Rhodium(III)-Catalyzed Direct Coupling of Quinoline-8-Carbaldehydes with (Het)Arylboronic Acids for the Synthesis of 8-Aryloylquinolines

Supporting Information

Xue-Li Lyu, † Shi-Sheng Huang, † Yuan-Qiong Huang, † Yong-Qiang Li, † Hong-Jian Song, *† Yu-Xiu Liu*† and Qing-Min Wang*†‡

†State Key Laboratory of Elemento-Organic Chemistry, Research Institute of Elemento-Organic Chemistry, College of Chemistry, Nankai University, Tianjin 300071, People's Republic of China

‡Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Tianjin 300071, People's Republic of China

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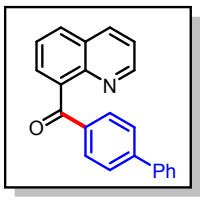
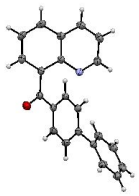
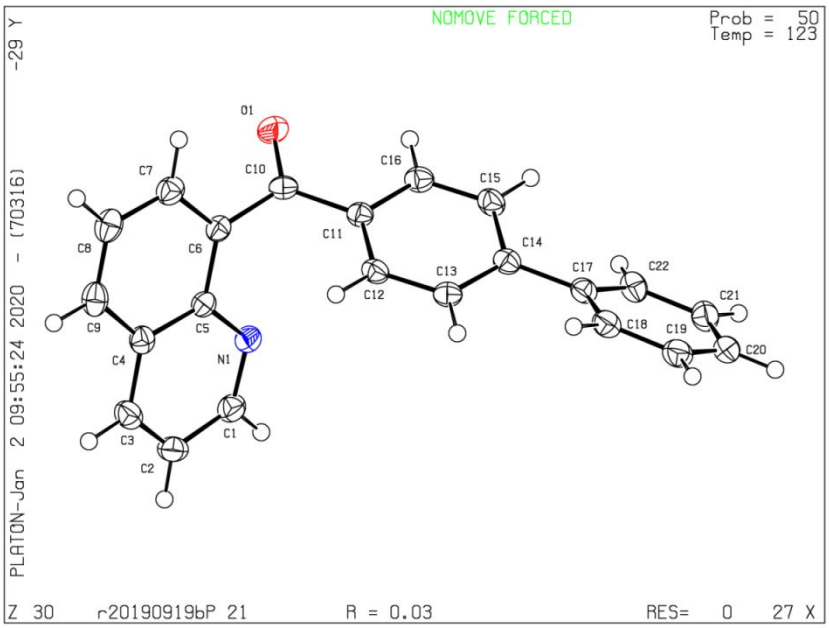
1. X-ray single crystal data for product 3ah.





ORTEP diagram of **3ah**. Thermal ellipsoids are shown at the 50% probability level. Carbon: grey; nitrogen: purple; oxygen: red; hydrogen: offwhite; CCDC 1966228 contains the supplementary crystallographic data for this paper. These data can obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.

By slowly volatilizing the DCM solvent, single crystals **3ah** suitable for X-ray analysis were obtained. The detailed characteristics and data are shown below.



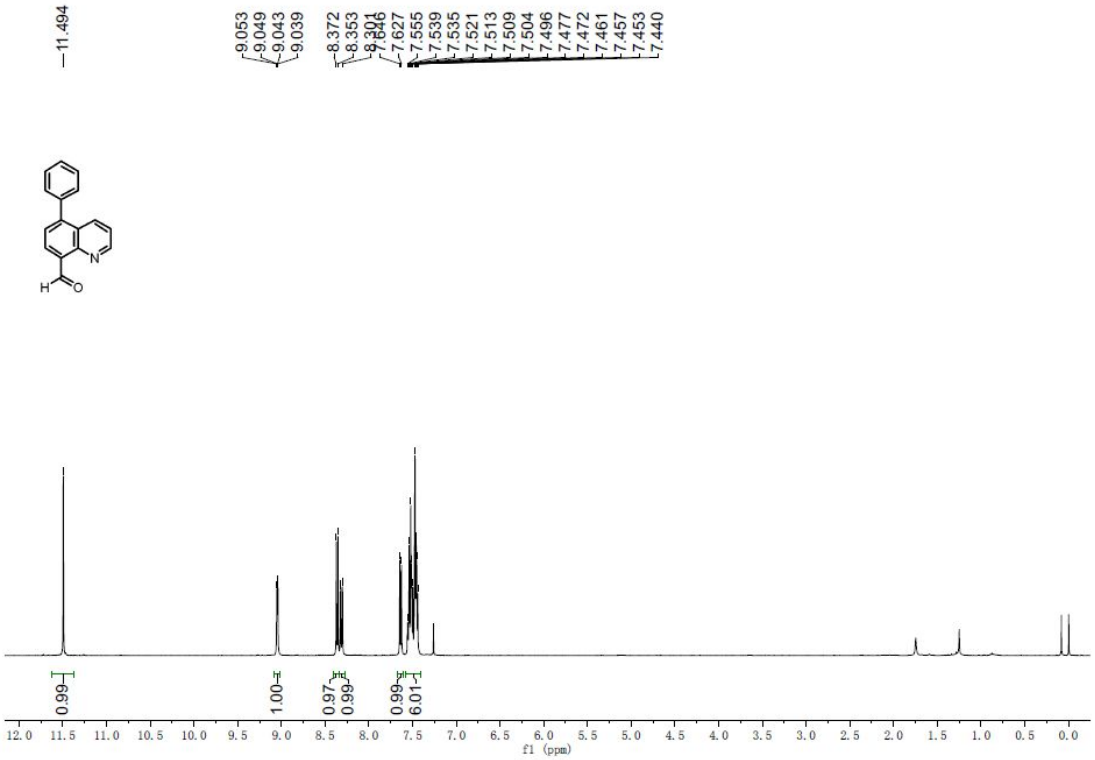
Identification code	**3ah**	
Empirical formula	$C_{22}H_{15}NO$	
Formula weight	309.12	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P2(1)	
	a = 7.6652(3) Å	alpha = 90 deg.
Unit cell dimensions	b = 10.2251(3) Å	beta = 97.411(3) deg.
	c = 10.0678(4) Å	gamma = 90 deg.
Volume	782.50(5) $Å^3$	

Z, Calculated density	16, 1.313 Mg/m^3
Absorption coefficient	0.080 mm^{-1}
F(000)	324
Crystal size	0.200 x 0.180 x 0.150 mm
Theta range for data collection	2.040 to 26.370 deg.
Limiting indices	-9<=h<=9, -12<=k<=12, -12<=l<=12
Reflections collected / unique	8399 / 3196 [R(int) = 0.0316]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8359
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3196/ 1 / 218
Goodness-of-fit on F^2	1.001
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0834
R indices (all data)	R1 = 0.0334, wR2 = 0.0855
Absolute structure parameter	1.5(7)
Extinction coefficient	0.082(11)
Largest diff. peak and hole	0.159 and -0.127 e. $Å^{-3}$

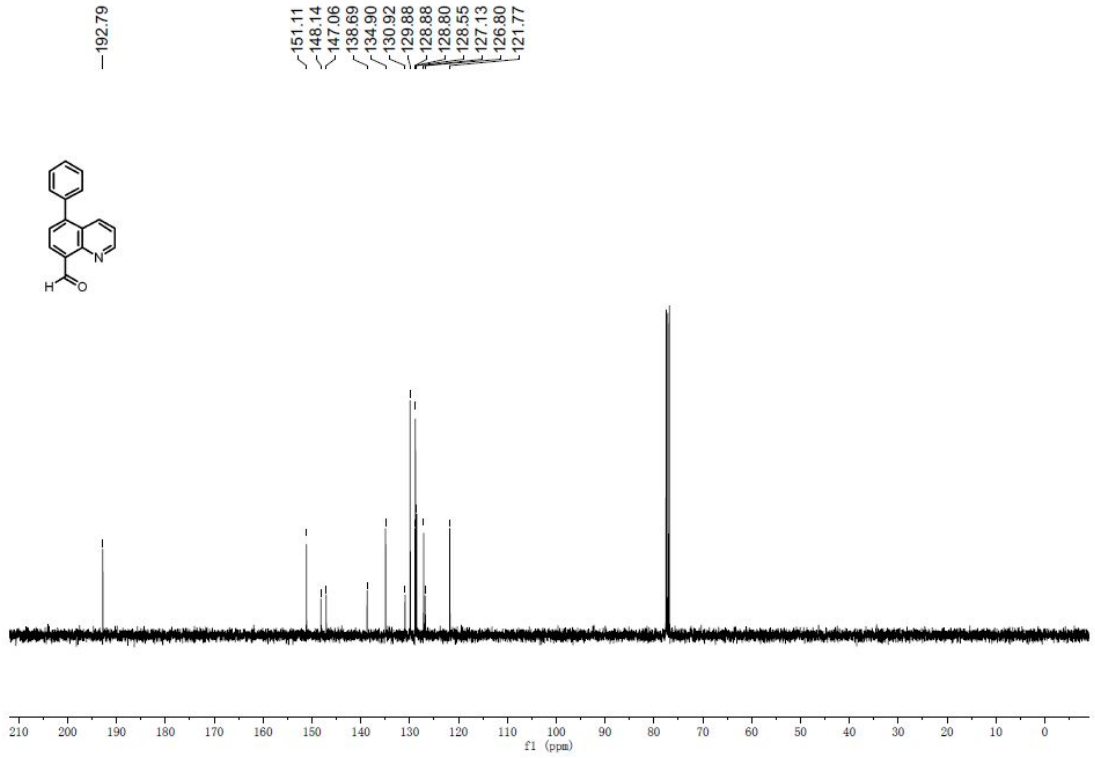
2. NMR spectra of starting materials and products.

(1) NMR spectra of starting materials.

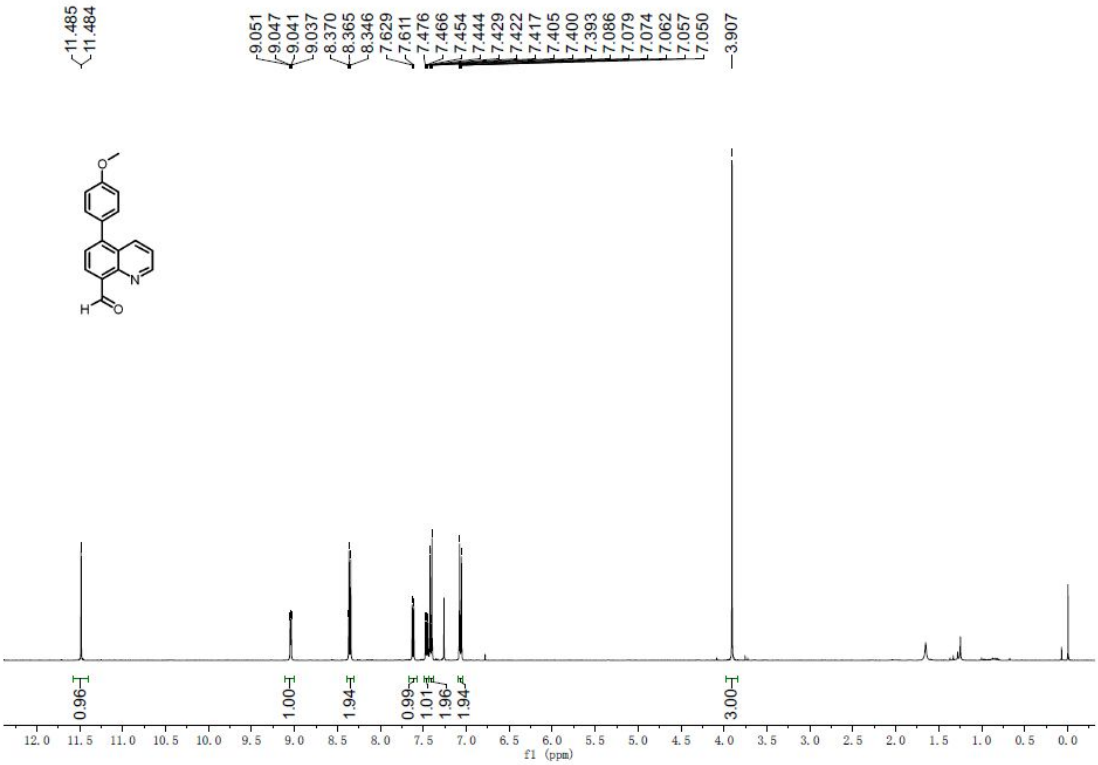
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1b



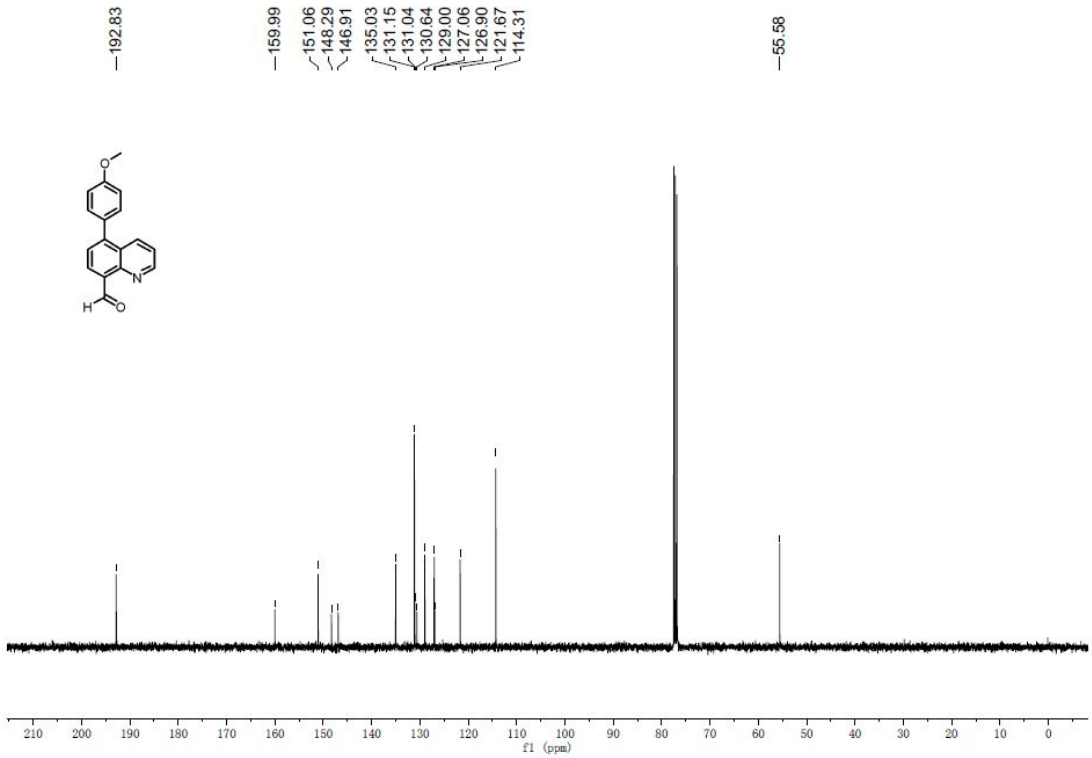
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1b



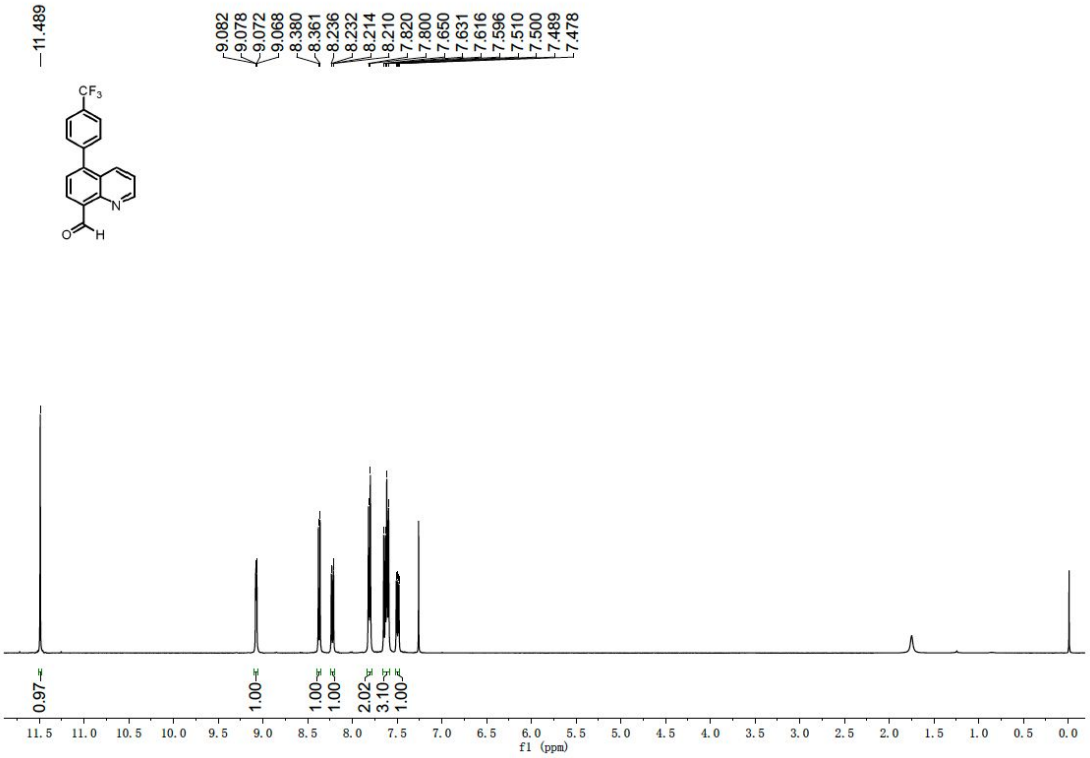
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1c



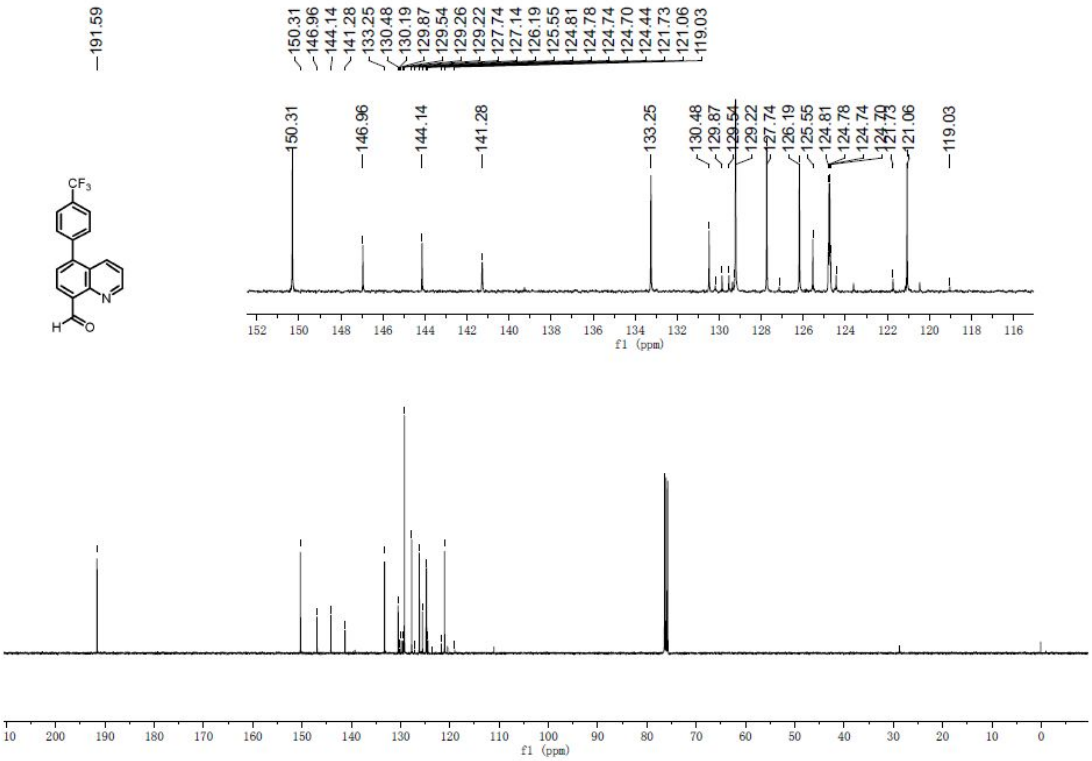
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1c



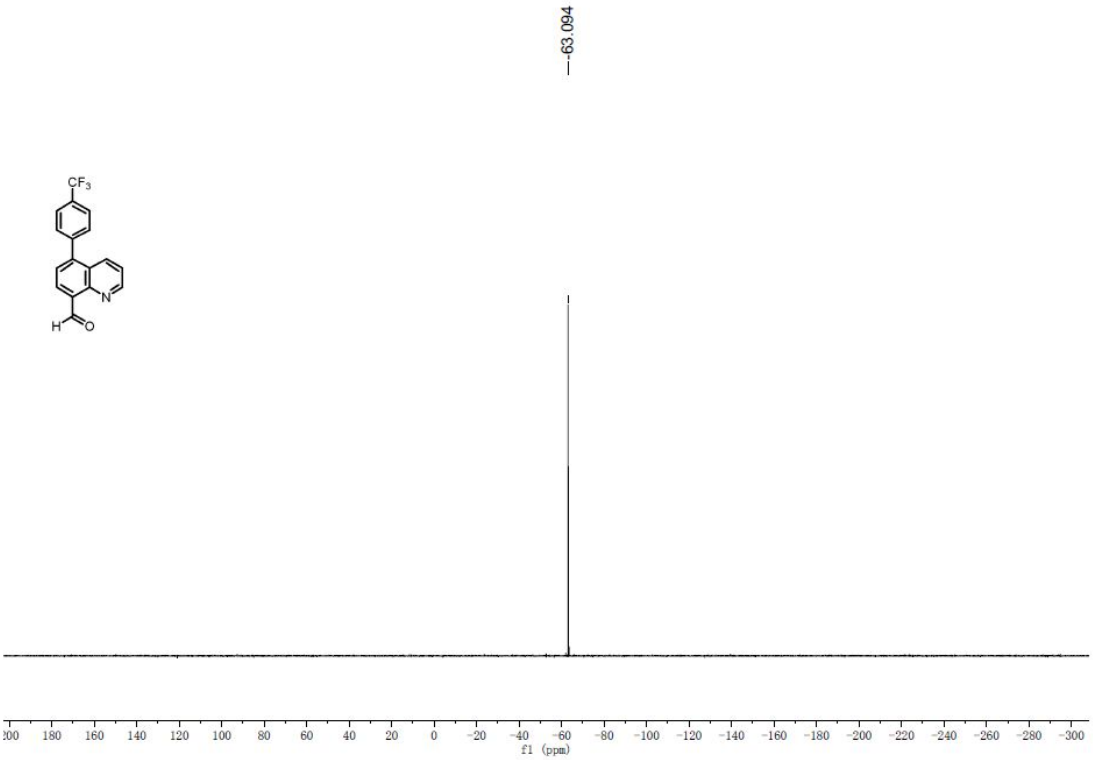
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1d



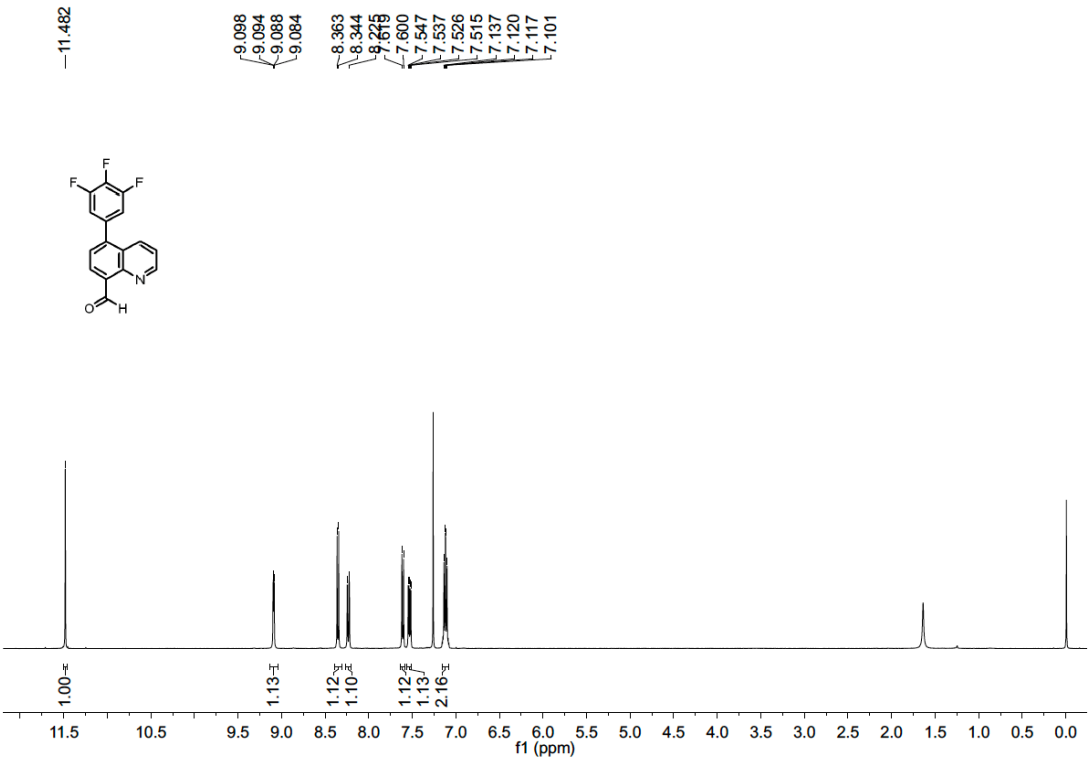
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1d



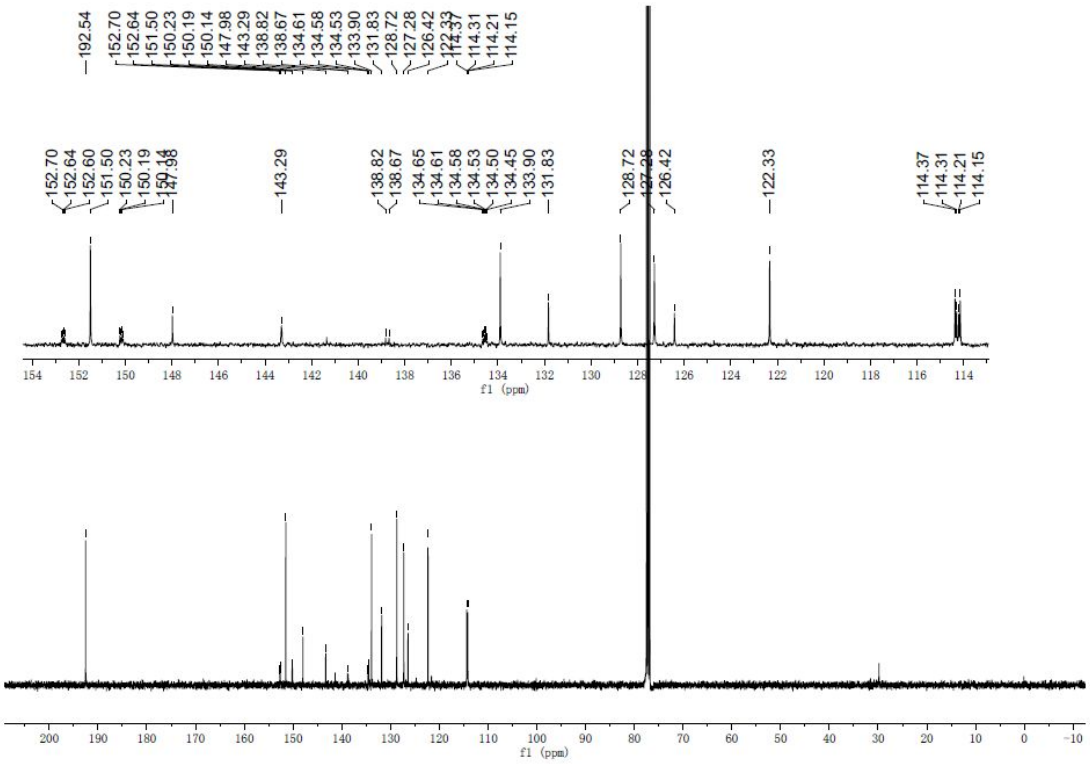
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 1d



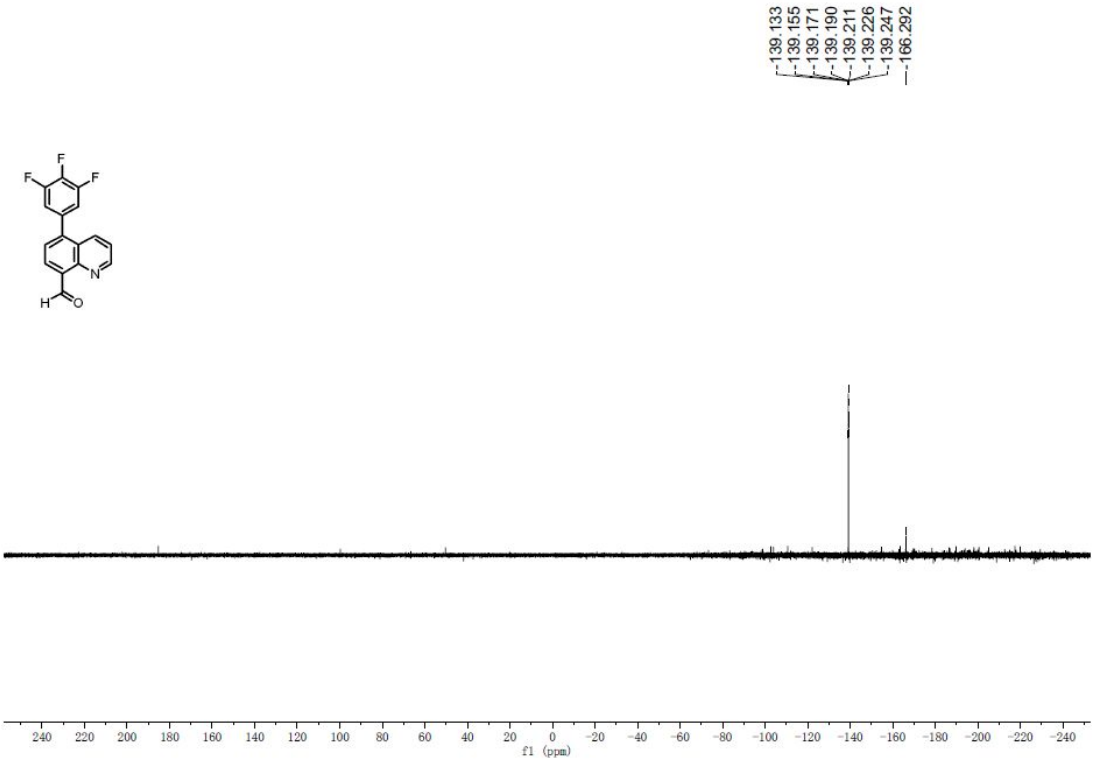
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1e



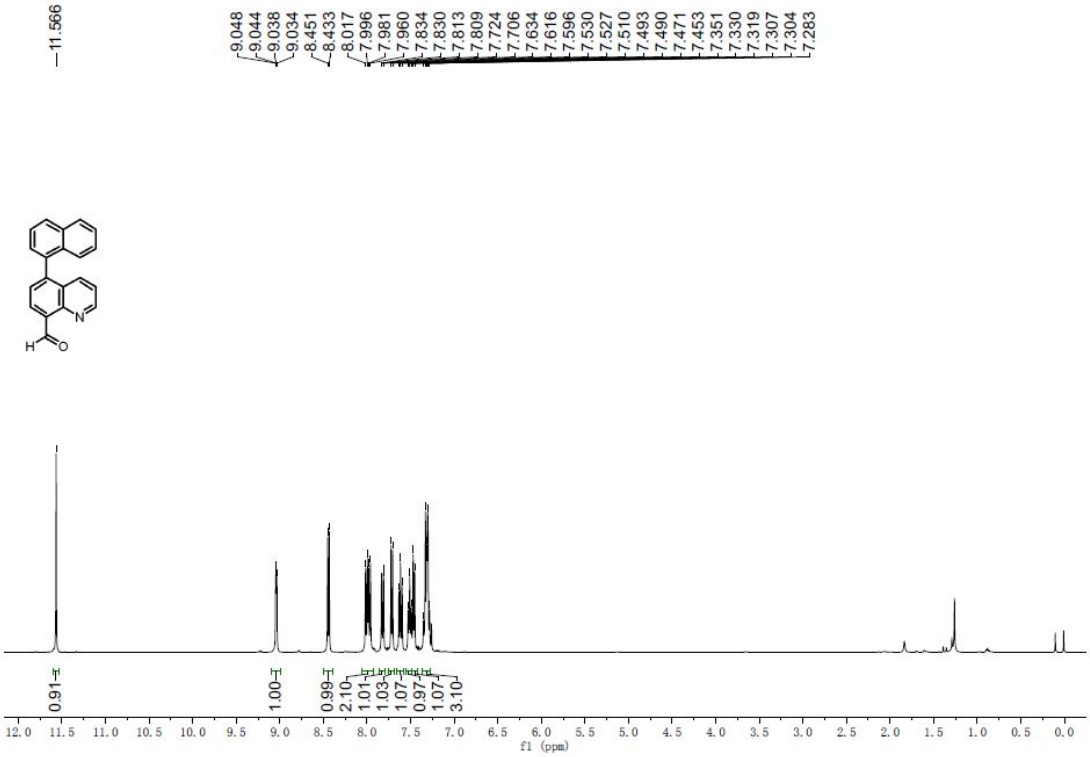
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1e



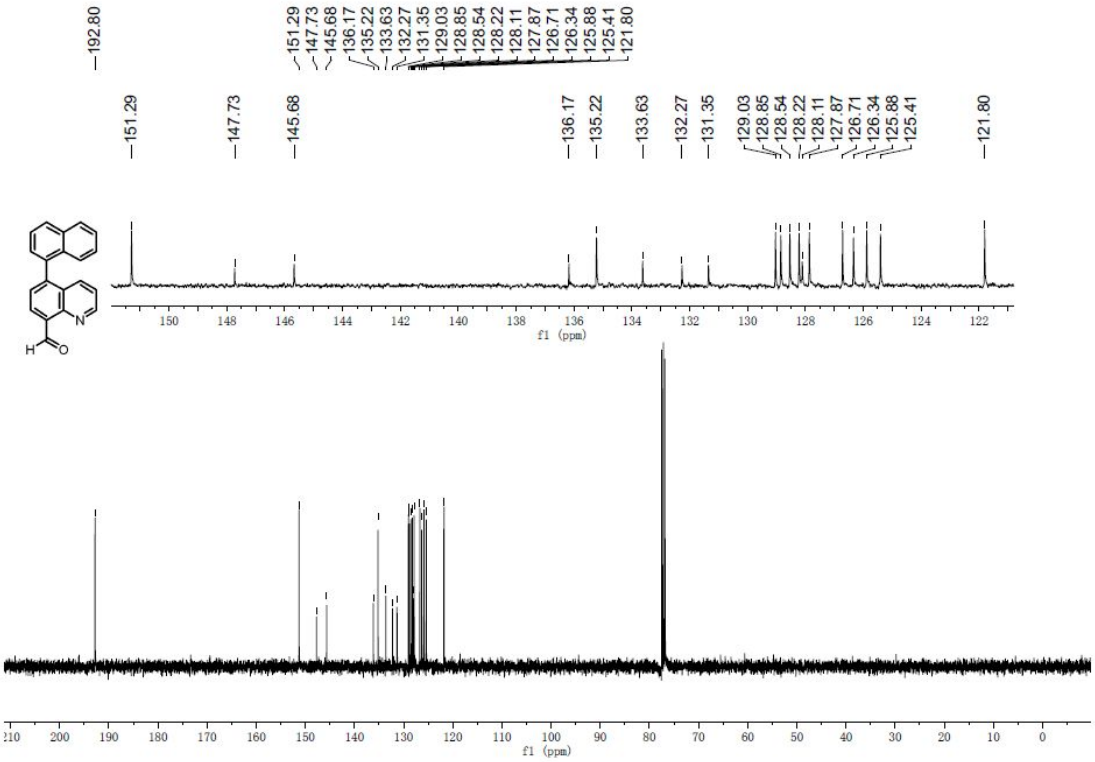
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 1e



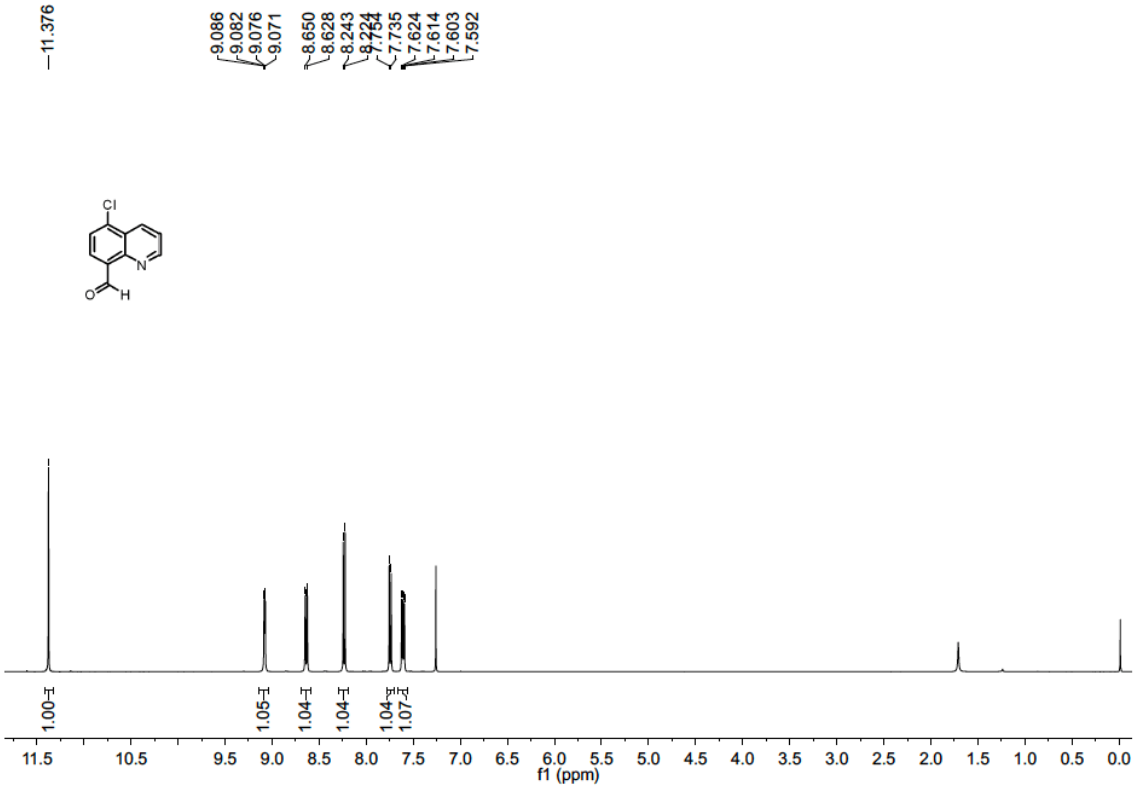
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1f



