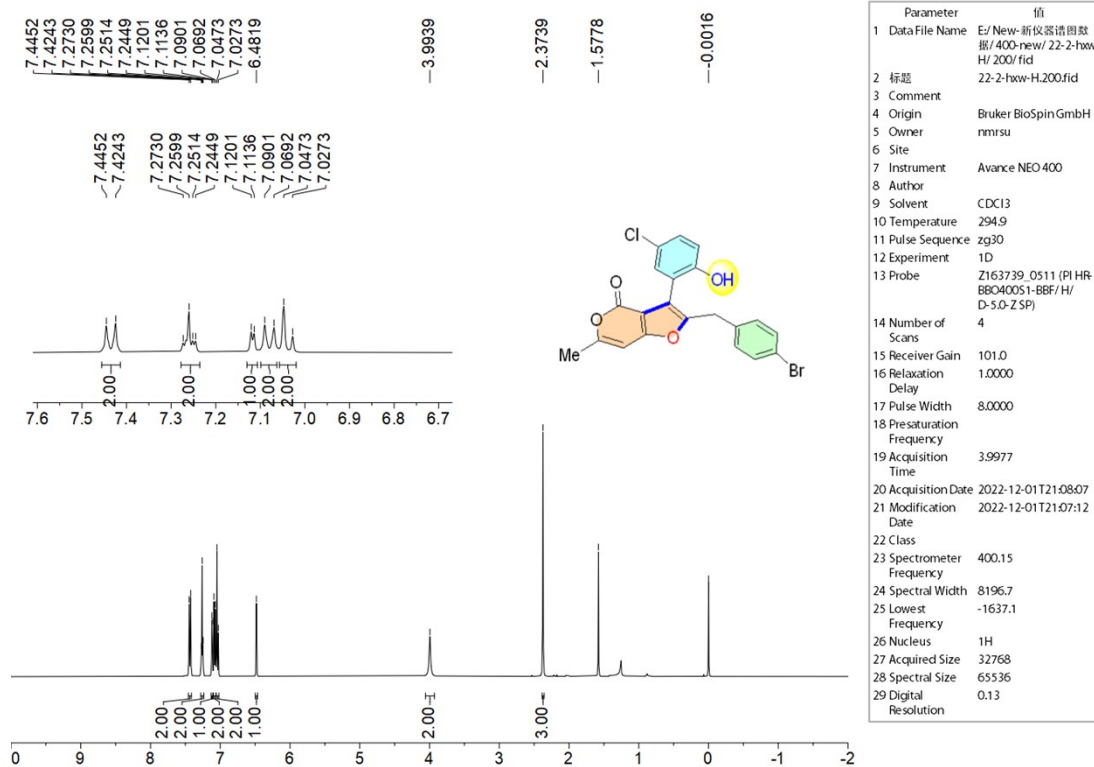
Cc1cc2c(c3cc(OC)c(Cc4ccc(Cl)cc4)c3c2=O)c1-c1ccc(Cl)cc1

¹H NMR Spectrum (CDCl₃):

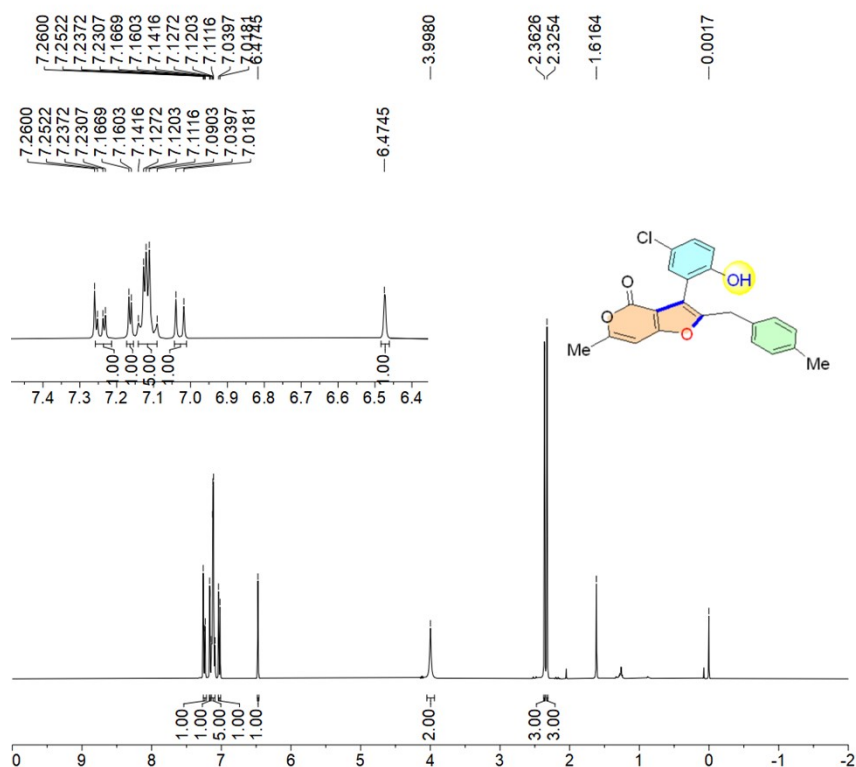
Chemical Shift (ppm)	Integration
7.2818, 7.2602, 7.2296, 7.2230, 7.2080, 7.2014, 7.1367, 7.1170, 6.9839, 6.9620, 6.4666	3.00, 2.00, 2.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00, 0.00
3.9936	2.00
2.3548	3.00
-0.0007	0.00



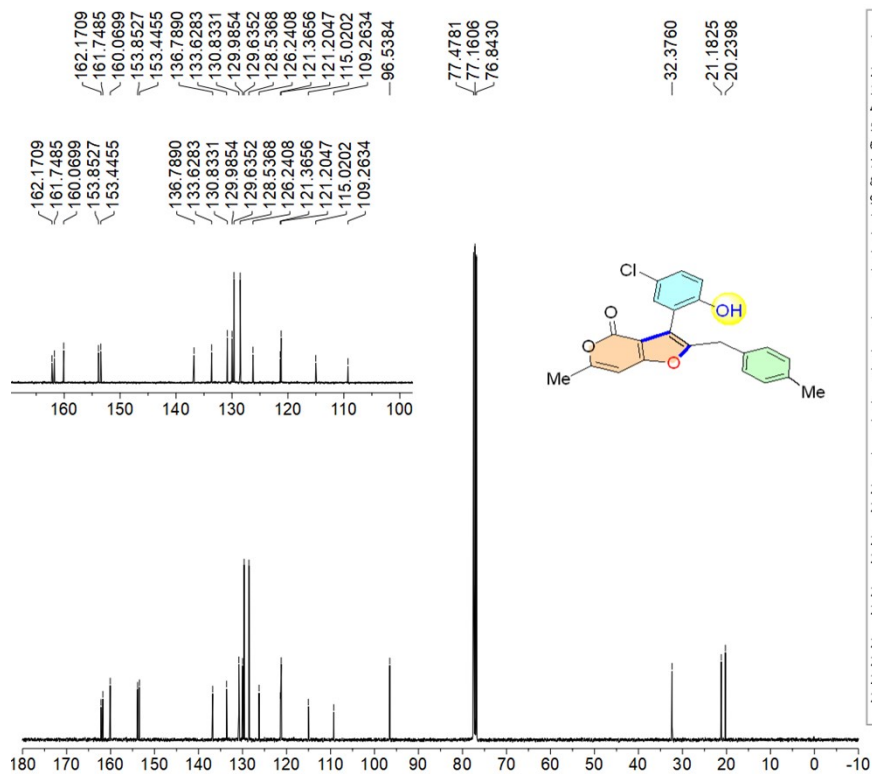
2-(4-Bromobenzyl)-3-(5-chloro-2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one
(product 3ed)



3-(5-Chloro-2-hydroxyphenyl)-6-methyl-2-(4-methylbenzyl)-4H-furo[3,2-c]pyran-4-one (3el)

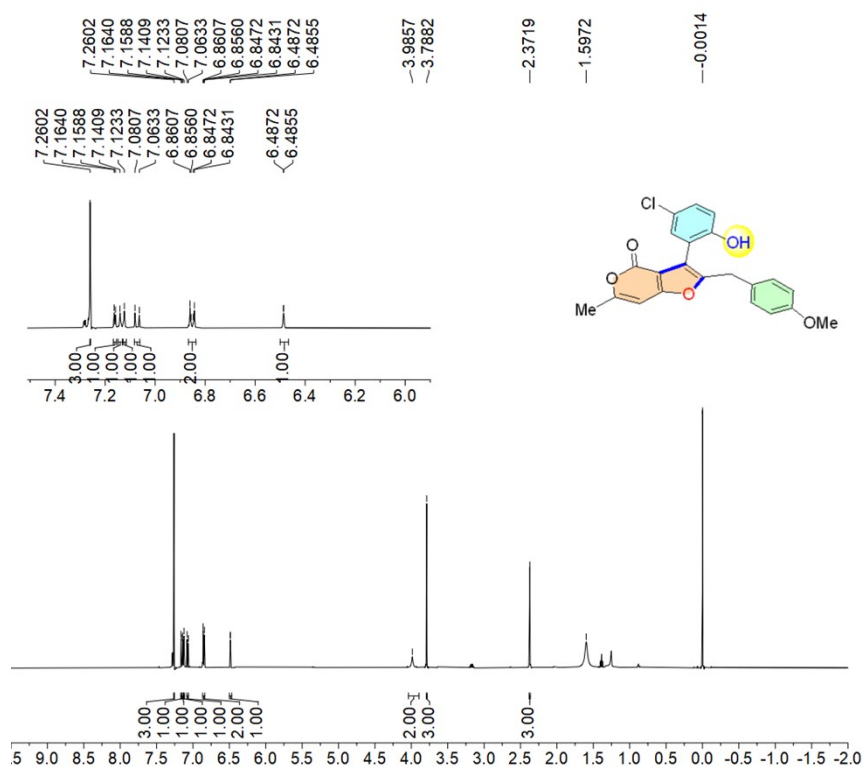


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1 Data File Name	E:/Old-新仪器谱图数据/2023-1-hxw-H/1/fid
2 标题	2023-1-hxw-H.1.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	293.9
11 Pulse Sequence	zg30
12 Experiment	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	2023-02-16T10:29:32
21 Modification Date	2023-02-16T10:29:18
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

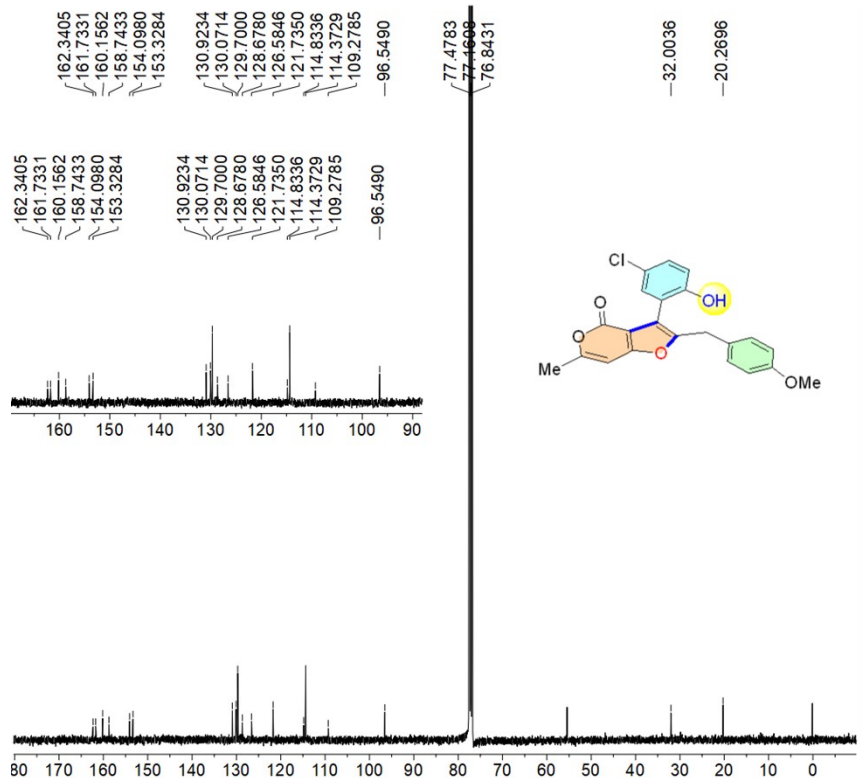


Parameter	值
1 Data File Name	E:/New-新仪器谱图数据/23-1-hxw-C/6/fid
2 标题	23-1-hxw-C.6.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BB040051-BBF/H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	12.6
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-02-22T22:03:54
21 Modification Date	2023-02-22T22:03:48
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

**3-(5-Chloro-2-hydroxyphenyl)-2-(4-methoxybenzyl)-6-methyl-4H-furo[3,2-c]pyran-4-one
(3em)**

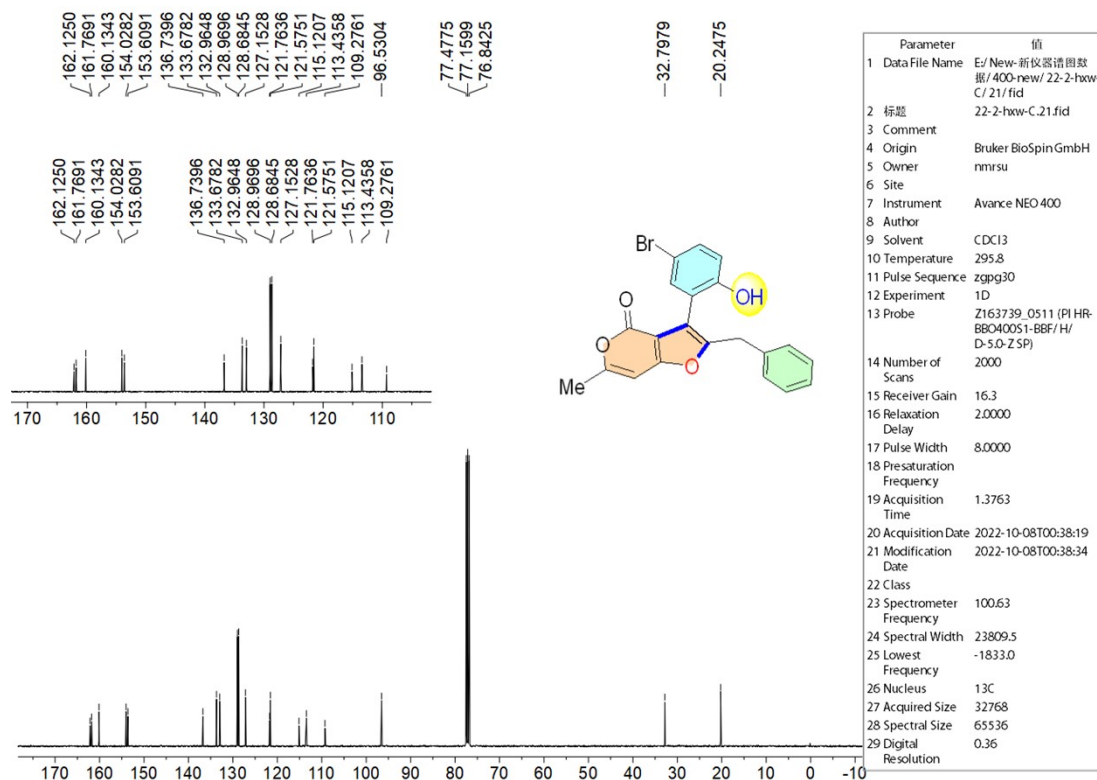
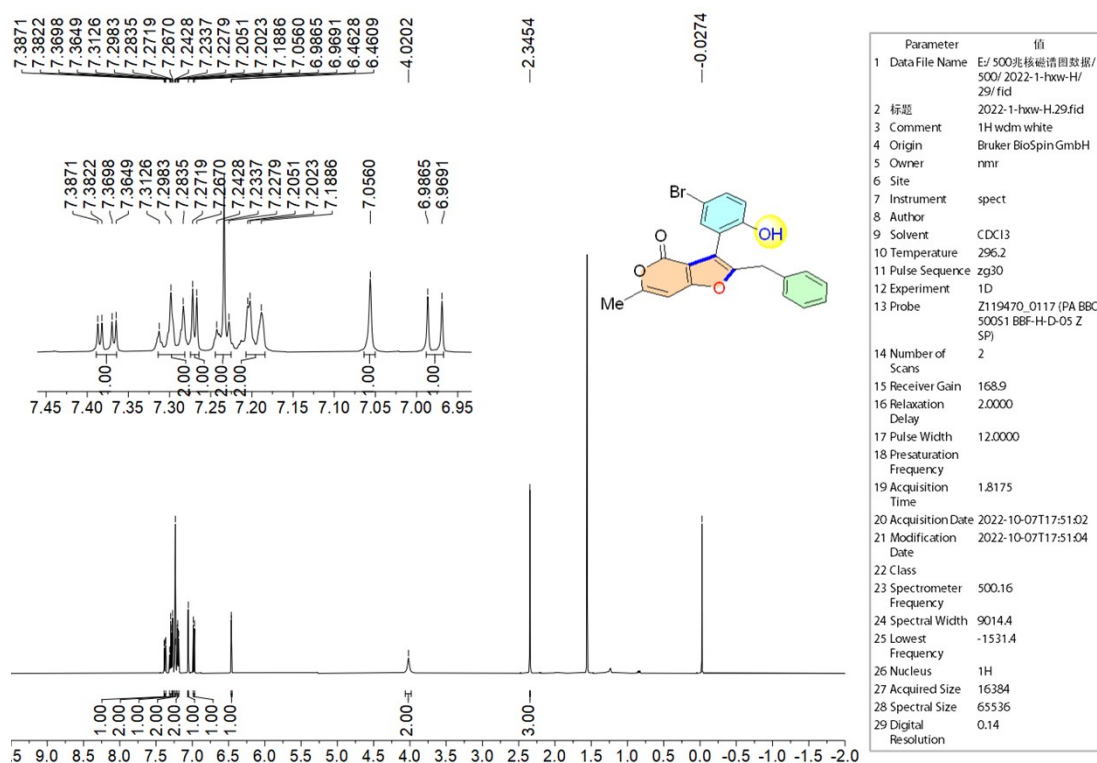


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1 Data File Name	E:/ 500兆核磁谱图数据/ 500/ 2022-1-hw-H-48/ f1d
2 标题	2022-1-hw-H-48.f1d
3 Comment	1H wdm cheng
4 Origin	Bruker BioSpin GmbH
5 Owner	nmr
6 Site	
7 Instrument	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	296.4
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z119470_0117 (PA BBO 500S1 BBF-H-D-05 Z SP)
14 Number of Scans	2
15 Receiver Gain	188.8
16 Relaxation Delay	2.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	1.8175
20 Acquisition Date	2022-11-24T21:17:47
21 Modification Date	2022-11-24T21:17:48
22 Class	
23 Spectrometer Frequency	500.16
24 Spectral Width	9014.4
25 Lowest Frequency	-1531.4
26 Nucleus	¹ H
27 Acquired Size	16384
28 Spectral Size	65536
29 Digital Resolution	0.14

