

Supporting Information

Phosphine-Catalyzed [4+2] Cyclization of *para*-Quinone Methide Derivatives with Allenes

Fu-Ru Yuan,^a Fei Jiang,^a Ke-Wei Chen,^a Guang-Jian Mei,^a Qiong Wu*^b and Feng Shi*^a

^a*School of Chemistry and Materials Science, Jiangsu Normal University, Xuzhou, 221116, China.*

E-mail: fshi@jsnu.edu.cn.

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

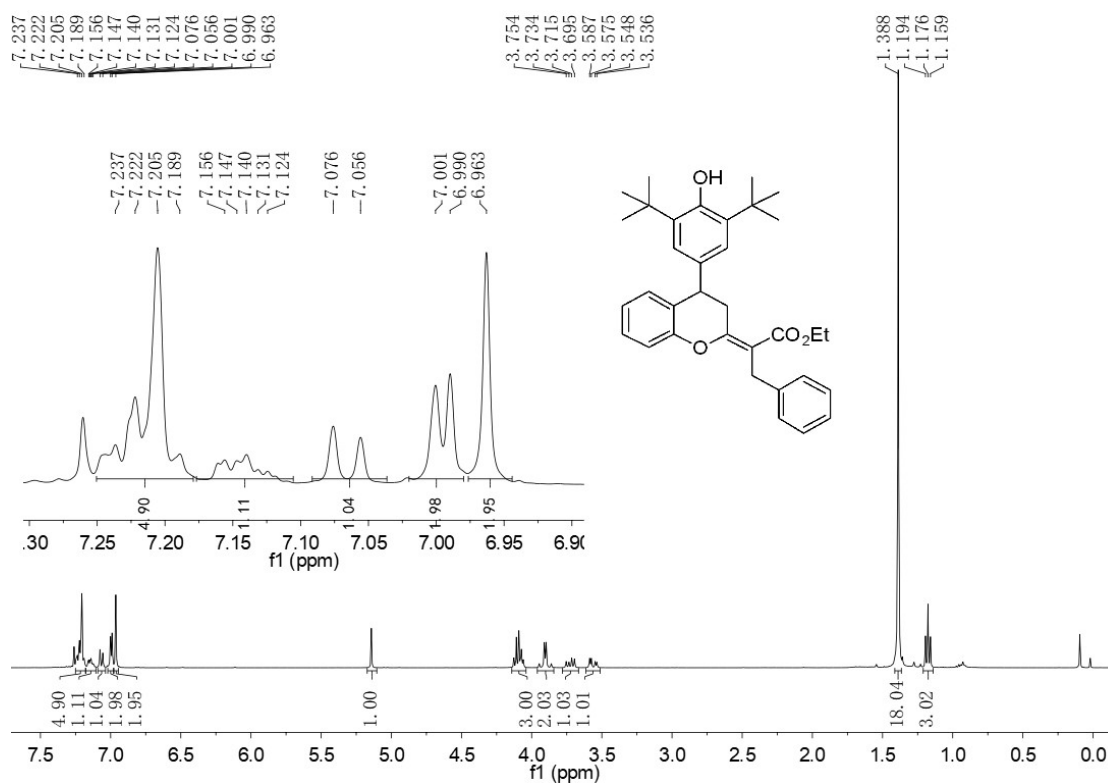
221018, China. E-mail: hgwuqiong@xzit.edu.cn.

Contents:

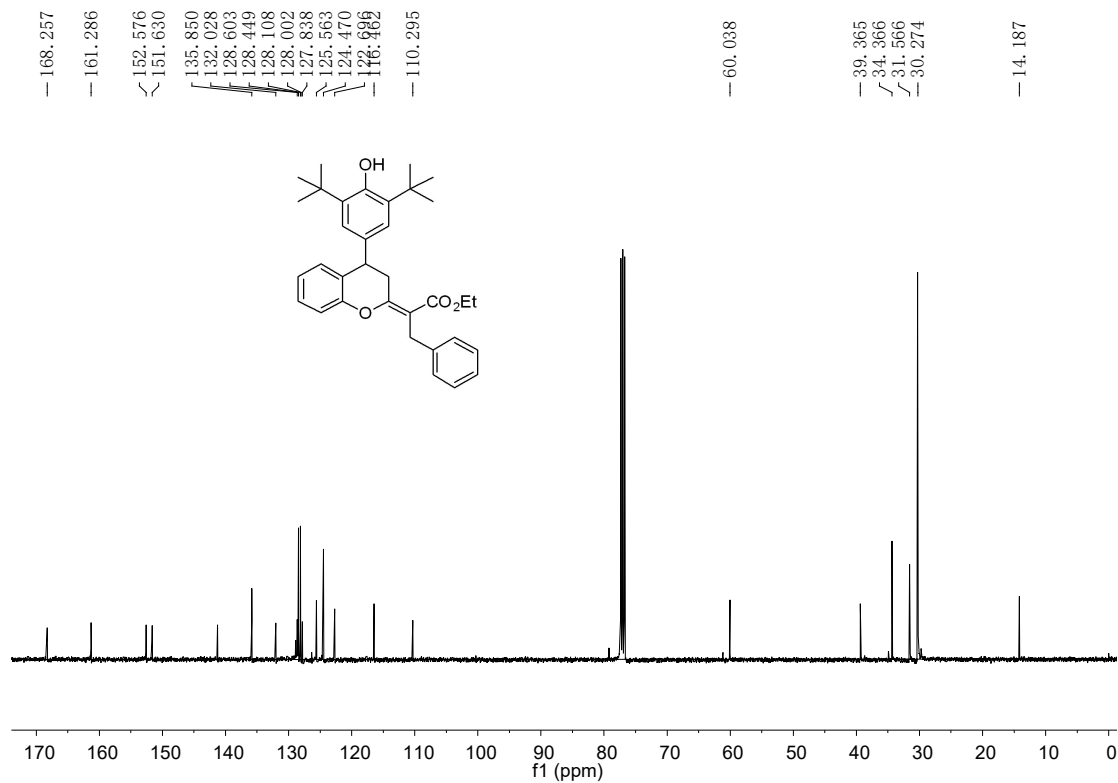
- 1. NMR spectra of products 3 (S1-S27)**
- 2. HPLC spectra of product 3aa (S28)**
- 3. X-ray single crystal data for compound 3aa (S29-S30)**

1. NMR spectra of products 3

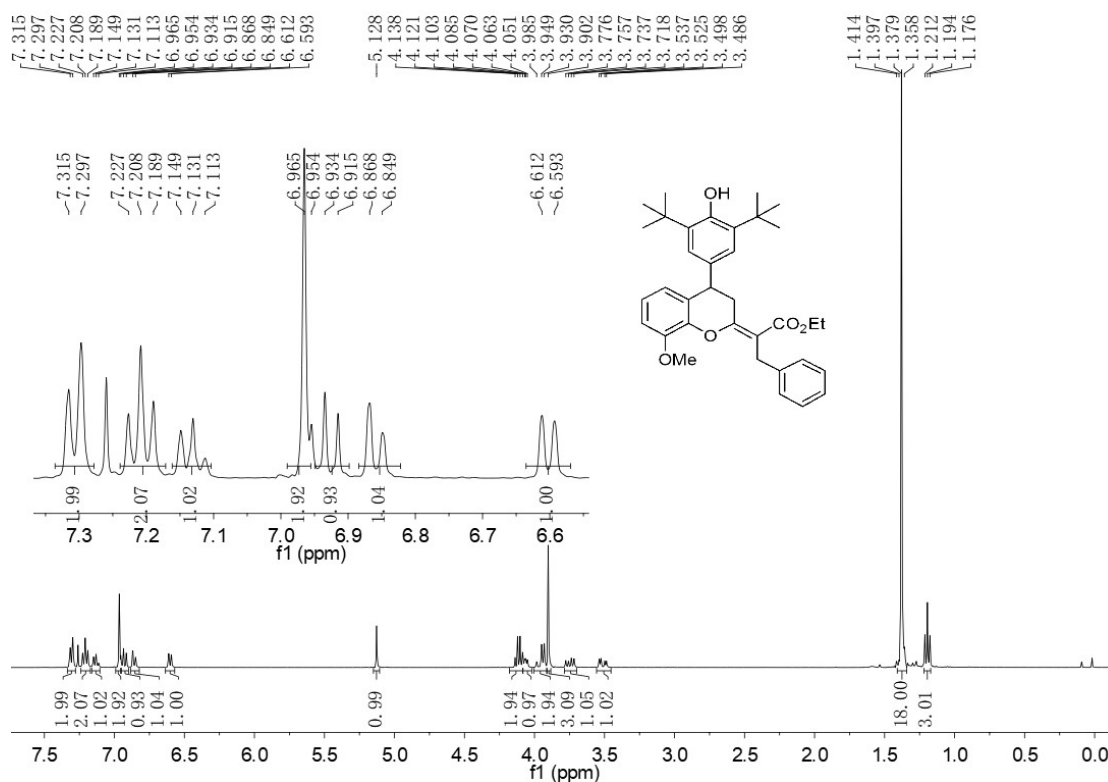
^1H NMR (400 MHz, CDCl_3) of compound **3aa**



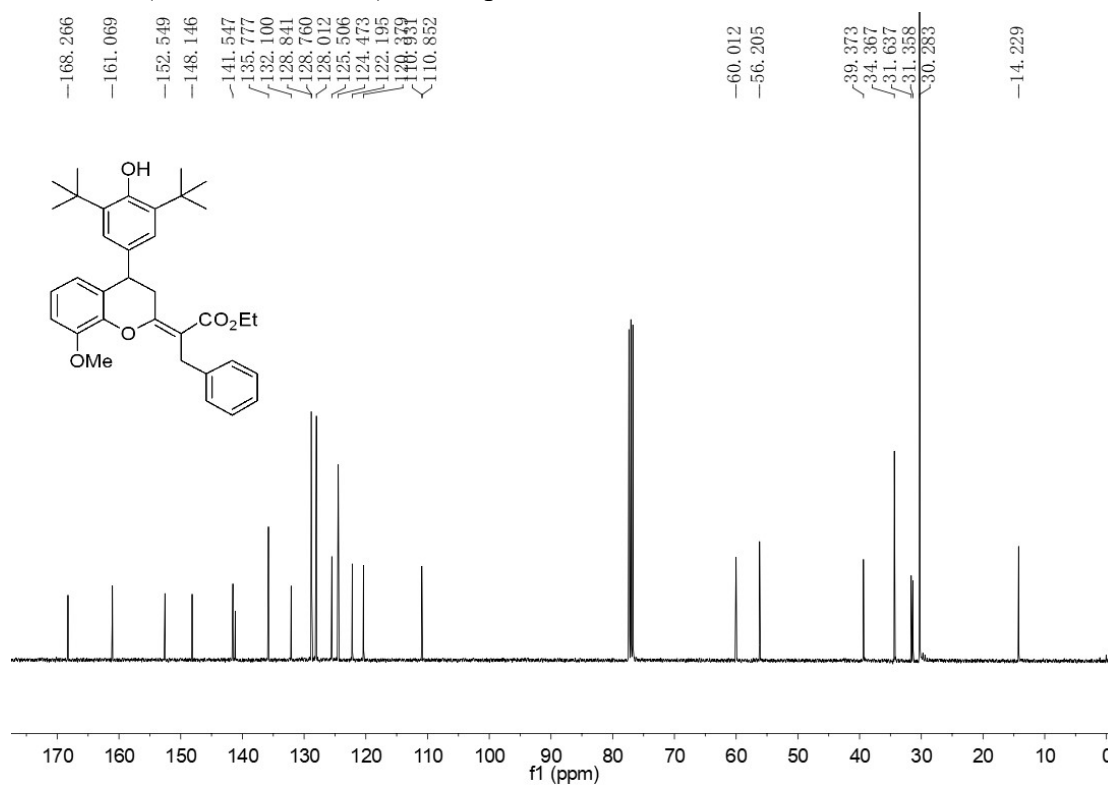
^{13}C NMR (100 MHz, CDCl_3) of compound **3aa**



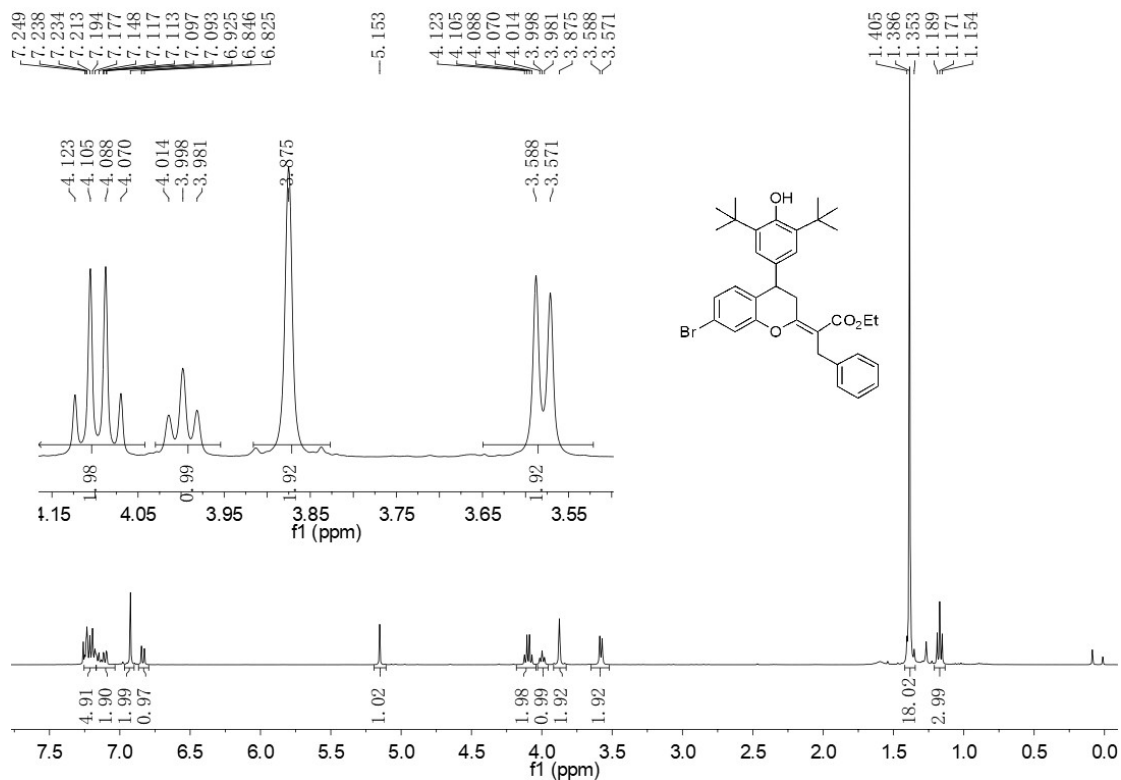
^1H NMR (400 MHz, CDCl_3) of compound **3ba**



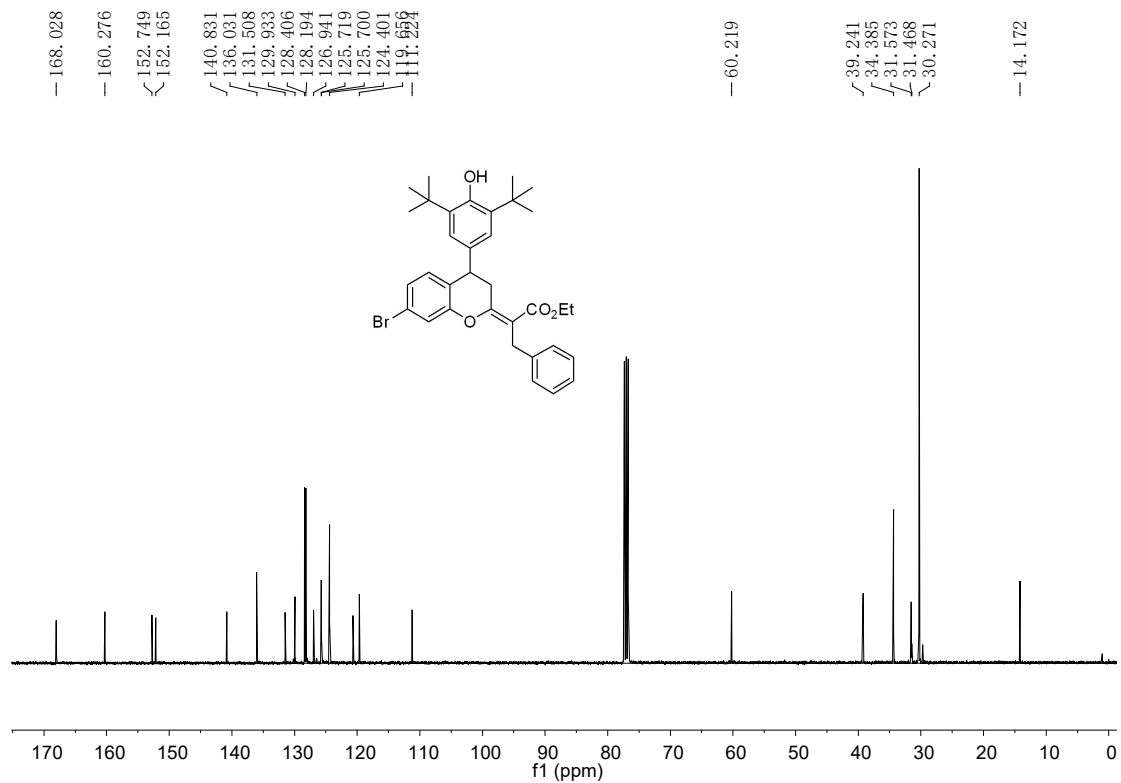
^{13}C NMR (100 MHz, CDCl_3) of compound **3ba**



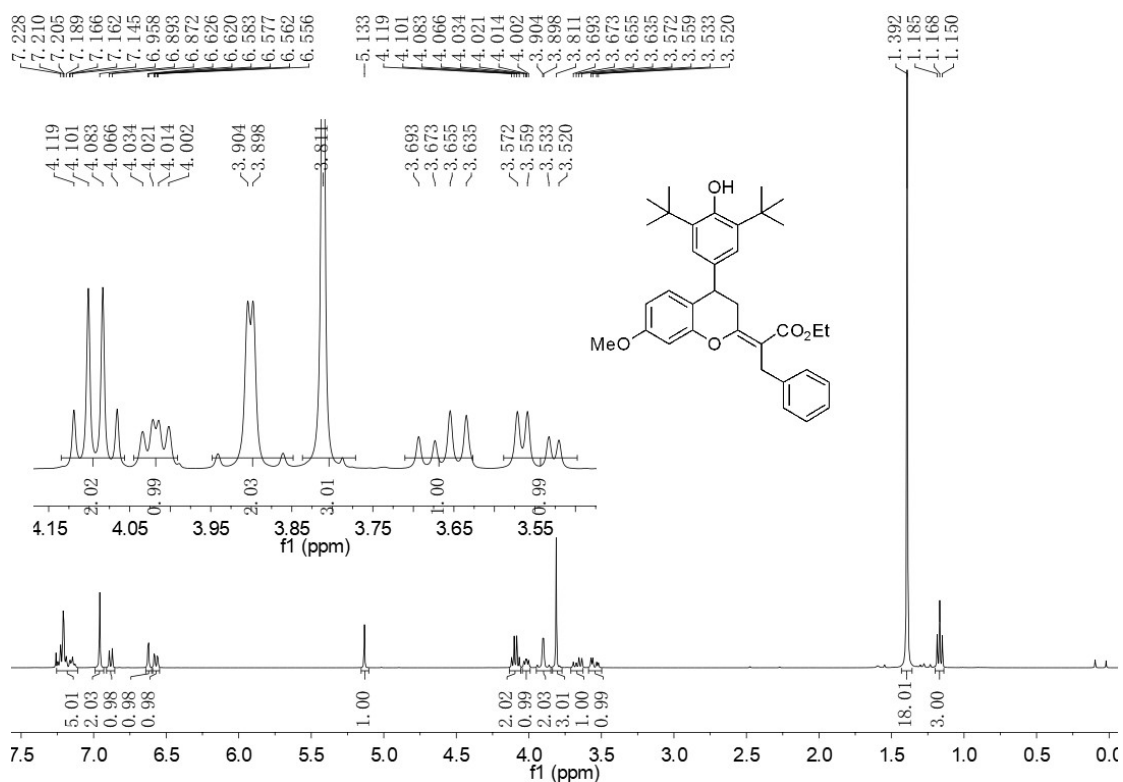
¹H NMR (400 MHz, CDCl₃) of compound **3ca**



