

# Supporting Information

## Iridium (I)-Catalyzed Isoindolinone-Directed Branched-Selective Aromatic C–H Alkylation with Simple Al- kenes

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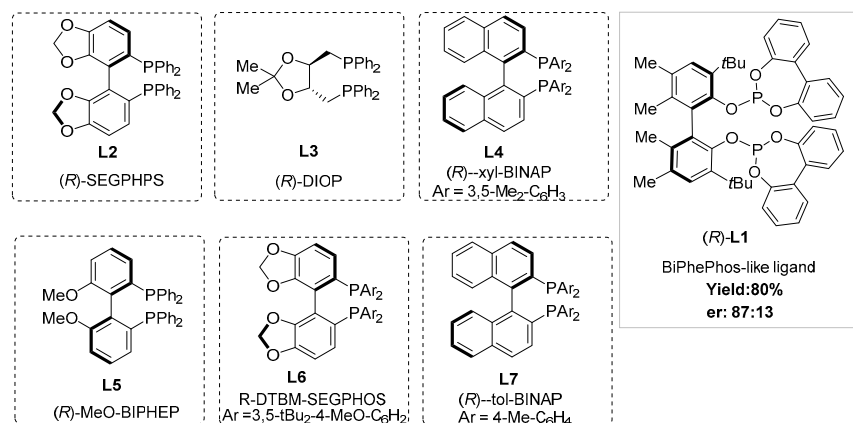
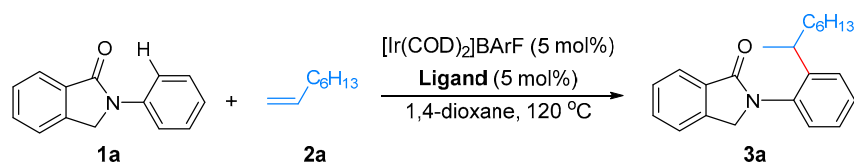
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## 1. Screening of Chiral Ligands and Condition Optimizations<sup>a</sup>

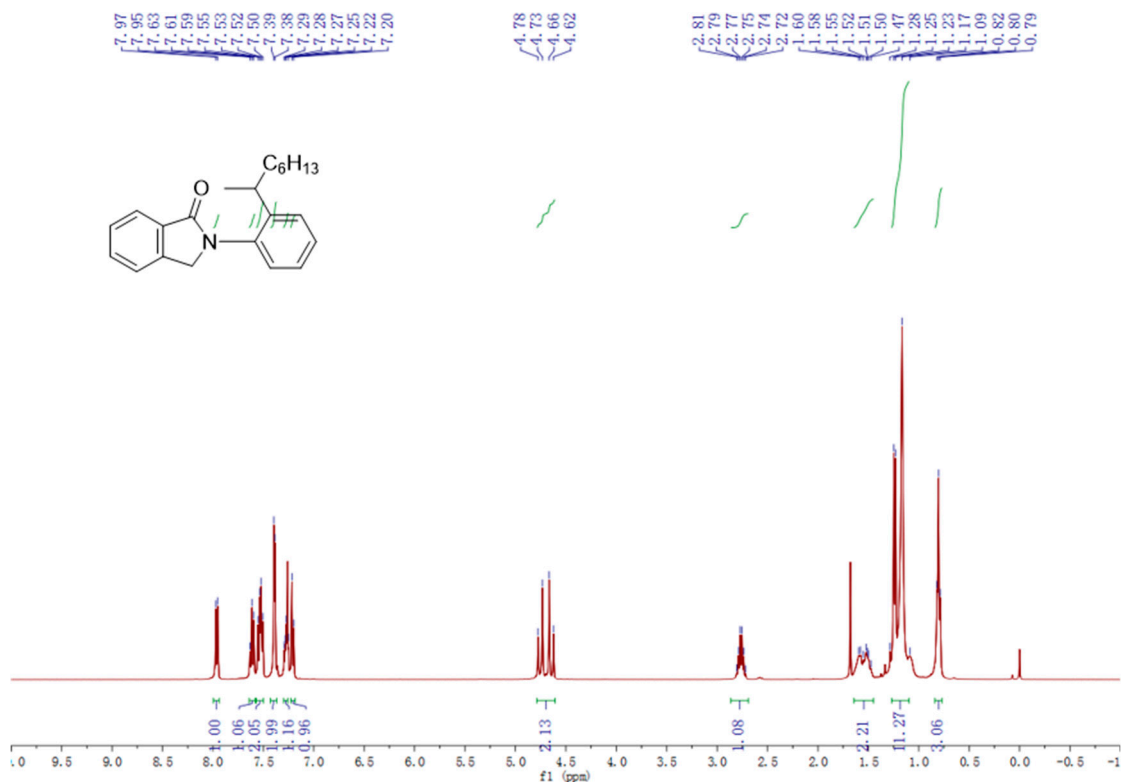


Entry	Ligand	solvent	Yield (%) <sup>b</sup>	er <sup>c</sup>	b/l <sup>d</sup>
1	<b>(R)-L1</b>	1,4-dioxane	81%	86:14	>20:1
2	<b>L2</b>	1,4-dioxane	21%	54:46	>20:1
3	<b>L3</b>	1,4-dioxane	56%	56:44	13:1
4	<b>L4</b>	1,4-dioxane	16%	65:35	18:1
5	<b>L5</b>	1,4-dioxane	42%	68:32	10:1
6	<b>L6</b>	1,4-dioxane	Trace		
7	<b>L7</b>	1,4-dioxane	11%	60:40	7:1
8	<b>(R)-L1</b>	CPME	80	87:13	> 20:1
9	<b>(R)- L1</b>	toluene	55	86:14	>20:1
10	<b>(R)- L1</b>	DCE	53	86:14	>20:1
11	<b>(R)- L1</b>	PhCl	61	86:14	>20:1
12	<b>(R)- L1</b>	<i>m</i> -xylene	60	86:14	>20:1
13	<b>(R)- L1</b>	DME	48	84:16	>20:1
14	<b>(S)-L1</b>	CPME	79	14:86	>20:1

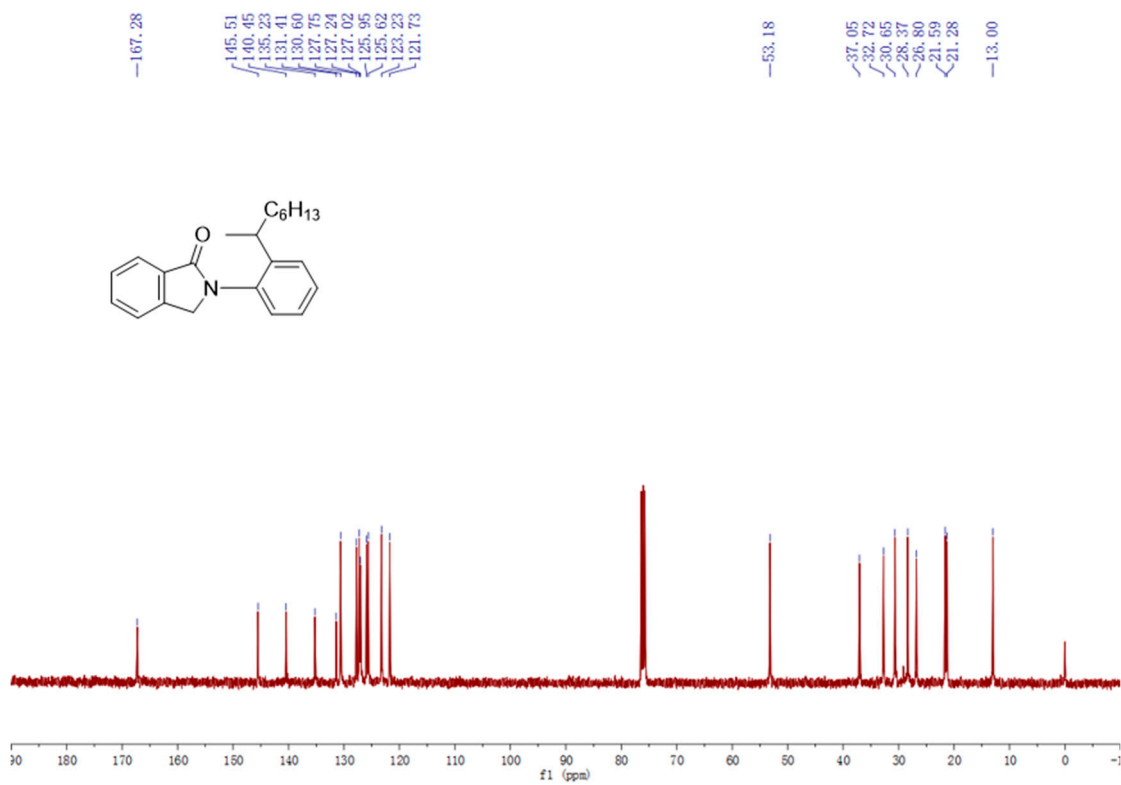
<sup>a</sup>Reaction conditions: **1a** (0.1mmol), **2a** (0.5 mmol),  $[\text{Ir}(\text{COD})_2]\text{BARF}$  (5 mol %), Ligand(5 mol%), solvent (0.2 mL), 120 °C, 48 h, <sup>b</sup>isolated yield for branched-selective product, <sup>c</sup>The er value of the product was determined by chiral HPLC analysis. <sup>d</sup>The linear/branched (l/b) ratio was determined by GC.

## 2. NMR Spectra

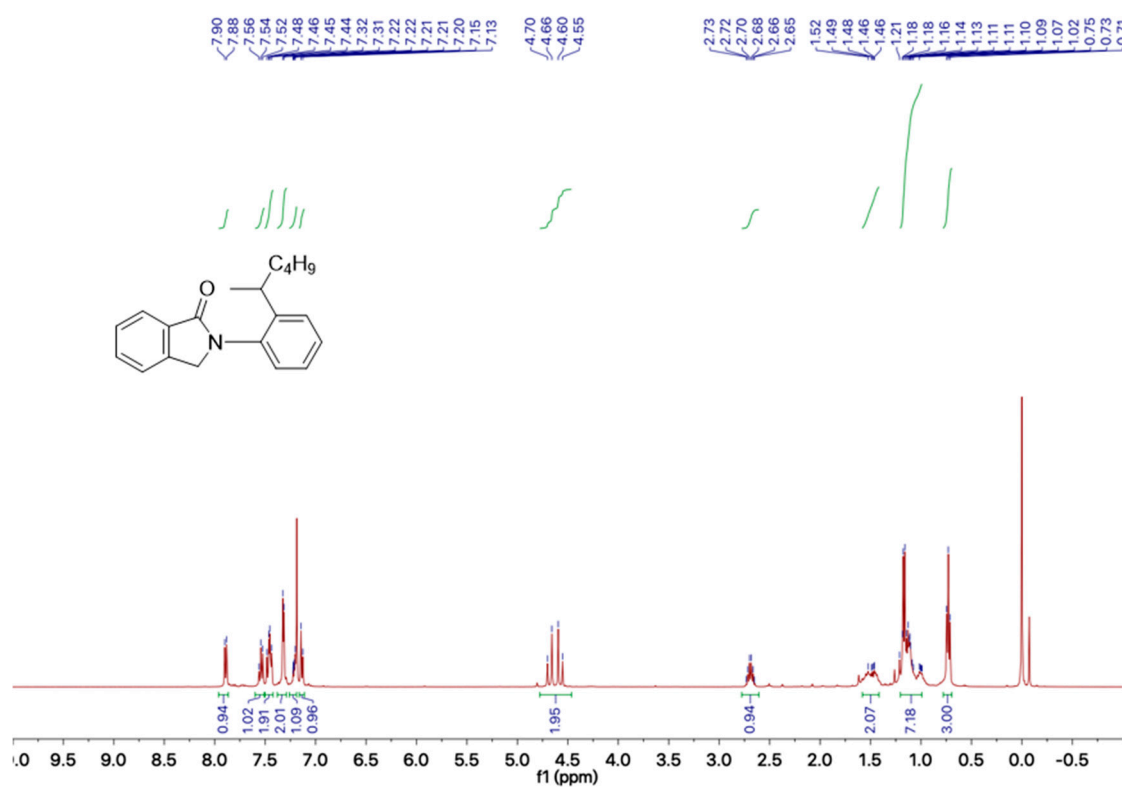
### $^1\text{H}$ NMR Spectrum of Compound **3a**



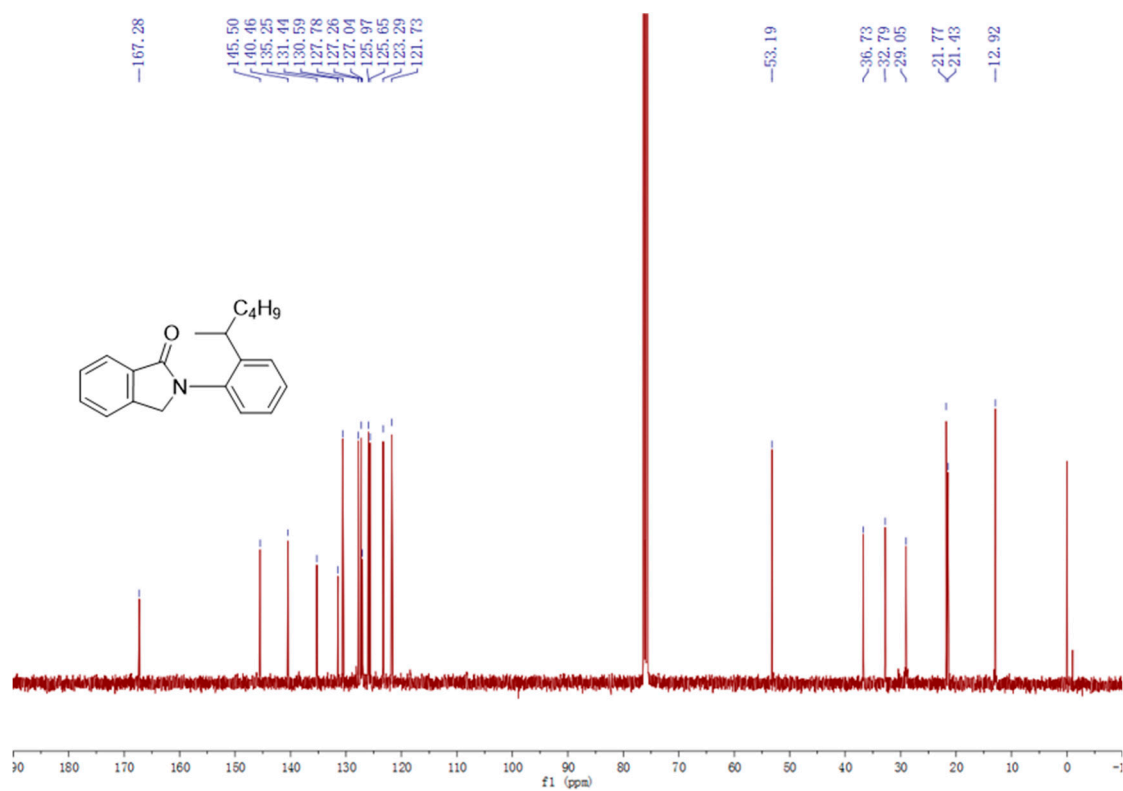
### $^{13}\text{C}$ NMR Spectrum of Compound **3a**