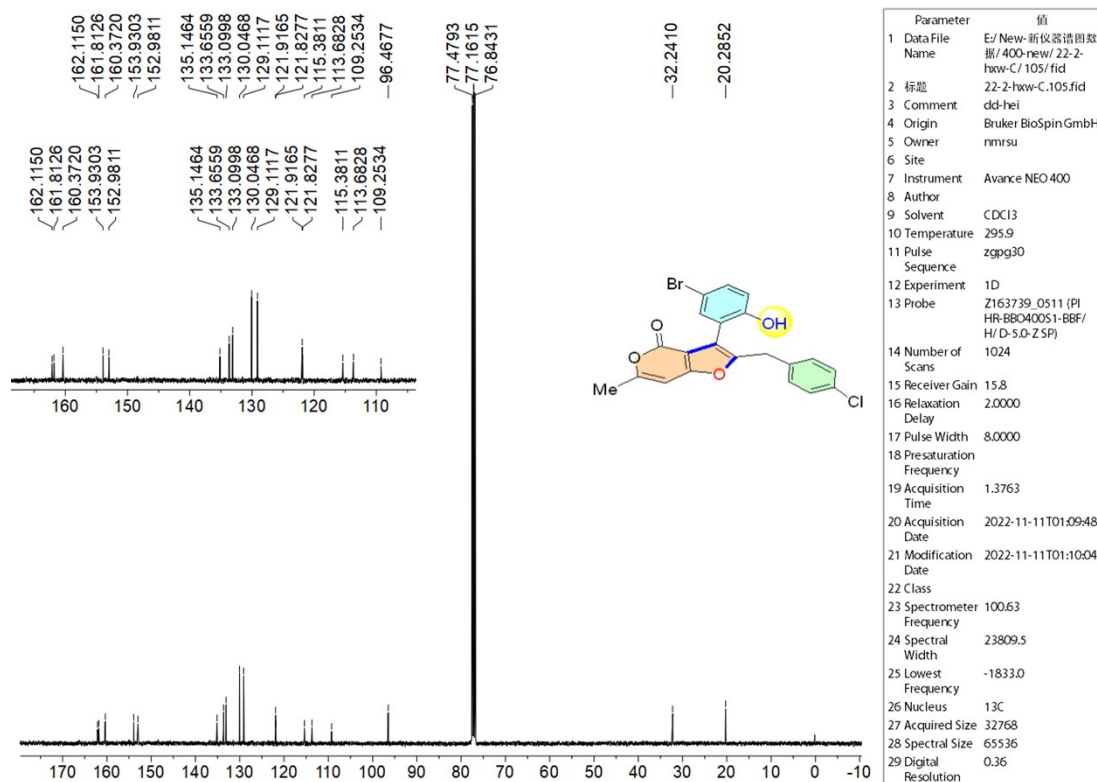
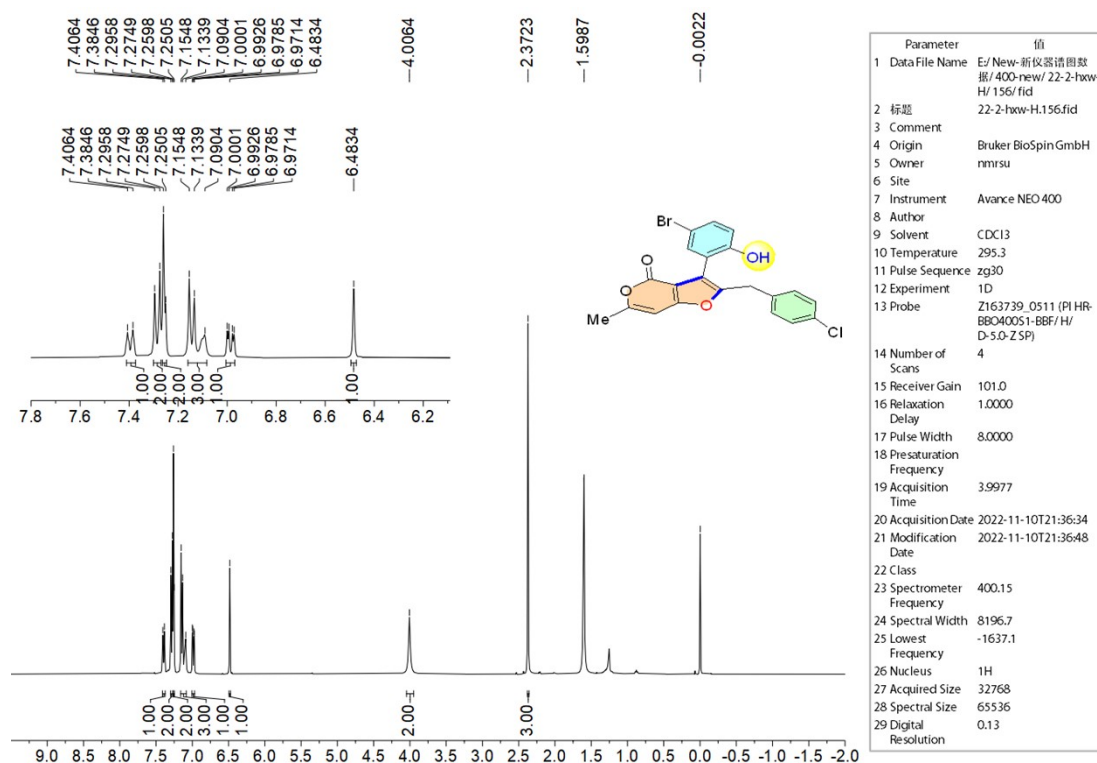


Parameter	值
1 Data File Name	E:/ New-新仪器谱图数据/ 22-2-HXWC/ 143/ f1d
2 标题	22-2-hw-C-143.f1d
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/ D-5.0-Z SP)
14 Number of Scans	3500
15 Receiver Gain	15.8
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-11-27T01:37:31
21 Modification Date	2022-11-27T01:37:34
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

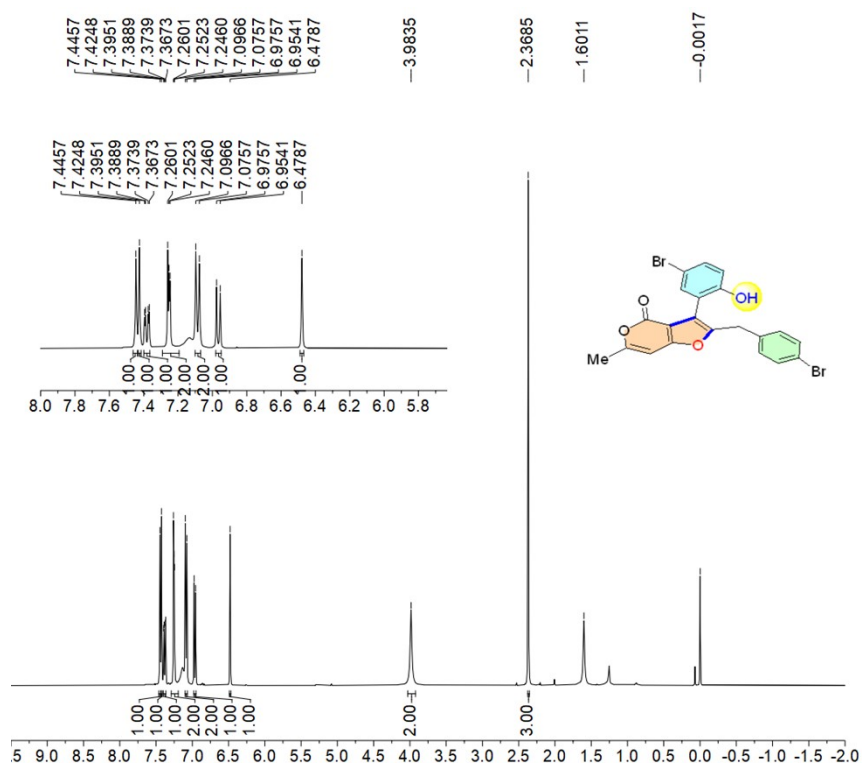
2-Benzyl-3-(5-bromo-2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3fa)



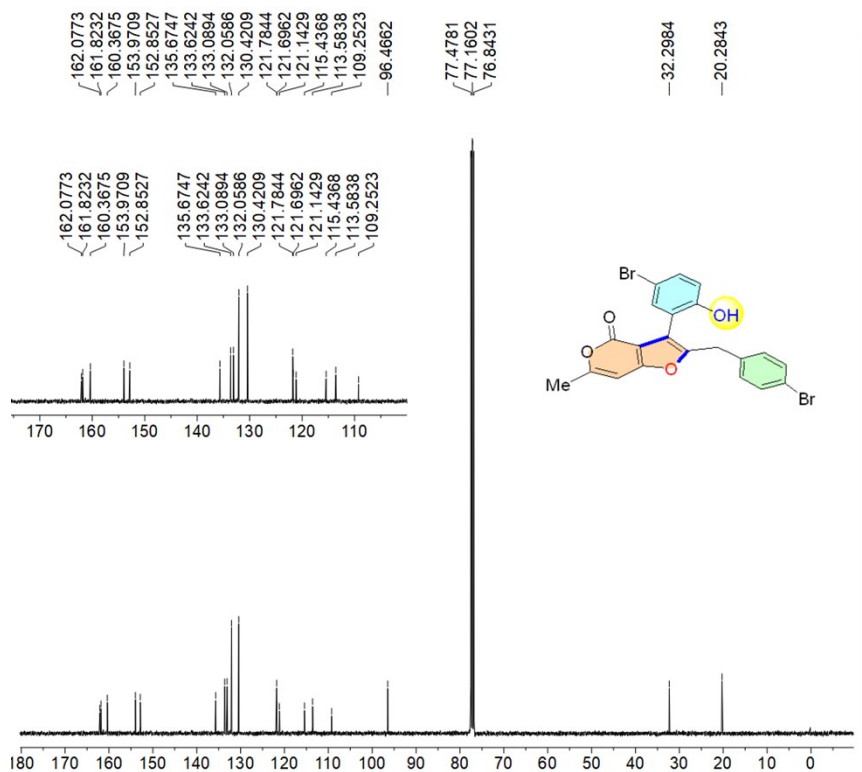
3-(5-Bromo-2-hydroxyphenyl)-2-(4-chlorobenzyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3fc)



3-(5-Bromo-2-hydroxyphenyl)-2-(4-bromobenzyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3fd)

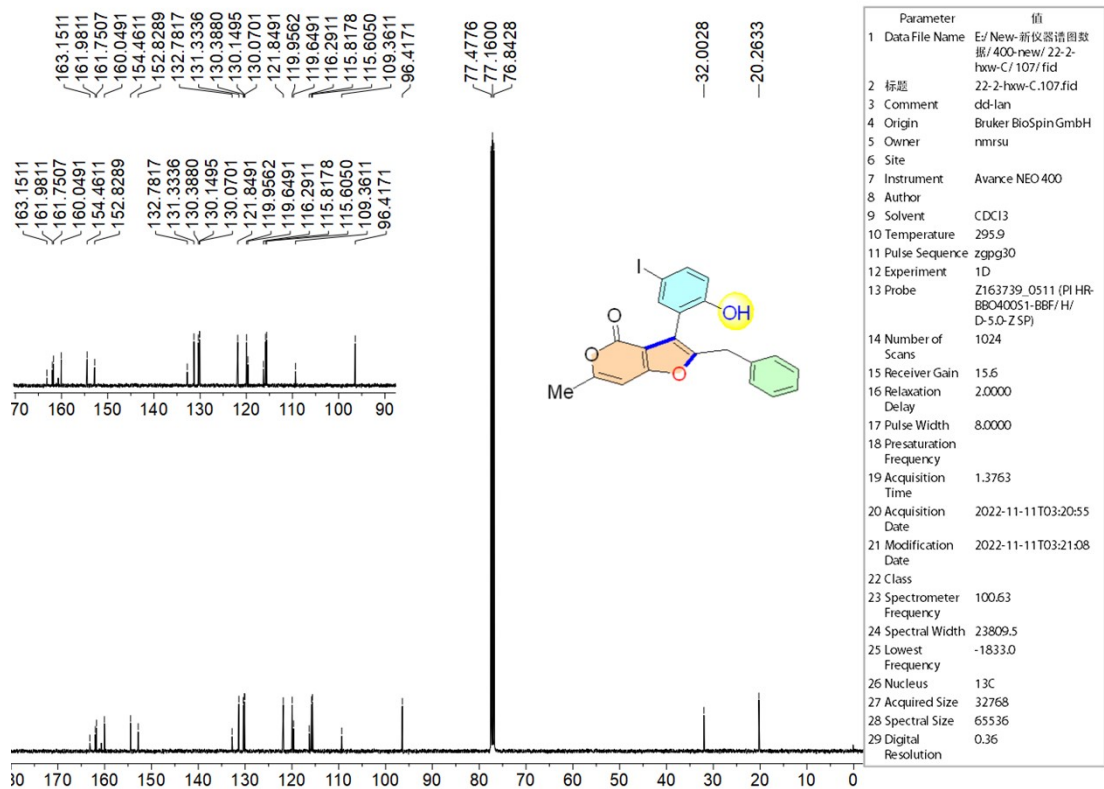


Parameter	值
1 Data File Name	E:/ New-前仪器谱图数据/ 400-new/ 22-2-hxw-H/ 162/ fid
2 标题	22-2-hxw-H.162.fid
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (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	2022-11-15T20:45:27
21 Modification Date	2022-11-15T20:45:42
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

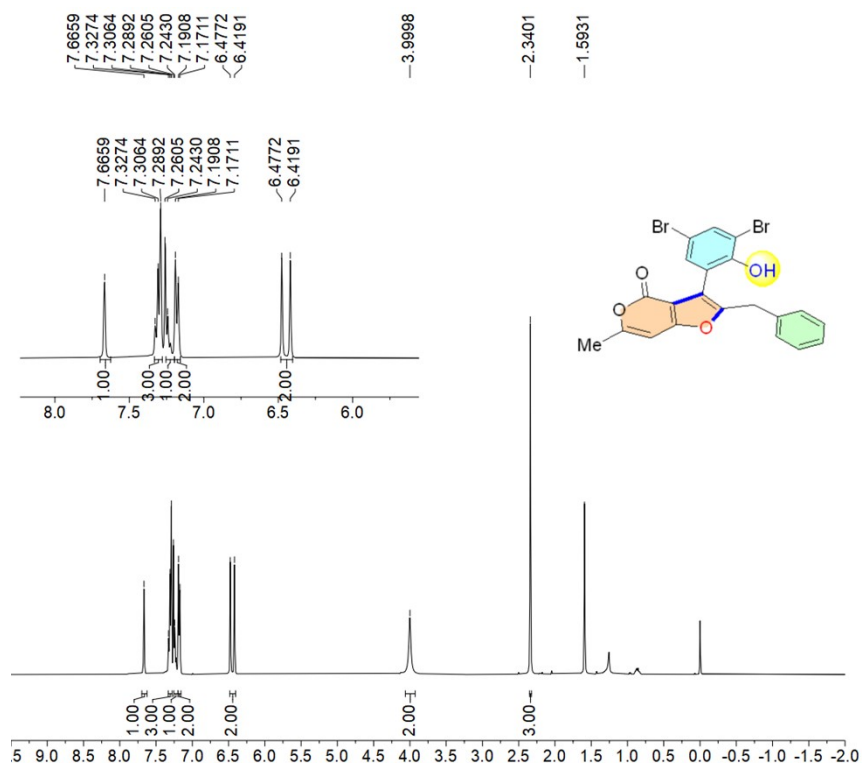


Parameter	值
1 Data File Name	E:/ New-前仪器谱图数据/ 22-2HXWC/ 114/ fid
2 标题	dd-bai
3 Comment	
4 Origin	Brucker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-11-16T03:02:29
21 Modification Date	2022-11-16T03:02:44
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

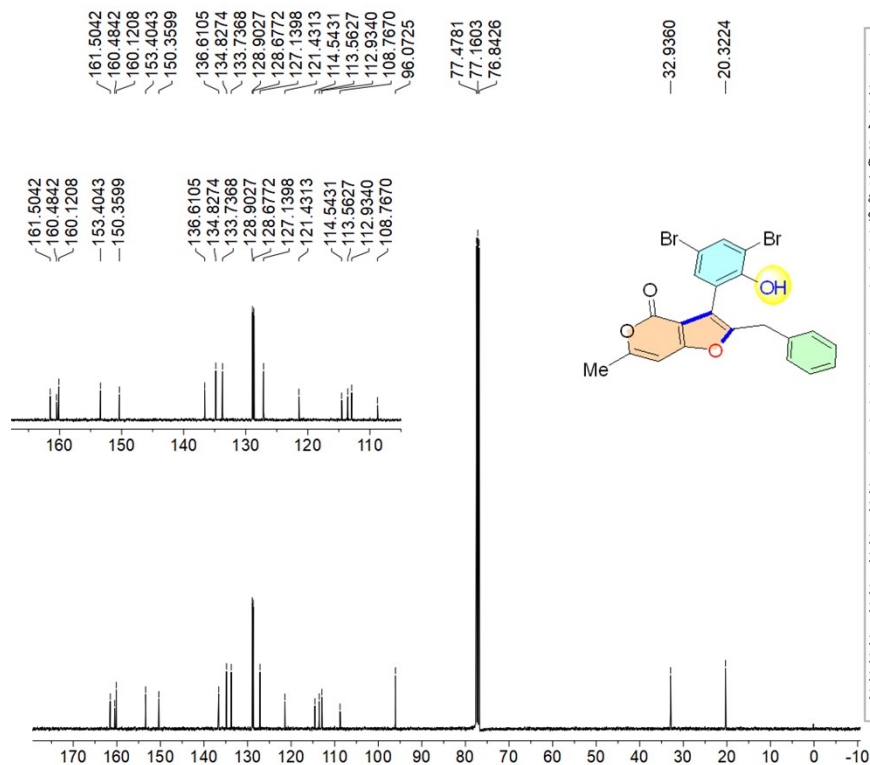
Figure 1 displays the ^1H NMR spectra of compound 22-2. The top spectrum shows the ^1H NMR in CDCl_3 , and the bottom spectrum shows the ^1H NMR in $\text{DMSO}-d_6$. The chemical structure of 22-2 is shown in the middle, featuring a benzofuran core with a 4-iodophenyl group, a 4-hydroxyphenyl group, and a 4-methylphenyl group.



