

## *Supporting Information*

### **A chemo- and regioselective C6-functionalization of 2,3-disubstituted indoles: highly efficient synthesis of diarylindol-6-ylmethanes**

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and Yan Chen\*

*School of Chemistry and Chemical Engineering, Xuzhou University of Technology, Xuzhou*

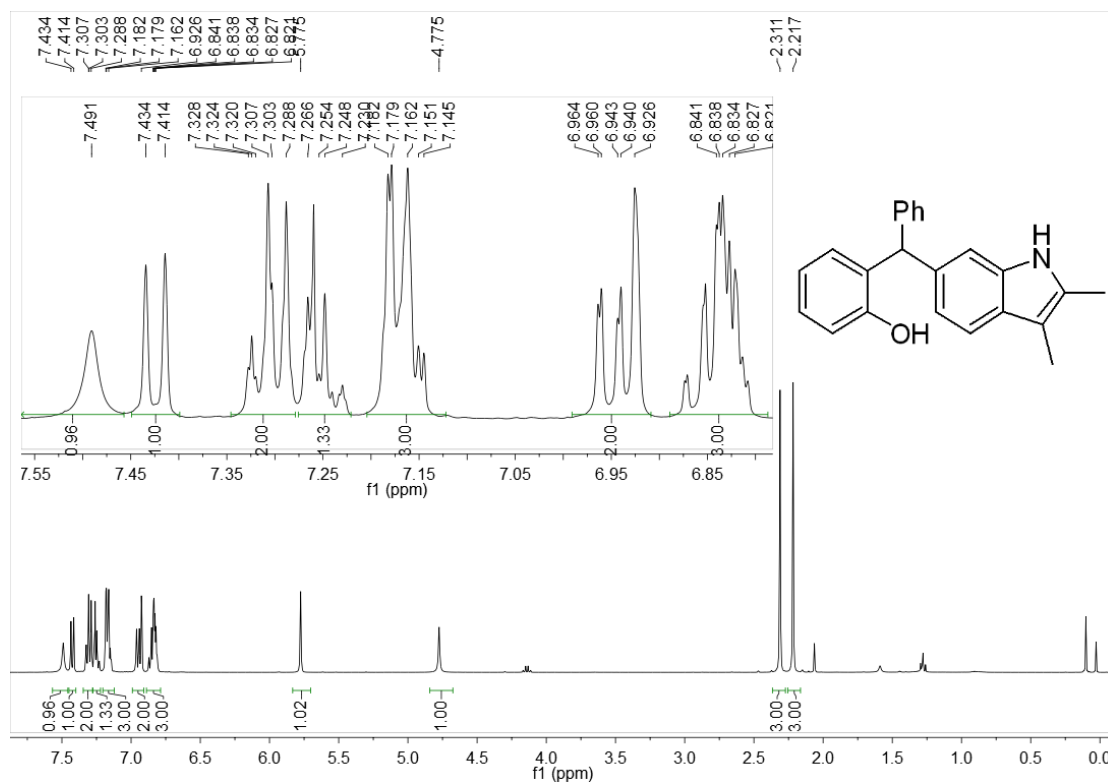
*221018, China. E-mail: [hgwuqiong@xzit.edu.cn](mailto:hgwuqiong@xzit.edu.cn).*

#### **Contents:**

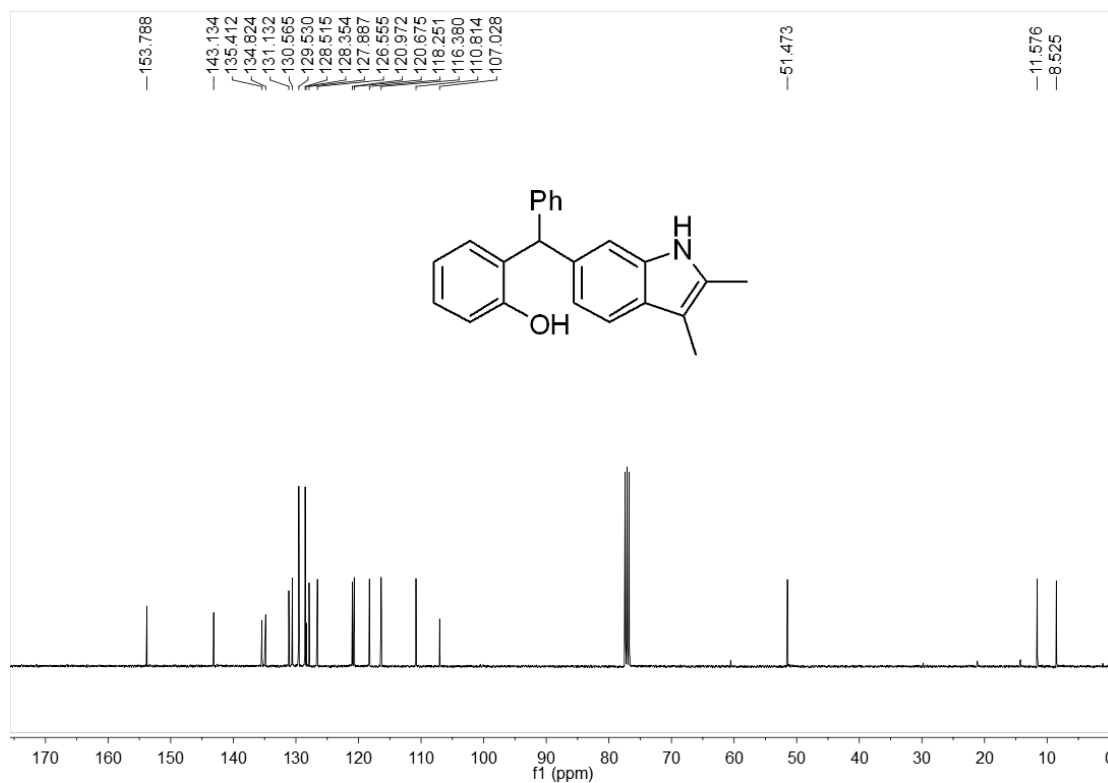
- 1. NMR spectra of products 3 (S2-S23)**
- 2. HPLC spectra of product 3aa (S24)**
- 3. X-ray single crystal data for compound 3ae (S25-S26)**

# 1.NMR spectra of products 3

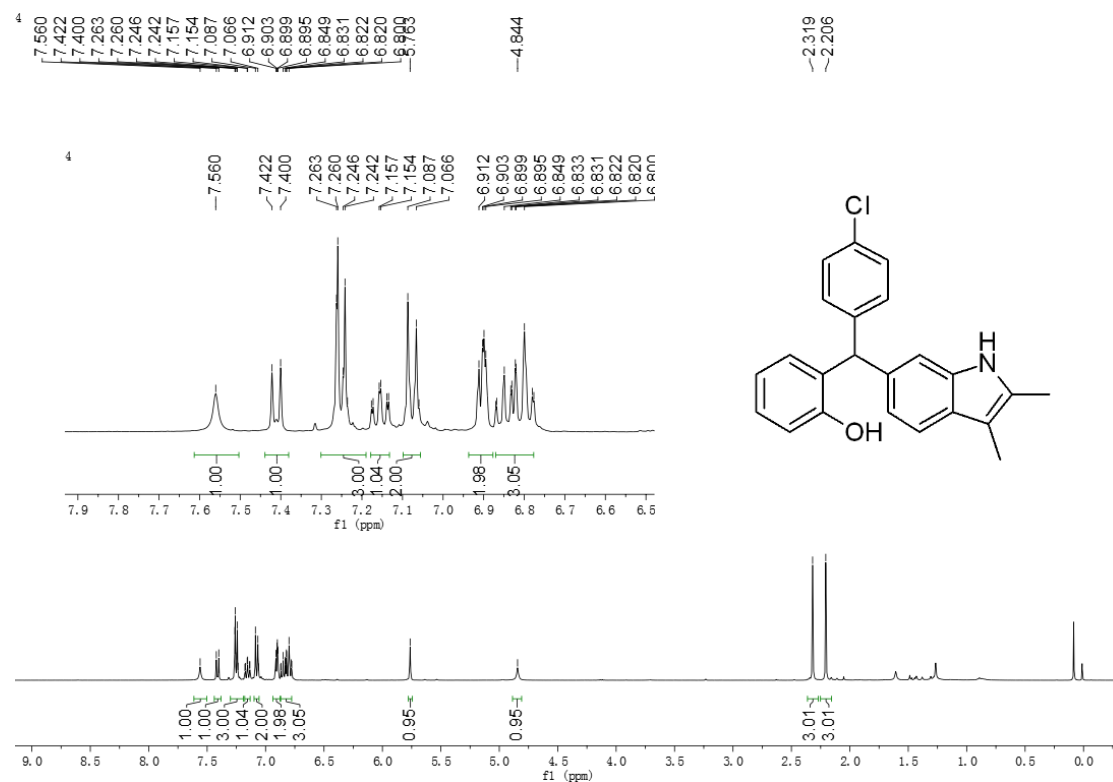
## <sup>1</sup>H NMR of compound 3aa



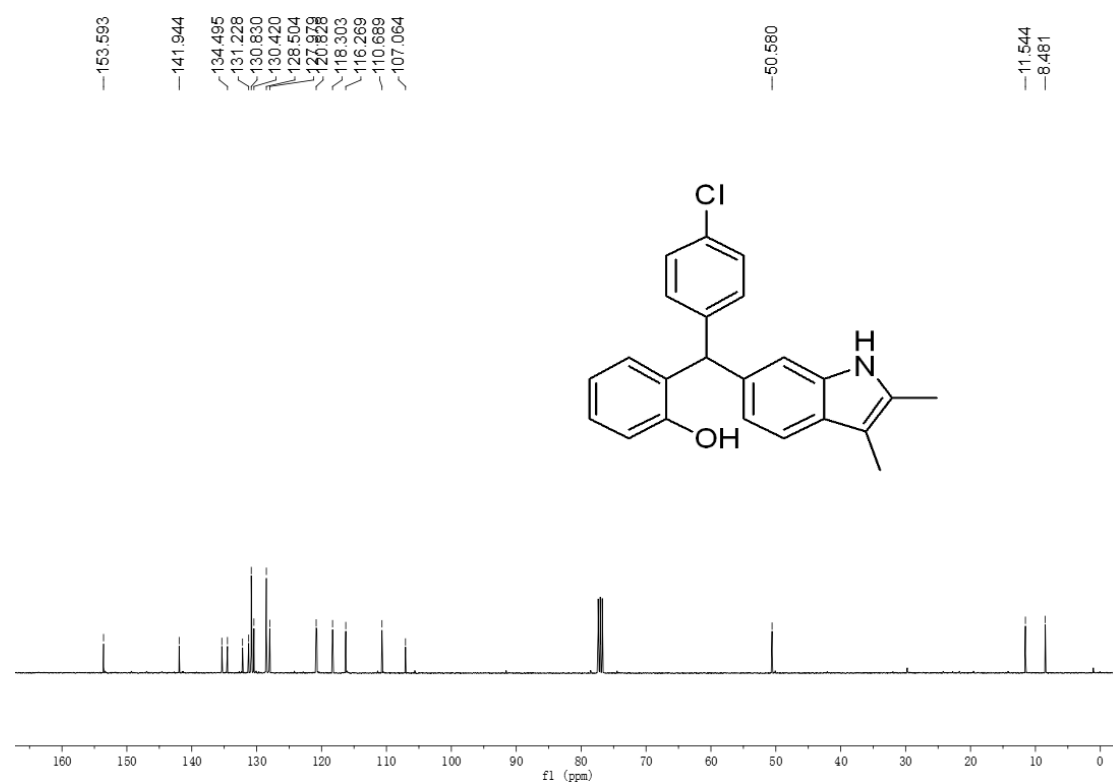
## <sup>13</sup>C NMR of compound 3aa



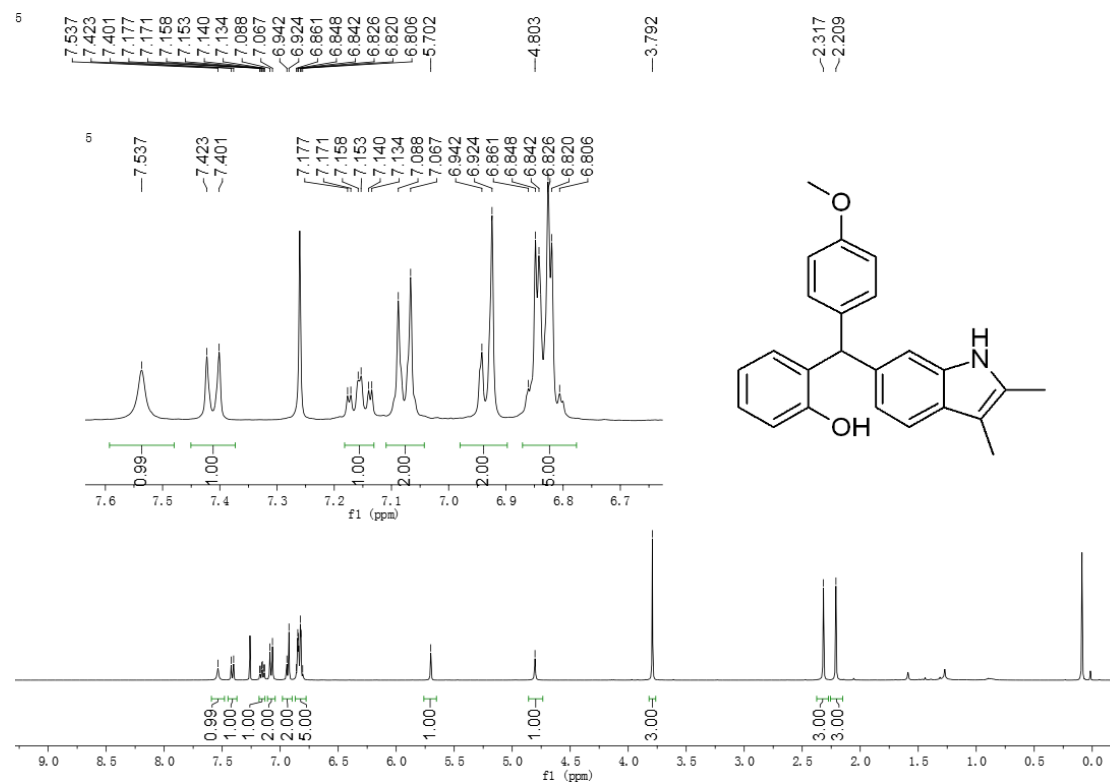
### $^1\text{H}$ NMR of compound **3ba**



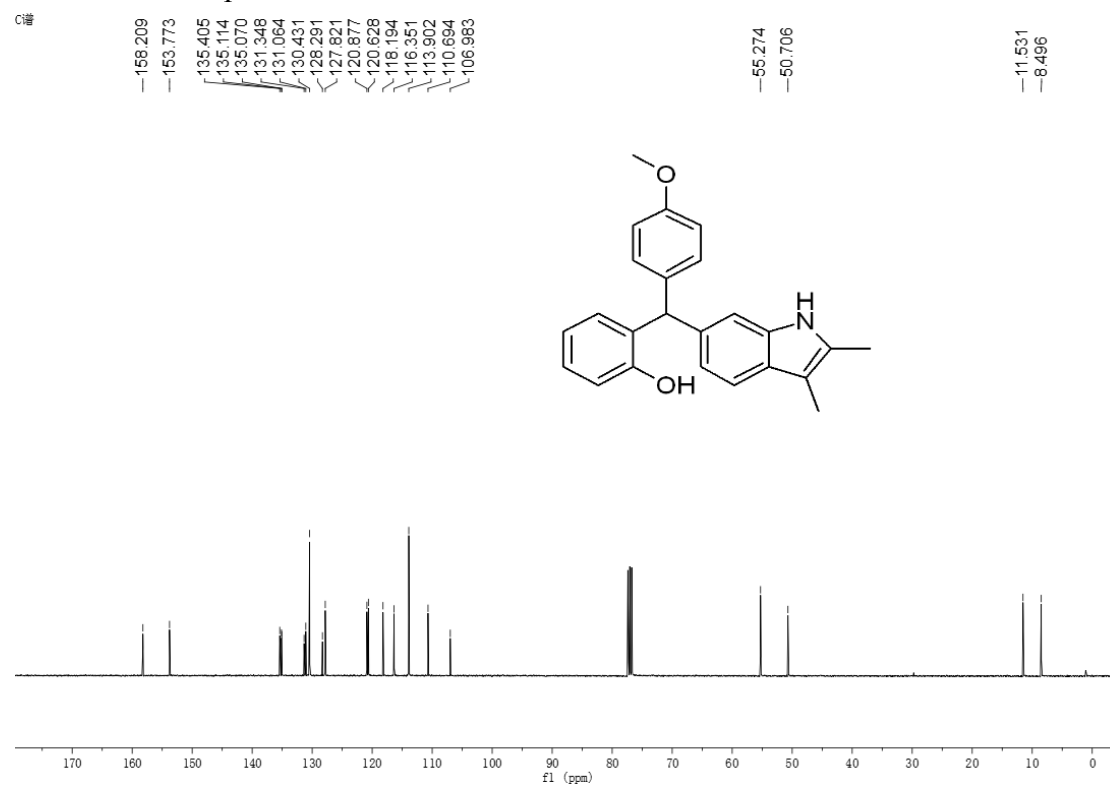
### $^{13}\text{C}$ NMR of compound **3ba**



