Supporting Information

Phosphine-Catalyzed Regiospecific (3+2) Cyclization of 3-Nitroindoles with Allene Esters

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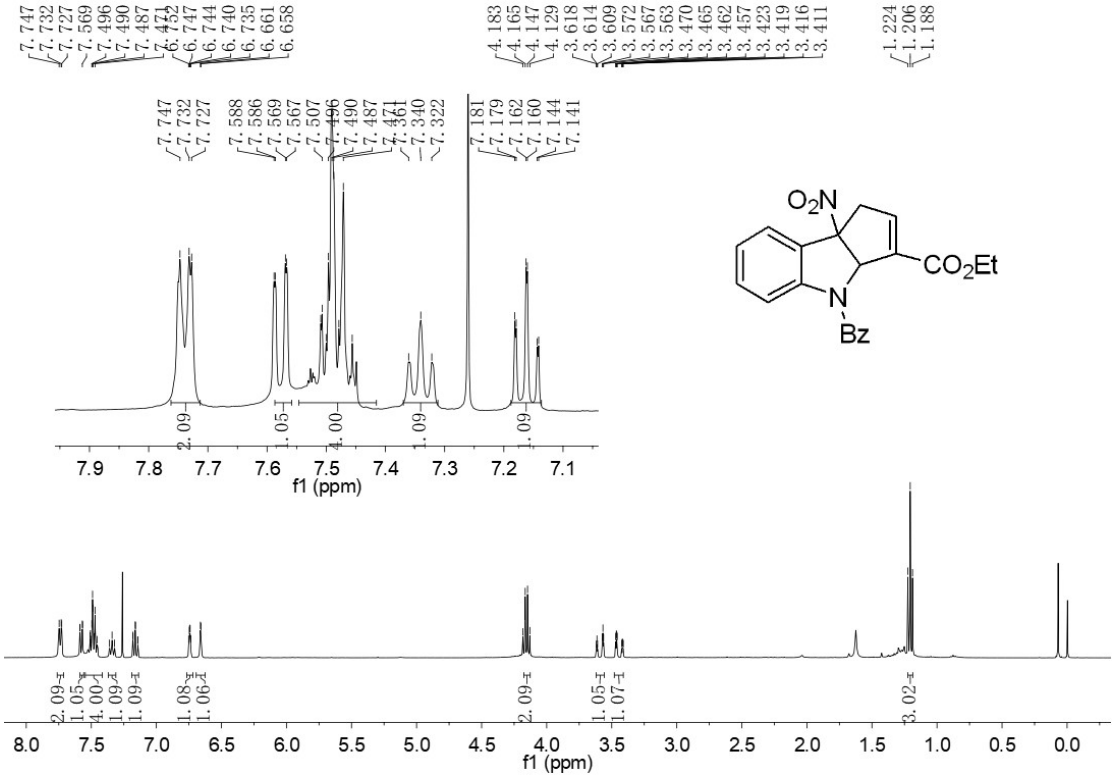
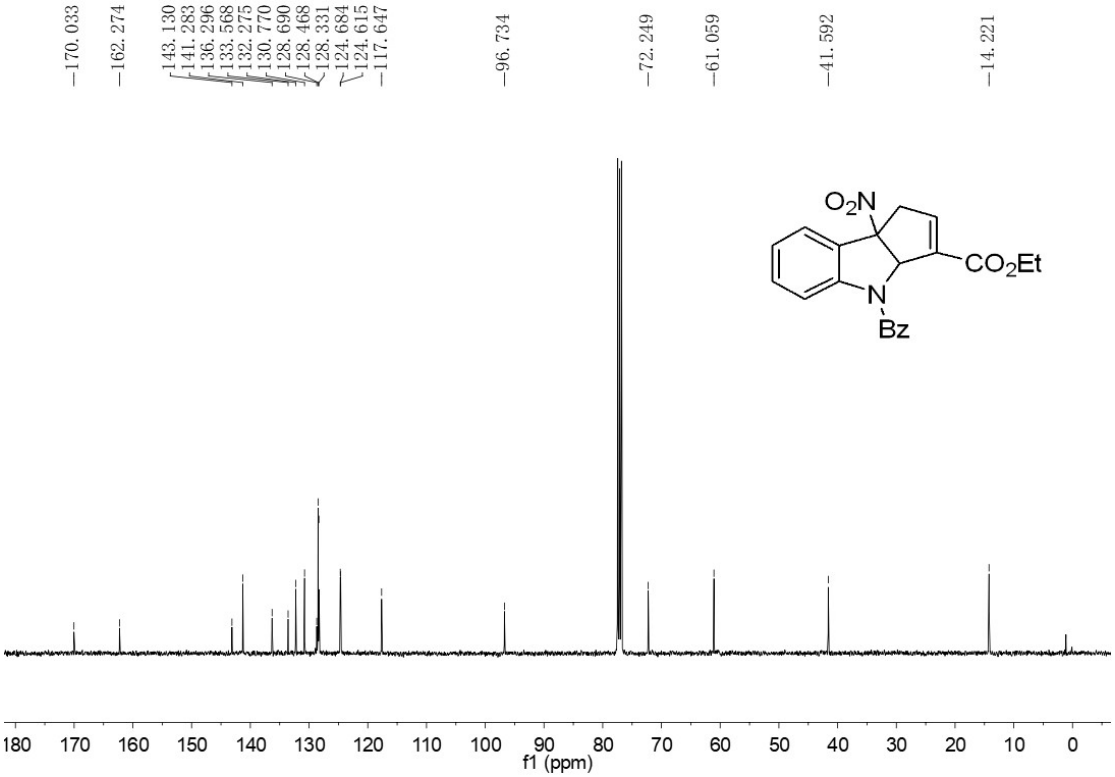
NMR spectra of products 3

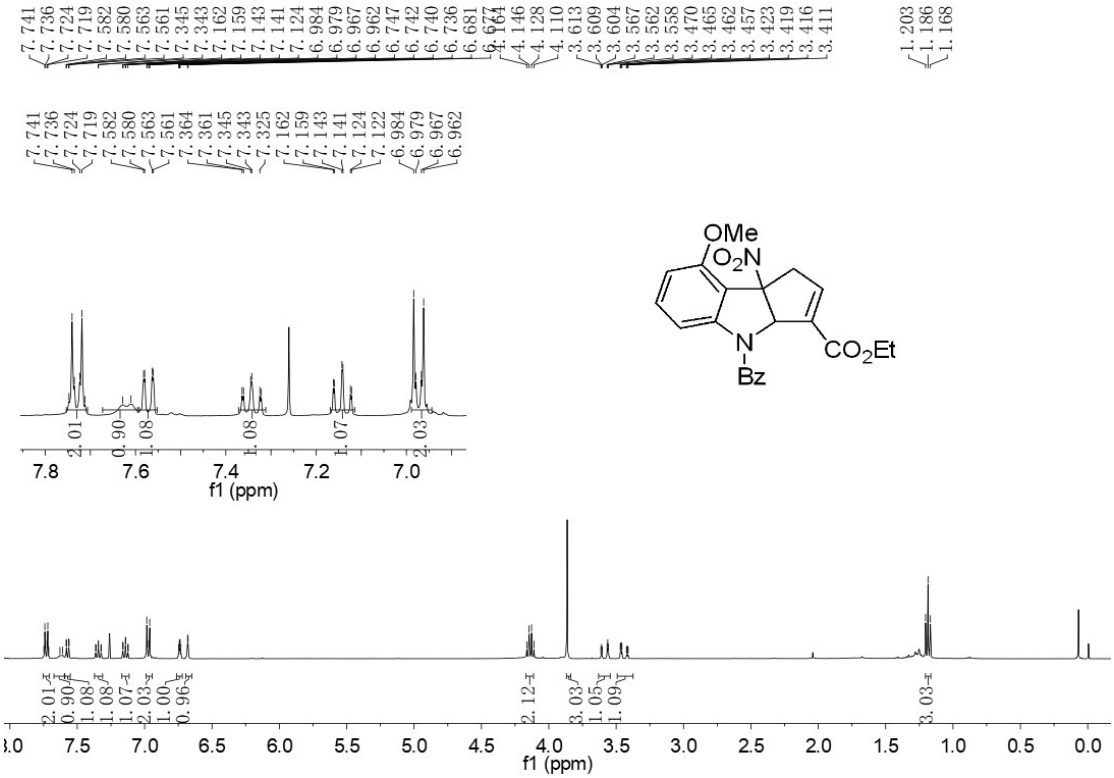
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aa**



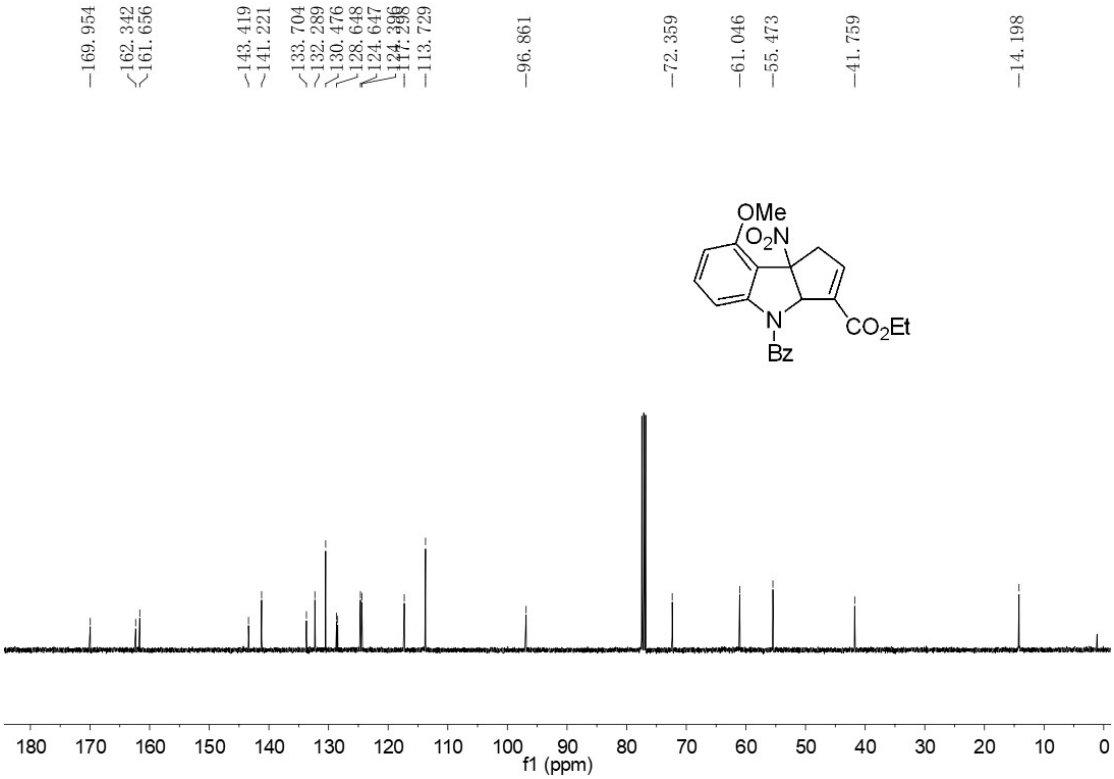
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aa**



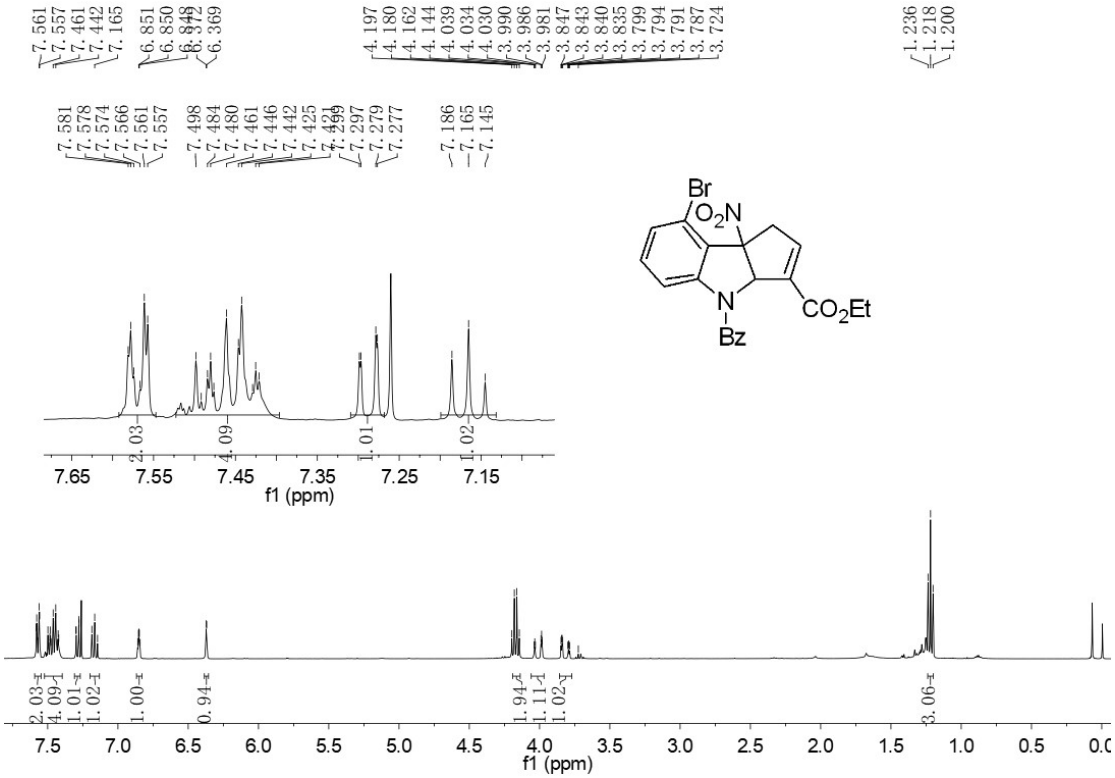
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ba**



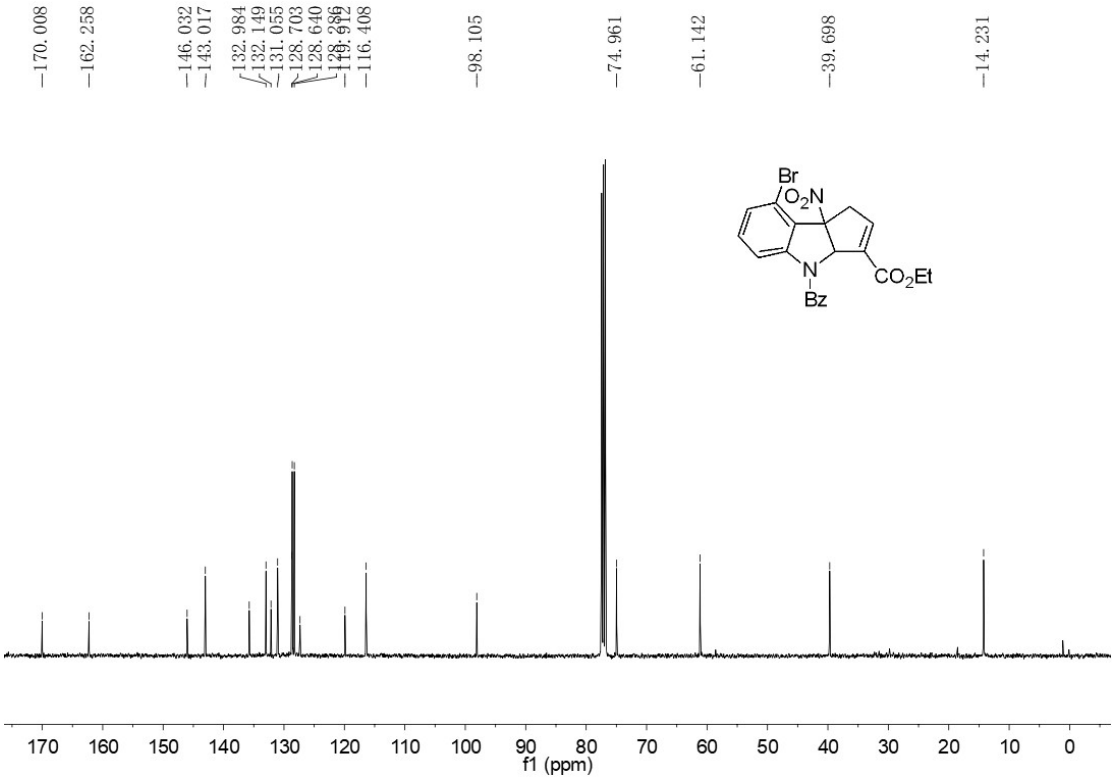
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ba**