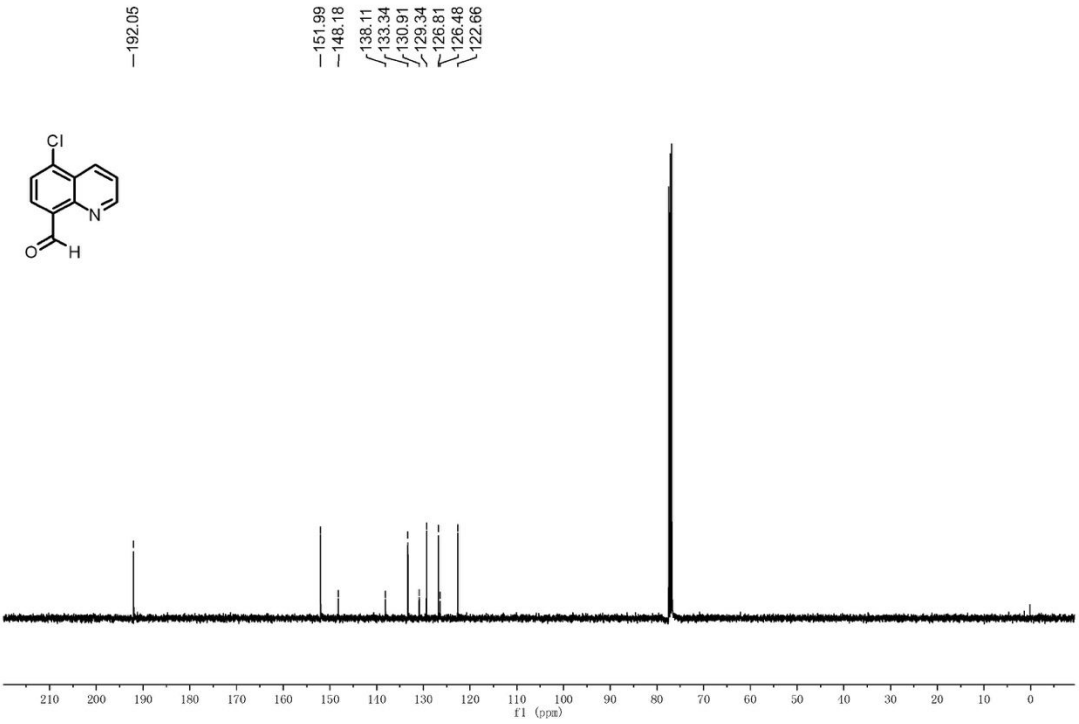
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1f



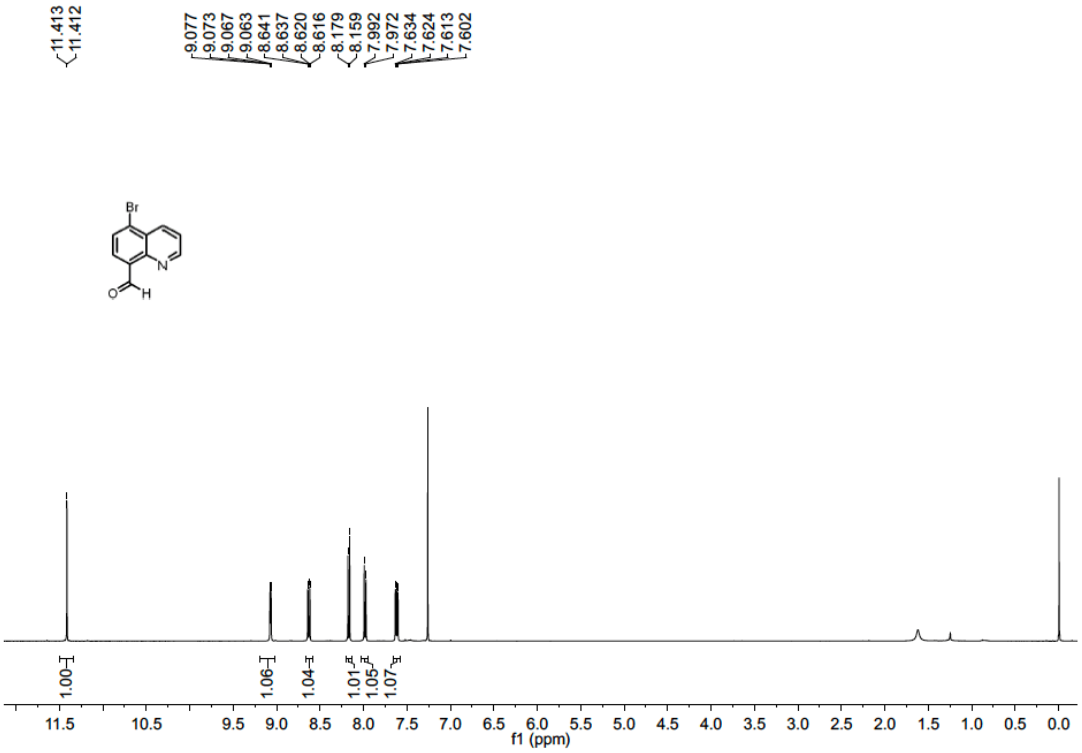
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1g



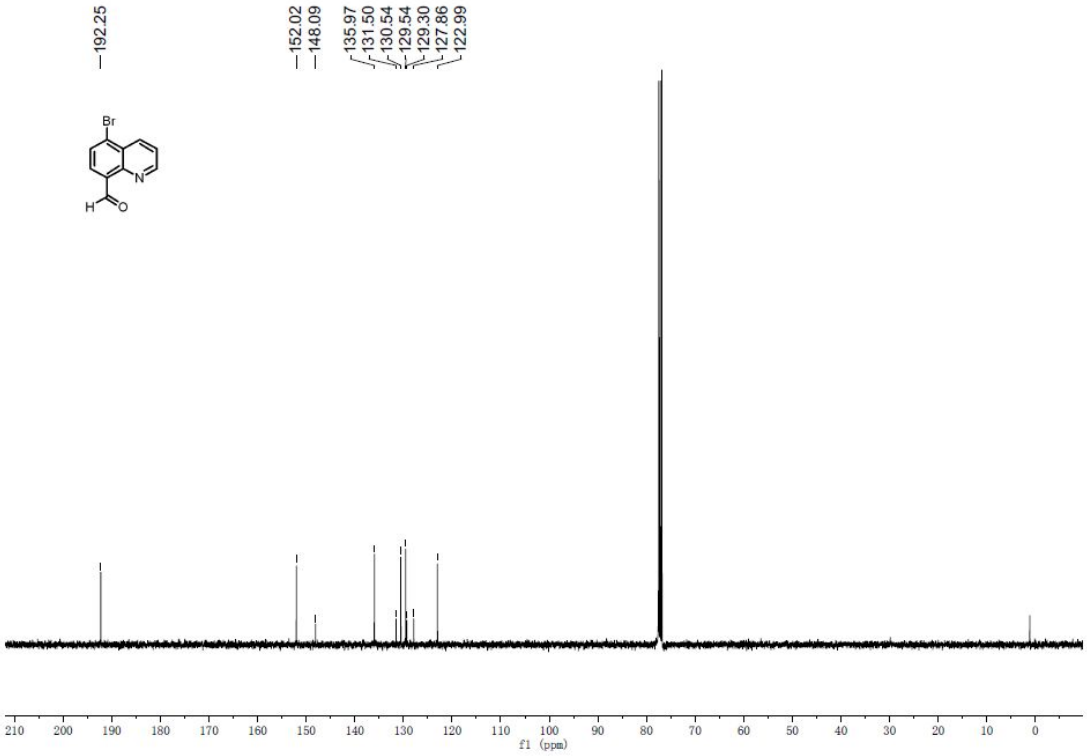
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1g



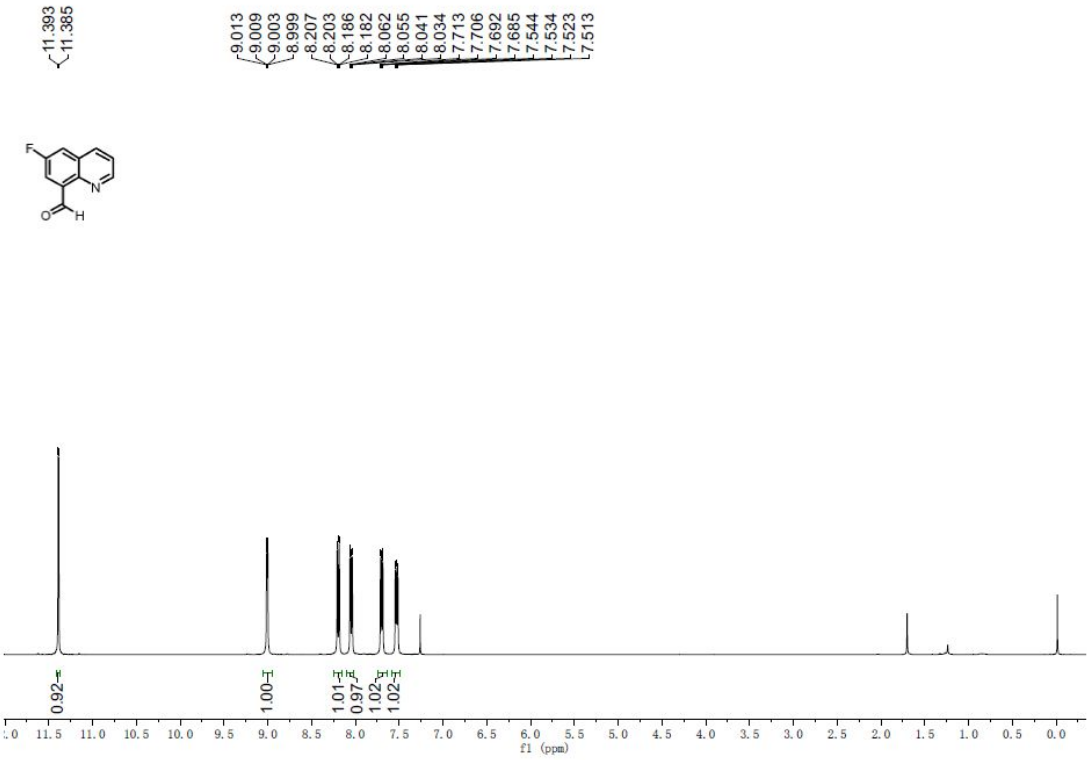
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1h



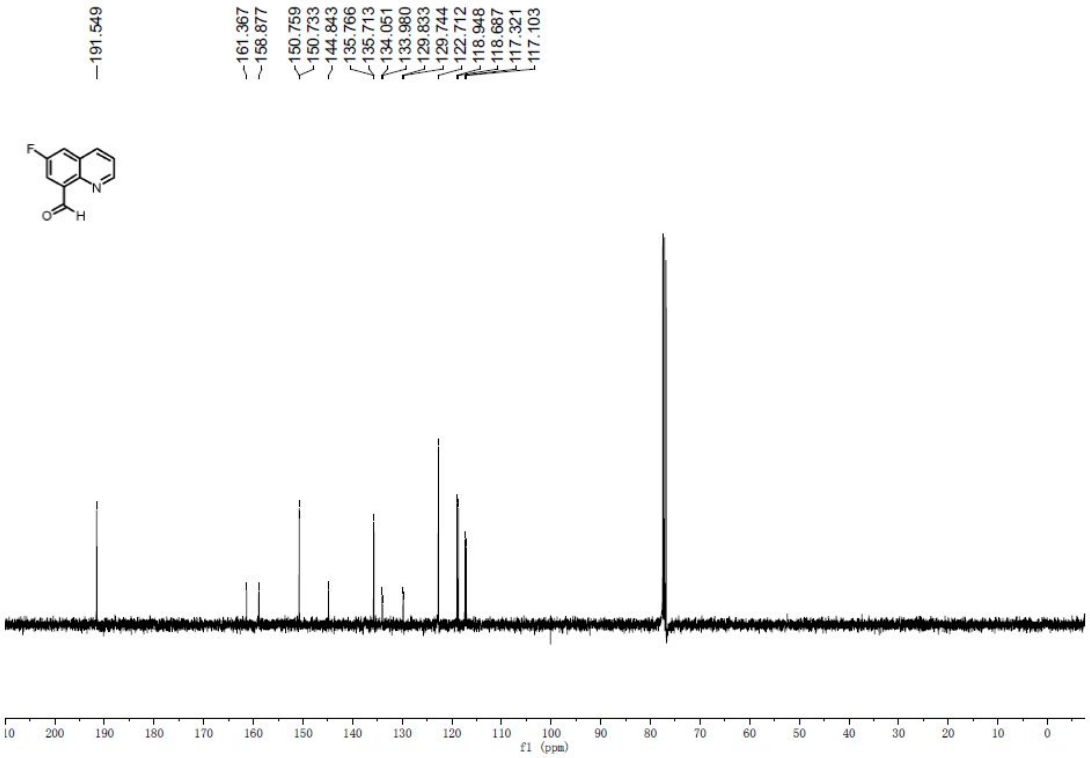
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1h



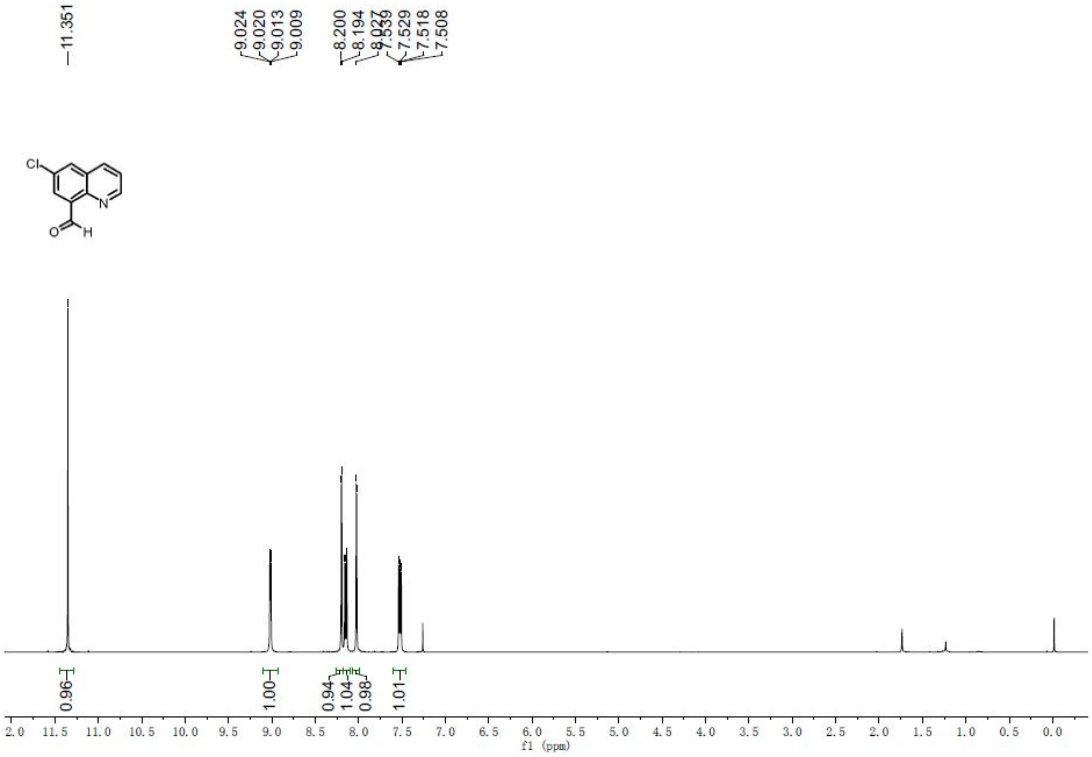
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1i



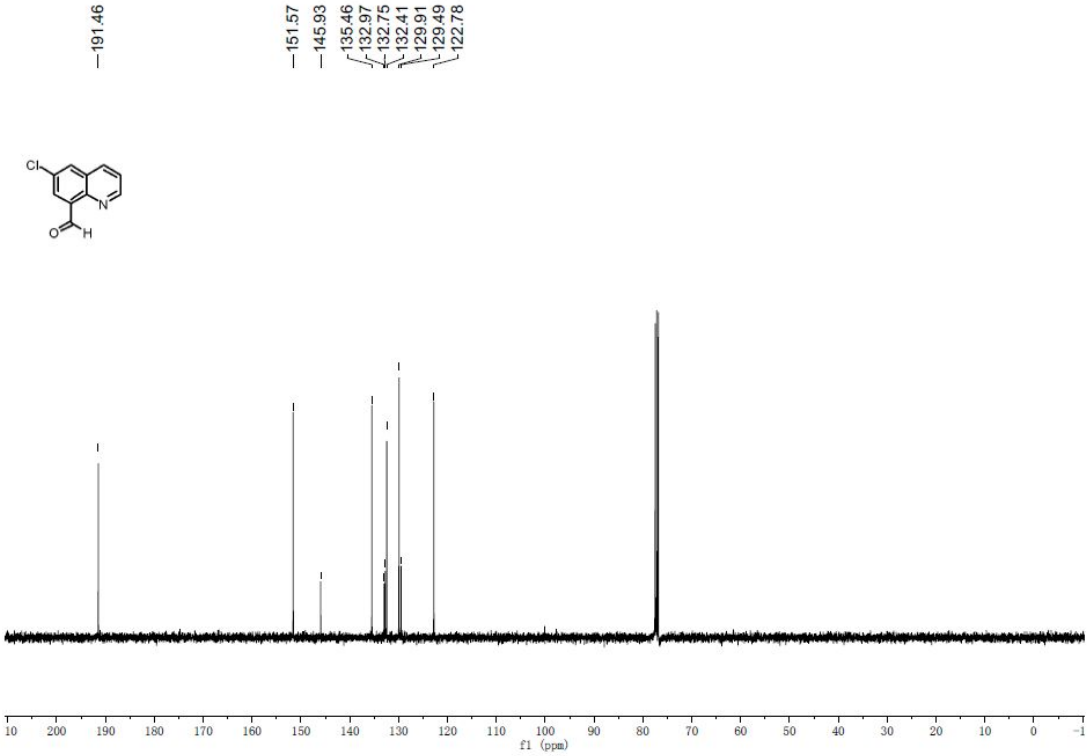
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1i



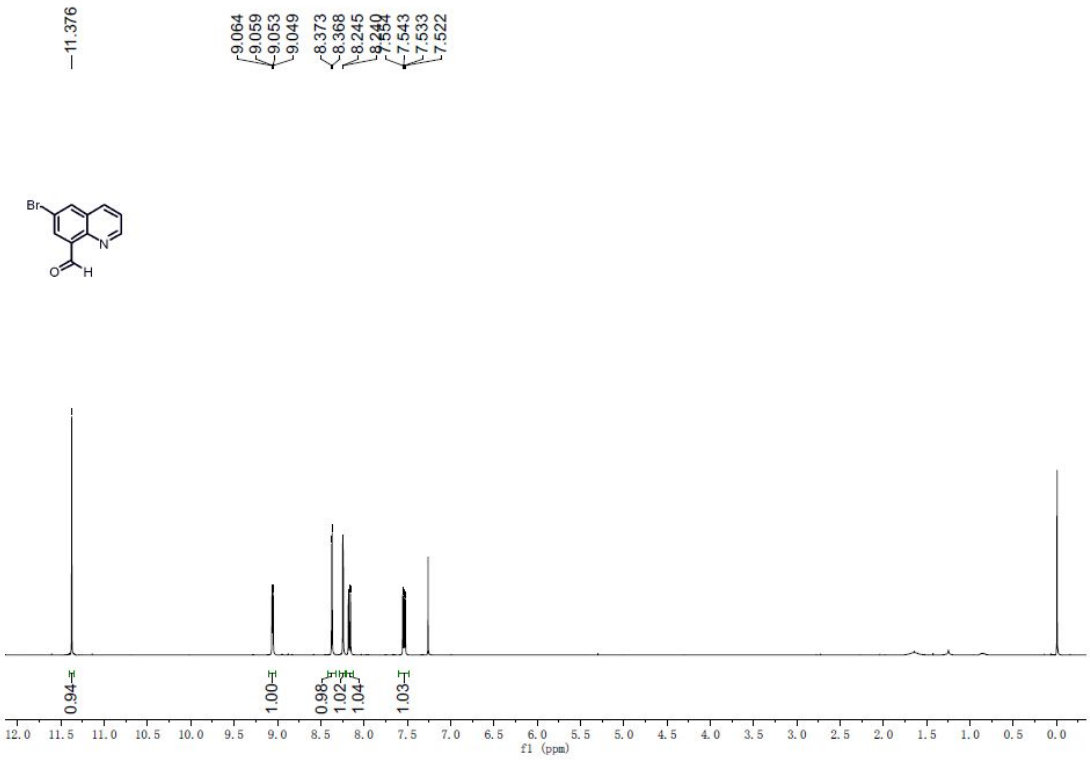
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1j



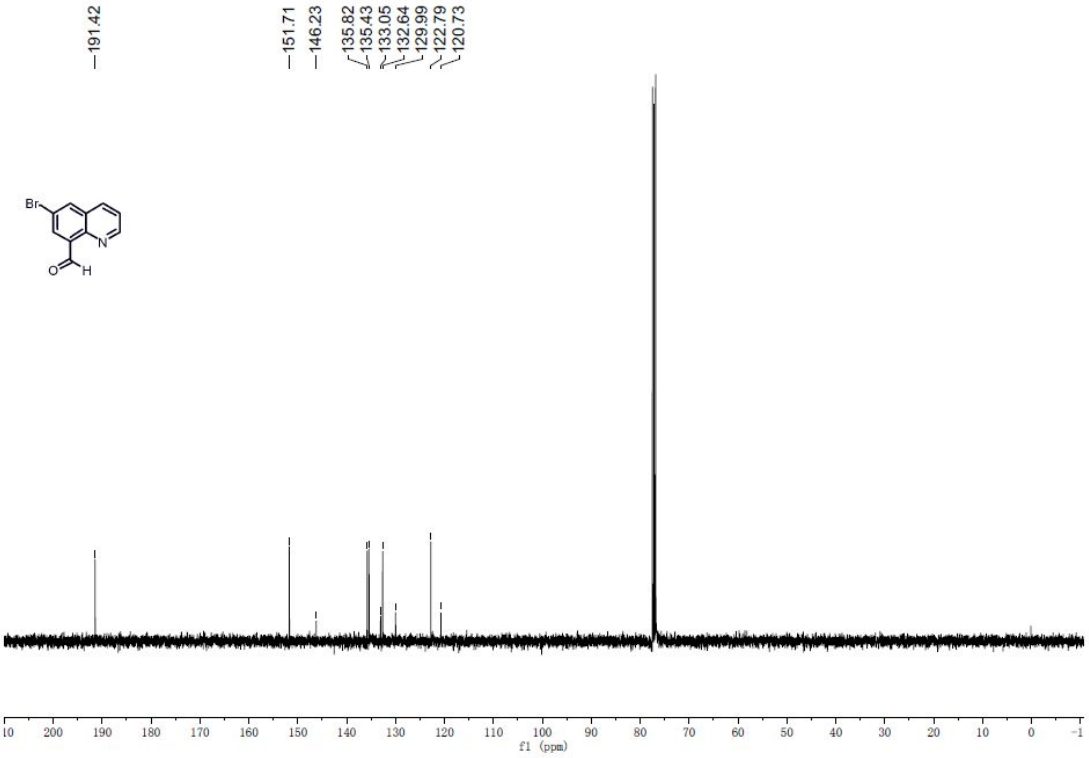
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1j



^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1k

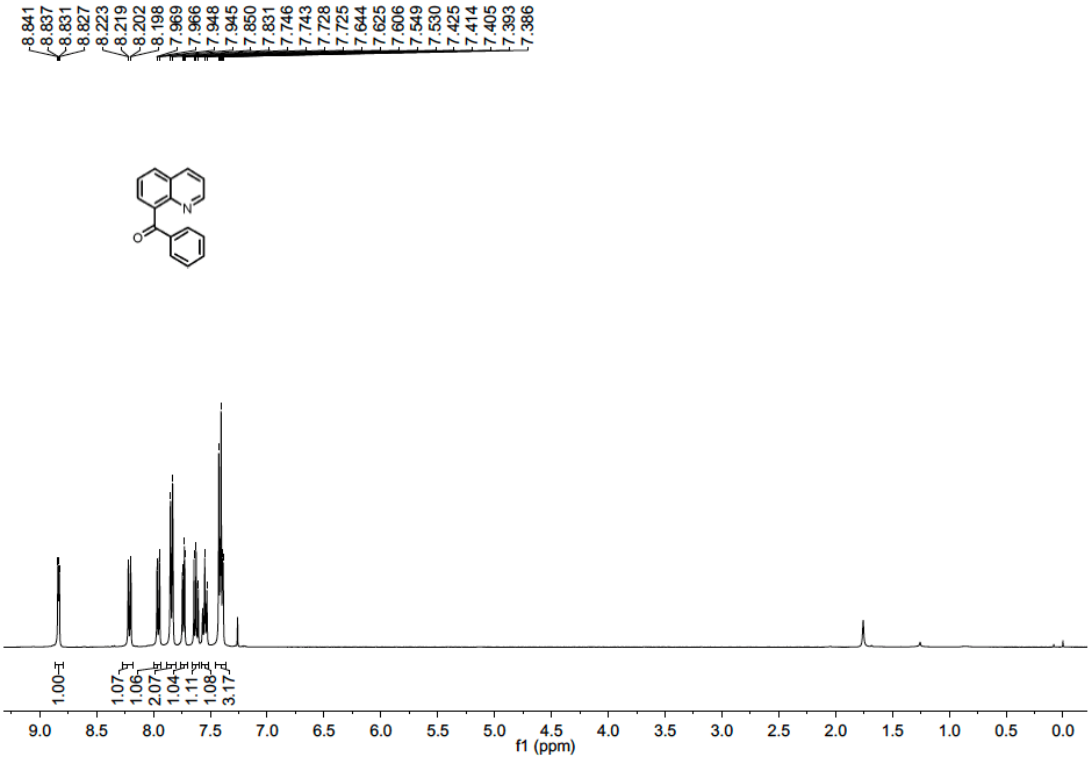


^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1k

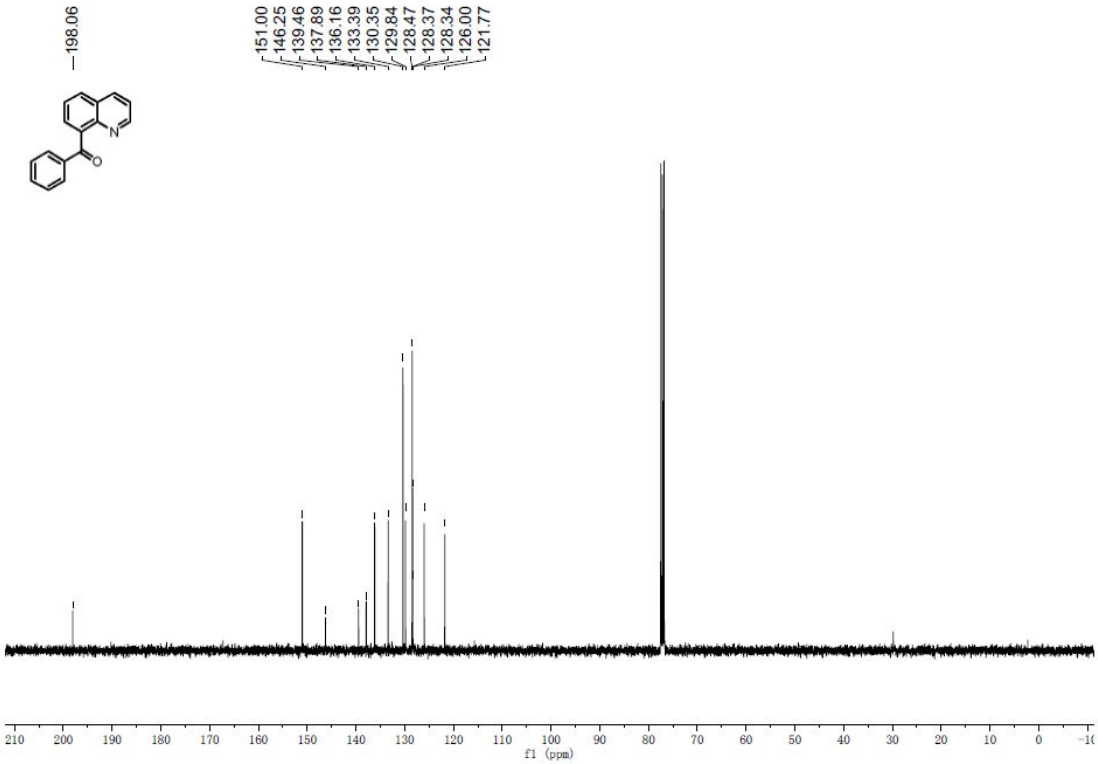


(2) NMR spectra of products.

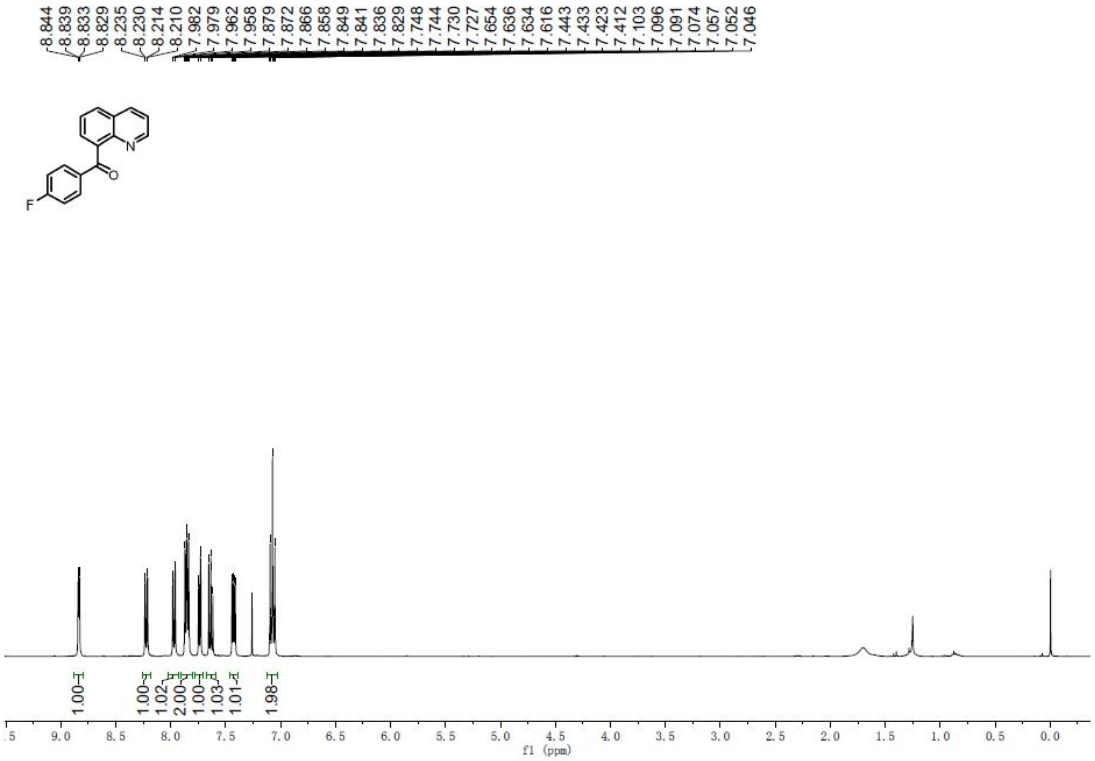
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3aa



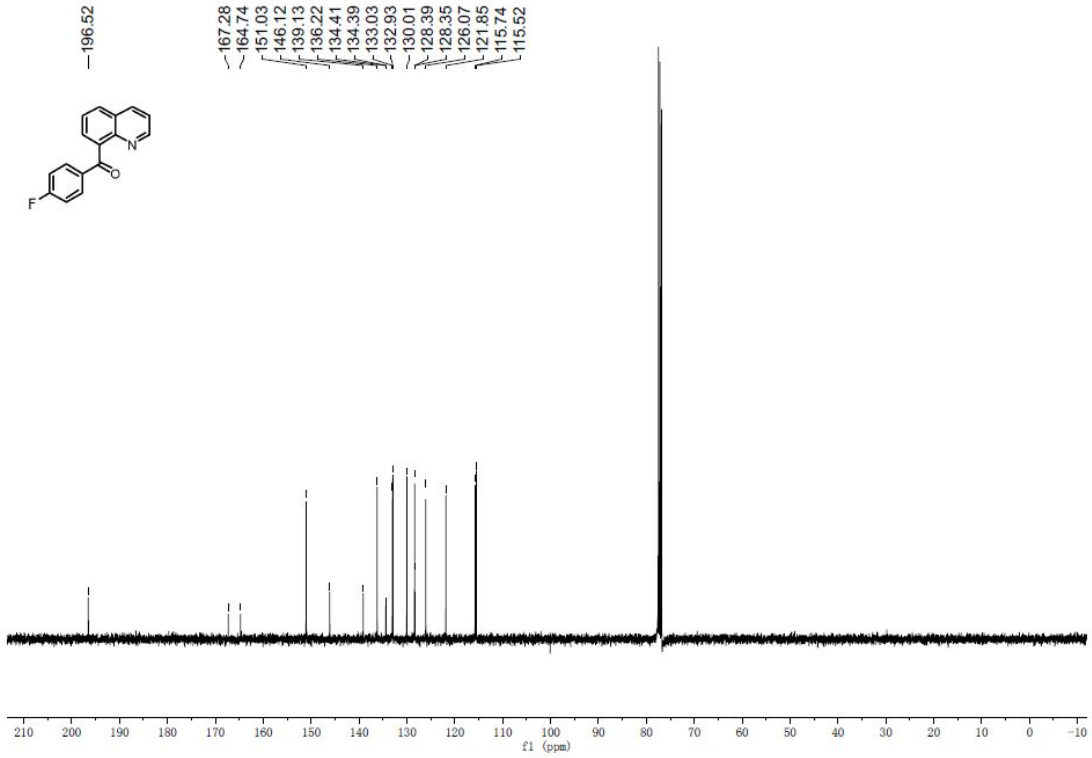
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3aa



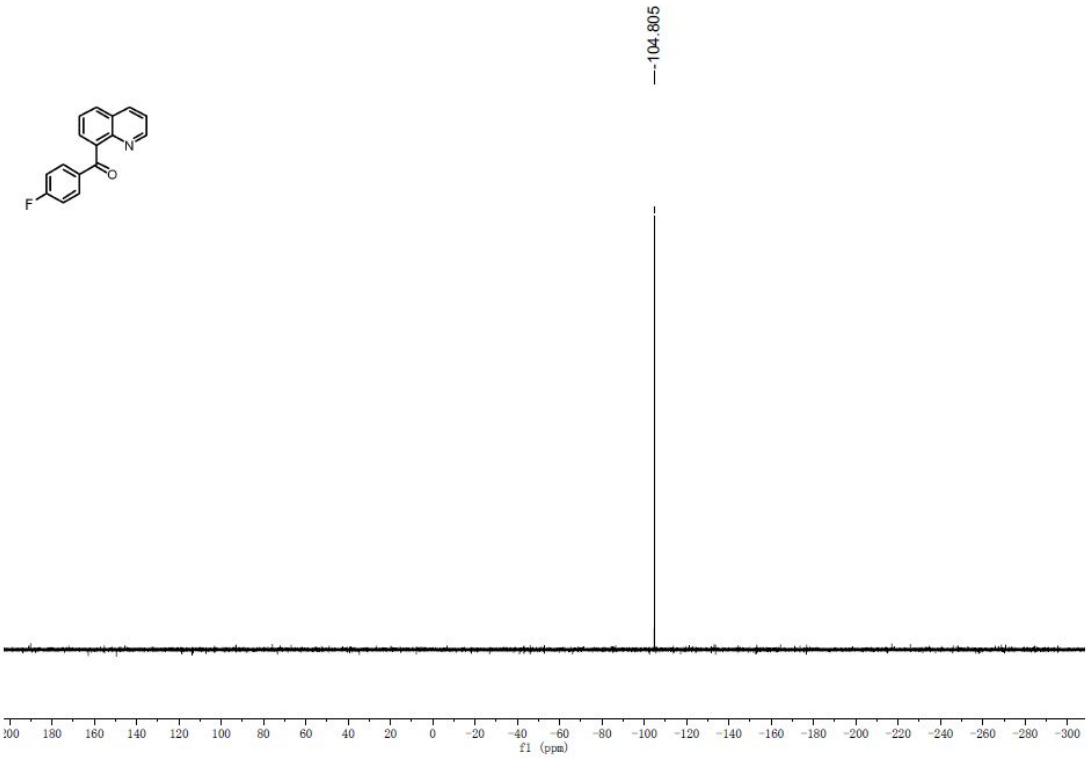
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ab



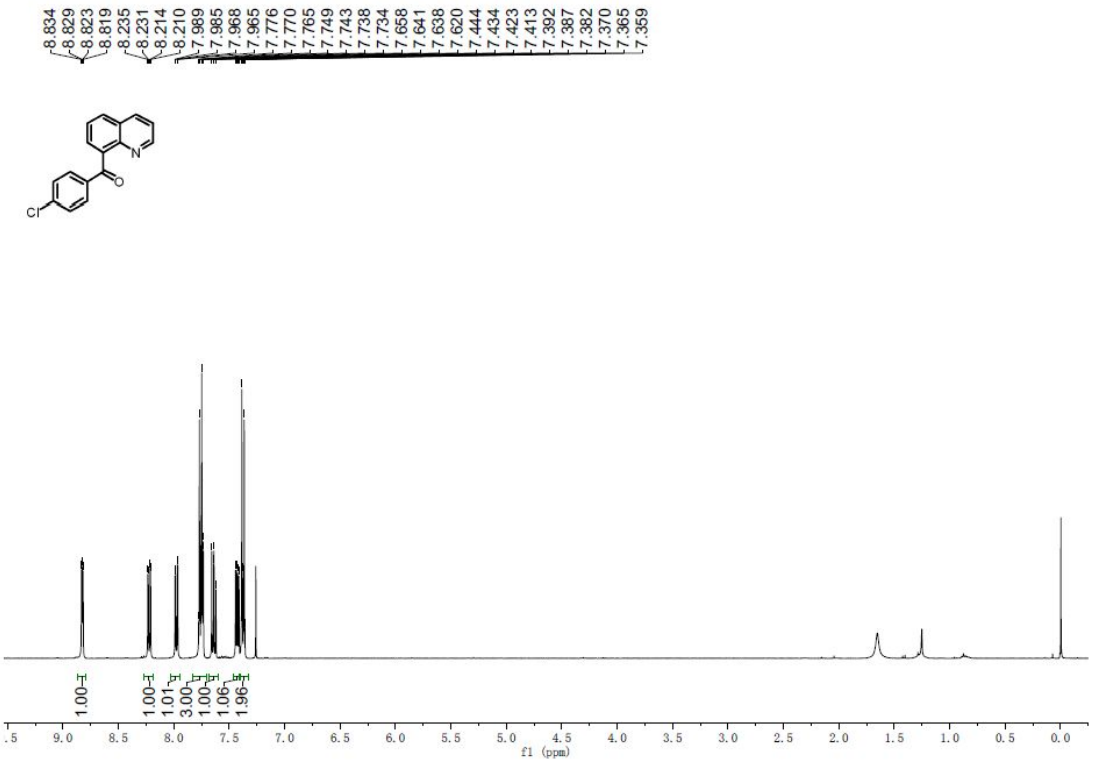
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ab