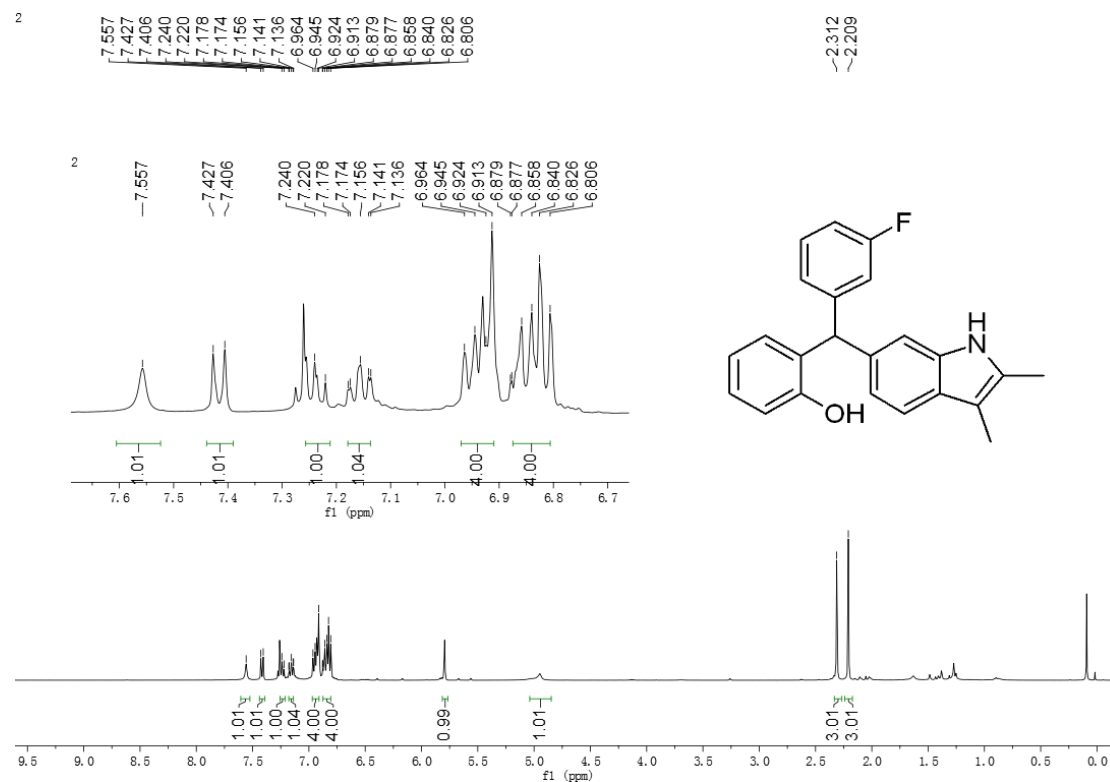
### <sup>1</sup>H NMR of compound 3ca



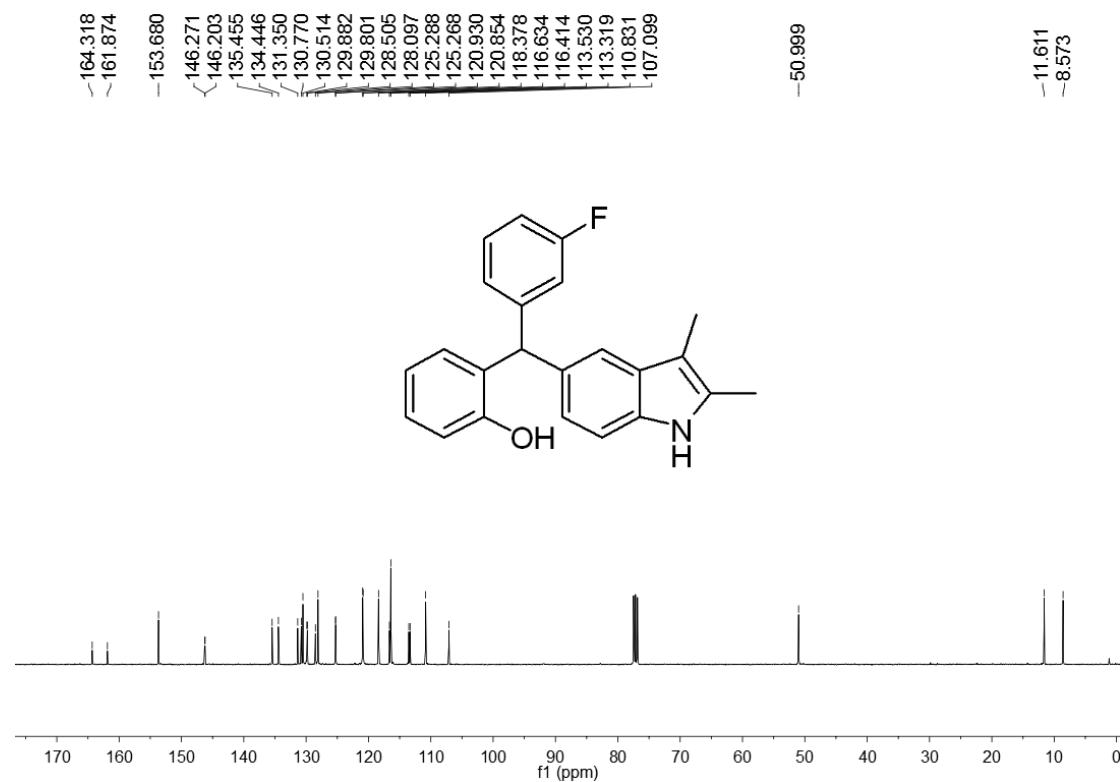
### <sup>13</sup>C NMR of compound 3ca



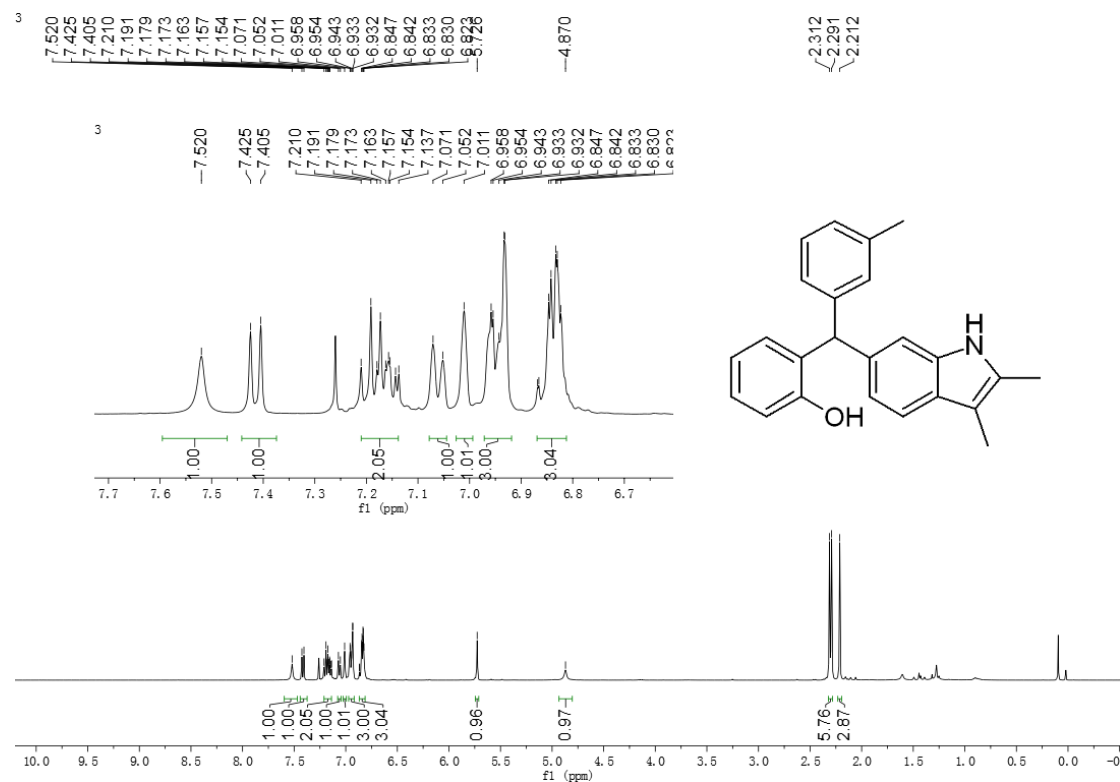
### <sup>1</sup>H NMR of compound 3da



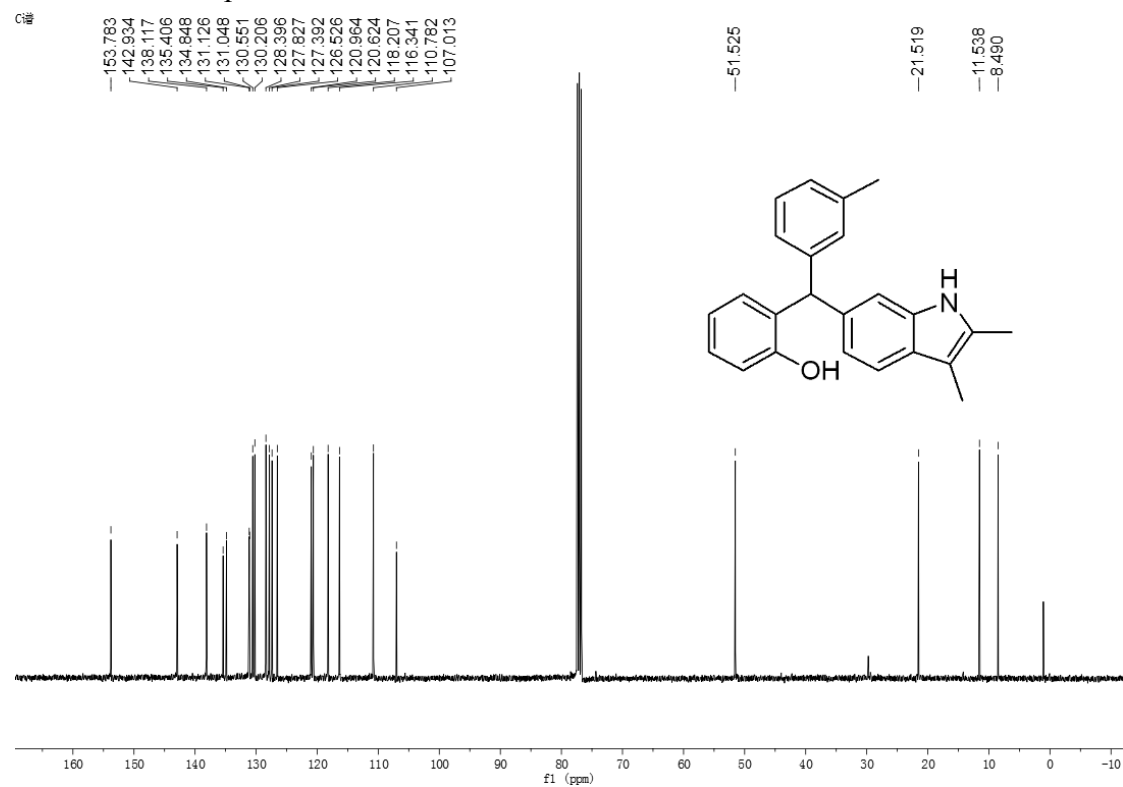
### <sup>13</sup>C NMR of compound 3da



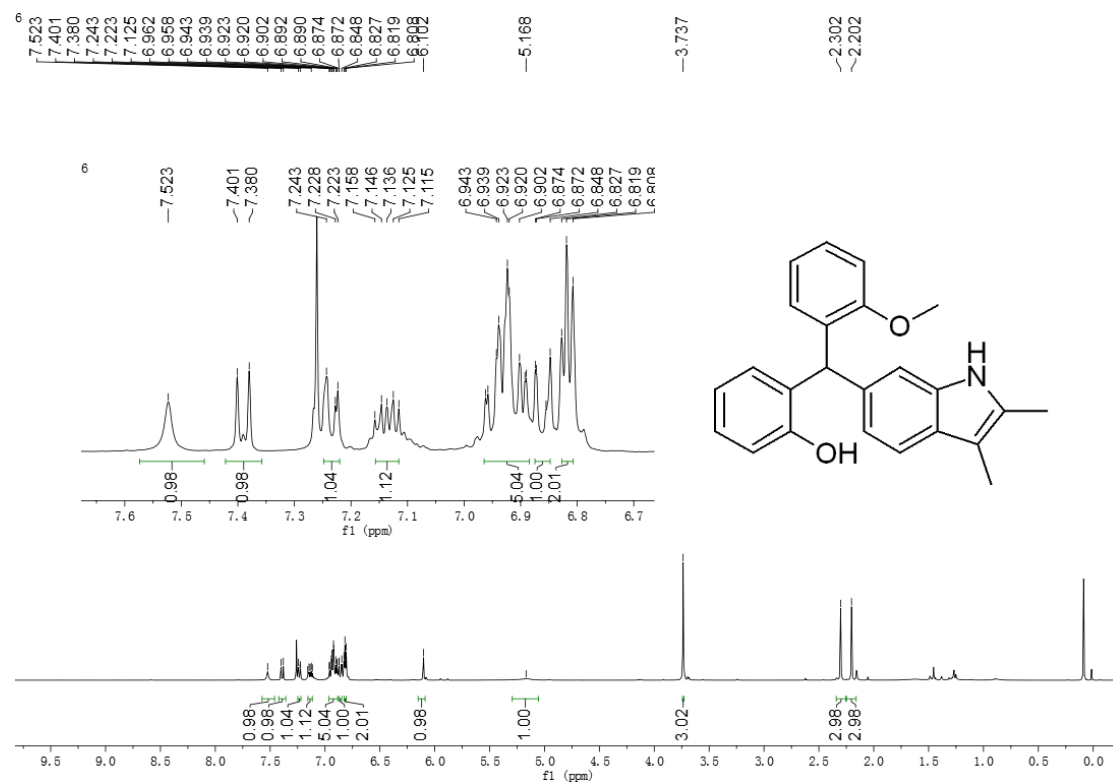
### <sup>1</sup>H NMR of compound 3ea



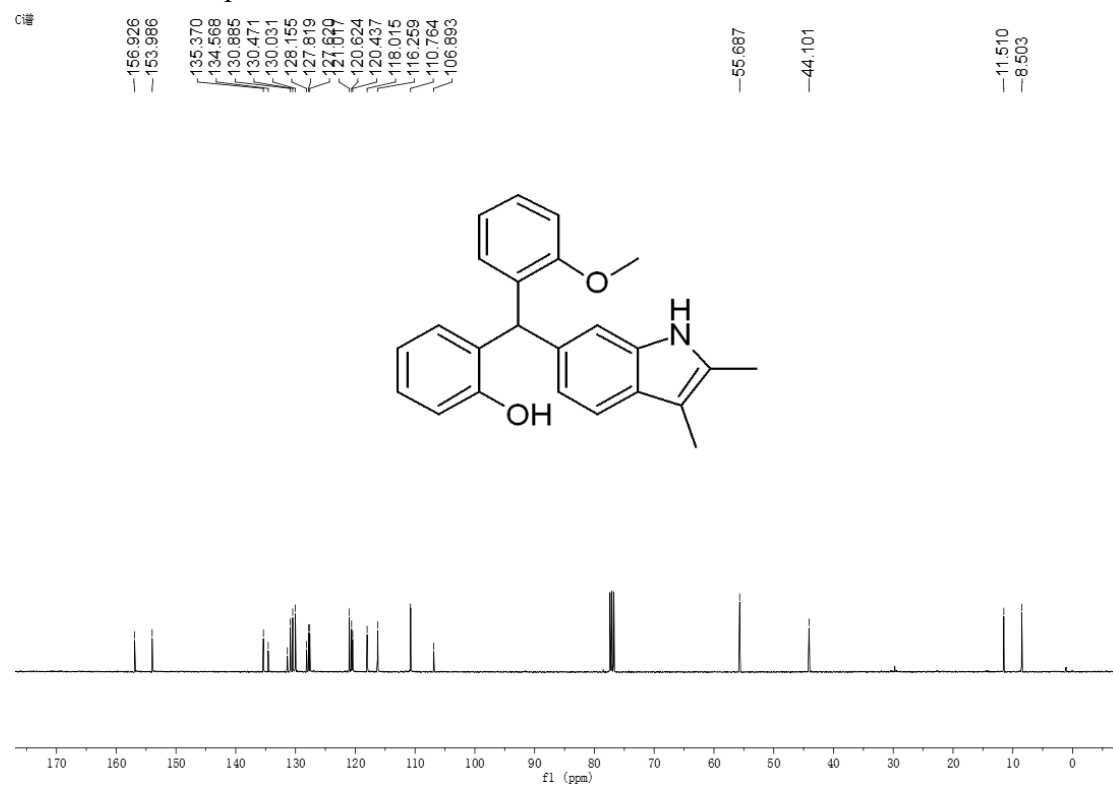