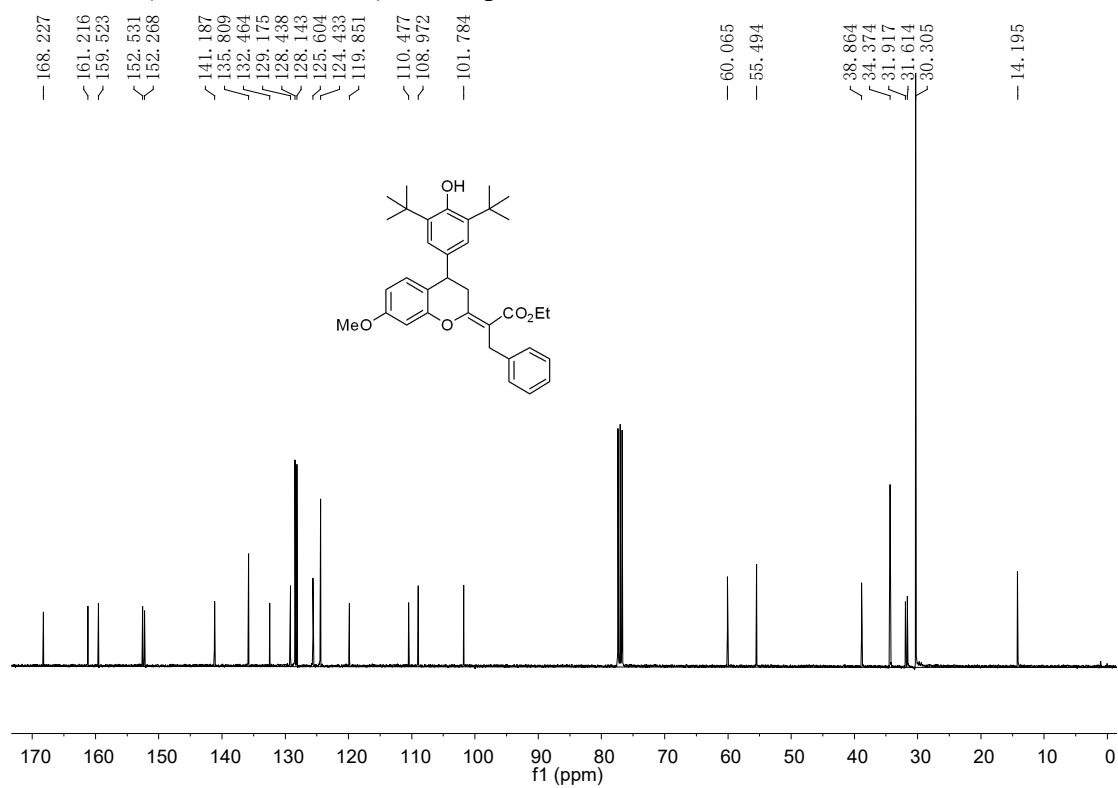
¹³C NMR (100 MHz, CDCl₃) of compound **3ca**



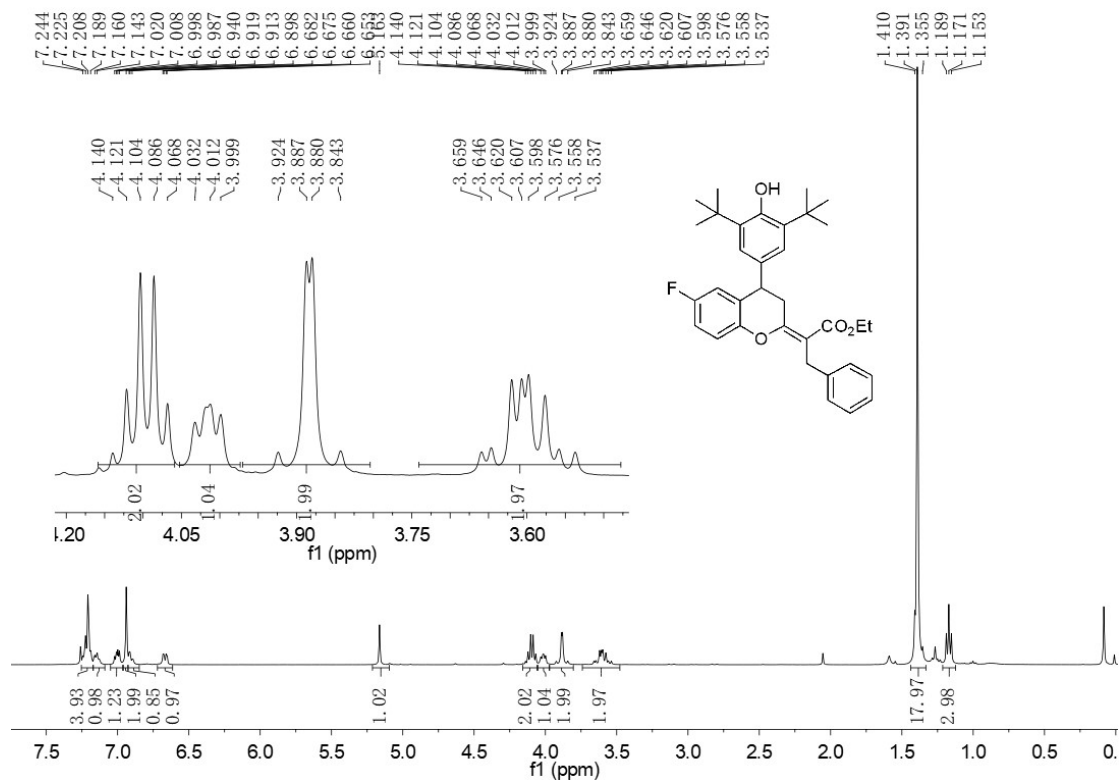
¹H NMR (400 MHz, CDCl₃) of compound **3da**



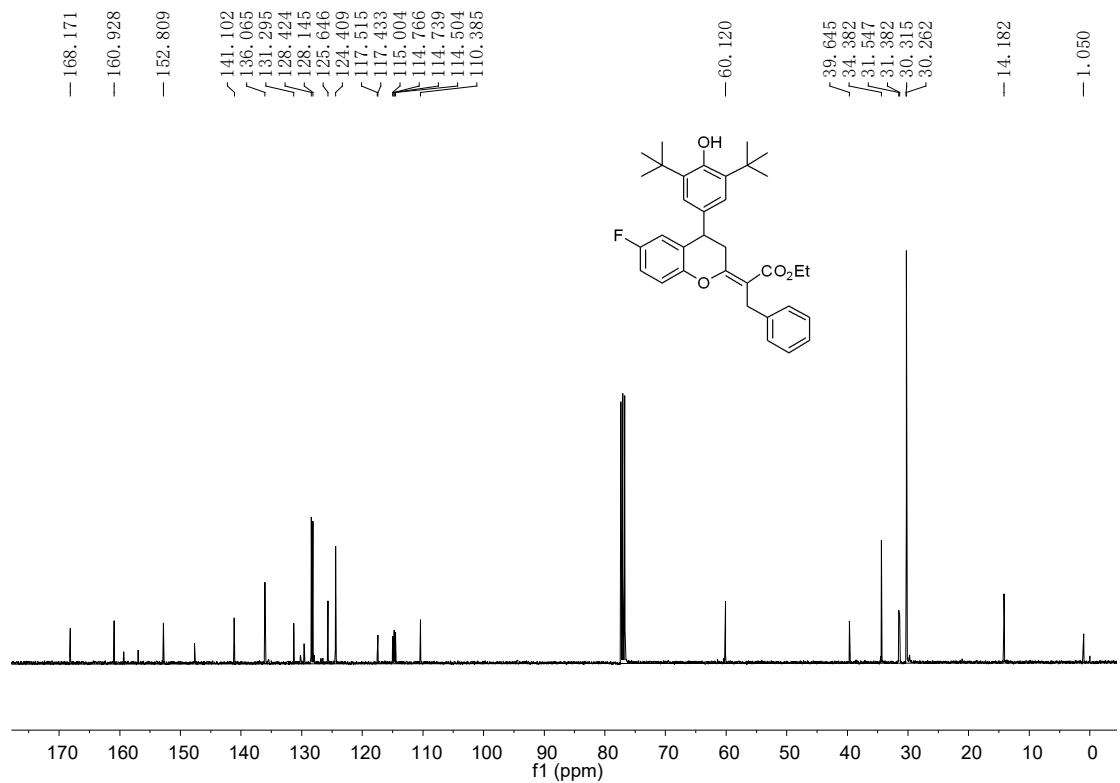
¹³C NMR (100 MHz, CDCl₃) of compound **3da**



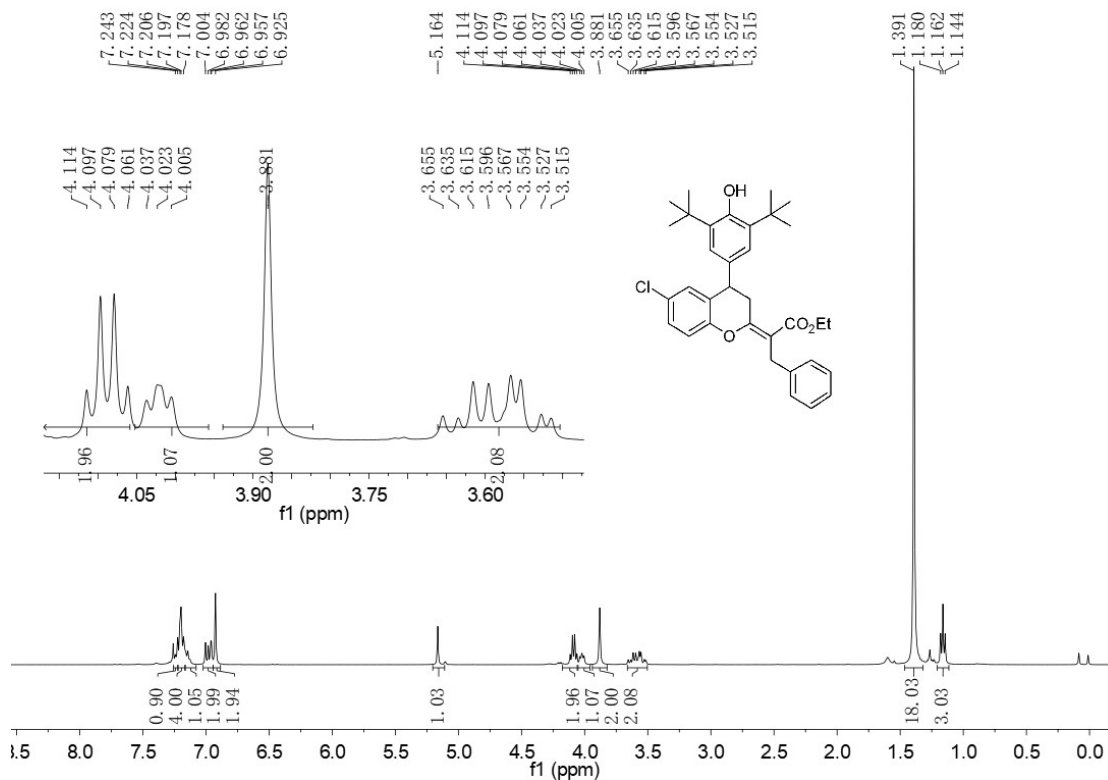
¹H NMR (400 MHz, CDCl₃) of compound **3ea**



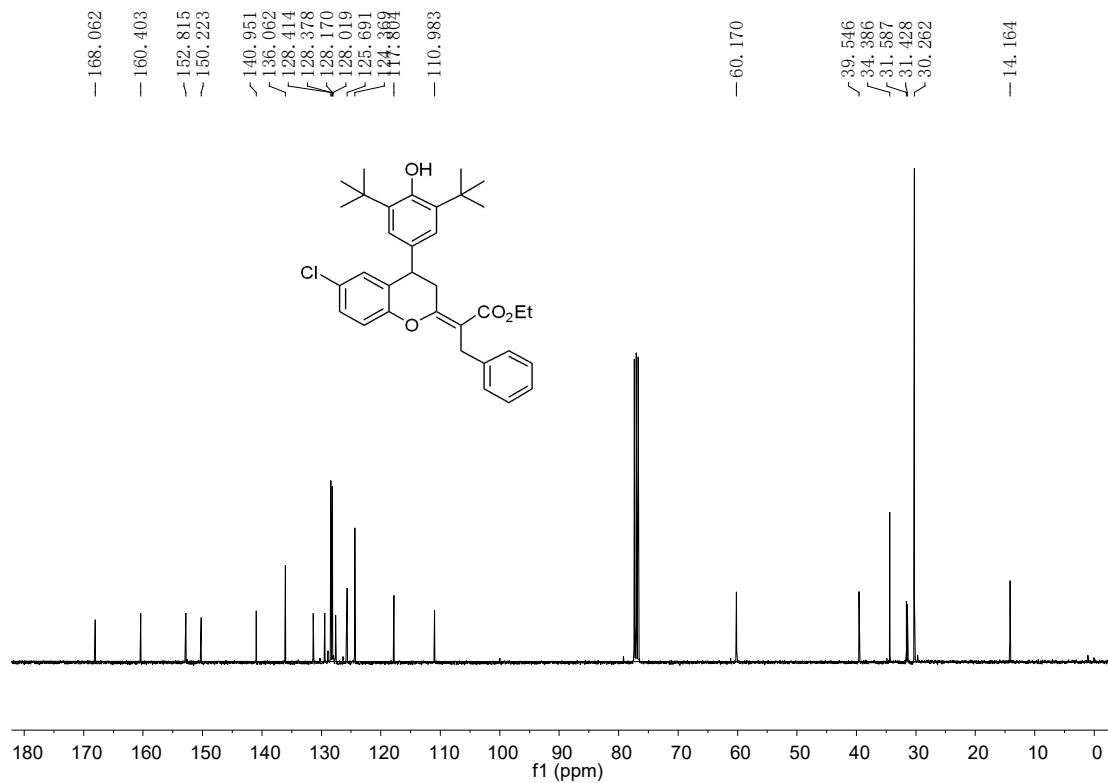
¹³C NMR (100 MHz, CDCl₃) of compound **3ea**



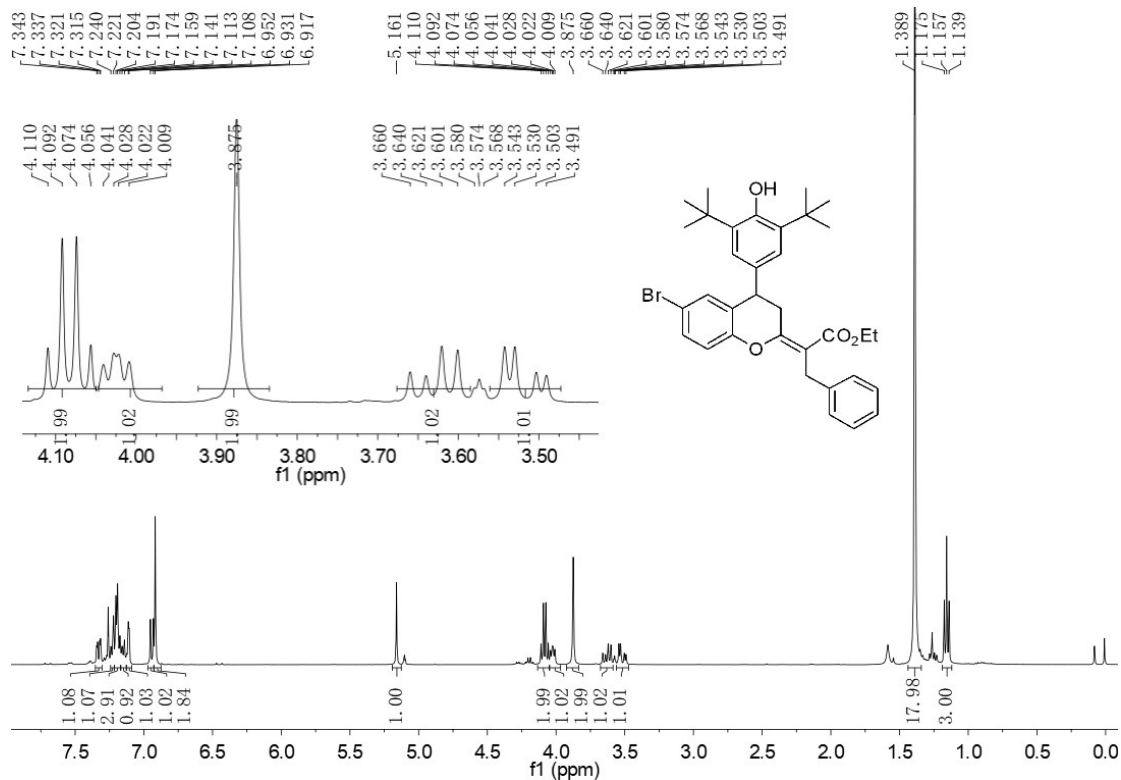
¹H NMR (400 MHz, CDCl₃) of compound **3fa**



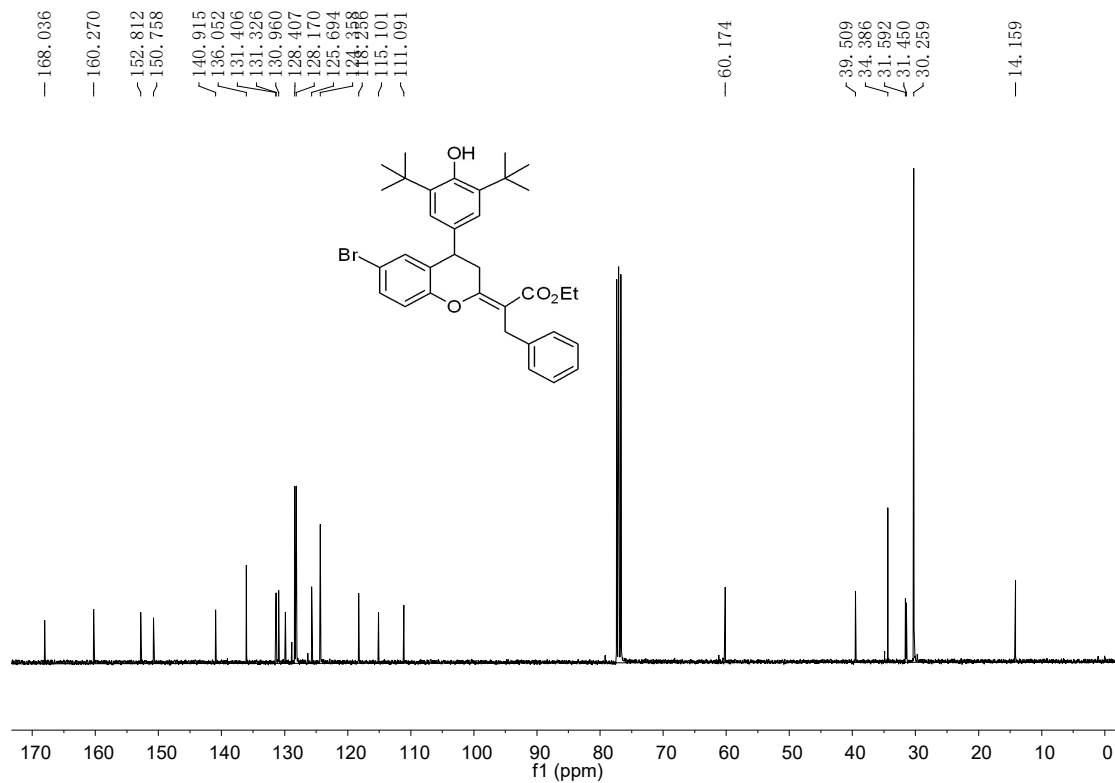
¹³C NMR (100 MHz, CDCl₃) of compound **3fa**