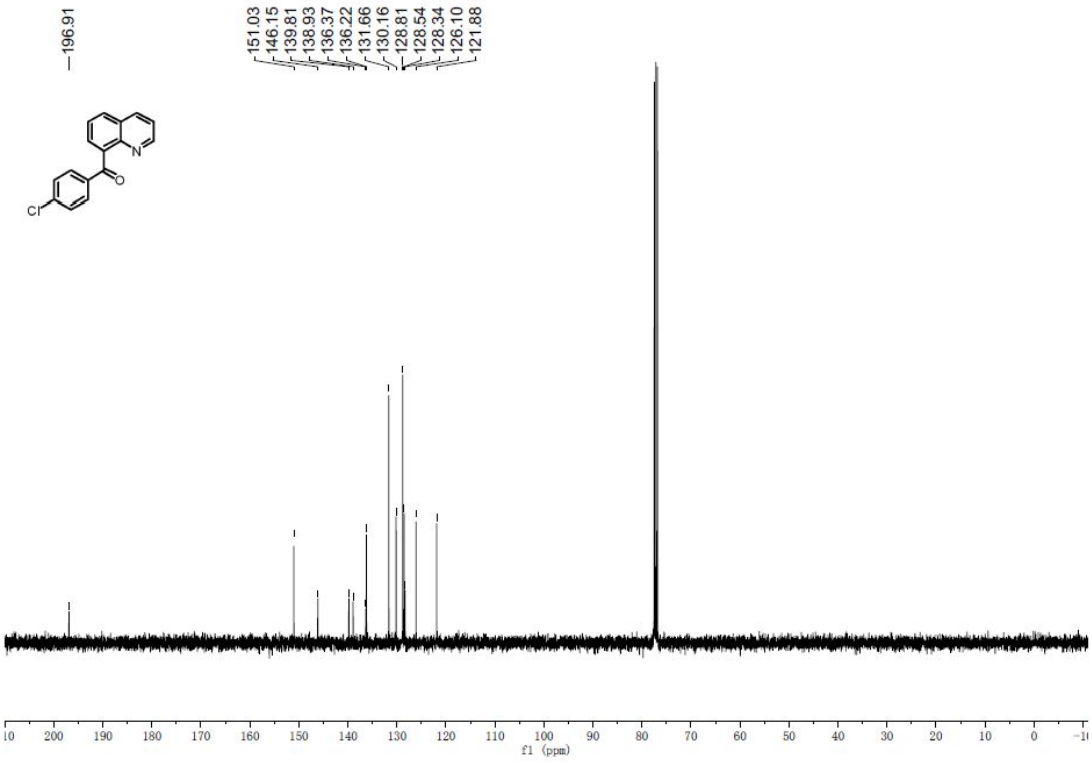
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 3ab



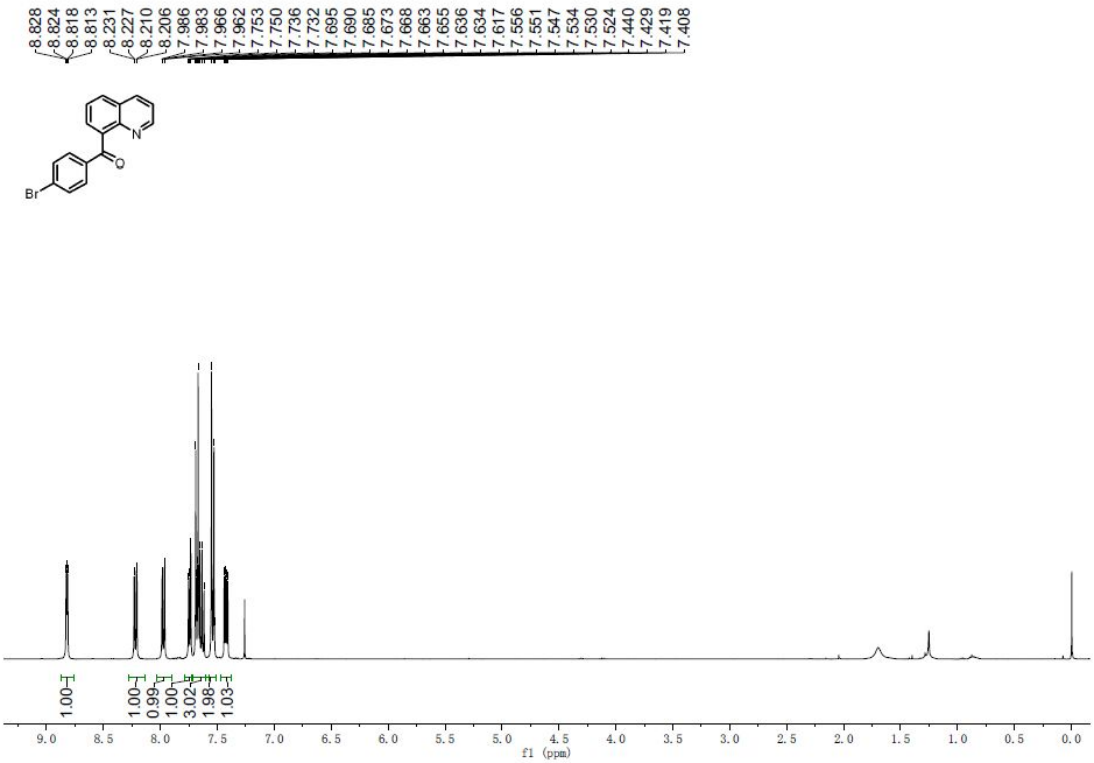
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ac



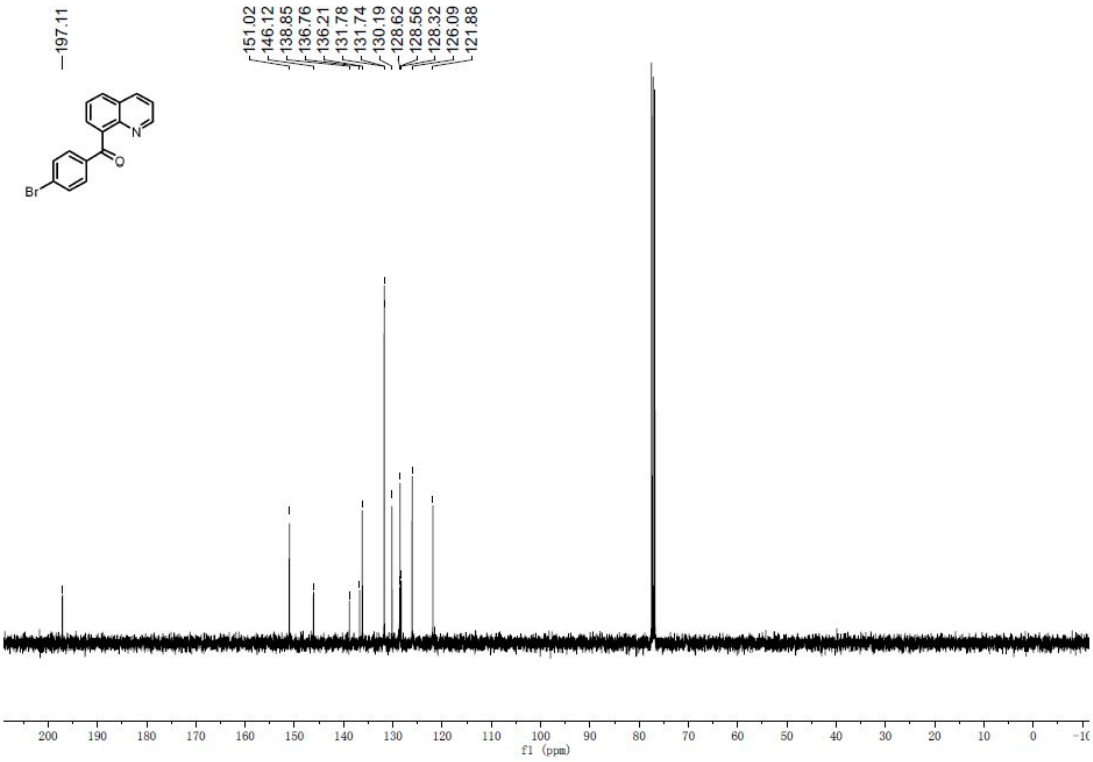
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ac



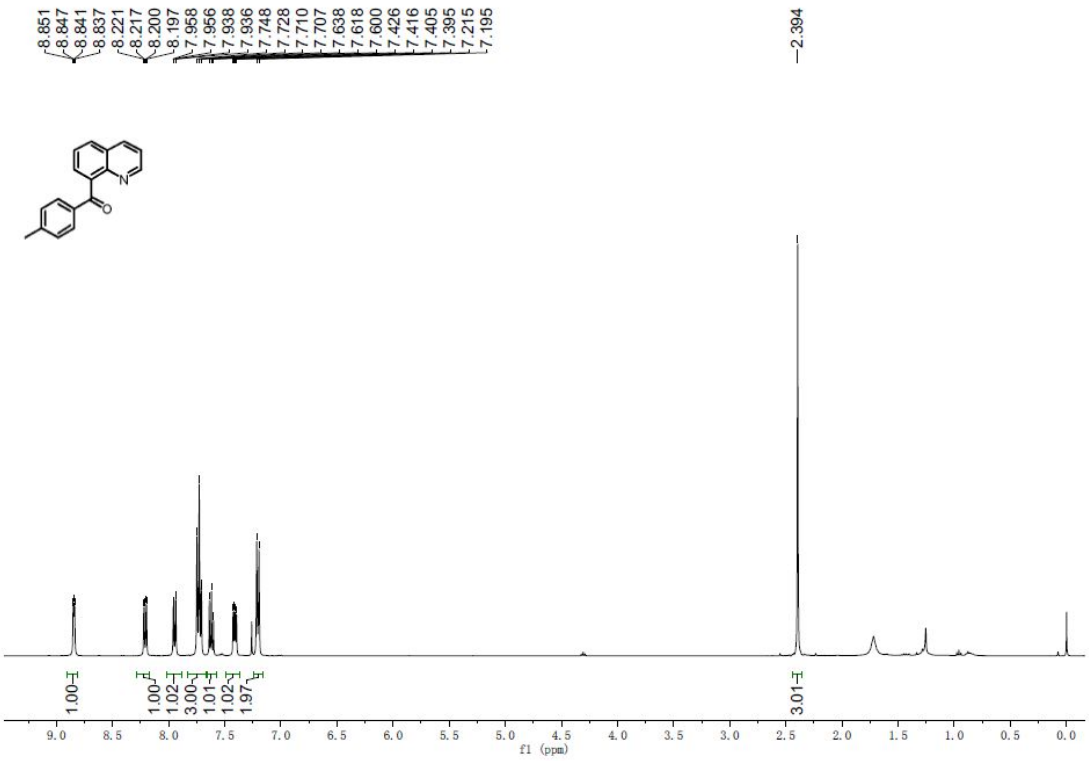
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ad



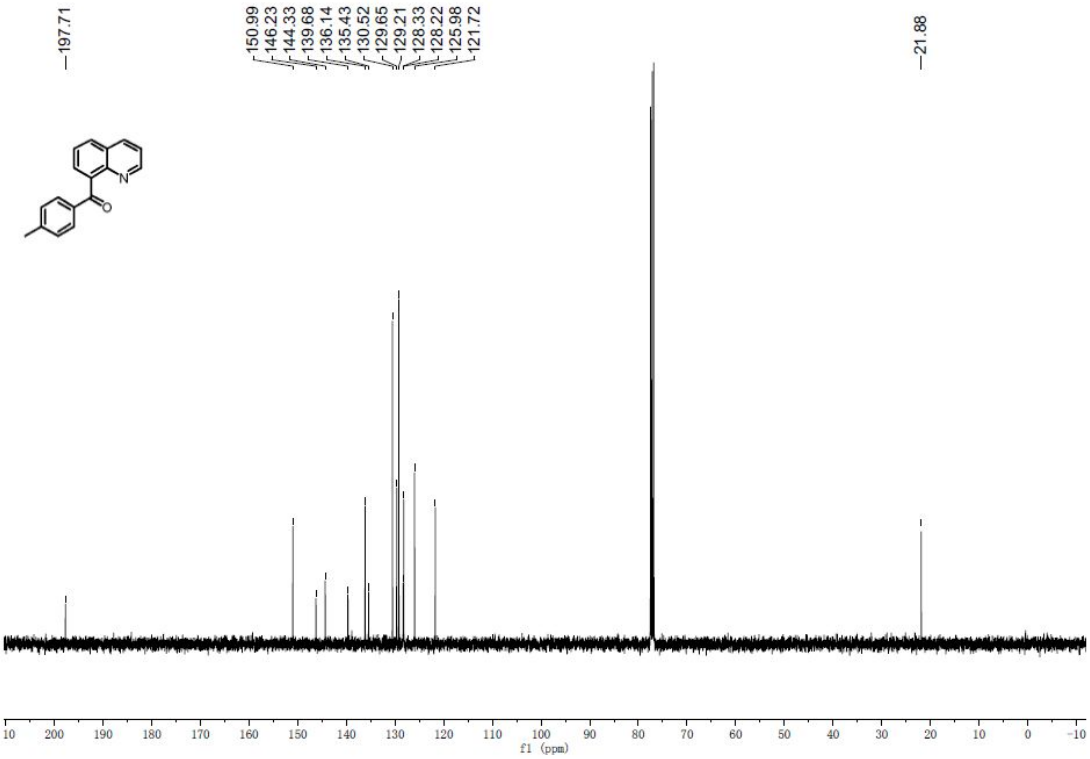
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ad



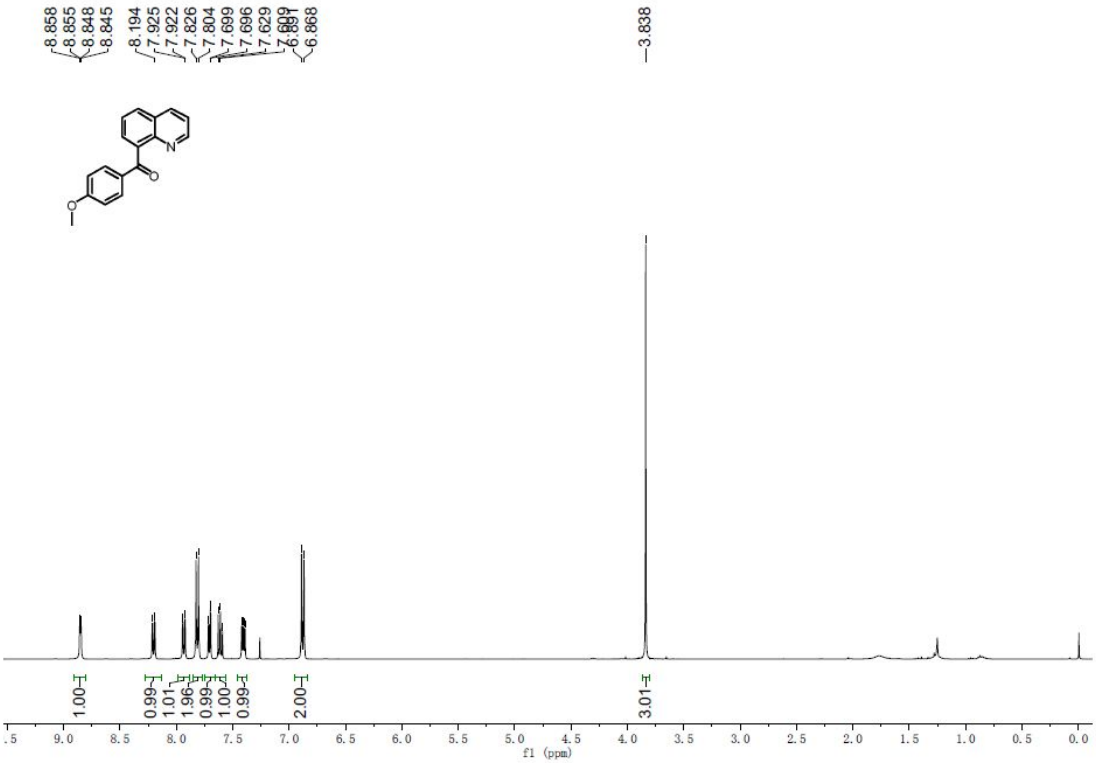
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ae



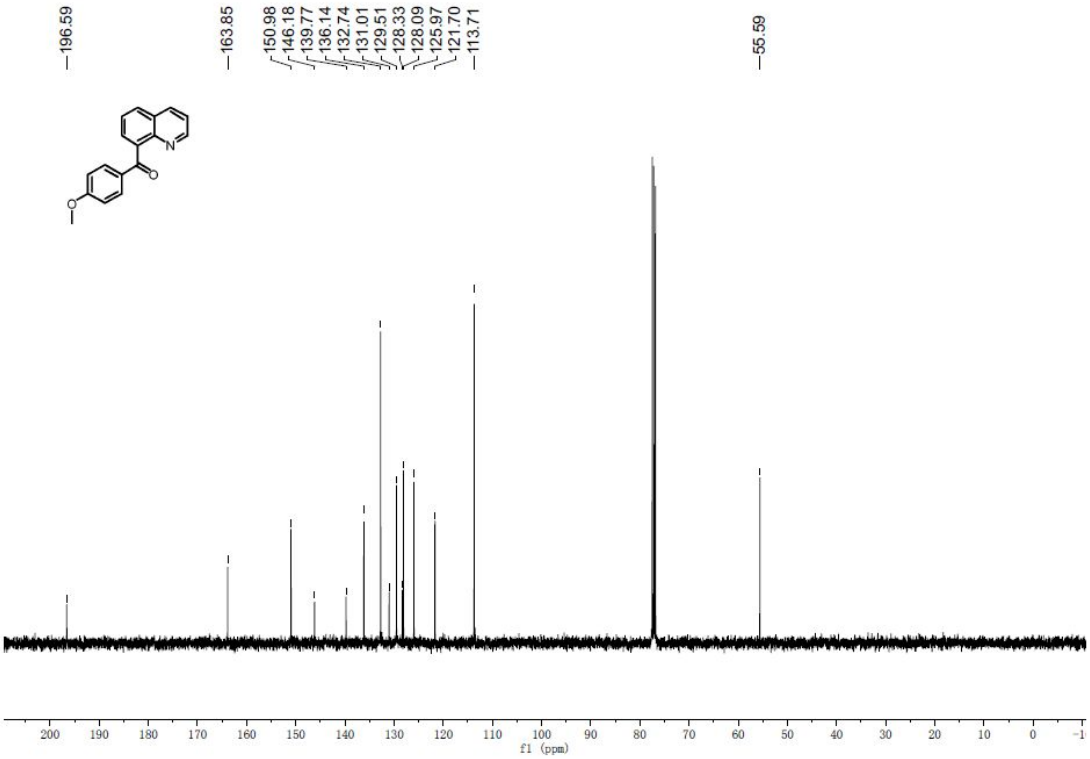
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ae



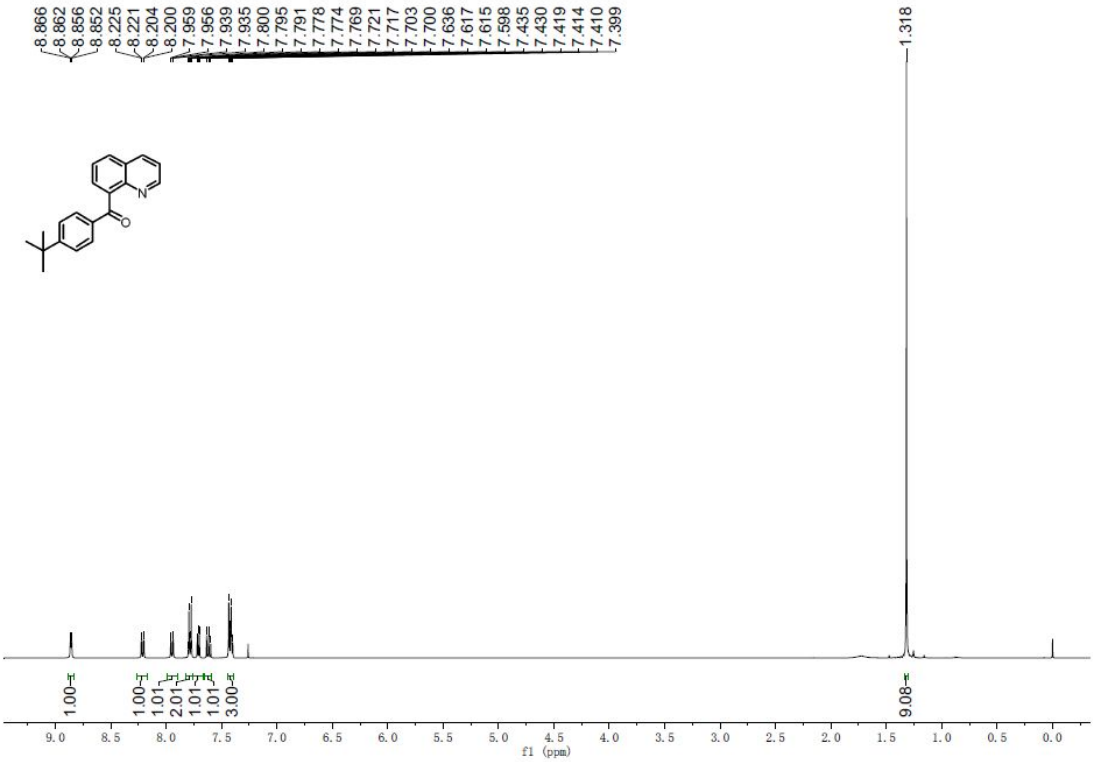
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3af



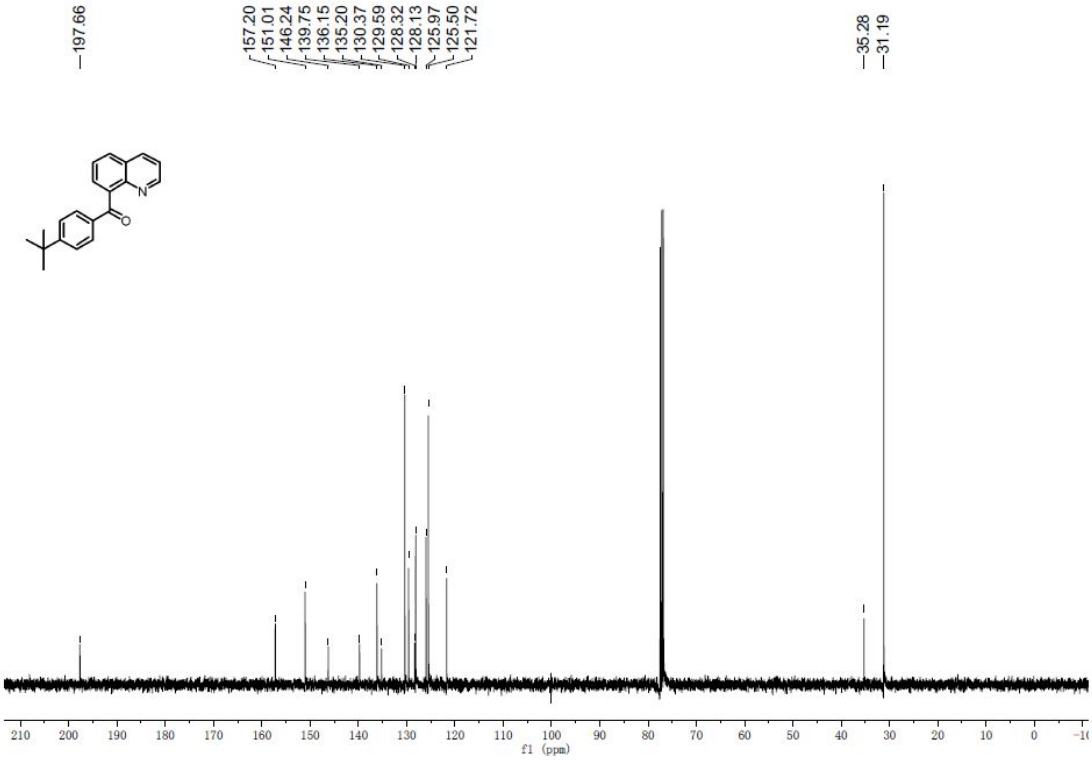
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3af



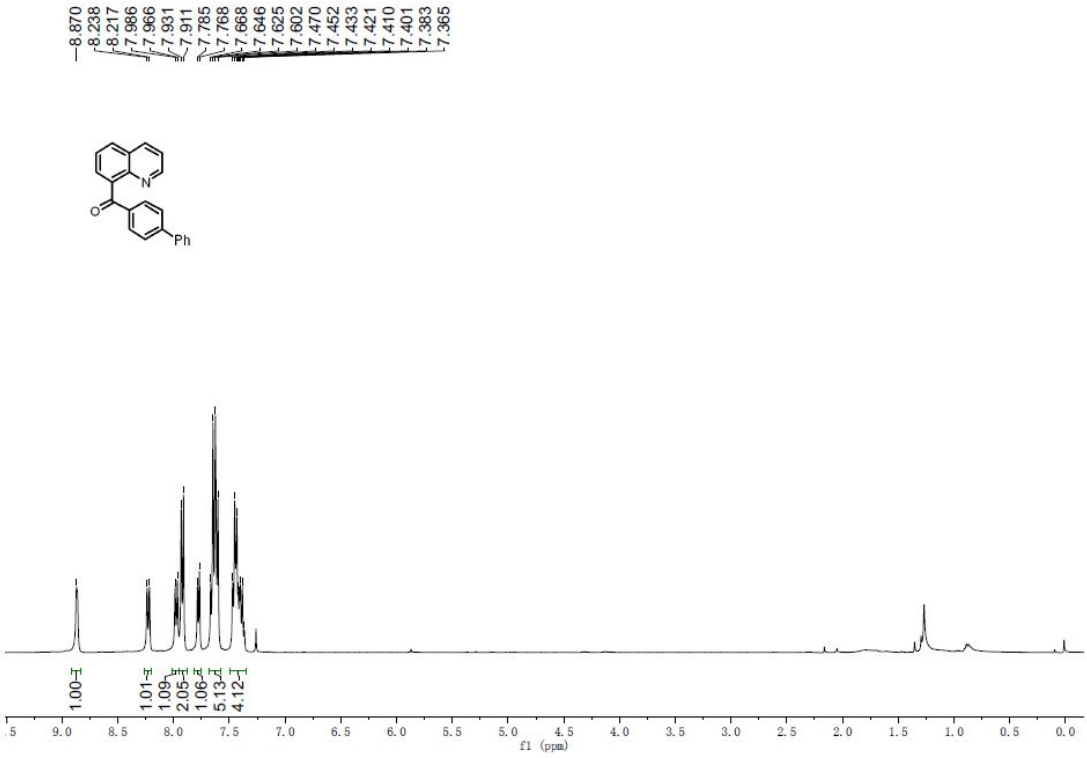
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ag



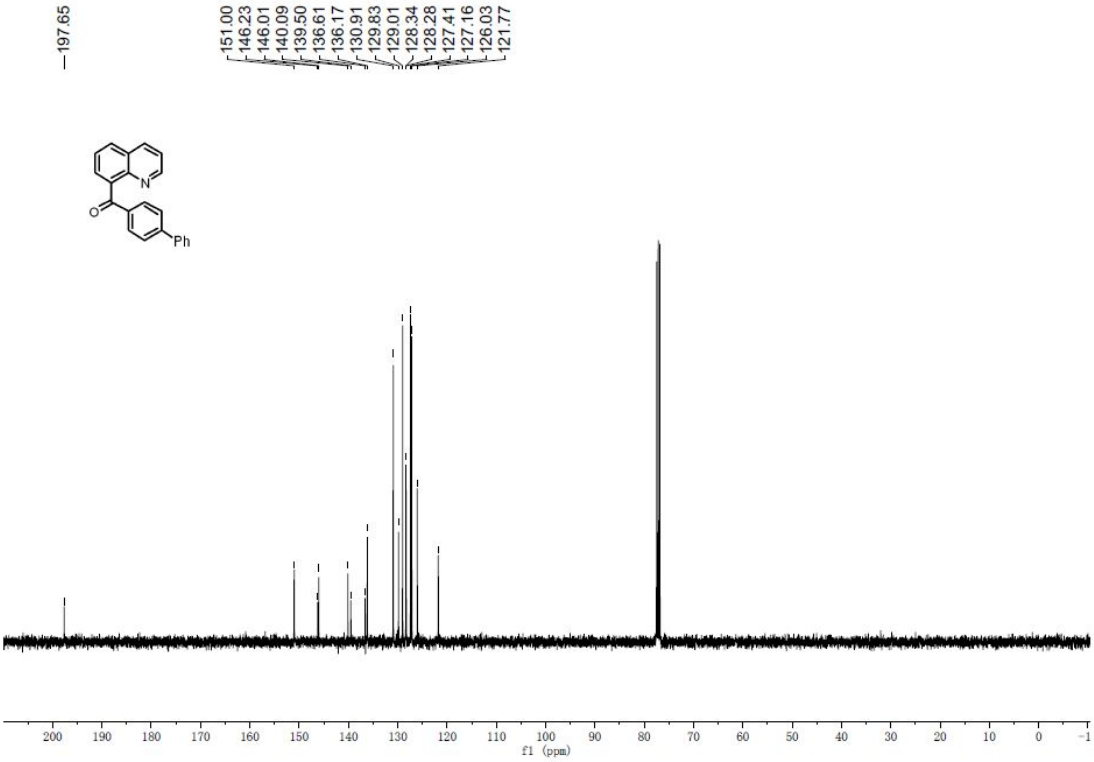
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ag



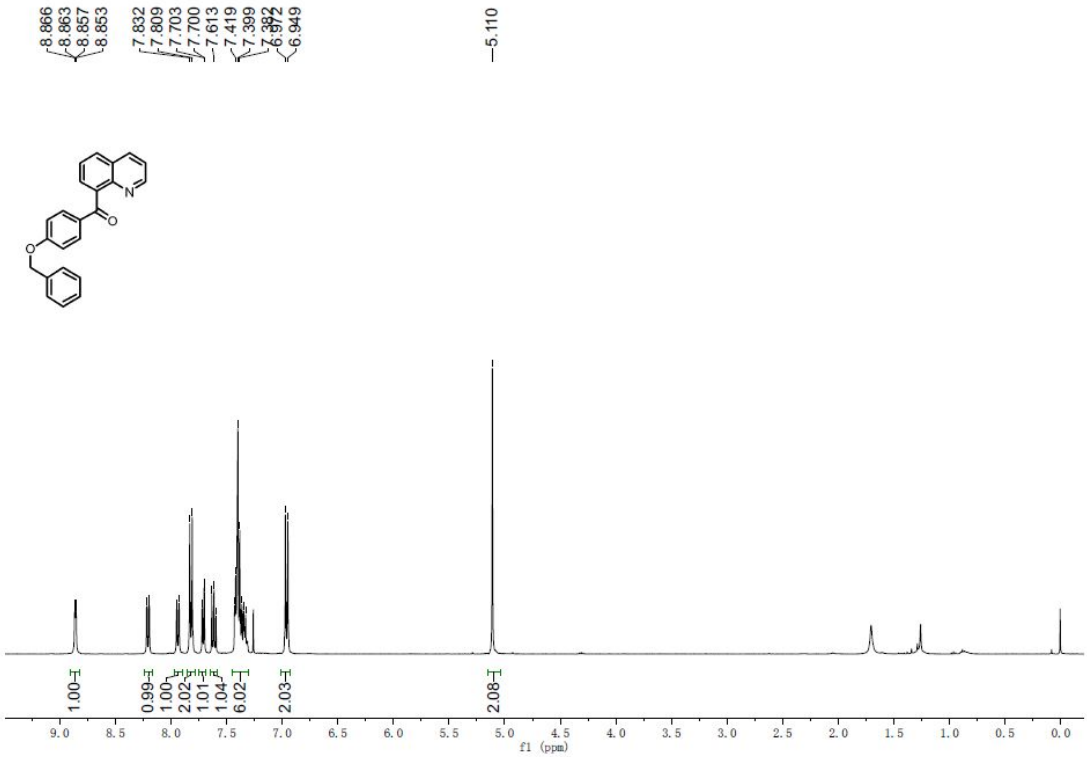
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ah



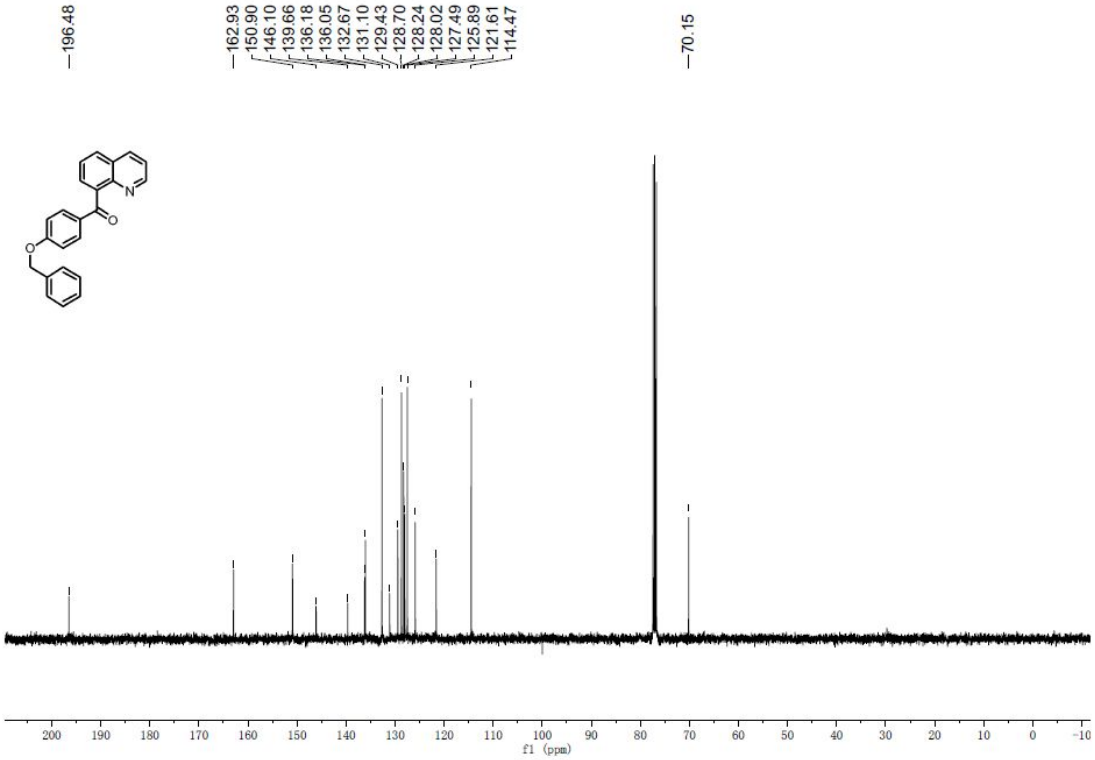
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ah



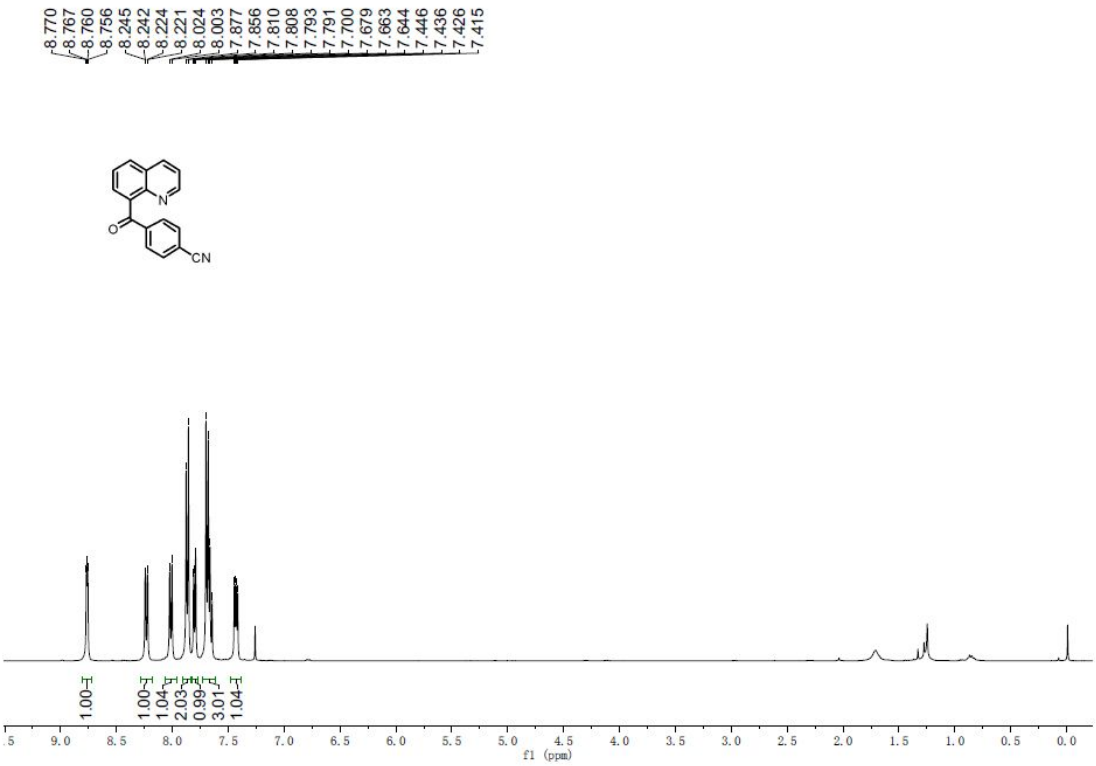
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ai



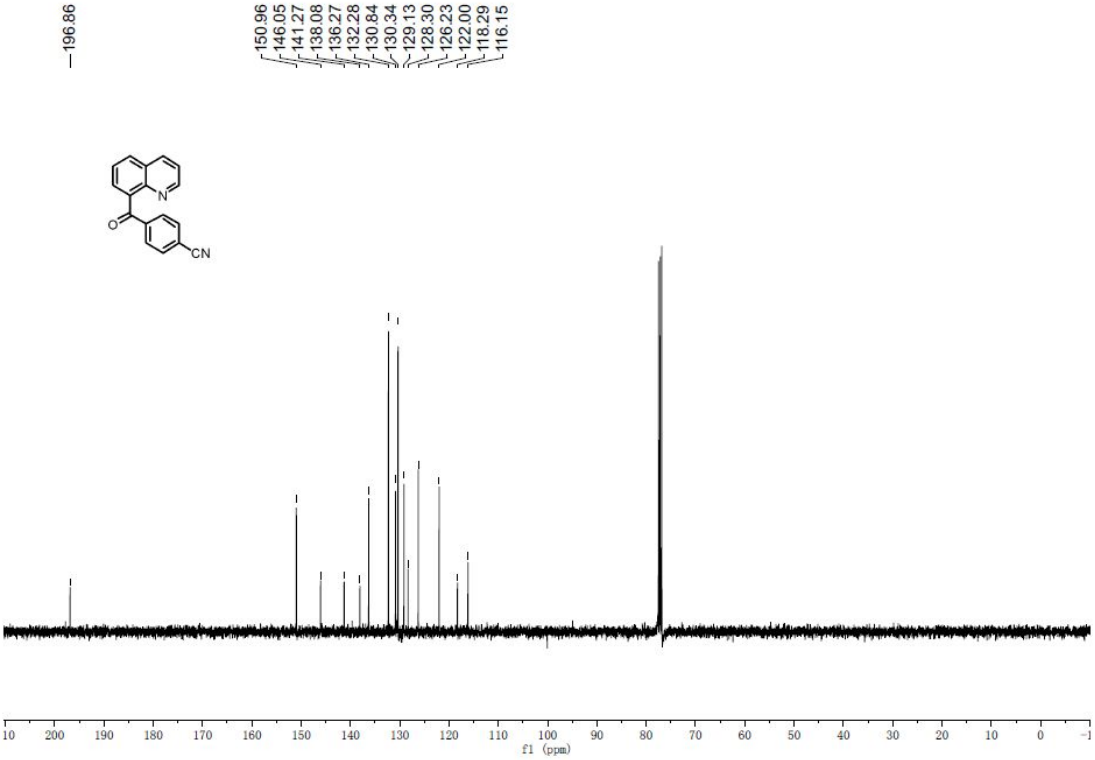
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ai



