Supporting Information

Visible-Light-Induced Acylation/Cyclization of Active Alkenes: Facile Access to Acylated Isoquinolinones

Yang Guo,† Peng-Fei Huang,† Yu Liu and Bin-Hong He*

[a] Department of Chemistry and Chemical Engineering, Hunan Institute of Science and Technology, Yueyang 414006, China

[phone and fax number: +86073-0864-0122 and E-mail addresses: hbhhd@126.com

List of Contents

1. General Information

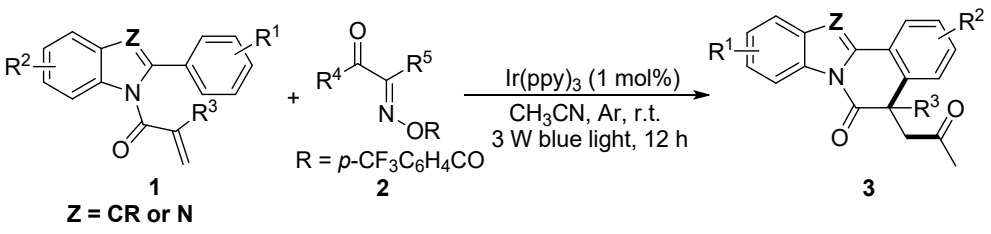
Unless otherwise stated, all commercial reagents were used as received. Propiophenone , aldehydes (Innochem, >98%), Phenylhydrazine hydrochloride and o-Phenylenediamine were used without further treatment. All reagents and solvents were commercially available and used without any further purification unless specified. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (0.25mm, 300-400 mesh). Analytical thin-layer chromatography was performed using glass plates pre-coated with 0.25mm 300-400 mesh silica gel impregnated with a fluorescent indicator (254 nm). All reactions were carried out with magnetic stirring and in dried glassware. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz, 376 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quated in Hz. The solvent peak was used as a reference value, for ^{1}H NMR: TMS = 0.00 ppm, for ^{13}C NMR: $CDCl_3$ = 77.00 ppm. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, dd = doublet of doublet, t = triplet, td = triplet of doublet, q = quartet, m = multiplet, and br = broad. High-resolution mass spectra (HRMS) were obtained on an Agilent mass spectrometer using ESI-TOF (electrospray ionization-time of flight).

2. Experiment Section

2.1. General Procedure for the Synthesis of Substrates

All 2-aryl indoles **1**[1] and acyl oxime esters **2**[2-3] were synthesized according to the known methods.

2.2. Typical Experimental Procedure



To a Schlenk tube were added 2-aryl indoles **1** (0.2 mmol, 0.1 M), acyl oxime esters **2** (0.3 mmol, 1.5 equiv), $Ir(ppy)_3$ (1mol %) and MeCN (2 mL) at room temperature under irradiation of 3 W blue light for 12 h. Until complete consumption of the starting material was observed by TLC and/or GC-MS analysis. After the reaction was finished, the reaction mixture removal of the solvent, the crude product was purified by column chromatography (petroleum ether/ethyl acetate, 5 : 1) to provide the desired products **3**. A scaled-up experiment conducted in the presence of **1a** (1 mmol), **2a** (1.5 mmol, 1.5 equiv), $Ir(ppy)_3$ (0.01 mmol, 1 mol %) and MeCN (10 mL) at 25 °C under irradiation of 3 W blue light for 12 h gave the target product **3aa** in 77% yield.

The light source bought from SANYI (https://item.taobao.com/item.htm?spm=a1z09.2.0.0.42672e8dv2Chsz&id=35497290577&_u=j35sh1qt9325), 3 W blue LED light bulb (E27). The wavelength was about 460-470 nm and the wavelength of peak intensity was about 467.5 nm. The pictures of the visible-light source (Figure S1) were shown as follow:

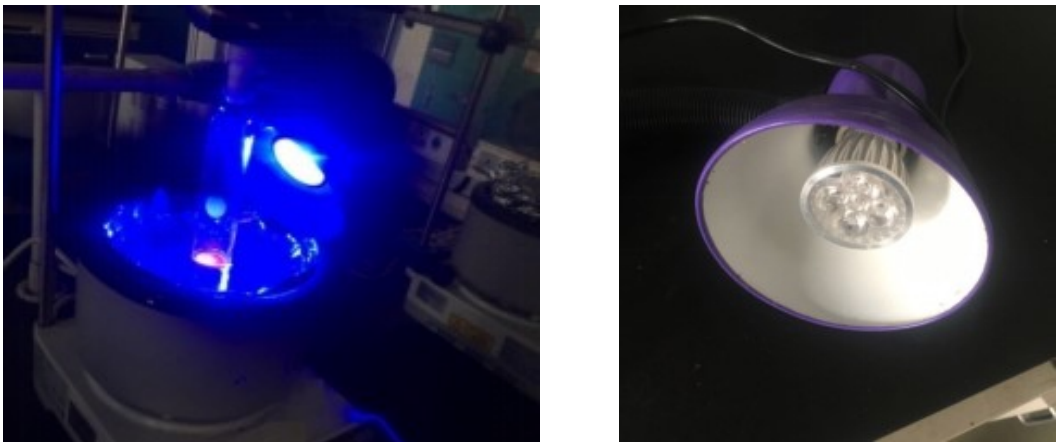
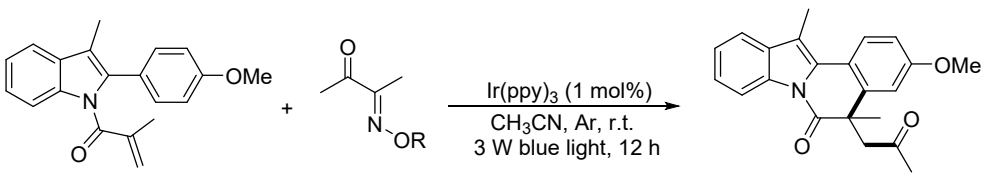


Figure S1. Pictures of Visible-Light Source.

2.3. Table S1: Screening of optimal *O*-benzoic acyl oxime [a]



1a **2** **3aa**

2a, R = *p*-$CF_3C_6H_4CO$
2a-1 R = 4-FC_6H_4CO
2a-2 R = 4-$NO_2C_6H_4CO$
2a-3 R = 4-$OMeC_6H_4CO$
2a-4, R = C_6F_5CO
2a-5, R = C_6H_5CO
2a-6, R = CF_3CO

entry	variation from the standard conditions	yield (%)[b]

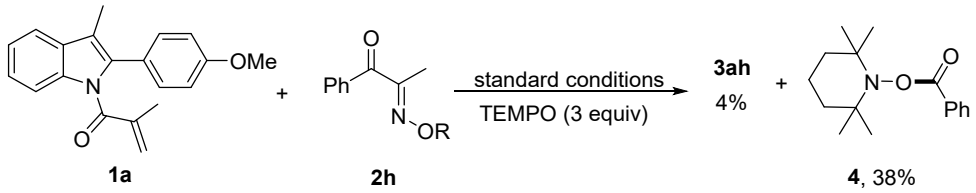
1	**2a**	93
2[c]	**2a-1** instead of **2a**	82
3	**2a-2** instead of **2a**	76
4	**2a-3** instead of **2a**	63
5	**2a-4** instead of **2a**	71
6	**2a-5** instead of **2a**	62
7[c]	**2a-6** instead of **2a**	72

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol, 1.5 equiv), $Ir(ppy)_3$ (1 mol%) and MeCN (2 mL) at 25 °C under irradiation of 3 W blue light for 12 h. [b] Isolated yield. [c] Most of starting materials were decomposed.

The results showed that the ester leaving groups had a significant impact on the reaction and none of these oxime esters gave better yield than that of *O*-4-$CF_3C_6H_4CO$ acyl oximes. Notably, *O*-acetic acyl oximes **2a-6** could undergo the acylation/cyclization and furnish the difunctional product **3aa** in 72% yeild (entry 7).

2.4 Control Experiments.

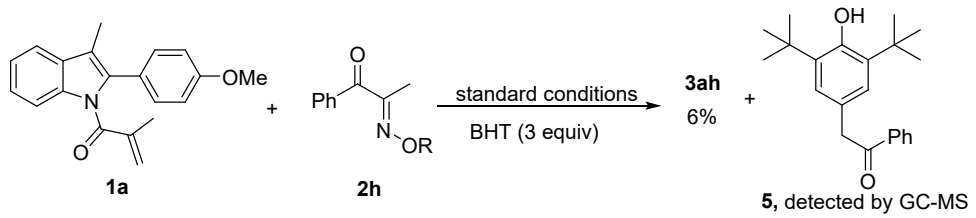
2.4.1 Using TEMPO as Radical Inhibitor



1a **2h** **4**, 38%

To a Schlenk tube were added 2-aryl indoles **1a** (0.2 mmol, 0.1 M), acyl oxime esters **2h** (0.3 mmol, 1,5 equiv), $Ir(ppy)_3$ (1mol%), TEMPO (3 equiv) and MeCN (2 mL) at room temperature under irradiation of 3 W blue light for 12 h. The GC-MS analysis of raw reaction mixture showed that onyl 4% yield of target product **3ah** was detected. Additionally, the Cyclohexan-trapping products **4** could be obtained in 38% yield.

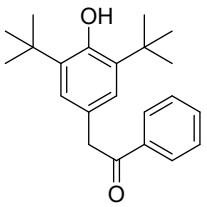
2.4.2 Using BHT as Radical Inhibitor



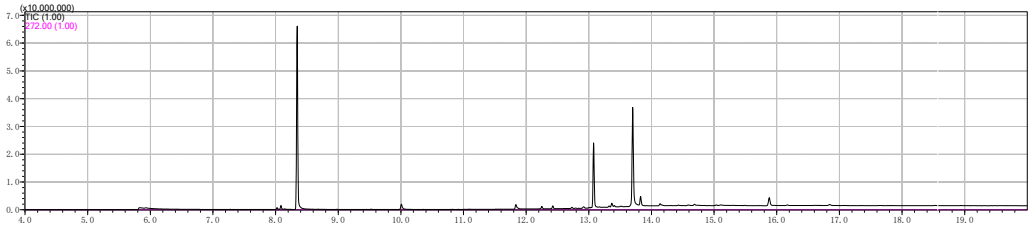
1a **2h** **5**, detected by GC-MS

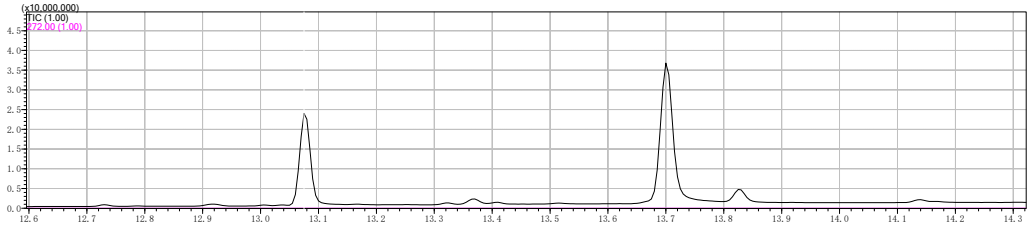
To a Schlenk tube were added 2-aryl indoles **1a** (0.2 mmol, 0.1 M), acyl oxime esters **2h** (0.3 mmol, 1.5 equiv), $Ir(ppy)_3$ (1mol %), BHT (3 equiv) and MeCN (2 mL) at room temperature under irradiation of 3 W blue light for 12 h. The GC-MS analysis of raw

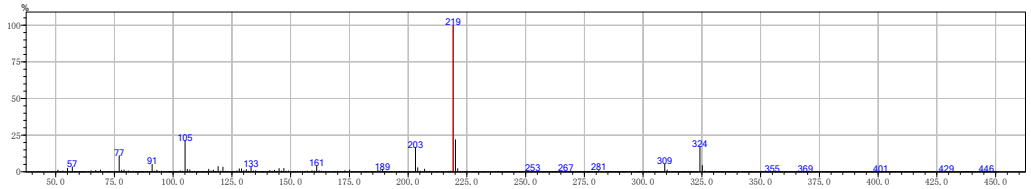
reaction mixture showed that onyl 6% yield of target product **3ah** was detected. Additionally, the Cyclohexan-trapping products **5** could be detected by GC-MS analysis of raw reaction mixture.



Chemical Formula: $C_{22}H_{28}O_2$
Exact Mass: 324.20893
Molecular Weight: 324.46400







[MS Spectrum]
# of Peaks 401
Raw Spectrum 13.075
(scan : 1816)
Background No
Background Spectrum
Base Peak m/z 219.15
(Inten : 8,126,740)
Event# 1
m/z Absolute Intensity
Relative Intensity

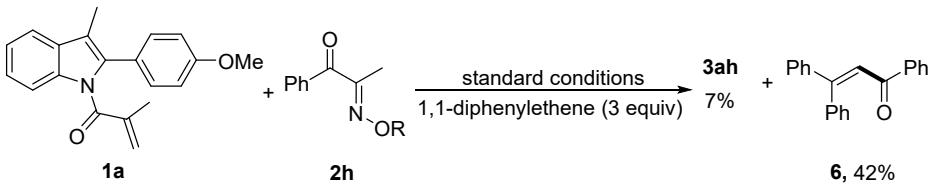
50.00	13796	0.17
51.00	94302	1.16
52.05	12733	0.16
53.05	50466	0.62
54.15	4698	0.06
55.05	199361	2.45
56.10	20294	0.25
57.10	264783	3.26
58.05	14683	0.18
59.05	14466	0.18
60.05	977	0.01
61.00	1258	0.02
61.95	1411	0.02
63.00	10023	0.12
64.00	6967	0.09
65.05	55123	0.68
66.05	9703	0.12
67.05	70010	0.86
68.10	5300	0.07
69.05	103757	1.28
70.05	6852	0.08
71.05	4358	0.05
72.00	2258	0.03
73.00	21858	0.27
74.00	5228	0.06
75.00	9017	0.11
76.05	26144	0.32
77.05	894066	11.00

78.05	84419	1.04	122.15	28168	0.35	166.05	8871	0.11
79.05	101254	1.25	123.15	30532	0.38	167.10	8065	0.10
80.05	28385	0.35	124.20	3406	0.04	168.10	2865	0.04
81.05	50667	0.62	125.15	2848	0.04	169.10	7657	0.09
82.10	7430	0.09	126.15	4566	0.06	170.10	33054	0.41
83.10	32425	0.40	127.10	46895	0.58	171.05	23321	0.29
84.05	2467	0.03	128.10	165895	2.04	172.10	7532	0.09
85.05	2406	0.03	129.10	167007	2.06	173.10	63905	0.79
86.05	1420	0.02	130.10	61473	0.76	174.10	21740	0.27
87.05	3128	0.04	131.10	128266	1.58	175.10	101194	1.25
88.15	4188	0.05	132.15	27698	0.34	176.10	18844	0.23
89.10	19870	0.24	133.15	251306	3.09	177.05	10279	0.13
90.15	8122	0.10	134.15	46999	0.58	178.05	18149	0.22
91.05	409645	5.04	135.15	65403	0.80	179.10	15684	0.19
92.05	41218	0.51	136.10	7556	0.09	180.05	4908	0.06
93.10	84231	1.04	137.10	3278	0.04	181.05	9719	0.12
94.10	17662	0.22	138.15	520	0.01	182.05	2867	0.04
95.10	38830	0.48	139.05	5238	0.06	183.05	5733	0.07
96.05	19005	0.23	140.15	2916	0.04	184.05	1939	0.02
97.05	11163	0.14	141.10	69783	0.86	185.10	21452	0.26
98.00	1108	0.01	142.10	42786	0.53	186.15	5623	0.07
99.00	918	0.01	143.10	82852	1.02	187.10	83794	1.03
100.15	776	0.01	144.10	34138	0.42	188.10	65183	0.80
101.15	4989	0.06	145.10	179671	2.21	189.10	127622	1.57
102.05	14124	0.17	146.10	45359	0.56	190.05	21846	0.27
103.05	51307	0.63	147.10	186410	2.29	191.00	30010	0.37
104.05	29386	0.36	148.10	30198	0.37	192.05	10650	0.13
105.05	1719710	21.16	149.10	45572	0.56	193.00	15473	0.19
106.05	142412	1.75	150.10	5554	0.07	194.05	6178	0.08
107.10	109340	1.35	151.05	3886	0.05	195.05	6364	0.08
108.10	13262	0.16	152.10	14982	0.18	196.05	1840	0.02
109.10	26700	0.33	153.05	22596	0.28	197.05	7930	0.10
110.15	3674	0.05	154.10	12855	0.16	198.05	1155	0.01
111.05	3950	0.05	155.10	33668	0.41	199.10	4364	0.05
112.15	764	0.01	156.10	31092	0.38	200.05	2210	0.03
113.15	1575	0.02	157.10	38057	0.47	201.10	6041	0.07
114.15	2521	0.03	158.10	15202	0.19	202.15	16303	0.20
115.10	139967	1.72	159.10	61177	0.75	203.10	1341182	16.50
116.10	47463	0.58	160.10	35369	0.44	204.10	230124	2.83
117.10	97487	1.20	161.10	306918	3.78	205.10	35722	0.44
118.15	21576	0.27	162.10	56060	0.69	206.05	8071	0.10
119.15	290527	3.57	163.10	39820	0.49	207.00	151044	1.86
120.15	41763	0.51	164.10	5850	0.07	208.00	33476	0.41
121.15	258600	3.18	165.05	23411	0.29	209.05	34939	0.43

210.05	7257	0.09	254.10	6305	0.08	298.20	102	0.00
211.05	4571	0.06	255.10	1009	0.01	299.20	16	0.00
212.05	1530	0.02	256.10	239	0.00	300.20	2	0.00
213.10	6738	0.08	257.00	519	0.01	301.20	113	0.00
214.10	1294	0.02	258.15	903	0.01	302.20	34	0.00
215.10	8442	0.10	259.15	688	0.01	303.20	76	0.00
216.10	5210	0.06	260.10	550	0.01	304.20	49	0.00
217.10	34148	0.42	261.10	743	0.01	305.20	271	0.00
218.15	38402	0.47	262.15	571	0.01	306.20	801	0.01
219.15	8126740	100.00	263.10	1593	0.02	307.15	5745	0.07
220.15	1778861	21.89	264.15	1148	0.01	308.25	14035	0.17
221.10	176478	2.17	265.10	18254	0.22	309.20	420929	5.18
222.15	15442	0.19	266.10	10647	0.13	310.20	99578	1.23
223.10	10466	0.13	267.10	22057	0.27	311.20	12151	0.15
224.10	2484	0.03	268.10	6268	0.08	312.20	1278	0.02
225.10	33041	0.41	269.00	2930	0.04	313.20	52	0.00
226.10	6206	0.08	270.00	660	0.01	314.20	108	0.00
227.05	1373	0.02	271.10	338	0.00	315.20	33	0.00
228.05	1630	0.02	272.10	145	0.00	316.20	14	0.00
229.05	2924	0.04	273.10	343	0.00	317.20	55	0.00
230.15	1584	0.02	274.10	116	0.00	318.20	132	0.00
231.15	6791	0.08	275.10	1022	0.01	319.20	130	0.00
232.05	3073	0.04	276.25	259	0.00	320.20	108	0.00
233.10	9295	0.11	277.15	1207	0.01	321.15	1051	0.01
234.10	6631	0.08	278.10	398	0.00	322.20	3695	0.05
235.10	19441	0.24	279.15	2468	0.03	**323.25**	**6987**	**0.09**
236.10	4458	0.05	280.15	1220	0.02	**324.20**	**1391135**	**17.12**
237.10	7116	0.09	281.10	79183	0.97	**325.20**	**345222**	**4.25**
238.10	1710	0.02	282.10	20060	0.25	**326.20**	**41100**	**0.51**
239.10	3199	0.04	283.05	10439	0.13	327.15	5861	0.07
240.05	738	0.01	284.10	2190	0.03	328.05	896	0.01
241.15	924	0.01	285.05	611	0.01	329.10	306	0.00
242.05	668	0.01	286.10	132	0.00	330.10	134	0.00
243.15	1824	0.02	287.10	134	0.00	331.10	106	0.00
244.15	1267	0.02	288.10	60	0.00	332.10	22	0.00
245.10	1798	0.02	289.10	490	0.01	333.10	63	0.00
246.05	745	0.01	290.10	105	0.00	334.10	57	0.00
247.05	1453	0.02	291.15	2856	0.04	335.10	52	0.00
248.05	1343	0.02	292.20	722	0.01	336.10	111	0.00
249.05	10392	0.13	293.15	21595	0.27	337.10	308	0.00
250.05	3632	0.04	294.15	5133	0.06	338.10	100	0.00
251.05	8335	0.10	295.15	5004	0.06	338.95	467	0.01
252.05	3144	0.04	296.05	1501	0.02	340.15	233	0.00
253.10	33044	0.41	297.20	364	0.00	341.05	3990	0.05

342.10	1708	0.02	348.00	31	0.00	354.10	188	0.00
343.00	1068	0.01	349.00	78	0.00	355.05	7521	0.09
344.00	201	0.00	350.00	73	0.00	356.10	2646	0.03
345.00	170	0.00	351.00	183	0.00	357.10	1897	0.02
346.00	76	0.00	352.00	52	0.00			
347.00	81	0.00	353.00	140	0.00			

2.4.3 Using 1,1-diphenylethene as Radical Inhibitor



To a Schlenk tube were added 2-aryl indoles **1h** (0.2 mmol, 0.1 M), acyl oxime esters **2h** (0.3 mmol, 1.5 equiv), $Ir(ppy)_3$ (1mol%), 1,1-diphenylethene (3 equiv) and MeCN (2 mL) at room temperature under irradiation of 3 W blue light for 12 h. The GC-MS analysis of raw reaction mixture showed that onyl 7% yield of target product **3ah** was detected. The benzoyl-trapping products **6** could be obtained in 42% yield.

3. References

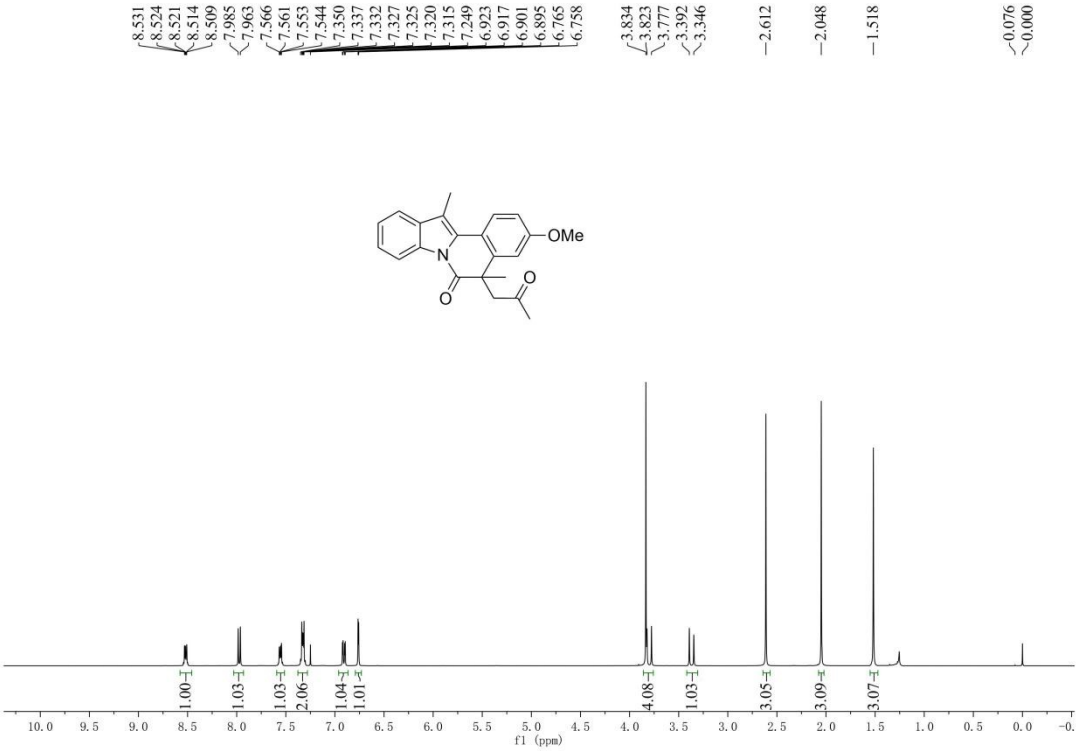
[1] Y.-L. Wei, J.-Q. Chen, B. Sun, P.-F. Xu, *Chem. Commun.* 2019, **55**, 5922.

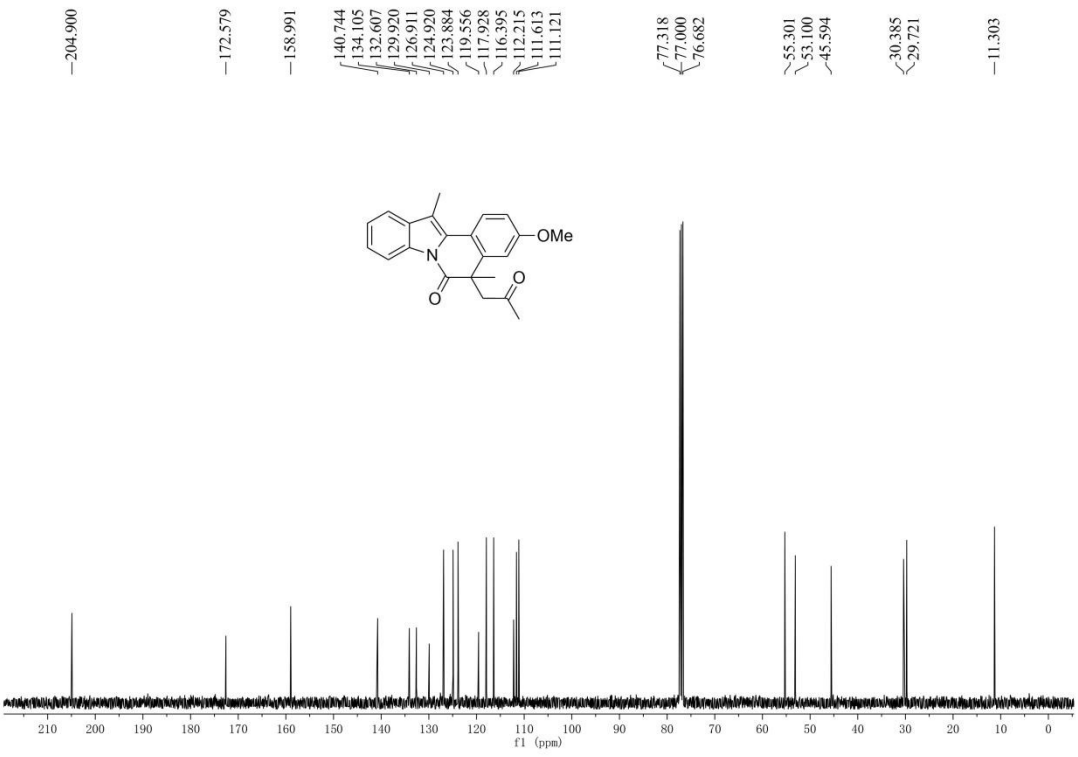
[2] P. Chen, J. Xie, Z. Chen, B.-Q. Xiong, Y. Liu, C.-A. Yang and K.-W. Tang, *Adv. Synth. Catal.,* 2021, **363**, 4440.

[3] X. Fan, T. Lei, B. Chen, C.-H. Tung and L.-Z. Wu, *Org. Lett.,* 2019, **21**, 4153.

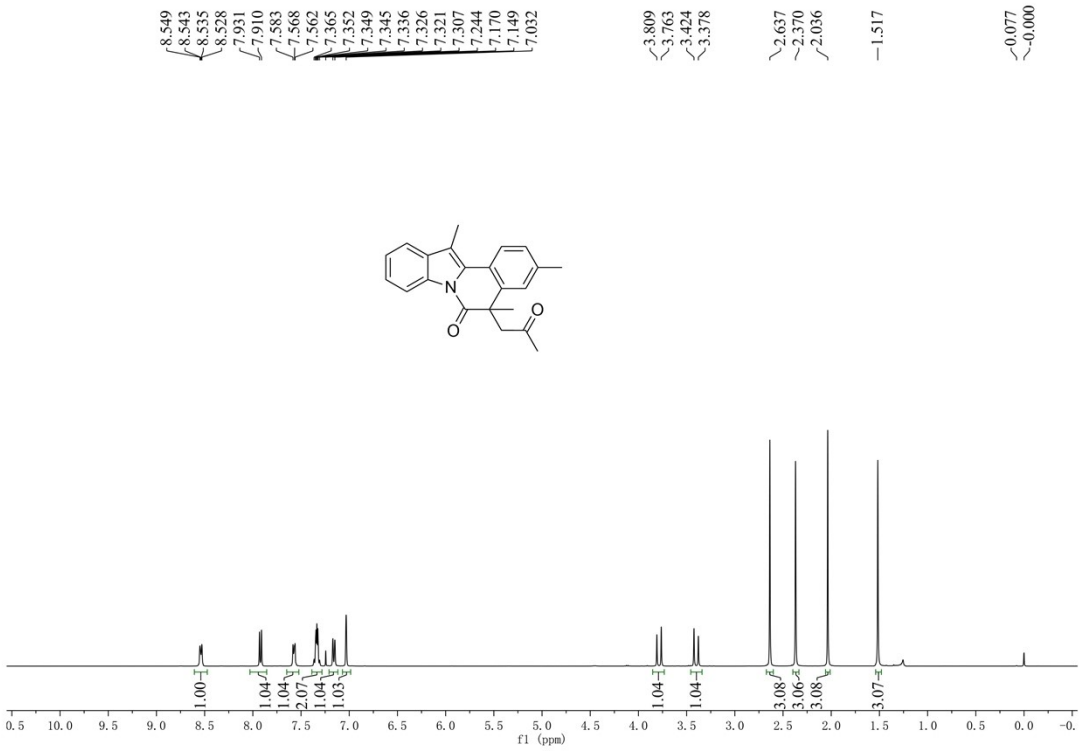
4. Spectra

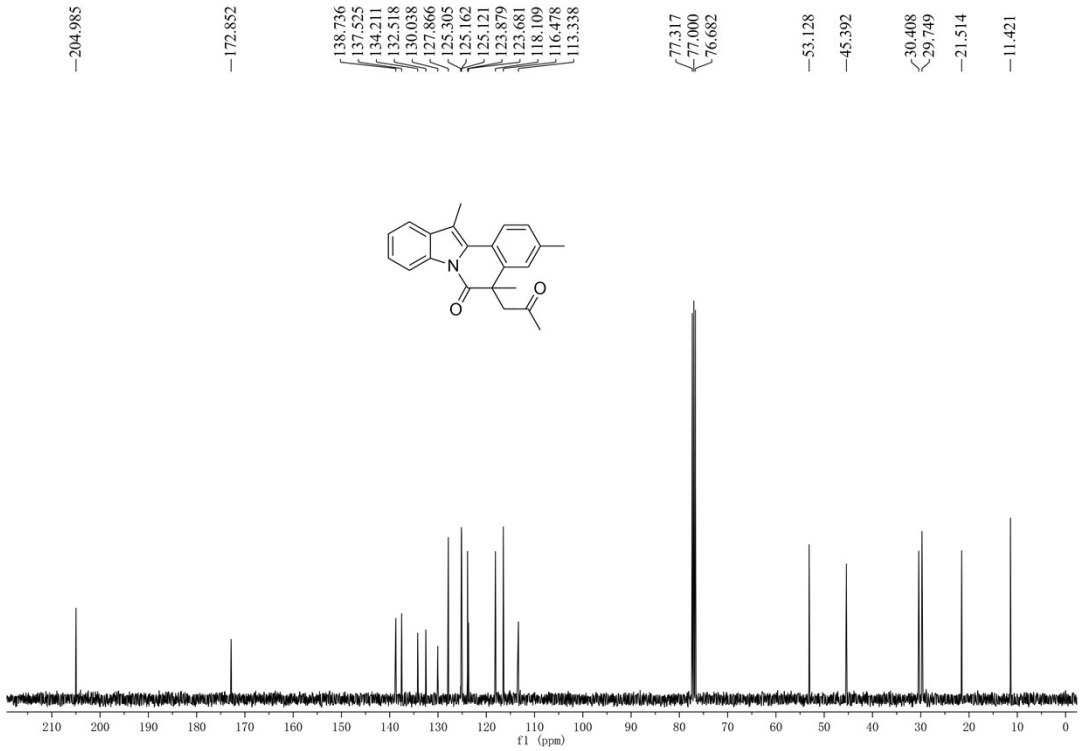
3-Methoxy-5,12-dimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3aa)



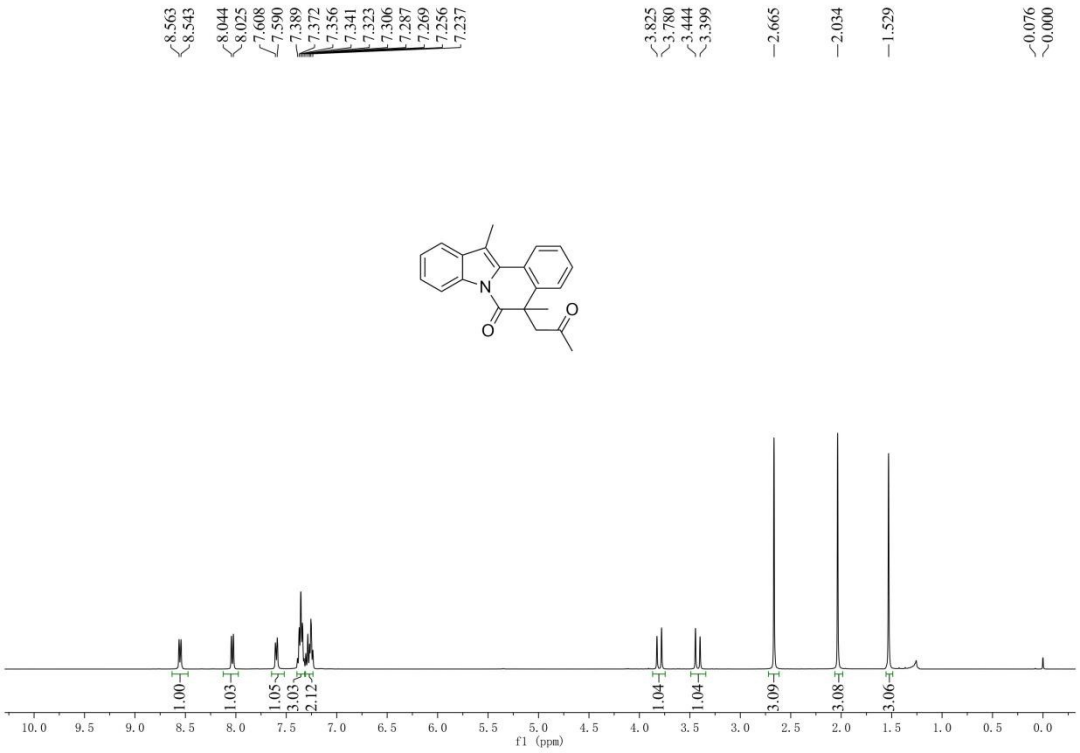


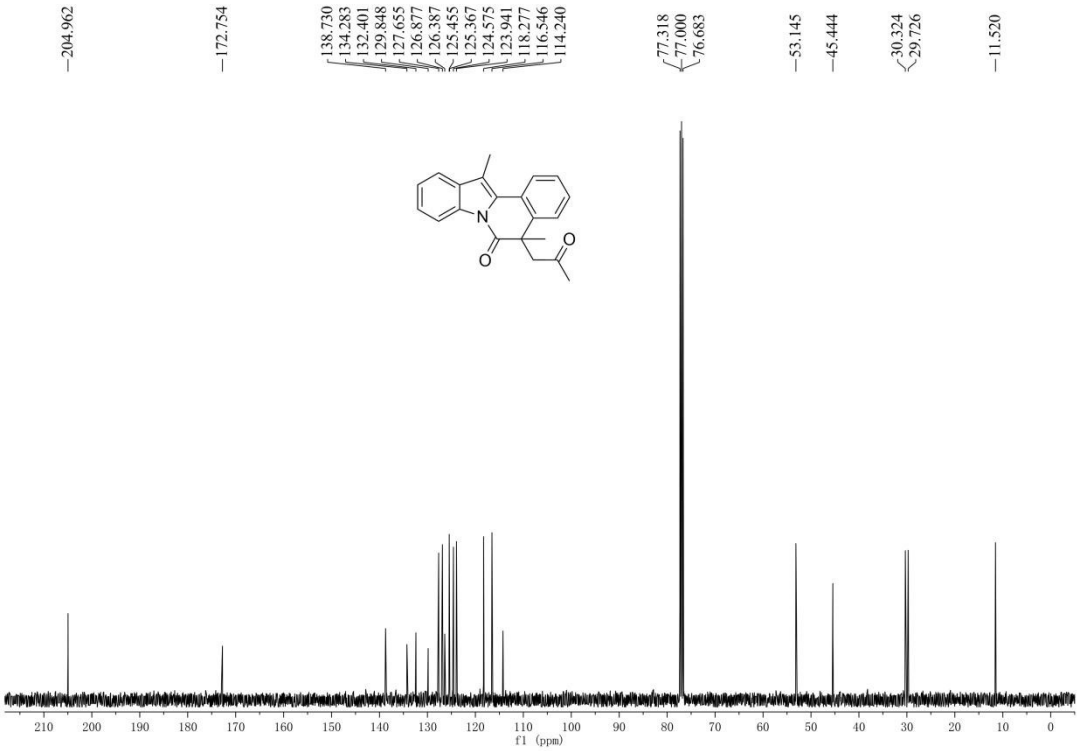
3,5,12-Trimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ba)