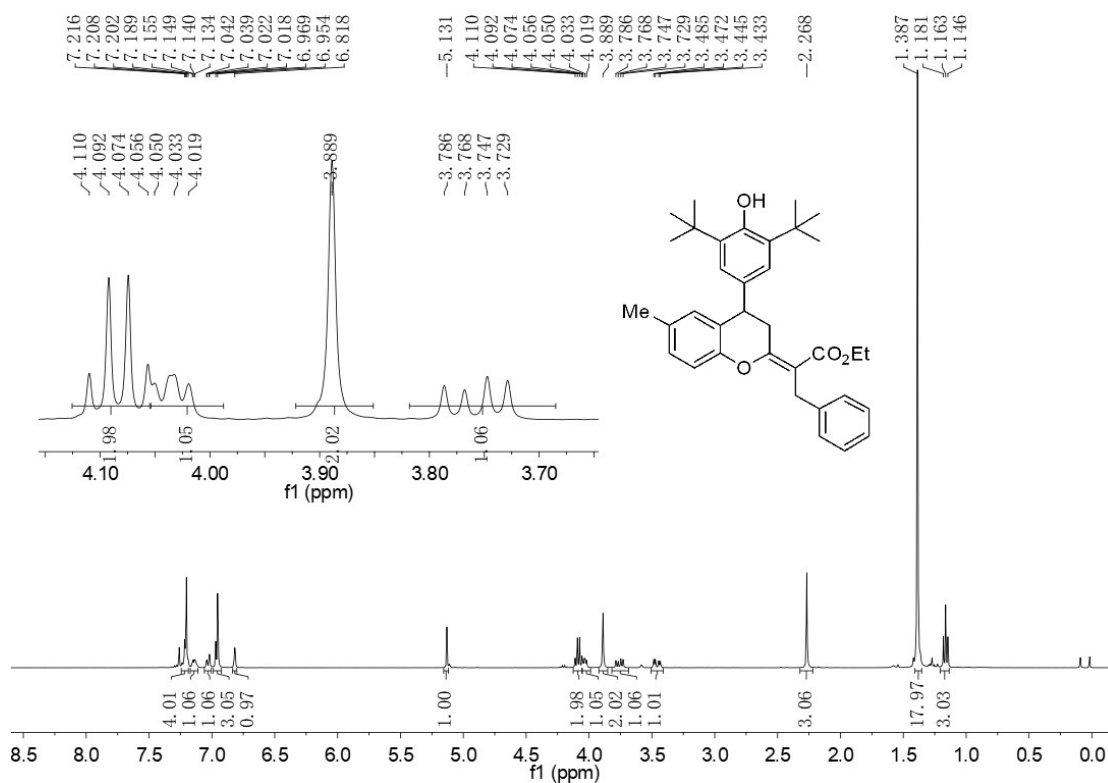
¹H NMR (400 MHz, CDCl₃) of compound **3ga**



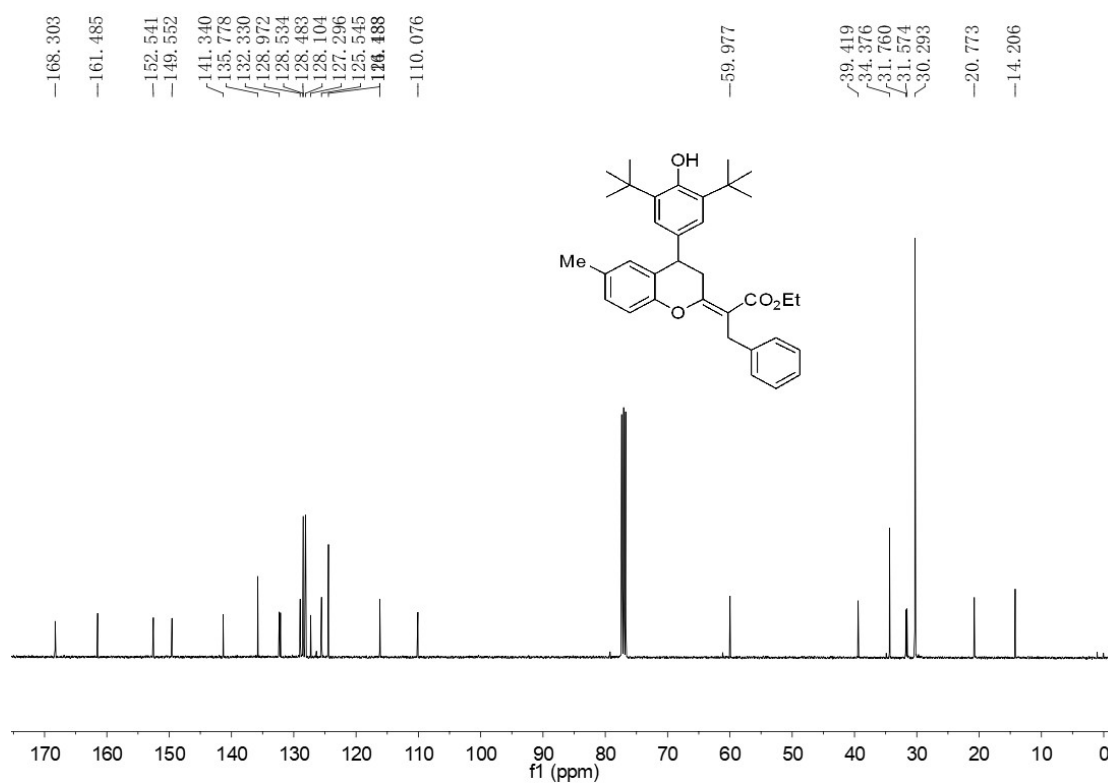
¹³C NMR (100 MHz, CDCl₃) of compound **3ga**



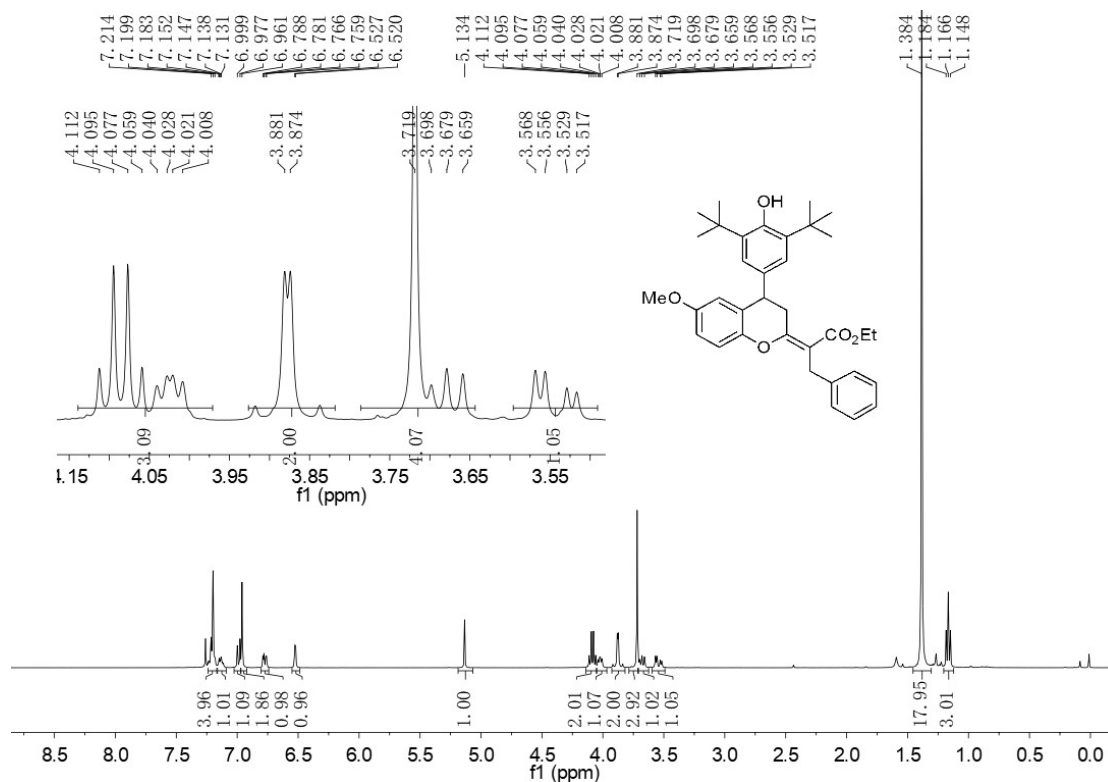
^1H NMR (400 MHz, CDCl_3) of compound **3ha**



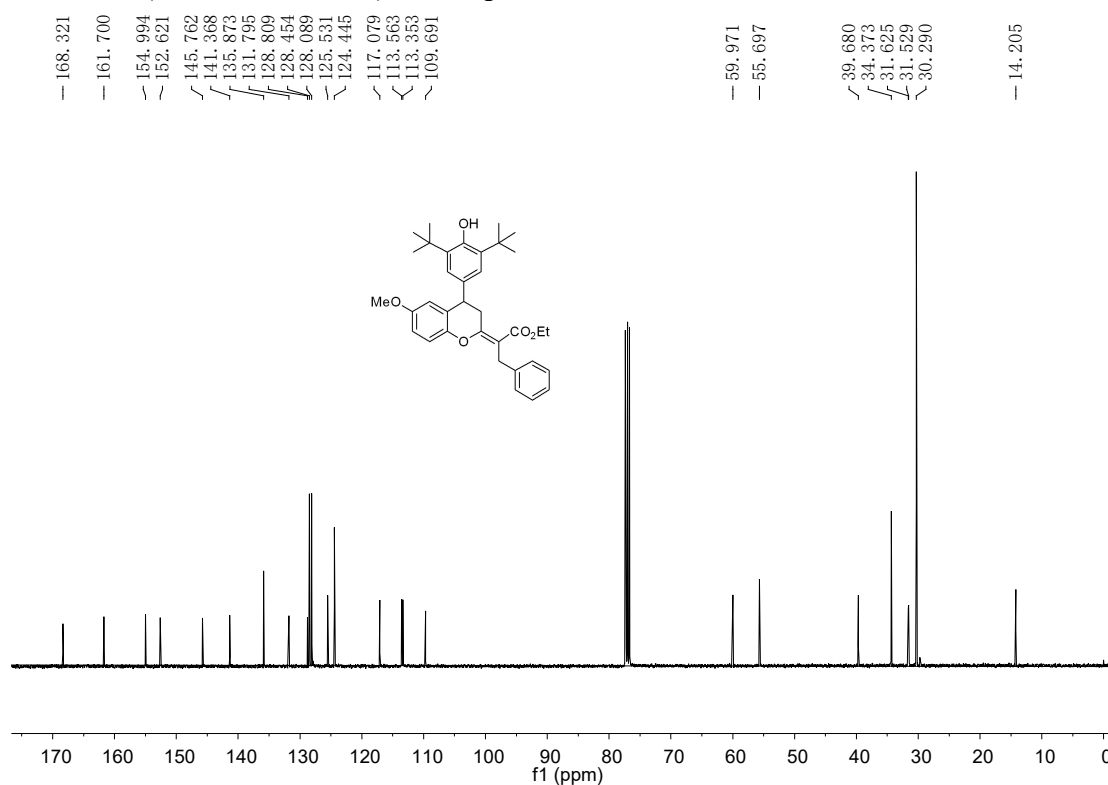
^{13}C NMR (100 MHz, CDCl_3) of compound **3ha**



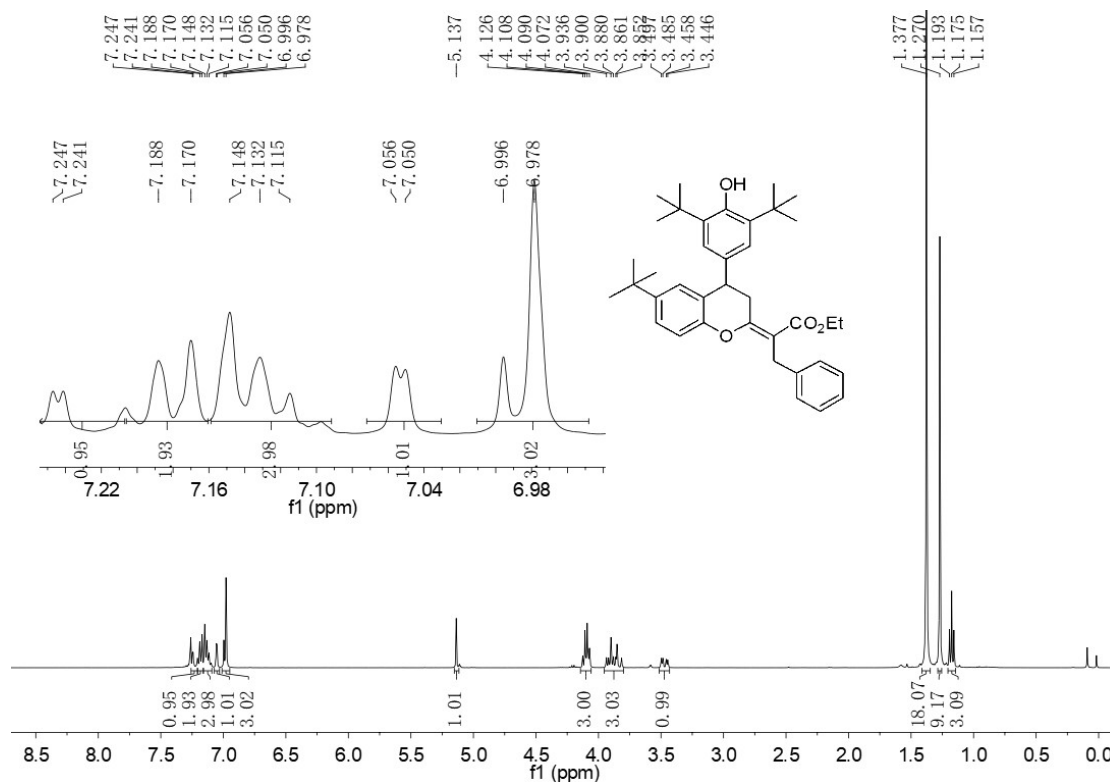
¹H NMR (400 MHz, CDCl₃) of compound **3ia**



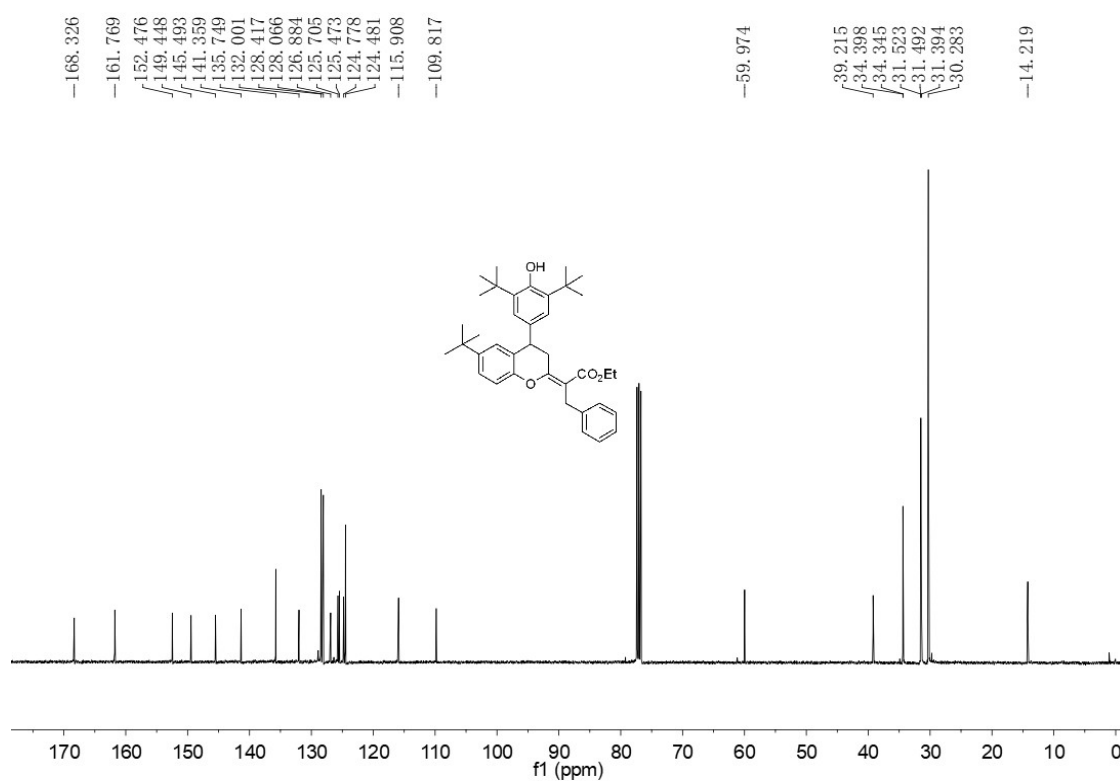
¹³C NMR (100 MHz, CDCl₃) of compound **3ia**



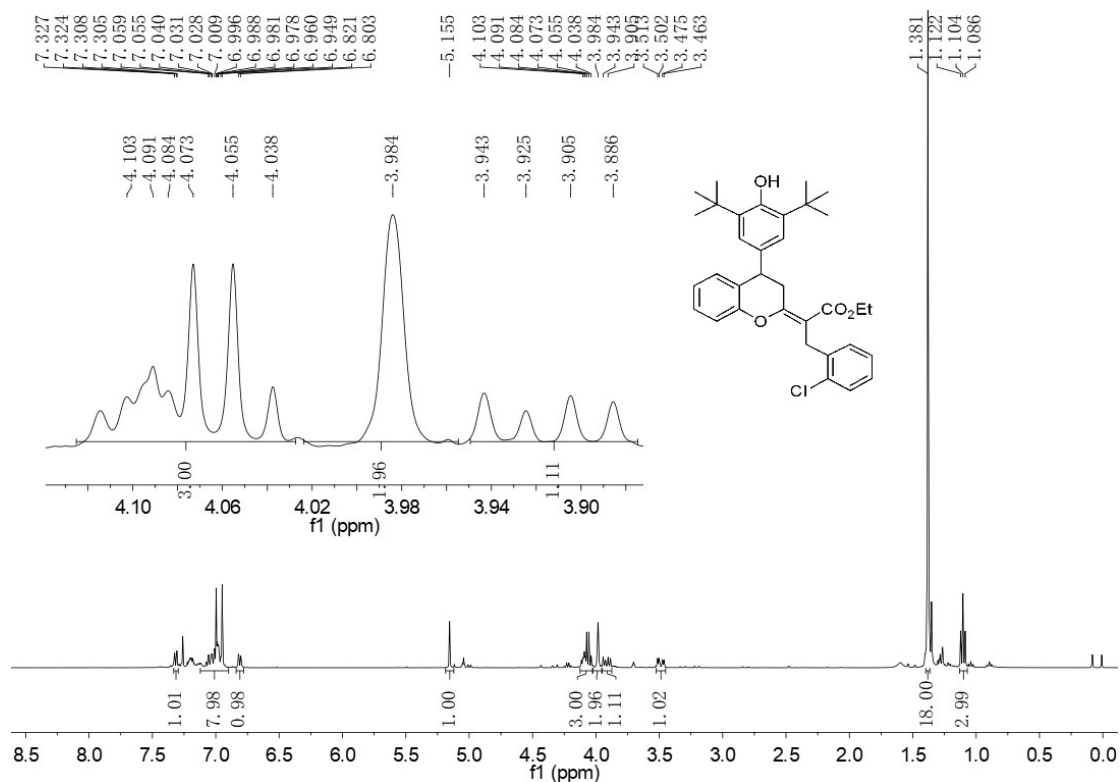
¹H NMR (400 MHz, CDCl₃) of compound **3ja**



