

Supporting Information

Metal-Free Iodine(III)-Promoted Synthesis of Isoquinolones

Zhi-Wei Chen, Yi-Zhou Zhu,* Jin-Wang Ou, Ya-Ping Wang, and Jian-Yu Zheng*

State Key Laboratory and Institute of Elemento-Organic Chemistry, Collaborative Innovation Center of

Chemical Science and Engineering (Tianjin), Nankai University, Tianjin 300071, China

zhuyizhou@nankai.edu.cn; jyzheng@nankai.edu.cn

Table of Contents

1. Optimization of the catalytic oxidation system	S2
2. Copies of NMR spectra of 3 and 4a	S3

1. Optimization of the catalytic oxidation system

Table S1 Screening of Temperature^a

	1a	2a	3aa
Entry	T(°C)		Yield(%) ^b
1	rt		56
2	0		55
3	-20		59
4	-40		51
5	-60		48

^aAll reactions were carried out with **1a** (0.17 mmol), **2a** (0.17 mmol), PIFA (0.17 mmol), TFA (0.17 mmol) under argon atmosphere and at room temperature. The concentration of **2a** was 0.1 M. ^bIsolated yield

Table S2 Screening of the Equivalent Ratio and Concentration of Reactants^a

	1a	2a	3aa		
Entry	1a	2a	PIFA	TFA	Yield(%) ^b
1	1	1	1	1	59
2	1	1	2	1	60
3	1	1	3	1	61
4	1	2	1	1	59
5	1	3	1	1	58
6	1.5	1	1	1	62.
7	1.5	2	1	1	64
8	1.5	3	1	1	64
9	1.5	1	2	1	69
10	1.5	1	3	1	70
11	1.5	1	2	3	72
12	1.5	1	2	5	78
13	1.5	1	2	7	74
14	1.5	1	2	10	63
15^c	1.5	1	2	5	84
16 ^d	1.5	1	2	10	72

^aUnless otherwise mentioned, all reactions were carried out under Argon atmosphere and at -20 °C. The concentration of **2a** was 0.1 M. ^bIsolated yield. ^cThe concentration of **2a** was 0.05 M. ^dThe concentration of **2a** was 0.025 M.

2. Copies of NMR spectra of 3 and 4a

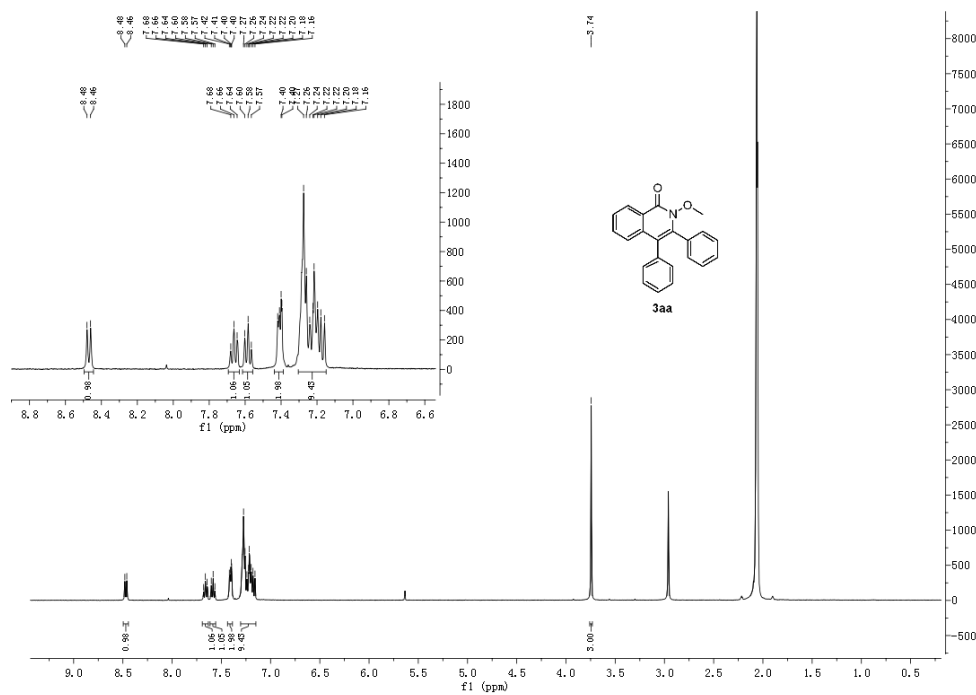


Figure S1 ¹H NMR spectra of compound **3aa** (400 MHz, Acetone-d₆)

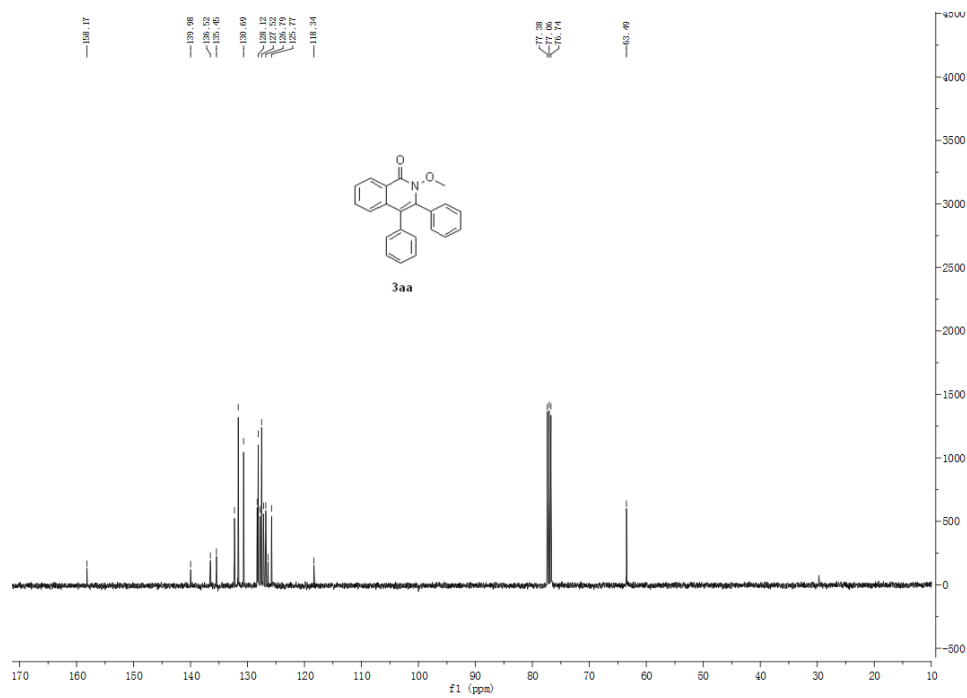


Figure S2 ^{13}C NMR spectra of compound **3aa** (101 MHz, CDCl_3)

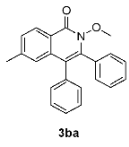


Figure S3 ^1H NMR spectra of compound **3ba** (400 MHz, CDCl_3)

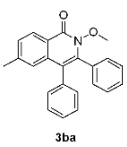


Figure S4 ^{13}C NMR spectra of compound **3ba** (101 MHz, CDCl_3)

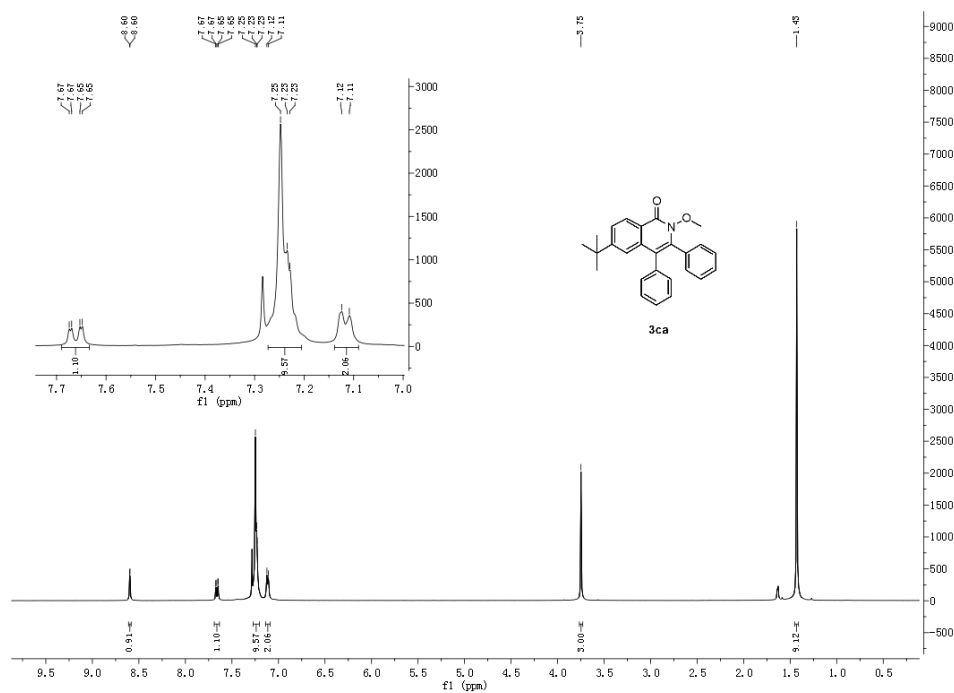


Figure S5 ¹H NMR spectra of compound **3ca** (400 MHz, CDCl₃)

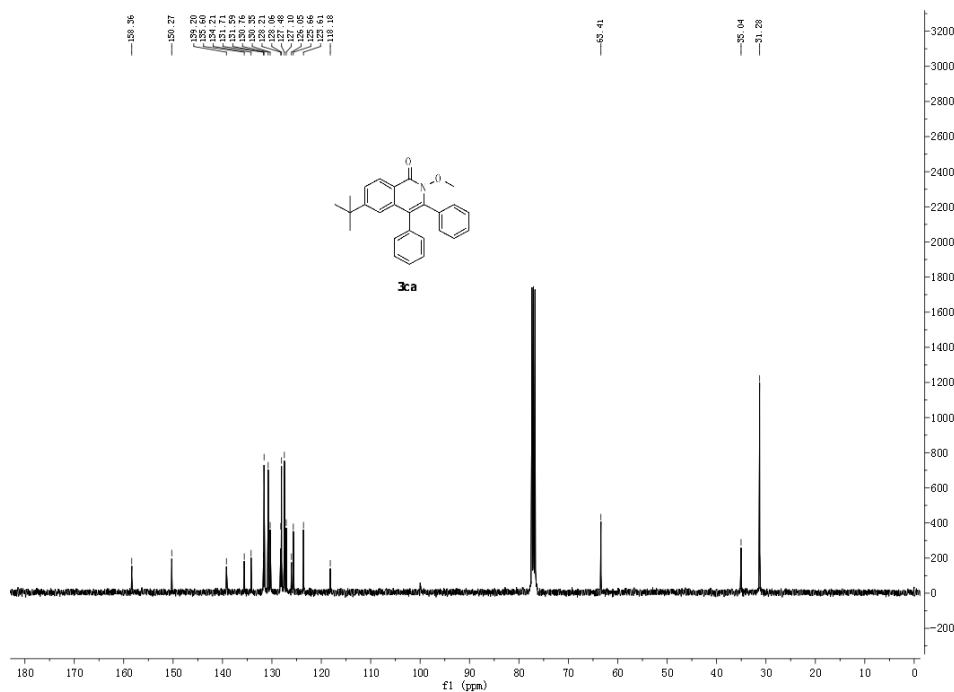


Figure S6 ¹³C NMR spectra of compound **3ca** (101 MHz, CDCl₃)

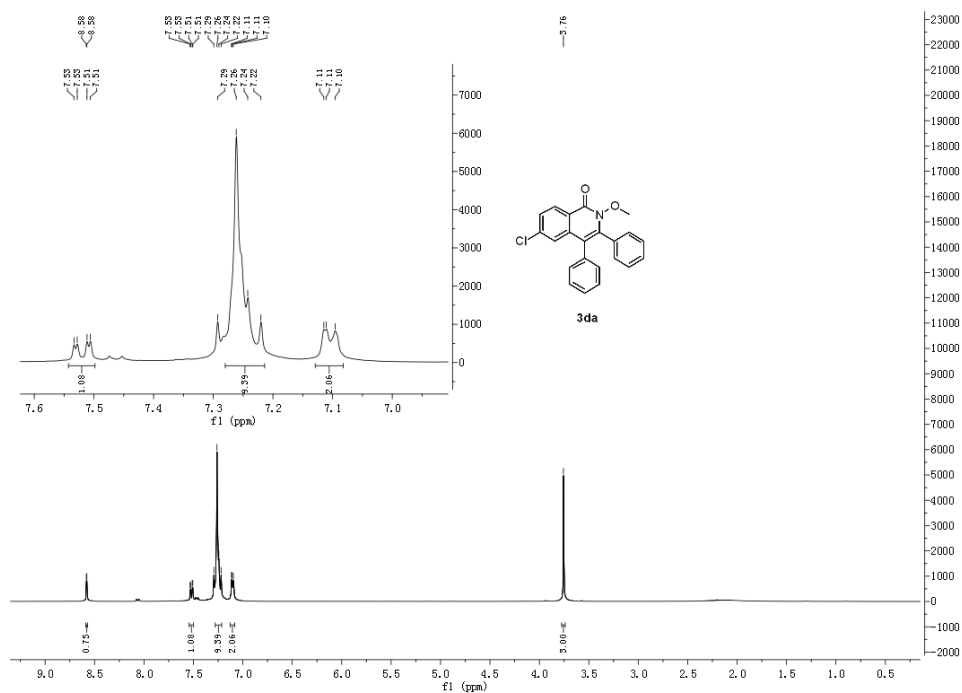


Figure S7 ¹H NMR spectra of compound **3da** (400 MHz, CDCl₃)

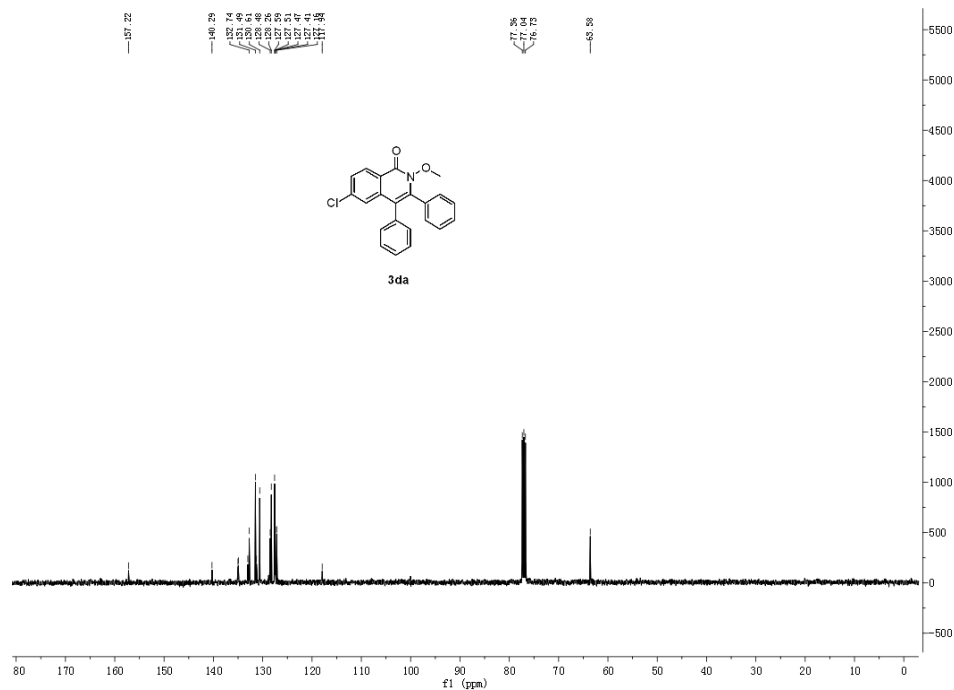


Figure S8 ¹³C NMR spectra of compound **3da** (101 MHz, CDCl₃)