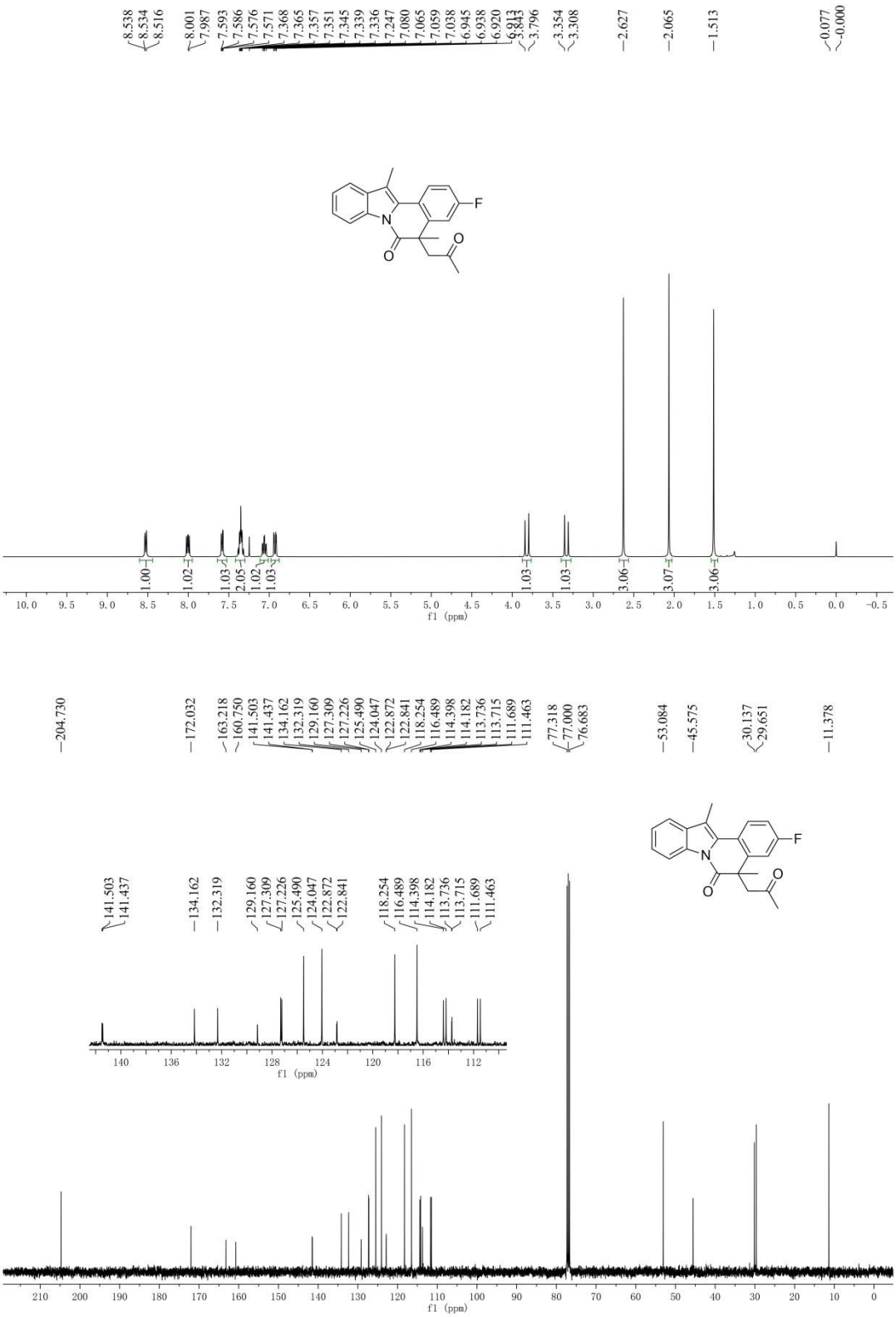


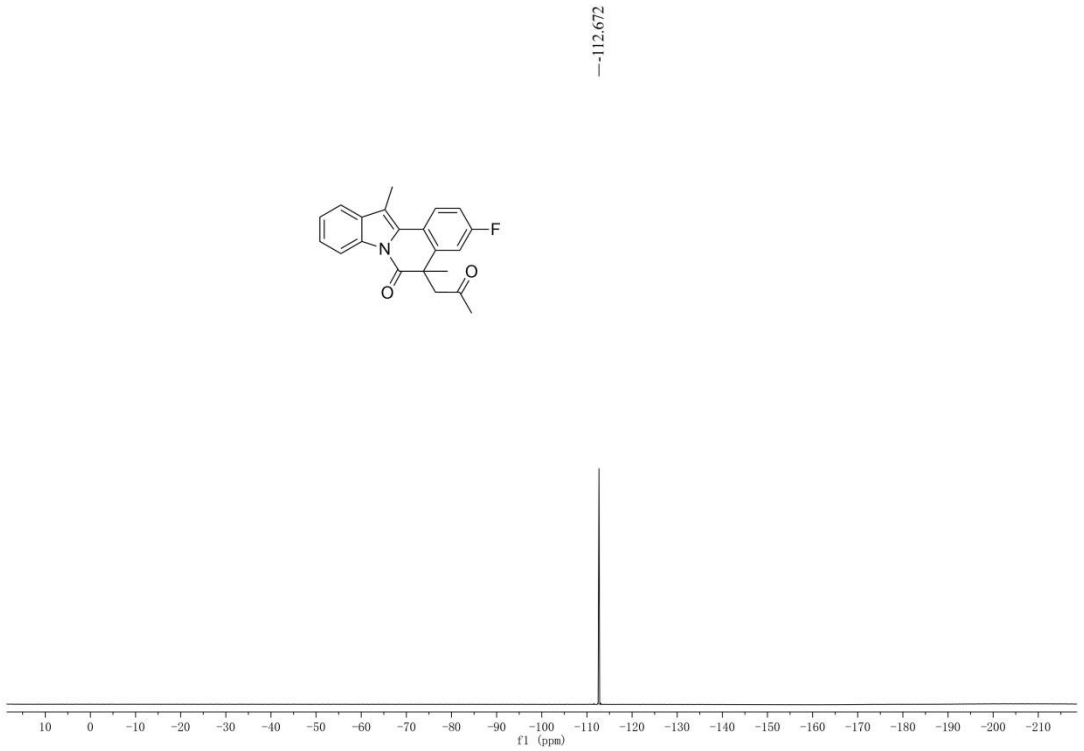
5,12-Dimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ca)



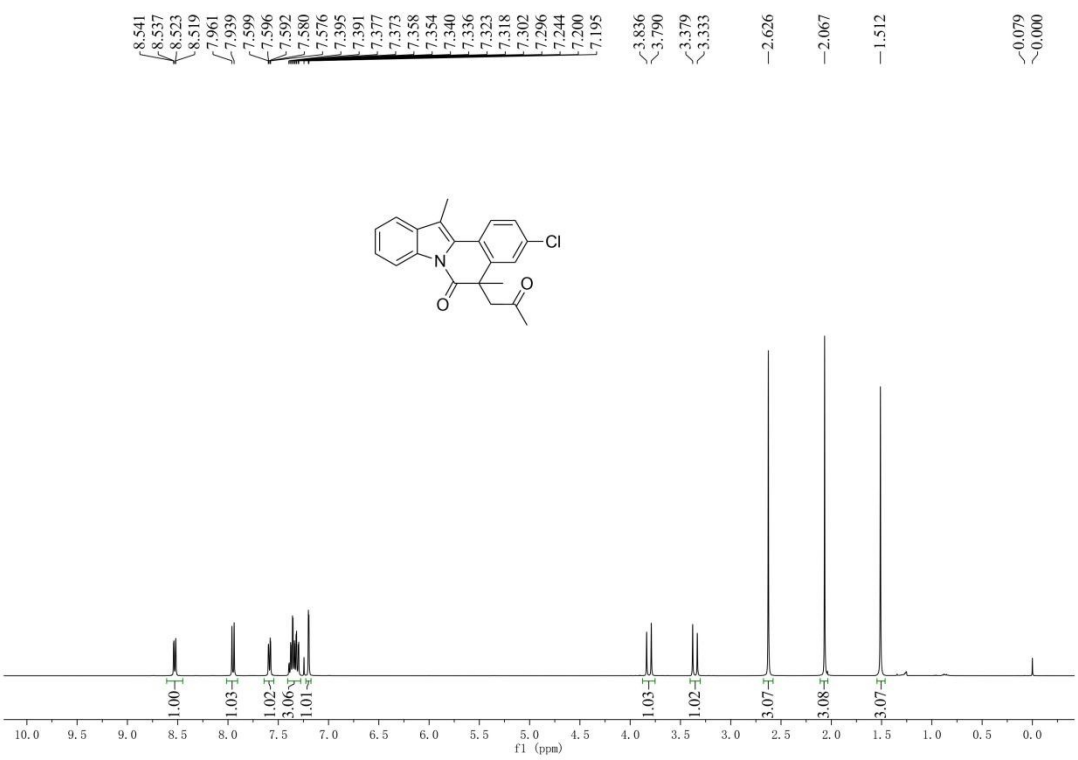


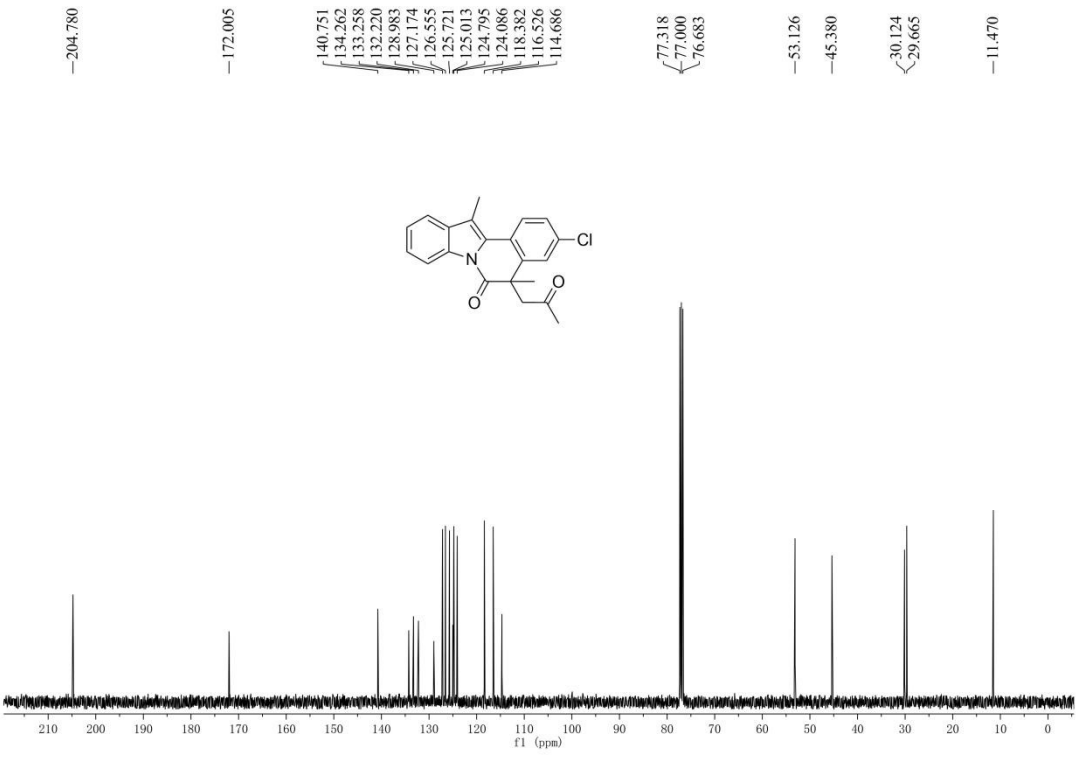
3-Fluoro-5,12-dimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3da)



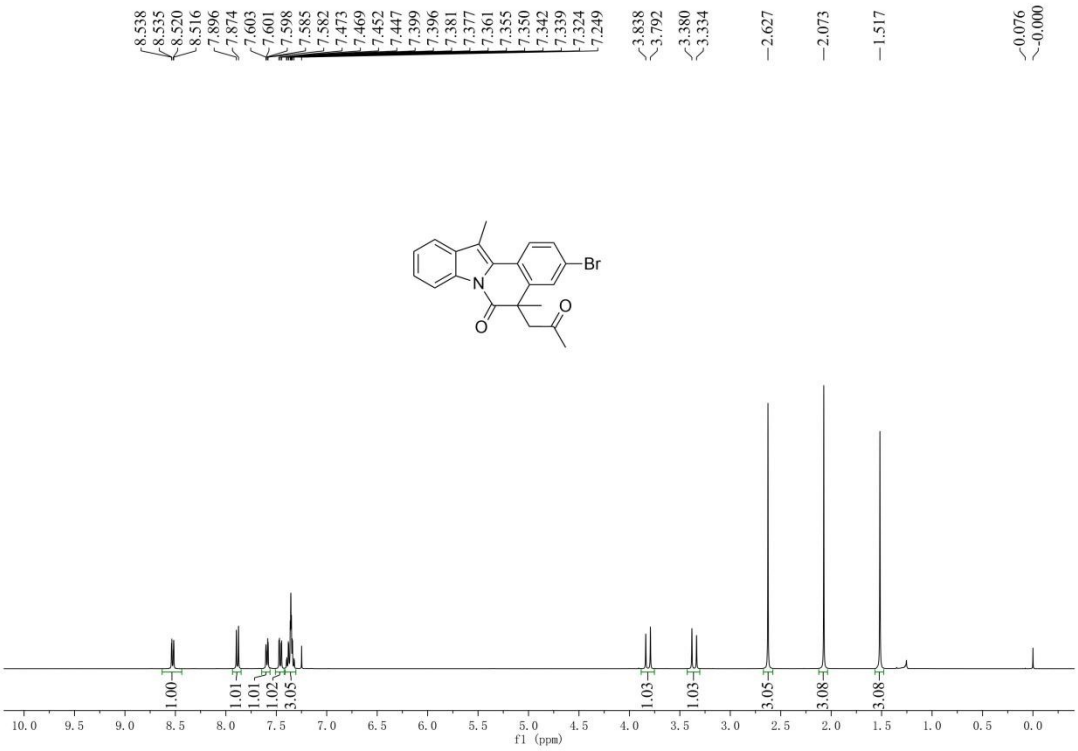

-112.672
F
N
O
O
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

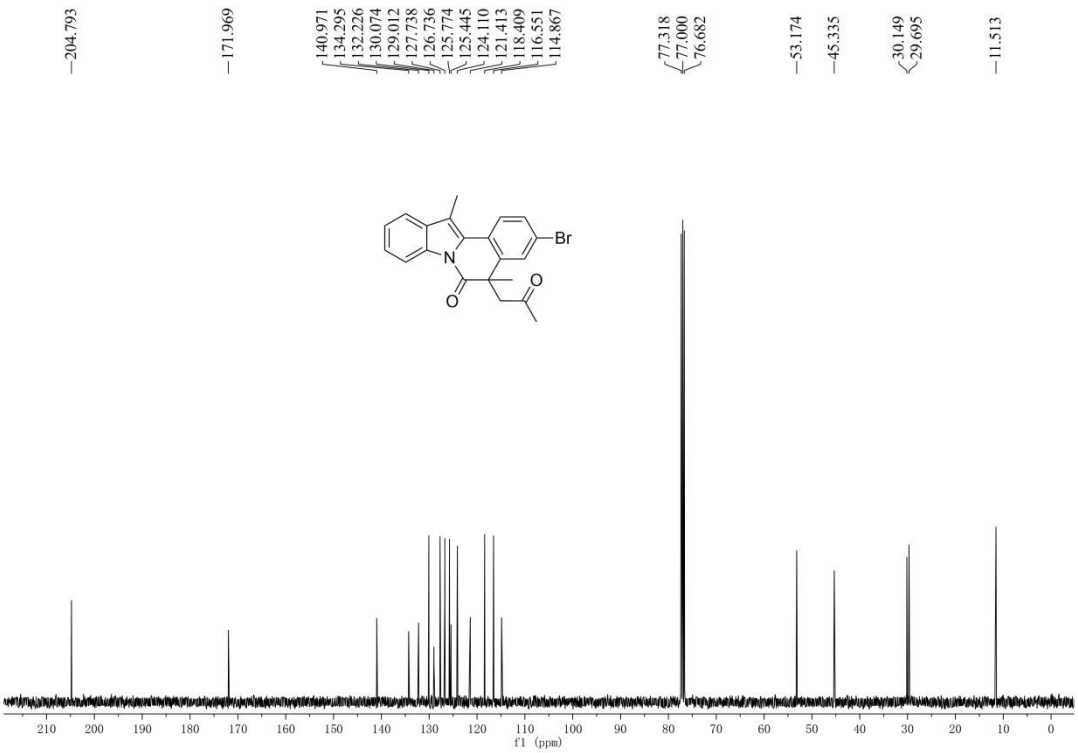
3-Chloro-5,12-dimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ea)



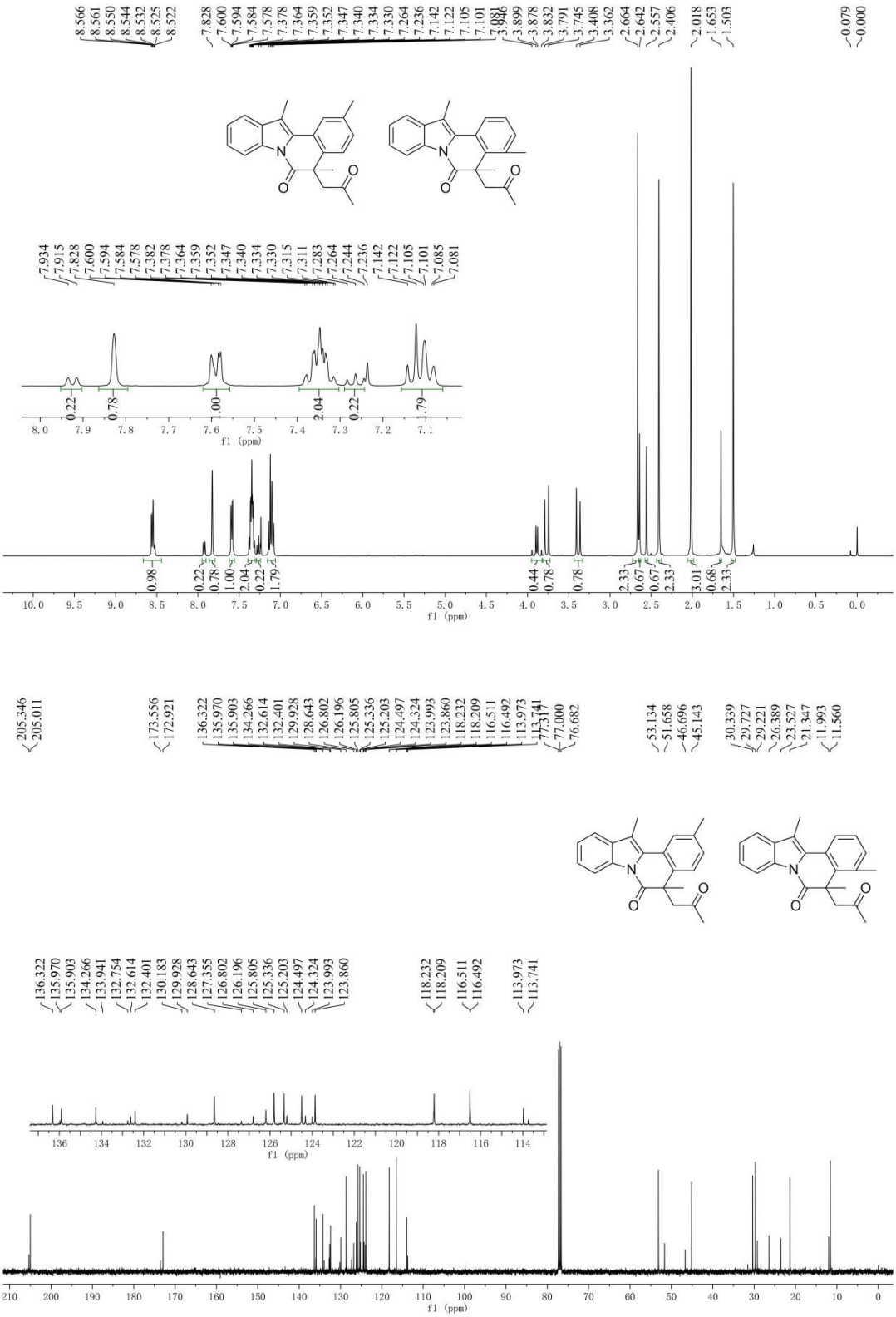


3-Bromo-5,12-dimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3fa)

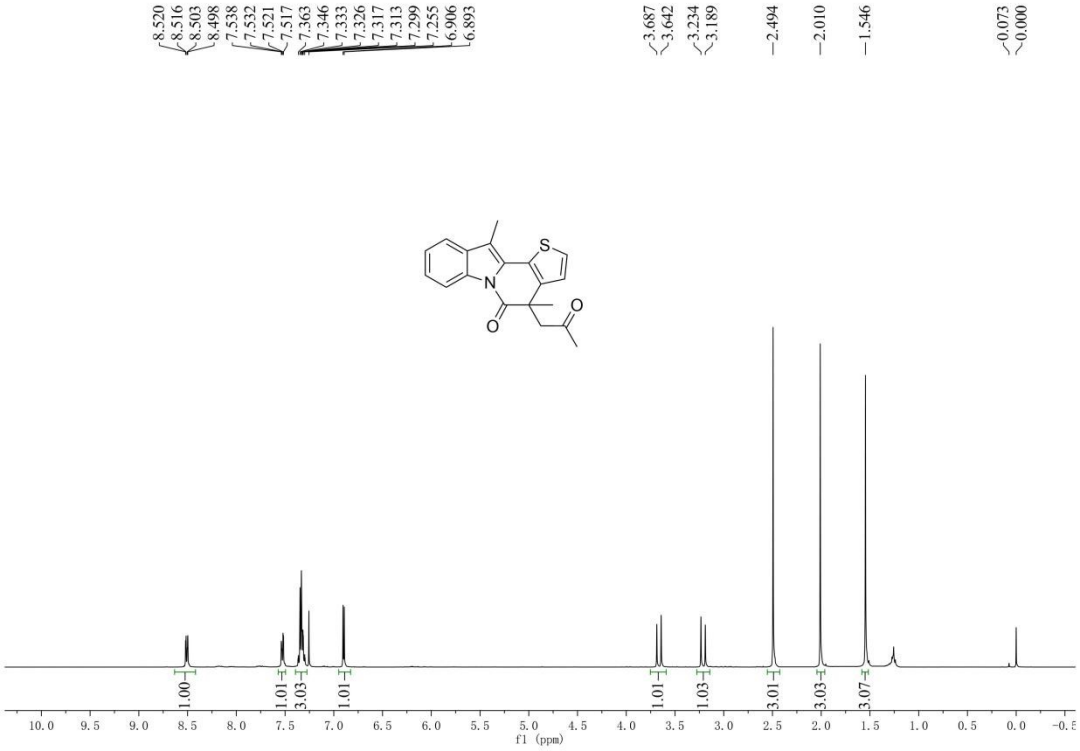


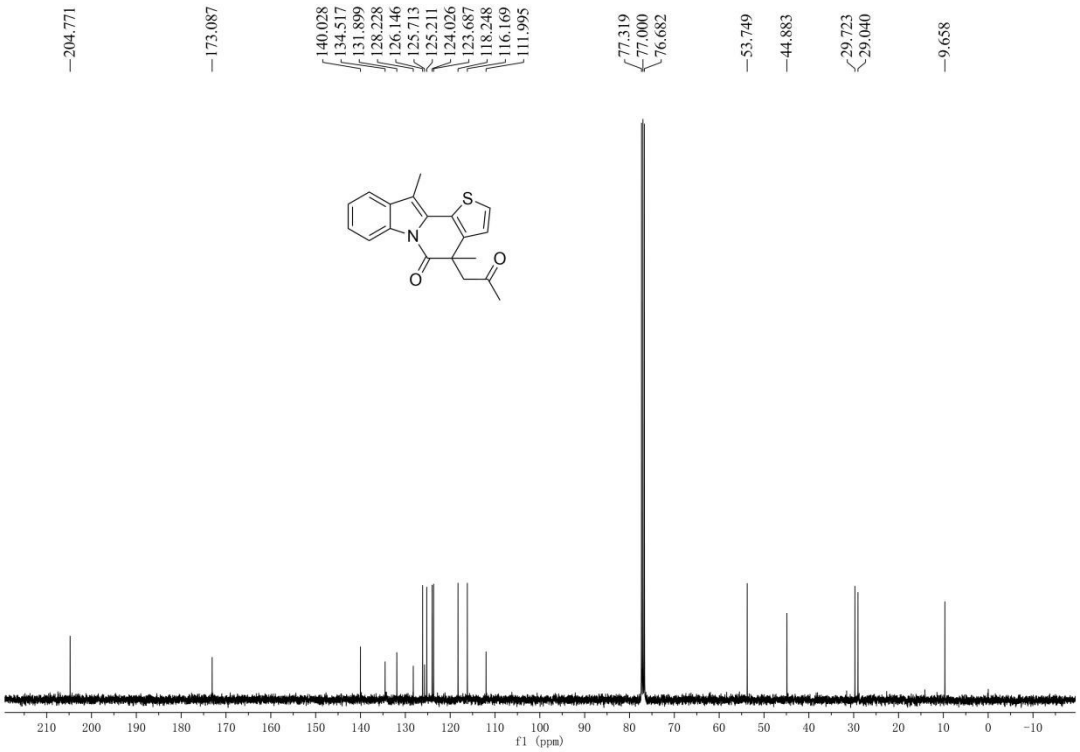


2,5,12-Trimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ga) and 4,5,12-Trimethyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ga')

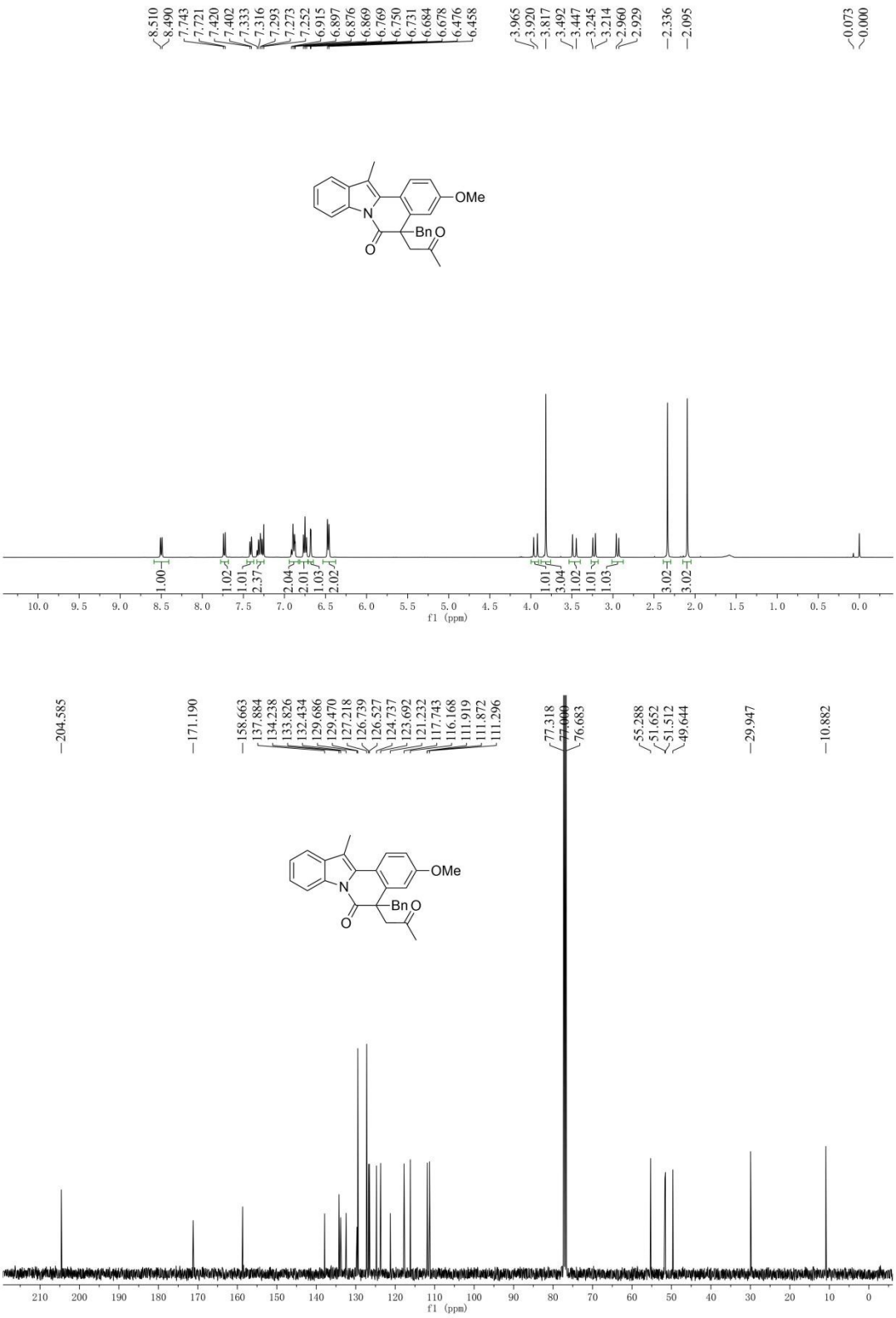


4,11-Dimethyl-4-(2-oxopropyl)thieno[2',3':3,4]pyrido[1,2-*a*]indol-5(4*H*)-one (3ha)

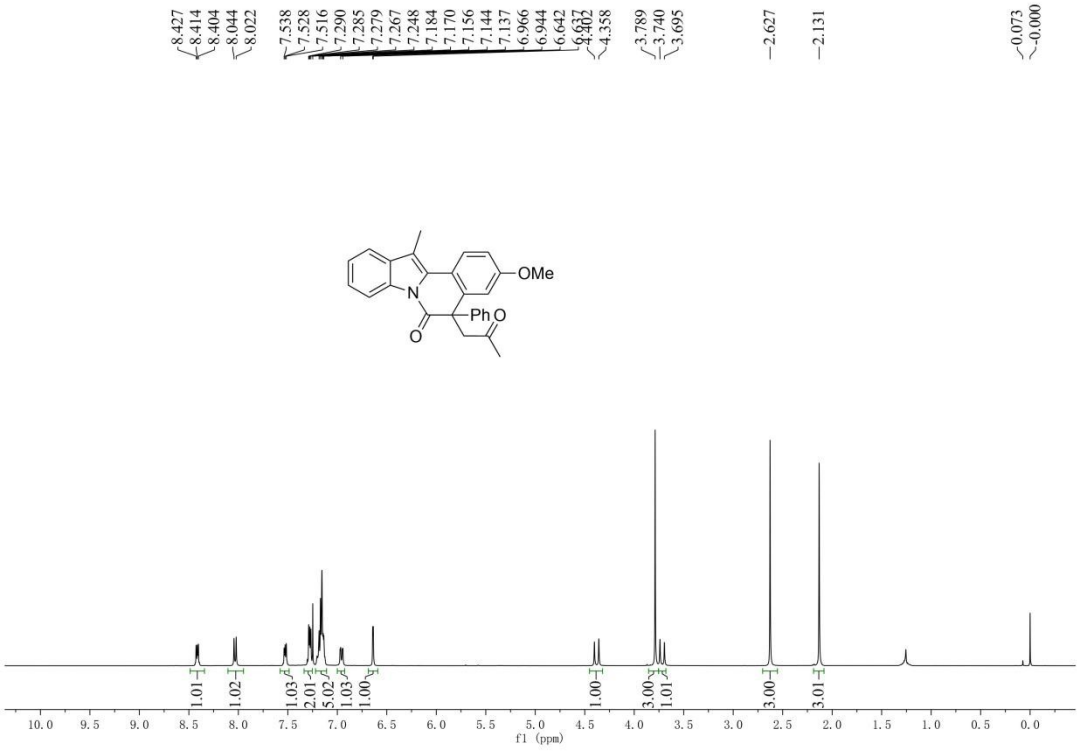


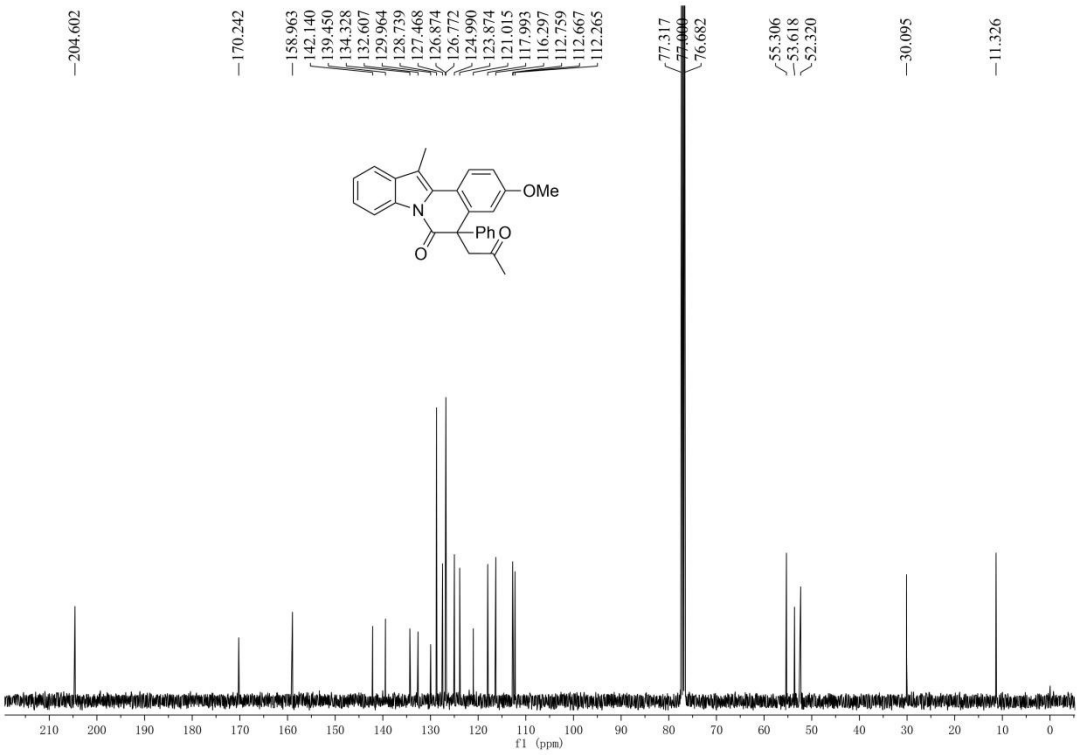


5-Benzyl-3-methoxy-12-methyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ia)

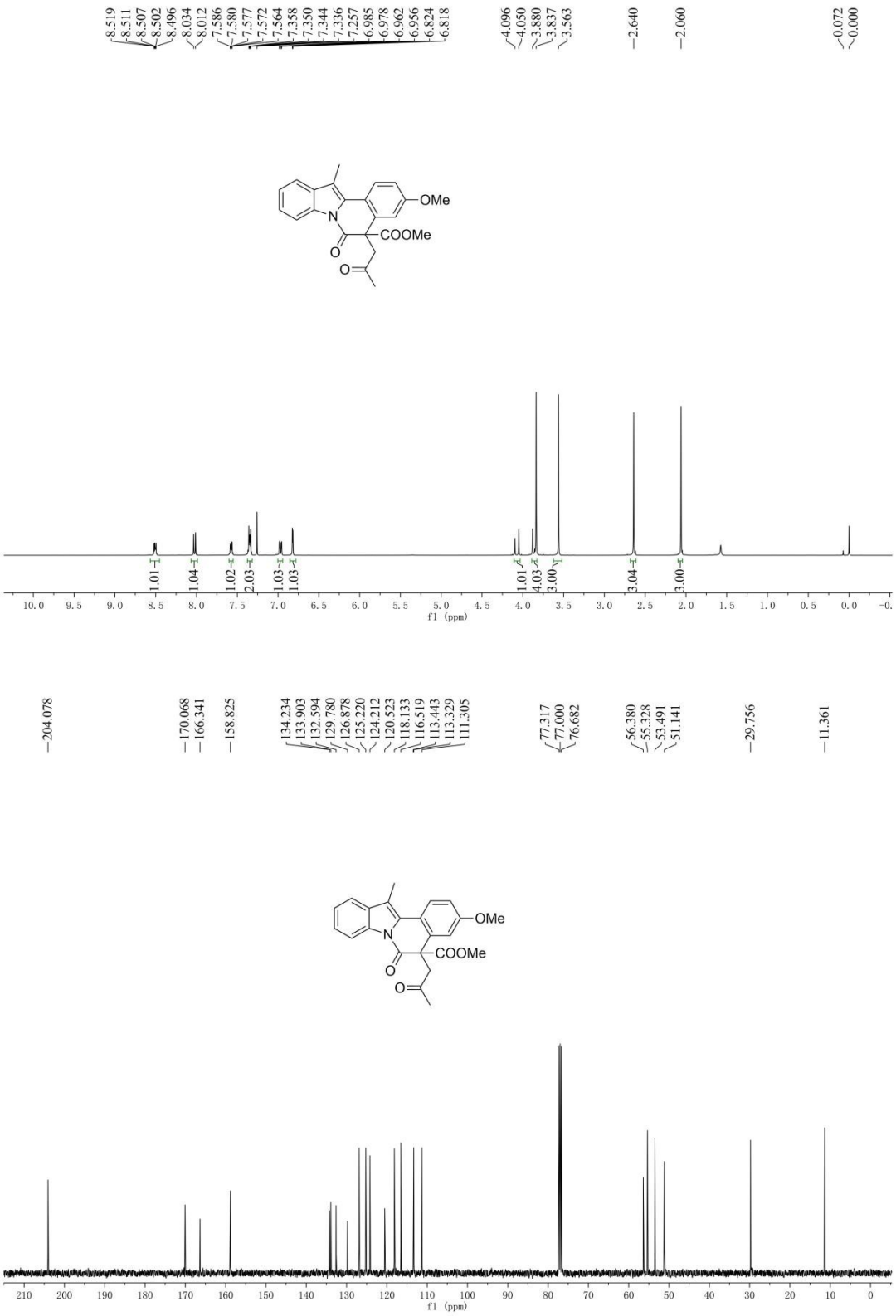


3-Methoxy-12-methyl-5-(2-oxopropyl)-5-phenylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ja)