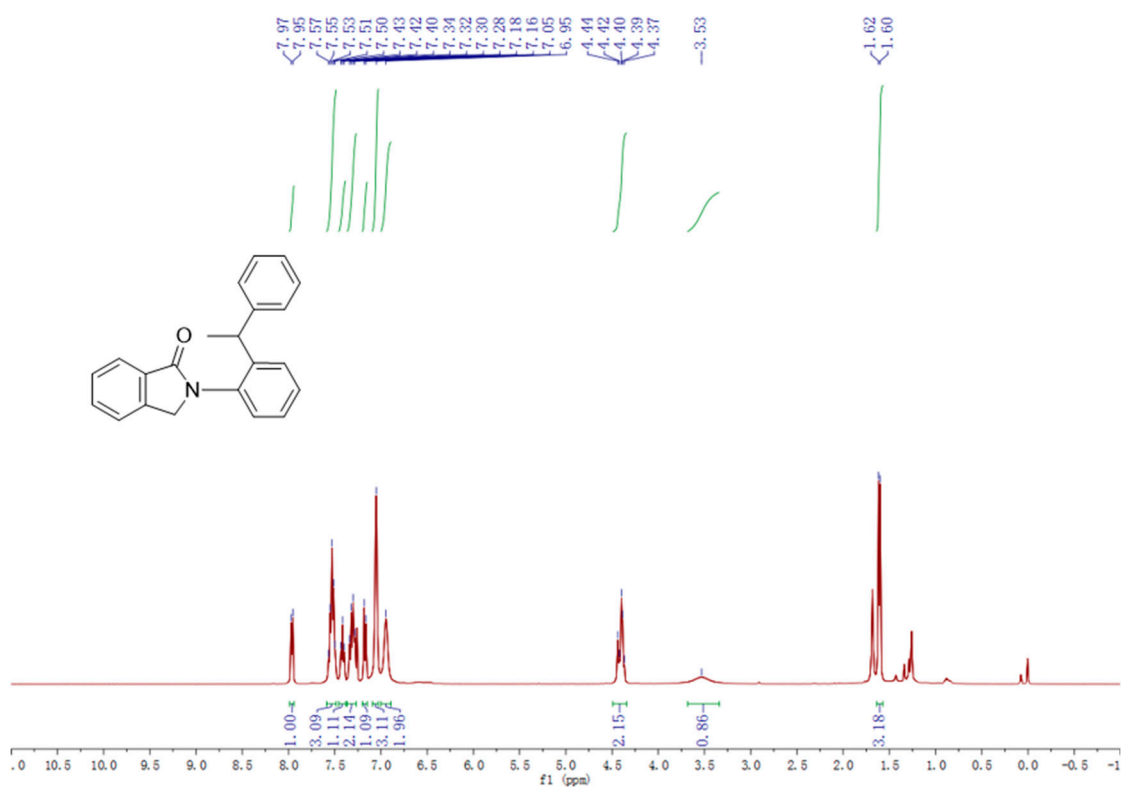
# <sup>1</sup>H NMR Spectrum of Compound **3b**



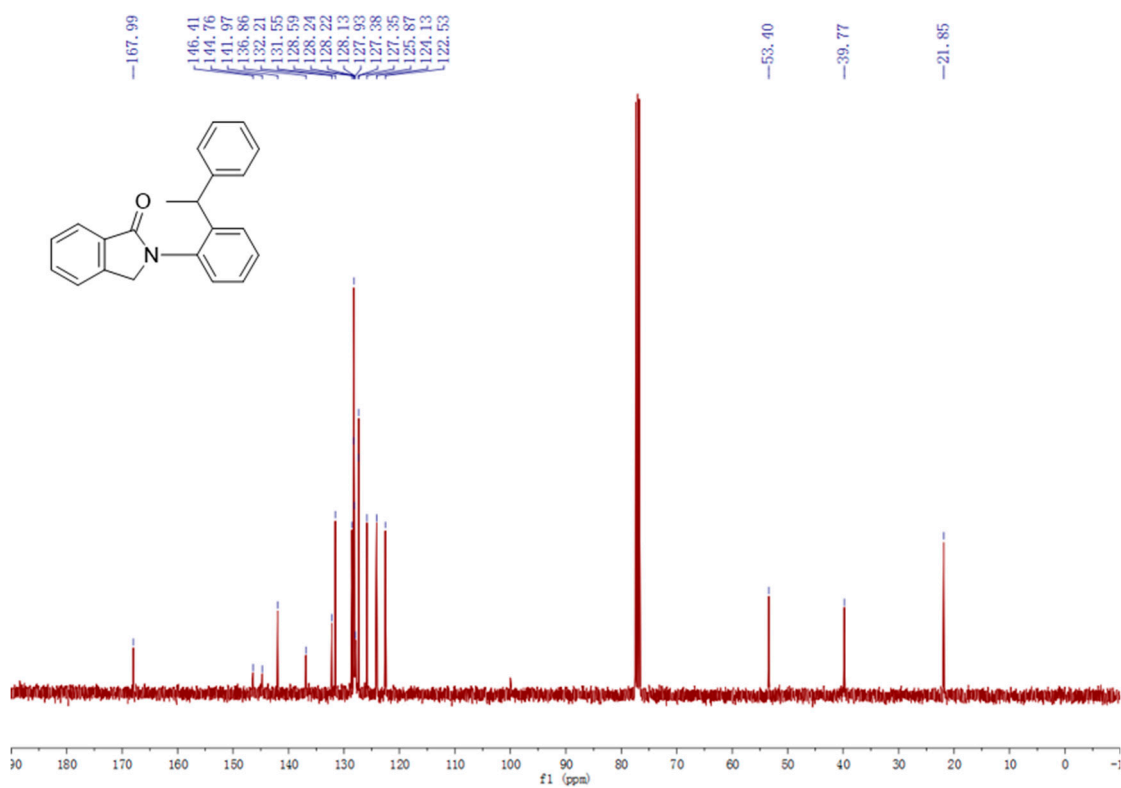
# <sup>13</sup>C NMR Spectrum of Compound **3b**



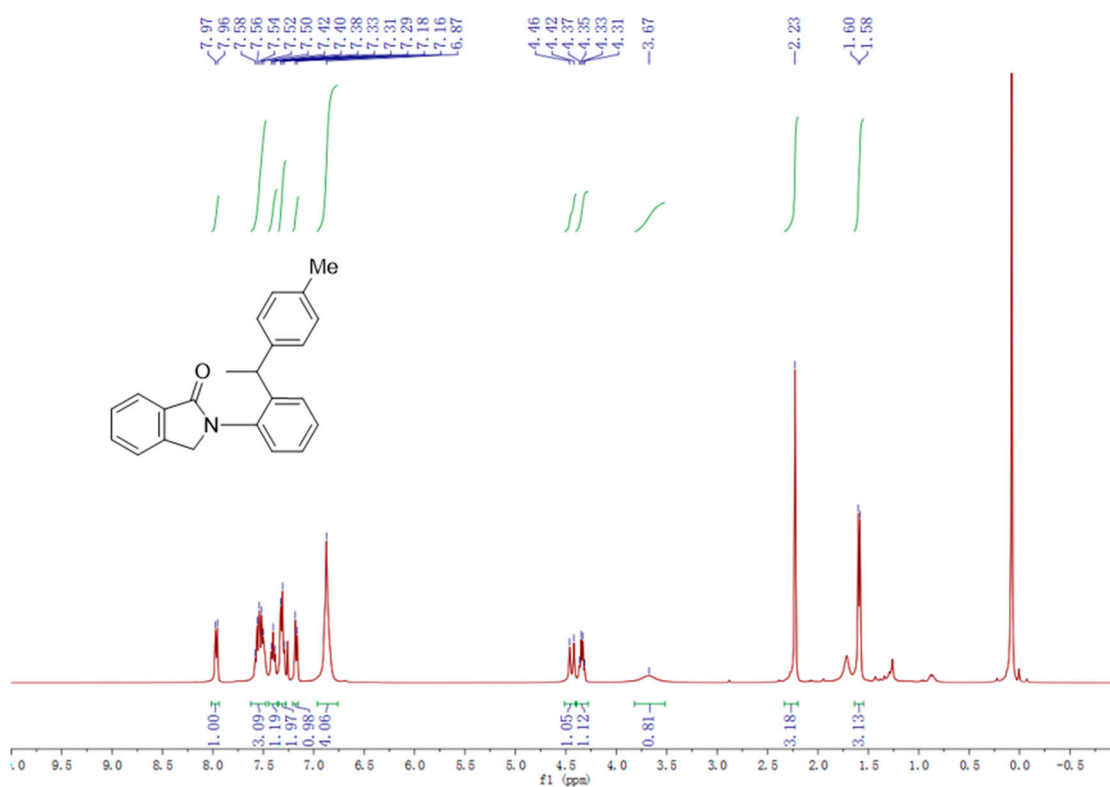
# <sup>1</sup>H NMR Spectrum of Compound **3c**



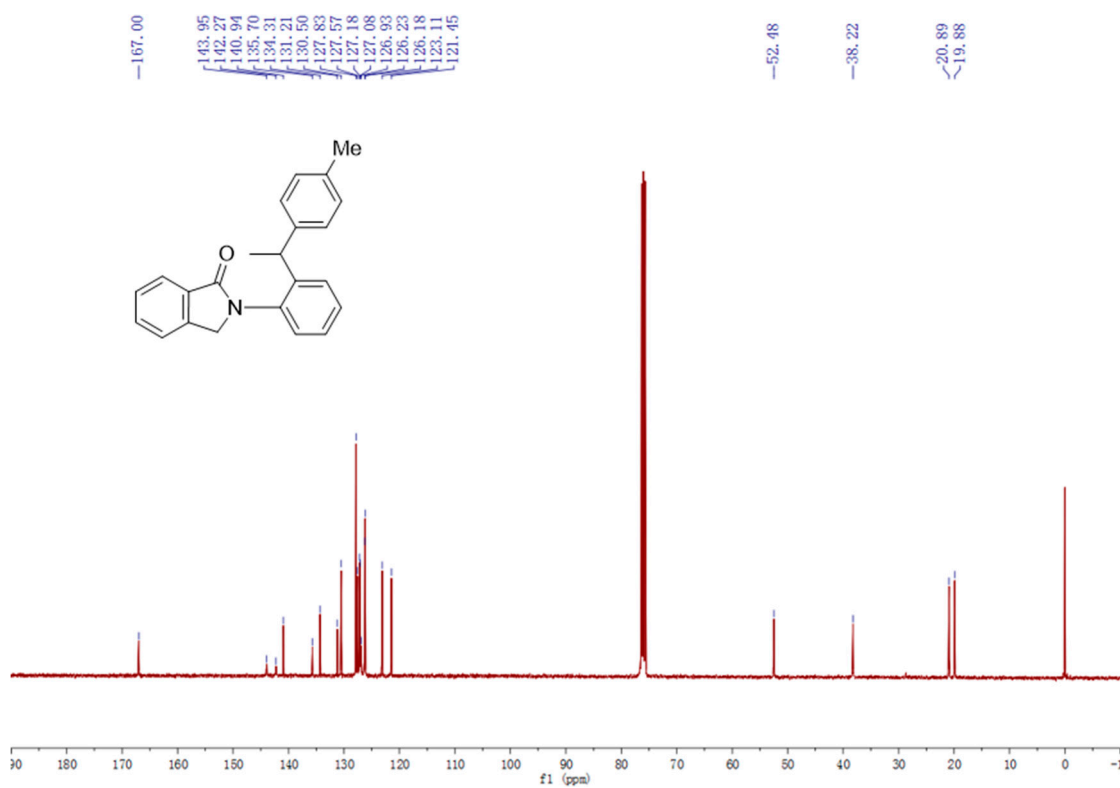
# <sup>13</sup>C NMR Spectrum of Compound **3c**