2-Benzyl-3-(3,5-dibromo-2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3ha)

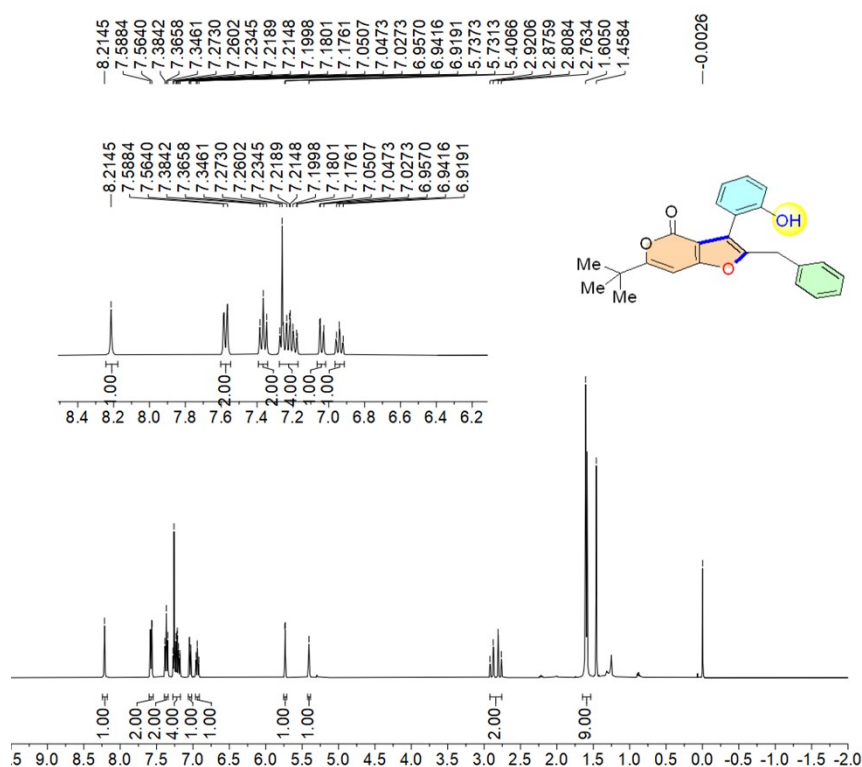


Parameter	值
1 Data File Name	E:/ New-前仪器谱图数据/ 400-new/ 22-2-hxw-H/ 184/ fid
2 标题	22-2-hxw-H.184.fid
3 Comment	
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI 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	2022-11-22T21:24:53
21 Modification Date	2022-11-22T21:25:14
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

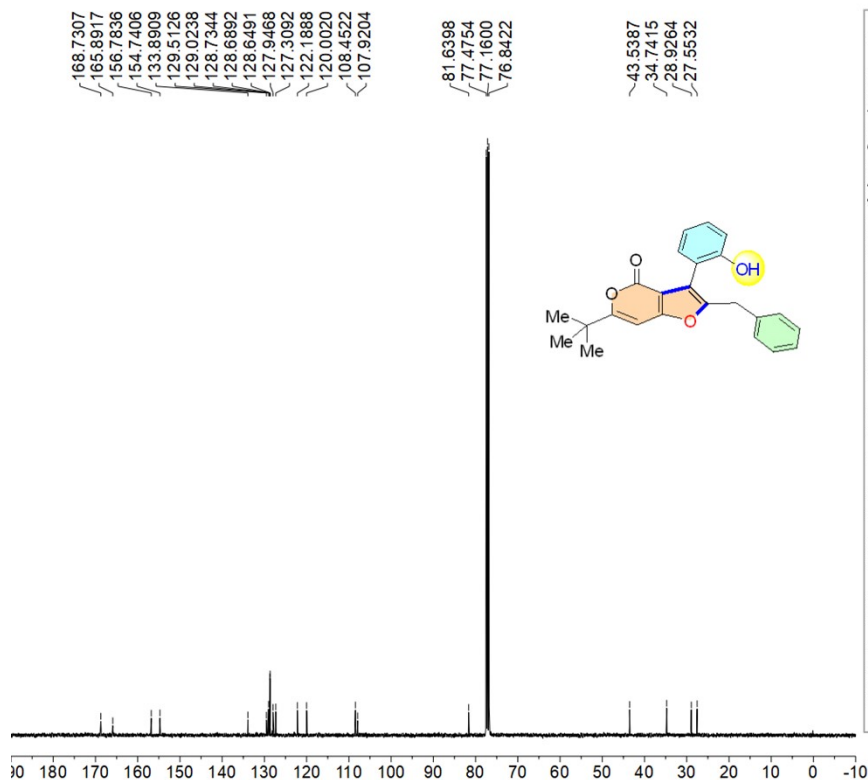


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2 标题	22-2-hxw-C.137.fid
3 Comment	DD-bai
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2022-11-25T23:49:06
21 Modification Date	2022-11-25T23:49:08
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

2-Benzyl-6-(*tert*-butyl)-3-(2-hydroxyphenyl)-4*H*-furo[3,2-*c*]pyran-4-one (3a**b**)



Parameter	值
1 Data File Name	E:/ 2023.8.8核磁数据/ New folder/ 152/ fid
2 标题	2023-1-hww-H.152.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	293.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-51-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	2023-07-20T08:02:21
21 Modification Date	2023-07-20T08:02:06
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



Parameter	值
1 Data File Name	E:/ 2023.8.8核磁数据/ New folder/ 43/ fid
2 标题	2023-1-hww-C.43.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-51-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	12.1
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-07-21T03:39:11
21 Modification Date	2023-07-21T03:38:52
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.5
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

¹H NMR (400 MHz, CDCl₃)

Chemical shift (ppm): 7.8, 7.6, 7.4, 7.2, 7.0, 6.8, 6.6, 6.4, 6.2

Integration values: 1.00, 1.00, 3.00, 4.00, 1.00, 1.00, 1.00, 2.00, 3.00

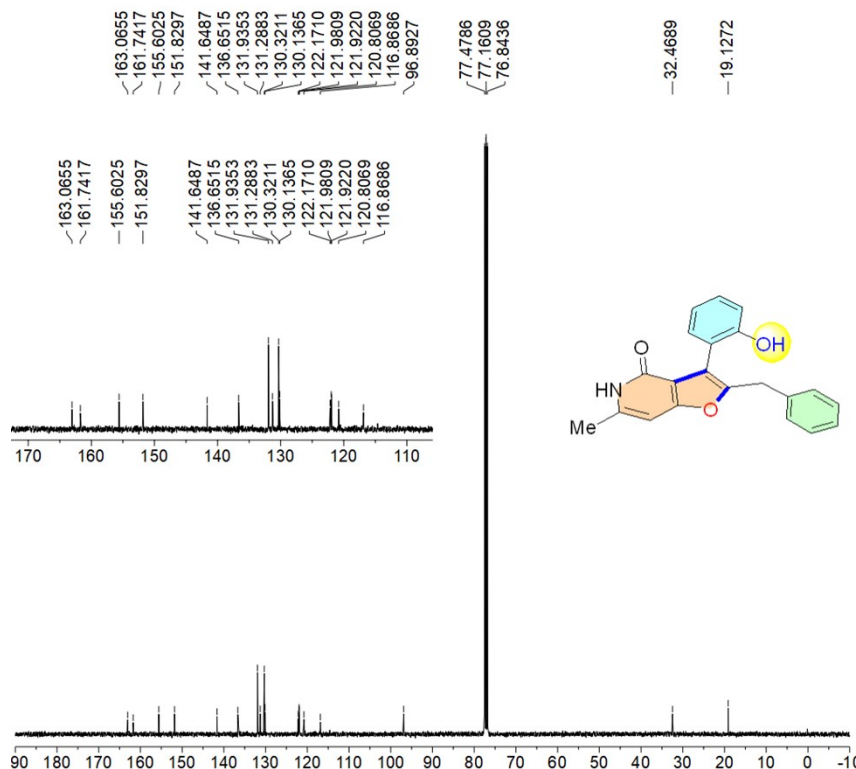
¹³C NMR (100 MHz, CDCl₃)

Chemical shift (ppm): 13, 12, 11, 10, 9, 8, 7, 6, 5, 4, 3, 2, 1, 0, -1, -2

Chemical Structure of Compound 10:

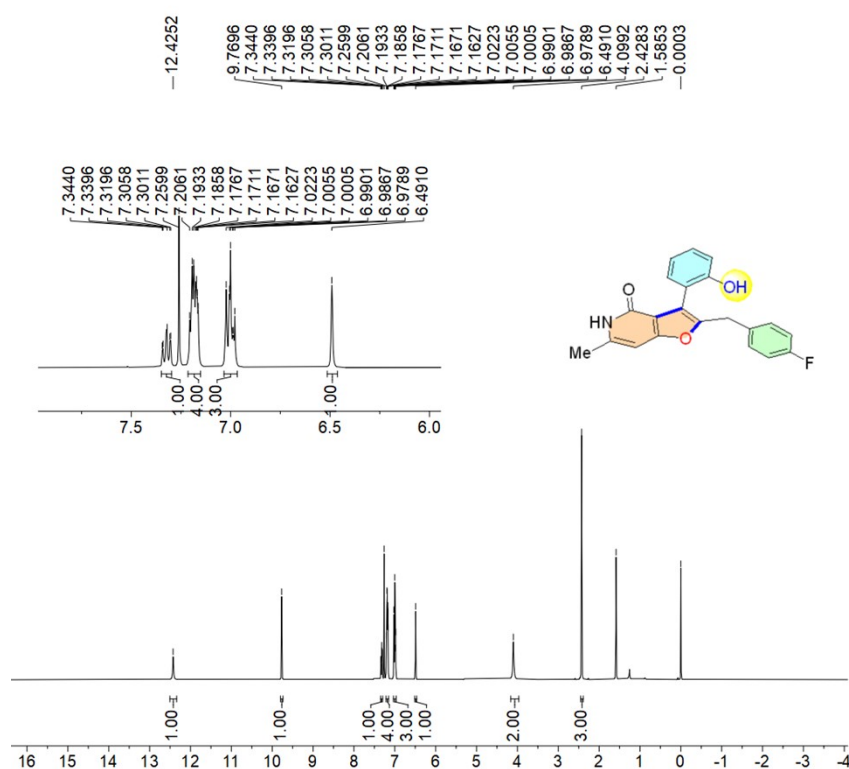
Cc1c[nH]c(=O)c2c(c1)c(c3ccccc3O)c(oc2Cc4ccccc4)c5ccccc5

Parameter	值
1 Data File Name	E/-New-新仪器请留数据/ 23-1-hww-C/ 33/fid
2 标题	23-1-hww-C.33.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	295.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HRBBO400S1-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	2023-03-08T22:00:05
21 Modification Date	2023-03-08T21:59:12
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

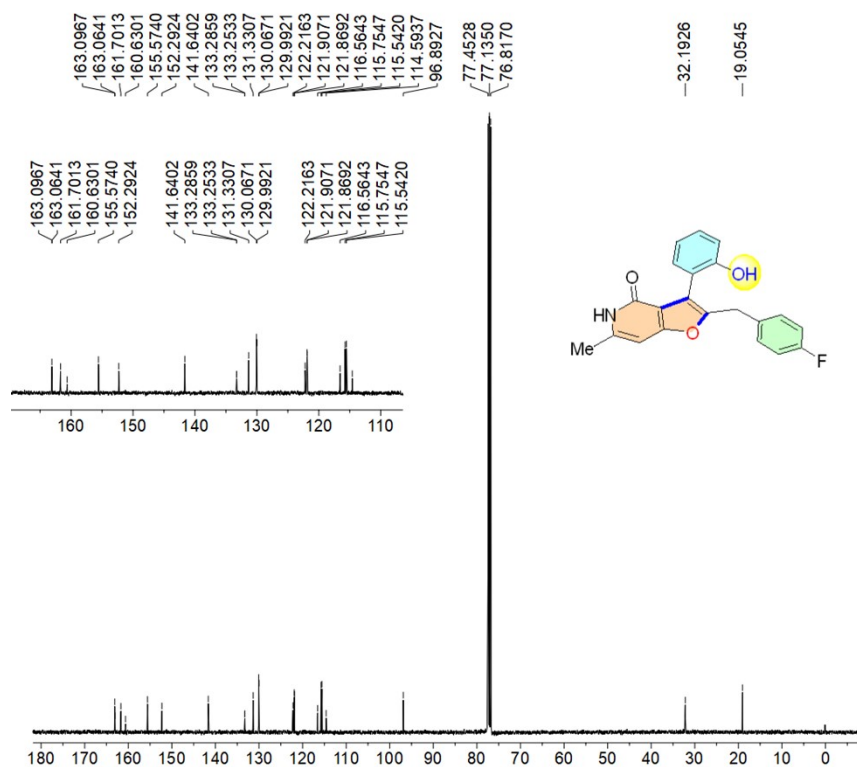


Parameter	值
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2 标题	23-1-hww-C_40.fid
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4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDC13
10 Temperature	295.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BB0400S1-BBF/H-D-5-O-Z SP)
14 Number of Scans	1024
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-10T23:42:39
21 Modification Date	2023-03-10T23:41:48
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

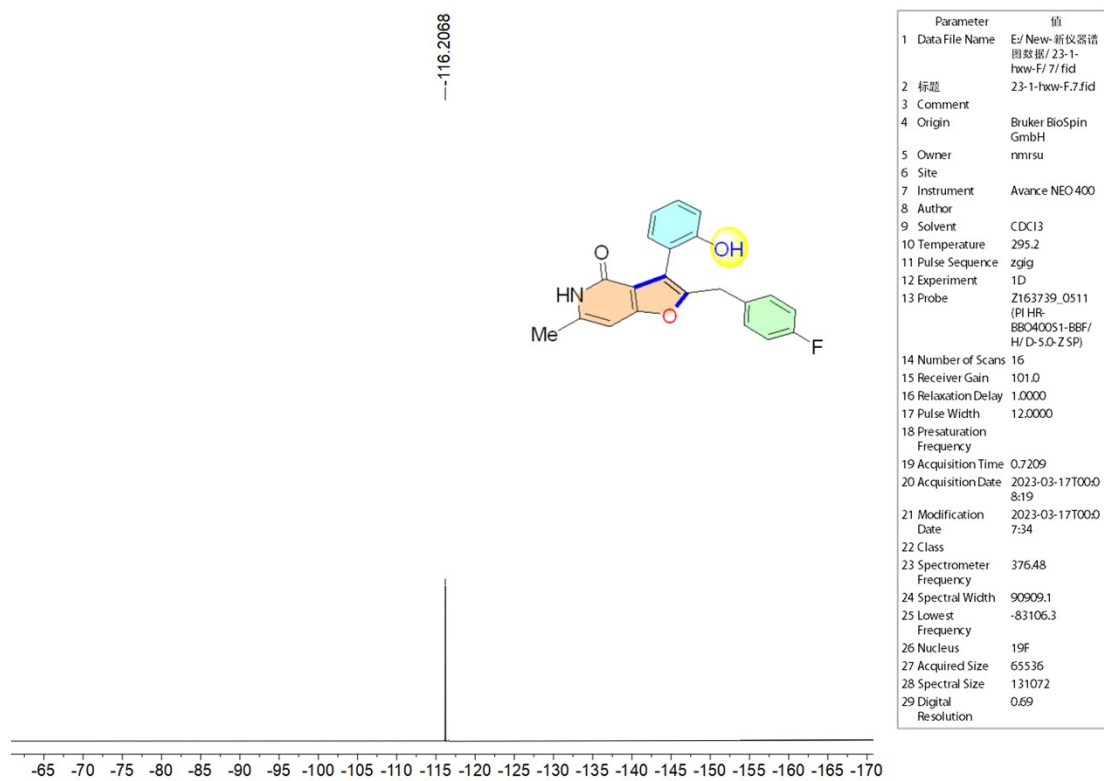
2-(4-Fluorobenzyl)-3-(2-hydroxyphenyl)-6-methylfuro[3,2-c]pyridin-4(5H)-one (5ab)



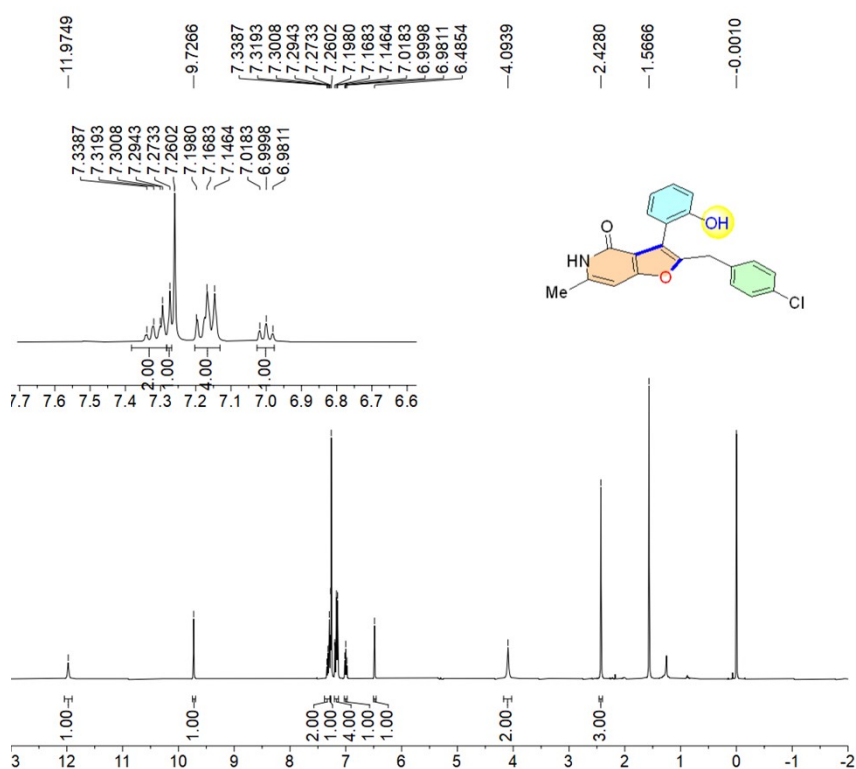
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1 Data File Name	E:/New-新仪器谱图数据/23-1-hw-H/53/fid
2 标题	23-1-hw-H.53.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.9
11 Pulse Sequence	zg30
12 Experiment	1D
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	2023-03-16T02:39:30
21 Modification Date	2023-03-16T02:38:44
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



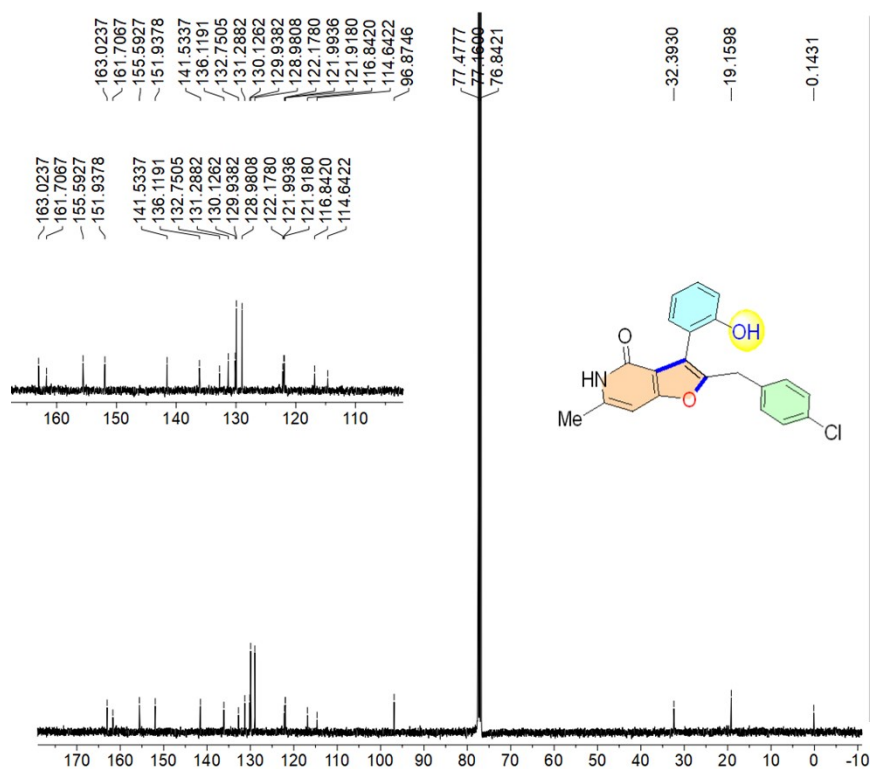
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2 标题	23-1-hw-H.53.fid
3 Comment	DD-ZI
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	15.1
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-17T01:10:12
21 Modification Date	2023-03-17T01:09:30
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36



2-(4-Chlorobenzyl)-3-(2-hydroxyphenyl)-6-methylfuro[3,2-c]pyridin-4(5H)-one (5ac)