### <sup>13</sup>C NMR of compound 3ea



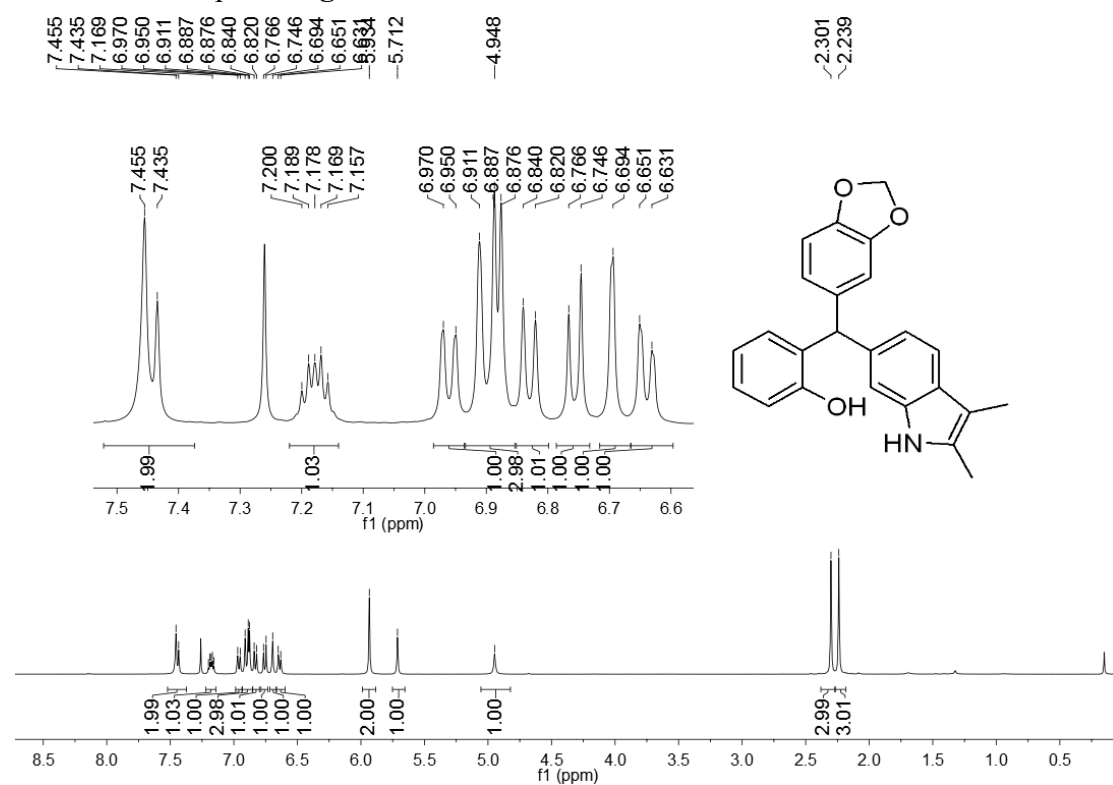
<sup>1</sup>H NMR of compound **3fa**



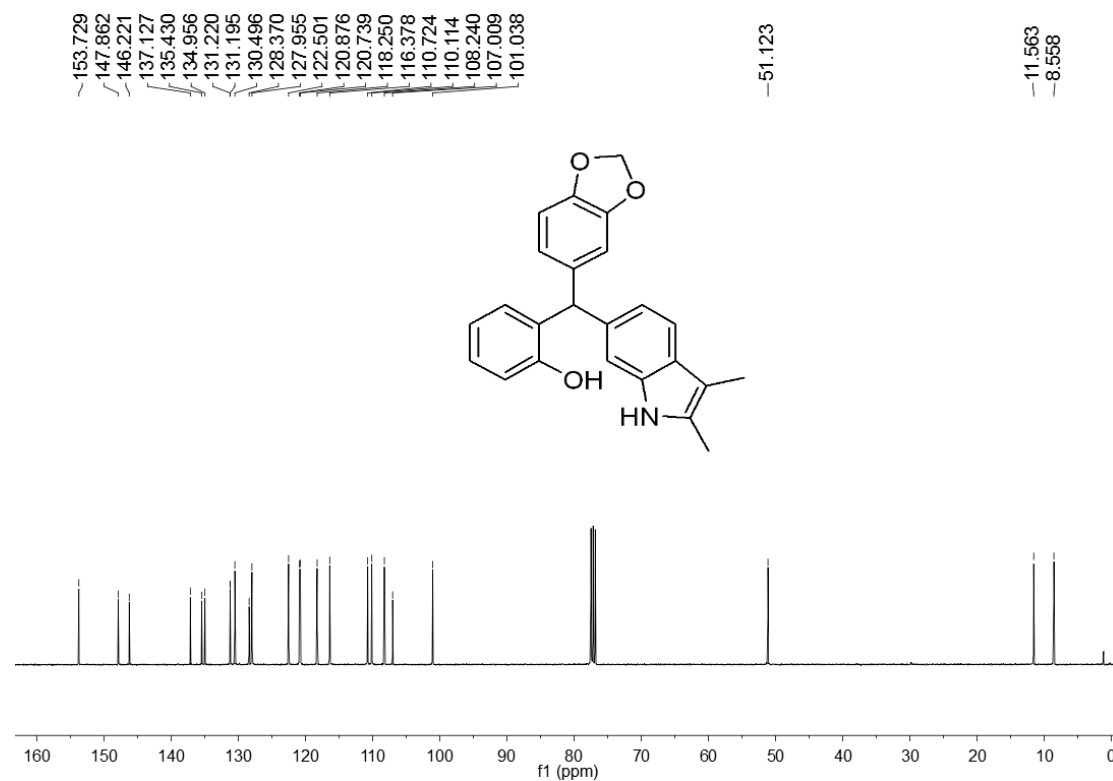
<sup>13</sup>C NMR of compound **3fa**



<sup>1</sup>H NMR of compound **3ga**

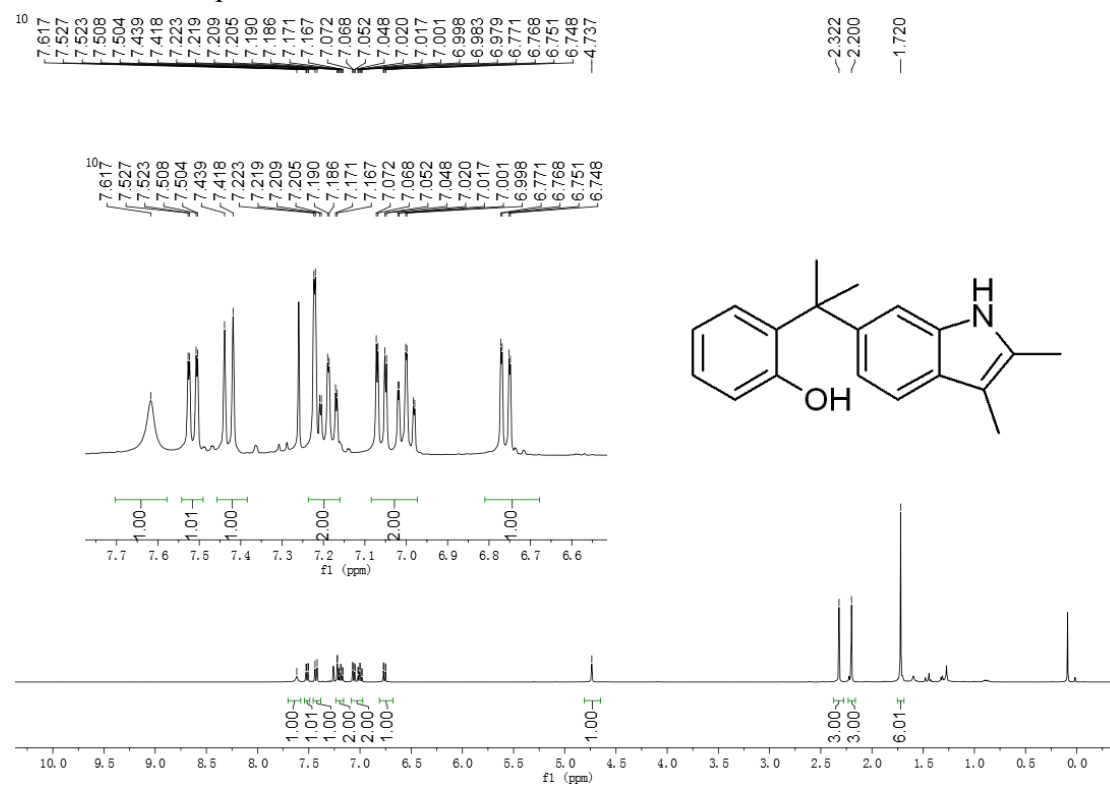


<sup>13</sup>C NMR of compound **3ga**

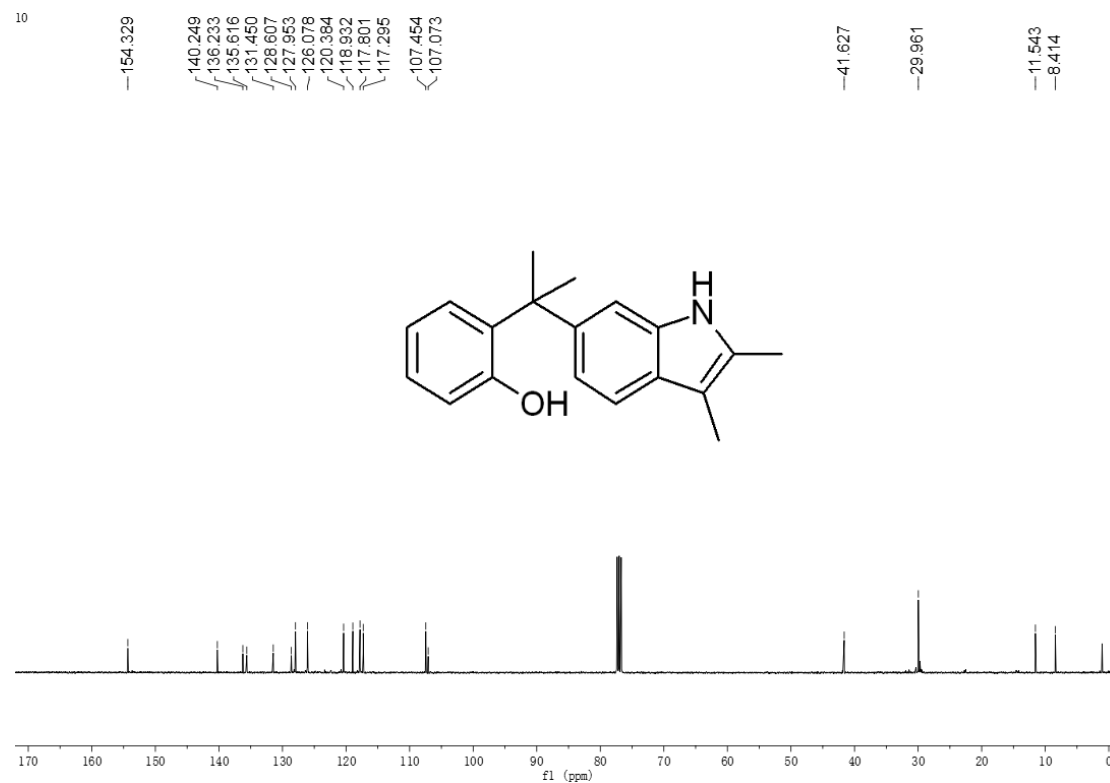




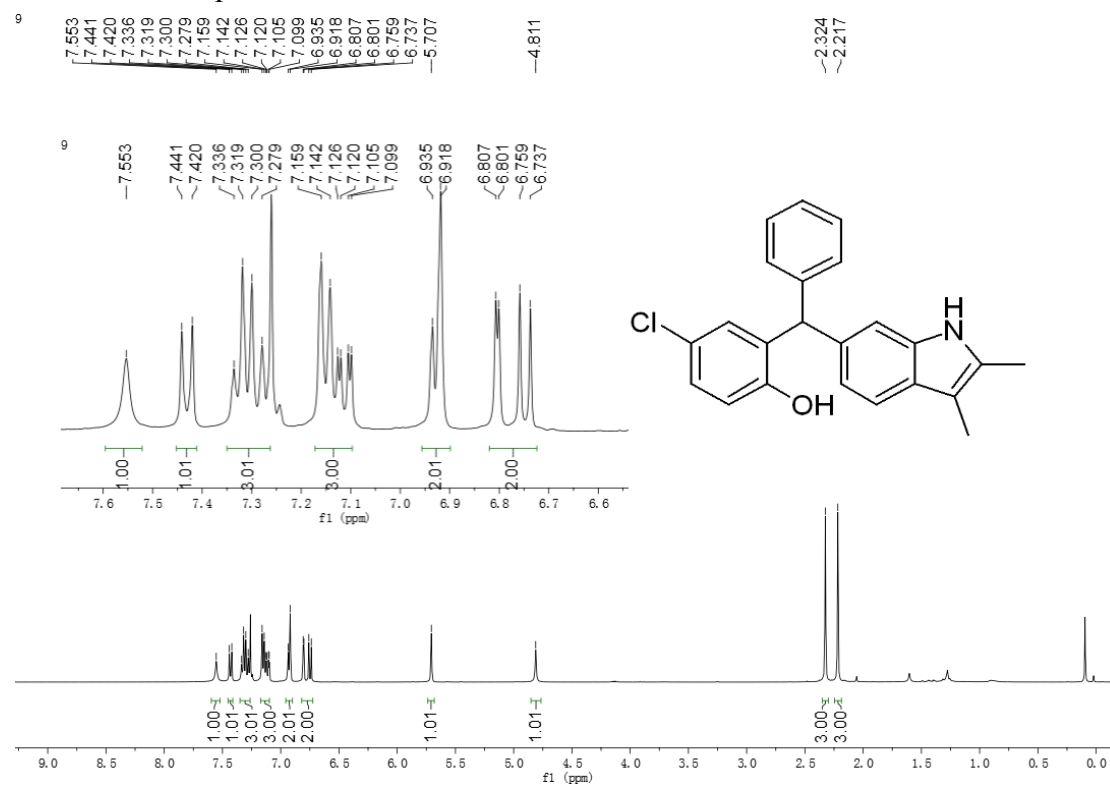
<sup>1</sup>H NMR of compound **3ha**



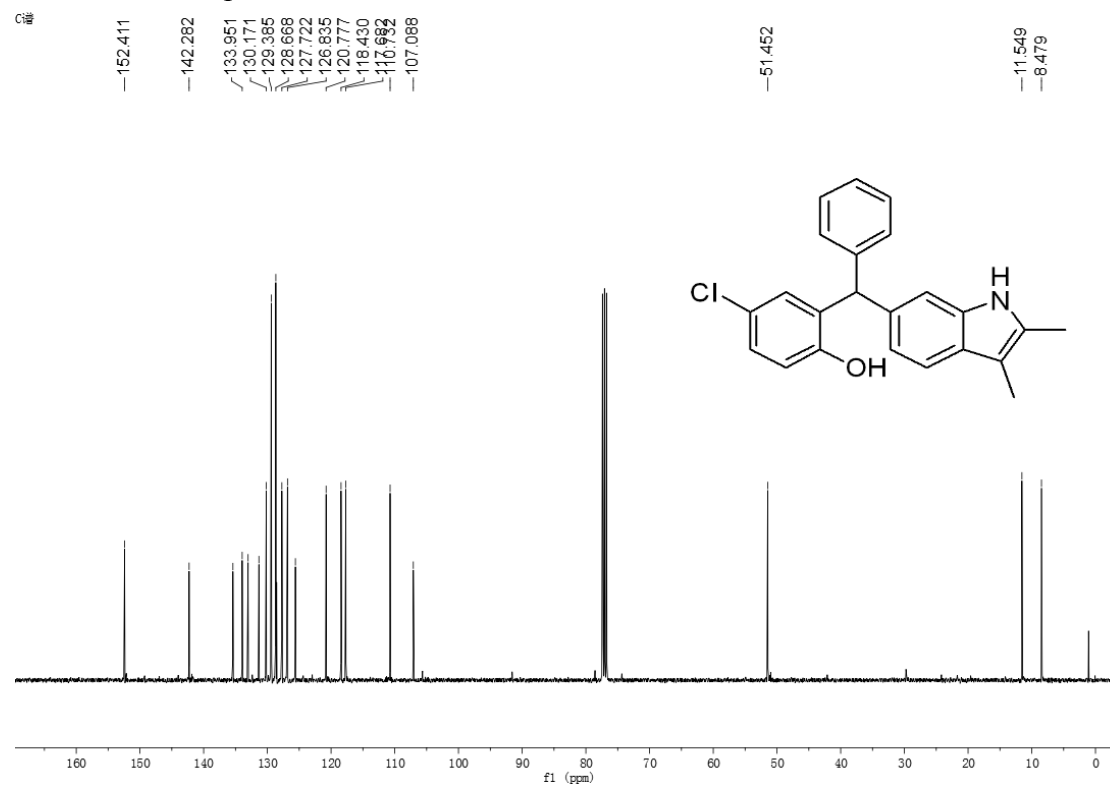