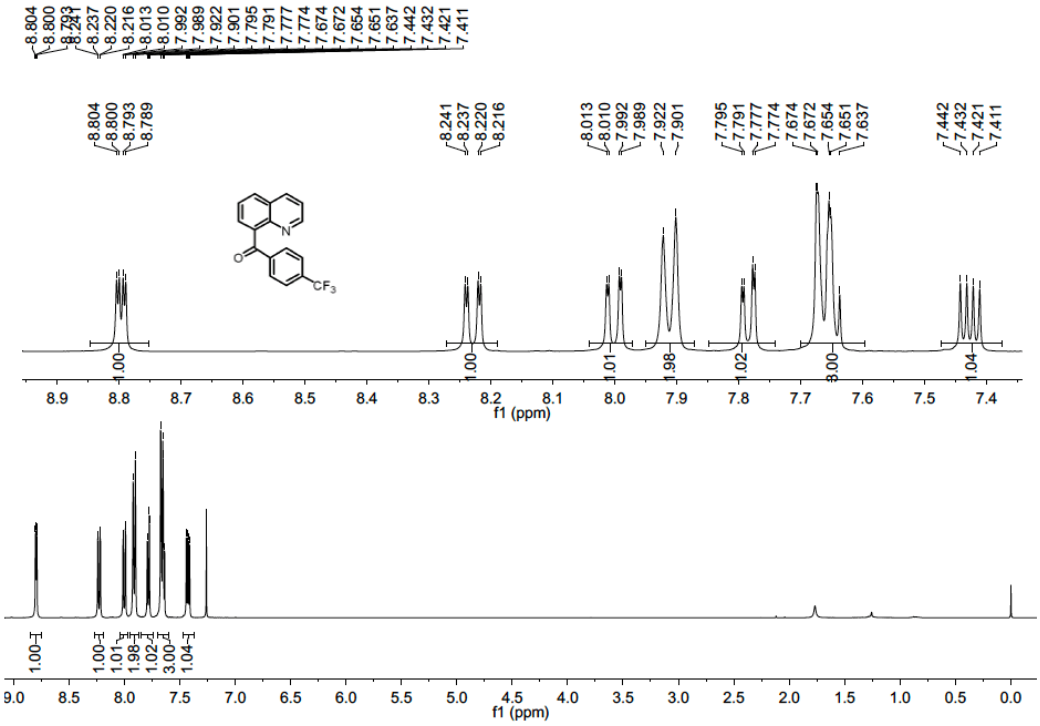
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3aj



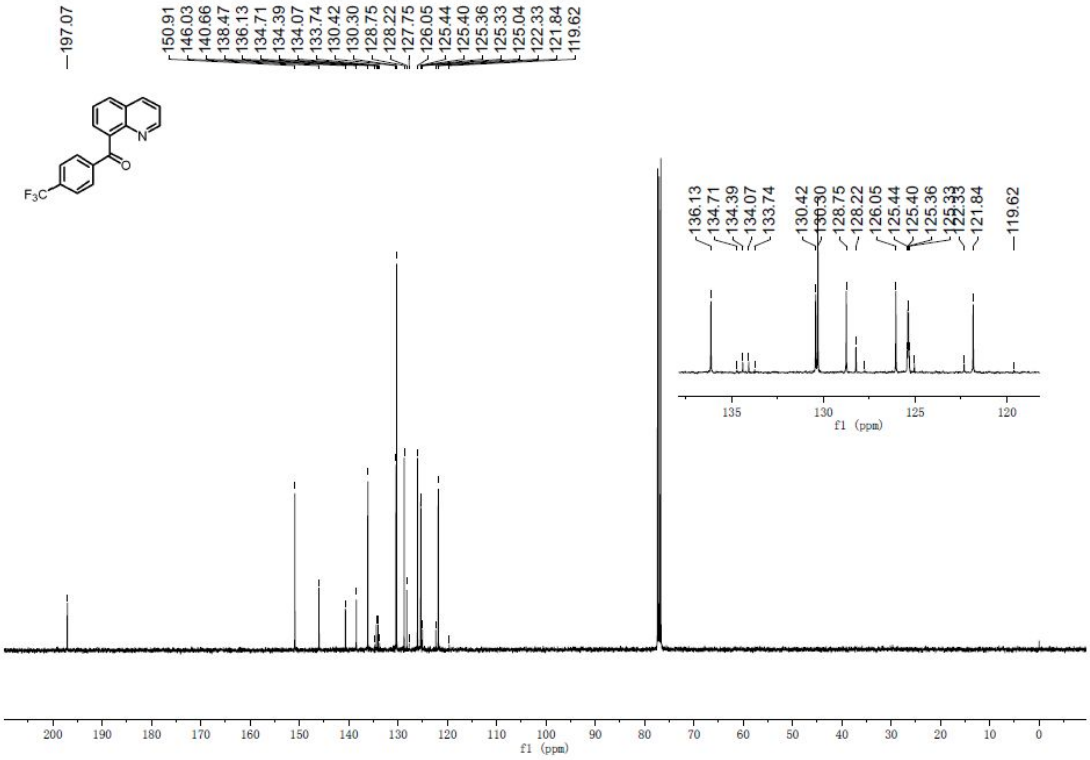
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3aj



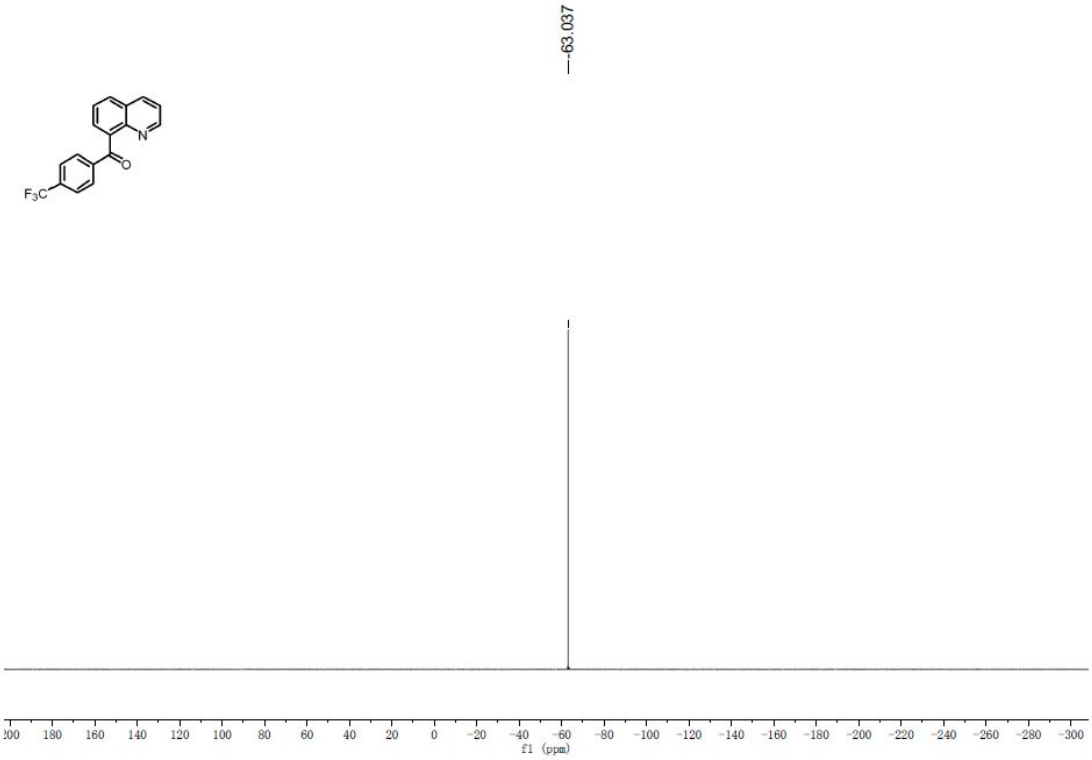
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ak



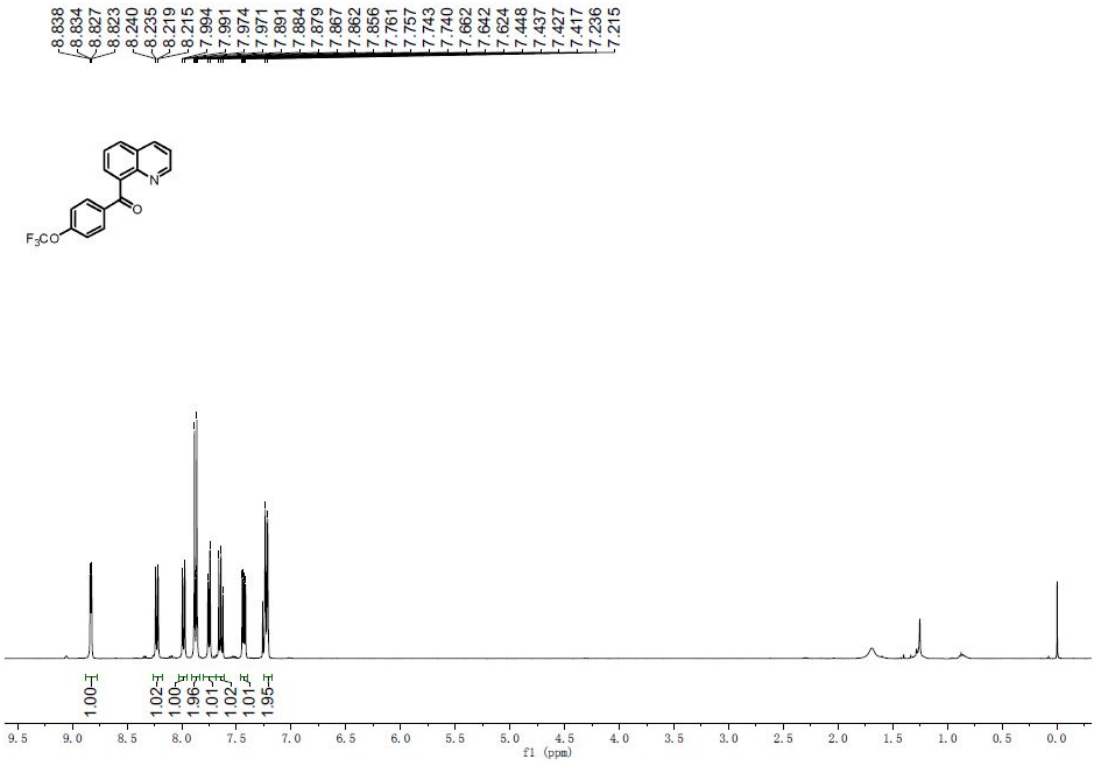
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ak



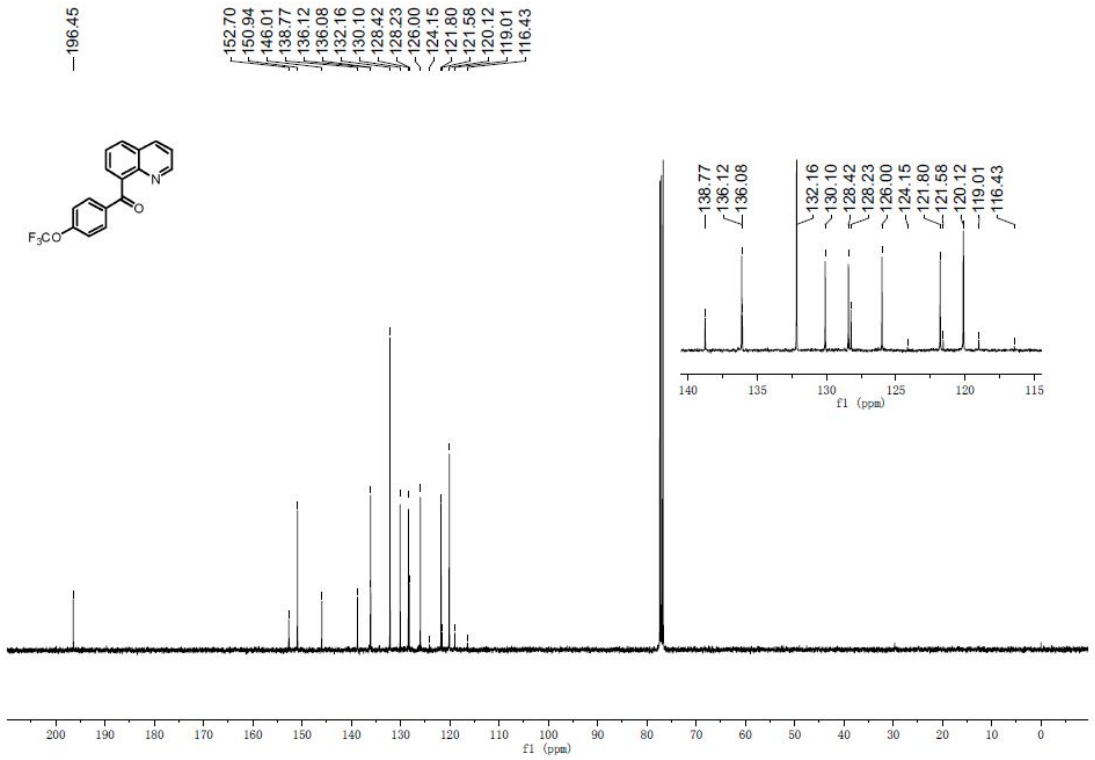
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 3ak



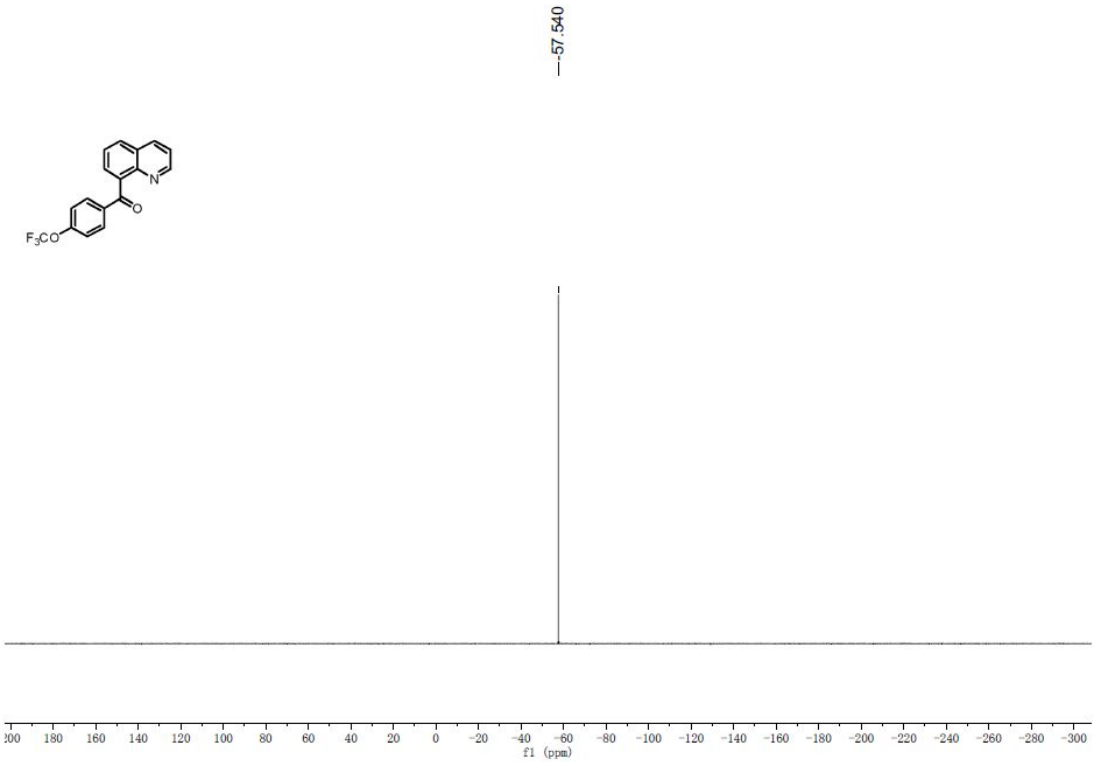
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3al



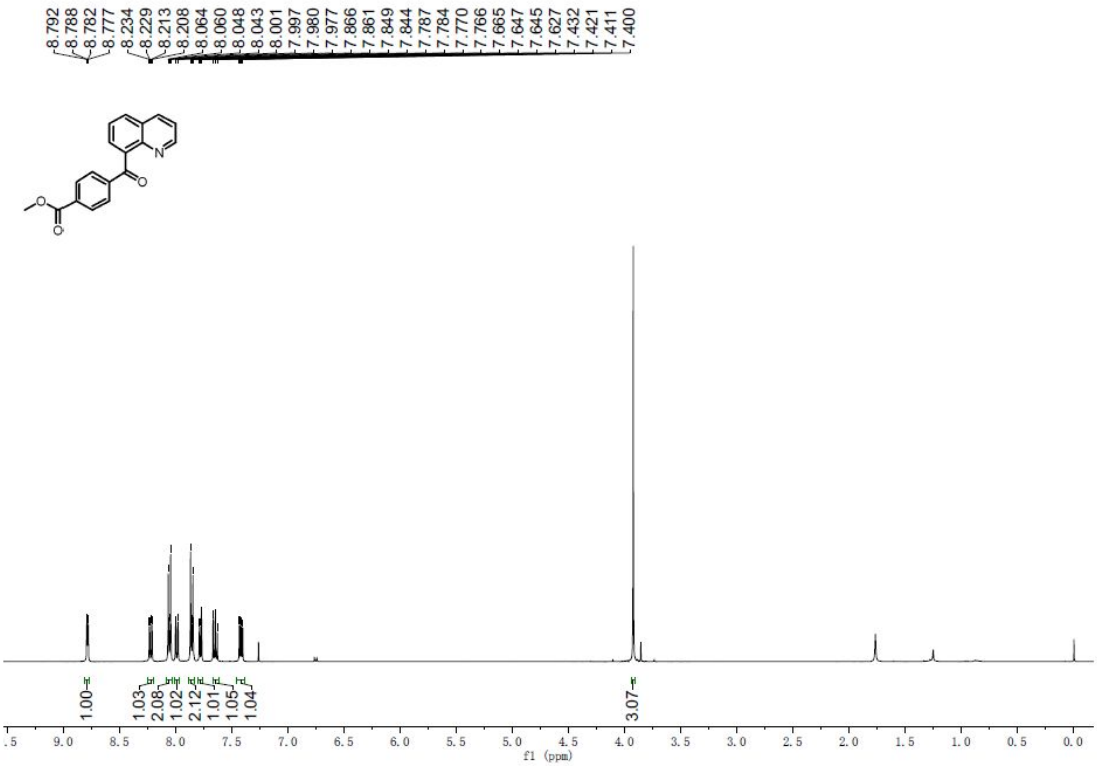
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3al



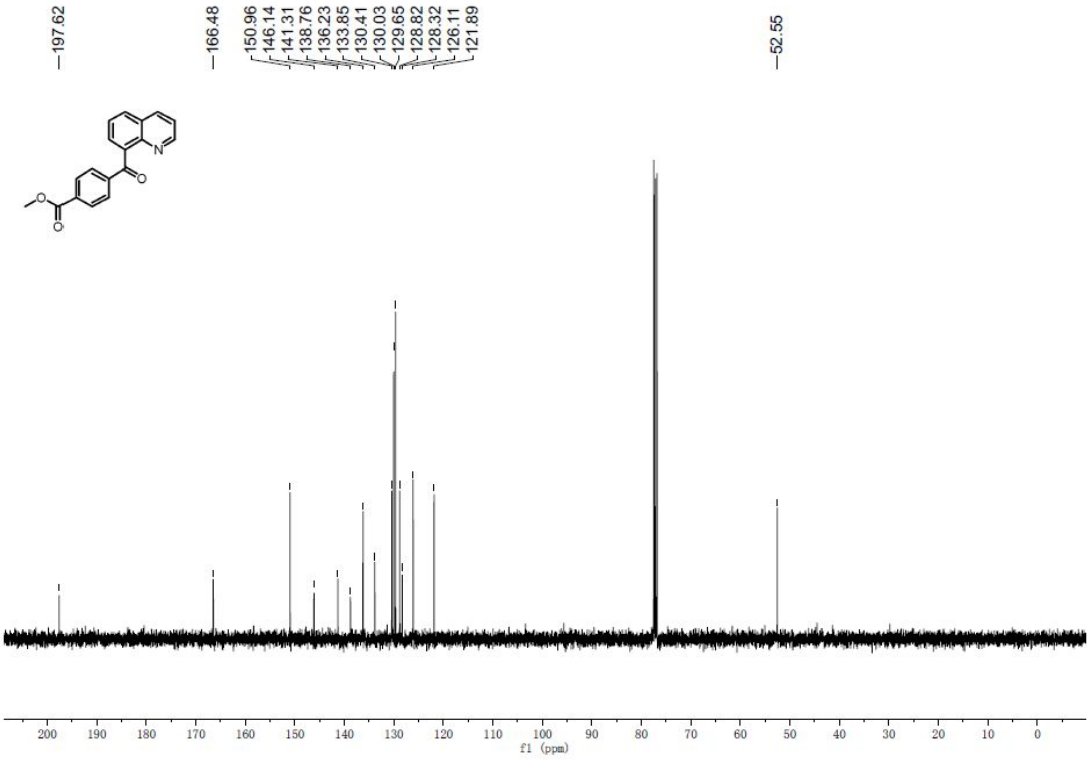
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 3al



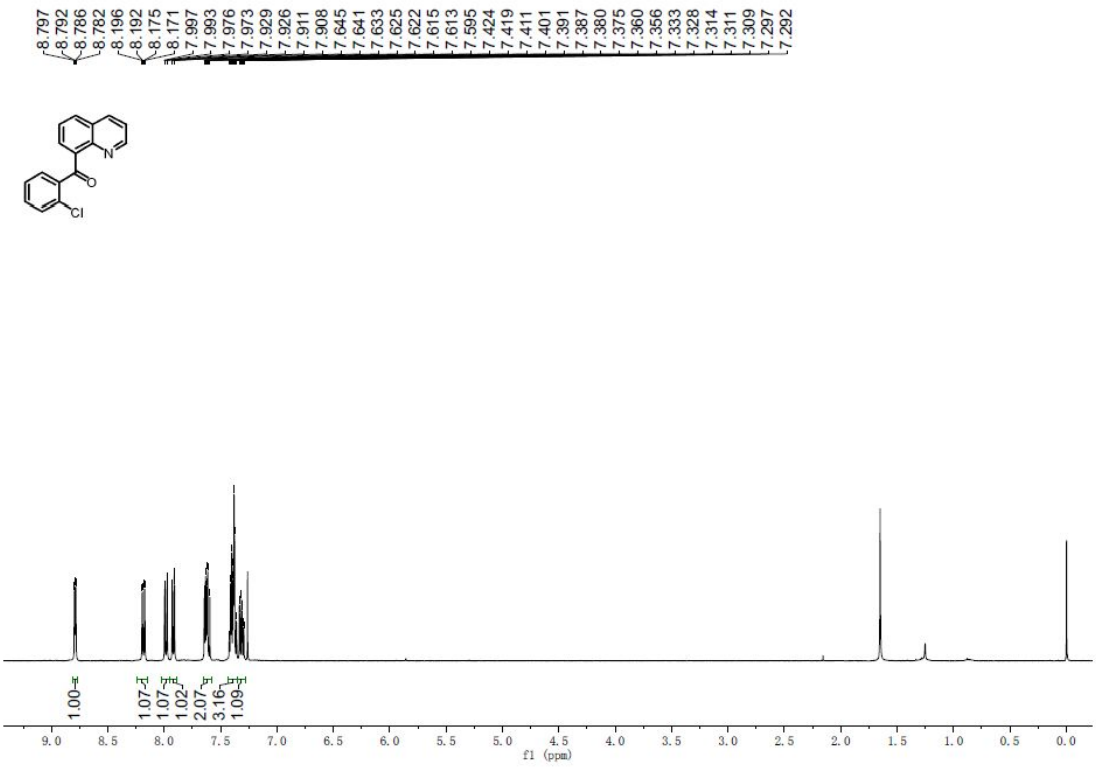
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3am



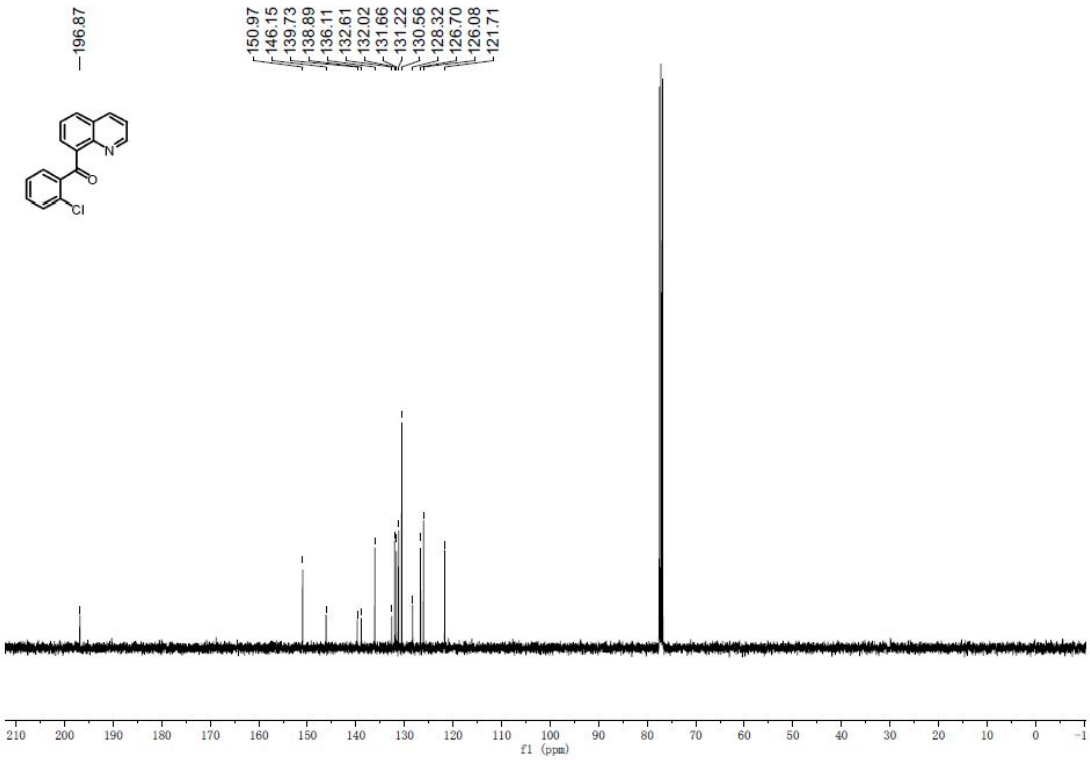
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3am



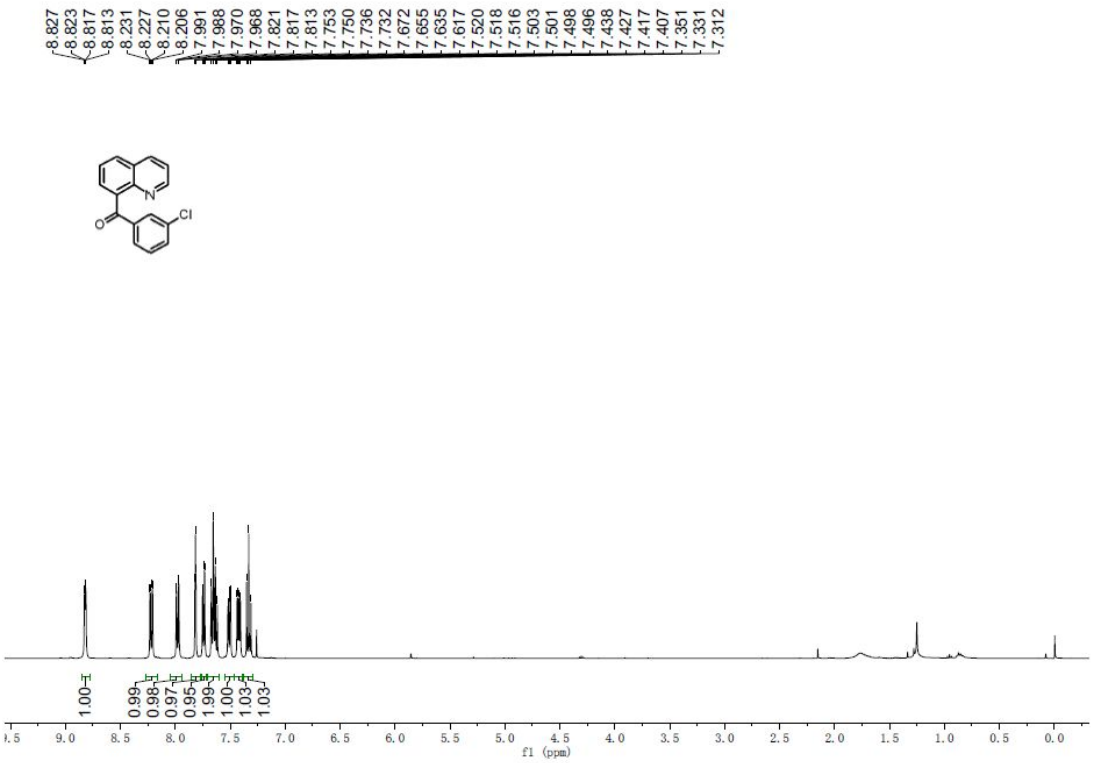
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3an



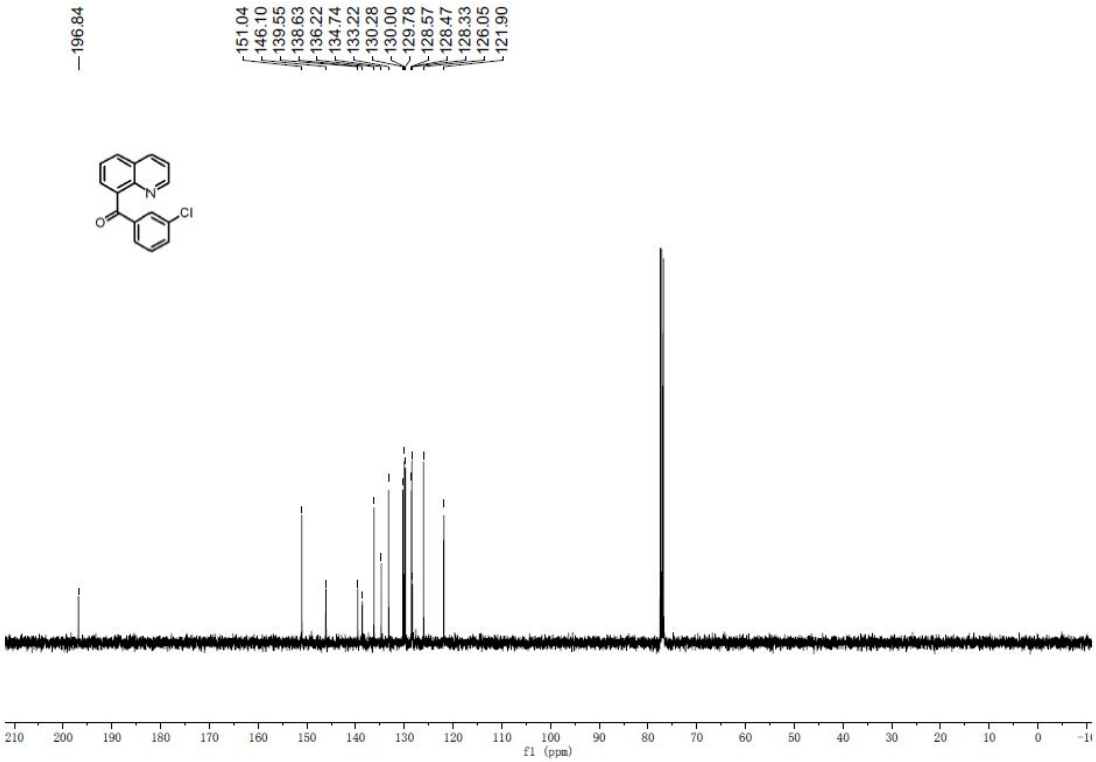
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3an



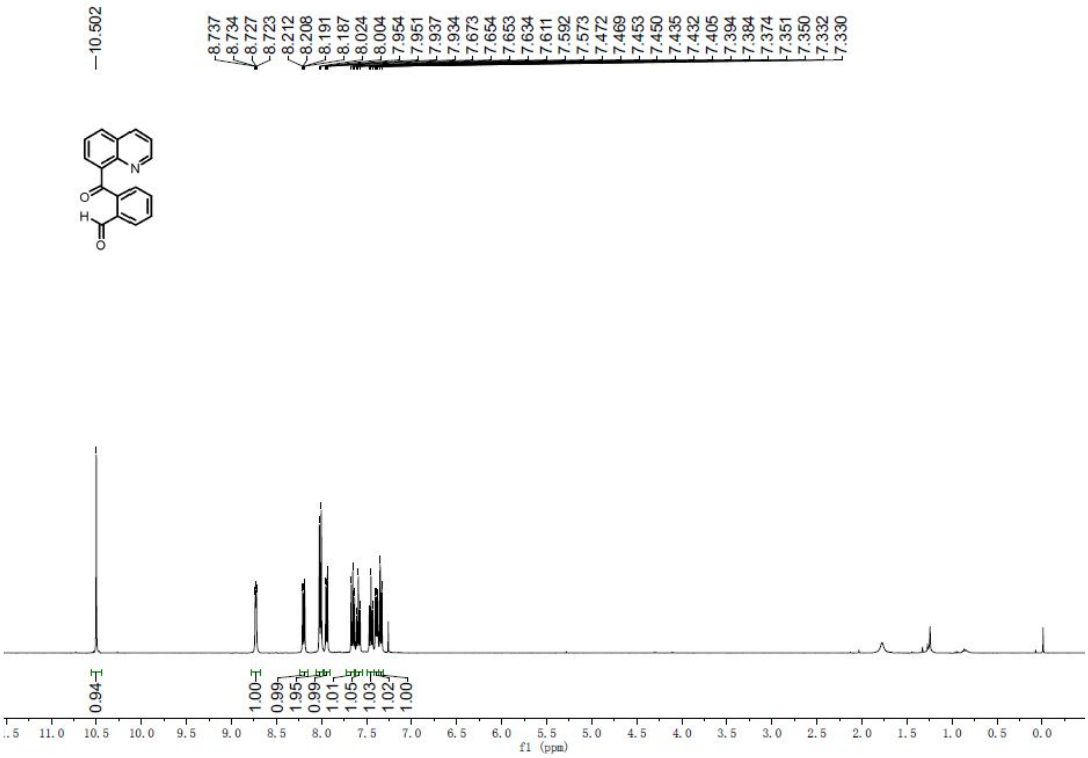
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ao



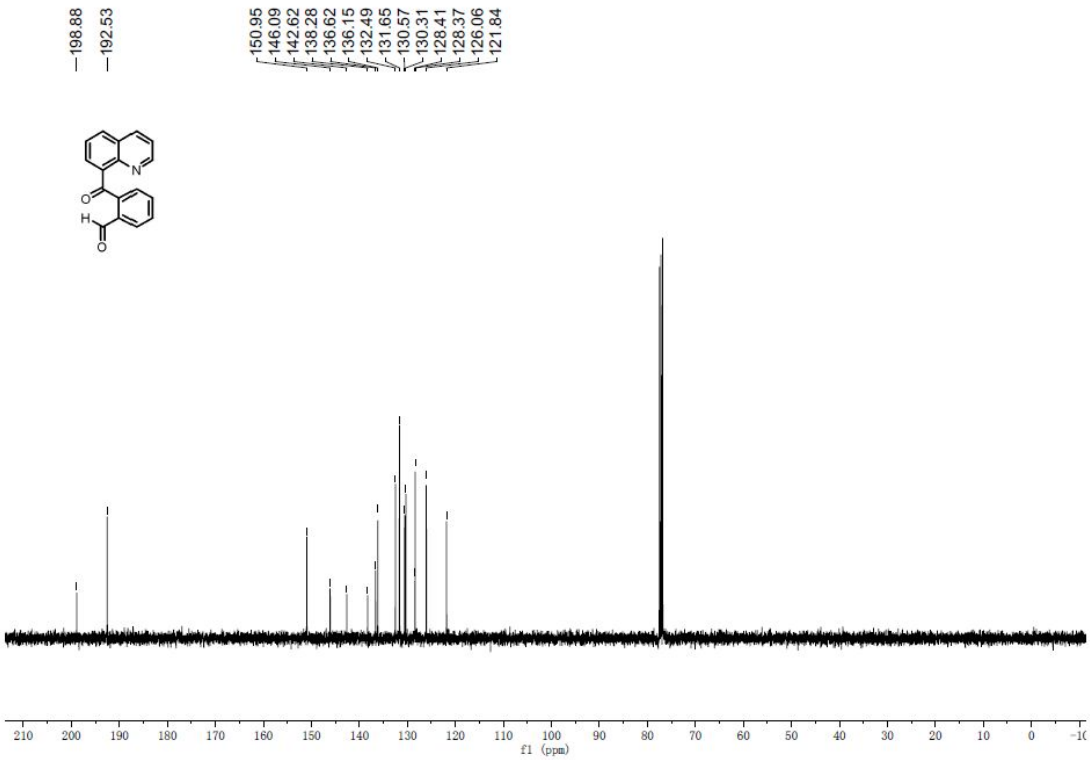
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ao



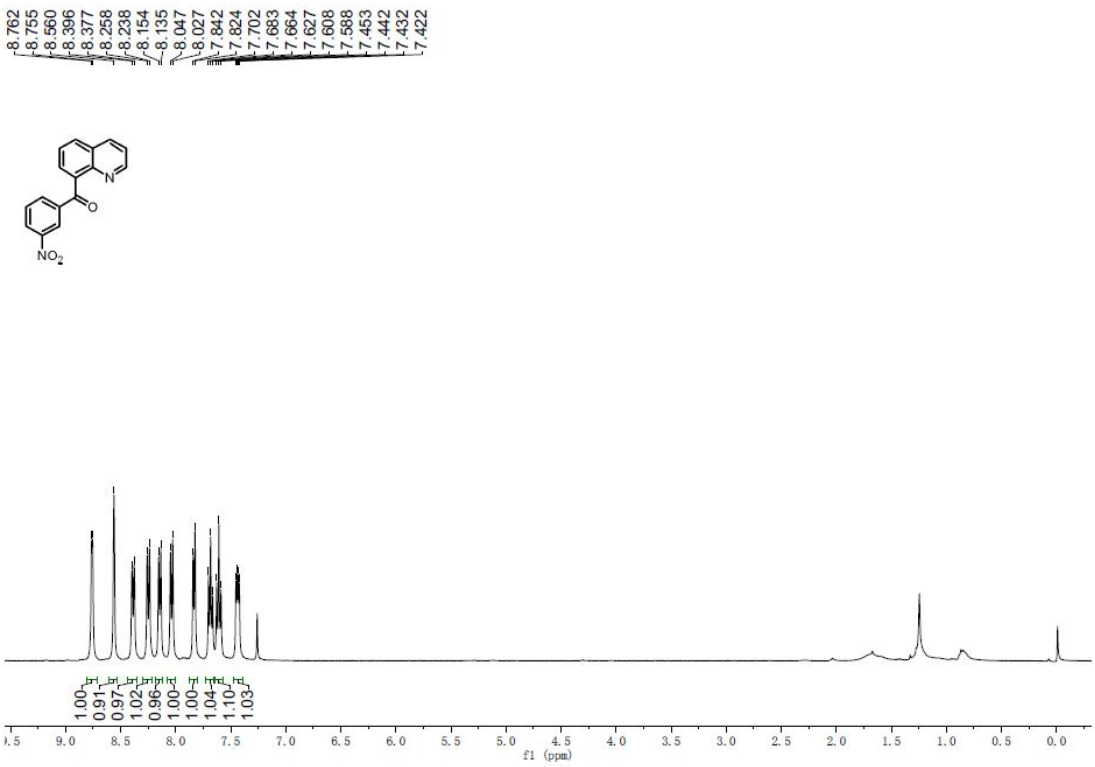
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ap