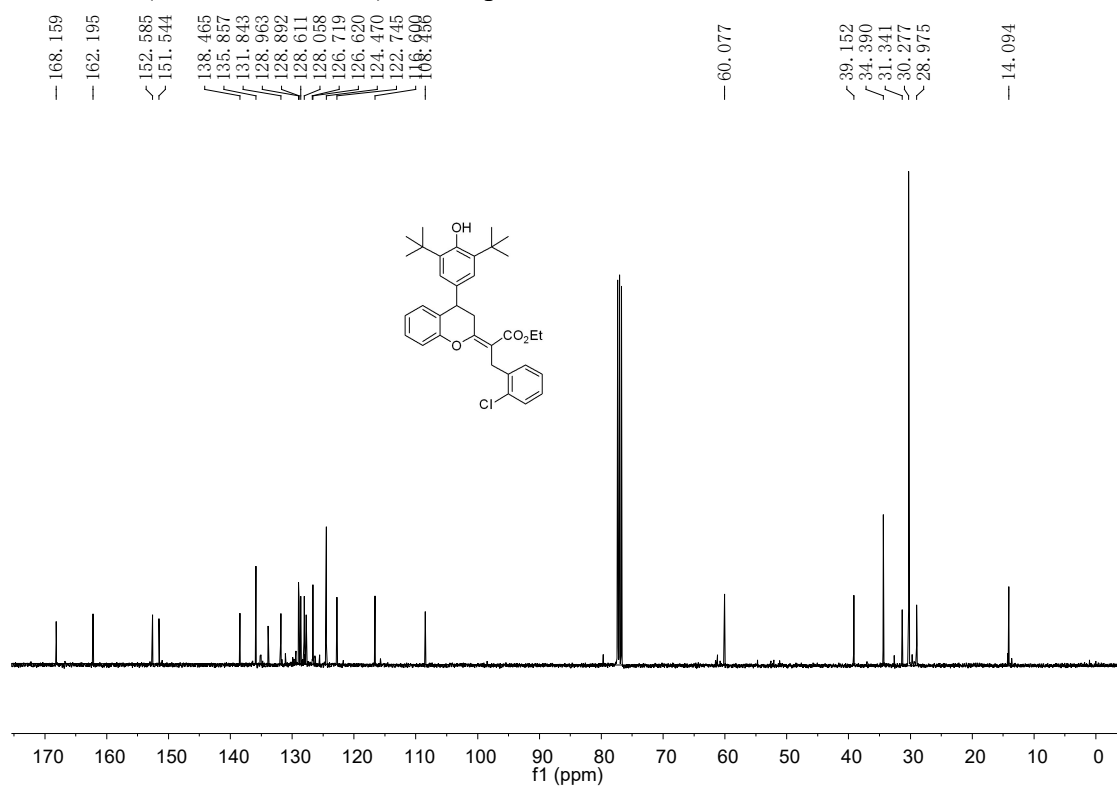
¹³C NMR (100 MHz, CDCl₃) of compound **3ja**



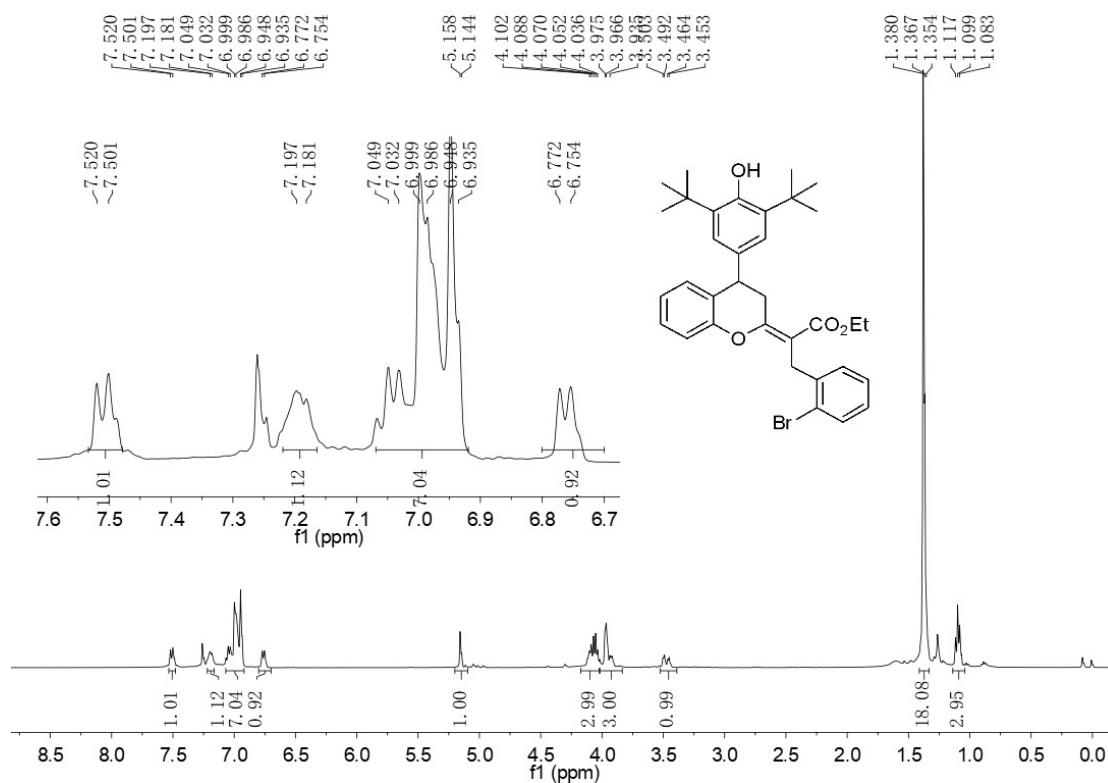
¹H NMR (400 MHz, CDCl₃) of compound **3ab**



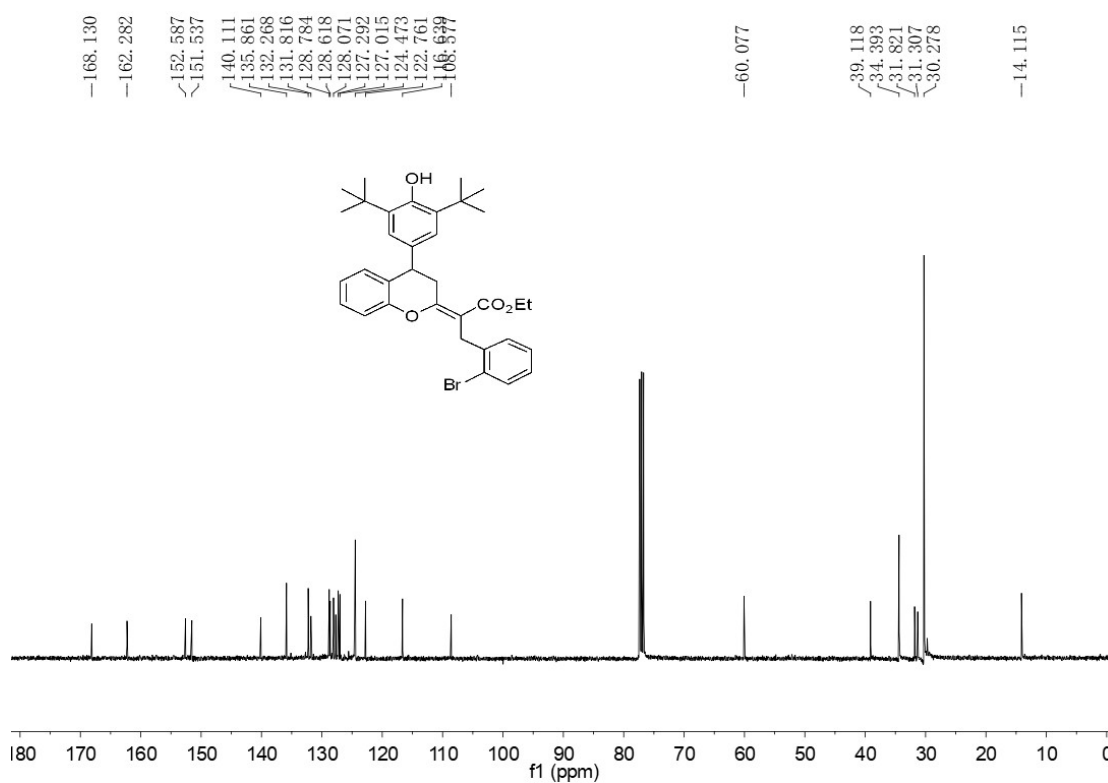
¹³C NMR (100 MHz, CDCl₃) of compound **3ab**



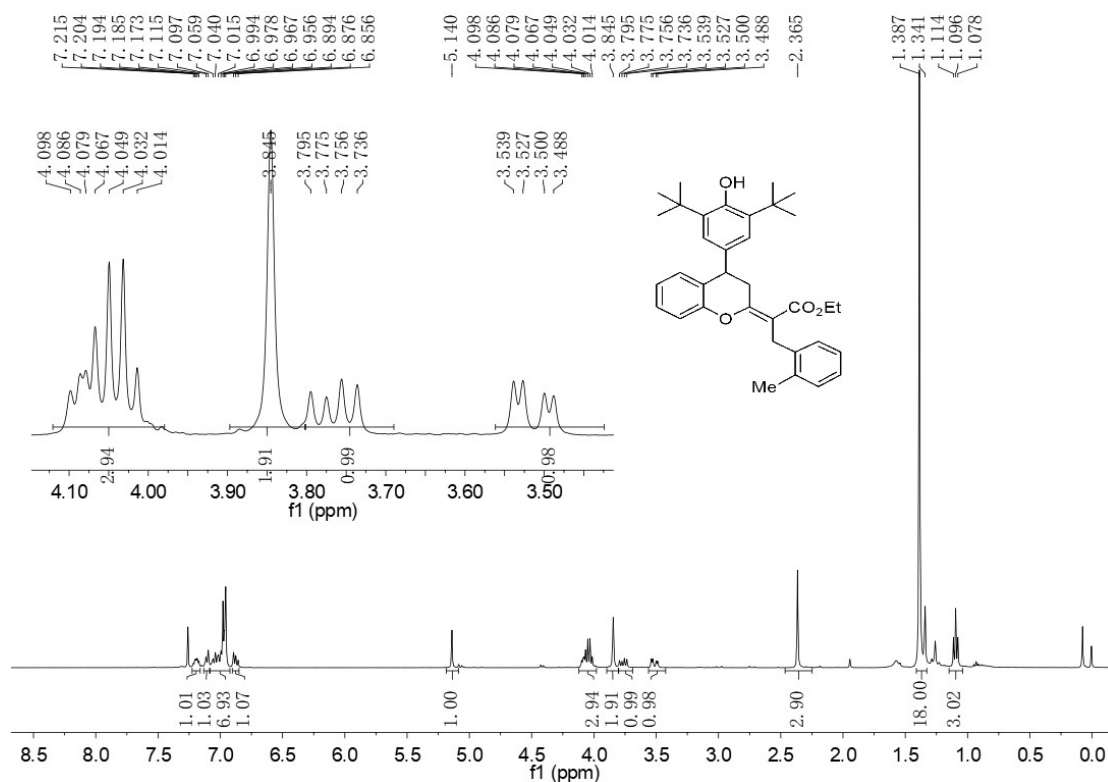
¹H NMR (400 MHz, CDCl₃) of compound **3ac**



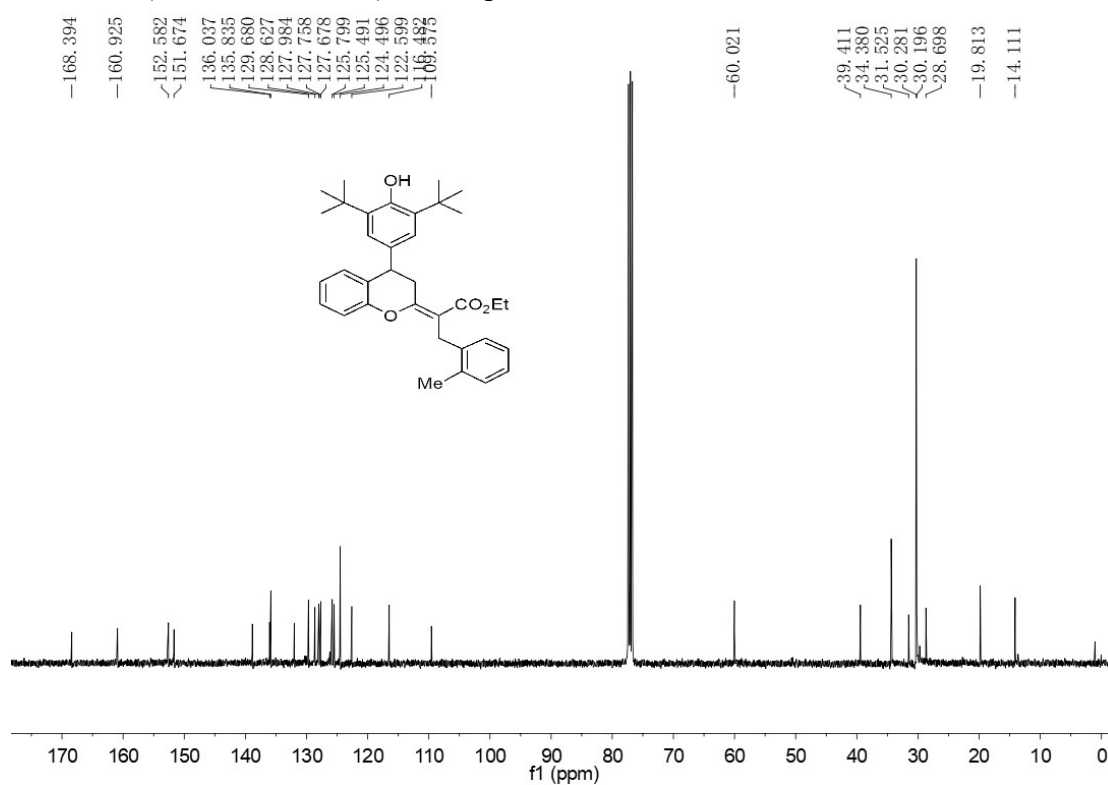
¹³C NMR (100 MHz, CDCl₃) of compound **3ac**



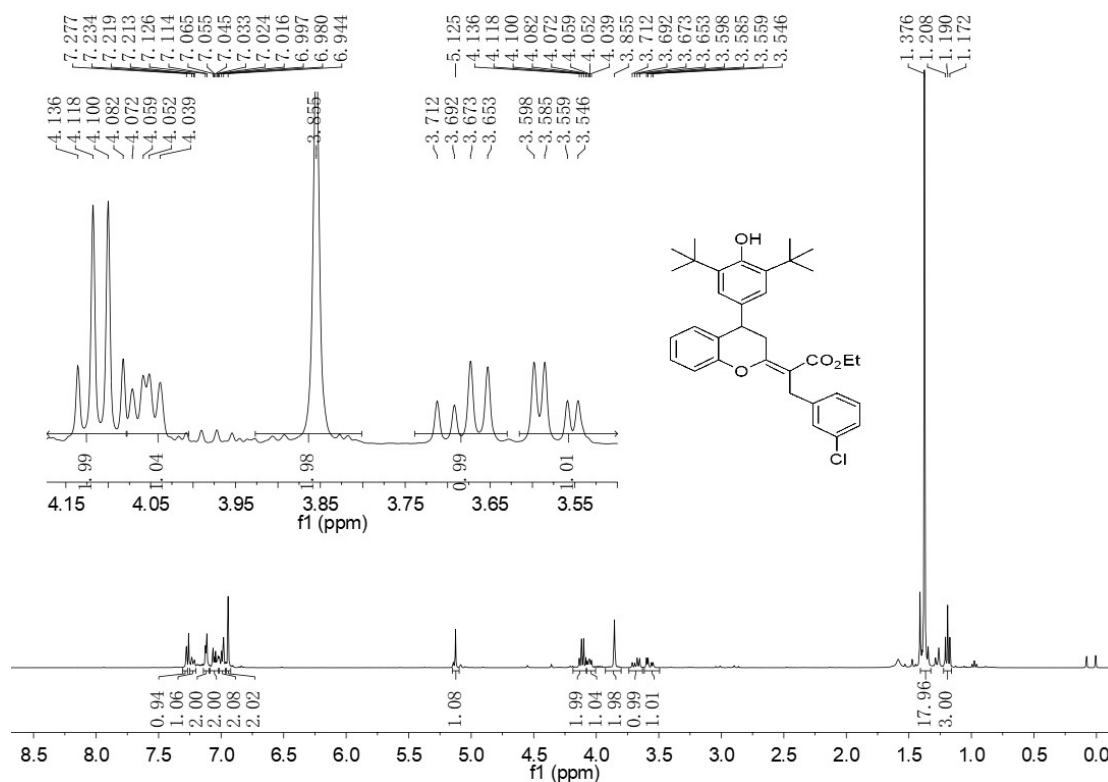
¹H NMR (400 MHz, CDCl₃) of compound **3ad**



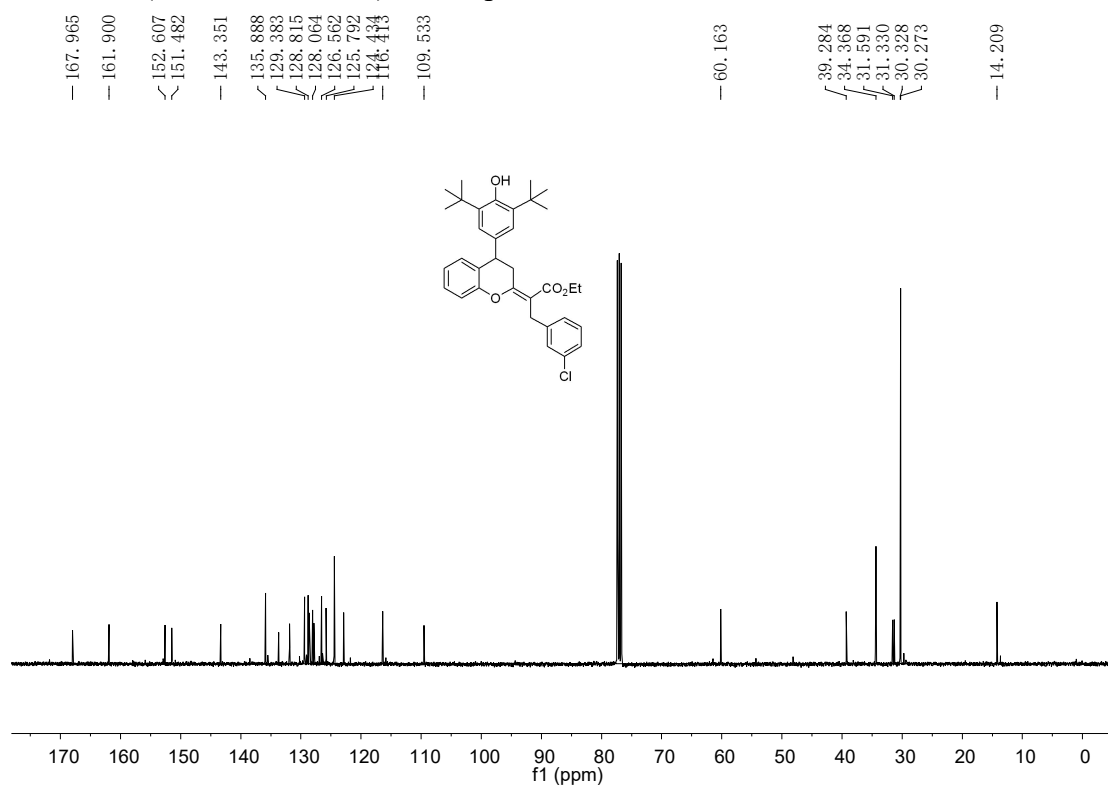
¹³C NMR (100 MHz, CDCl₃) of compound **3ad**



