Supporting Information

Redox-Neutral Palladium-Catalyzed C-H Functionalization to Form Isoindolinones with Carboxylic Acids or Anhydrides as Readily Available Starting Materials

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Table of Contents

Materials and Methods.....S2

Preparation of Substrates.....S3

Palladium-Catalyzed C-H Functionalization to Form Isoindolinones..... S4

Deuteration and Competition Experiments.....S22

^{1}H and ^{13}C NMR Spectra.....S24

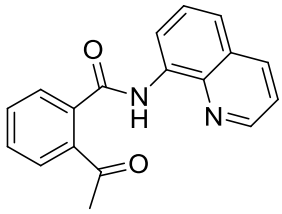
Materials and Methods

General. All reactions dealing with air- and moisture-sensitive compounds were carried out in dry reaction vessels under a nitrogen atmosphere. ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded on Agilent 600 MHz NMR spectrometer. ^{1}H and ^{13}C NMR spectra are reported in parts per million (ppm) downfield from an internal standard, tetramethylsilane (0 ppm) and $CHCl_3$ (77.0 ppm), respectively. ESI high-resolution mass spectra (HRMS) were recorded on a Waters SYNPAT G2. Melting points were determined using a capillary melting point apparatus and are uncorrected.

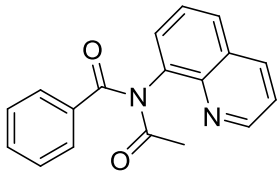
Materials. Unless otherwise noted, materials were purchased from commercial suppliers and were used as received. Anhydrous toluene was distilled over CaH_2 and stored under Ar.

Preparation of Substrates

All carboxamides were synthesized by the reactions between the corresponding acyl chlorides or acids and aminoquinolines according to the literature procedures.[1] Below are summaried characterization data for newly synthesized carboxamides. ^{1}H and ^{13}C NMR spectra data for the rest of the carboxamides showed good agreement with the literature data.



2-Acetyl-N-(quinolin-8-yl)benzamide (6): White solid; Mp = 91–92 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.80–8.75 (m, 1H), 8.07–7.99 (m, 2H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.58–7.51 (m, 2H), 7.40 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.14 (d, *J* = 8.2 Hz, 1H), 7.04 (t, *J* = 8.0 Hz, 1H), 6.03 (d, *J* = 7.7 Hz, 1H), 2.15 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.7, 150.6, 147.6, 138.9, 138.7, 136.2, 134.6, 130.2, 128.4, 127.6, 126.9, 126.0, 122.1, 121.5, 117.7, 109.9, 95.6, 29.4; **HRMS** (ESI): Calcd for $C_{18}H_{14}N_2O_2$ $[M + Na]^+$ 313.0953, found 313.0959.

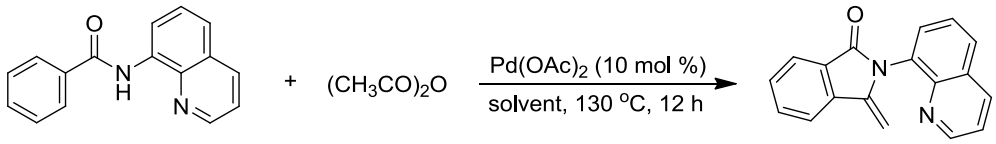


N-Acetyl-N-(quinolin-8-yl)benzamide (7): White solid; Mp = 85–87 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.96–8.93 (m, 1H), 8.13 (d, *J* = 8.3 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.65 (d, *J* = 8.3 Hz, 2H), 7.56 (d, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.42 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.30 (dd, *J* = 10.8, 4.2 Hz, 1H), 7.18 (t, *J* = 7.7 Hz, 2H), 2.53 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 174.3, 173.2, 150.8, 143.8, 137.3, 136.1, 135.7, 131.4, 130.0, 129.1, 128.7, 128.5, 127.8, 126.1, 121.8, 25.7; **HRMS** (ESI): Calcd for $C_{18}H_{14}N_2O_2$ $[M + Na]^+$313.0953, found 313.0958.

[1] Grigorjeva, L.; Daugulis, O. *Org. Lett.* **2014**, *16*, 4684.

Palladium-Catalyzed C-H Functionalization to Form Isoindolinones

Table S1. Screening of Different Solvents[a]



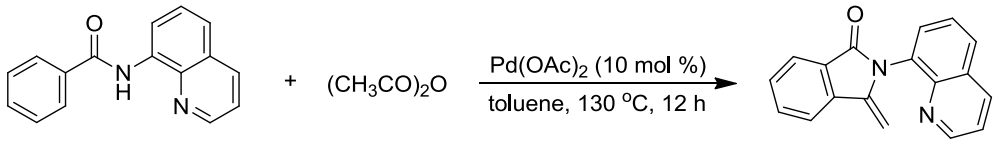
1a **2a** **3aa**

entry	solvent	yield (%)[b]
1	toluene	17
2	MeCN	trace
3	dioxane	0
4	DMF	0
5	DMSO	0
6	DCE	trace

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (1 equiv), $Pd(OAc)_2$ (10 mol %), solvent (2 mL), 130 °C, 12 h.

[b] Determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard.

Table S2. Screening of the Amount of Acetic Anhydride 2a[a]



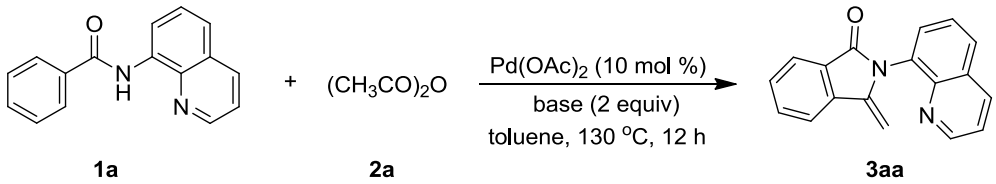
1a **2a** **3aa**

entry	**2a** (x equiv)	yield (%)[b]
1	1	17
2	2	59
3	3	64
4	5	87
5	5	99[c]

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (x equiv), $Pd(OAc)_2$ (10 mol %), toluene (2 mL), 130 °C, 12 h.

[b] Determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. [c] Reaction was run for 24 h.

Table S3. Screening of Different Bases[a]

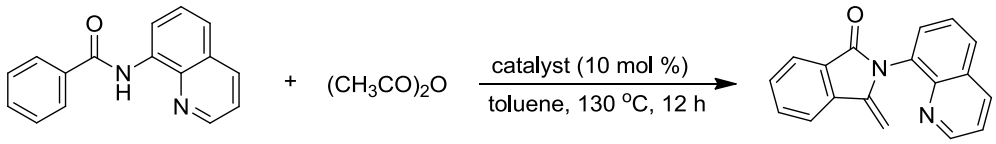


1a **2a** **3aa**

entry	base	yield (%)[b]
1	none	59
2	NaOAc	17
3	K_2CO_3	trace
4	K_3PO_4	trace
5	$NaHCO_3$	14
6	*t*BuOK	trace

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2 equiv), $Pd(OAc)_2$ (10 mol %), base (2 equiv), toluene (2 mL), 130 °C, 12 h. [b] Determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard.

Table S4. Screening of Different Catalyst[a]

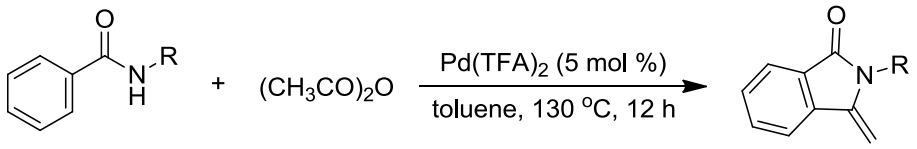


1a **2a** **3aa**

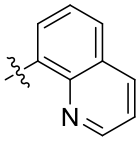
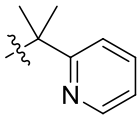
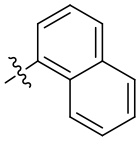
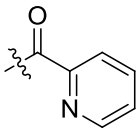
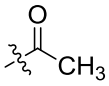
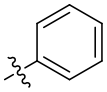
entry	catalyst	yield (%)[b]
1	$Pd(OAc)_2$	59
2	$Pd(MeCN)_2Cl_2$	86
3	$Pd(TFA)_2$	99
4	$Pd(TFA)_2$	99 (99)[c]
5	$Pd(TFA)_2$	49[d]
6	$Pd_2(dba)_3$	0
7	$Pd(PPh_3)_4$	0
8	$Cp^*Rh(CH_3CN)_2][SbF_6]_2$	0[e]
9	$[RuCl_2(p\text{-cymene})]_2$	0[e]
10	$AuCl_3$	0
11	$FeCl_3$	0
12	$Zn(OAc)_2$	0

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (2 equiv), catalyst (10 mol %), toluene (2mL), 130 °C, 12 h. [b] Determined by ^{1}H NMR spectroscopy using 1,1,2,2-tetrachloroethane as an internal standard. Value given in the parenthesis refers to isolated yield. [c] $Pd(TFA)_2$ (5 mol %). [d] Reaction was run at 110 °C. [e] Catalyst (5 mol %).

Table S5. The Effect of Substituents on Nitrogen Atom



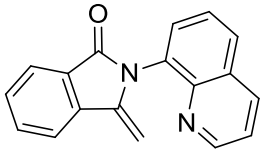
1 **2a** (2 equiv) **3**

			
99%	82%	0	0
			
0	0	0	0

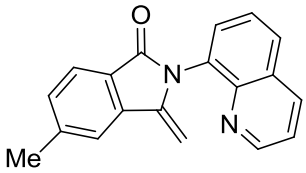
A General Procedure

For reactions carried with anhydrieds: A 10 mL of Schlenk tube equipped with a stirrer bar was charged with carboxamide (0.2 mmol) and $Pd(TFA)_2$ (5 mol %) under Ar. Then, the Schlenk tube was quickly evacuated and refilled with Ar for three times, followed by addition of toluene (2 mL) and anhydride (2 equiv). The Schlenk tube was sealed with a Teflon screwcap and the reaction mixture was stirred at 130 ℃ for 12 h. Upon cooling to room temperature, the reaction mixture was diluted with 10 mL of ethyl acetate, filtered through a pad of silica gel, followed by washing the pad of the silica gel with ethyl acetate (20 mL). Subsequently, the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the isoindolinones.

For reactions carried with carboxylic acids: A 10 mL of Schlenk tube equipped with a stirrer bar was charged with carboxamide (0.2 mmol), carboxylic acid (2 equiv), and $Pd(TFA)_2$ (10 mol %) under Ar. Then, the Schlenk tube was quickly evacuated and refilled with Ar for three times, followed by addition of toluene (2 mL) and pivalic anhydride (2 equiv). Then, the Schlenk tube was sealed with a Teflon screwcap and the reaction mixture was stirred at 130 ℃ for 12 h. Upon cooling to room temperature, the reaction mixture was diluted with 10 mL of ethyl acetate, filtered through a pad of silica gel, followed by washing the pad of the silica gel with ethyl acetate (20 mL). Subsequently, the filtrate was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel to afford the isoindolinones.

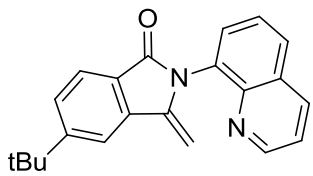


3-Methylene-2-(quinolin-8-yl)isoindolin-1-one (3aa): White solid (99% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 183–184 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 9.00–8.81 (m, 1H), 8.24 (d, *J* = 8.3 Hz, 1H), 7.97 (t, *J* = 8.6 Hz, 2H), 7.79 (dd, *J* = 17.3, 7.4 Hz, 2H), 7.71–7.63 (m, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.44 (dd, *J* = 8.3, 4.1 Hz, 1H), 5.19 (d, *J* = 1.8 Hz, 1H), 4.41 (d, *J* = 1.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.4, 151.1, 144.8, 144.1, 136.7, 136.2, 132.6, 132.1, 130.9, 129.6, 129.5, 129.5, 129.3, 126.2, 123.7, 121.8, 120.3, 90.2; **HRMS** (ESI): Calcd for $C_{18}H_{12}N_2O$ $[M + H]^+$ 273.1028, found 273.1031.

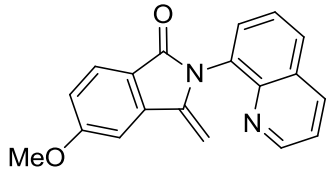


5-Methyl-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (3ba): Yellow solid; (99% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 185–186 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (dd, *J* = 4.0, 1.5 Hz, 1H), 8.23 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.95 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.86 (d, *J* = 7.7 Hz, 1H), 7.76 (dd, *J* = 7.2, 1.0 Hz, 1H), 7.67 (t, *J* = 7.7 Hz, 1H), 7.59 (s, 1H), 7.43 (dd, *J* = 8.3, 4.1 Hz, 1H), 7.39 (d, *J* = 7.7 Hz, 1H), 5.14 (d, *J* = 2.0 Hz, 1H), 4.36 (d, *J* = 1.9 Hz, 1H), 2.53 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.5, 151.1, 144.8, 144.2, 142.8, 137.1, 136.2, 132.8, 130.9, 130.6, 129.5, 129.2, 127.1, 126.2, 123.5, 121.7, 120.6, 89.7, 22.1; **HRMS** (ESI): Calcd for

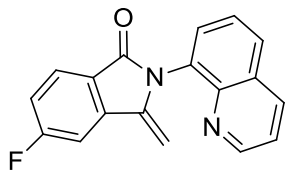
$C_{19}H_{14}N_2O$ [M + H]$^+$ 287.1184, found 287.1185.



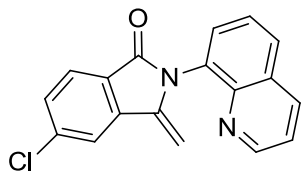
5-(Tert-butyl)-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3ca**): Yellow solid; (84% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 215–216 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.90 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.23 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.96 (d, *J* = 8.2 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.81 (s, 1H), 7.76 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.71 – 7.66 (m, 1H), 7.63 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.43 (dd, *J* = 8.3, 4.1 Hz, 1H), 5.19 (d, *J* = 2.1 Hz, 1H), 4.37 (d, *J* = 2.0 Hz, 1H), 1.42 (s, 9H); **^{13}C NMR** (150 MHz,$CDCl_3$): δ 167.5, 156.1, 151.1, 144.9, 144.4, 136.7, 136.2, 132.7, 130.9, 129.5, 129.2, 127.2, 127.0, 126.3, 123.4, 121.7, 117.0, 89.6, 35.5, 31.4; **HRMS** (ESI): Calcd for $C_{22}H_{20}N_2O$ [M + H]$^+$ 329.1654, found 329.1655.



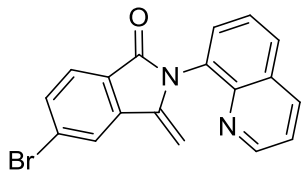
5-Methoxy-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3da**): Yellow solid; (85% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 179–180 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.90 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.23 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.94 (d, *J* = 7.9 Hz, 1H), 7.88 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 6.9 Hz, 1H), 7.67 (t, *J* = 7.7 Hz, 1H), 7.42 (dd, *J* = 8.3, 4.1 Hz, 1H), 7.25 (d, *J* = 1.9 Hz, 1H), 7.10 (dd, *J* = 8.4, 2.1 Hz, 1H), 5.13 (d, *J* = 2.0 Hz, 1H), 4.37 (d, *J* = 2.0 Hz, 1H), 3.93 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.3, 163.4, 151.1, 144.9, 144.0, 138.9, 136.2, 132.8, 130.9, 129.5, 129.2, 126.1, 125.2, 122.3, 121.7, 116.5, 104.6, 89.8, 55.8; **HRMS** (ESI): Calcd for $C_{19}H_{14}N_2O_2$ [M + Na]$^+$ 325.0953, found 325.0952.



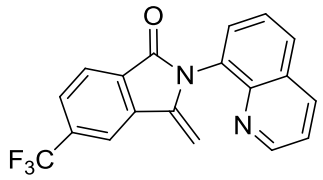
5-Fluoro-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3ea**): White solid; (90% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 214–215 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.90 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.24 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.99–7.94 (m, 2H), 7.76 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.71 – 7.66 (m, 1H), 7.45 (dt, *J* = 8.2, 3.3 Hz, 2H), 7.29–7.27 (m, 1H), 5.16 (d, *J* = 2.3 Hz, 1H), 4.45 (d *J* = 2.3 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 166.5, 164.8 (d, $^1J_{C\text{-}F}$ = 250.1 Hz), 151.2, 144.7, 143.2 (d, $^6J_{C\text{-}F}$ = 3.6 Hz), 139.1 (d, $^4J_{C\text{-}F}$ = 10.4 Hz), 136.2, 132.3, 130.8, 129.5, 129.5 126.3, 125.9 (d, $^5J_{C\text{-}F}$ = 9.8 Hz), 125.5 (d, $^7J_{C\text{-}F}$ = 2.0 Hz), 121.9, 117.3 (d, $^3J_{C\text{-}F}$ = 23.7 Hz), 107.4 (d, $^2J_{C\text{-}F}$ = 24.5 Hz), 91.3; **HRMS** (ESI): Calcd for $C_{18}H_{11}FN_2O$ [M + H]$^+$ 291.0934, found 291.0931.



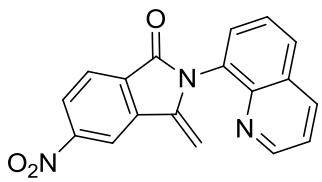
5-Chloro-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3fa**): Yellow solid; (80% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 248–249 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (d, *J* = 4.0 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 7.5 Hz, 2H), 7.69 (t, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.45 (dd, *J* = 8.3, 4.1 Hz, 1H), 5.18 (d, *J* = 2.1 Hz, 1H), 4.45 (d, *J* = 2.1 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 166.5, 151.2, 144.6, 143.0, 138.6, 138.2, 136.4, 132.2, 130.8, 130.0, 129.5, 129.5, 127.8, 126.3, 125.0, 121.9, 120.7, 91.4; **HRMS** (ESI): Calcd for $C_{18}H_{11}ClN_2O$ $[M + Na]^+$ 329.0458, found 329.0458.



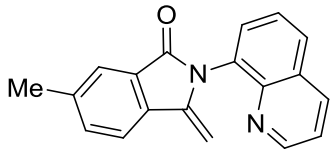
5-Bromo-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3ga**): Yellow solid; (91% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 230–231 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (d, *J* = 2.8 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 7.98 (d, *J* = 8.2 Hz, 1H), 7.94 (s, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 7.1 Hz, 1H), 7.70 (dd, *J* = 17.5, 8.7 Hz, 2H), 7.45 (dd, *J* = 8.2, 4.0 Hz, 1H), 5.18 (s, 1H), 4.46 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 166.5, 151.2, 144.6, 142.9, 141.9, 138.3, 136.3, 132.8, 132.2, 130.8, 129.5, 128.2, 126.9, 126.2, 125.2, 123.6, 121.9, 91.4; **HRMS** (ESI): Calcd for $C_{18}H_{11}BrN_2O$ $[M + H]^+$ 351.0133, found 351.0131.



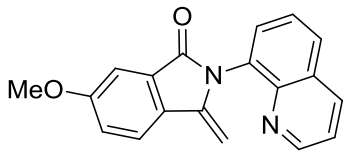
3-Methylene-2-(quinolin-8-yl)-5-(trifluoromethyl)isoindolin-1-one (3ha): White solid; (80% yield, eluent = petroleum ether/EtOAc (5:1)); Mp = 210–211 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (dd, *J* = 4.1, 1.5 Hz, 1H), 8.26 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.10 (d, *J* = 7.9 Hz, 1H), 8.06 (s, 1H), 7.99 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.85 (d, *J* = 7.9 Hz, 1H), 7.82–7.76 (m, 1H), 7.70 (t, *J* = 7.7 Hz, 1H), 7.46 (dd, *J* = 8.3, 4.1 Hz, 1H), 5.29 (d, *J* = 2.4 Hz, 1H), 4.53 (d, *J* = 2.4 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 166.1, 151.2, 144.5, 143.0, 136.9, 136.3, 134.2 (q, $^{2}J_{C\text{-}F}$ = 32.4 Hz), 132.2, 132.0, 130.8, 129.6, 129.5, 126.5 (q, $^{3}J_{C\text{-}F}$ = 3.6 Hz), 126.2, 124.7 (q, $^{1}J_{C\text{-}F}$ = 271.2 Hz), 124.3, 121.9, 117.7 (q, $^{3}J_{C\text{-}F}$ = 3.9 Hz), 92.0; **HRMS** (ESI): Calcd for $C_{19}H_{11}F_3N_2O$ $[M + Na]^+$ 363.0721, found 363.0721.



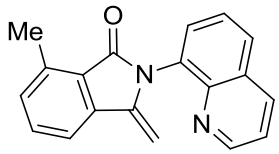
3-Methylene-5-nitro-2-(quinolin-8-yl)isoindolin-1-one (**3ia**): Following the general procedure but the reaction was run using **2a** (7 equiv) and $Pd(TFA)_2$ (20 mol %); Yellow solid; (61% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 208–209 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (dd, *J* = 4.1, 1.3 Hz, 1H), 8.65 (s, 1H), 8.45 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.27 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.14 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 6.6 Hz, 1H), 7.72 (t, *J* = 7.7 Hz, 1H), 7.48 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.37 (d, *J* = 2.6 Hz, 1H), 4.61 (d, *J* = 2.6 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 165.2, 151.3, 150.7, 144.3, 142.4, 137.5, 136.3, 134.0, 131.7, 130.6, 129.9, 129.5, 126.3, 124.9, 124.7, 122.1, 116.1, 93.3; **HRMS** (ESI): Calcd for $C_{18}H_{11}N_3O_3$ $[M + H]^+$ 318.0879, found 318.0800.



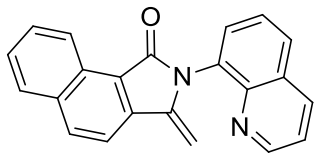
6-Methyl-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3ja**): White solid; (60% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 145–146 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (dd, *J* = 4.1, 1.5 Hz, 1H), 8.23 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.94 (dd, *J* = 8.2, 0.8 Hz, 1H), 7.82–7.72 (m, 2H), 7.67 (t, *J* = 7.8 Hz, 2H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.42 (dd, *J* = 8.3, 4.1 Hz, 1H), 5.12 (d, *J* = 2.0 Hz, 1H), 4.35 (d, *J* = 1.9 Hz, 1H), 2.51 (s, 3H); **^{13}C NMR (150 MHz, $CDCl_3$)**: δ 167.6, 151.1, 144.8, 144.1, 139.9, 136.2, 134.3, 133.1, 132.7, 130.9, 129.7, 129.5, 129.2, 126.2, 123.8, 121.7, 120.1, 89.4, 21.6; **HRMS** (ESI): Calcd for $C_{19}H_{14}N_2O$ $[M + H]^+$ 287.1184, found 287.1185.



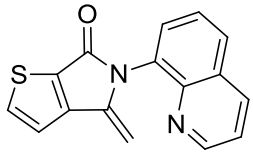
6-Methoxy-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3ka**): Following the general procedure but the reaction was run using $Pd(TFA)_2$ (10 mol %); Yellow solid; (81% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 210–211 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (dd, *J* = 4.1, 1.5 Hz, 1H), 8.23 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.75 (dd, *J* = 7.2, 1.0 Hz, 1H), 7.67 (t, *J* = 7.6 Hz, 2H), 7.42 (dd, *J* = 9.2, 3.2 Hz, 2H), 7.19 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.05 (d, *J* = 2.1 Hz, 1H), 4.31 (d, *J* = 2.0 Hz, 1H), 3.91 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.4, 161.3, 151.2, 144.8, 143.8, 136.2, 132.6, 131.1, 130.9, 129.5, 129.5, 129.3, 126.2, 121.8, 121.6, 120.7, 106.1, 89.1, 55.8; **HRMS** (ESI): Calcd for $C_{19}H_{14}N_2O_2$ $[M + Na]^+$ 325.0953, found 325.0954.



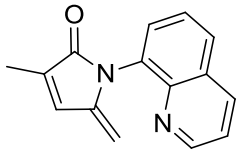
7-Methyl-3-methylene-2-(quinolin-8-yl)isoindolin-1-one (**3la**): Yellow solid; (90% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 184–185 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.94 (dd, *J* = 4.1, 1.3 Hz, 1H), 8.24 (d, *J* = 8.3 Hz, 1H), 7.95 (d, *J* = 8.2 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.68 (t, *J* = 7.7 Hz, 1H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.44 (dd, *J* = 8.3, 4.1 Hz, 1H), 7.31 (d, *J* = 7.6 Hz, 1H), 5.13 (d, *J* = 1.9 Hz, 1H), 4.34 (d, *J* = 1.9 Hz, 1H), 2.77 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.2, 151.2, 144.9, 143.9, 137.8, 137.2, 136.3, 132.7, 131.6, 131.6, 131.0, 129.5, 129.2, 126.6, 126.3, 121.7, 117.7, 89.2, 17.5; **HRMS** (ESI): Calcd for $C_{19}H_{14}N_2O$ $[M + H]^+$ 287.1184, found 287.1184.



3-Methylene-2-(quinolin-8-yl)-2,3-dihydro-1H-benzo[e]isoindol-1-one (**3ma**): Yellow solid; (80% yield, eluent = petroleum ether/EtOAc (2:1)); Mp = 170–171 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 9.18 (d, *J* = 8.3 Hz, 1H), 8.94–8.86 (m, 1H), 8.25 (d, *J* = 8.3 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.99–7.93 (m, 2H), 7.87–7.81 (m, 2H), 7.73–7.65 (m, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.44 (dd, *J* = 8.3, 4.1 Hz, 1H), 5.32 (d, *J* = 1.7 Hz, 1H), 4.56 (d, *J* = 1.8 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.3, 151.2, 145.1, 144.2, 136.3, 136.2, 134.2, 132.9, 132.7, 131.1, 129.5, 129.2, 129.1, 128.3, 128.2, 126.9, 126.4, 124.7, 123.5, 121.8, 117.4, 91.8; **HRMS** (ESI): Calcd for $C_{22}H_{14}N_2O$ $[M + Na]^+$ 345.1004, found 345.1004.

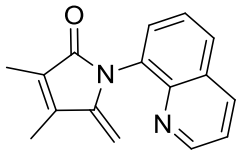


4-Methylene-5-(quinolin-8-yl)-4H-thieno[2,3-c]pyrrol-6(5H)-one (**3na**): Following the general procedure but the reaction was run using $Pd(TFA)_2$ (10 mol %); Yellow solid; (21% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 198–200 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.95 (d, *J* = 3.6 Hz, 1H), 8.25 (d, *J* = 7.9 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.77 (d, *J* = 7.4 Hz, 1H), 7.71 (d, *J* = 4.8 Hz, 1H), 7.68 (t, *J* = 7.5 Hz, 1H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.30 (d, *J* = 4.8 Hz, 1H), 5.01 (d, *J* = 1.8 Hz, 1H), 4.40 (d, *J* = 1.7 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 162.7, 151.2, 148.3, 145.0, 141.5, 136.3, 135.4, 132.6, 131.2, 129.5, 129.3, 126.2, 121.8, 119.2, 110.0, 92.5; **HRMS** (ESI): Calcd for $C_{16}H_{10}N_2OS$ $[M + Na]^+$ 301.0412, found 301.0412.

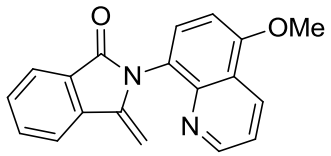


3-Methyl-5-methylene-1-(quinolin-8-yl)-1H-pyrrol-2(5H)-one (**3oa**): Following the general

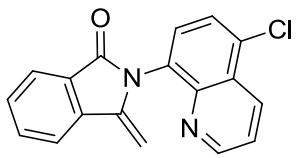
procedure but the reaction was run using **2a** (5 equiv) and $Pd(TFA)_2$ (10 mol %); Yellow solid; (66% yield, eluent = petroleum ether/EtOAc (6:1)); Mp = 190–191 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.93 (d, *J* = 2.7 Hz, 1H), 8.21 (d, *J* = 7.0 Hz, 1H), 7.91 (d, *J* = 8.7 Hz, 1H), 7.69–7.61 (m, 2H), 7.43 (dd, *J* = 8.3, 4.1 Hz, 1H), 6.93 (s, 1H), 4.72 (s, 1H), 4.36 (s, 1H), 2.12 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.1, 151.1, 146.3, 145.0, 136.2, 134.5, 132.6, 131.8, 130. 8, 129.5, 129.0, 126.2, 121.6, 95.6, 11.1; **HRMS** (ESI): Calcd for $C_{15}H_{12}N_2O$ $[M + H]^+$ 237.1028, found 237.1029.



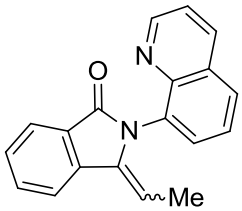
3,4-Dimethyl-5-methylene-1-(quinolin-8-yl)-1H-pyrrol-2(5H)-one (**3pa**): Yellow solid; (57% yield, eluent = petroleum ether/EtOAc (6:1)); Mp = 127–128 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.93 (d, *J* = 4.1 Hz, 1H), 8.20 (d, *J* = 8.3 Hz, 1H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.67–7.59 (m, 2H), 7.41 (dd, *J* = 8.2, 4.1 Hz, 1H), 4.77 (s, 1H), 4.29 (s, 1H), 2.15 (s, 3H), 2.02 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 171.0, 151.0, 148.4, 145.1, 139.8, 136.2, 133.0, 130.8, 129.5, 129.1, 128.8, 126.2, 121.6, 92.2, 10.1, 8.9; **HRMS** (ESI): Calcd for $C_{16}H_{14}N_2O$ $[M + Na]^+$ 273.1004, found 273.1010.



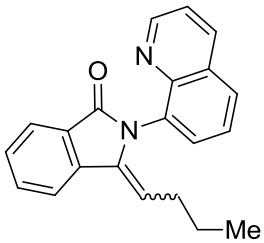
2-(5-Methoxyquinolin-8-yl)-3-methyleneisoindolin-1-one (**3qa**): Yellow solid; (90% yield, eluent = petroleum ether/EtOAc (2:1)); Mp = 185–186 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.87 (dd, *J* = 4.1, 1.1 Hz, 1H), 8.63 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 7.6 Hz, 1H), 7.68–7.62 (m, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.40 (dd, *J* = 8.5, 4.2 Hz, 1H), 6.97 (d, *J* = 8.2 Hz, 1H), 5.16 (d, *J* = 1.5 Hz, 1H), 4.42 (d, *J* = 1.5 Hz, 1H), 4.07 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.7, 155.9, 151.3, 145.3, 144.3, 136.6, 132.0, 131.1, 131.0, 129.5, 129.4, 124.7, 123.6, 121.7, 120.8, 120.3, 103.8, 90.1, 56.0; **HRMS** (ESI): Calcd for $C_{19}H_{14}N_2O_2$ $[M + Na]^+$ 325.0953, found 325.0954.



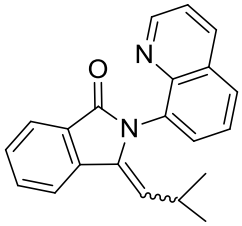
2-(5-Chloroquinolin-8-yl)-3-methyleneisoindolin-1-one (**3ra**): White solid; (96% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 179–180 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.93 (dd, *J* = 4.0, 1.3 Hz, 1H), 8.64 (dd, *J* = 8.6, 1.3 Hz, 1H), 7.97 (d, *J* = 7.5 Hz, 1H), 7.81–7.77 (m, 2H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.55 (dd, *J* = 8.6, 4.1 Hz, 1H), 5.19 (d, *J* = 2.2 Hz, 1H), 4.41 (d, *J* = 2.1 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.4, 151.7, 145.3, 143.9, 136.6, 133.3, 132.6, 132.3, 131.8, 130.7, 129.7, 129.2, 127.5, 126.4, 123.7, 122.6, 120.3, 90.2; **HRMS** (ESI): Calcd for $C_{18}H_{11}ClN_2O$ $[M + Na]^+$ 329.0458, found 329.0459.



3-Ethylidene-2-(quinolin-8-yl)isoindolin-1-one (**3ab**): Approx. 1.3:1 mixture of *E* and *Z* isomers; Yellow solid; (92% yield, eluent = petroleum ether/EtOAc (3:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): *E* isomer: δ 8.91–8.89 (m, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 7.5 Hz, 1H), 7.95 (t, *J* = 8.4 Hz, 2H), 7.75–7.46 (m, 4H), 7.44–7.41 (m, 1H), 5.05 (q, *J* = 7.6 Hz, 1H), 2.11 (d, *J* = 7.6 Hz, 3H); *Z* isomer: δ 8.91–8.89 (m, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 7.95 (t, *J* = 8.4 Hz, 2H), 7.80 (d, *J* = 7.1 Hz, 1H), 7.74–7.46 (m, 4H), 7.44–7.41 (m, 1H), 5.73 (q, *J* = 7.5 Hz, 1H), 1.03 (d, *J* = 7.6 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.3, 166.8, 151.2, 145.5, 145.1, 138.4, 138.3, 136.3, 136.2, 136.0, 135.2, 134.2, 133.0, 131.9, 131.8, 131.4, 130.7, 130.5, 129.5, 129.3, 129.1, 128.6, 128.3, 128.1, 126.3, 126.2, 123.9, 123.8, 123.6, 123.5, 121.7, 119.1, 107.6, 103.3, 12.9, 11.4; **HRMS** (ESI): Calcd for $C_{19}H_{14}N_2O$ $[M + Na]^+$ 309.1004, found 309.1003.

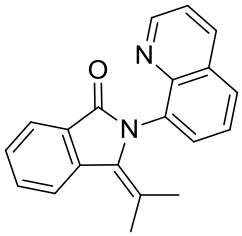


3-Butylidene-2-(quinolin-8-yl)isoindolin-1-one (**3ac**): Approx. 1:1 mixture of *E* and *Z* isomers; Yellow solid; (93% yield, eluent = petroleum ether/EtOAc (3:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): *E* isomer: δ 8.91–8.89 (m, 1H), 8.23 (d, *J* = 8.3 Hz, 1H), 8.02 (d, *J* = 7.5 Hz, 1H), 7.96–7.94 (m, 2H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.68–7.66 (m, 2H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.43–7.42(m, 1H), 4.96 (t, *J* = 7.7 Hz, 1H), 2.57–2.54(m, 2H), 1.39–1.37 (m, 1H), 1.09–1.07 (m, 1H), 0.89 (t, *J* = 7.4 Hz, 3H); *Z* isomer: δ 8.91–8.89 (m, 1H), 8.23 (d, *J* = 8.3 Hz, 1H), 7.96–7.94 (m, 2H), 7.80 (d, *J* = 7.2 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.68–7.66 (m, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.43–7.41 (m, 1H), 5.63 (t, *J* = 7.9 Hz, 1H), 1.46–1.44 (m, 2H), 1.21–1.19 (m, 1H), 1.03–1.02 (m, 1H), 0.46 (t, *J* = 7.3 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.4, 166.7, 151.2, 151.1, 145.5, 145.1, 138.5, 137.5, 136.2, 136.1, 136.0, 135.5, 135.3, 134.2, 133.0, 131.9, 131.8, 131.3, 130.7, 130.5, 129.5, 129.2, 129.1, 128.6, 128.3, 128.1, 126.3, 126.1, 123.9, 123.8, 123.6, 123.5, 121.8, 121.7, 119.2, 113.9, 109.4, 77.2, 77.0, 76.8, 29.2, 27.6, 23.1, 22.8, 13.8, 13.4; **HRMS** (ESI): Calcd for $C_{21}H_{18}N_2O$ $[M + Na]^+$ 337.1317, found 337.1321.

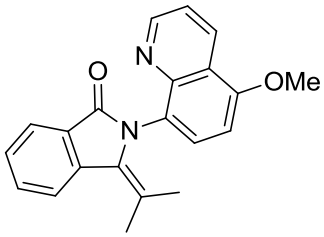


3-(2-Methylpropylidene)-2-(quinolin-8-yl)isoindolin-1-one (**3ad**): Approx. 1.3:1 mixture of *E*

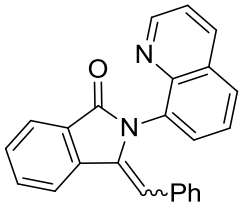
and *Z* isomers; Yellow solid; (90% yield, eluent = petroleum ether/EtOAc (3:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): *E* isomer: δ 8.91–8.90 (m, 1H), 8.24–8.23 (m, 1H), 8.02 (d, *J* = 7.5 Hz, 1H), 7.97–7.91 (m, 2H), 7.74–7.72 (m, 1H), 7.68–7.66 (m, 2H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.42 (dd, *J* = 8.2, 4.1 Hz, 1H), 4.82 (d, *J* = 9.6 Hz, 1H), 3.35–7.32 (m, 1H), 1.09 (d, *J* = 6.7 Hz, 3H), 1.00 (d, *J* = 6.6 Hz, 3H); Z isomer: δ 8.91–8.90 (m, 1H), 8.24–8.22 (m, 1H), 7.96–7.92 (m, 2H), 7.82–7.80 (m, 1H), 7.74–7.72 (m, 1H), 7.67 (dt, *J* = 13.5, 7.6 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.42 (dd, *J* = 8.2, 4.1 Hz, 1H), 5.43 (d, *J* = 10.6 Hz, 1H), 1.61–1.59 (m, 1H), 0.74 (d, *J* = 6.6 Hz, 3H), 0.38 (d, *J* = 6.5 Hz, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.4, 166.7, 151.1, 151.0, 145.4, 145.0, 135.8, 135.4, 133.6, 132.9, 132.0, 131.8, 131.4, 130.6, 130.5, 129.5, 129.3, 129.2, 128.6, 128.3, 126.3, 126.2, 123.9, 123.6, 123.4, 121.8, 121.7, 121.4, 119.2, 26.6, 25.1, 23.3, 23.2, 23.1, 22.8; **HRMS** (ESI): Calcd for $C_{21}H_{18}N_2O$ $[M + Na]^+$ 337.1317, found 337.1320.



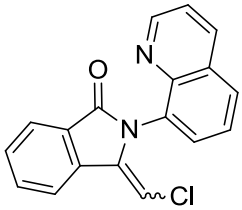
3-(Propan-2-ylidene)-2-(quinolin-8-yl)isoindolin-1-one (**3ae**): Yellow solid; (90% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 174–175 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.91 (d, *J* = 2.9 Hz, 1H), 8.20 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 7.5 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.69 (d, *J* = 7.0 Hz, 1H), 7.62 (t, *J* = 7.7 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.41 (dd, *J* = 8.3, 4.1 Hz, 1H), 2.26 (s, 3H), 1.19 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.1, 151.1, 145.5, 137.8, 136.9, 136.2, 132.8, 131.9, 130.3, 129.4, 129.2, 128.6, 127.4, 126.2, 124.0, 123.9, 121.6, 119.1, 23.5, 22.7; **HRMS** (ESI): Calcd for $C_{20}H_{16}N_2O$ $[M + Na]^+$ 323.1160, found 323.1160.