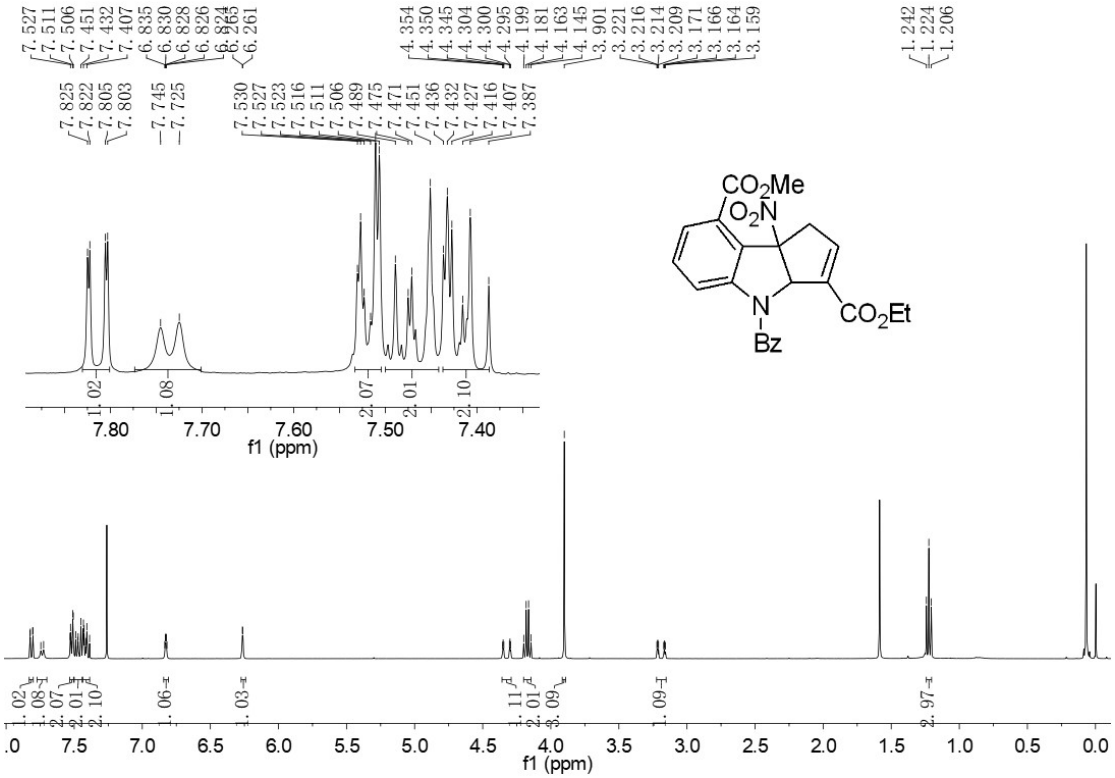
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ca**



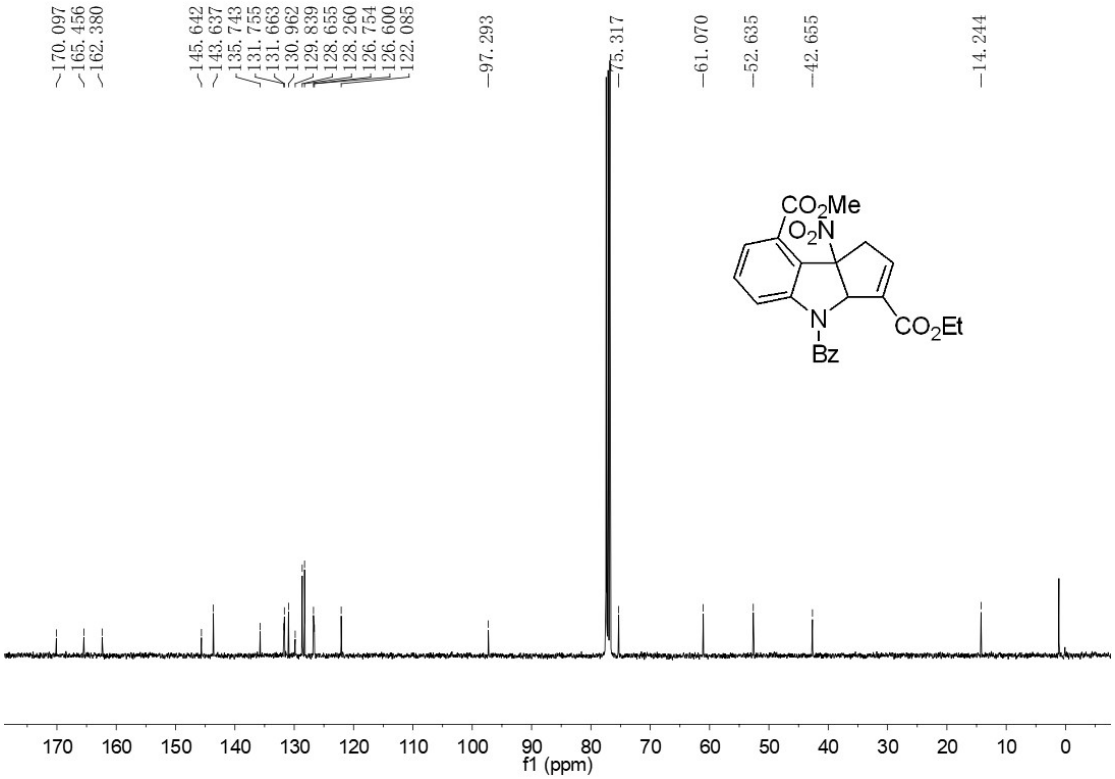
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ca**



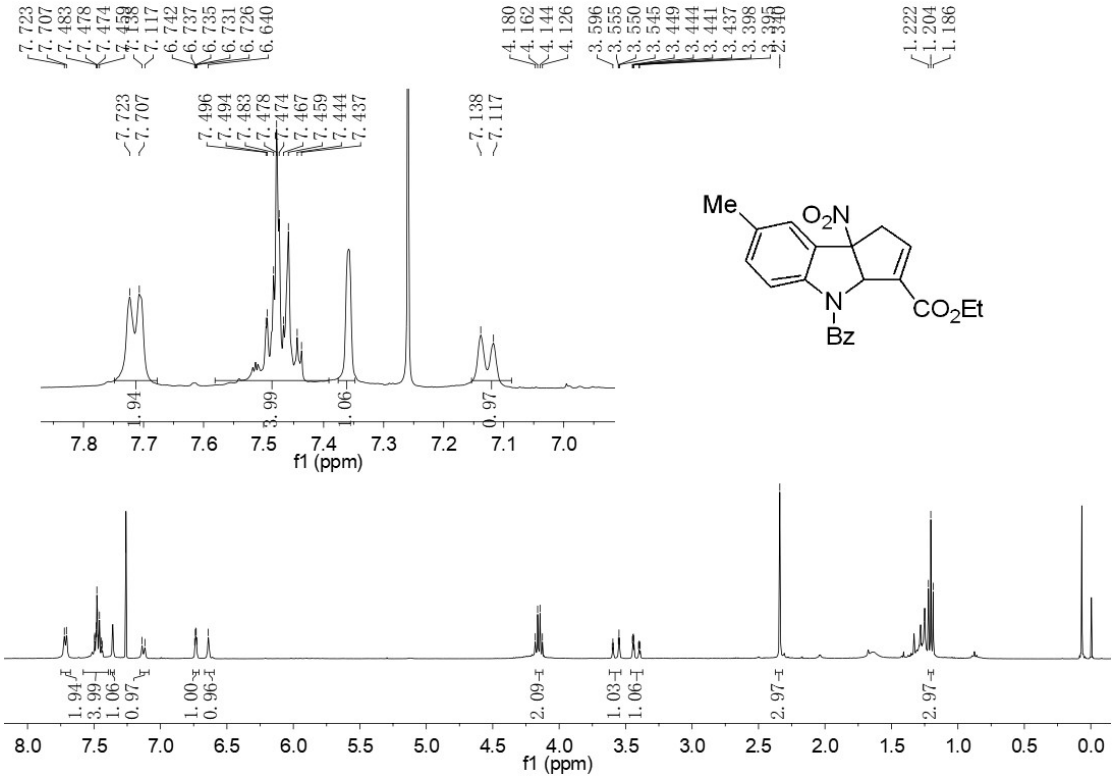
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3da**



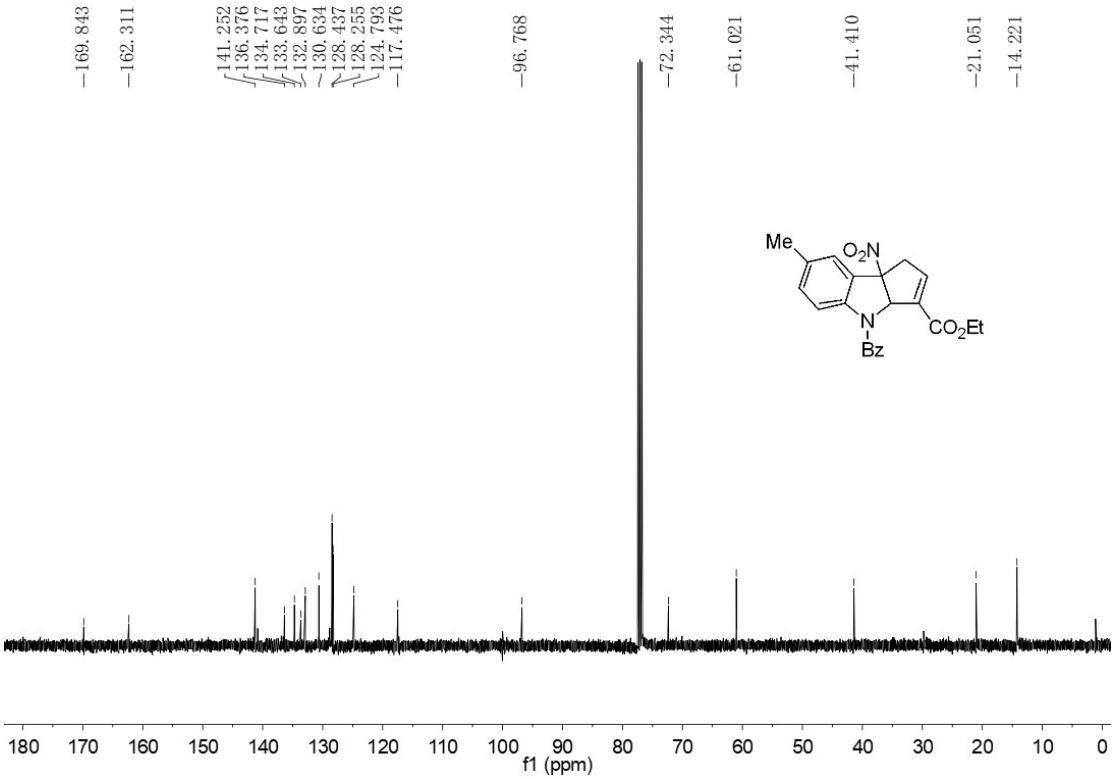
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3da**



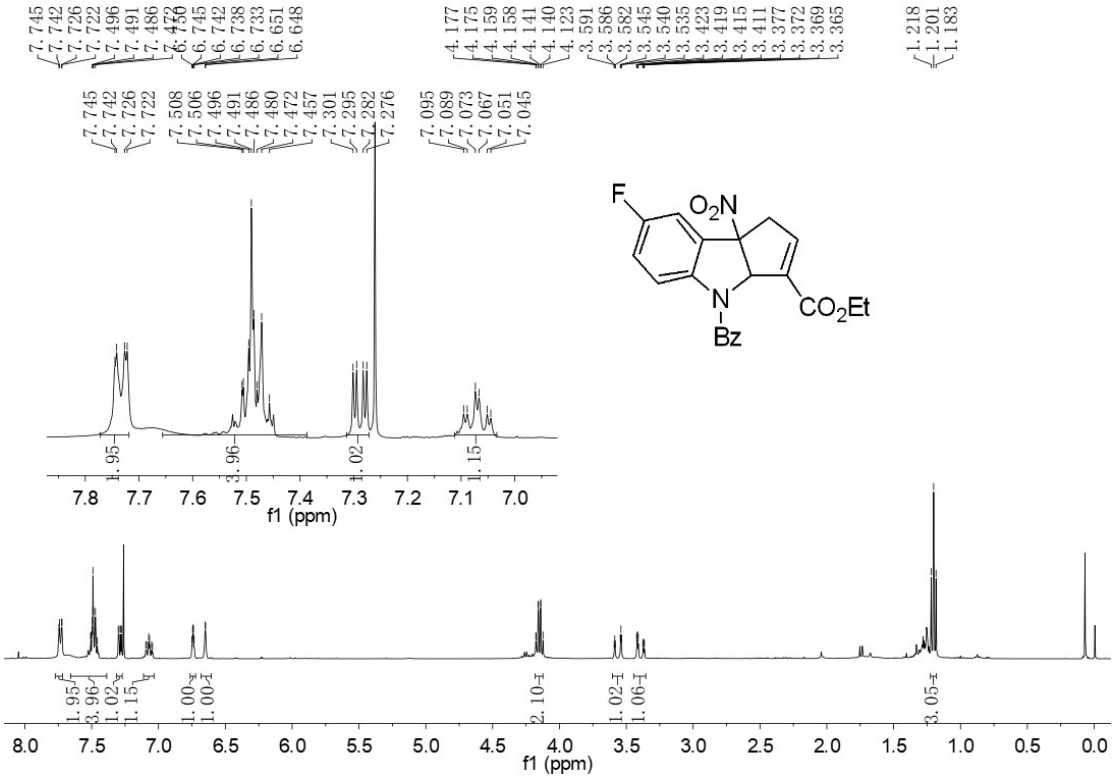
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ea**



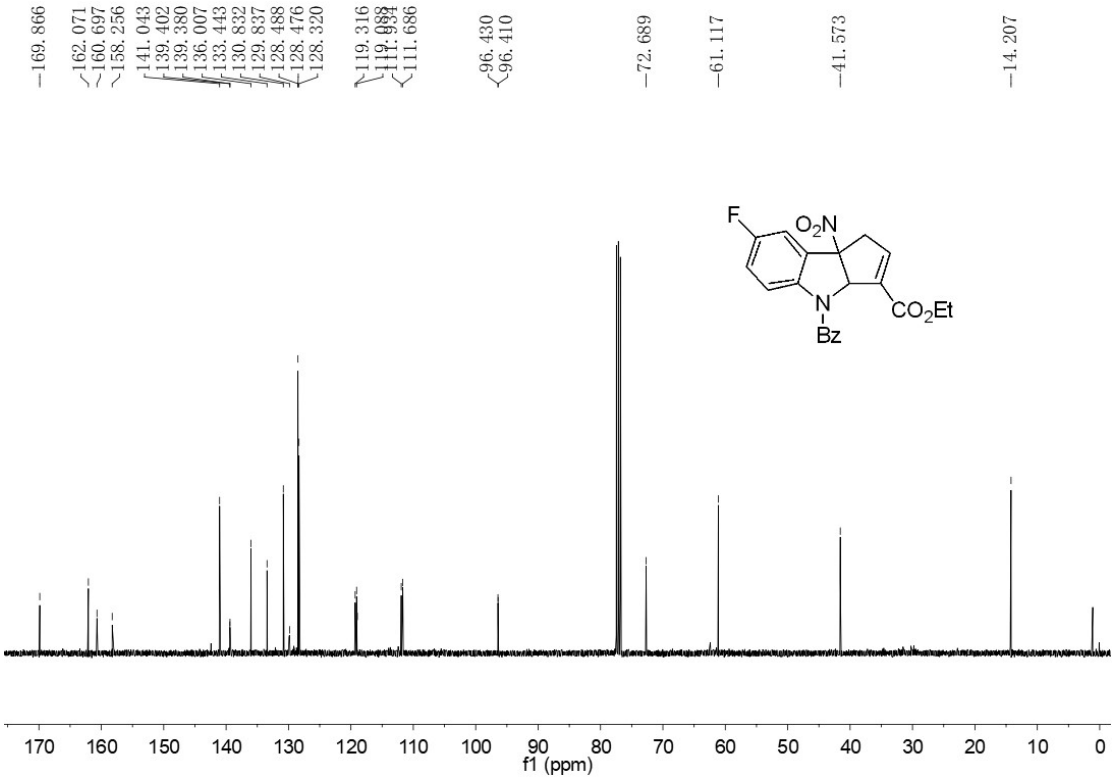
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ea**