<sup>13</sup>C NMR of compound **3ha**



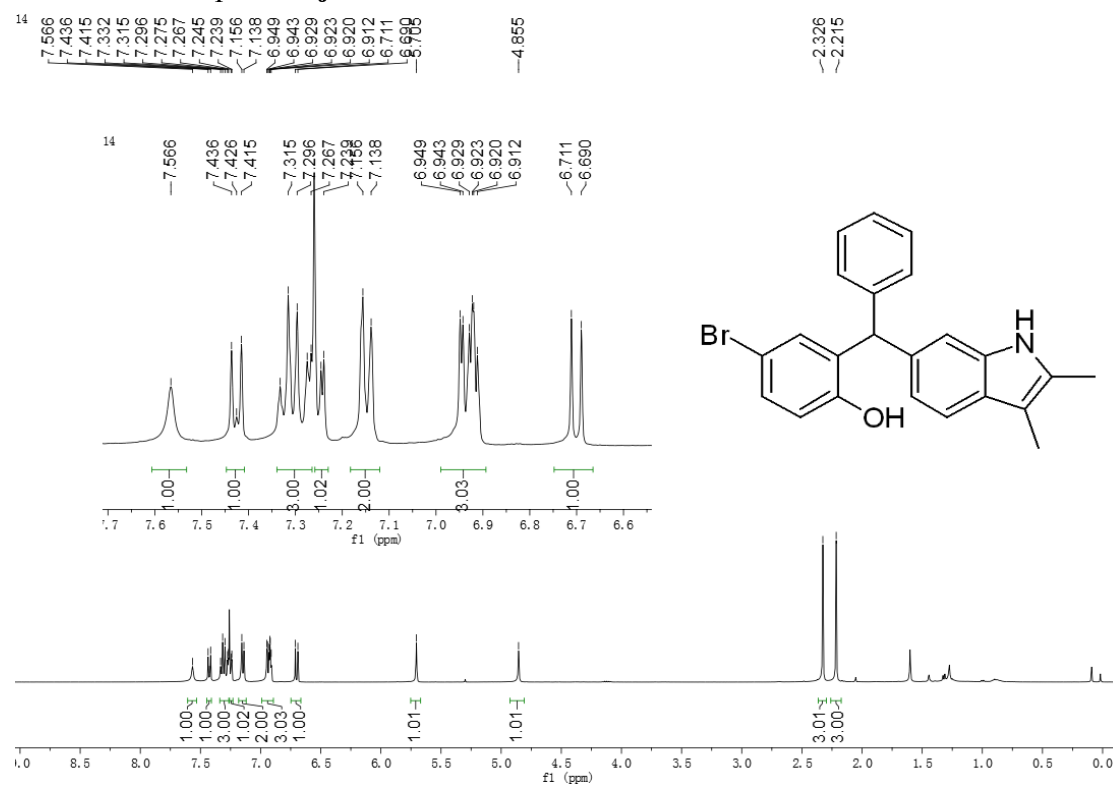
### <sup>1</sup>H NMR of compound **3ia**



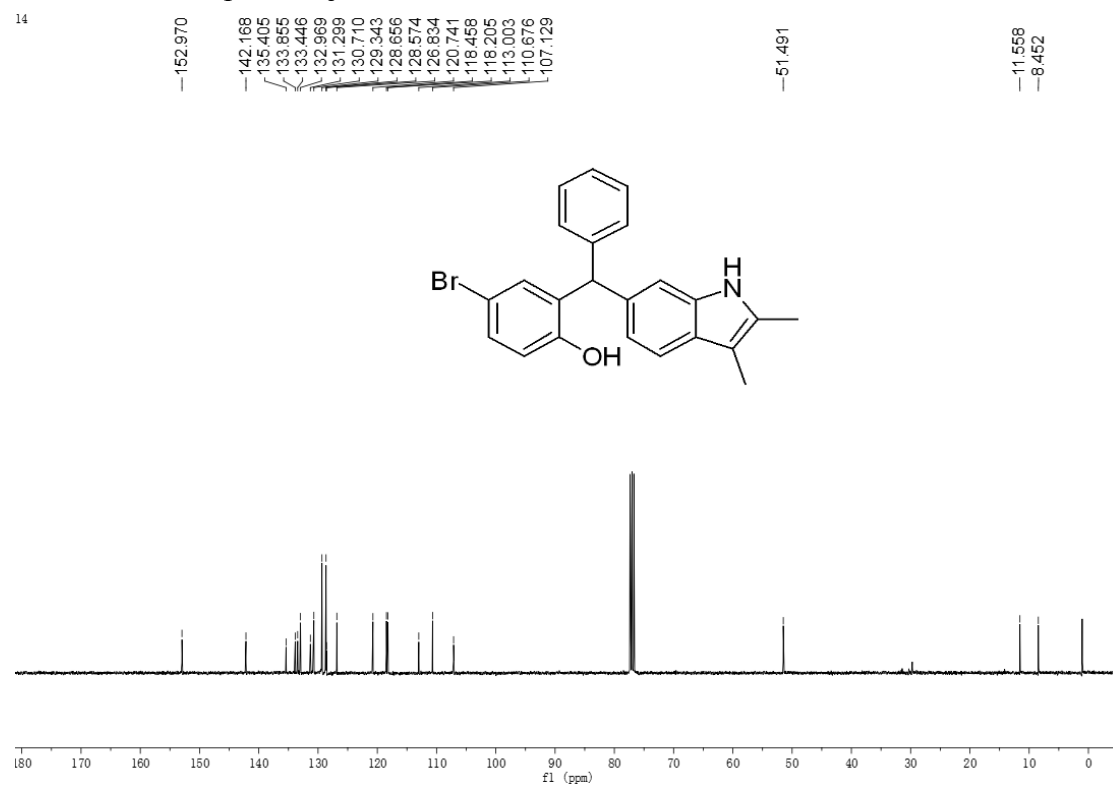
### <sup>13</sup>C NMR of compound **3ia**



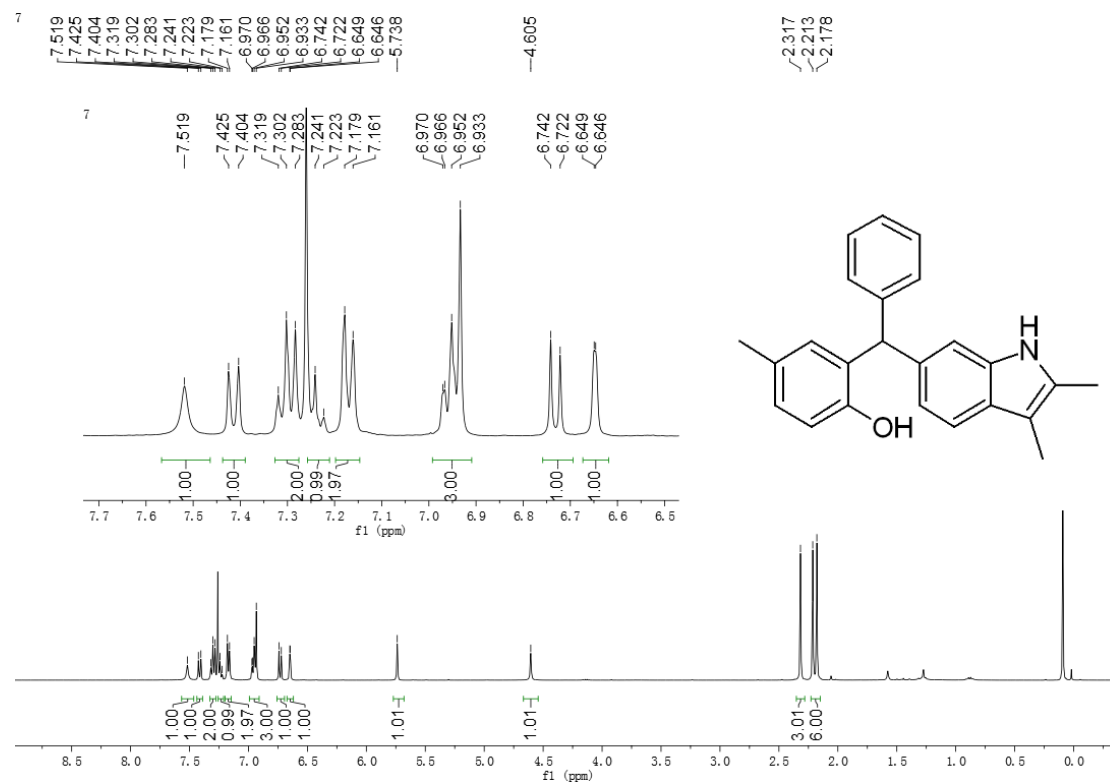
<sup>1</sup>H NMR of compound **3ja**



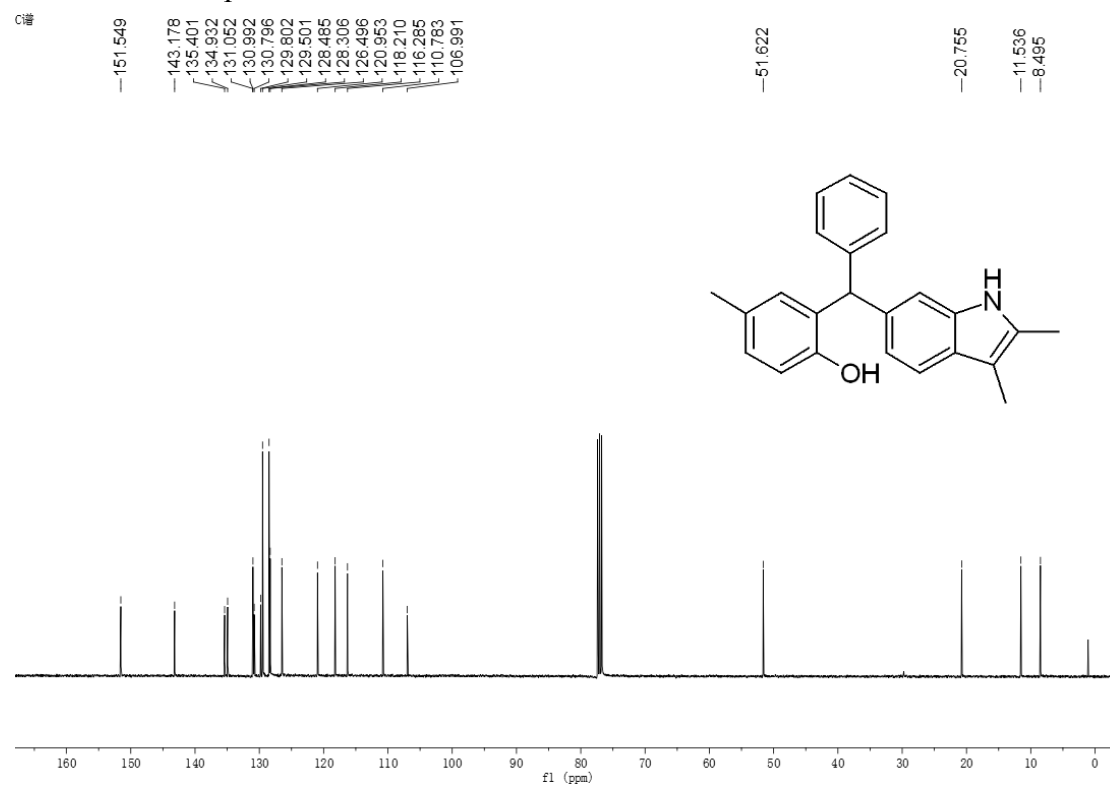
<sup>13</sup>C NMR of compound **3ja**



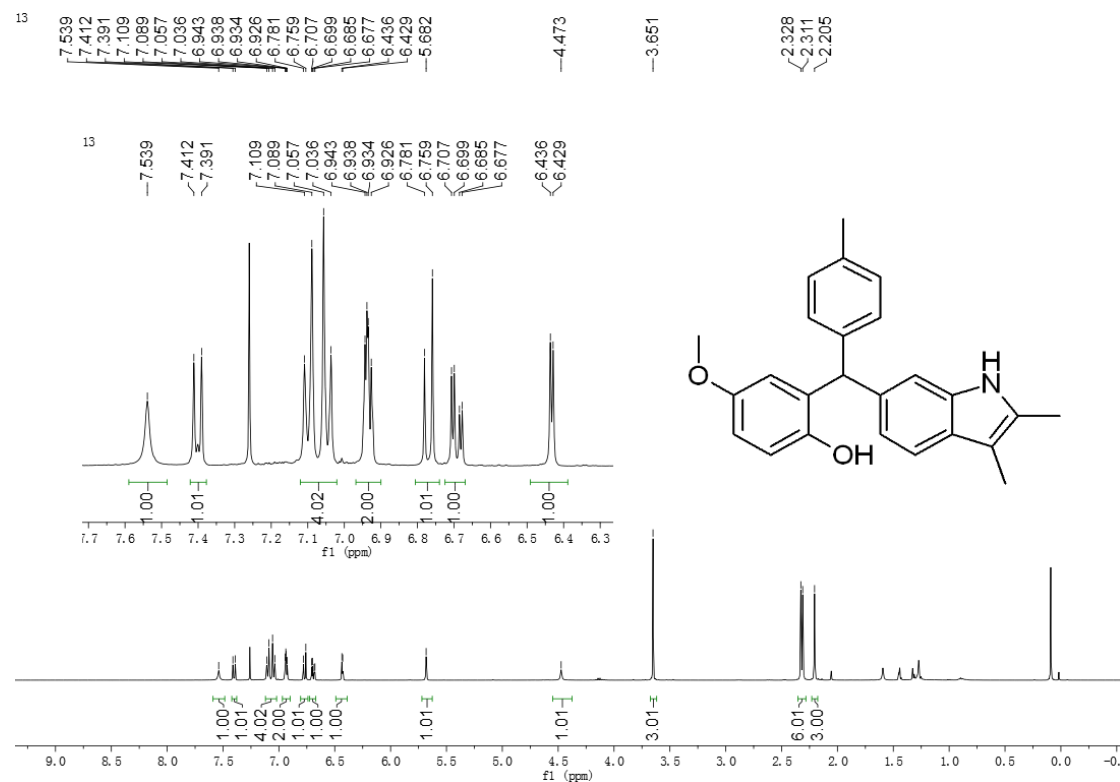
### <sup>1</sup>H NMR of compound **3ka**