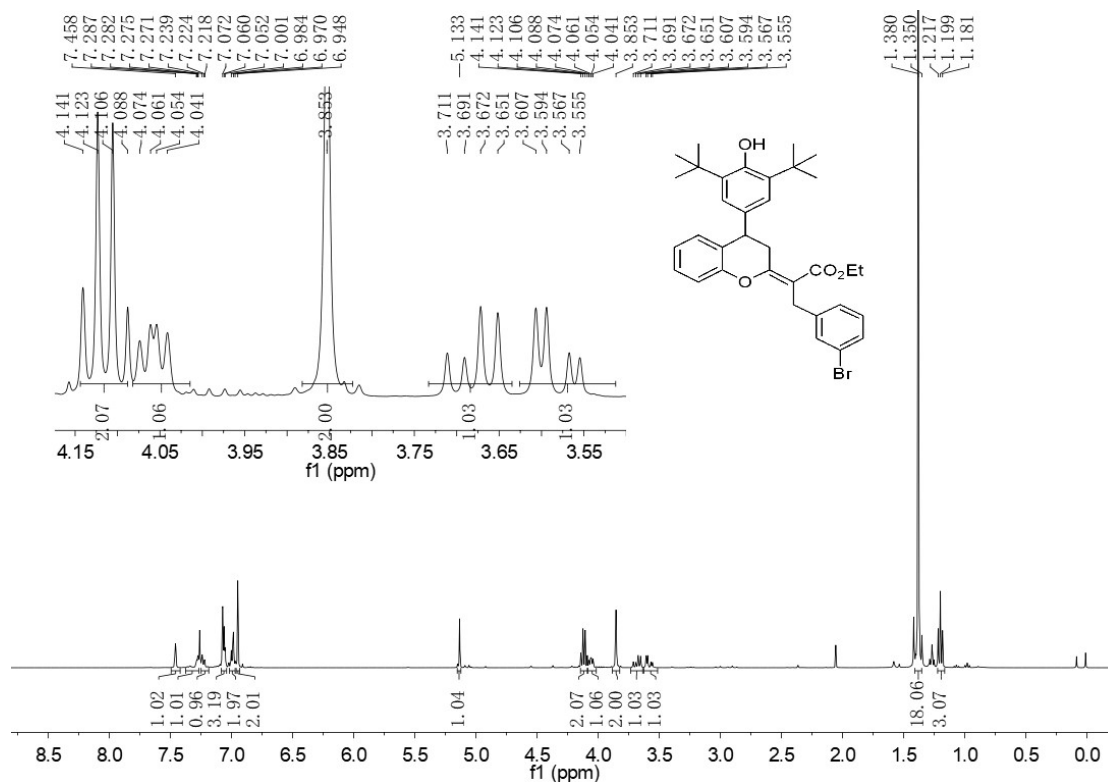
¹H NMR (400 MHz, CDCl₃) of compound **3ae**



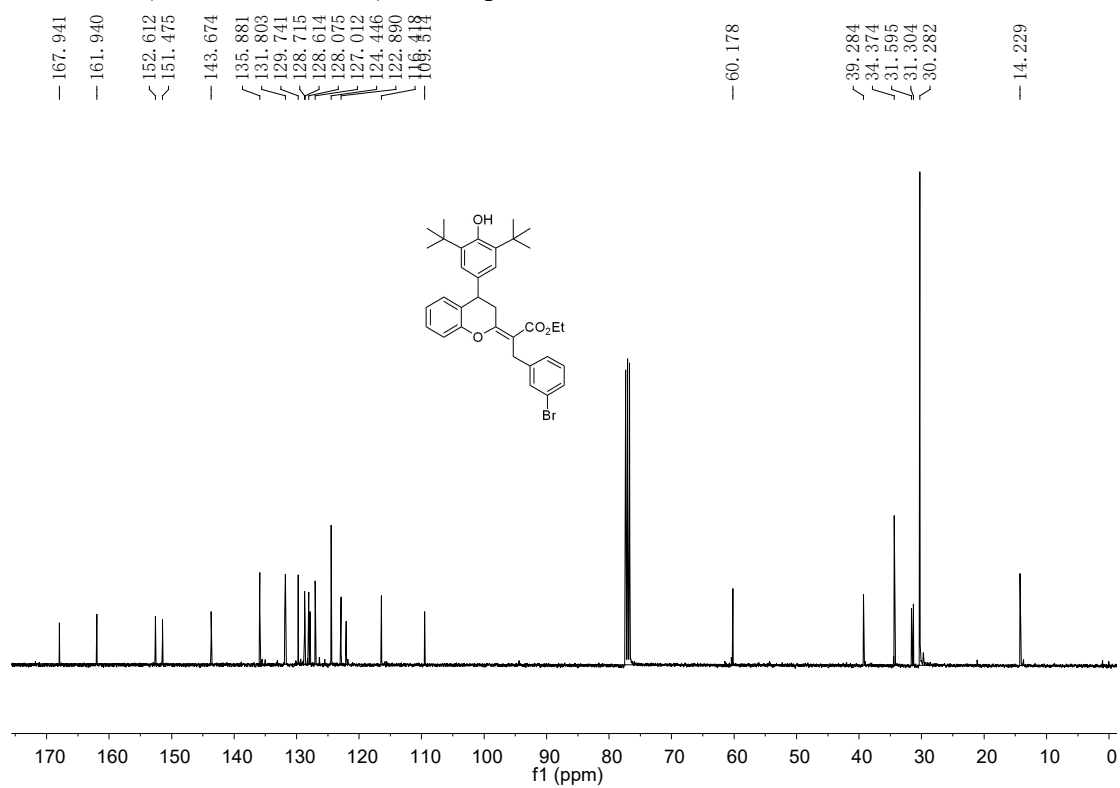
¹³C NMR (100 MHz, CDCl₃) of compound **3ae**



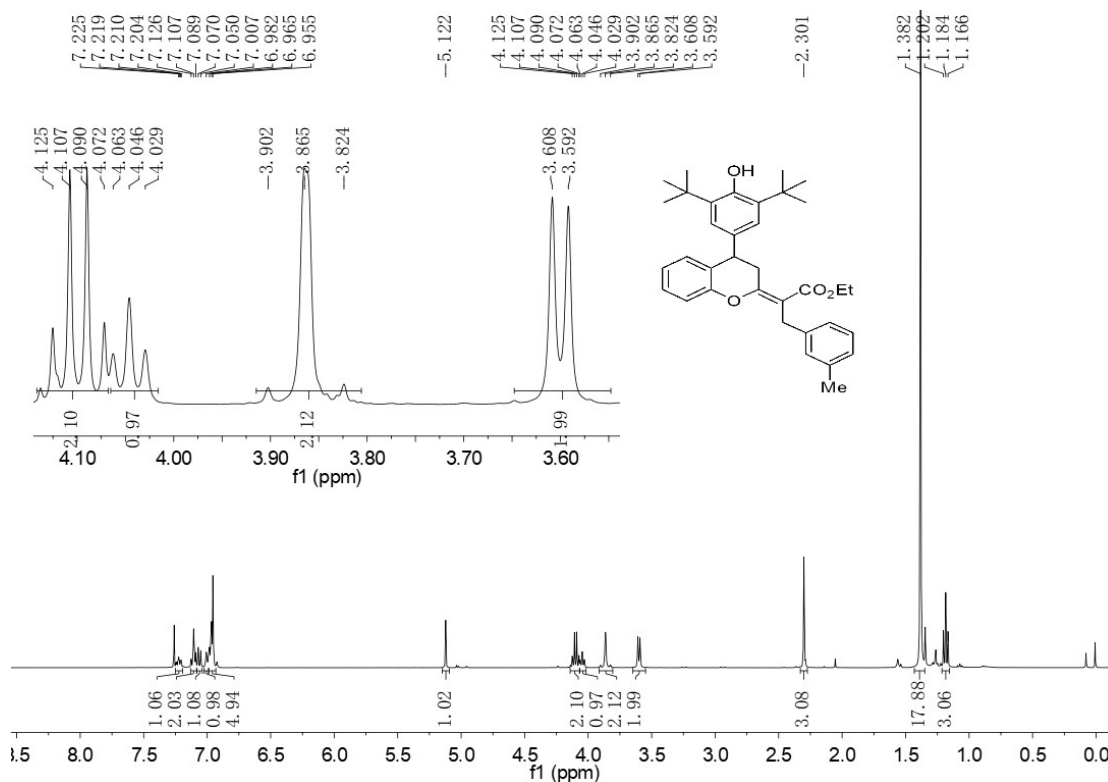
¹H NMR (400 MHz, CDCl₃) of compound **3af**



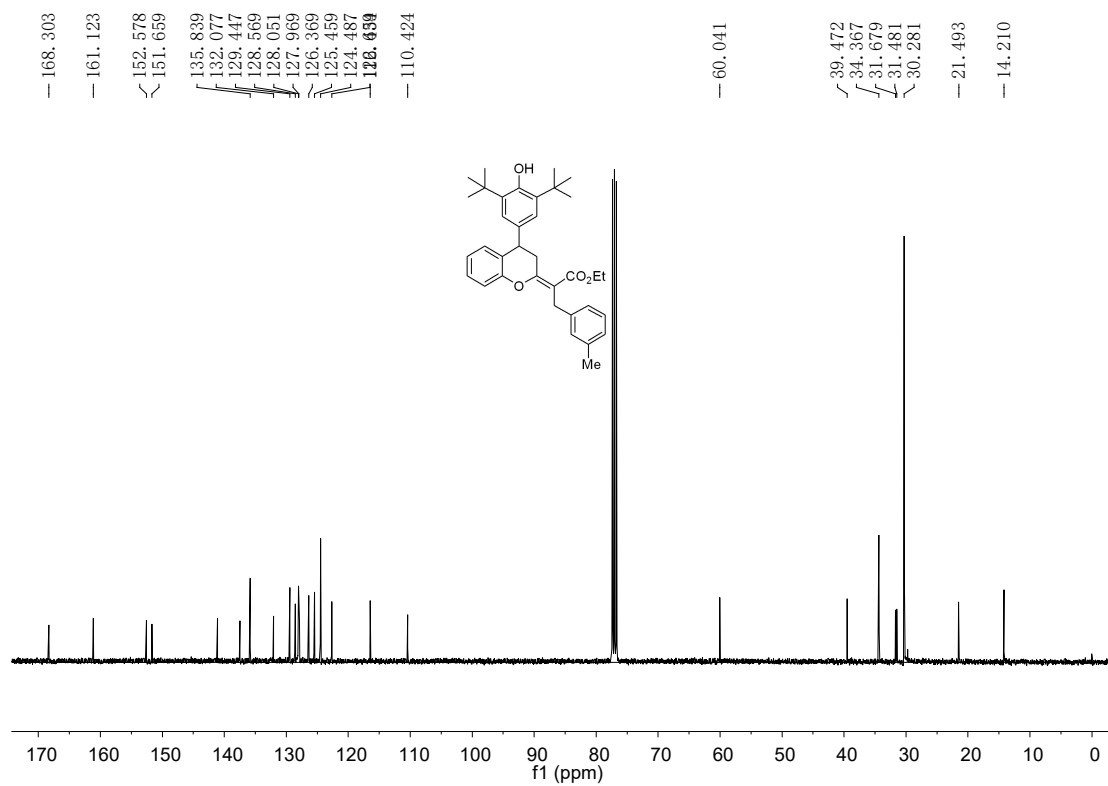
¹³C NMR (100 MHz, CDCl₃) of compound **3af**



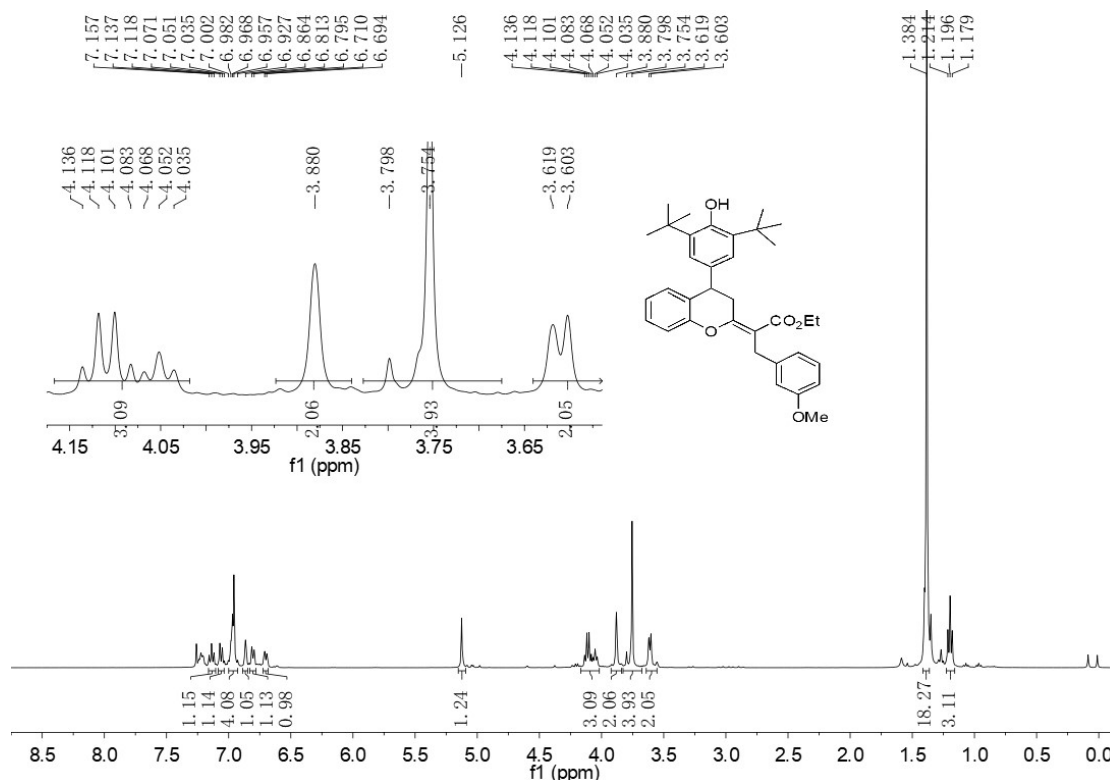
^1H NMR (400 MHz, CDCl_3) of compound **3ag**



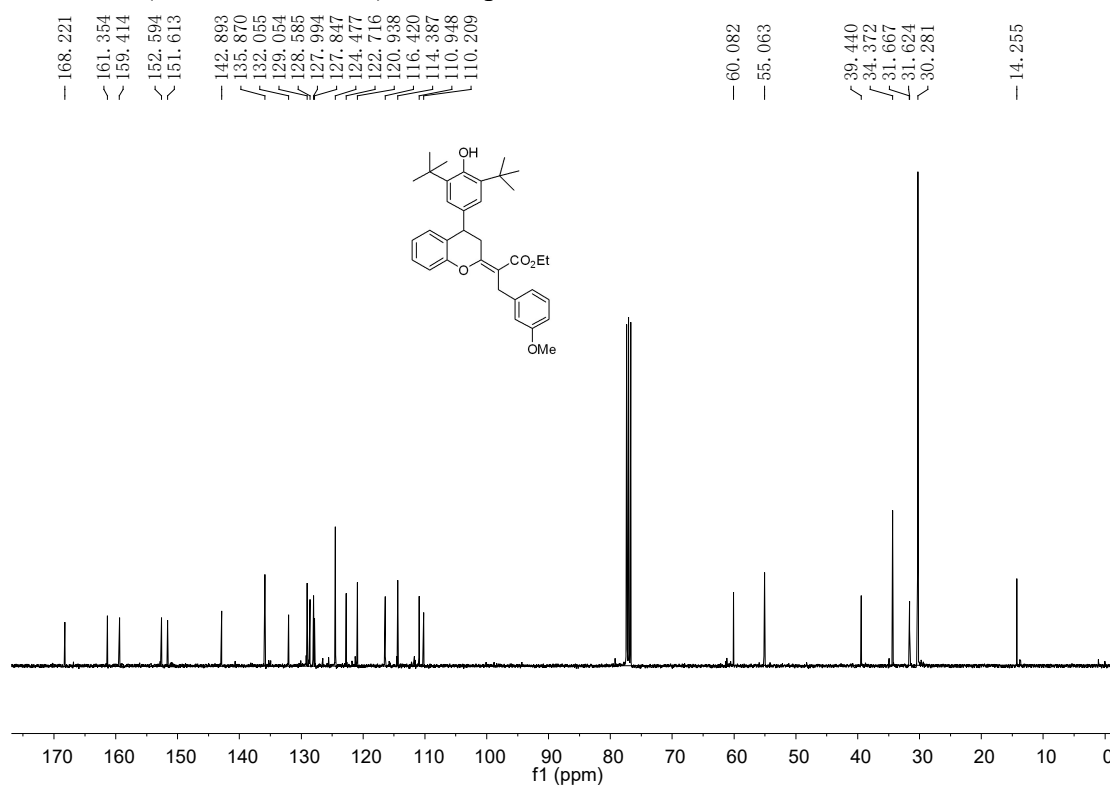
^{13}C NMR (100 MHz, CDCl_3) of compound **3ag**



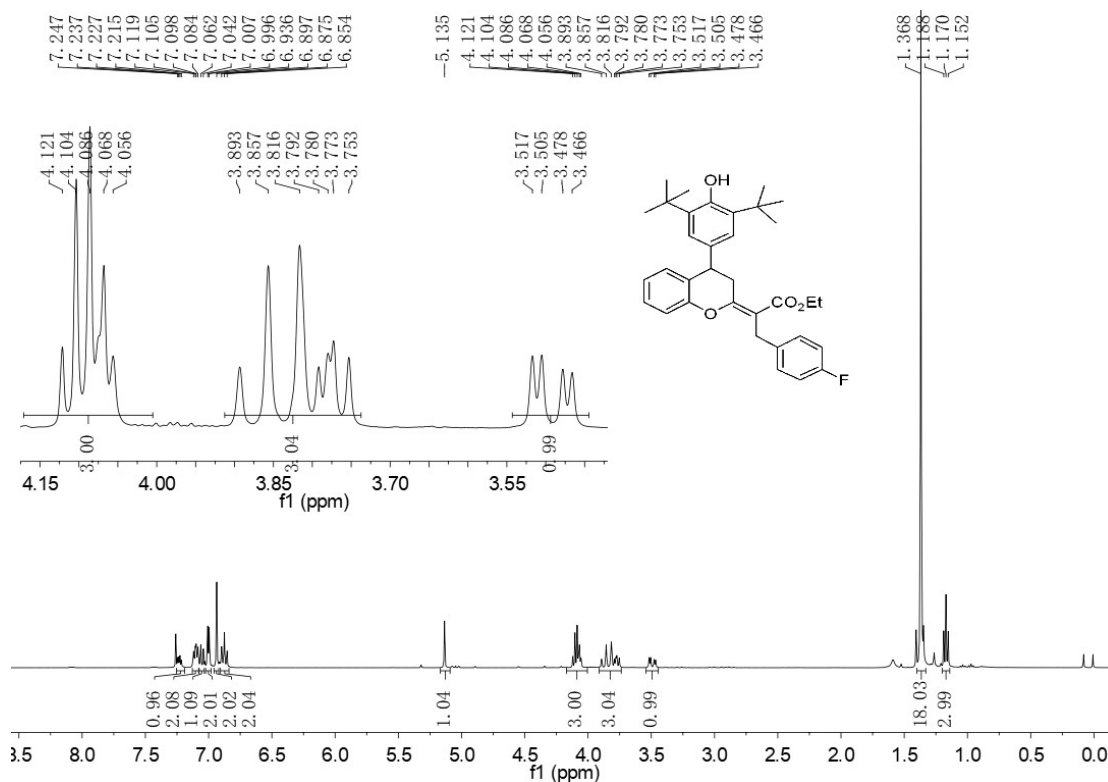
^1H NMR (400 MHz, CDCl_3) of compound **3ah**