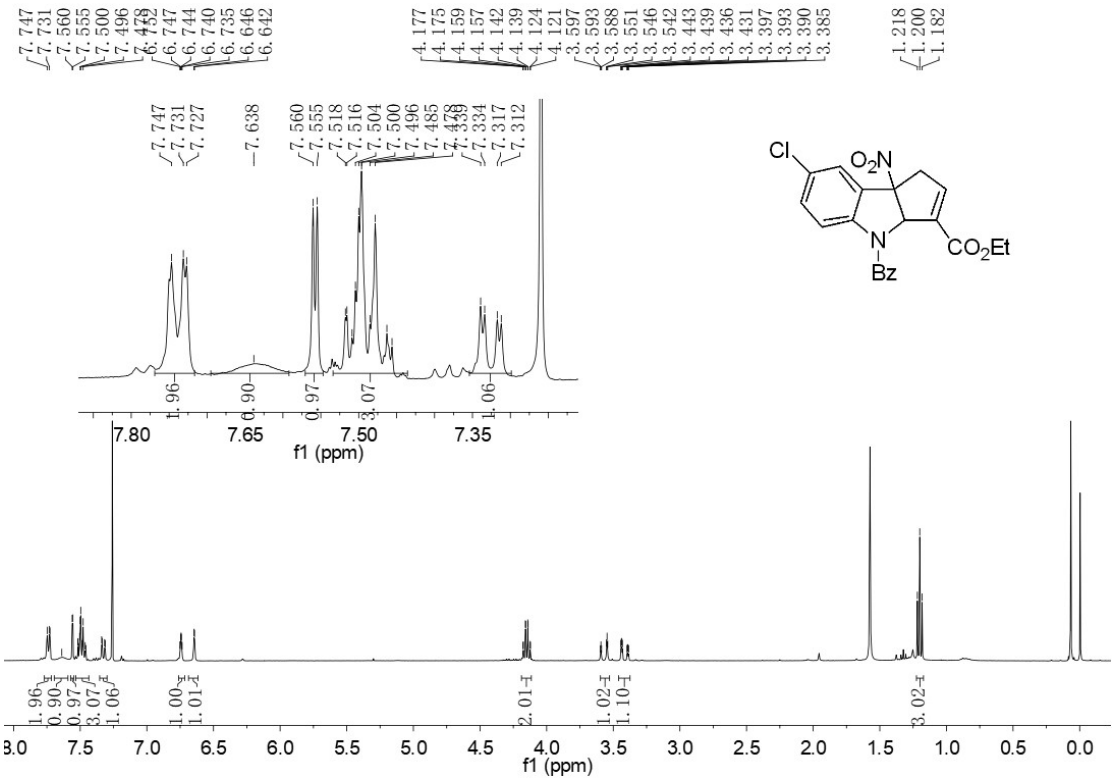
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3fa**



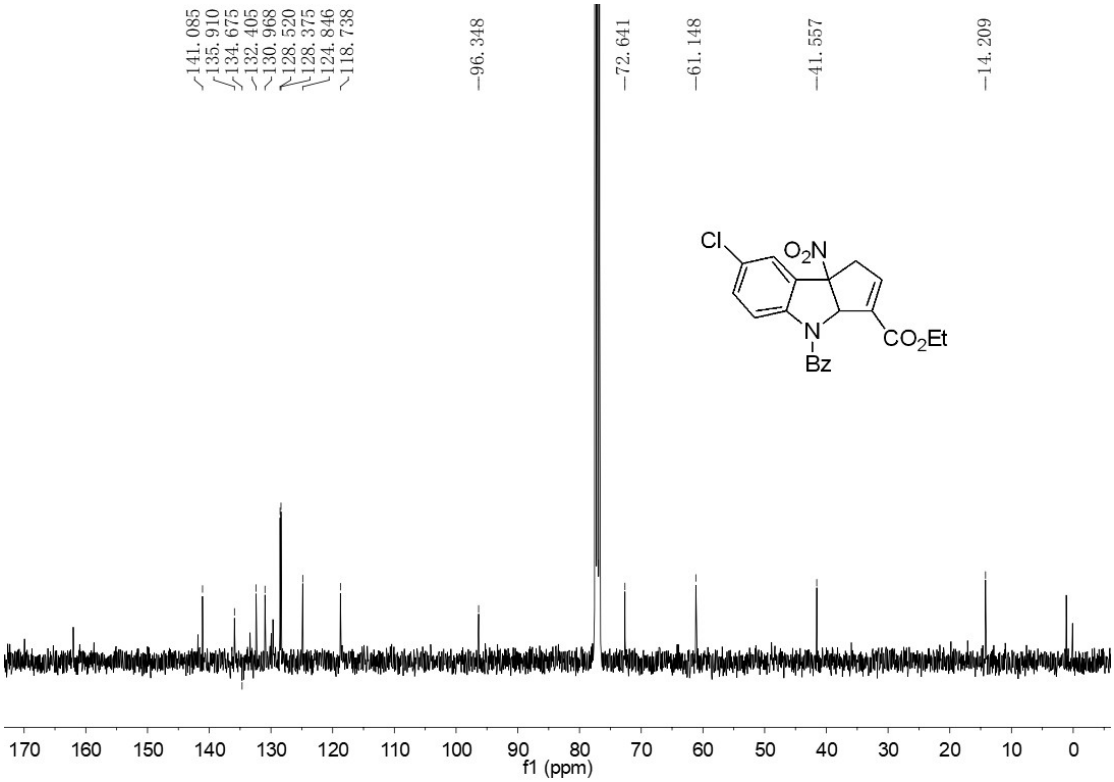
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3fa**



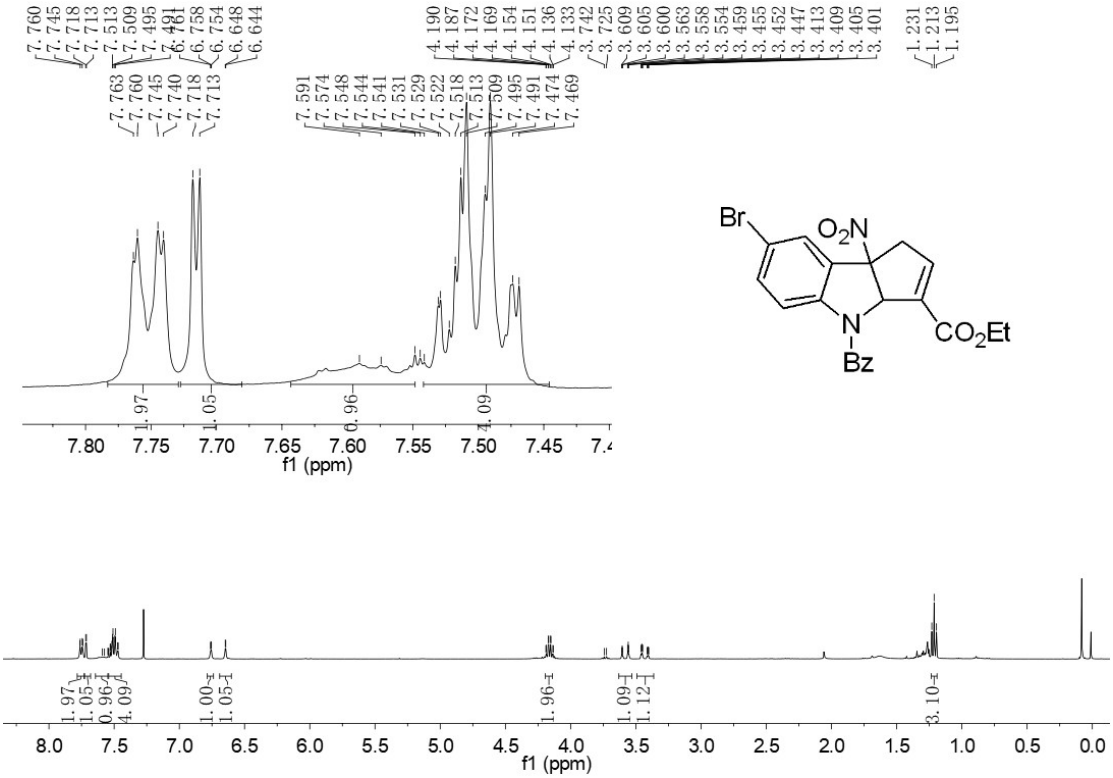
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ga**



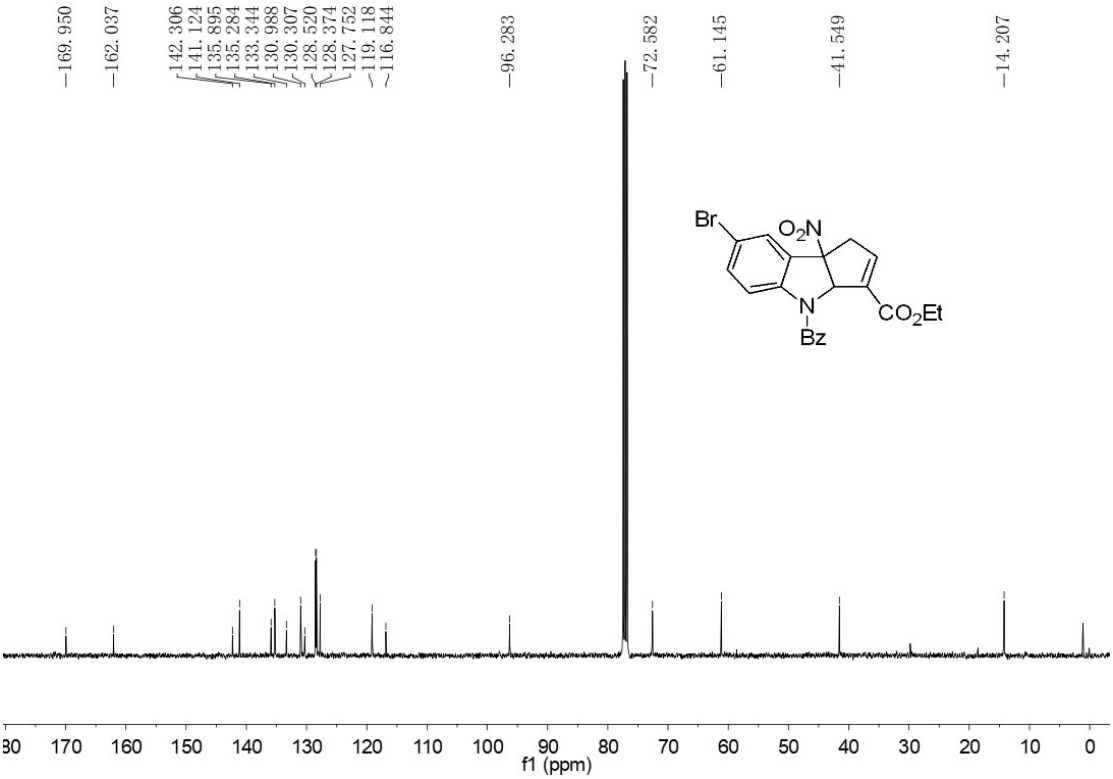
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ga**



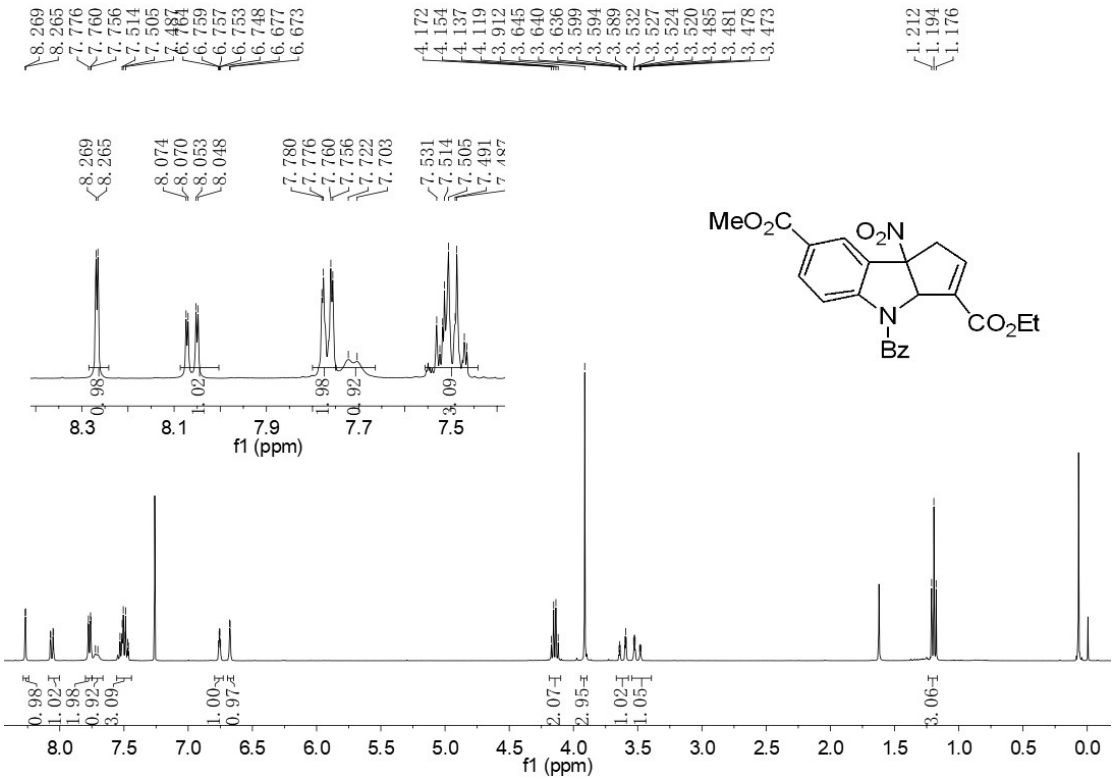
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ha**



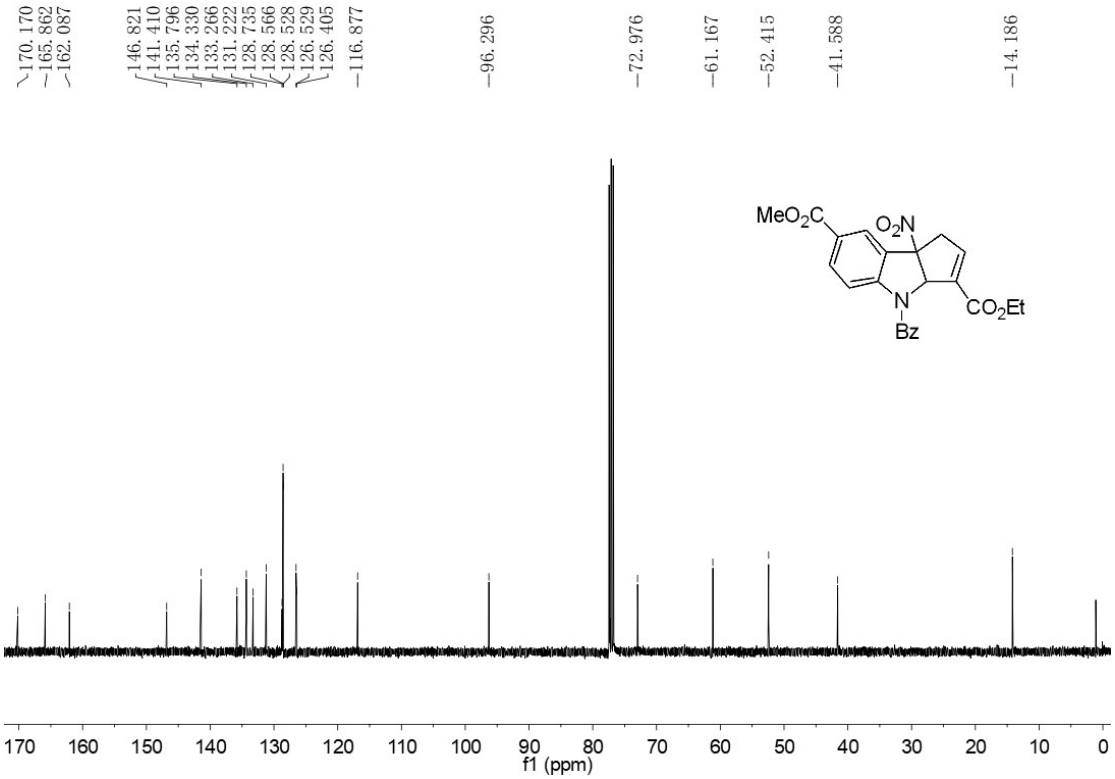
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ha**