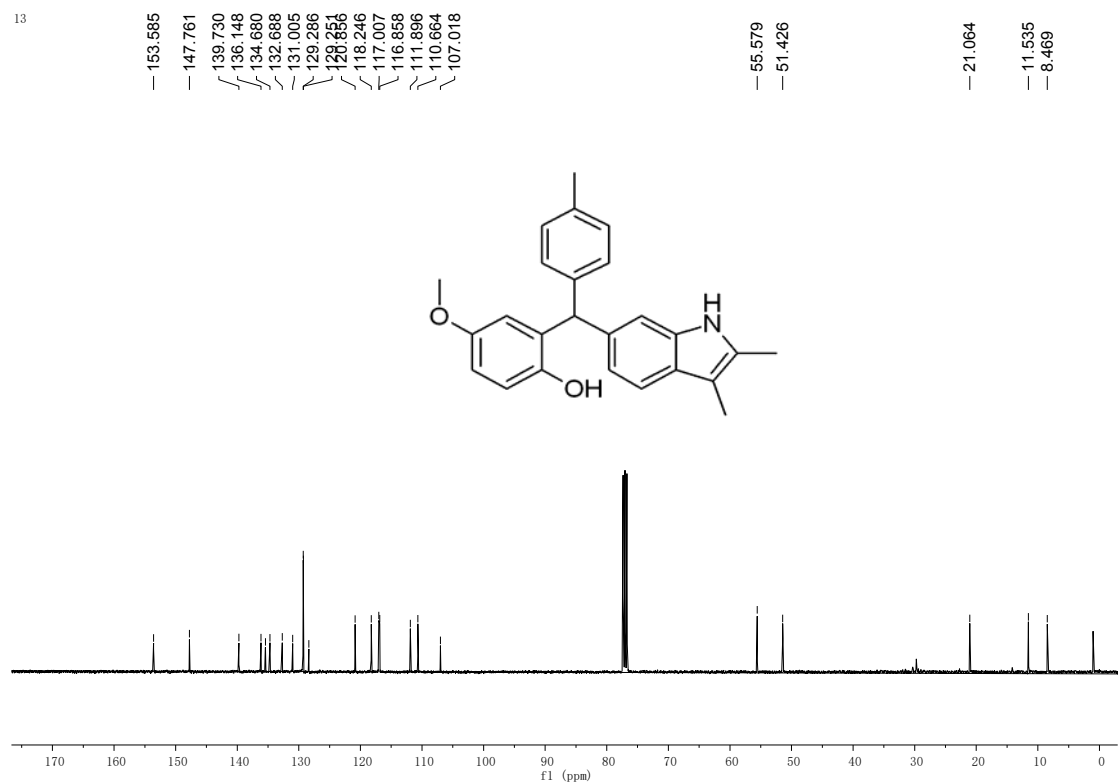
### <sup>13</sup>C NMR of compound **3ka**



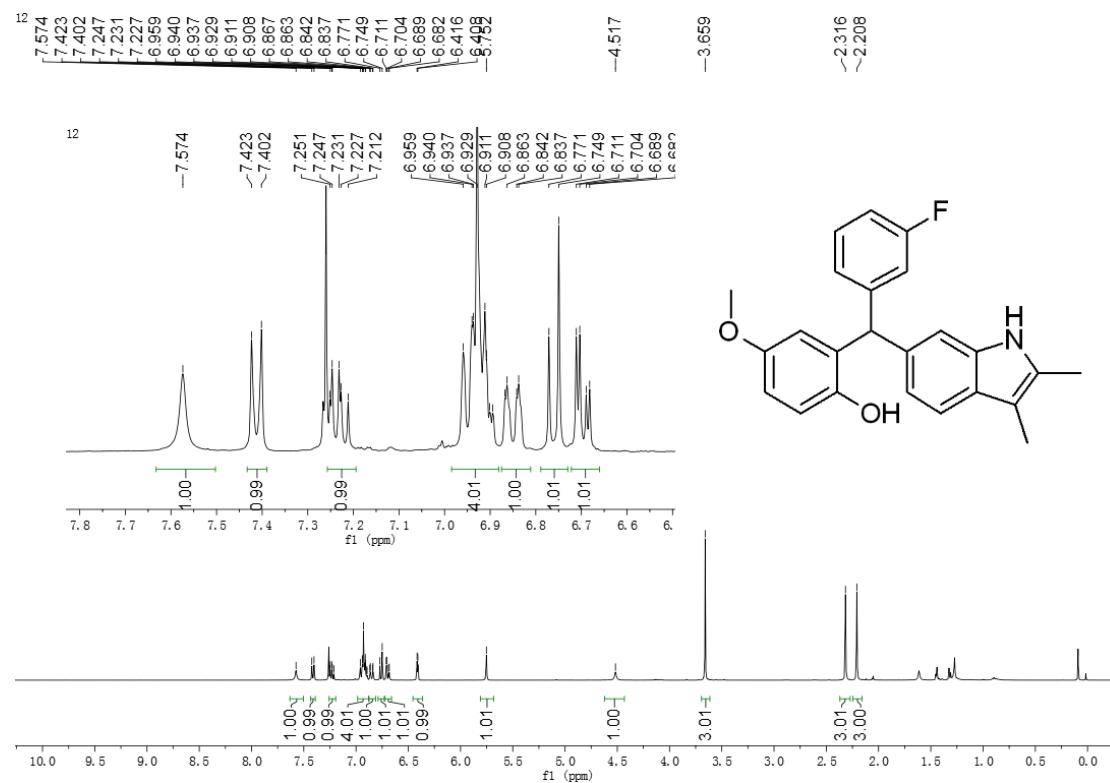
### <sup>1</sup>H NMR of compound **3la**



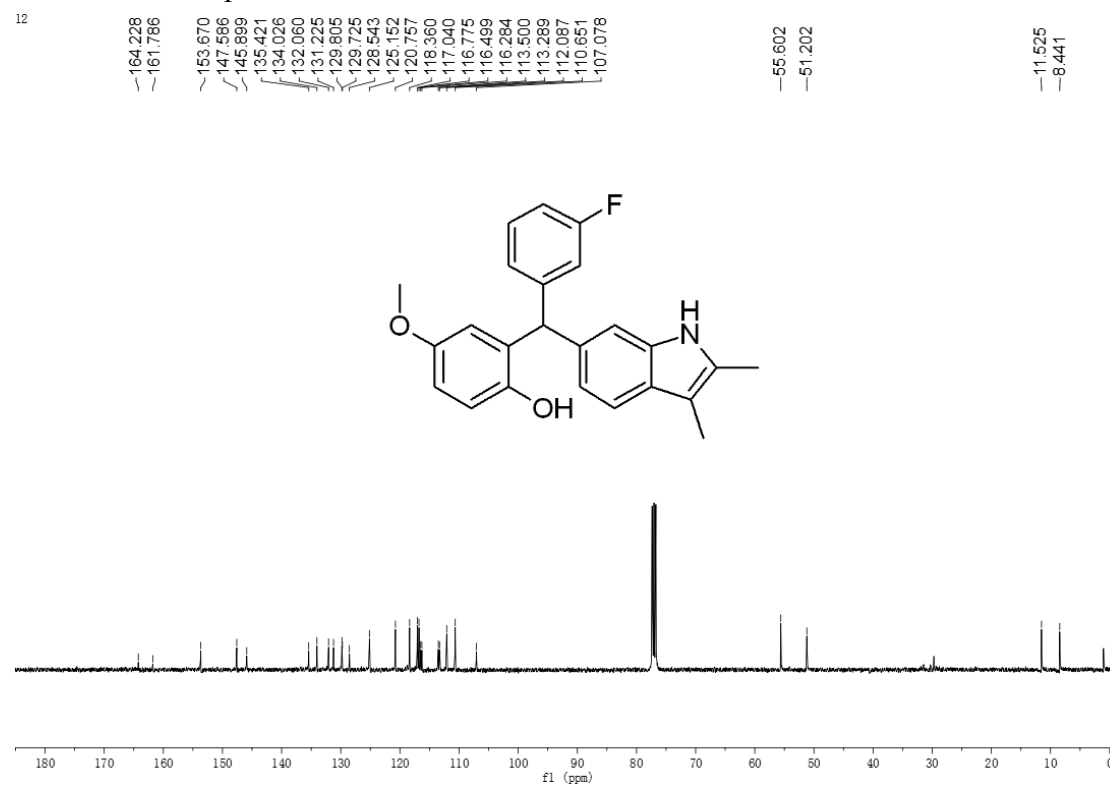
### <sup>13</sup>C NMR of compound **3la**



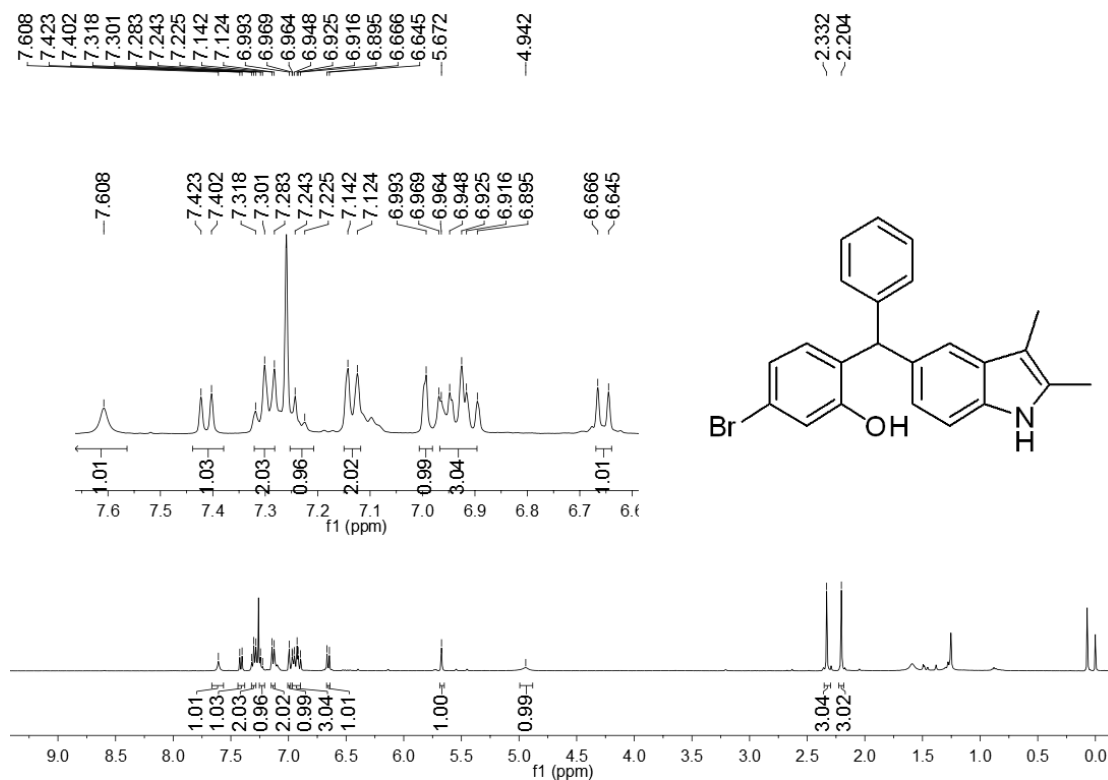
<sup>1</sup>H NMR of compound **3ma**



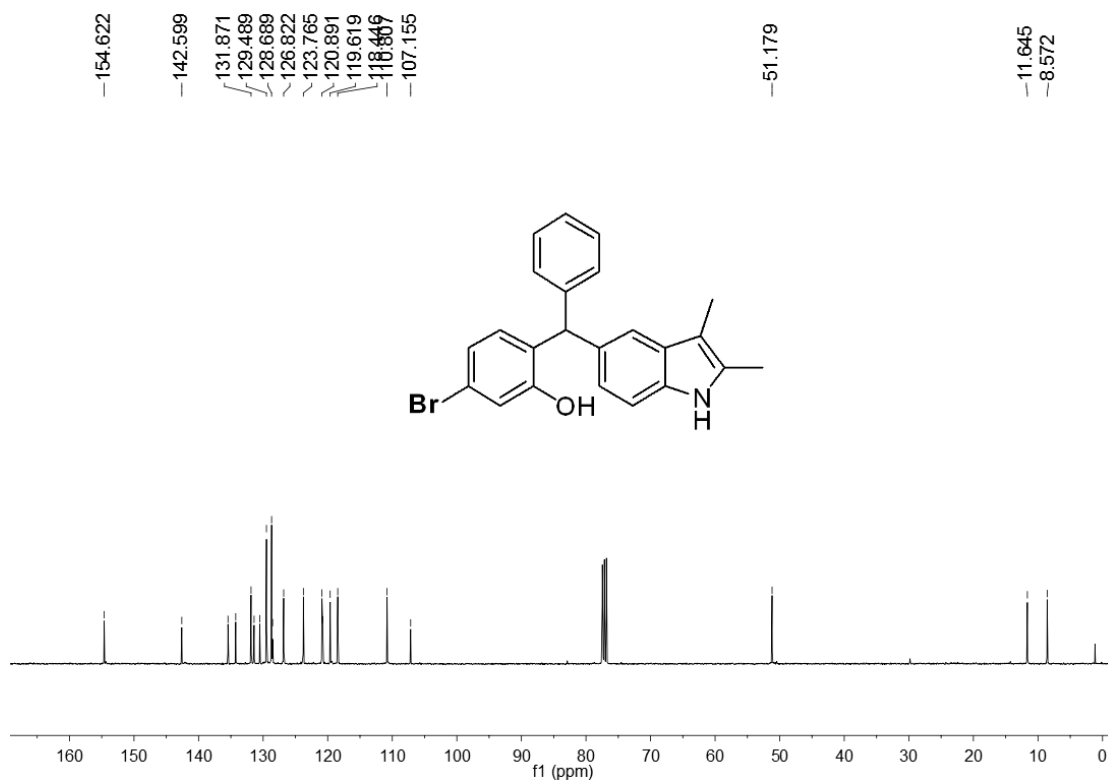
<sup>13</sup>C NMR of compound **3ma**



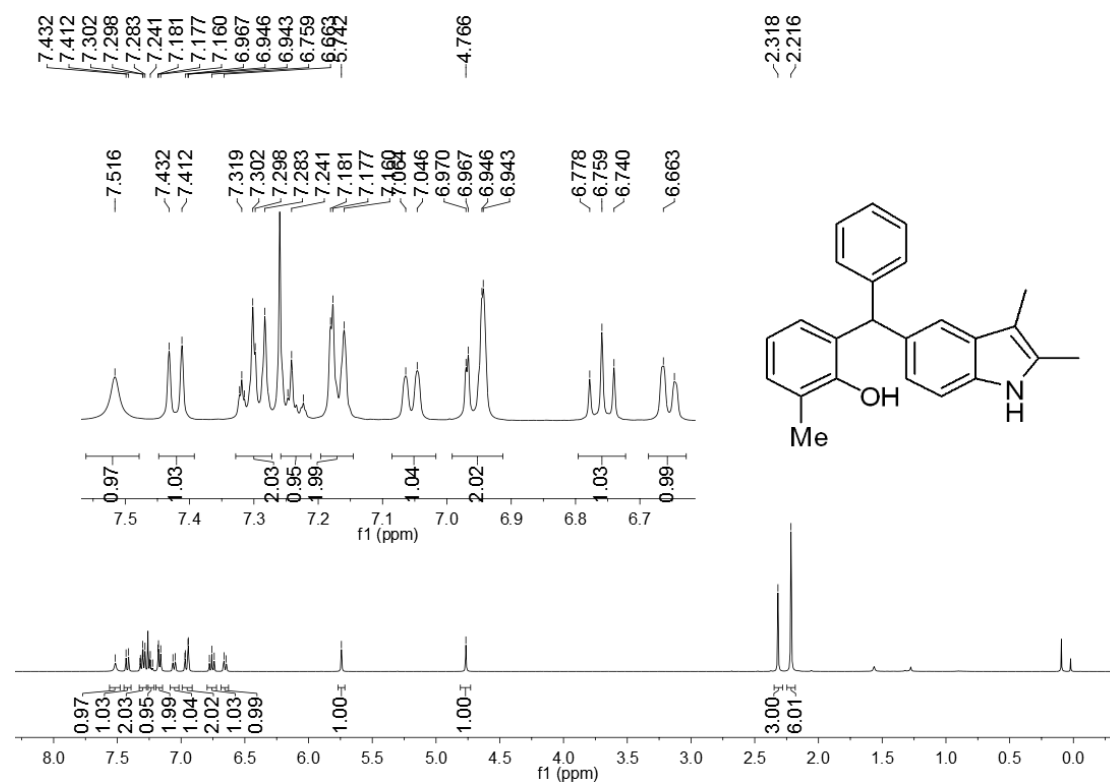
### <sup>1</sup>H NMR of compound **3na**