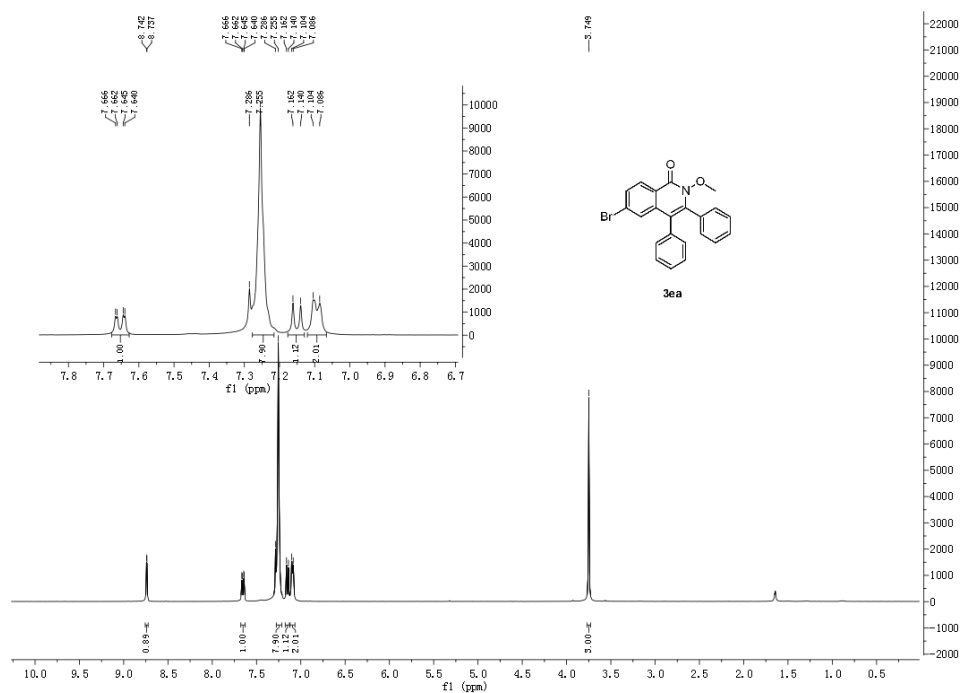


Figure S9 ^1H NMR spectra of compound **3ea** (400 MHz, CDCl_3)

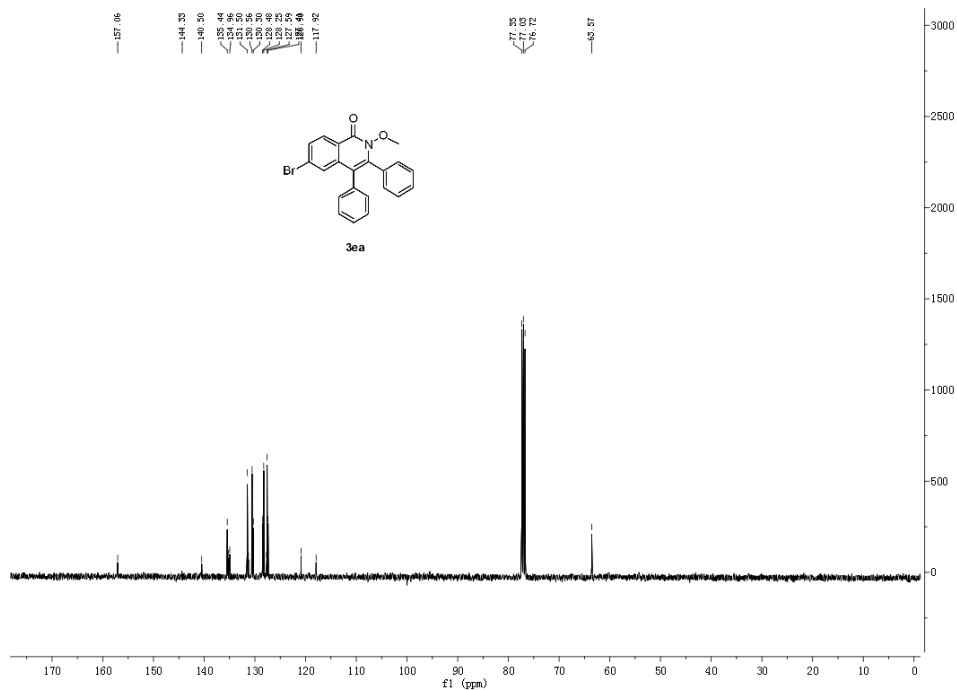


Figure S10 ^{13}C NMR spectra of compound **3ea** (101 MHz, CDCl_3)

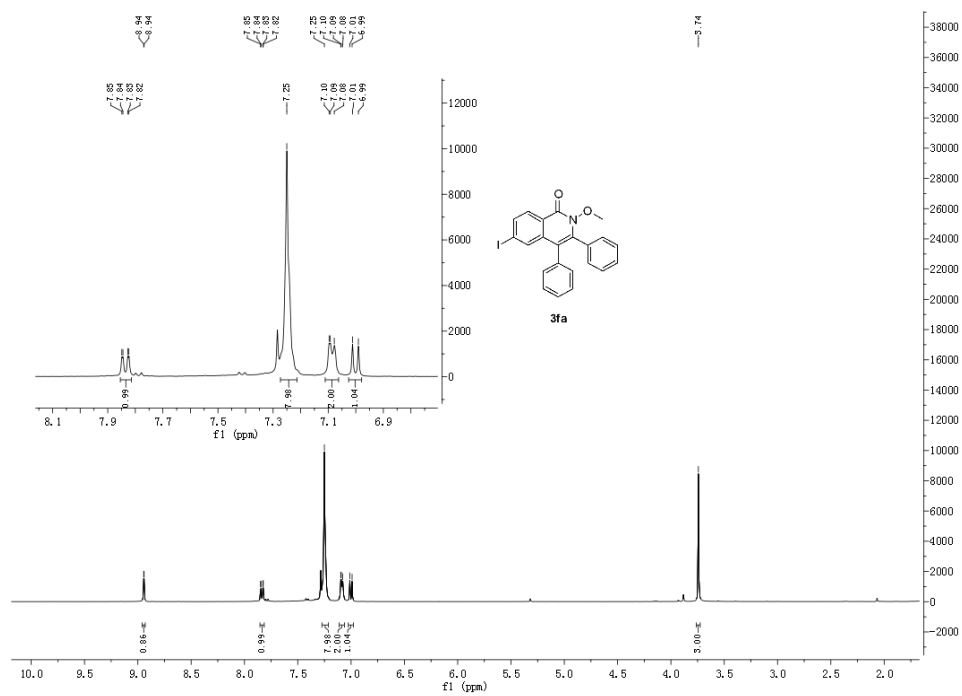


Figure S11 ¹H NMR spectra of compound **3fa** (400 MHz, CDCl₃)

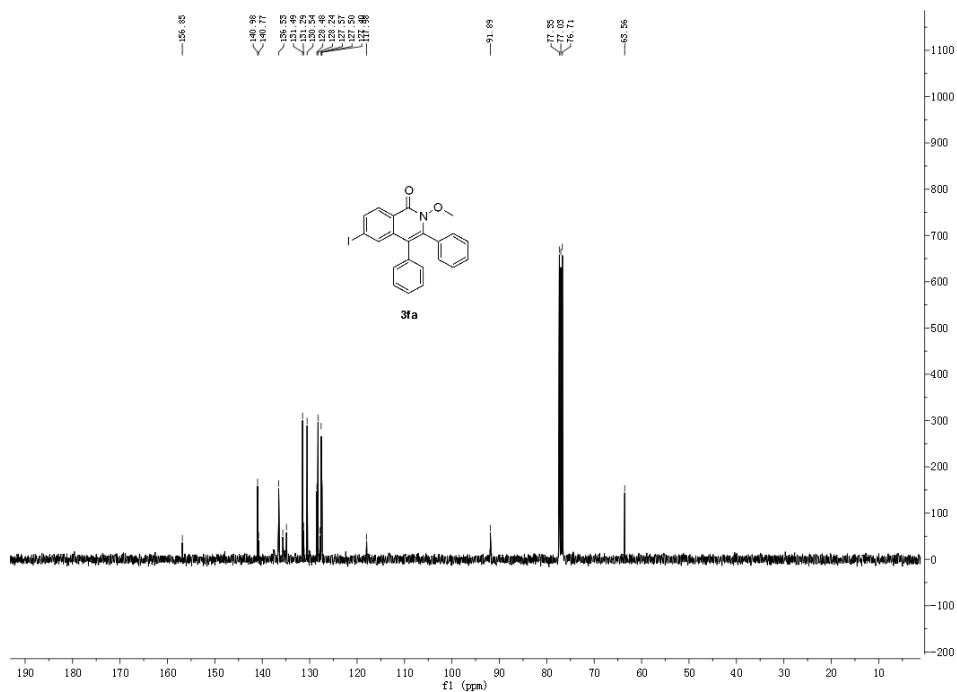


Figure S12 ¹³C NMR spectra of compound **3fa** (101 MHz, CDCl₃)

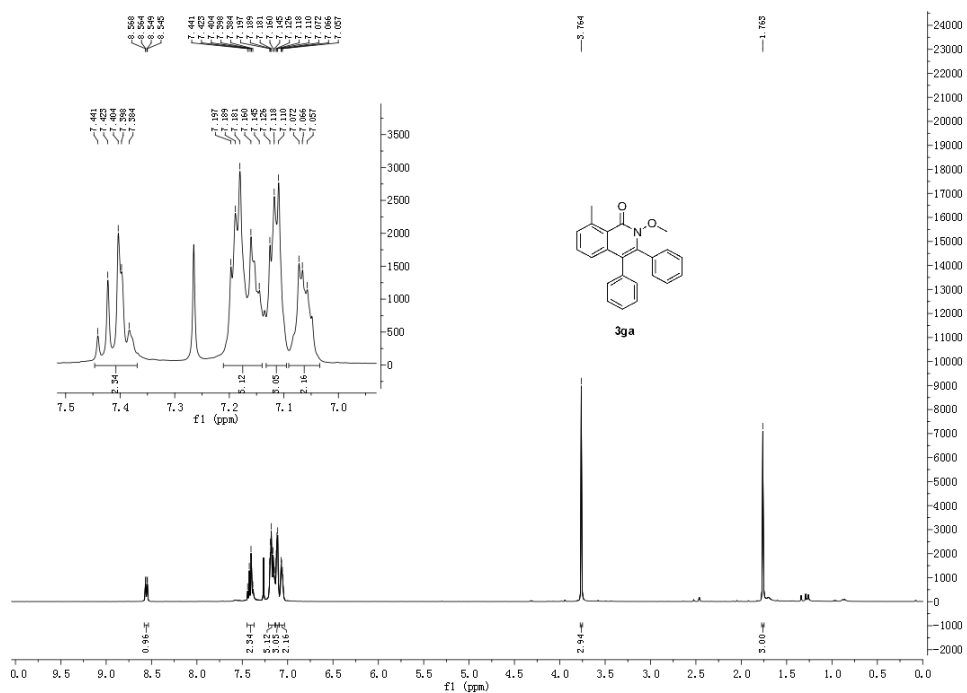


Figure S13 ¹H NMR spectra of compound **3ga** (400 MHz, CDCl₃)

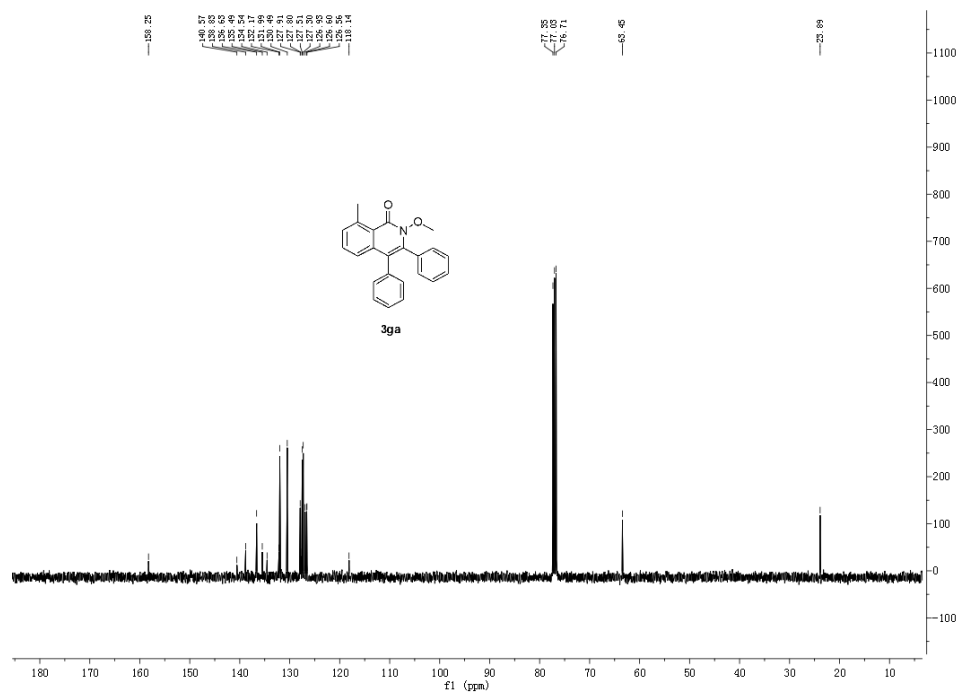


Figure S14 ¹³C NMR spectra of compound **3ga** (101 MHz, CDCl₃)

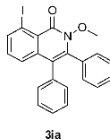


Figure S17 ^1H NMR spectra of compound **3ia** (400 MHz, CDCl_3)

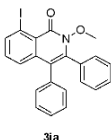


Figure S18 ^{13}C NMR spectra of compound **3ia** (101 MHz, CDCl_3)

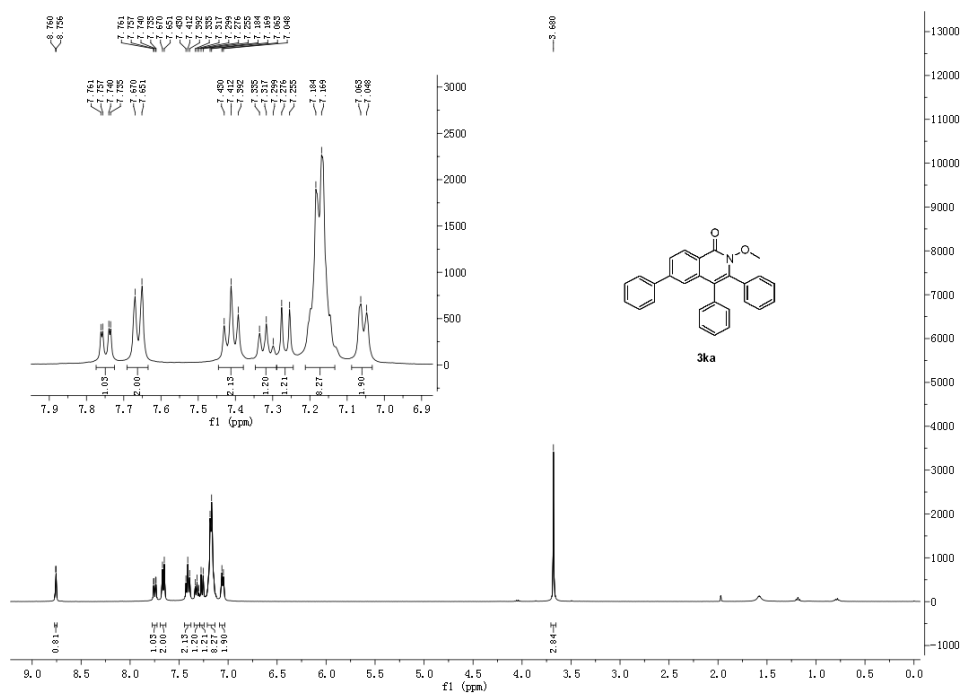


Figure S19 ¹H NMR spectra of compound **3ka** (400 MHz, CDCl₃)

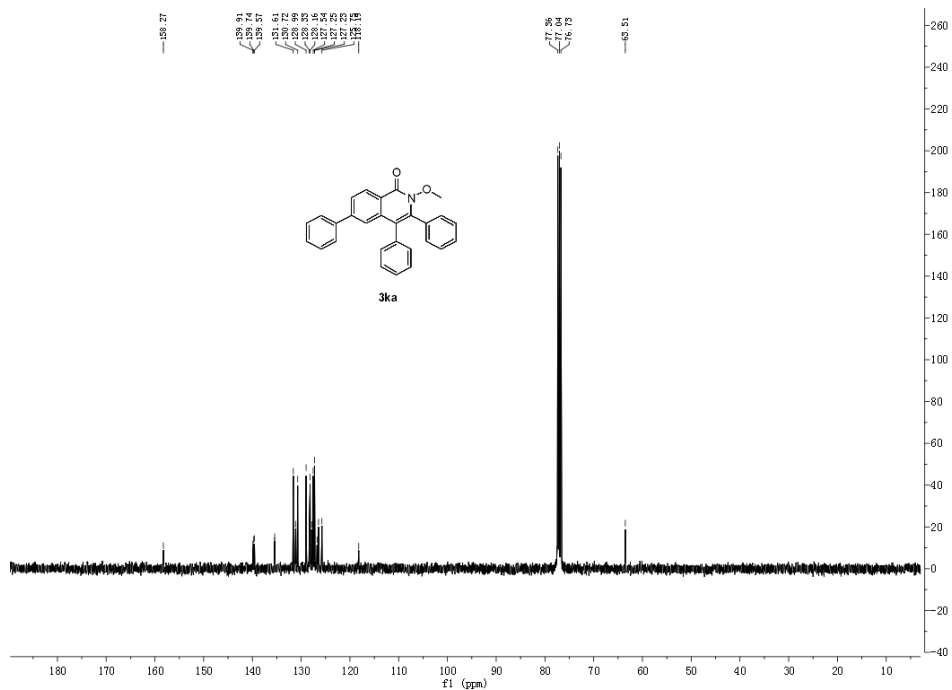


Figure S20 ¹³C NMR spectra of compound **3ka** (101 MHz, CDCl₃)