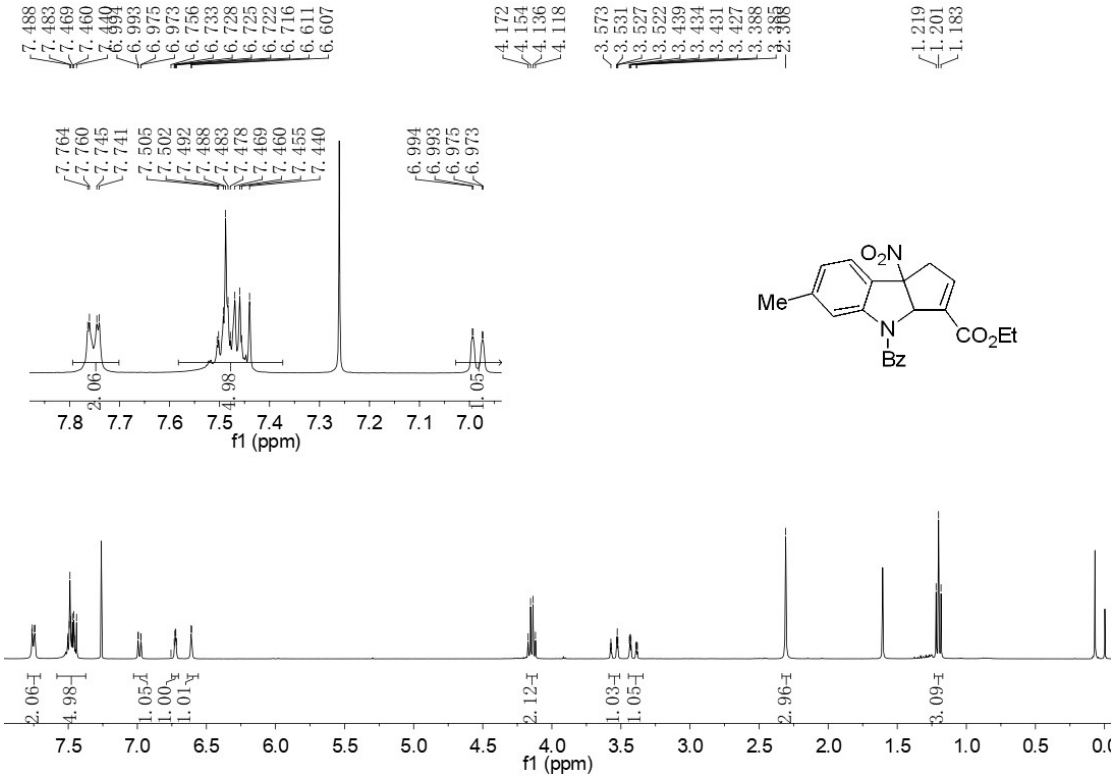
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ia**



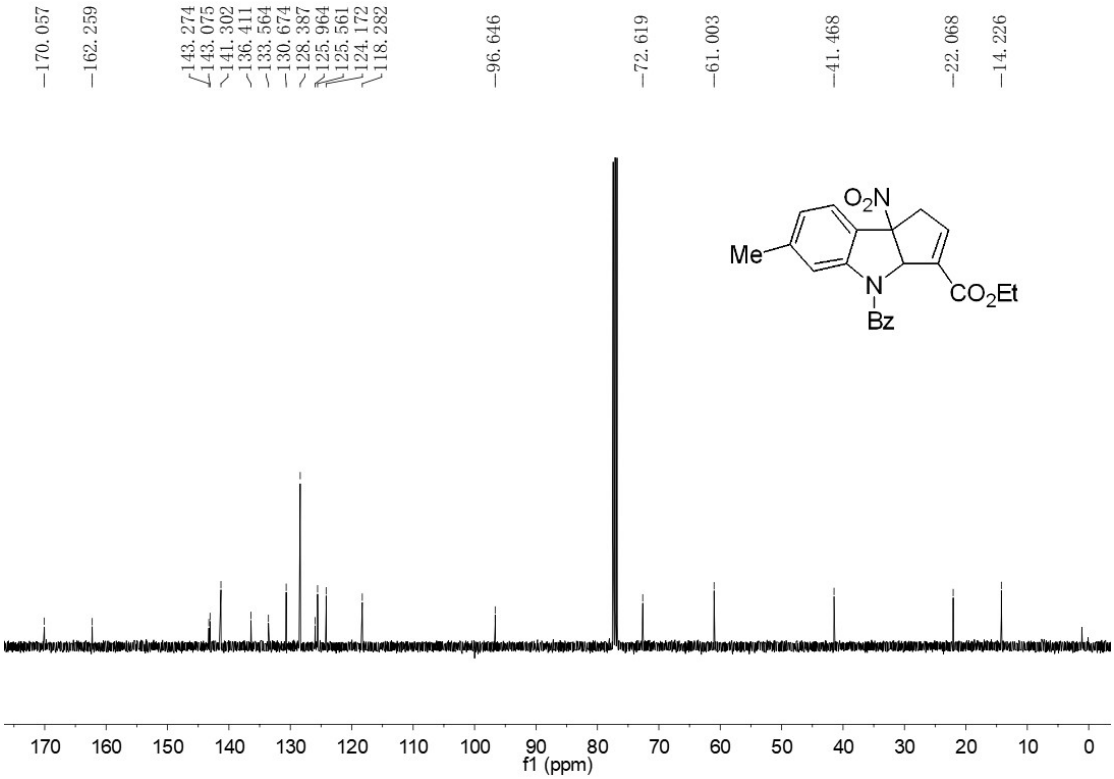
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ia**



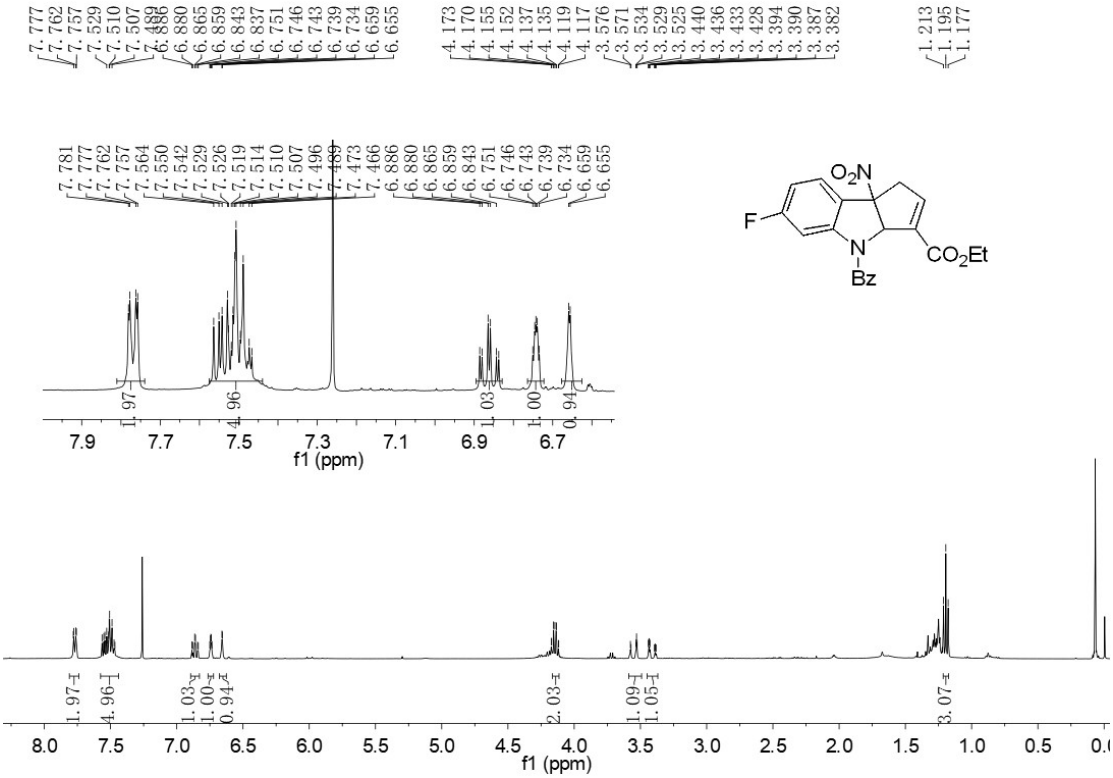
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ja**



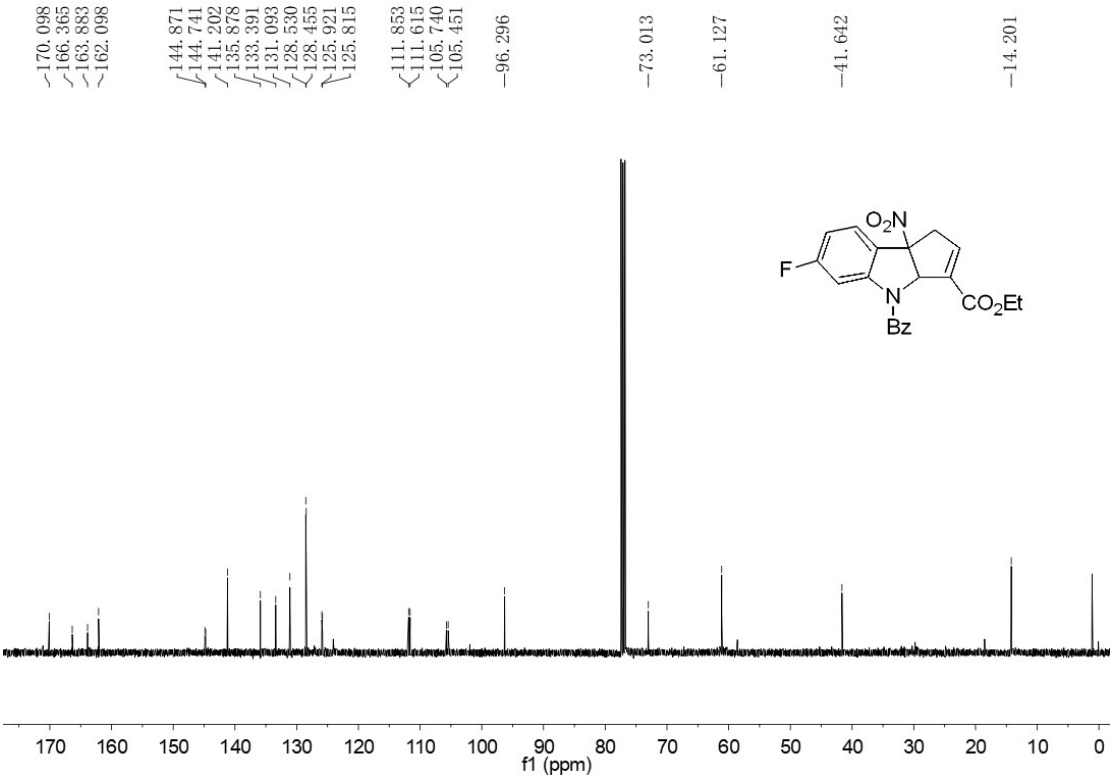
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ja**



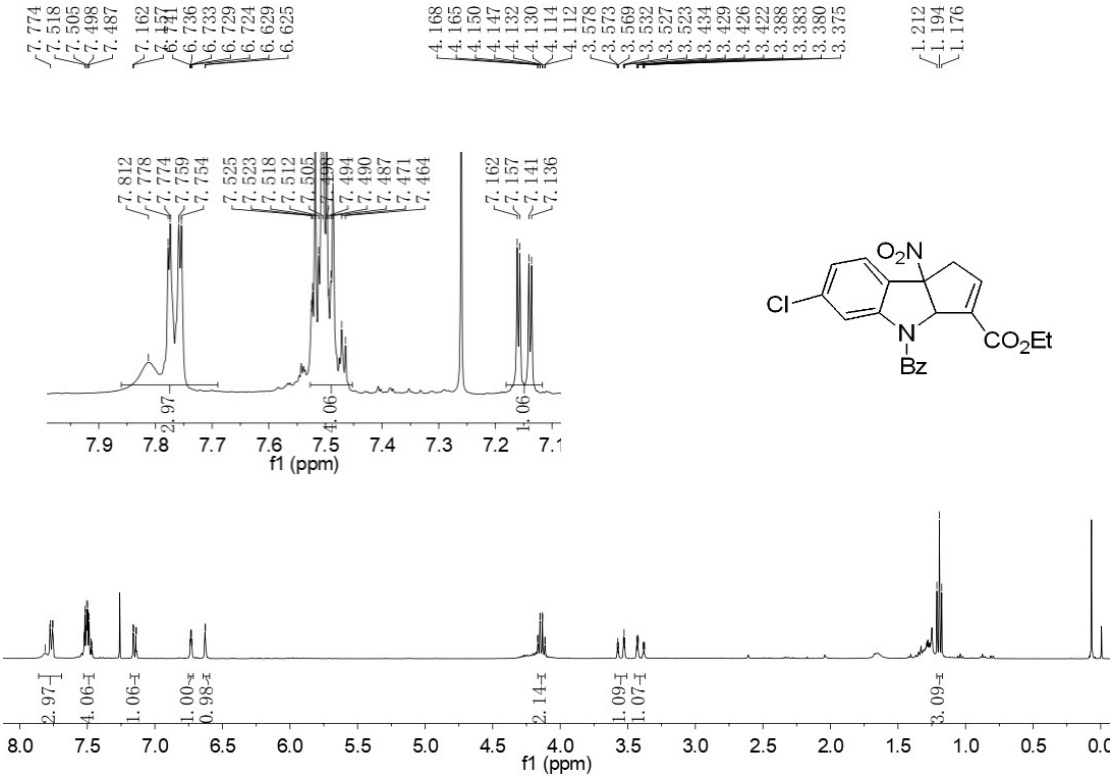
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ka**



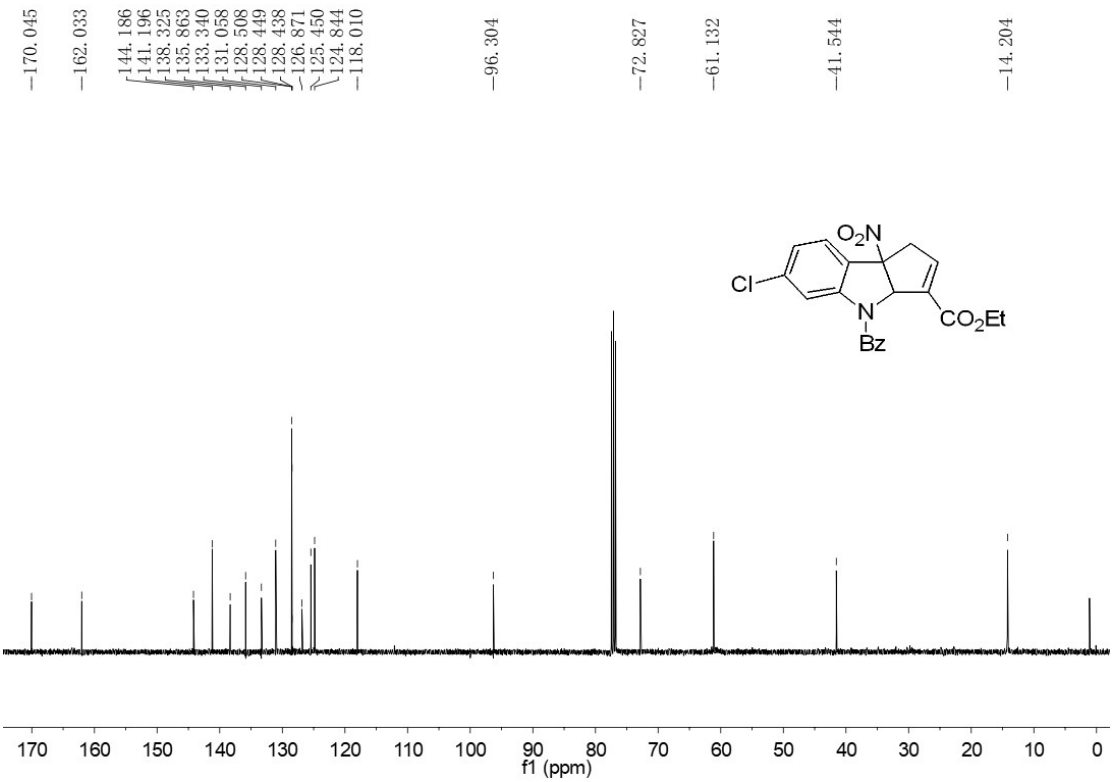
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ka**