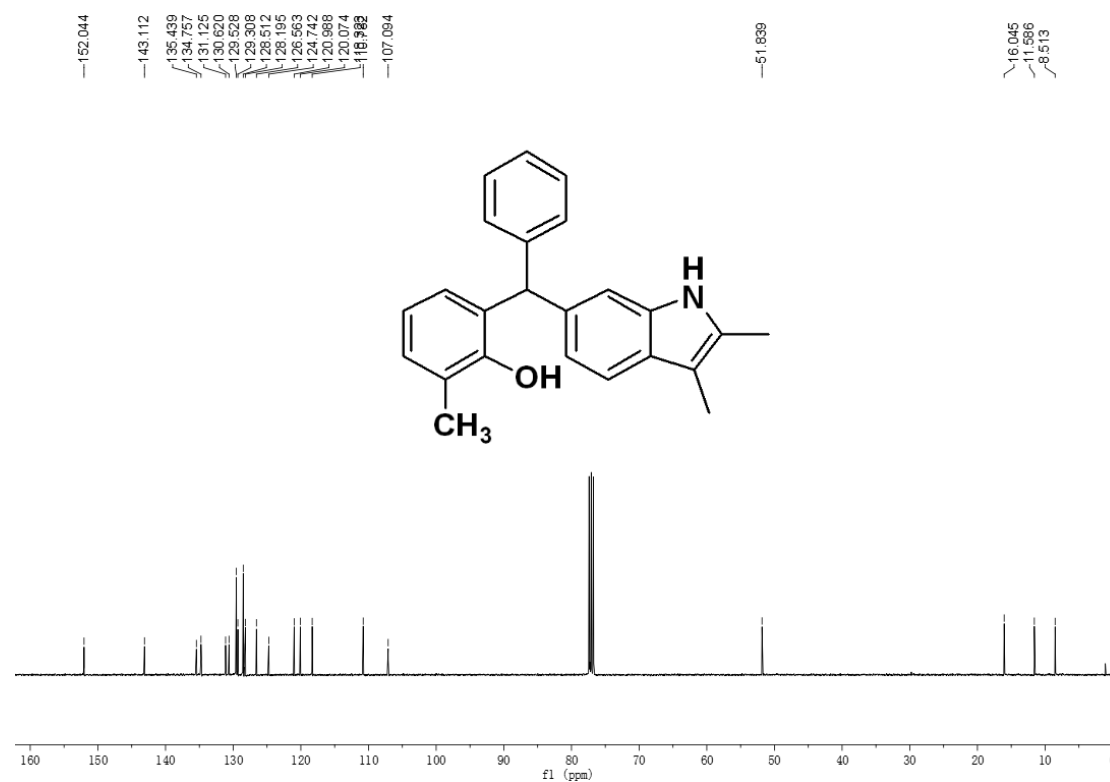
### <sup>13</sup>C NMR of compound **3na**



<sup>1</sup>H NMR of compound **30a**

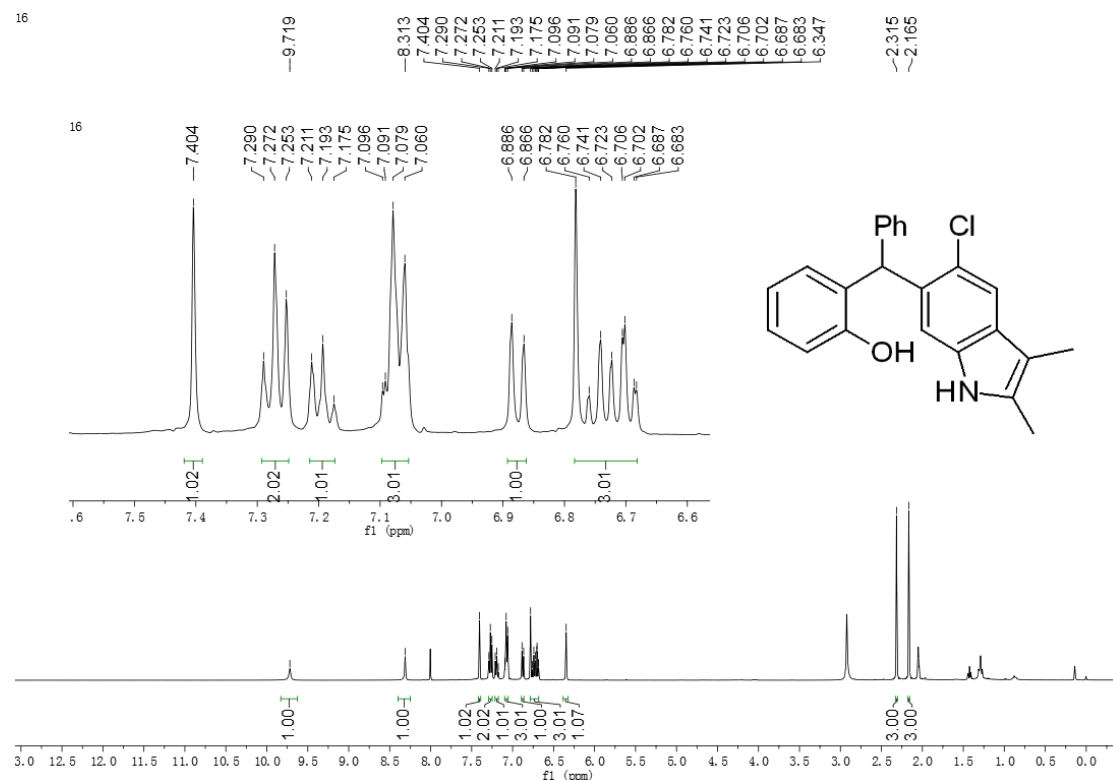


<sup>13</sup>C NMR of compound **30a**

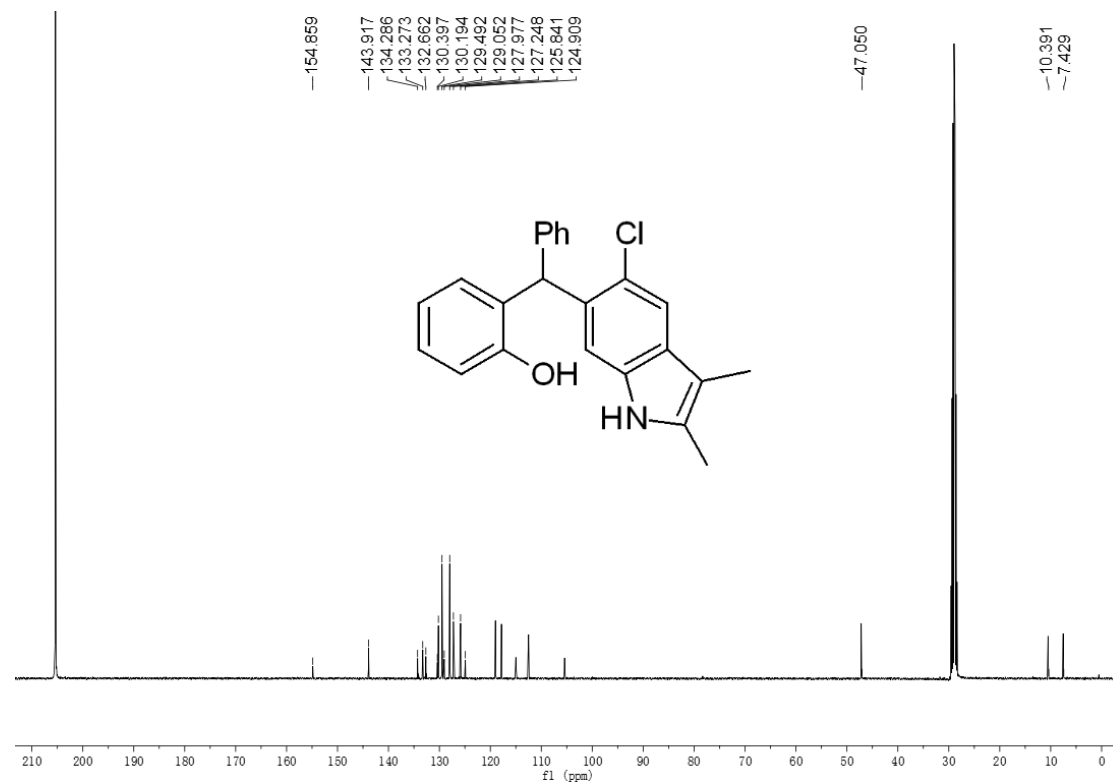




# <sup>1</sup>H NMR of compound **3ab**



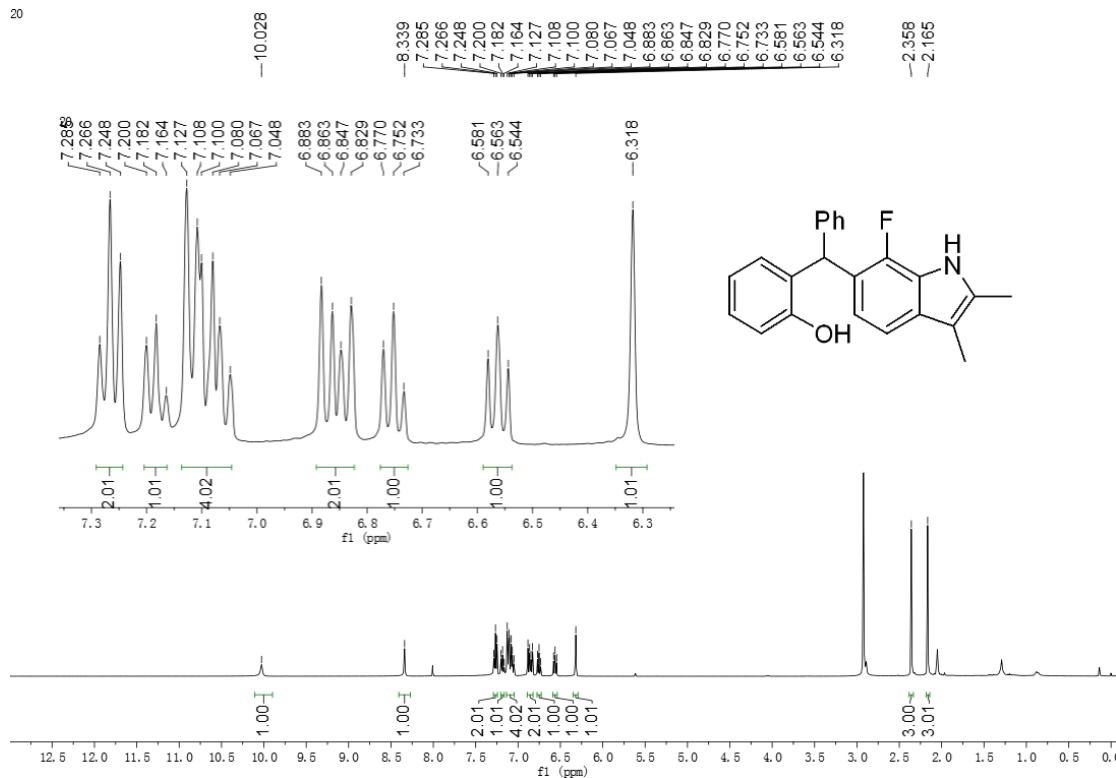
# <sup>13</sup>C NMR of compound **3ab**