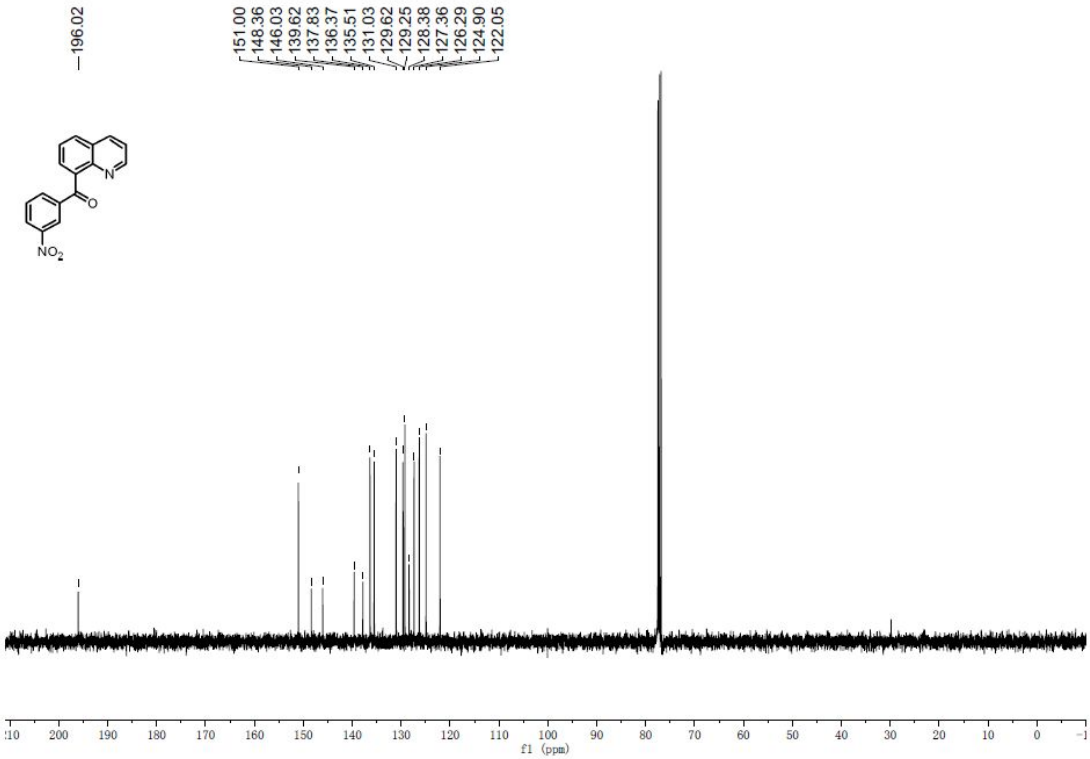
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ap



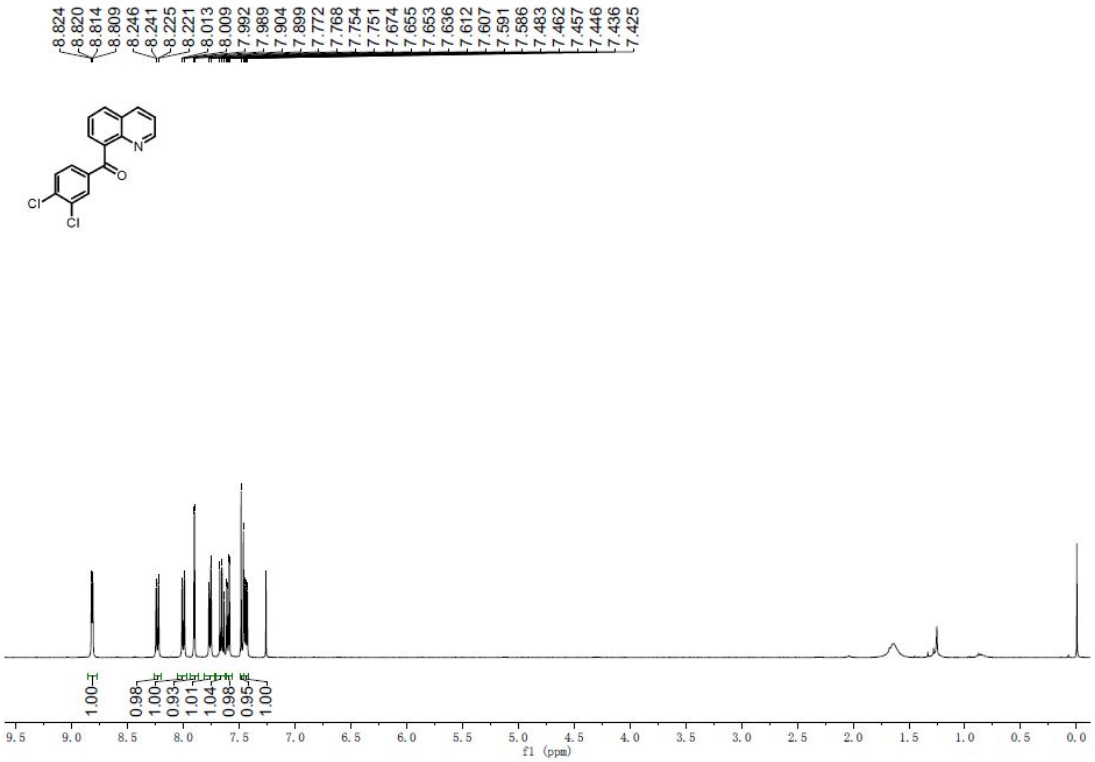
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3aq



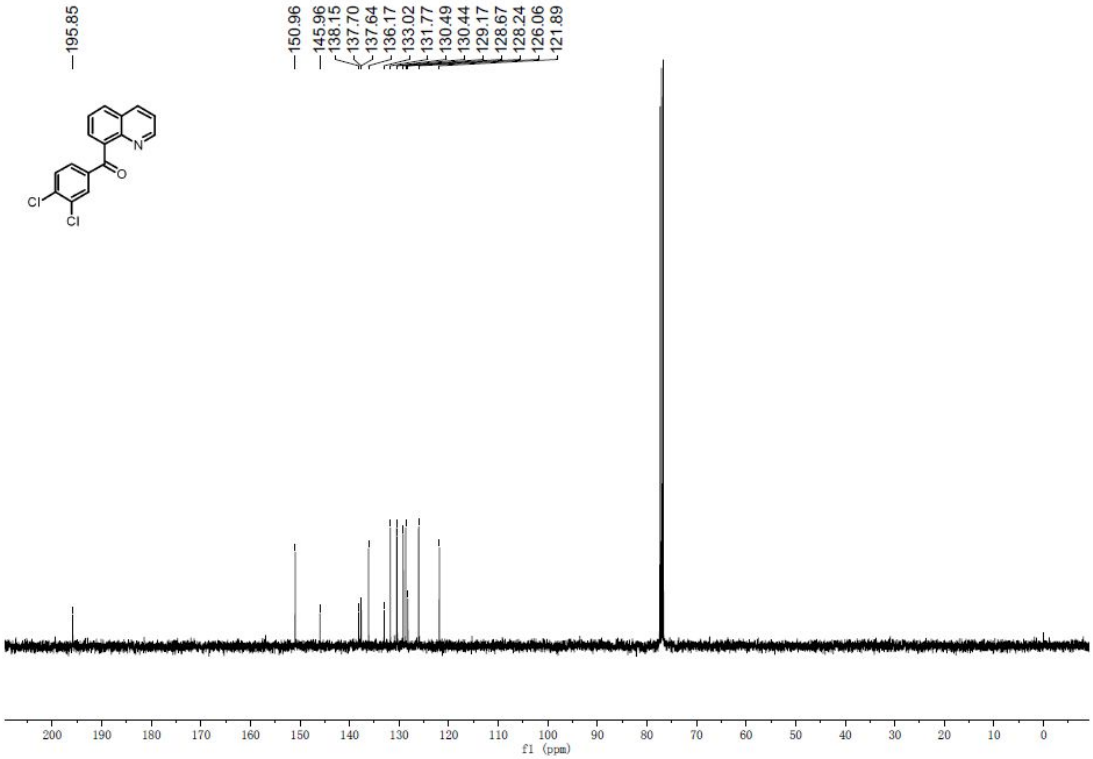
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3aq



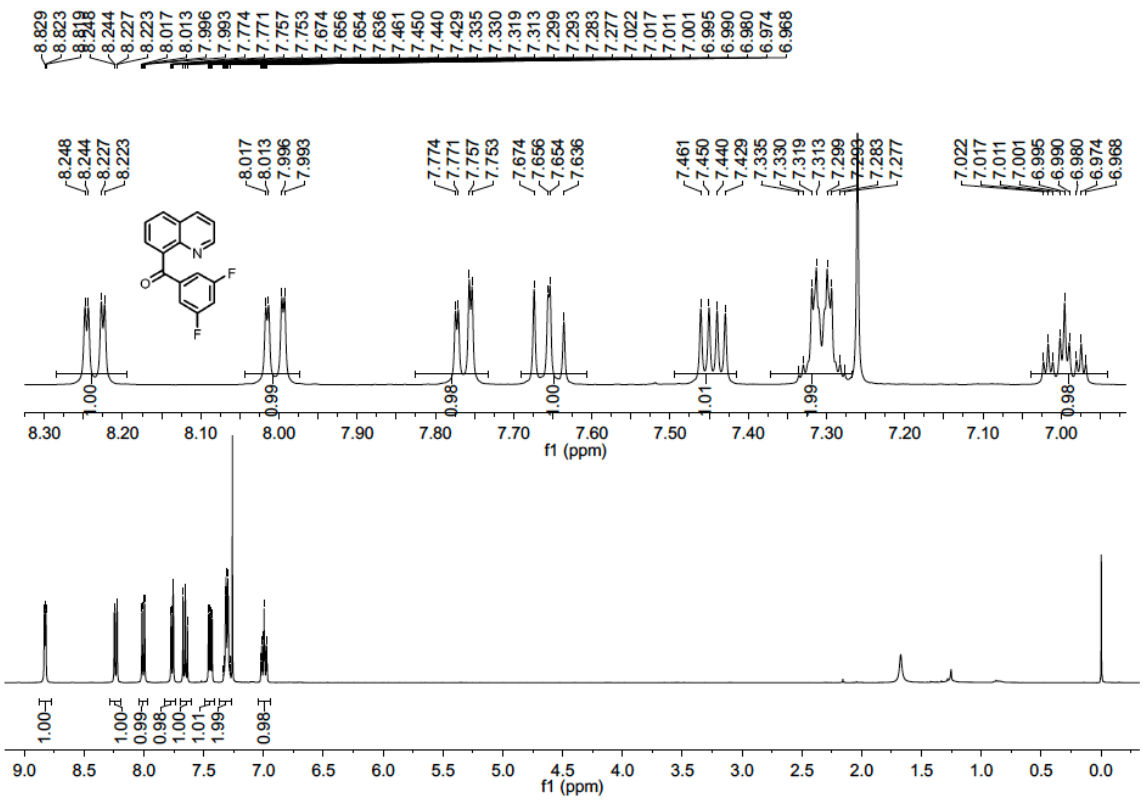
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ar



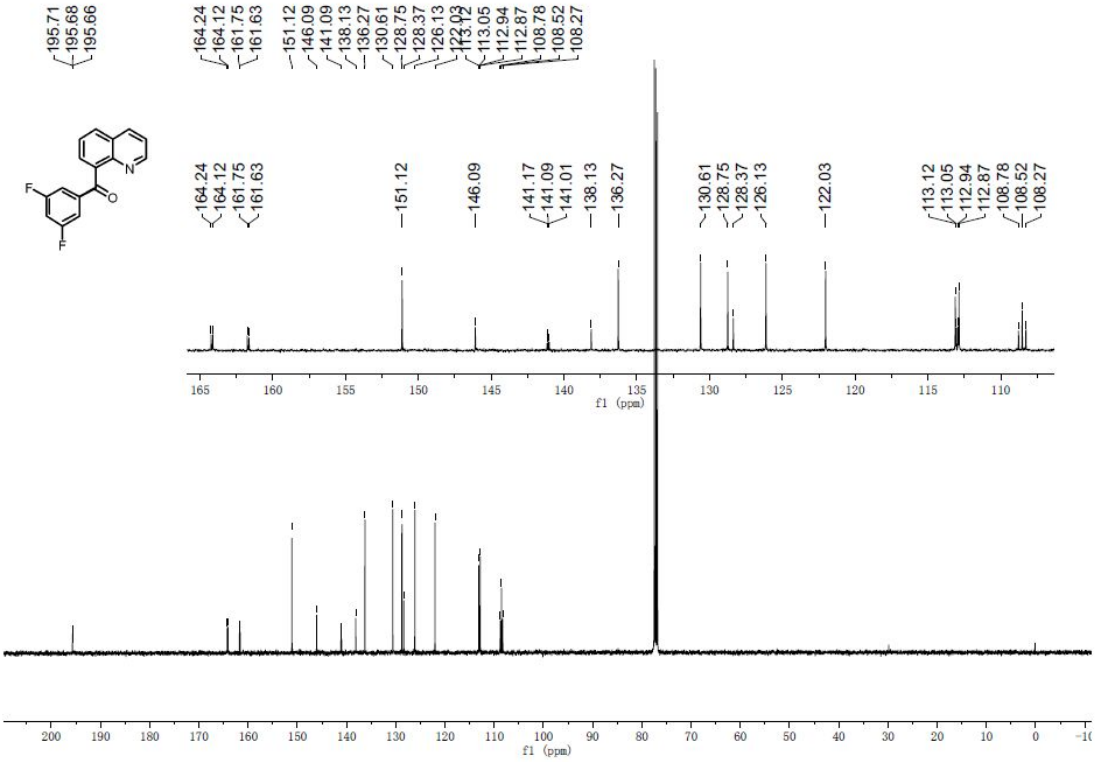
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ar



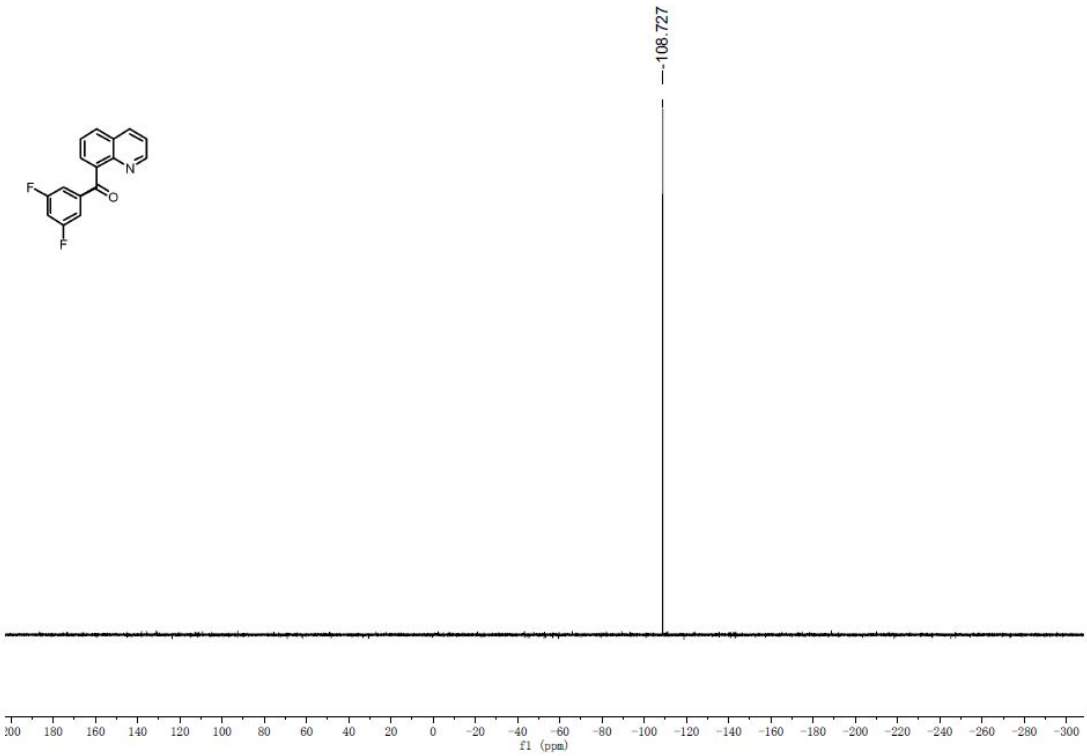
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3as



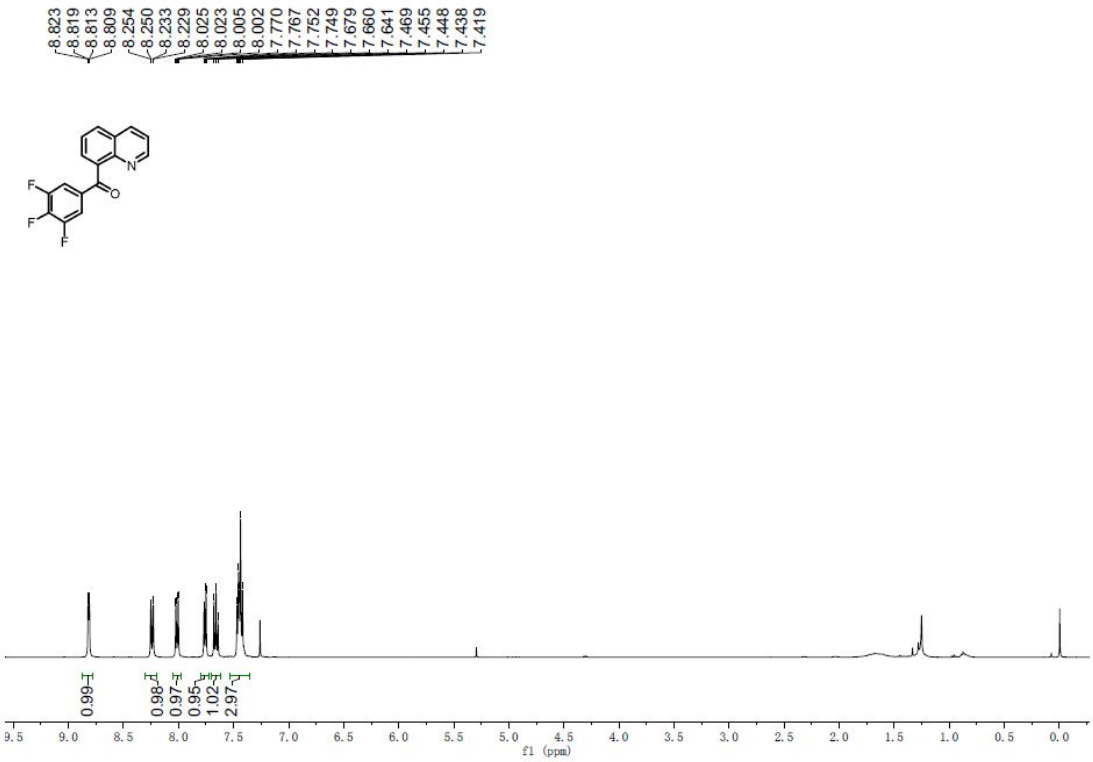
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3as



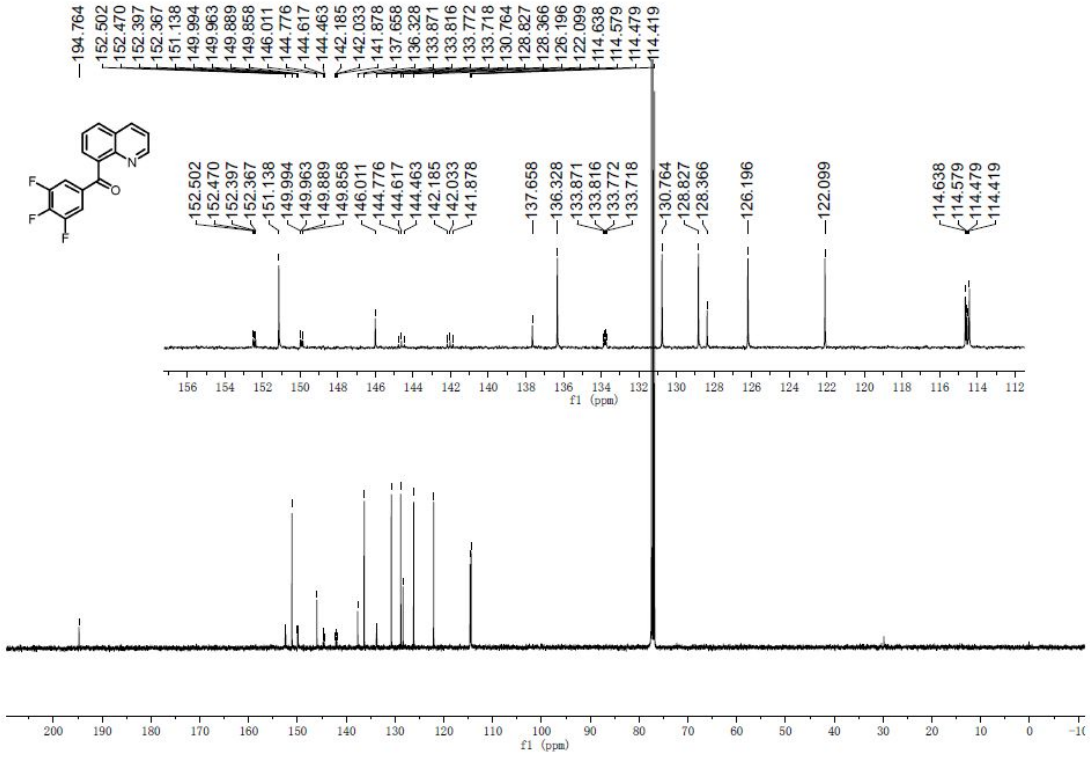
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 3as



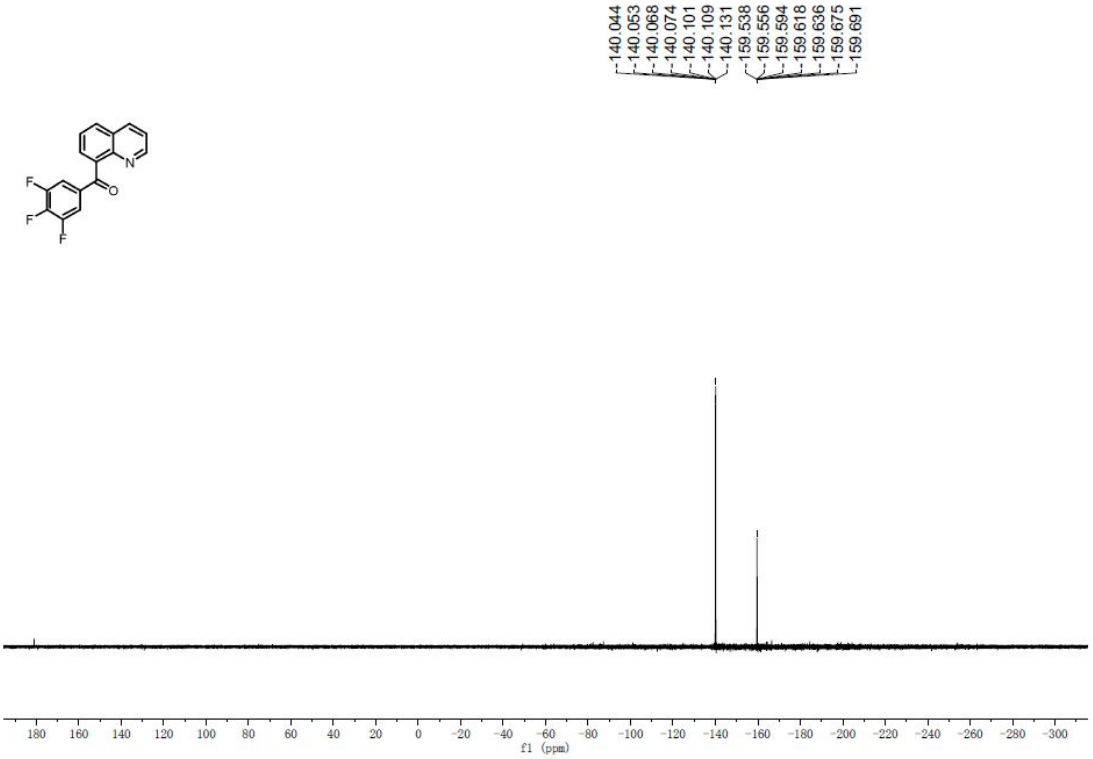
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3at



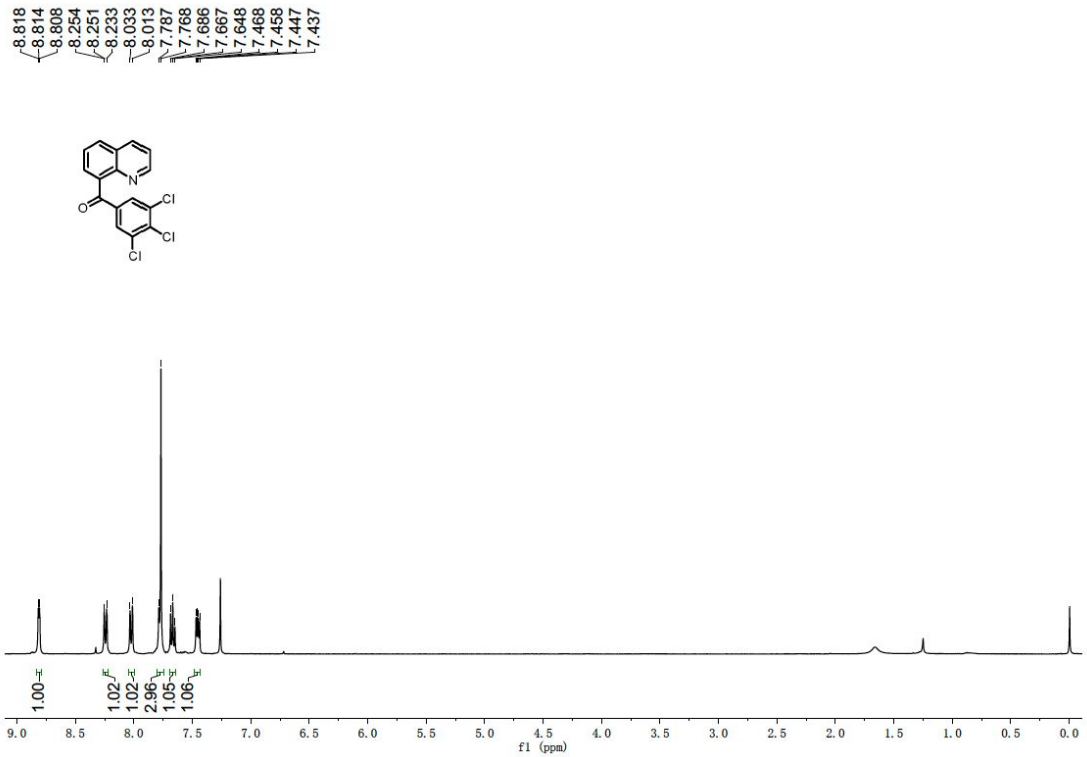
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3at



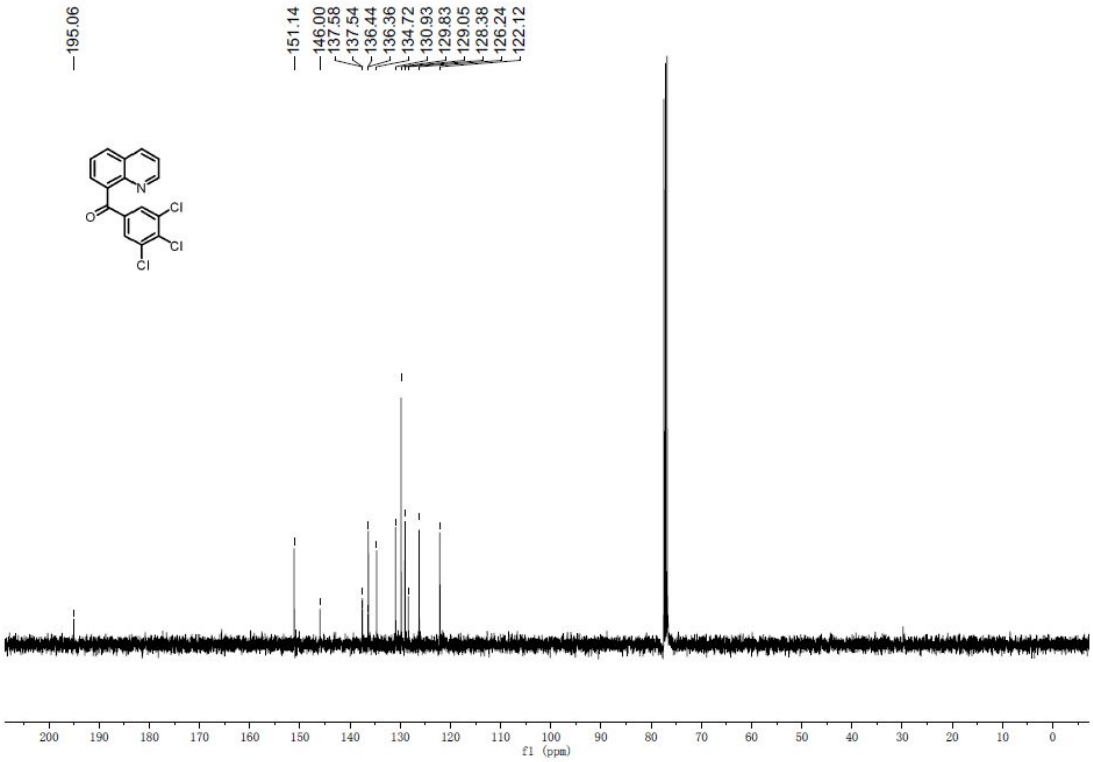
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 3at



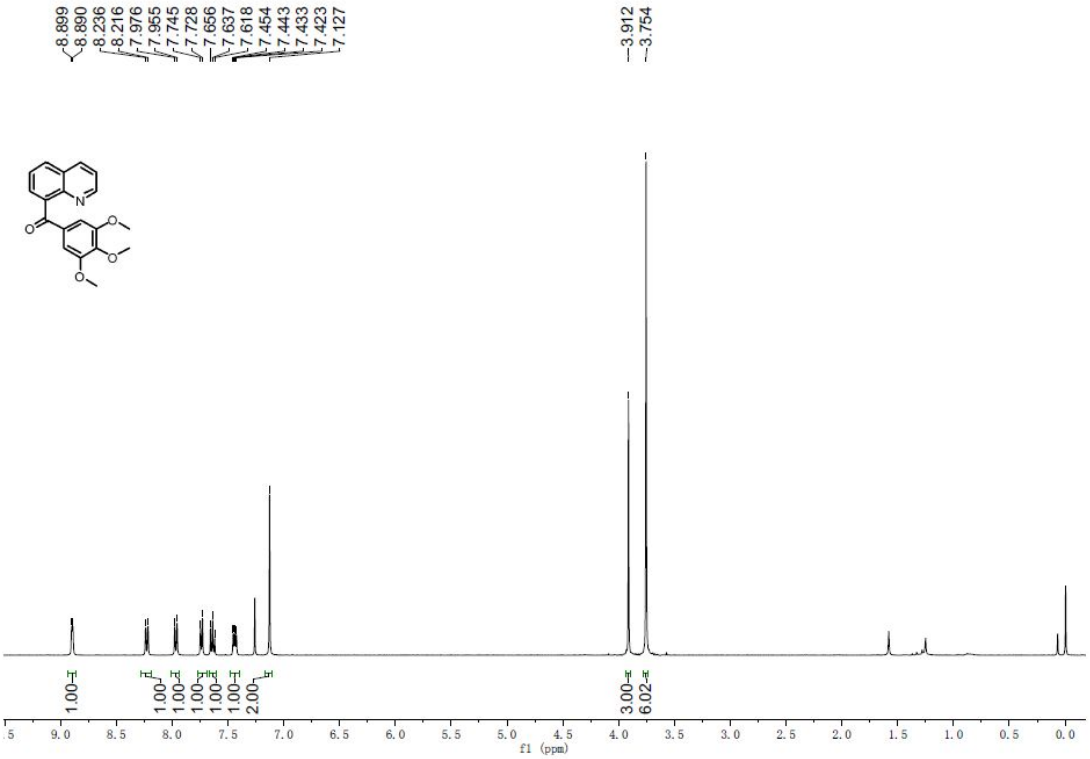
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3au



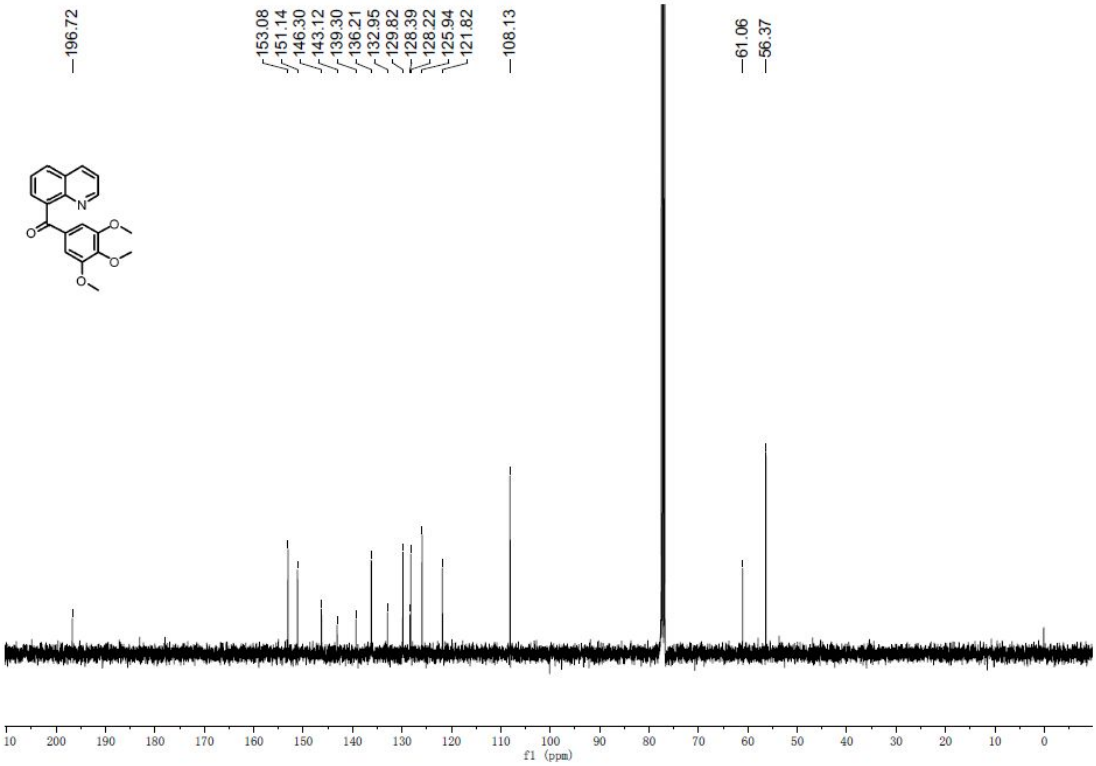
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3au



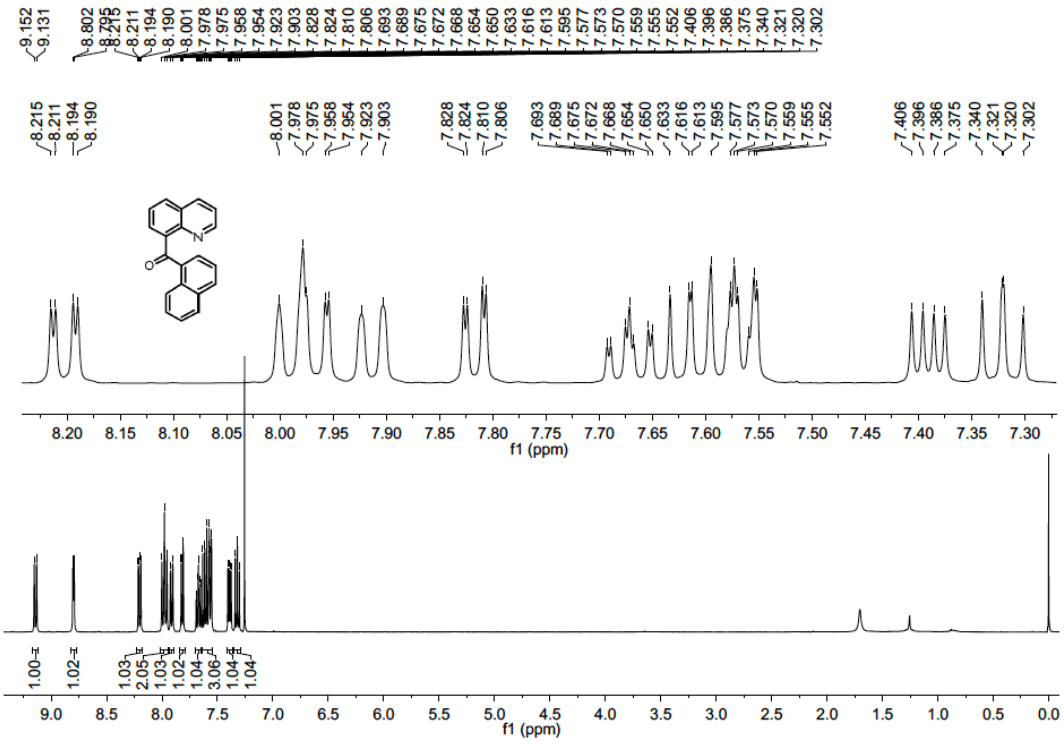
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3av