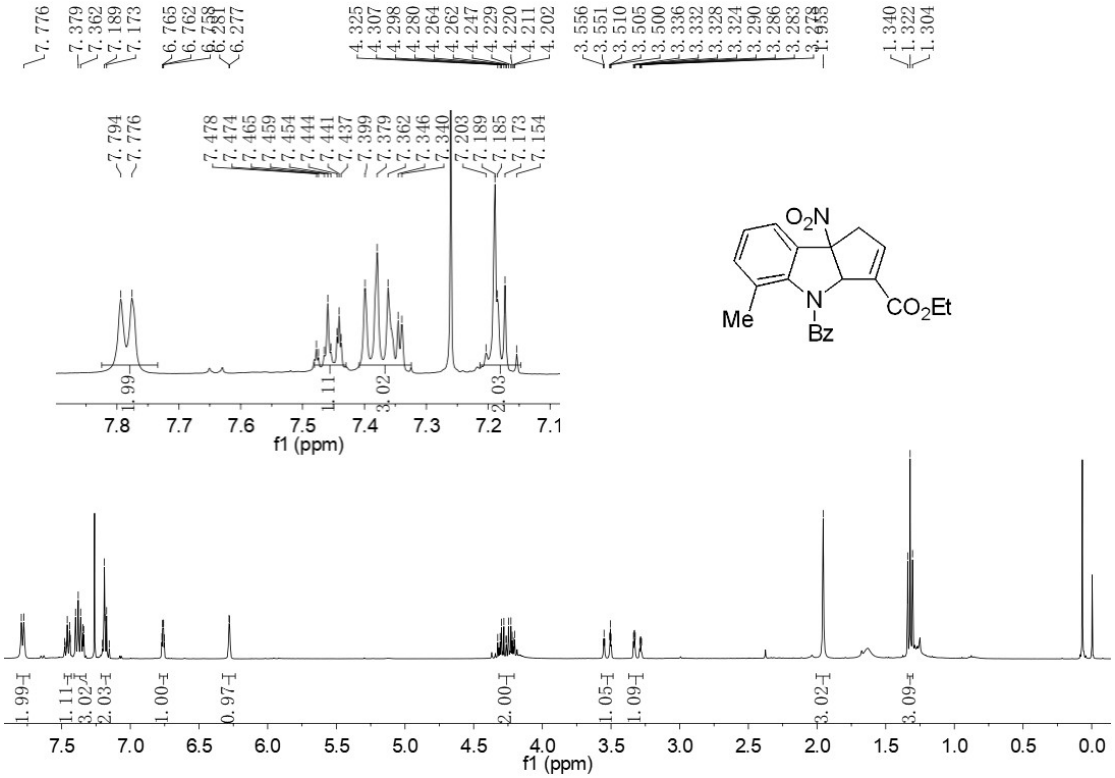
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3la**



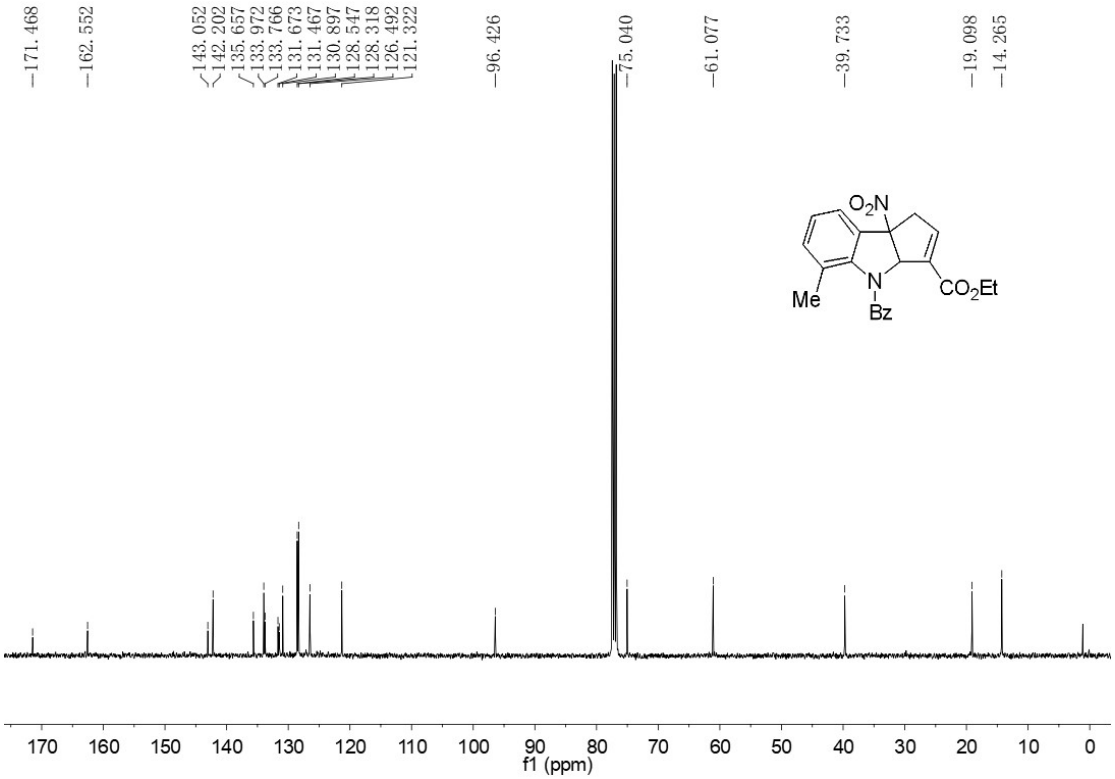
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3la**



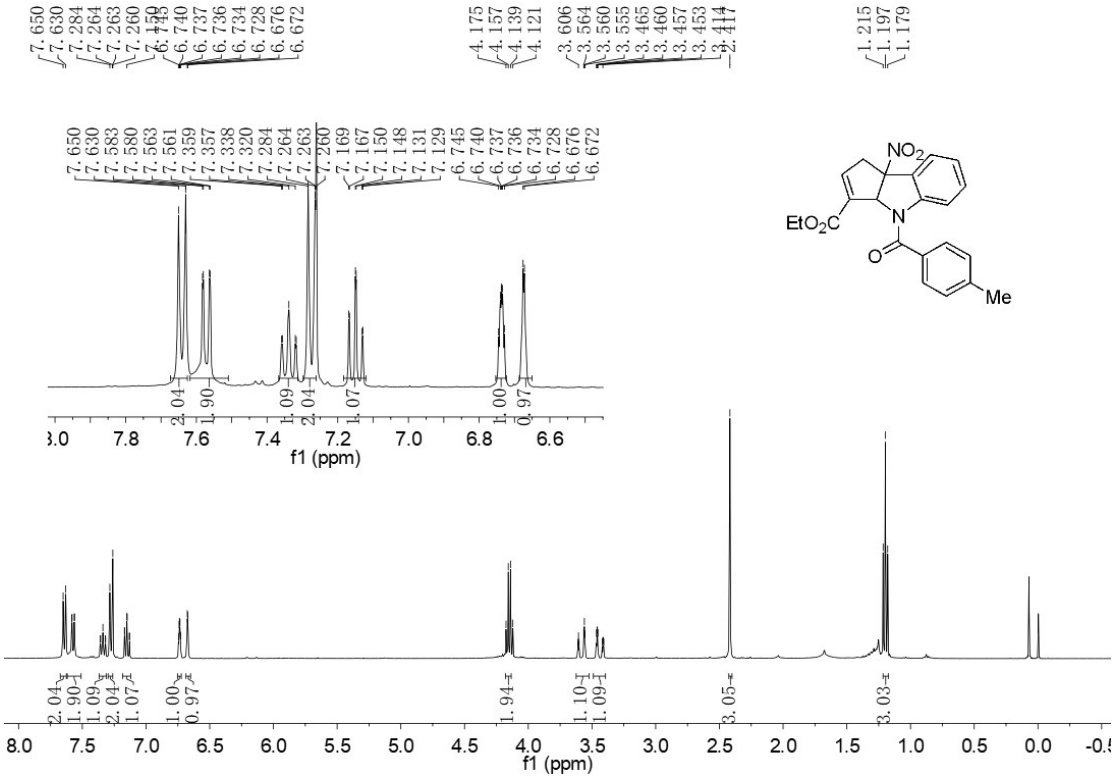
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ma**



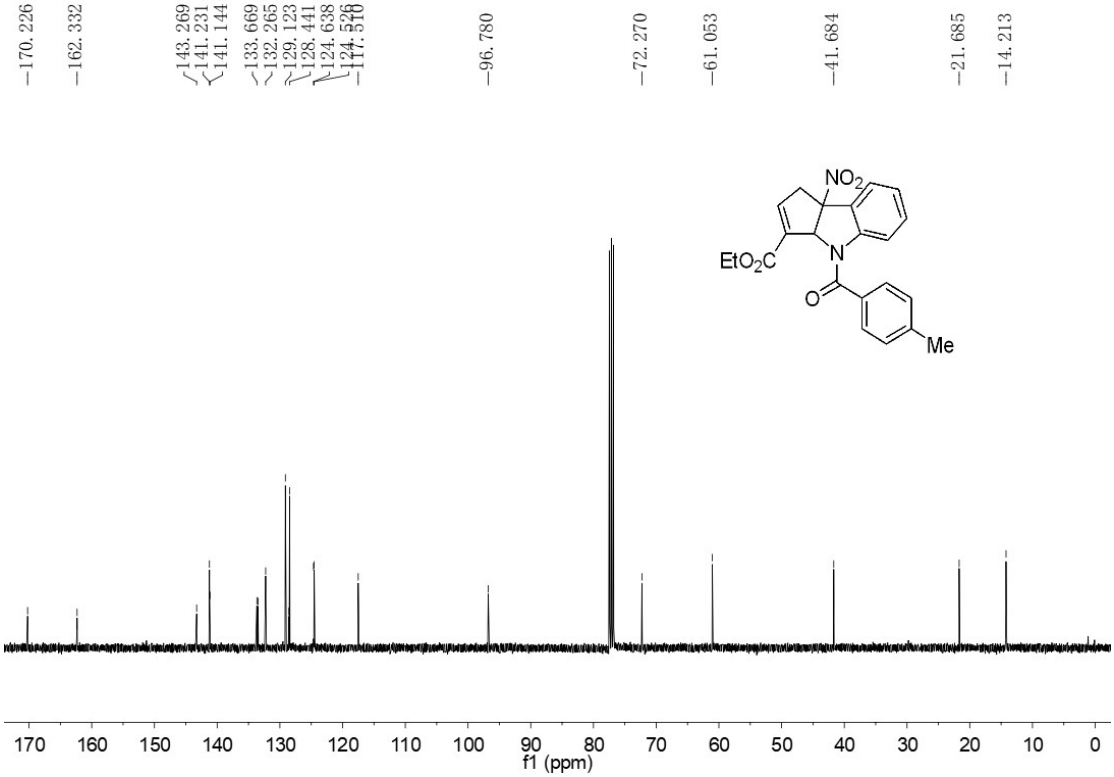
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ma**



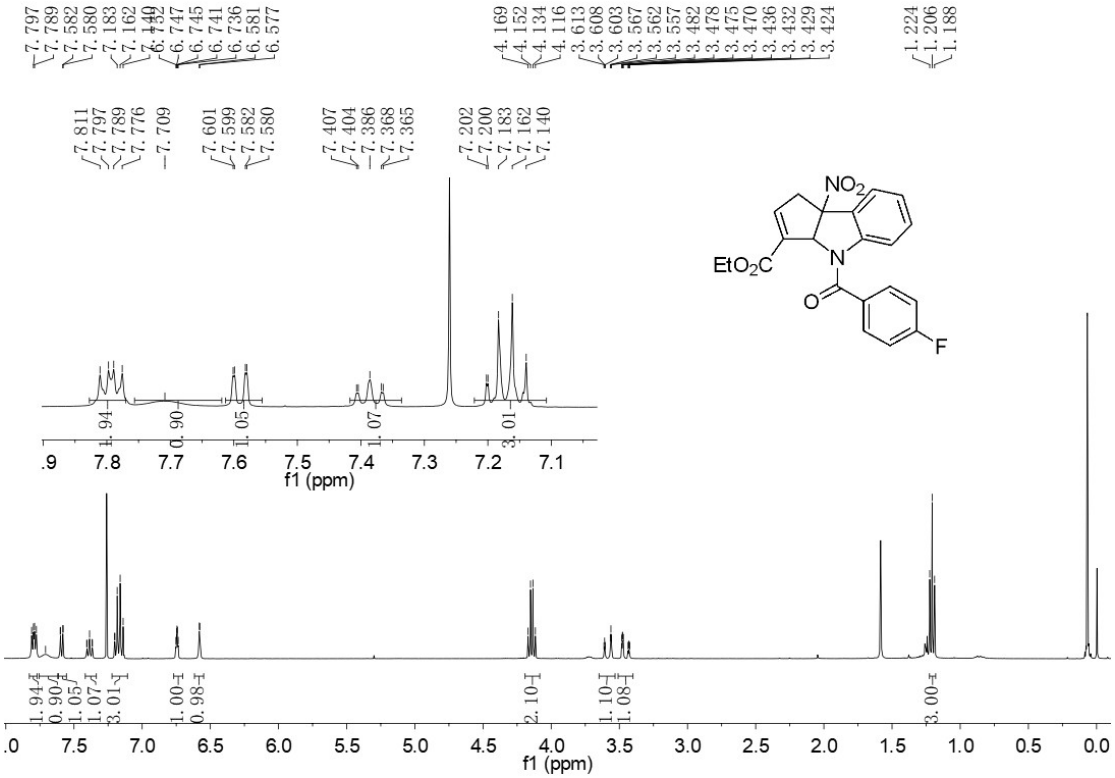
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3na**



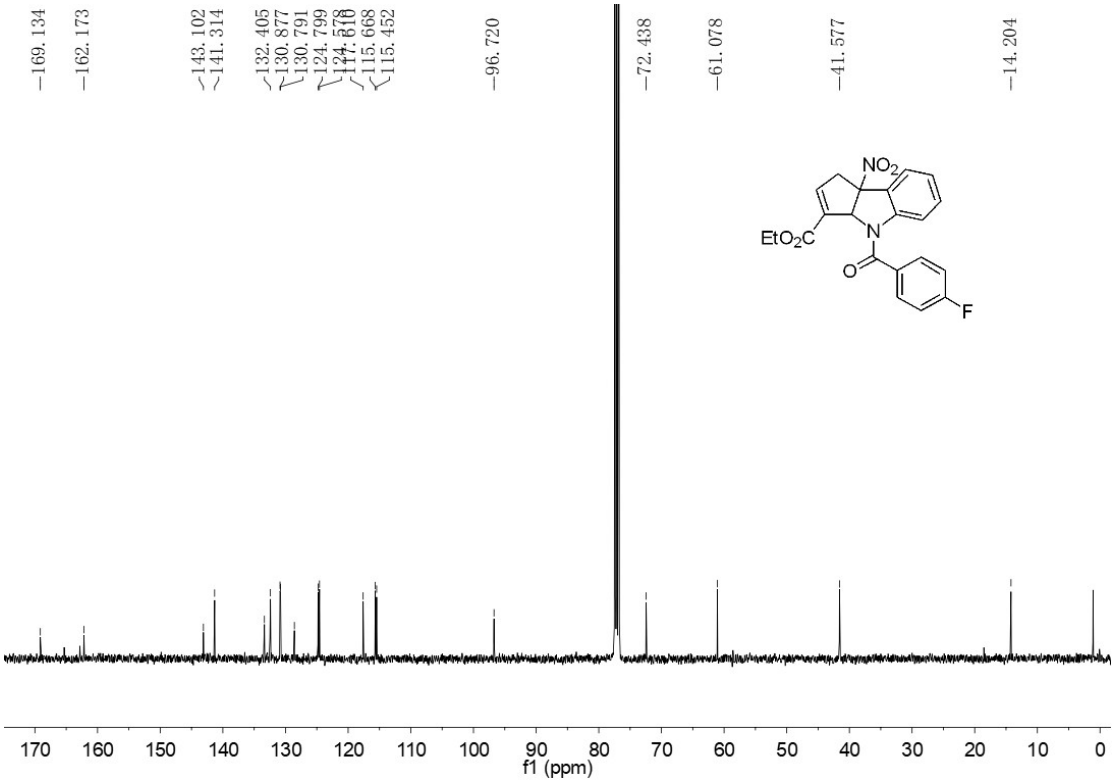
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3na**