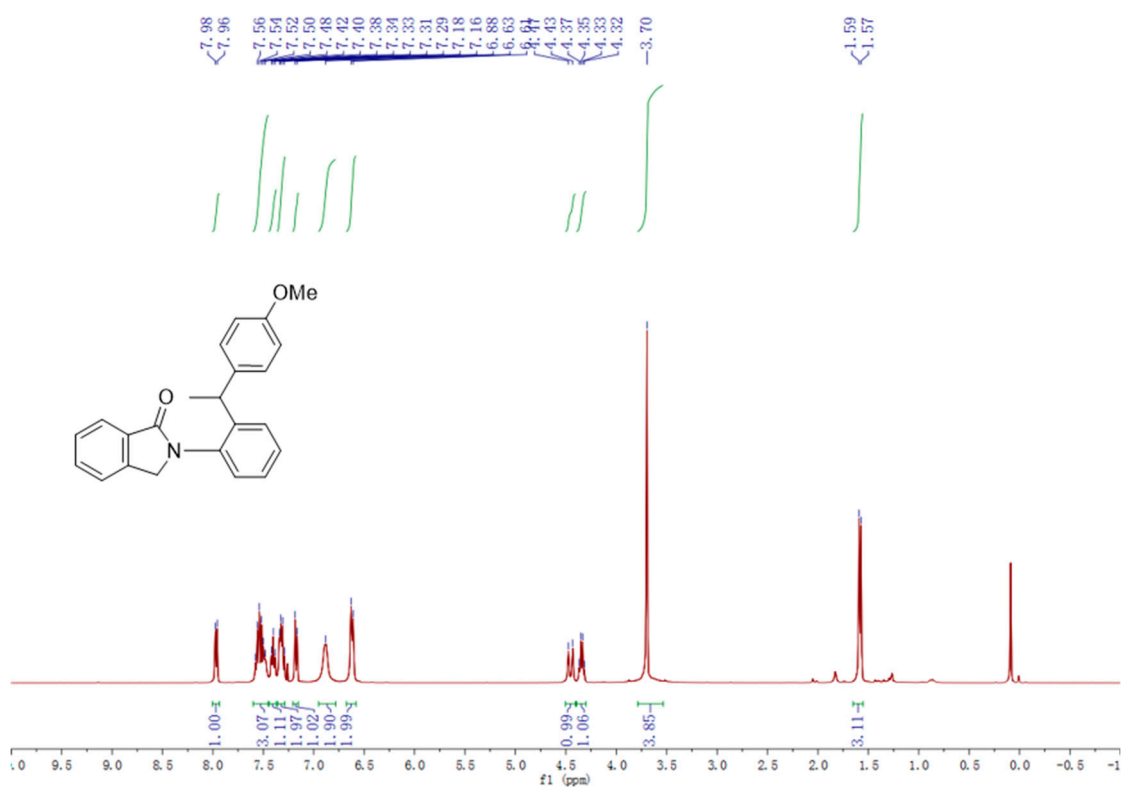
# <sup>1</sup>H NMR Spectrum of Compound **3d**



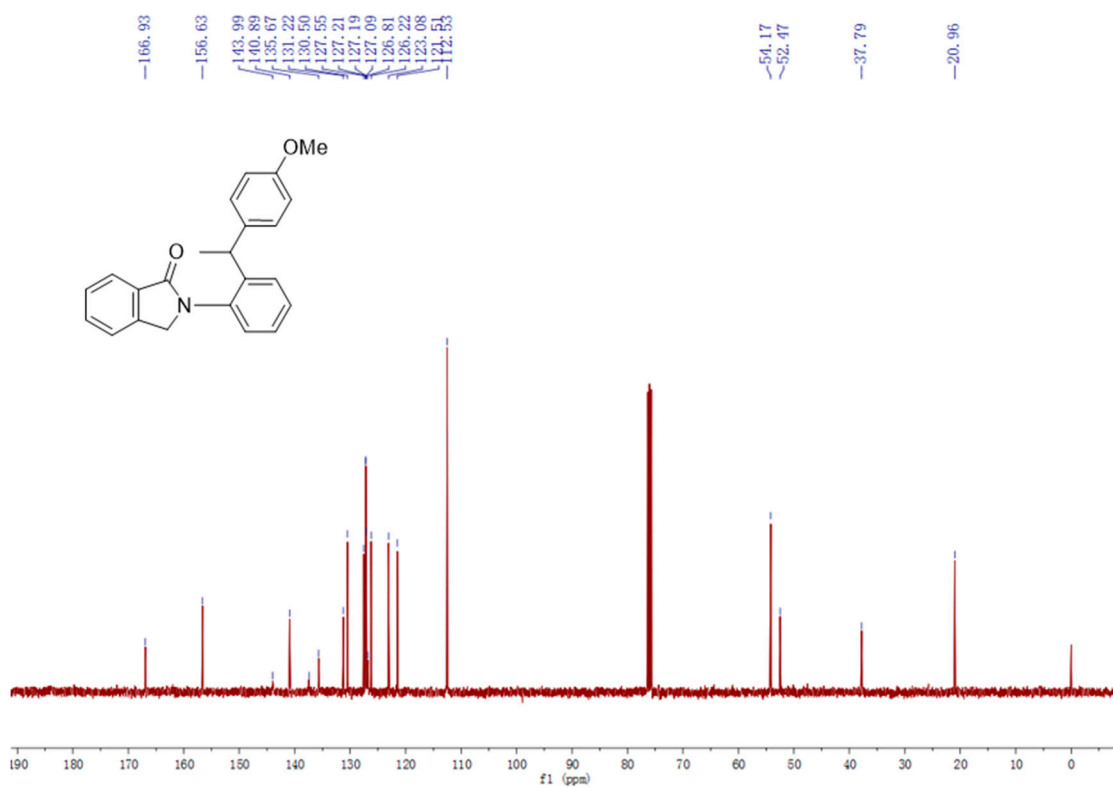
# <sup>13</sup>C NMR Spectrum of Compound **3d**



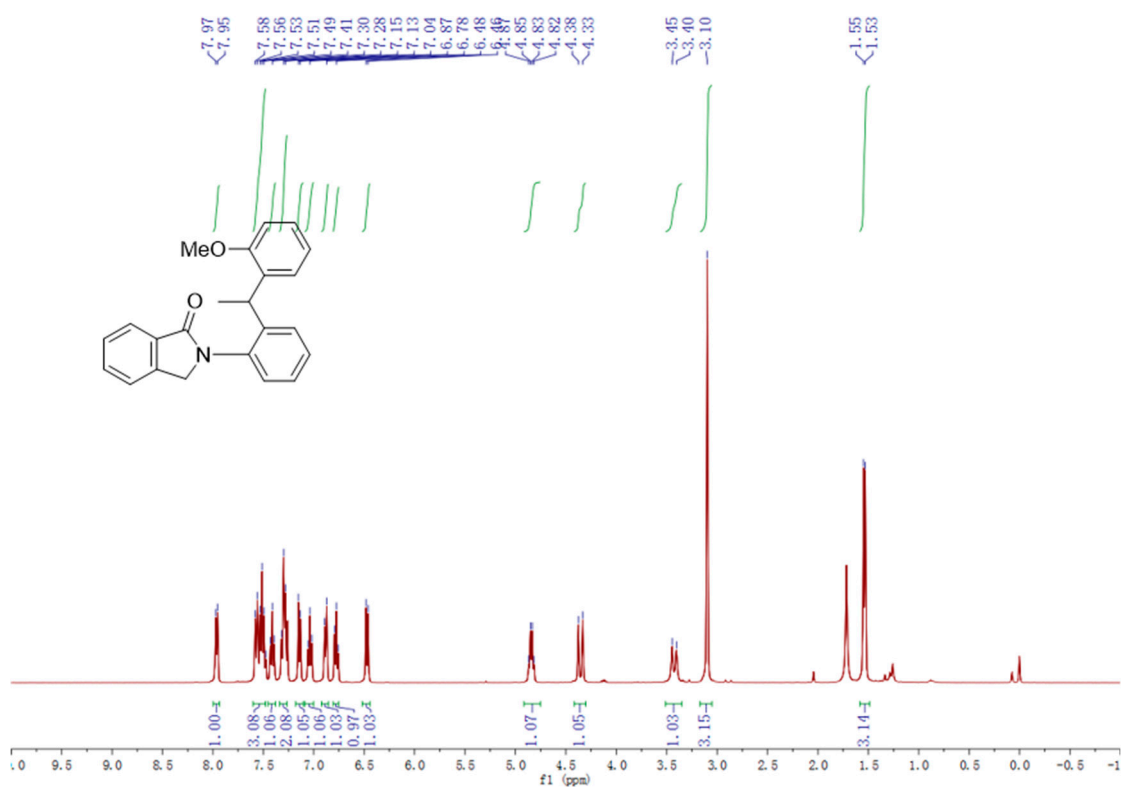
# <sup>1</sup>H NMR Spectrum of Compound 3e



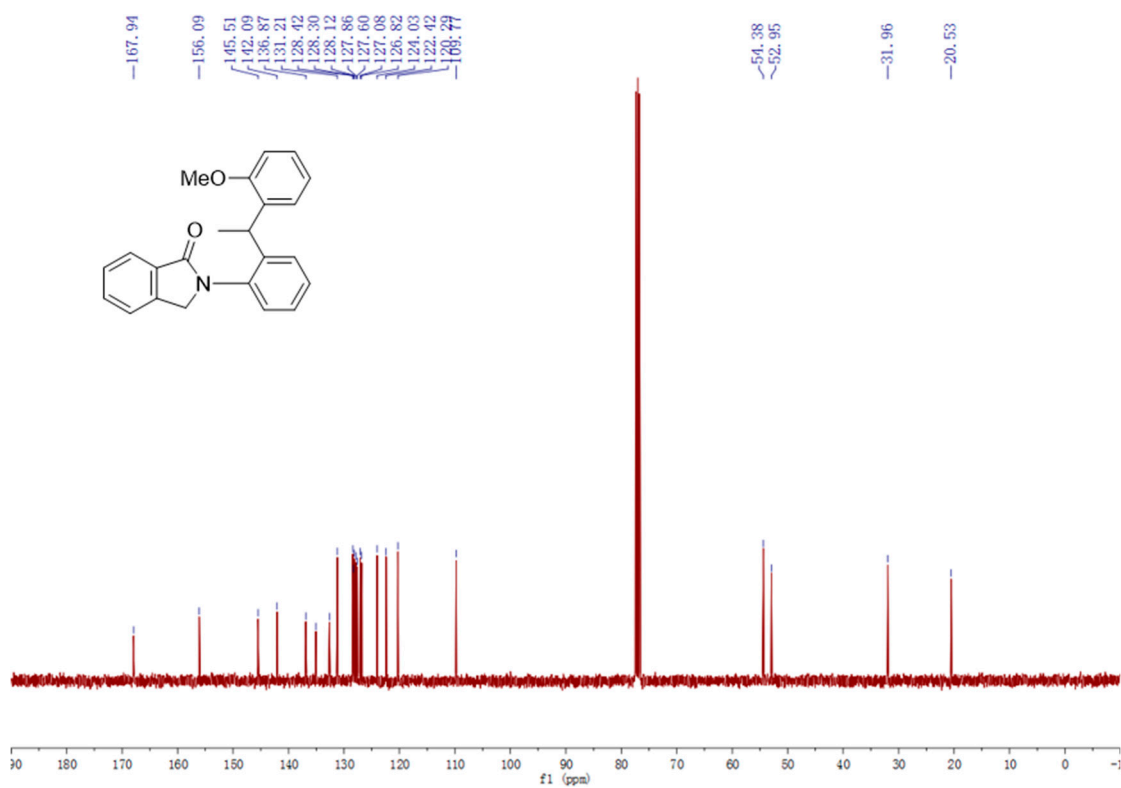
# <sup>13</sup>C NMR Spectrum of Compound 3e