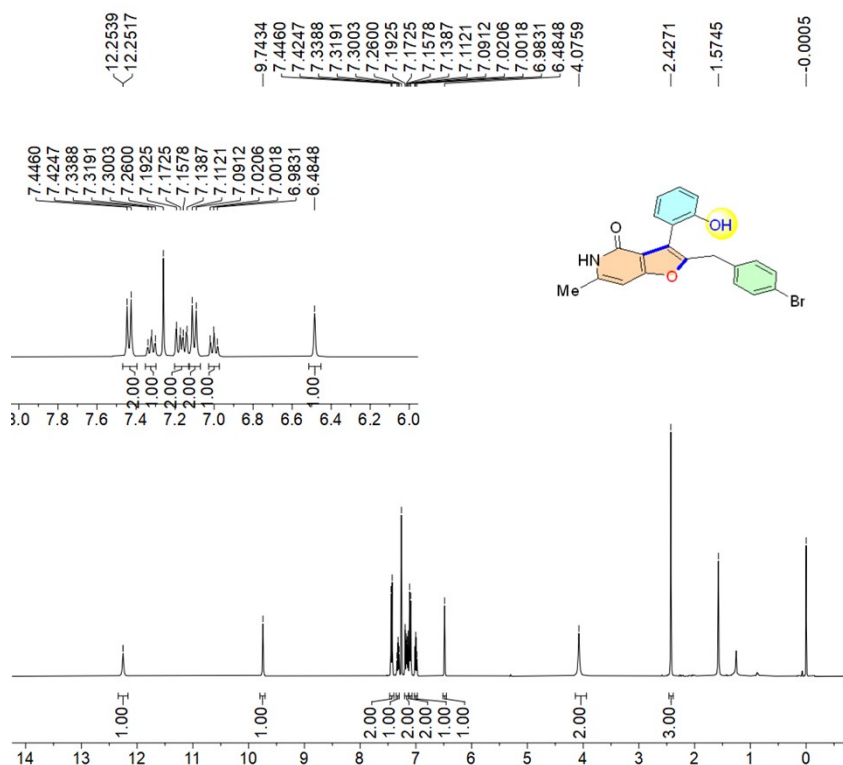


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2 标题	23-1-hww-H.57.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z 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	2023-03-16T04:59:50
21 Modification Date	2023-03-16T04:59:04
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

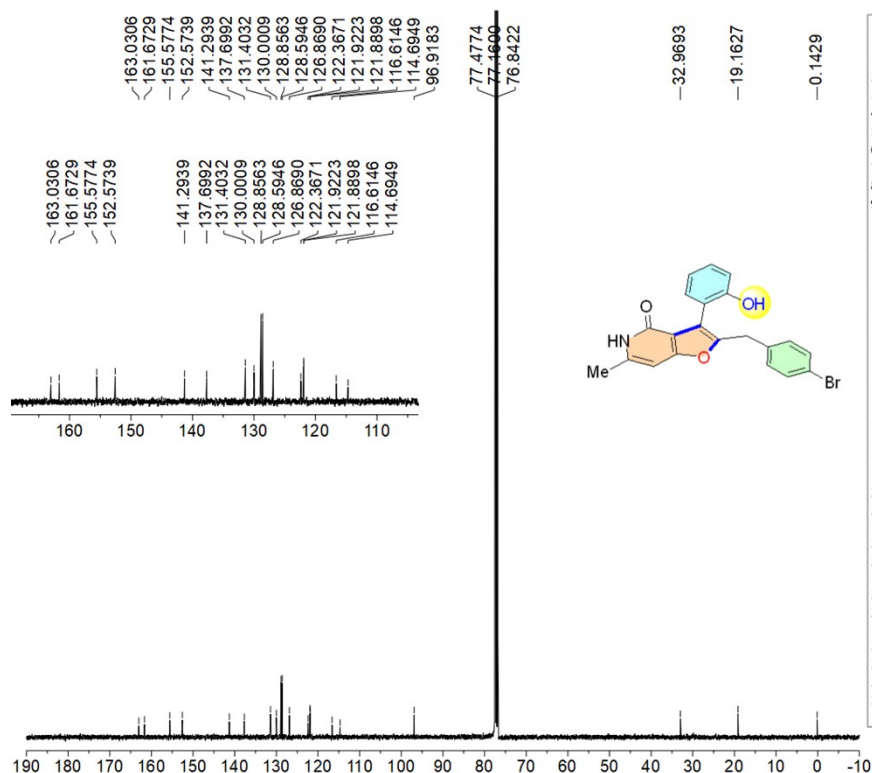


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1 Data File Name	E:/ New-前仪器谱图数据/ 23-1-hww-H/ 52/ fid
2 标题	23-1-hww-H.52.fid
3 Comment	DD-HET
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	11.8
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-17T00:02:57
21 Modification Date	2023-03-17T00:02:14
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

2-(4-Bromobenzyl)-3-(2-hydroxyphenyl)-6-methylfuro[3,2-c]pyridin-4(5H)-one (5ad)

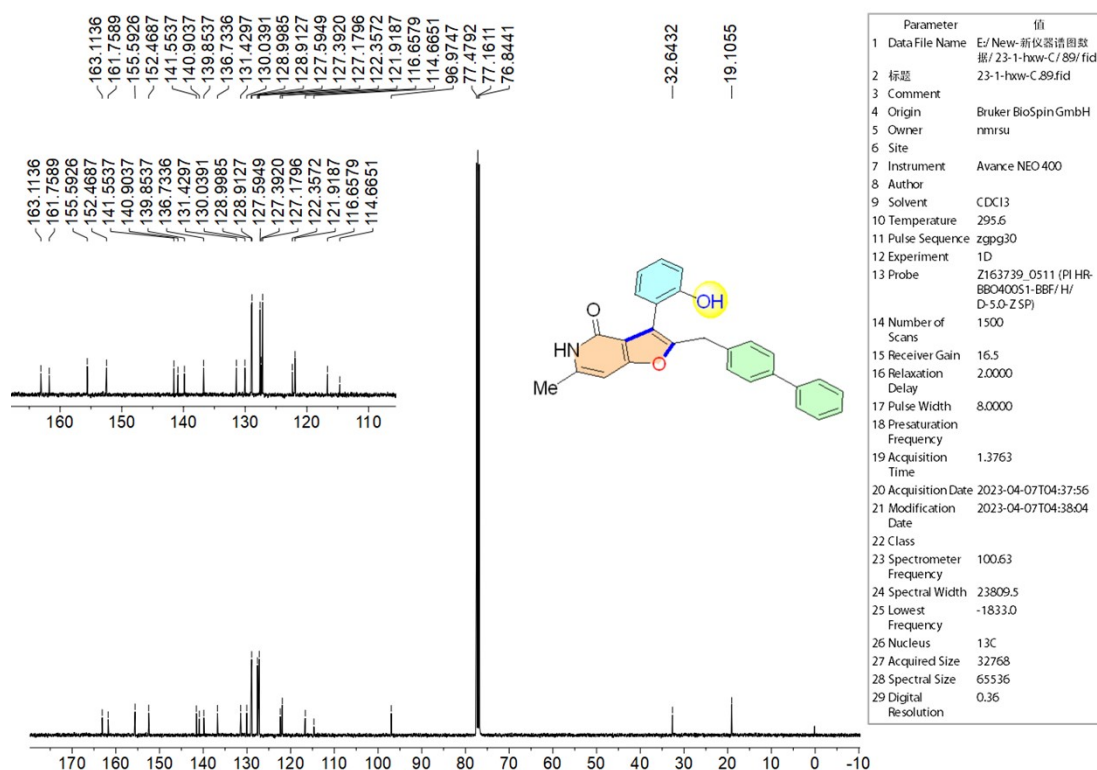
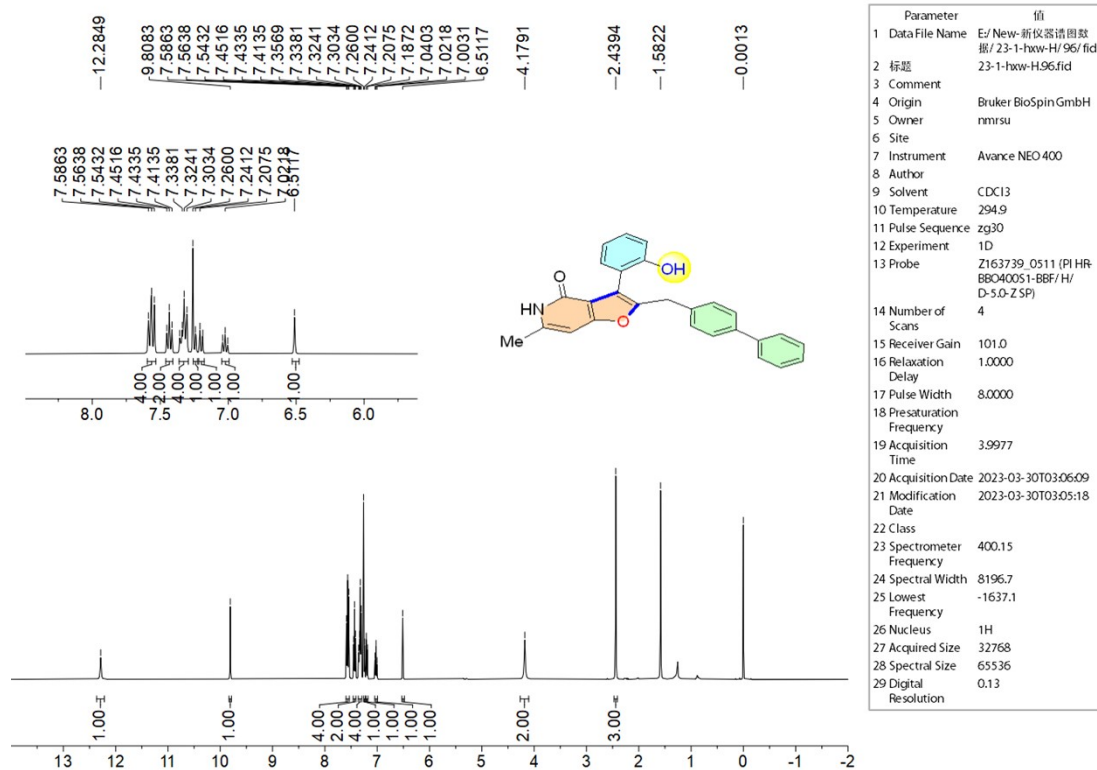


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1 Data File Name	E:/New-新仪器谱图数据/23-1-hw-H/49/fid
2 标题	23-1-hw-H49.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.4
11 Pulse Sequence	zg30
12 Experiment	1D
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	2023-03-10T21:26:05
21 Modification Date	2023-03-10T21:25:14
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

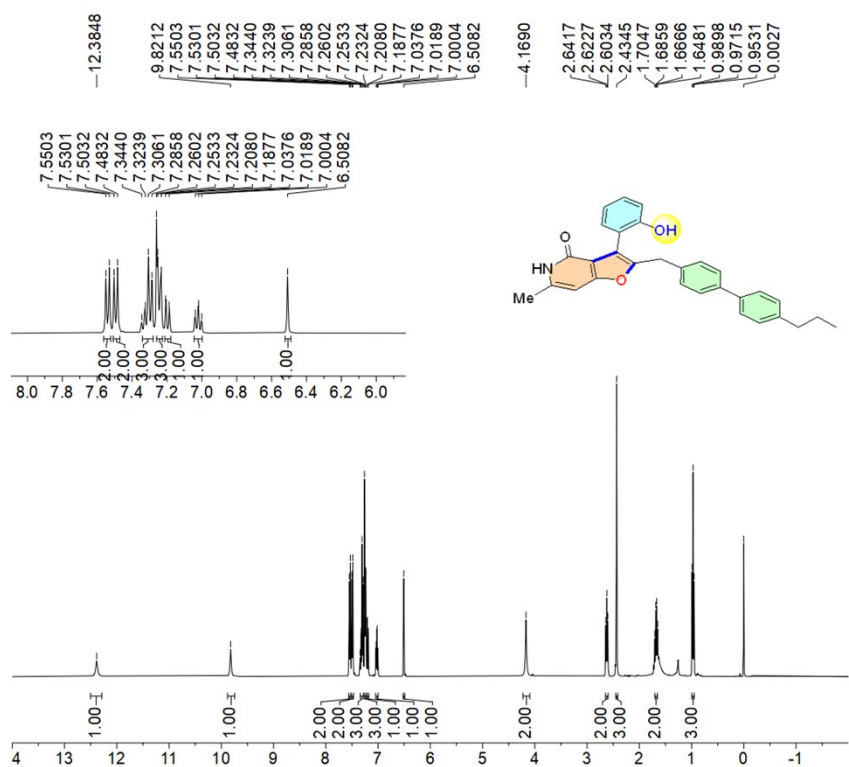


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3 Comment	DD-HOMG
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.8
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	2000
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-15T23:26:37
21 Modification Date	2023-03-15T23:25:50
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

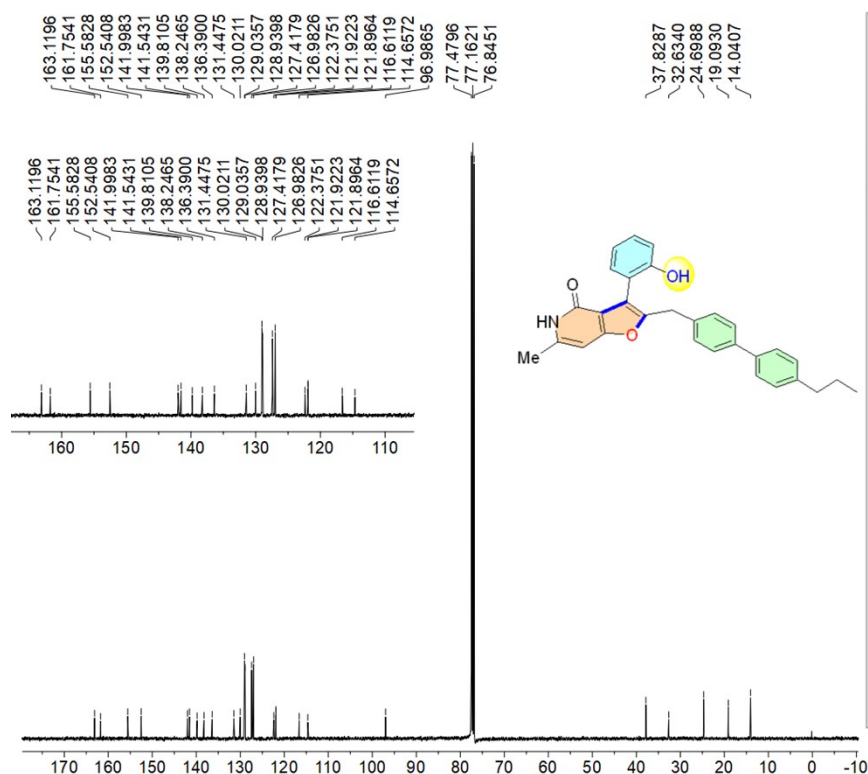
2-([1,1'-Biphenyl]-4-ylmethyl)-3-(2-hydroxyphenyl)-6-methylfuro[3,2-c]pyridin-4(5H)-one (5af)



3-(2-Hydroxyphenyl)-6-methyl-2-((4'-propyl-[1,1'-biphenyl]-4-yl)methyl)furo[3,2-c]pyridin-4(5H)-one (5ag)



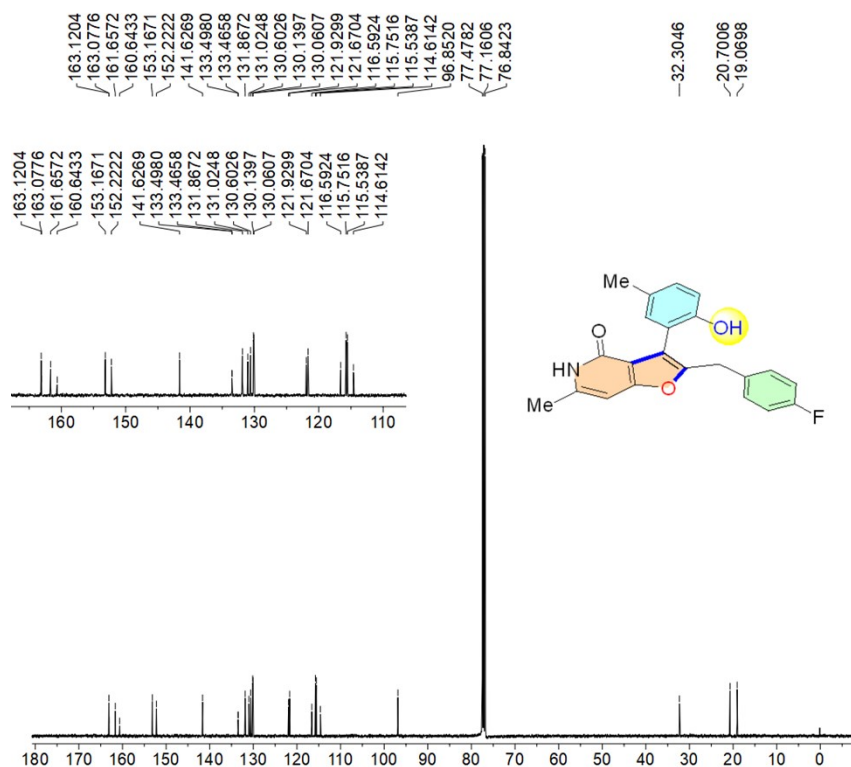
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3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of 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	2023-03-21T08:25:05
21 Modification Date	2023-03-21T08:25:10
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



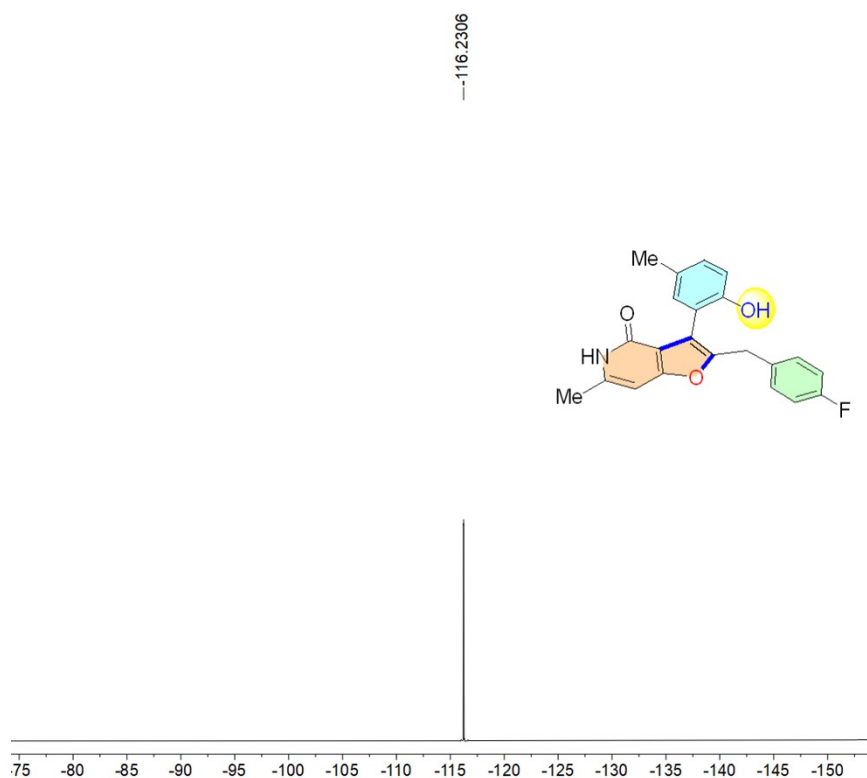
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1 Data File Name	E:/ New-前仪器谱图数据/ 23-1-hww-C/ 73/ fid
2 标题	23-1-hww-C.73.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1181
15 Receiver Gain	16.3
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-24T07:34:08
21 Modification Date	2023-03-24T07:34:12
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

Chemical structure of compound 10 is shown in the top right corner. The structure is a benzofuran derivative with a methyl group (Me) at the 2-position, a 4-methylphenyl group at the 3-position, and a 4-fluorophenyl group at the 4-position. The chemical shift values (ppm) are listed above the spectrum, and the integration values are shown below the spectrum.

