Supporting Information

Construction of 1-Acryloyl-2-cyanoindoles: Unveiling Their Potential in Radical Cascade Cyclization

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1. General Information

1.1 Materials and Instruments

All reagents were purchased from commercial suppliers and used without further purification unless otherwise stated. TLC was performed on silica gel plates (GF254, 200-300 mesh) using UV light (254/366 nm) for detection. Products were purified by column chromatography using silica gel (200-300 mesh) purchased from Qing Dao Hai Yang Chemical Industry Co. The ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on Bruker Avance 400 MHz spectrometer. Proton chemical shifts (δ) were reported in parts per million (ppm) using tetramethylsilane as an internal standard. All NMR spectra were recorded in $CDCl_3$ at room temperature (20 ± 3 °C). High-resolution mass spectra (HRMS) were acquired using an Agilent Infinity II Q-TOF G6545 equipped with electrospray ionization (ESI) technique.

1.2 Spectrum of Our Lamp and Visible-Light Irradiation Instrument

Photochemical reaction was carried out under visible light irradiation by a blue LED at 25 ºC. RLH-18 8-position Photo Reaction System manufactured by Beijing Roger Tech Ltd. was used in this system. Eight 10 W blue LEDs were equipped in this Photo reactor. The blue LED's energy peak wavelength is 460 nm, peak width at half-height is 23.4 nm, lirradiance@10 W is 195.55 mW/cm^2. The reaction vessel is a borosilicate glass test tube and the distance between it and the lamp is 15 mm, no filter applied.

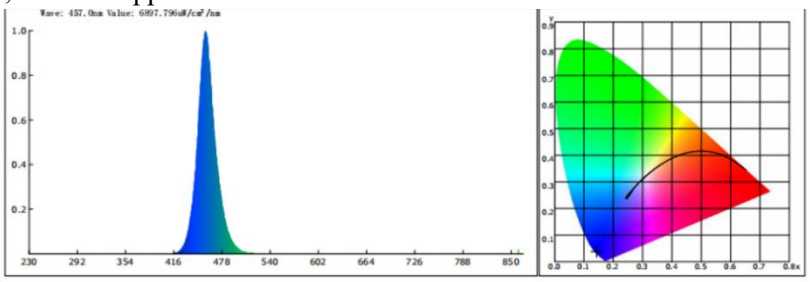
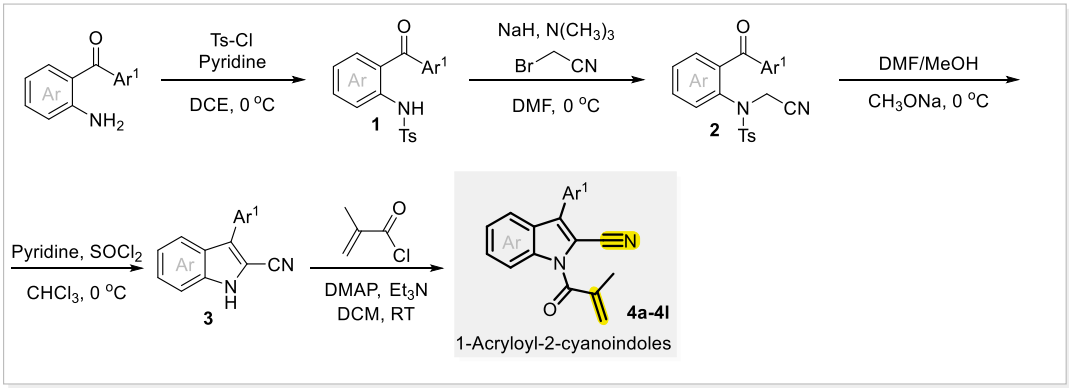


Figure S1a. The spectrum of our lamp (blue LED)