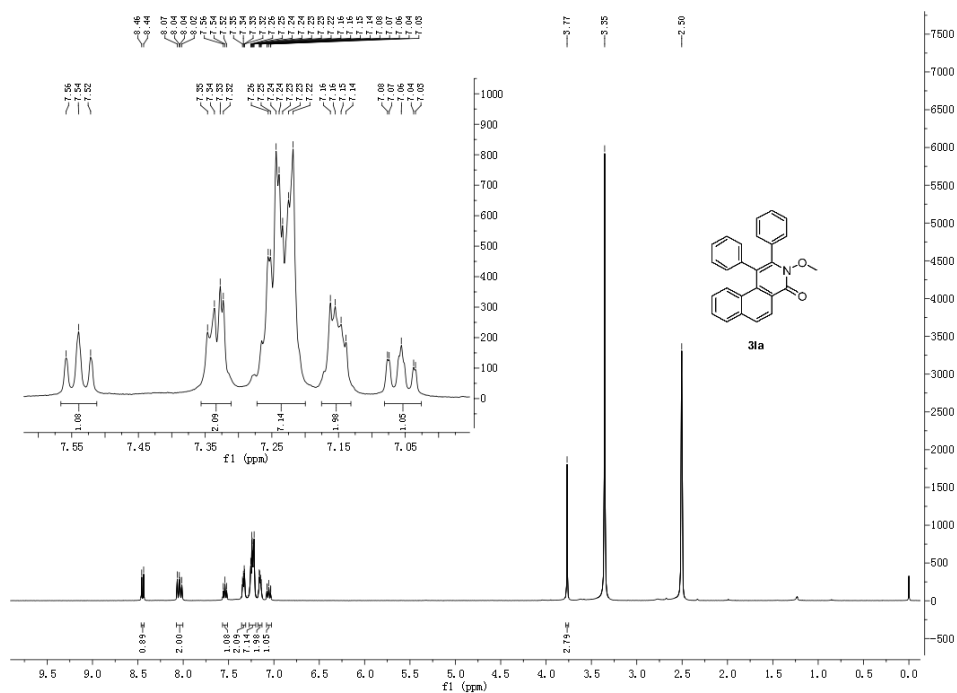


Figure S21 ¹H NMR spectra of compound **3la** (400 MHz, DMSO-d₆)

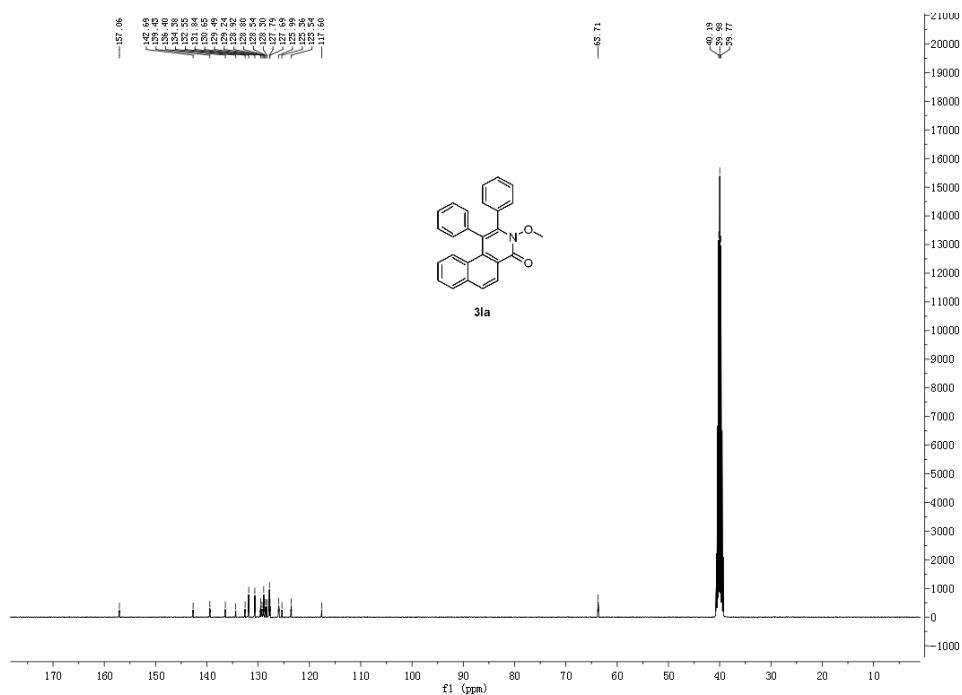


Figure S22 ¹³C NMR spectra of compound **3la** (101 MHz, DMSO-d₆)

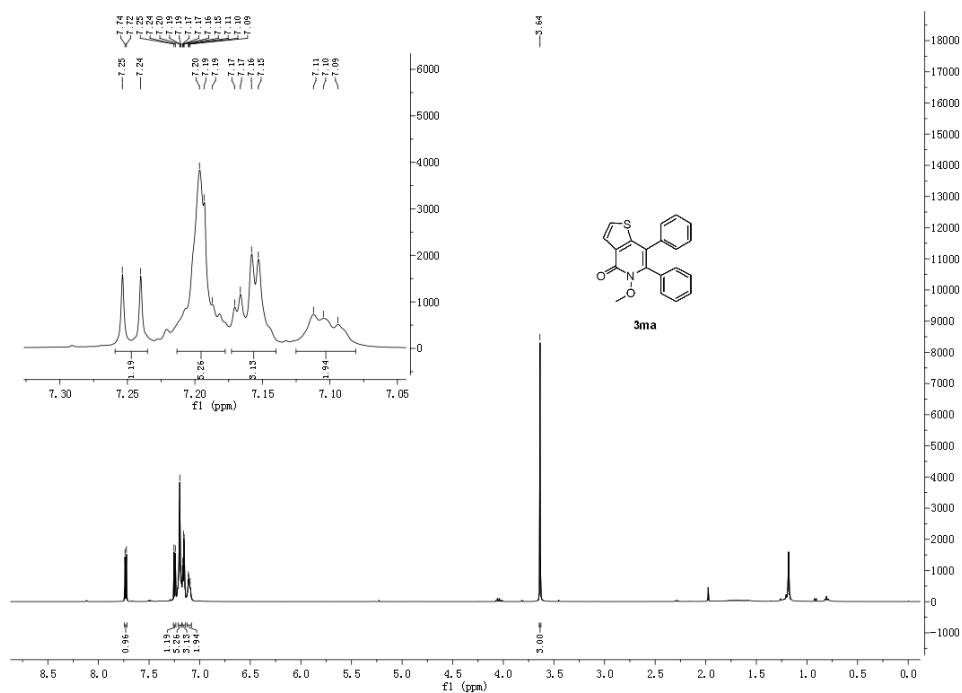


Figure S23 ^1H NMR spectra of compound **3ma** (400 MHz, CDCl_3)

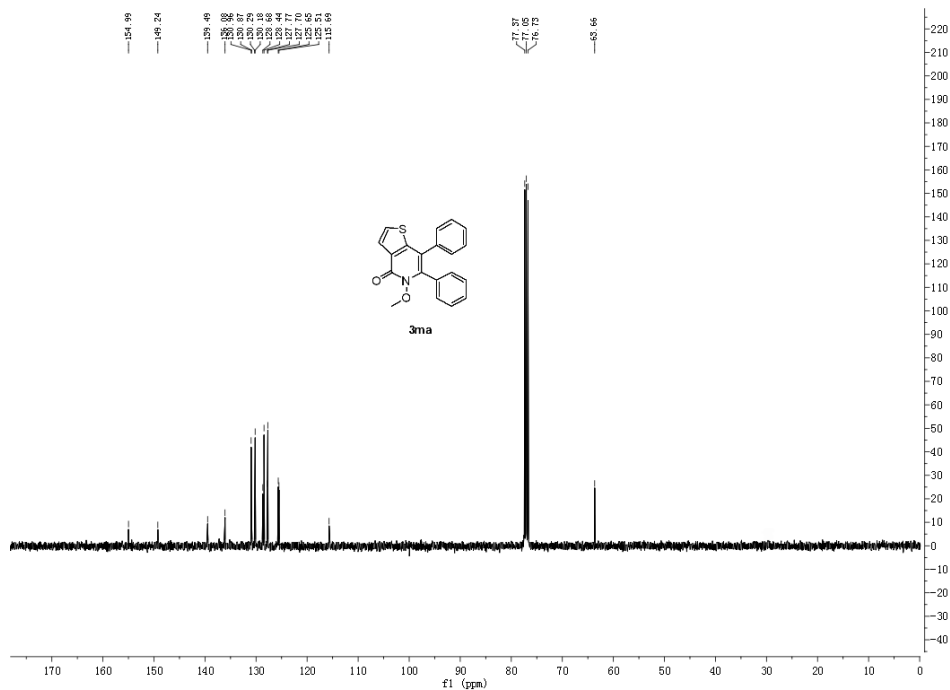


Figure S24 ^{13}C NMR spectra of compound **3ma** (101 MHz, CDCl_3)

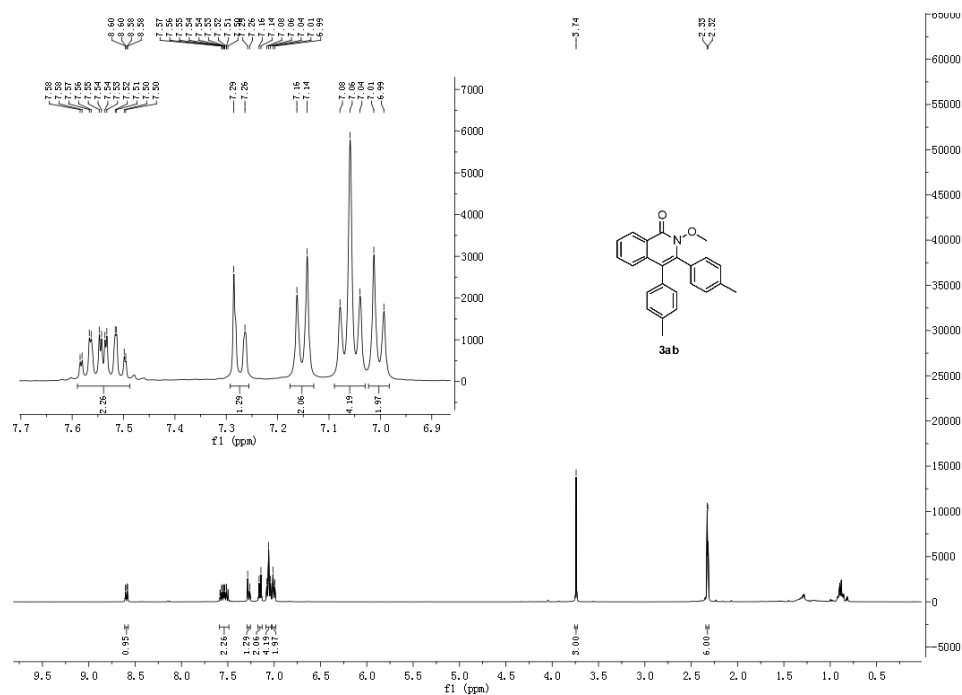


Figure S25 ¹H NMR spectra of compound **3ab** (400 MHz, CDCl₃)

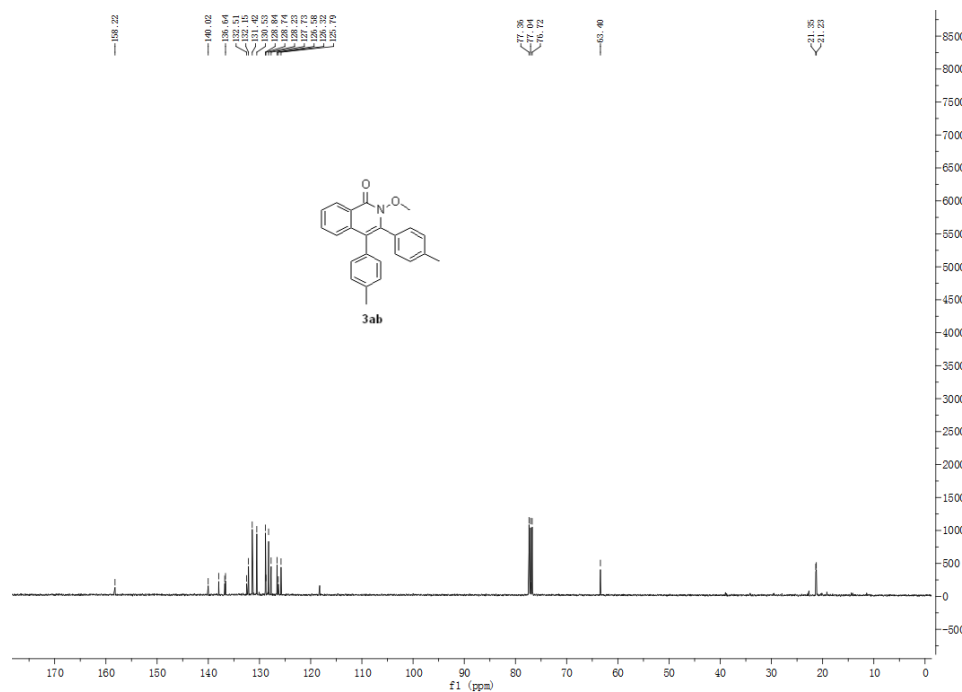


Figure S26 ¹³C NMR spectra of compound **3ab** (101 MHz, CDCl₃)

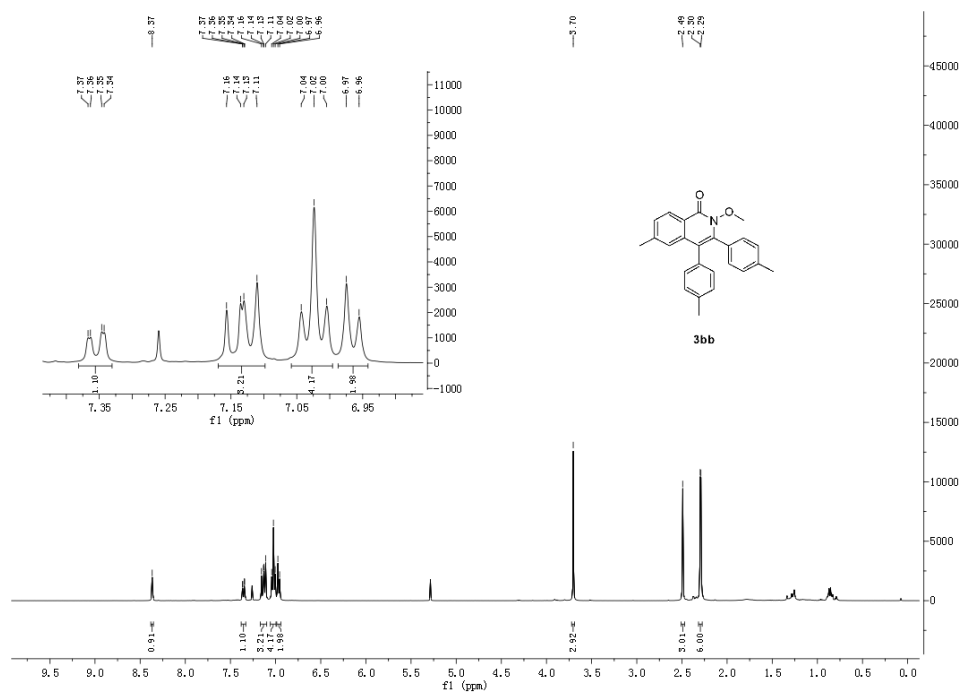


Figure S27 ¹H NMR spectra of compound **3bb** (400 MHz, CDCl₃)