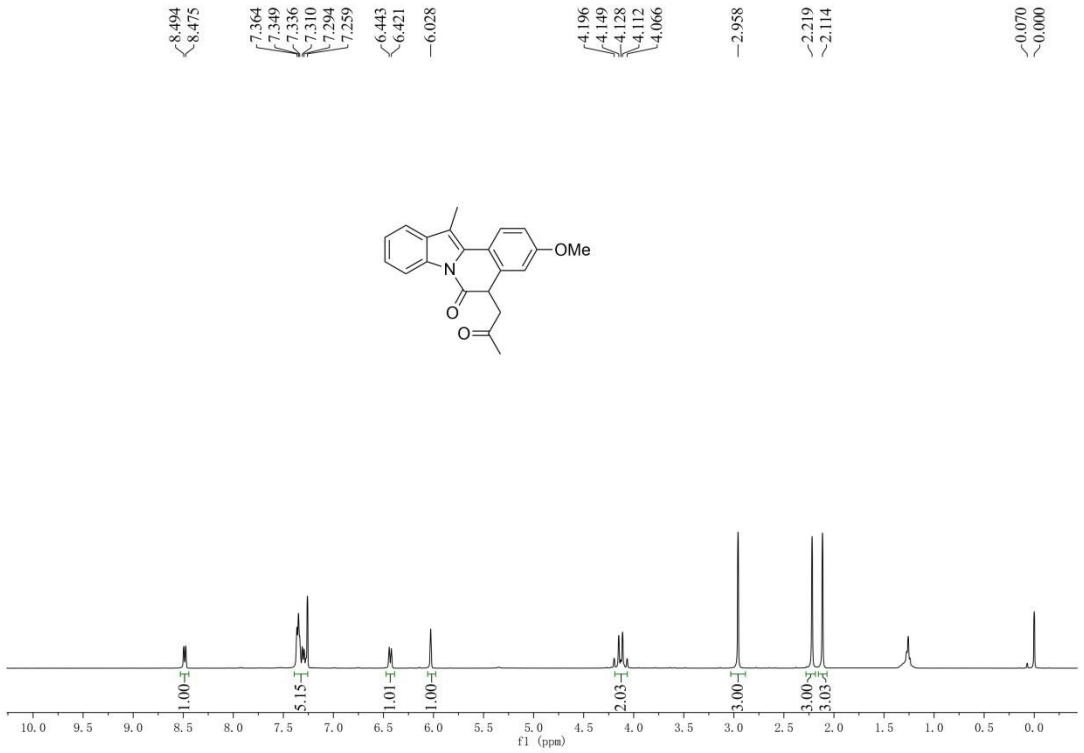


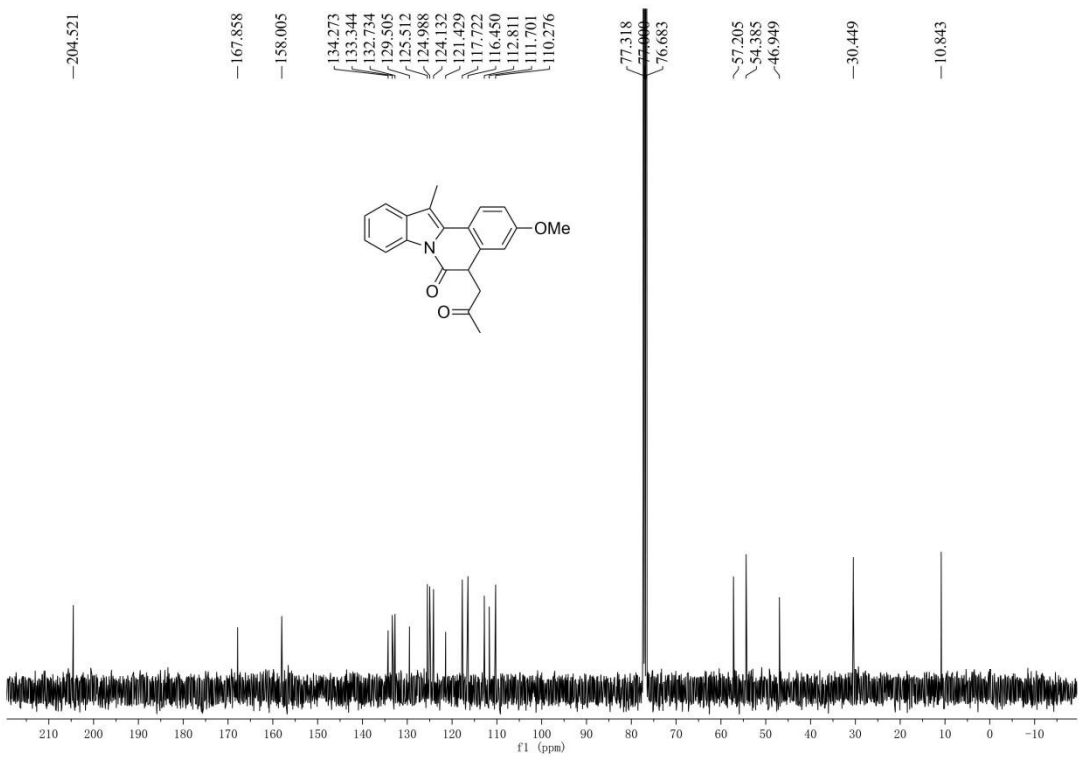


Methyl 3-methoxy-12-methyl-6-oxo-5-(2-oxopropyl)-5,6-dihydroindolo[2,1-*a*]isoquinoline-5-carboxylate (3ka)

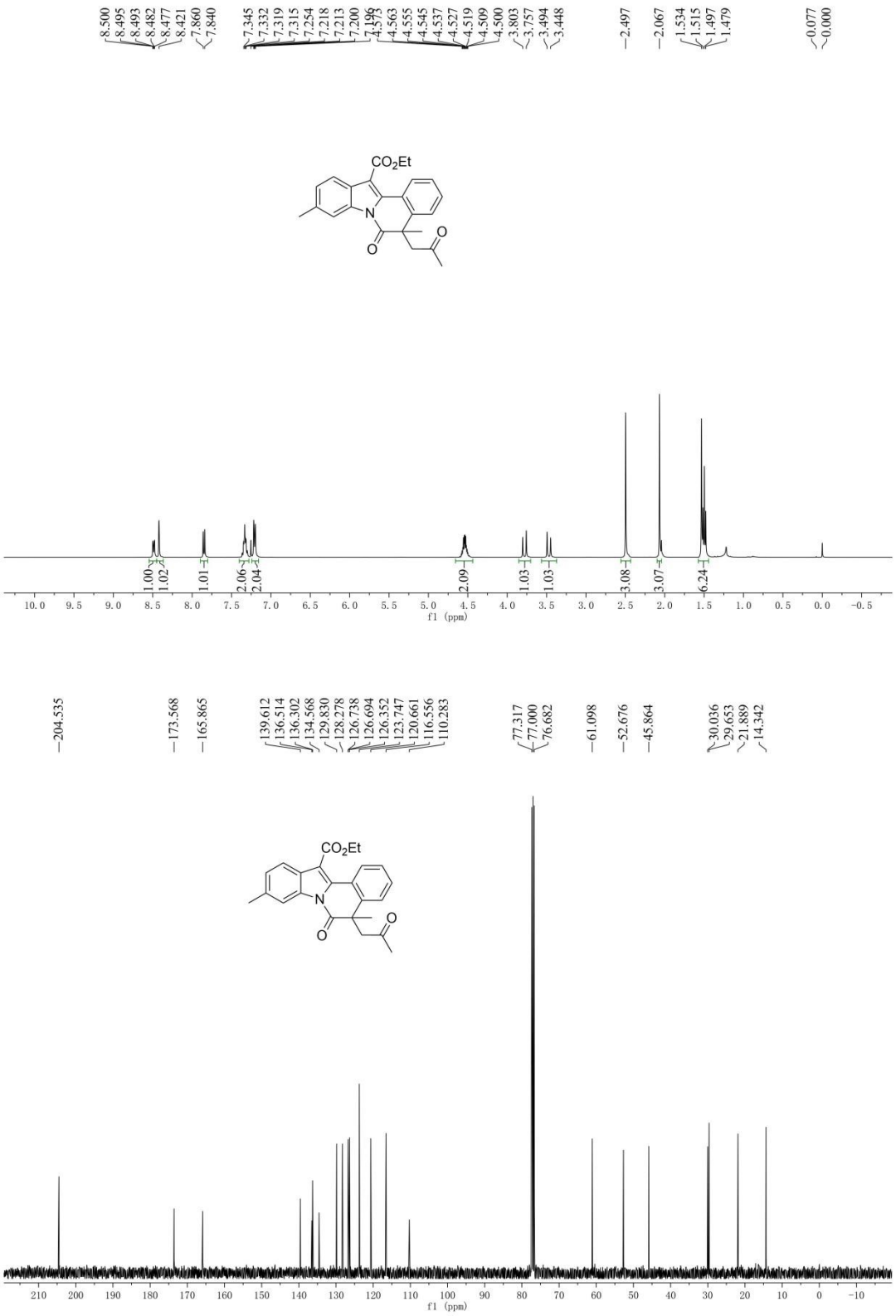


3-Methoxy-12-methyl-5-(2-oxopropyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3la)

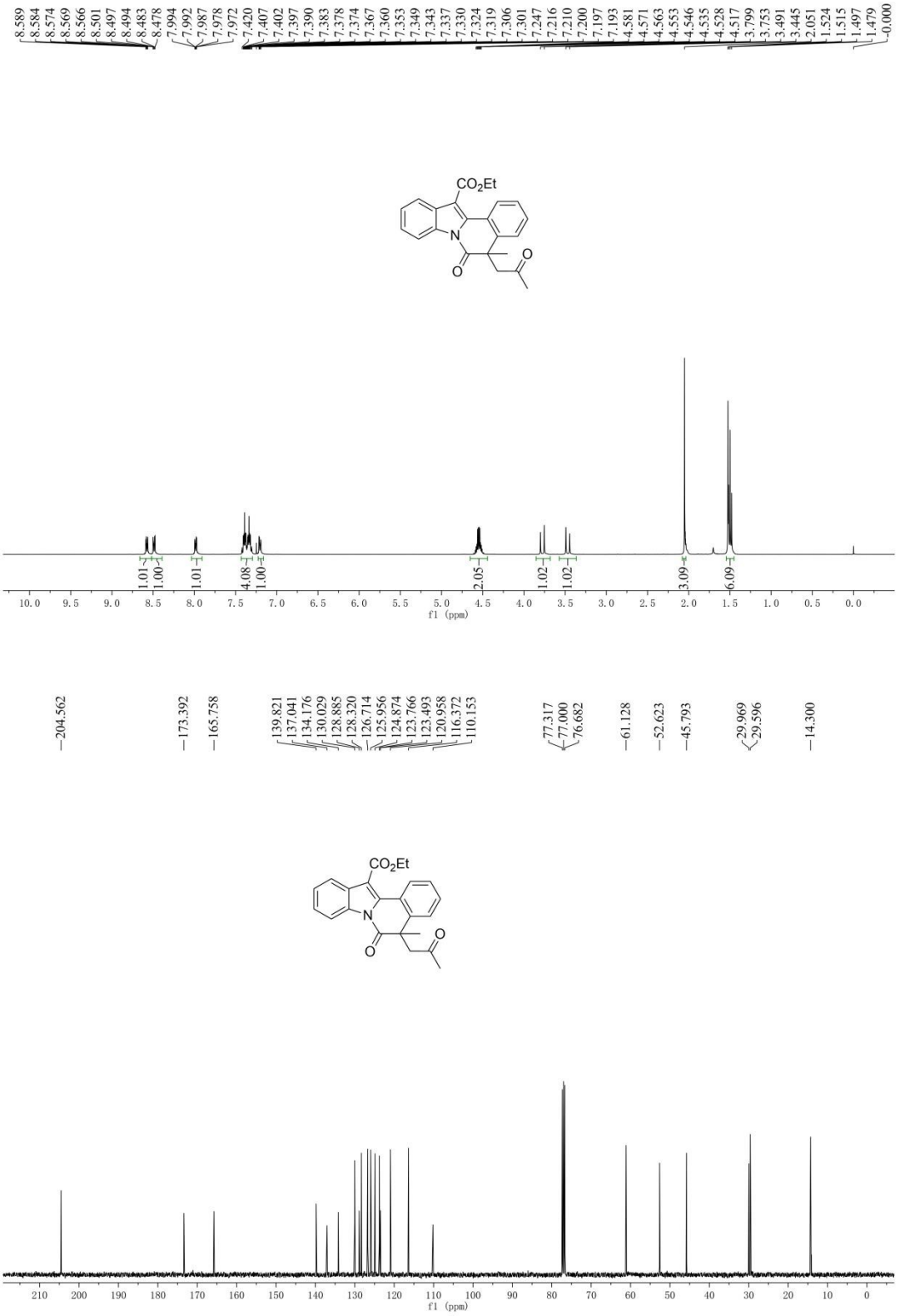




Ethyl 5,9-dimethyl-6-oxo-5-(2-oxopropyl)-5,6-dihydroindolo[2,1-*a*]isoquinoline-12-carboxylate (3ma)

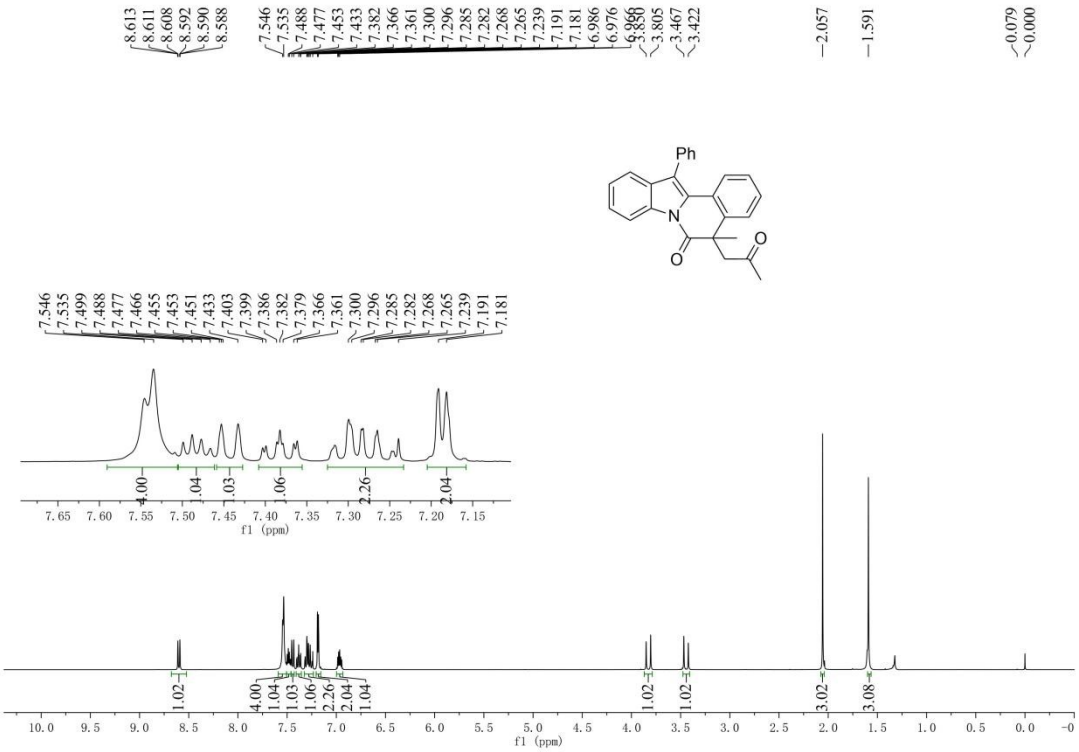


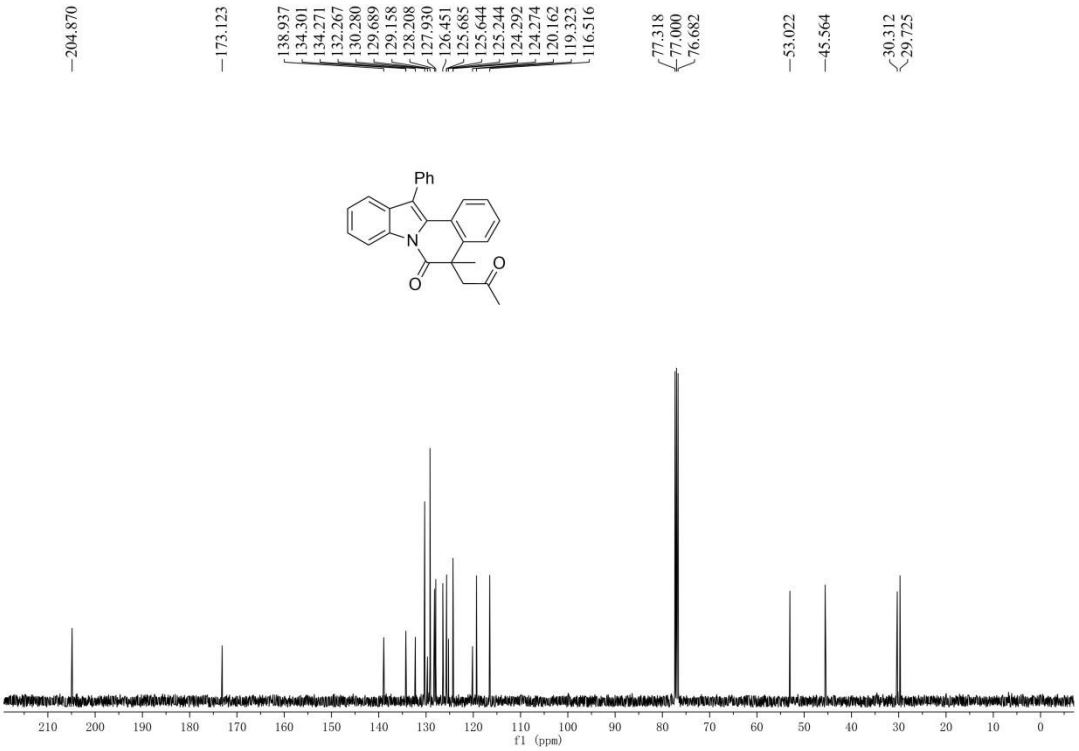
Ethyl 5-methyl-6-oxo-5-(2-oxopropyl)-5,6-dihydroindolo[2,1-*a*]isoquinoline-12-carboxylate (3na)



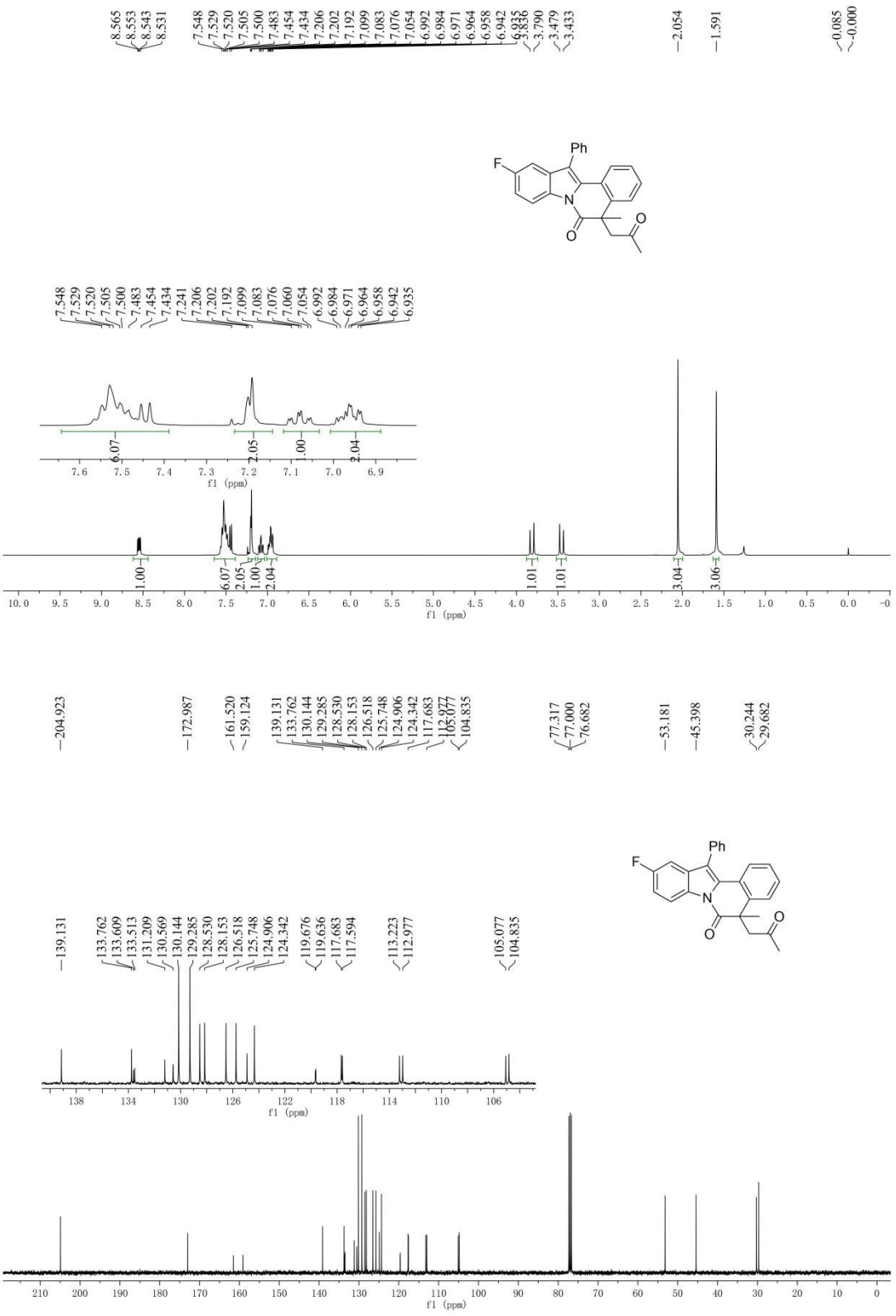
5,10-Dimethyl-5-(2-oxopropyl)-12-phenylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3oa)

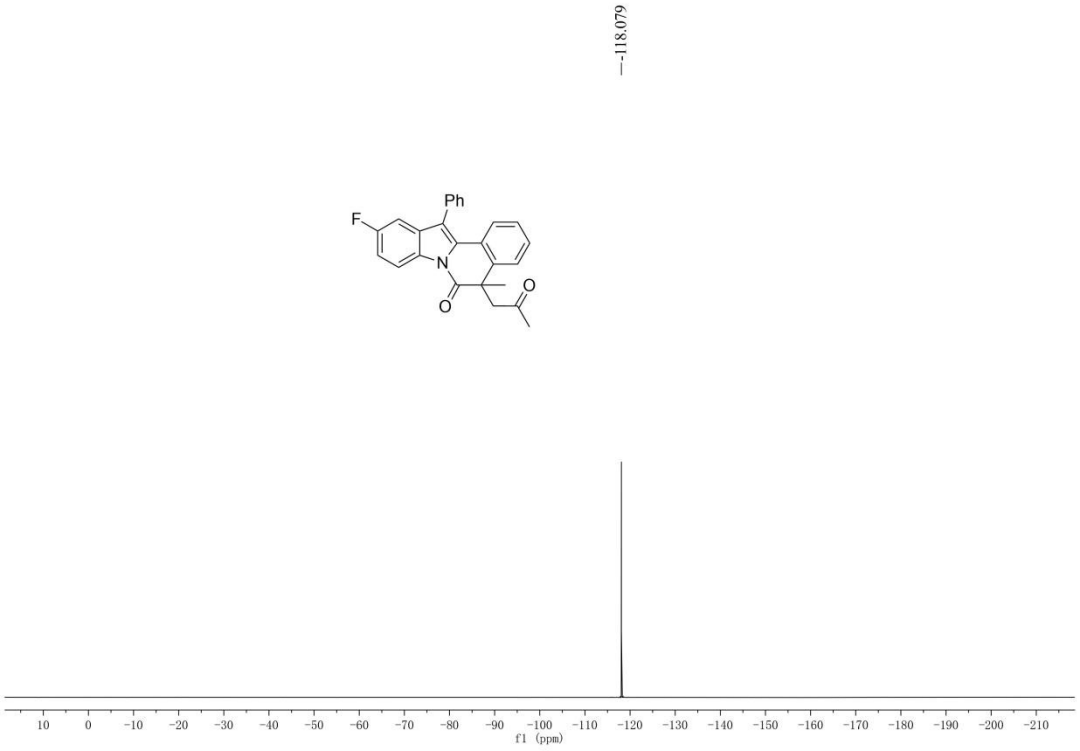
5-Methyl-5-(2-oxopropyl)-12-phenylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3pa)



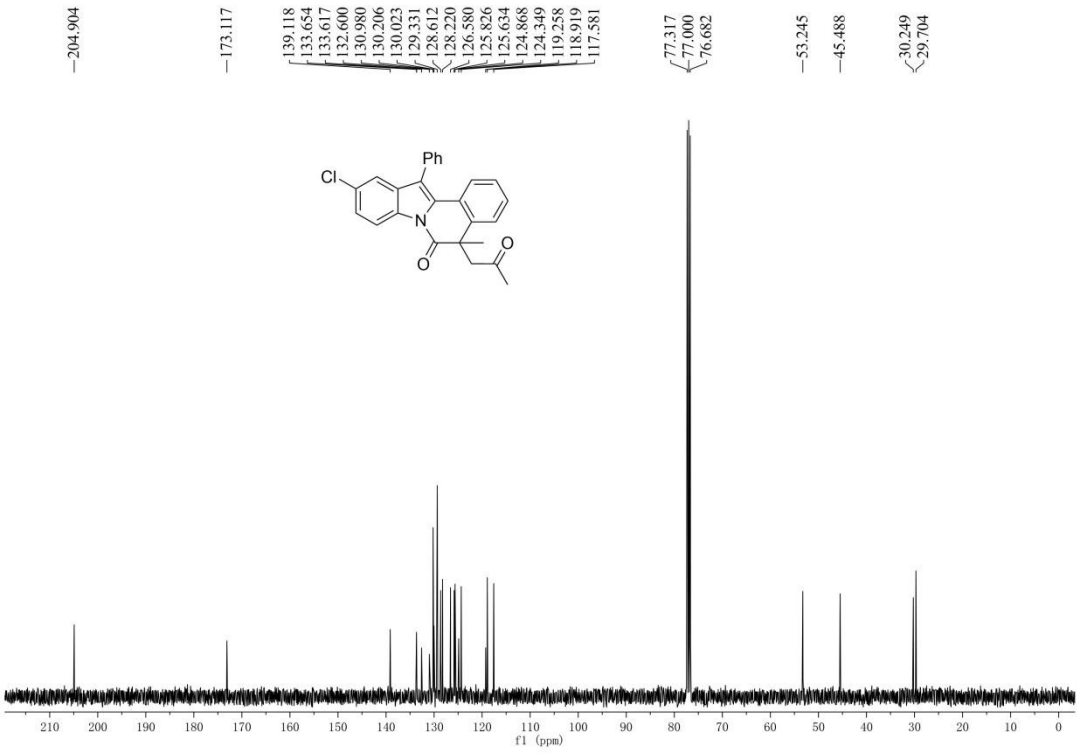


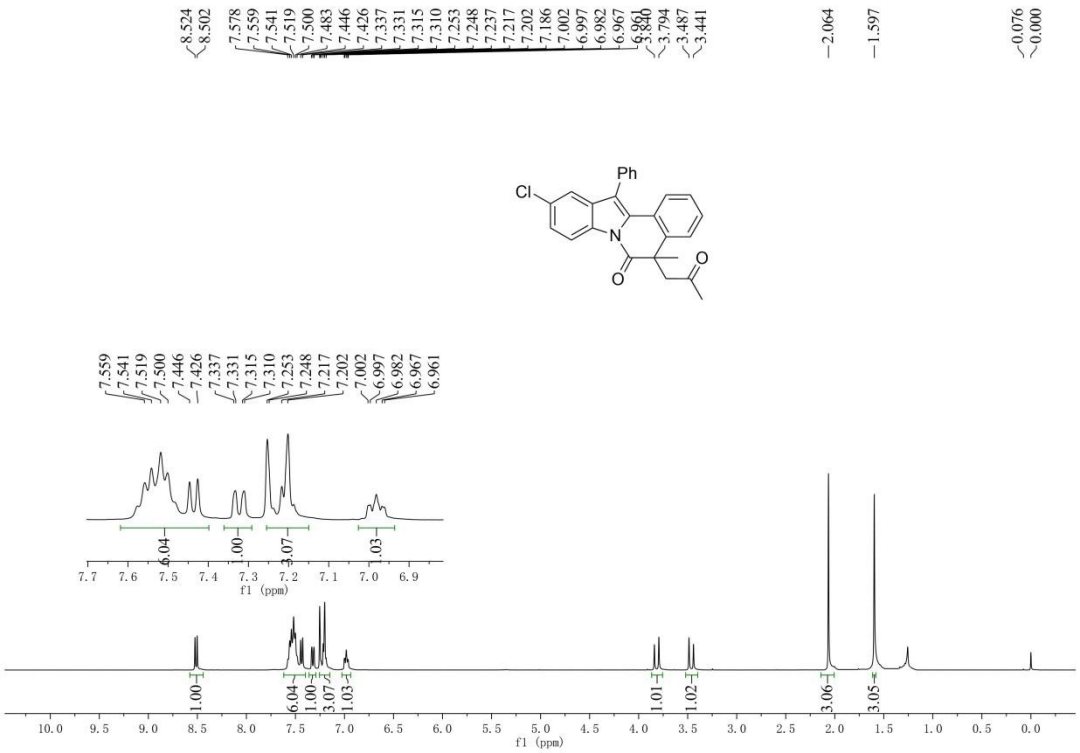
10-Fluoro-5-methyl-5-(2-oxopropyl)-12-phenylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3qa)



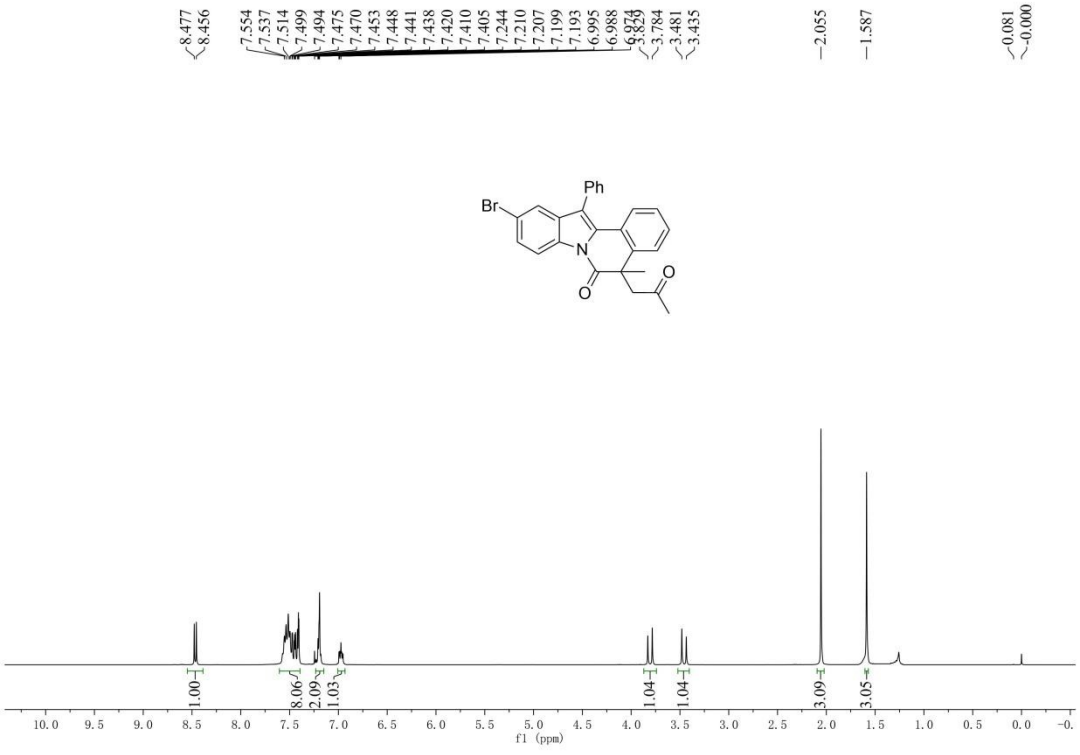

-118.079
Ph
F
N
O
O
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

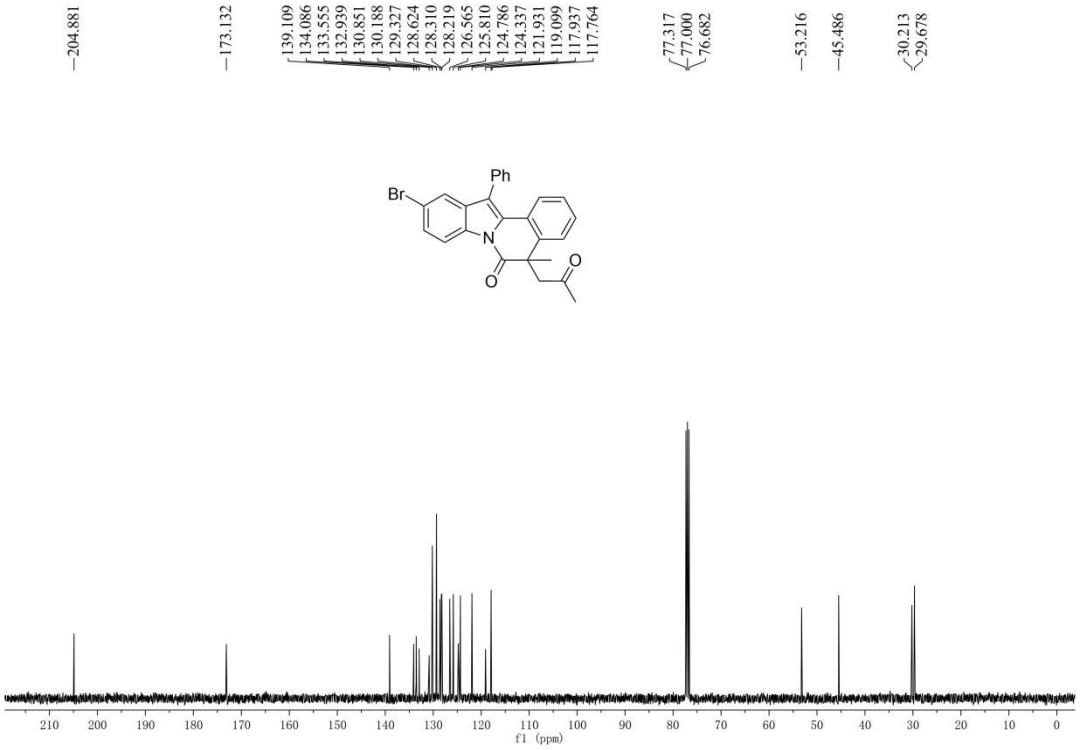
10-Chloro-5-methyl-5-(2-oxopropyl)-12-phenylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ra)