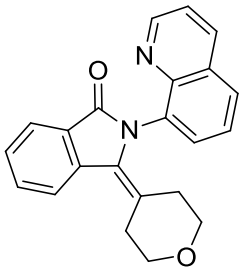
2-(5-Methoxyquinolin-8-yl)-3-(propan-2-ylidene)isoindolin-1-one (**3qe**): White solid; (68% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 230–231 ^oC; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.90 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.62 (dd, *J* = 8.5, 1.6 Hz, 1H), 7.98 (d, *J* = 7.3 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.64–7.59 (m, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.40 (dd, *J* = 8.5, 4.2 Hz, 1H), 6.93 (d, *J* = 8.2 Hz, 1H), 4.05 (s, 3H), 2.27 (s, 3H), 1.26 (s, 3H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.4, 155.4, 151.3, 145.9, 137.7, 132.7, 131.8, 131.1, 130.3, 129.4, 129.1, 127.3, 123.9 (two signals are overlapped), 121.4, 120.7, 119.0, 103.8, 55.9, 23.7, 22.4; **HRMS** (ESI): Calcd for $C_{21}H_{18}N_2O_2$ $[M + H]^+$ 331.1447, found 331.1448.



3-Benzylidene-2-(quinolin-8-yl)isoindolin-1-one (**3af**): Following the general procedure but the reaction was run using $Pd(TFA)_2$ (10 mol %); Yellow solid; (For reactions carried with anhydrieds: Approx. 1:1 mixture of *E* and *Z* isomers; 50% yield; For reactions carried with carboxylic acids: Approx. 1:1 mixture of *E* and *Z* isomers; 83% yield; eluent = petroleum ether/EtOAc (3:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): *E* isomer: δ 8.94 (d, *J* = 2.9 Hz, 1H), 8.26 (d, *J* = 8.2 Hz, 1H), 8.00–7.96 (m, 2H), 7.86 (d, *J* = 6.8 Hz, 2H), 7.74–7.66 (m, 6H), 7.53–7.27 (m, 2H), 6.68 (t, *J* = 7.2 Hz, 1H), 6.02 (s, 1H); *Z* isomer: δ 8.88 (d, *J* = 3.4 Hz, 1H), 8.02 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 7.8 Hz, 2H), 7.59–7.57 (m, 2H), 7.54–7.28 (m, 4H), 6.82 (s, 1H), 6.68 (t, *J* = 7.2 Hz, 1H), 6.58 (d, *J* = 7.4 Hz, 2H), 6.53 (t, *J* = 7.6 Hz, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168. 2, 167.0, 151.1, 150.0, 144.8, 138.8, 138.7, 136.5, 136.1, 135.5, 135.3, 133.5, 132.7, 132.3, 131.7, 131.5, 130.4, 130.3, 129.6, 129.4, 129.3, 129.1, 128.9, 128.4, 128.3, 128.2, 128.1, 127.5, 126.4, 126.3, 126.0, 125.9, 123.9, 123.8, 123.2, 121.8, 121.2, 119.6, 112.1, 107.4; **HRMS** (ESI): Calcd for $C_{24}H_{16}N_2O$ $[M + Na]^+$ 371.1160, found 371.1161.

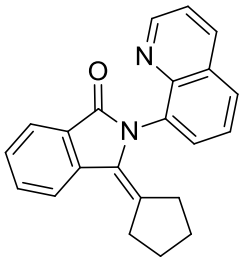


3-(Chloromethylene)-2-(quinolin-8-yl)isoindolin-1-one (**3ag**): Following the general procedure but the reaction was run using anhydride **2g** (5 equiv); Approx. 3:1 mixture of *E* and *Z* isomers; Yellow solid; (86% yield, eluent = petroleum ether/EtOAc (5:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): *E* isomer: δ 8.92–8.89 (m, 1H), 8.48 (d, *J* = 7.9 Hz, 1H), 8.25 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 7.5 Hz, 1H), 7.98 (d, *J* = 8.8 Hz, 1H), 7.77 (d, *J* = 7.1 Hz, 1H), 7.75–7.61 (m, 3H), 7.46 (dd, *J* = 8.3, 4.1 Hz, 1H), 5.58 (s, 1H); *Z* isomer: δ 8.88 (d, *J* = 2.8 Hz, 1H), 8.23 (d, *J* = 8.6 Hz, 1H), 7.96 (d, *J* = 6.9 Hz, 2H), 7.82 (d, *J* = 7.4 Hz, 1H), 7.75–7.61 (m, 3H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.44–7.41 (m, 1H), 6.26 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 166.4, 151.4, 144.6, 139.0, 136.3, 134.5, 132.6, 132.0, 131.1, 130.1, 129.8, 129.6, 129.3, 126.3, 126.0, 124.8, 124.1, 122.0, 121.7, 119.2, 102.3; **HRMS** (ESI): Calcd for $C_{18}H_{11}ClN_2O$ $[M + Na]^+$ 329.0458, found 329.0461.

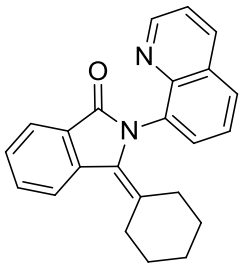


3-(Dihydro-2H-pyran-4(3H)-ylidene)-2-(quinolin-8-yl)isoindolin-1-one (**3ah**): Yellow solid;

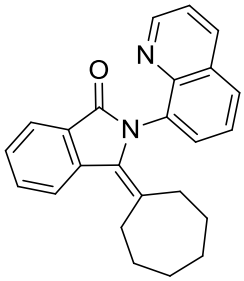
(89% yield, eluent = petroleum ether/EtOAc (2:1)); Mp = 180–181 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.91 (dd, *J* = 4.1, 1.6 Hz, 1H), 8.22 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.99 (t, *J* = 7.4 Hz, 2H), 7.91 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.74 (dd, *J* = 7.3, 1.2 Hz, 1H), 7.67 – 7.58 (m, 2H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 3.85–3.81 (m, 1H), 3.76–3.72 (m, 1H), 3.23–3.19 (m, 1H), 3.08–3.04 (m, 1H), 2.97–2.93 (m, 1H), 2.90–2.86 (m, 1H), 1.82–1.78 (m, 1H), 1.64–1.61 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.1, 151.0, 144.9, 137.7, 136.9, 136.3, 132.2, 132.0, 130.0, 129.8, 129.3, 128.8, 128.0, 126.4, 124.2, 123.8, 121.9, 121.8, 68.1, 67.2, 31.8, 30.8; **HRMS** (ESI): Calcd for $C_{22}H_{18}N_2O_2$ $[M + H]^+$ 343.1447, found 343.1451.



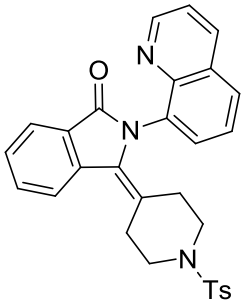
3-Cyclopentylidene-2-(quinolin-8-yl)isoindolin-1-one (**3ai**): Yellow solid; (90% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 179–180 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.93 (d, *J* = 2.6 Hz, 1H), 8.23 (d, *J* = 8.2 Hz, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.82 (d, *J* = 7.9 Hz, 1H), 7.74 (d, *J* = 7.1 Hz, 1H), 7.66–7.63 (m, 2H), 7.48 (t, *J* = 7.4 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.1 Hz, 1H), 2.88 (s, 2H), 1.77–1.74 (m, 1H), 1.67–1.64 (m, 2H), 1.39–1.37 (m, 1H), 1.29–1.27 (m, 1H), 1.22–1.20 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.0, 151.1, 145.7, 137.6, 136.4, 135.8, 131.9, 131.0, 129.6, 129.4, 129.2, 129.1, 129.0, 127.4, 126.1, 123.9, 123.3, 121.7, 33.5, 32.1, 26.7, 26.3; **HRMS** (ESI): Calcd for $C_{22}H_{18}N_2O$ $[M + Na]^+$ 349.1317, found 349.1320.



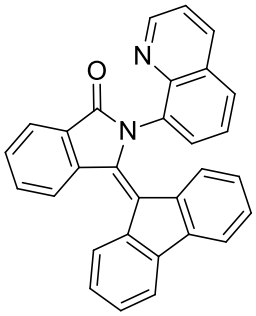
3-Cyclohexylidene-2-(quinolin-8-yl)isoindolin-1-one (**3aj**): Yellow solid; (90% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 182–183 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.98 (s, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 8.03 (d, *J* = 8.1 Hz, 1H), 7.97 (d, *J* = 7.3 Hz, 1H), 7.91 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.65 (t, *J* = 7.7 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.48–7.46 (m, 2H), 2.88–2.85 (m, 2H), 1.74–1.70 (m, 2H), 1.64–1.62 (m, 1H), 1.56–1.54 (m, 1H), 1.45–1.41 (m, 2H), 1.09–1.07 (m, 1H), 0.89–0.86 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.3, 150.4, 144.1, 138.2, 137.3, 136.9, 132.1, 130.8, 130.0, 129.6, 129.3, 129.2, 128.4, 127.5, 126.7, 124.0, 123.8, 121.8, 31.7, 31.2, 27.7, 26.8, 25.8; **HRMS** (ESI): Calcd for $C_{23}H_{20}N_2O$ $[M + Na]^+$ 363.1473, found 363.1473.



3-Cycloheptylidene-2-(quinolin-8-yl)isoindolin-1-one (**3ak**): Yellow solid; (80% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 175–176 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.93 (d, *J* = 2.7 Hz, 1H), 8.22 (d, *J* = 8.2 Hz, 1H), 7.99 (d, *J* = 7.5 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.65–7.60 (m, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.43 (dd, *J* = 8.2, 4.1 Hz, 1H), 2.93–2.81 (m, 2H), 1.87–1.78 (m, 3H), 1.69–1.64 (m, 1H), 1.53–1.50 (m, 2H), 1.34–1.26 (m, 2H), 1.12–1.03 (m, 1H), 0.92 (d, *J* = 6.5 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.3, 150.9, 145.1, 137.6, 137.3, 136.4, 133.0, 132.1, 130.2, 129.8, 129.4, 129.2, 128.5, 127.9, 127.4, 126.3, 124.0, 121.7, 33.0, 32.3, 29.3, 27.8, 26.9, 26.8; **HRMS** (ESI): Calcd for $C_{24}H_{22}N_2O$ $[M + Na]^+$ 377.1630, found 377.1631.

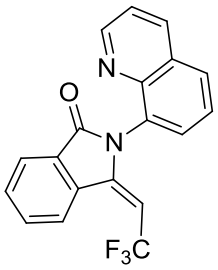


2-(quinolin-8-yl)-3-(1-tosylpiperidin-4-ylidene)isoindolin-1-one (**3al**): Yellow solid; (43% yield, eluent = petroleum ether/EtOAc (1:1)); Mp = 215–216 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.65 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.18 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.94 (d, *J* = 7.4 Hz, 1H), 7.92–7.86 (m, 2H), 7.66 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.62–7.56 (m, 2H), 7.48–7.44 (m, 3H), 7.31 (dd, *J* = 8.3, 4.1 Hz, 1H), 7.25 (d, *J* = 8.2 Hz, 2H), 3.35–3.30 (m, 1H), 3.16–3.11 (m, 1H), 2.97–2.88 (m, 2H), 2.64–2.62 (m, 1H), 2.40 (s, 3H), 1.99–1.94 (m, 1H), 1.85–1.80 (m, 1H), 1.68–1.64 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.0, 150.8, 144.6, 143.6, 137.4, 136.4, 136.3, 132.7, 132.7, 132.4, 130.1, 129.7, 129.6, 129.2, 128.9, 128.3, 127.5, 126.5, 124.2, 123.8, 121.8, 119.9, 46.5, 45.5, 30.0, 28.9, 21.5; **HRMS** (ESI): Calcd for $C_{29}H_{25}N_3O_3S$ $[M + Na]^+$ 518.1514, found 518.1514.

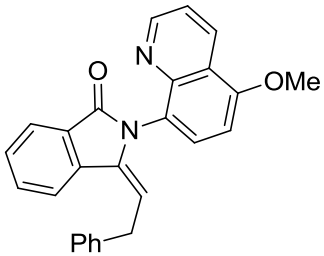


3-(9H-Fluoren-9-ylidene)-2-(quinolin-8-yl)isoindolin-1-one (**3am**): Yellow solid; (62% yield,

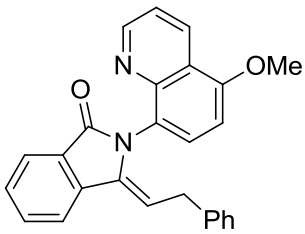
eluent = petroleum ether/EtOAc (2:1)); Mp = 150–152 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.99 (s, 1H), 8.60 (d, *J* = 7.9 Hz, 1H), 8.45 (d, *J* = 7.5 Hz, 1H), 8.17 (d, *J* = 8.3 Hz, 1H), 8.02 (d, *J* = 7.5 Hz, 1H), 7.73–7.63 (m, 3H), 7.59 (t, *J* = 7.4 Hz, 2H), 7.50 (d, *J* = 7.5 Hz, 1H), 7.44 (dd, *J* = 8.0, 3.9 Hz, 1H), 7.32 (dt, *J* = 17.0, 7.8 Hz, 3H), 6.94 (t, *J* = 7.4 Hz, 1H), 6.81 (d, *J* = 7.9 Hz, 1H), 6.41 (t, *J* = 7.6 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.3, 150.7, 140.5, 139.0, 137.8, 137.6, 136.3, 136.0, 132.5, 130.3, 129.2, 128.3, 128.1, 127.7, 126.9, 126.5, 126.0, 125.9, 125.8, 124.7, 124.6, 121.5, 119.9, 119.1; **HRMS** (ESI): Calcd for $C_{30}H_{18}N_2O$ [M + H]$^+$ 423.1497, found 423.1494.



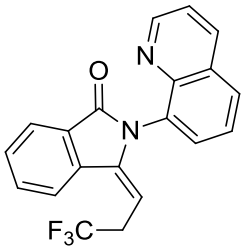
(*E*)-2-(Quinolin-8-yl)-3-(2,2,2-trifluoroethylidene)isoindolin-1-one (**3an**): Following the general procedure but the reaction was run using carboxylic acid **2o** (4 equiv) and $Pd(TFA)_2$ (20 mol %); Yellow solid; (54% yield, eluent = petroleum ether/EtOAc (2:1)); Mp = 170–171 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (dd, *J* = 4.1, 1.4 Hz, 1H), 8.26 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 8.01 (t, *J* = 6.7 Hz, 2H), 7.77–7.68 (m, 4H), 7.46 (dd, *J* = 8.3, 4.1 Hz, 1H), 4.98 (q, *J* = 9.2 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.0, 151.5, 144.4, 136.5, 135.0, 133.1, 132.9 (q, $^{1}J_{C\text{-}F}$ = 231.8 Hz), 131.4, 131.2, 130.2, 130.1, 130.0, 129.6, 126.3, 125.0 (q, $^{3}J_{C\text{-}F}$ = 5.4 Hz), 124.1, 122.2, 97.1, 96.6 (q, $^{2}J_{C\text{-}F}$ = 38.6 Hz); **HRMS** (ESI): Calcd for $C_{19}H_{11}F_3N_2O$ [M + Na]$^+$ 363.0721, found 363.0720.



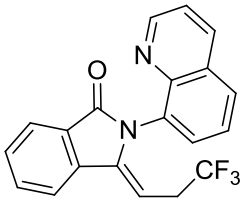
(*E*)-2-(5-Methoxyquinolin-8-yl)-3-(2-phenylethylidene)isoindolin-1-one (**3qo**): Yellow solid; (39% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 175–176 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.89 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.61 (dd, *J* = 8.5, 1.7 Hz, 1H), 8.05 (d, *J* = 7.6 Hz, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 8.2 Hz, 1H), 7.65–7.61 (m, 1H), 7.57 (t, *J* = 7.5 Hz, 1H), 7.39 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.26–7.15 (m, 5H), 6.94 (d, *J* = 8.2 Hz, 1H), 5.16 (t, *J* = 8.0 Hz, 1H), 4.04 (s, 3H), 4.00–3.93 (m, 2H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 167.0, 155.9, 151.3, 145.4, 139.7, 138.6, 135.7, 132.0, 131.4, 131.1, 130.8, 128.9, 128.5, 128.3, 126.3, 124.9, 124.0, 123.3, 121.8, 120.8, 111.3, 103.9, 55.9, 33.2; **HRMS** (ESI): Calcd for $C_{26}H_{20}N_2O_2$ [M + Na]$^+$ 415.1422, found 415.1422.



(*Z*)-2-(5-Methoxyquinolin-8-yl)-3-(2-phenylethylidene)isoindolin-1-one (**3qo'**): Yellow solid; (33% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 180–181 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.90 (dd, *J* = 4.1, 1.5 Hz, 1H), 8.61 (dd, *J* = 8.4, 1.5 Hz, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.72 (dd, *J* = 12.1, 8.0 Hz, 2H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.41 (dd, *J* = 8.5, 4.2 Hz, 1H), 7.16–7.09 (m, 3H), 6.92 (d, *J* = 8.2 Hz, 1H), 6.81 (d, *J* = 7.3 Hz, 2H), 5.76 (t, *J* = 7.8 Hz, 1H), 4.05 (s, 3H), 2.90 (dd, *J* = 16.5, 8.0 Hz, 1H), 2.68 (dd, *J* = 16.5, 7.6 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.7, 155.9, 151.5, 145.8, 140.1, 138.4, 135.8, 131.9, 131.2, 130.7, 128.5, 128.3, 128.3, 128.2, 127.2, 126.0, 123.6, 121.5, 120.9, 119.3, 107.3, 103.8, 55.9, 31.7. **HRMS** (ESI): Calcd for $C_{26}H_{20}N_2O_2$ $[M + Na]^+$ 415.1422, found 415.1422.

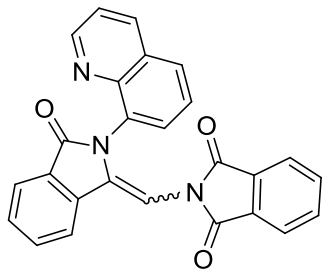


(*E*)-2-(Quinolin-8-yl)-3-(3,3,3-trifluoropropylidene)isoindolin-1-one (**3ap**): Following the general procedure but the reaction was run using carboxylic acid **2p** (4 equiv) and $Pd(TFA)_2$ (20 mol %); Yellow solid; (46% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 171–172 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.90 (d, *J* = 2.6 Hz, 1H), 8.27 (d, *J* = 8.3 Hz, 1H), 8.05 (d, *J* = 7.5 Hz, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.71 (t, *J* = 7.7 Hz, 2H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.46 (dd, *J* = 8.2, 4.1 Hz, 1H), 4.84 (t, *J* = 7.8 Hz, 1H), 3.53–3.46 (m, 1H), 3.34–3.29 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 166.7, 151.2, 144.6, 141.4, 136.5, 134.9, 132.4, 132.1, 131.4, 130.8, 129.8, 129.7, 129.6, 126.4, 124.8 (q, $^{1}J_{C\text{-}F}$ = 275.5 Hz), 124.4, 123.1, 121.9, 98.7 (q, $^{3}J_{C\text{-}F}$ = 3.9 Hz), 32.5 (q, $^{2}J_{C\text{-}F}$ = 30.6 Hz); **HRMS** (ESI): Calcd for $C_{20}H_{13}F_3N_2O$ $[M + Na]^+$ 377.0878, found 377.0886.

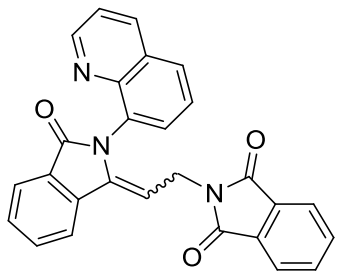


(*Z*)-2-(Quinolin-8-yl)-3-(3,3,3-trifluoropropylidene)isoindolin-1-one (**3ap'**): Following the general procedure but the reaction was run using carboxylic acid **2p** (4 equiv) and $Pd(TFA)_2$ (20 mol %); Yellow solid; (35% yield, eluent = petroleum ether/EtOAc (3:1)); Mp = 169–170 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.91 (d, *J* = 2.7 Hz, 1H), 8.27 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 8.2 Hz,

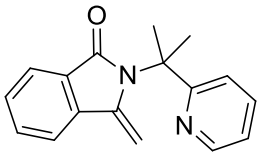
1H), 7.95 (d, J = 7.5 Hz, 1H), 7.83 (d, J = 7.2 Hz, 1H), 7.79 (d, J = 7.7 Hz, 1H), 7.72–7.66 (m, 2H), 7.57 (t, J = 7.5 Hz, 1H), 7.47 (dd, J = 8.2, 4.1 Hz, 1H), 5.52 (dd, J = 8.1, 7.0 Hz, 1H), 2.27–2.19 (m, 1H), 2.06–1.98 (m, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.4, 151.5, 145.0, 139.2, 137.8, 136.4, 134.0, 132.4, 131.1, 129.8, 129.4, 129.2, 128.2, 126.4, 126.3 (q, $^1J_{C\text{-}F}$ = 275.7 Hz), 123.8, 122.1, 119.7, 94.0 (q, $^3J_{C\text{-}F}$ = 4.0 Hz), 30.6 (q, $^2J_{C\text{-}F}$ = 30.2 Hz); **HRMS** (ESI): Calcd for $C_{20}H_{13}F_3N_2O$ $[M + Na]^+$ 377.0878, found 377.0886.



2-((3-Oxo-2-(quinolin-8-yl)isoindolin-1-ylidene)methyl)isoindoline-1,3-dione (**3aq**): Approx. 1:1.6 mixture of *E* and *Z* isomers; White solid; (76% yield, eluent = petroleum ether/EtOAc (3:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): *E* isomer: δ 8.96 (dd, J = 4.1, 1.4 Hz, 1H), 8.24 (dd, J = 8.3, 1.3 Hz, 1H), 8.02–7.96 (m, 2H), 7.79–7.74 (m, 3H), 7.56–7.52 (m, 4H), 7.46 (dd, J = 8.3, 4.2 Hz, 1H), 7.33–7.23 (m, 2H), 5.66 (s, 1H); *Z* isomer: δ 8.84 (dd, J = 4.1, 1.3 Hz, 1H), 7.93–7.88 (m, 3H), 7.70 (q, J = 7.6 Hz, 3H), 7.61 (t, J = 7.5 Hz, 1H), 7.56–7.52 (m, 4H), 7.35–7.22 (m, 2H), 6.30 (s, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.1, 166.8, 166.6, 151.4, 151.3, 144.5, 144.2, 140.6, 139.1, 136.4, 136.2, 135.2, 134.6, 134.0, 133.7, 132.7, 132.5, 132.2, 132.0, 131.9, 130.14, 129.7, 129.6, 128.6, 128.4, 128.2, 126.3, 125.5, 124.1, 124.0, 123.9, 122.7, 122.0, 121.7, 120.6, 99.8, 95.0; **HRMS** (ESI): Calcd for $C_{26}H_{15}N_3O_3$ $[M + Na]^+$ 440.1011, found 440.1014.



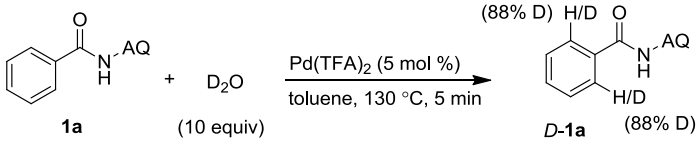
2-(2-(3-Oxo-2-(quinolin-8-yl)isoindolin-1-ylidene)ethyl)isoindoline-1,3-dione (**3ar**): Approx. 1:1 mixture of *E* and *Z* isomers; White solid; (49% yield, eluent = petroleum ether/EtOAc (3:1)); **^{1}H NMR** (600 MHz, $CDCl_3$): *E* isomer: δ 9.14 (dd, J = 4.2, 1.6 Hz, 1H), 8.56 (d, J = 7.9 Hz, 1H), 8.42 (dd, J = 8.3, 1.5 Hz, 1H), 8.16–8.11 (m, 2H), 8.01–7.78 (m, 7H), 7.72 (t, J = 7.4 Hz, 1H), 7.61 (dd, J = 8.3, 4.1 Hz, 1H), 5.16 (dd, J = 15.4, 8.6 Hz, 1H), 4.96 (dd, J = 15.4, 6.9 Hz, 1H), 3.70 (dd, J = 16.2, 5.4 Hz, 1H); *Z* isomer: δ 9.05 (dd, J = 4.1, 1.6 Hz, 1H), 8.46 (dd, J = 8.3, 1.5 Hz, 1H), 8.26–8.19 (m, 3H), 8.00–7.78 (m, 8H), 7.67 (dd, J = 8.3, 4.2 Hz, 1H), 5.74 (dd, J = 8.3, 5.4 Hz, 1H), 5.23 (dd, J = 8.4, 7.0 Hz, 1H), 3.89 (dd, J = 16.2, 8.3 Hz, 1H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.4, 167.8, 167.5, 167.0, 151.5, 151.2, 145.2, 144.8, 140.0, 137.9, 136.9, 136.3, 135.1, 134.3, 134.0, 132.4, 132.3, 132.2, 132.0, 131.9, 131.6 131.3, 130.6, 129.6, 129.5, 129.3, 129.1, 128.3, 126.5, 126.3, 124.3, 124.1, 123.8, 123.3, 123.2, 122.0, 121.8, 119.7, 105.4, 101.5, 35.1, 33.7; **HRMS** (ESI): Calcd for $C_{27}H_{17}N_3O_3$ $[M + Na]^+$ 454.1168, found 454.1172.



3-Methylene-2-(2-(pyridin-2-yl)propan-2-yl)isoindolin-1-one (**4**): White solid; (82% yield, eluent = petroleum ether/EtOAc (8:1)); Mp = 85–86 ^{o}C; **^{1}H NMR** (600 MHz, $CDCl_3$): δ 8.58 (d, 1H), 7.80 (d, *J* = 7.5 Hz, 1H), 7.60 (t, *J* = 8.0, 1.6 Hz, 1H), 7.53 (d, *J* = 4.2 Hz, 2H), 7.49–7.45 (m, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.16 (dd, *J* = 6.9, 5.4 Hz, 1H), 5.01 (d, *J* = 2.3 Hz, 1H), 4.09 (d, *J* = 2.3 Hz, 1H), 2.10 (s, 6H); **^{13}C NMR** (150 MHz, $CDCl_3$): δ 168.7, 165.4, 148.4, 141.2, 136.6, 133.7, 131.9, 129.6, 129.2, 122.9, 121.7, 120.9, 119.1, 94.1, 63.9, 28.4; **HRMS** (ESI): Calcd for $C_{17}H_{16}N_2O$ $[M + Na]^+$ 287.1160, found 287.1163.

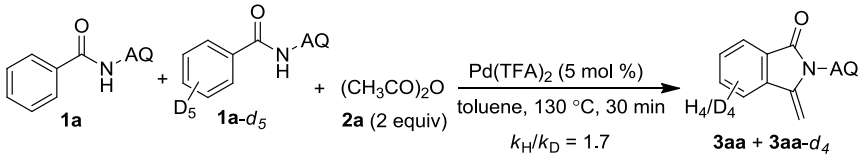
Deuteration and Competition Experiments

(A) H/D exchange reaction



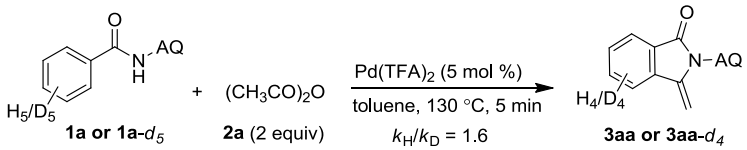
The reaction between **1a** (0.2 mmol) and D_2O (10 equiv) was carried out in the presence of $Pd(TFA)_2$ (5 mol%) with toluene (2 mL) as a solvent at 130 ^oC for 5 min. After standard workup and purification, a mixture of **1a** and *D*-**1a** was obtained. ^{1} H NMR analysis of the mixture showed 88% D was incorporated into the two *ortho* positions of the carboxyamide aryl ring (see the attached spectrum).

(B) Intermolecular competition reaction

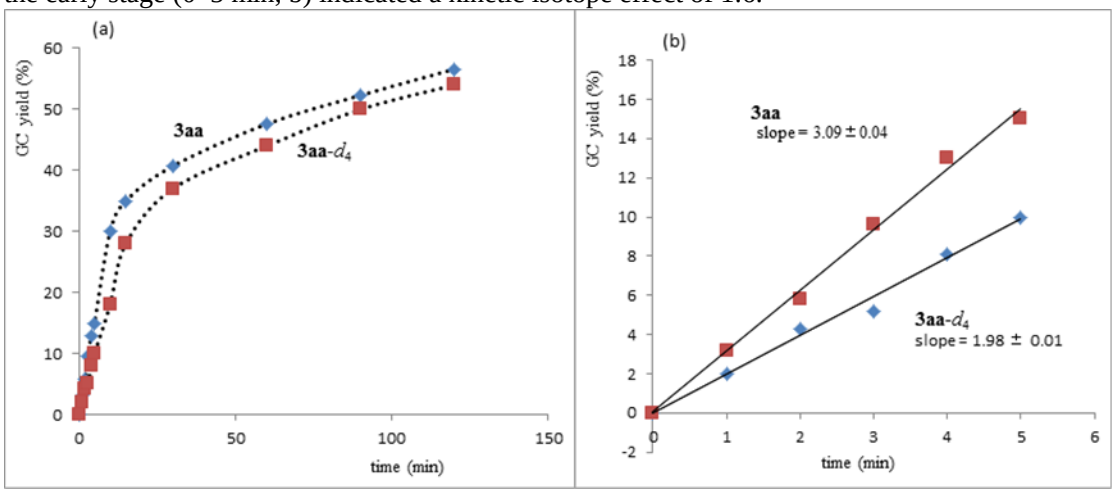


A mixture of **1a** and **1a**-d_5 (0.2 mmol each) was subjected to the standard reaction conditions for 30 min. After standard workup and purification, a mixture of **3aa** and **3aa**-d_4 was obtained**.** ^{1} H NMR analysis of the mixture showed a modest value of k_H/k_D = 1.7 (see the attached spectrum).

(C) Parallel reactions

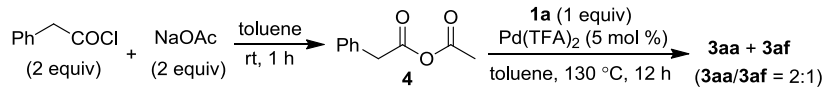


Parallel individual reactions of **1a** and **1a**-d_5 under the standard conditions were monitored by GC analysis of periodically taken aliquots (0–120 min, a). Comparison of the reaction progress in the early stage (0–5 min, b) indicated a kinetic isotope effect of 1.6.



(D) Selectivity investigation

(d) Selectivity investigation

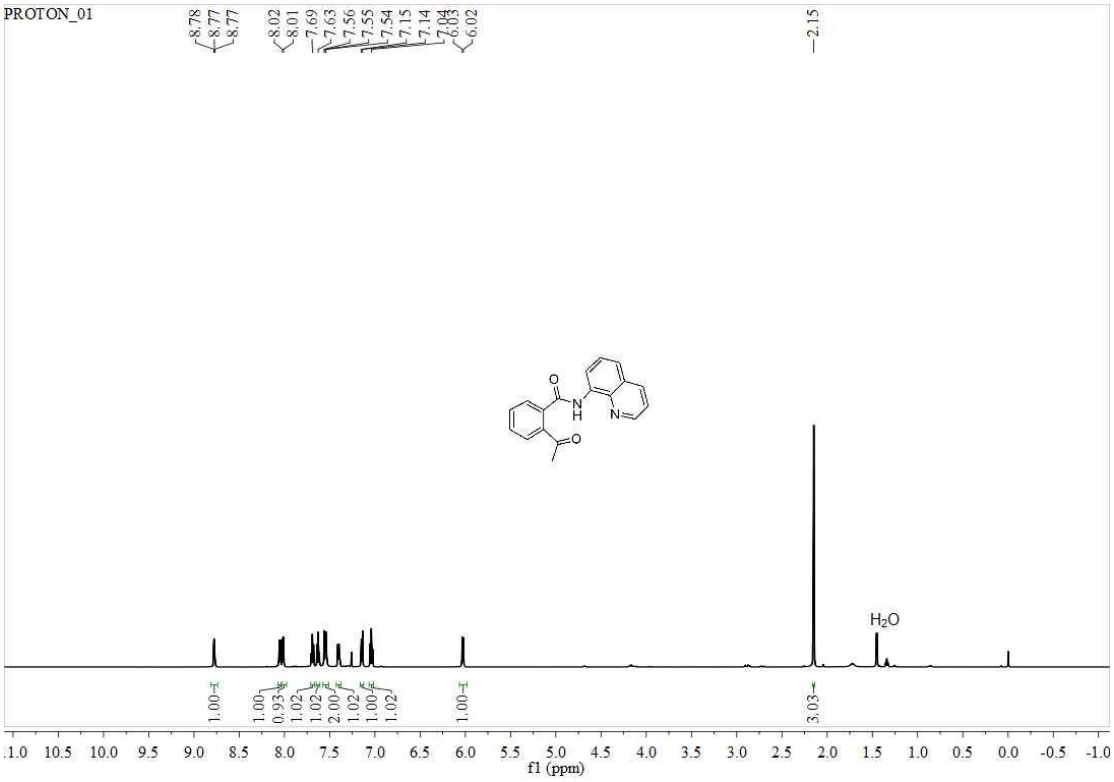


A 10 mL of Schlenk tube equipped with a stirrer bar was charged with phenylacetyl chloride

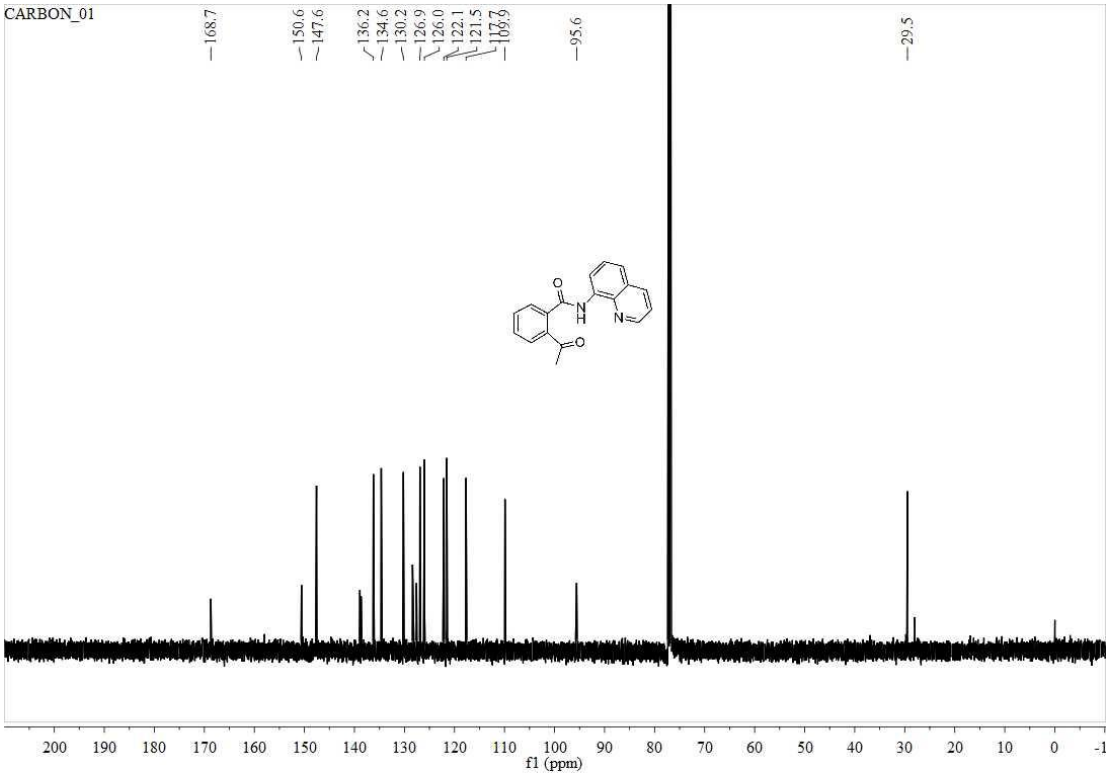
(0.4 mmol) and NaOAc (0.4 mmol). Then, the Schlenk tube was quickly evacuated and refilled with Ar for three times, followed by addition of toluene (1 mL). The reaction was run at room temperature for 1 h. Subsequently, **1a** (0.2 mmol) and $Pd(TFA)_2$ (0.01mmol) were added into the Schlenk tube under Ar. The Schlenk tube was sealed with a Teflon screwcap and the reaction mixture was stirred at 130 ^{o}C for 12h. ^{1}H NMR analysis of the mixture showed that the ratio of **3aa** and **3af** was 2:1.