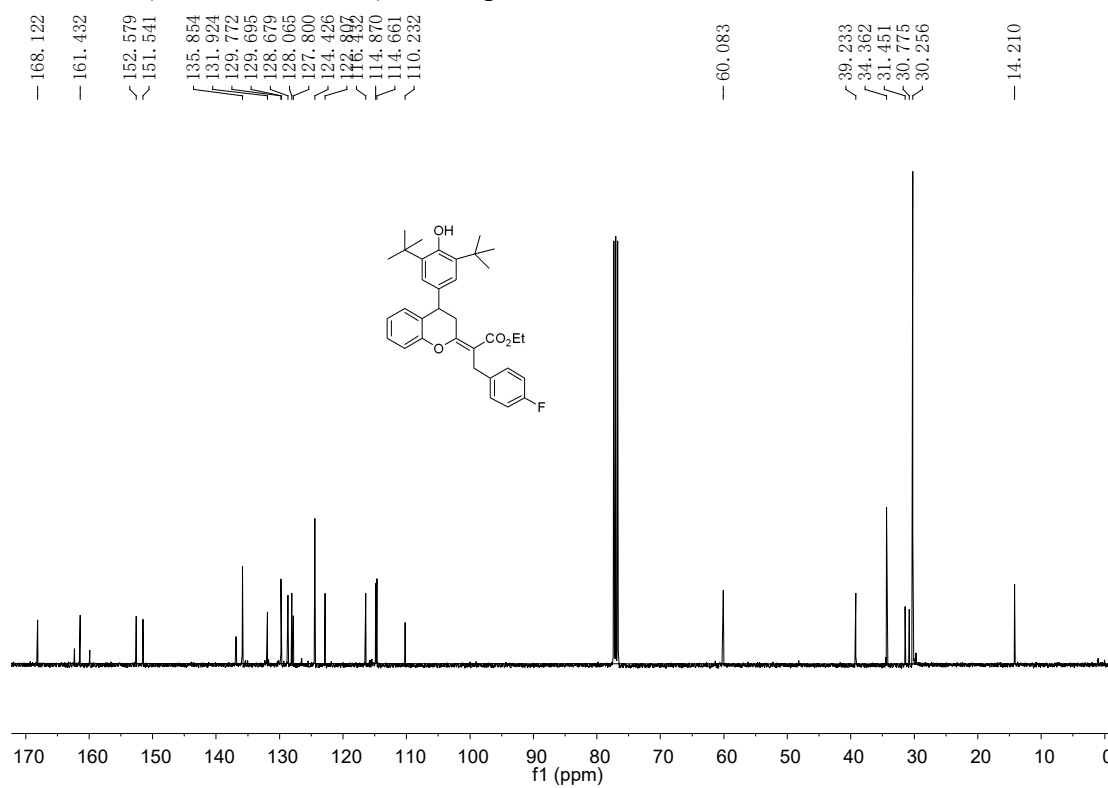
^{13}C NMR (100 MHz, CDCl_3) of compound **3ah**



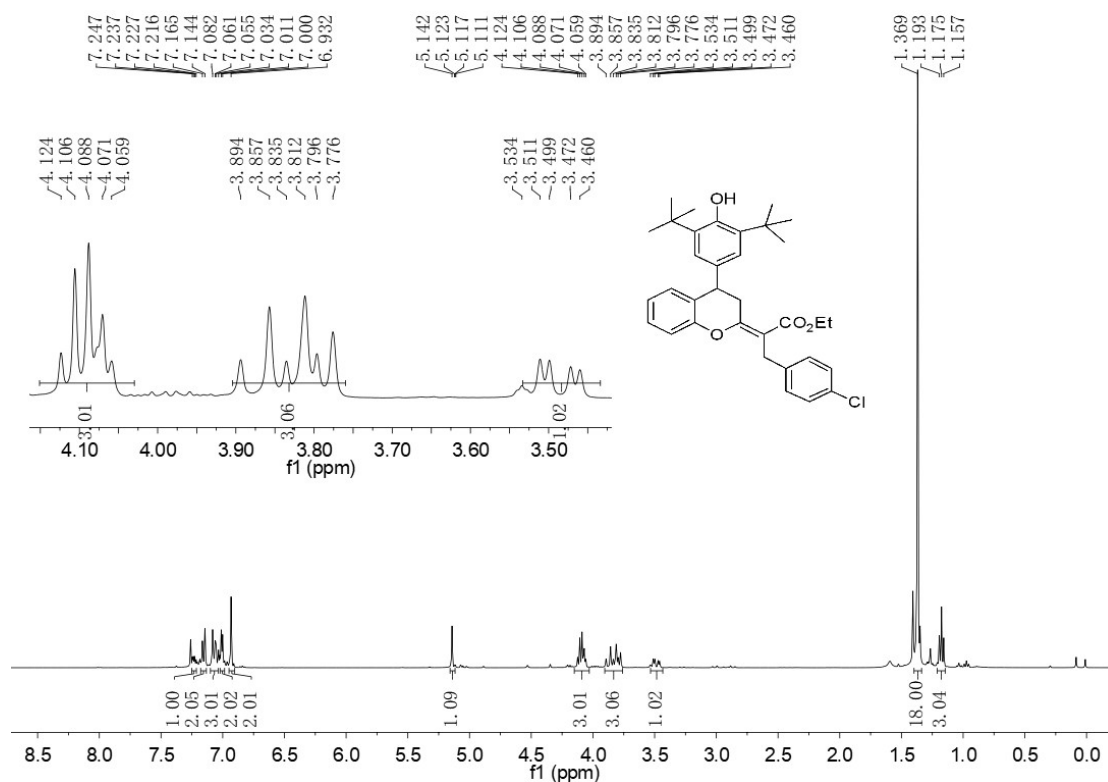
¹H NMR (400 MHz, CDCl₃) of compound **3ai**



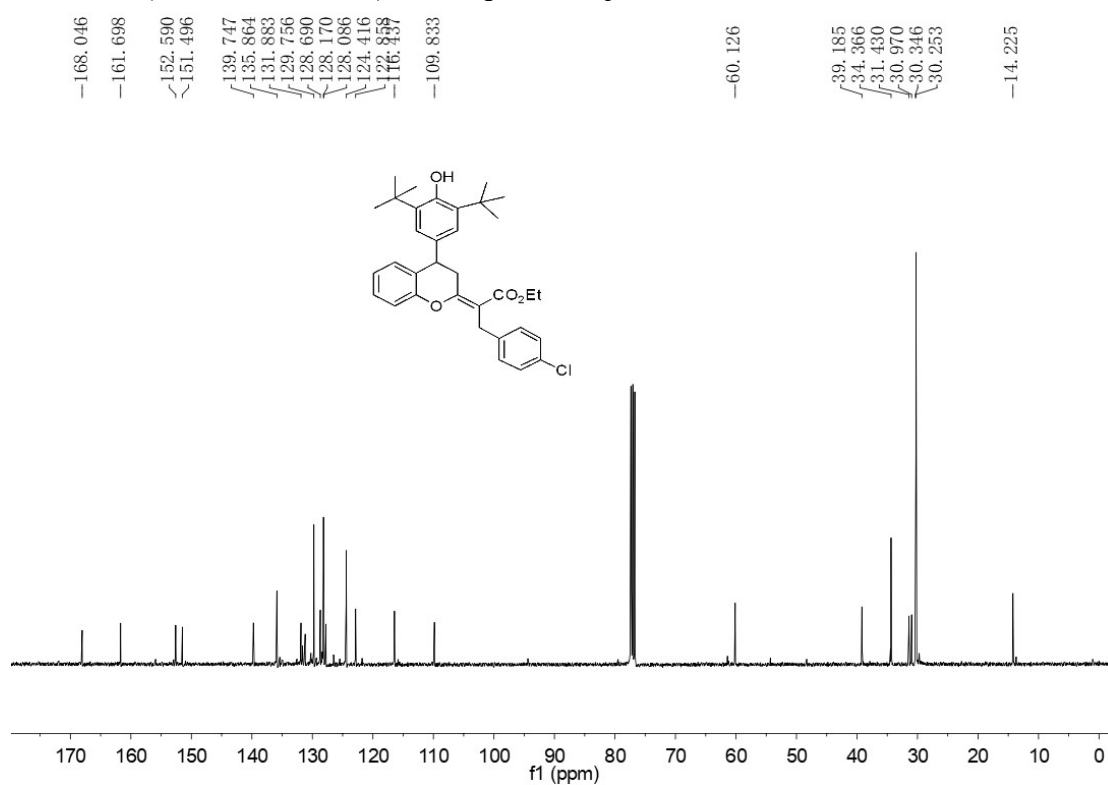
¹³C NMR (100 MHz, CDCl₃) of compound **3ai**



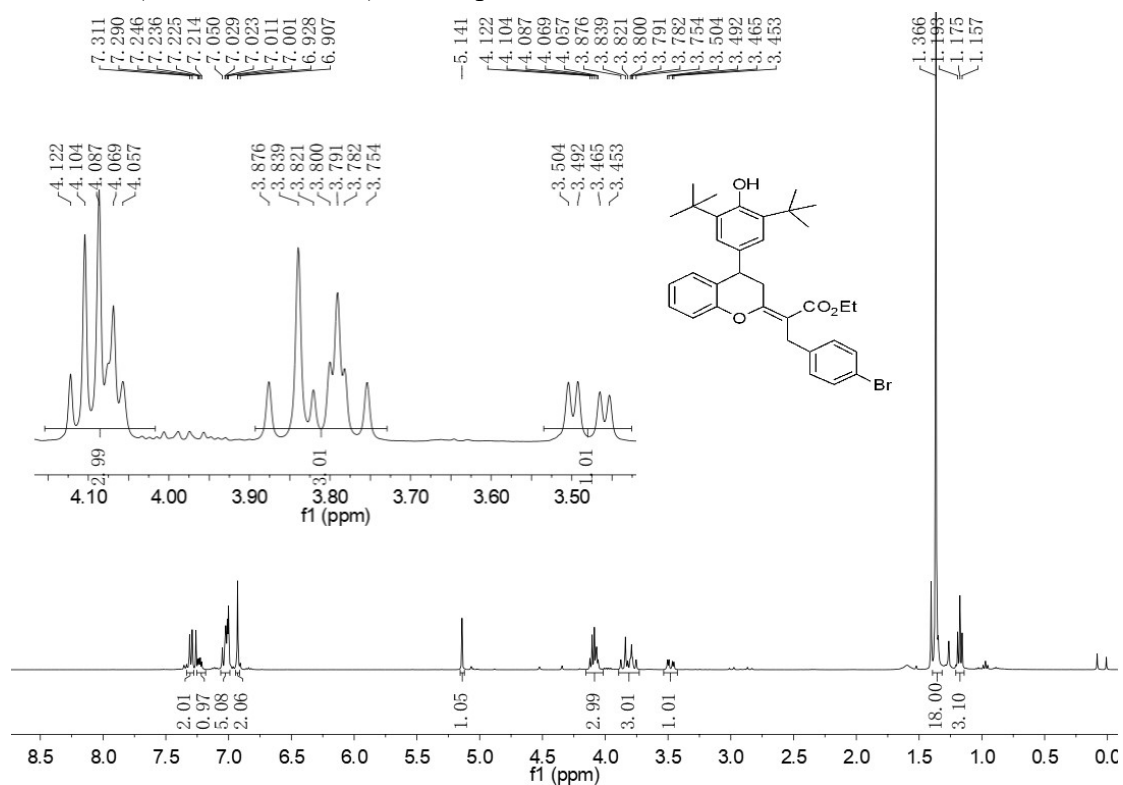
¹H NMR (400 MHz, CDCl₃) of compound **3aj**



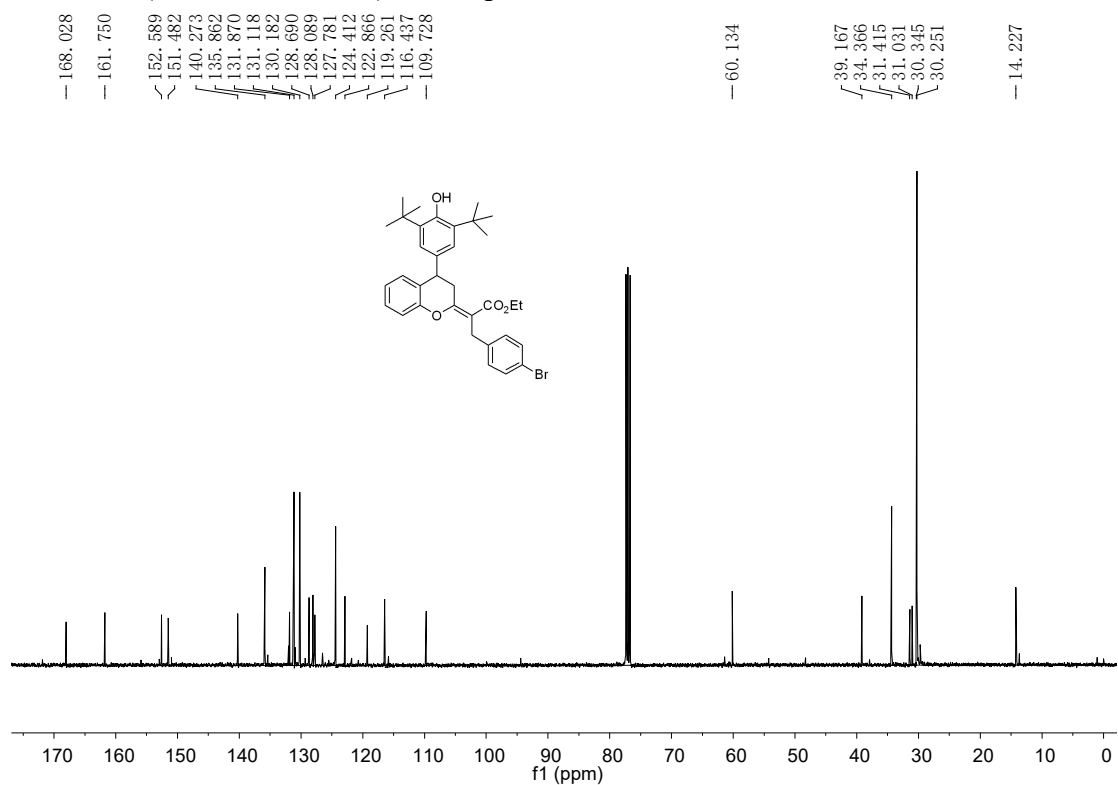
¹³C NMR (100 MHz, CDCl₃) of compound **3aj**



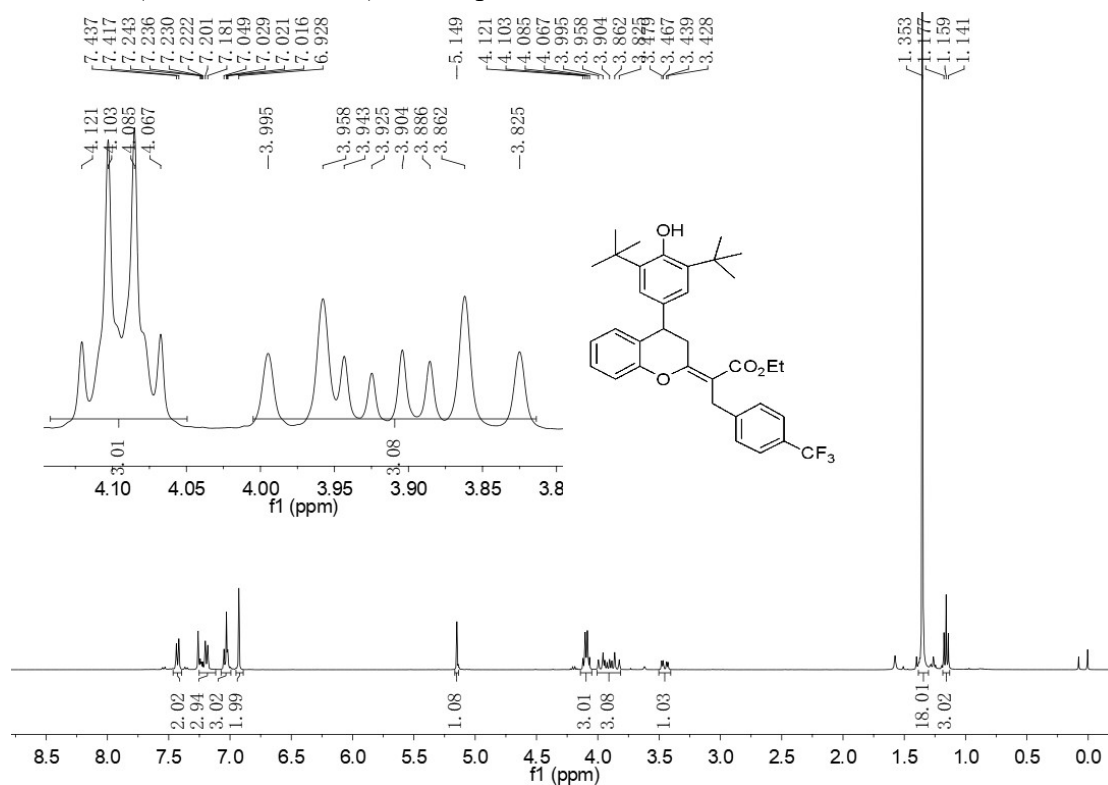
¹H NMR (400 MHz, CDCl₃) of compound **3ak**



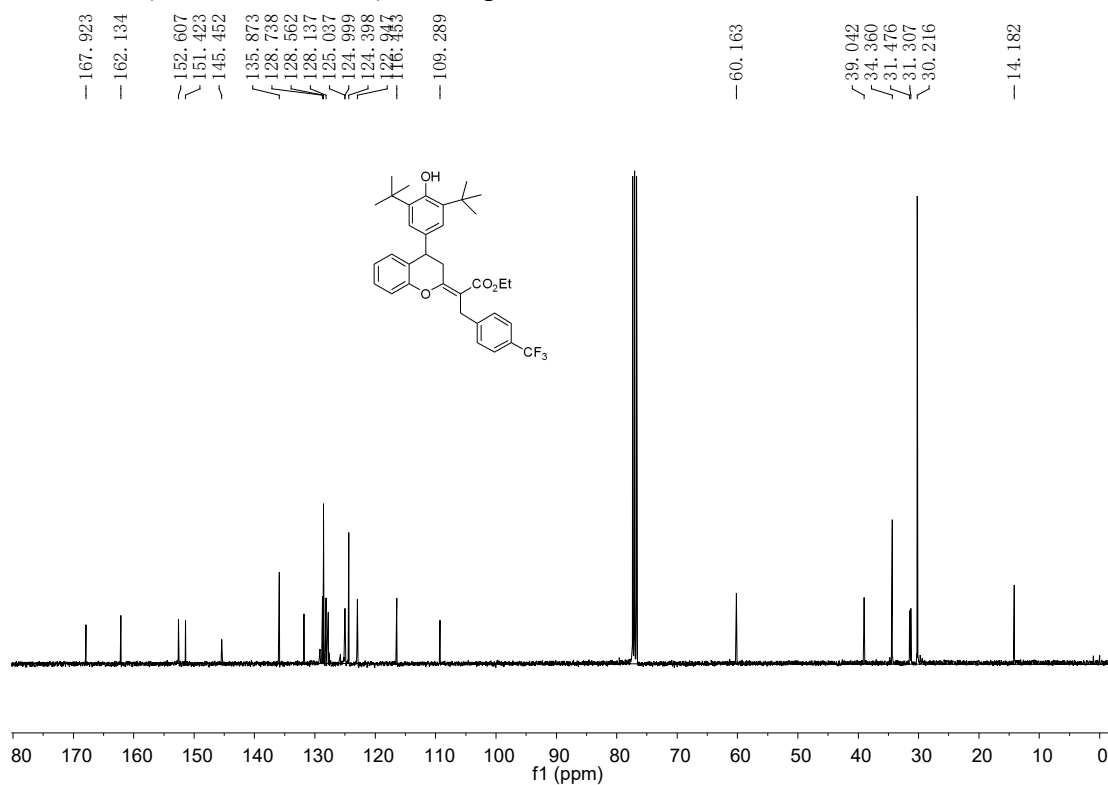
¹³C NMR (100 MHz, CDCl₃) of compound **3ak**