Parameter	值
1 DataFile Name	E:/New-新仪器谱图数据/23-1-hw-H/64/fid
2 标题	23-1-hw-H.64.fid
3 Comment	DD-HUANG
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.5
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 Prestaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-03-16T21:44:33
21 Modification Date	2023-03-16T21:43:46
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

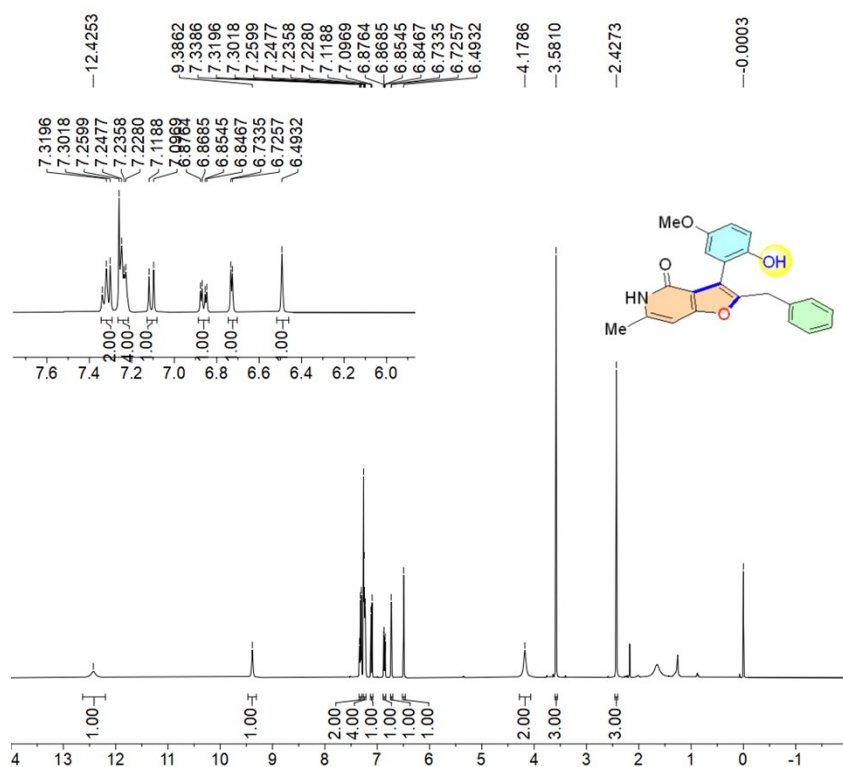


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1 DataFile Name	E:/New-前仪器谱图数据/23-1-hww-C/68/fid
2 标题	23-1-hww-C.68.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BB0400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1978
15 Receiver Gain	16.8
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-23T08:03:36
21 Modification Date	2023-03-23T08:03:38
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

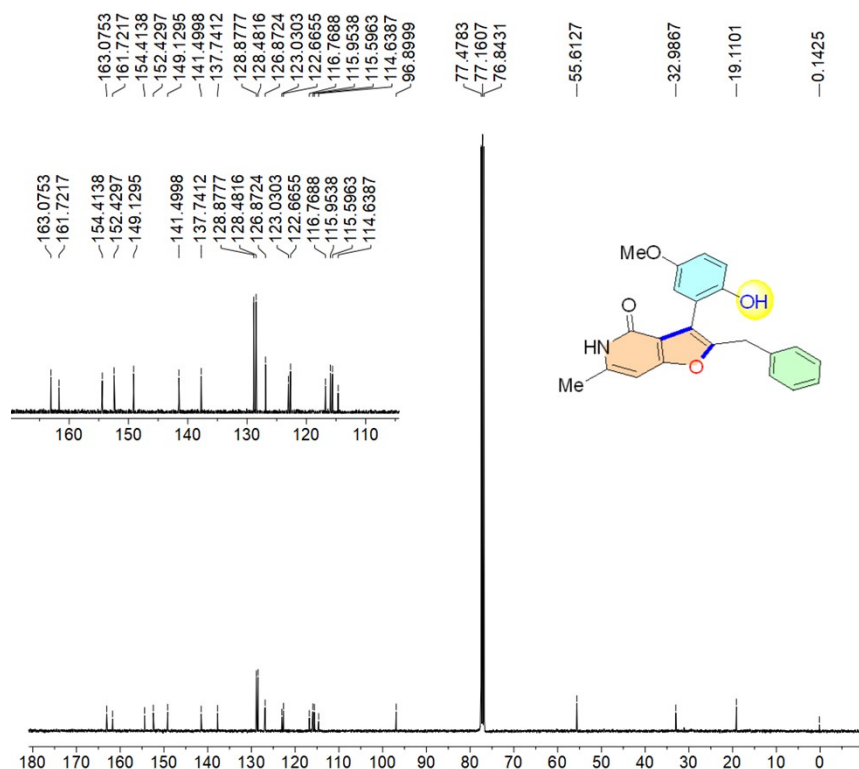


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4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO40051-BBF/H/ D-5-D-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2023-03-16T21:42:49
21 Modification Date	2023-03-16T21:42:04
22 Class	
23 Spectrometer Frequency	376.48
24 Spectral Width	90909.1
25 Lowest Frequency	-83106.3
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	131072
29 Digital Resolution	0.69

2-Benzyl-3-(2-hydroxy-5-methylphenyl)-6-methylfuro[3,2-c]pyridin-4(5H)-one (5ca)

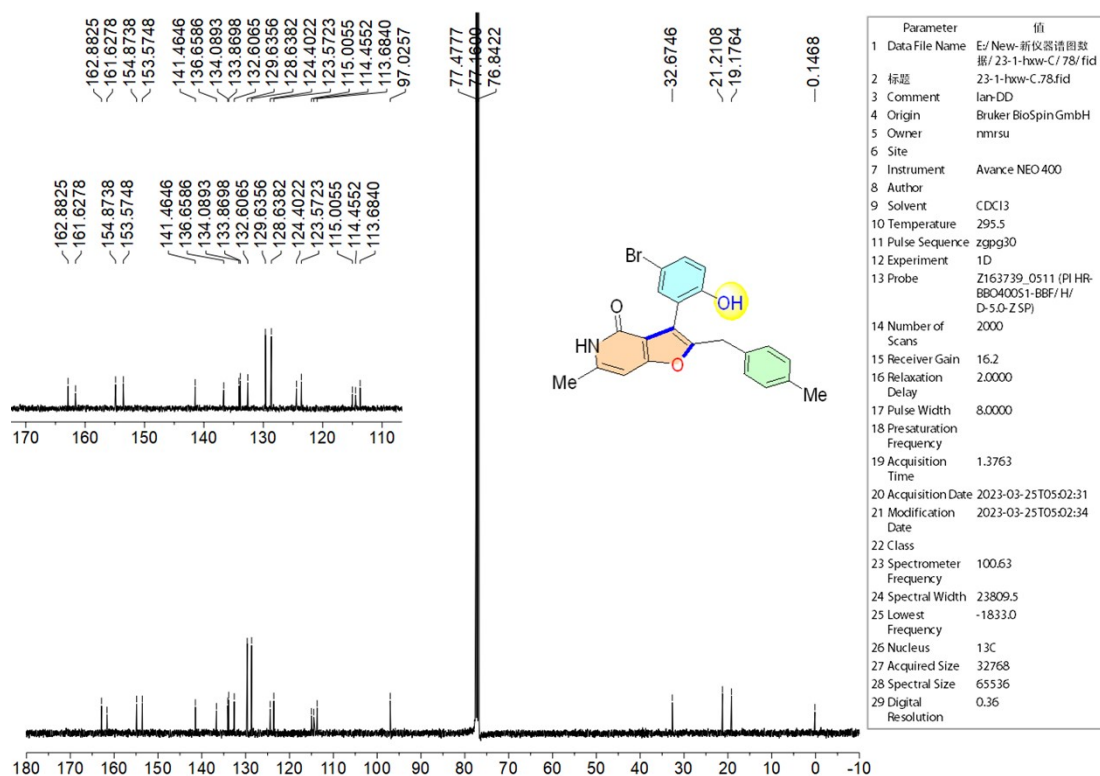
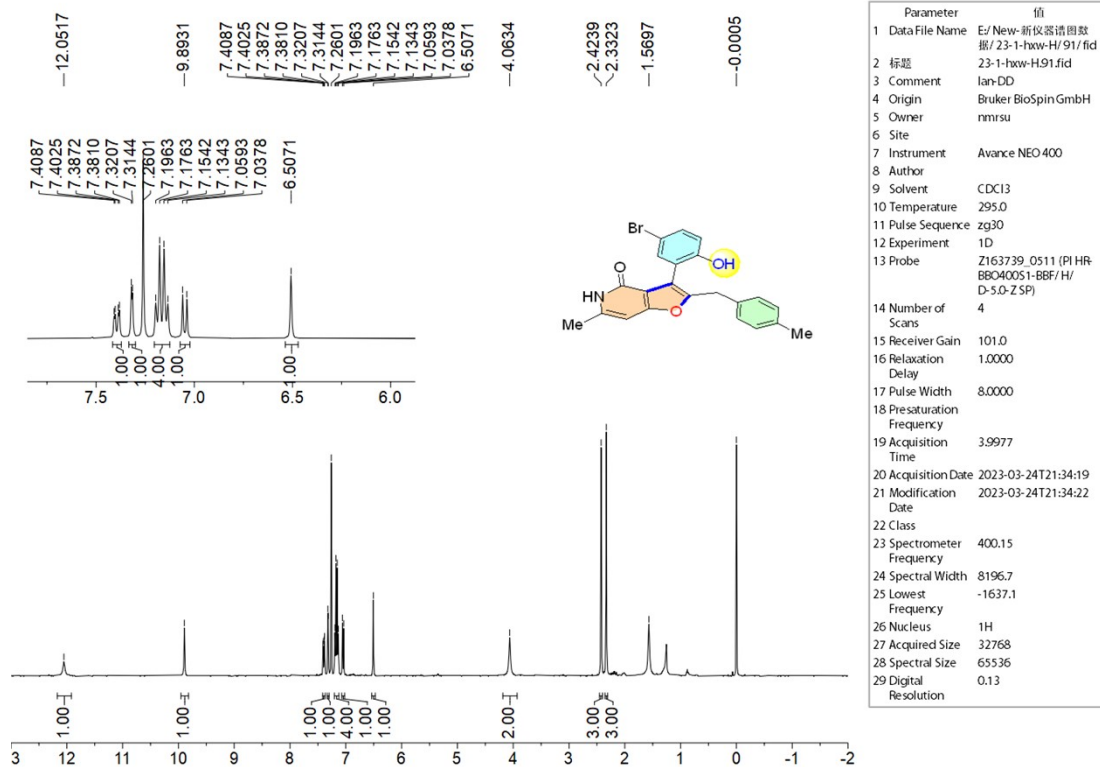


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3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.8
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	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	2023-03-21T08:34:35
21 Modification Date	2023-03-21T08:34:40
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

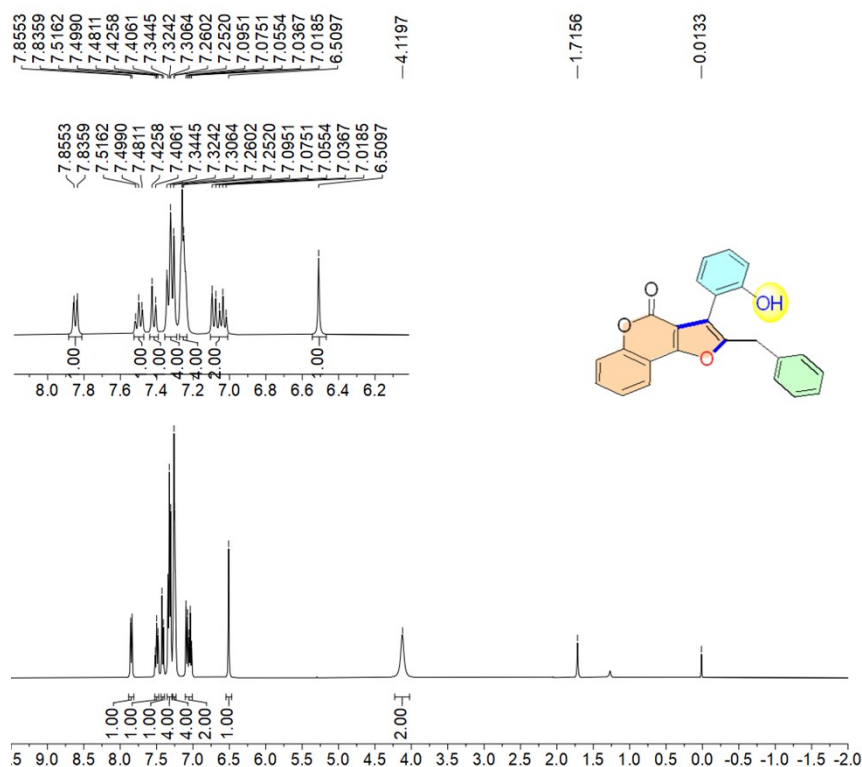


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2 标题	23-1-hww-C.91.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.6
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	15.3
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-07T07:11:03
21 Modification Date	2023-04-07T07:11:14
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

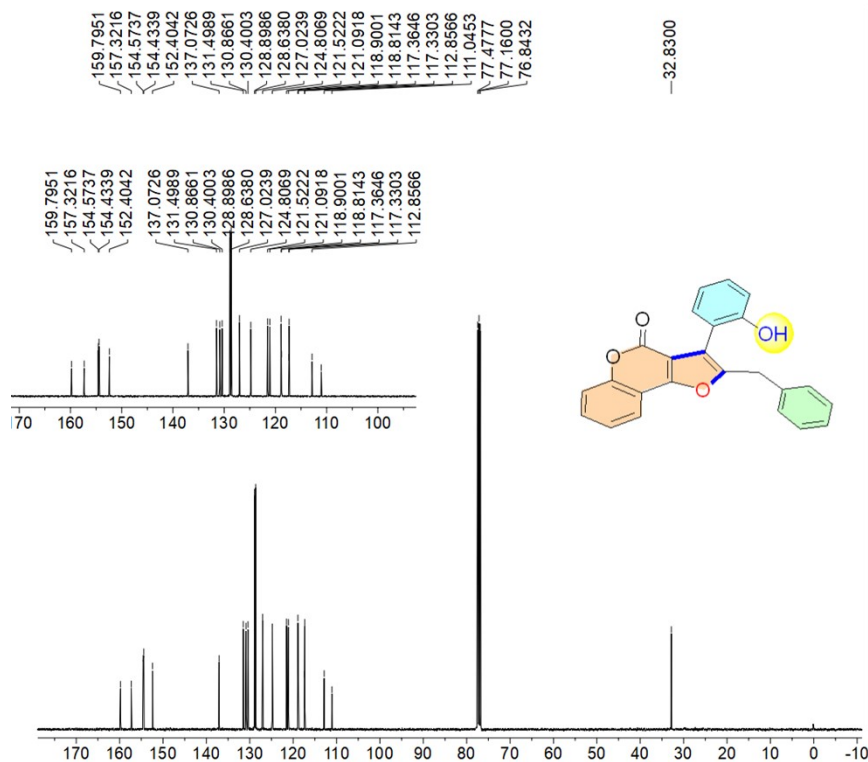
3-(5-Bromo-2-hydroxyphenyl)-6-methyl-2-(4-methylbenzyl)furo[3,2-c]pyridin-4(5H)-one (product 5fl)



2-Benzyl-3-(2-hydroxyphenyl)-4H-furo[3,2-c]chromen-4-one (7)



Parameter	值
1 Data File Name	E:/Old-新仪器谱图数据/2023-1-hxw-H/ 52/ fid
2 标题	2023-1-hxw-H.52.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.4
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	2023-04-24T16:22:37
21 Modification Date	2023-04-24T16:22:06
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



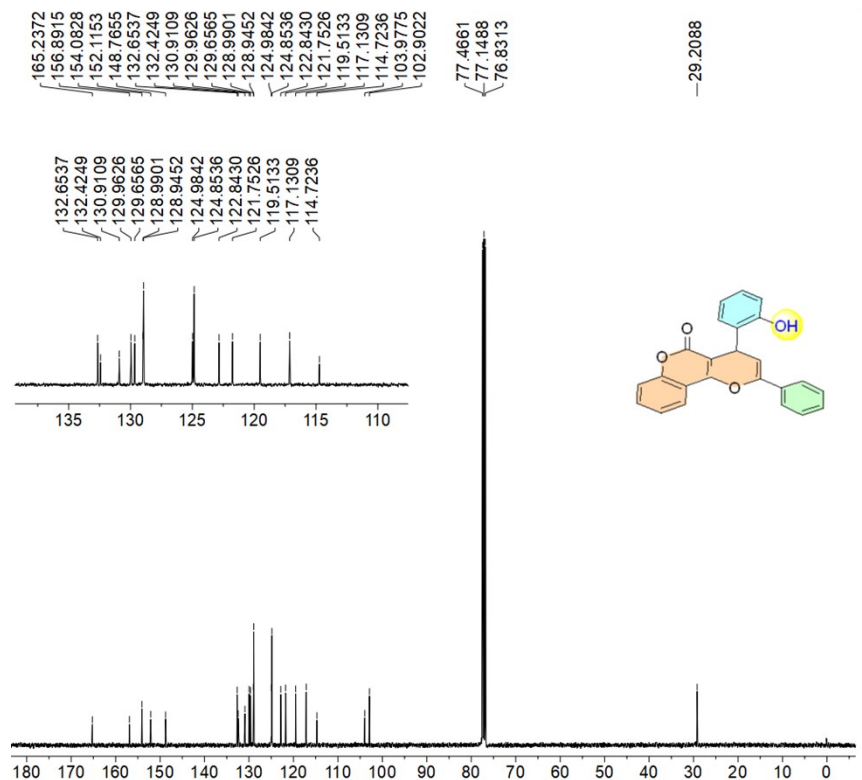
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2 标题	23-1-hxw-C.128.fid
3 Comment	HONG
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	296.3
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1500
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-21T05:07:29
21 Modification Date	2023-04-21T05:07:52
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

Chemical structure: c1ccc(cc1)-c2cc3ccccc3oc2-c2cc3ccccc3oc21

¹H NMR spectrum (CDCl₃) of 2,2'-bis(4-phenyl)-6,6'-bibenzofuran. The spectrum shows peaks from 8.5 to 6.6 ppm (aromatic protons) and 7.4 to 6.9 ppm (aromatic protons). Integration values are provided below the peaks.