# <sup>1</sup>H NMR Spectrum of Compound **3f**

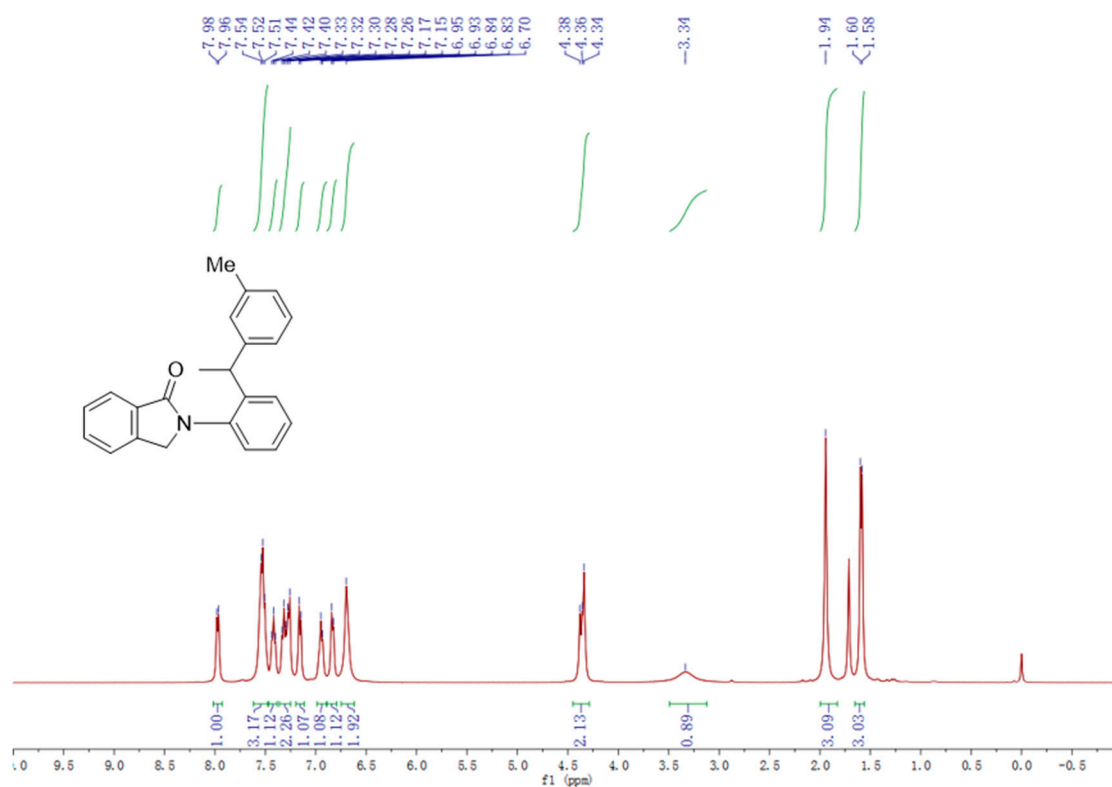


# <sup>13</sup>C NMR Spectrum of Compound **3f**

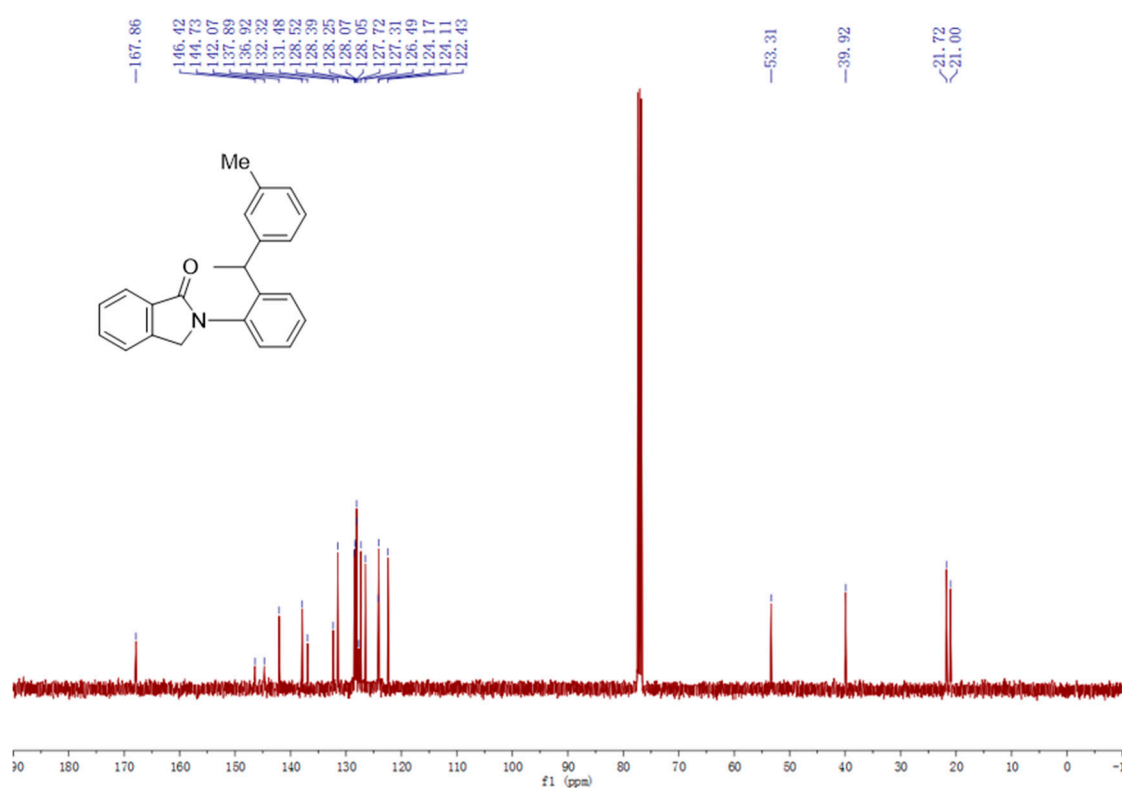




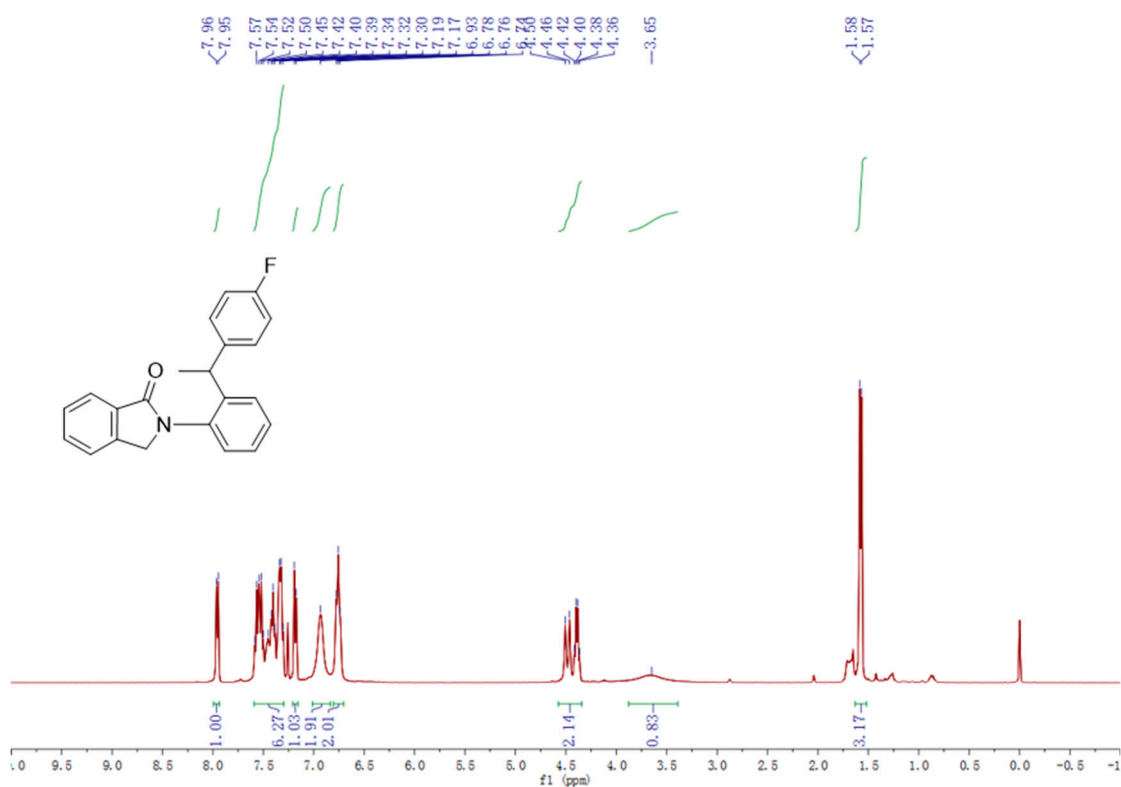
# <sup>1</sup>H NMR Spectrum of Compound **3g**



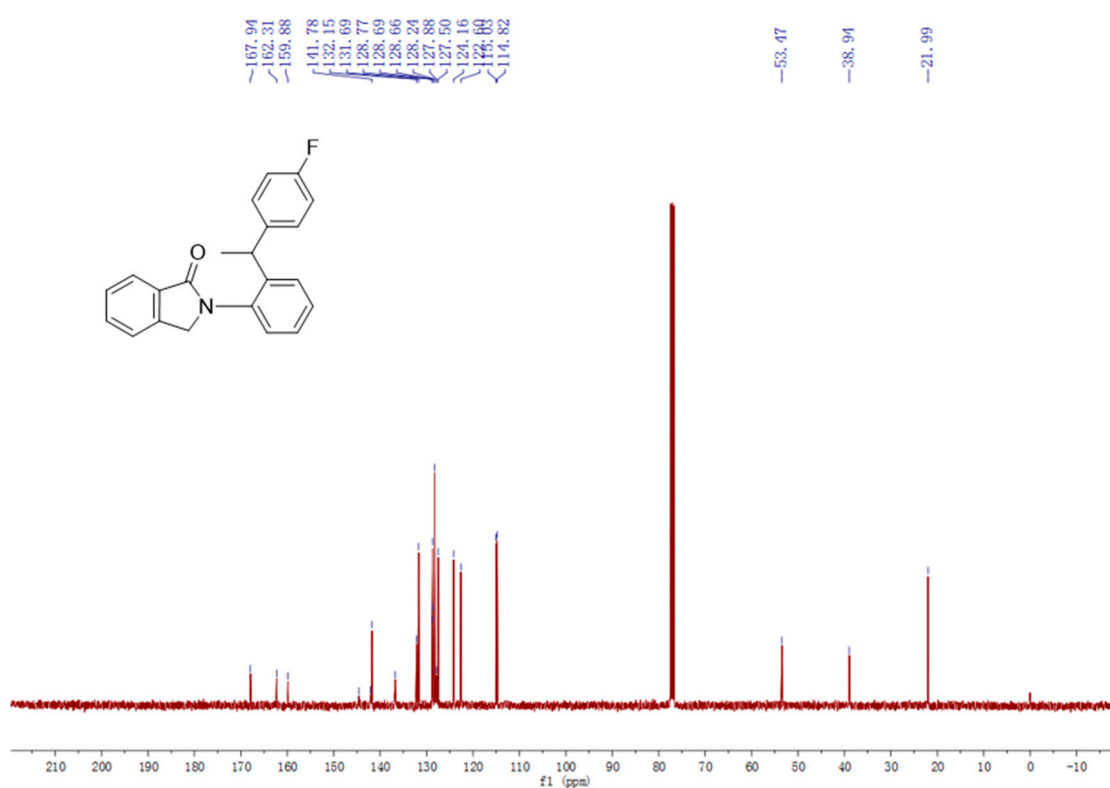
# <sup>13</sup>C NMR Spectrum of Compound **3g**



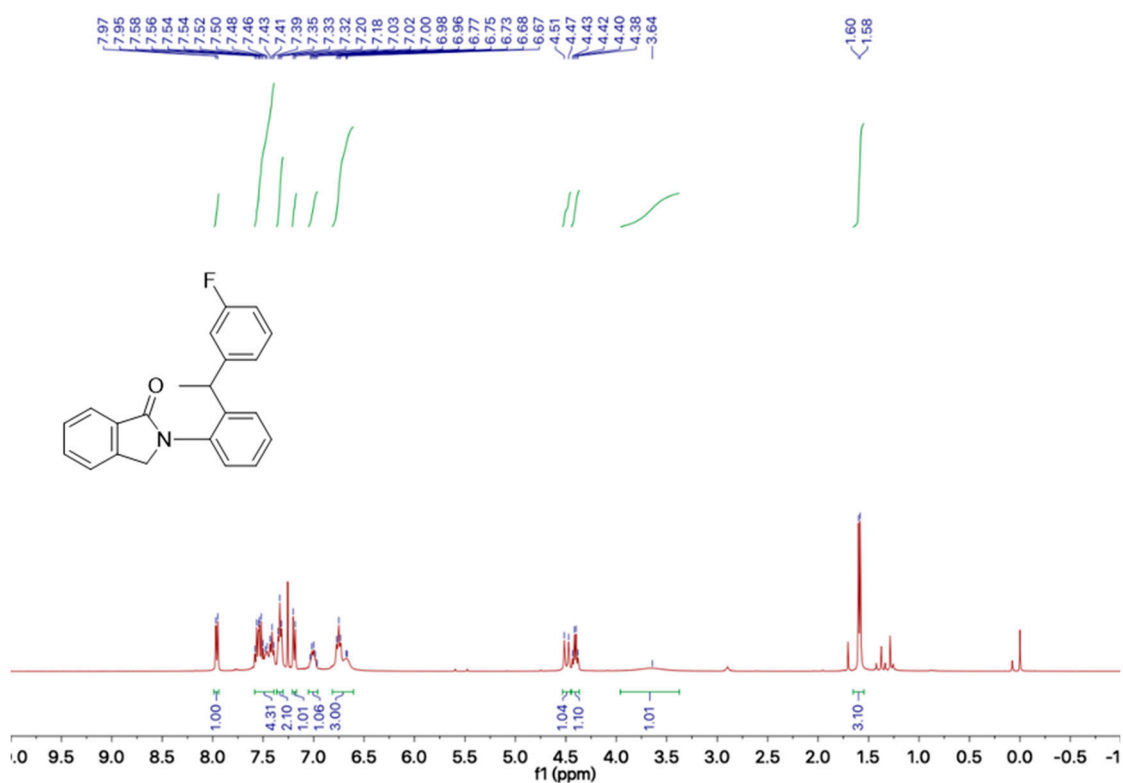
# <sup>1</sup>H NMR Spectrum of Compound **3h**



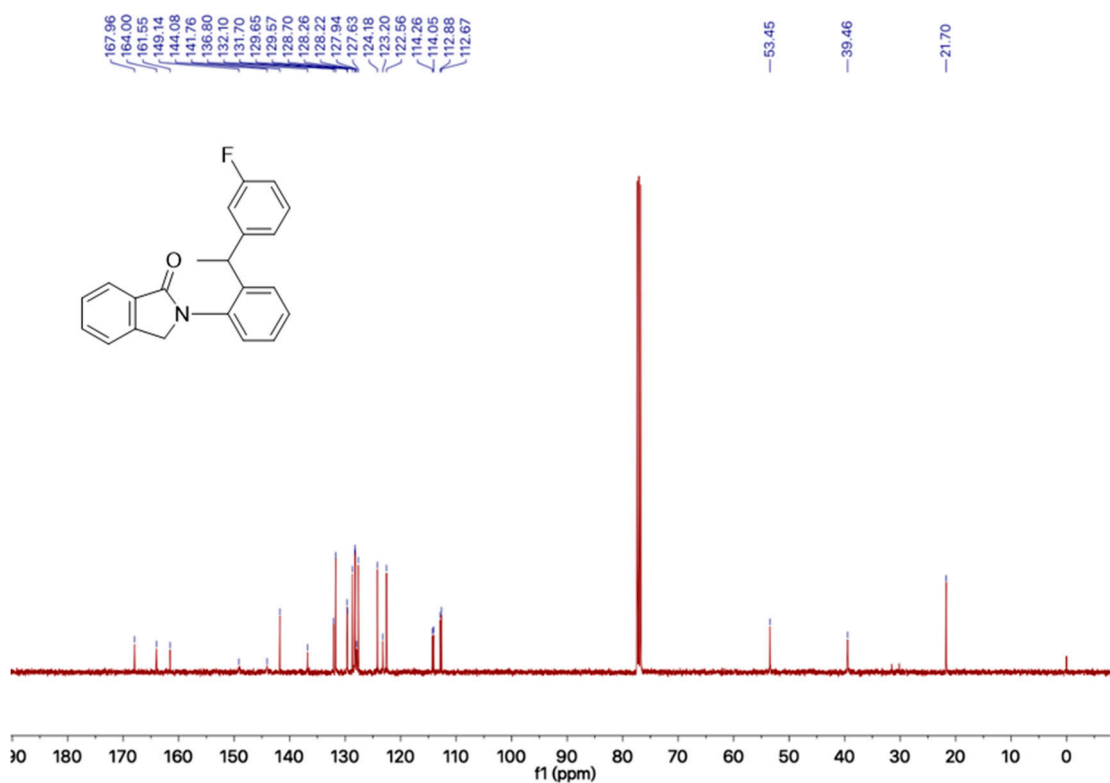
# <sup>13</sup>C NMR Spectrum of Compound **3h**