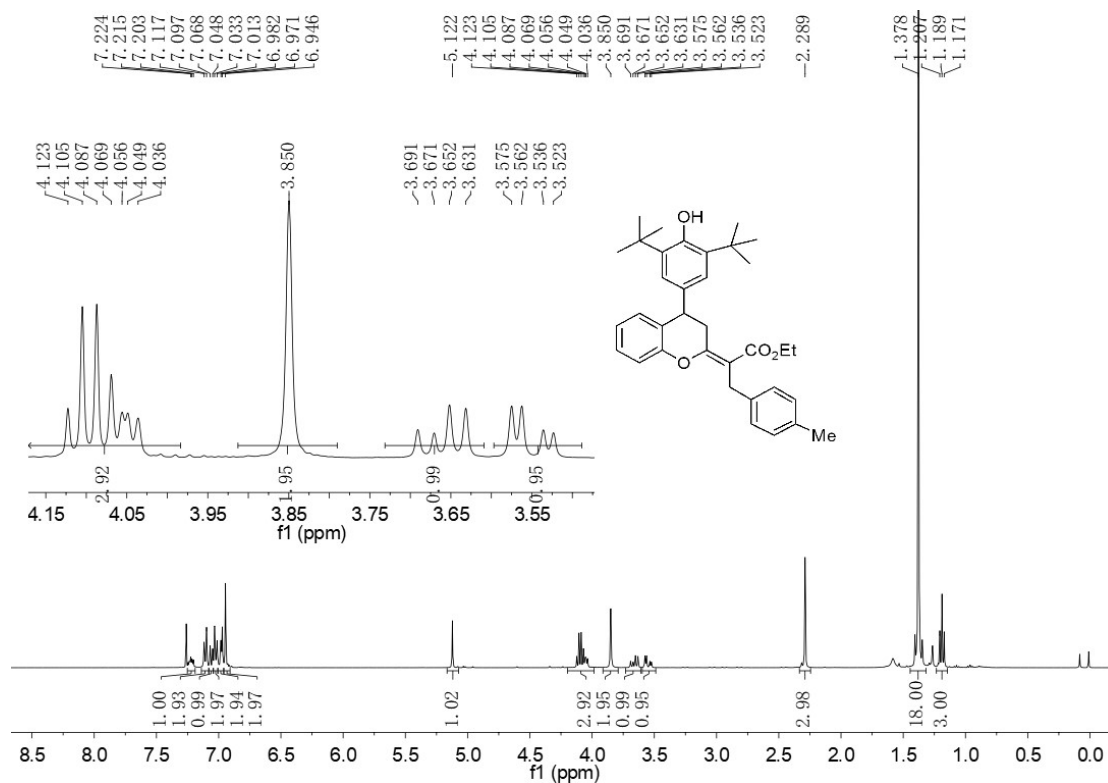
^1H NMR (400 MHz, CDCl_3) of compound **3al**



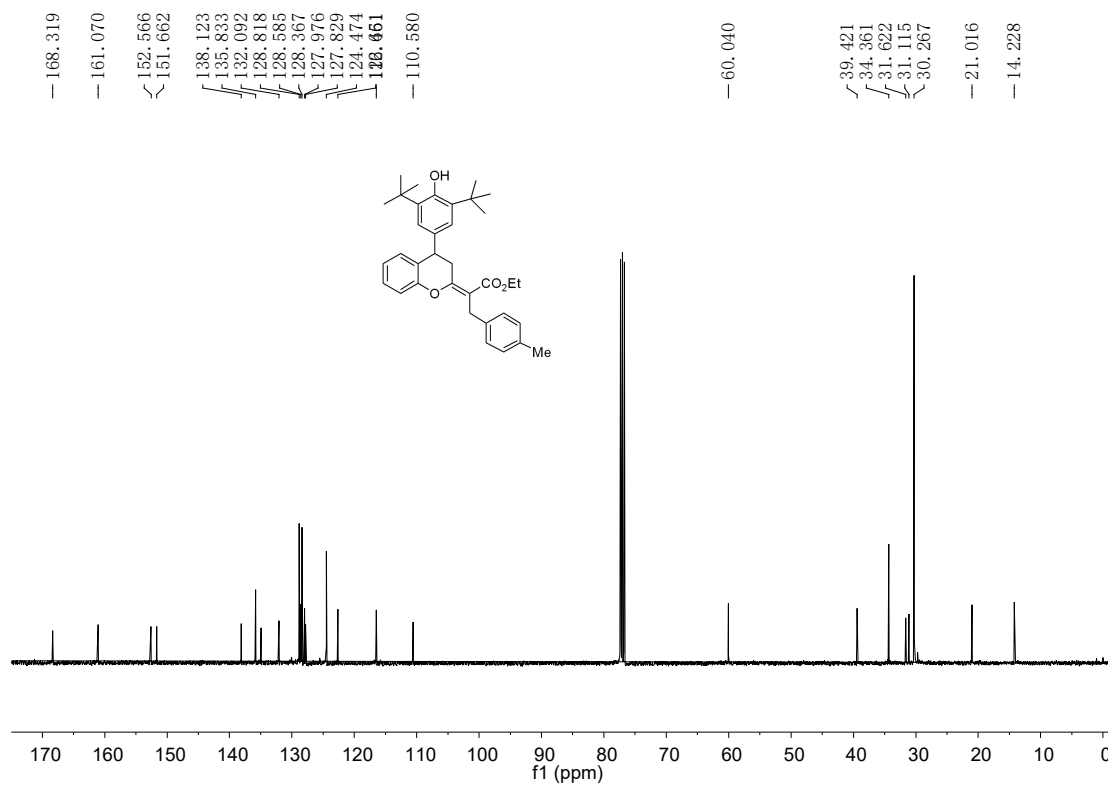
^{13}C NMR (100 MHz, CDCl_3) of compound **3al**



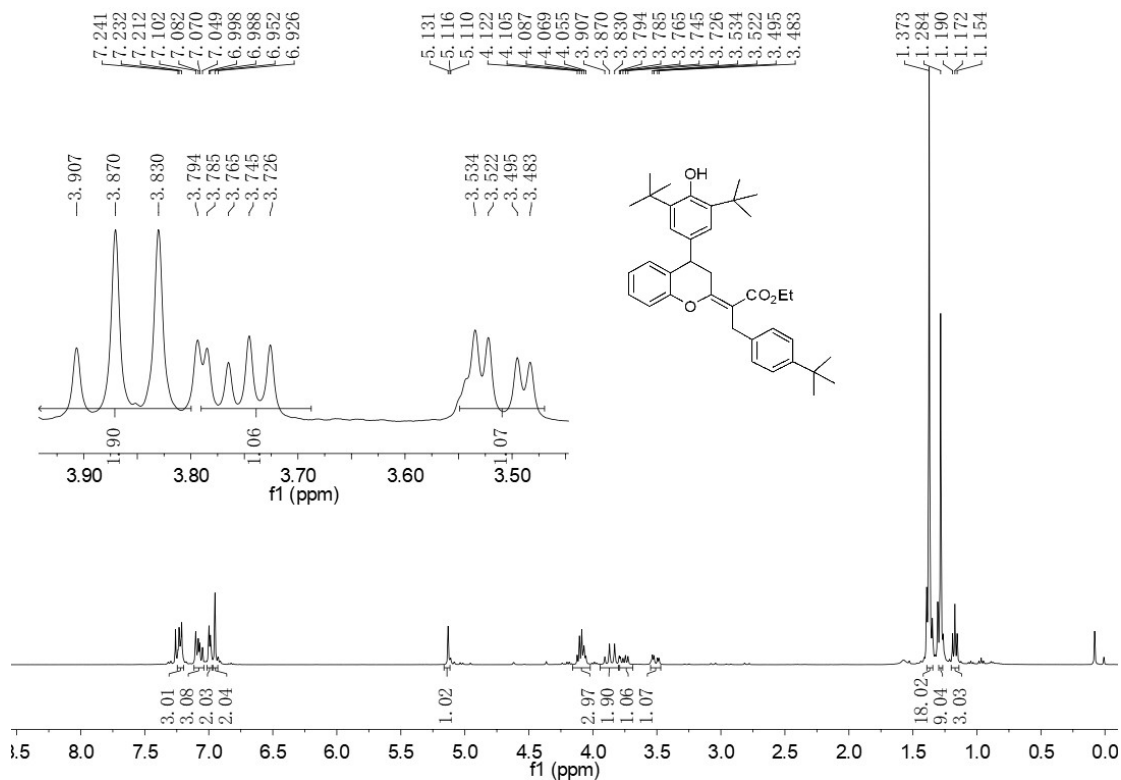
¹H NMR (400 MHz, CDCl₃) of compound **3am**



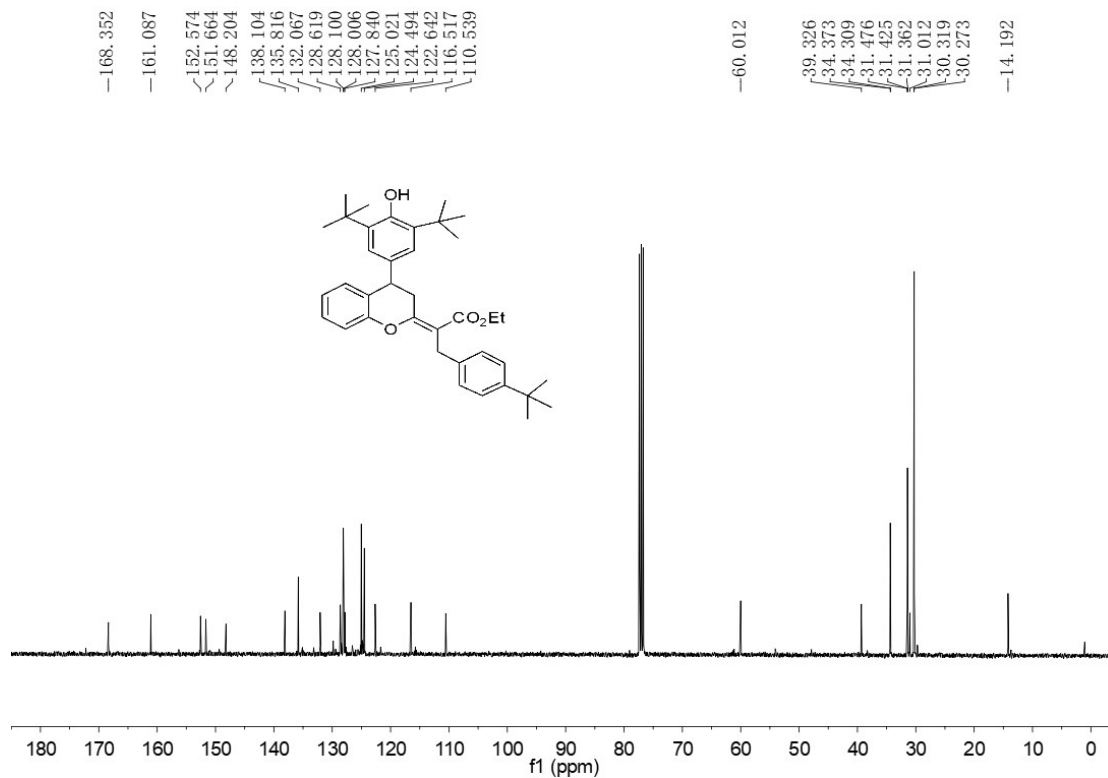
¹³C NMR (100 MHz, CDCl₃) of compound **3am**



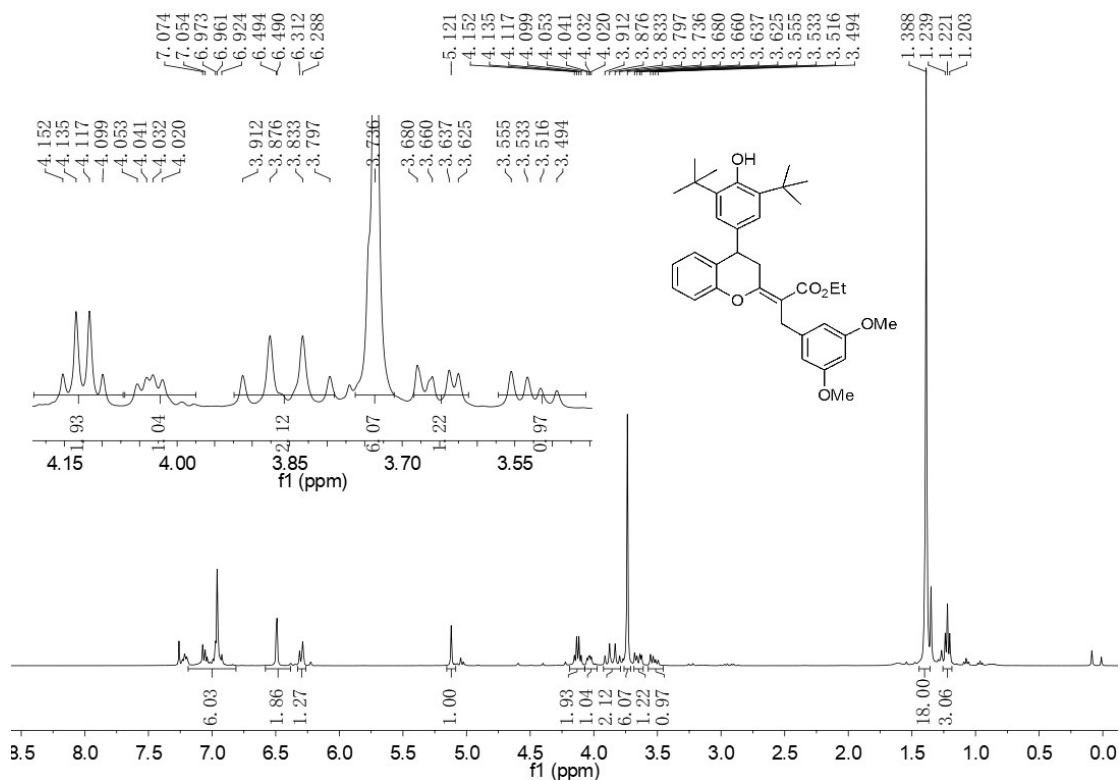
¹H NMR (400 MHz, CDCl₃) of compound **3an**



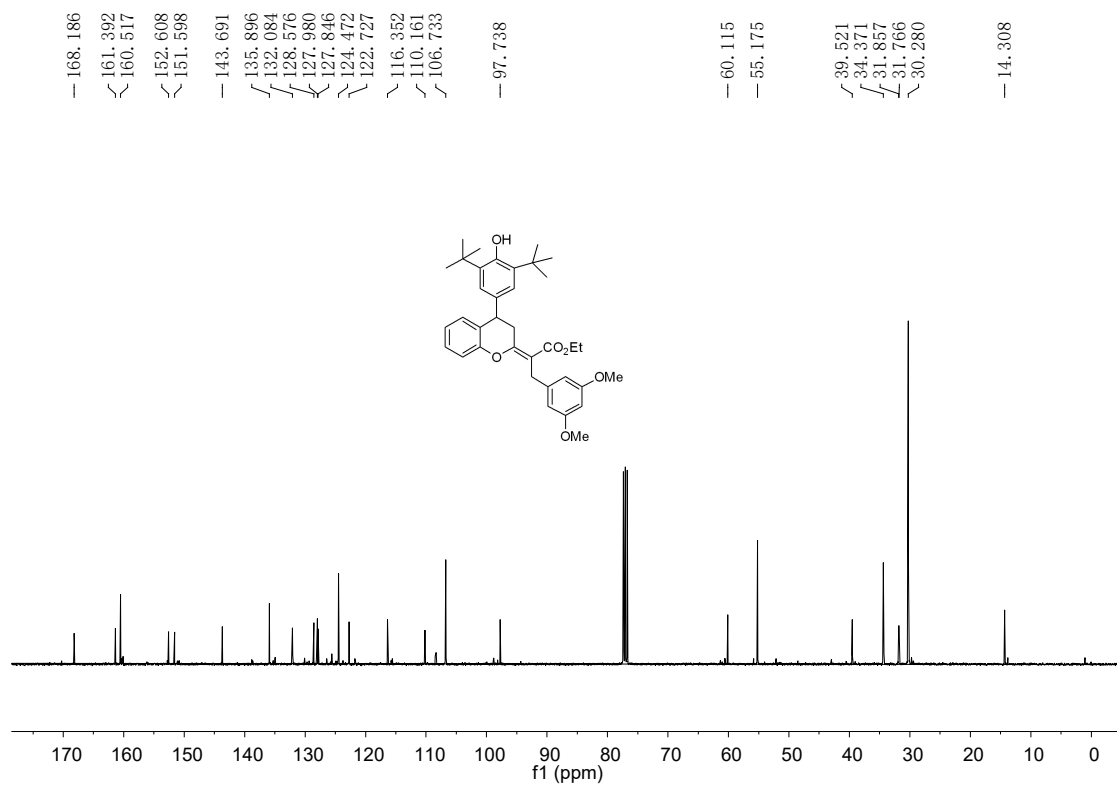
¹³C NMR (100 MHz, CDCl₃) of compound **3an**