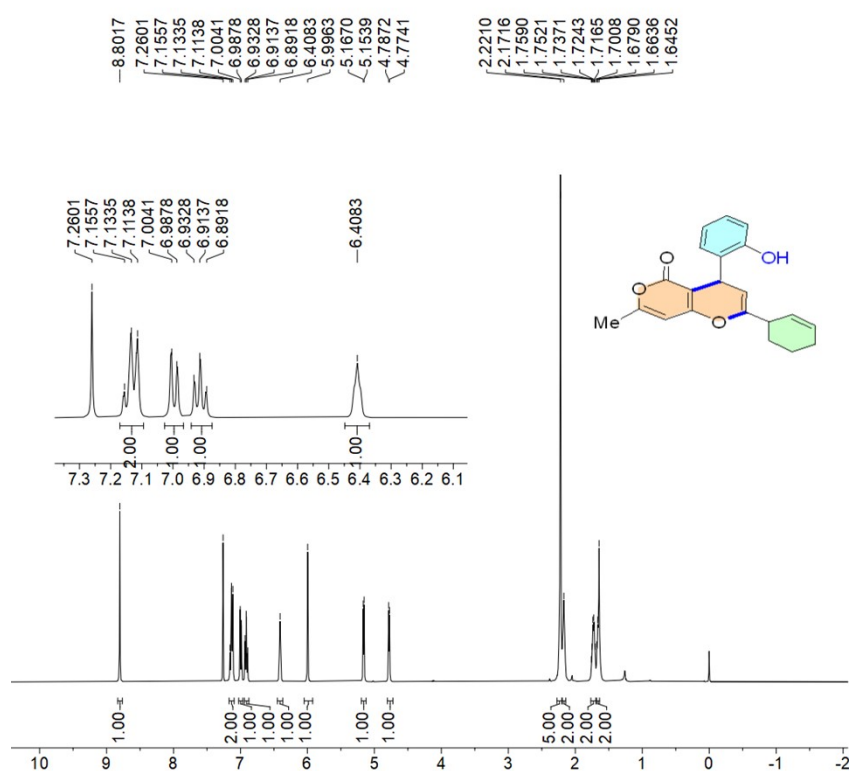
Chemical structure: c1ccc(cc1)-c2cc3ccccc3oc2-c2cc3ccccc3oc21

Parameter	值
1 Data File Name	Gz/2023-hww-H/1/fid
2 标题	2023-hww-H.1.fid
3 Comment	
4 Origin	Braker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDC13
10 Temperature	294.5
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	ZH673739_0032 (PI H1R-400-S1-BBF/H/ D-5.0-Z-SP)
14 Number of Scans	4
15 Receiver Gain	101.0
16 Relaxation Delay	1.00000
17 Pulse Width	10.00000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-04-24T16:26:29
21 Modification Date	2023-04-24T16:25:58
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
29 Digital Resolution	0.13

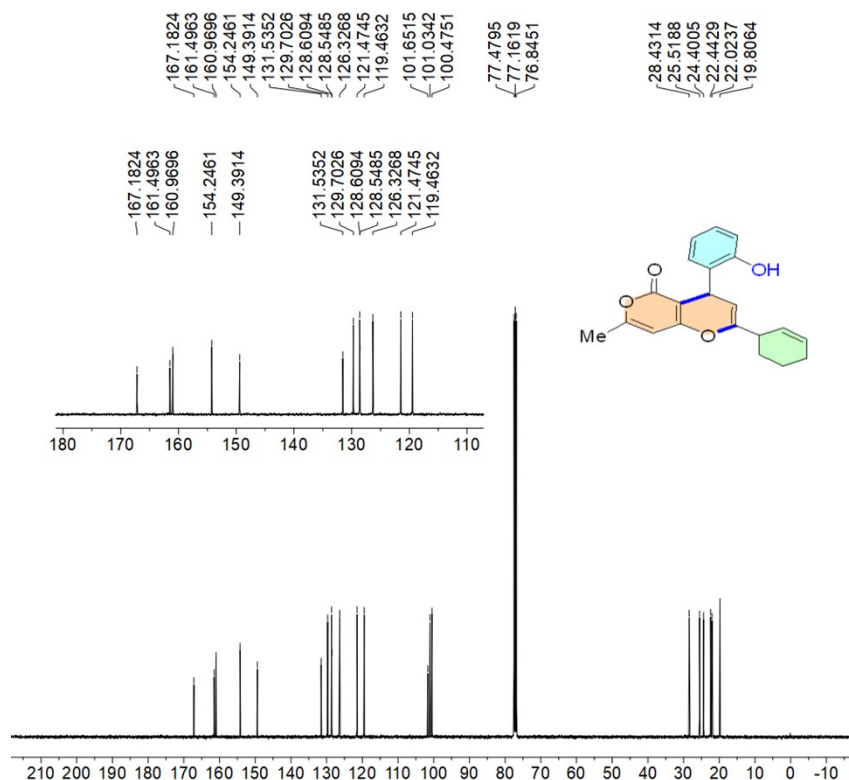


Parameter	值
1 Data File Name	E:/ New-新仪器清菌数据/ 23-1-hwx-C / 131/
2 标题	fid-131-hwx-C.131.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsru
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.7
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	2163739_0511 (PI HRB040051-BBF/ H/-D5.0-S ZSP)
14 Number of Scans	600
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-24T17:34:42
21 Modification Date	2023-04-24T17:34:46
22 Class	
23 Spectrometer Frequency	10063
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65336
29 Digital Resolution	0.36

2-(Cyclohex-2-en-1-yl)-4-(2-hydroxyphenyl)-7-methyl-4H,5H-pyrano[4,3-b]pyran-5-one (8a)

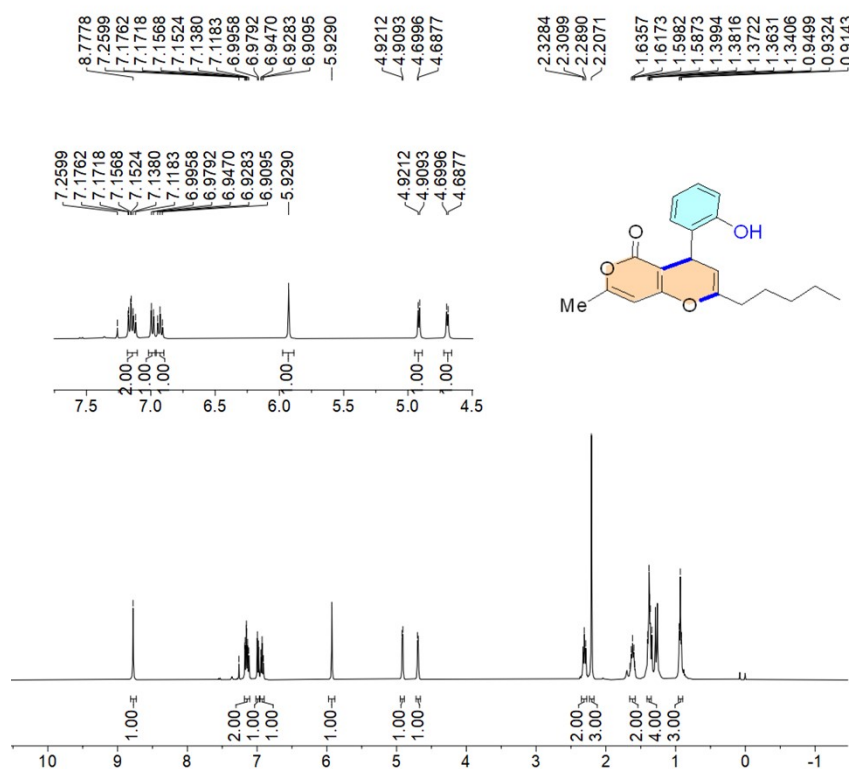


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2 标题	2023-2-hww-H.33.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	296.6
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/H/D-5.0-Z 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	2023-10-24T14:45:33
21 Modification Date	2023-10-24T14:45:10
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

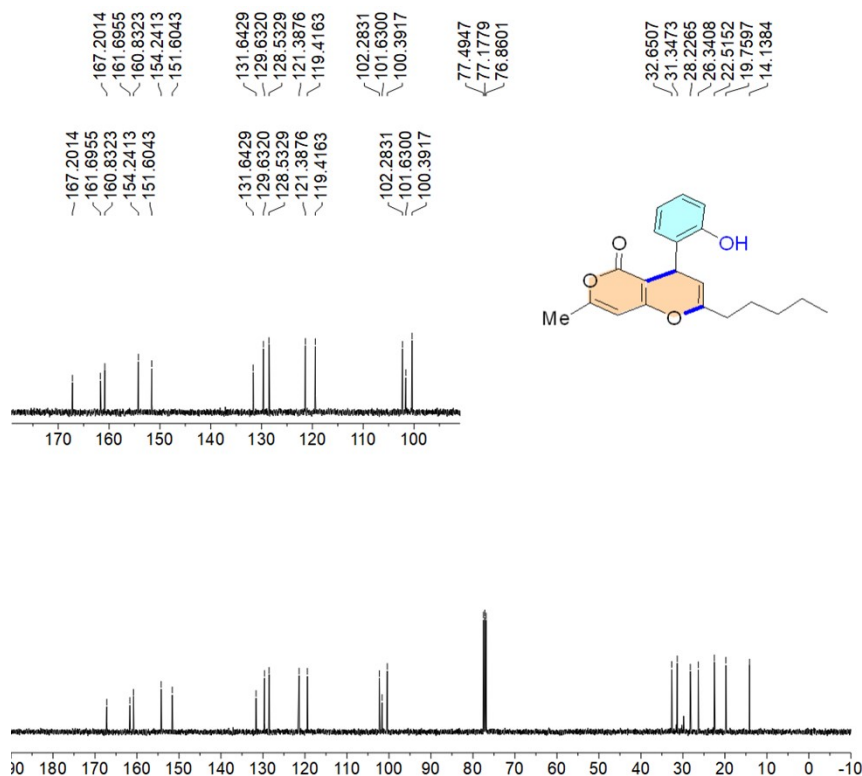


Parameter	值
1 Data File Name	G:/ 23-2-hww-C.14.fid
2 标题	23-2-hww-C.14.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	297.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BB0400S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	26.4
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-10-24T15:59:09
21 Modification Date	2023-10-24T15:58:34
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

4-(2-Hydroxyphenyl)-7-methyl-2-pentyl-4*H*,5*H*-pyrano[4,3-*b*]pyran-5-one (8b)



Parameter	值
1 Data File Name	G/ 2023-2-hww-H 31/ fid
2 标题	2023-2-hww-H.31.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	296.7
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	57.8
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-10-23T16:45:22
21 Modification Date	2023-10-23T16:45:04
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
29 Digital Resolution	0.13

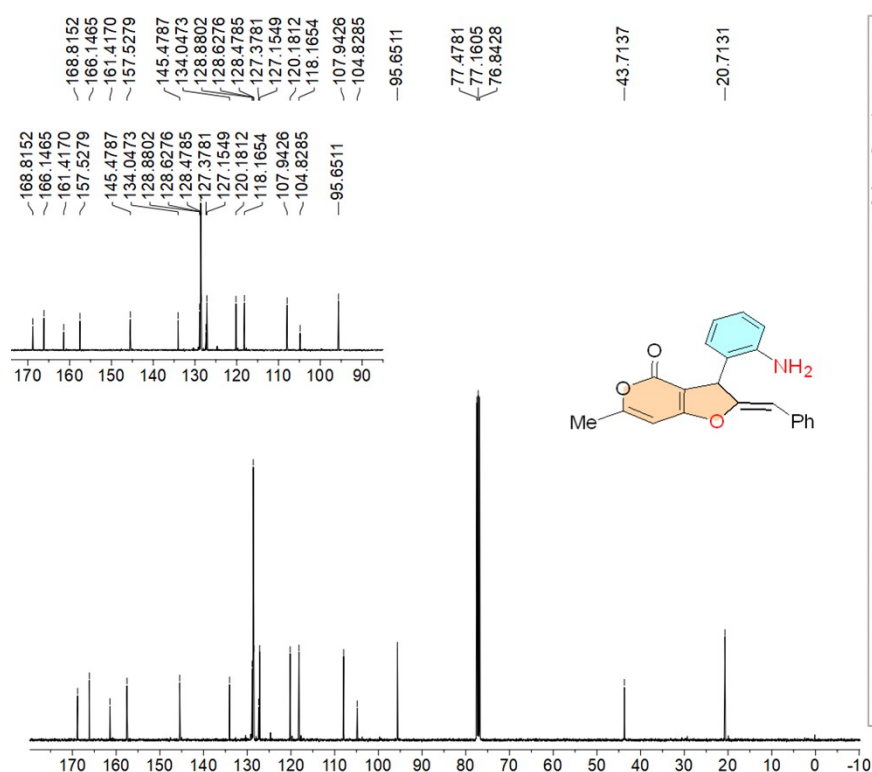


Parameter	值
1 Data File Name	G/ 23-2-hww-C 5/ fid
2 标题	2023-2-hww-C.5.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.9
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	64
15 Receiver Gain	17.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-10-23T17:49:00
21 Modification Date	2023-10-23T17:48:42
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.5
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

Chemical structure of compound 10: Cc1cc2c(c1)oc(C=Cc3ccccc3)c2c1ccccc1N

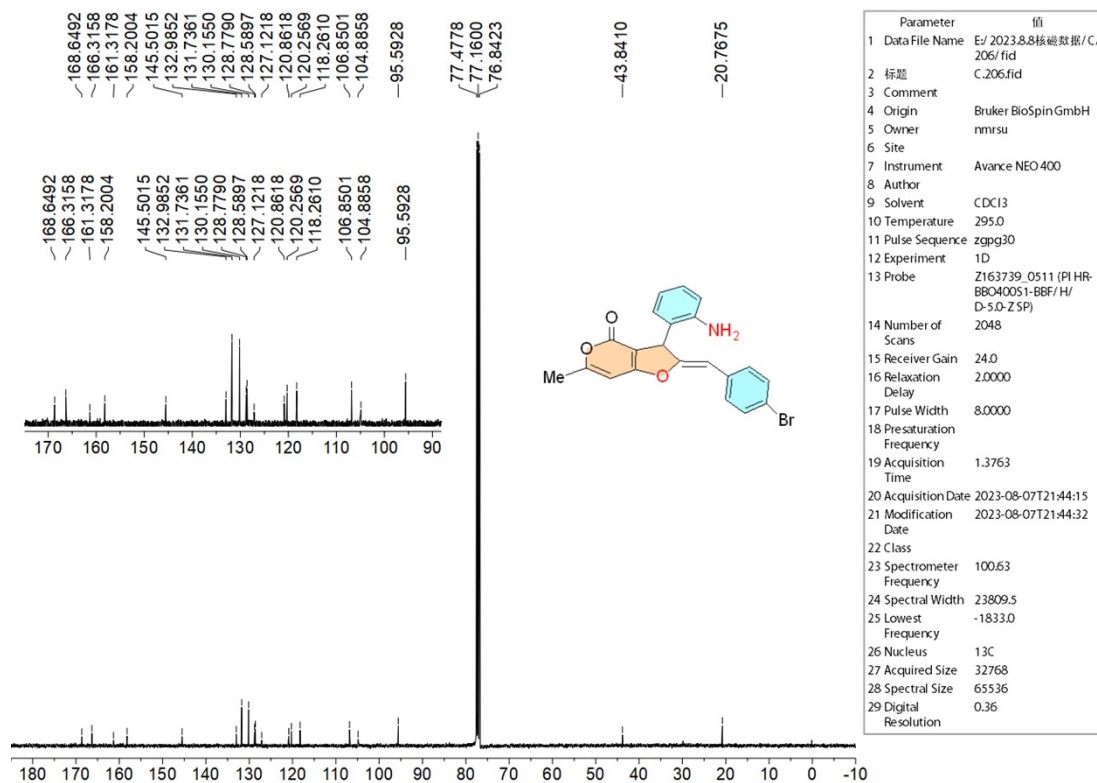
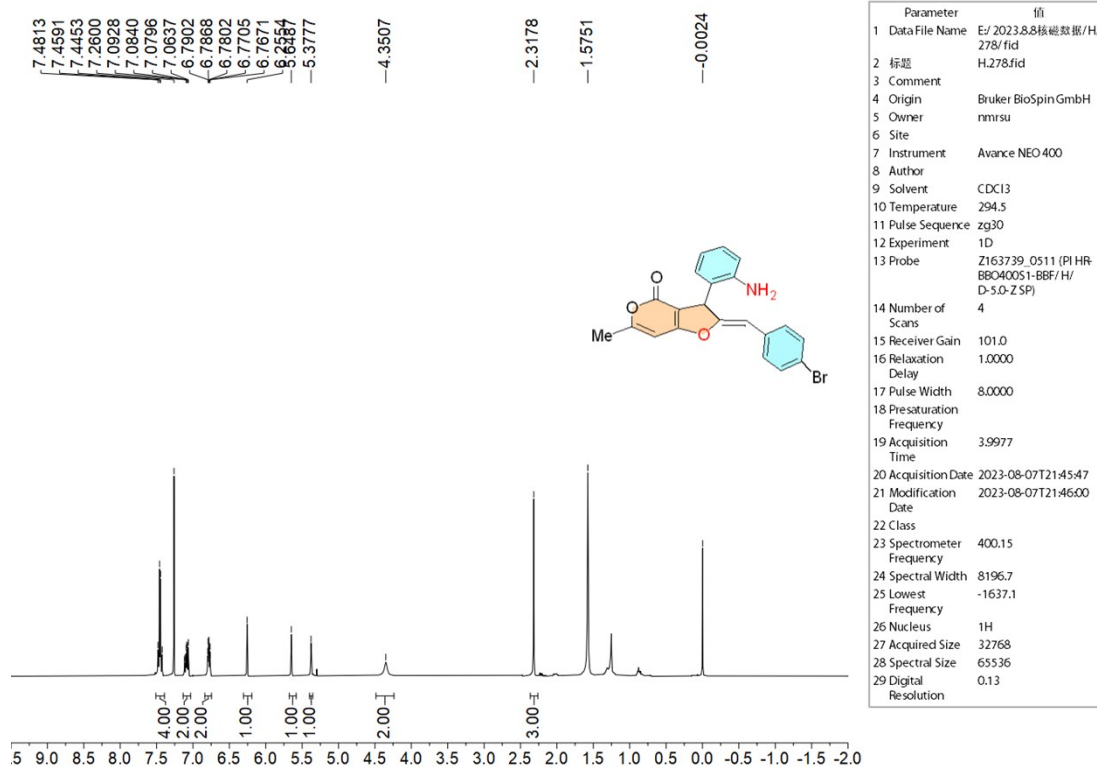
¹H NMR spectrum (CDCl₃) of compound 10. The x-axis ranges from -2.0 to 10.0 ppm. The spectrum shows several peaks in the aromatic region (6.5-7.6 ppm) and a peak at 2.3104 ppm. Integration values are shown below the peaks: 2.00, 2.00, 1.00, 2.00, 2.00, 1.00, 1.00, 1.00, 2.00, 3.00. A chemical structure of compound 10 is shown in the top right corner.