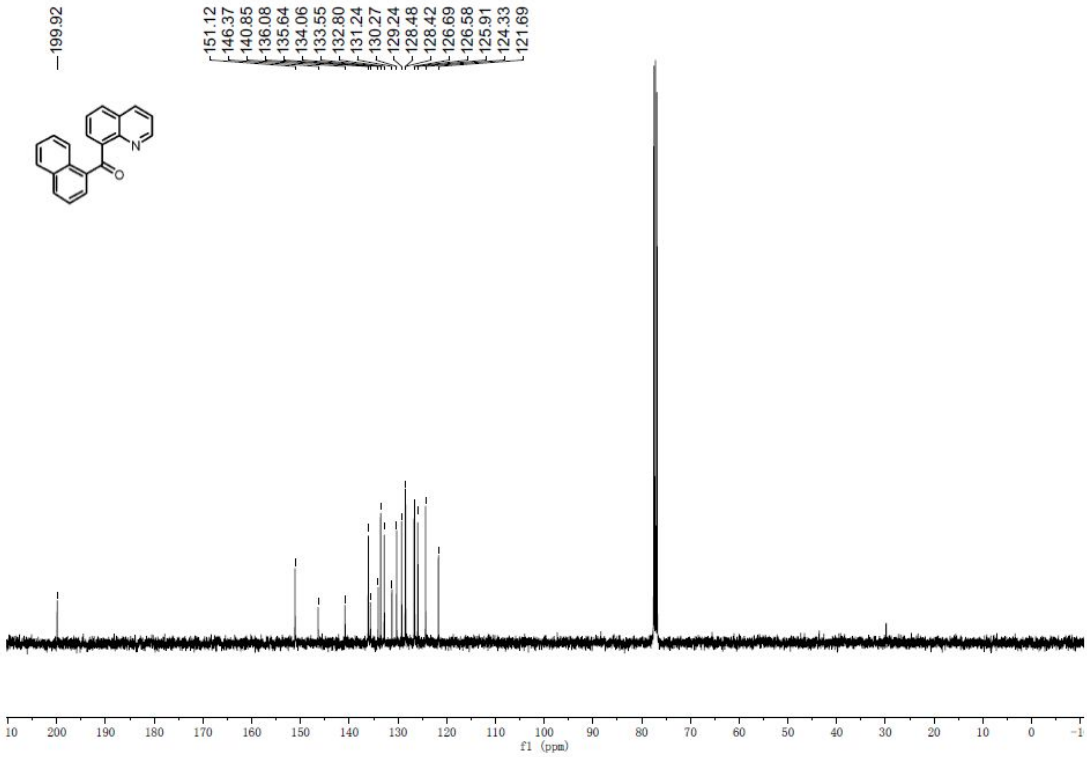
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3av



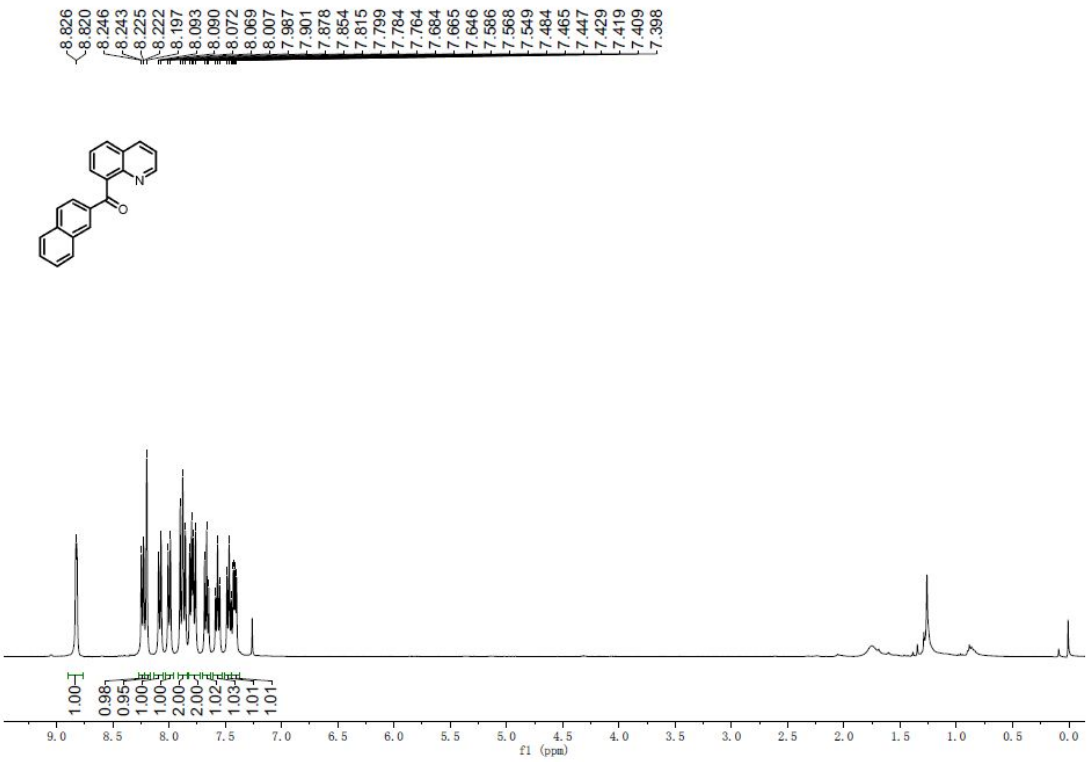
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3aw



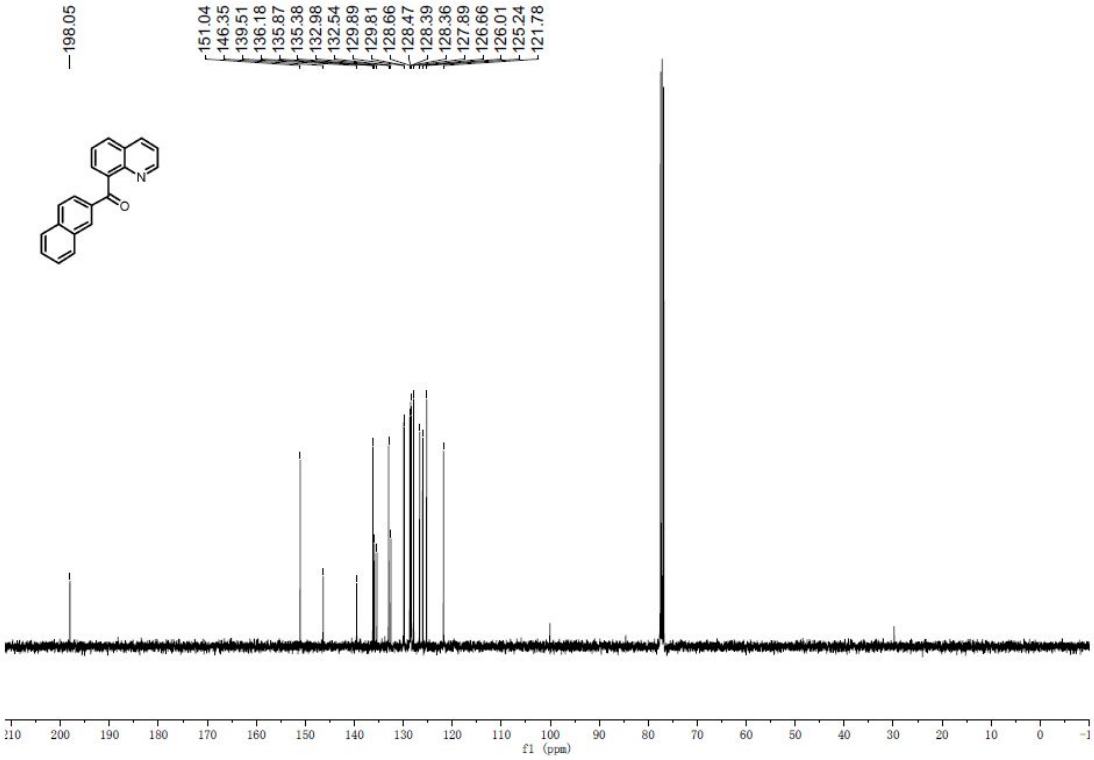
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3aw



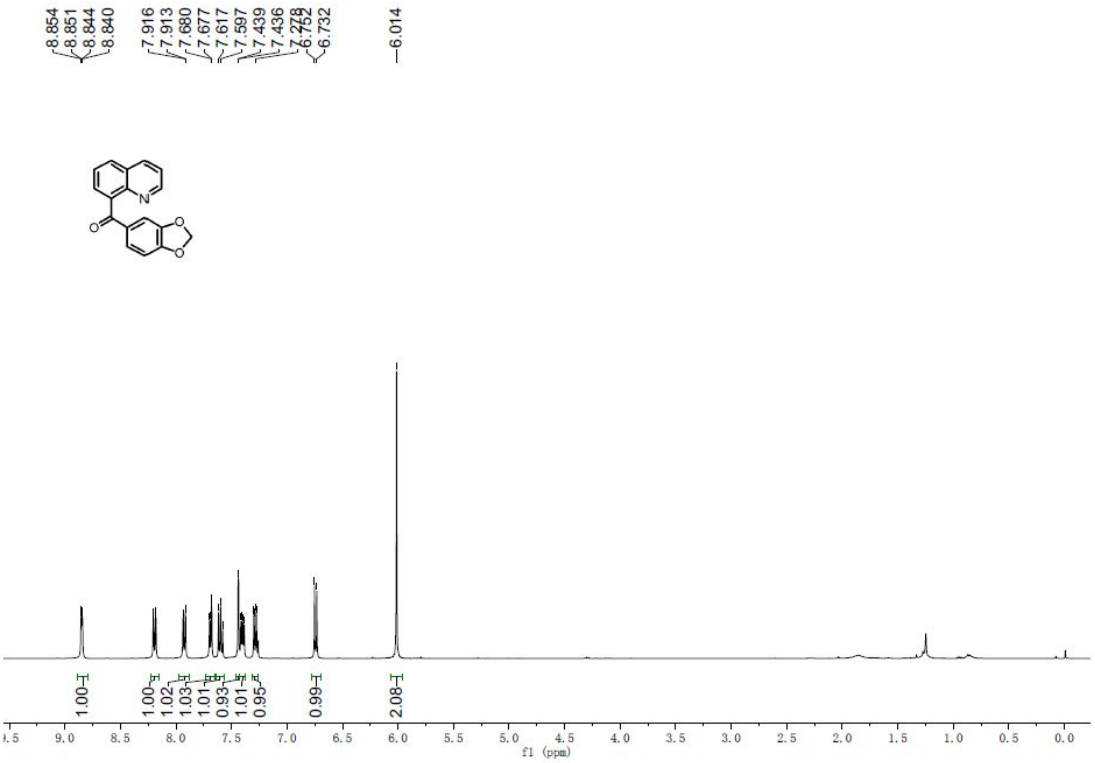
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ax



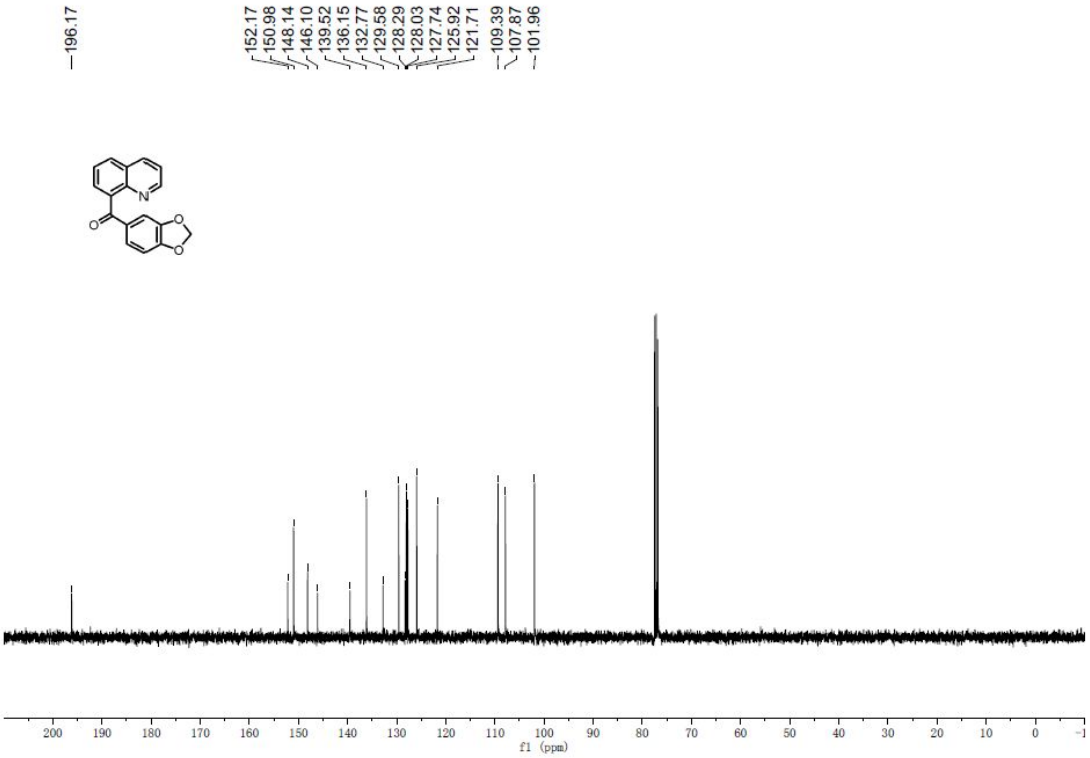
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ax



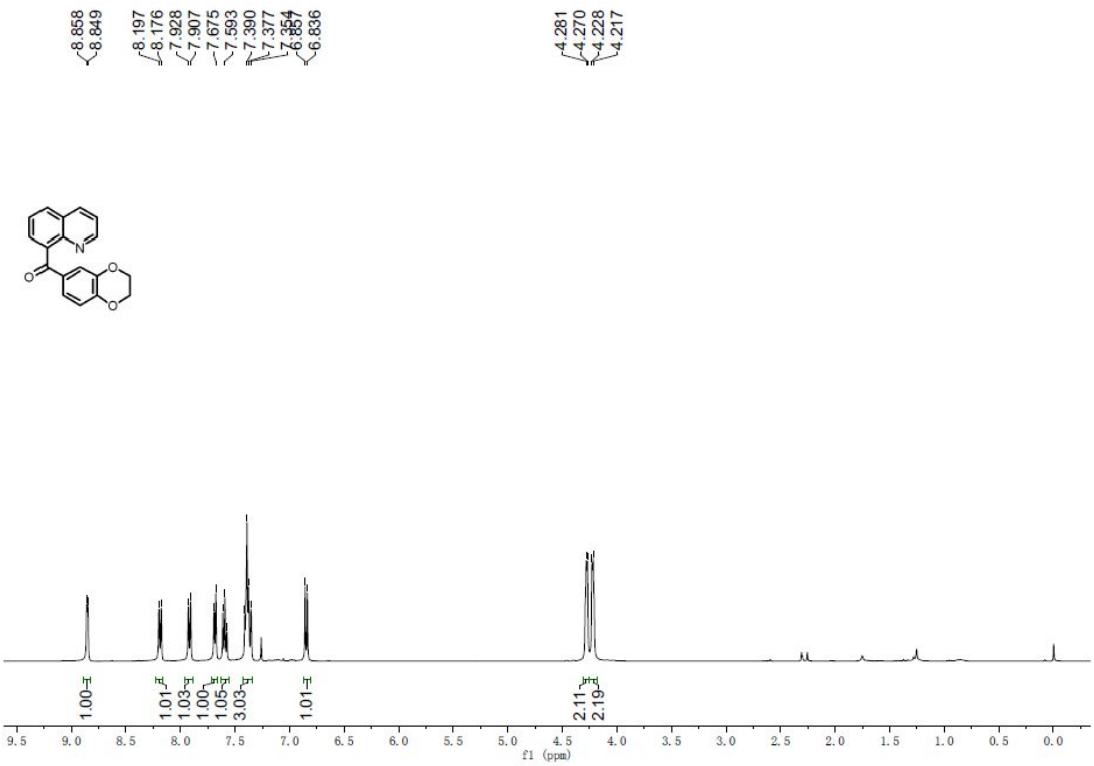
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ay



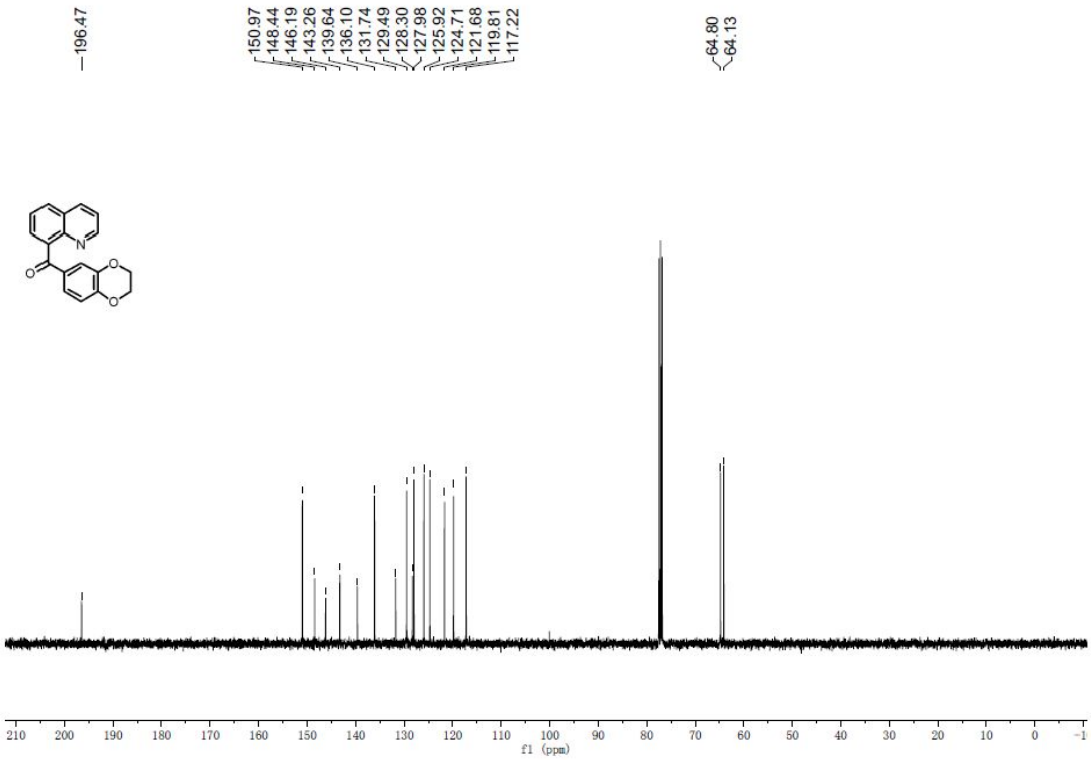
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ay



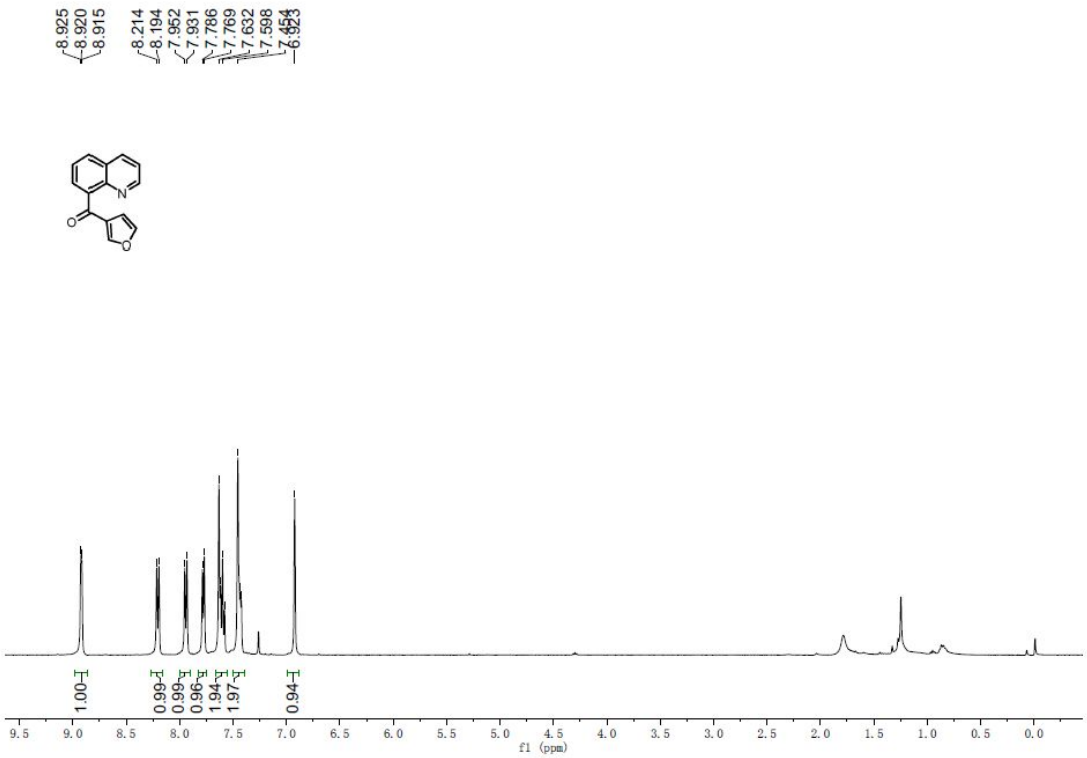
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3az



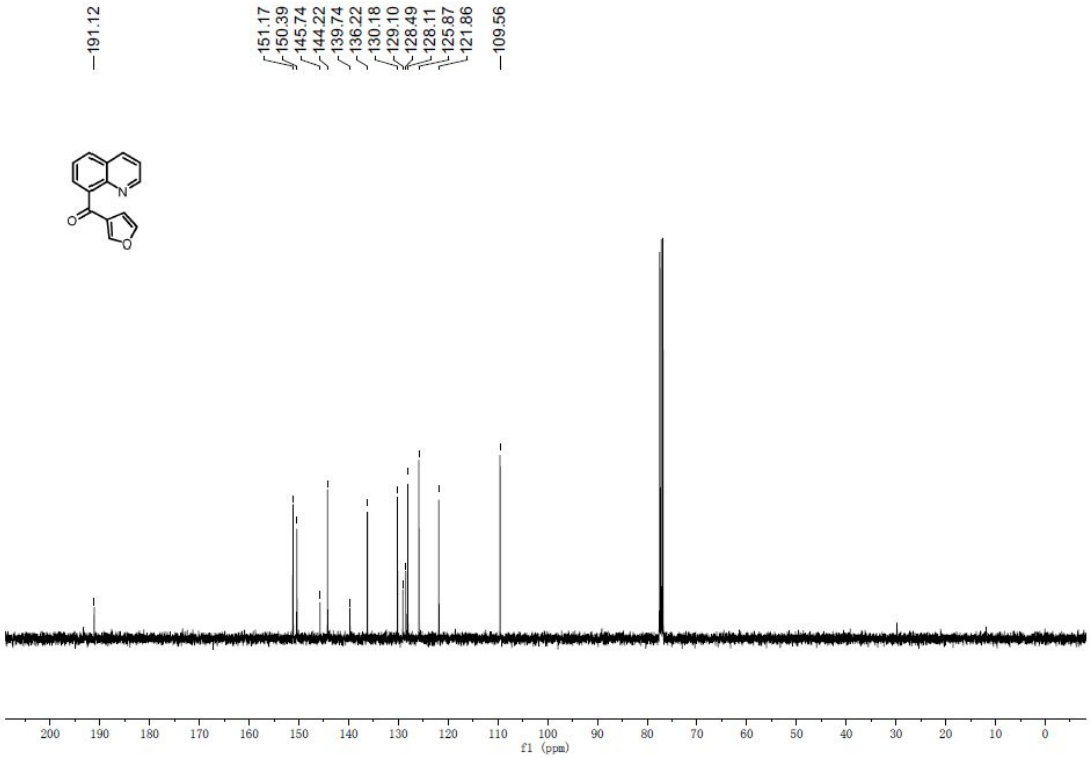
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3az



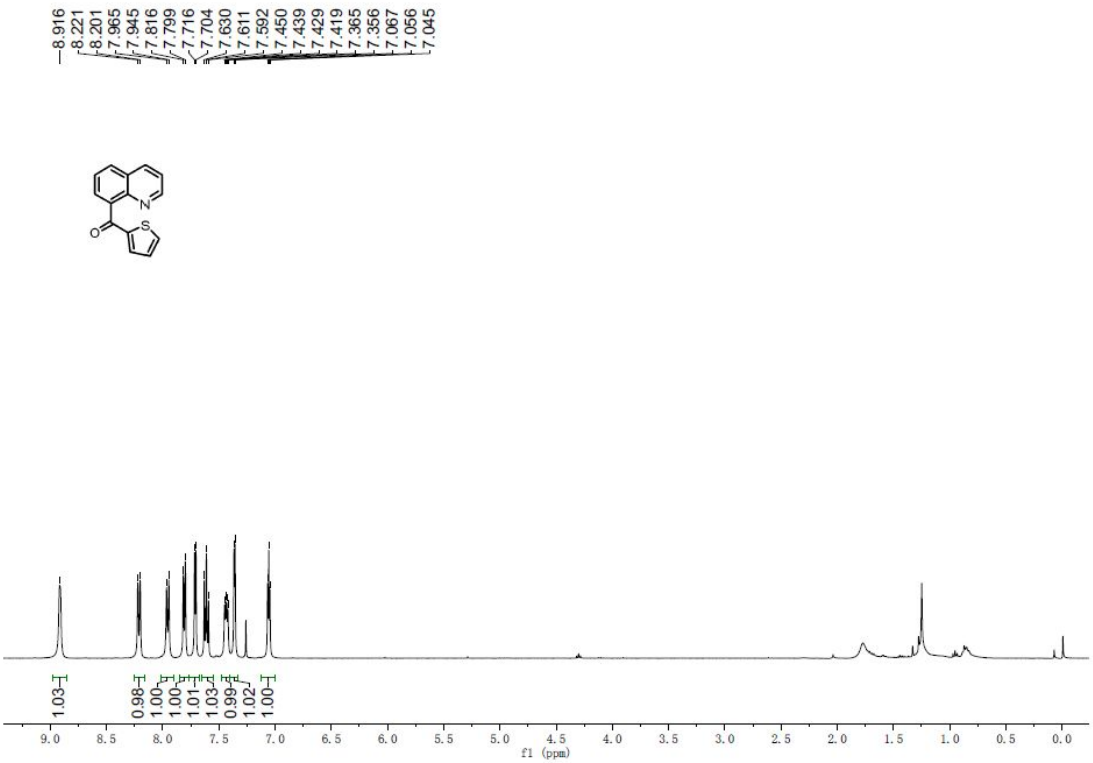
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3aaa



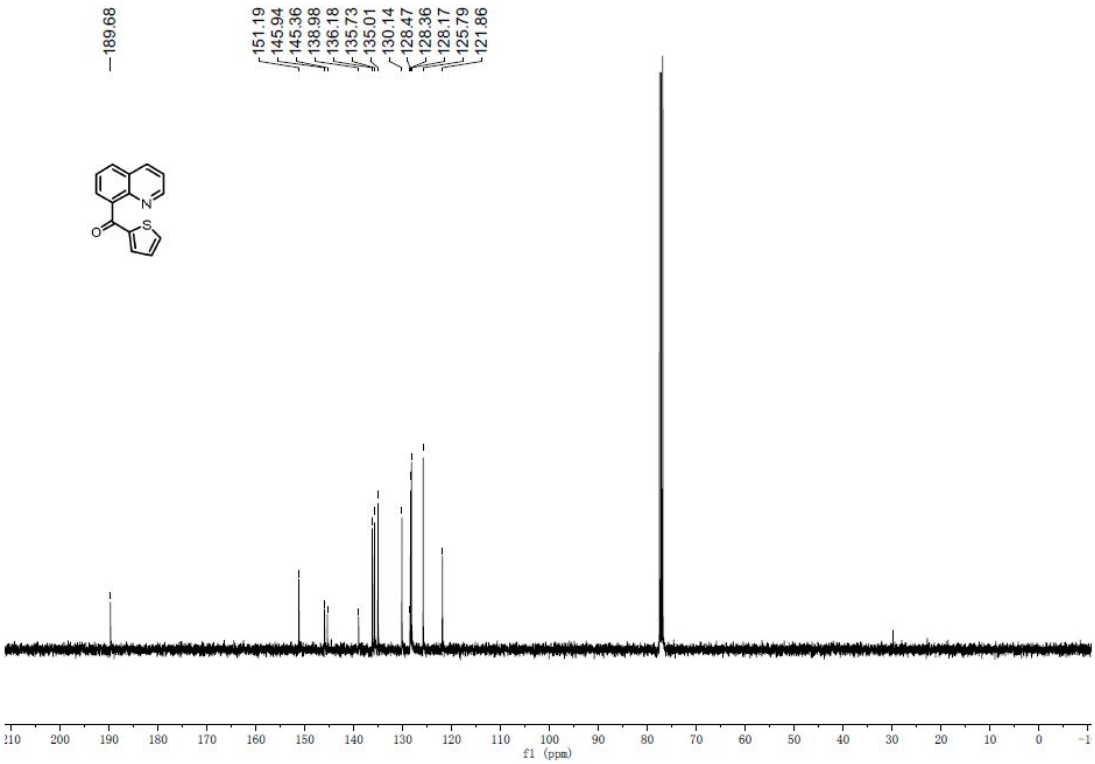
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3aaa



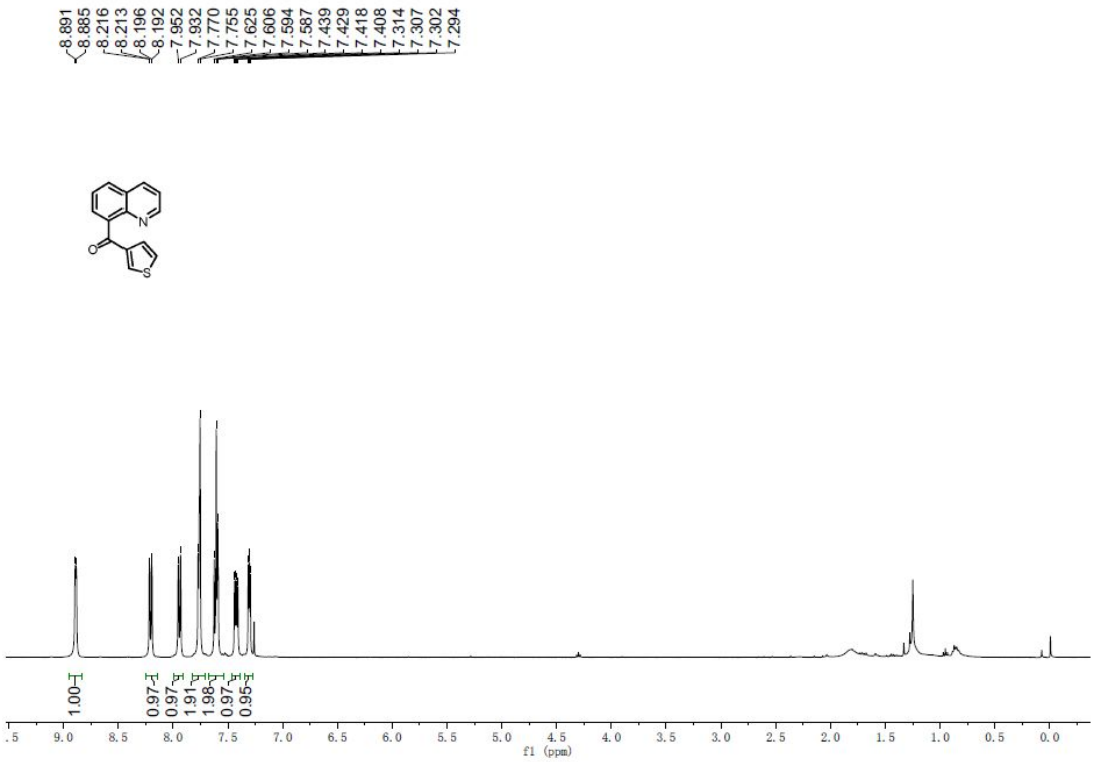
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3aab



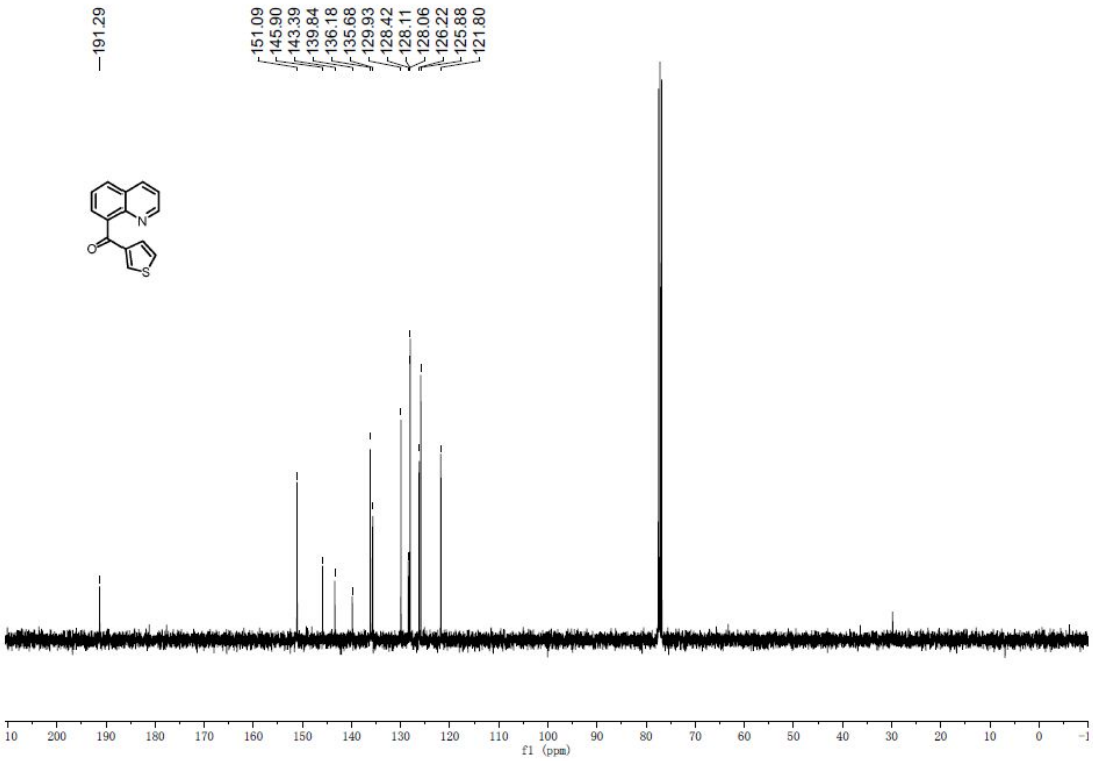
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3aab



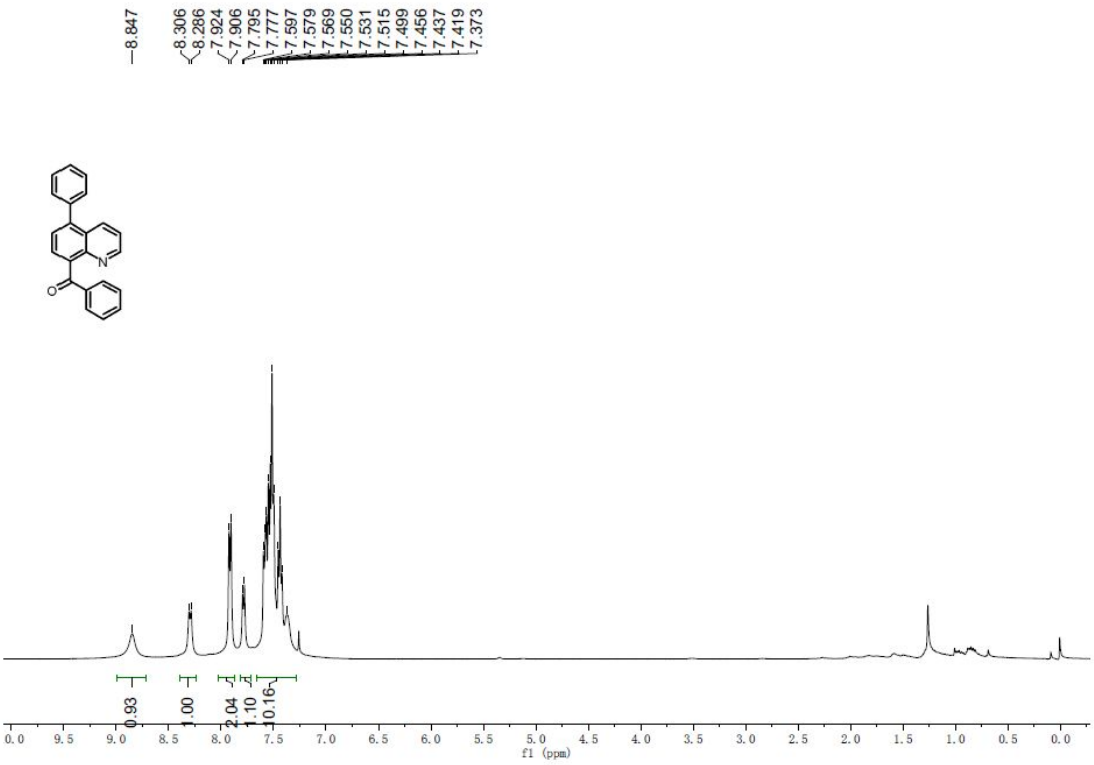
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3aac



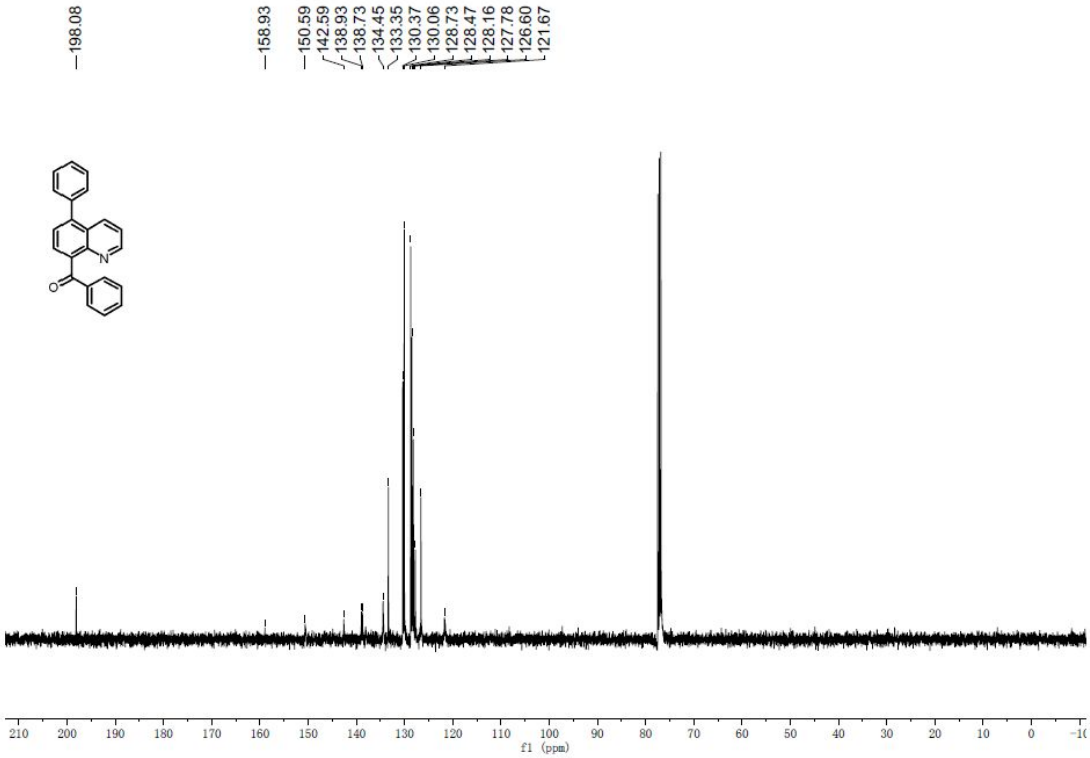
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3aac