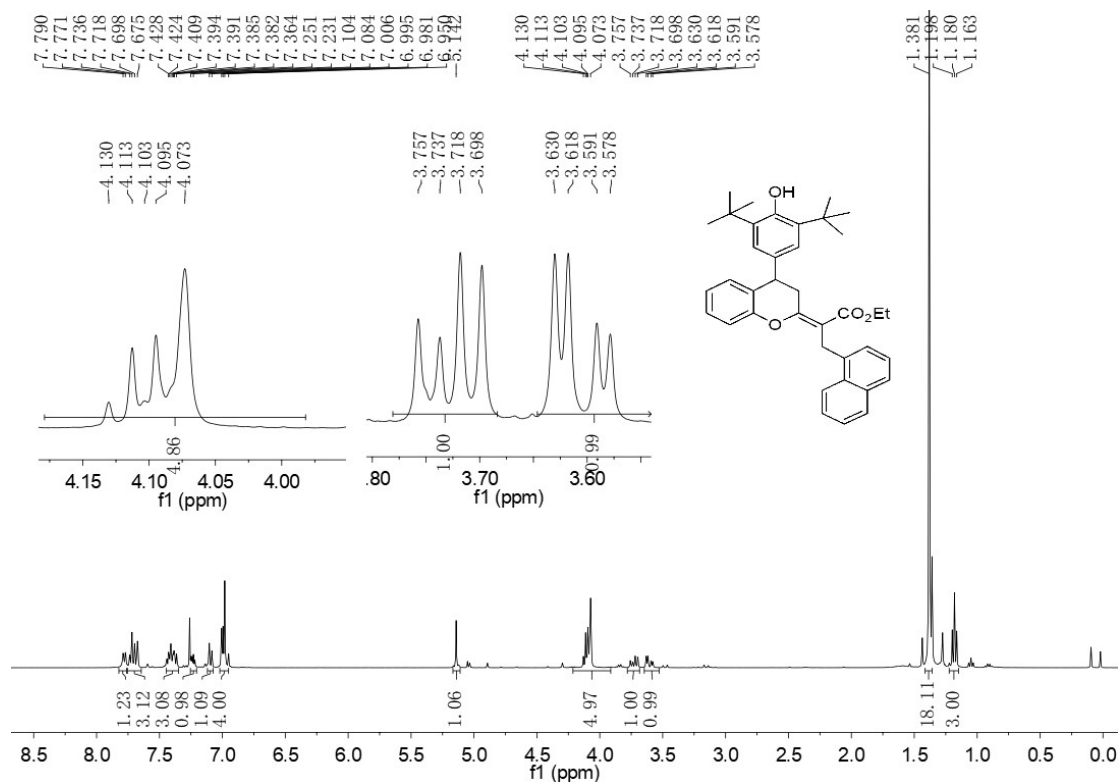
^1H NMR (400 MHz, CDCl_3) of compound **3ao**



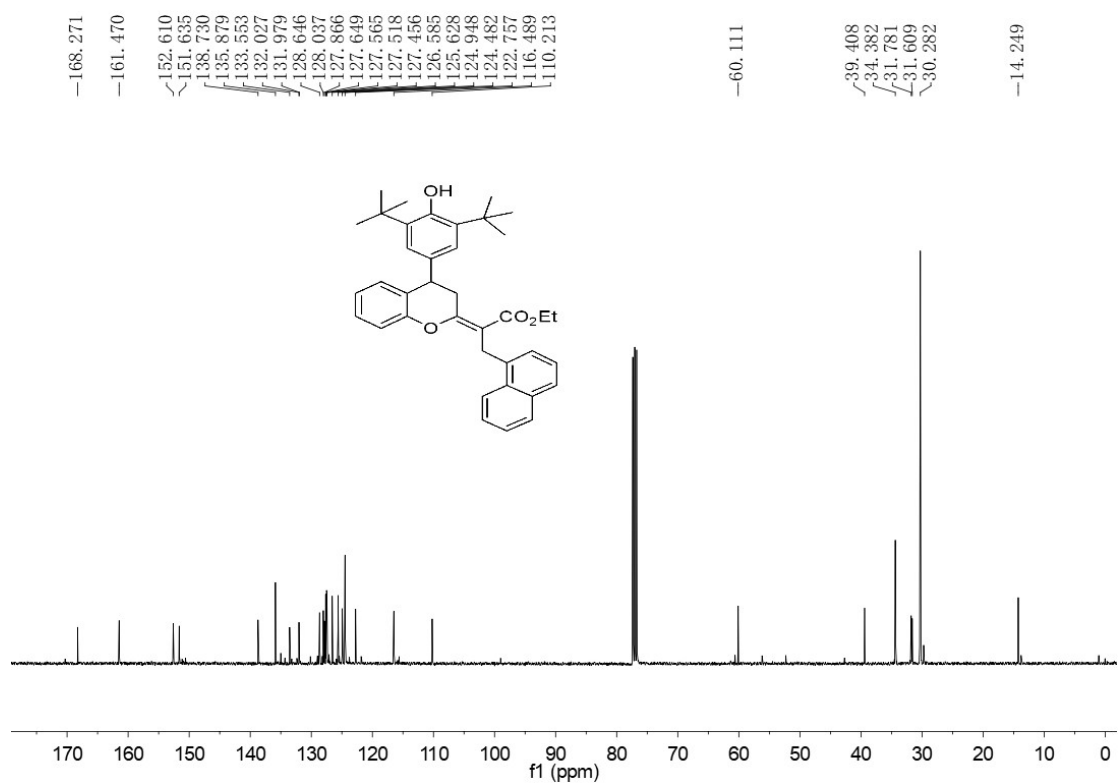
^{13}C NMR (100 MHz, CDCl_3) of compound **3ao**



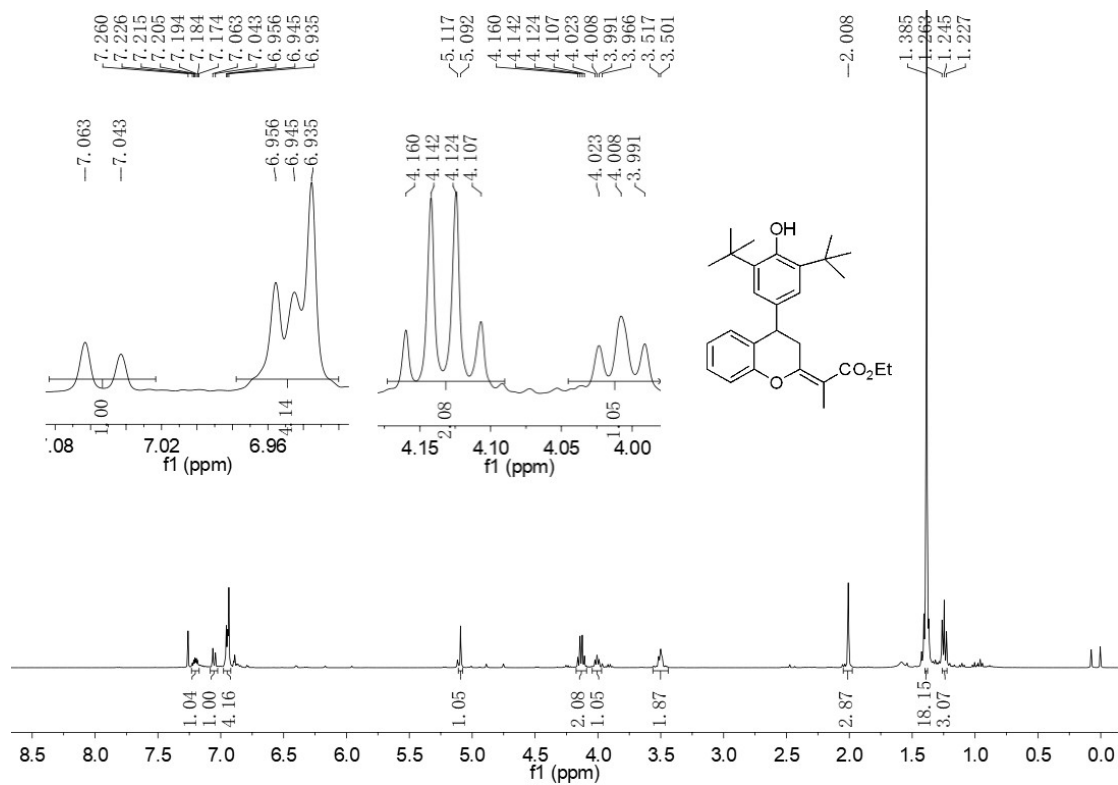
¹H NMR (400 MHz, CDCl₃) of compound **3ap**



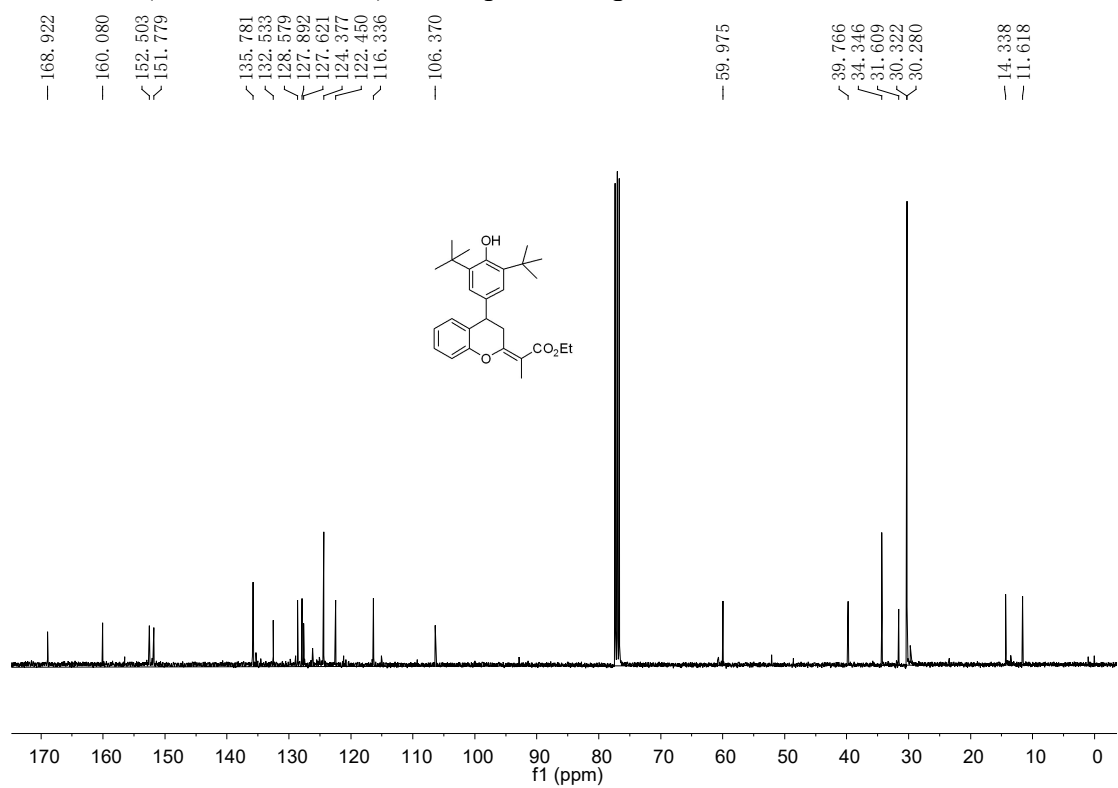
¹³C NMR (100 MHz, CDCl₃) of compound **3ap**



¹H NMR (400 MHz, CDCl₃) of compound **3aq**

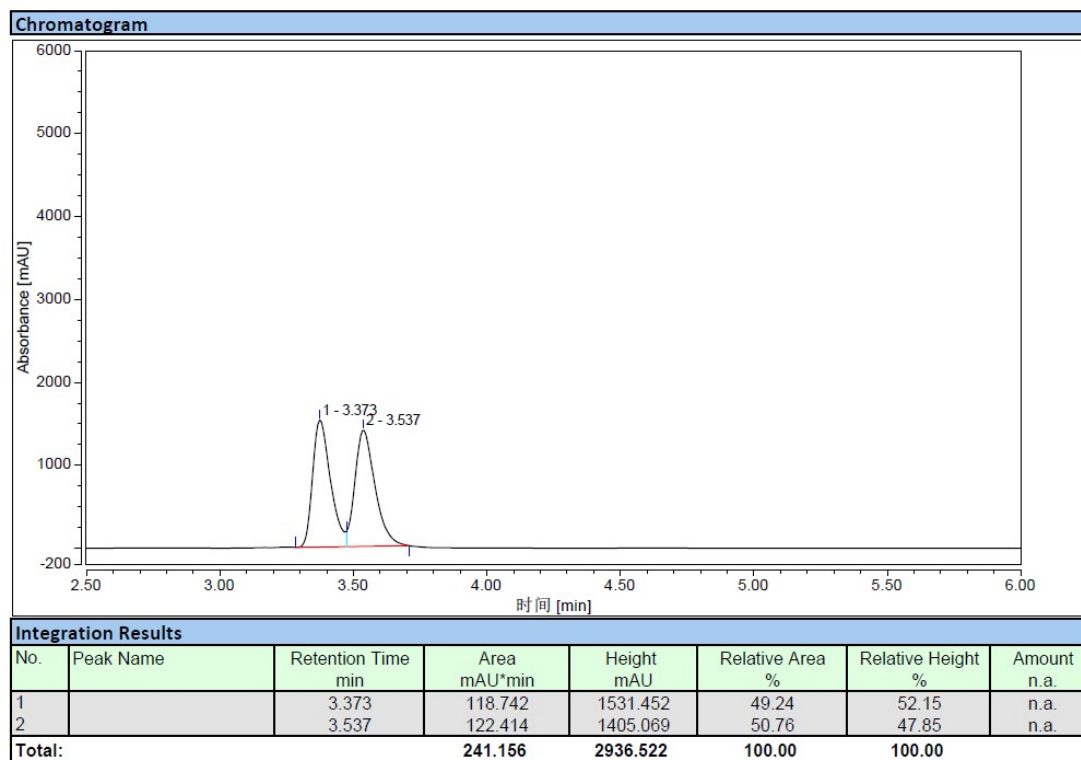


¹³C NMR (100 MHz, CDCl₃) of compound **3aq**

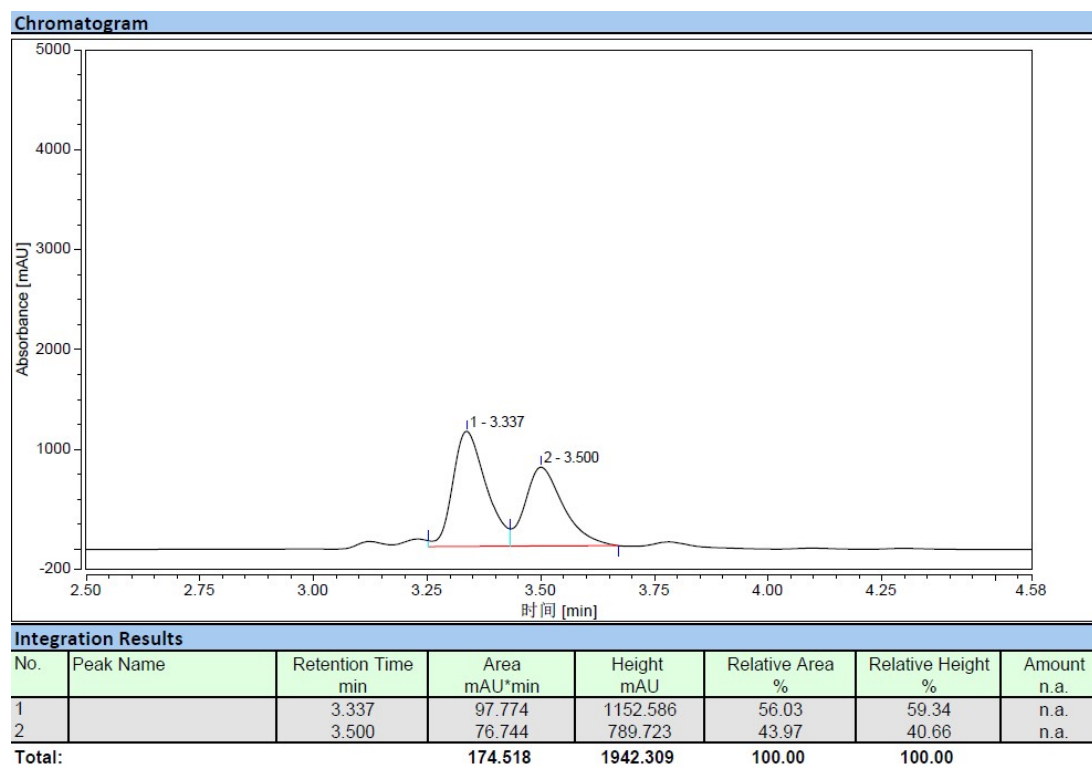


2. HPLC spectra of product 3aa

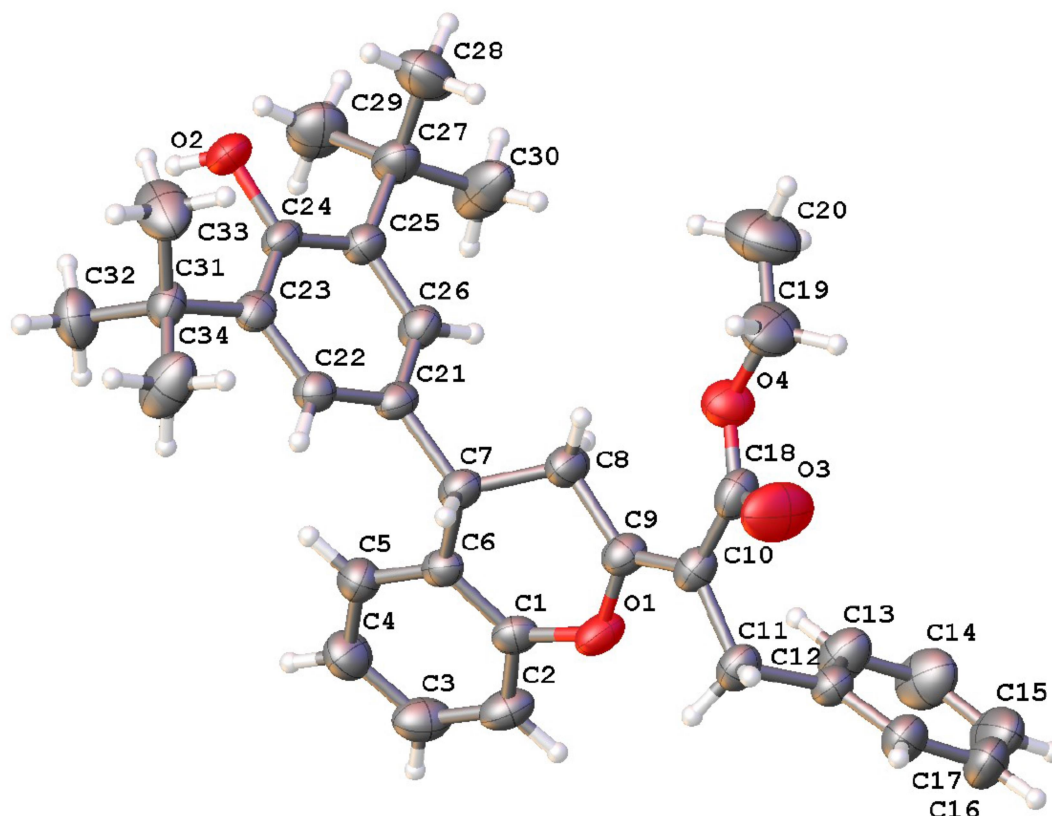
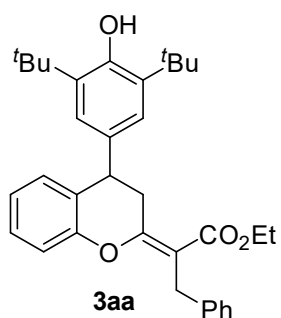
Racemic:



Enantioselective: 12% ee



3. X-ray single crystal data for compound 3aa



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

Empirical formula	C ₁₇ H ₂₀ O ₂	
Formula weight	256.33	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.090(3) Å	α = 63.859(3)°.
	b = 12.294(3) Å	β = 70.176(3)°.
	c = 12.543(3) Å	γ = 61.173(3)°.
Volume	1447.2(6) Å ³	
Z	4	

Density (calculated)	1.176 Mg/m ³
Absorption coefficient	0.075 mm ⁻¹
F(000)	552
Crystal size	0.3 x 0.3 x 0.1 mm ³
Theta range for data collection	2.882 to 26.991°.
Index ranges	-15<=h<=12, -15<=k<=9, -16<=l<=15
Reflections collected	8425
Independent reflections	6083 [R(int) = 0.0265]
Completeness to theta = 25.242°	97.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7455 and 0.6316
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6083 / 0 / 351
Goodness-of-fit on F ²	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0680, wR2 = 0.1447
R indices (all data)	R1 = 0.1393, wR2 = 0.1806
Extinction coefficient	n/a
Largest diff. peak and hole	0.203 and -0.254 e.Å ⁻³