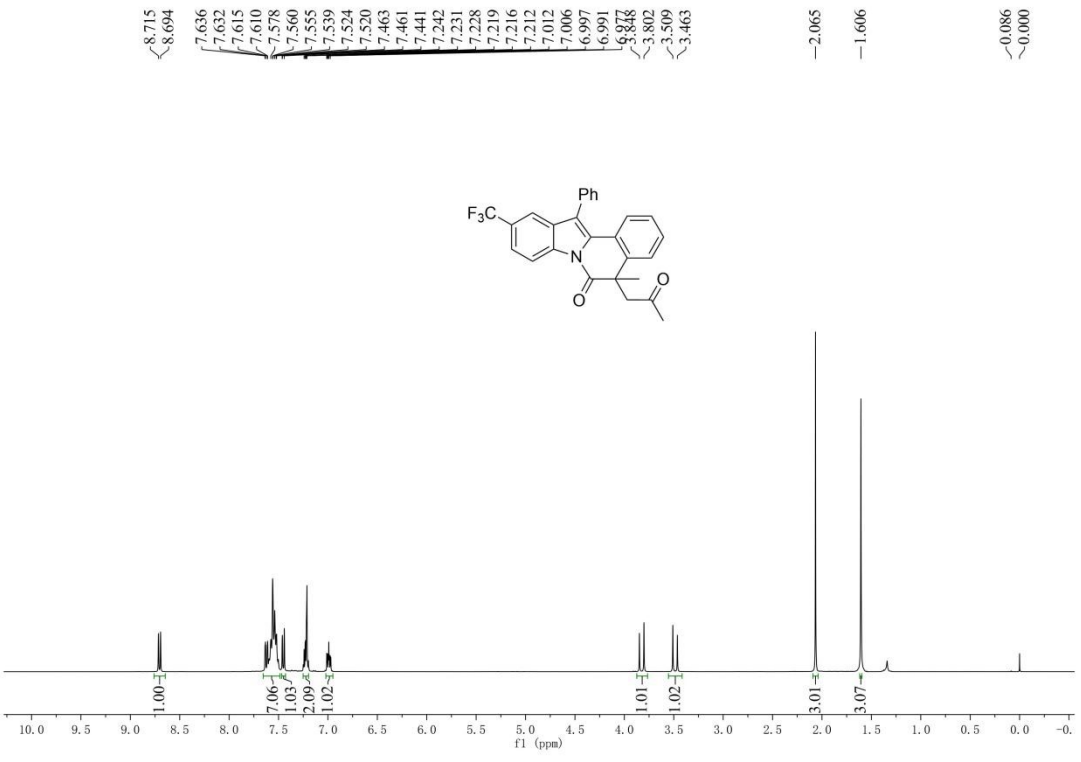


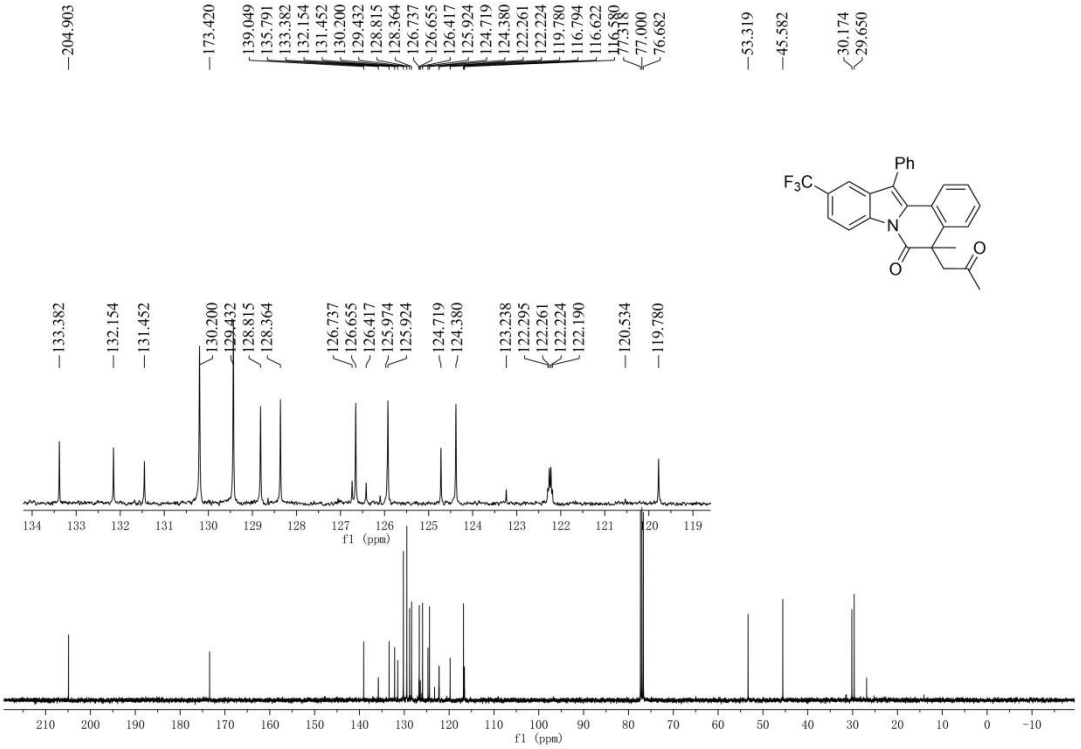
10-Bromo-5-methyl-5-(2-oxopropyl)-12-phenylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3sa)

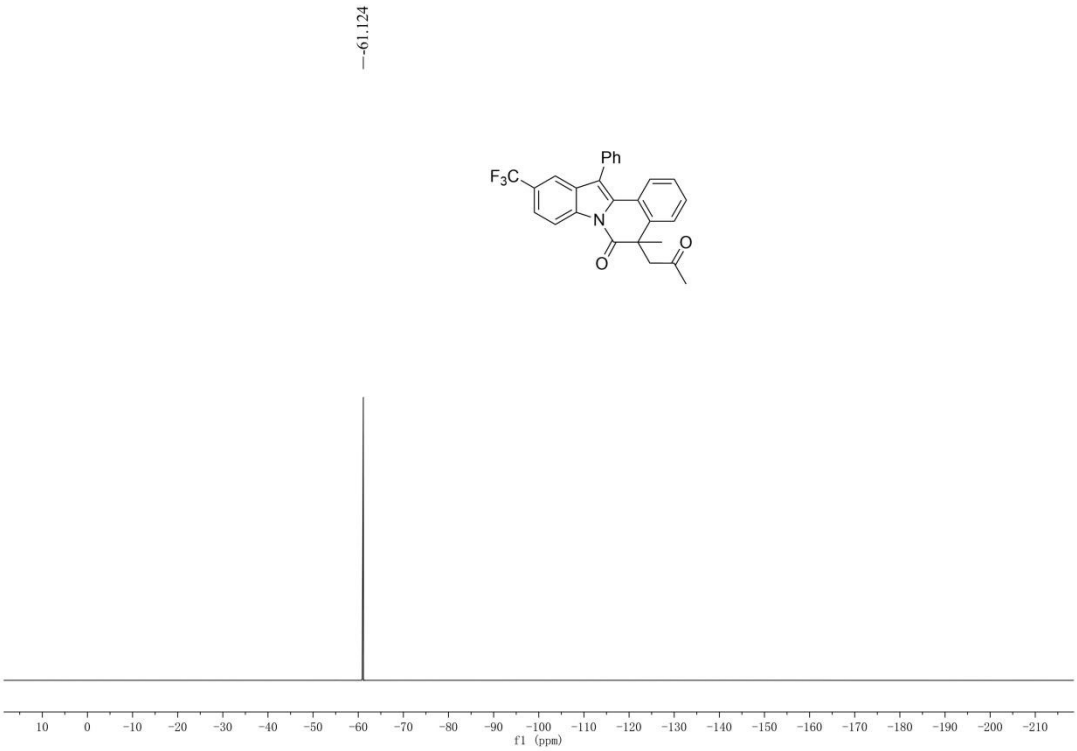




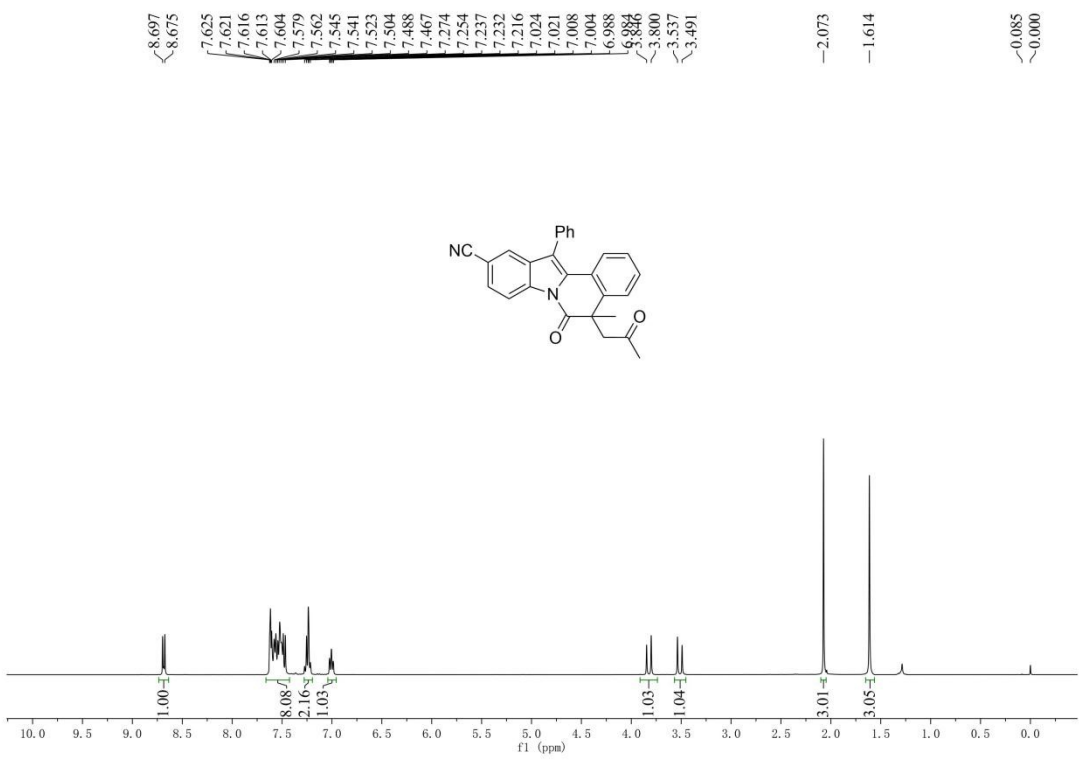
5-Methyl-5-(2-oxopropyl)-12-phenyl-10-(trifluoromethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ta)

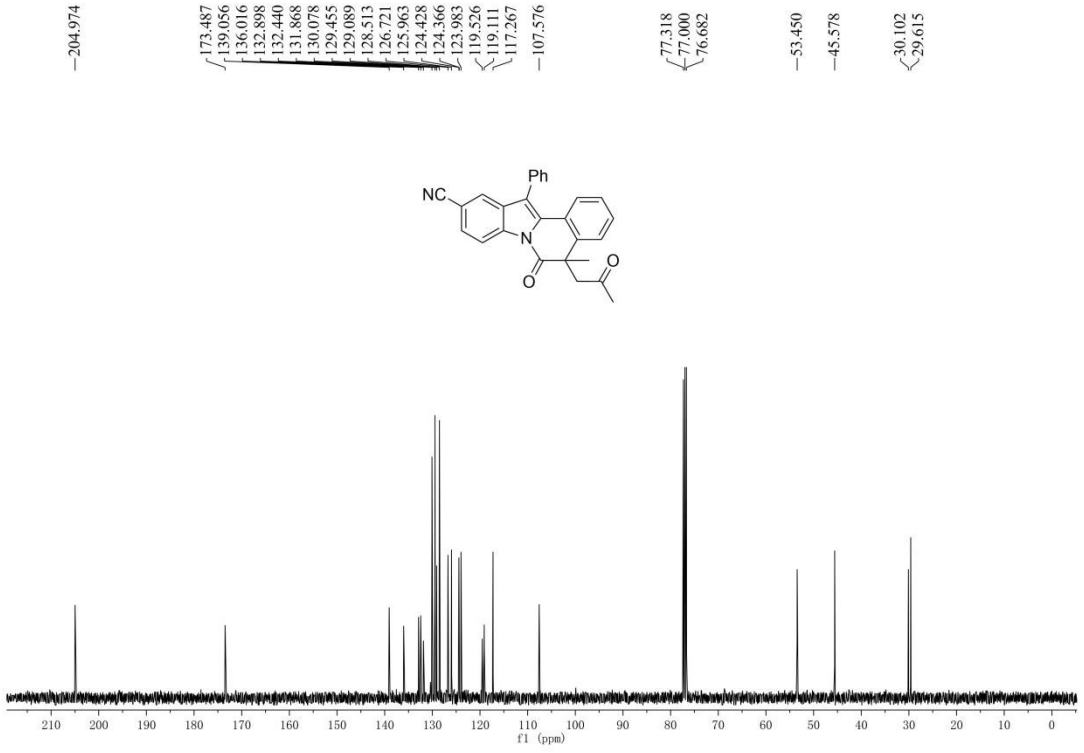




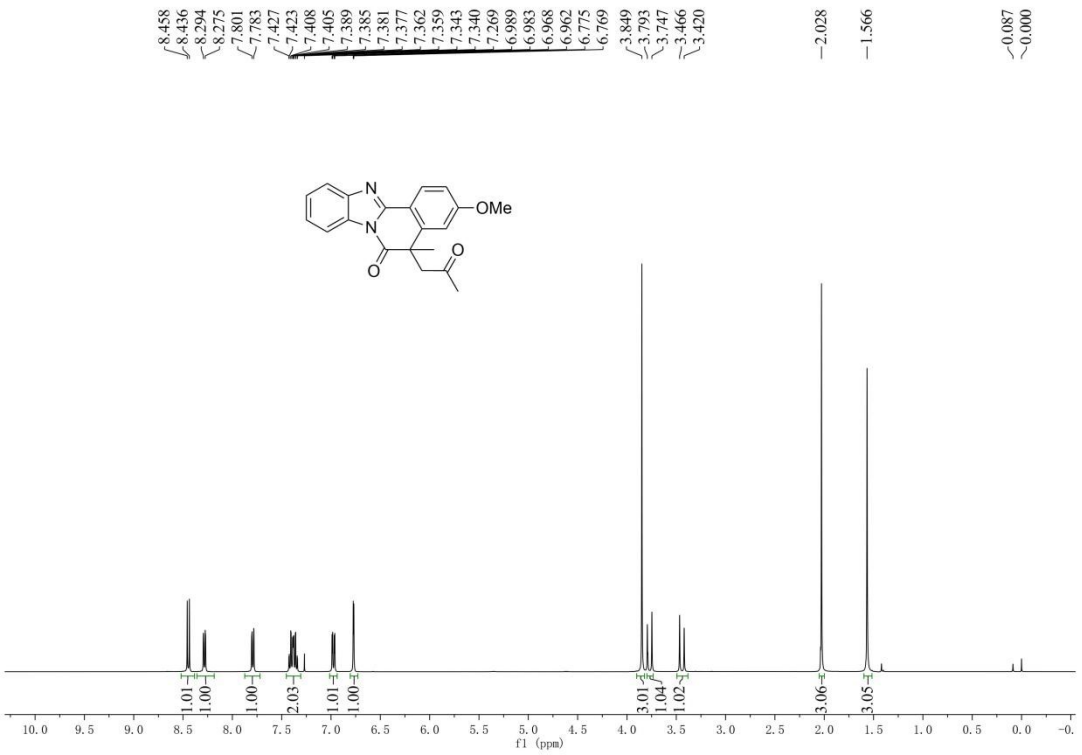

-61.124
Ph
F3C
N
O
O
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

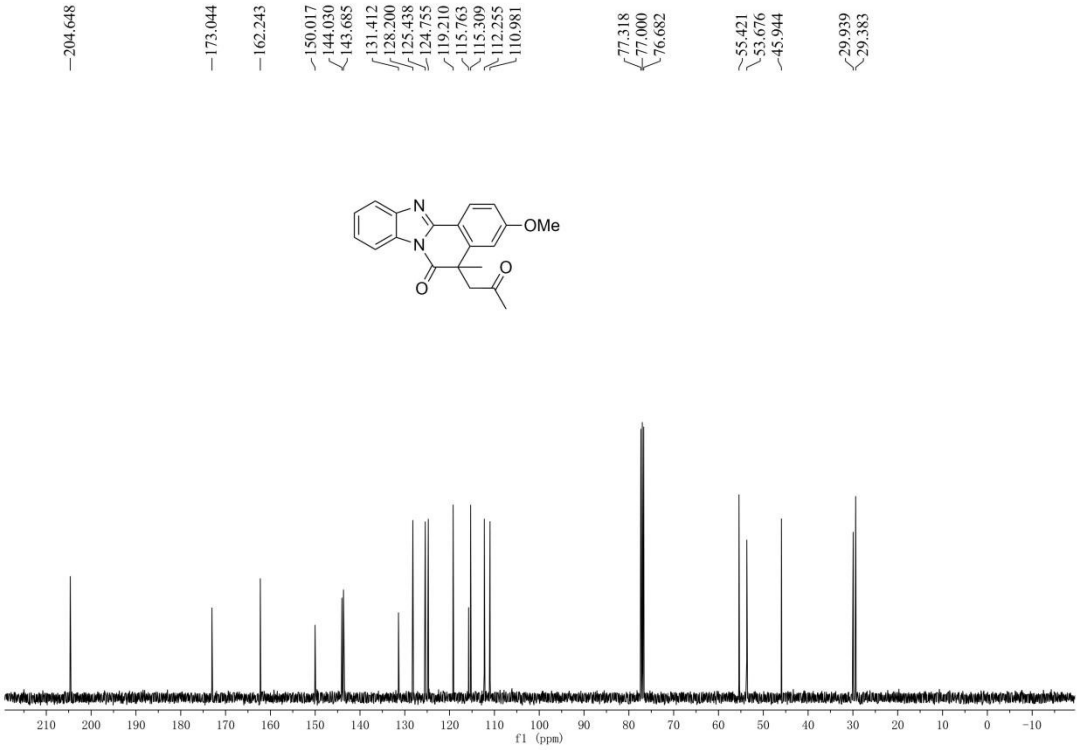
5-Methyl-6-oxo-5-(2-oxopropyl)-12-phenyl-5,6-dihydroindolo[2,1-*a*]isoquinoline-10-carbonitrile (3ua)



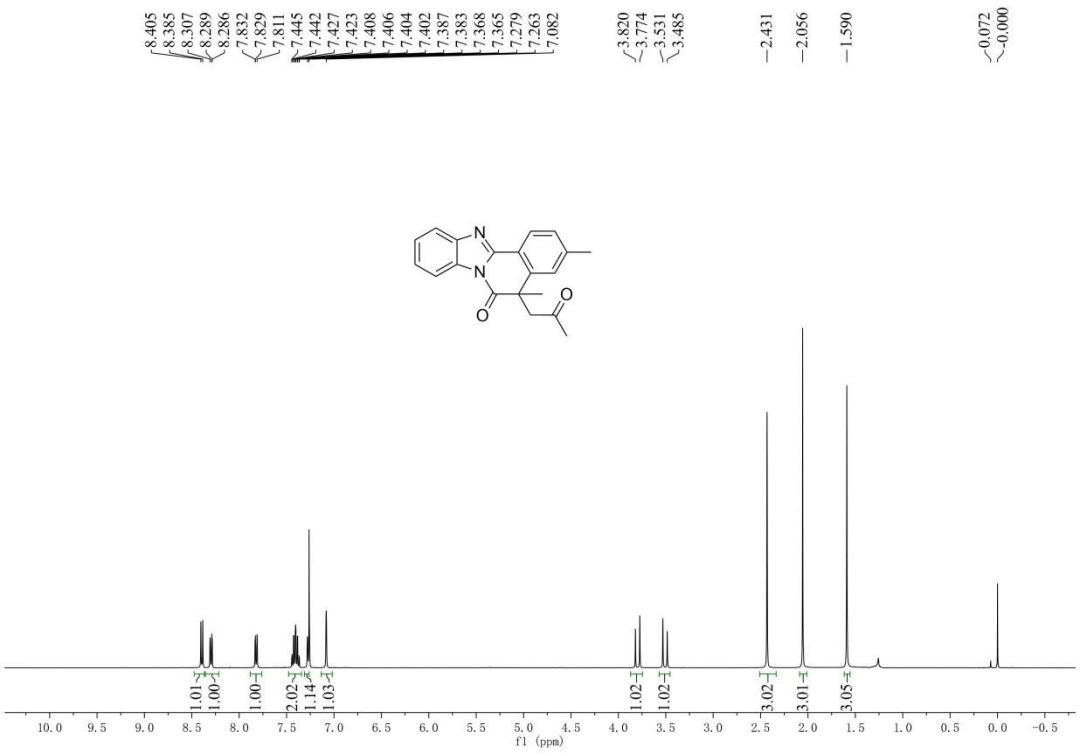


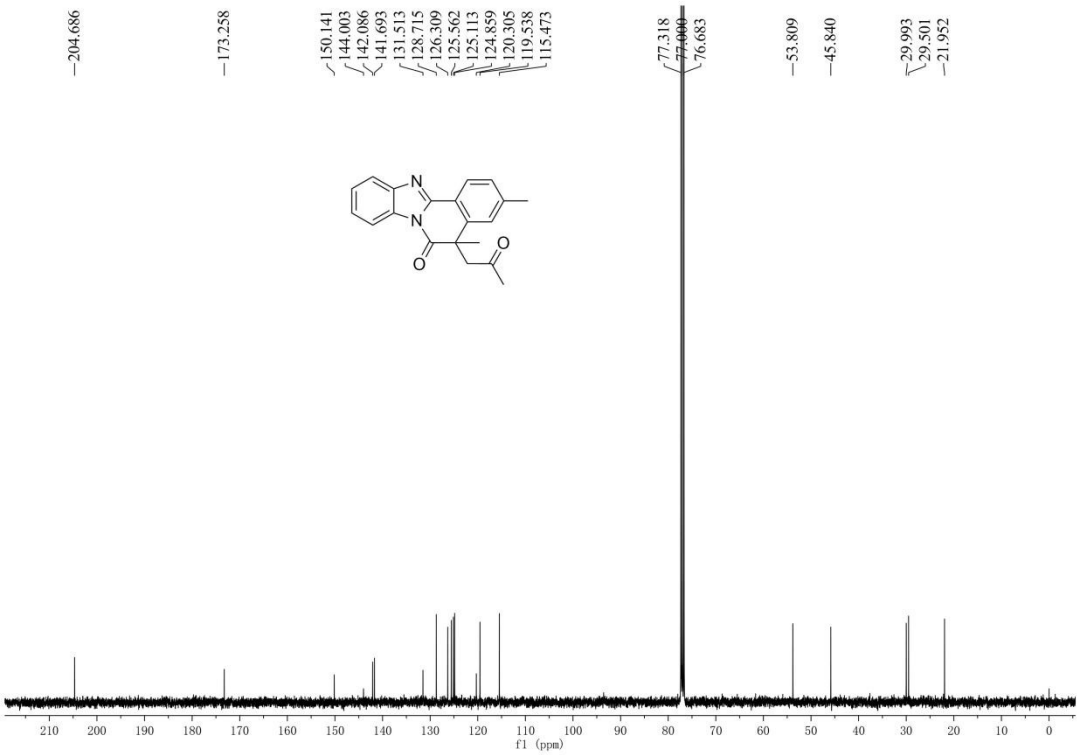
3-Methoxy-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3va)



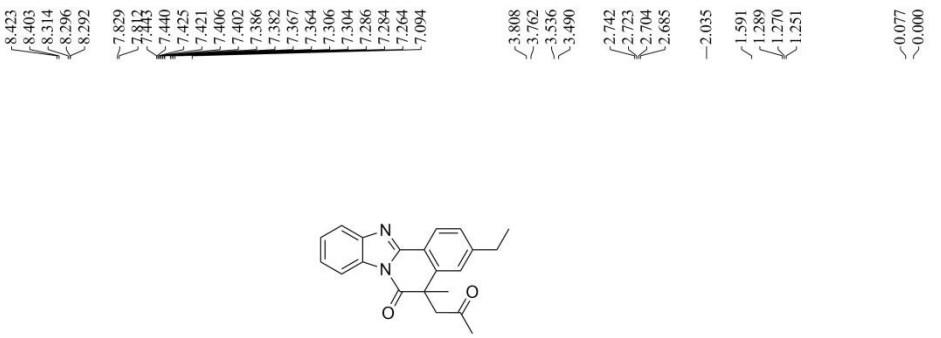


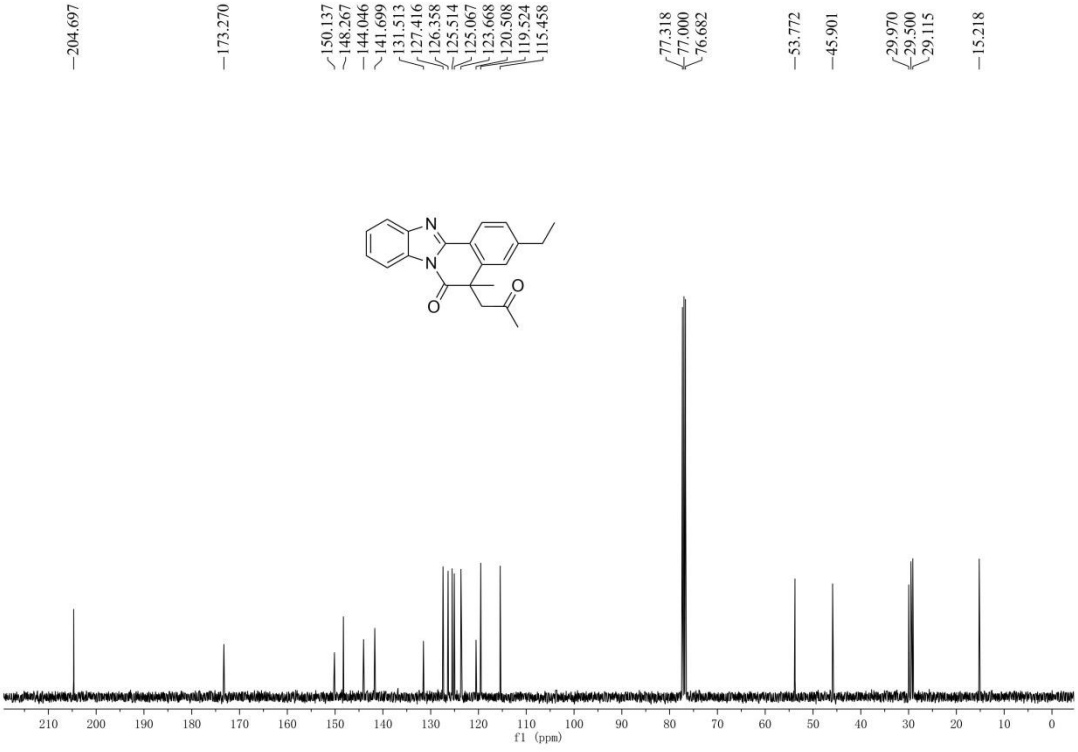
3,5-Dimethyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3wa)



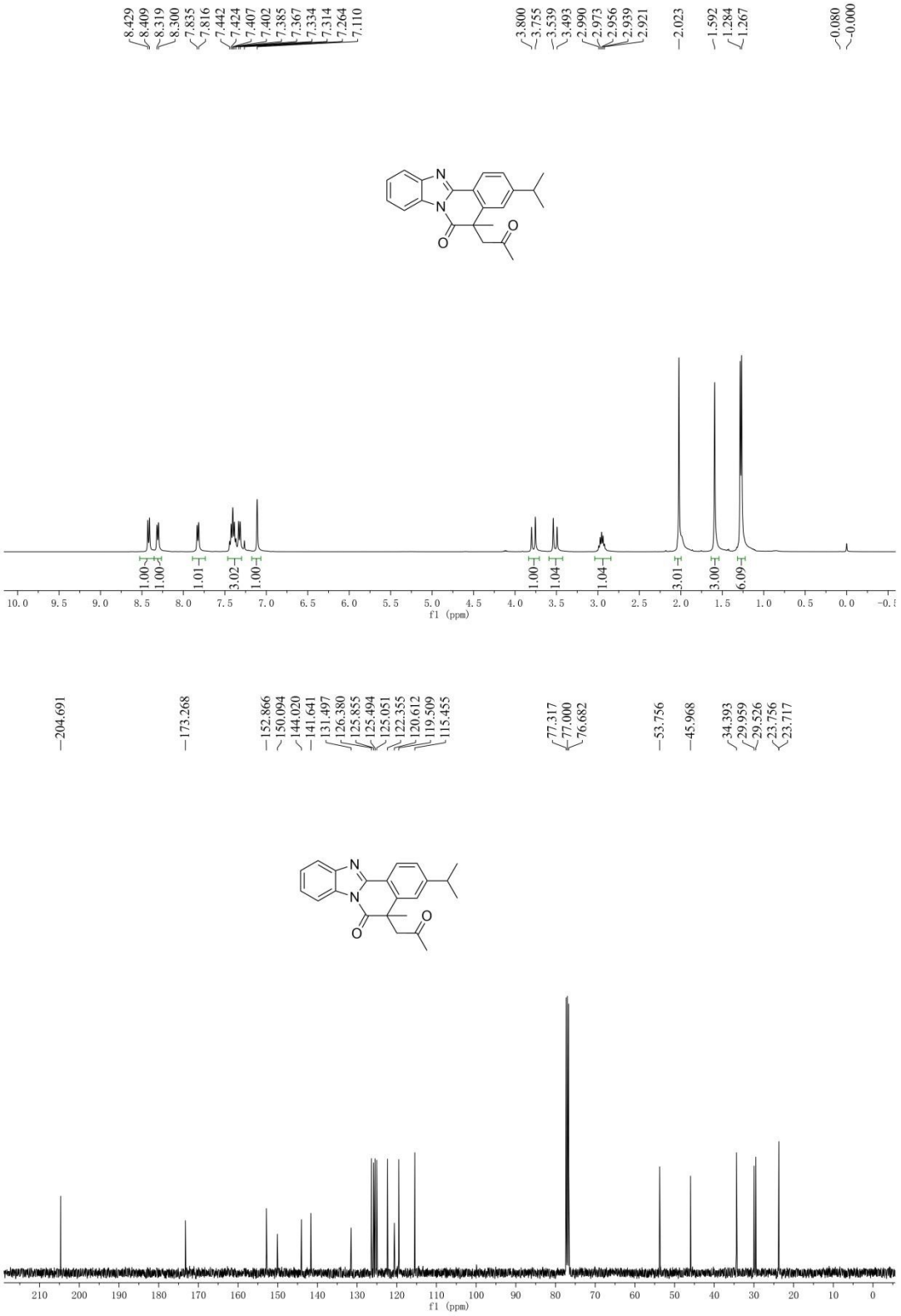


3-Ethyl-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3xa)

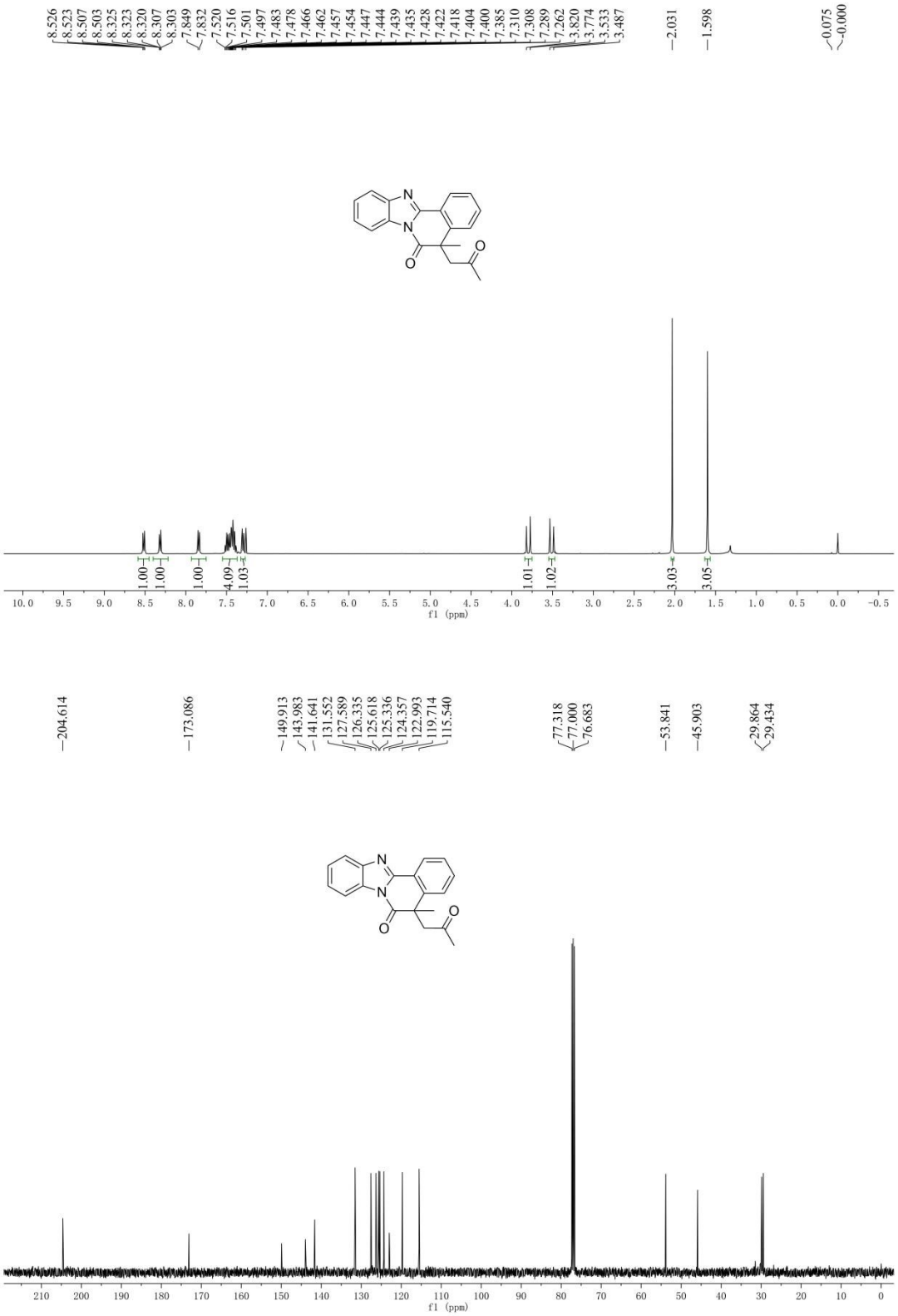




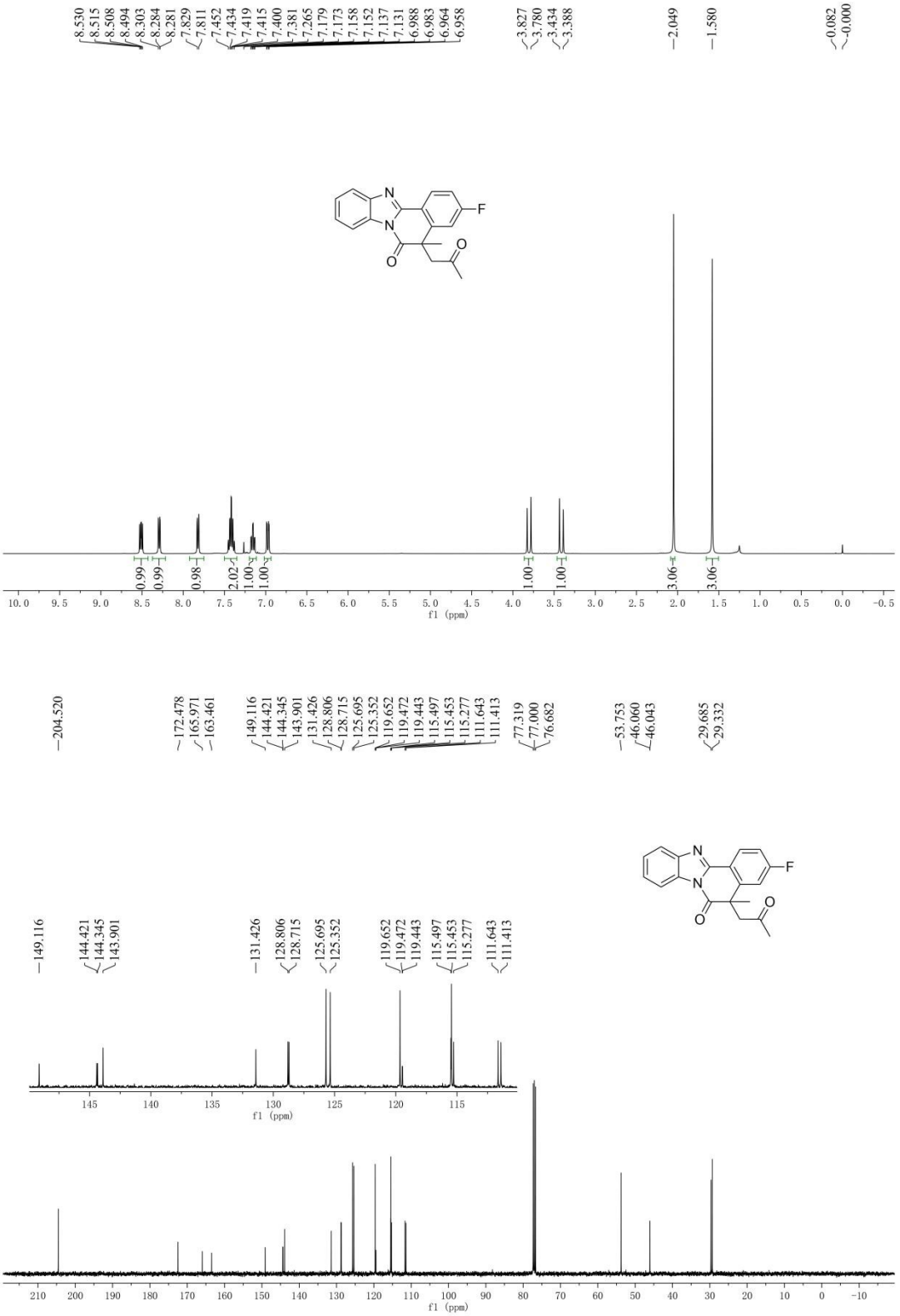
3-Isopropyl-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3ya)