^{1}H and ^{13}C NMR Spectra

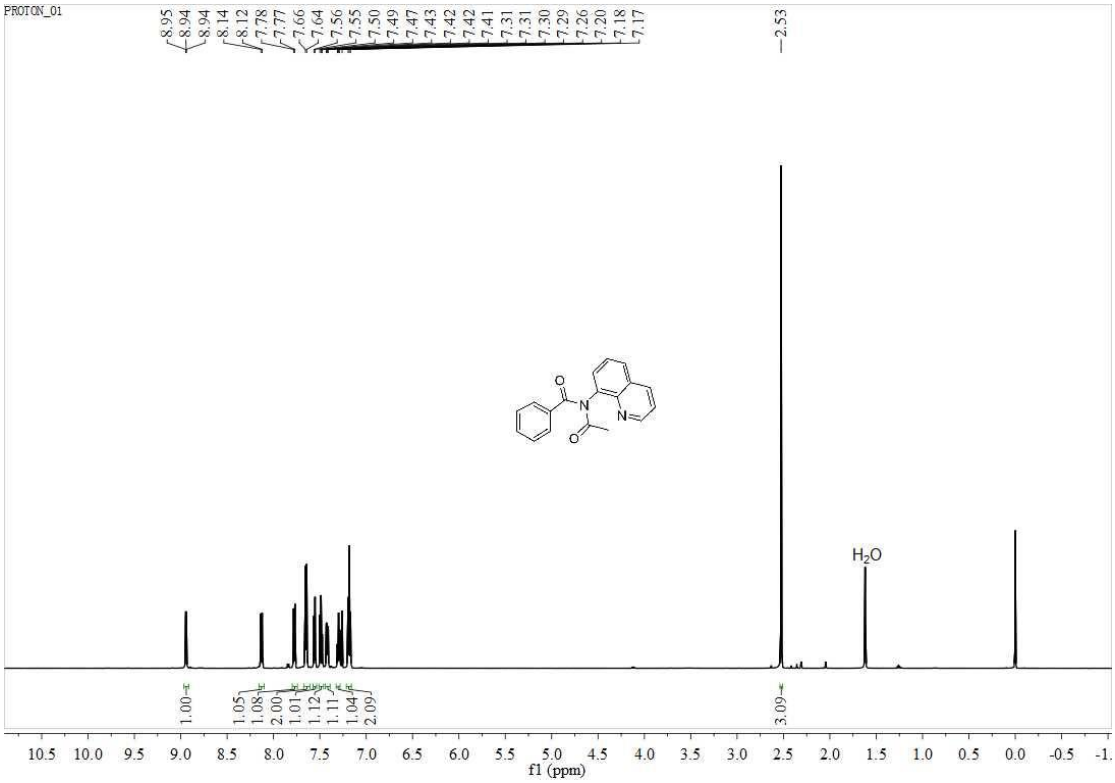
^{1}H NMR Spectrum of 6



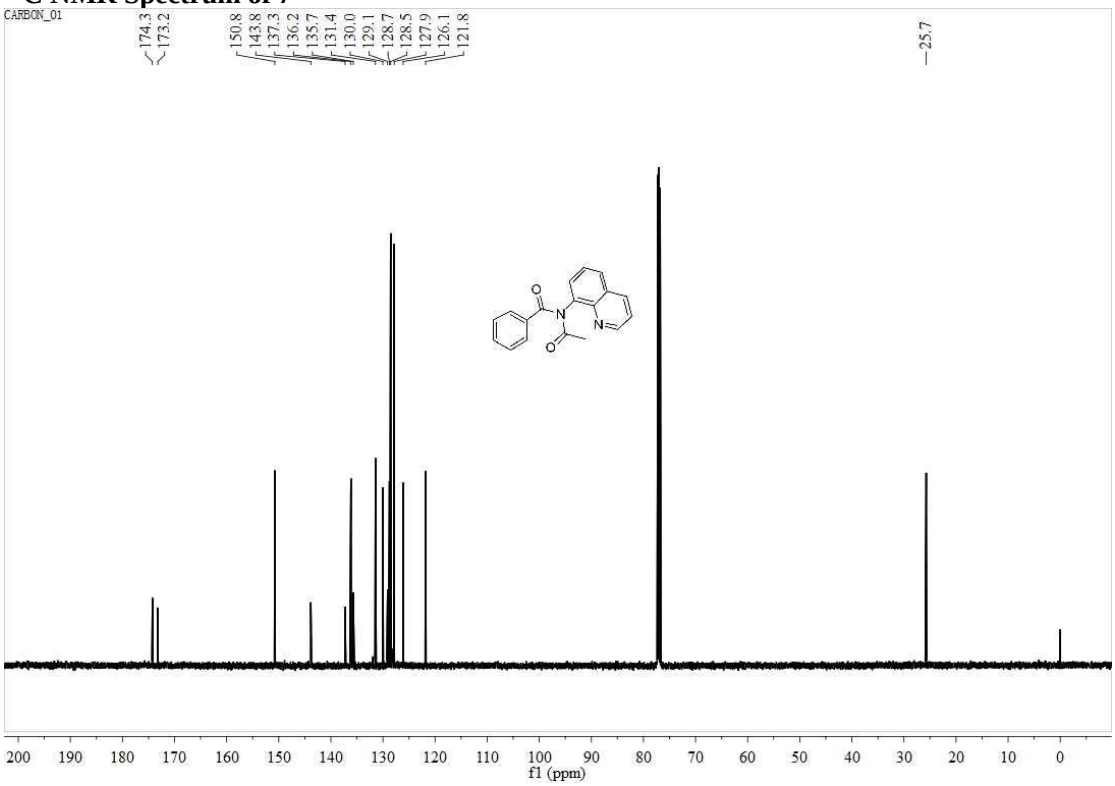
^{13}C NMR Spectrum of 6



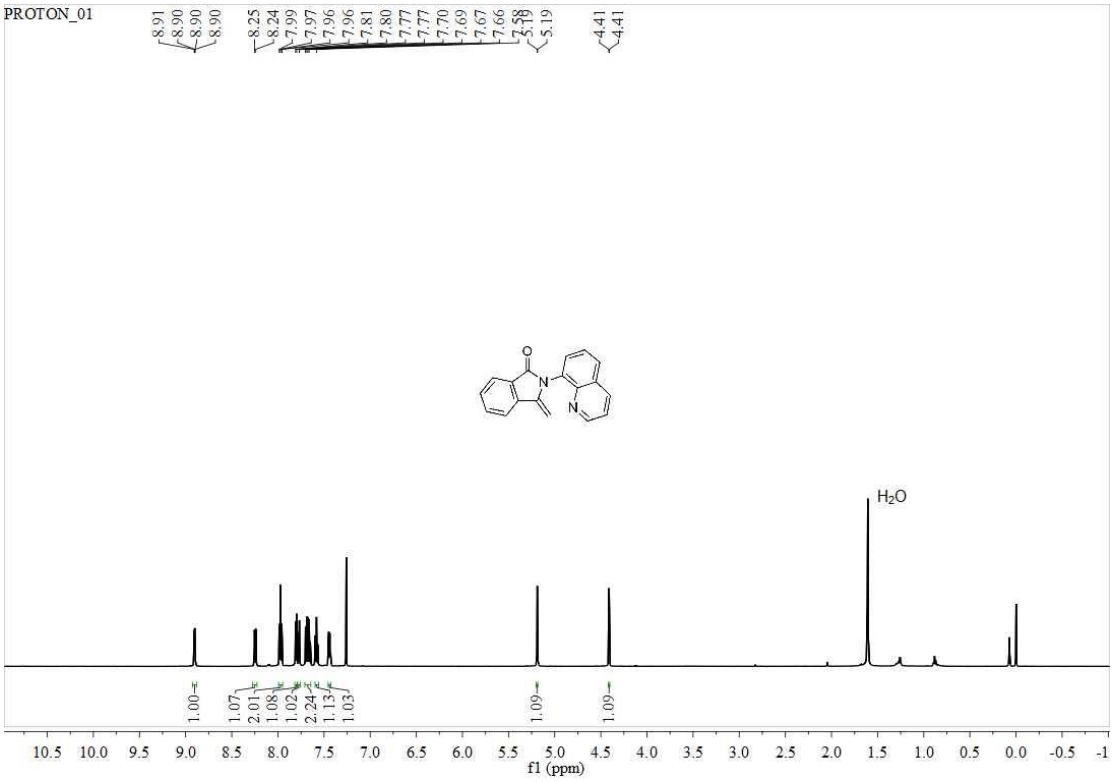
^{1}H NMR Spectrum of 7



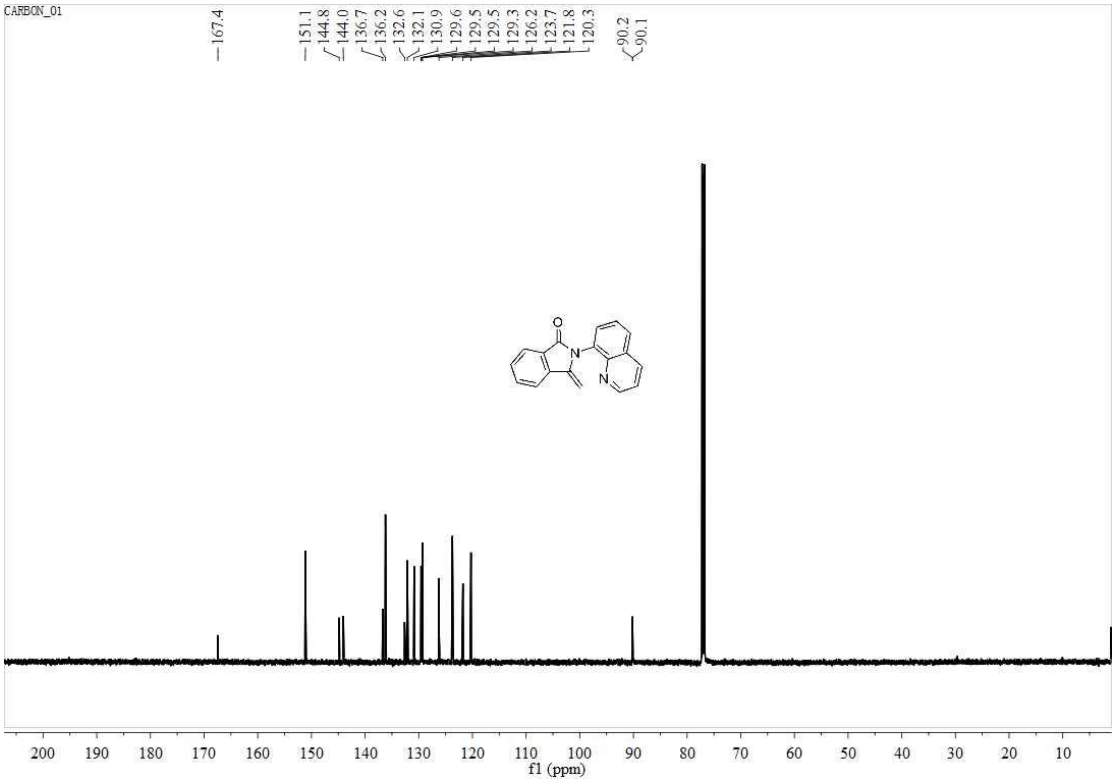
^{13}C NMR Spectrum of 7



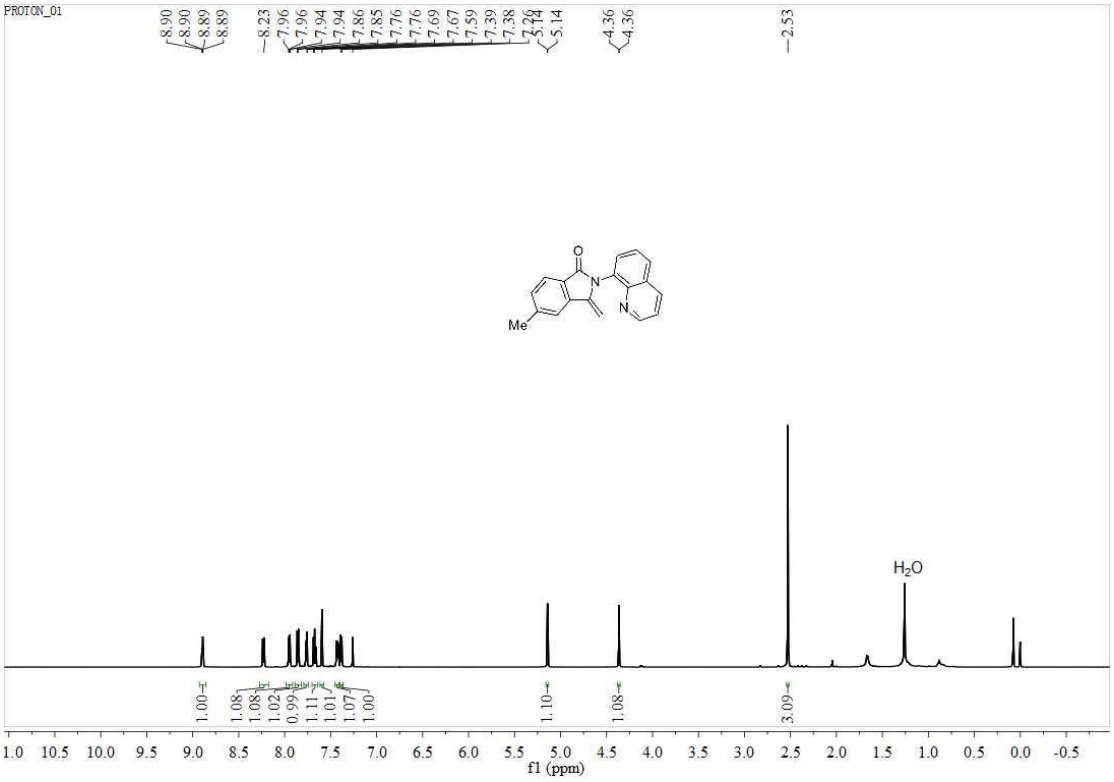
^{1}H NMR Spectrum of 3aa



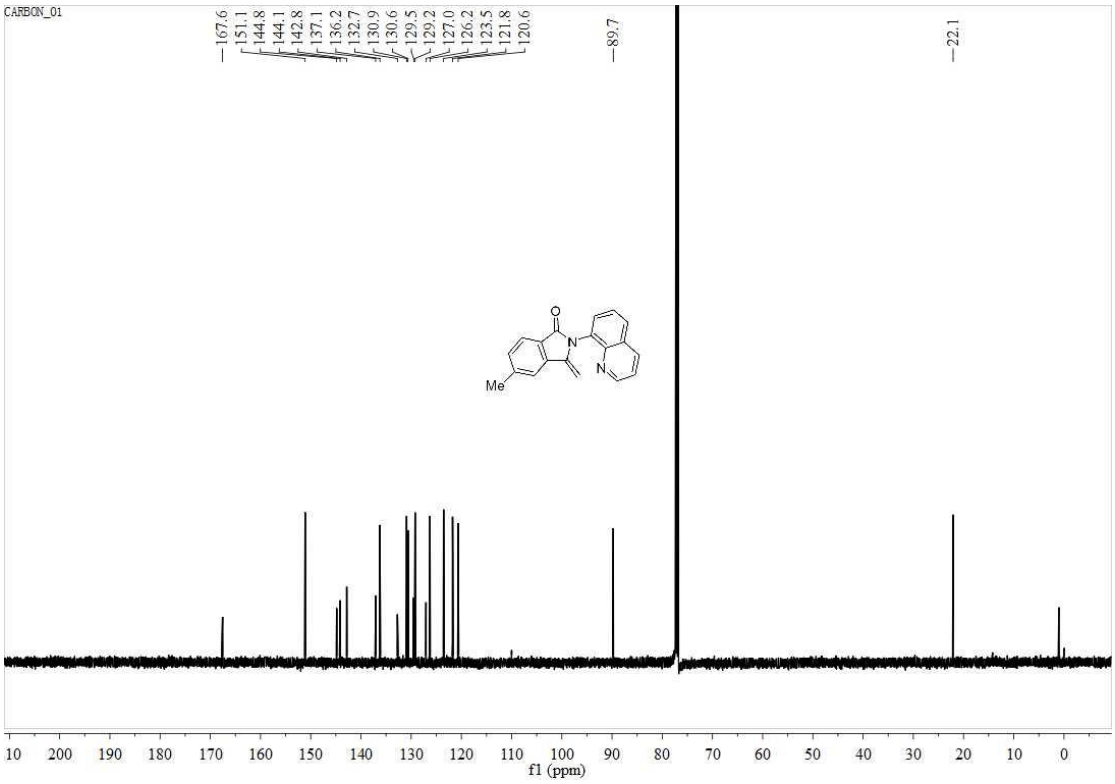
^{13}C NMR Spectrum of 3aa



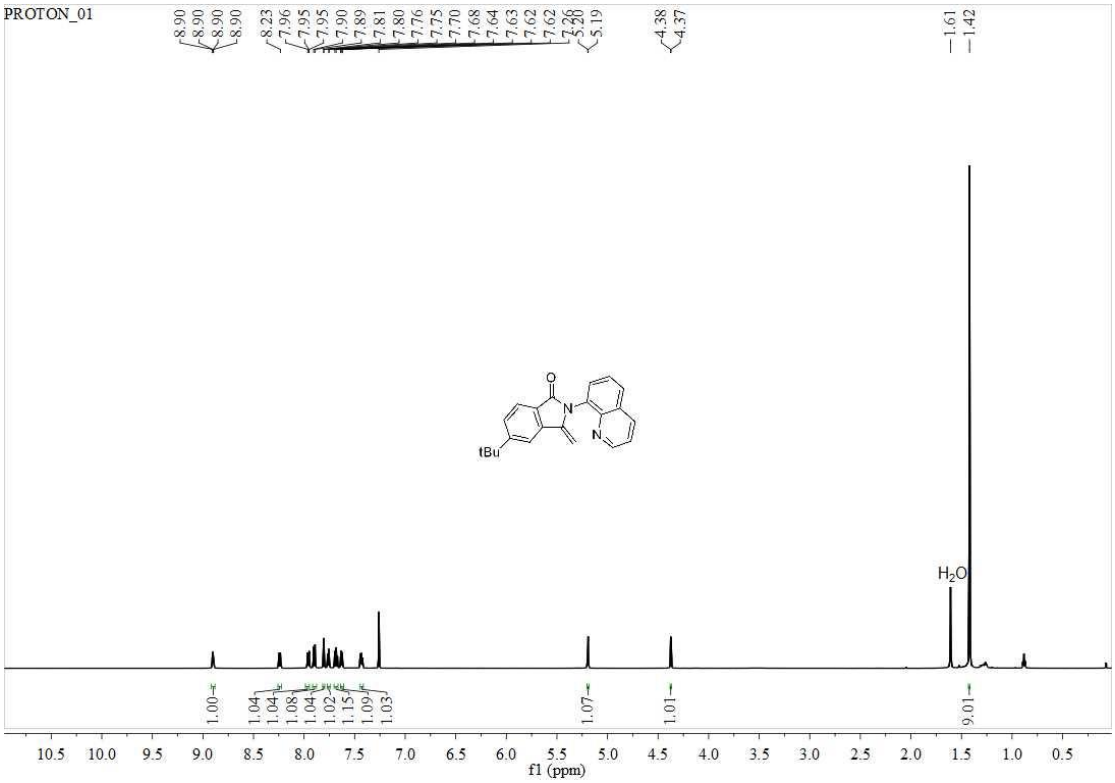
^{1}H NMR Spectrum of 3ba



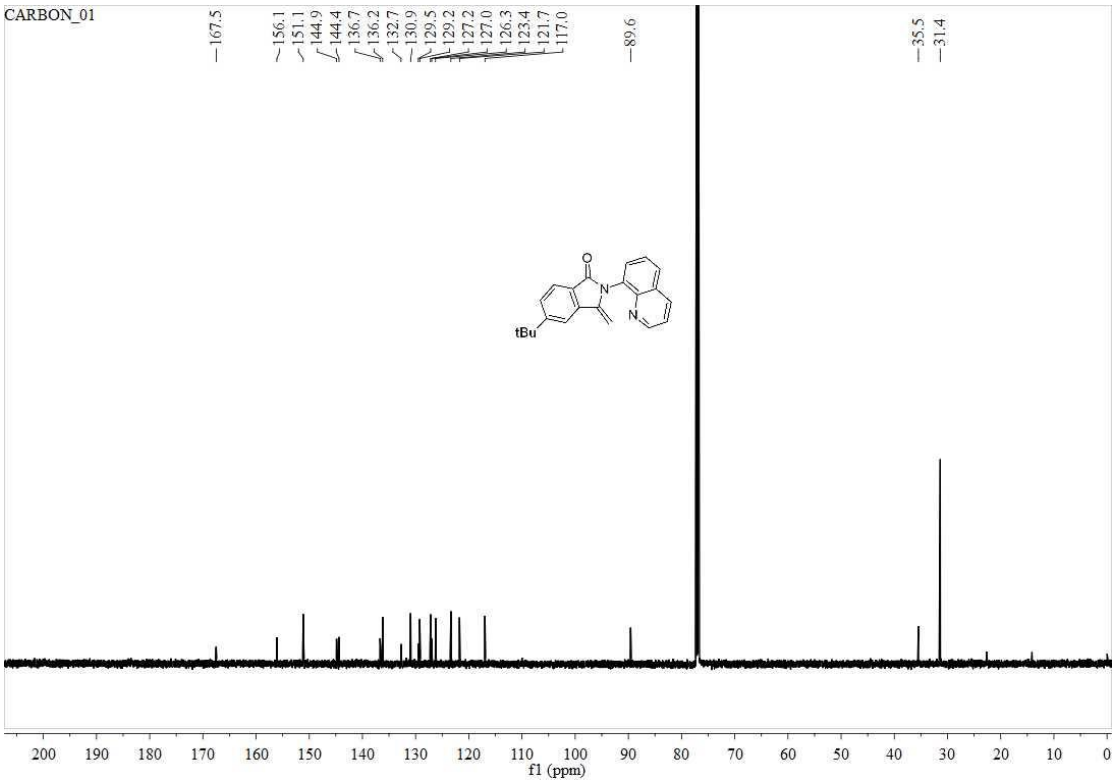
^{13}C NMR Spectrum of 3ba



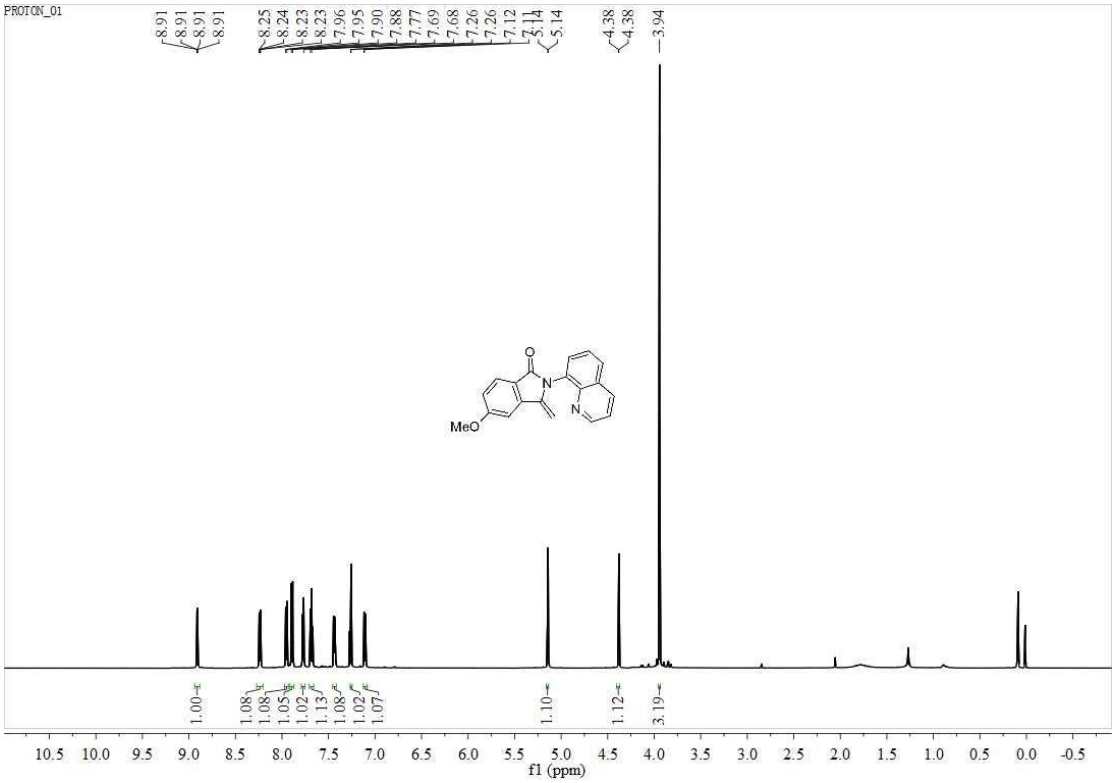
^{1}H NMR Spectrum of 3ca



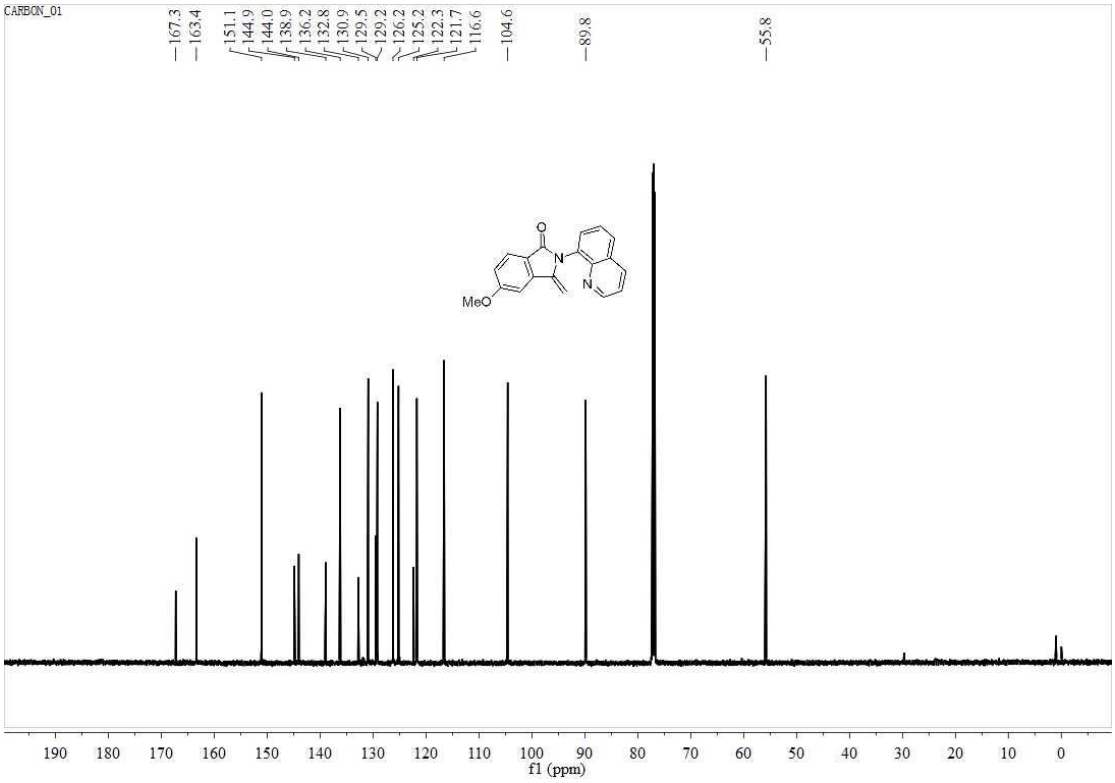
^{13}C NMR Spectrum of 3ca



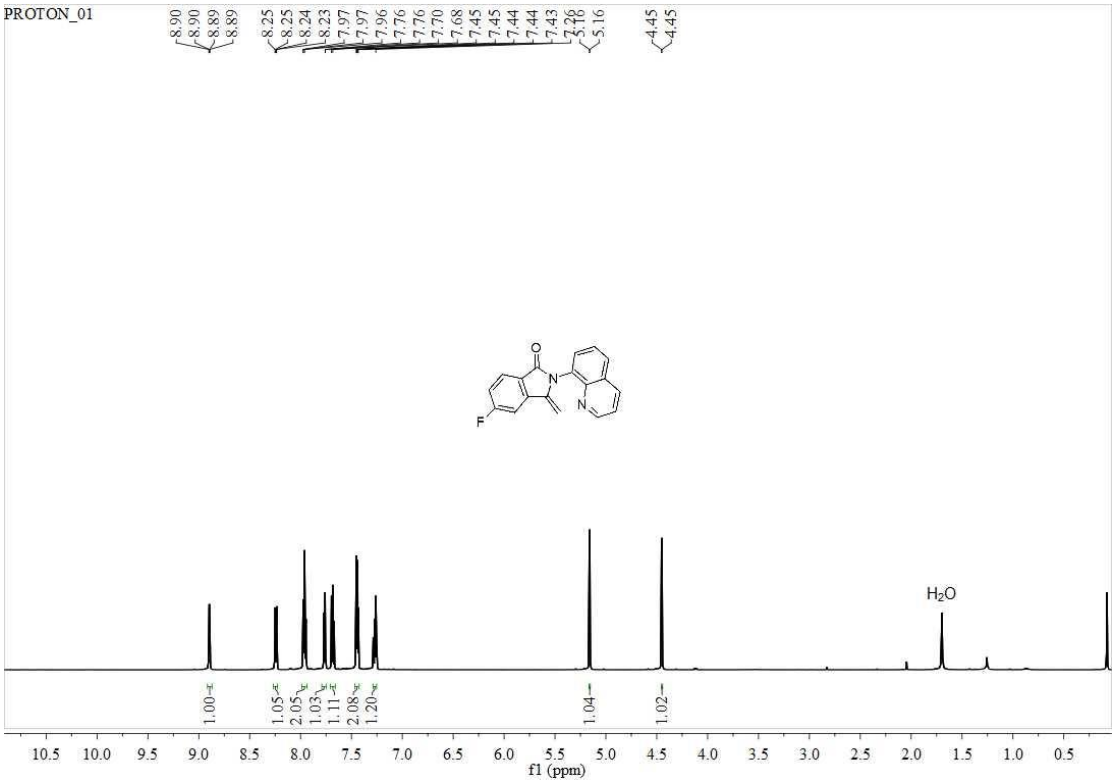
^{1}H NMR Spectrum of 3da



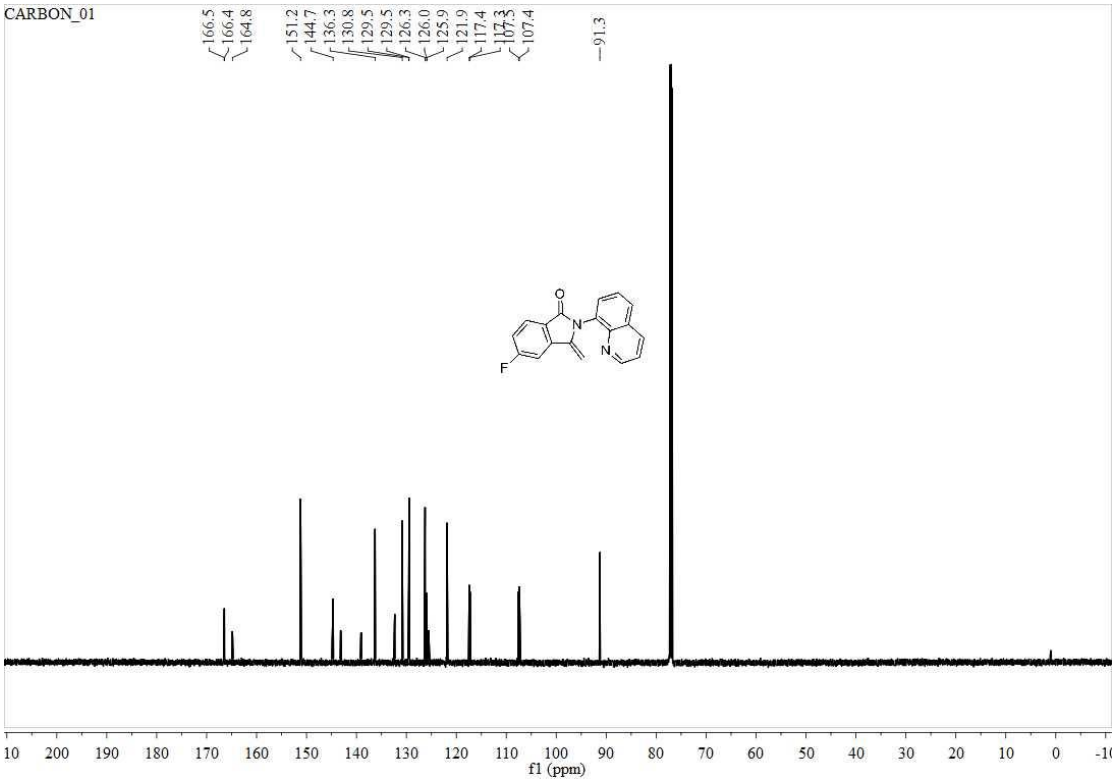
^{13}C NMR Spectrum of 3da



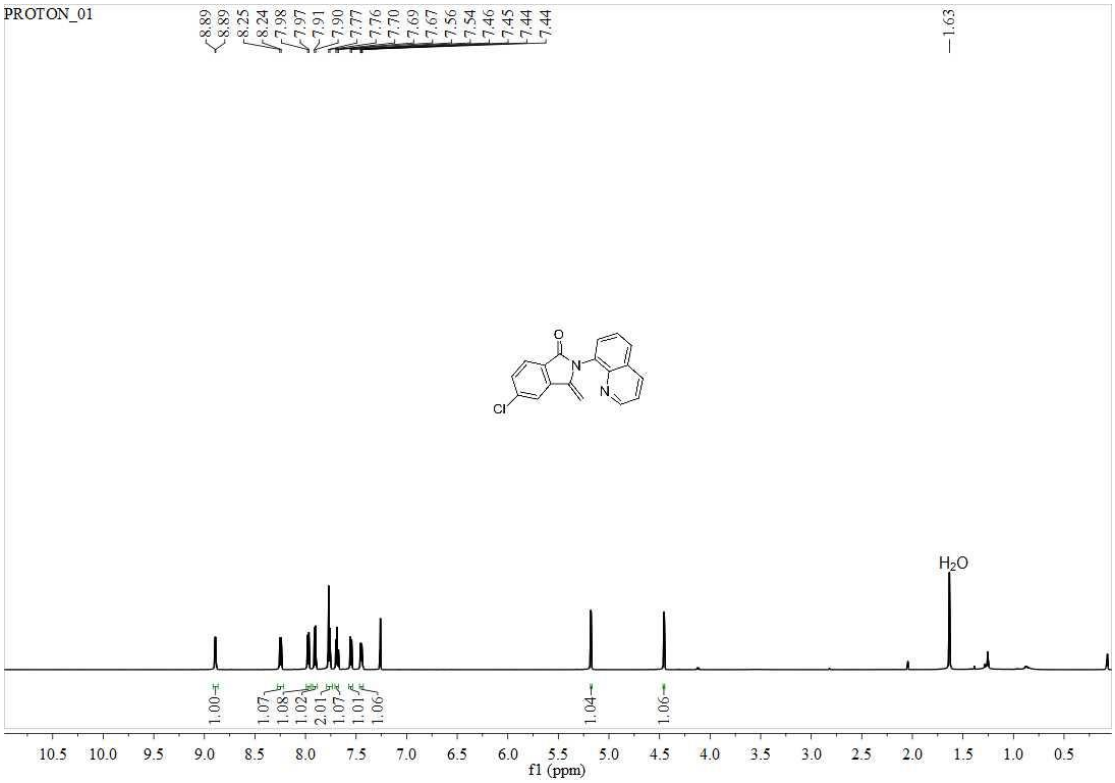
^{1}H NMR Spectrum of 3ea



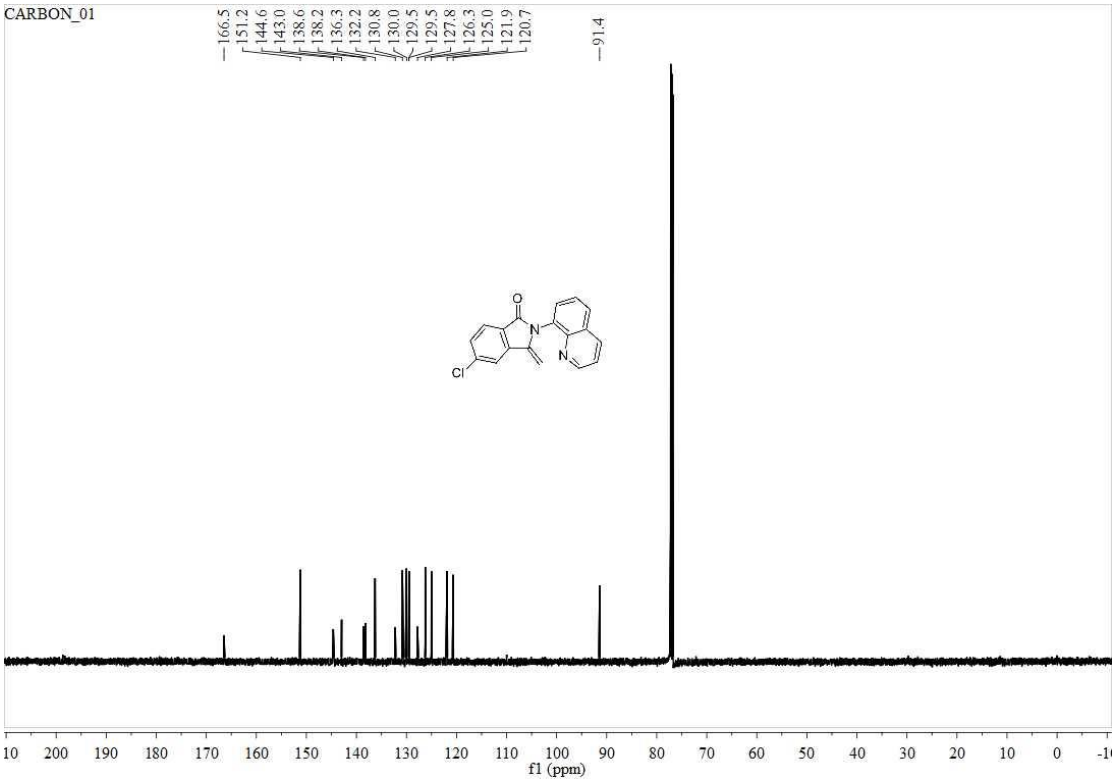
^{13}C NMR Spectrum of 3ea



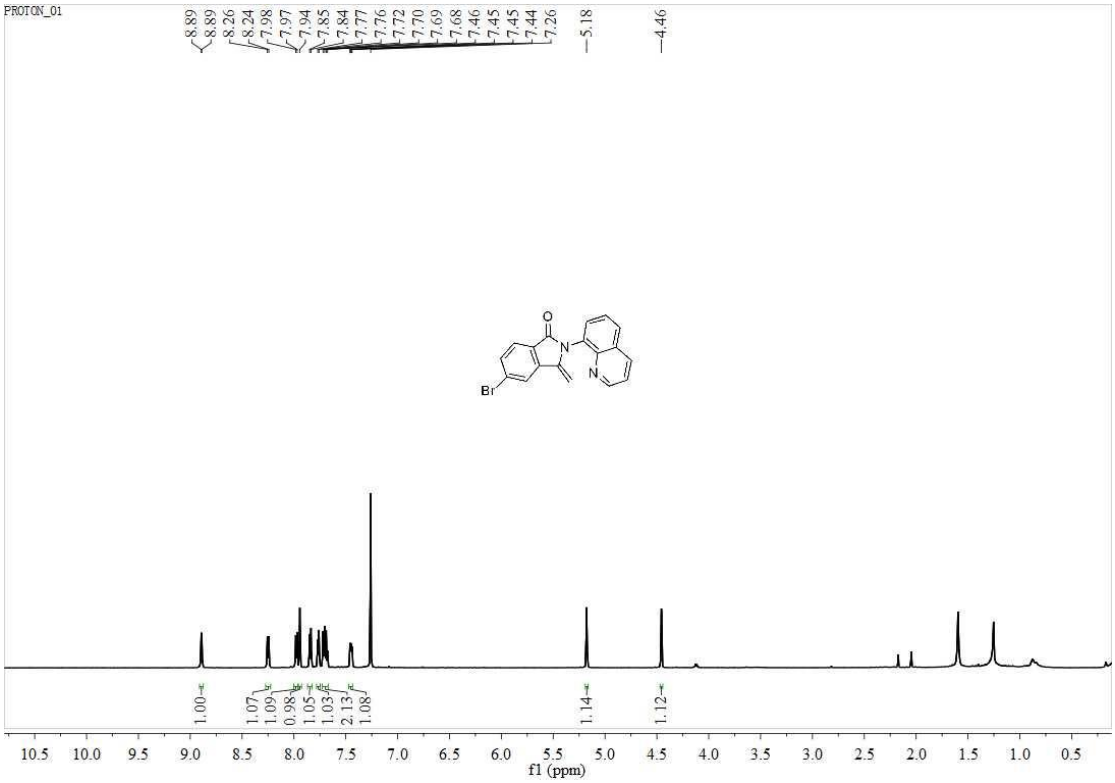