Figure S1b. The visible-light irradiation instrument

2. Experimental Procedures

2.1 General Method for the Synthesis of 1-Acryloyl-2-cyanoindoles (4a-4l)



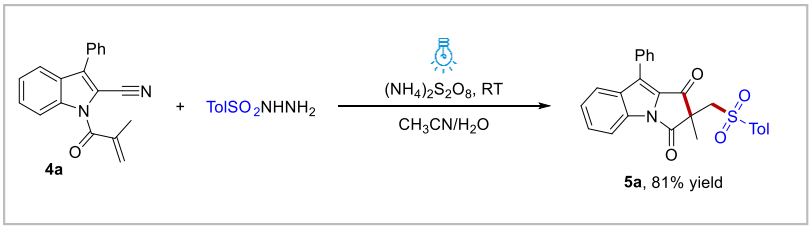
In a 250 mL round-bottom flask, 2-amino phenyl benzophenone (40.6 mmol) was added to 80 mL of 1,2-dichloroethane at 0 °C, followed by the addition of pyridine (9.7 g, 122 mmol) and p-toluenesulfonyl chloride (8.1 g, 42.6 mmol). The reaction mixture was stirred at 0 °C for 12 hours. Subsequently, the reaction mixture was poured into saturated brine (100 mL) and extracted with dichloromethane (3 × 50 mL). The organic phase was combined, washed with saturated brine (2 × 100 mL), dried over anhydrous Na_2SO_4, and concentrated using a rotary evaporator. The crude product was purified through silica gel column chromatography to obtain compound **1**.

In a 100 mL round-bottom flask, compound **1** (20 mmol) was dissolved in 50 mL of N,N-dimethylformamide at room temperature, and the temperature of the reaction mixture was subsequently lowered to 0 °C. Sodium hydride (0.7 g, 30.0 mmol), bromoacetonitrile (4.8 g, 40.0 mmol), and trimethylamine (2 mol/L in THF, 40.0 mmol) were added slowly. The reaction mixture was stirred at room temperature for 1.5 hours. After completion of the reaction, the mixture was poured into saturated brine (50 mL) and extracted with ethyl acetate (3 × 50 mL). The organic phase was combined, washed with saturated brine (2 × 100 mL), dried over anhydrous Na_2SO_4, and concentrated using a rotary evaporator. The crude product was purified through silica gel column chromatography to obtain compound **2**.

In a 100 mL round-bottom flask, compound **2** (10.0 mmol) was dissolved in a mixed solvent of N,N-dimethylformamide/methanol (v/v = 9:25, 68 mL). A solution of sodium methoxide (10 mL, 5 M) was added dropwise at 0 °C, and the mixture was stirred for 10 minutes. Following the completion of the reaction, the mixture was poured into saturated brine (50 mL) and extracted with ethyl acetate (3 × 50 mL). The organic phase was combined, washed with saturated brine (2 × 100 mL), dried over anhydrous Na_2SO_4, and concentrated using a rotary evaporator. The resulting crude product was used without further purification. Subsequently, the crude product was dissolved in 40 mL of chloroform, and at 0 °C, pyridine (2.4 g, 30.0 mmol) and dichlorosulfoxide (2.4 g, 20.0 mmol) were added sequentially. The mixture was stirred for 10 minutes; upon completion of the reaction, it was poured into saturated brine (50 mL) and extracted with dichloromethane (2 × 50 mL). The organic phase was combined, washed with saturated brine (2 × 100 mL), dried over anhydrous Na_2SO_4, and concentrated using a rotary evaporator. The crude product was purified through silica gel column chromatography to obtain compound **3**.

In a 50 mL round-bottom flask, compound **3** (5.0 mmol) and 4-dimethylaminopyridine (0.1 g, 1.0 mmol) were dissolved in 10 mL of dichloromethane. At 0 °C, triethylamine (0.6 g, 10.0 mmol) and acryloyl chloride (1.1 g, 10.0 mmol) were added sequentially. The reaction was allowed to proceed at room temperature for 12–24 hours. After completion, the reaction mixture was poured into a saturated sodium bicarbonate solution (10 mL) and extracted with dichloromethane (3 × 10 mL). The organic phase was combined, washed with saturated brine (2 × 10 mL), dried over anhydrous Na_2SO_4, and concentrated using a rotary evaporator. The resulting crude product was purified through silica gel column chromatography to give the target compounds **4a-4l**.