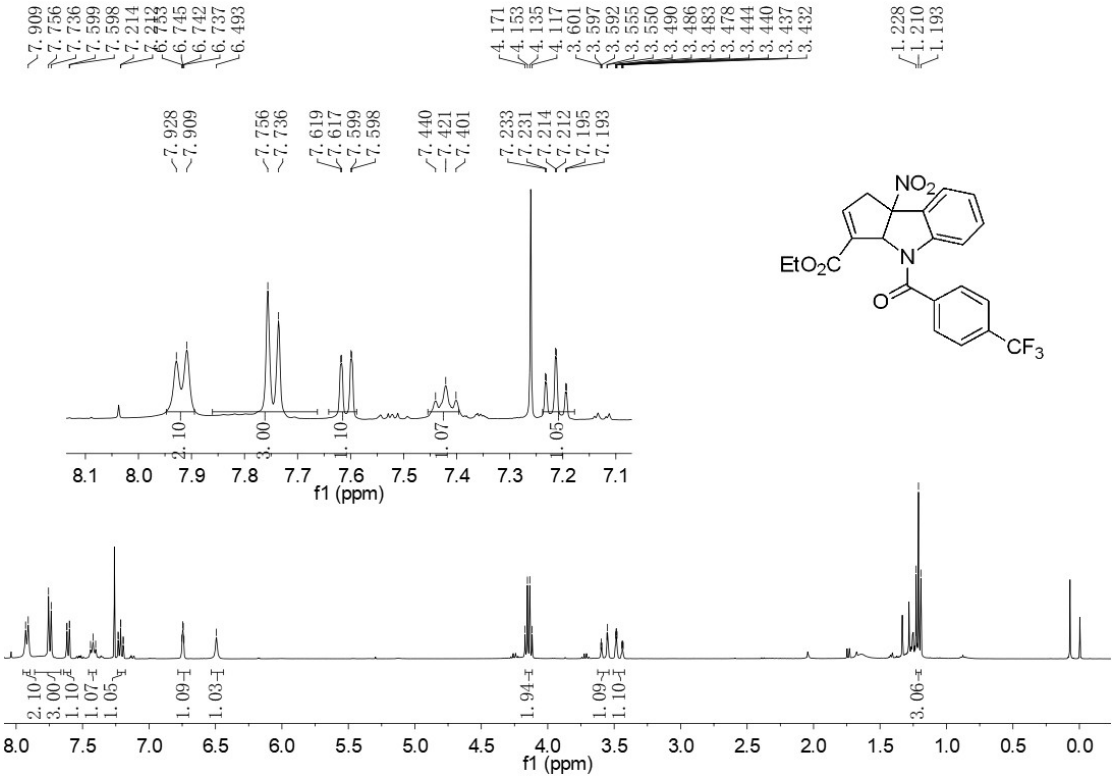
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3oa**



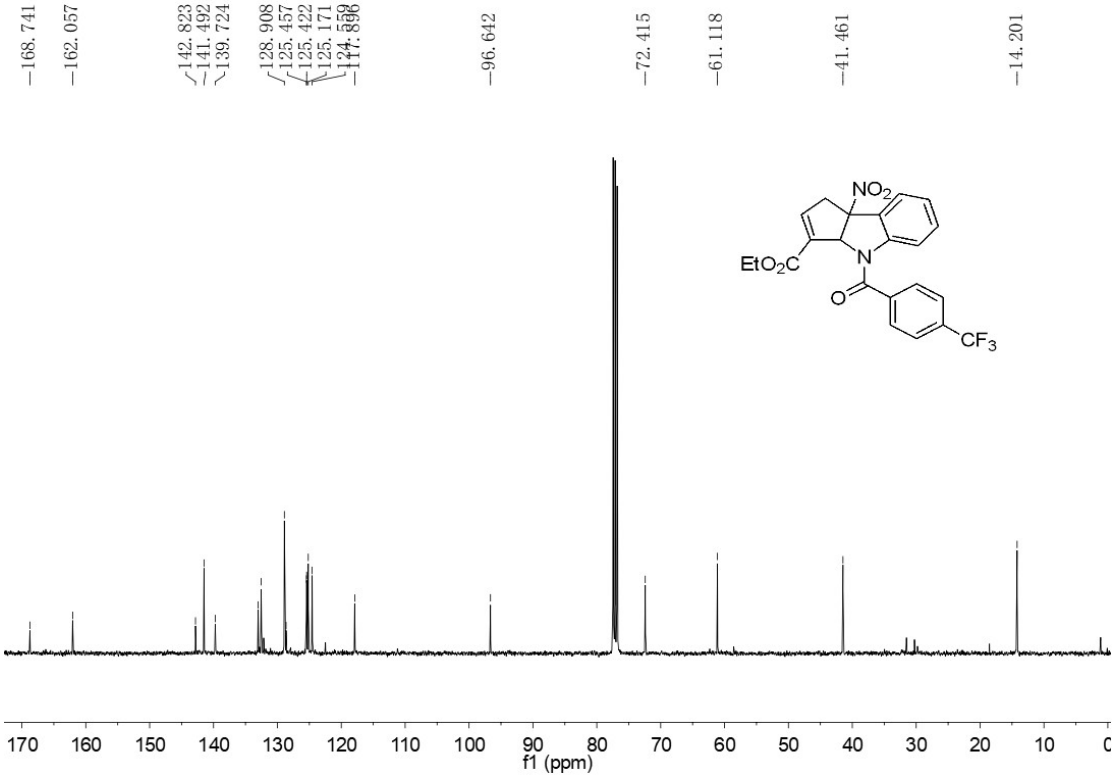
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3oa**



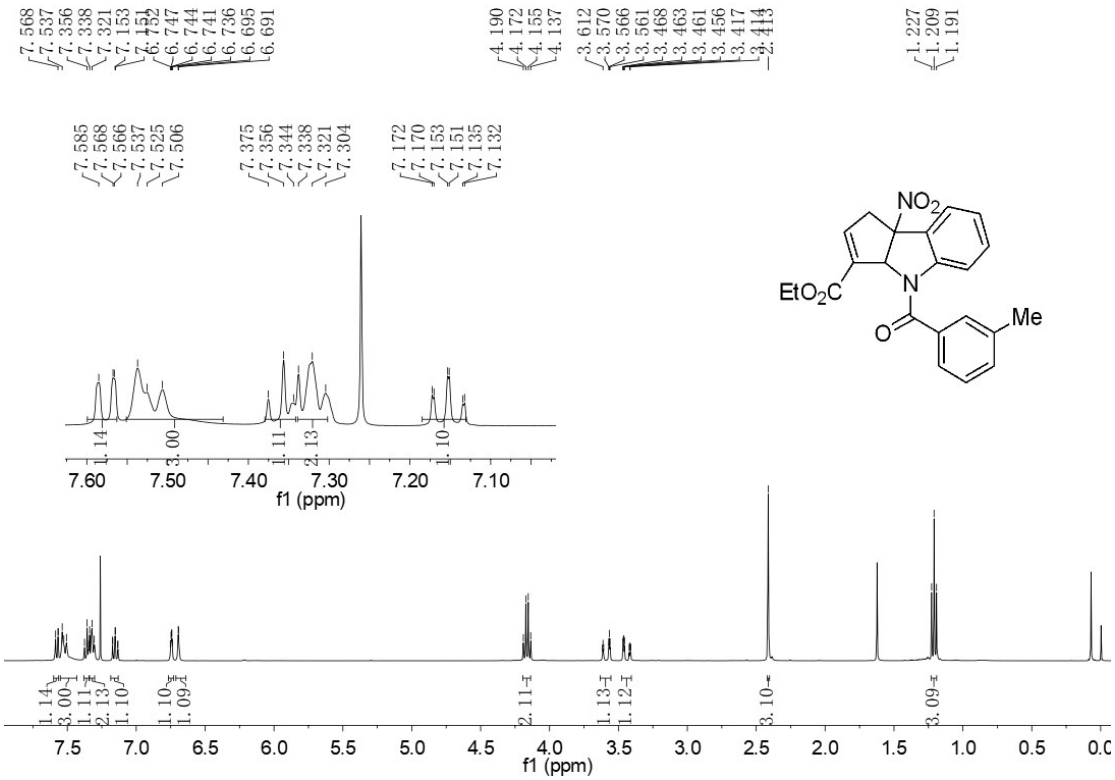
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3pa**



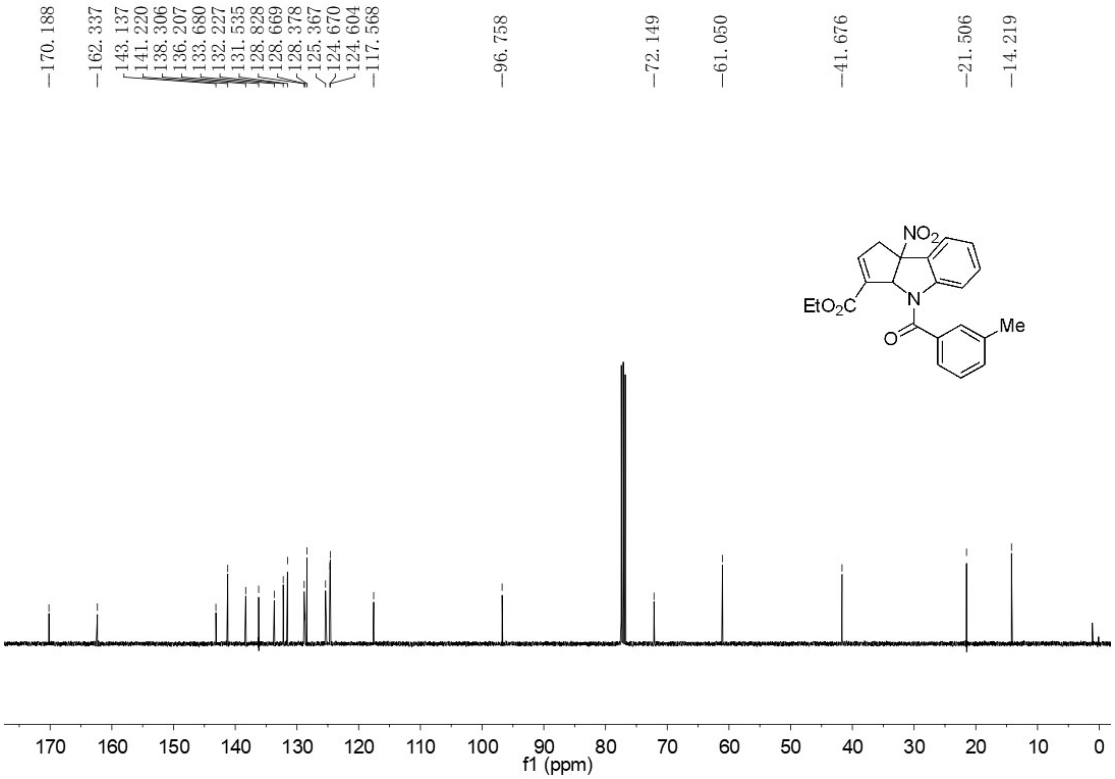
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3pa**



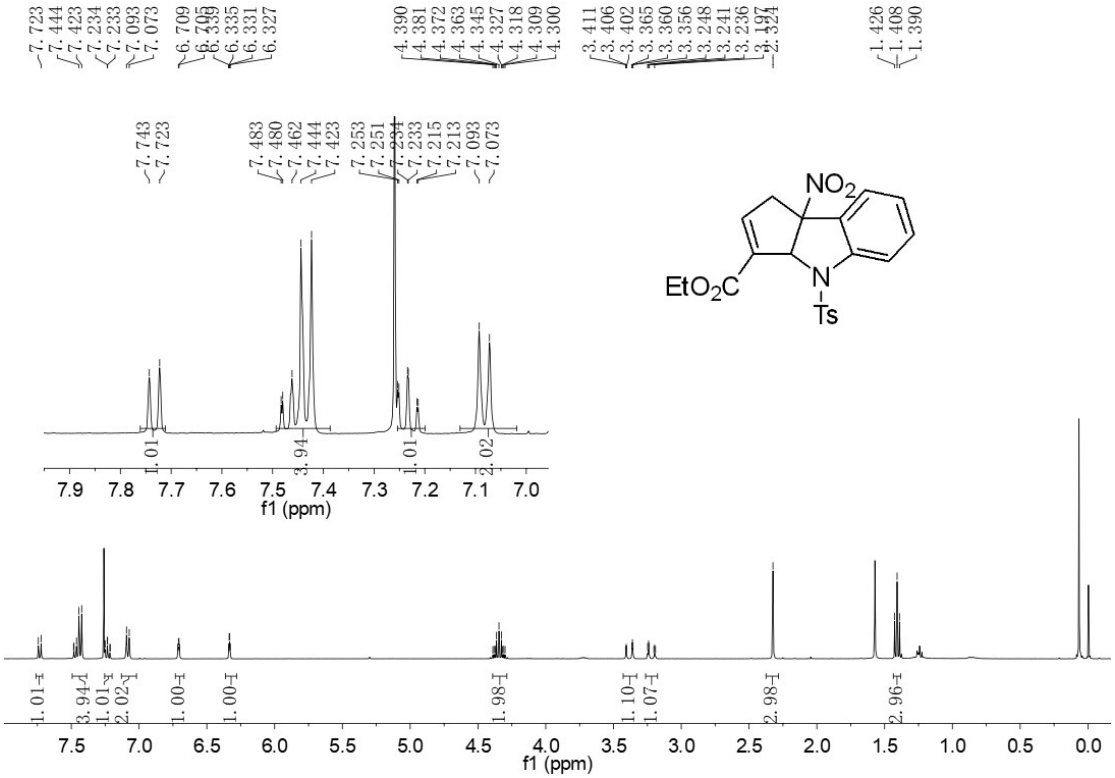
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3qa**