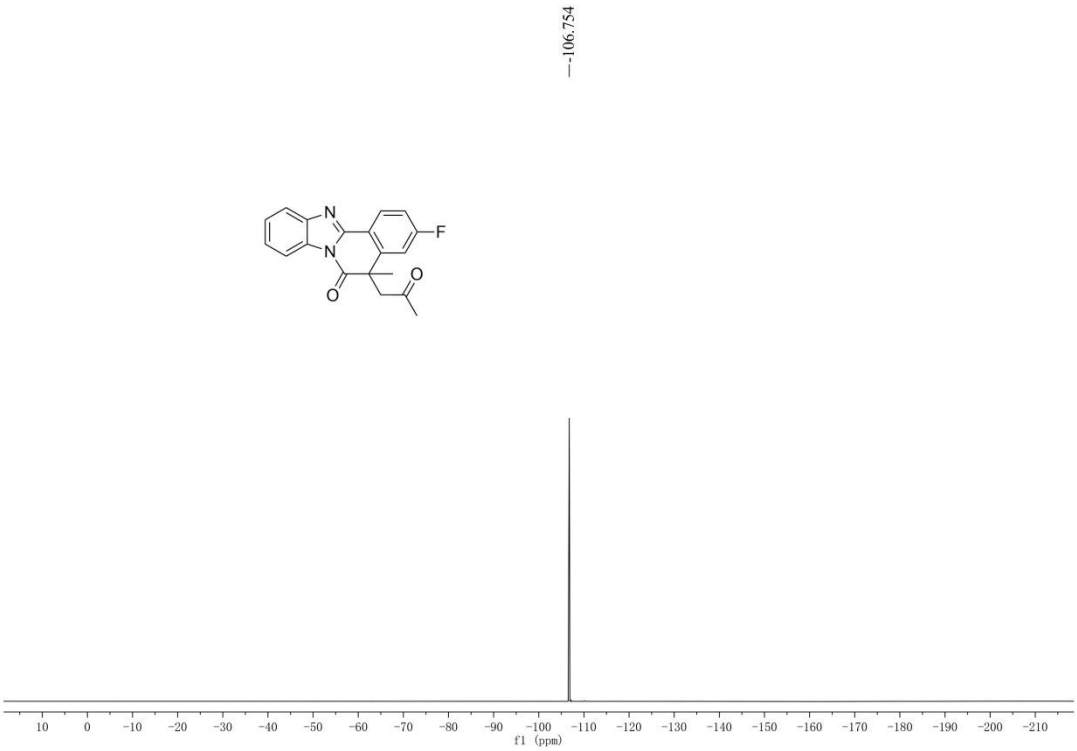


5-Methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3za)

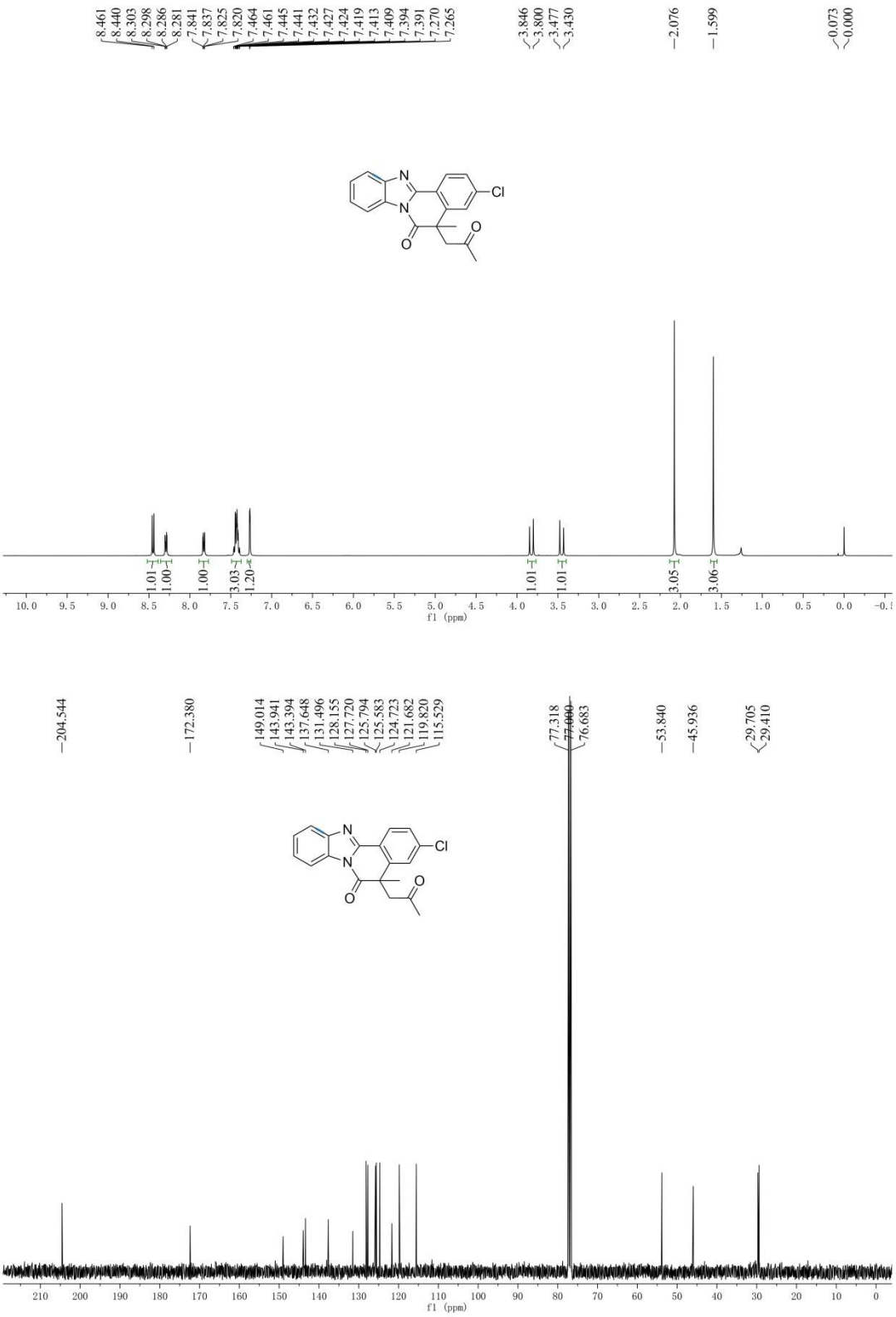


3-Fluoro-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aaa)

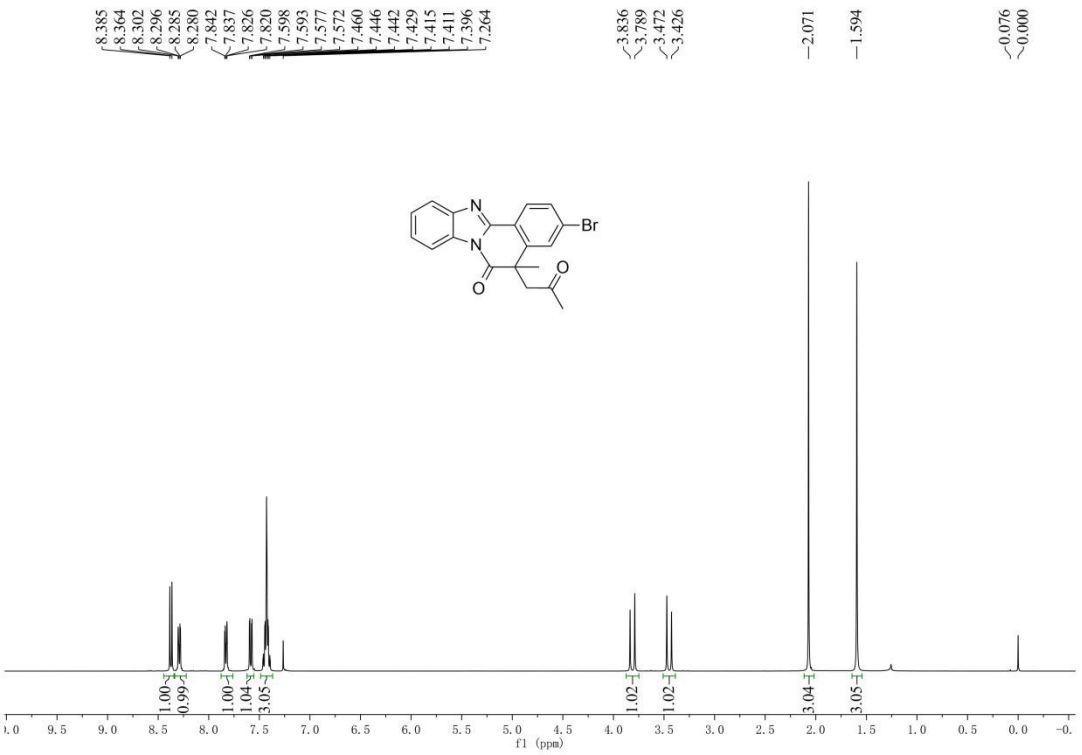


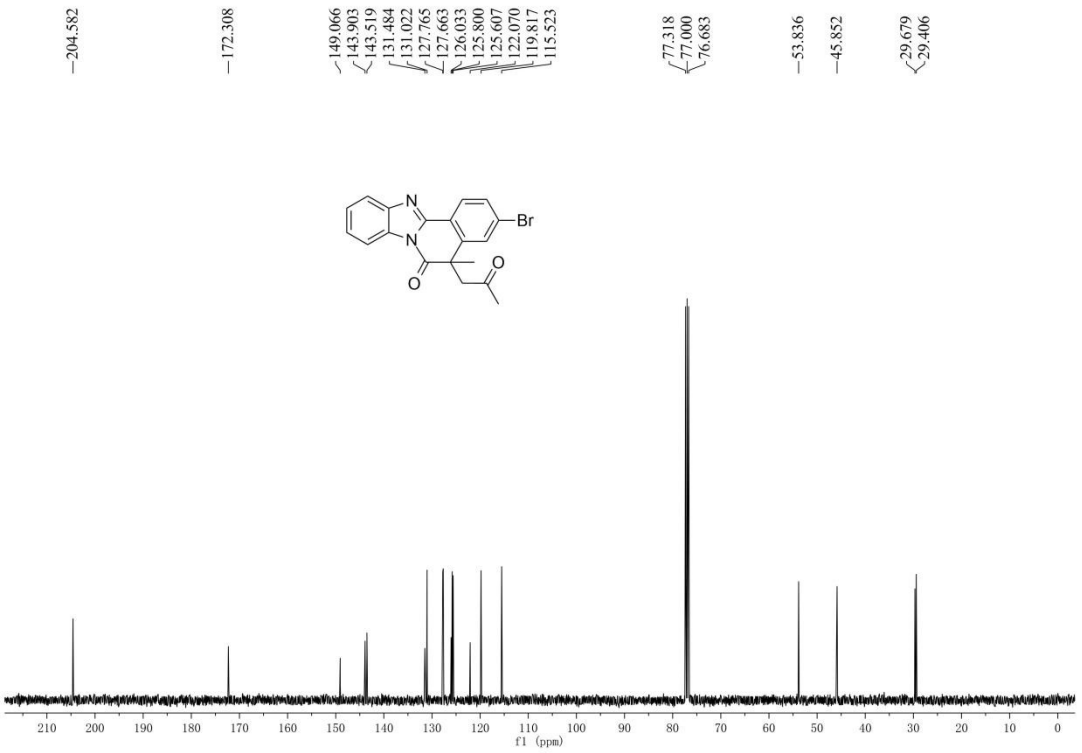

-106.754
N
N
F
O
O
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

3-Chloro-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aba)

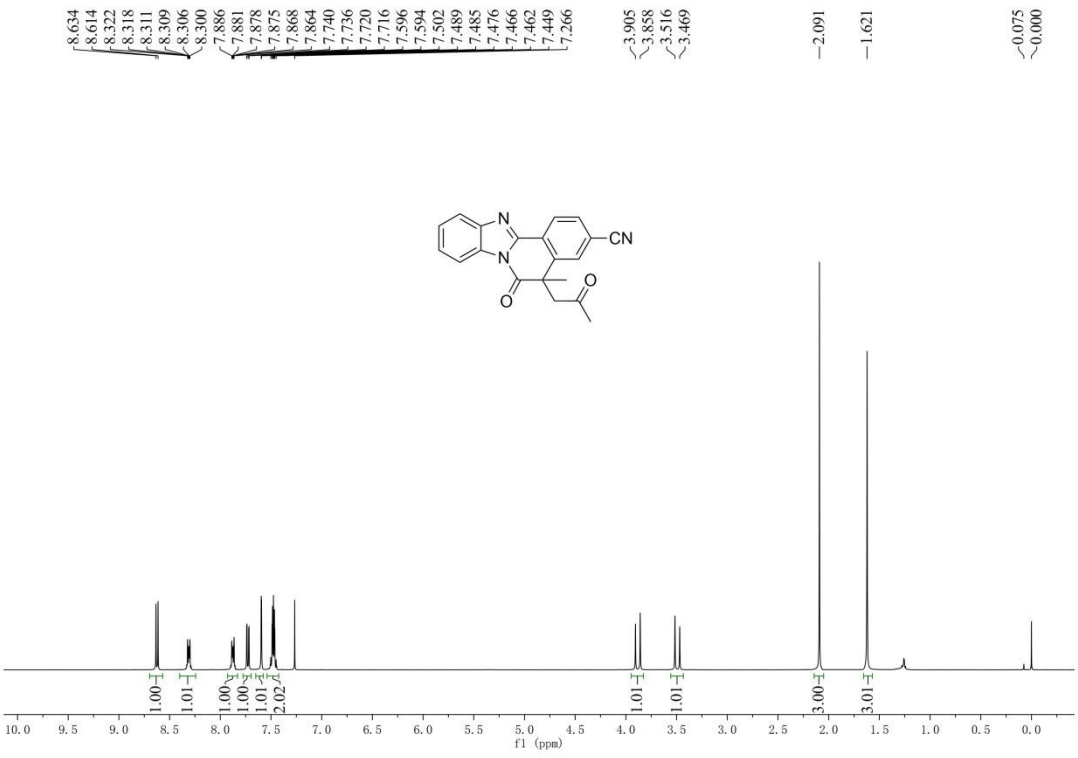


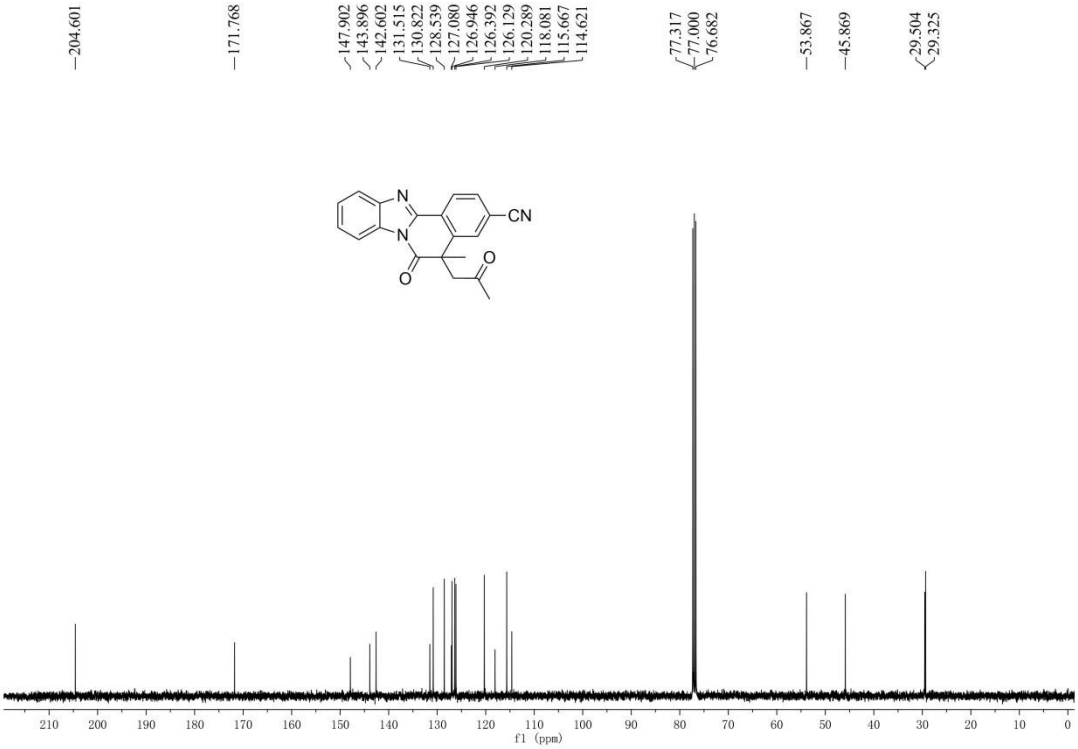
3-Bromo-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aca)



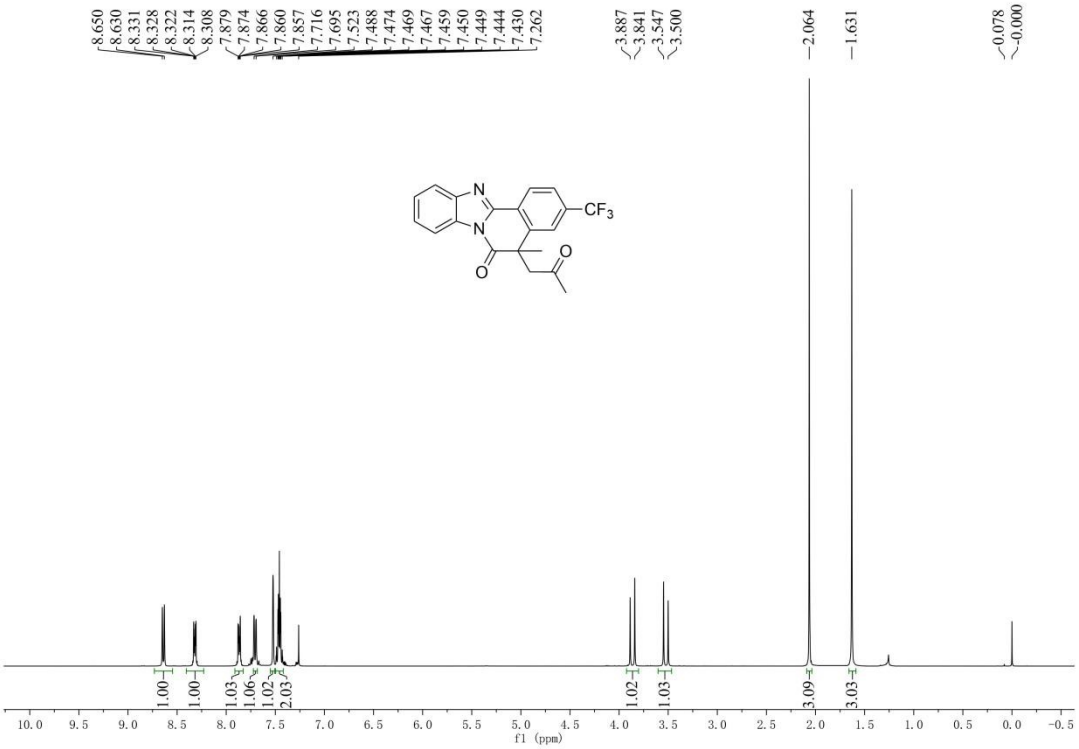


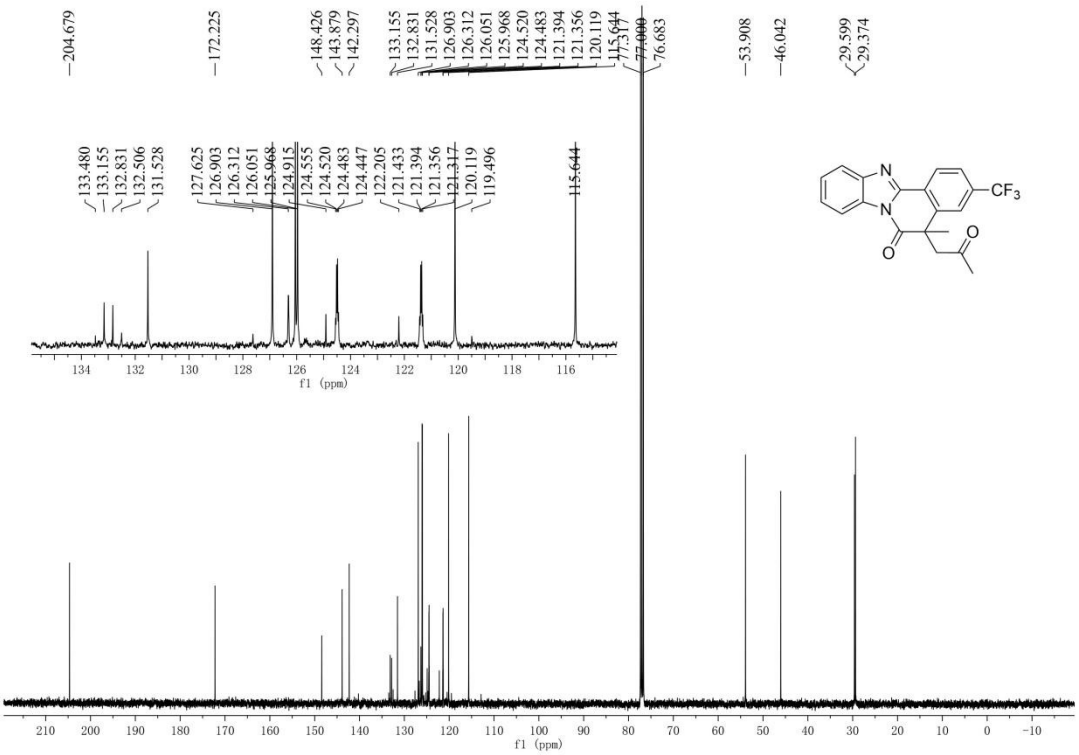
5-Methyl-6-oxo-5-(2-oxopropyl)-5,6-dihydrobenzo[4,5]imidazo[2,1-*a*]isoquinoline-3-carbonitrile (3ada)

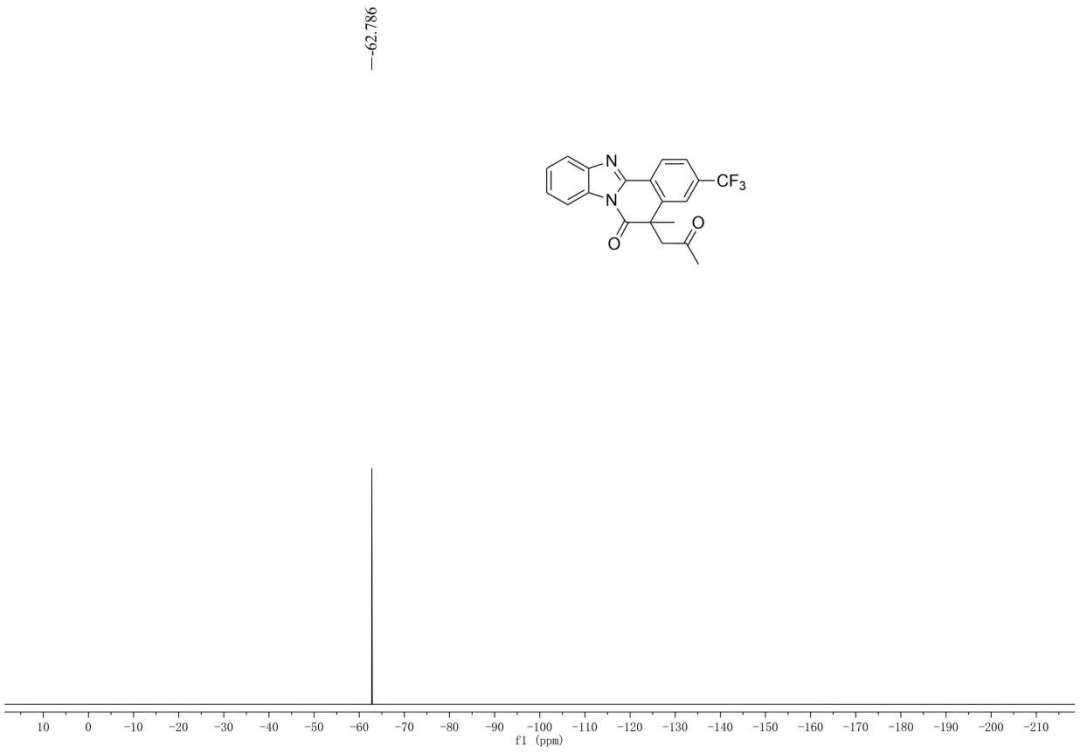




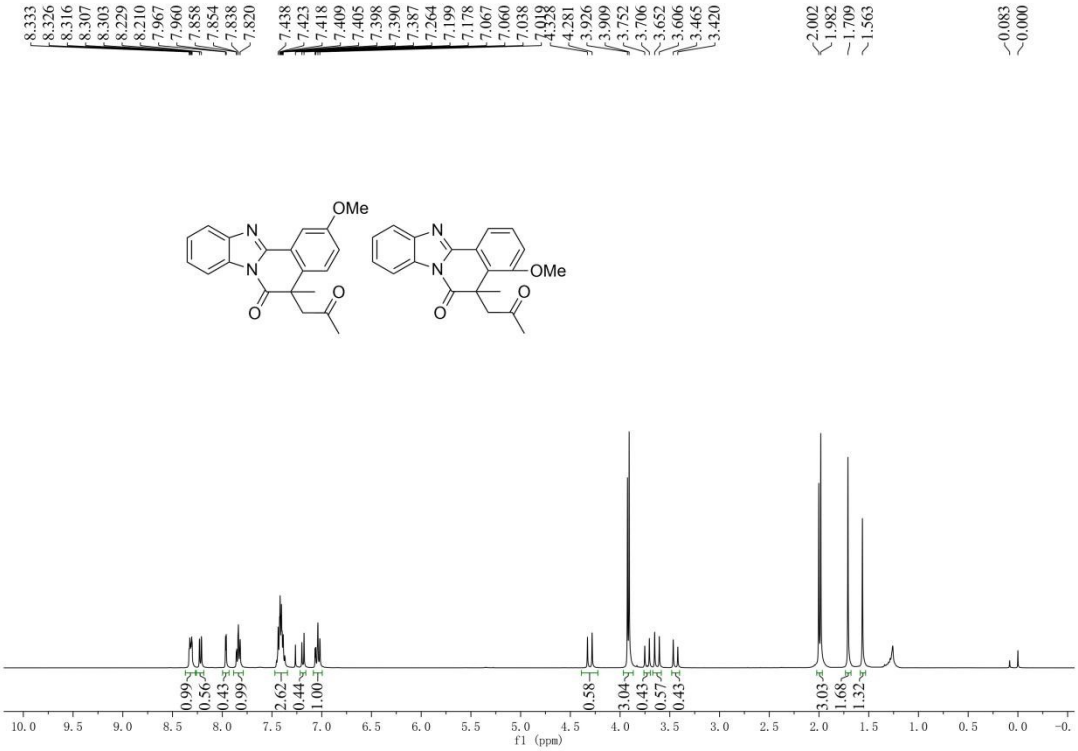
5-Methyl-5-(2-oxopropyl)-3-(trifluoromethyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aea)

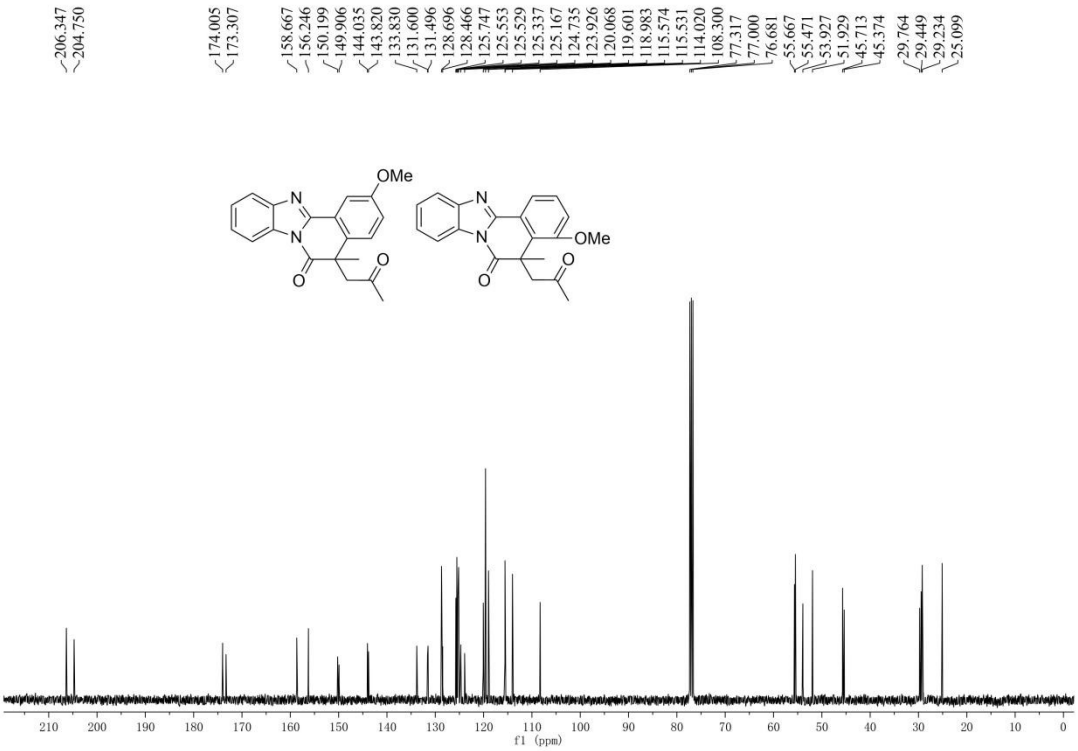




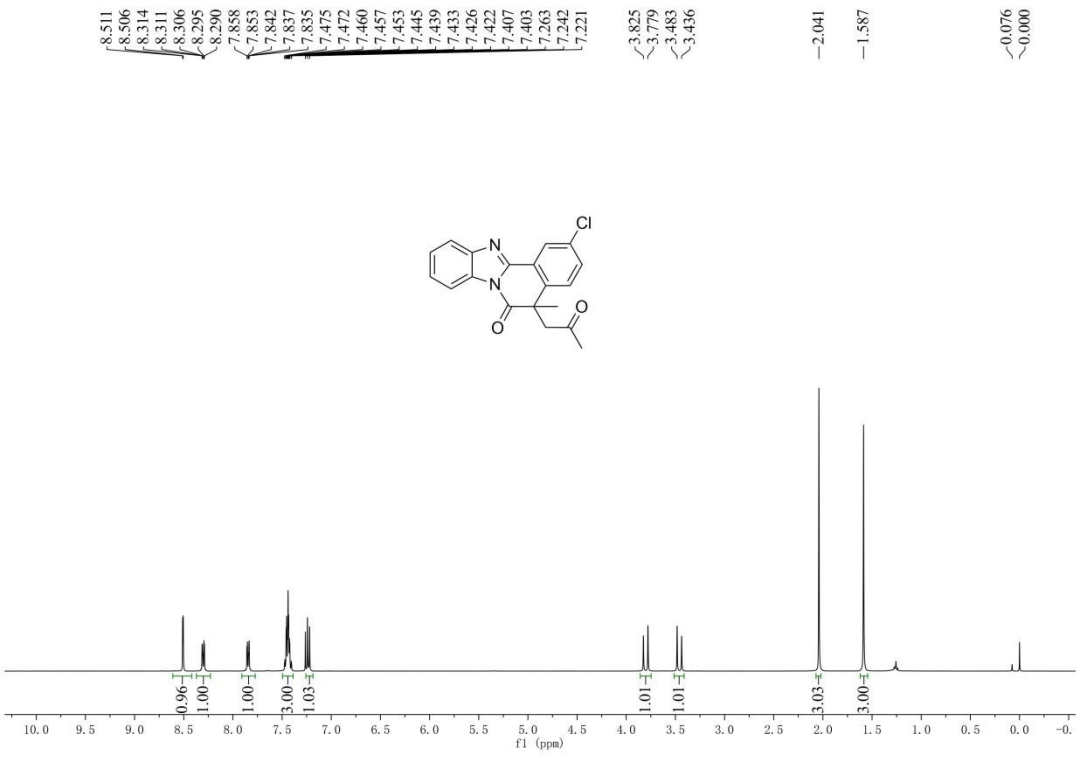

−62.786
N
N
CF3
O
O
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

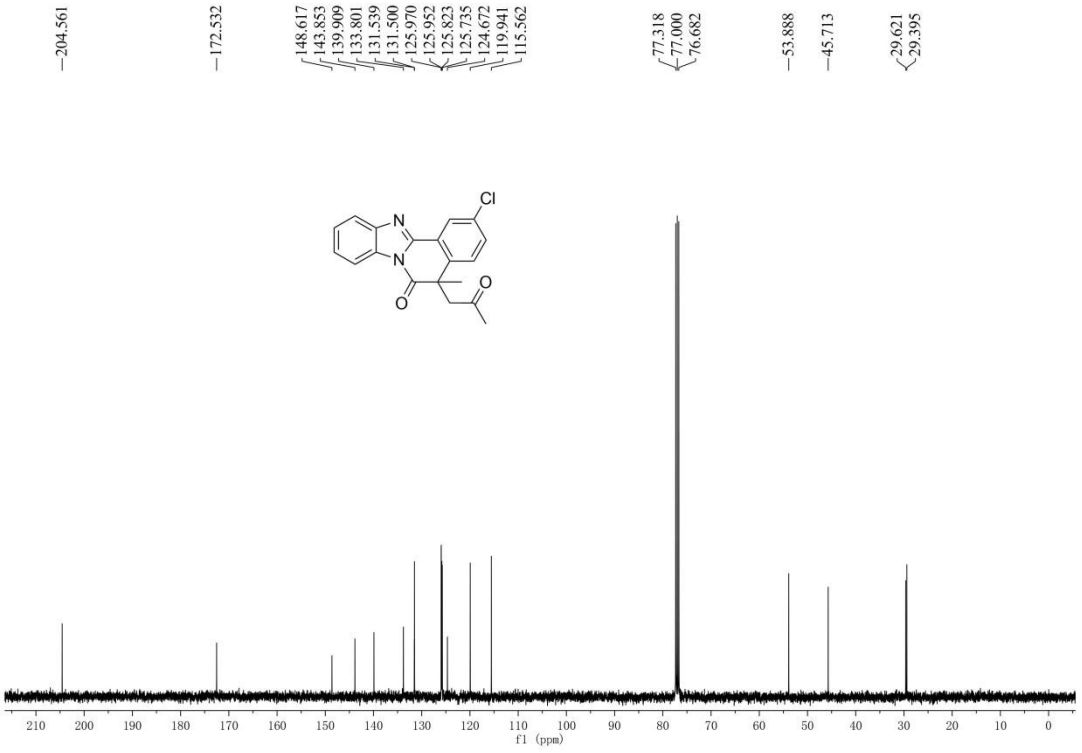
2-Methoxy-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3afa) and 4-Methoxy-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3afa')



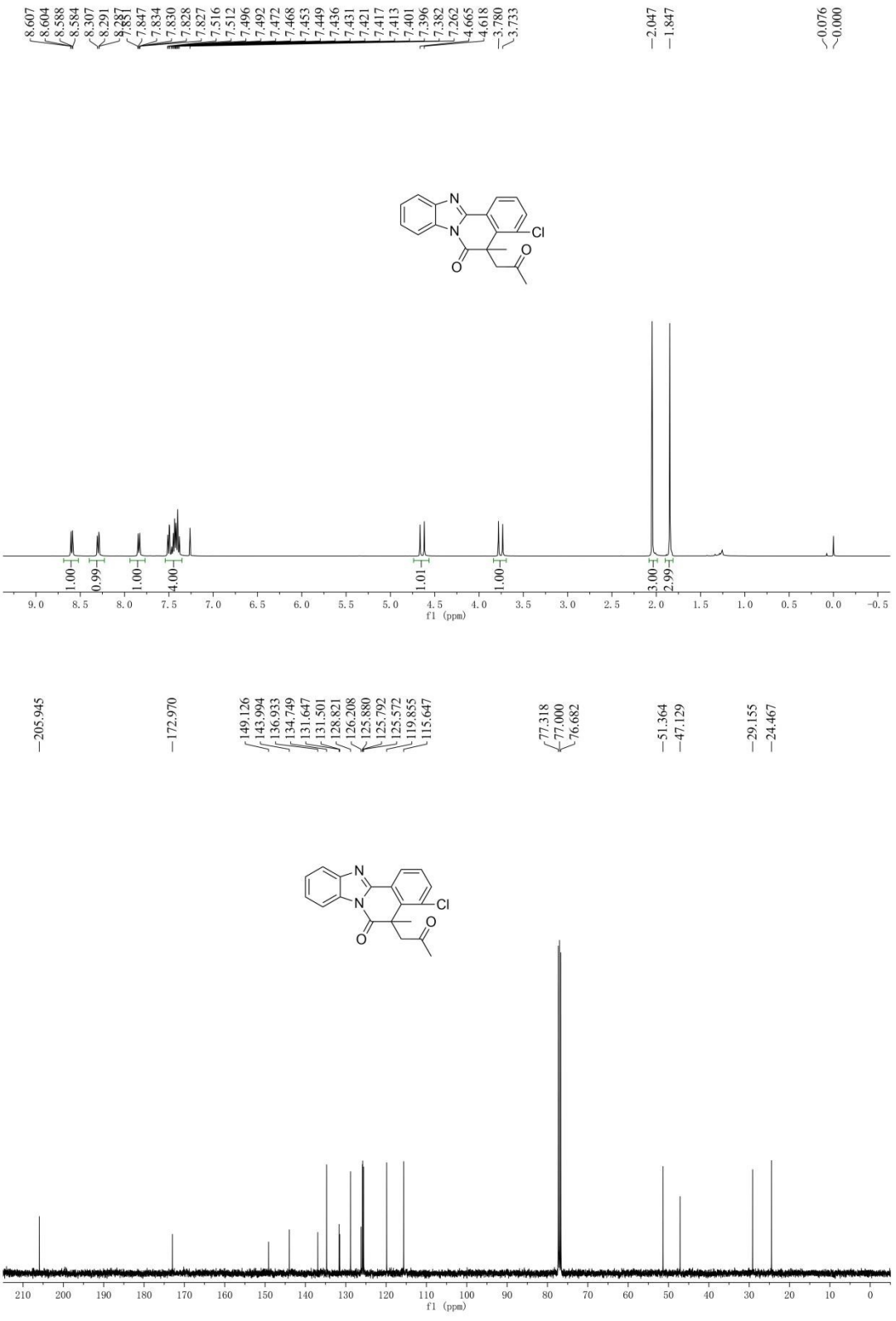


2-Chloro-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aga)