2.2 Visible Light-Induced Cascade Cyclization Reaction



1-methylacryloyl-2-cyano-3-phenylindole **4a** (0.1 mmol), p-toluenesulfonyl hydrazine (0.2 mmol), ammonium persulfate (0.2 mmol), and the solvent acetonitrile/water (v/v = 3:1, 1 mL) were added into a Schlenk reaction vessel. The mixture was freeze-degassed and nitrogen-purged three times before sealing and irradiating with 10 W 460 nm blue light at room temperature for 12 hours. Upon completion of the reaction, a saturated sodium chloride solution and dichloromethane extraction were used, followed by rotary evaporation of the organic solvent to yield the crude product, which was then purified by silica gel column chromatography to obtain the final target product **5a** as a white solid with a yield of 81%, melting point 206 – 208 ºC, R_f = 0.4 (PE:EA = 5:1). ^{1}H NMR (400 MHz, Chloroform-d) δ 8.20 (d, J = 8.3 Hz, 1H), 8.05 (d, J = 8.2 Hz, 1H), 7.95 – 7.91 (m, 2H), 7.67 – 7.62 (m, 1H), 7.57 – 7.53 (m, 4H), 7.50 – 7.45 (m, 2H), 7.14 (d, J = 8.1 Hz, 2H), 3.85 (s, 2H), 2.35 (s, 3H), 1.50 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-d) δ 187.8, 168.3, 145.2, 136.2, 132.88, 132.85, 130.4, 130.1, 129.9, 129.6, 129.3, 129.1, 128.8, 128.0, 125.8, 125.5, 123.6, 115.7, 60.3, 54.3, 22.2, 21.6. HRMS (ESI-TOF) m/z: $[M + H]^+$, calculated for $C_{26}H_{22}NO_4S$, 444.1264, found: 444.1269.

2.3 Characterization Data of Products

1-methacryloyl-3-phenyl-1*H*-indole-2-carbonitrile (**4a**)
white solid, yield 87%; mp 153 – 155 ºC, R_f = 0.4 (PE:EA = 6:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (dt, *J* = 8.5, 0.8 Hz, 1H), 7.80 – 7.76 (m, 1H), 7.73 – 7.68 (m, 2H), 7.61 – 7.46 (m, 4H), 7.41 – 7.37 (m, 1H), 5.93 (q, *J* = 1.5 Hz, 1H), 5.70 (d, *J* = 0.9 Hz, 1H), 2.28 – 2.26 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.7, 140.0, 137.4, 136.0, 129.9, 129.3, 129.20, 129.16, 128.7, 127.0, 126.6, 124.8, 121.6, 115.7, 113.3, 106.1, 19.0. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{15}N_2O$, 287.1179, found: 287.1179.

1-methacryloyl-3-(p-tolyl)-1*H*-indole-2-carbonitrile (**4b**)
white solid, yield 85%; mp 161 – 163 ºC, R_f = 0.5 (PE:EA = 10:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 8.5 Hz, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.64 – 7.58 (m, 2H), 7.56 – 7.52 (m, 1H), 7.40 – 7.36 (m, 3H), 5.92 (d, *J* = 1.5 Hz, 1H), 5.69 (d, *J* = 0.7 Hz, 1H), 2.45 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.8, 140.0, 139.5, 137.4, 136.1, 129.9, 129.1, 128.6, 127.1, 127.0, 126.5, 124.7, 121.6, 115.7, 113.5, 105.9, 21.4, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{20}H_{16}N_2NaO$, 323.1155, found: 323.1154.