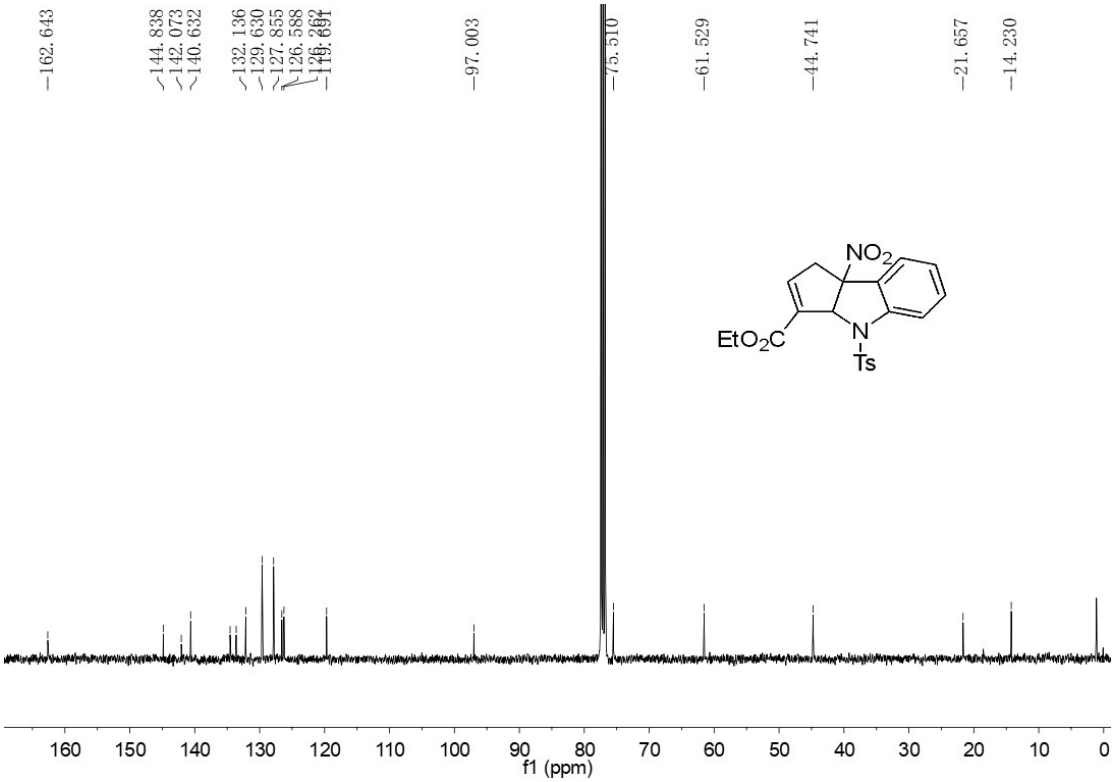
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3qa**



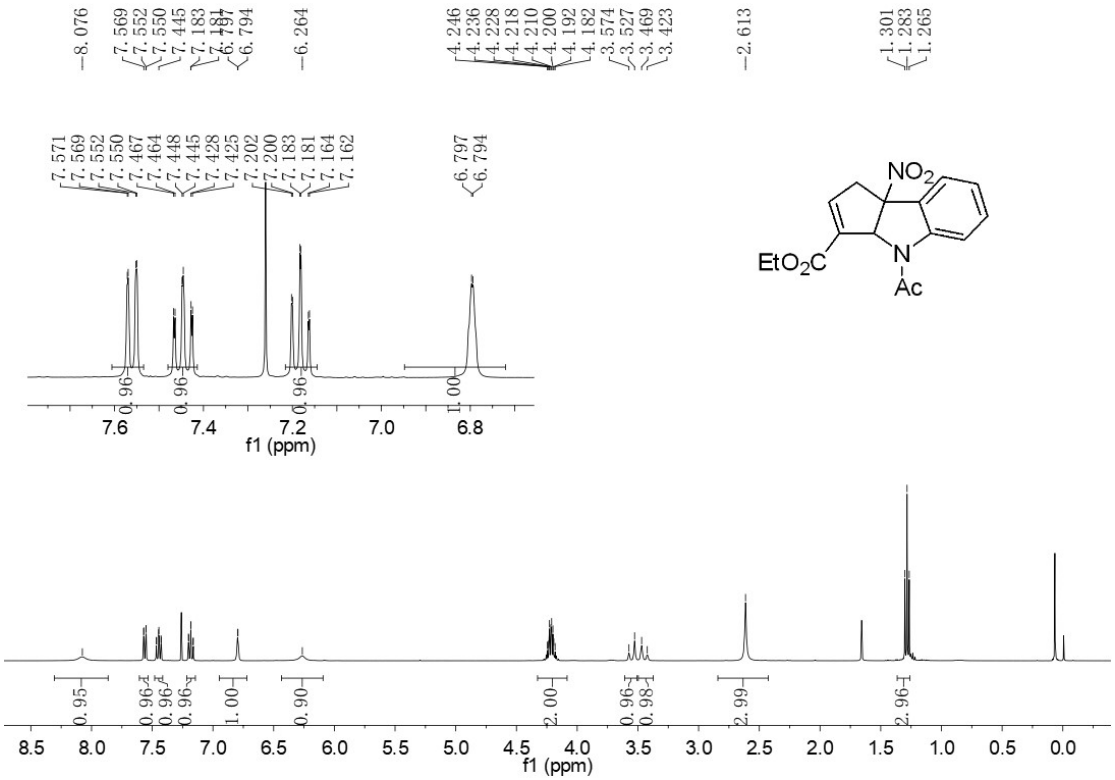
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ra**



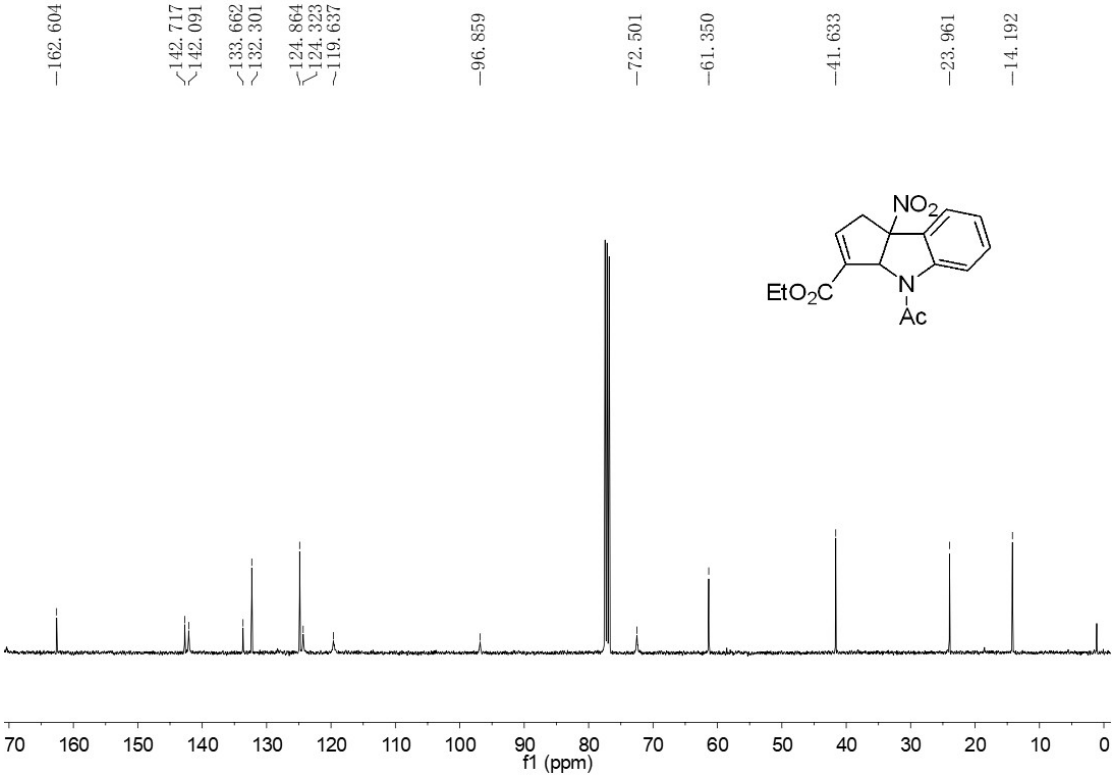
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ra**



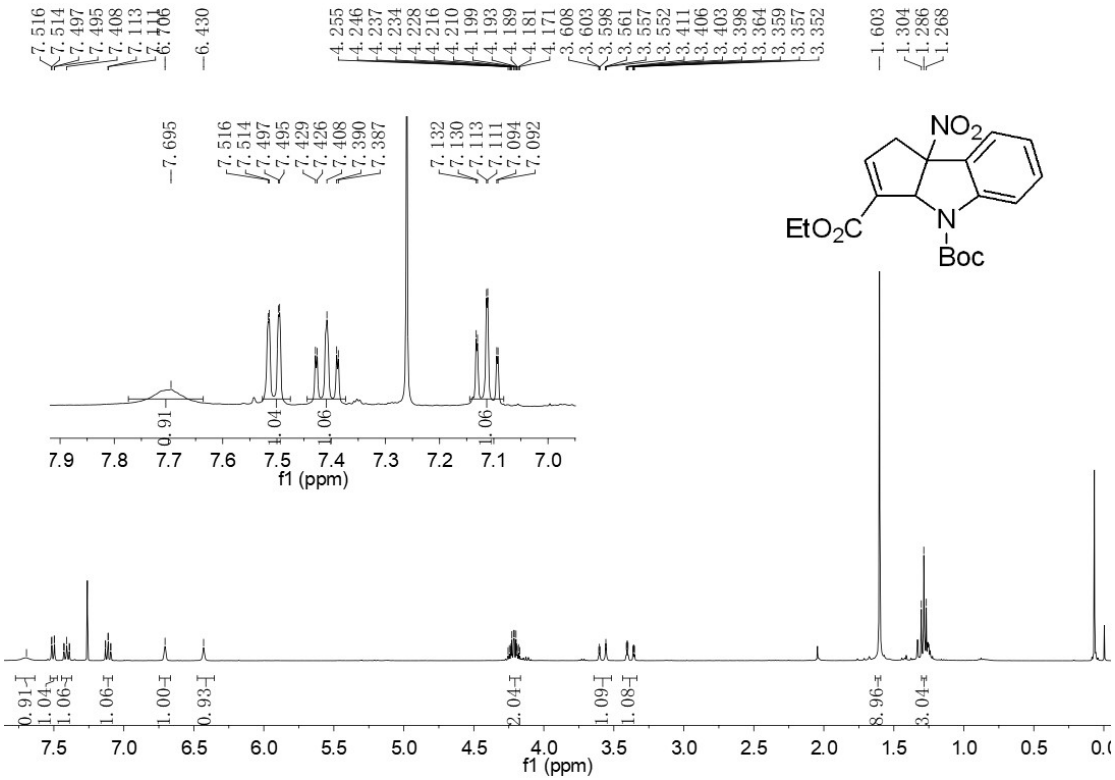
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3sa**



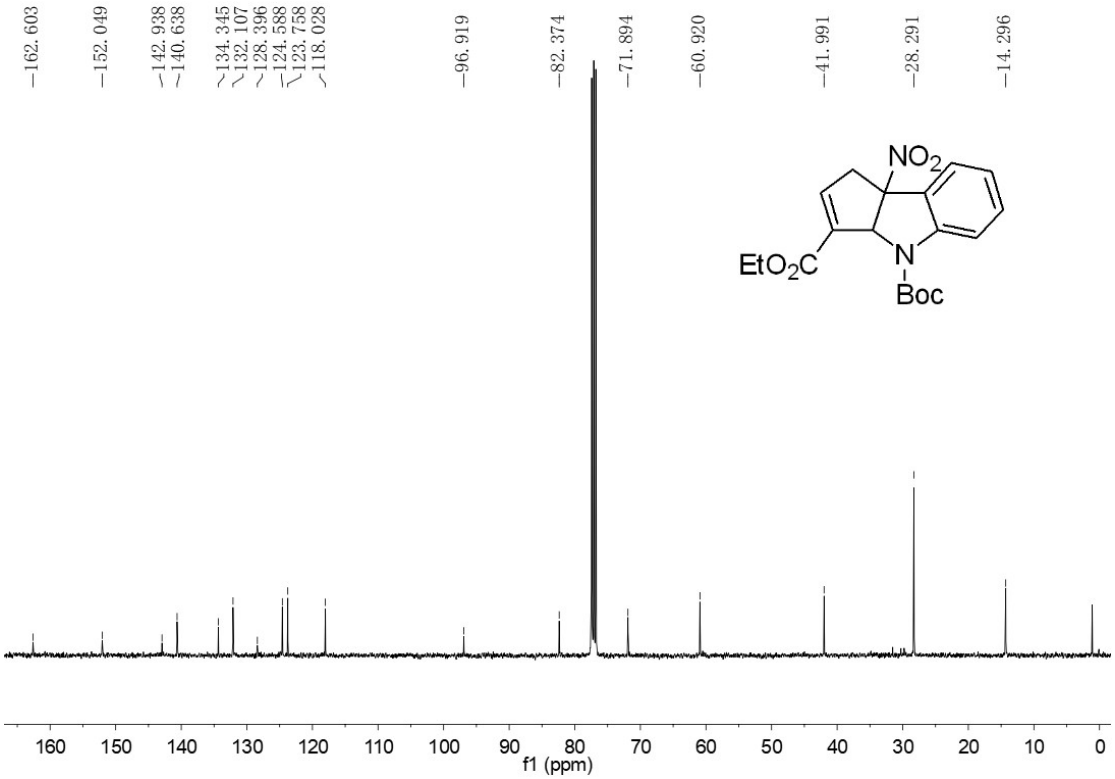
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3sa**



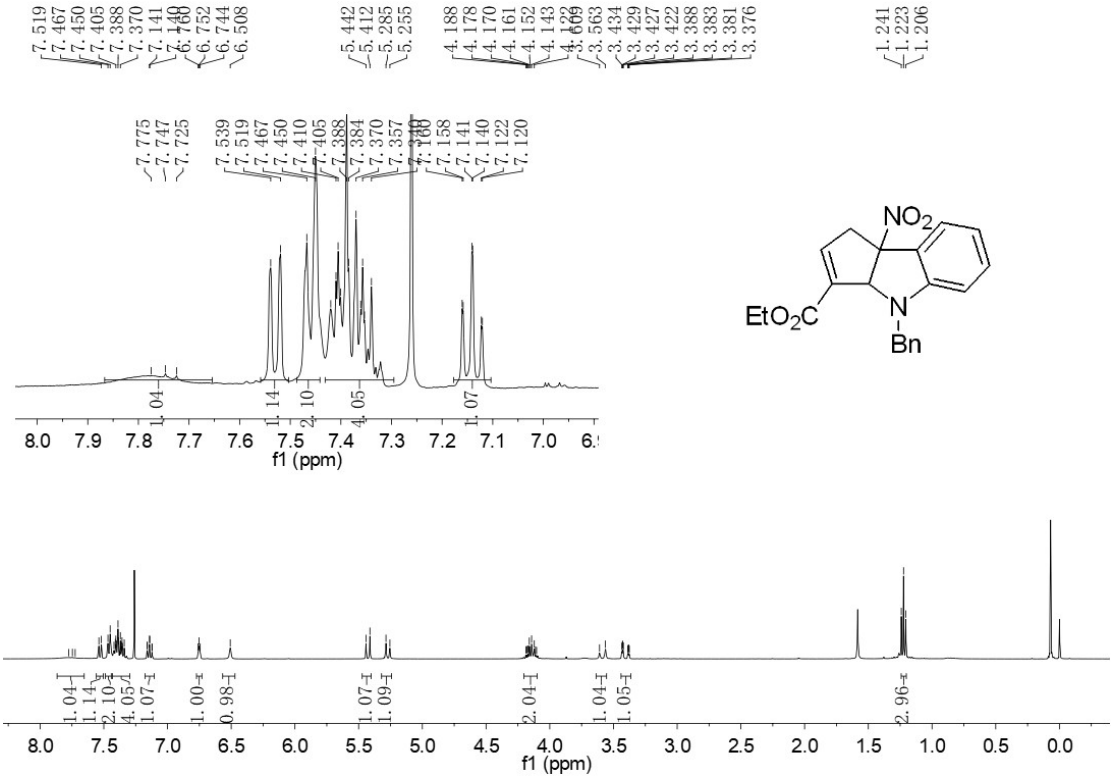
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ta**