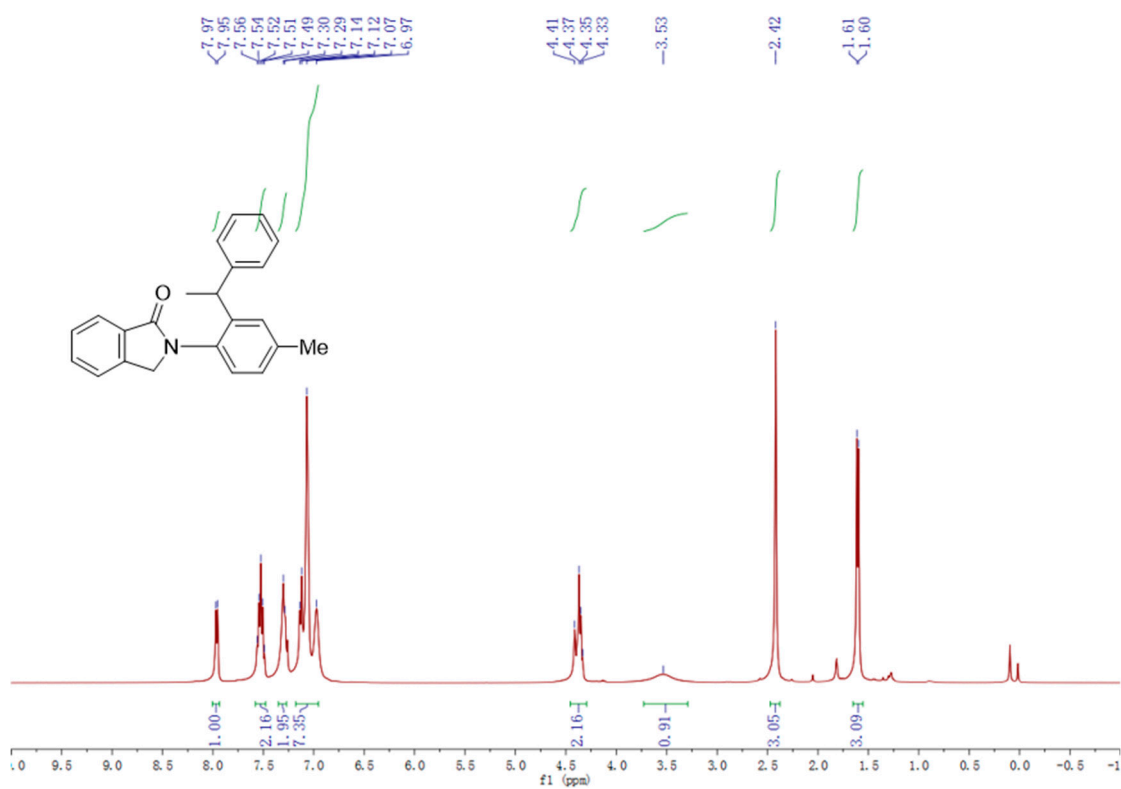
# <sup>1</sup>H NMR Spectrum of Compound **3i**



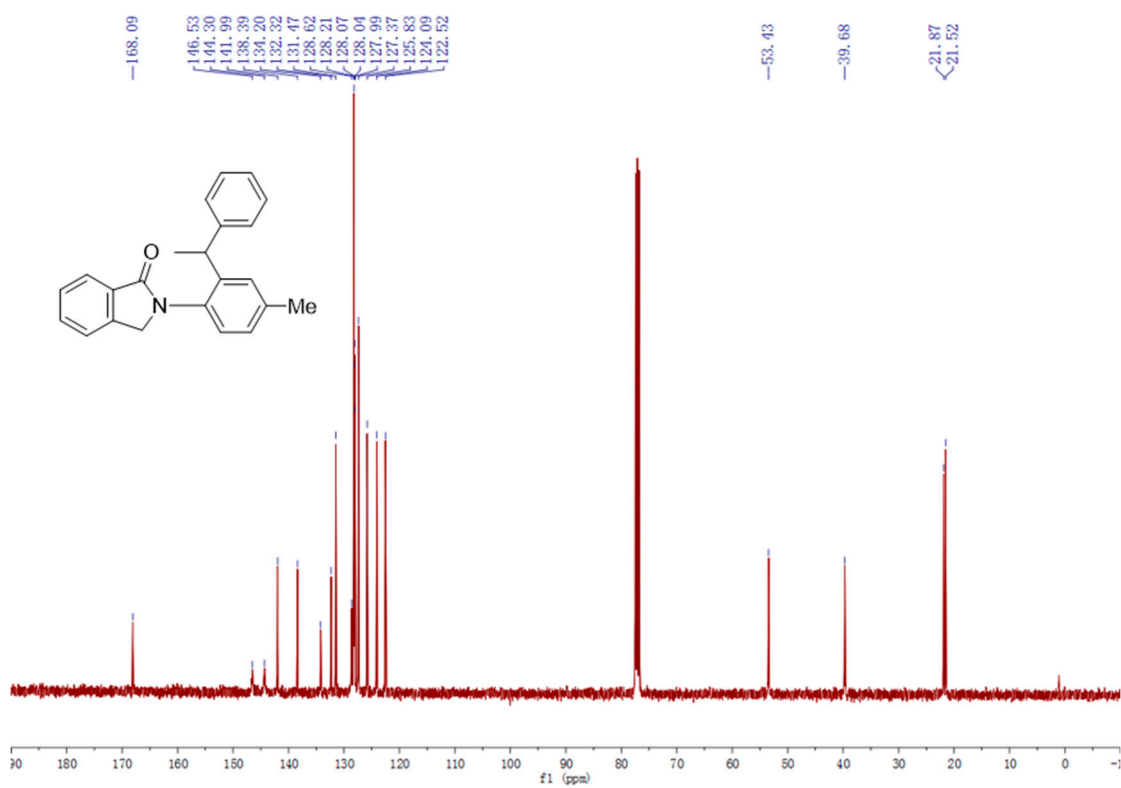
# <sup>13</sup>C NMR Spectrum of Compound **3i**



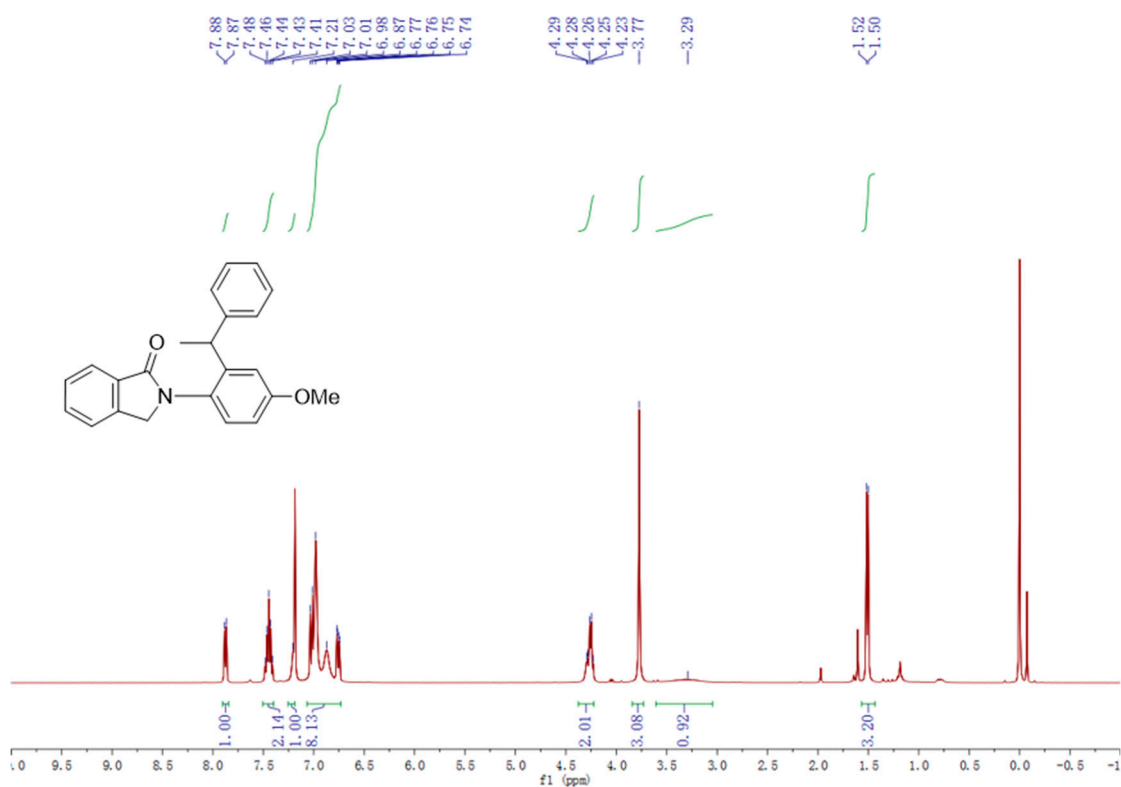
# <sup>1</sup>H NMR Spectrum of Compound **3j**



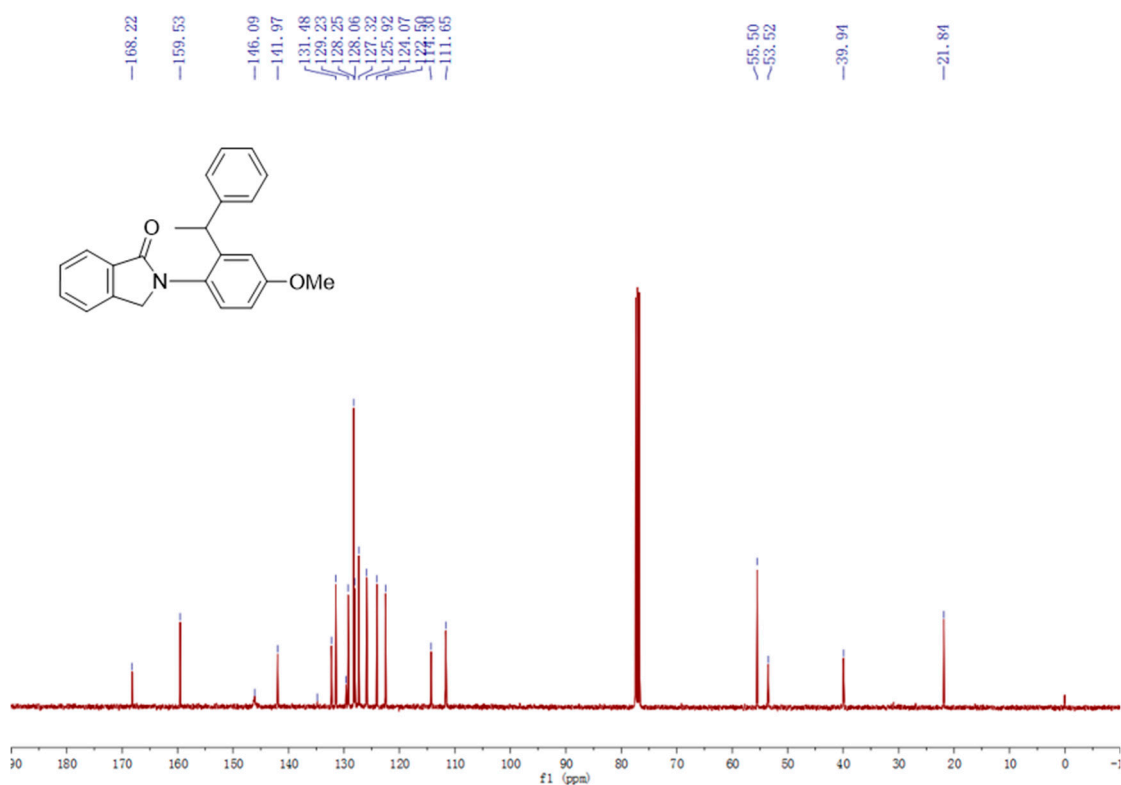
# <sup>13</sup>C NMR Spectrum of Compound **3j**