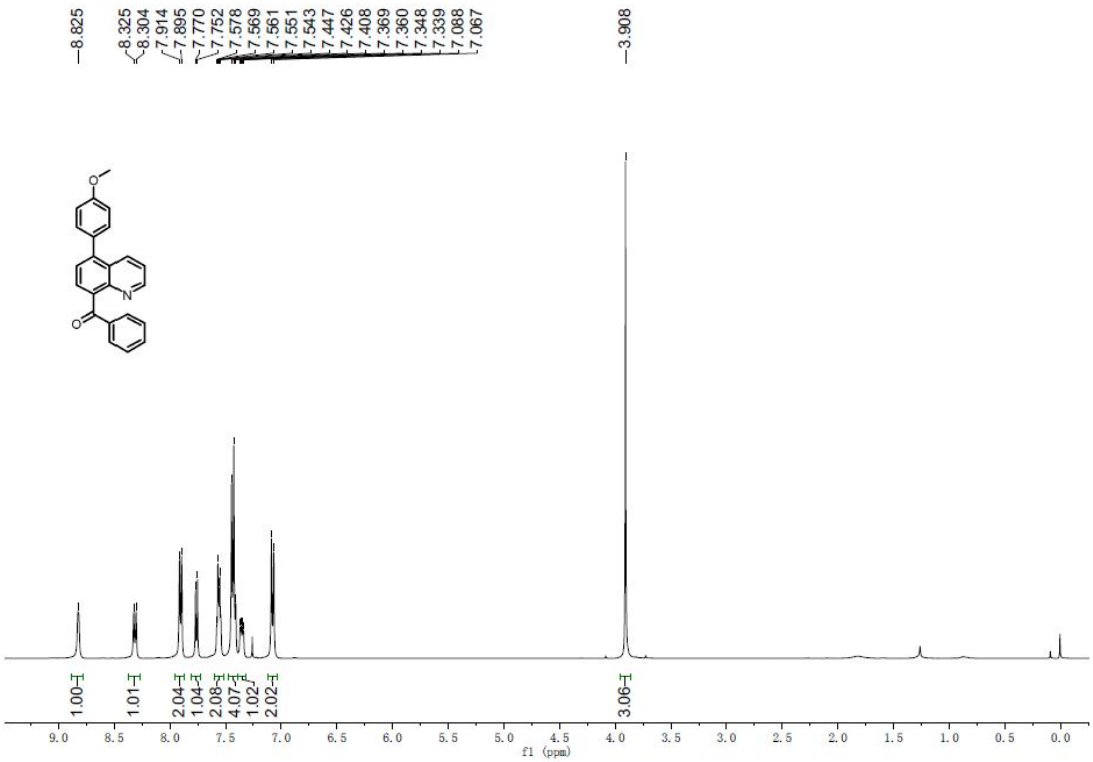
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ba



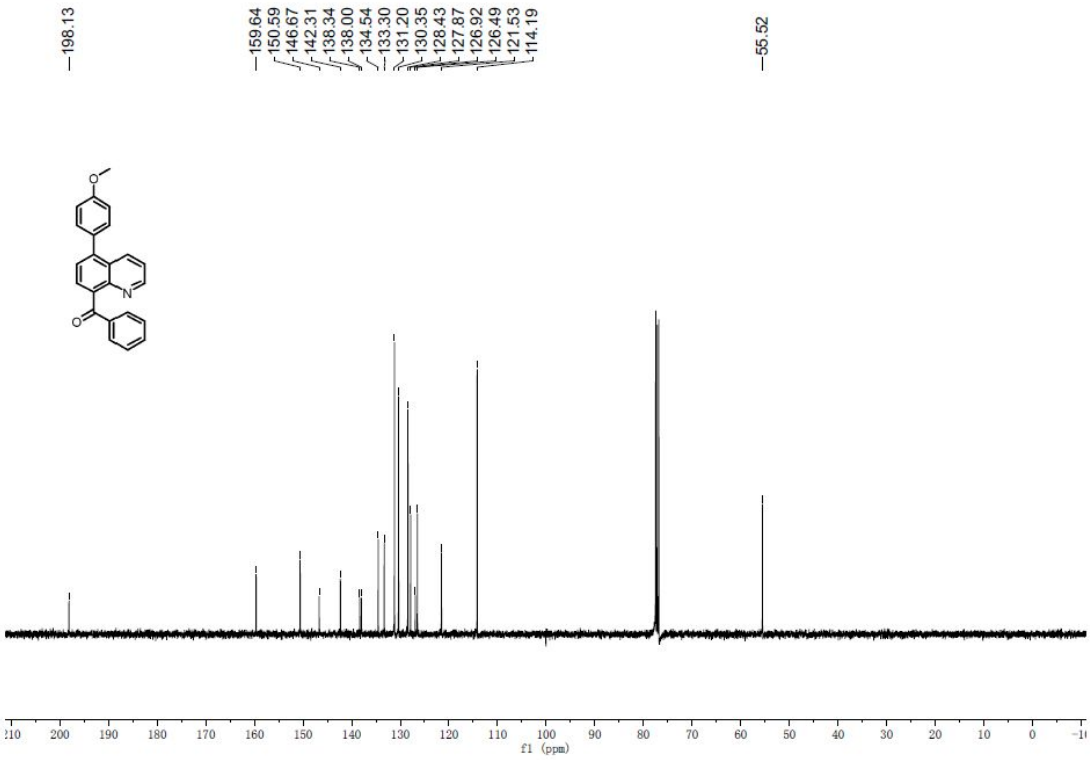
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ba



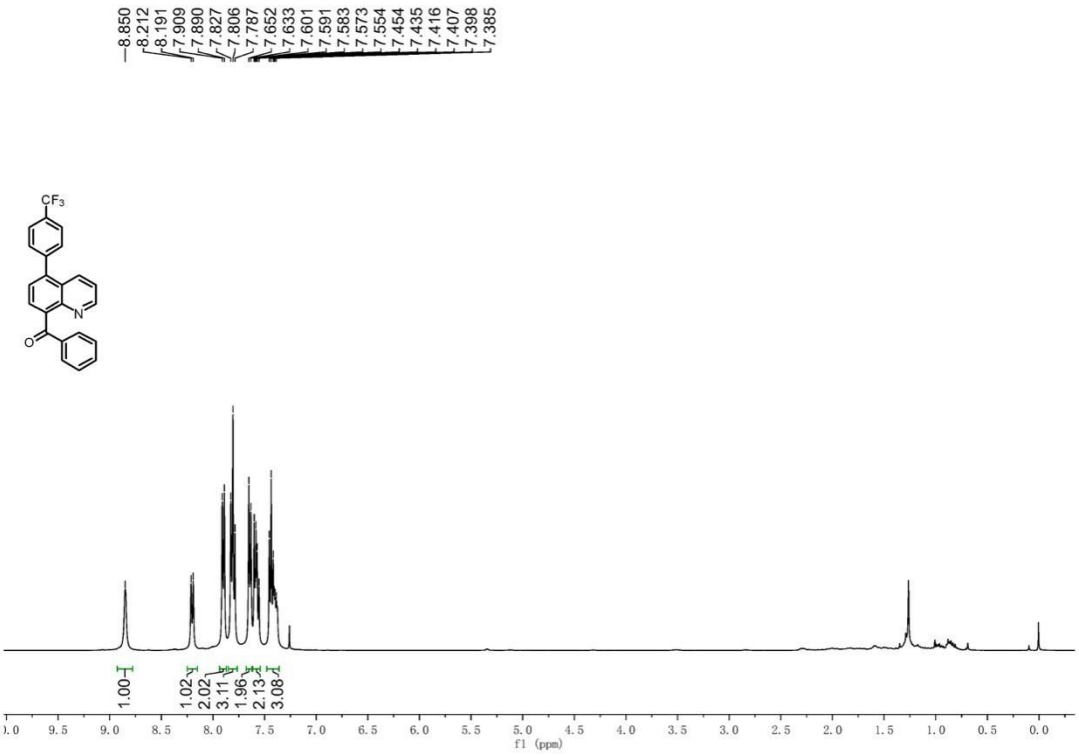
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ca



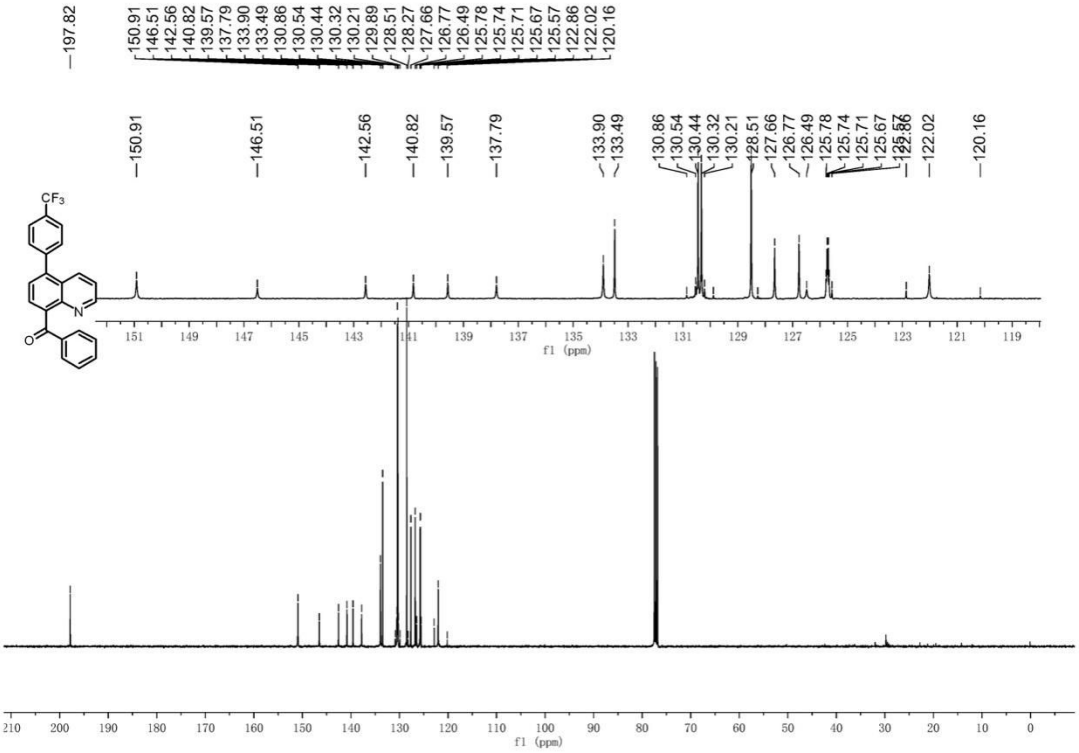
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ca



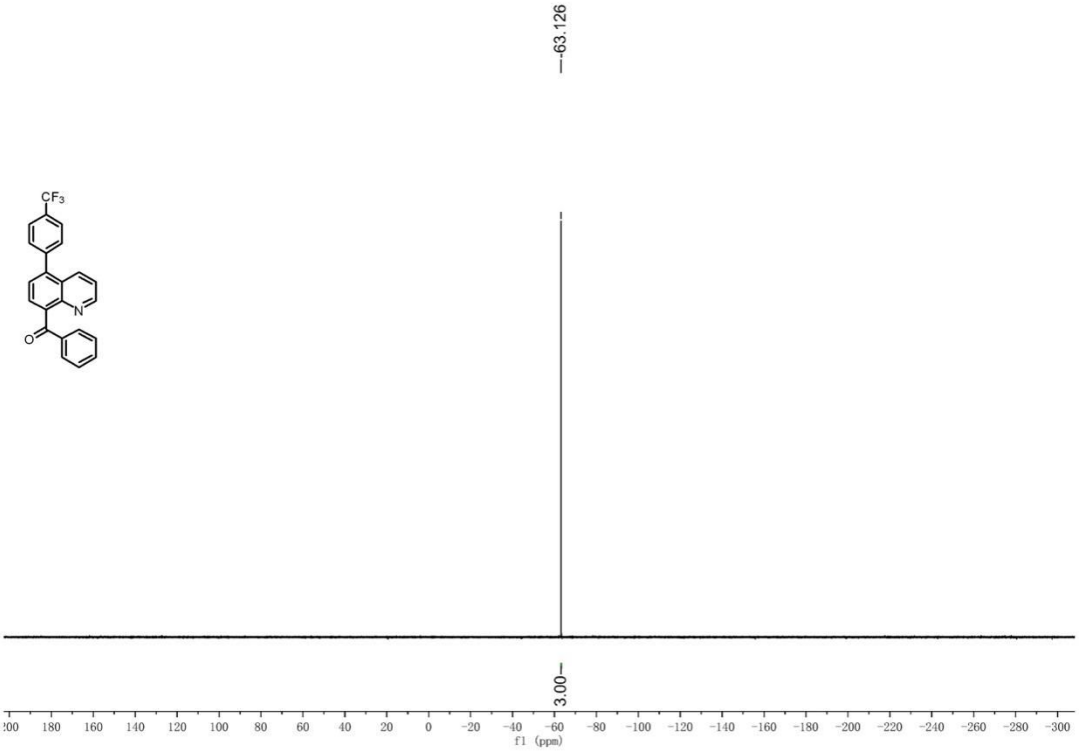
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3da



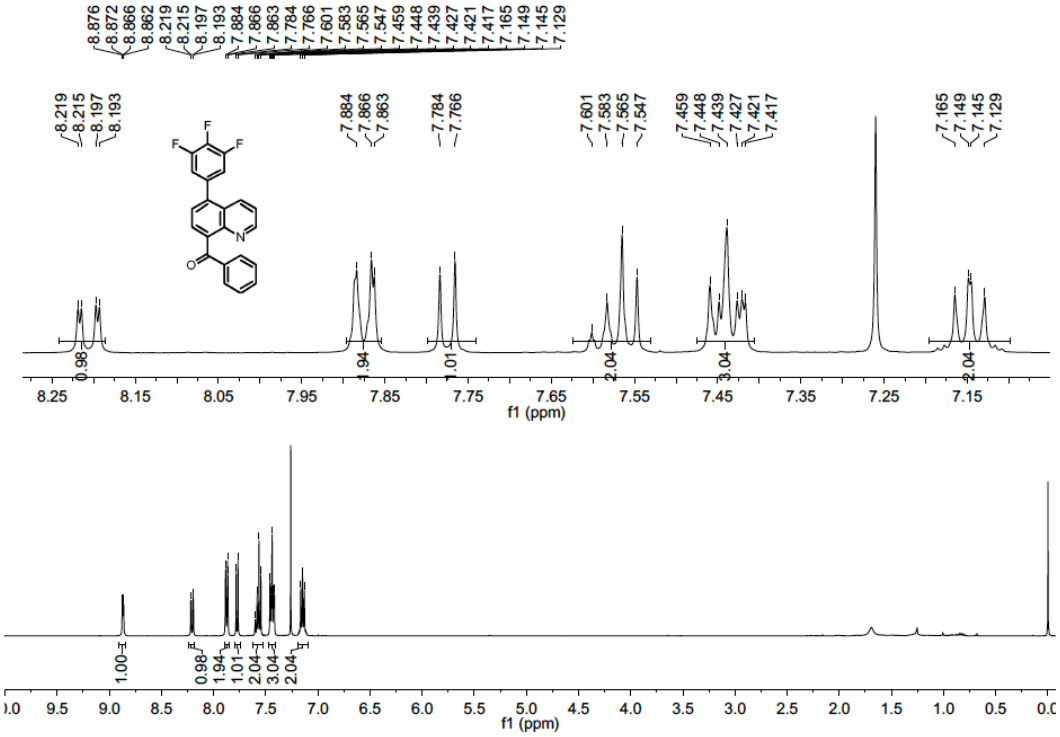
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3da



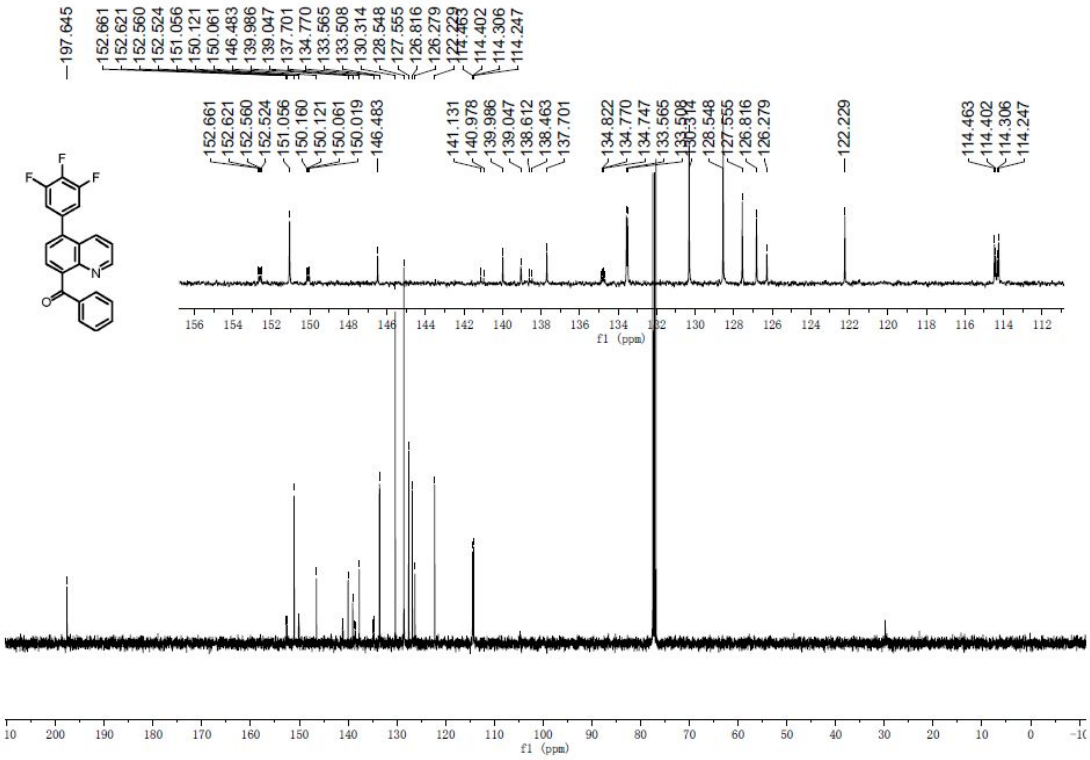
^{19}F NMR spectrum (376 MHz, $CDCl_3$, 23 ºC) of 3da



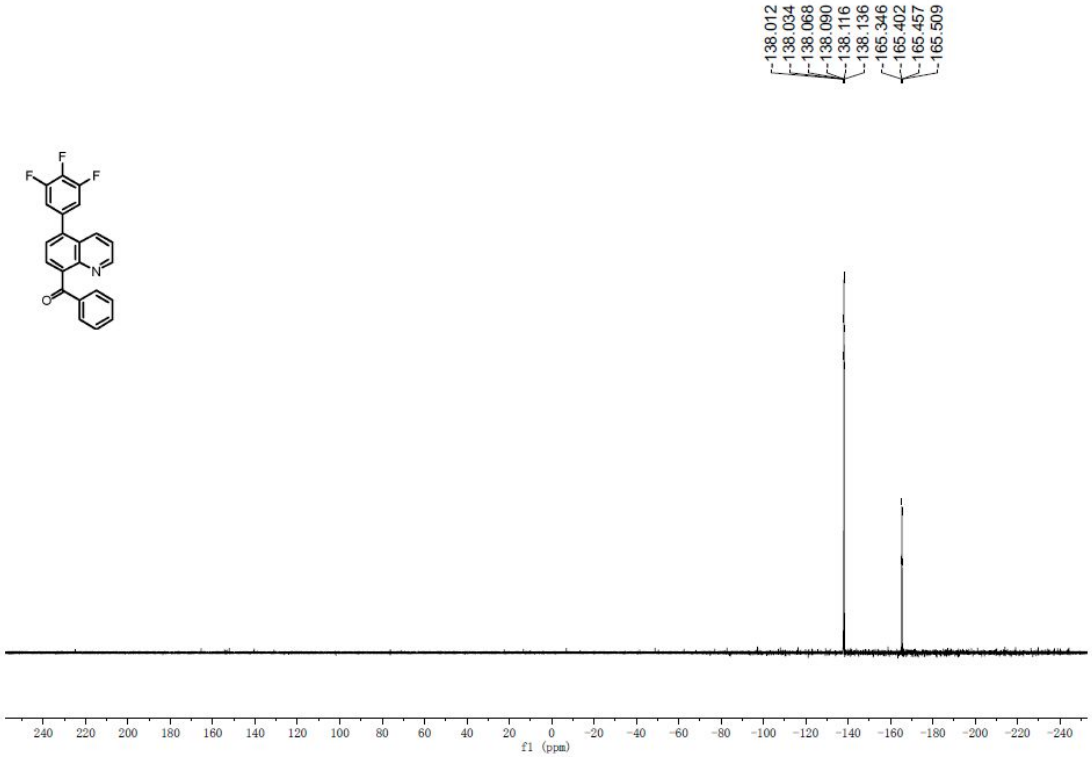
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ea



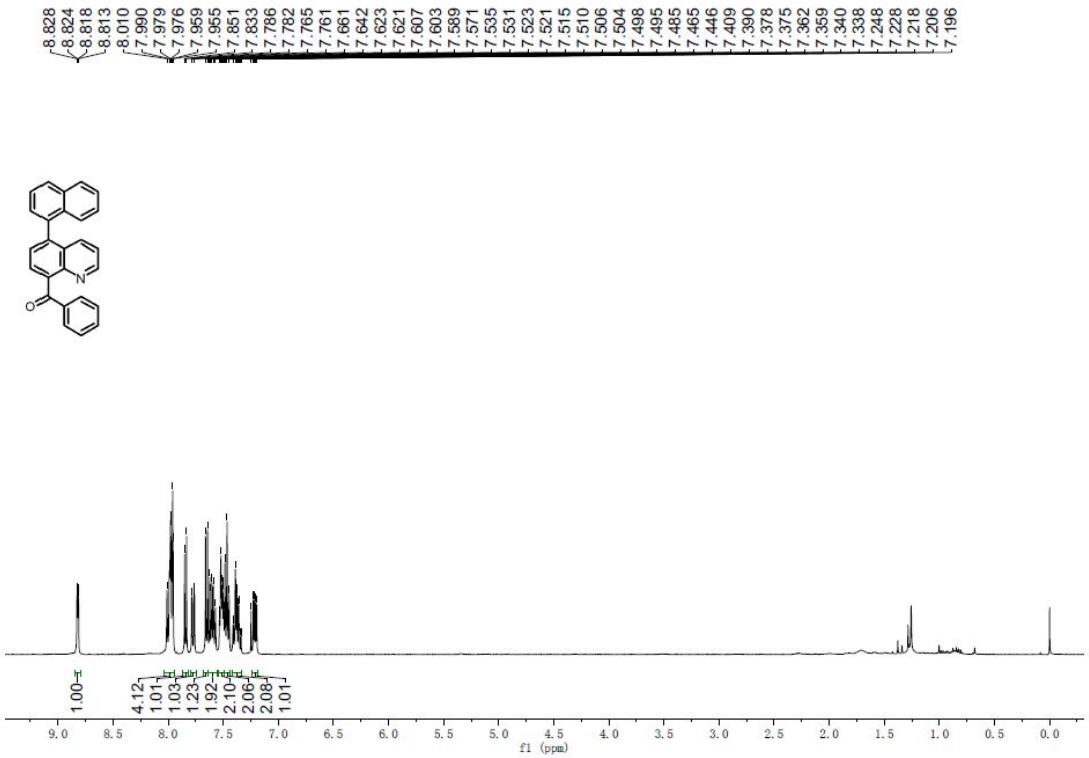
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ea



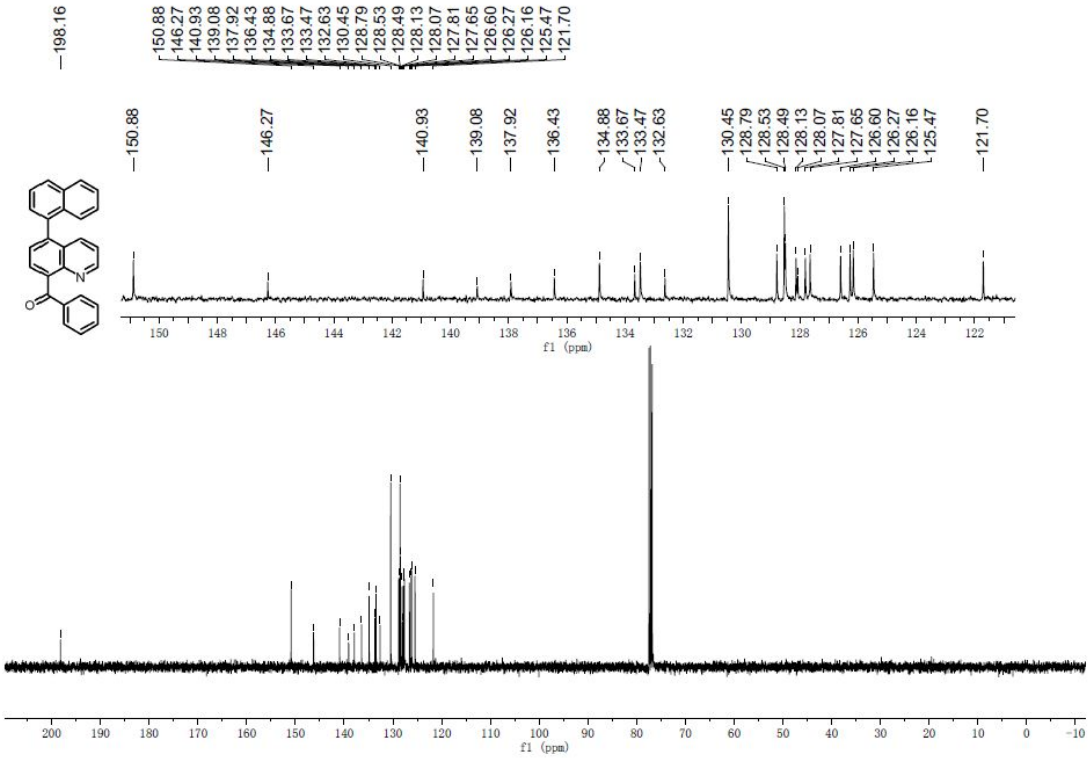
^{19}F NMR spectrum (376MHz, $CDCl_3$, 23 ºC) of 3ea



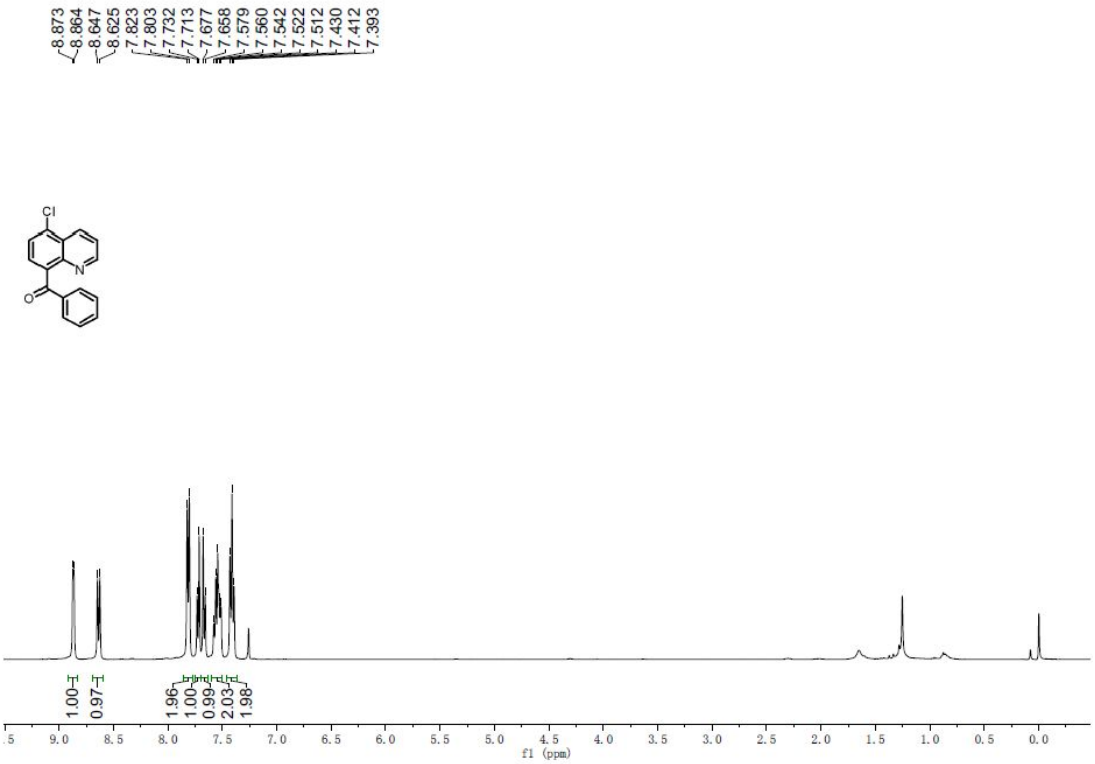
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3fa



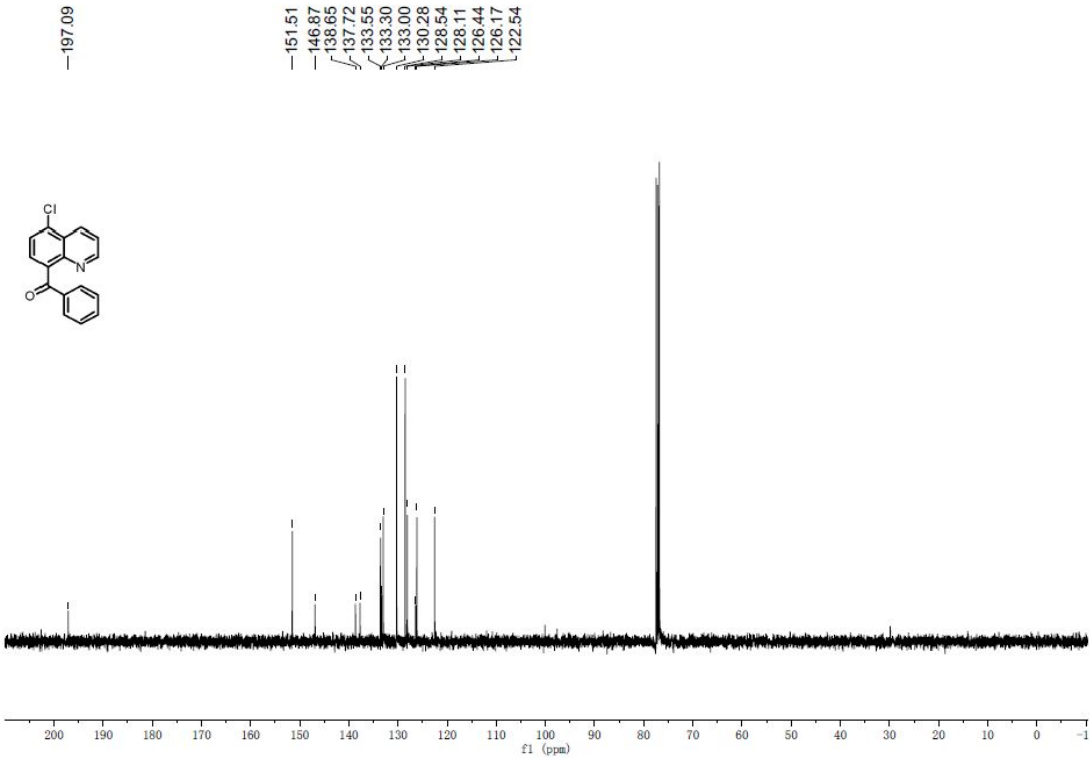
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3fa



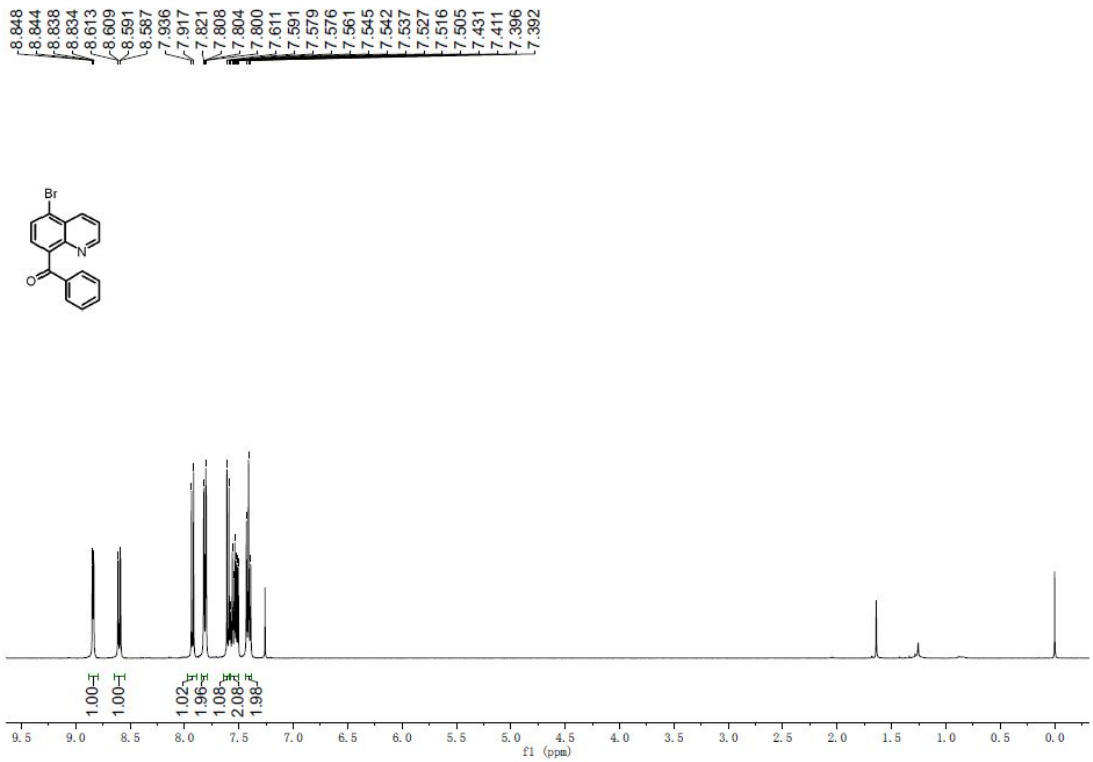
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ga



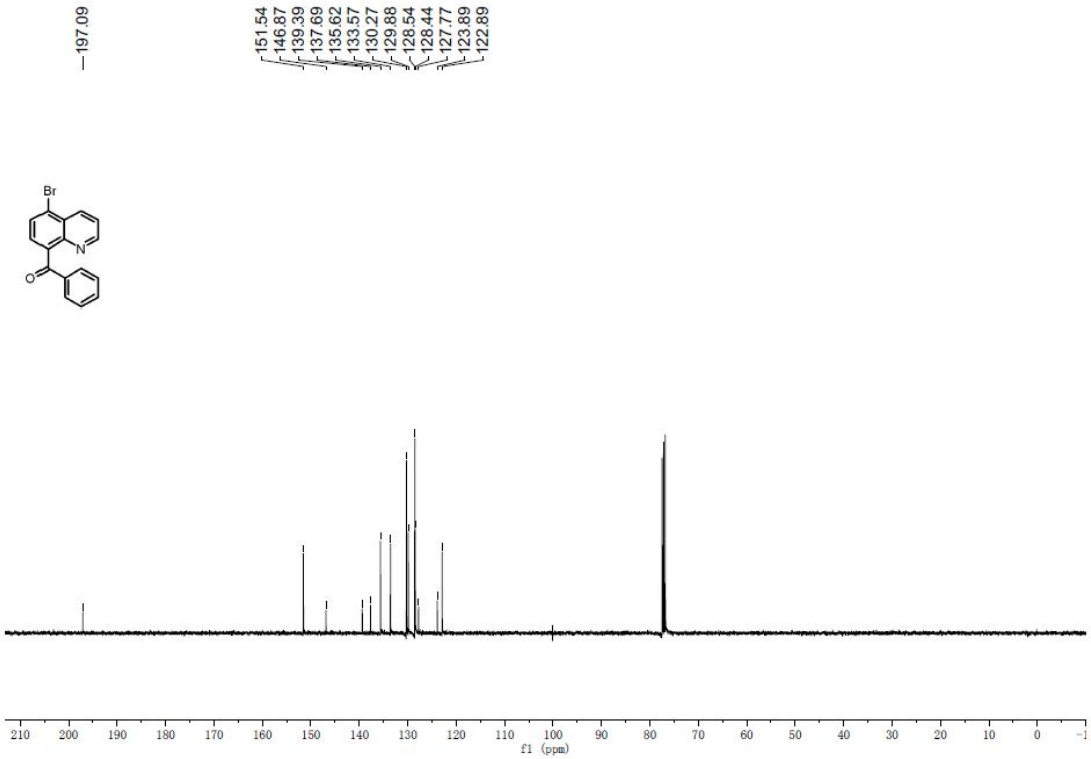
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ga



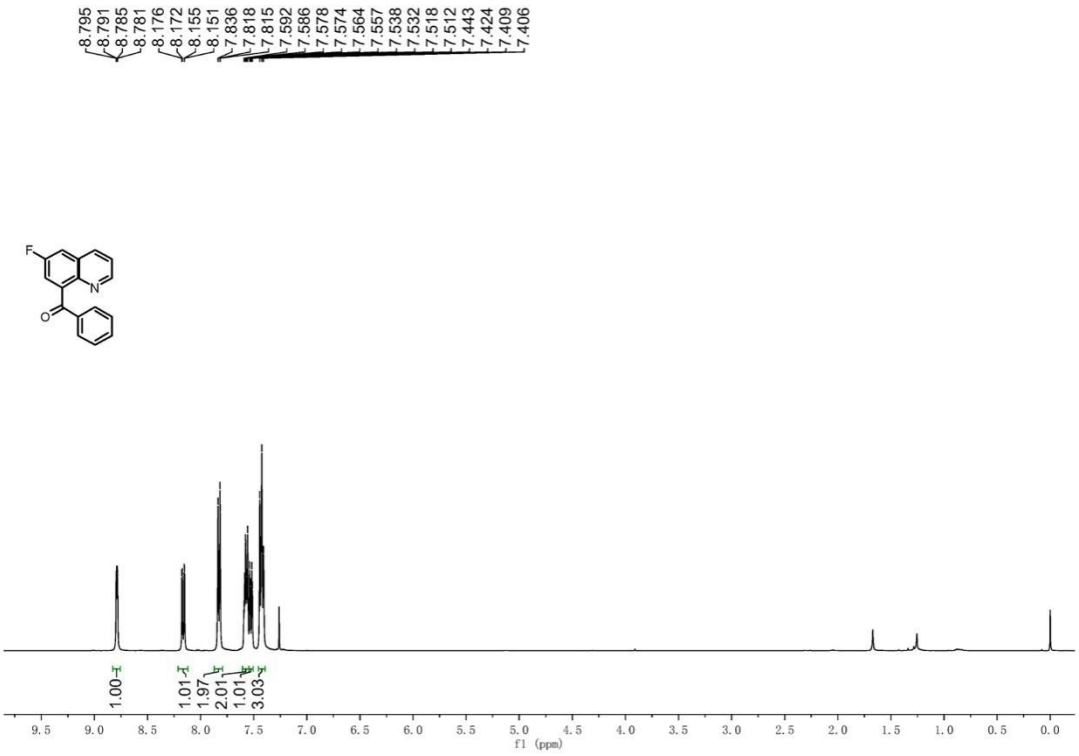
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ha