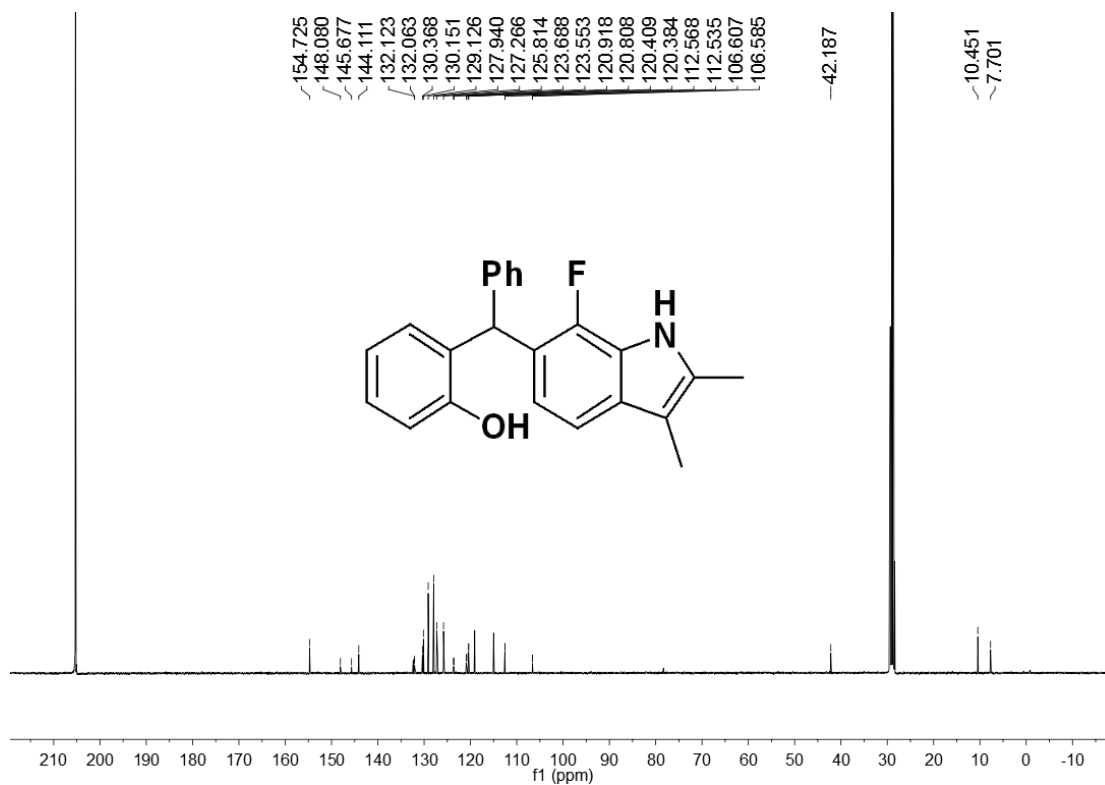


# <sup>1</sup>H NMR of compound 3ad

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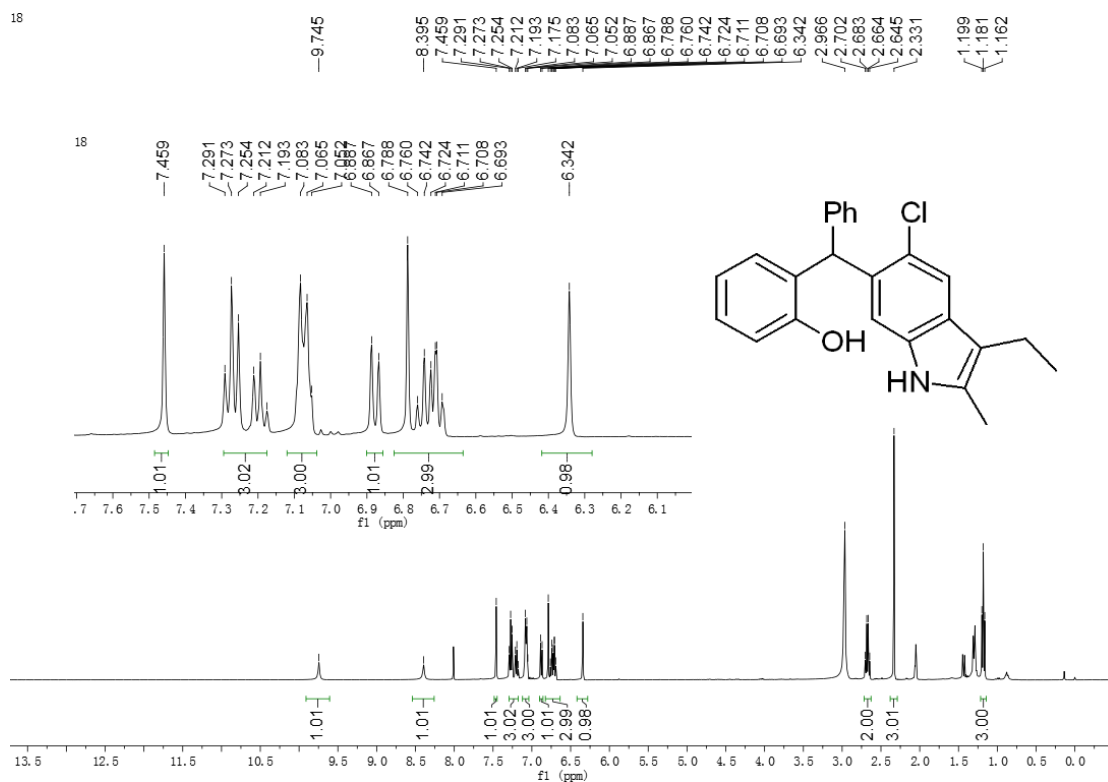