^{1}H NMR Spectrum of 3fa



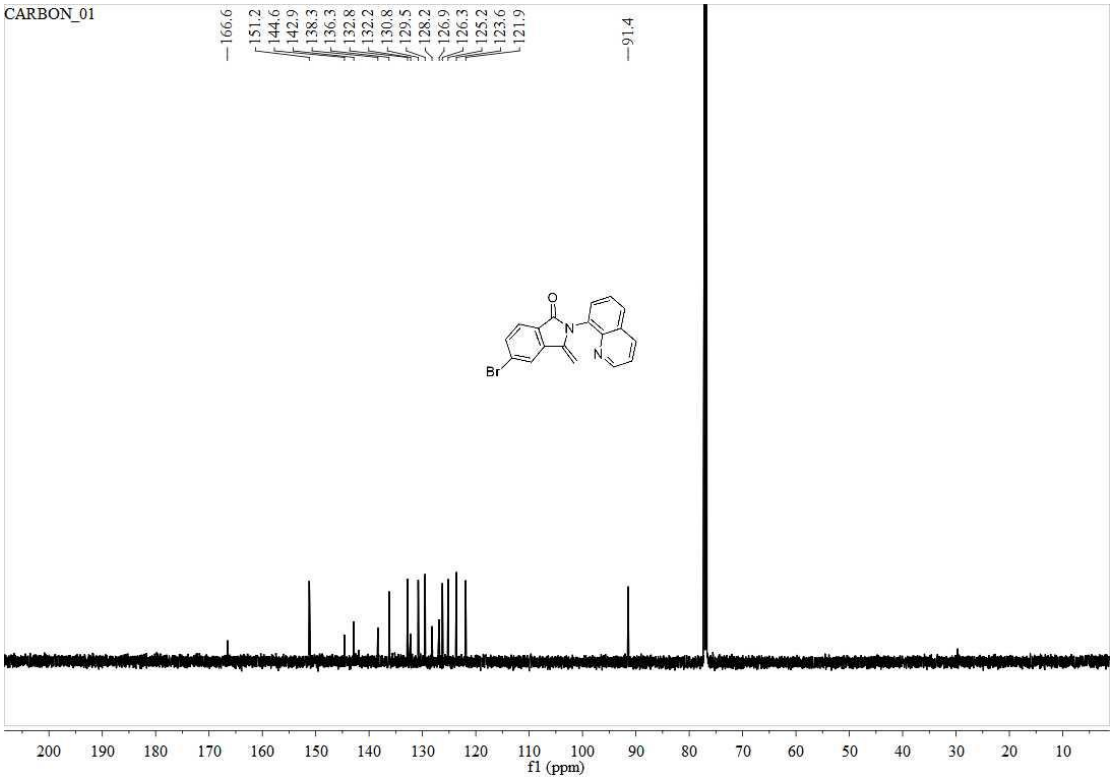
^{13}C NMR Spectrum of 3fa



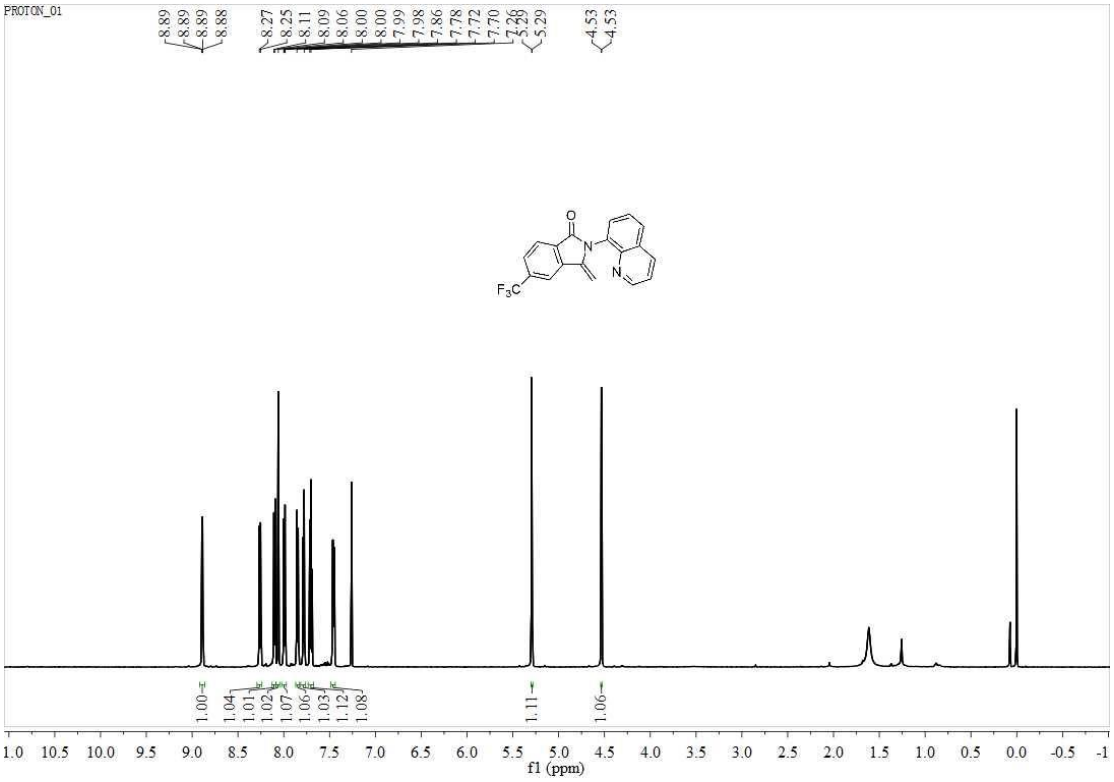
^{1}H NMR Spectrum of 3ga



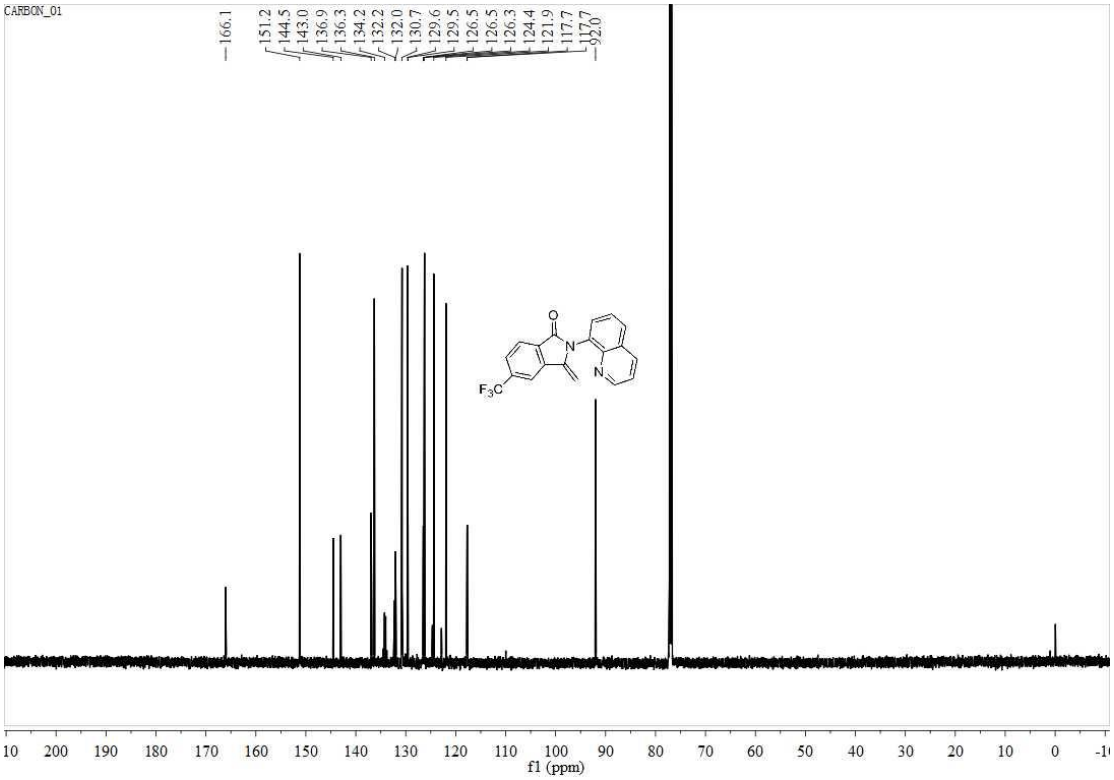
^{13}C NMR Spectrum of 3ga



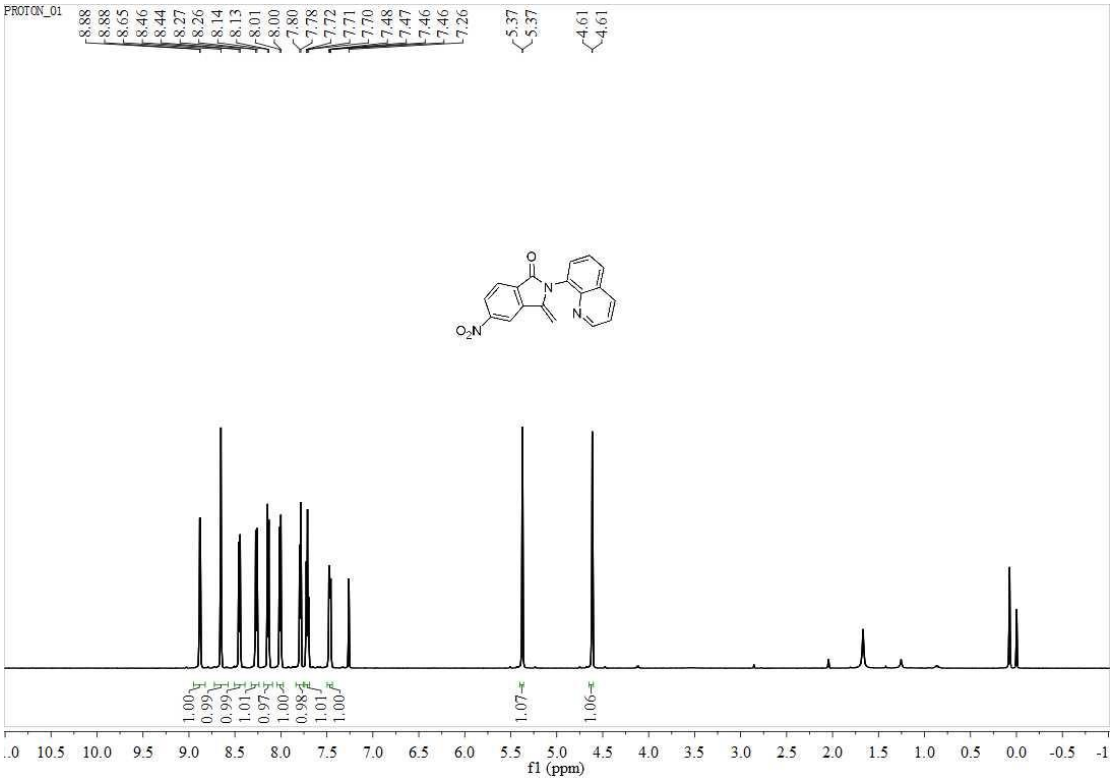
^{1}H NMR Spectrum of 3ha



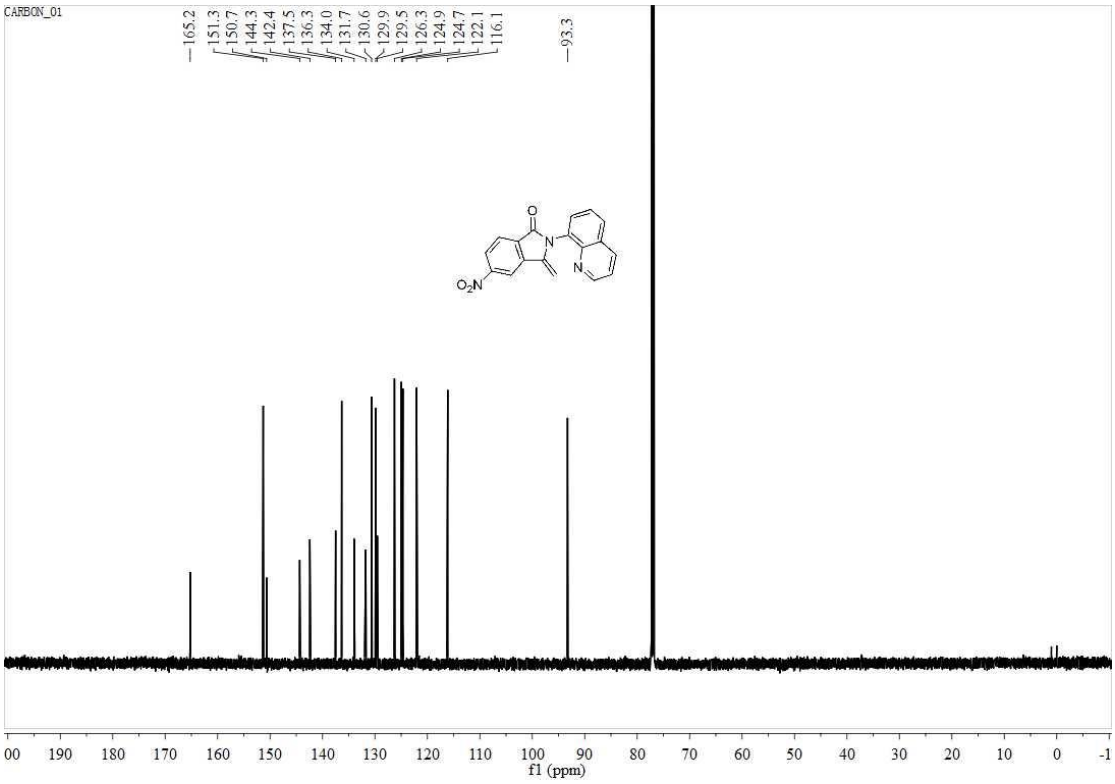
^{13}C NMR Spectrum of 3ha



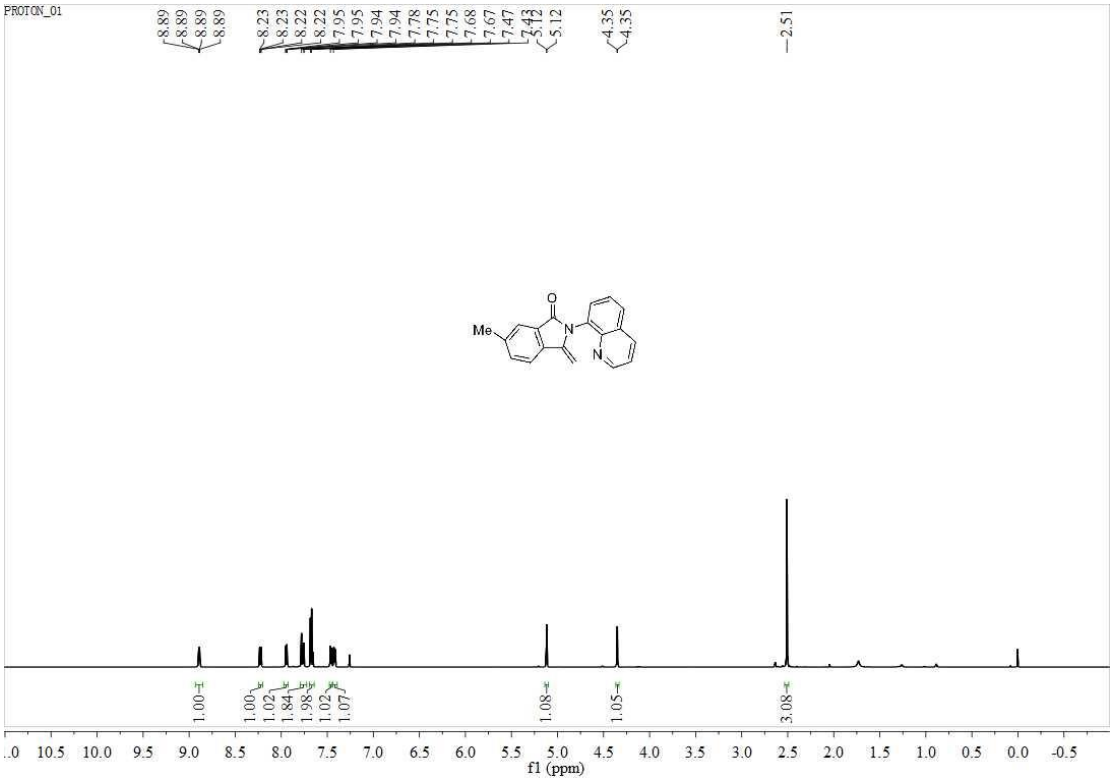
^{1}H NMR Spectrum of 3ia



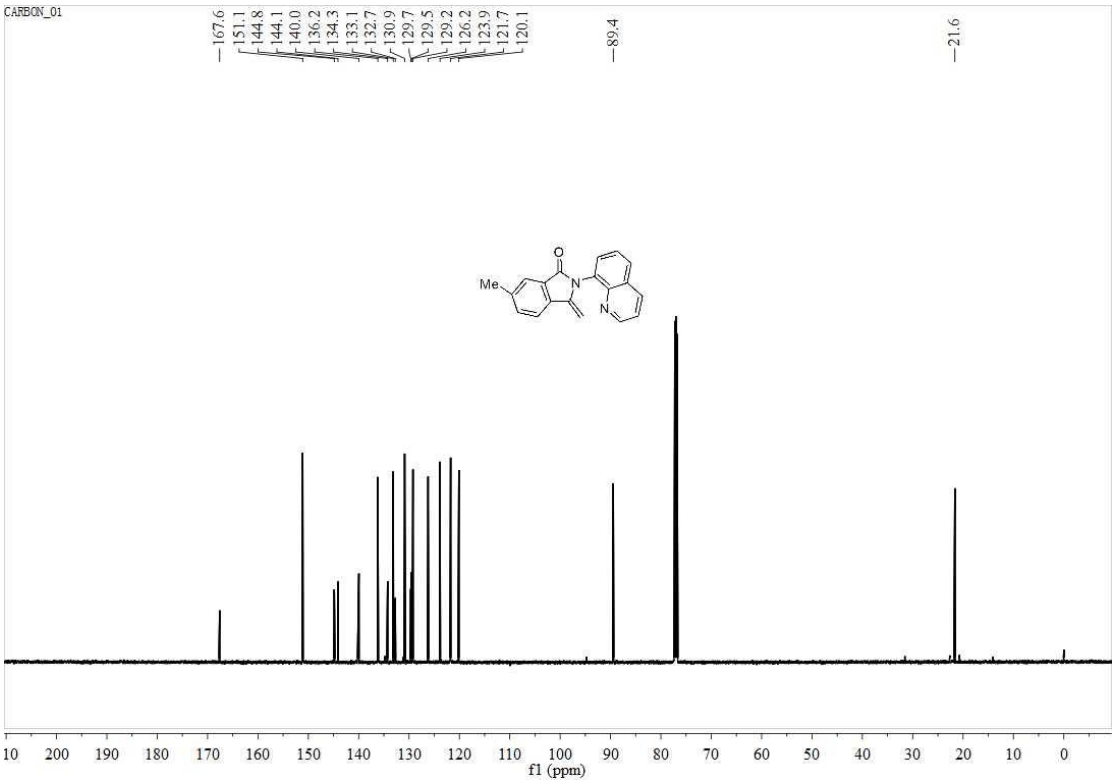
^{13}C NMR Spectrum of 3ia



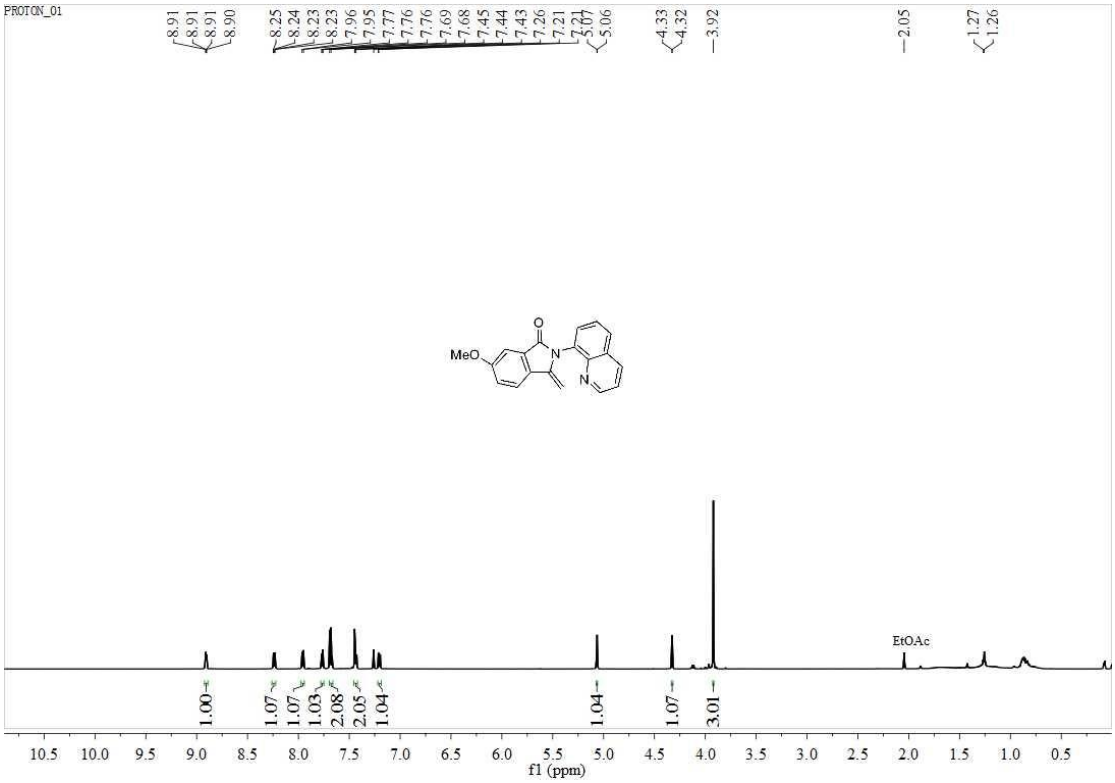
^{1}H NMR Spectrum of 3ja



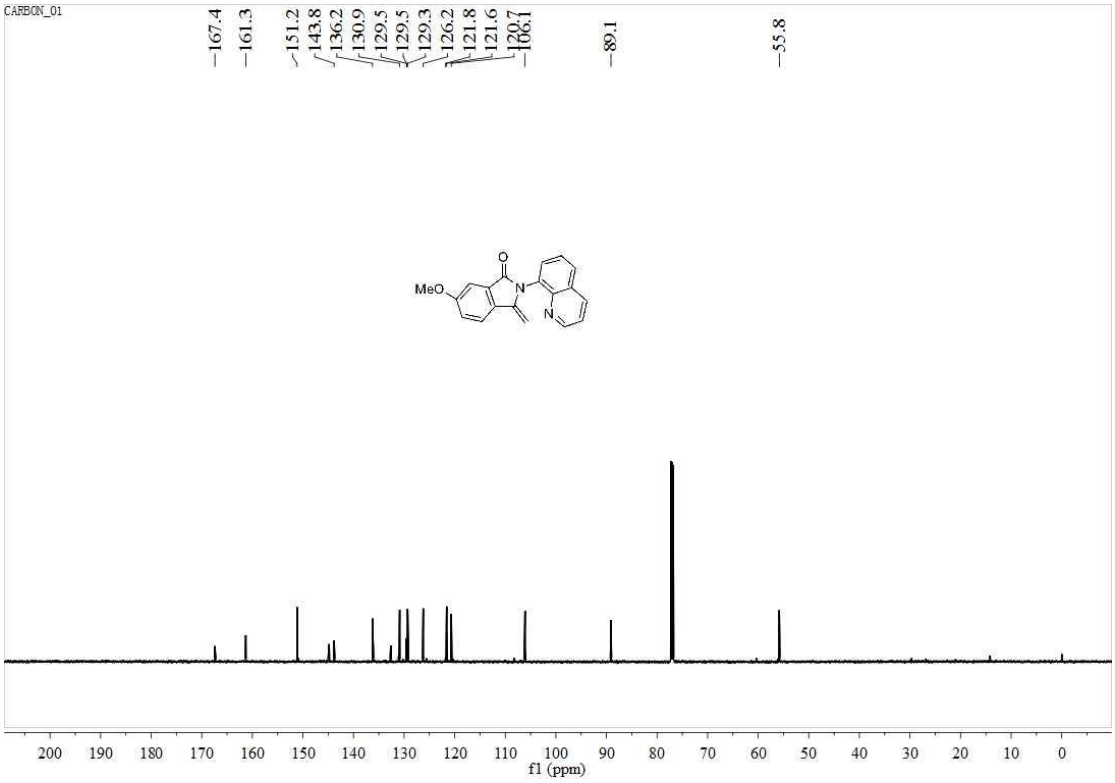
^{13}C NMR Spectrum of 3ja



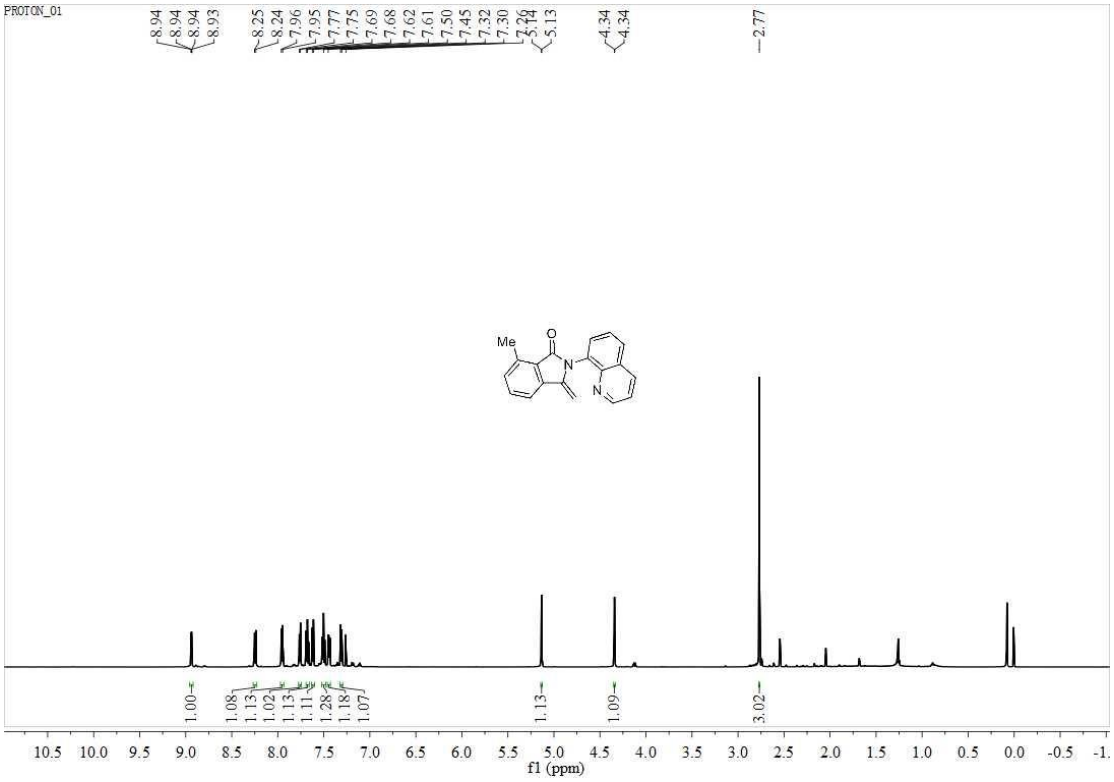
^{1}H NMR Spectrum of 3ka



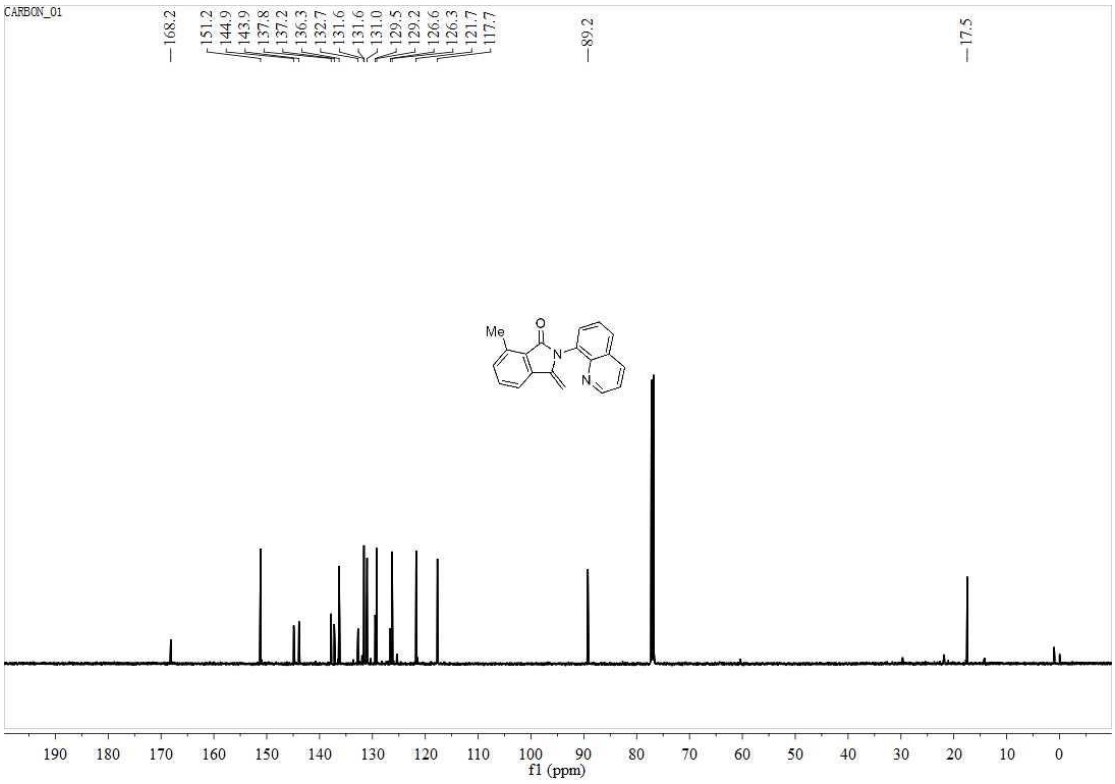
^{13}C NMR Spectrum of 3ka



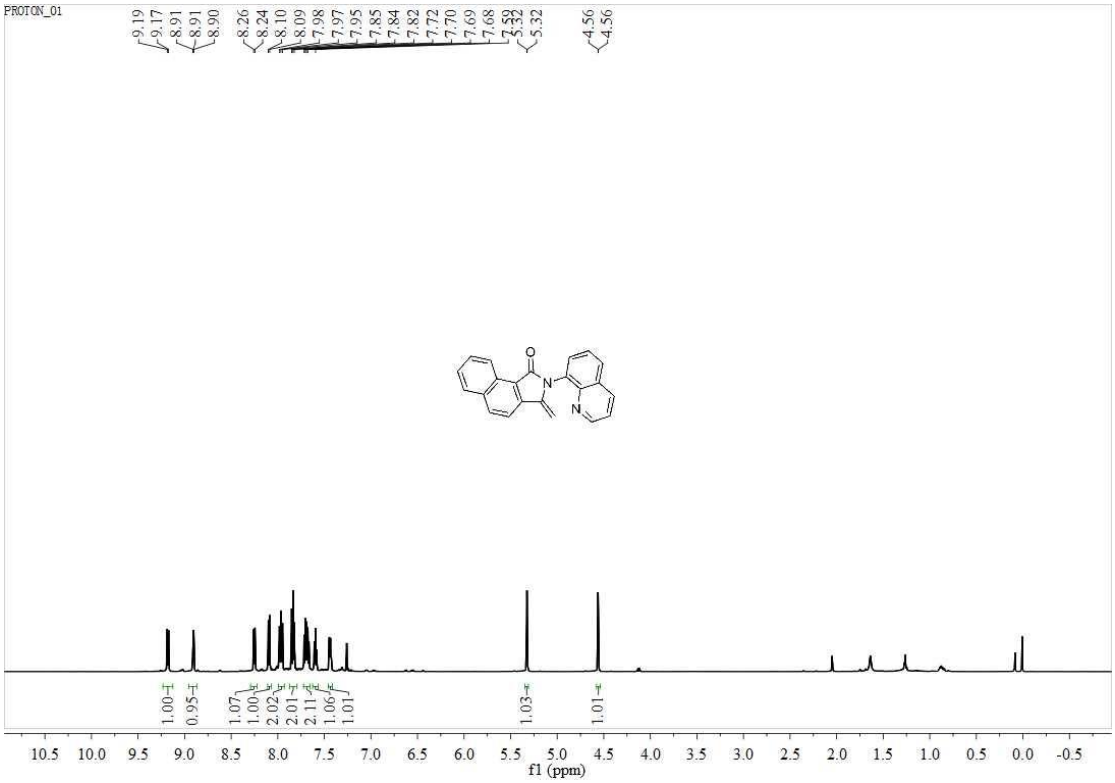
^{13}C NMR Spectrum of 3la



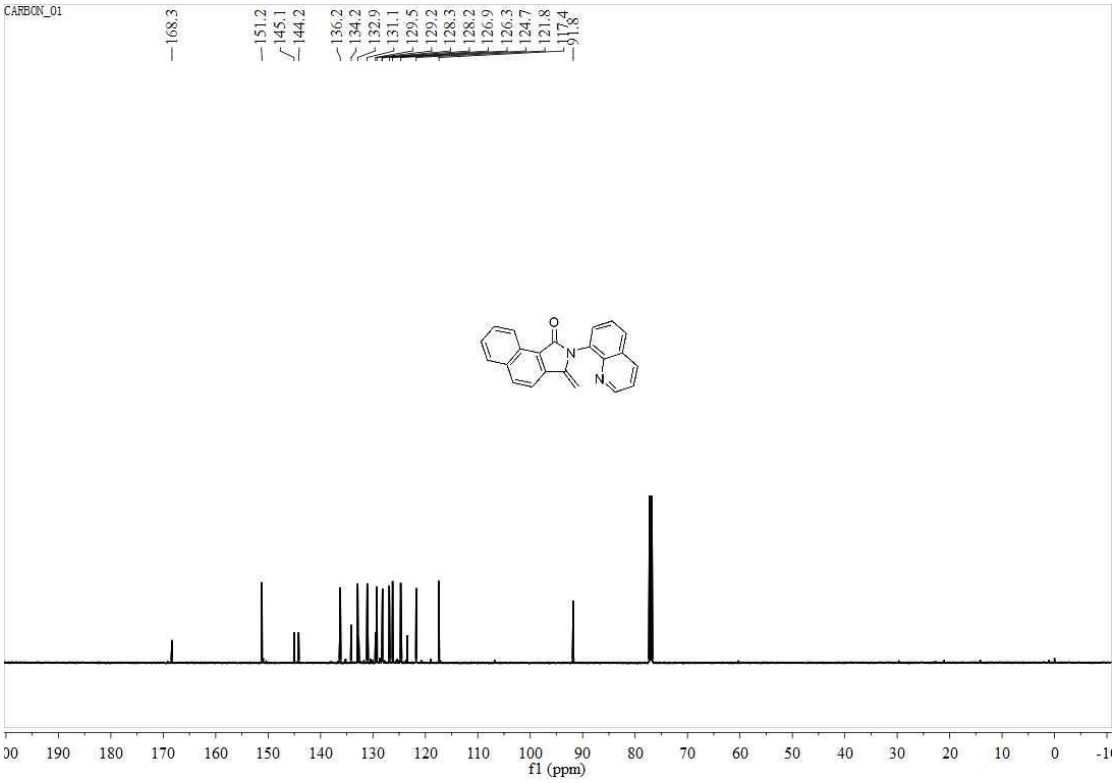
^{13}C NMR Spectrum of 3la



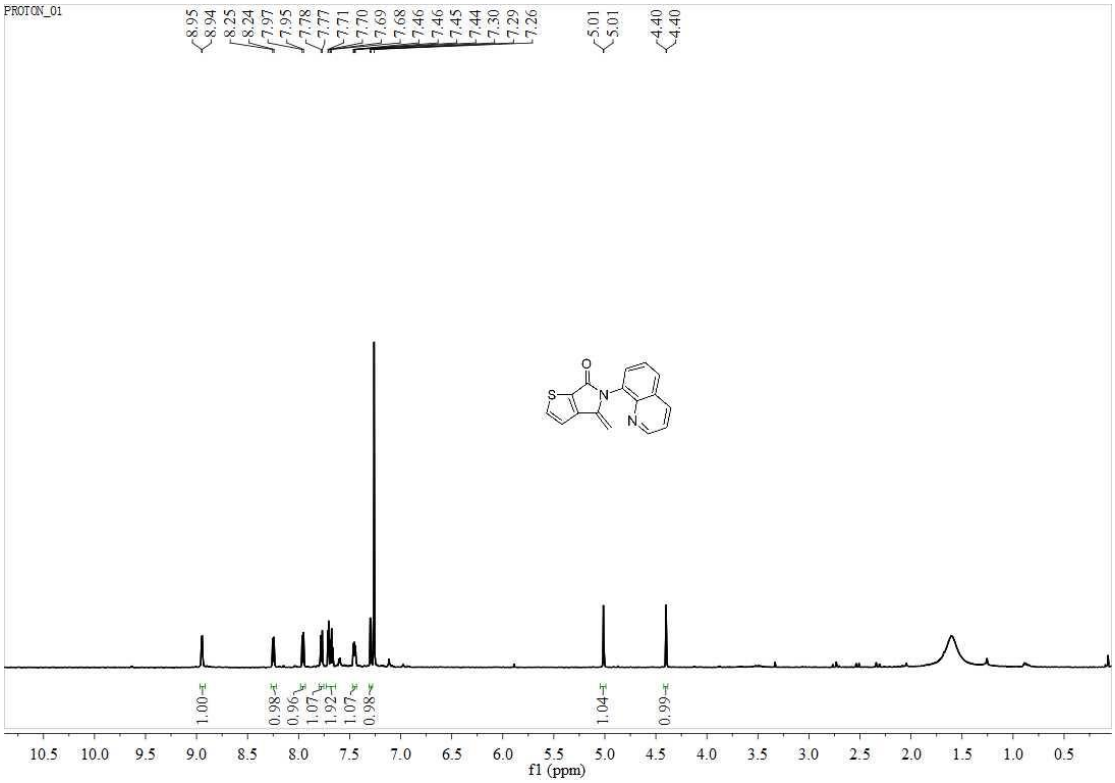
^{1}H NMR Spectrum of 3ma