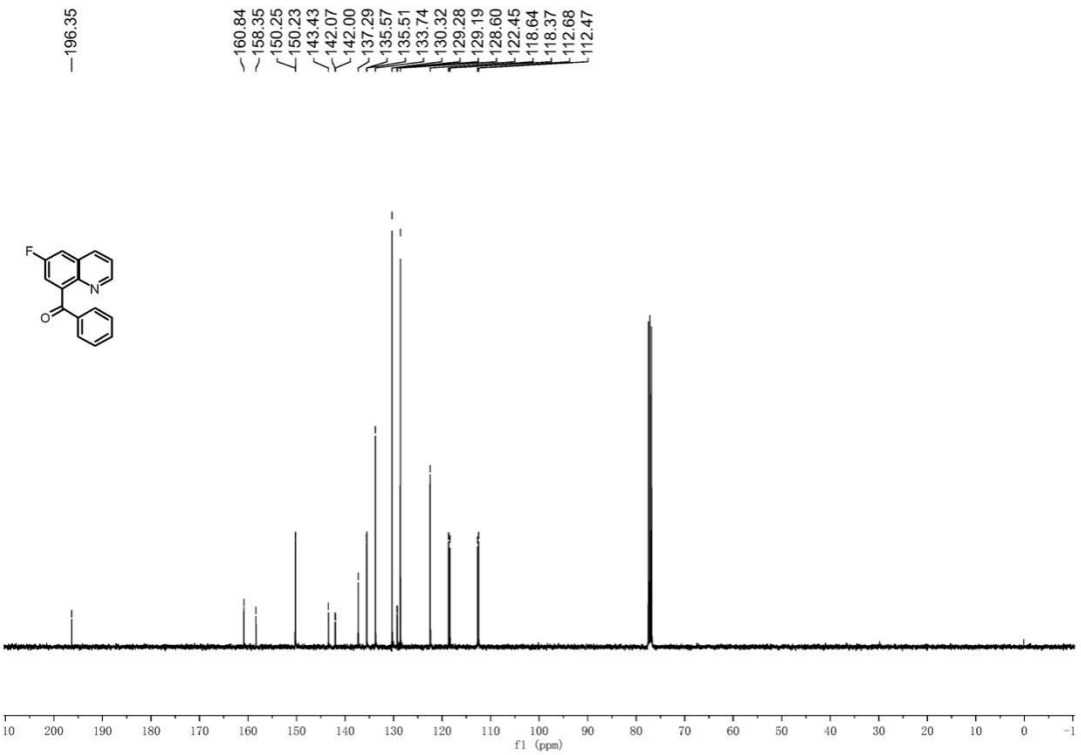
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ha



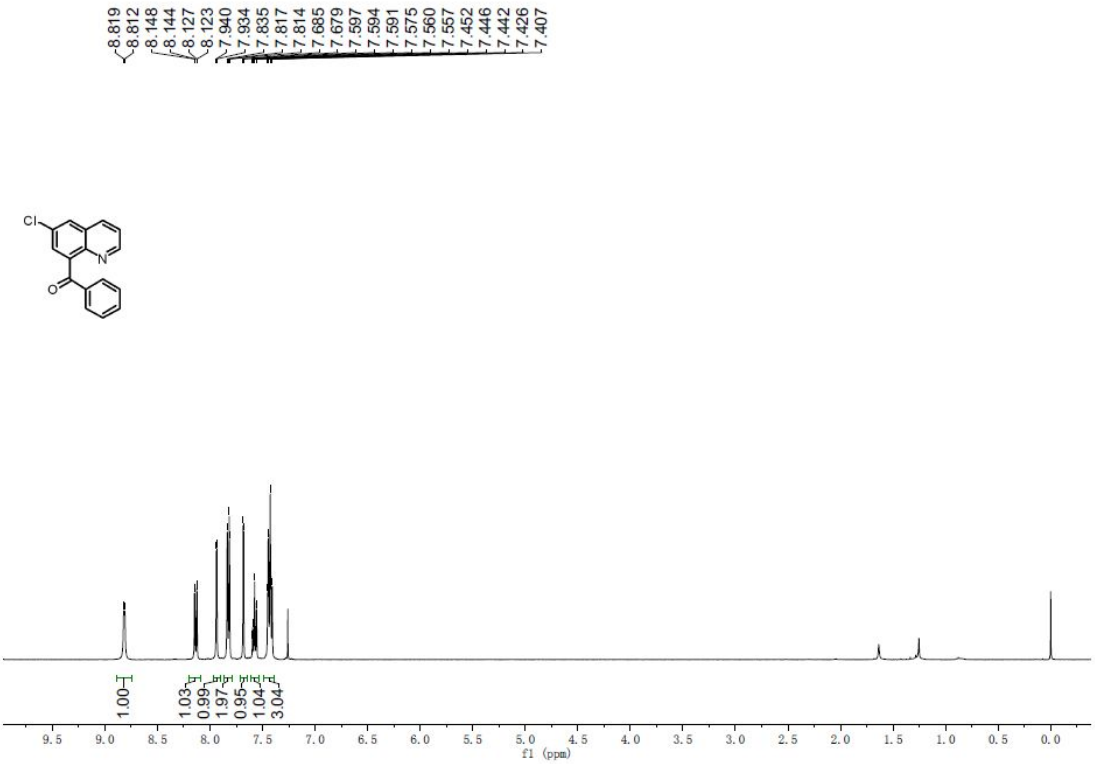
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ia



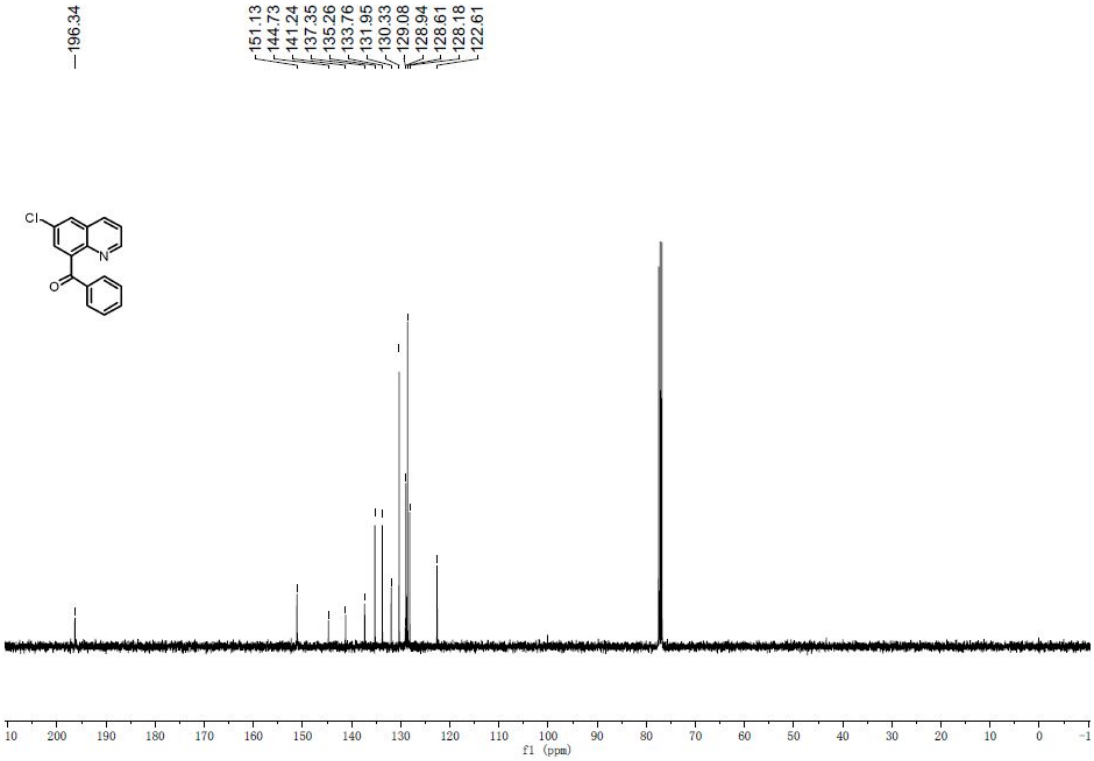
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ia



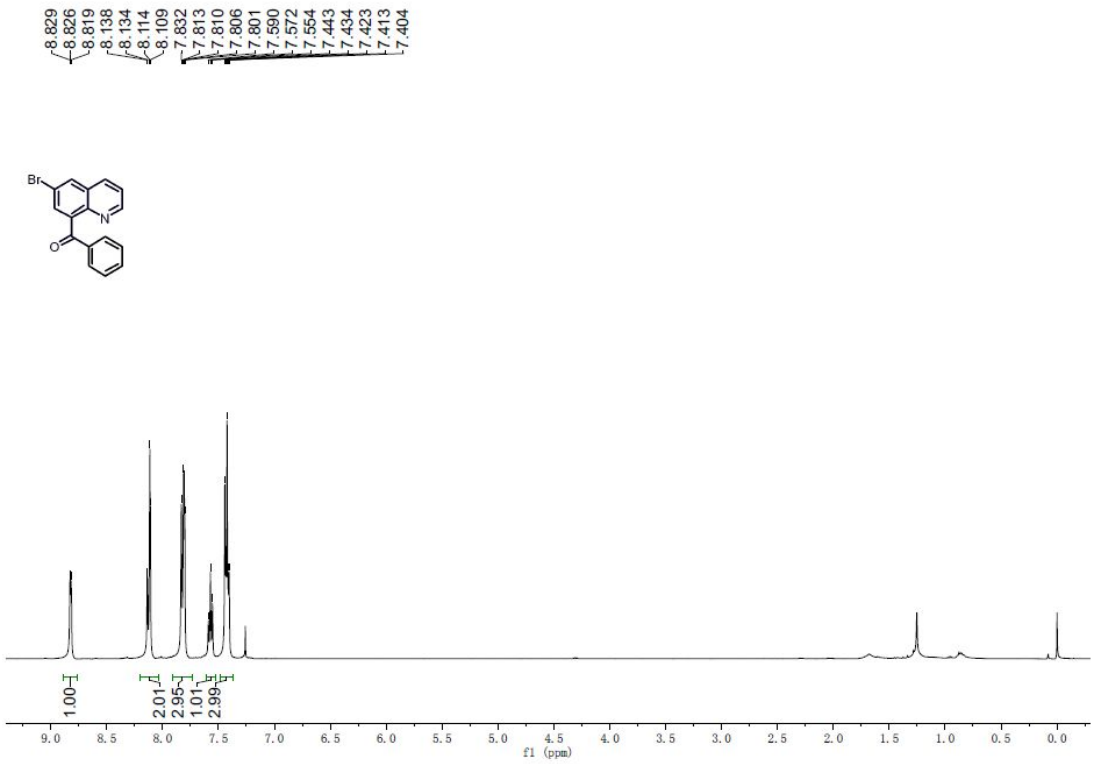
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ja



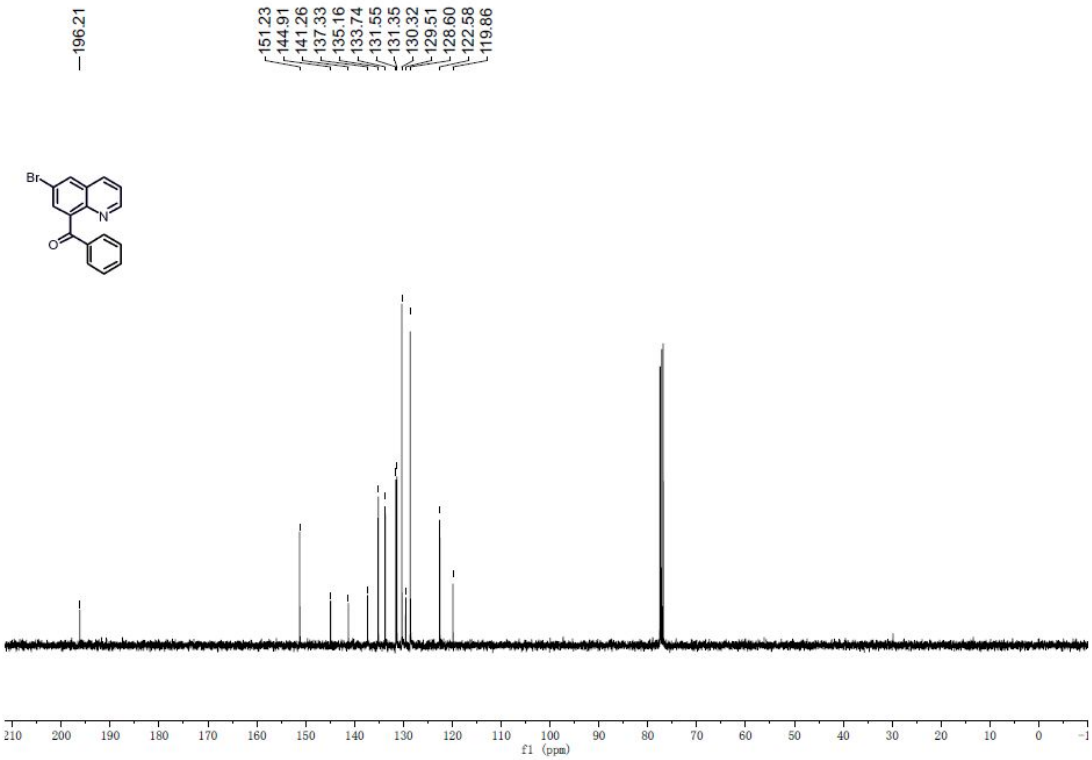
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ja



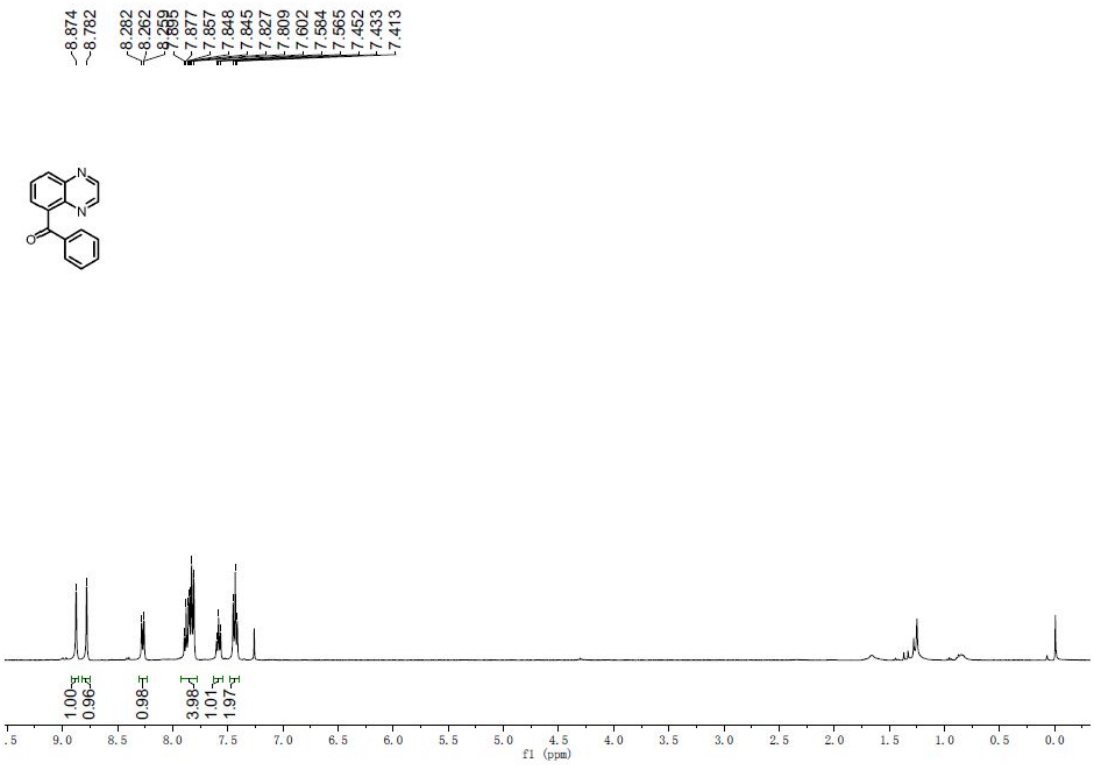
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ka



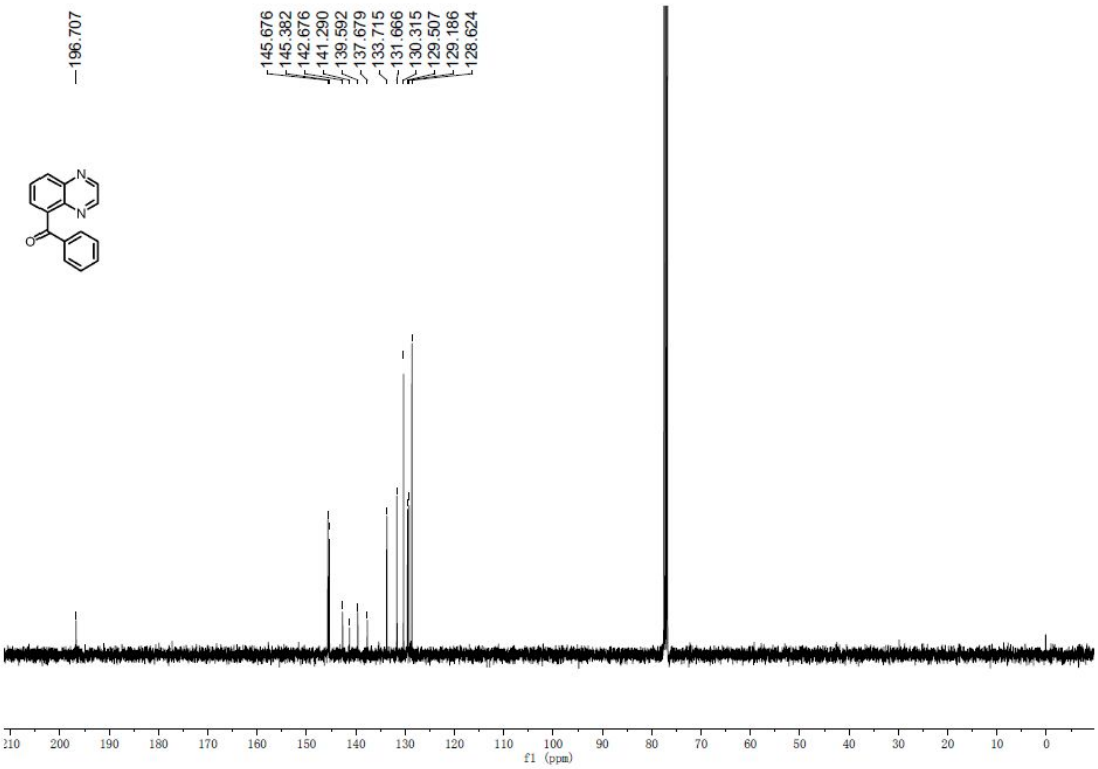
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ka



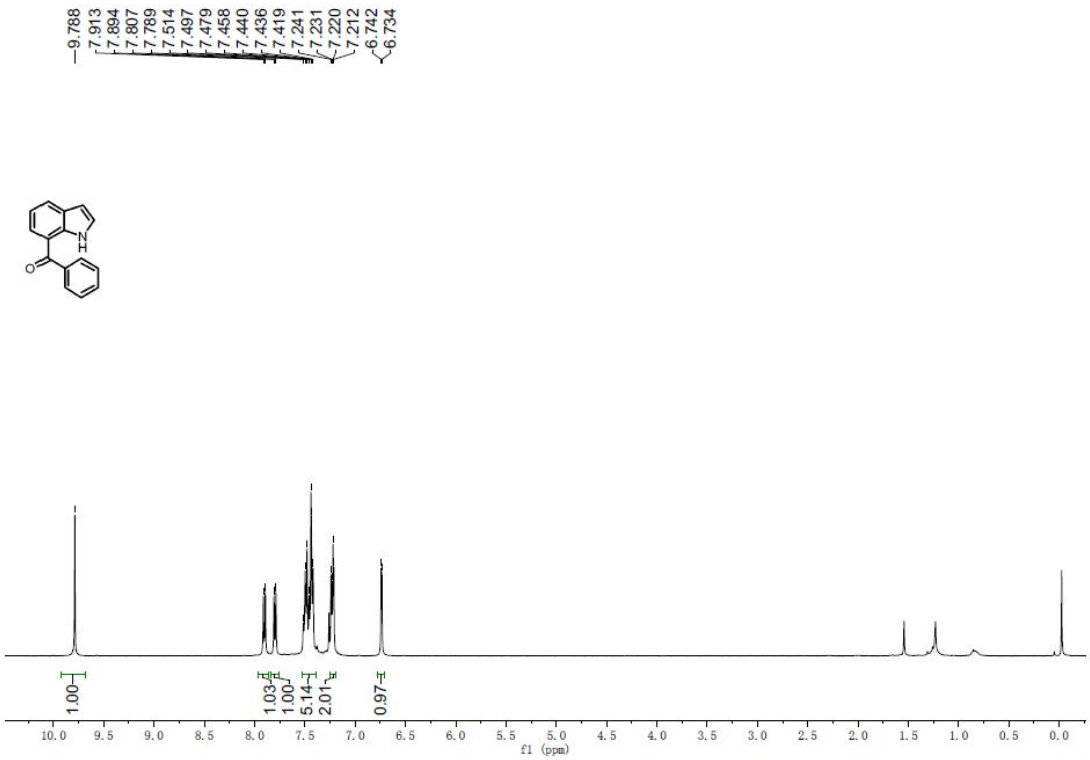
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3la



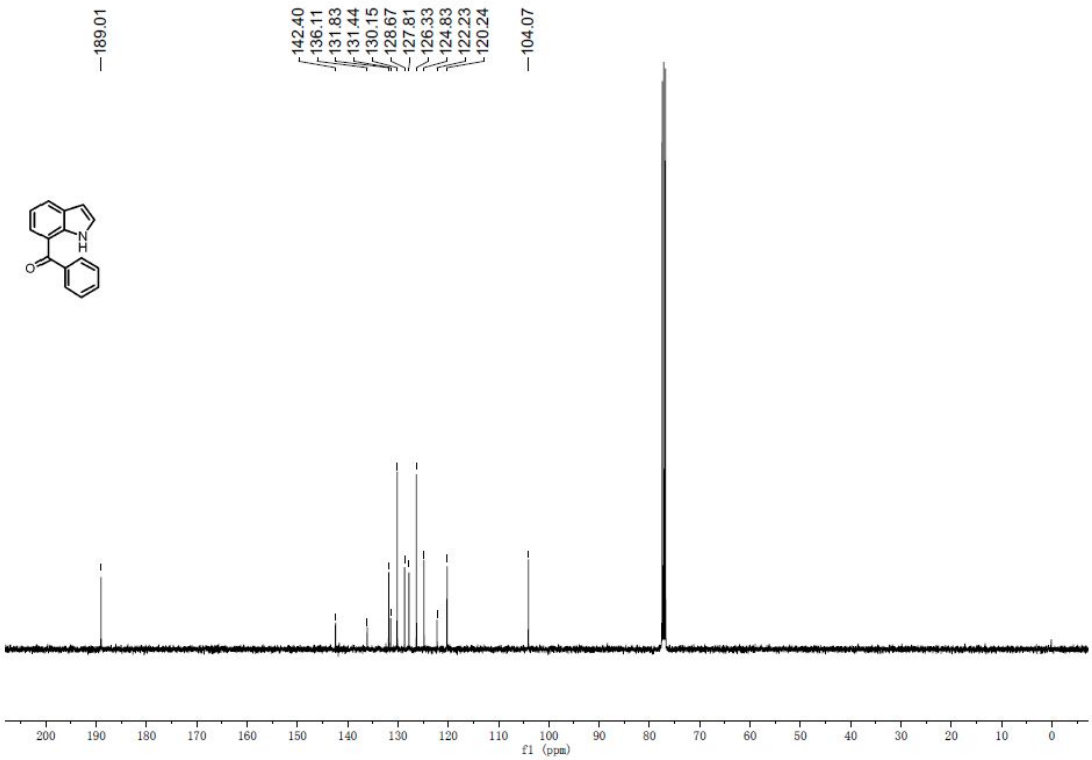
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3la



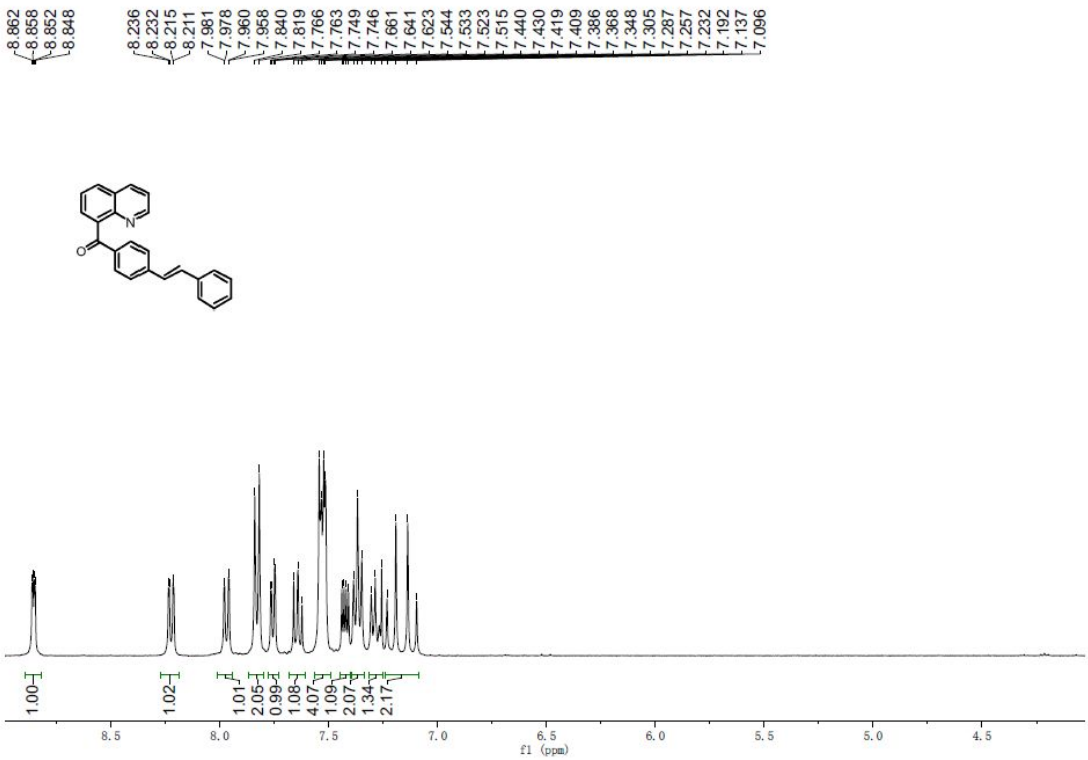
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ma



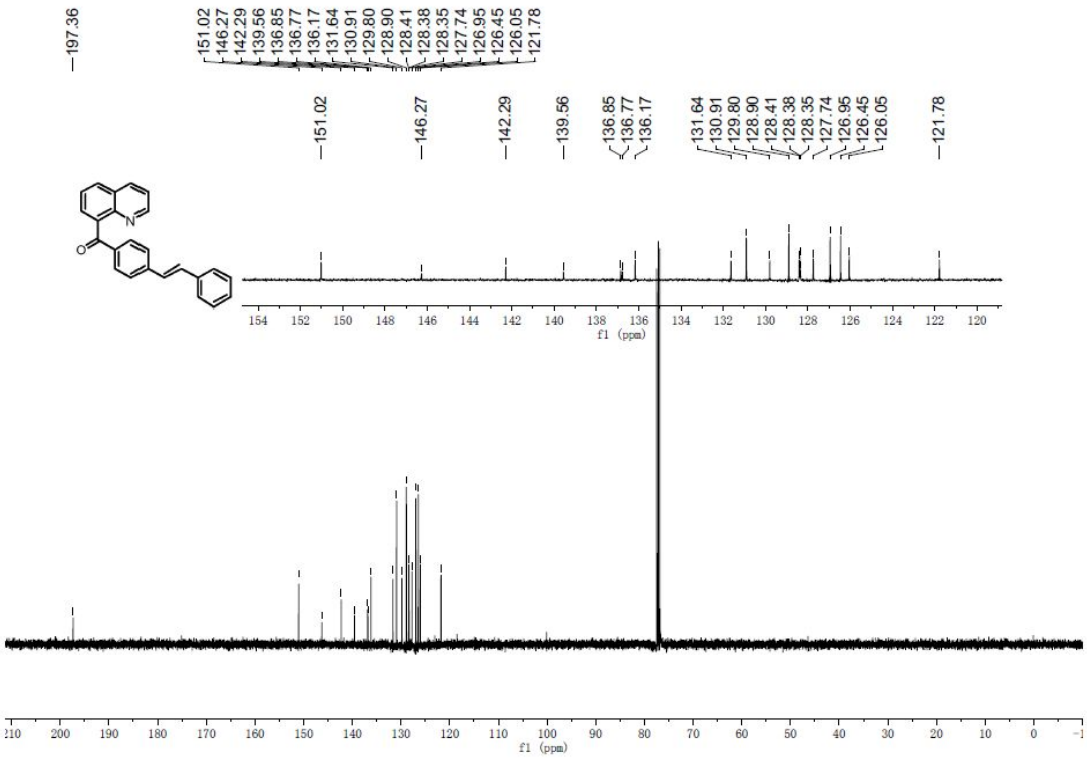
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ma



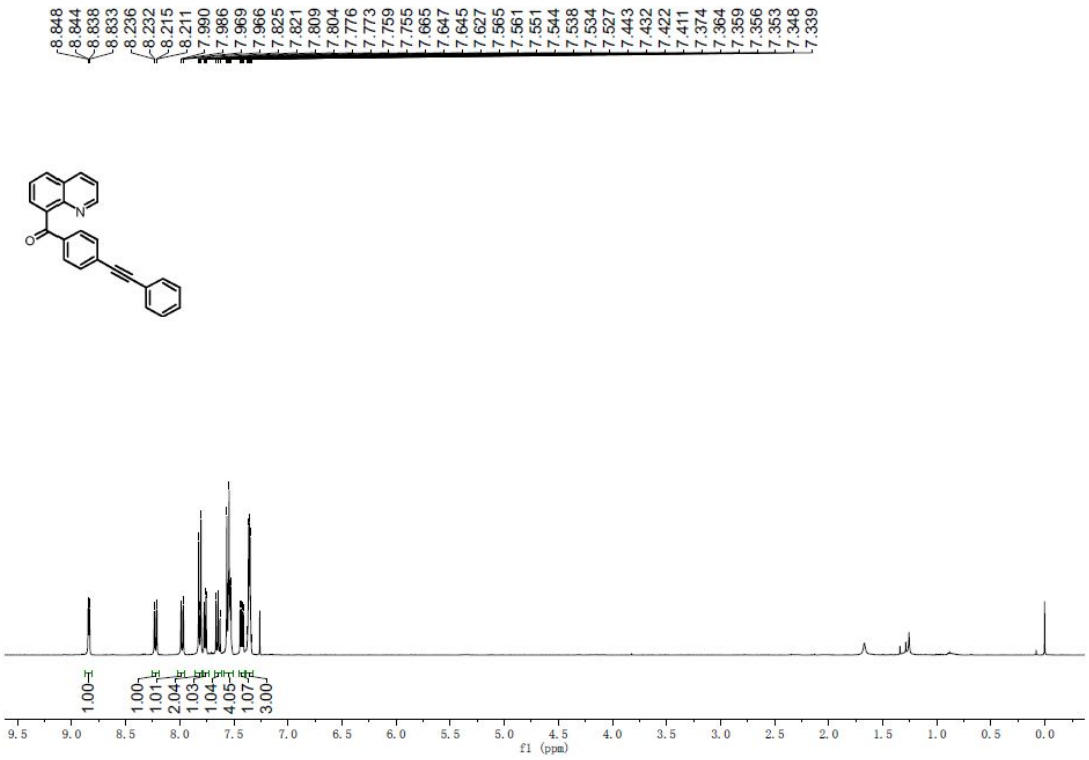
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ad'



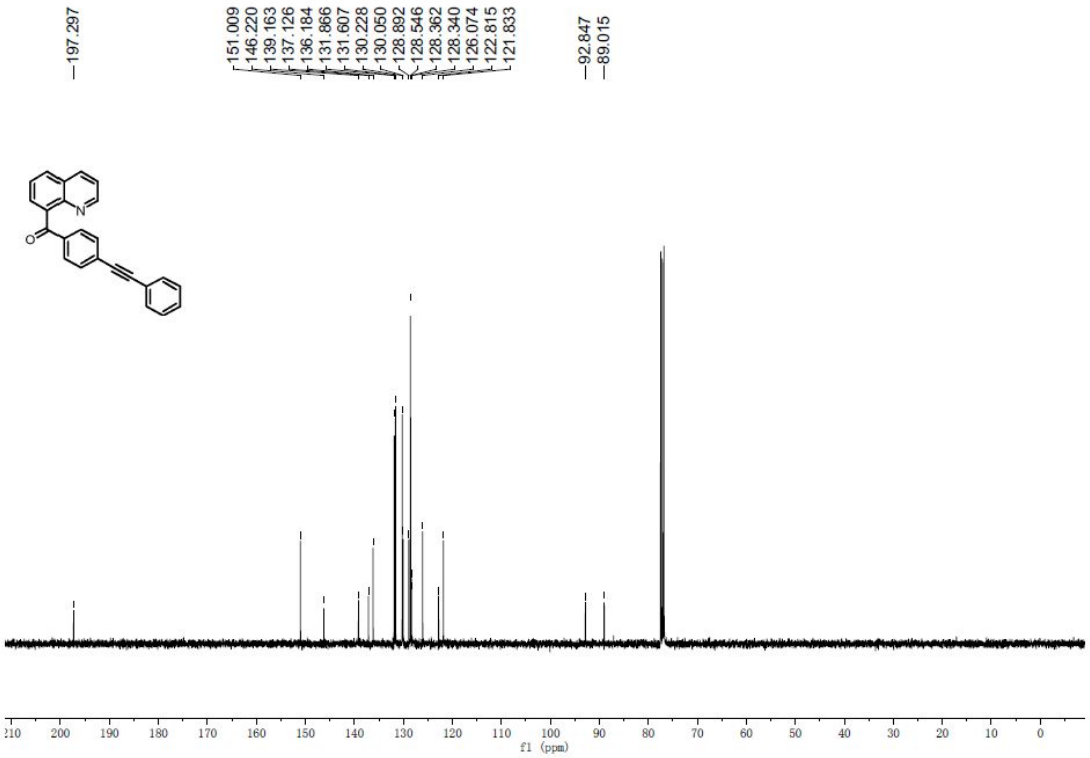
^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ad'



^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 3ad''

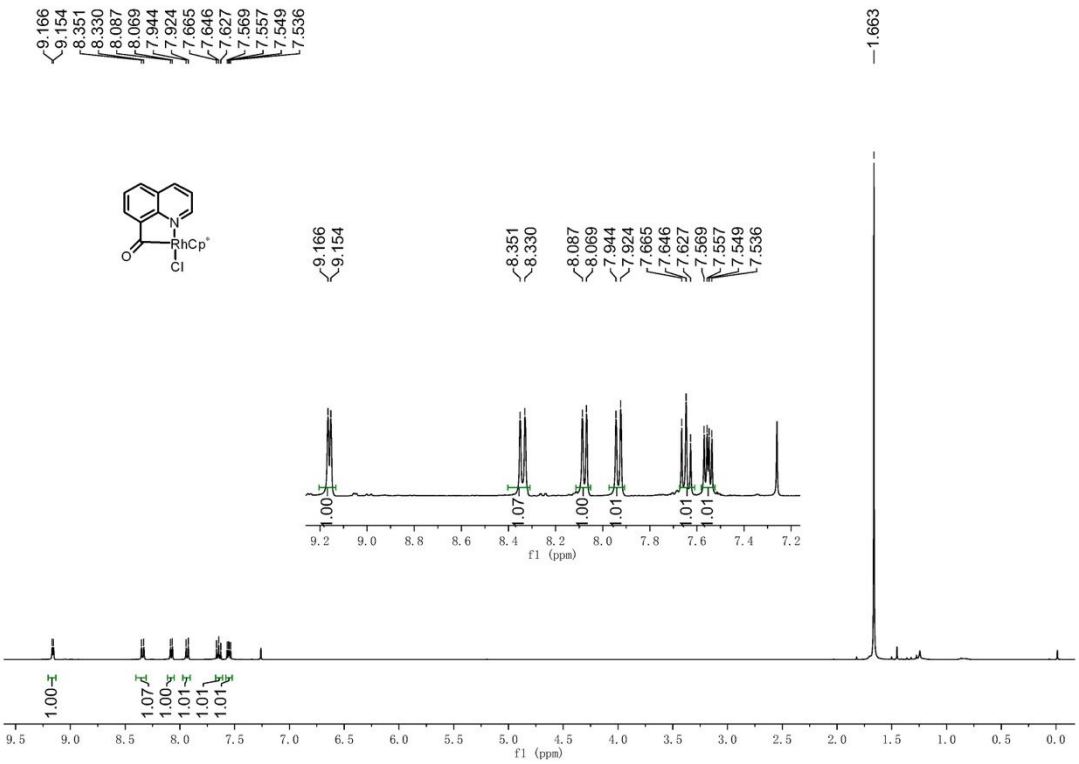
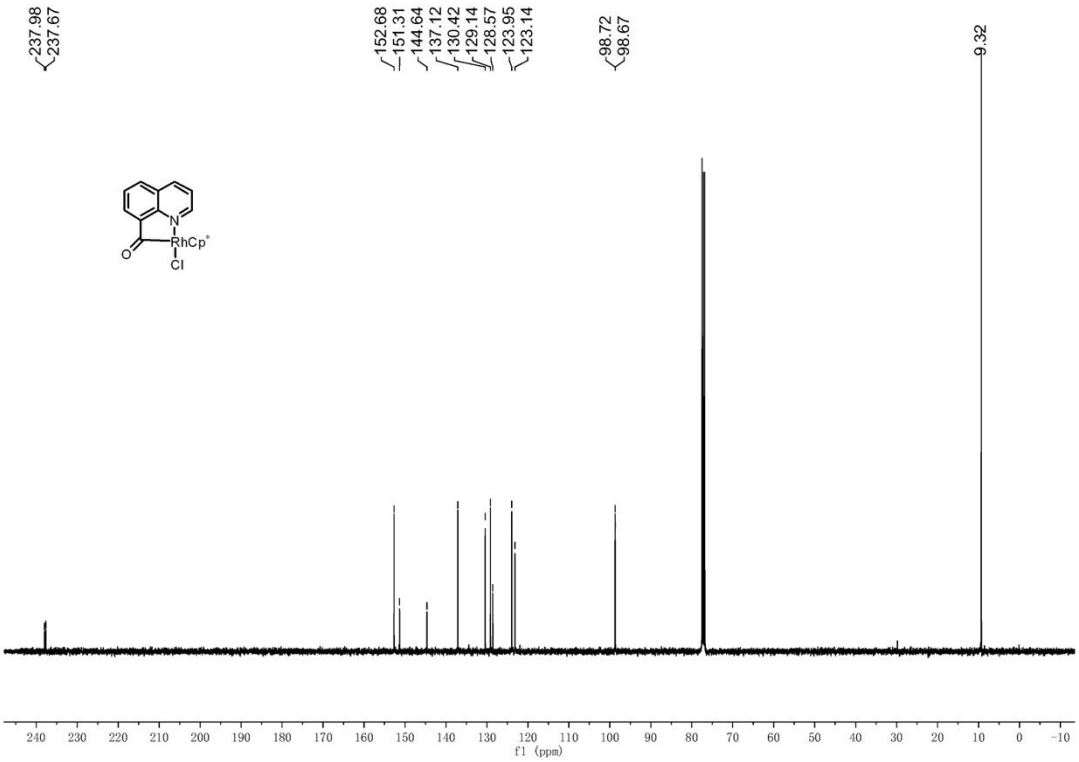


^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 3ad''



(3) NMR spectra of 1a-Rh-Int.

^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ºC) of 1a-Rh-Int



^{13}C NMR spectrum (100 MHz, $CDCl_3$, 23 ºC) of 1a-Rh-Int