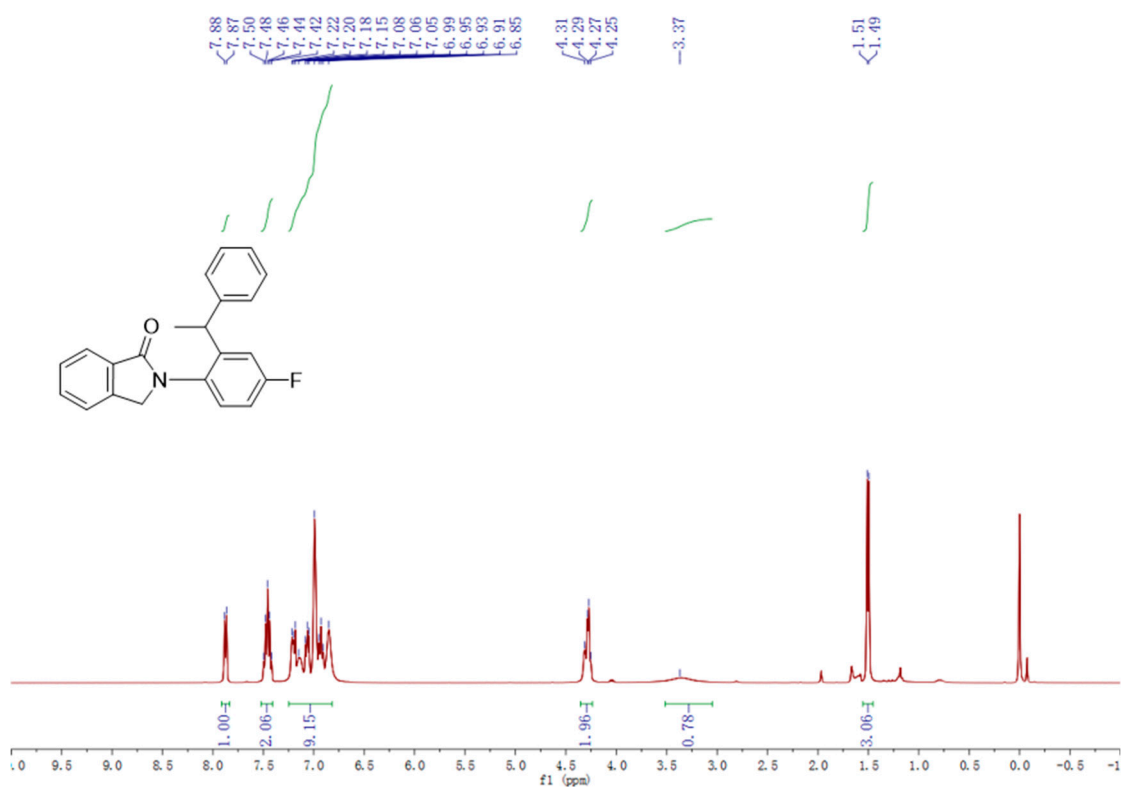
# <sup>1</sup>H NMR Spectrum of Compound **3k**



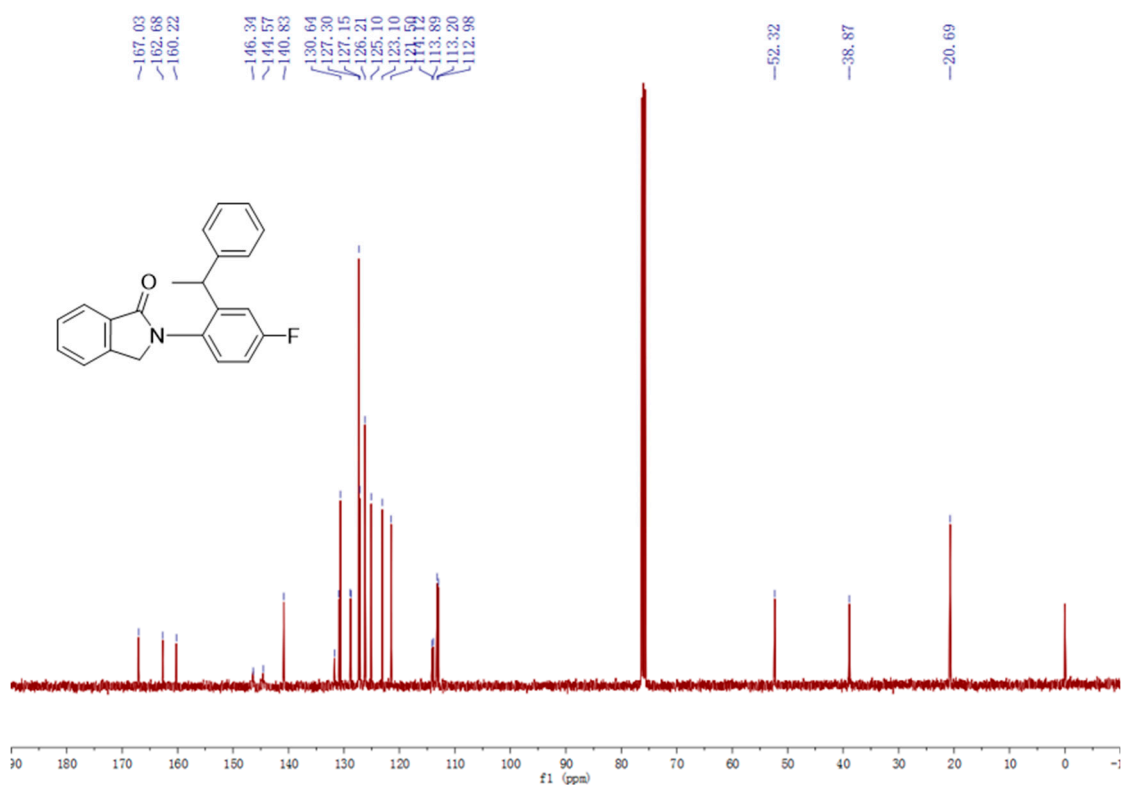
# <sup>13</sup>C NMR Spectrum of Compound **3k**



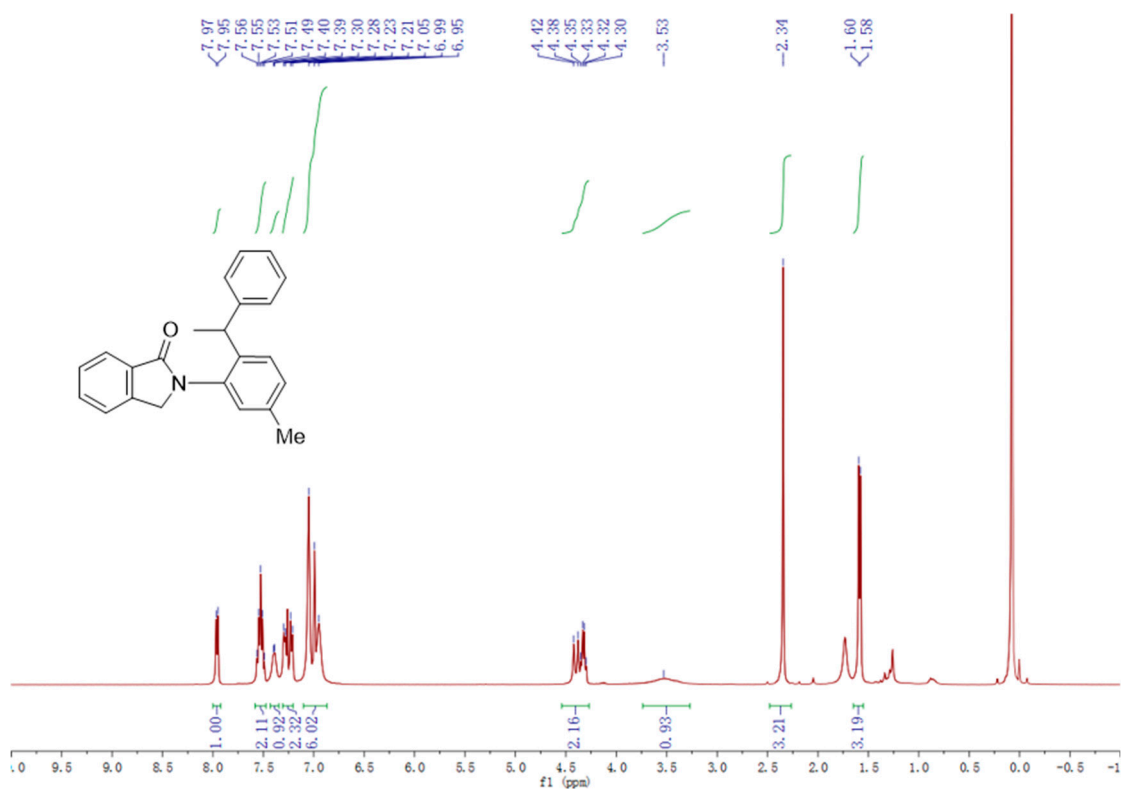
# <sup>1</sup>H NMR Spectrum of Compound **31**



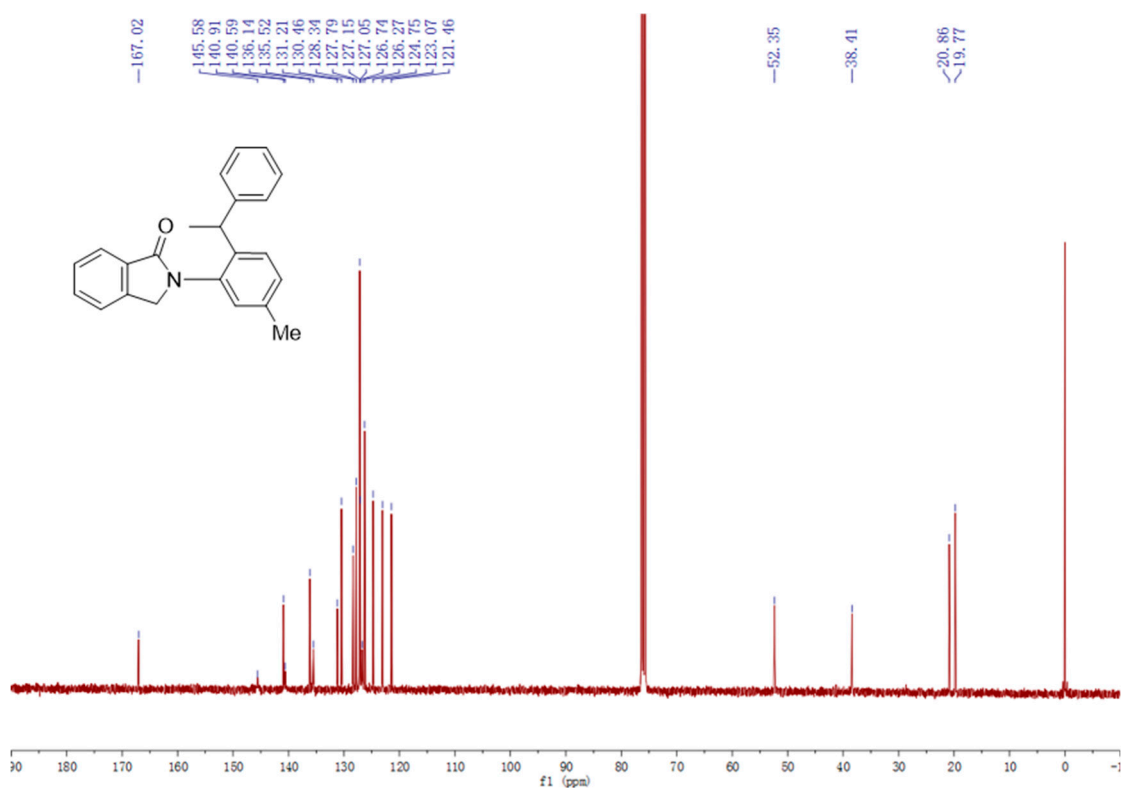
# <sup>13</sup>C NMR Spectrum of Compound **31**



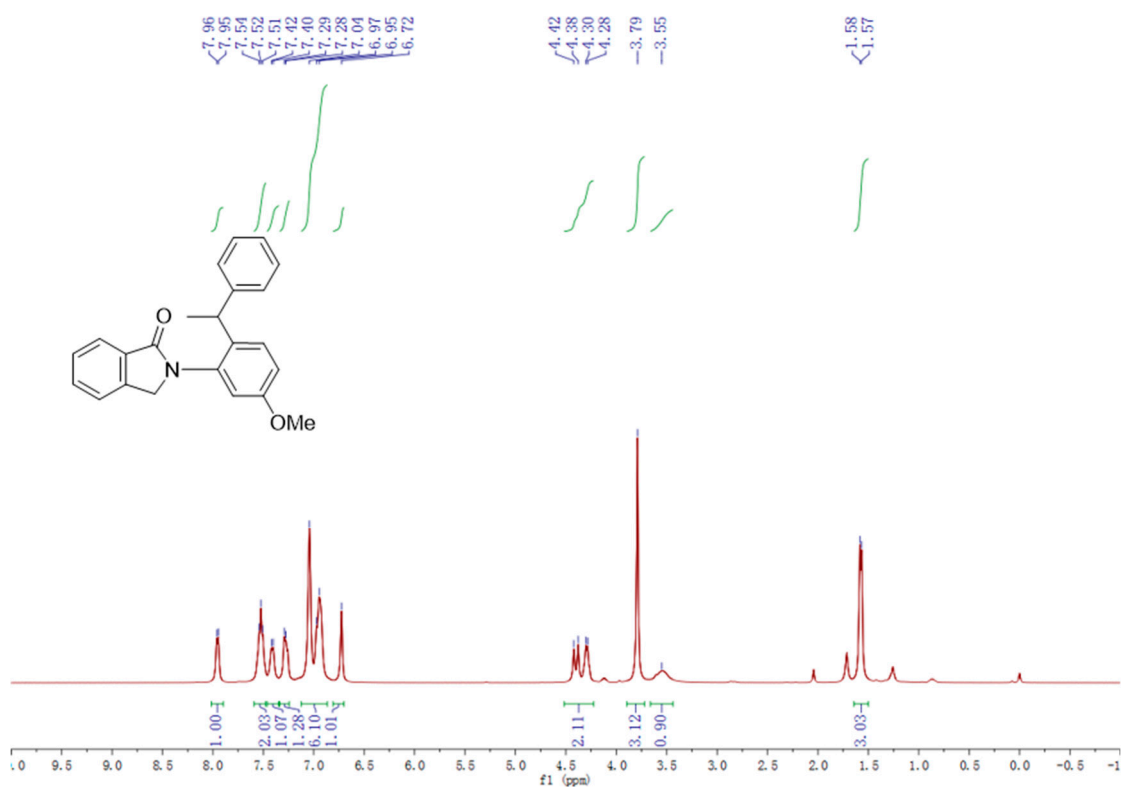
<sup>1</sup>H NMR Spectrum of Compound **3m**