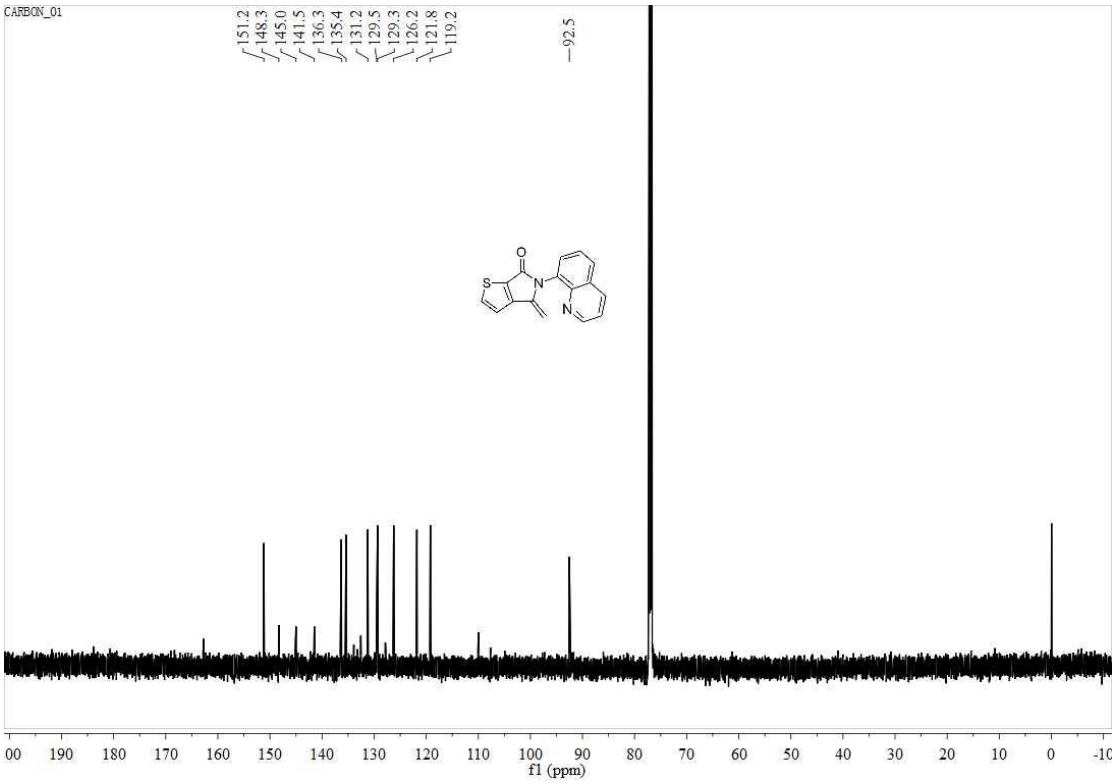
^{13}C NMR Spectrum of 3ma



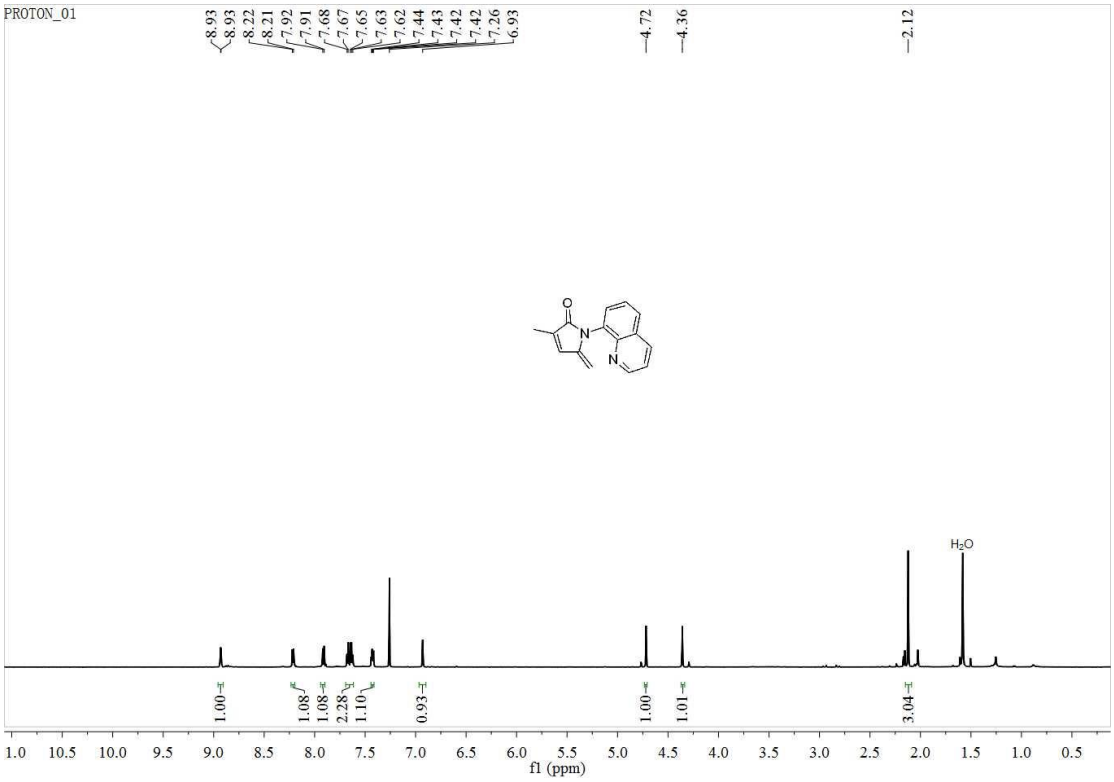
^{1}H NMR Spectrum of 3na



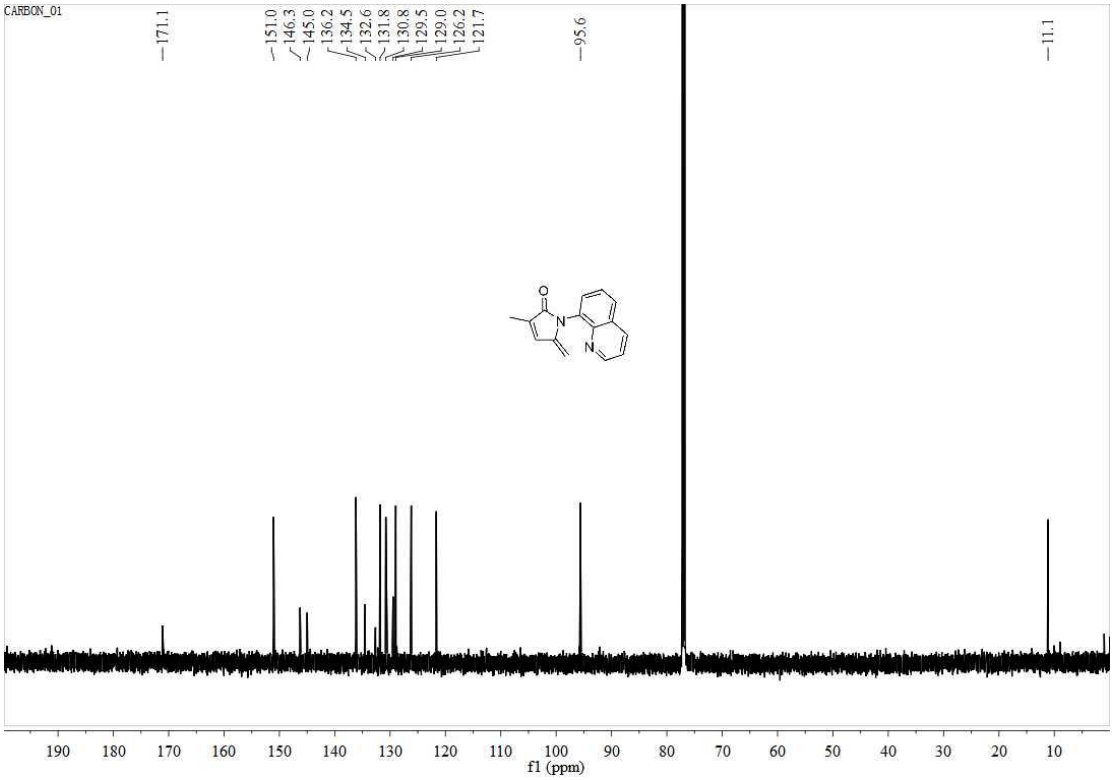
^{13}C NMR Spectrum of 3na



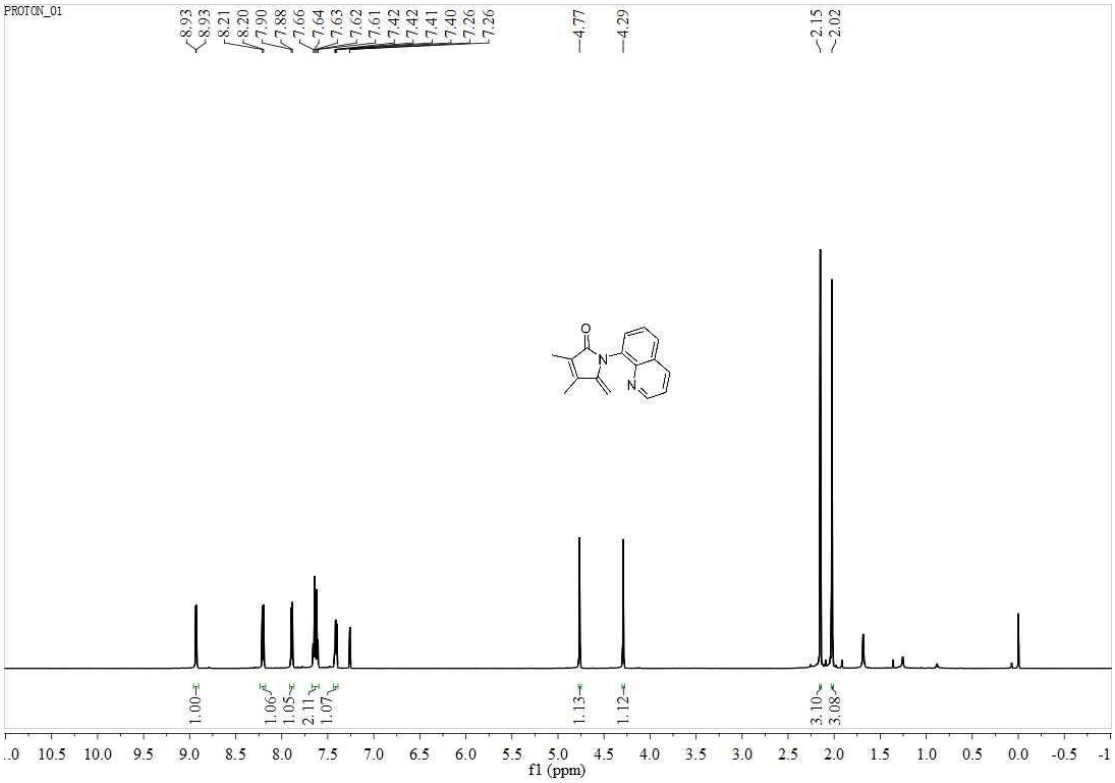
^{1}H NMR Spectrum of 3oa



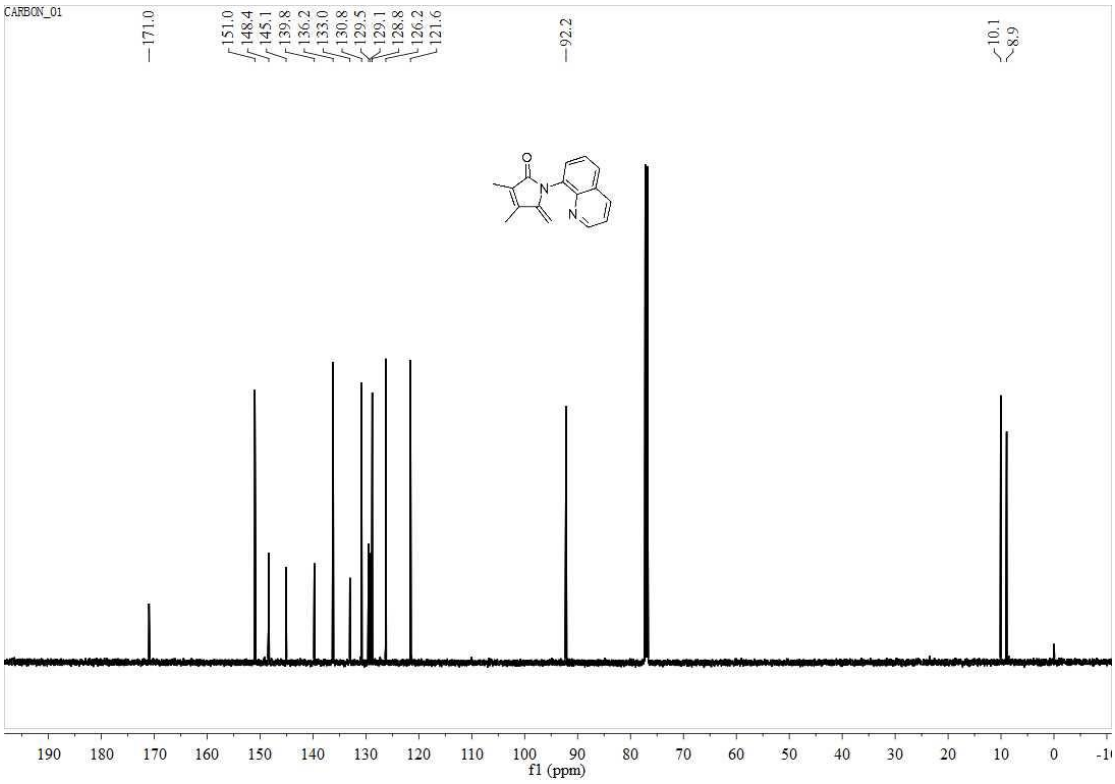
^{13}C NMR Spectrum of 3oa



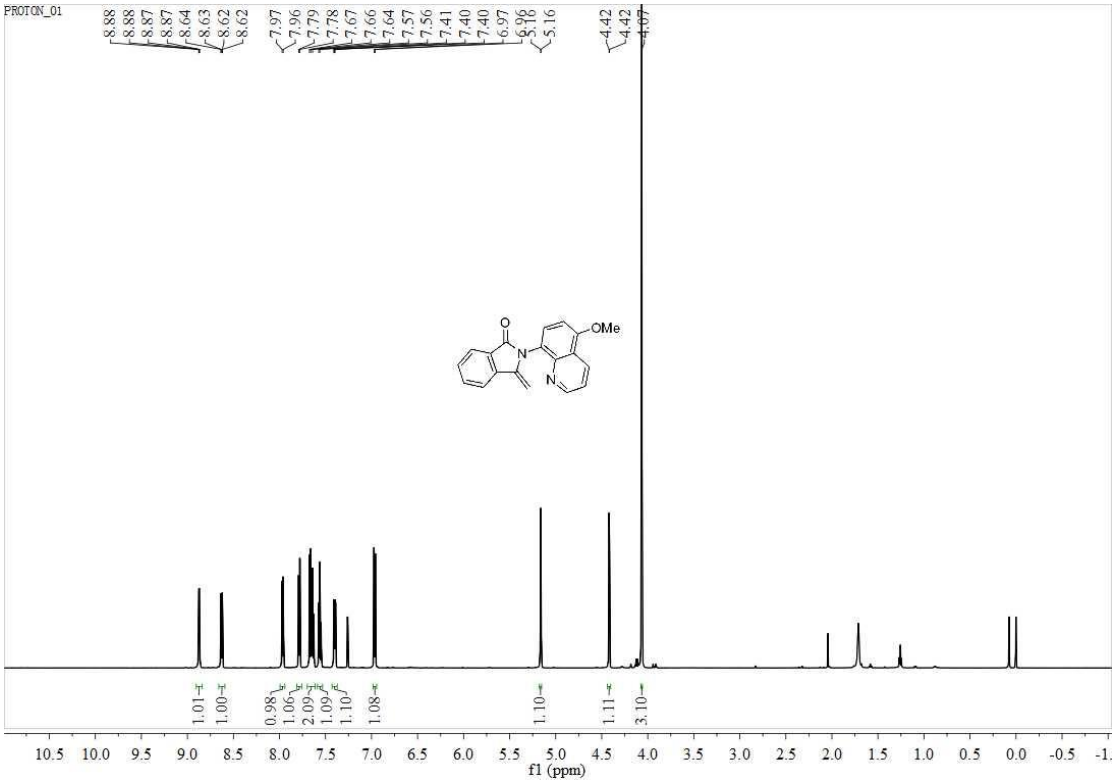
^{1}H NMR Spectrum of 3pa



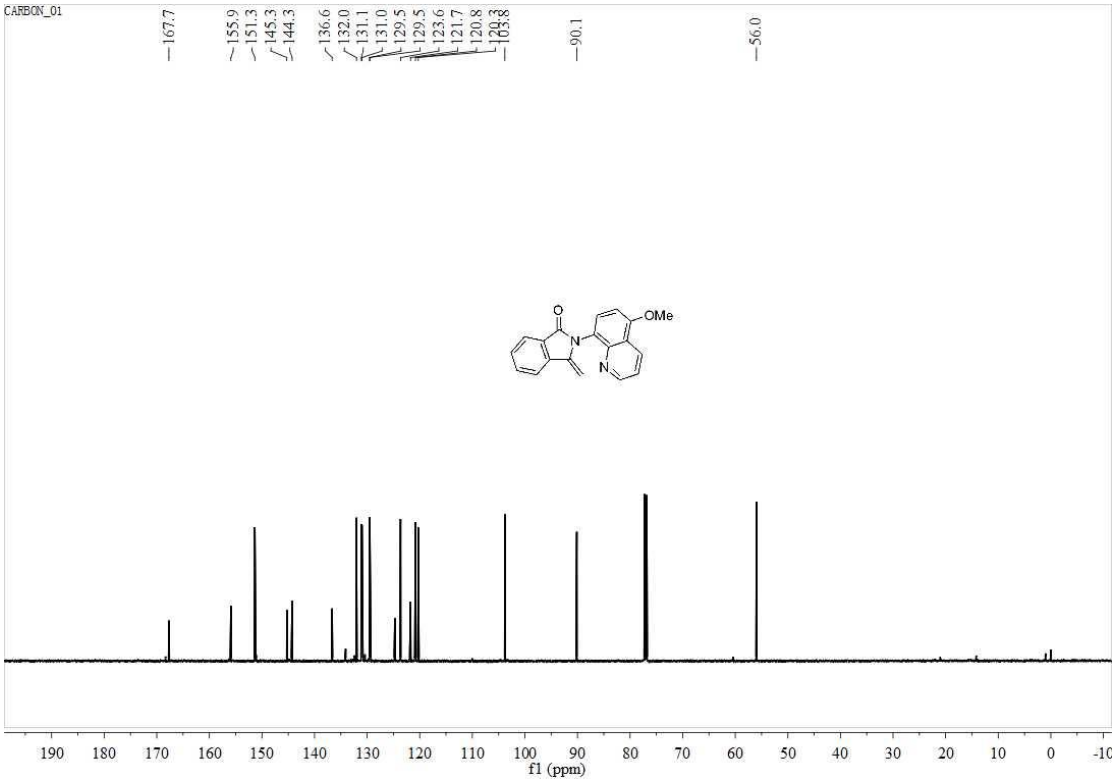
^{13}C NMR Spectrum of 3pa



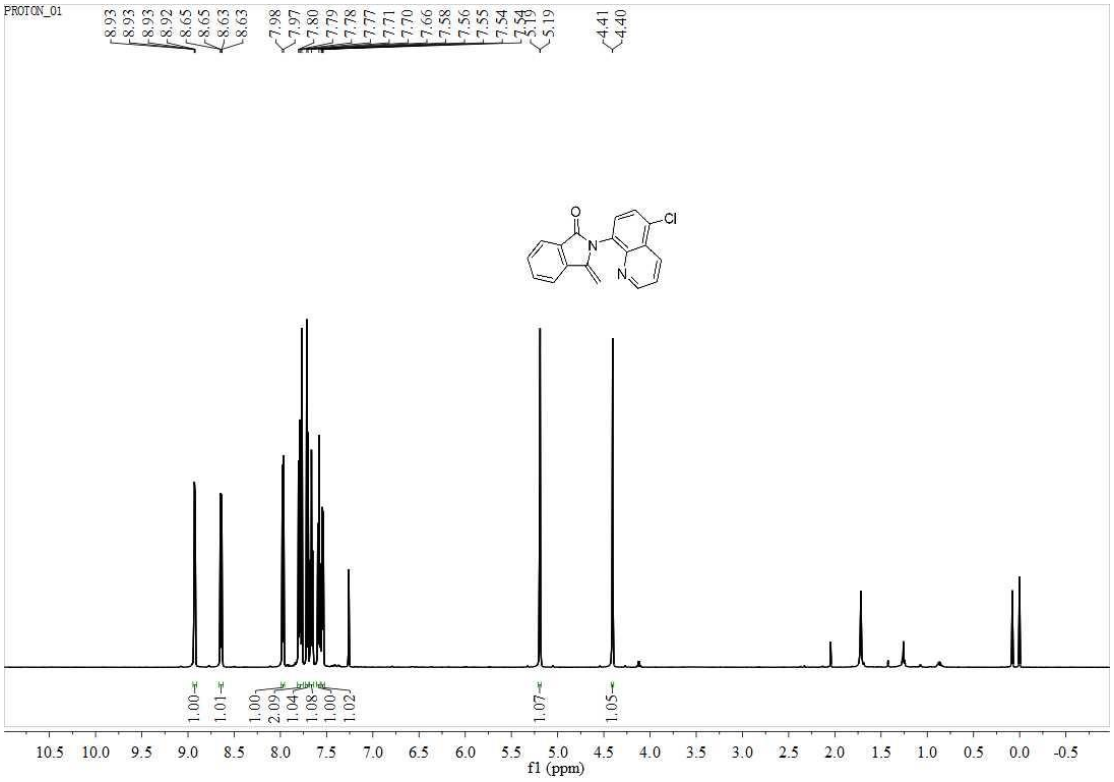
^{1}H NMR Spectrum of 3qa



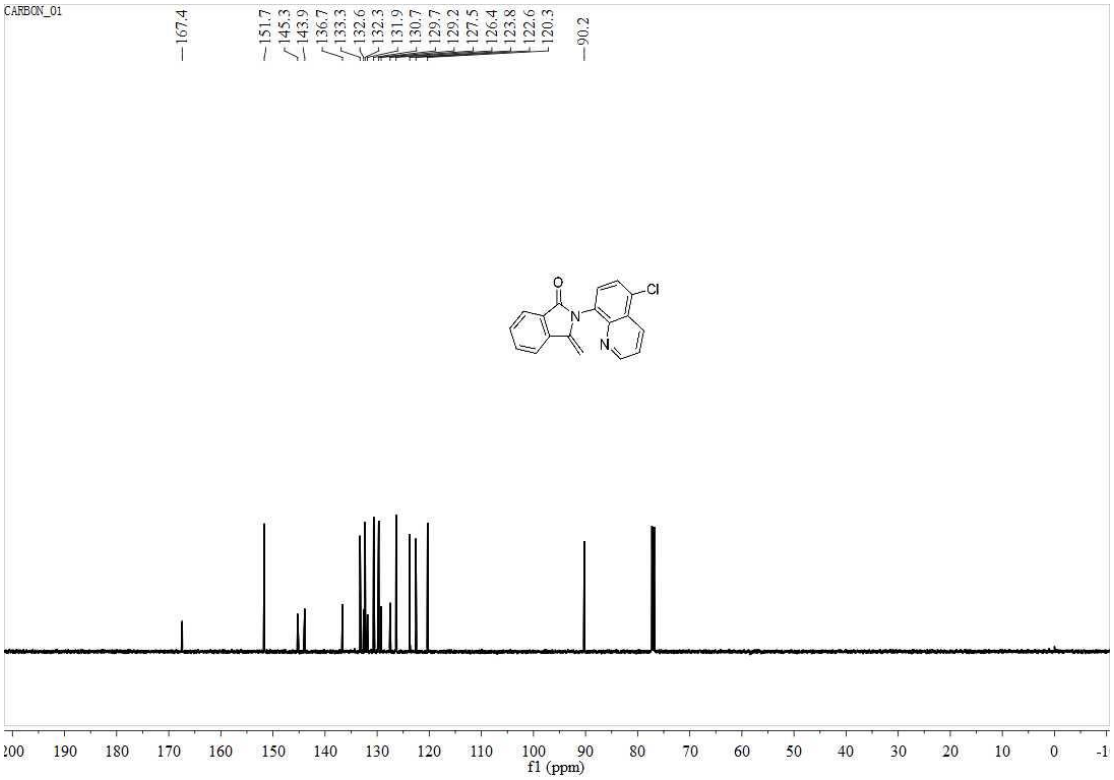
^{13}C NMR Spectrum of 3qa



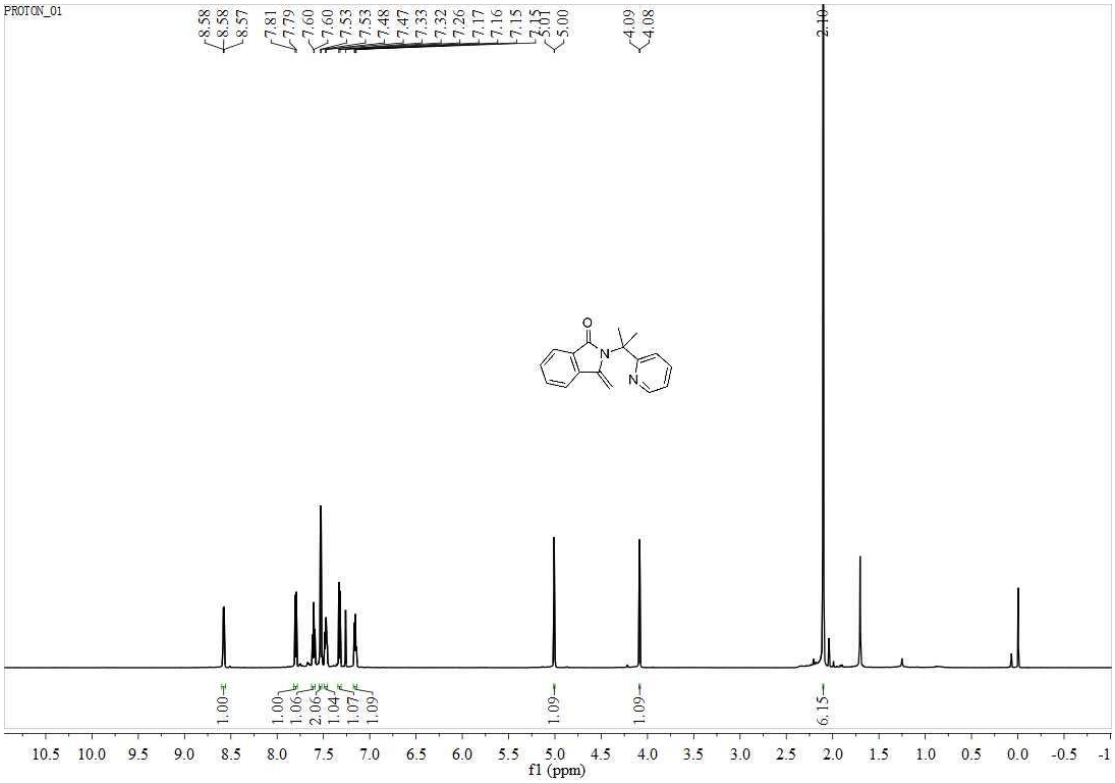
^{1}H NMR Spectrum of 3ra



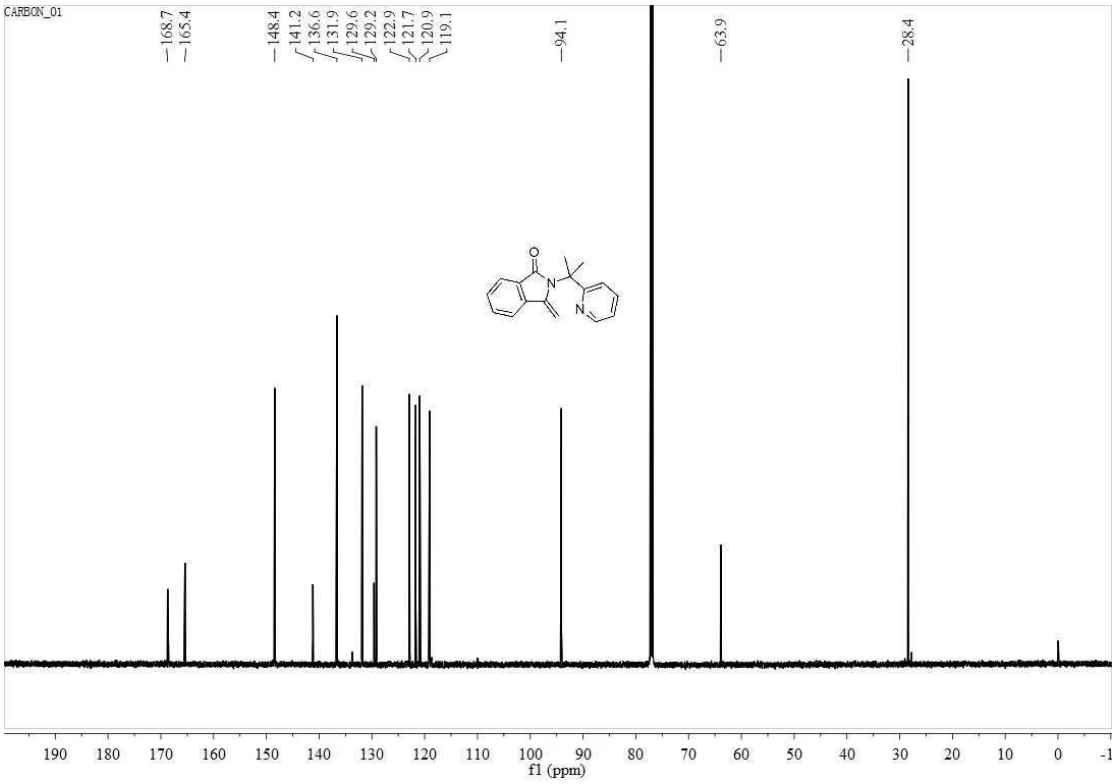
^{13}C NMR Spectrum of 3ra



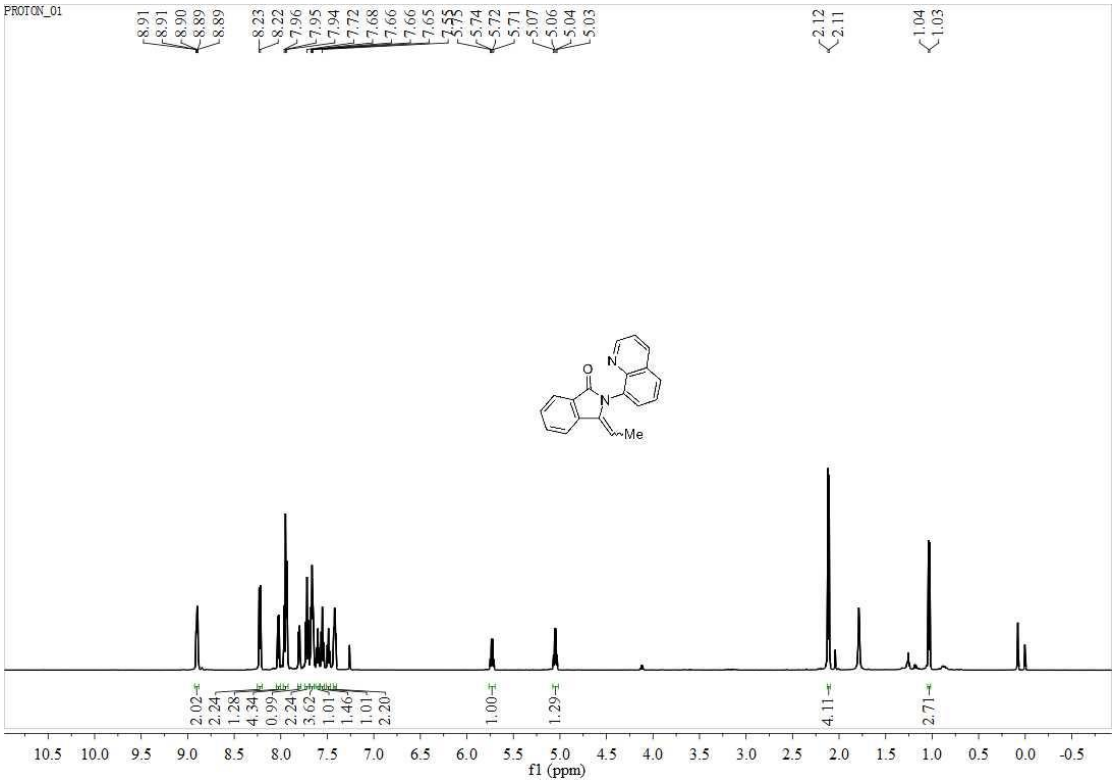
^{1}H NMR Spectrum of 4



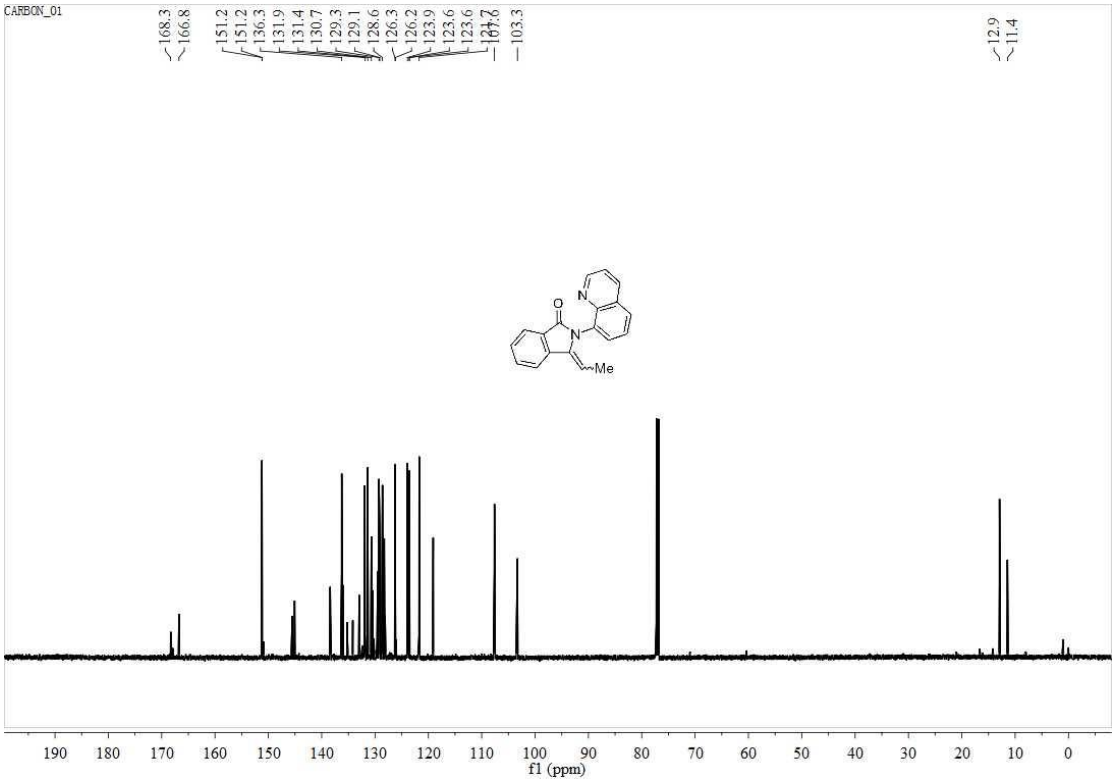
^{13}C NMR Spectrum of 4



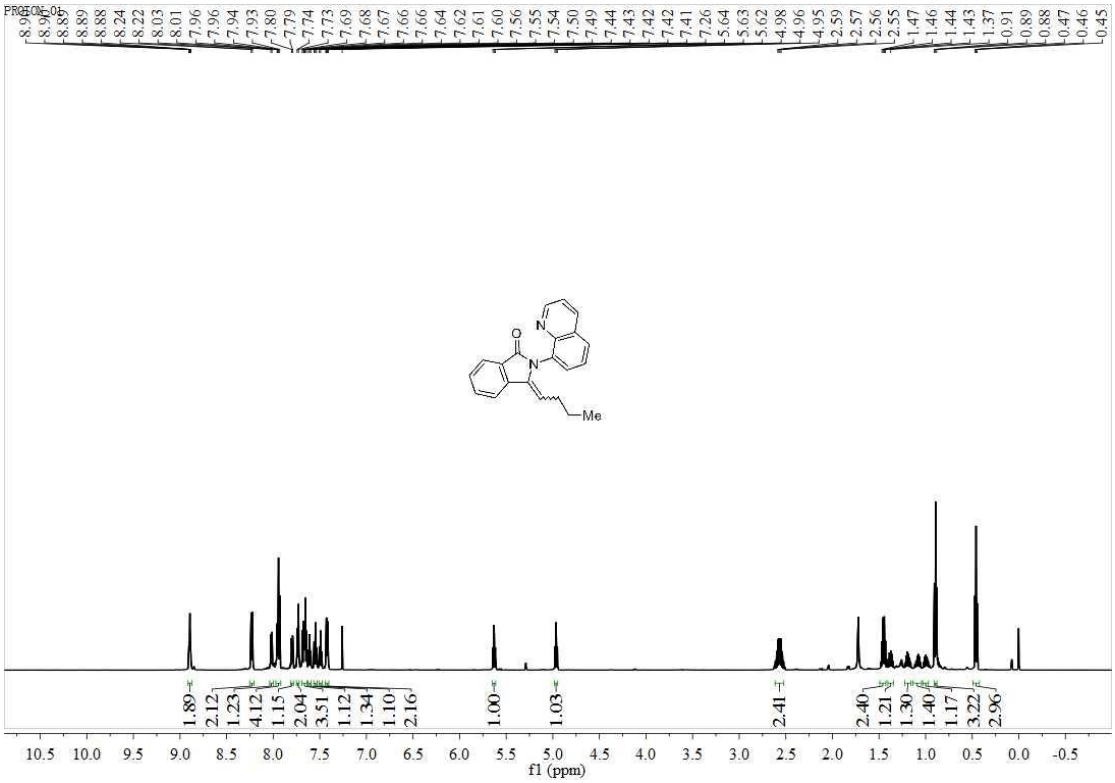
^{1}H NMR Spectrum of 3ab



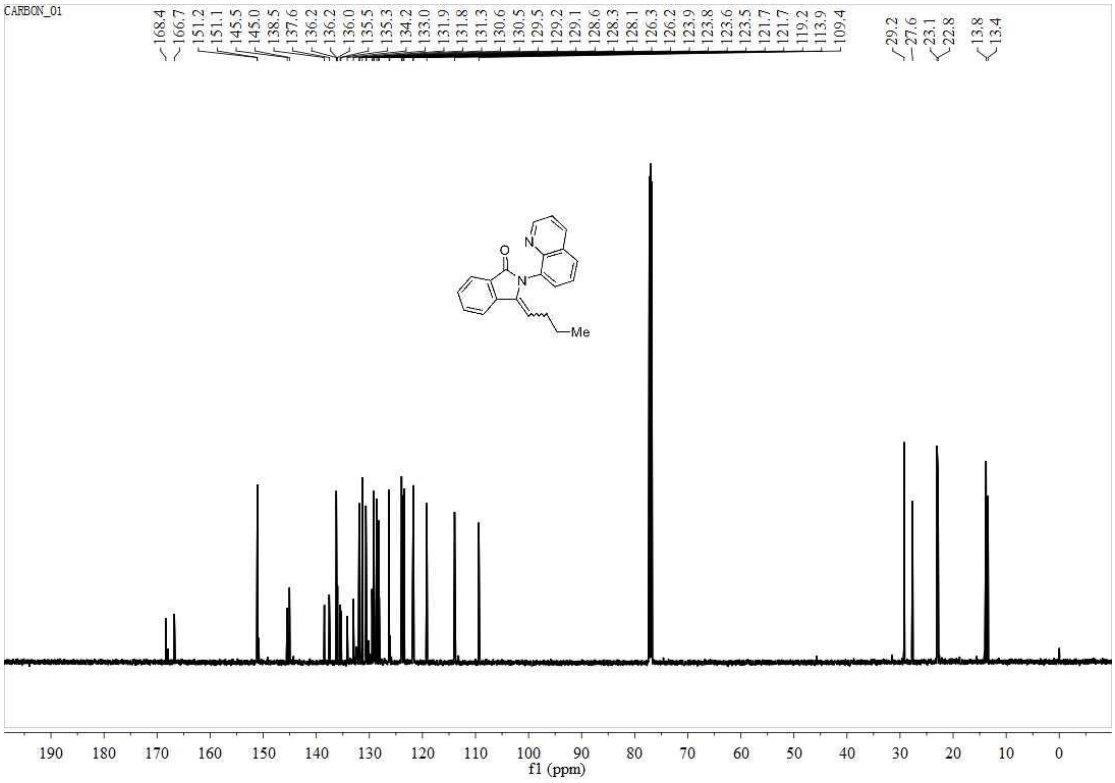