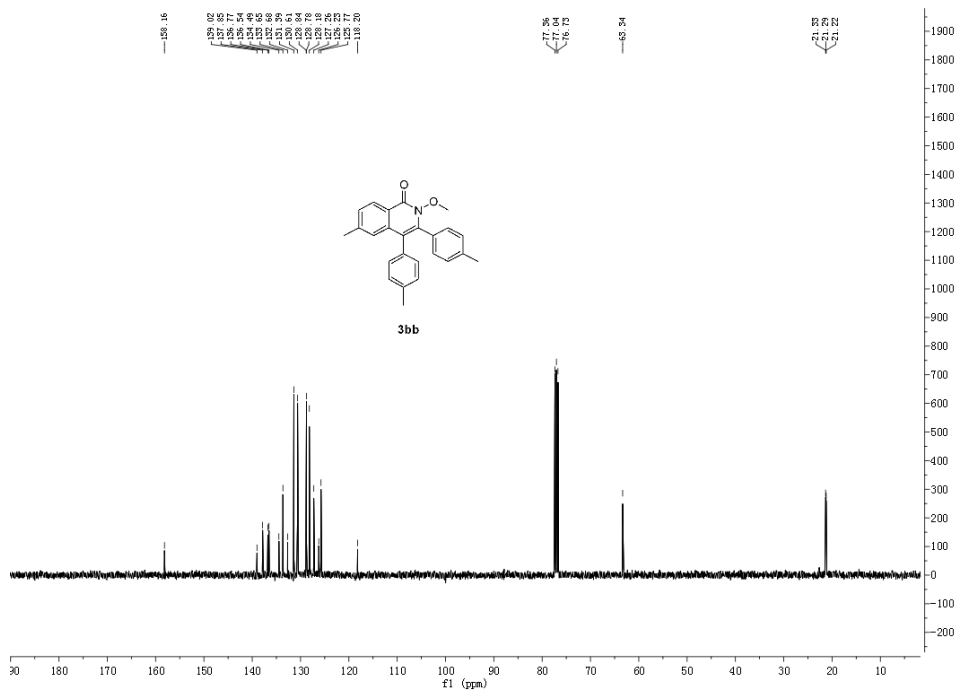


Figure S28 ¹³C NMR spectra of compound **3bb** (101 MHz, CDCl₃)

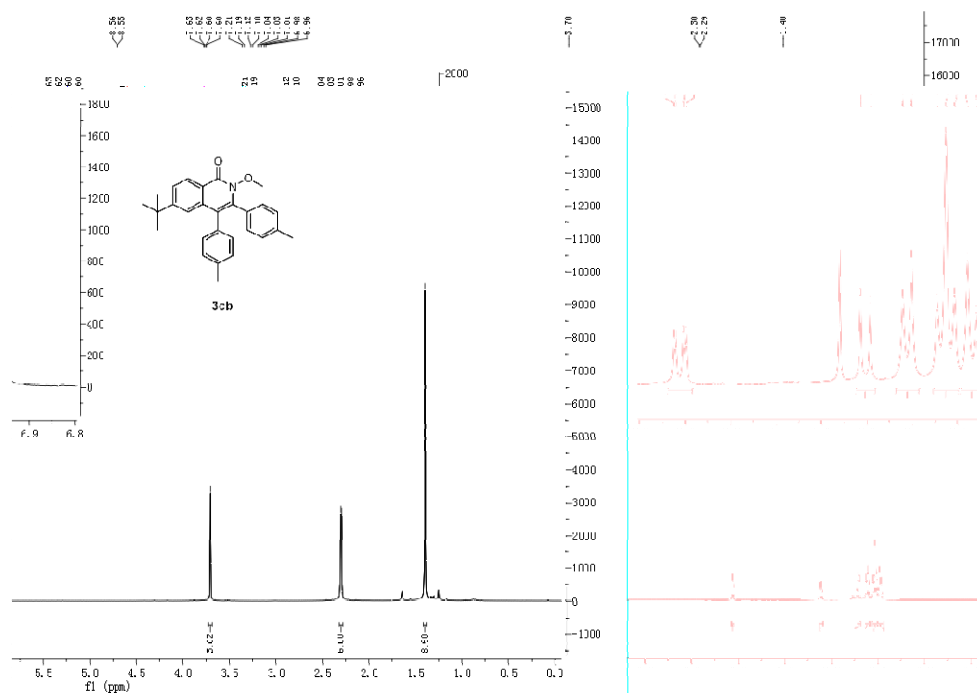


Figure S29 ^1H NMR spectra of compound **3cb** (400 MHz, CDCl_3)

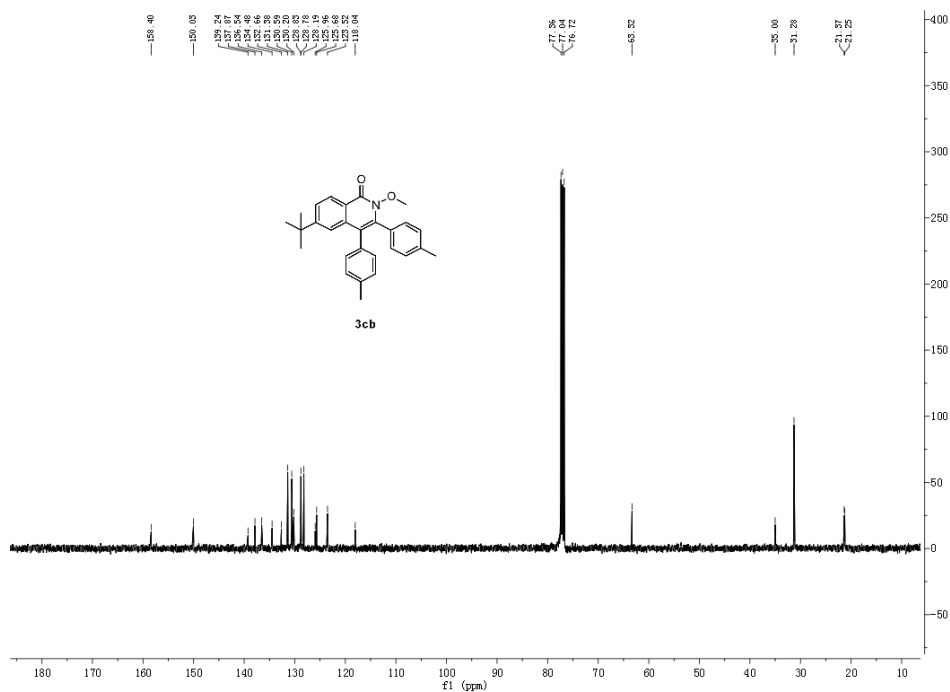


Figure S30 ^{13}C NMR spectra of compound **3cb** (101 MHz, CDCl_3)

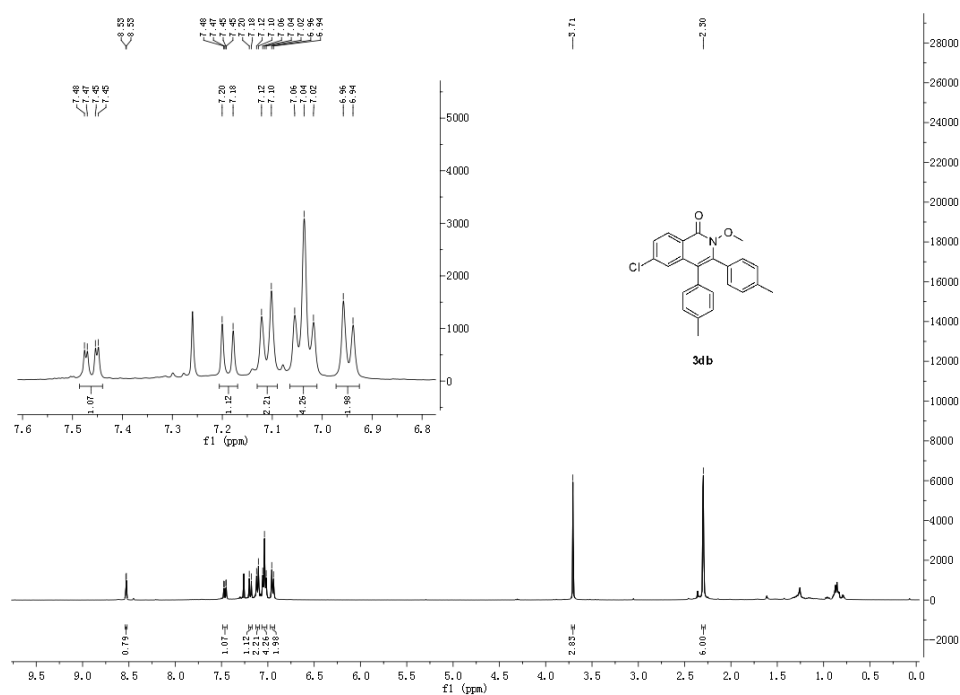


Figure S31 ^1H NMR spectra of compound **3db** (400 MHz, CDCl_3)

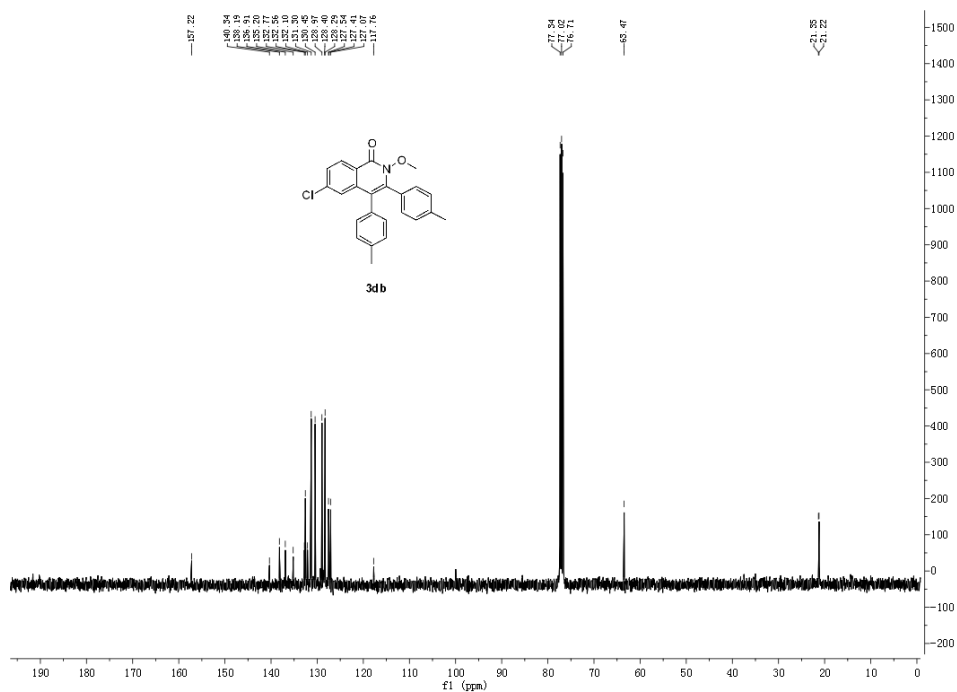


Figure S32 ^{13}C NMR spectra of compound **3db** (101 MHz, CDCl_3)

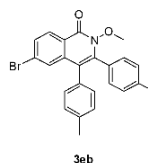


Figure S33 ^1H NMR spectra of compound **3eb** (400 MHz, CDCl_3)

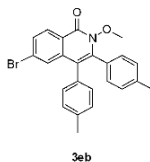


Figure S34 ^{13}C NMR spectra of compound **3eb** (101 MHz, CDCl_3)

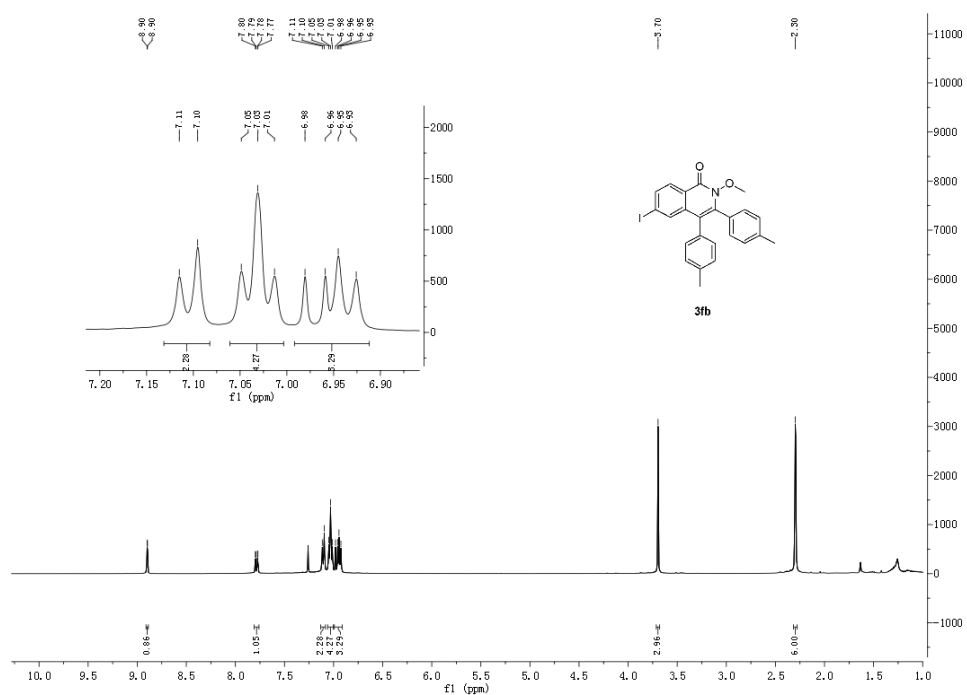


Figure S35 ^1H NMR spectra of compound **3fb** (400 MHz, CDCl_3)

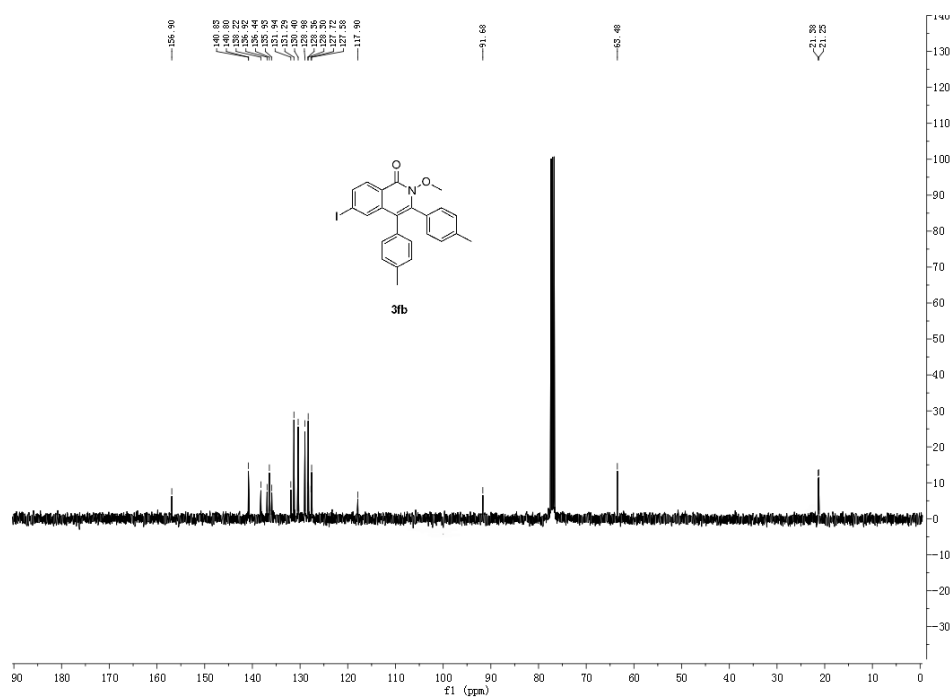


Figure S36 ^{13}C NMR spectra of compound **3fb** (101 MHz, CDCl_3)