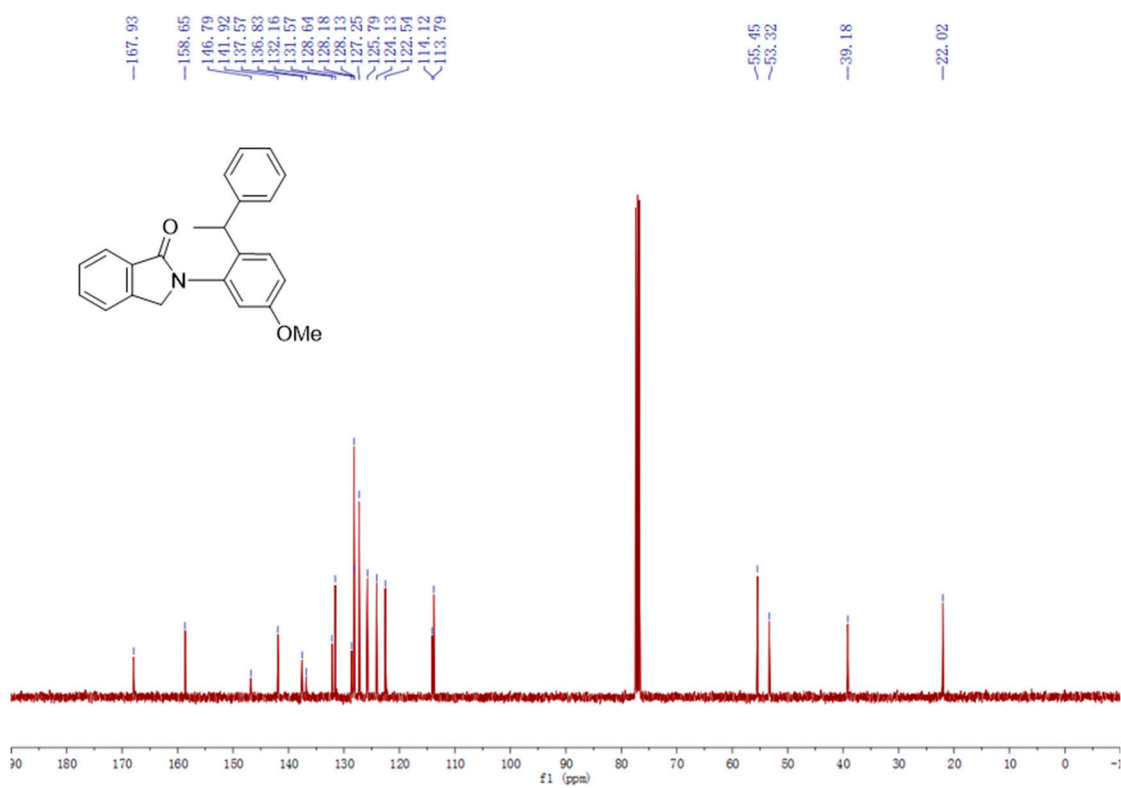
<sup>13</sup>C NMR Spectrum of Compound **3m**



# <sup>1</sup>H NMR Spectrum of Compound **3n**

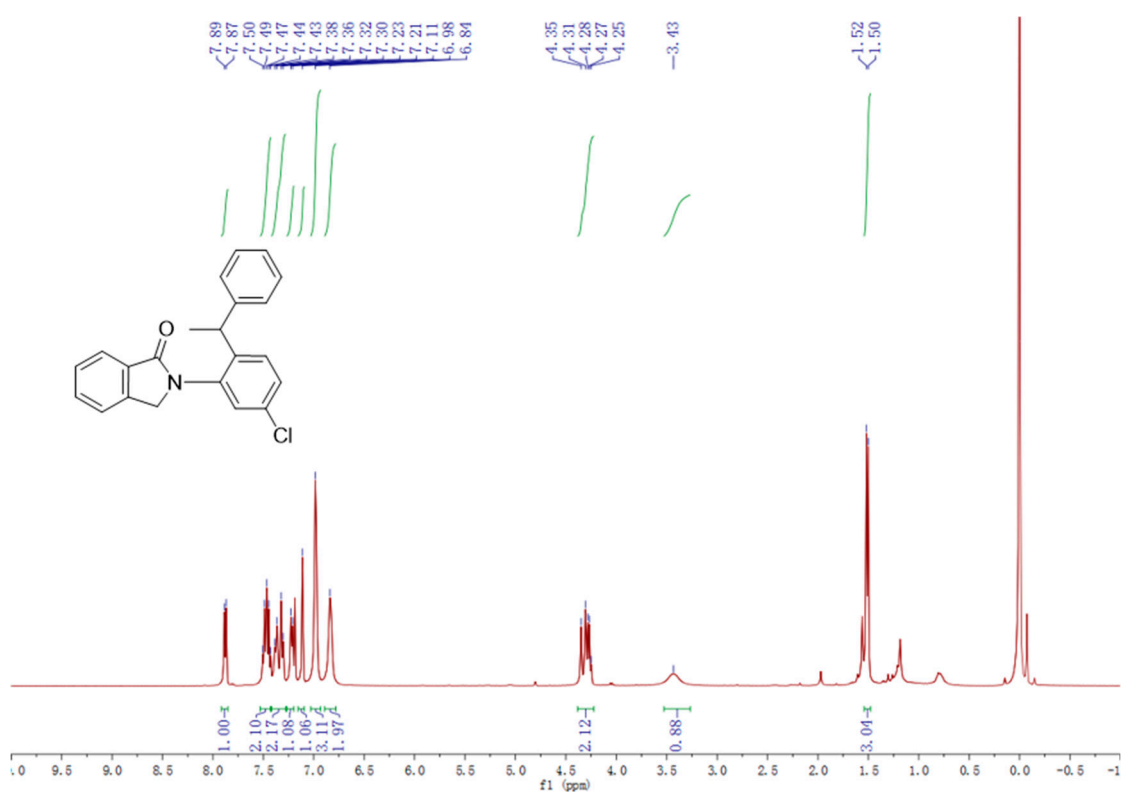


# <sup>13</sup>C NMR Spectrum of Compound **3n**

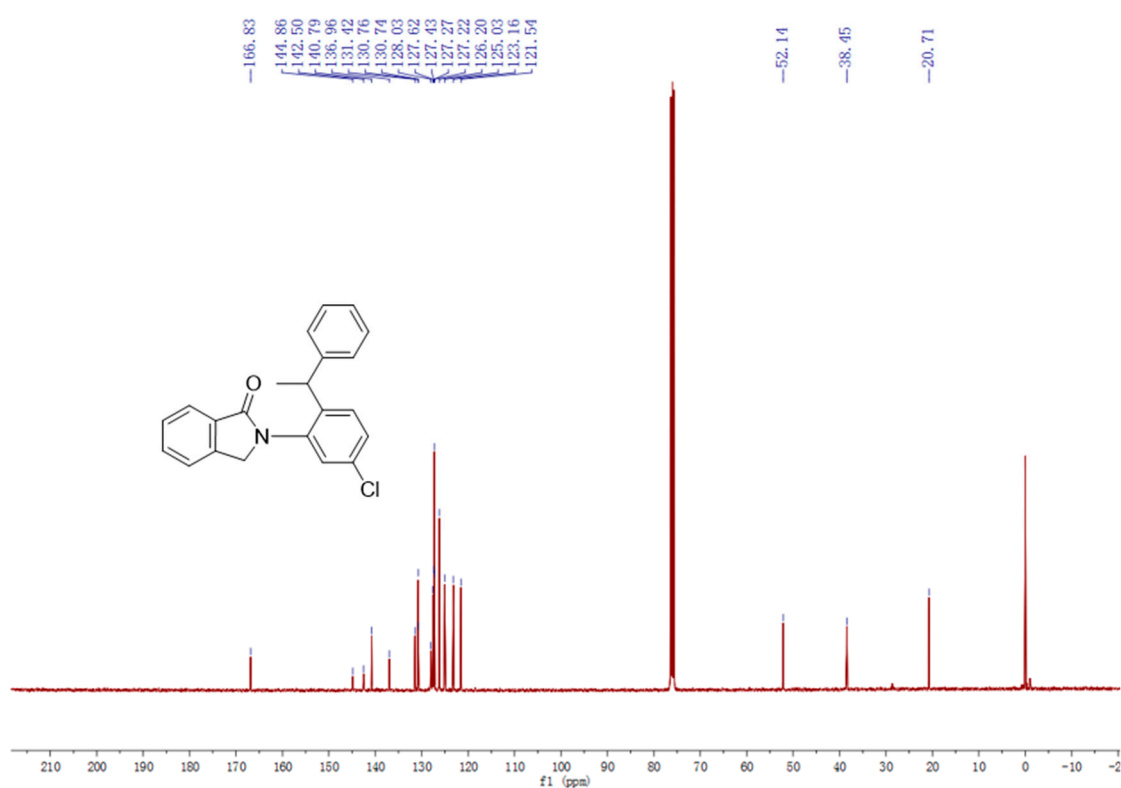




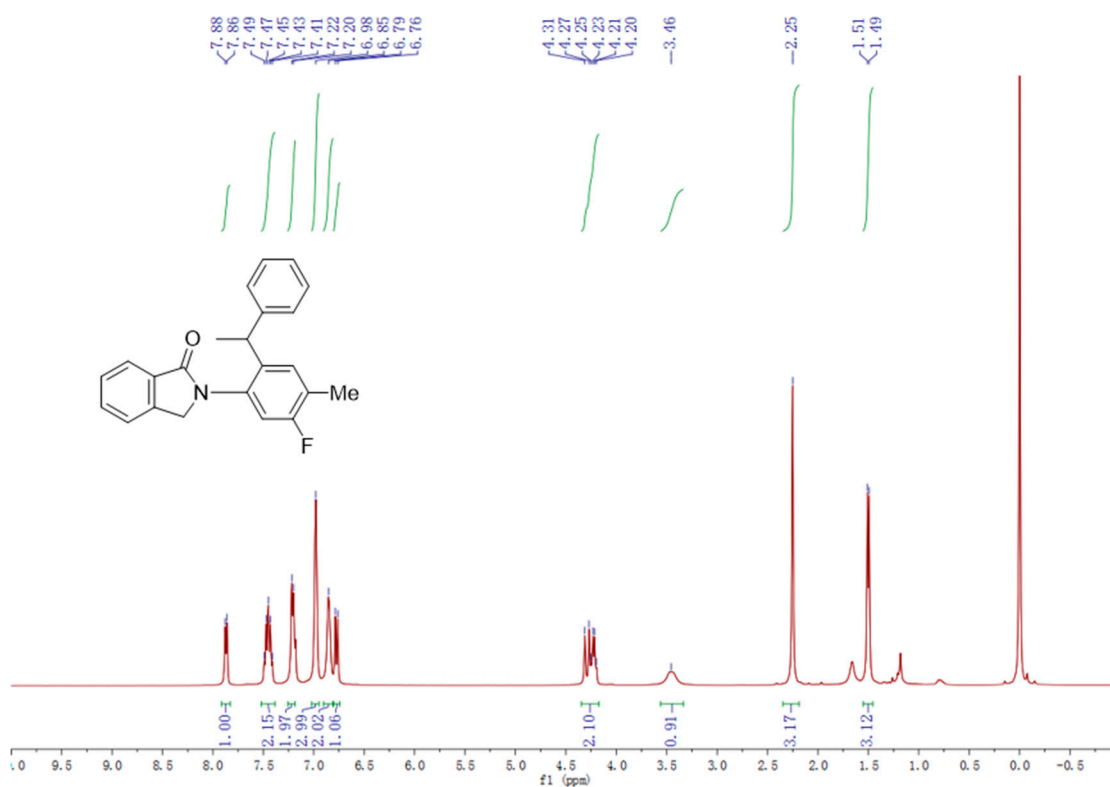
<sup>1</sup>H NMR Spectrum of Compound **3o**



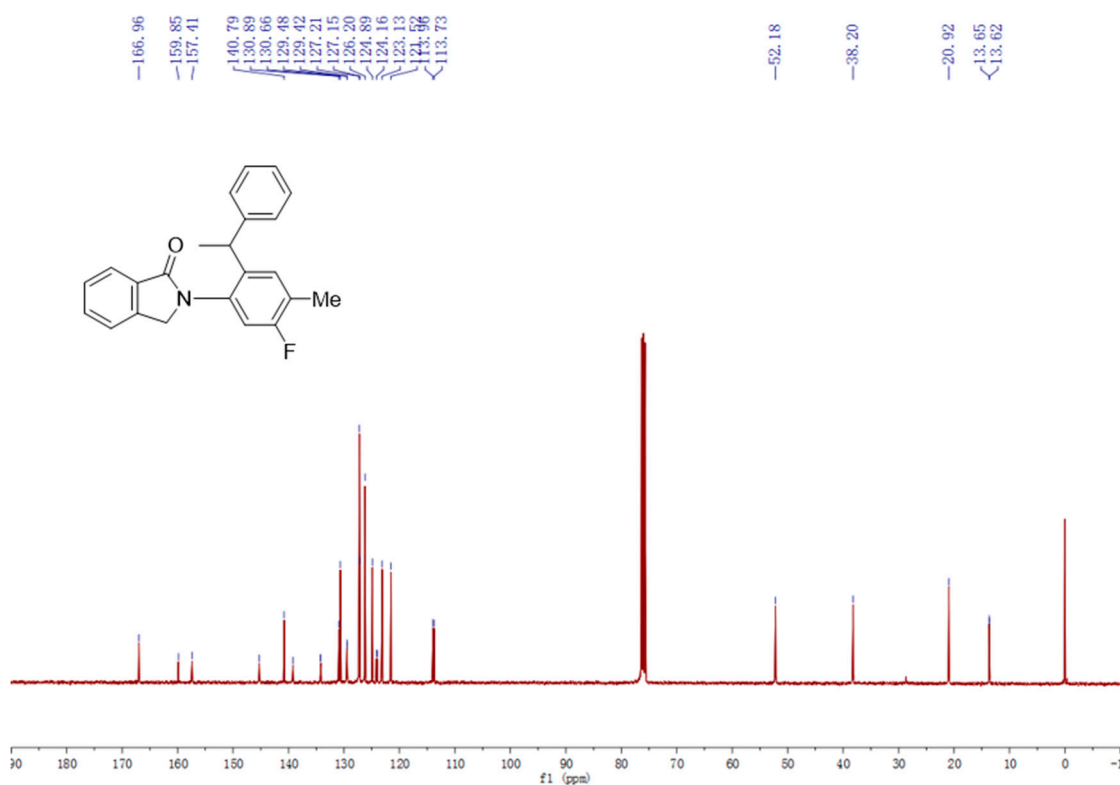
<sup>13</sup>C NMR Spectrum of Compound **3o**