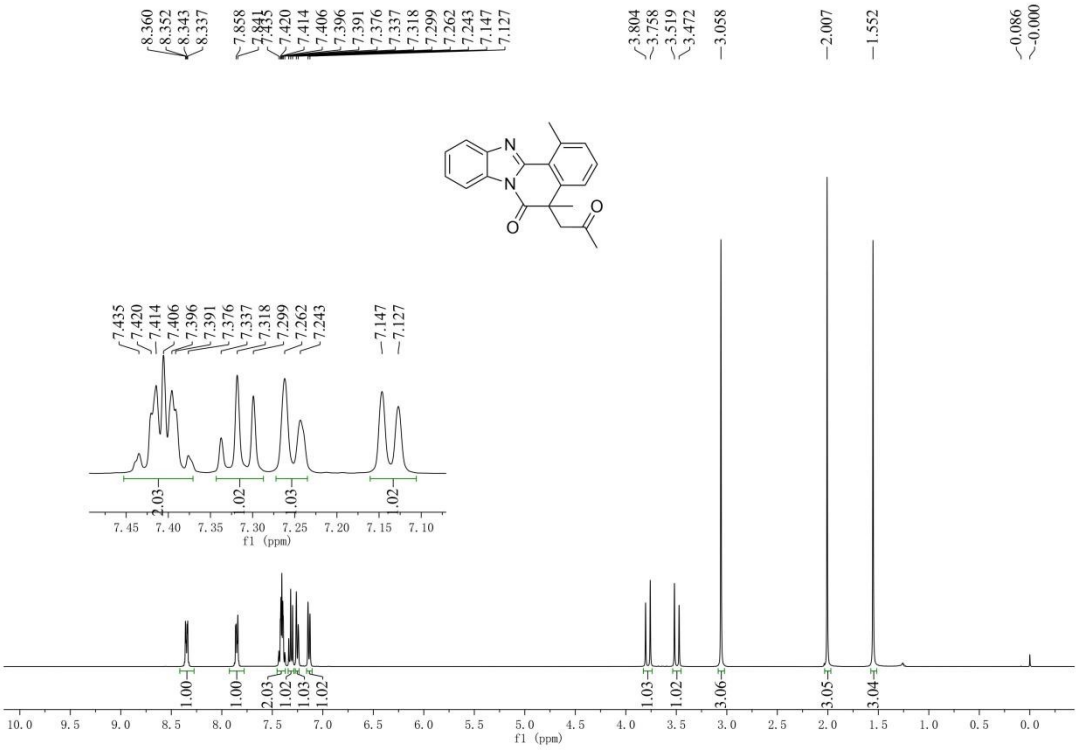


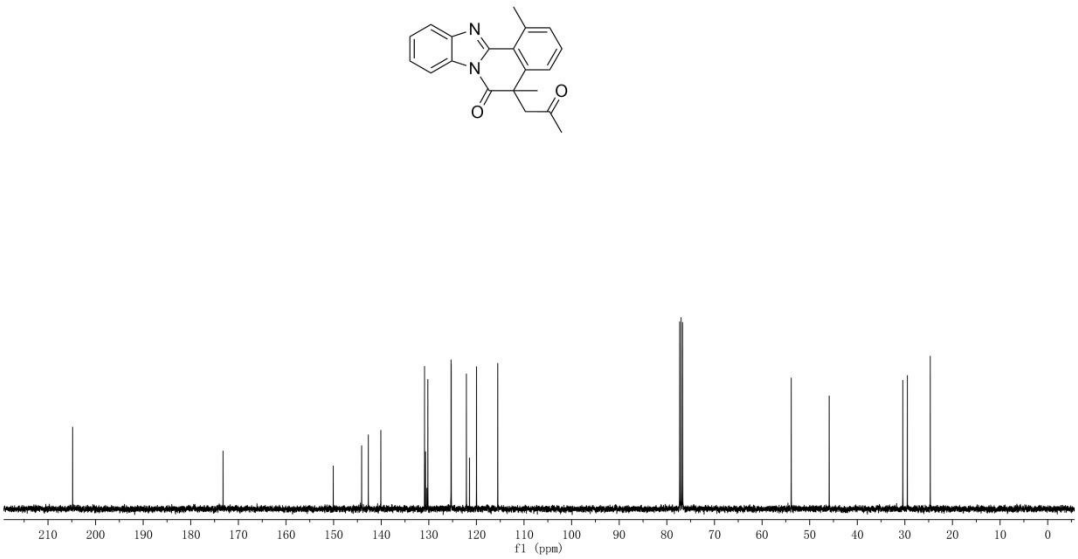


4-Chloro-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aga')

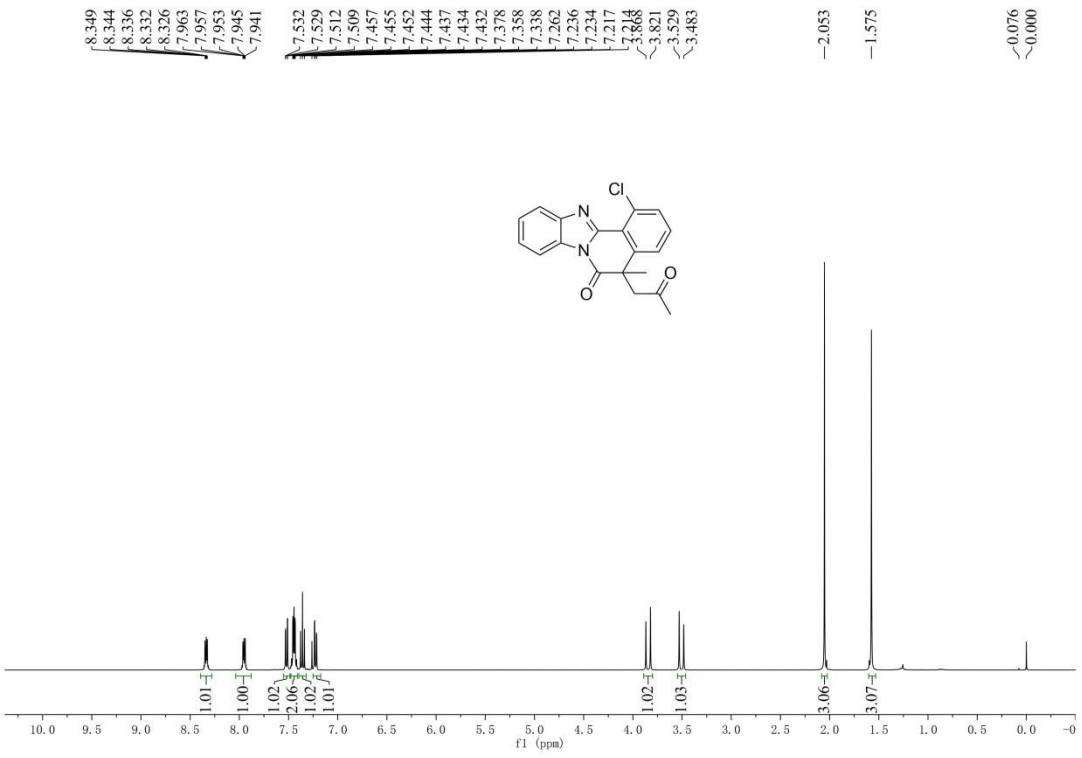


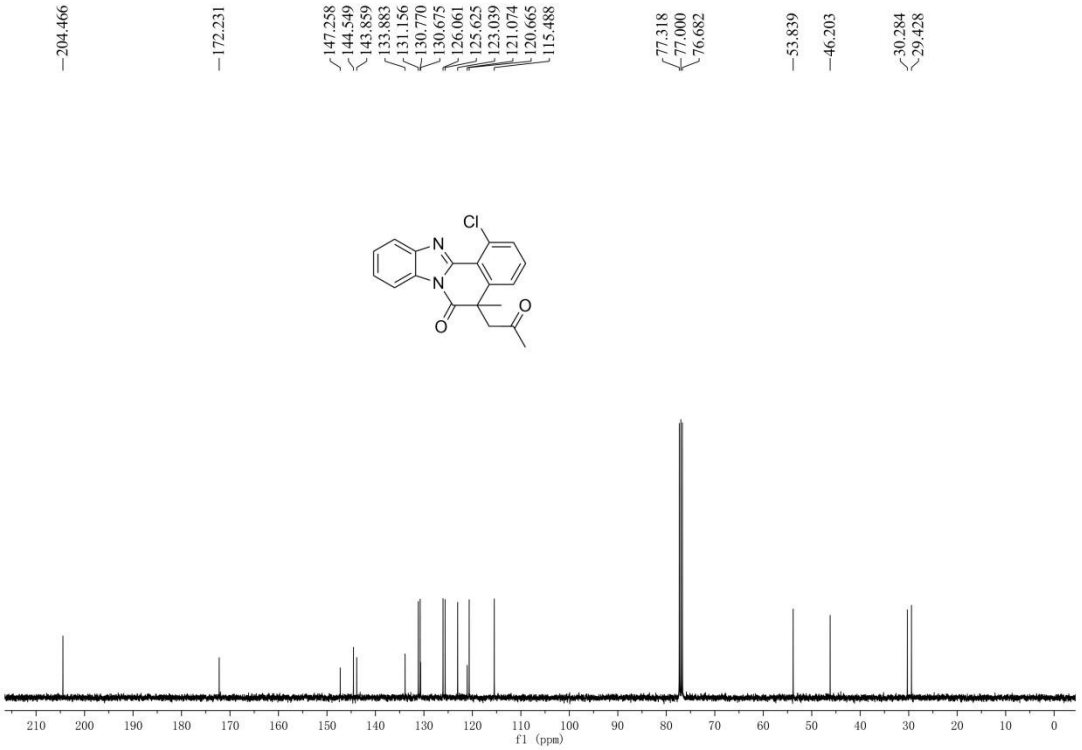
1,5-Dimethyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aha)



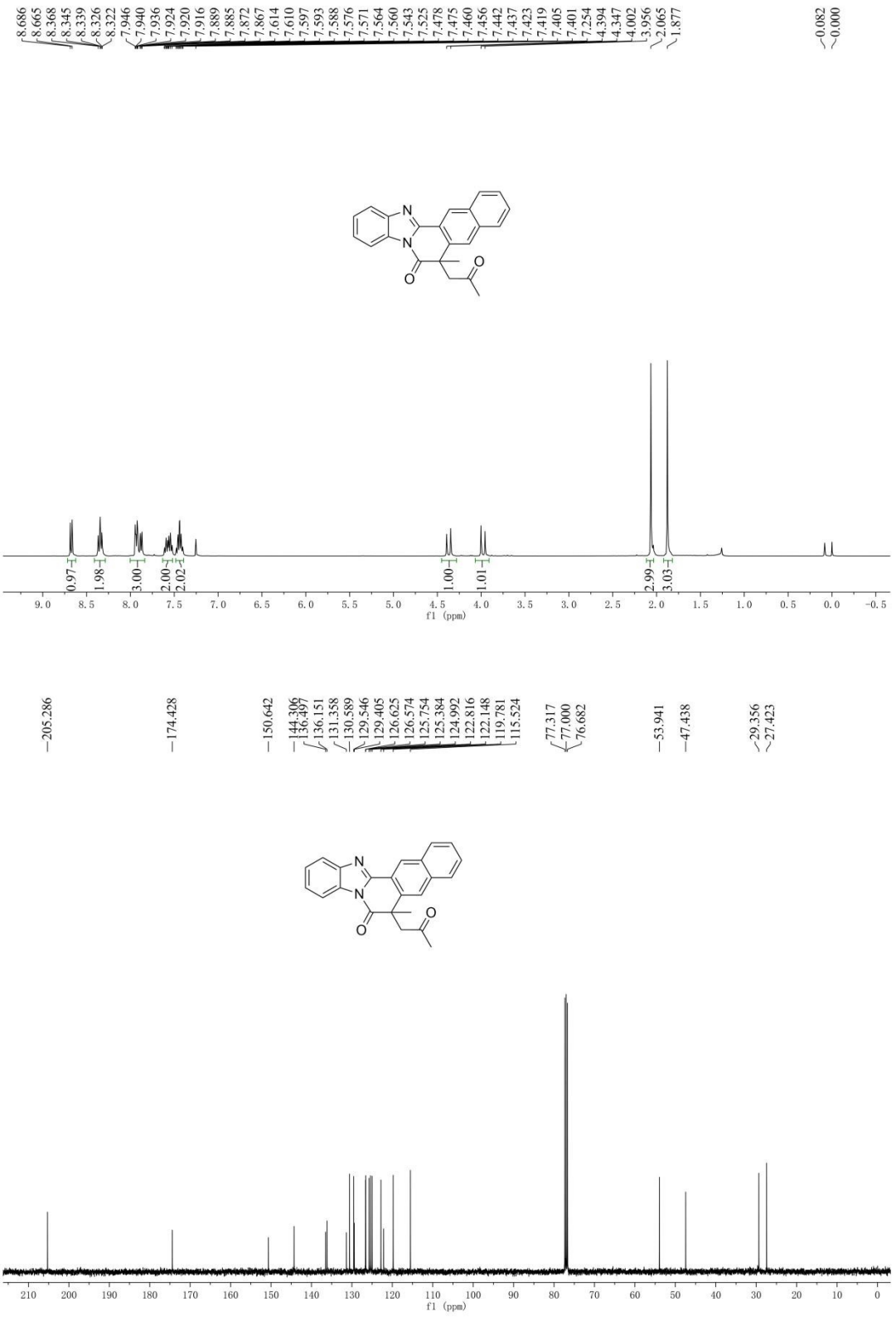


1-Chloro-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aia)

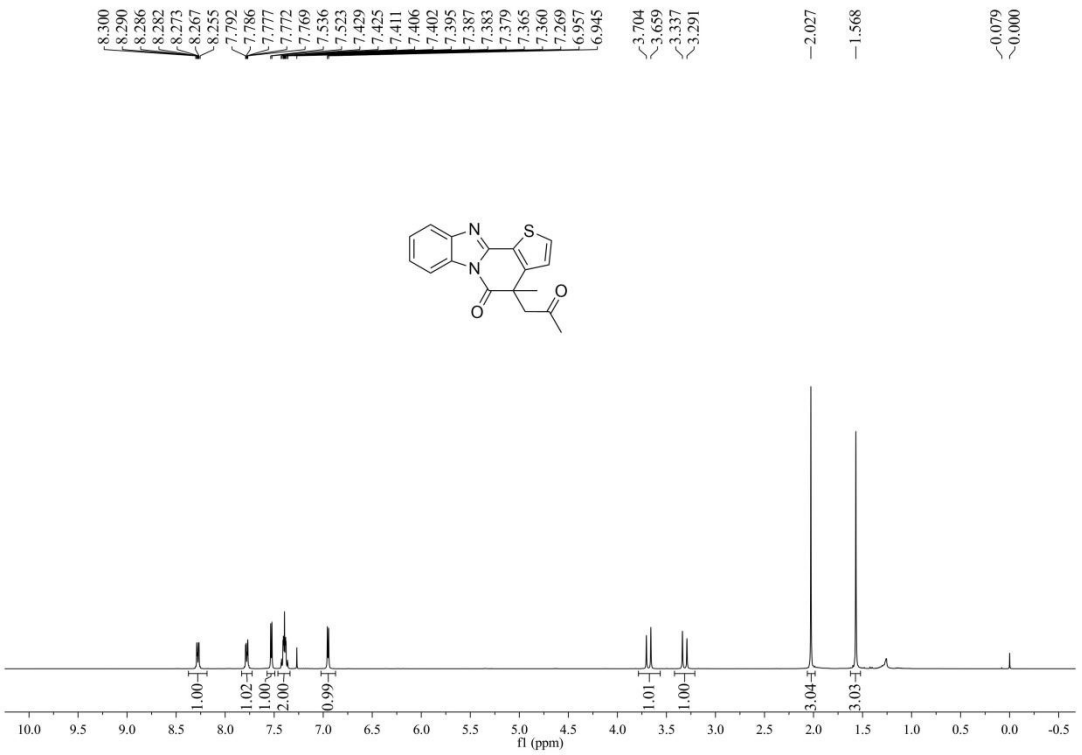


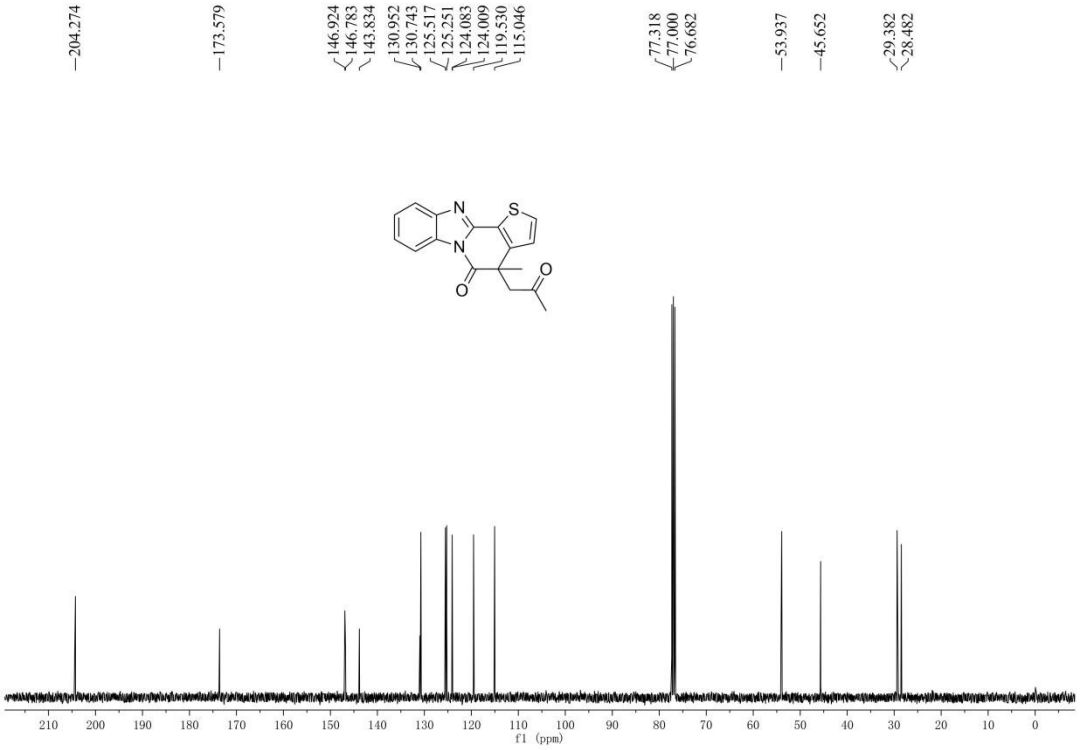


7-Methyl-7-(2-oxopropyl)benzo[g]benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(7*H*)-one (3aja)

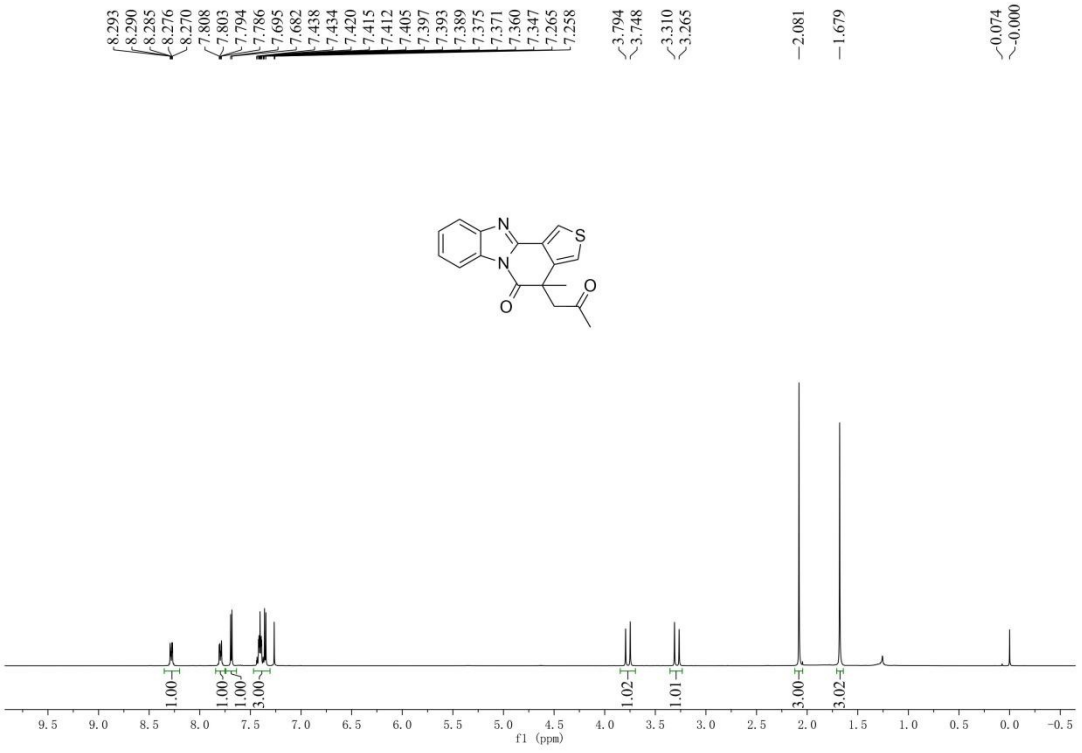


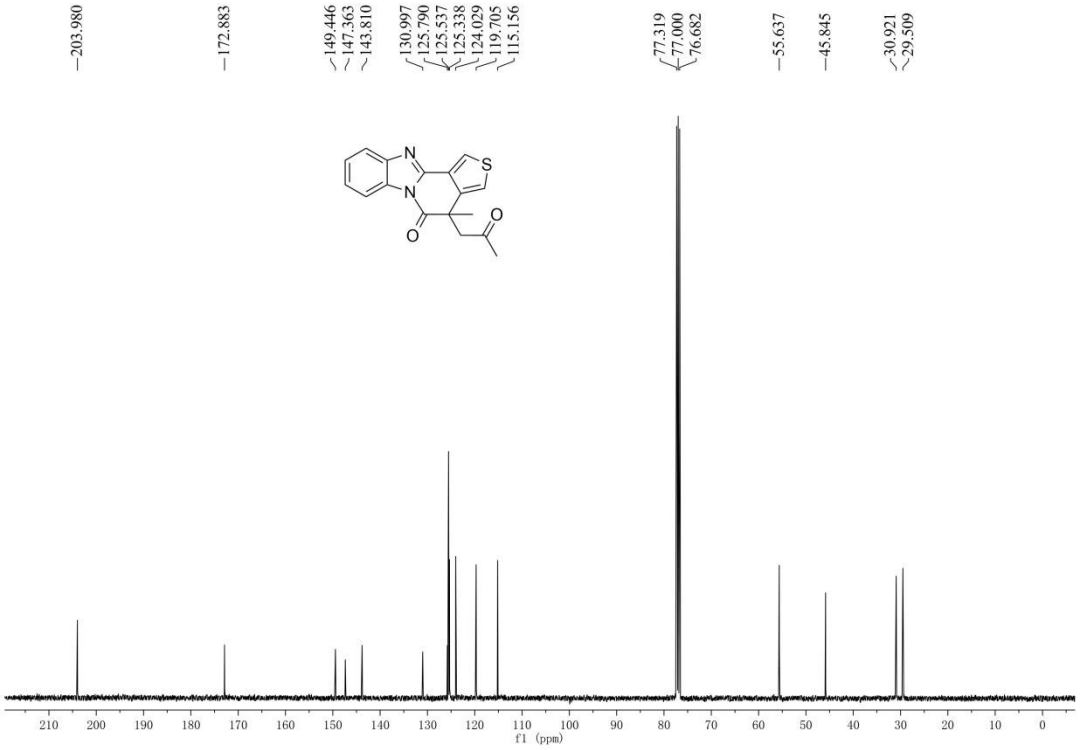
4-Methyl-4-(2-oxopropyl)benzo[4,5]imidazo[1,2-*a*]thieno[2,3-*c*]pyridin-5(4*H*)-one (3aka)



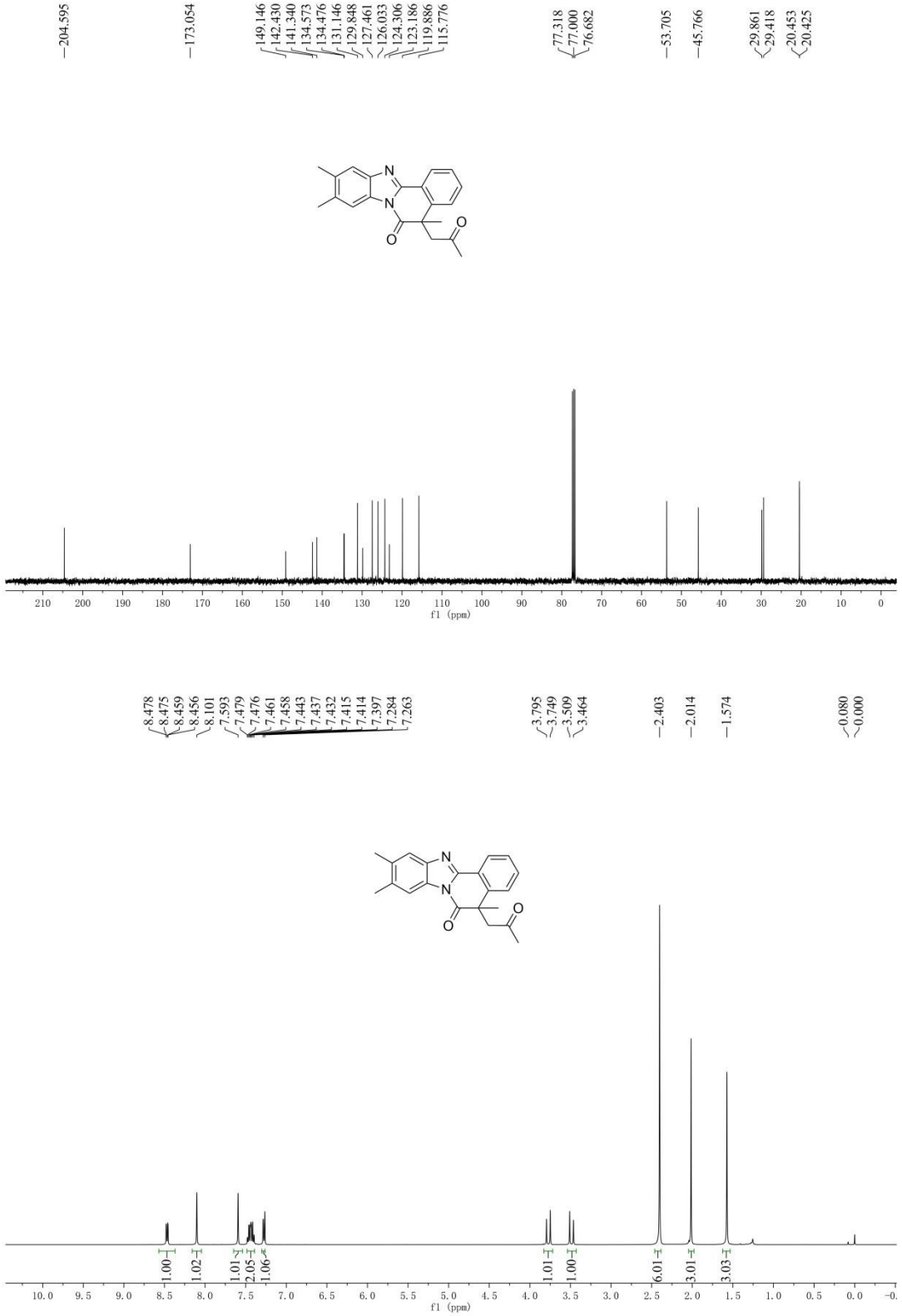


4-Methyl-4-(2-oxopropyl)benzo[4,5]imidazo[1,2-*a*]thieno[3,4-*c*]pyridin-5(4*H*)-one (3ala)

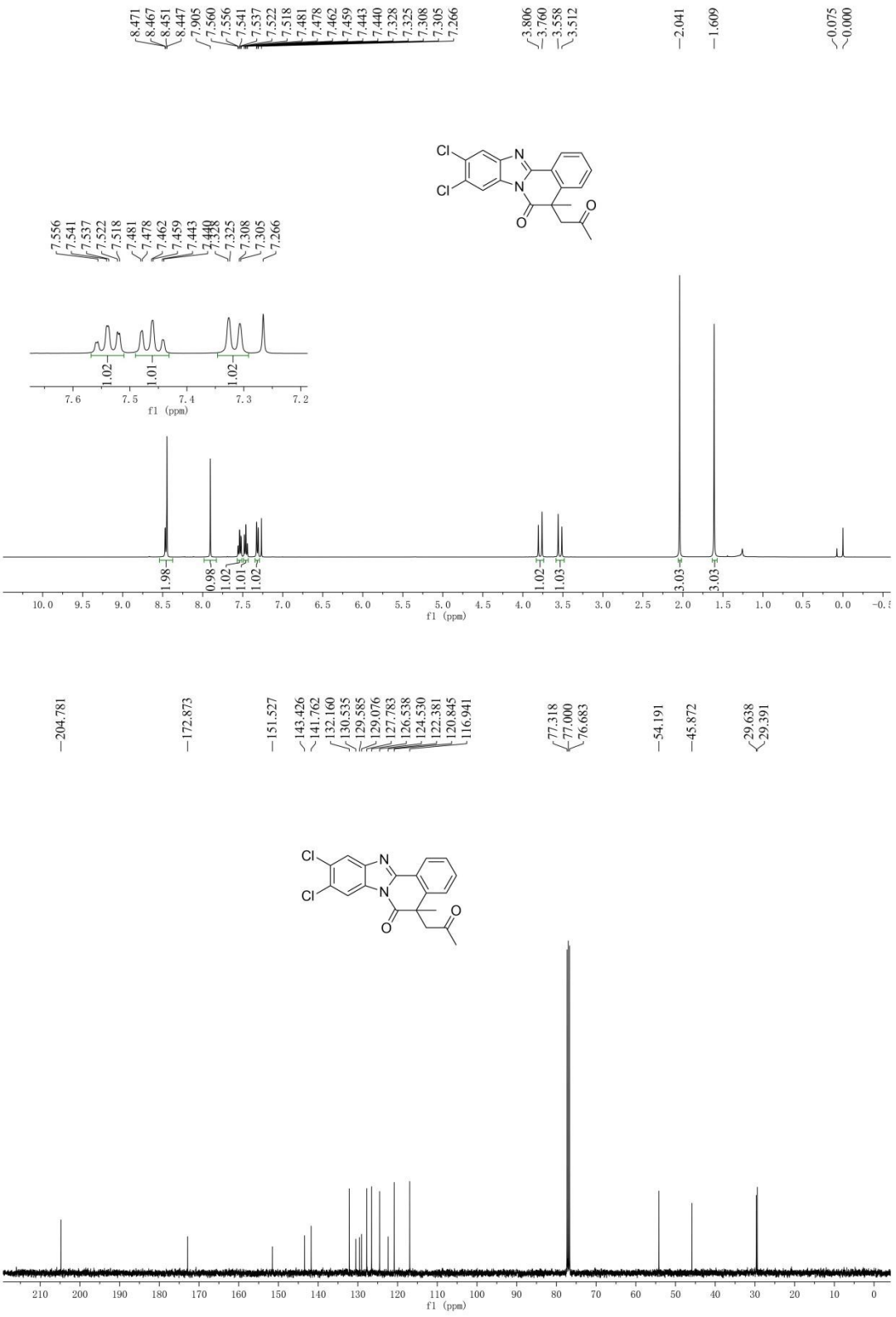




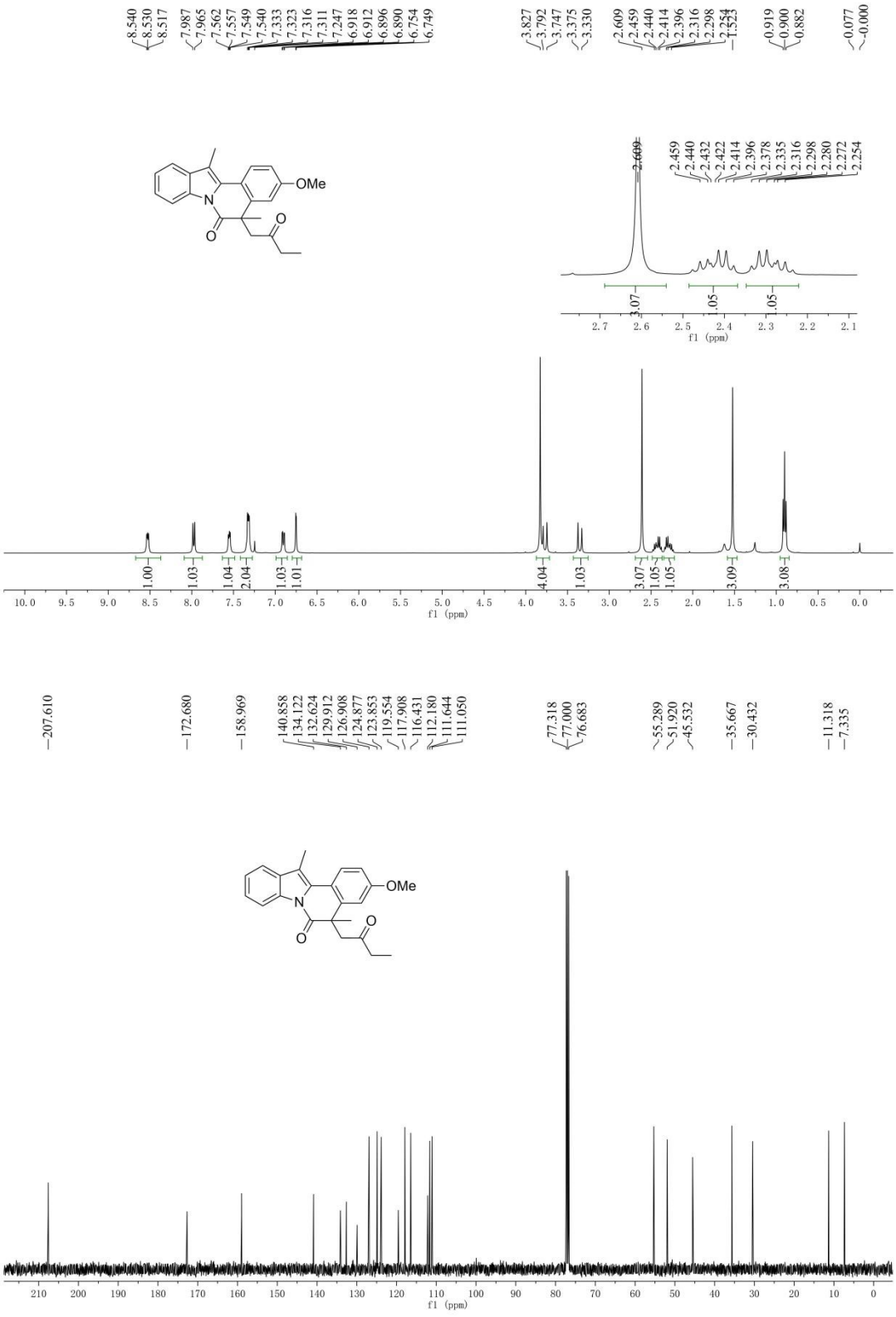
5,9,10-Trimethyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3ana)