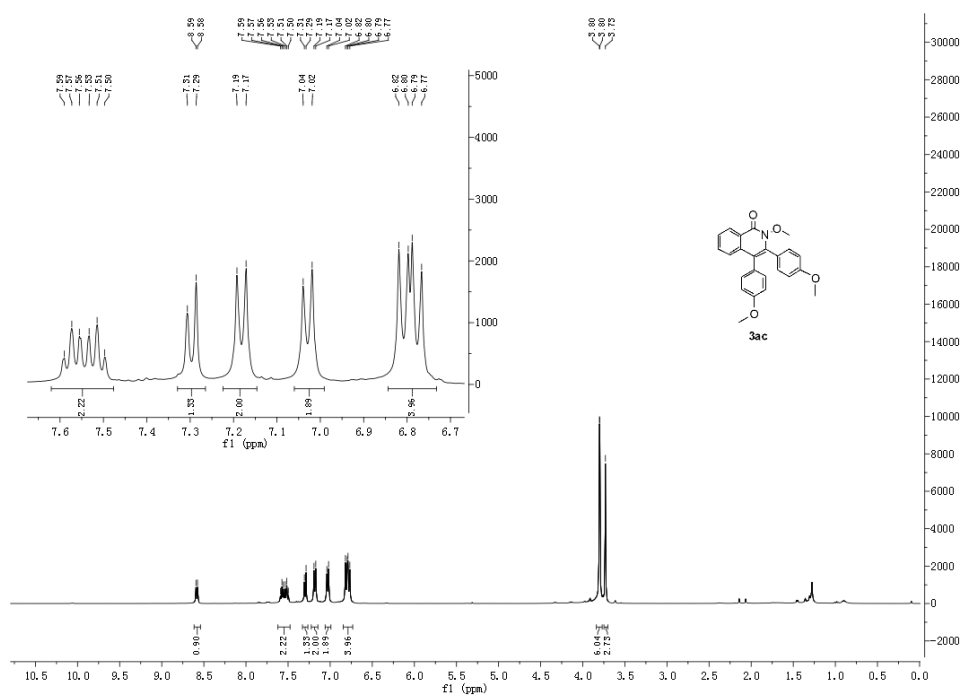


Figure S37 ^1H NMR spectra of compound **3ac** (400 MHz, CDCl_3)

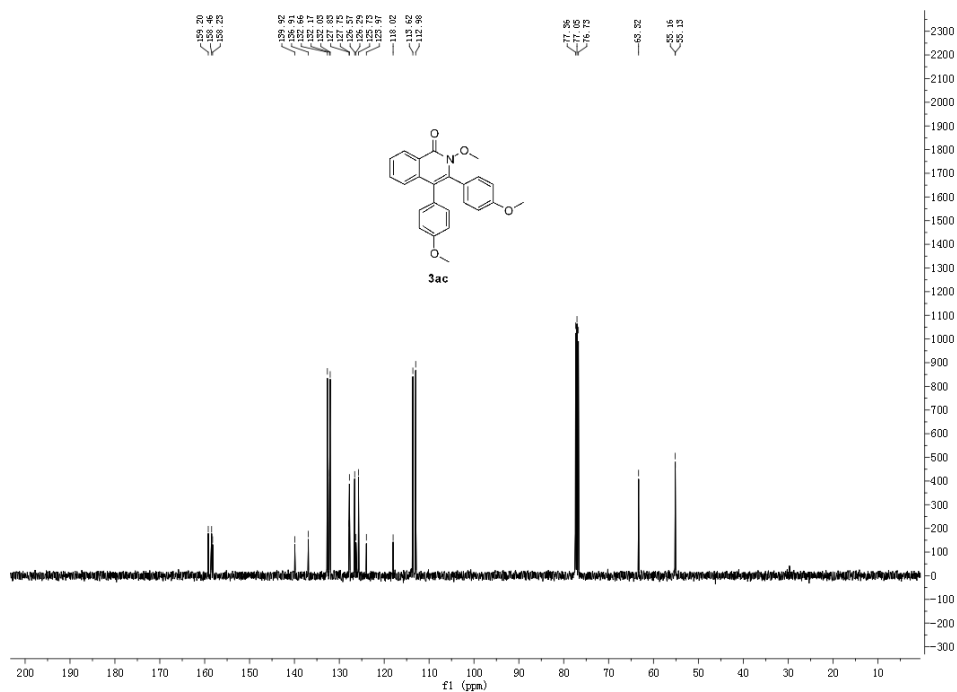


Figure S38 ^{13}C NMR spectra of compound **3ac** (101 MHz, CDCl_3)

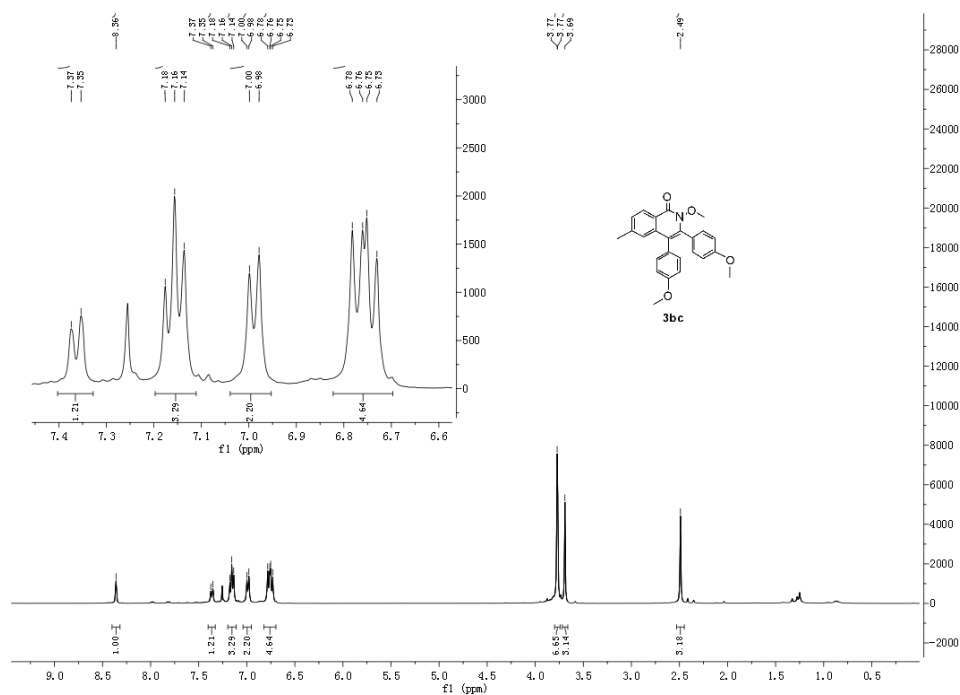


Figure S39 ¹H NMR spectra of compound **3bc** (400 MHz, CDCl₃)

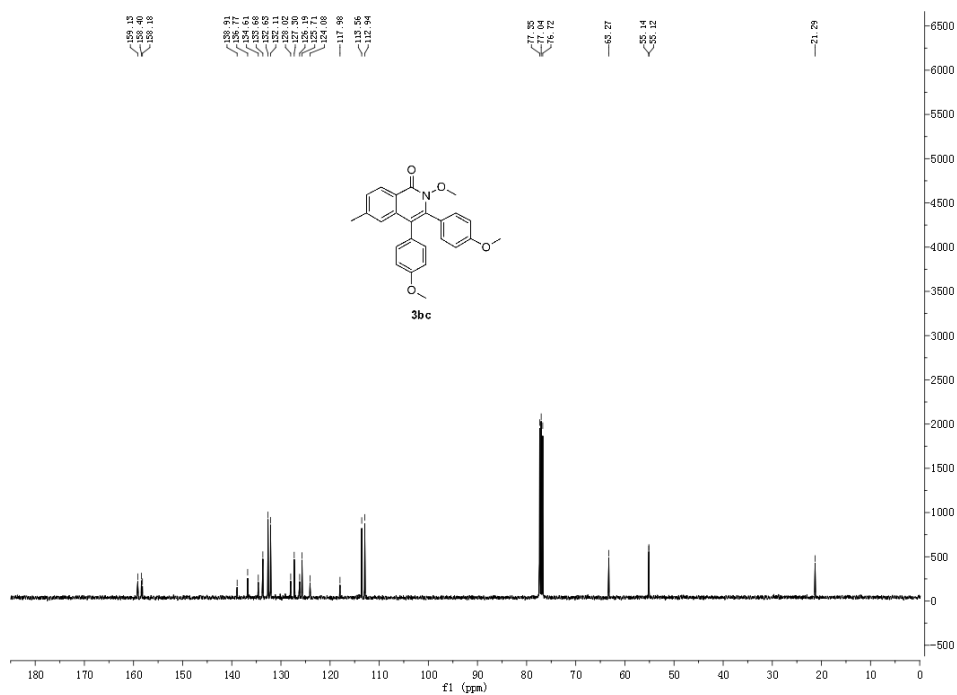


Figure S40 ¹³C NMR spectra of compound **3bc** (101 MHz, CDCl₃)

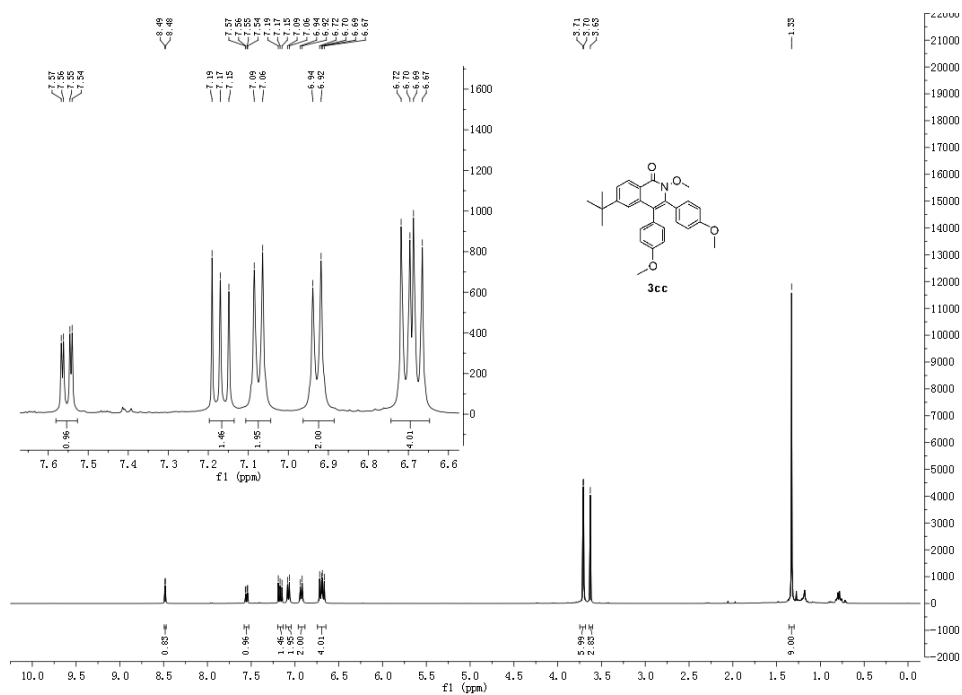


Figure S41 ^1H NMR spectra of compound **3cc** (400 MHz, CDCl_3)

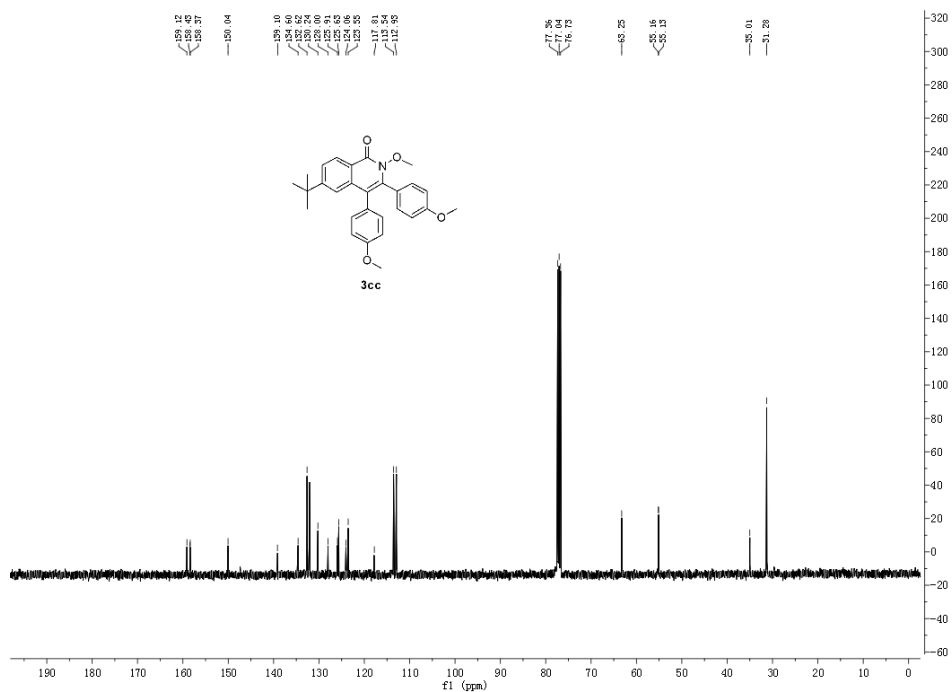


Figure S42 ^{13}C NMR spectra of compound **3cc** (101 MHz, CDCl_3)

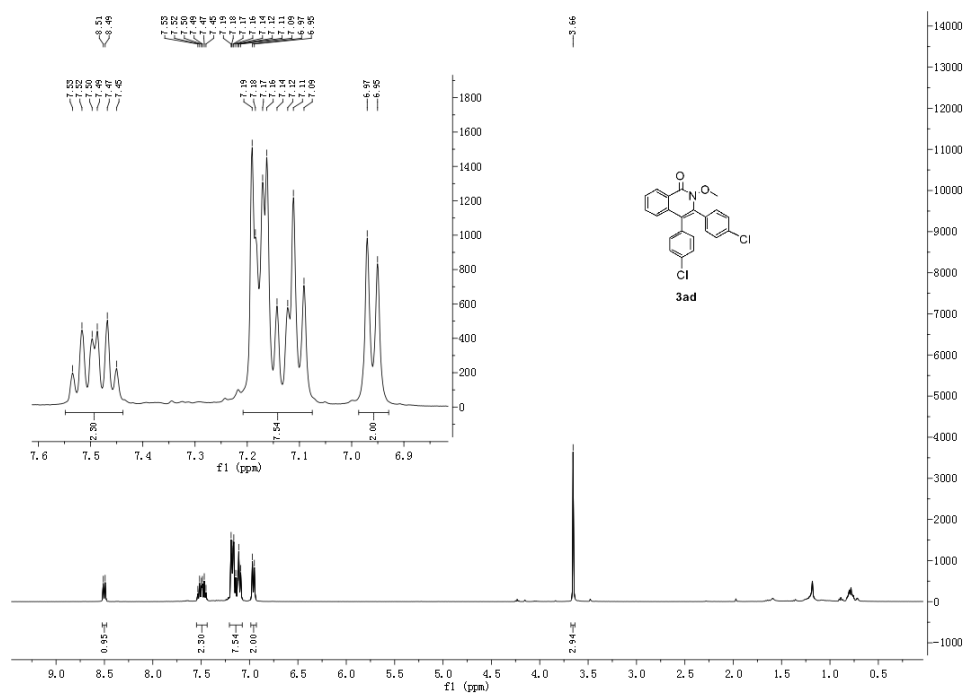
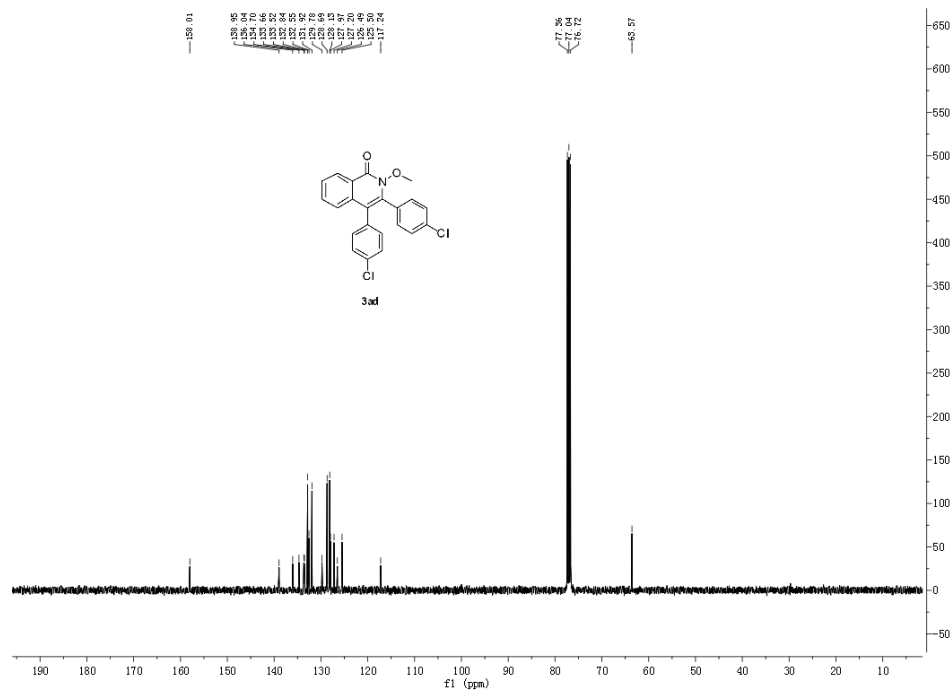