^{13}C NMR Spectrum of 3ab



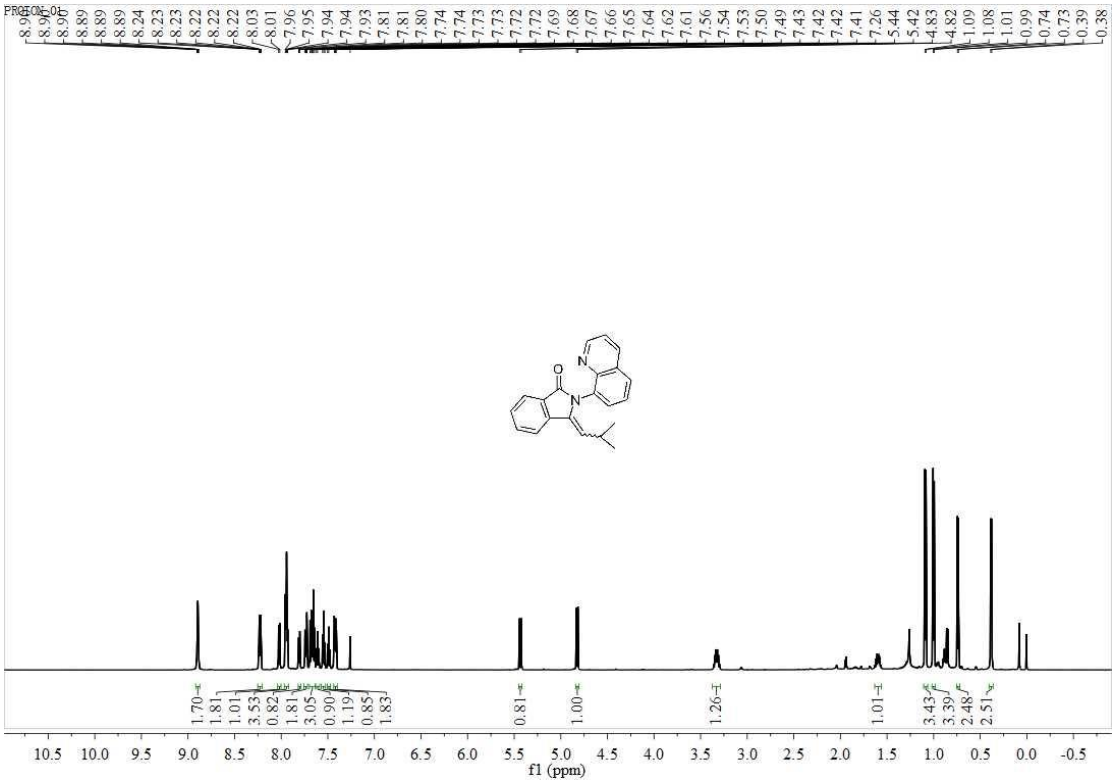
^{1}H NMR Spectrum of 3ac



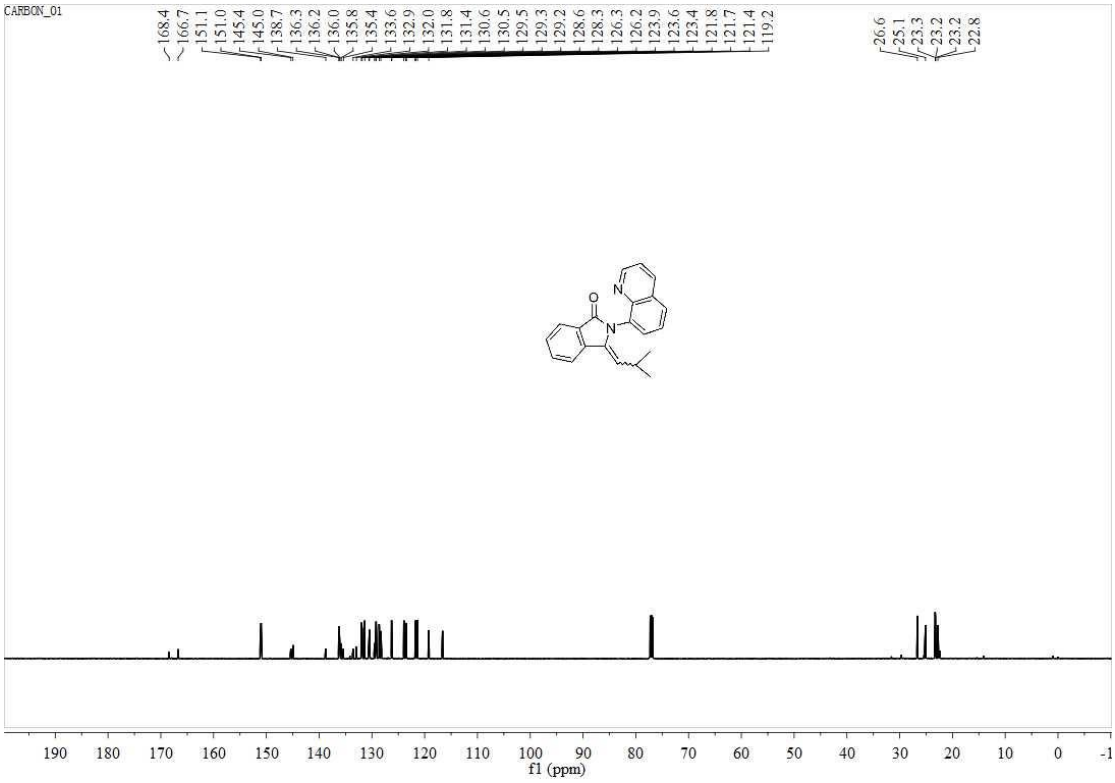
^{13}C NMR Spectrum of 3ac



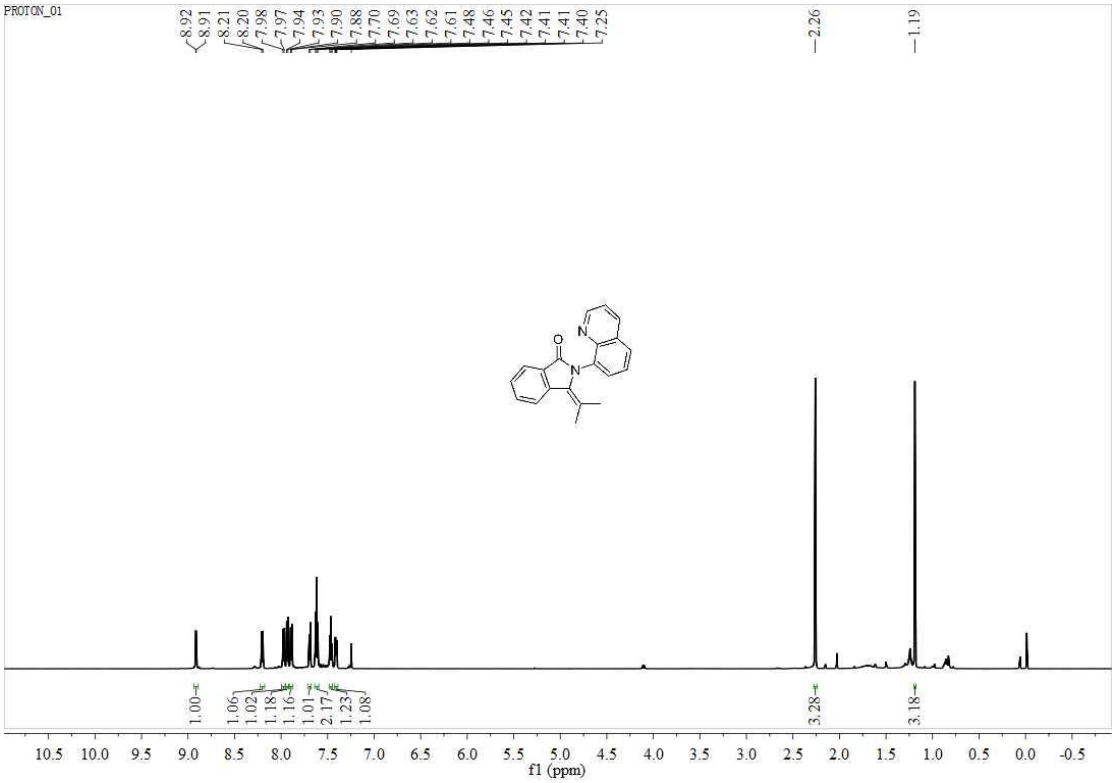
^{1}H NMR Spectrum of 3ad



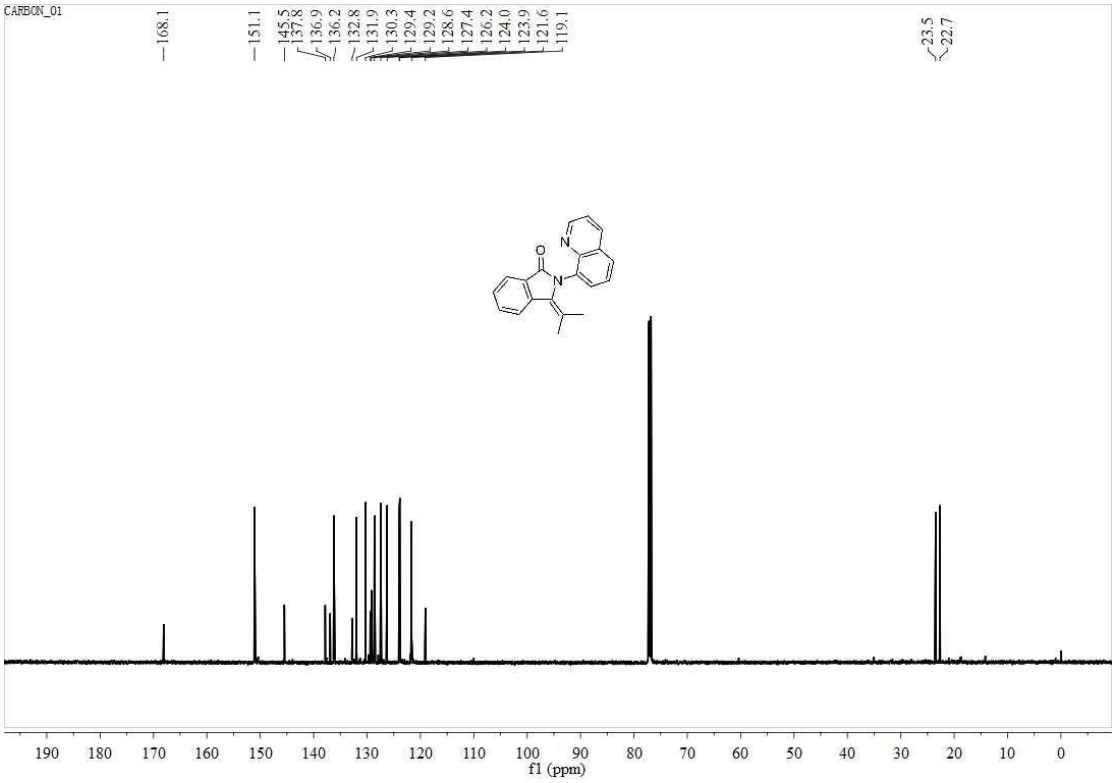
^{13}C NMR Spectrum of 3ad



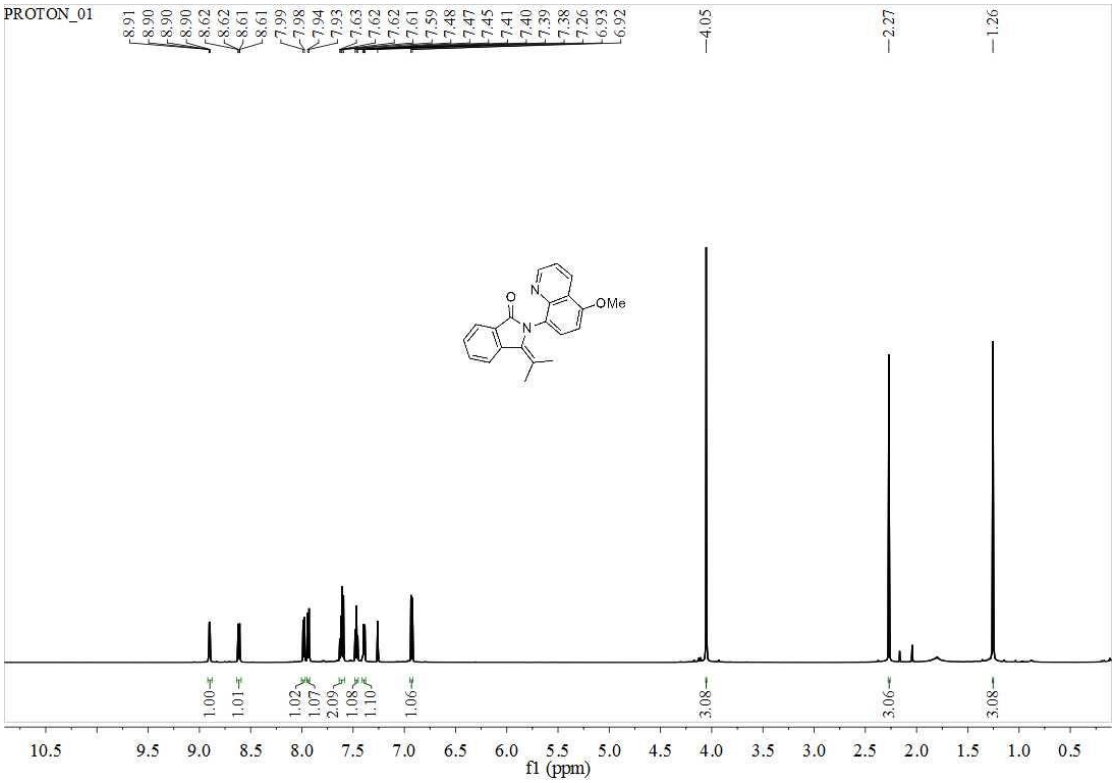
^{1}H NMR Spectrum of 3ae



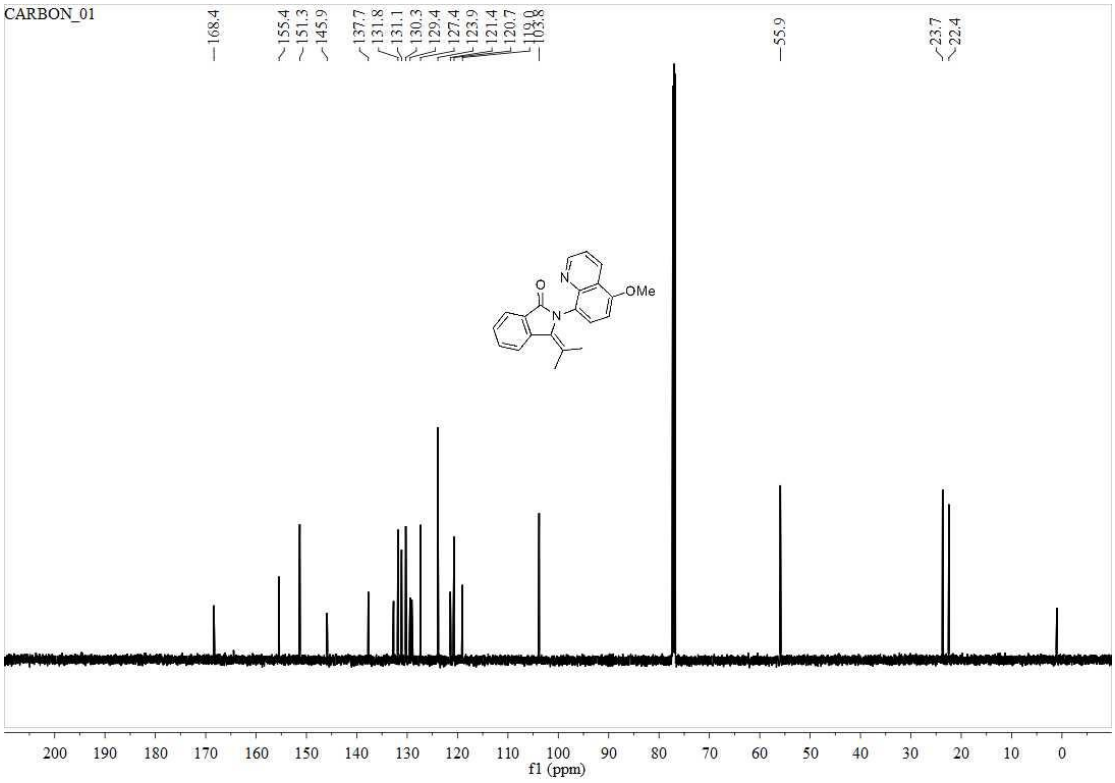
^{13}C NMR Spectrum of 3ae



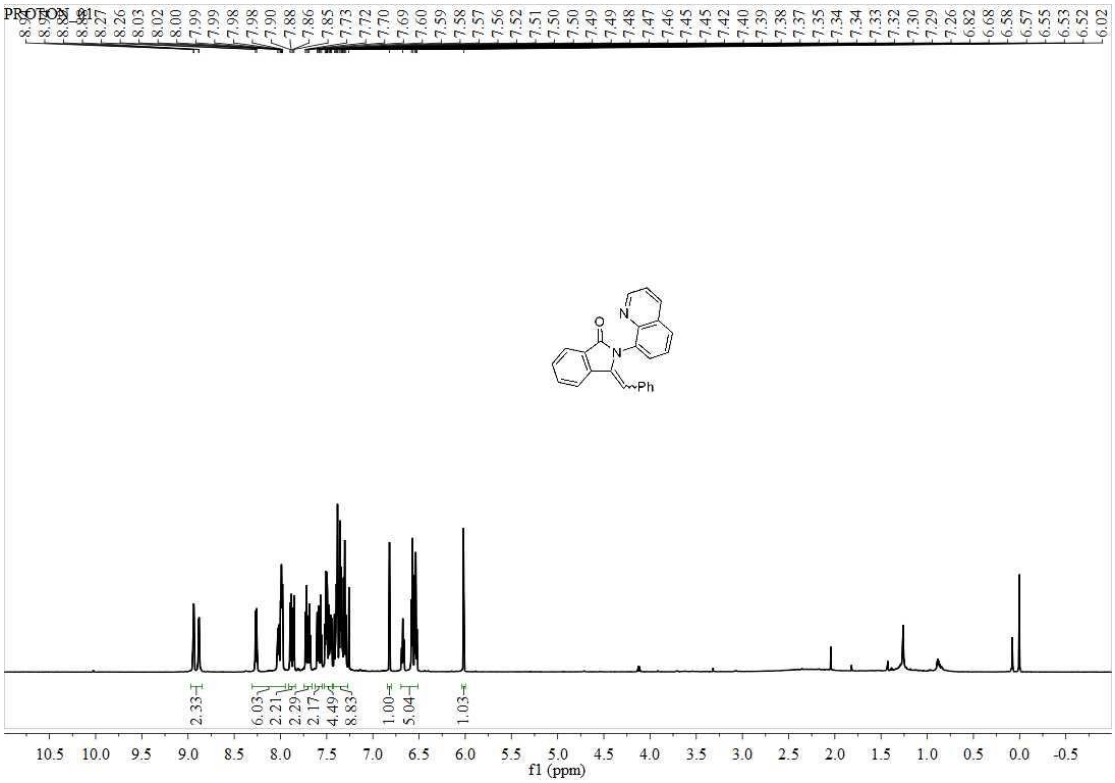
^{1}H NMR Spectrum of 3qe



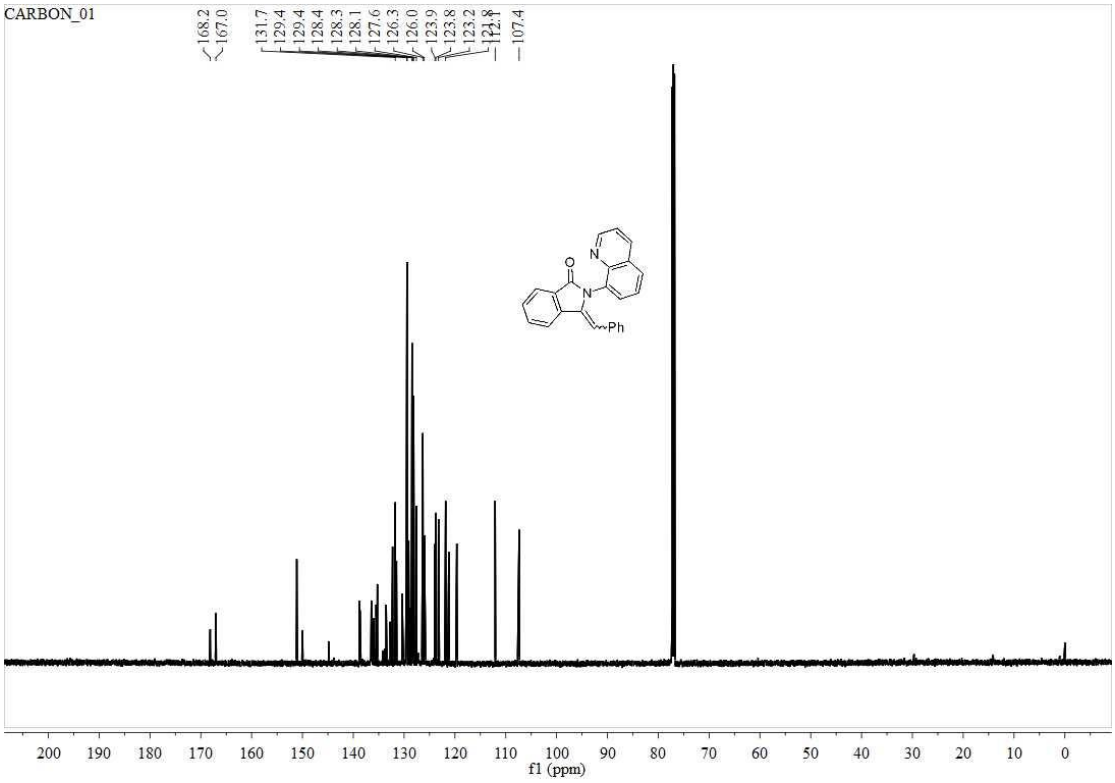
^{13}C NMR Spectrum of 3qe



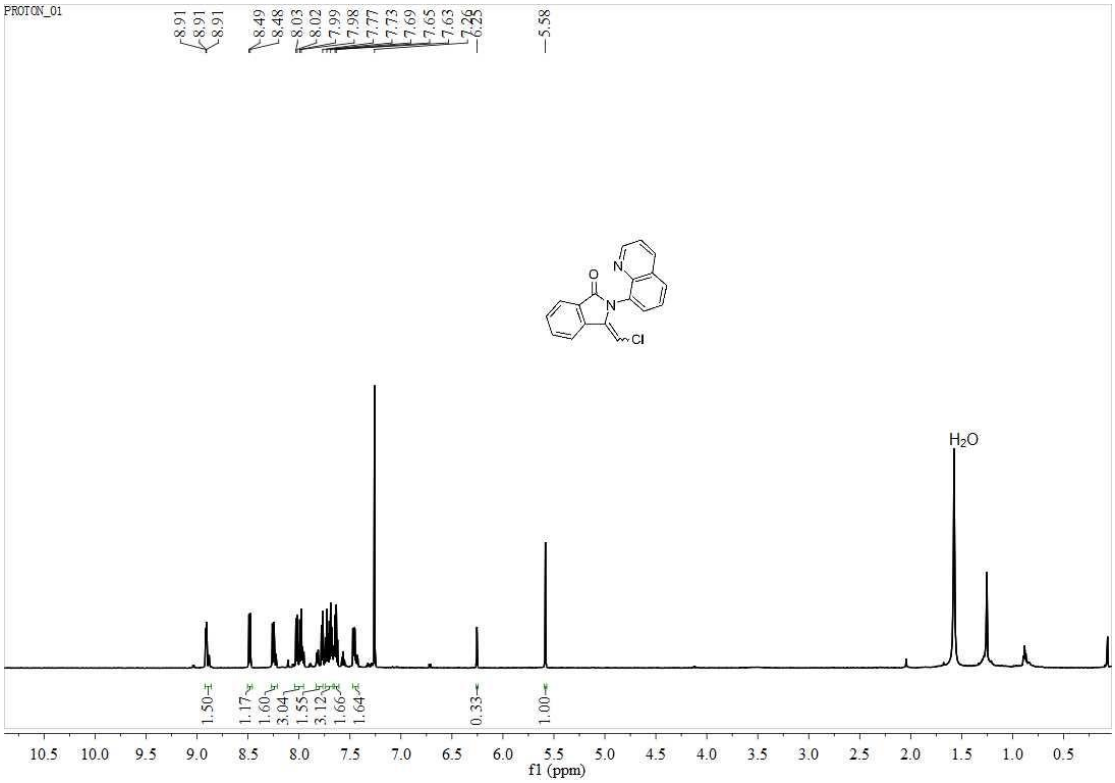
^{1}H NMR Spectrum of 3af



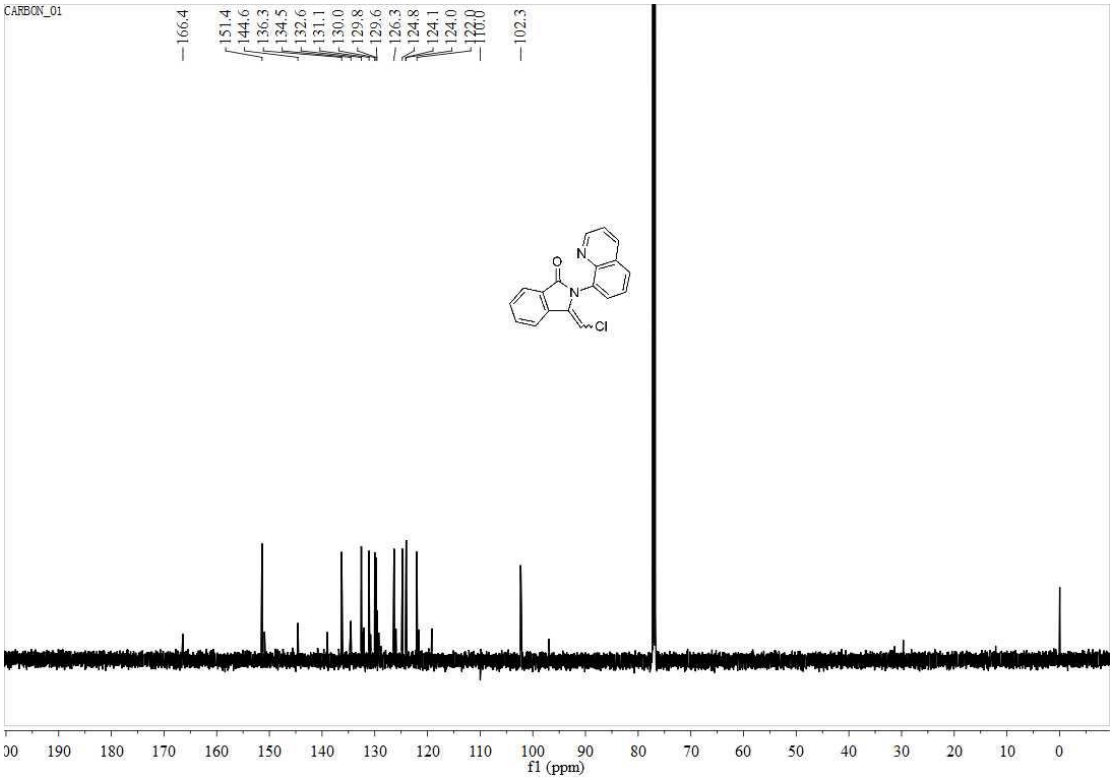
^{13}C NMR Spectrum of 3af



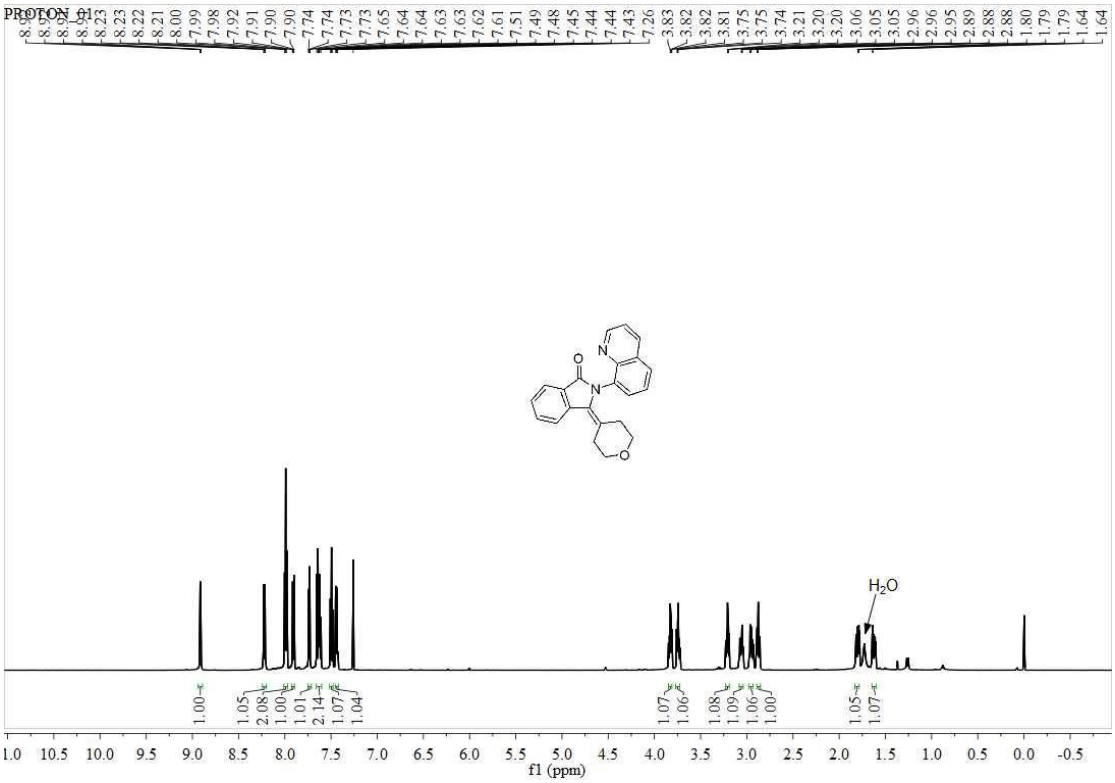
^{1}H NMR Spectrum of 3ag



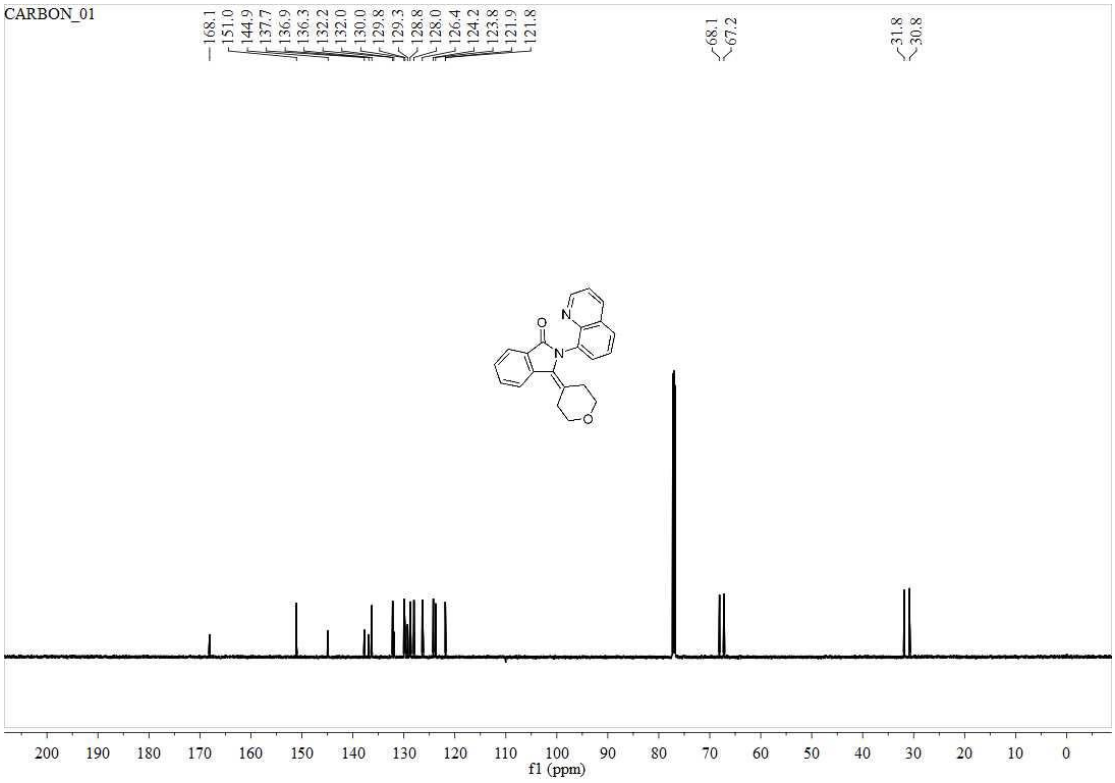
^{13}C NMR Spectrum of 3ag



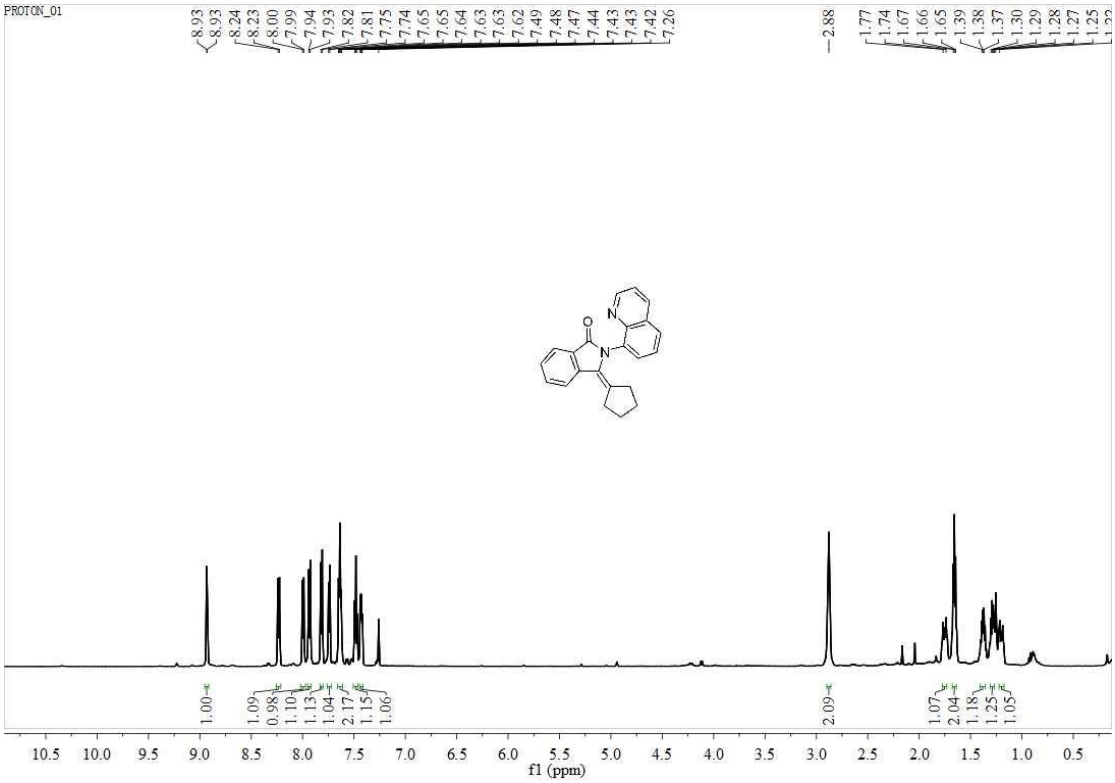
^{1}H NMR Spectrum of 3ah



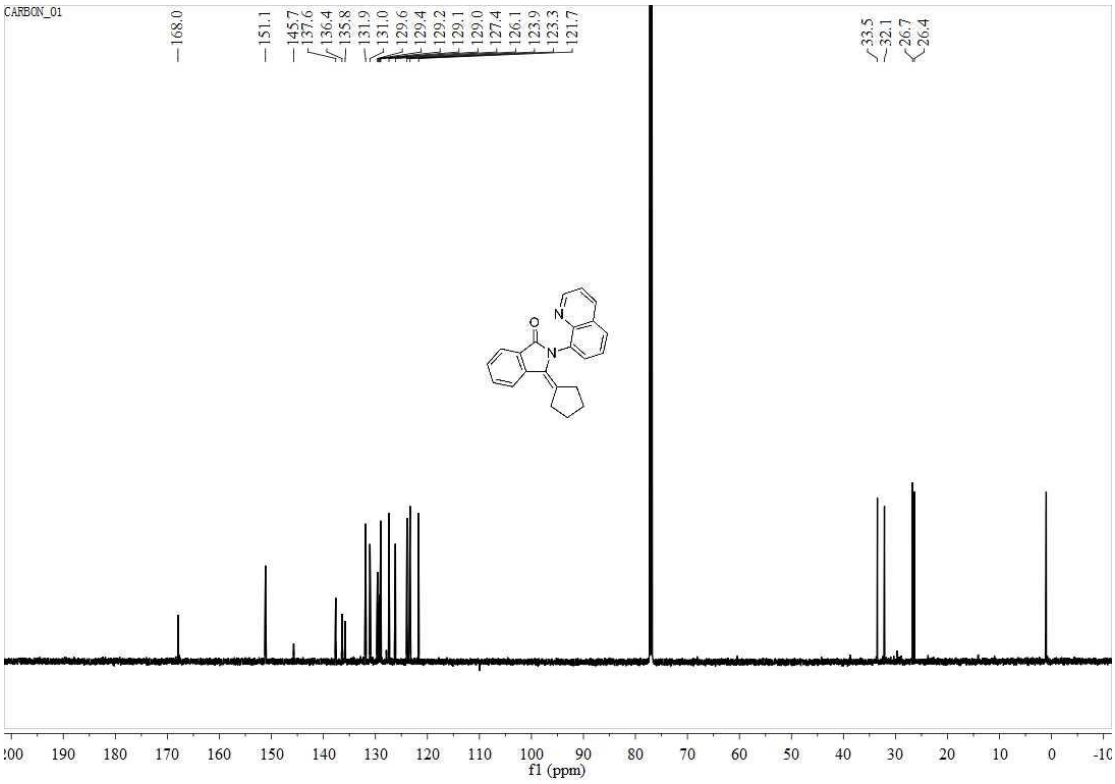
^{13}C NMR Spectrum of 3ah



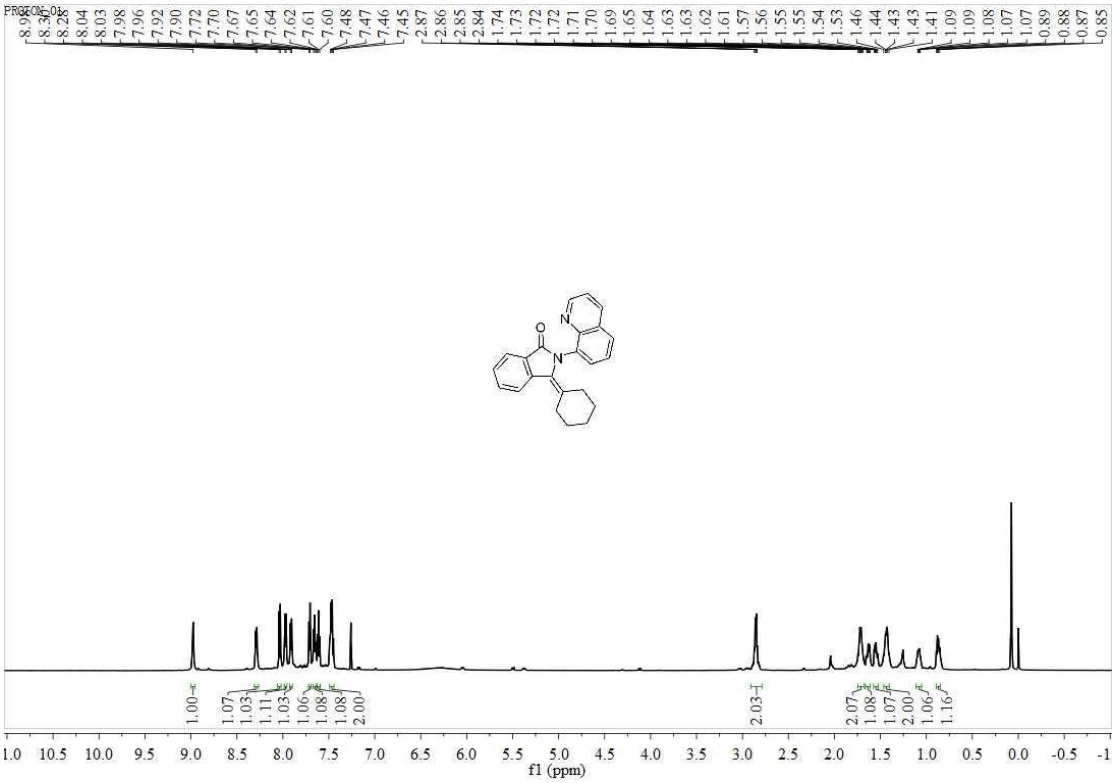