# <sup>1</sup>H NMR Spectrum of Compound **3p**



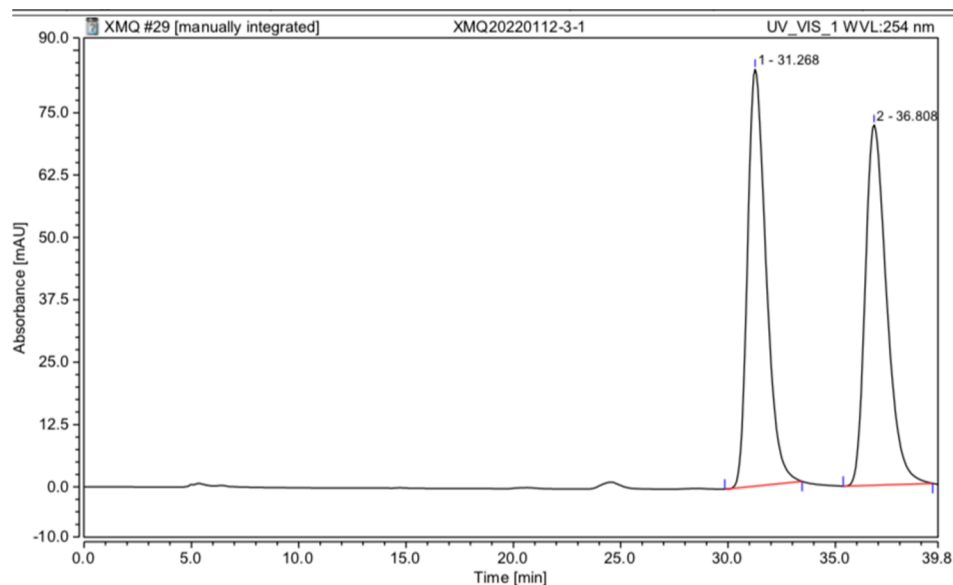
# <sup>13</sup>C NMR Spectrum of Compound **3p**



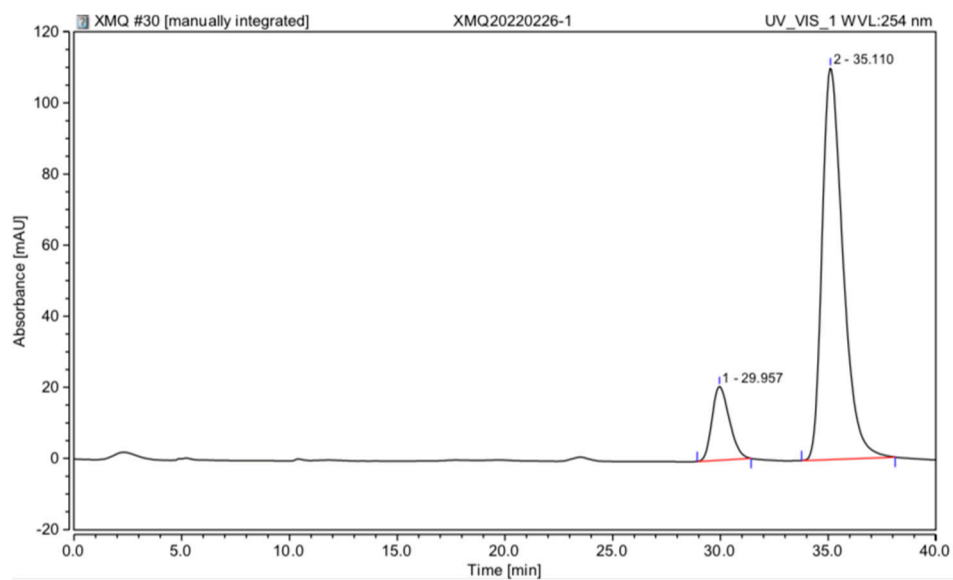
### 3. HPLC Spectra

HPLC spectra for compound *ent*-**3a** ((*R*)-L1)

Chiralcel IC column, *n*-hexane/*i*-PrOH = 100:6, flow rate = 1.0 mL/min,  $\lambda$  = 254 nm,  $t_R$  (major isomer) = 35.110 min,  $t_R$  (minor isomer) = 29.957 min.



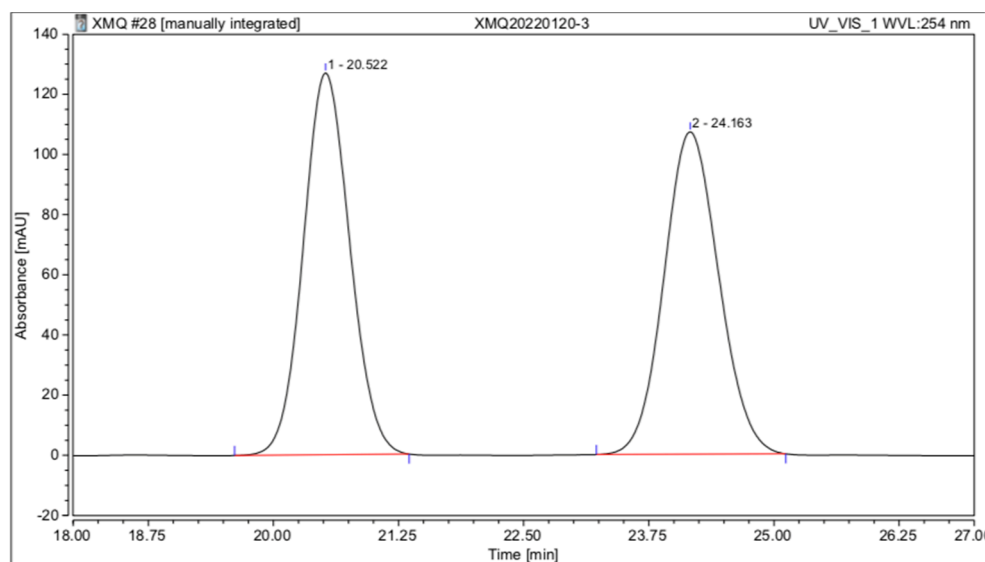
Integration Results						
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Amount n.a.
1		31.268	83.613	83.545	50.09	n.a.
2		36.808	83.321	72.234	49.91	n.a.
Total:			166.934	155.779	100.00	



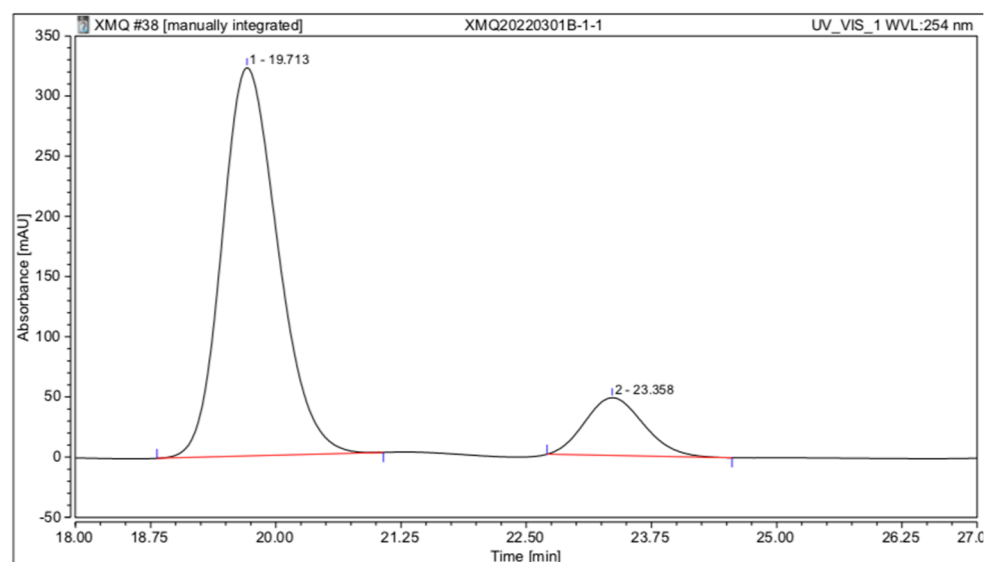
Integration Results						
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Amount n.a.
1		29.957	18.882	20.487	13.26	n.a.
2		35.110	123.481	110.165	86.74	n.a.
Total:			142.363	130.652	100.00	

HPLC spectra for compound *ent*-**3a** ((*S*)-L1)

Chiralcel IC column, *n*-hexane/*i*-PrOH = 100:10, flow rate = 1.0 mL/min,  $\lambda$  = 254 nm,  $t_R$  (major isomer) = 19.713 min,  $t_R$  (minor isomer) = 23.358 min.



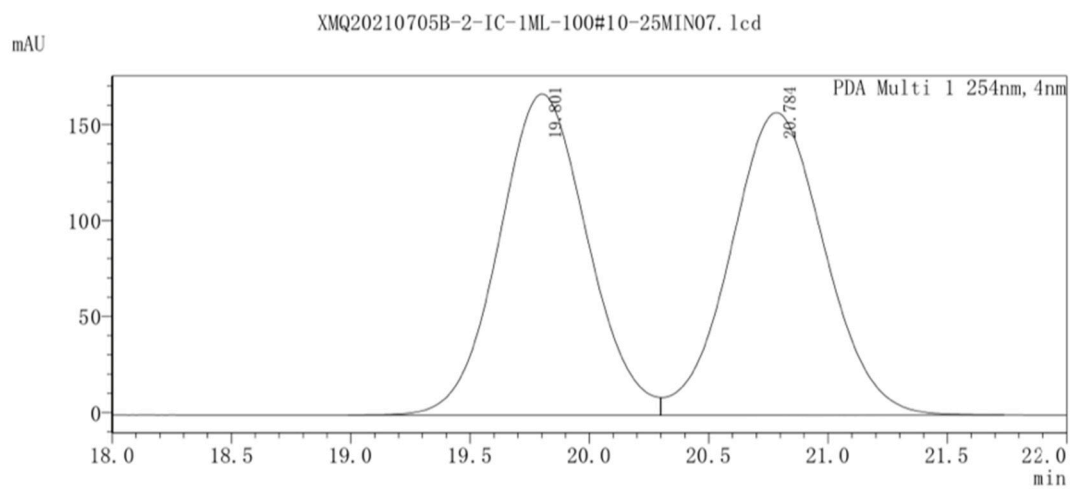
Integration Results						
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Amount n.a.
1		20.522	68.535	126.902	50.16	n.a.
2		24.163	68.106	107.134	49.84	n.a.
<b>Total:</b>			<b>136.641</b>	<b>234.036</b>	<b>100.00</b>	



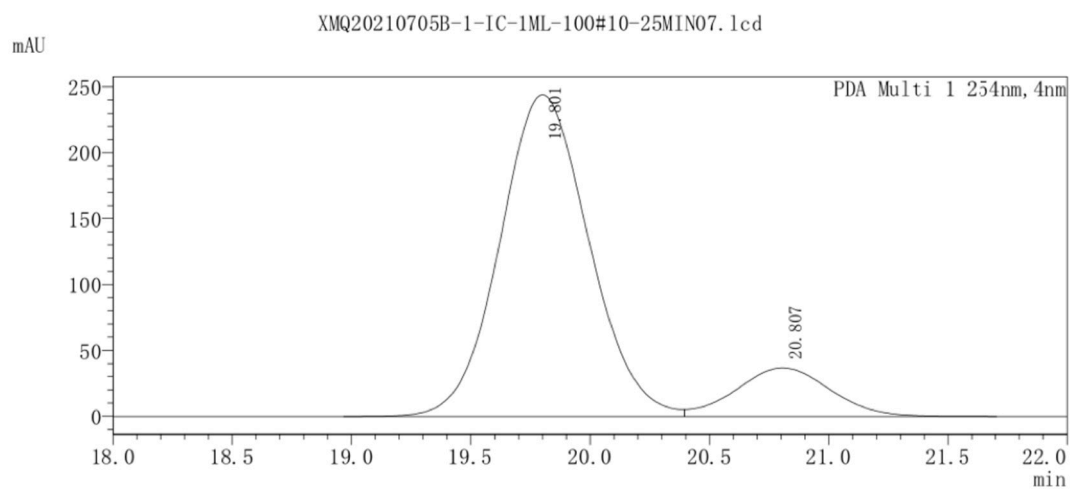
Integration Results						
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Amount n.a.
1		19.713	208.528	322.494	86.45	n.a.
2		23.358	32.687	47.981	13.55	n.a.
<b>Total:</b>			<b>241.214</b>	<b>370.475</b>	<b>100.00</b>	

HPLC spectra for compound *ent*-**3c** ((*R*)-L1)

Chiralcel IC column, *n*-hexane/*i*-PrOH = 100:10, flow rate = 1.0 mL/min,  $\lambda$  = 254 nm,  
 $t_R$  (major isomer) = 19.801 min,  $t_R$  (minor isomer) = 20.807 min.



Peak No	Retention time	Area	Area%	Height
1	19.801	4310259	49.987	167211
2	20.784	4312423	50.013	157449
Total		8622682	100.00	324660



Peak No	Retention time	Area	Area%	Height
1	19.801	6329235	86.258	244163
2	20.807	1008338	13.742	36855
Total		7337572	100.00	281018