Figure S43 ¹H NMR spectra of compound **3ad** (400 MHz, CDCl₃)



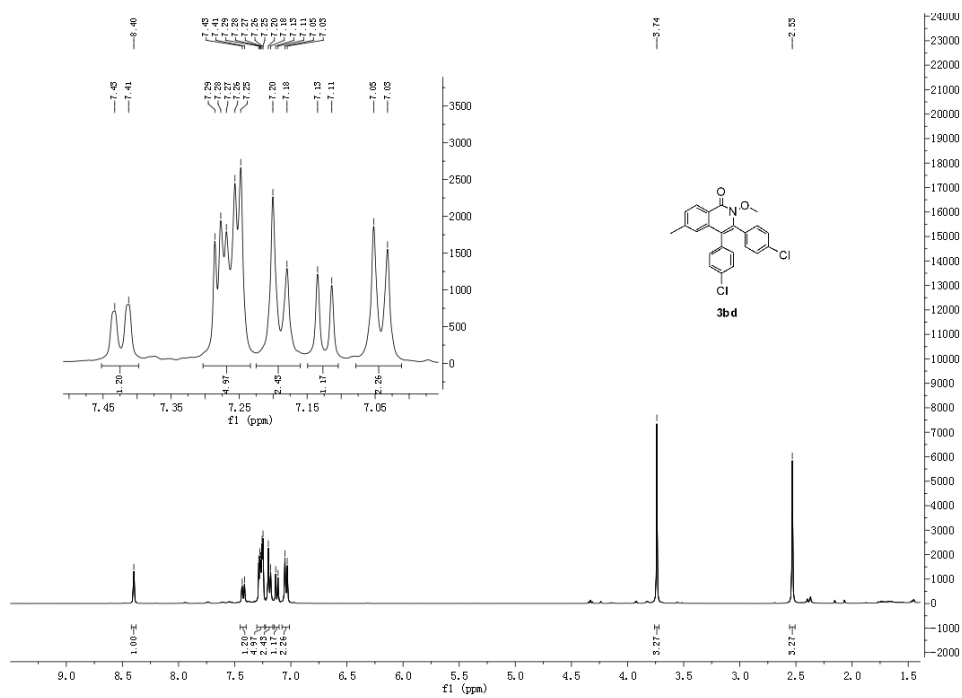


Figure S45 ^1H NMR spectra of compound **3bd** (400 MHz, CDCl_3)

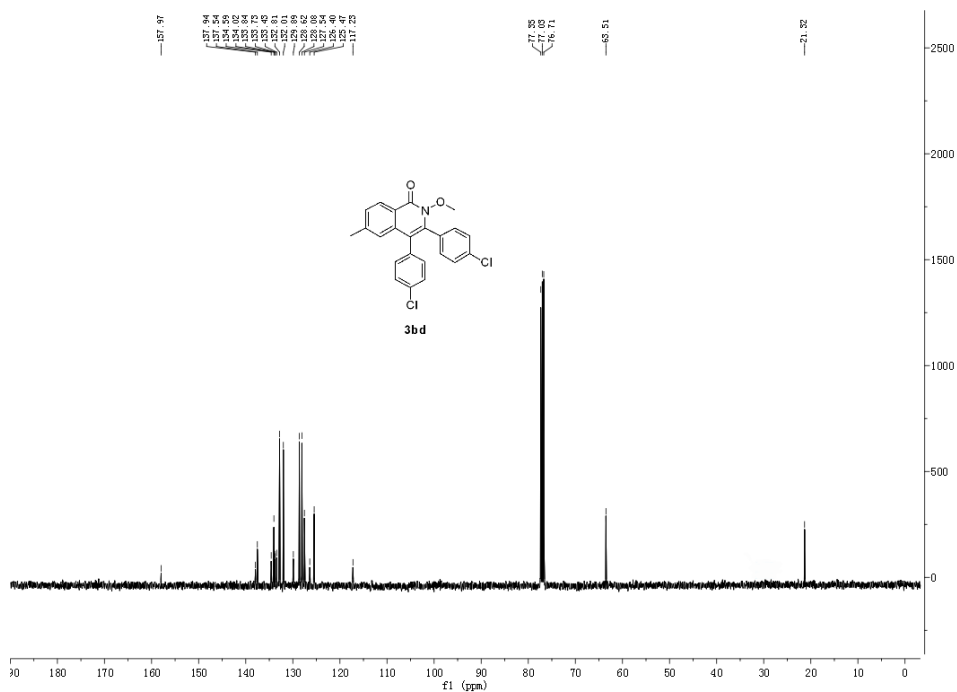


Figure S46 ^{13}C NMR spectra of compound **3bd** (101 MHz, CDCl_3)

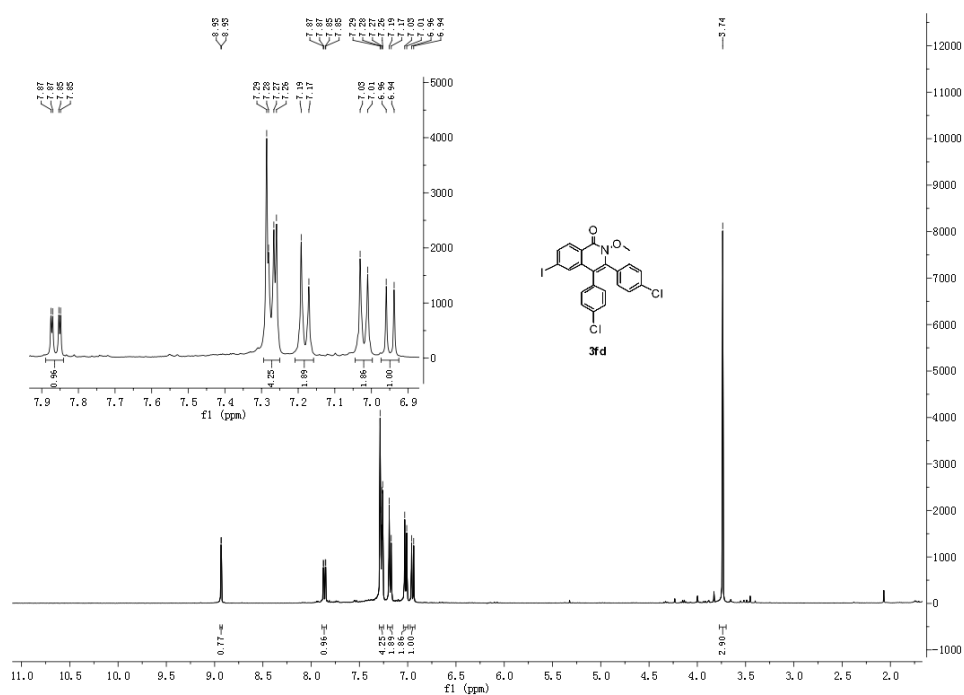


Figure S47 ¹H NMR spectra of compound **3fd** (400 MHz, CDCl₃)

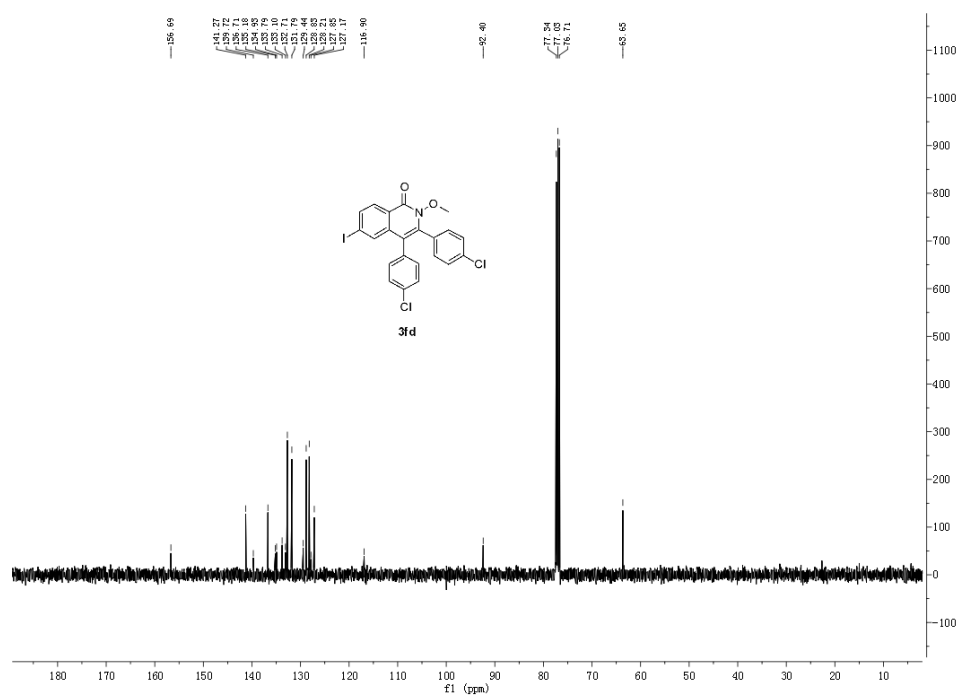


Figure S48 ¹³C NMR spectra of compound **3fd** (101 MHz, CDCl₃)

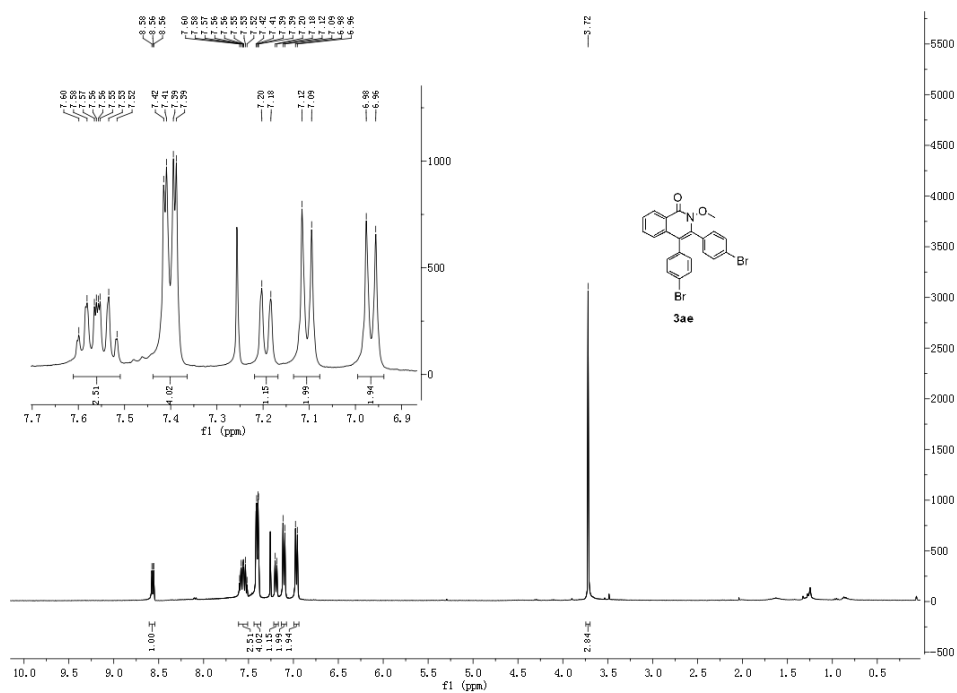


Figure S49 ¹H NMR spectra of compound **3ae** (400 MHz, CDCl₃)

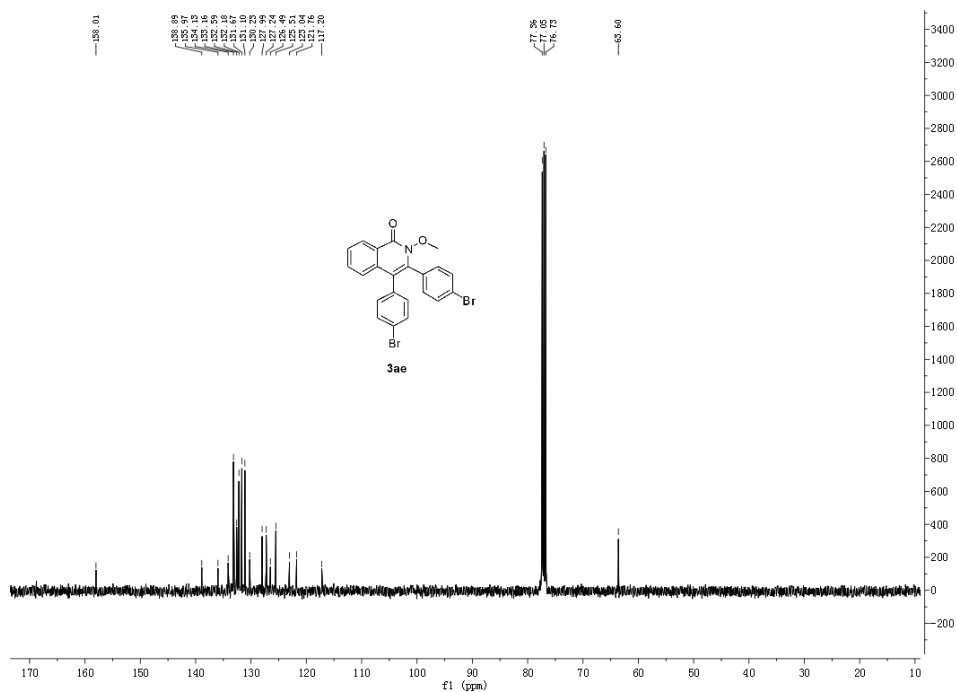


Figure S50 ¹³C NMR spectra of compound **3ae** (101 MHz, CDCl₃)

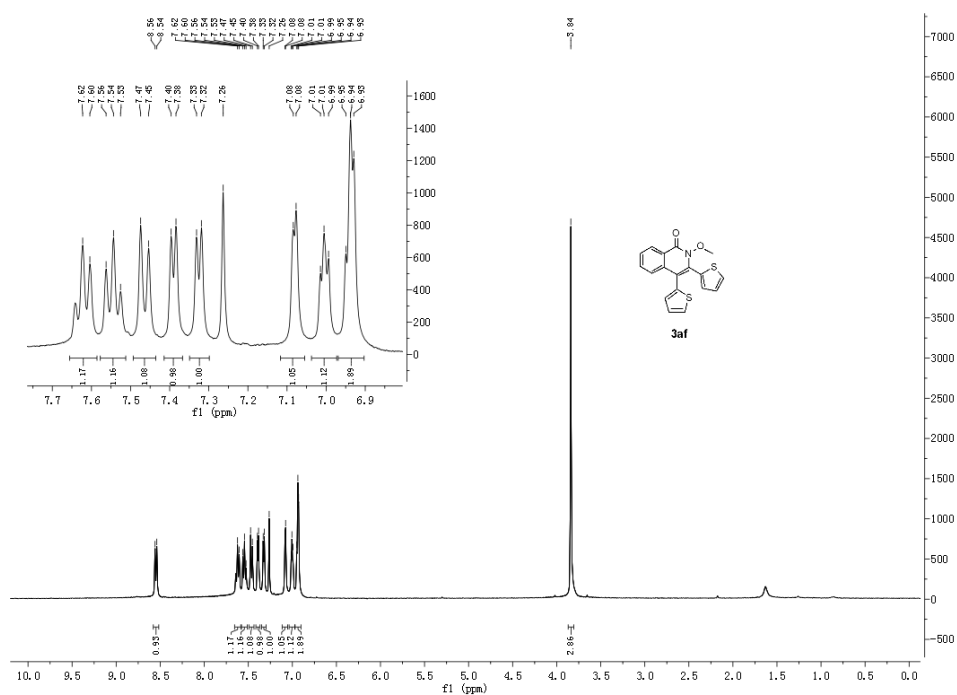


Figure S51 ¹H NMR spectra of compound **3af** (400 MHz, CDCl₃)