^{1}H NMR Spectrum of 3ai



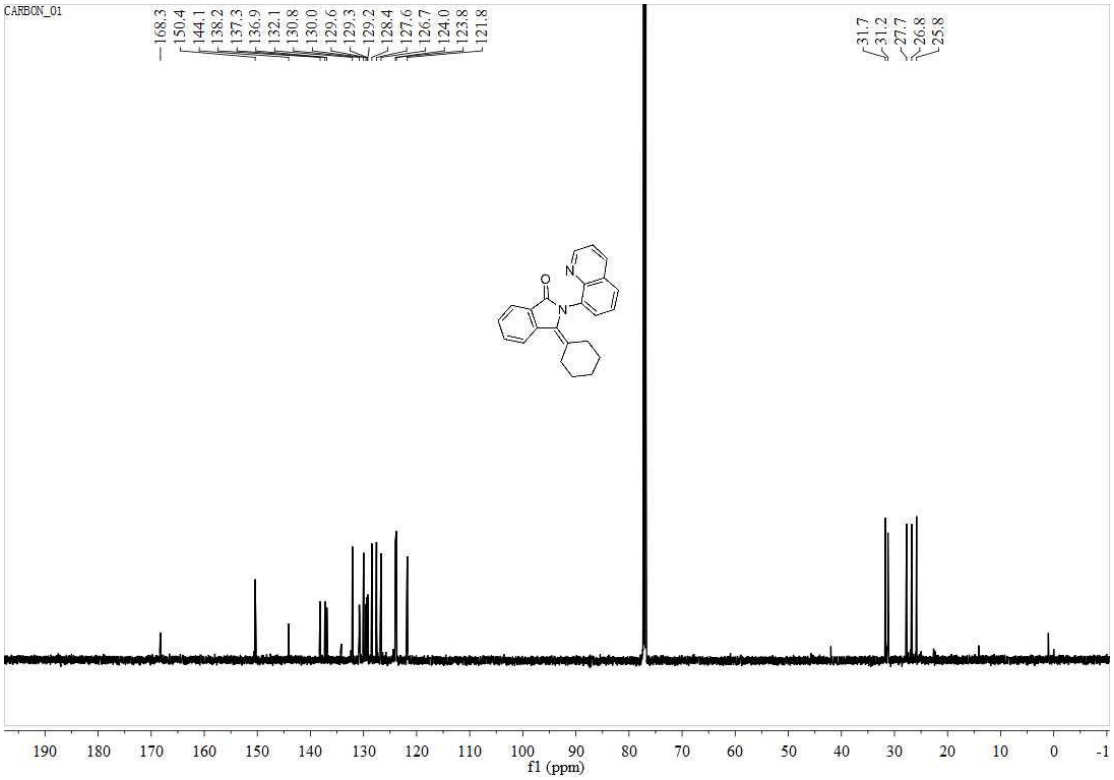
^{13}C NMR Spectrum of 3ai



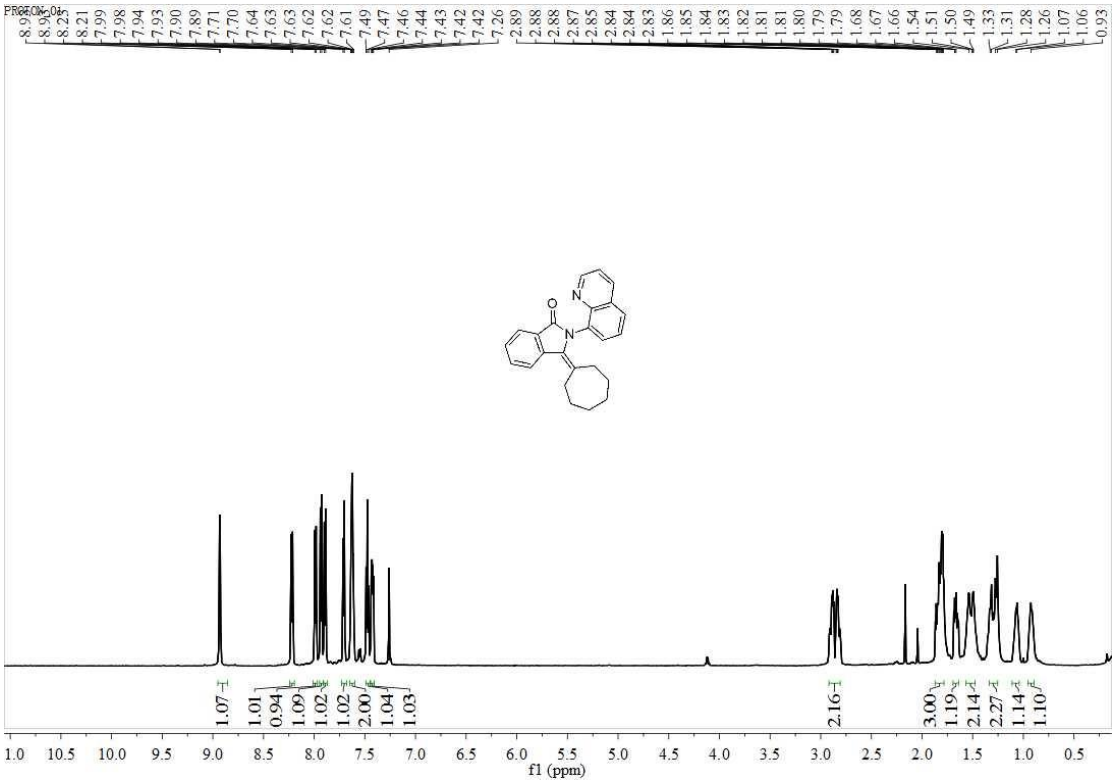
^{1}H NMR Spectrum of 3aj



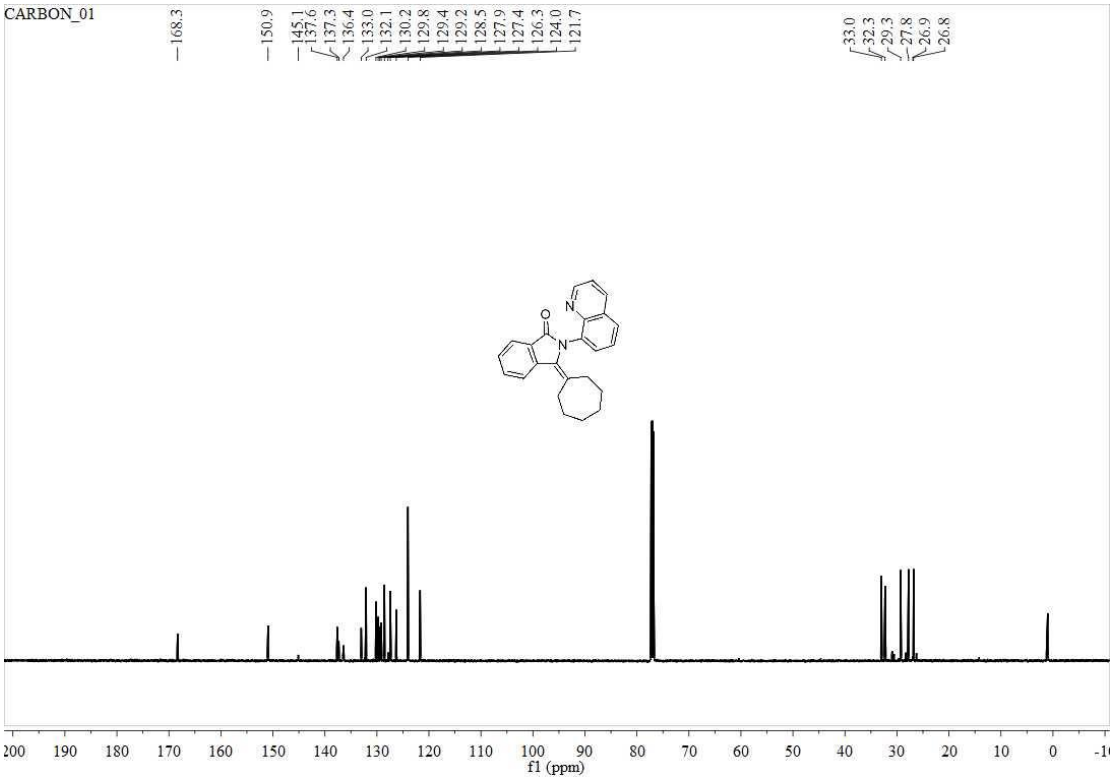
^{13}C NMR Spectrum of 3aj



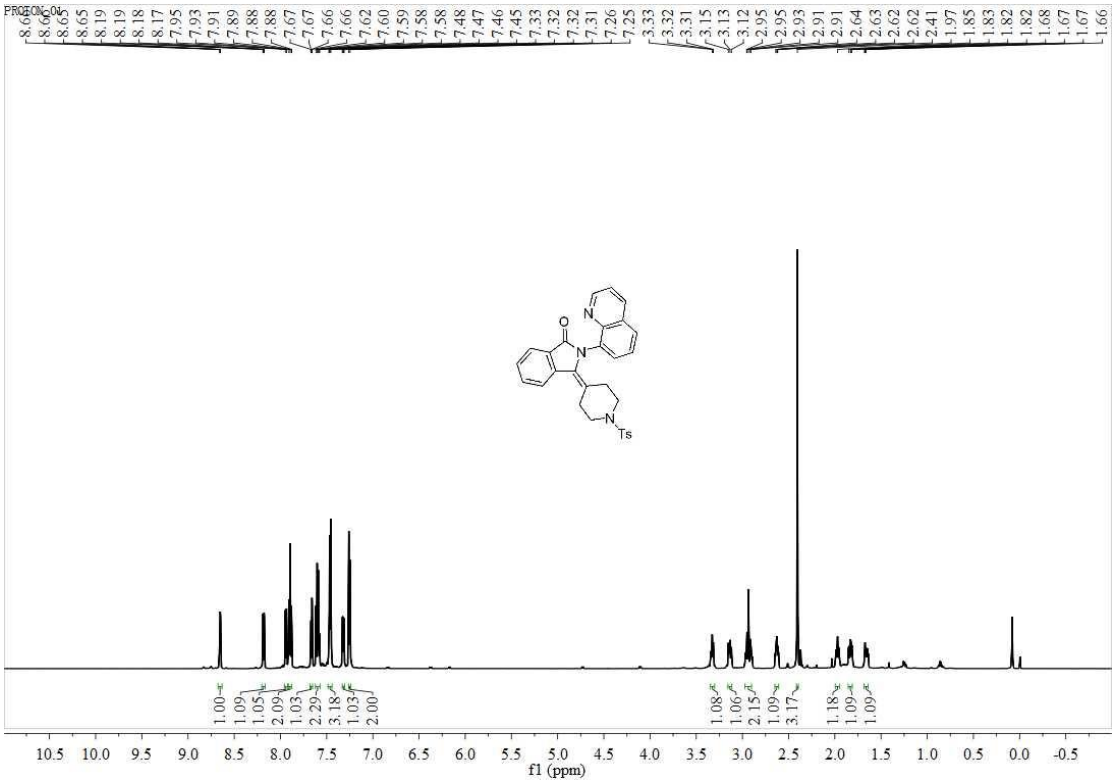
^{1}H NMR Spectrum of 3ak



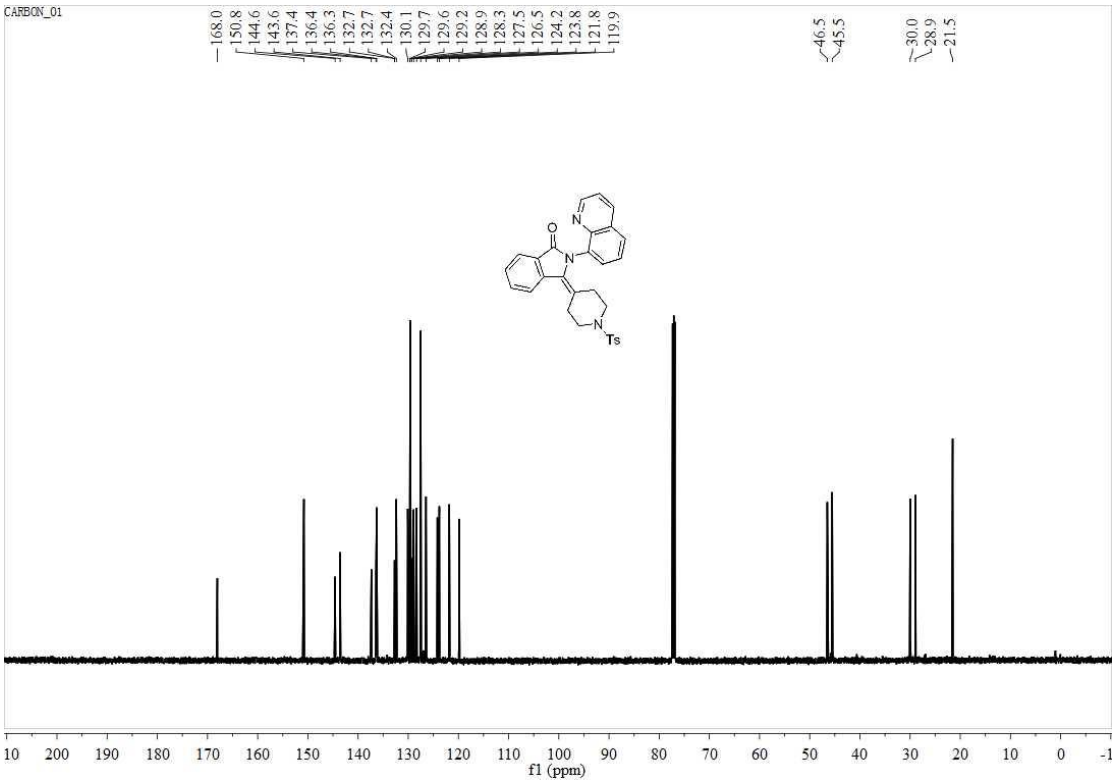
^{13}C NMR Spectrum of 3ak



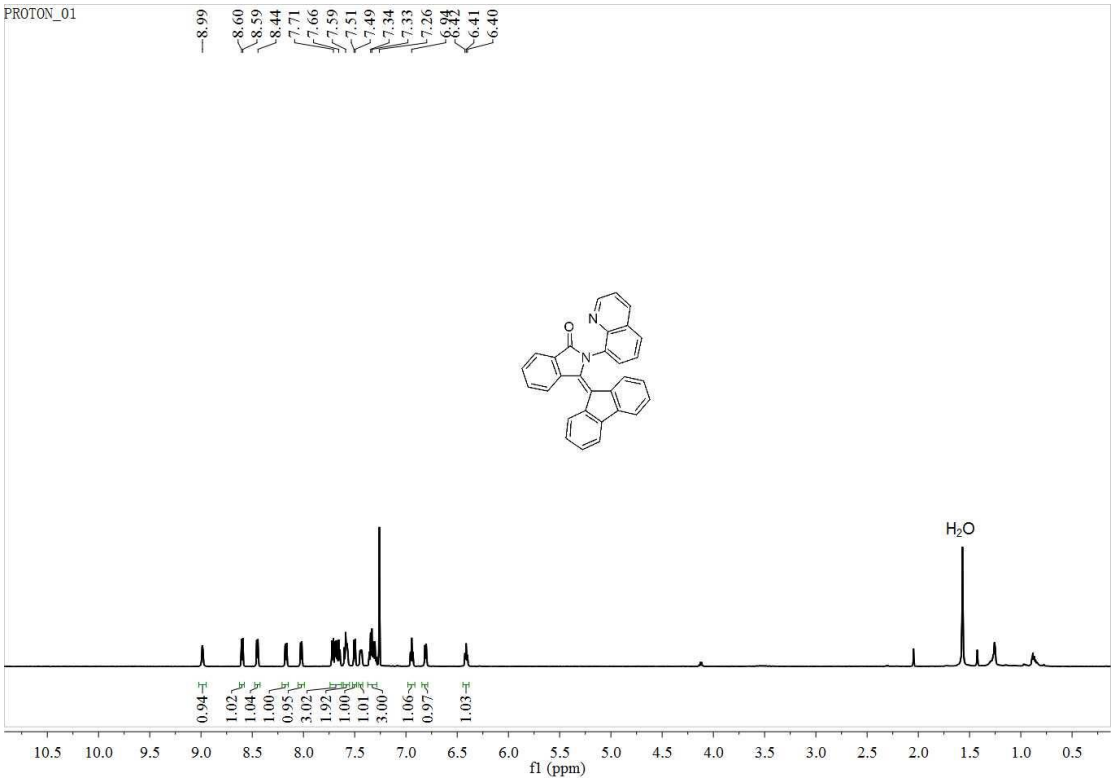
^{1}H NMR Spectrum of 3al



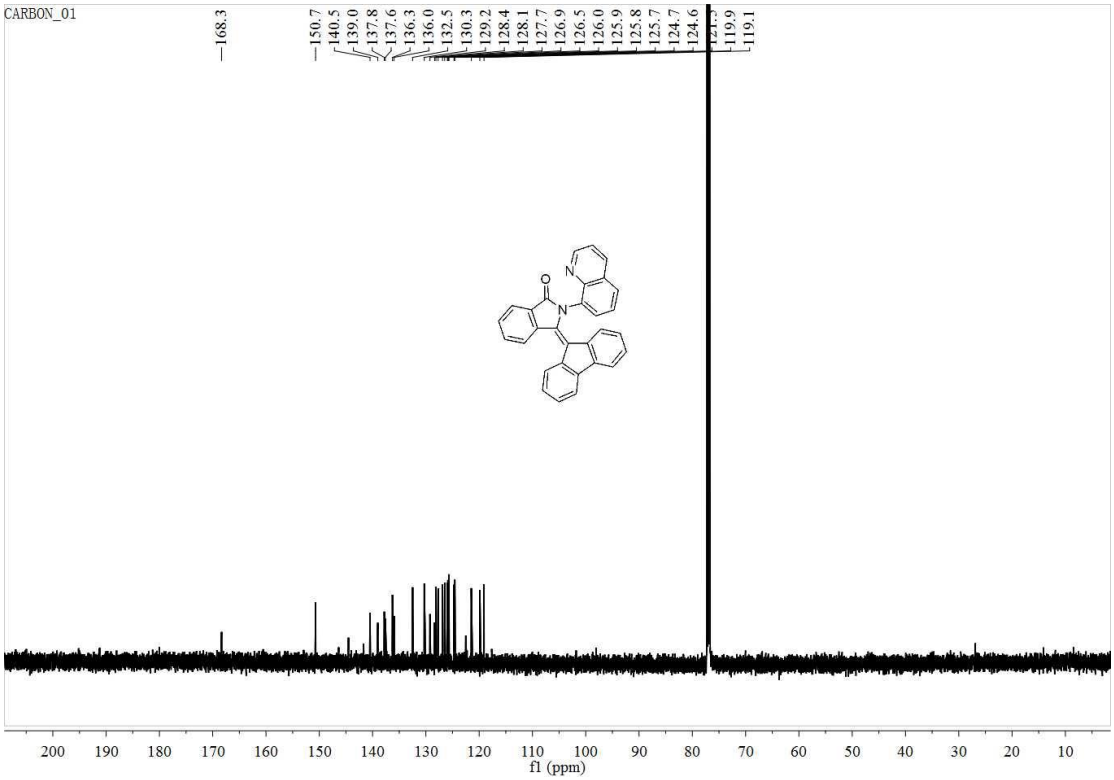
^{13}C NMR Spectrum of 3al



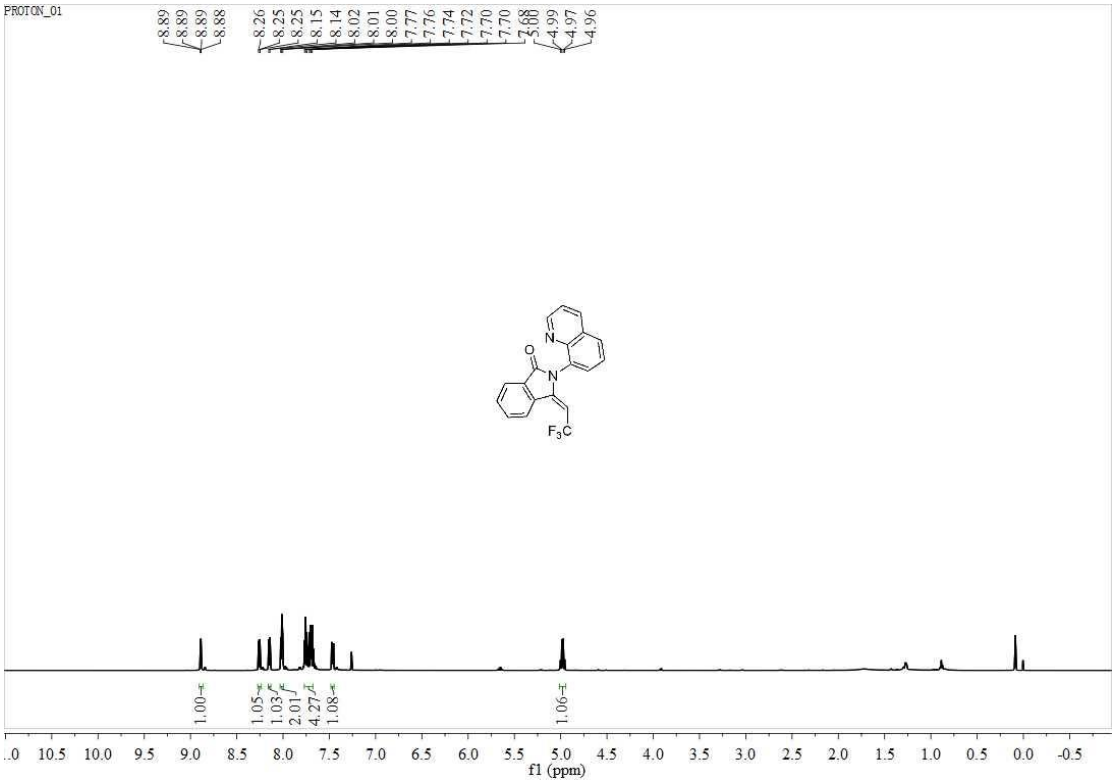
^{1}H NMR Spectrum of 3am



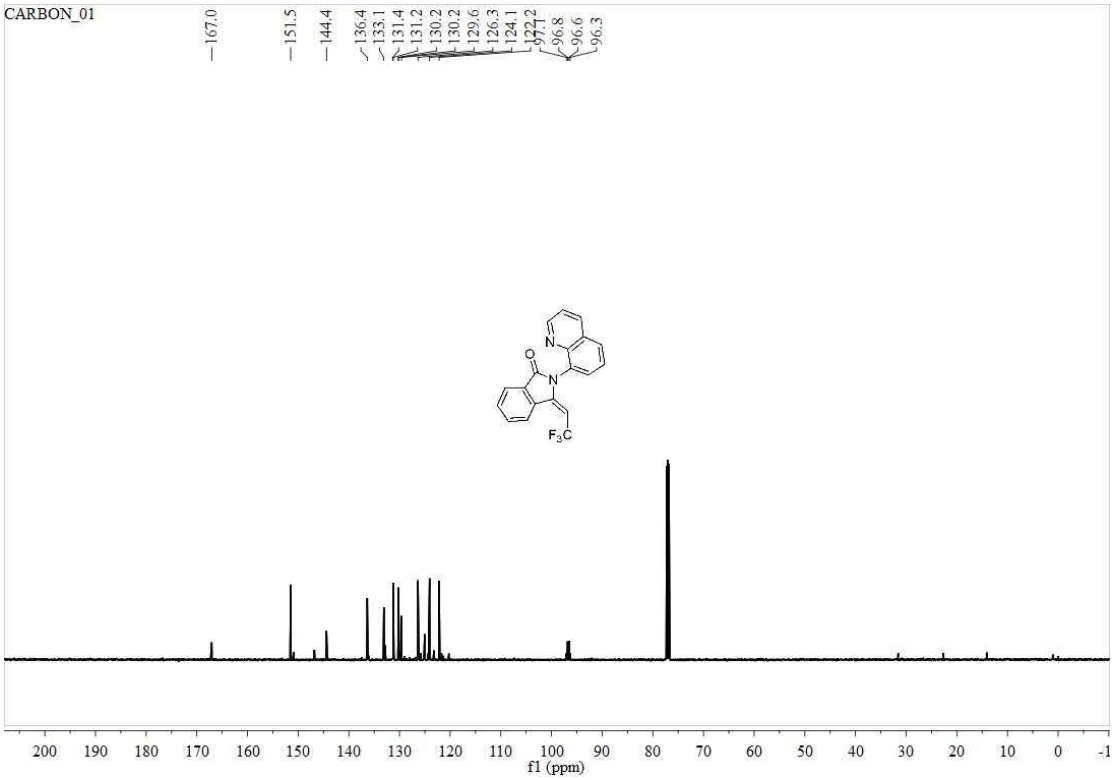
^{13}C NMR Spectrum of 3am



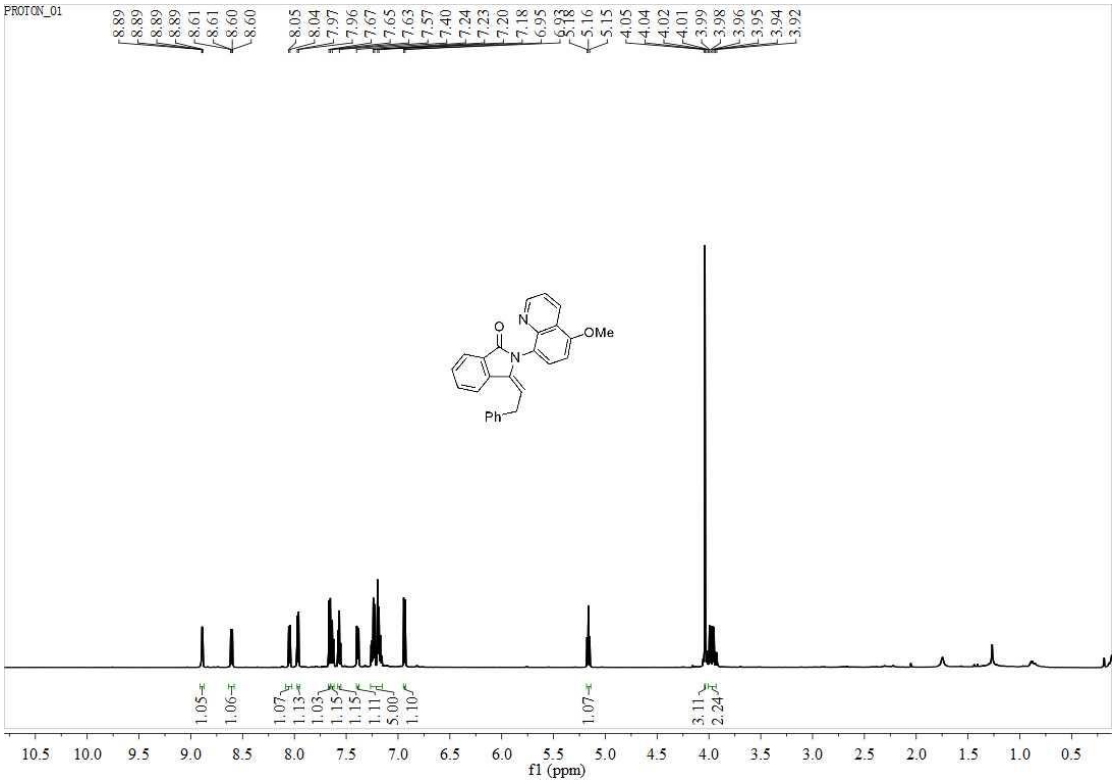
^{1}H NMR Spectrum of 3an



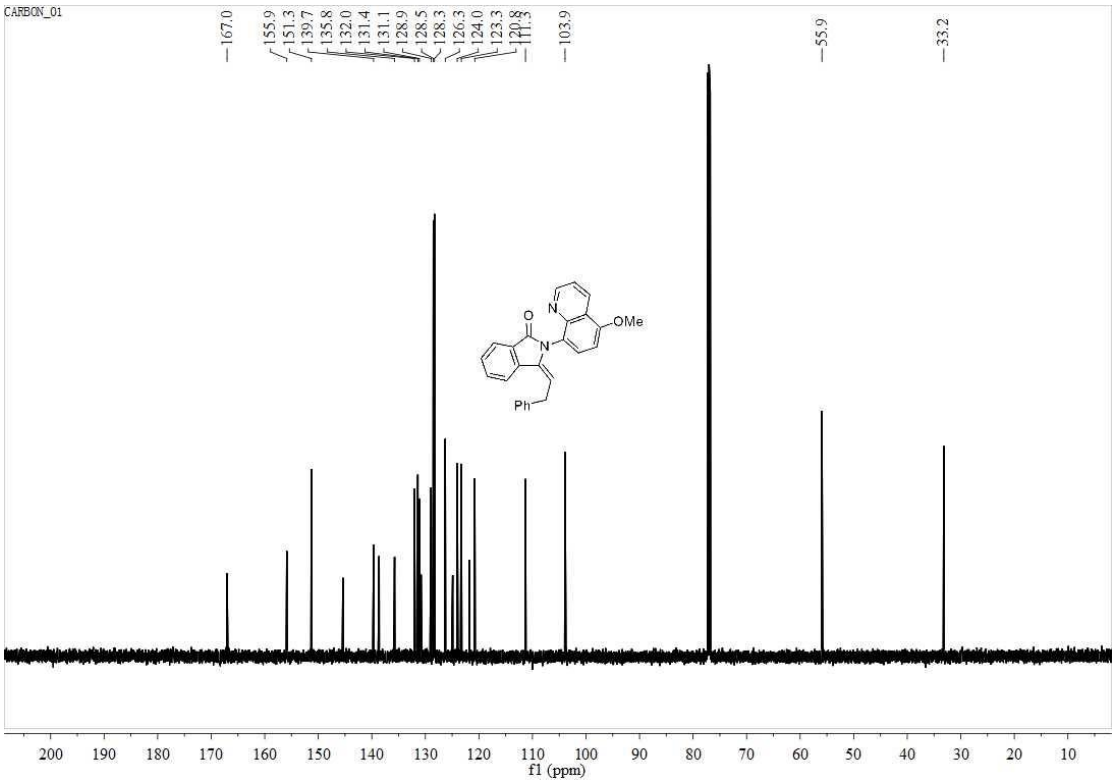
^{13}C NMR Spectrum of 3an



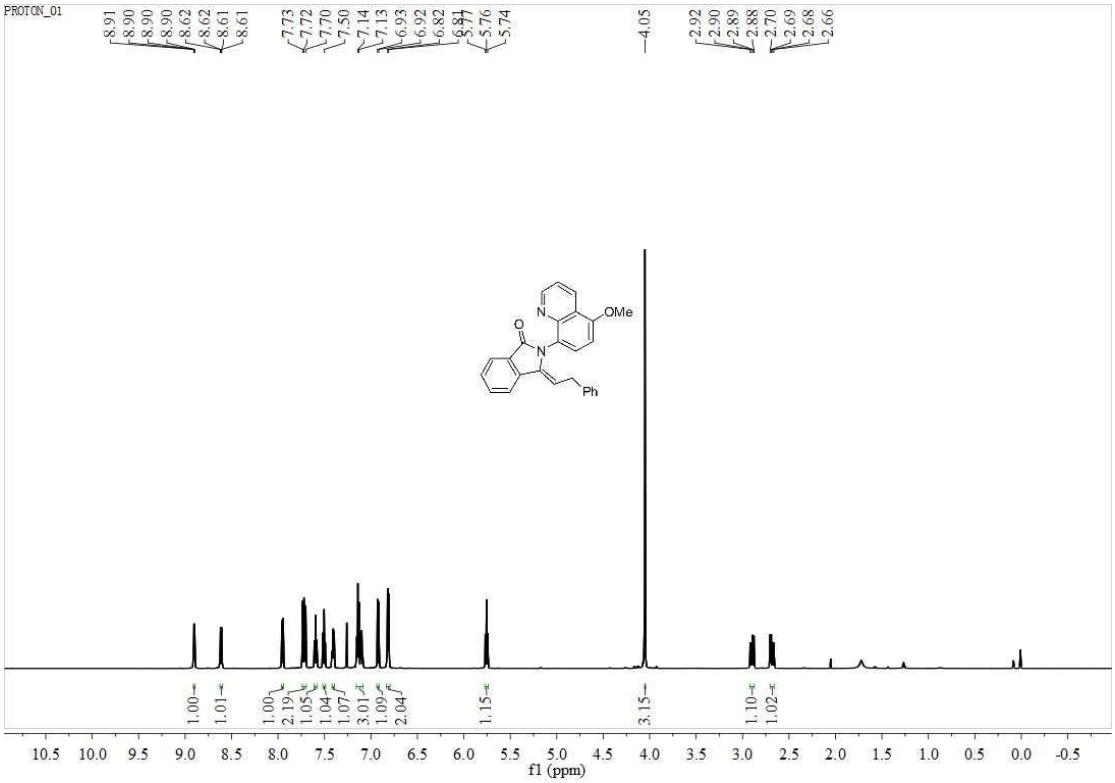
^{1}H NMR Spectrum of 3qo



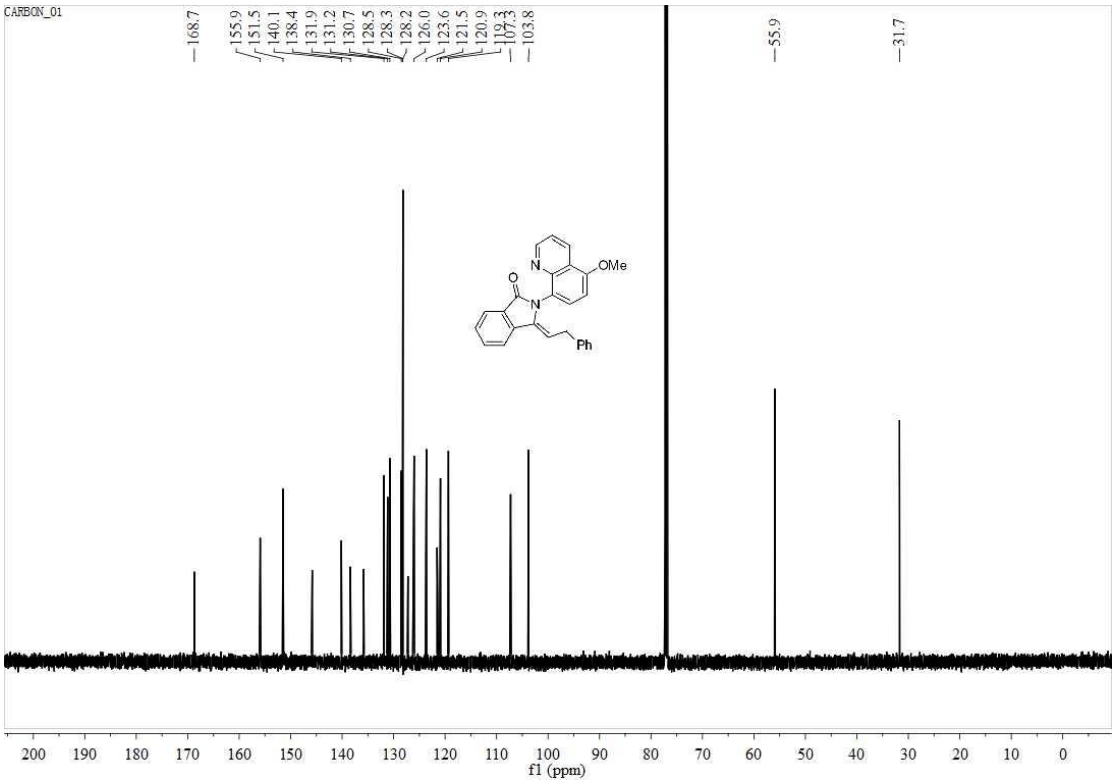
^{13}C NMR Spectrum of 3qo



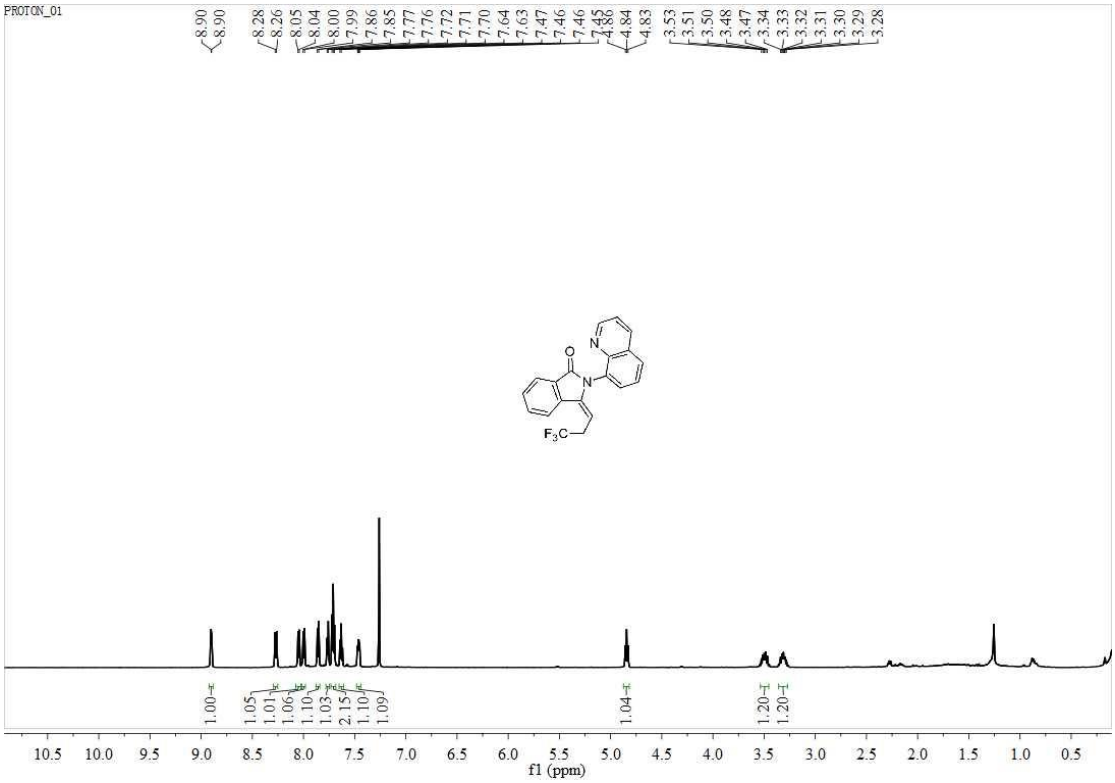
^{1}H NMR Spectrum of 3qo'