Parameter	值
1 Data File Name	E:/ 2023.6.28磁共振数据/23-1-hwx-H/182/fid
2 标题	23-1-hwx-H.182.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDC13
10 Temperature	293.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	BBC13739_0511 (PI HHRB040051-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	2023-05-20T07:41:00
21 Modification Date	2023-05-20T07:41:08
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	1H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

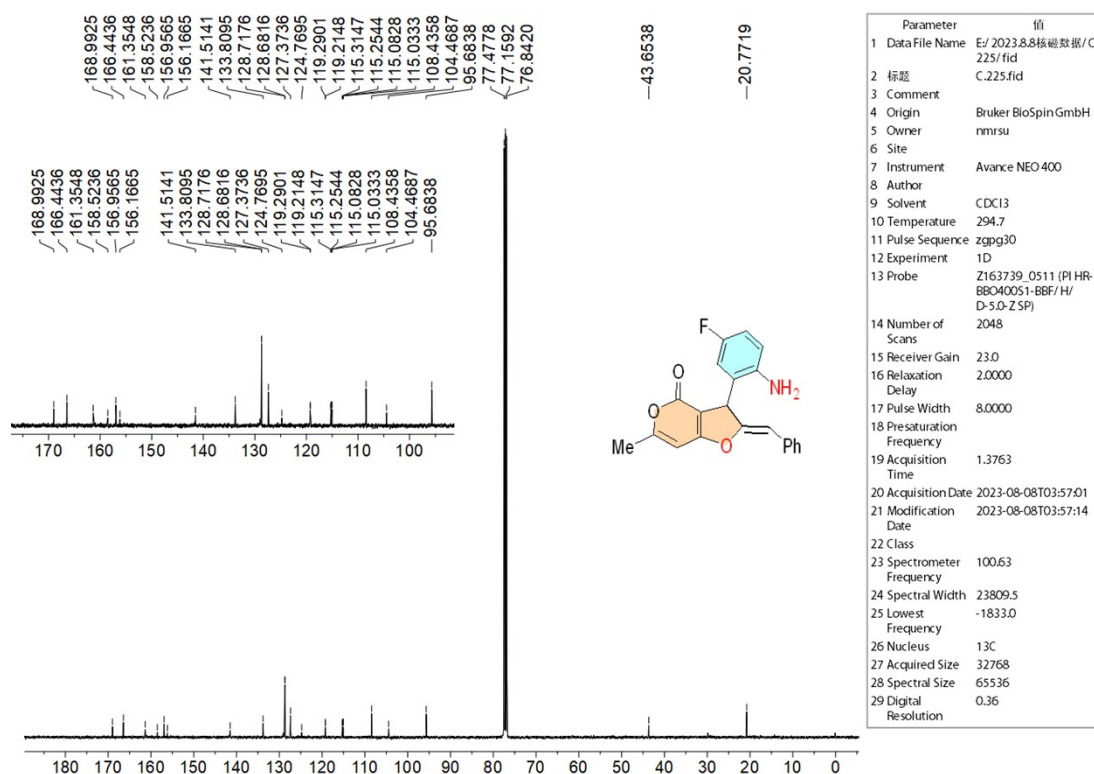
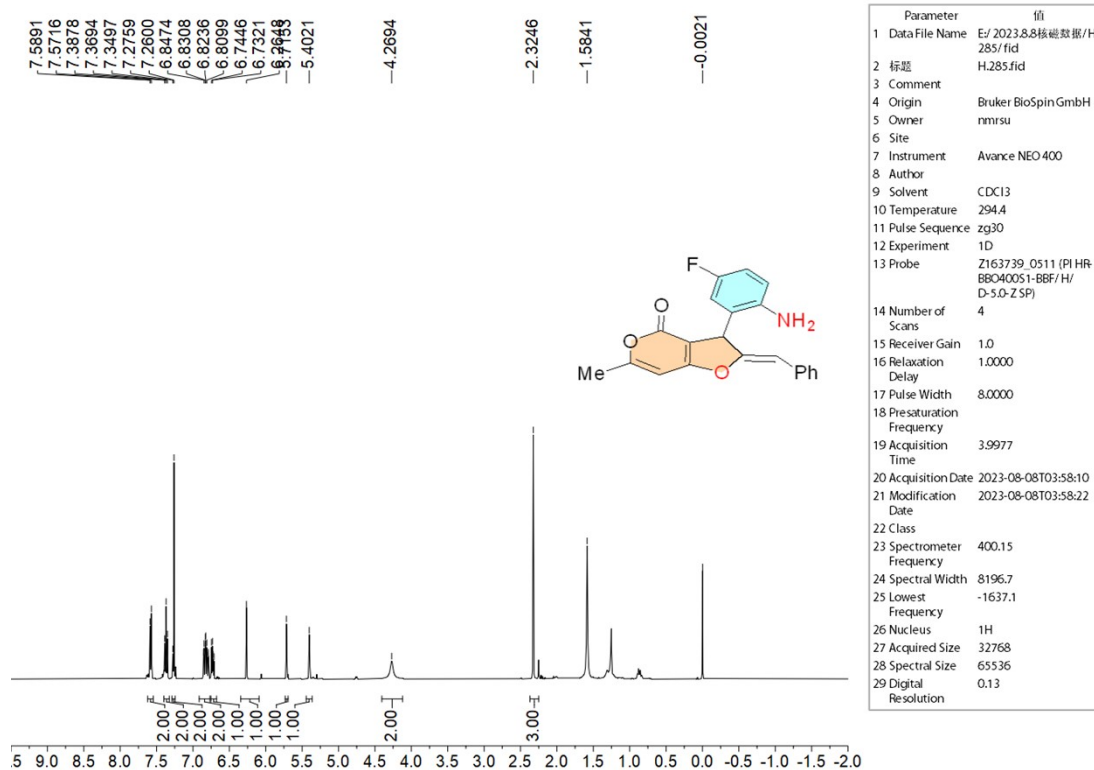


Parameter	值
1 Data File Name	E:/ 2023-6.28核磁数据/23-1-hw-C/167/fid
2 标题	23-1-hw-C.167.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	163739_0511 (PI HRB0400S-1-BBF/H/D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-06-02T02:01:31
21 Modification Date	2023-06-02T02:00:48
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

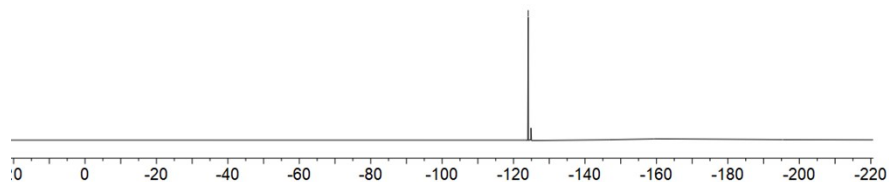
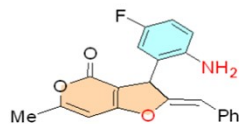
(Z)-3-(2-Aminophenyl)-2-(4-bromobenzylidene)-6-methyl-2,3-dihydro-4H-furo[3,2-c]pyran-4-one(10ad)



(Z)-3-(2-Amino-5-fluorophenyl)-2-benzylidene-6-methyl-2,3-dihydro-4H-furo[3,2-c]pyran-4-one(10da)

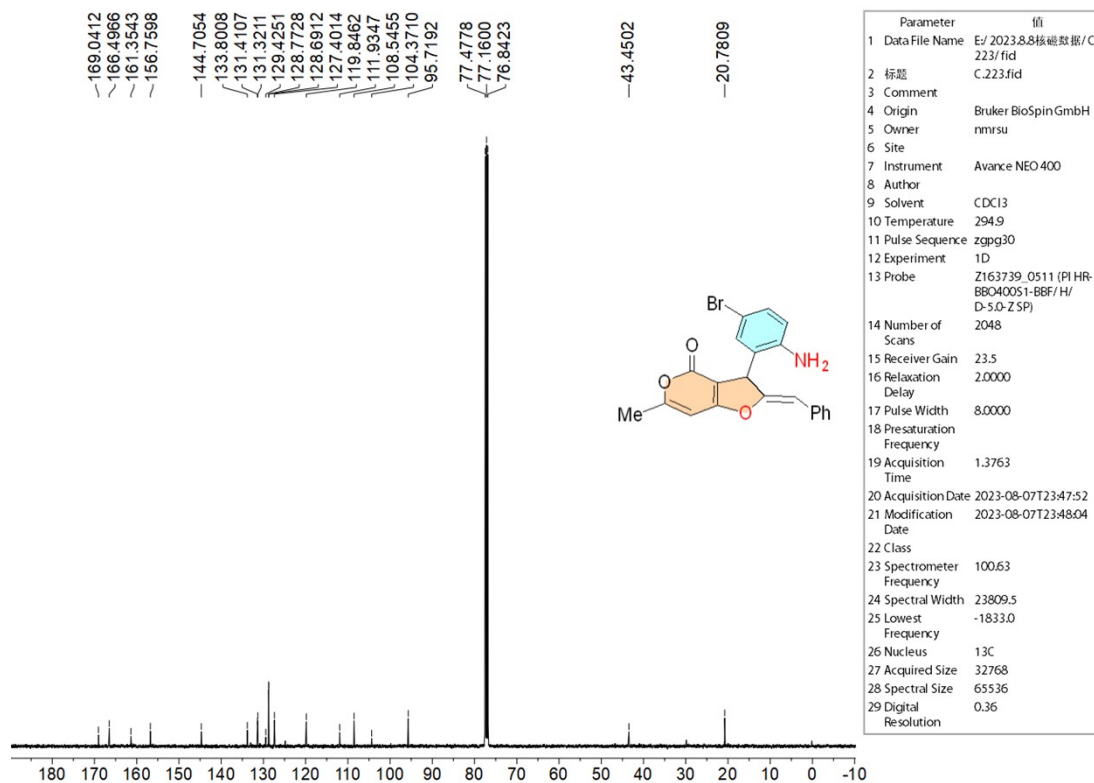
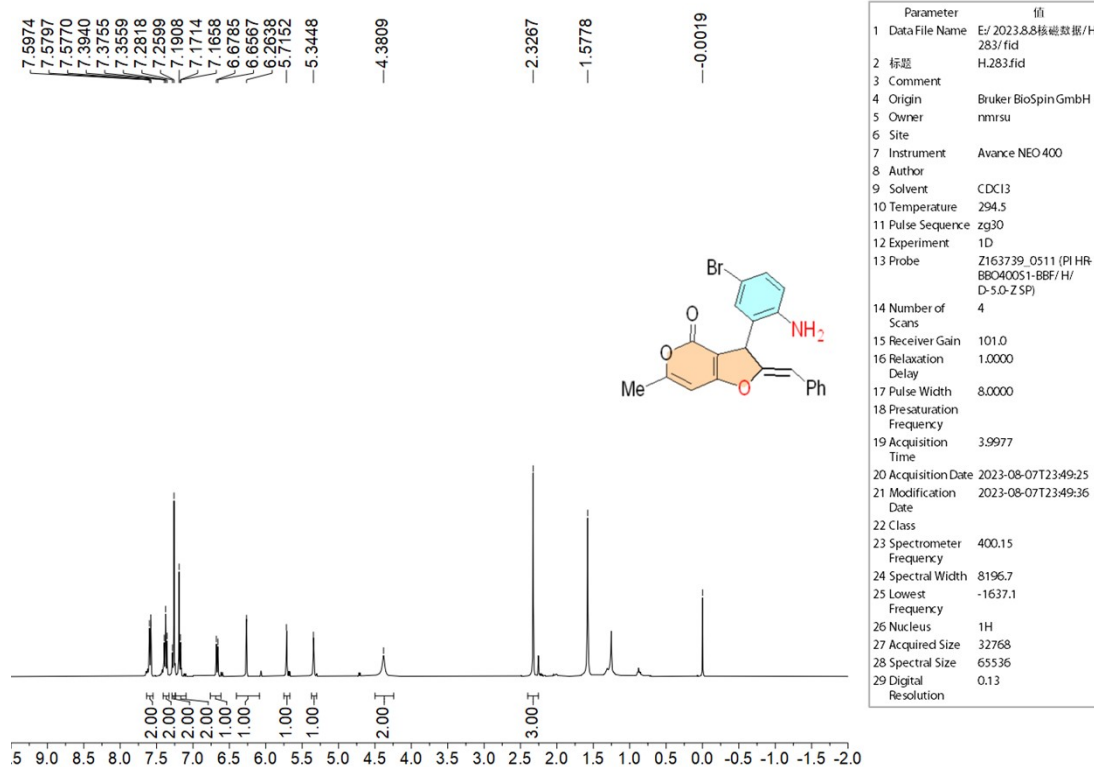


--124.0929

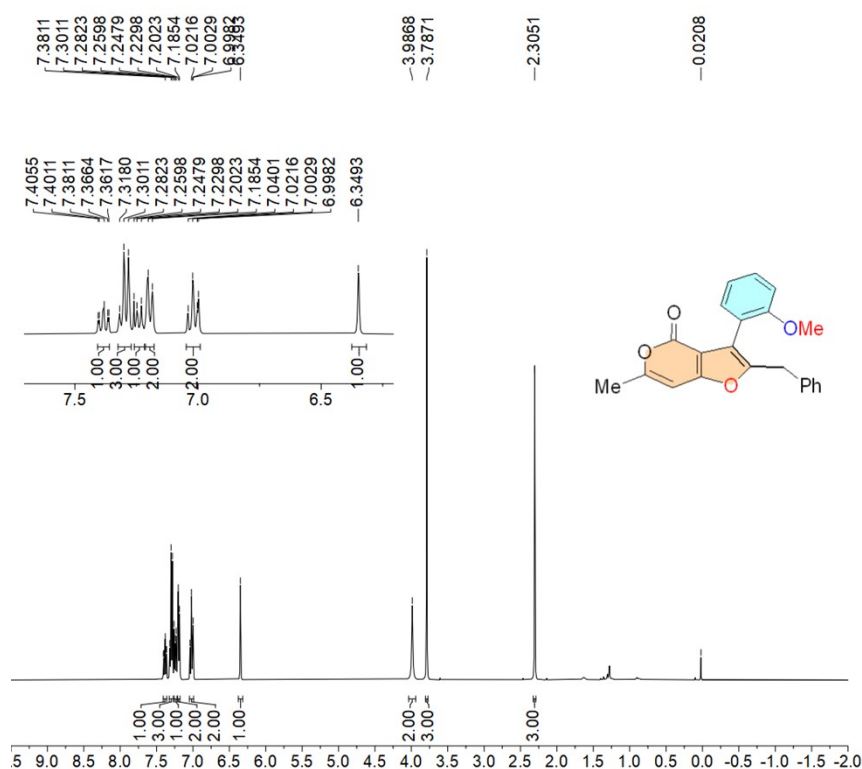


Parameter	值
1 Data File Name	E:/ 2023.8.8核磁数据/ 16/ fid
2 标题	2023.8.8核磁数据.16.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	294.3
11 Pulse Sequence	zgpg
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO400S1-BBF/H/ D-5.D-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	1.0000
17 Pulse Width	12.0000
18 Presaturation Frequency	
19 Acquisition Time	0.7209
20 Acquisition Date	2023-08-08T01:57:22
21 Modification Date	2023-08-08T01:57:34
22 Class	
23 Spectrometer Frequency	376.48
24 Spectral Width	90909.1
25 Lowest Frequency	-83106.3
26 Nucleus	19F
27 Acquired Size	65536
28 Spectral Size	131072
29 Digital Resolution	0.69

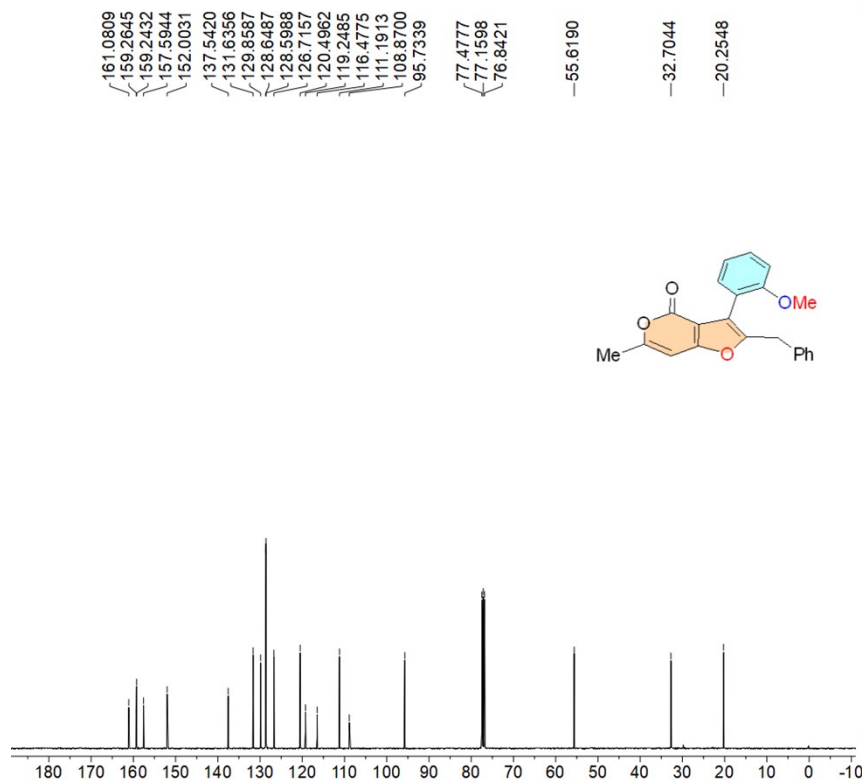
(Z)-3-(2-Amino-5-bromophenyl)-2-benzylidene-6-methyl-2,3-dihydro-4H-furo[3,2-c]pyran-4-one(10fa)



2-Benzyl-3-(2-methoxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (11)

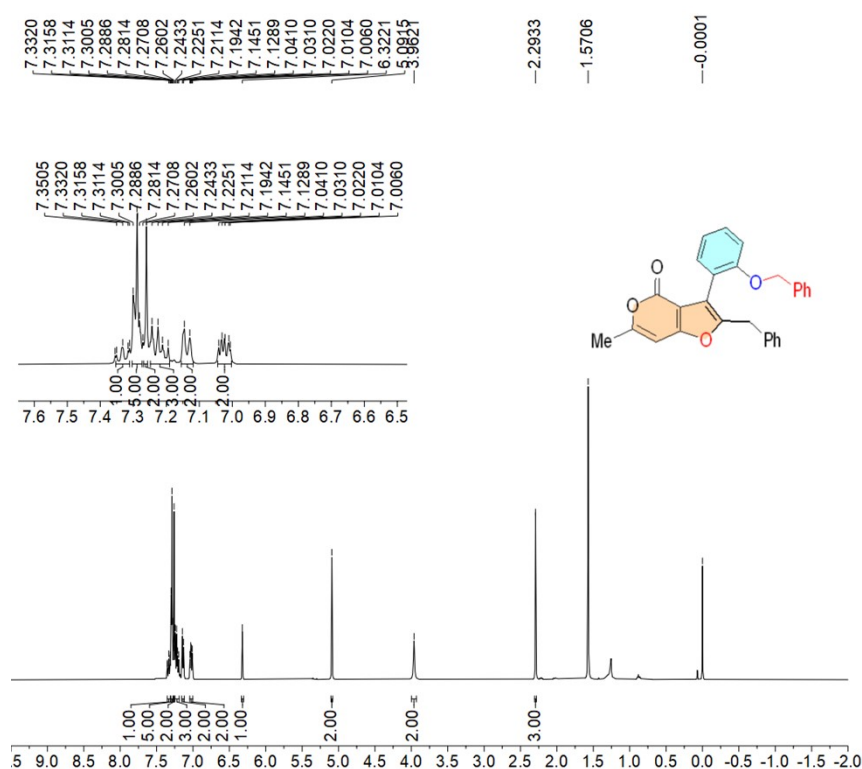


Parameter	值
1 Data File Name	E:/Old-老仪器谱图数据/2023-1-hww-H/ 20/ fid
2 标题	2023-1-hww-H.20.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.0
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-51-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	4
15 Receiver Gain	87.2
16 Relaxation Delay	1.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	3.9977
20 Acquisition Date	2023-03-07T07:39:01
21 Modification Date	2023-03-07T07:37:46
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
29 Digital Resolution	0.13

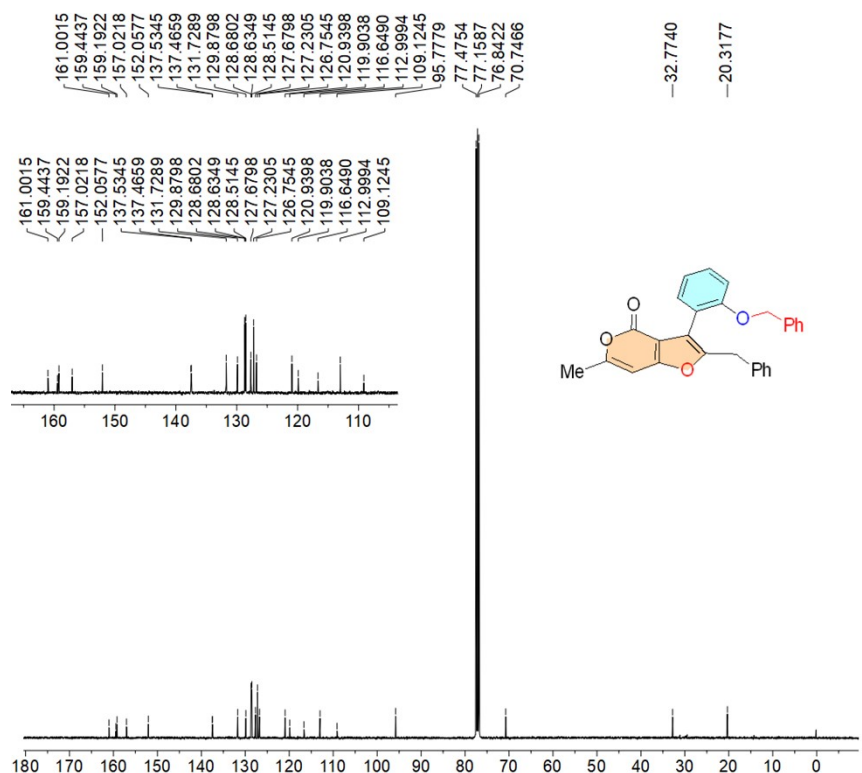


Parameter	值
1 Data File Name	E:/New-新仪器谱图数据/ 23-1-hww-C/ 37/ fid
2 标题	23-1-hww-C.37.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	296.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BB040051-BBF/ H/ D-5.0-Z SP)
14 Number of Scans	1024
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-09T01:11:28
21 Modification Date	2023-03-09T01:10:36
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	13C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