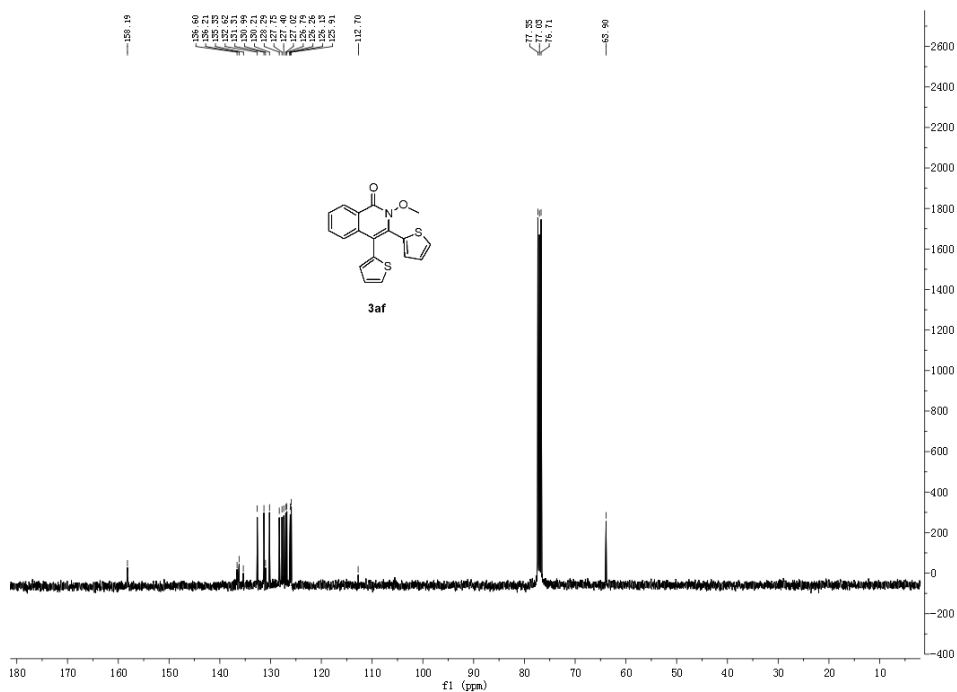


Figure S52 ¹³C NMR spectra of compound **3af** (101 MHz, CDCl₃)

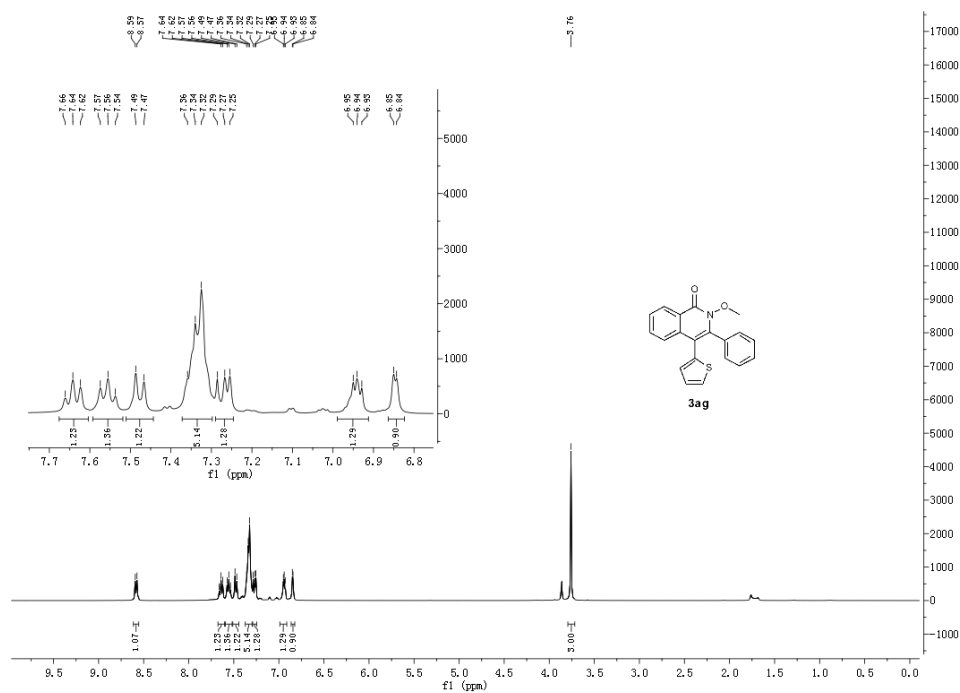


Figure S53 ¹H NMR spectra of compound **3ag** (400 MHz, CDCl₃)

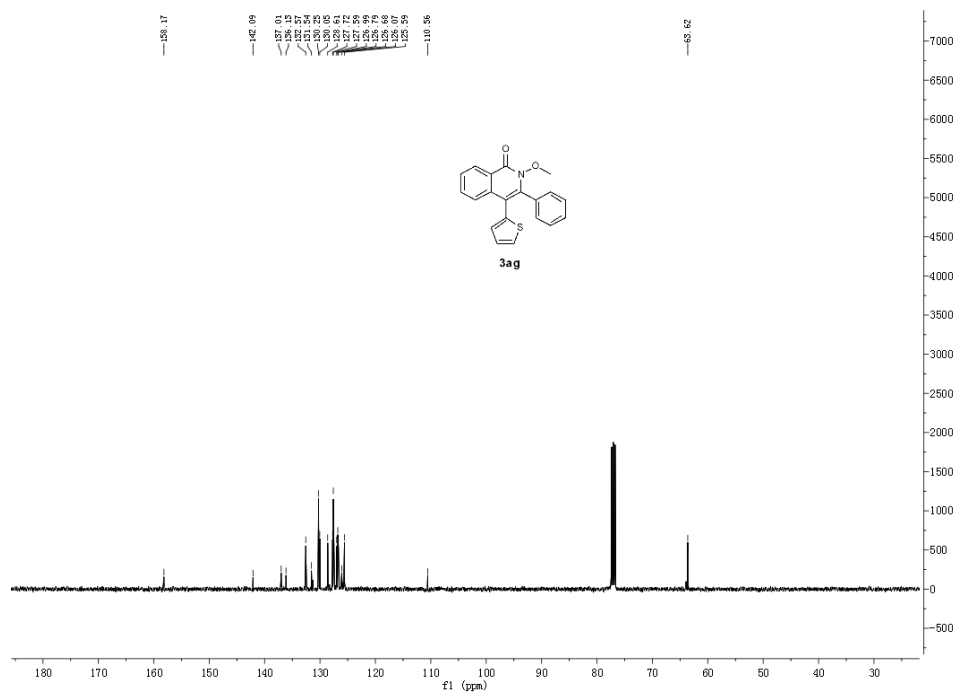


Figure S54 ¹³C NMR spectra of compound **3ag** (101 MHz, CDCl₃)

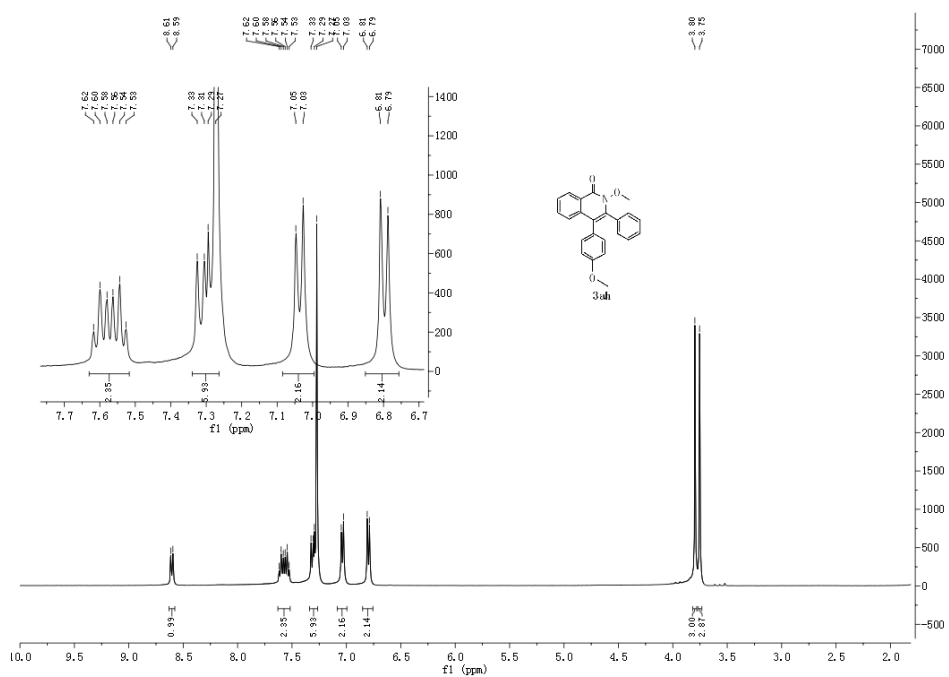


Figure S55 ¹H NMR spectra of compound **3ah** (400 MHz, CDCl₃)

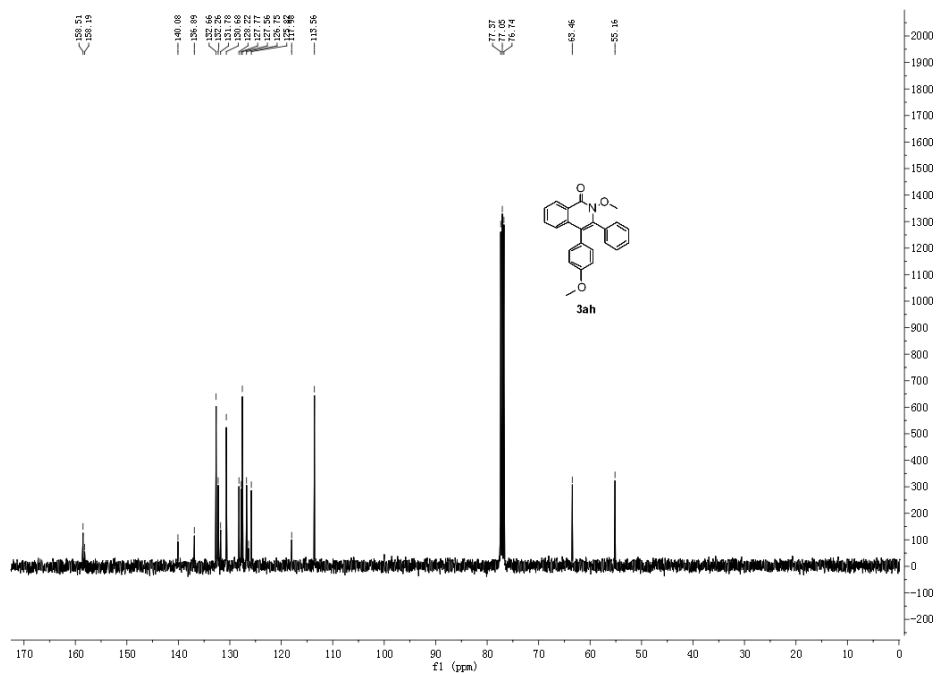


Figure S56 ¹³C NMR spectra of compound **3ah** (101 MHz, CDCl₃)

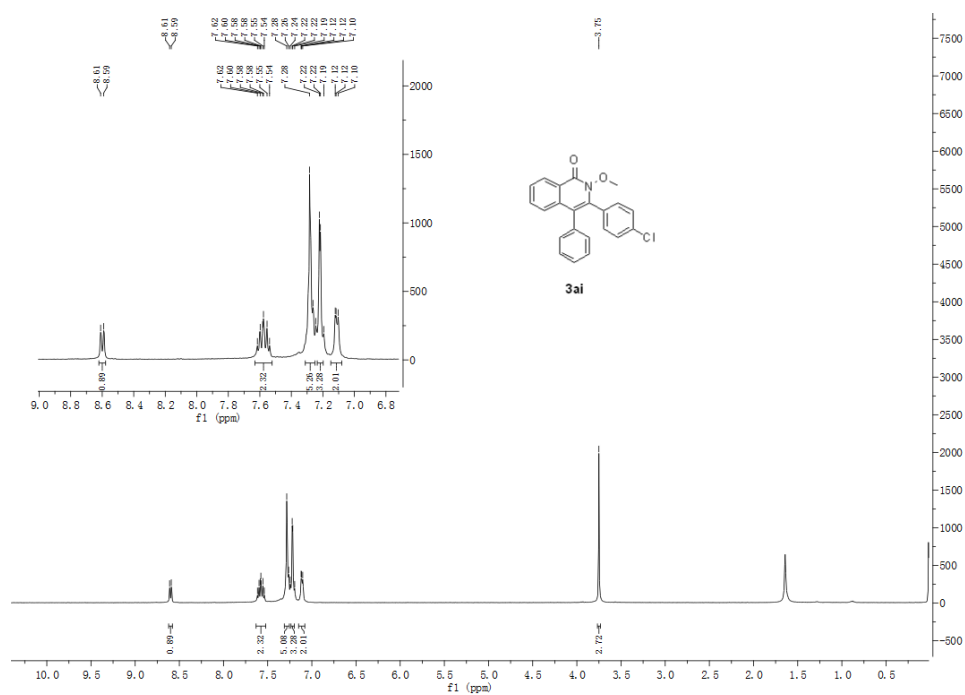


Figure S57 ¹H NMR spectra of compound **3ai** (400 MHz, CDCl₃)

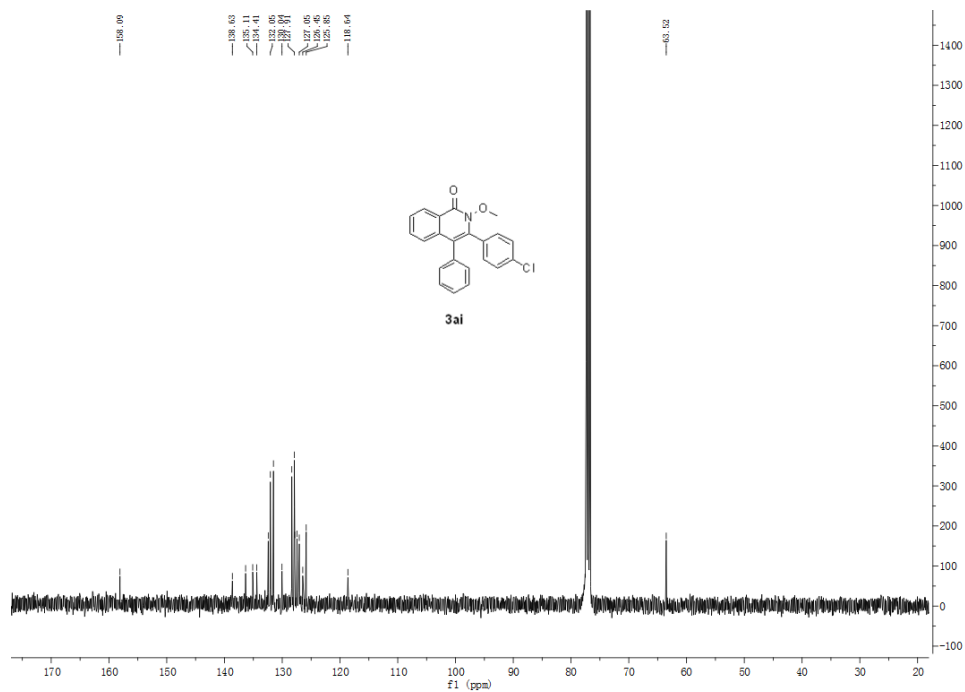
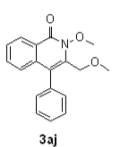
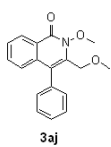


Figure S58 ¹³C NMR spectra of compound **3ai** (101 MHz, CDCl₃)



3aj

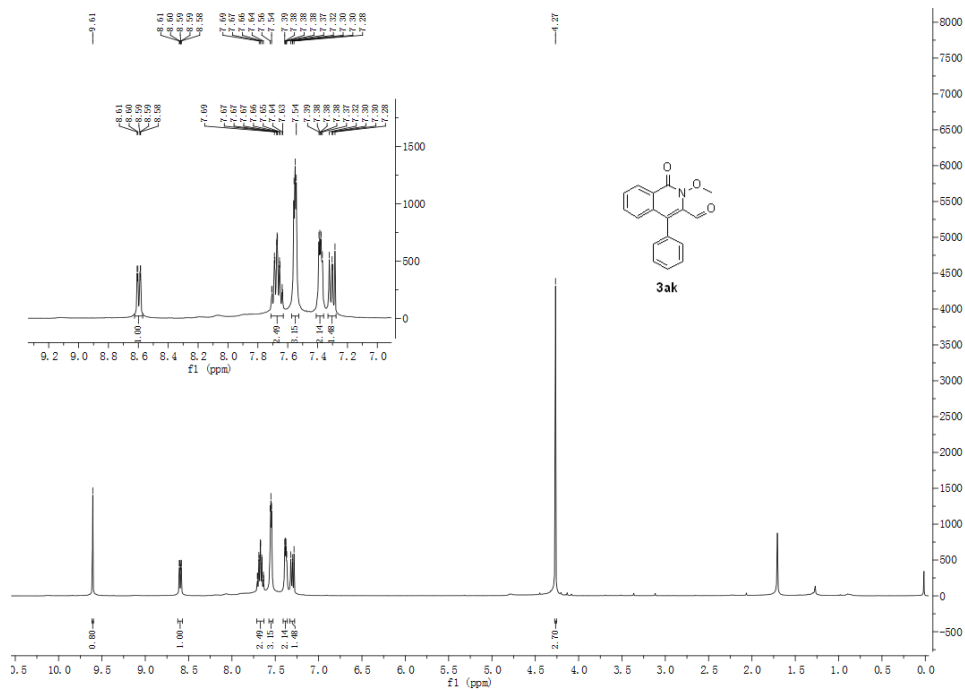


Figure S63 ¹H NMR spectra of compound **3ak** (400 MHz, CDCl₃)