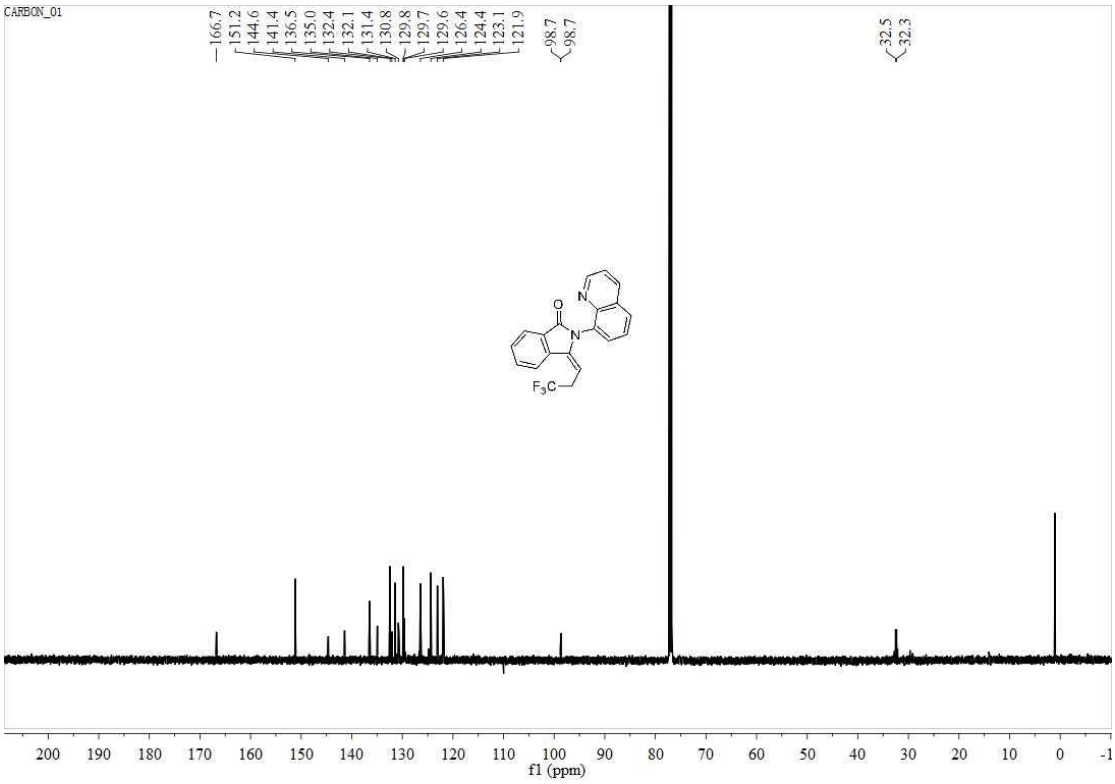
^{13}C NMR Spectrum of 3qo'



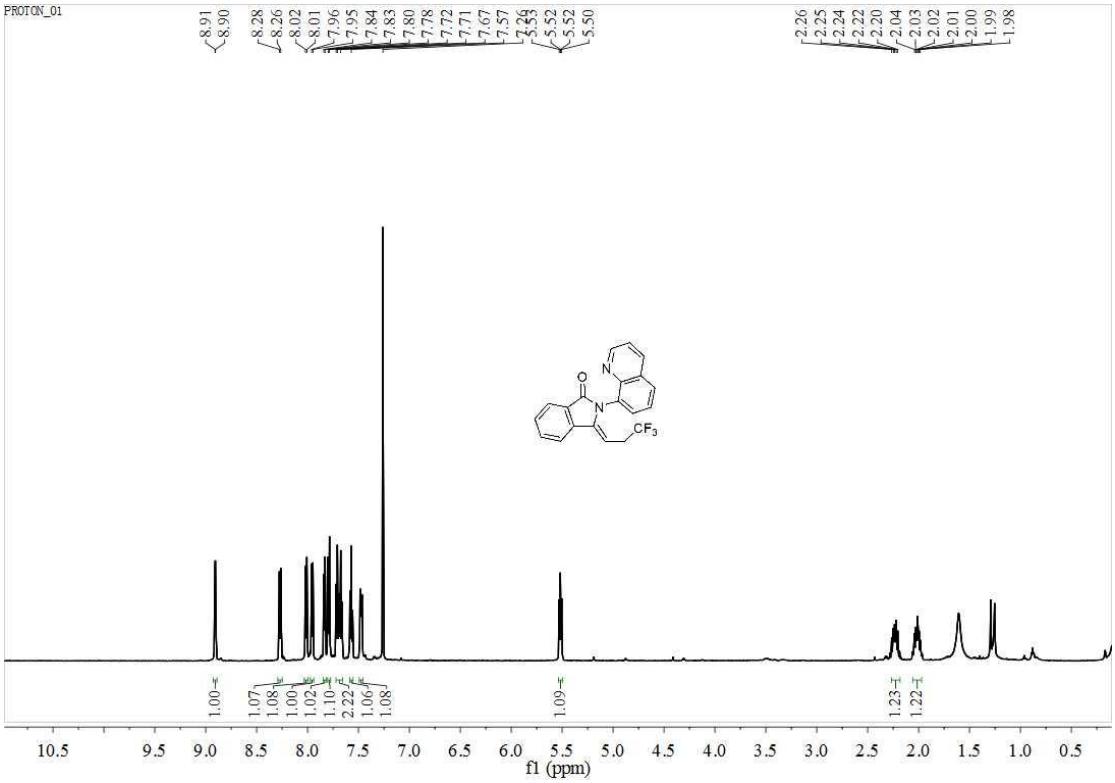
^{1}H NMR Spectrum of 3ap



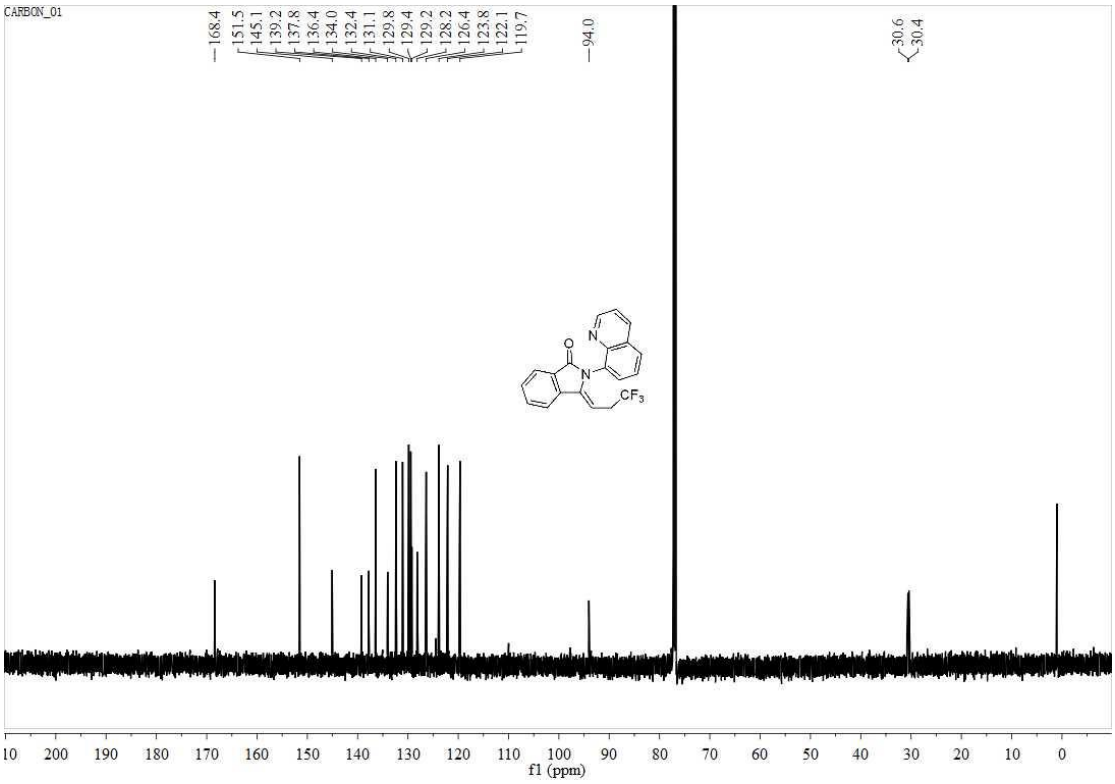
^{13}C NMR Spectrum of 3ap



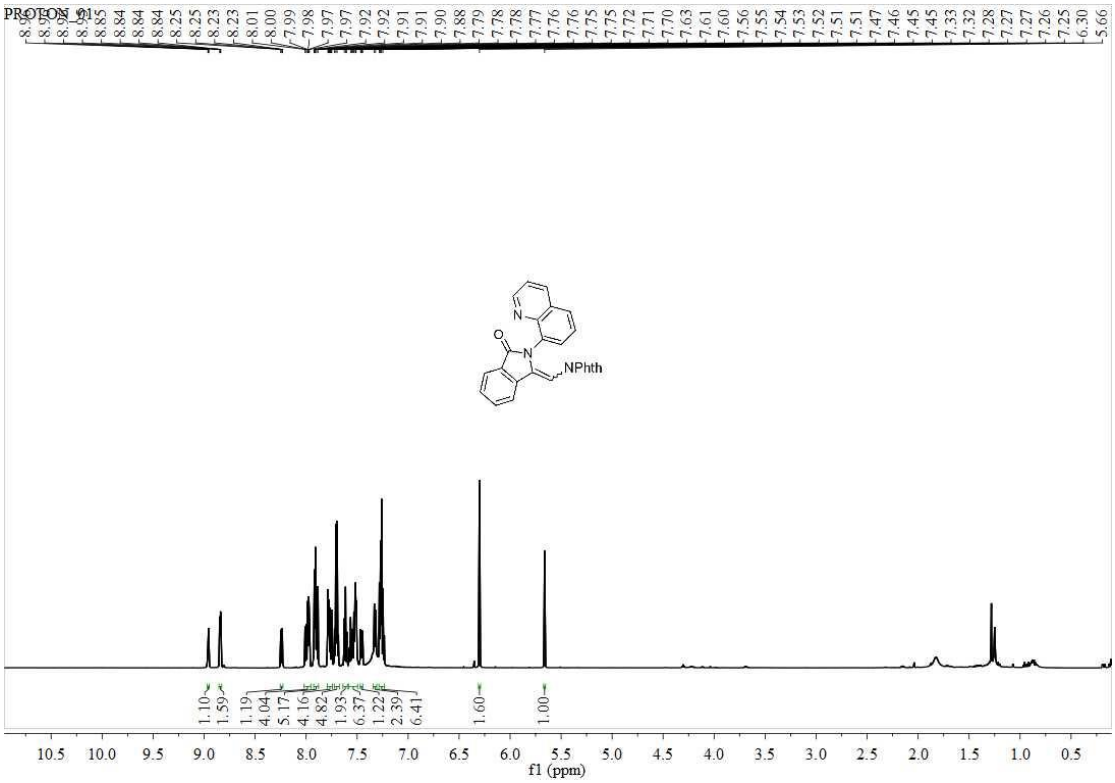
^{1}H NMR Spectrum of 3ap'



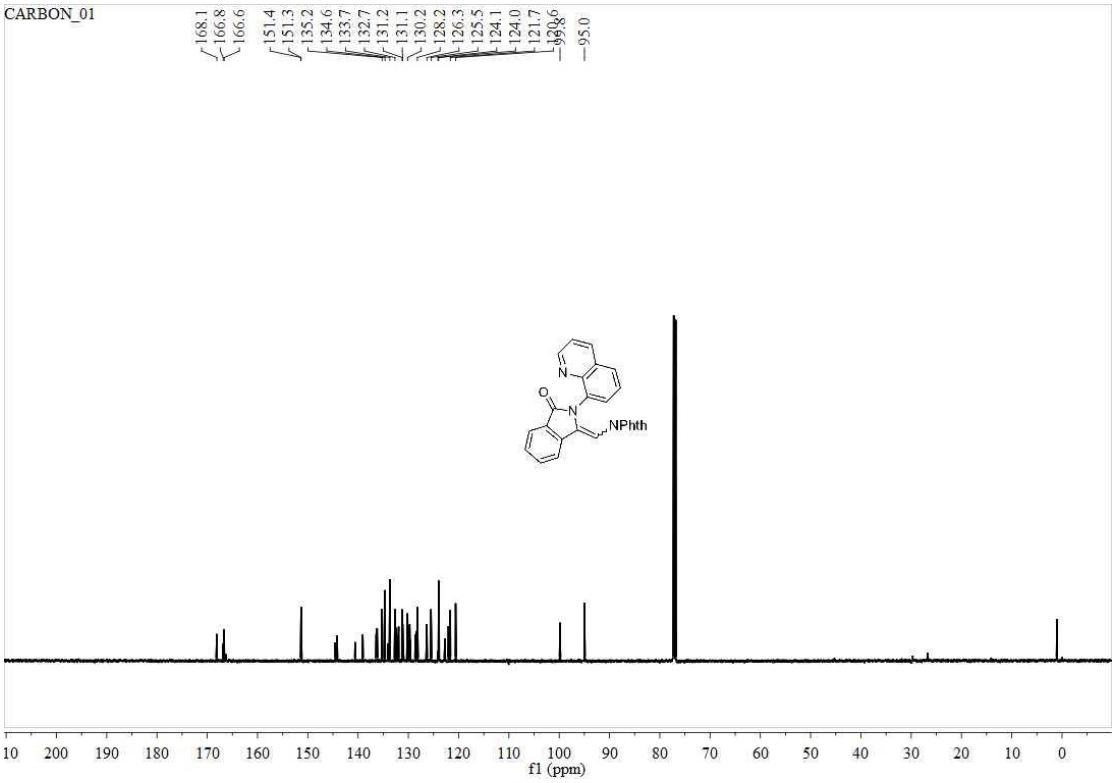
^{13}C NMR Spectrum of 3ap'



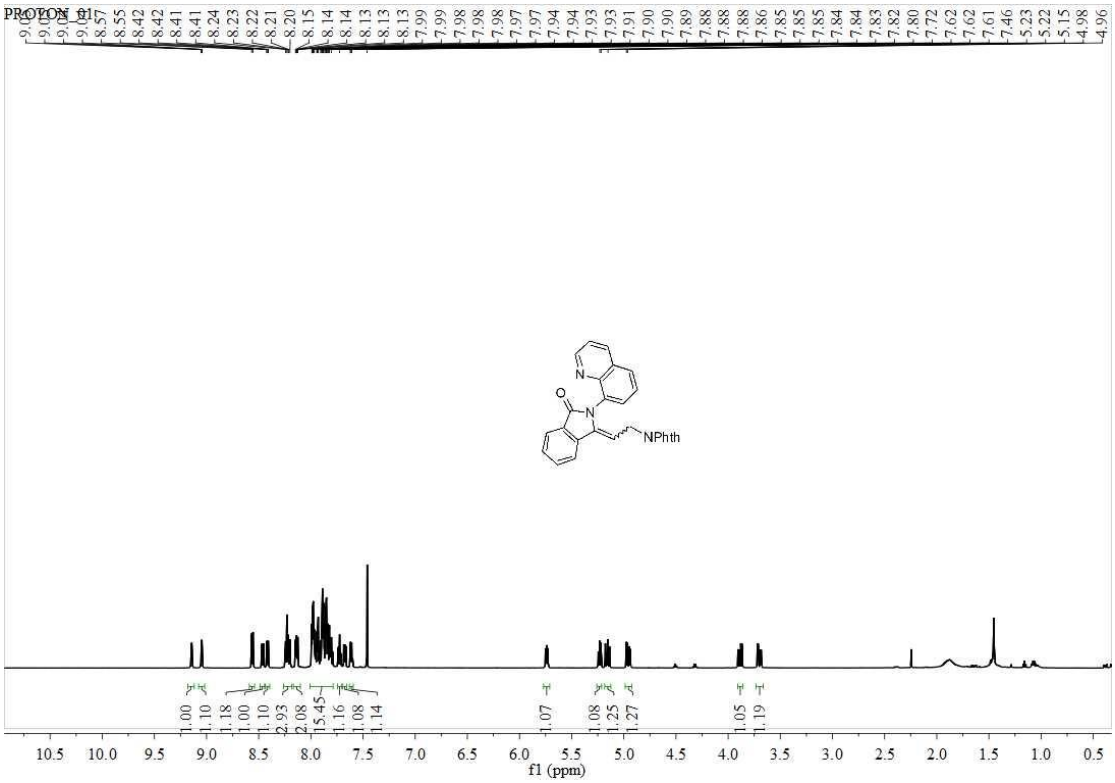
^{1}H NMR Spectrum of 3aq



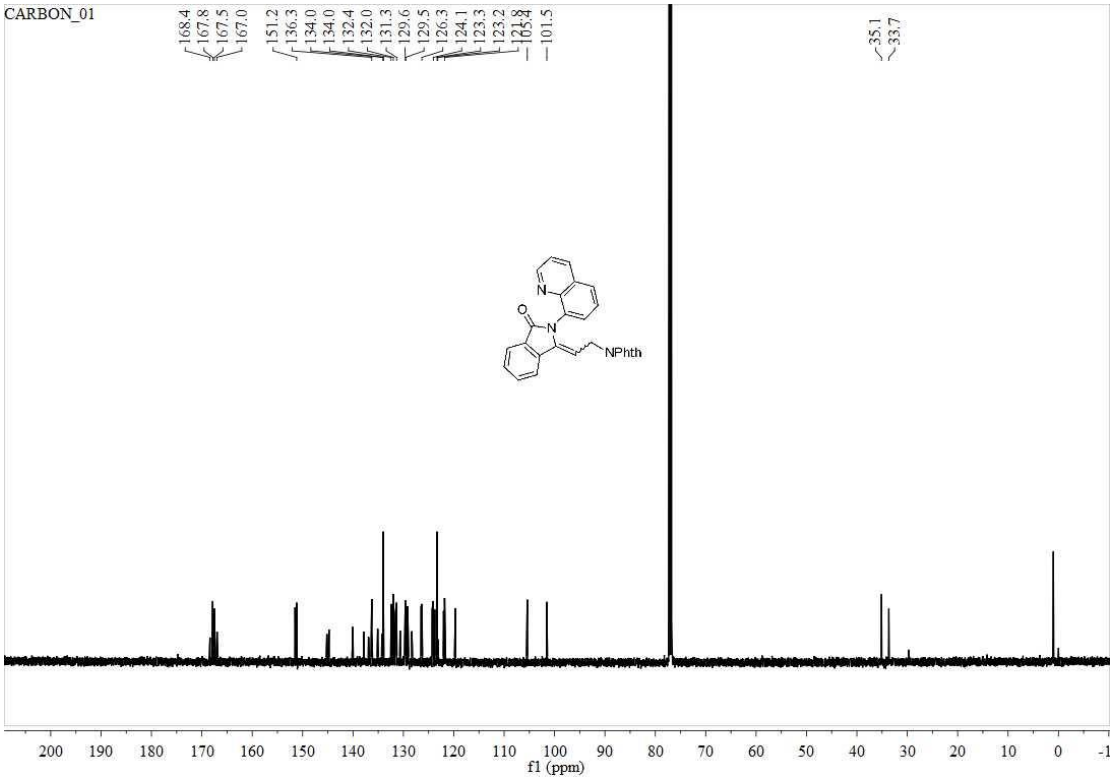
^{13}C NMR Spectrum of 3aq

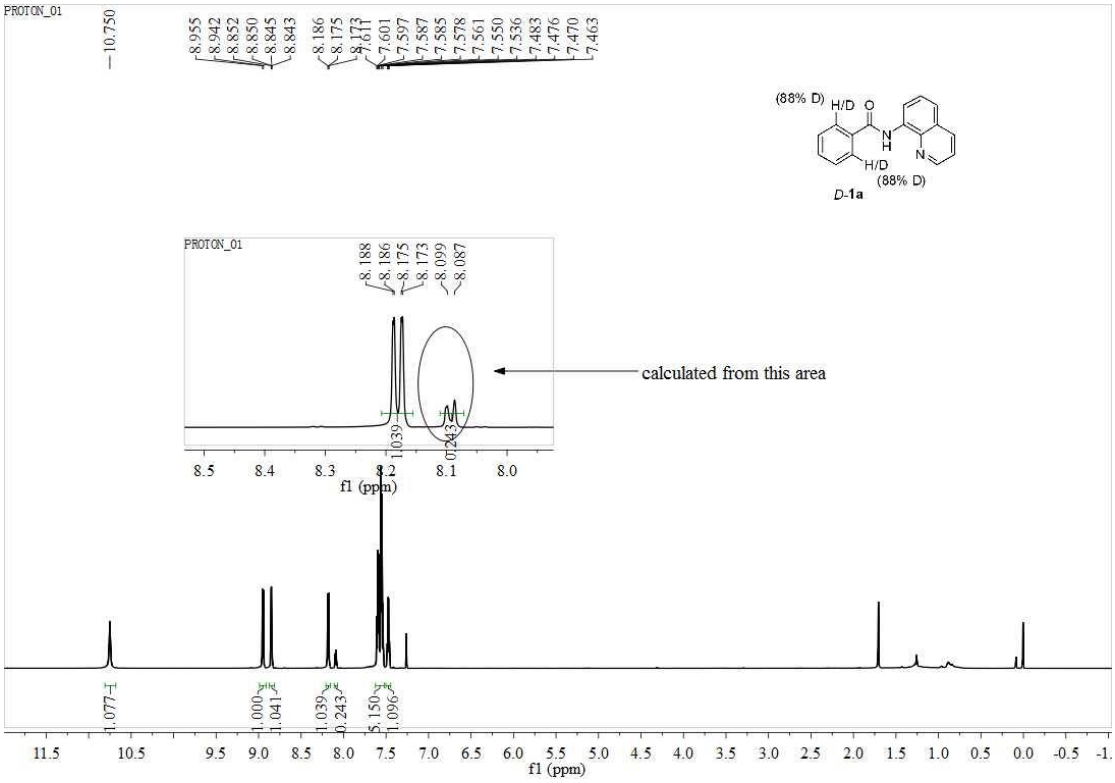


^{1}H NMR Spectrum of 3ar



^{13}C NMR Spectrum of 3ar

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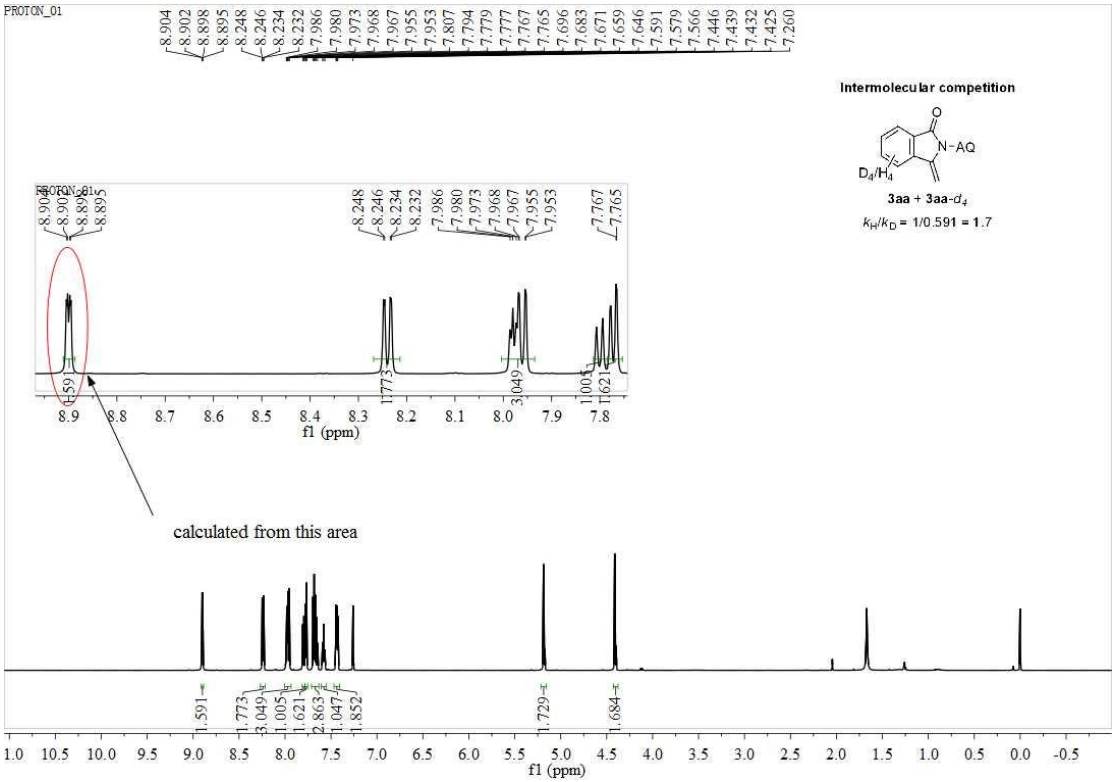
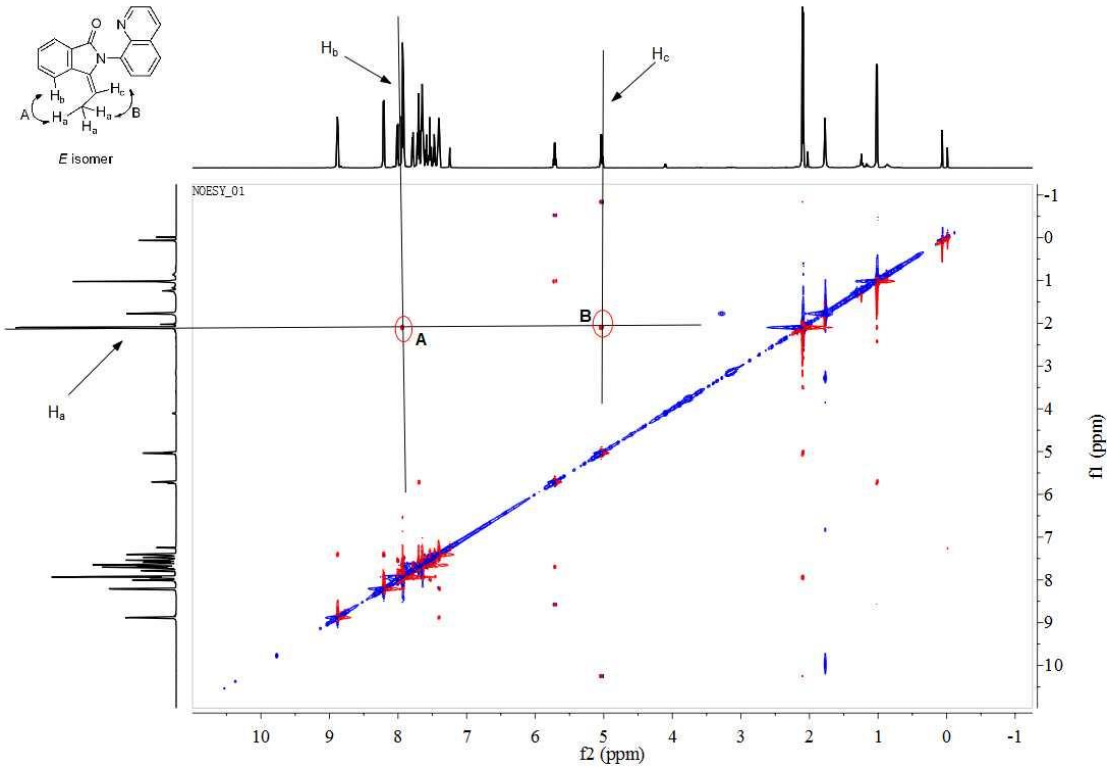
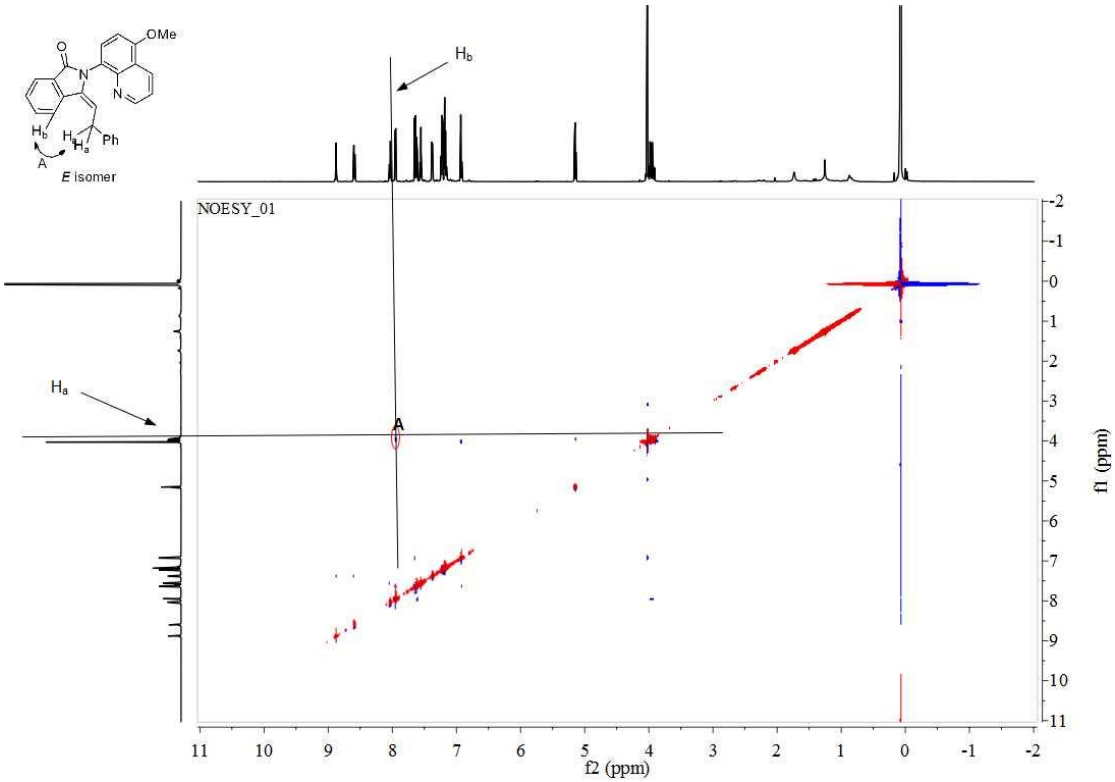
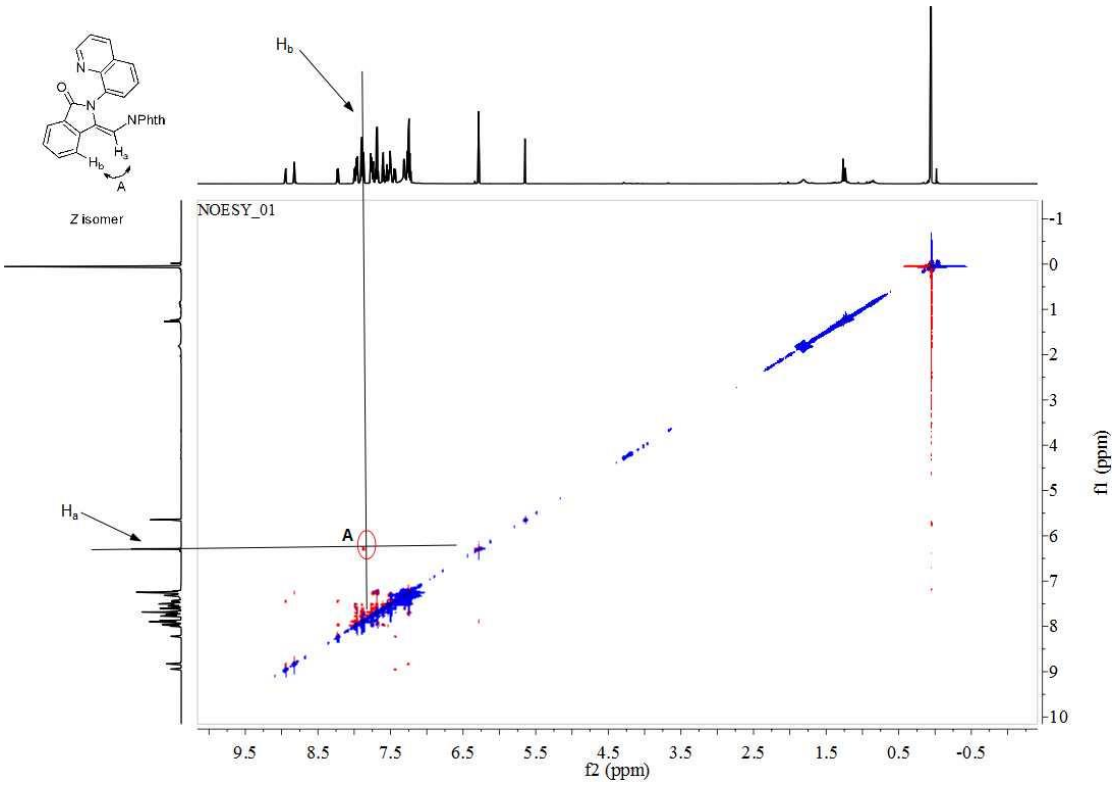
H/D
H/D
(88% D)
D-1a
calculated from this area
f1 (ppm)


PROTON_01
Intermolecular competition
N-AQ
3aa + 3aa-d4
kH/kD = 1/0.591 = 1.7
calculated from this area
f1 (ppm)

^{1}H - ^{1}H NOESY spectrum of 3ab



^{1}H - ^{1}H NOESY spectrum of 3qo



^{1}H - ^{1}H NOESY spectrum of 3aq