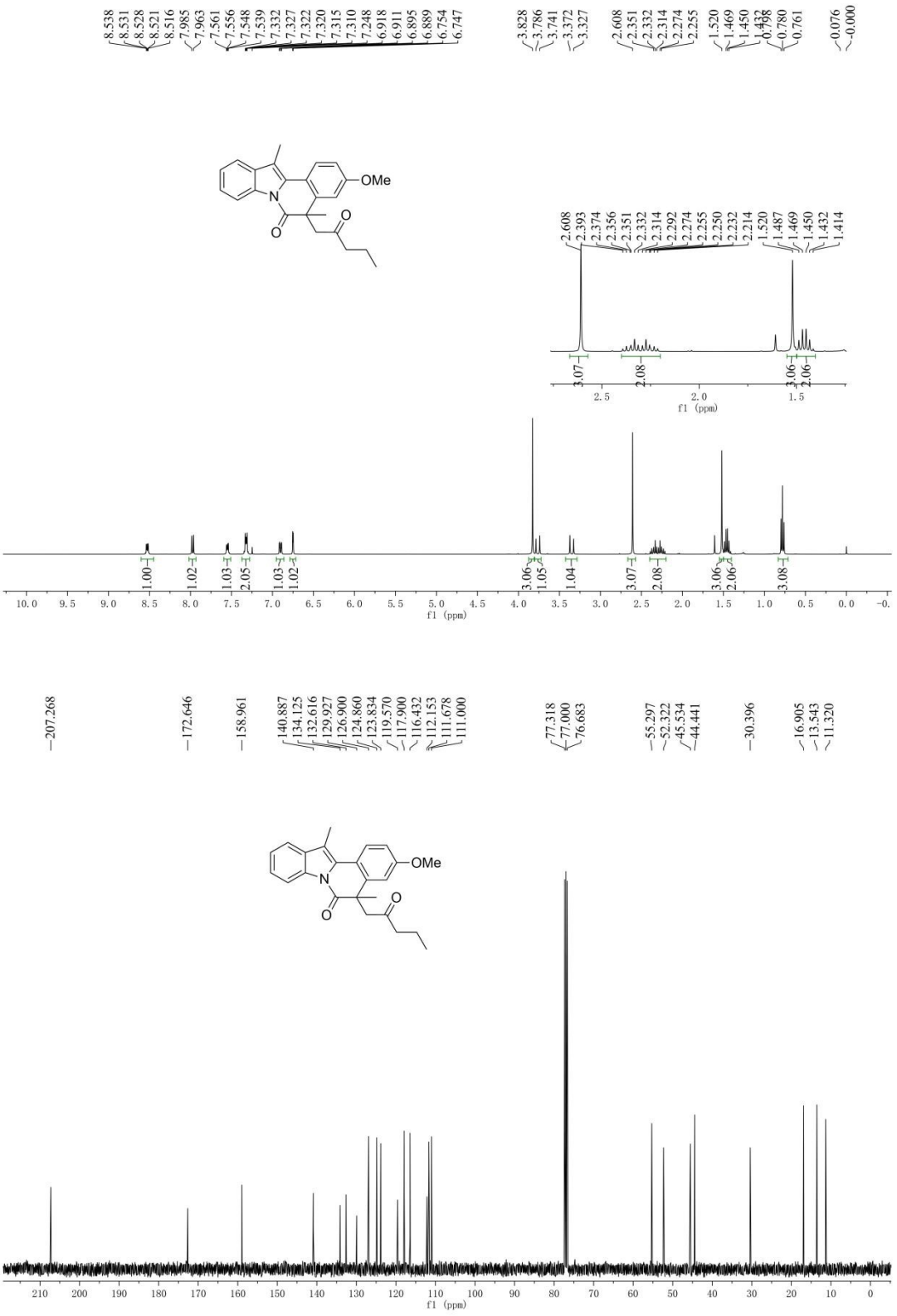
9,10-Dichloro-5-methyl-5-(2-oxopropyl)benzo[4,5]imidazo[2,1-*a*]isoquinolin-6(5*H*)-one (3aoa)



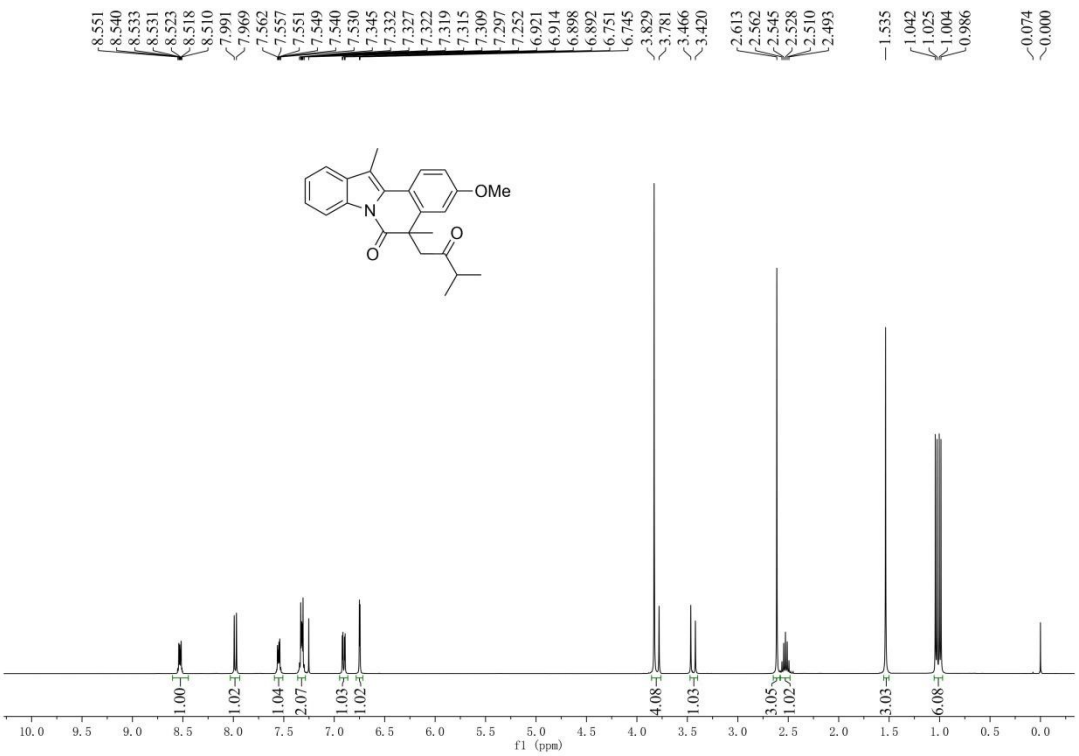
3-Methoxy-5,12-dimethyl-5-(2-oxobutyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ab)

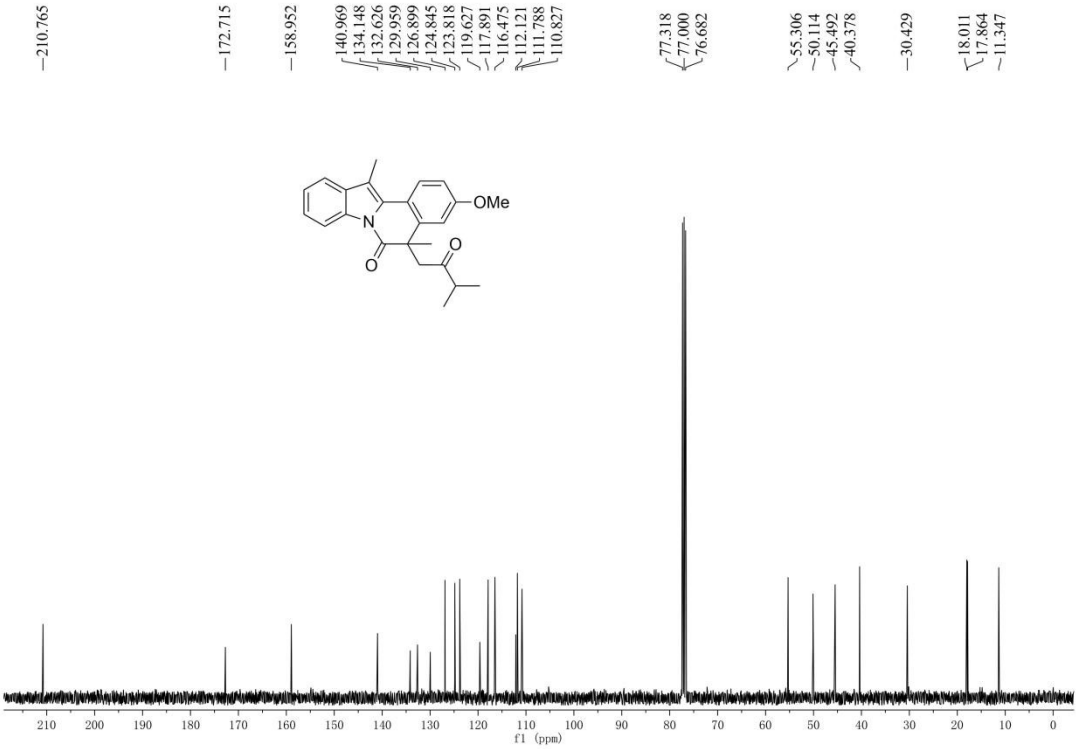


3-Methoxy-5,12-dimethyl-5-(2-oxopentyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ac)

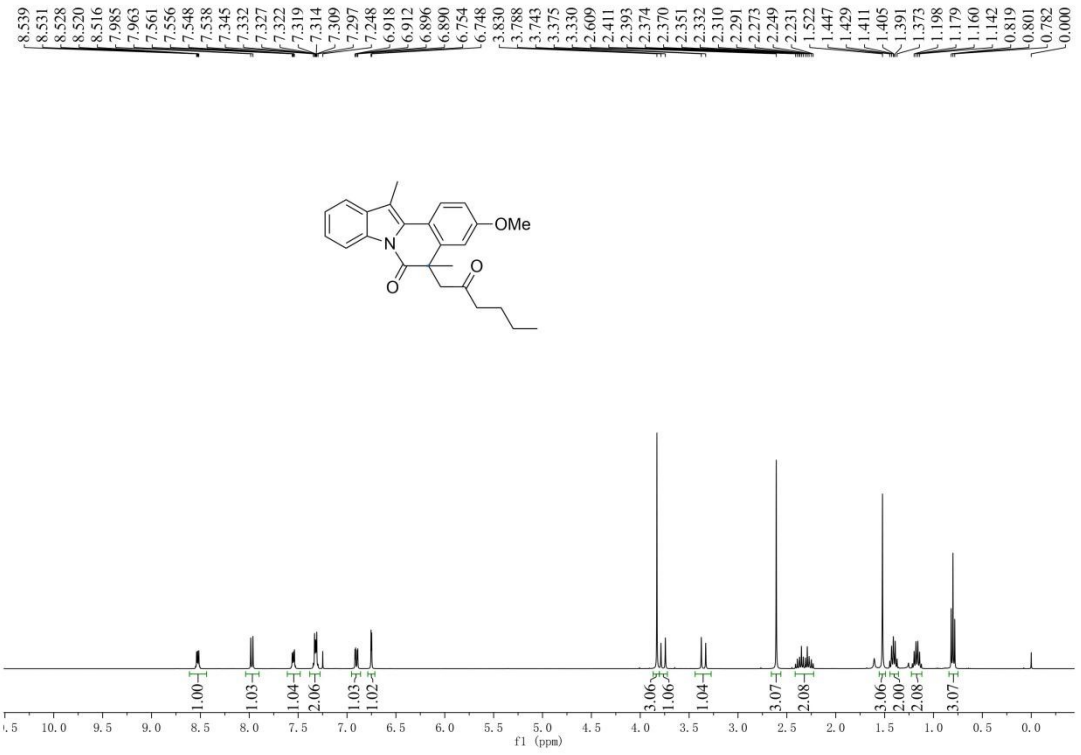


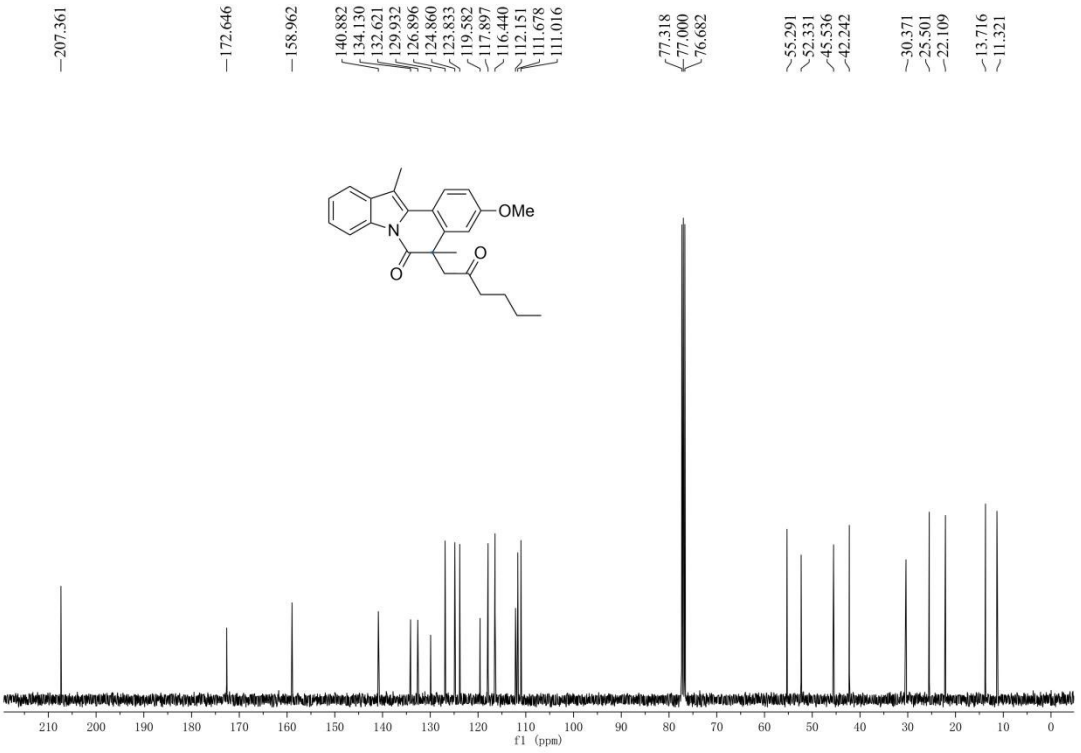
3-Methoxy-5,12-dimethyl-5-(3-methyl-2-oxobutyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ad)



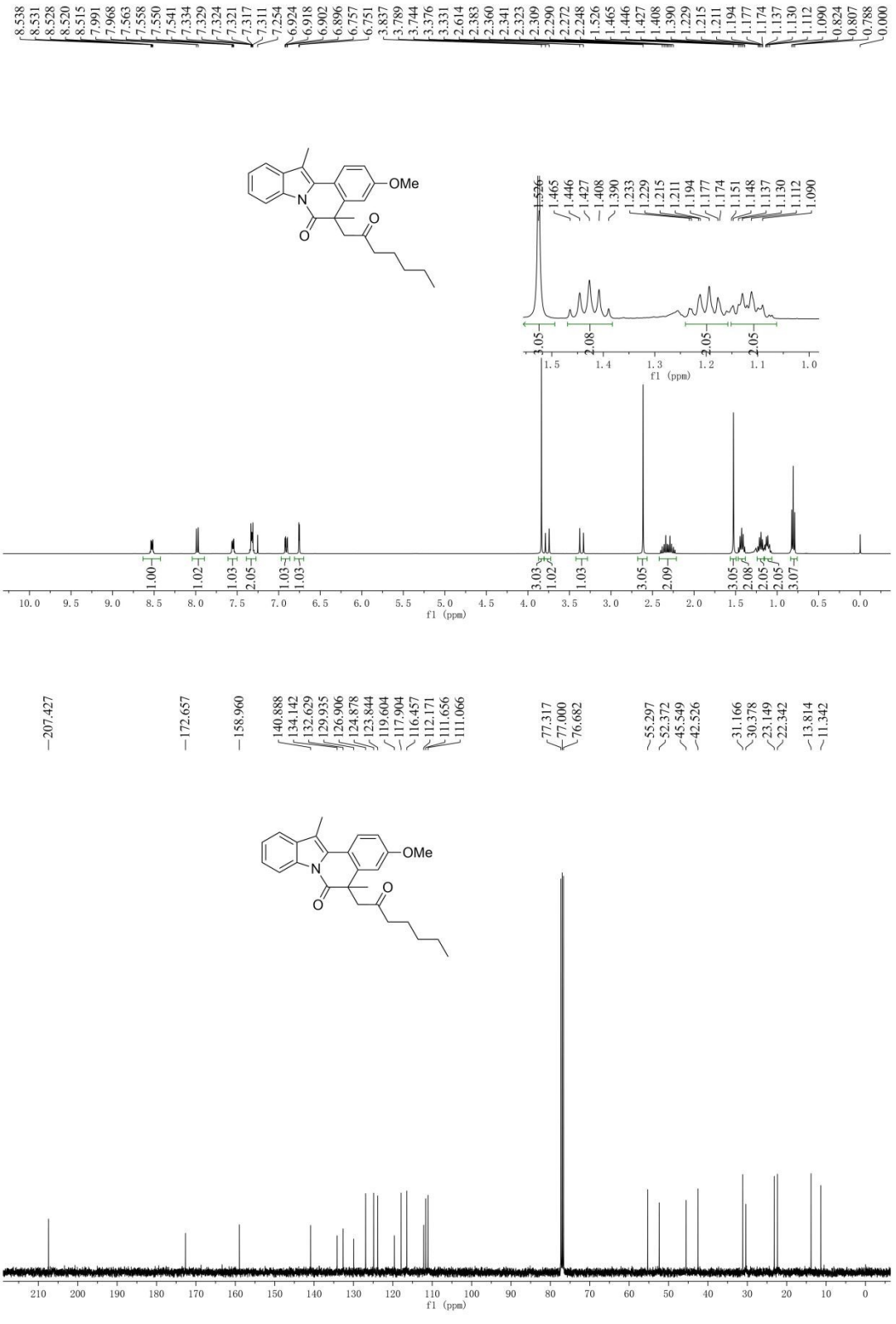


3-Methoxy-5,12-dimethyl-5-(2-oxohexyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ae)

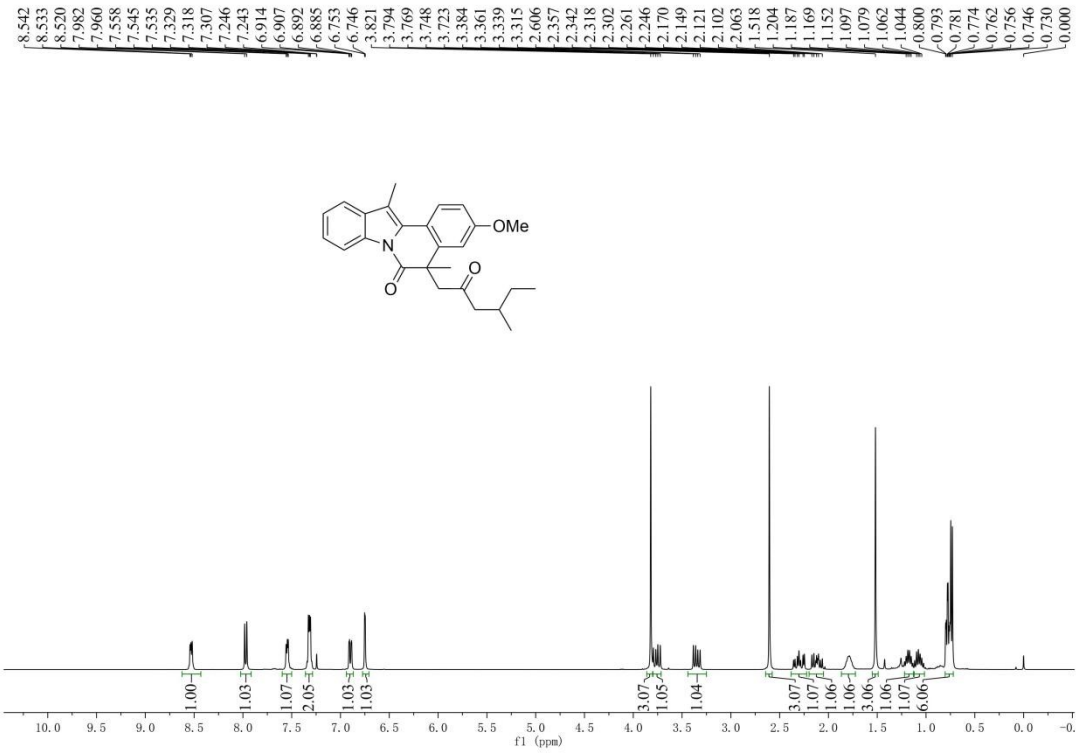


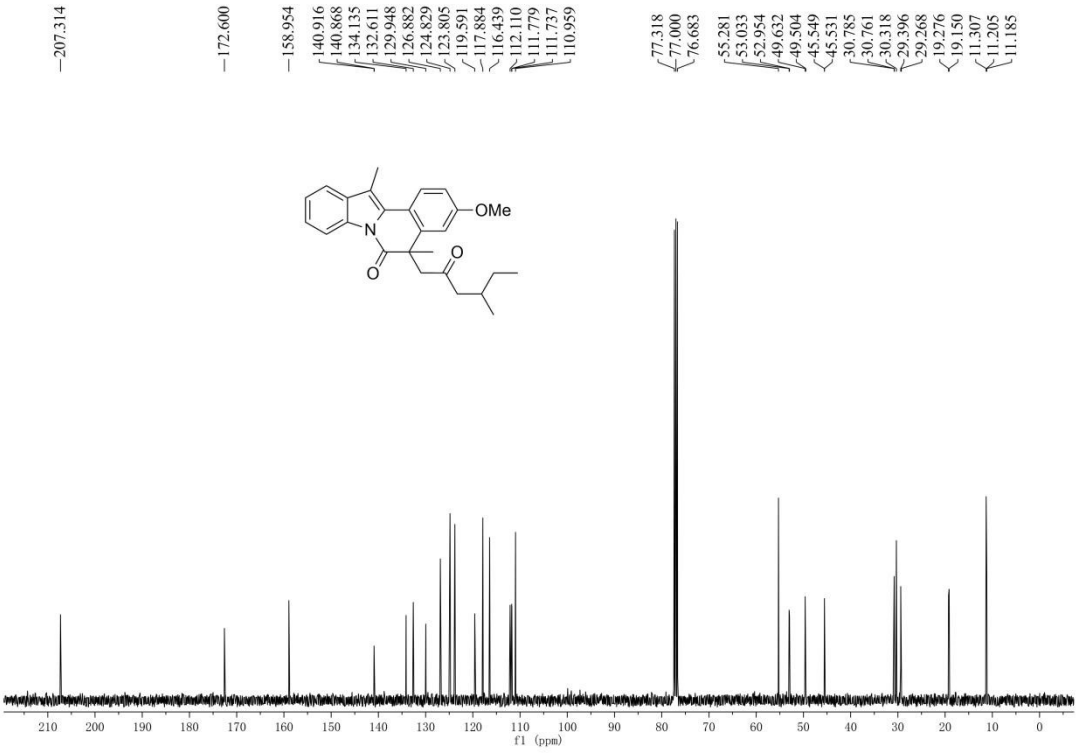


3-Methoxy-5,12-dimethyl-5-(2-oxoheptyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3af)

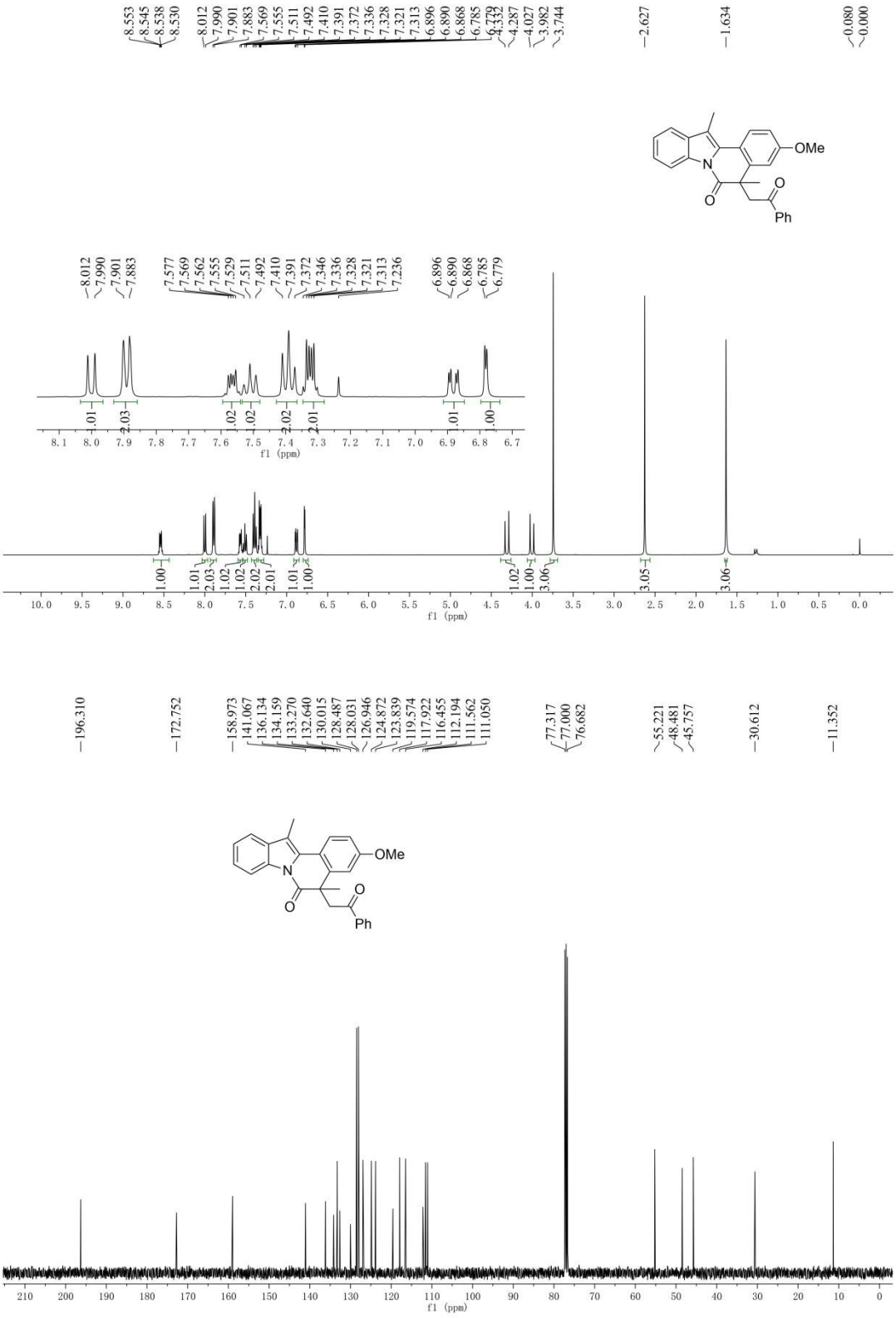


3-Methoxy-5,12-dimethyl-5-(4-methyl-2-oxohexyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ag)

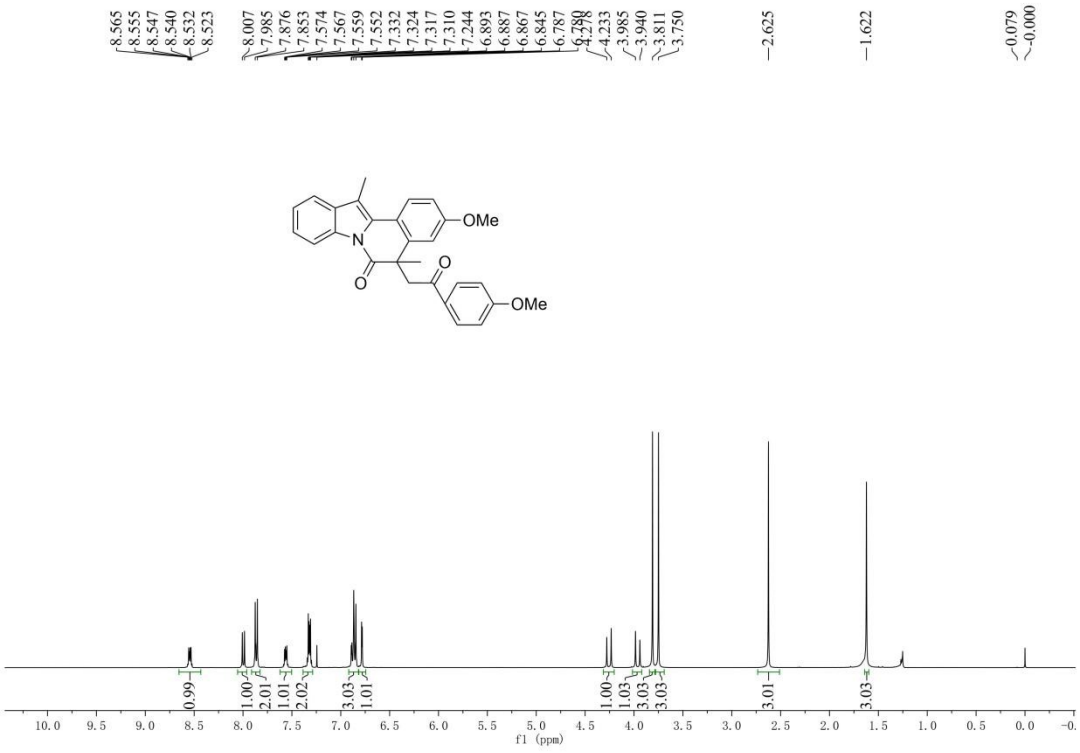


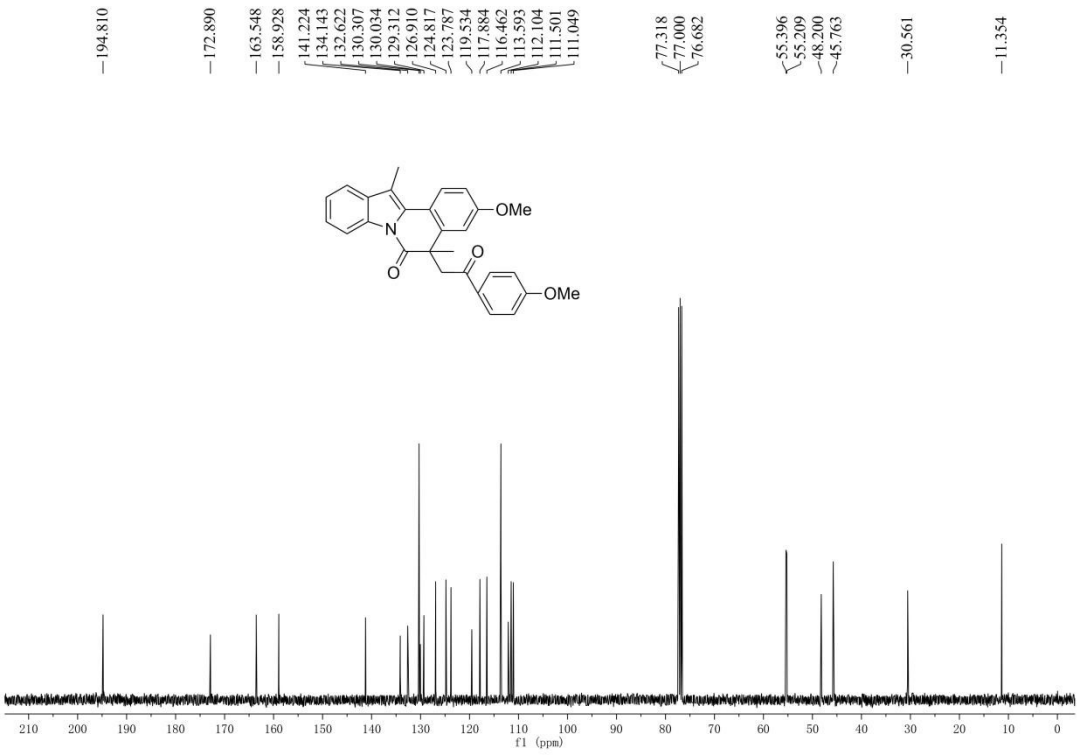


3-Methoxy-5,12-dimethyl-5-(2-oxo-2-phenylethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ah)

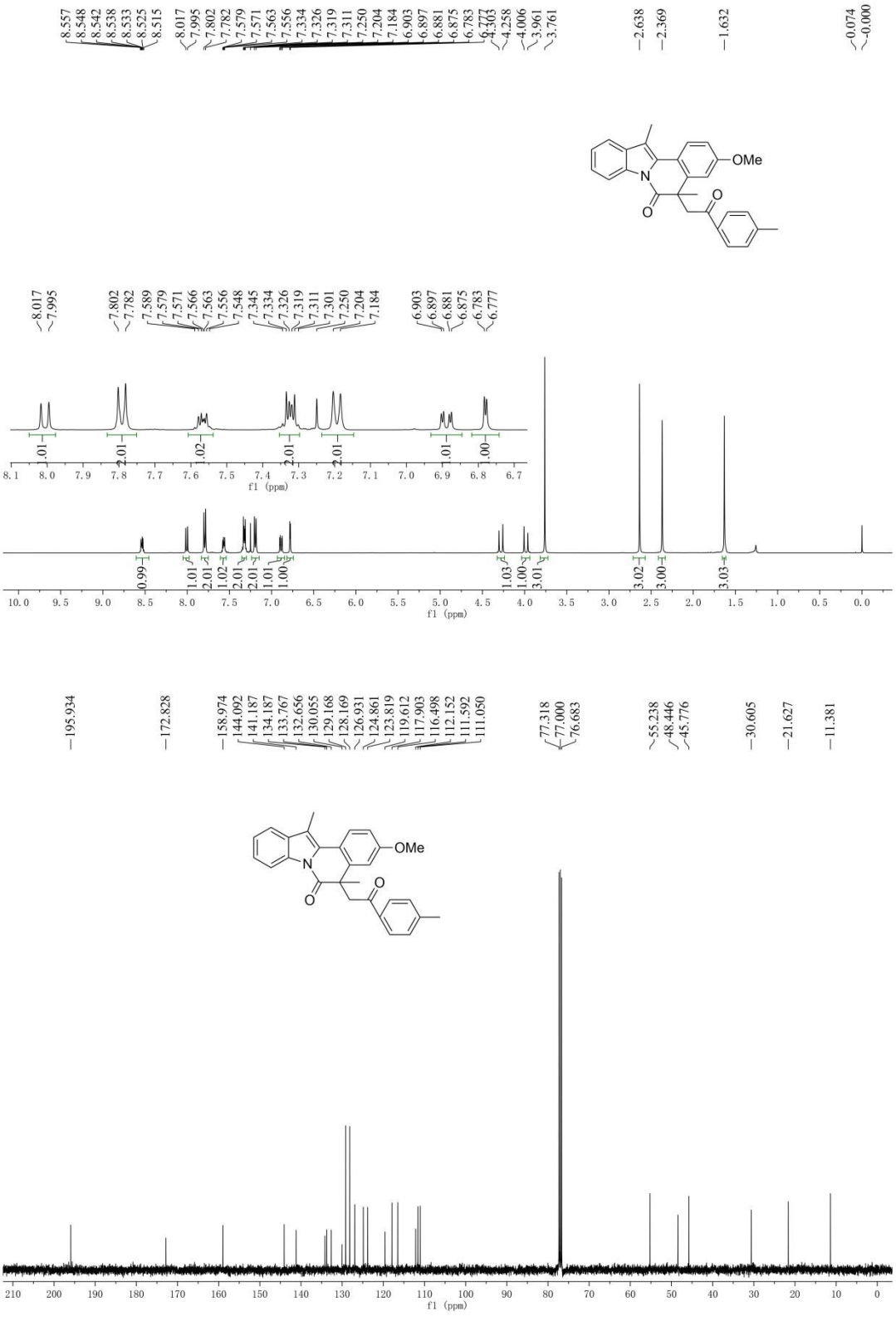


3-Methoxy-5-(2-(4-methoxyphenyl)-2-oxoethyl)-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ai)