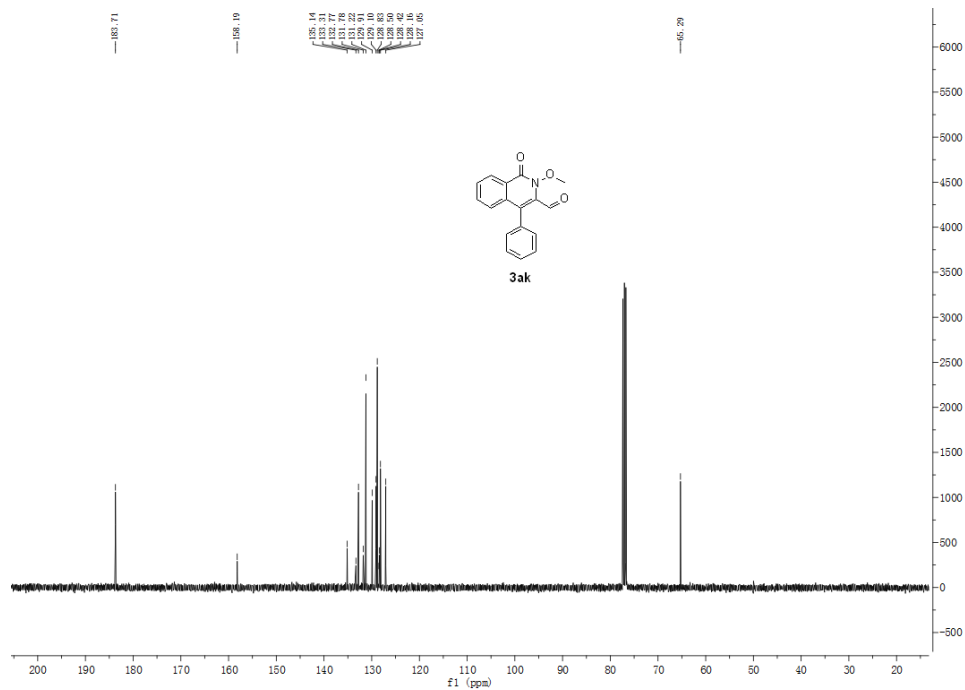


Figure S64 ¹³C NMR spectra of compound **3ak** (101 MHz, CDCl₃)

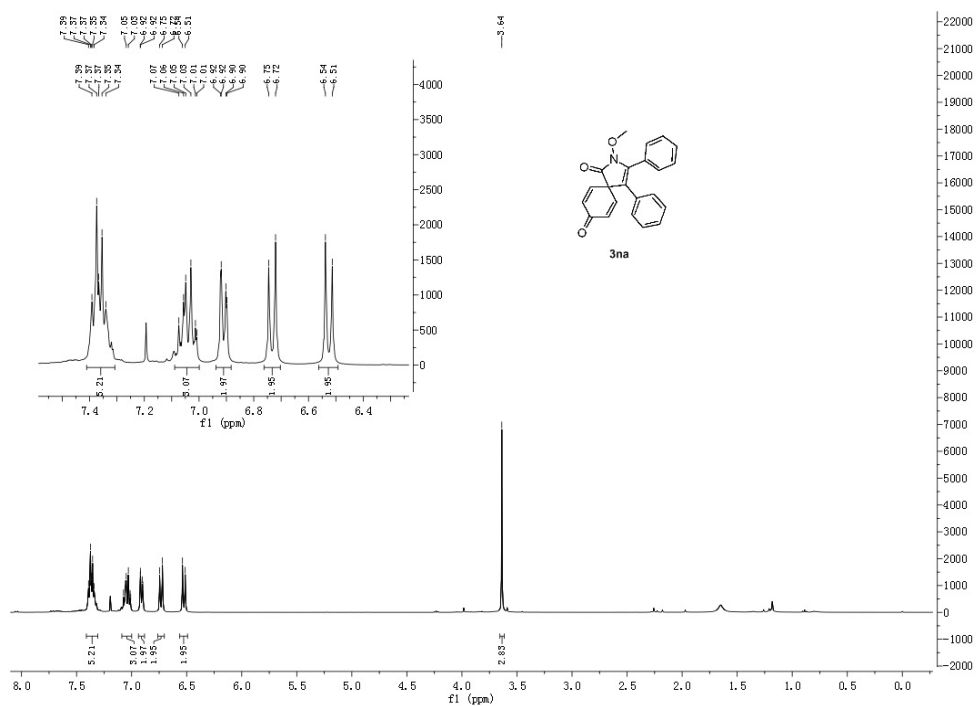


Figure S65 ¹H NMR spectra of compound **3na** (400 MHz, CDCl₃)

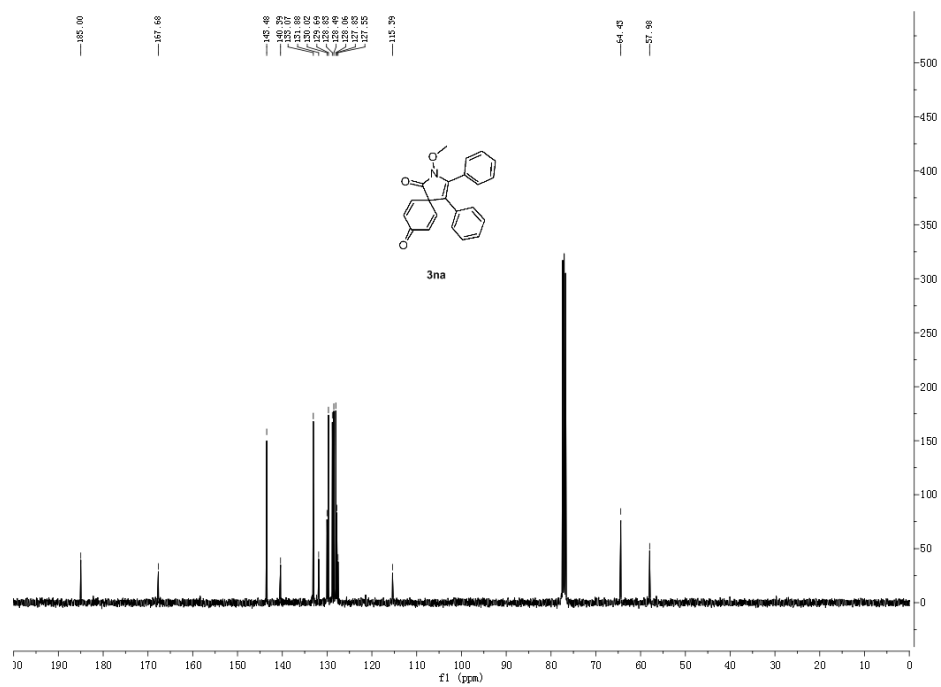


Figure S66 ¹³C NMR spectra of compound **3na** (101 MHz, CDCl₃)

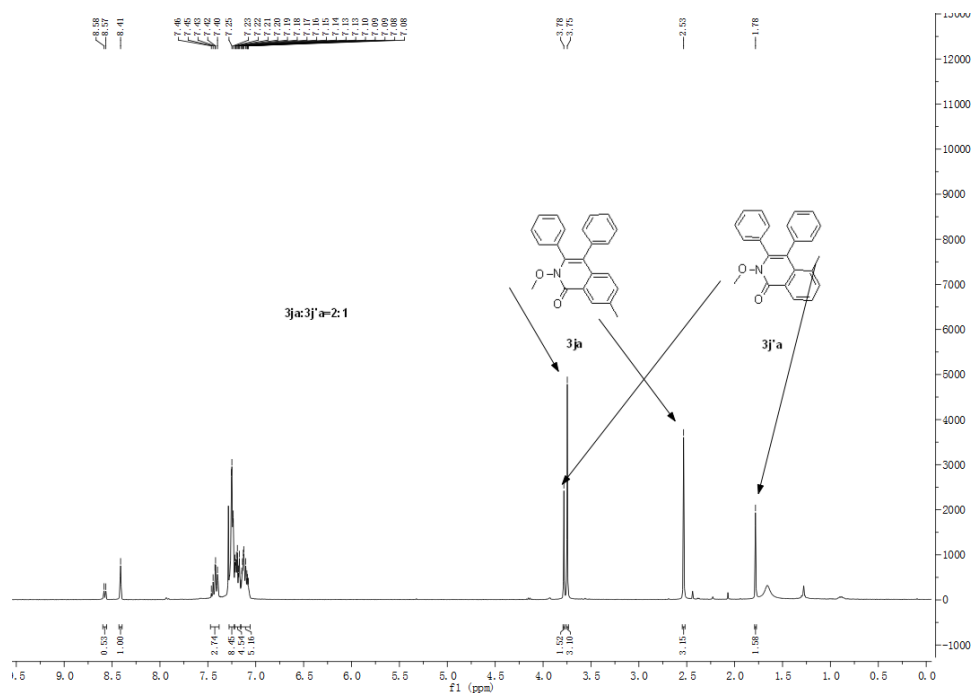


Figure S67 ^1H NMR spectra of compound **3ja** and **3ja'** (400 MHz, CDCl_3)

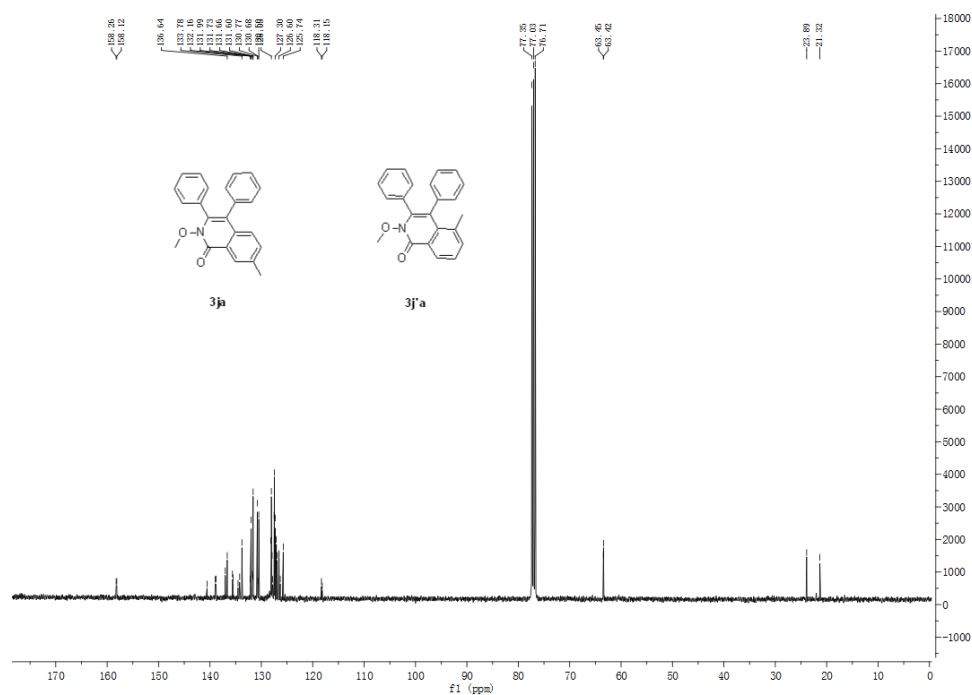


Figure S68 ^{13}C NMR spectra of compound **3ja** and **3ja'** (101 MHz, CDCl_3)

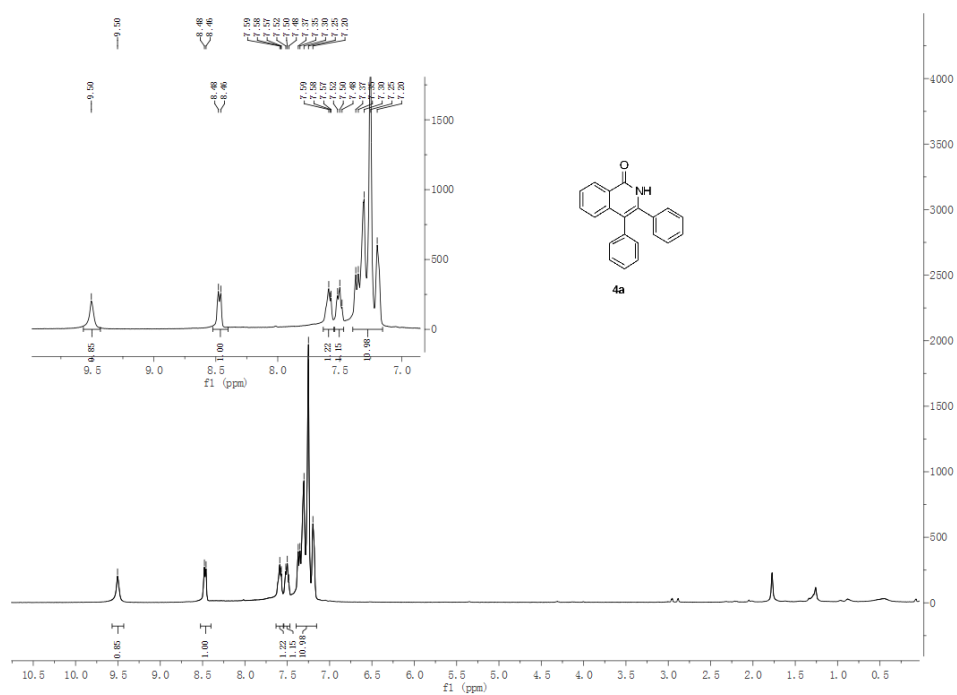


Figure S69 ¹H NMR spectra of compound **4a** (101 MHz, CDCl₃)

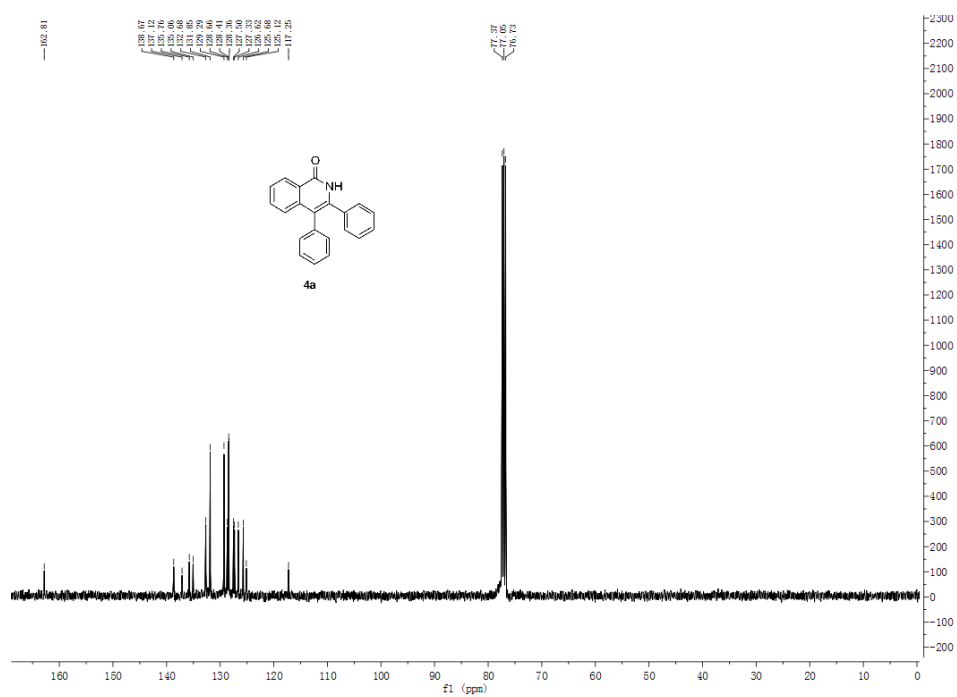


Figure S70 ¹³C NMR spectra of compound **4a** (CDCl₃)