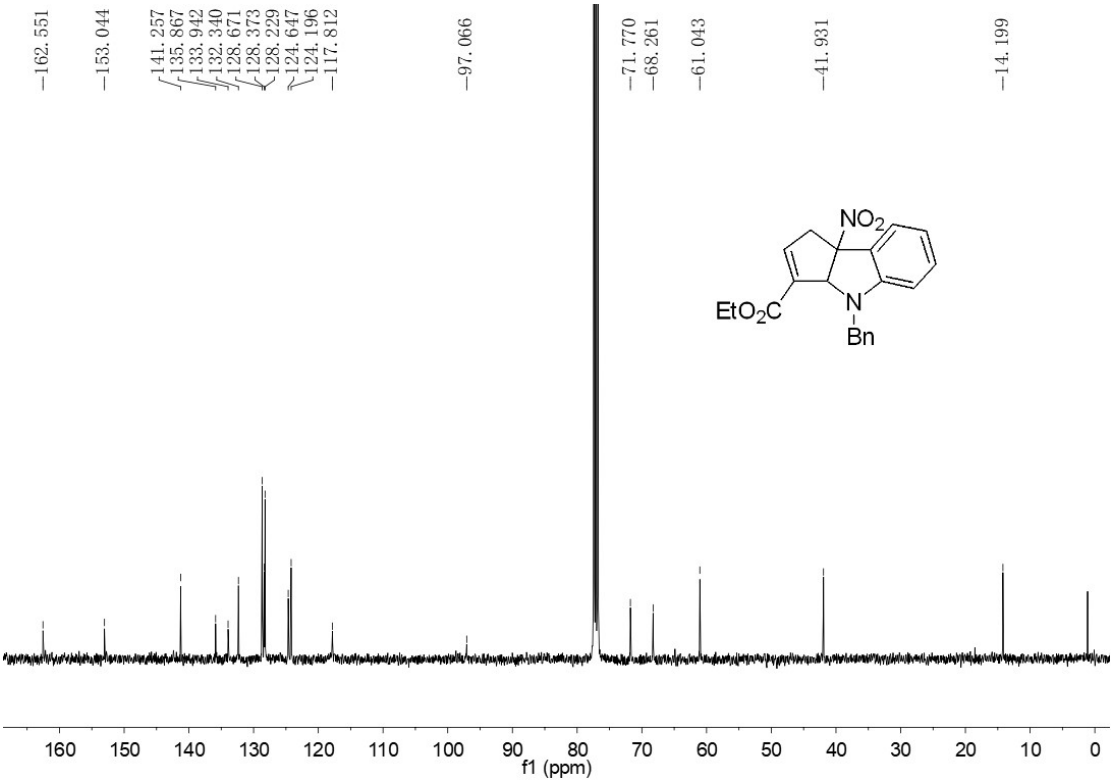
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ta**



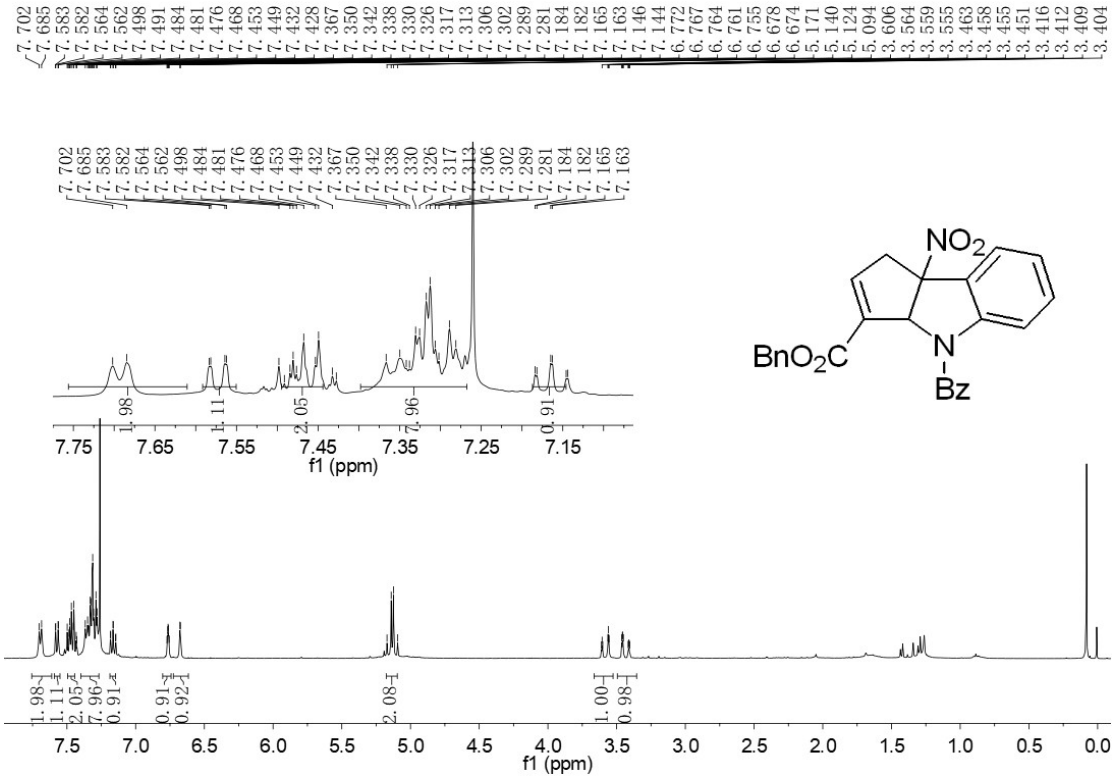
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ua**



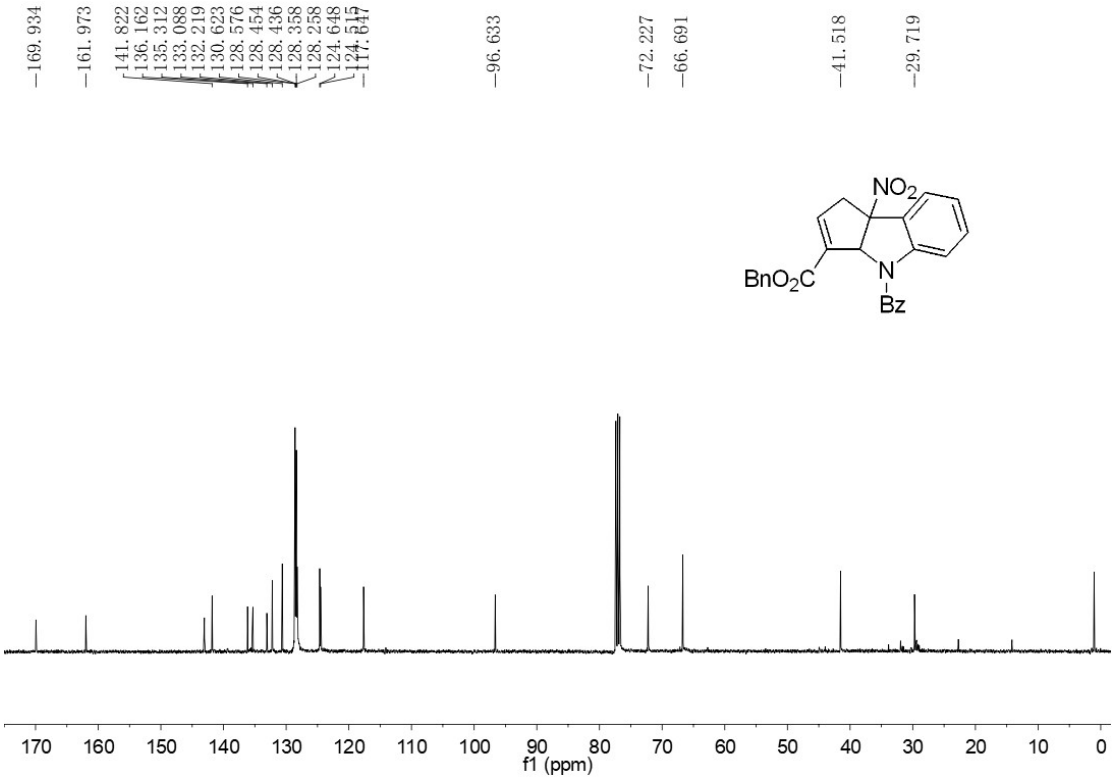
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ua**



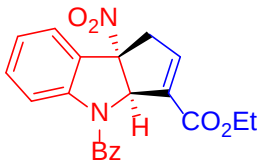
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ab**



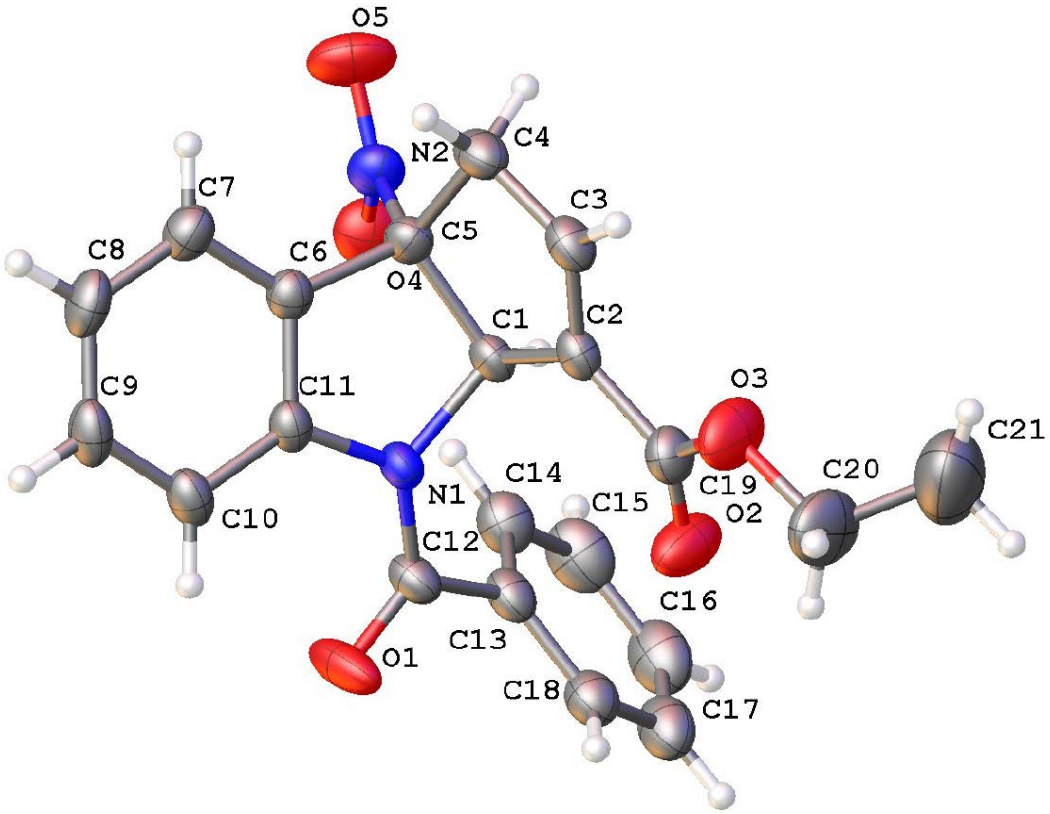
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ab**



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



(relative configuration)
3aa



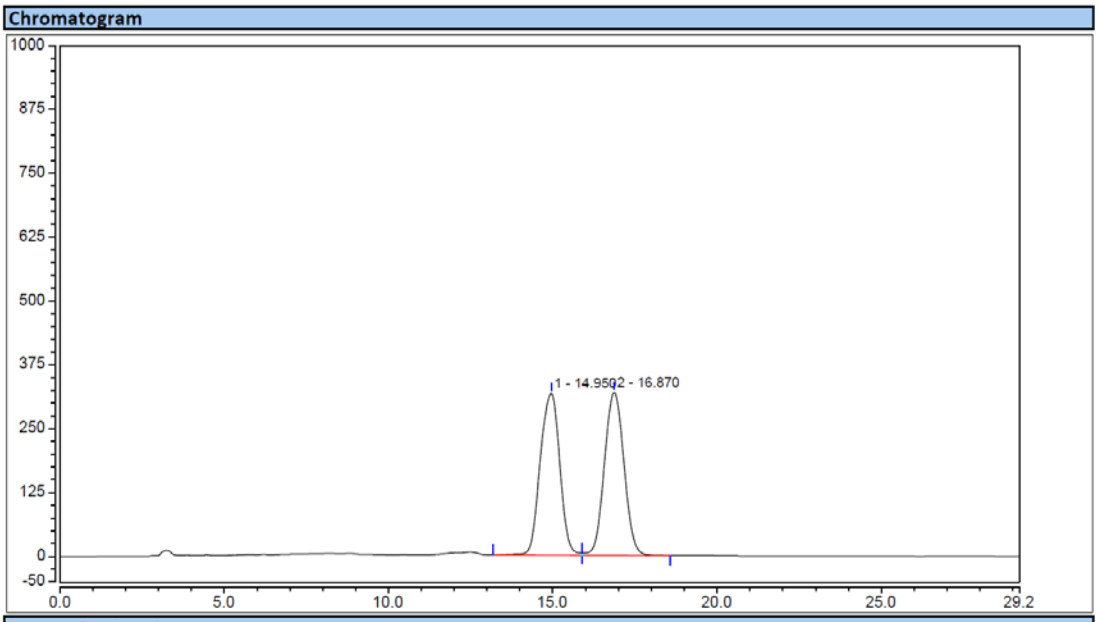
The thermal ellipsoid was drawn at the 30% probability level.

Empirical formula	C21 H18 N2 O5	
Formula weight	378.37	
Temperature	296.15 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 15.7507(18) Å	α= 90°.
	b = 9.3997(11) Å	β= 93.560(2)°.
	c = 12.8142(15) Å	γ = 90°.
Volume	1893.5(4) $Å^3$	
Z	4	
Density (calculated)	1.327 Mg/m^3	
Absorption coefficient	0.096 mm^{-1}	

F(000)	792
Crystal size	0.5 x 0.2 x 0.2 mm^3
Theta range for data collection	2.525 to 28.074°.
Index ranges	-19<=h<=20, -10<=k<=12, -16<=l<=16
Reflections collected	11052
Independent reflections	4370 [R(int) = 0.0255]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6661
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4370 / 19 / 254
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0715, wR2 = 0.2062
R indices (all data)	R1 = 0.1139, wR2 = 0.2455
Extinction coefficient	n/a
Largest diff. peak and hole	0.827 and -0.469 e.$Å^{-3}$

3. HPLC copies of product 3aa

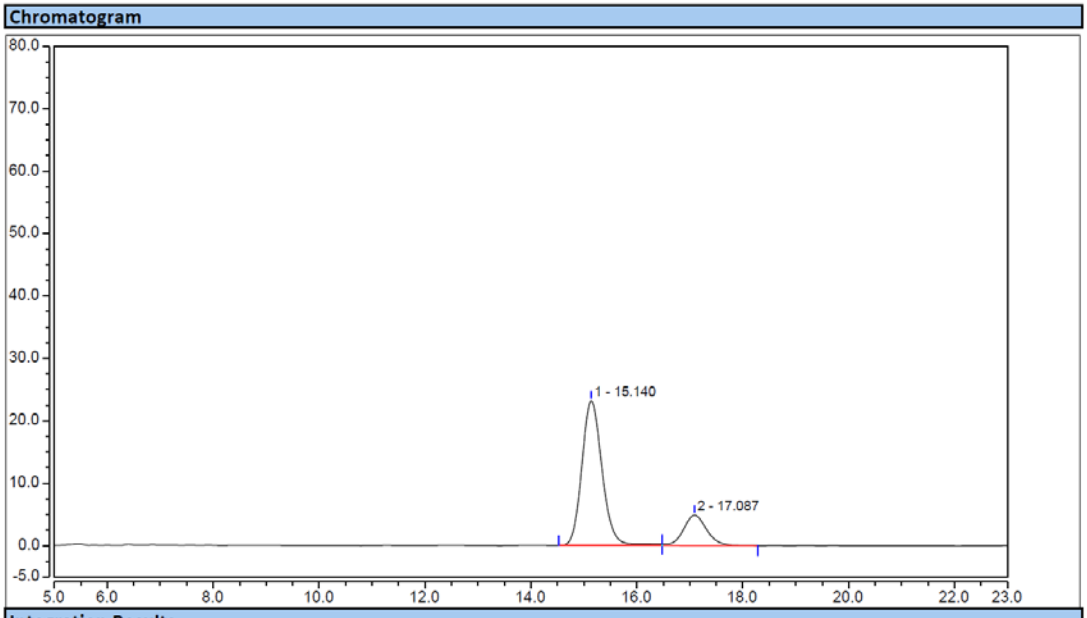
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.950	218.104	317.003	49.77	49.79	n.a.
2		16.870	220.109	319.630	50.23	50.21	n.a.
Total:			**438.213**	**636.633**	**100.00**	**100.00**	

Enantioselective:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.140	10.317	23.206	80.74	82.64	n.a.
2		17.087	2.461	4.874	19.26	17.36	n.a.
Total:			**12.778**	**28.080**	**100.00**	**100.00**	