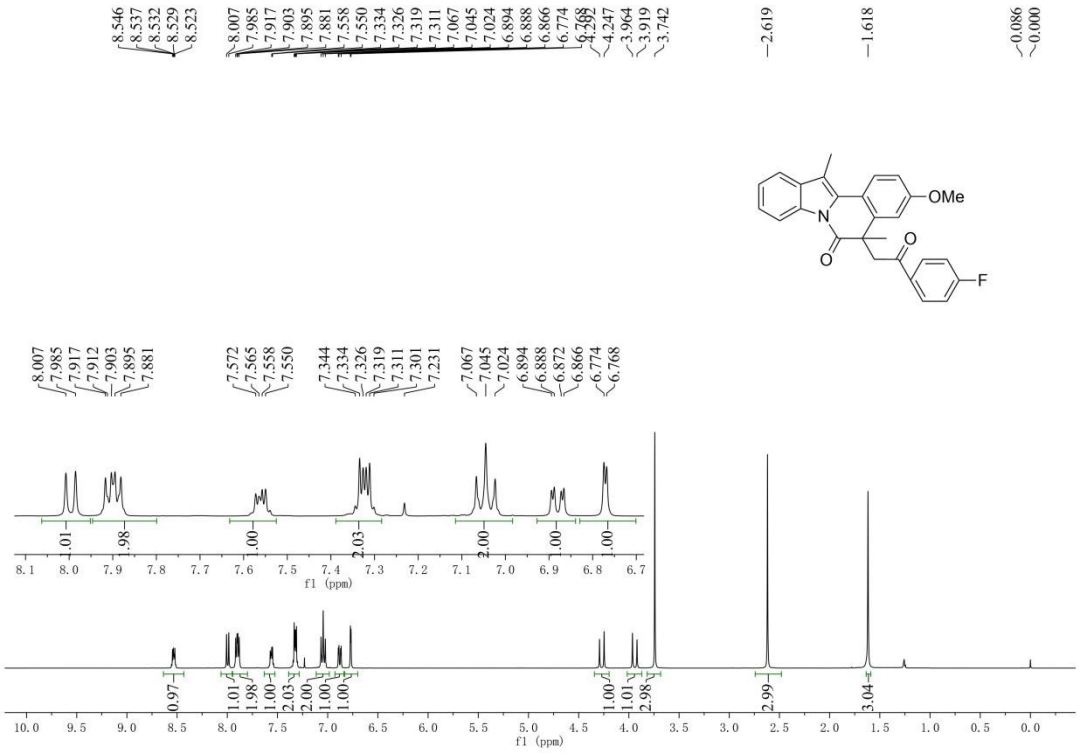


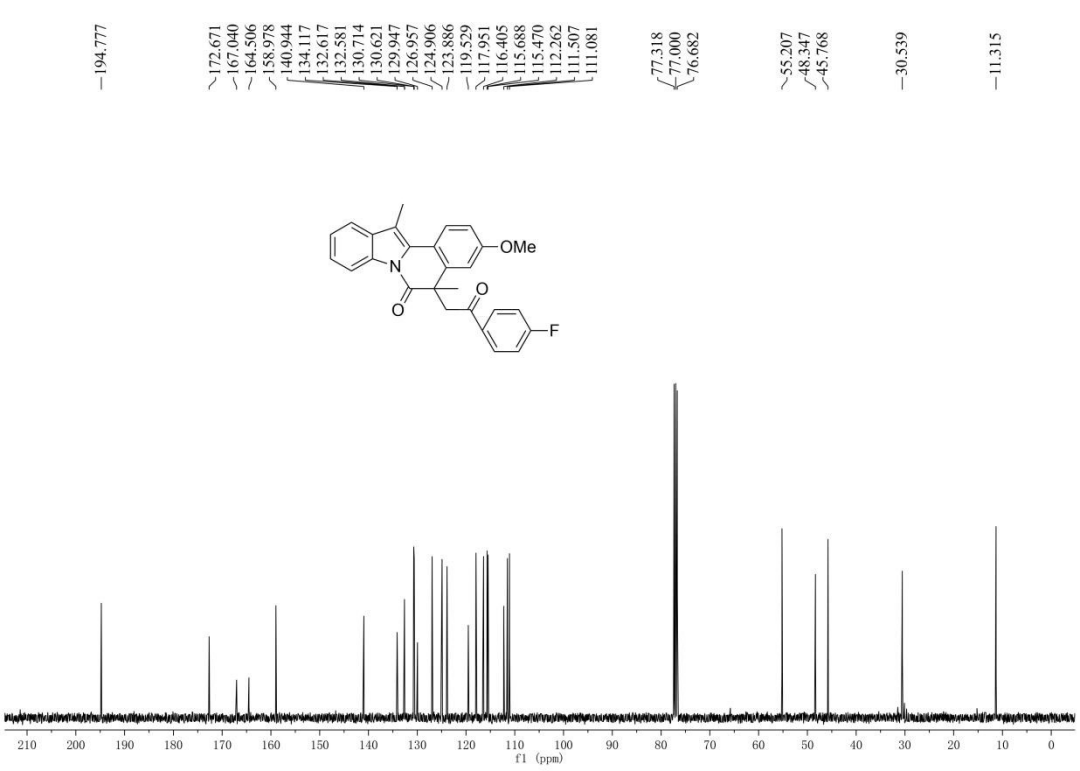


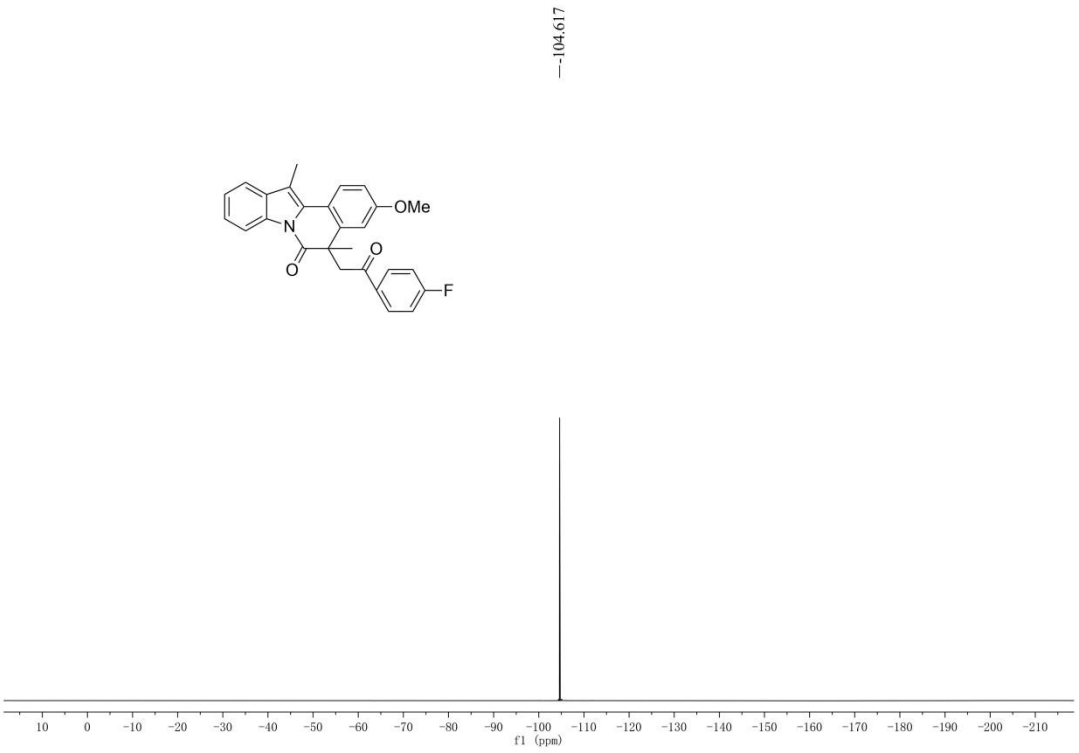
3-Methoxy-5,12-dimethyl-5-(2-oxo-2-(p-tolyl)ethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3aj)



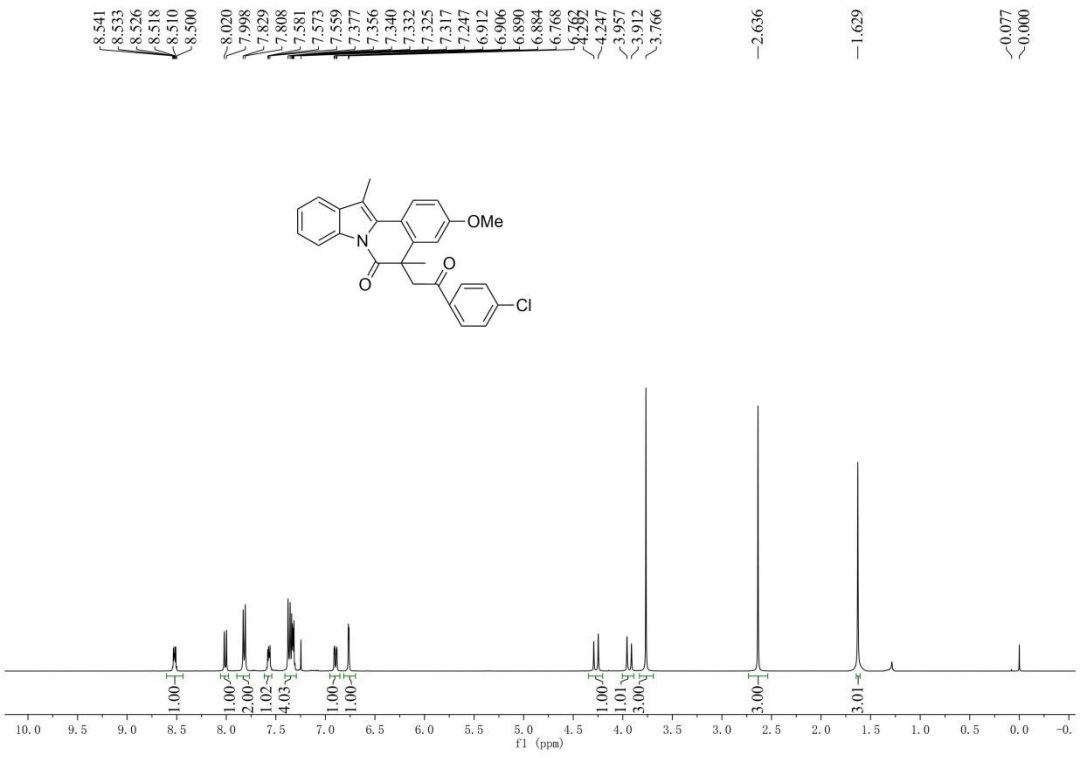
5-(2-(4-Fluorophenyl)-2-oxoethyl)-3-methoxy-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ak)

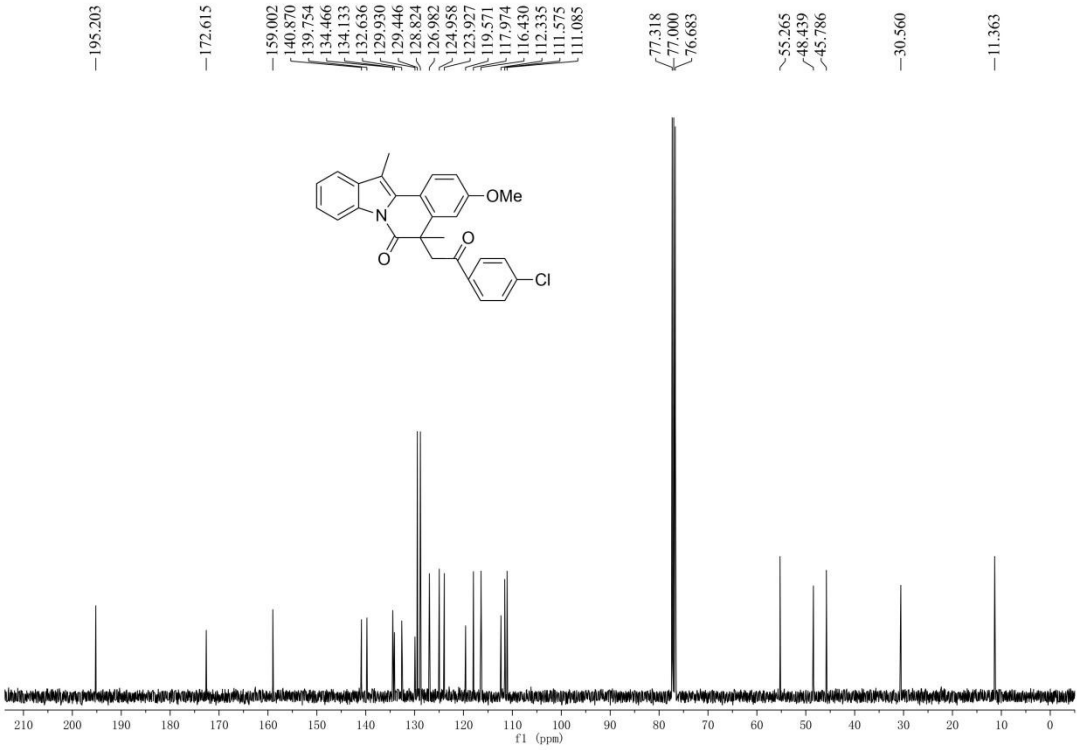

8.546
8.537
8.532
8.529
8.523
8.007
7.985
7.917
7.903
7.895
7.881
7.558
7.550
7.334
7.326
7.319
7.311
7.067
7.045
7.024
6.894
6.888
6.866
6.774
6.768
4.252
4.247
3.964
3.919
3.742
2.619
1.618
0.086
0.000
OMe
N
O
O
F
f1 (ppm)


194.777
172.671
167.040
164.506
158.978
140.944
134.117
132.617
132.581
130.714
130.621
129.947
126.957
124.906
123.886
119.529
117.951
116.405
115.688
115.470
112.262
111.507
111.081
77.318
77.000
76.682
55.207
48.347
45.768
30.539
11.315
OMe
N
O
O
F
f1 (ppm)

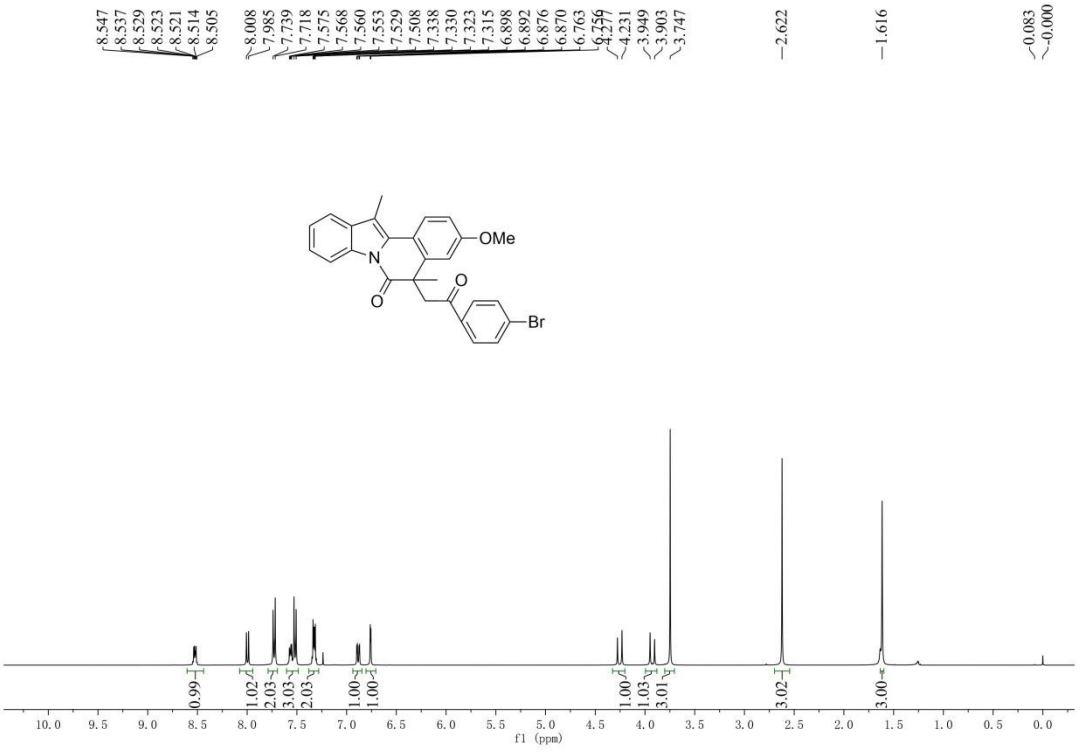

-104.617
OMe
N
O
O
F
10
0
−10
−20
−30
−40
−50
−60
−70
−80
−90
−100
−110
−120
−130
−140
−150
−160
−170
−180
−190
−200
−210
f1 (ppm)

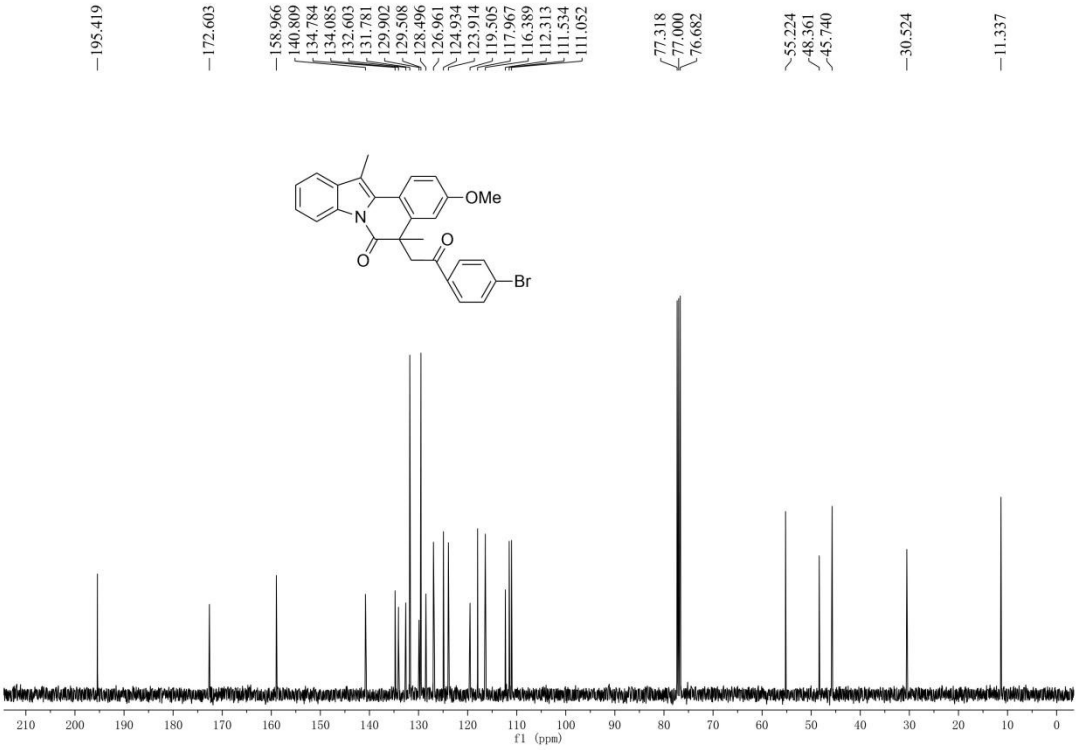
5-(2-(4-Chlorophenyl)-2-oxoethyl)-3-methoxy-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3al)



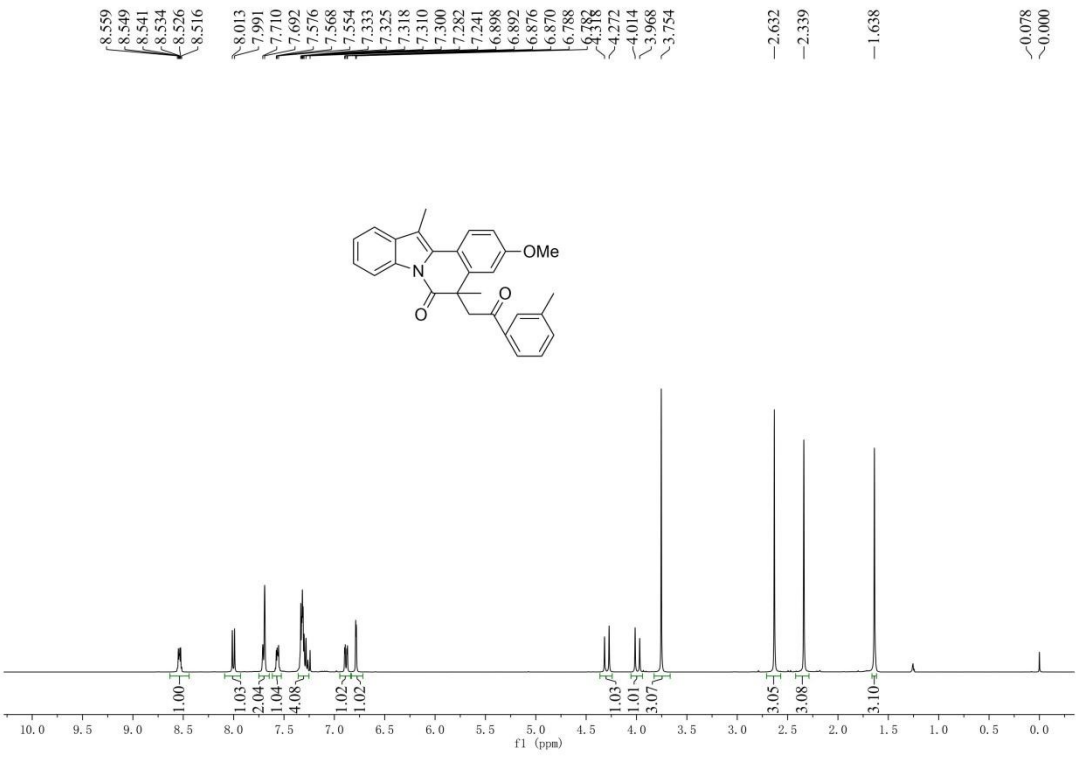


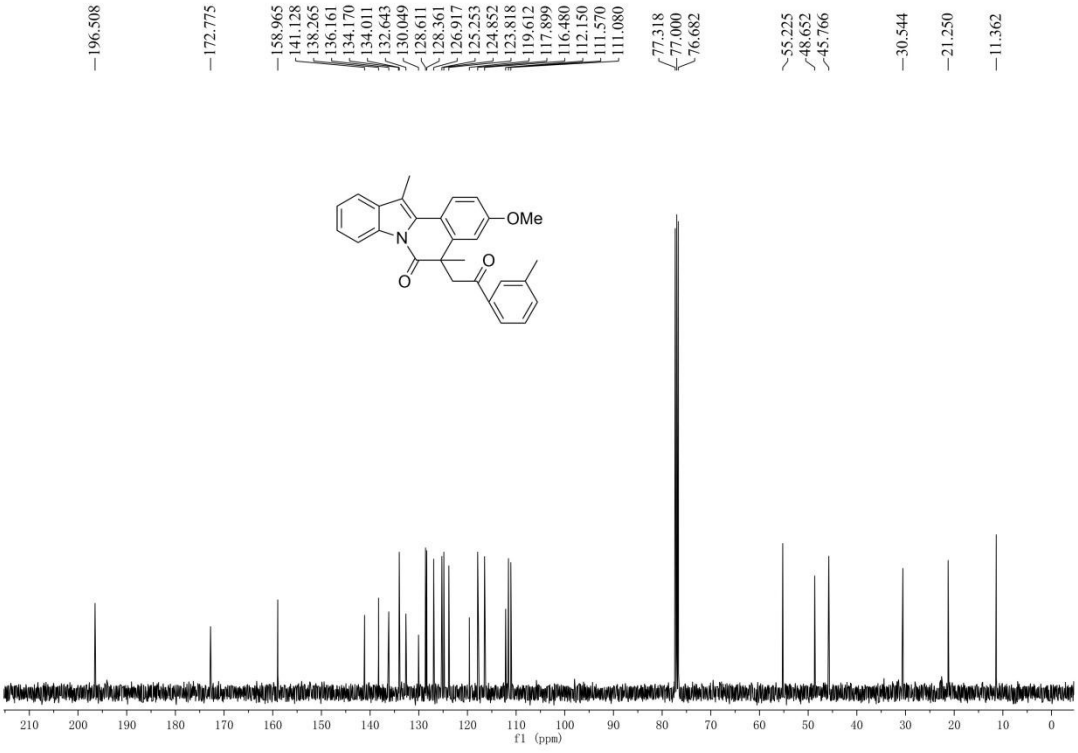
5-(2-(4-Bromophenyl)-2-oxoethyl)-3-methoxy-5,12-dimethylindolo[2,1-*a*]isoquinolin-6(5*H*)-one (3am)



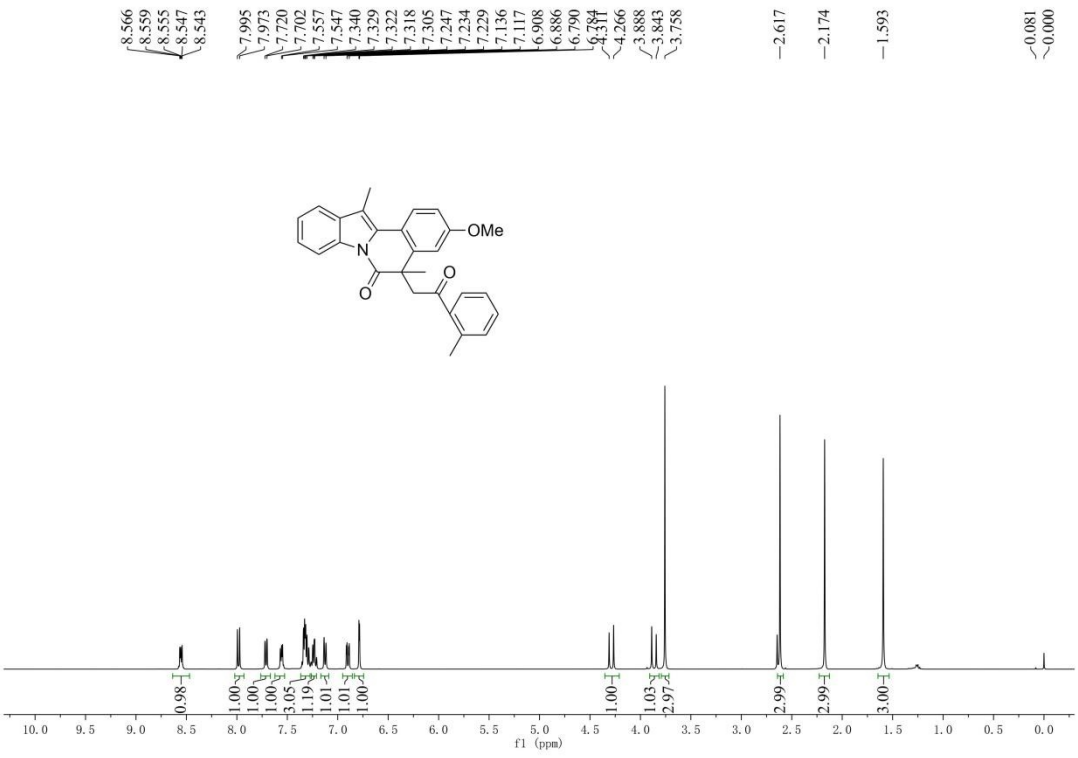


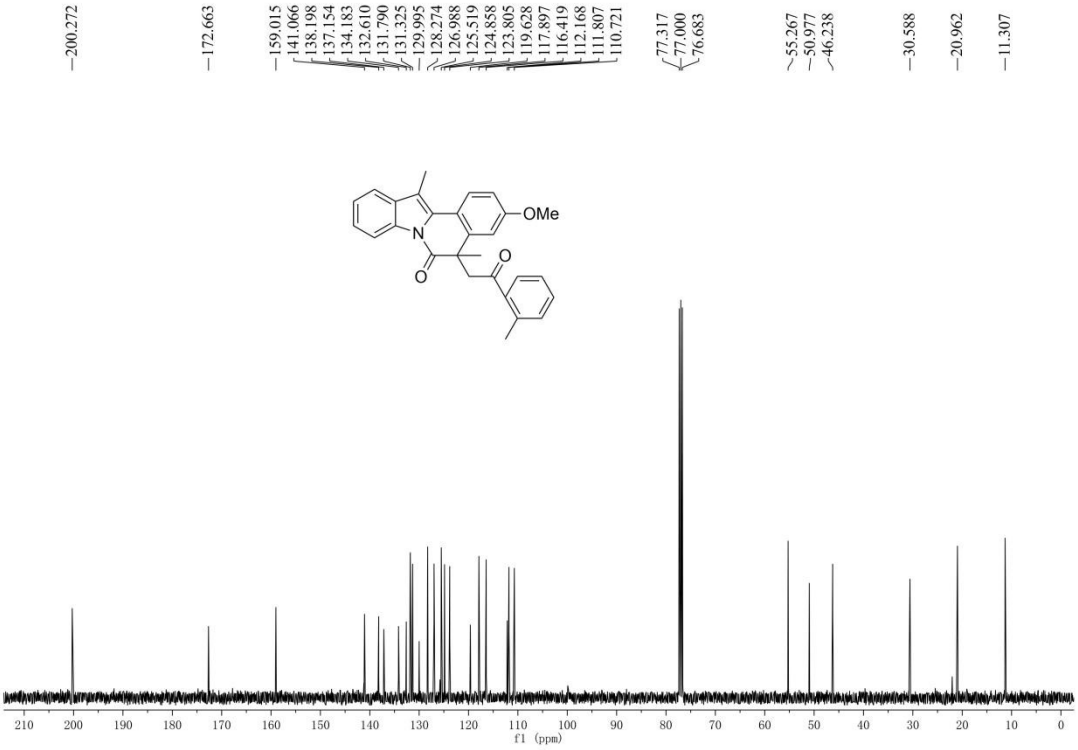
3-Methoxy-5,12-dimethyl-5-(2-oxo-2-(m-tolyl)ethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3an)



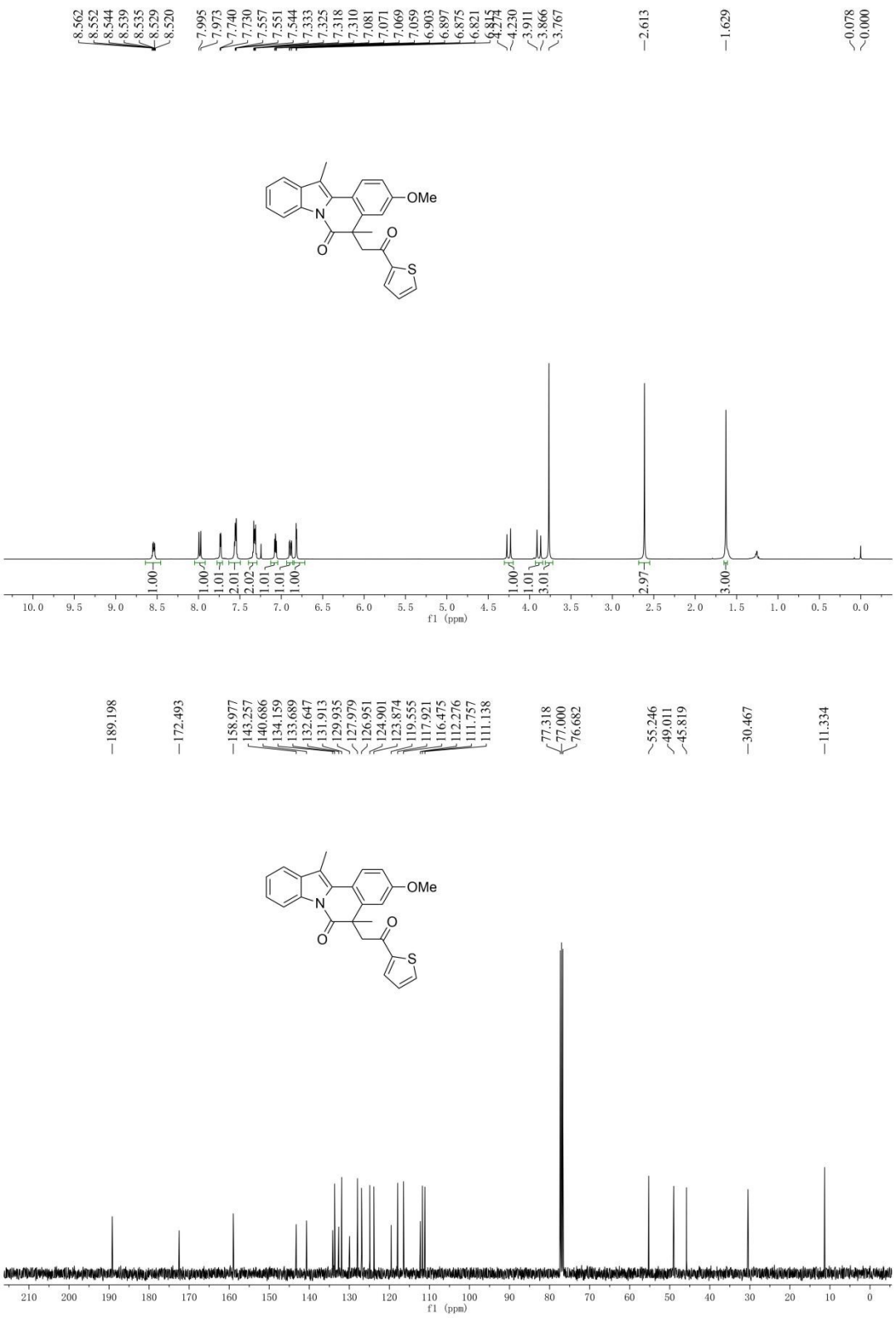


3-Methoxy-5,12-dimethyl-5-(2-oxo-2-(o-tolyl)ethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ao)

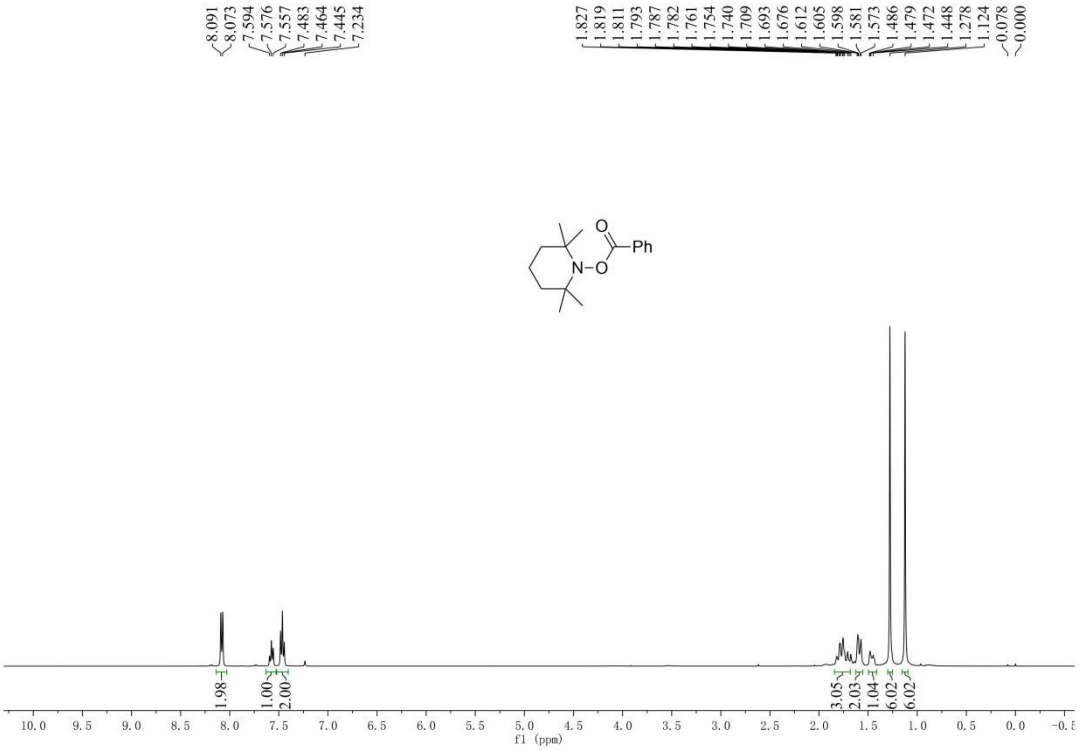


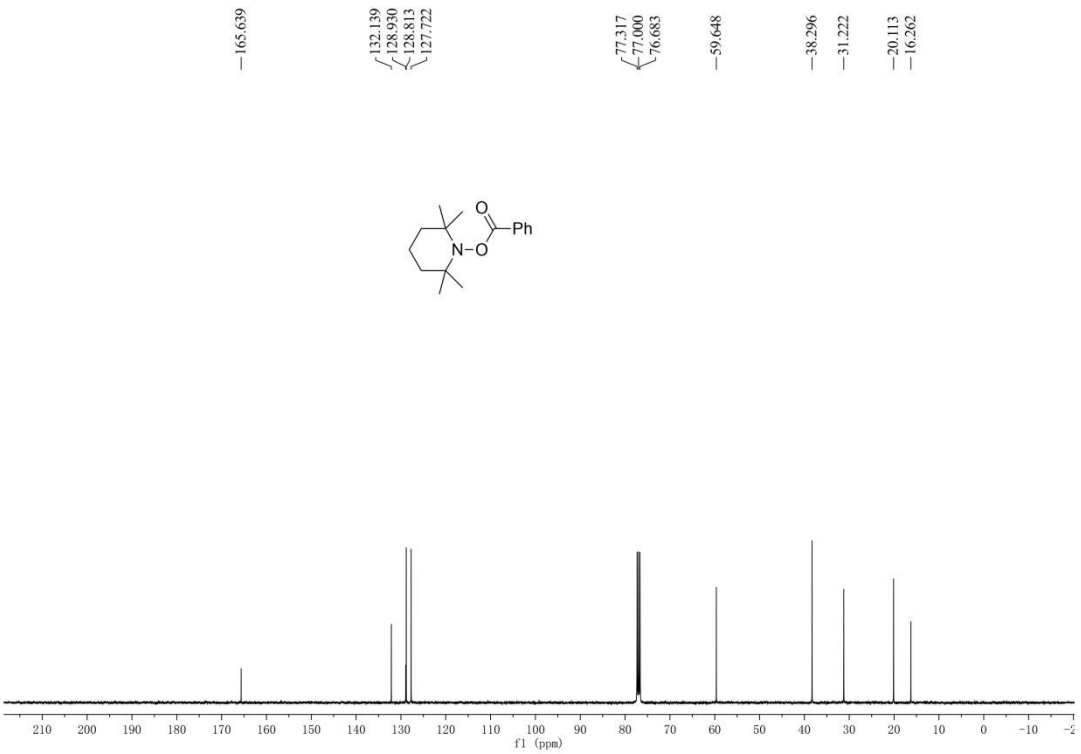


3-Methoxy-5,12-dimethyl-5-(2-oxo-2-(thiophen-2-yl)ethyl)indolo[2,1-*a*]isoquinolin-6(5*H*)-one (3ap)



2,2,6,6-Tetramethylpiperidin-1-yl benzoate (4)





1,3,3-Triphenylprop-2-en-1-one (6)