2-Benzyl-3-(2-(benzyloxy)phenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (12)

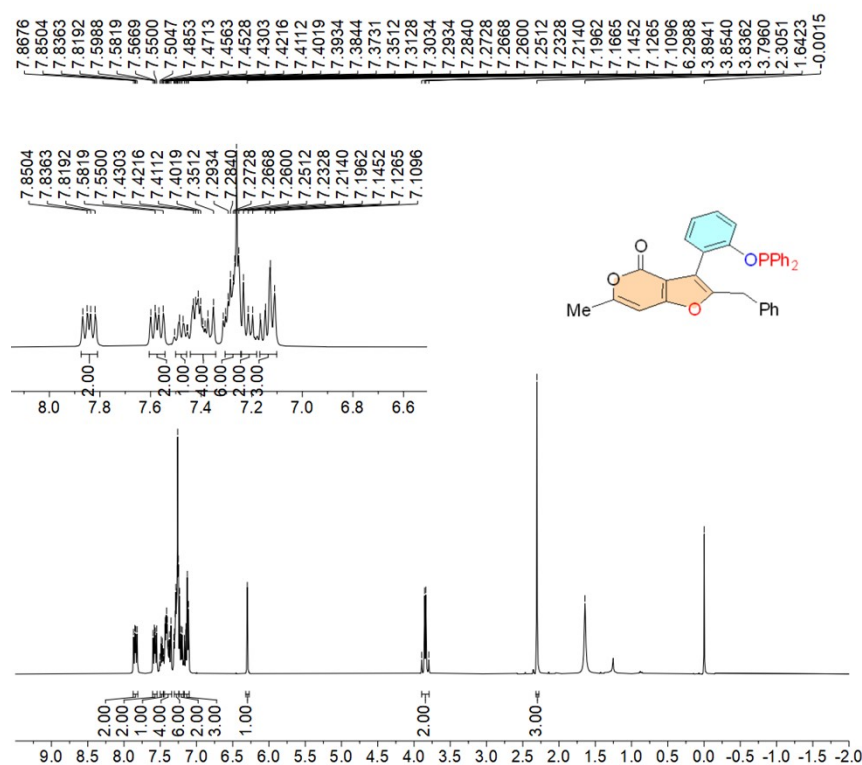


Parameter	值
1 Data File Name	E:/Old-老仪器谱图数据/2023-1-hw-H/34/fid
2 标题	2023-1-hw-H.34.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	294.9
11 Pulse Sequence	zg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/H/D-5.0-Z 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	2023-03-31T21:00:53
21 Modification Date	2023-03-31T21:00:04
22 Class	
23 Spectrometer Frequency	400.13
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.2
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13

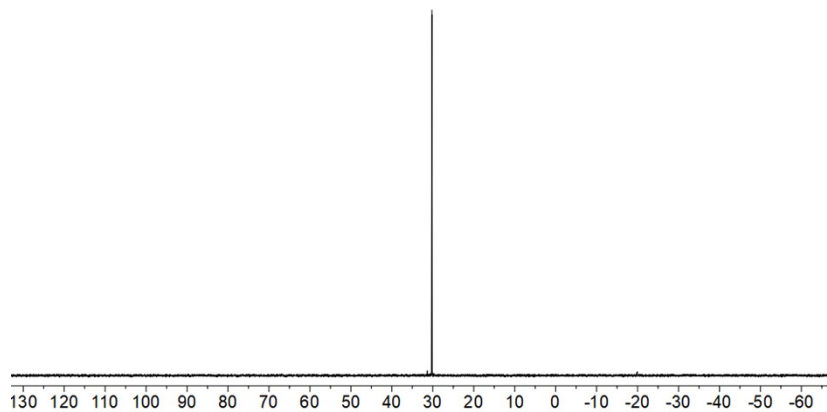
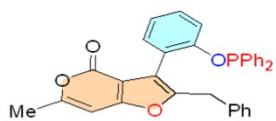


Parameter	值
1 Data File Name	E:/Old-老仪器谱图数据/2023-1-hw-C/4/fid
2 标题	2023-1-hw-C.4.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.5
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0032 (PI HR-400-S1-BBF/H/D-5.0-Z SP)
14 Number of Scans	3000
15 Receiver Gain	16.0
16 Relaxation Delay	2.0000
17 Pulse Width	10.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-04-01T06:42:47
21 Modification Date	2023-04-01T06:41:54
22 Class	
23 Spectrometer Frequency	100.62
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.5
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36

2-Benzyl-3-((diphenylphosphaneyl)oxy)phenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (13)

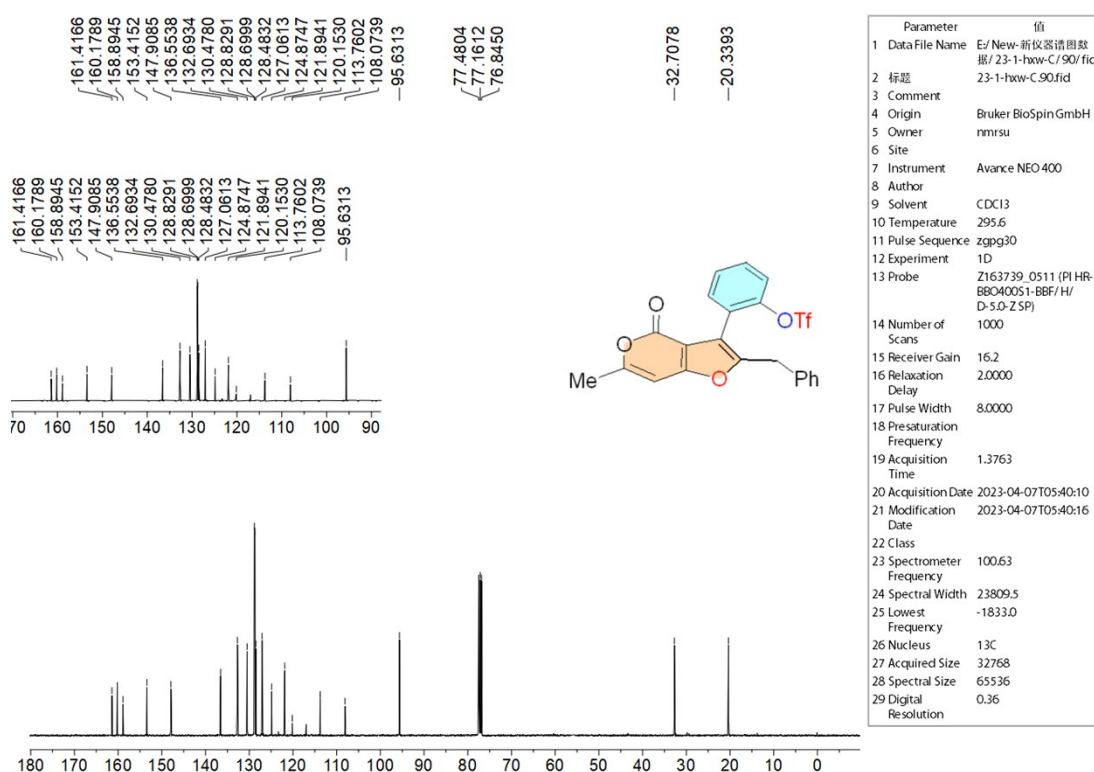
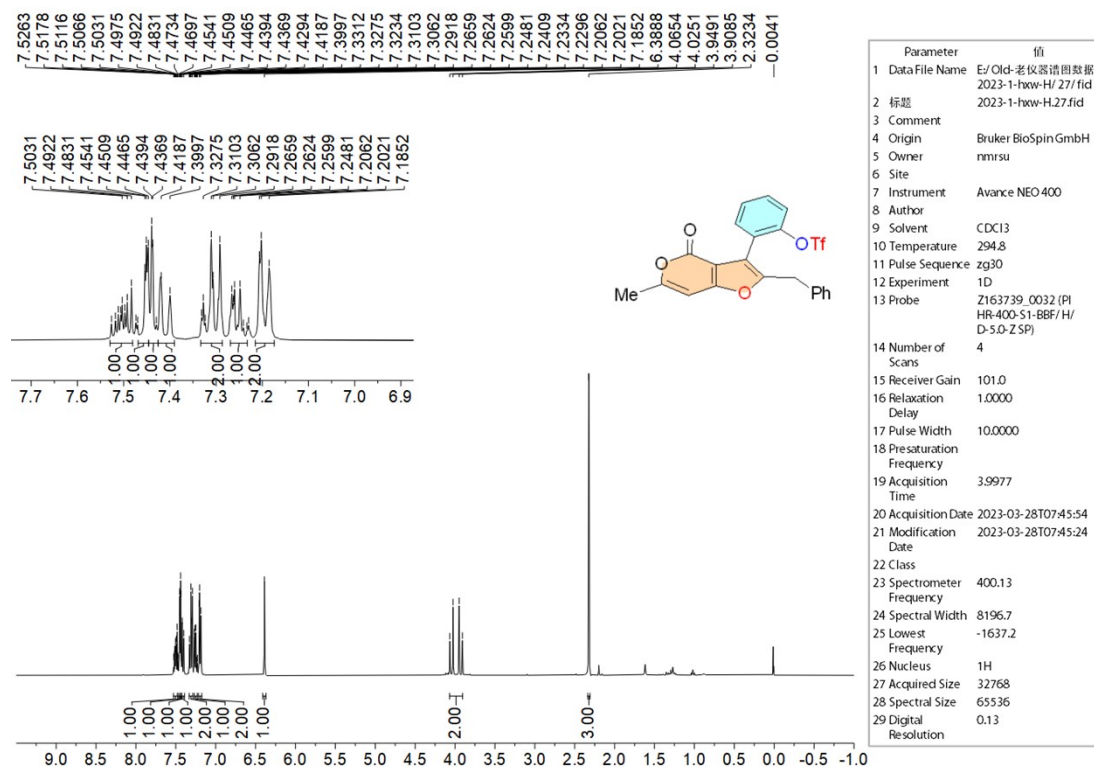


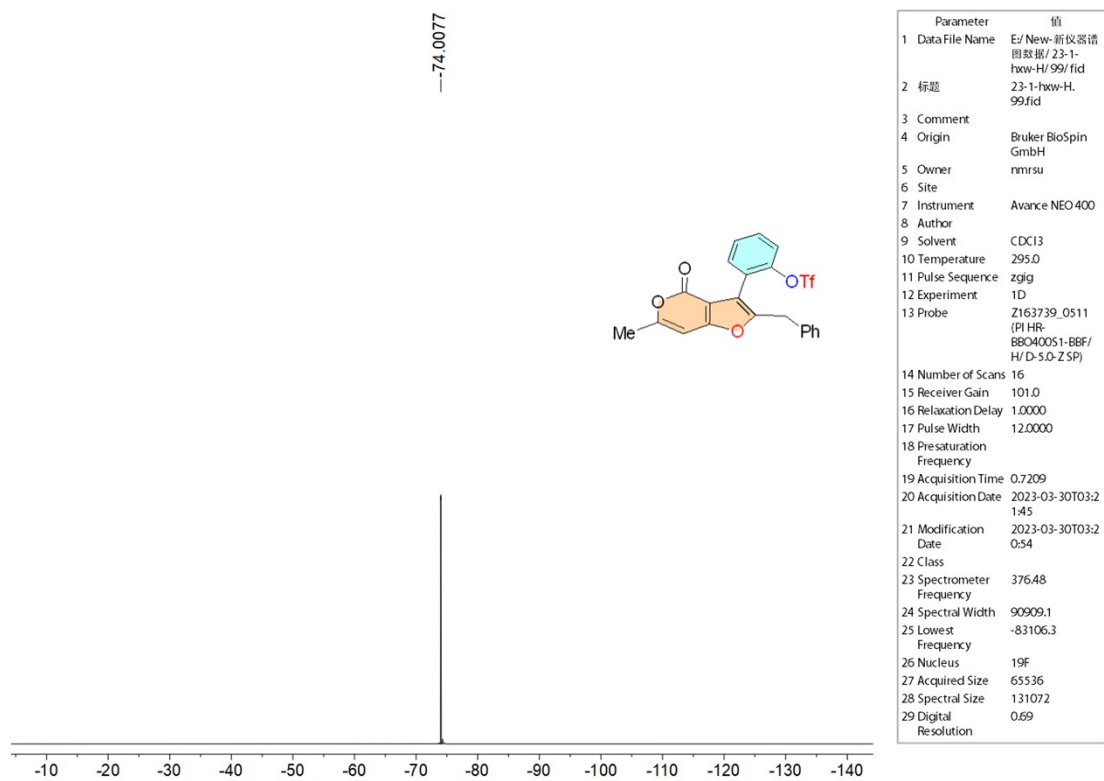
-30.2058



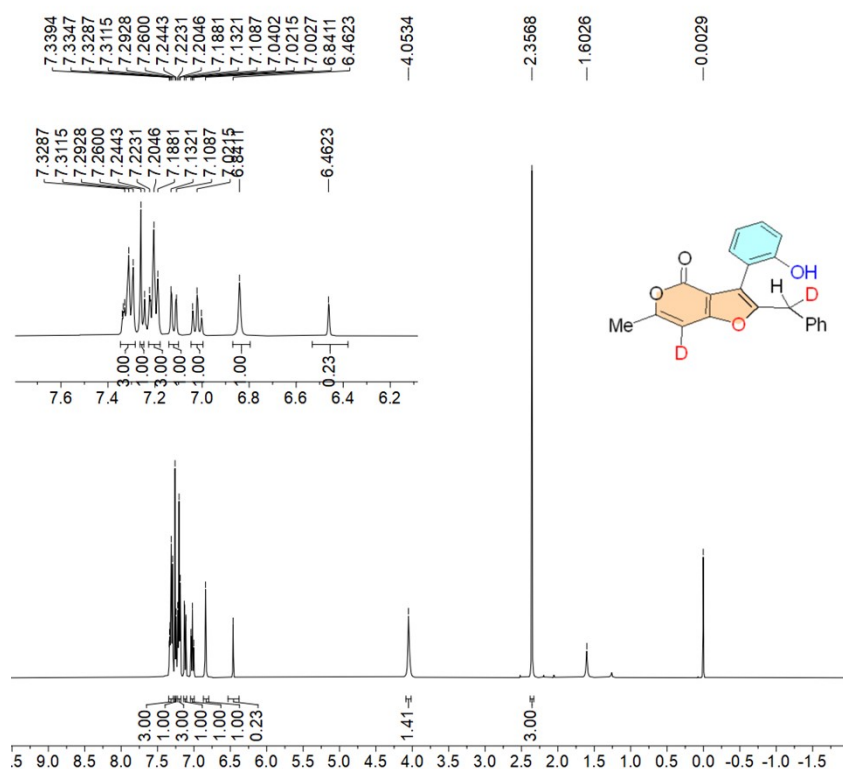
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1 Data File Name	E/ 2023.6.28核磁数据/ 23-1-hww-P/ 3/ fid
2 标题	23-1-hww-P.3.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl3
10 Temperature	295.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Probe	Z163739_0511 (PI HR-BBO40051-BBF/H/D-5.0-Z SP)
14 Number of Scans	16
15 Receiver Gain	101.0
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	0.4981
20 Acquisition Date	2023-03-30T08:13:38
21 Modification Date	2023-03-30T08:12:46
22 Class	
23 Spectrometer Frequency	161.98
24 Spectral Width	65789.5
25 Lowest Frequency	-40993.9
26 Nucleus	31P
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	1.00

2-(2-benzyl-6-methyl-4-oxo-4H-furo[3,2-c]pyran-3-yl)phenyl trifluoromethanesulfonate (14)

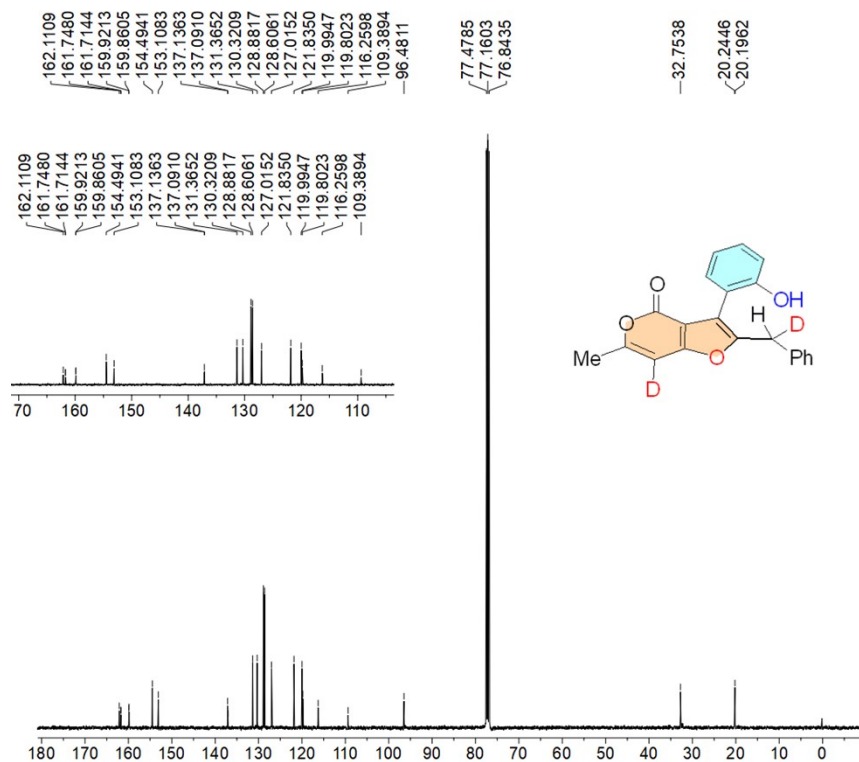




2-Benzyl-3-(2-hydroxyphenyl)-6-methyl-4H-furo[3,2-c]pyran-4-one (3aa-d)



Parameter	值
1 Data File Name	E:/ New-前仪器谱图数据/ 23-1-hww-H/ 33/ fid
2 标题	23-1-hww-H.33.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.4
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	2023-03-03T21:40:58
21 Modification Date	2023-03-03T21:40:00
22 Class	
23 Spectrometer Frequency	400.15
24 Spectral Width	8196.7
25 Lowest Frequency	-1637.1
26 Nucleus	¹ H
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.13



Parameter	值
1 Data File Name	E:/ New-前仪器谱图数据/ 23-1-hww-C/ 28/ fid
2 标题	23-1-hww-C.28.fid
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Instrument	Avance NEO 400
8 Author	
9 Solvent	CDCl ₃
10 Temperature	295.9
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	1024
15 Receiver Gain	16.2
16 Relaxation Delay	2.0000
17 Pulse Width	8.0000
18 Presaturation Frequency	
19 Acquisition Time	1.3763
20 Acquisition Date	2023-03-03T23:19:22
21 Modification Date	2023-03-03T23:18:28
22 Class	
23 Spectrometer Frequency	100.63
24 Spectral Width	23809.5
25 Lowest Frequency	-1833.0
26 Nucleus	¹³ C
27 Acquired Size	32768
28 Spectral Size	65536
29 Digital Resolution	0.36