# <sup>13</sup>C NMR of compound 3ad

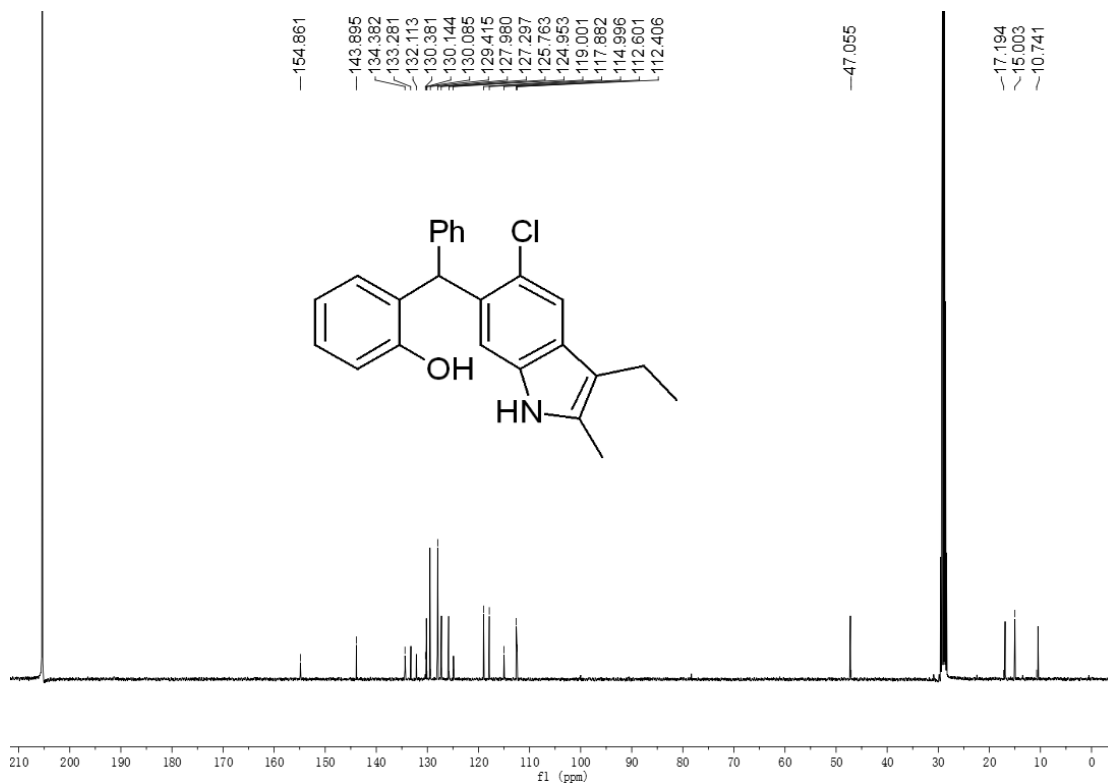


<sup>1</sup>H NMR of compound **3ae**

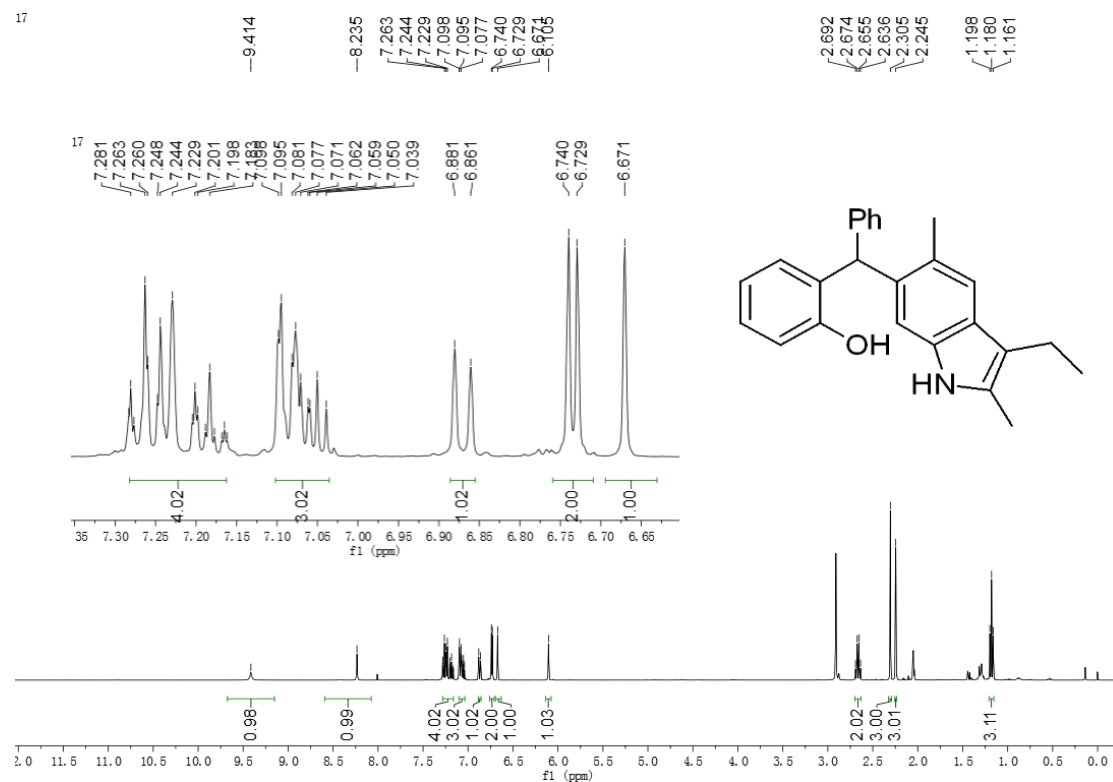
18



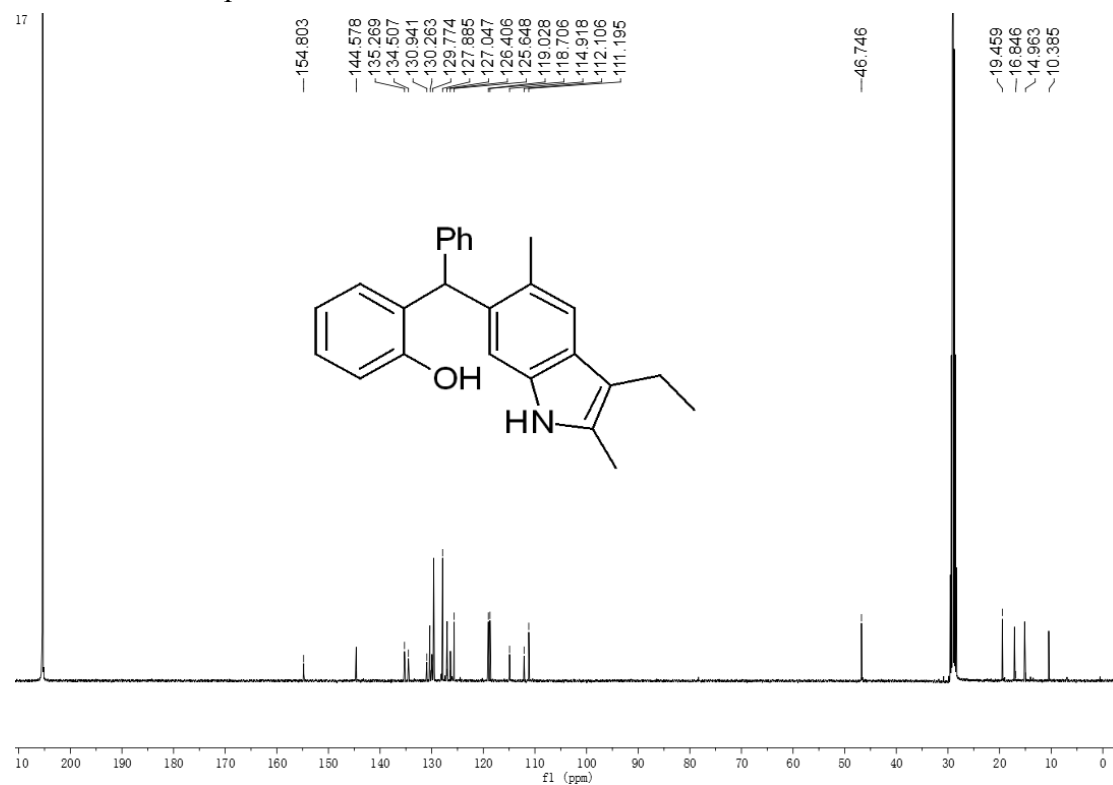
<sup>13</sup>C NMR of compound **3ae**



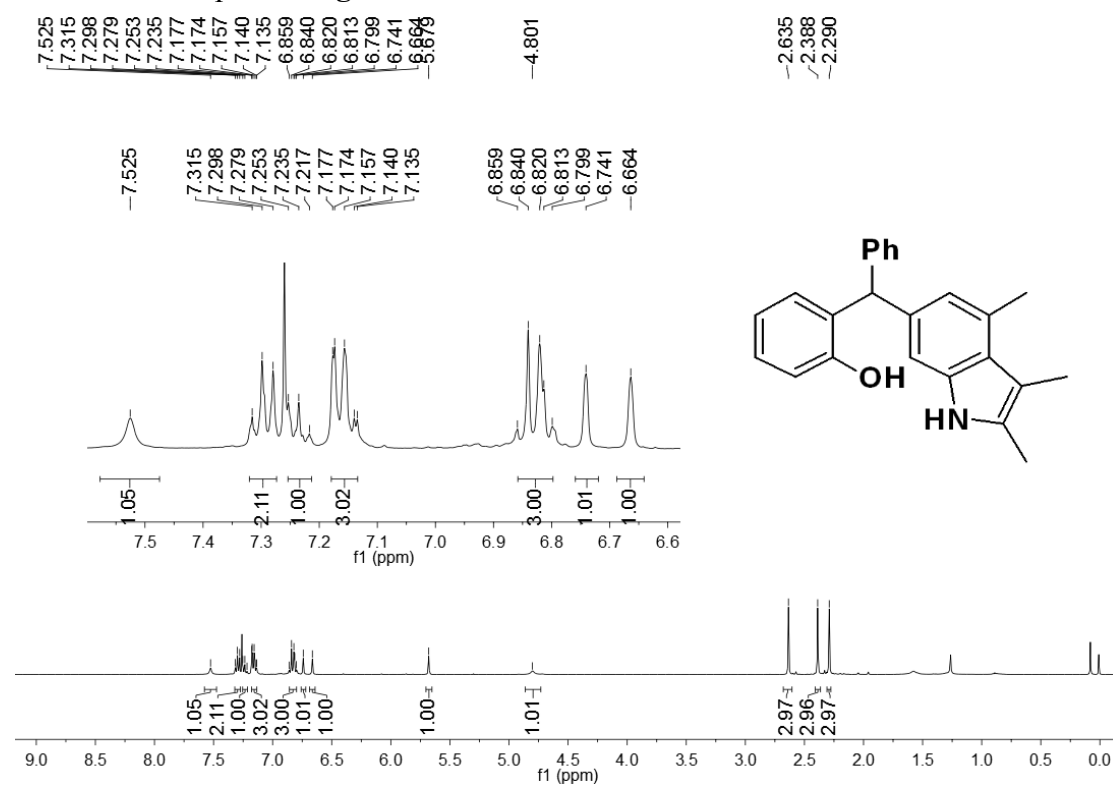
<sup>1</sup>H NMR of compound **3af**



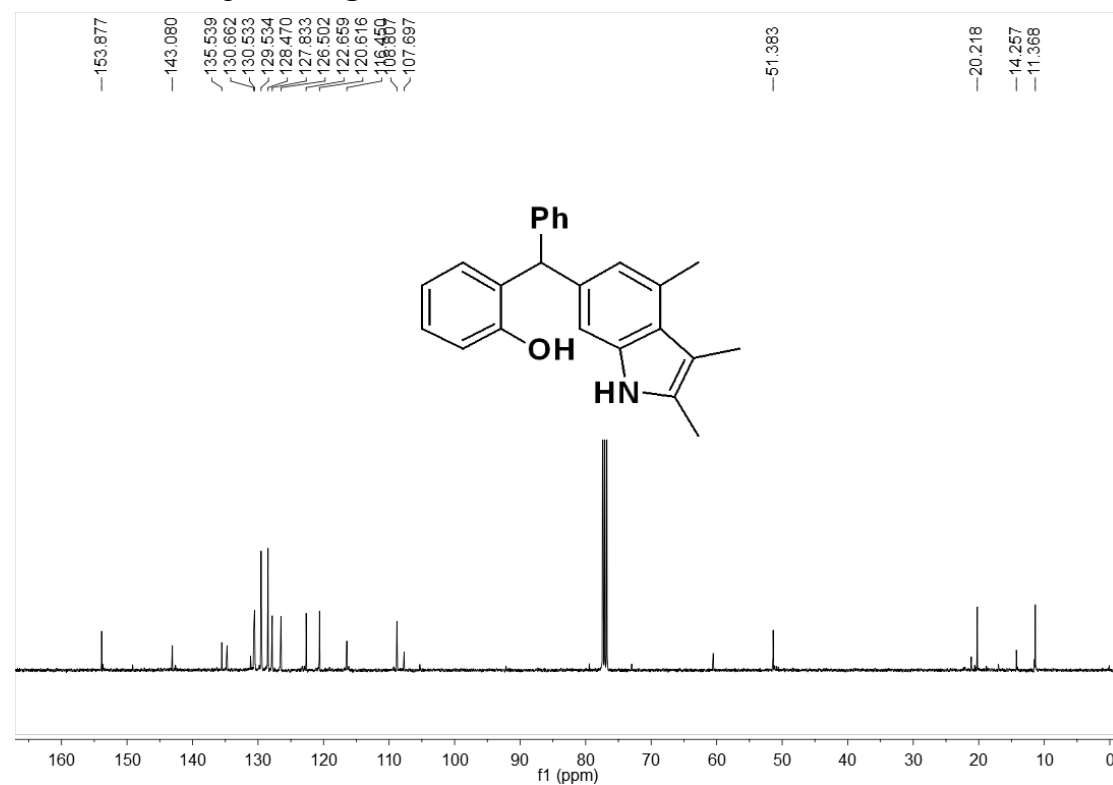
<sup>13</sup>C NMR of compound **3af**



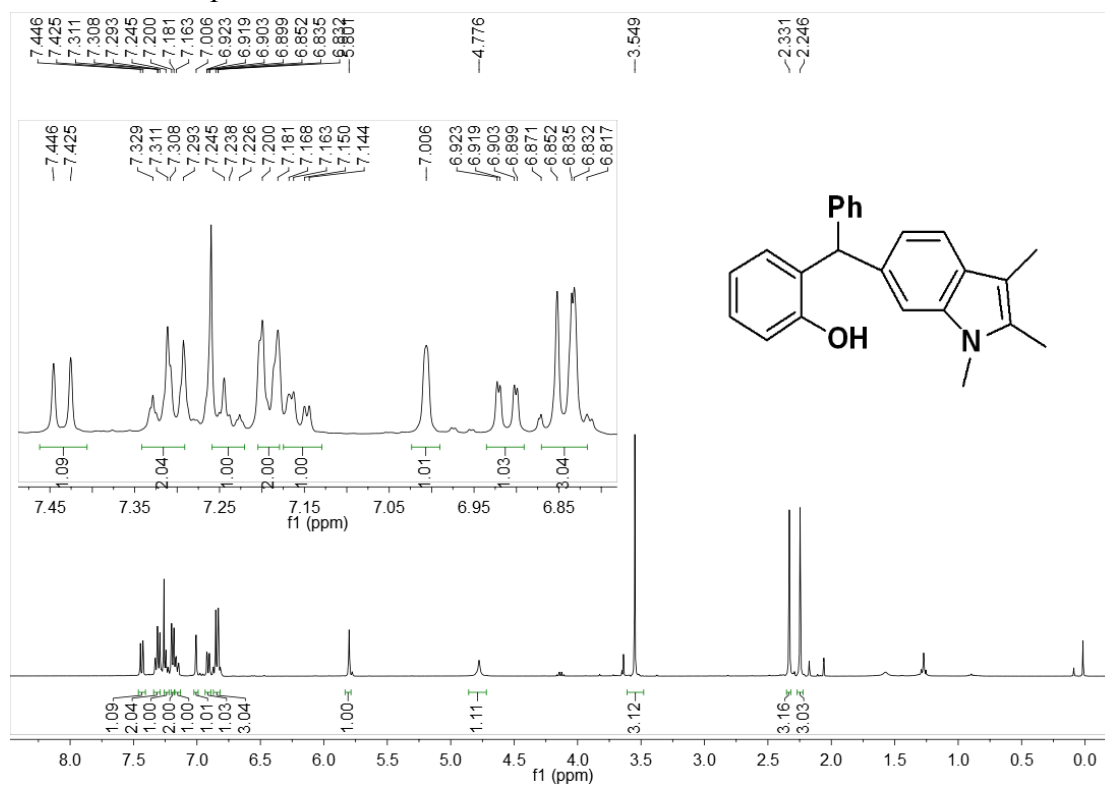
### <sup>1</sup>H NMR of compound **3ag**



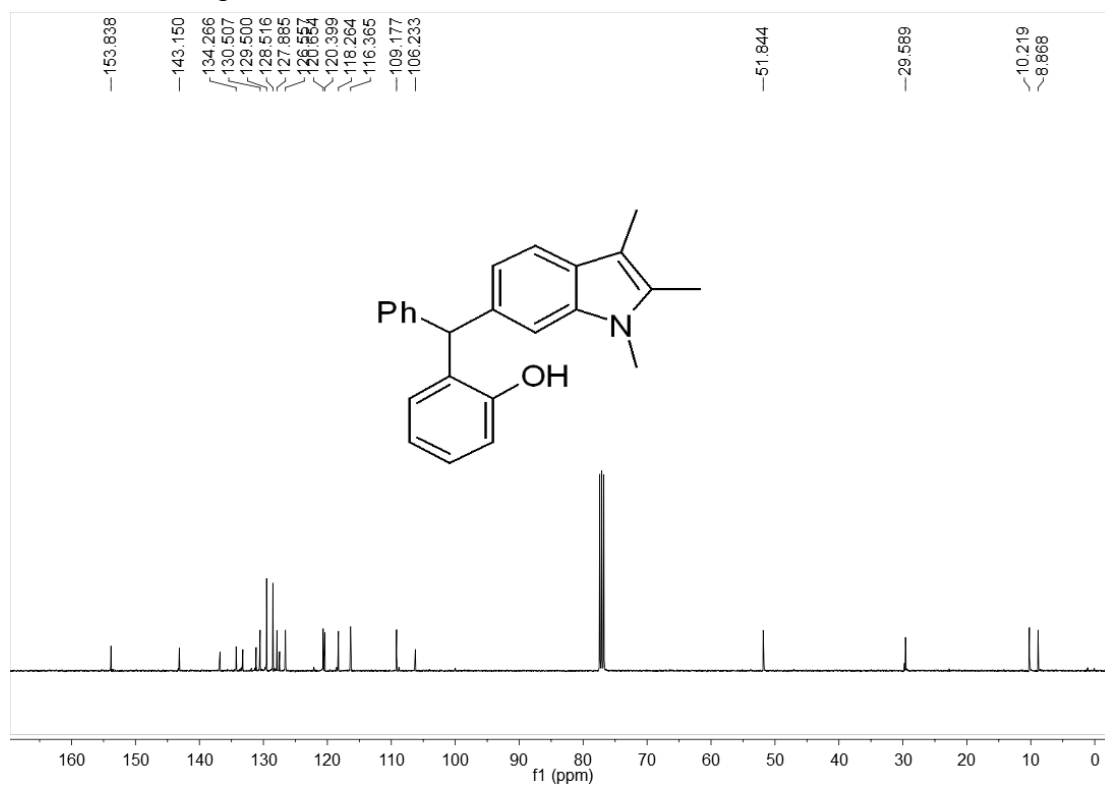
### <sup>13</sup>C NMR of compound **3ag**



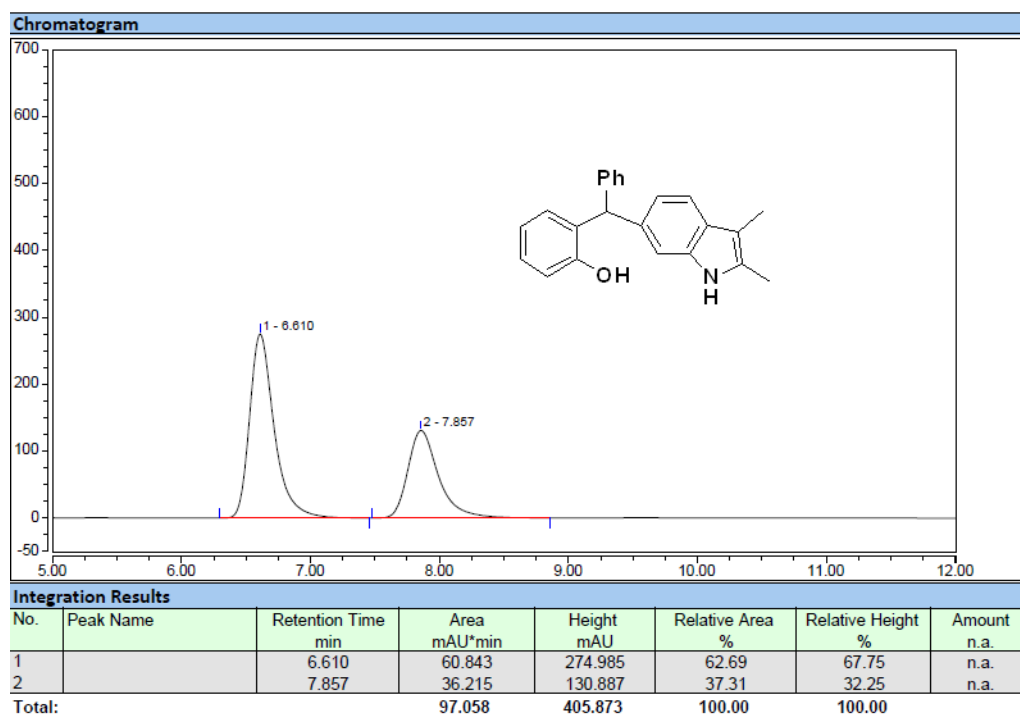
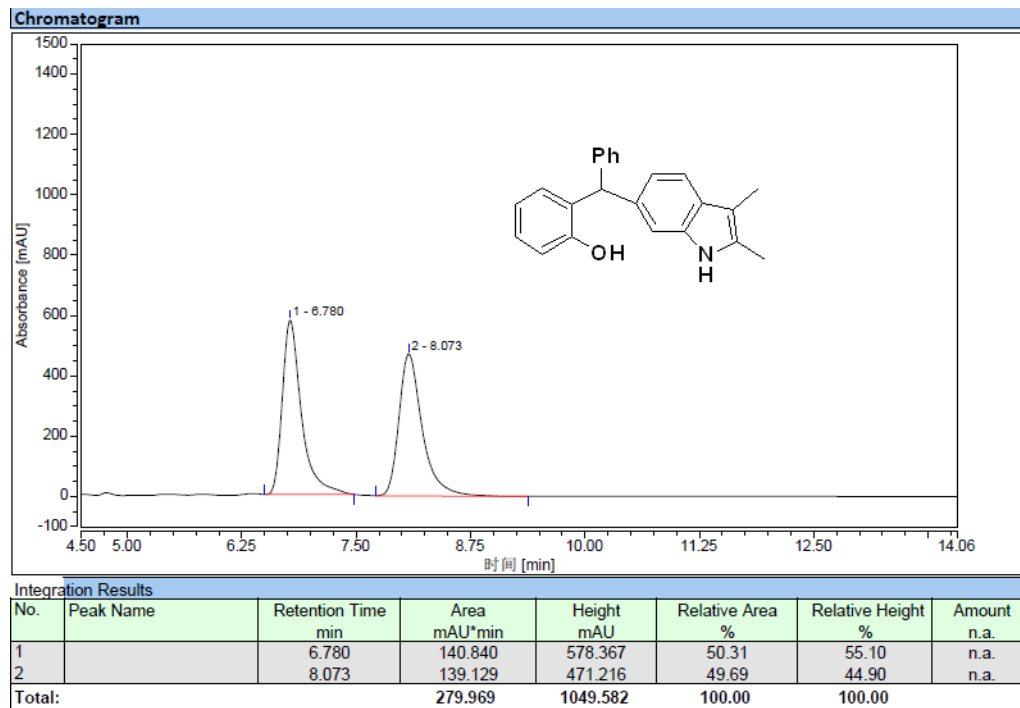
### <sup>1</sup>H NMR of compound **3ah**



### <sup>13</sup>C NMR of compound **3ah**

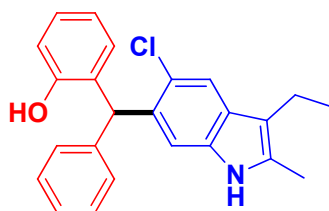


## 2. HPLC spectra of product 3aa

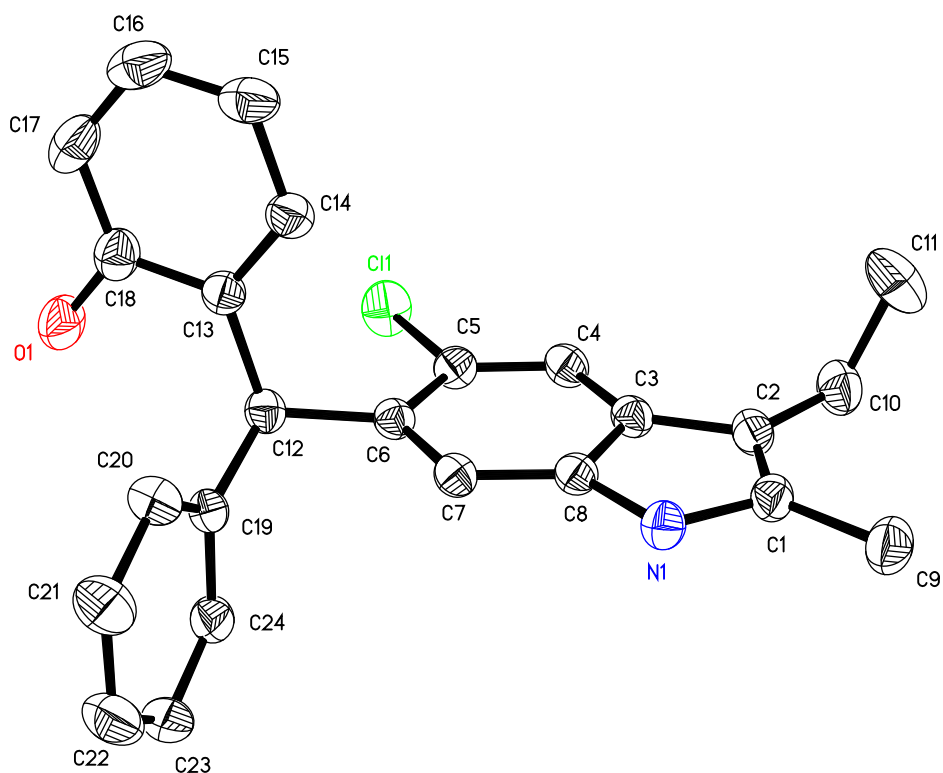




### 3. X-ray single crystal data for compound 3ae



3ae



The thermal ellipsoid was drawn at the 30% probability level.

Empirical formula	C <sub>24</sub> H <sub>22</sub> Cl N O
Formula weight	375.87
Temperature	296 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C 1 2/c 1
Unit cell dimensions	a = 17.424(3) Å      α = 90° b = 12.100(2) Å      β = 101.189(4)°

	$c = 19.028(3) \text{ \AA}$	$\gamma = 90^\circ$ .
Volume	$3935.4(12) \text{ \AA}^3$	
Z	8	
Density (calculated)	$1.269 \text{ Mg/m}^3$	
Absorption coefficient	$0.207 \text{ mm}^{-1}$	
F(000)	1584	
Crystal size	$0.25 \times 0.2 \times 0.15 \text{ mm}^3$	
Theta range for data collection	$2.062 \text{ to } 30.714^\circ$ .	
Index ranges	$-16 \leq h \leq 25, -17 \leq k \leq 17, -27 \leq l \leq 26$	
Reflections collected	19722	
Independent reflections	6111 [R(int) = 0.0432]	
Completeness to theta = $25.242^\circ$	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7461 and 0.6912	
Refinement method	Full-matrix least-squares on $F^2$	
Data / restraints / parameters	6111 / 0 / 257	
Goodness-of-fit on $F^2$	1.000	
Final R indices [ $I > 2\sigma(I)$ ]	$R1 = 0.0478, wR2 = 0.1126$	
R indices (all data)	$R1 = 0.1218, wR2 = 0.1450$	
Extinction coefficient	n/a	
Largest diff. peak and hole	$0.181 \text{ and } -0.307 \text{ e.\AA}^{-3}$	