1-methacryloyl-3-(m-tolyl)-1*H*-indole-2-carbonitrile (**4c**)
white solid, yield 89%; mp 118 – 120 ºC, R_f = 0.5 (PE:EA = 8:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.77 (dt, *J* = 8.1, 1.0 Hz, 1H), 7.56 – 7.48 (m, 3H), 7.47 – 7.42 (m, 1H), 7.42 – 7.36 (m, 1H), 7.34 – 7.29 (m, 1H), 5.92 (q, *J* = 1.5 Hz, 1H), 5.69 (d, *J* = 0.9 Hz, 1H), 2.46 (s, 3H), 2.29 – 2.25 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.8, 140.0, 138.9, 137.4, 136.2, 130.1, 129.83, 129.76, 129.1, 128.6, 127.1, 126.6, 126.3, 124.7, 121.7, 115.7, 113.3, 106.0, 21.5, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{20}H_{16}N_2NaO$, 323.1155, found: 323.1159.

1-methacryloyl-3-(4-methoxyphenyl)-1*H*-indole-2-carbonitrile (**4d**)
white solid, yield 91%; mp 165 – 167 ºC, R_f = 0.4 (PE:EA = 8:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (d, *J* = 8.5 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.69 – 7.62 (m, 2H), 7.67 – 7.63 (m, 1H), 7.42 – 7.34 (m, 1H), 7.14 – 7.03 (m, 2H), 5.91 (d, *J* = 1.6 Hz, 1H), 5.68 (d, *J* = 1.5 Hz, 1H), 3.89 (s, 3H), 2.26 (t, *J* = 1.0 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.7, 160.5, 140.0, 137.4, 135.9, 130.5, 128.6, 127.1, 126.4, 124.7, 122.1, 121.6, 115.7, 114.7, 113.6, 105.6, 55.4, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{20}H_{16}N_2NaO_2$, 339.1104, found: 339.1104.

1-methacryloyl-3-(3-methoxyphenyl)-1*H*-indole-2-carbonitrile (**4e**)

white solid, yield 81%; mp 107 – 109 °C, R_f = 0.4 (PE:EA = 9:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.43 – 7.36 (m, 1H), 7.29 – 7.26 (m, 2H), 7.07 – 7.02 (m, 1H), 5.93 (d, *J* = 1.5 Hz, 1H), 5.70 (d, *J* = 1.7 Hz, 1H), 3.89 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.7, 160.0, 140.0, 137.4, 135.8, 131.1, 130.2, 128.6, 127.0, 126.7, 124.8, 121.62, 121.57, 115.7, 115.1, 114.6, 113.2, 106.2, 55.5, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{20}H_{16}N_2NaO_2$, 339.1104, found: 339.1105.

3-(4-(tert-butyl)phenyl)-1-methacryloyl-1*H*-indole-2-carbonitrile (**4f**)
white solid, yield 85%; mp 131 – 133 °C, R_f = 0.5 (PE:EA = 10:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, *J* = 8.5 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.71 – 7.67 (m, 2H), 7.63 – 7.60 (m, 2H), 7.58 – 7.54 (m, 1H), 7.42 – 7.38 (m, 1H), 5.98 – 5.93 (m, 1H), 5.72 (d, *J* = 0.9 Hz, 1H), 2.32 – 2.29 (m, 3H), 1.44 (s, 9H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.7, 152.5, 140.0, 137.4, 136.0, 128.9, 128.6, 127.1, 127.0, 126.6, 126.2, 124.7, 121.8, 115.7, 113.6, 105.8, 34.9, 31.3, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{23}H_{22}N_2NaO$, 365.1624, found: 365.1627.

3-(4-fluorophenyl)-1-methacryloyl-1*H*-indole-2-carbonitrile (**4g**)
white solid, yield 51%; mp 153 – 155 °C, R_f = 0.5 (PE:EA = 9:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.75 – 7.65 (m, 3H), 7.57 – 7.53 (m, 1H), 7.42 – 7.36 (m, 1H), 7.30 – 7.22 (m, 2H), 5.93 (d, *J* = 1.5 Hz, 1H), 5.69 (d, *J* = 1.2 Hz, 1H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.6, 163.3 (d, *J* = 250.0 Hz), 139.9, 137.3, 134.9, 131.1 (d, *J* = 8.4 Hz), 128.8, 126.9, 126.7, 126.0 (d, *J* = 3.4 Hz), 124.9, 121.3, 116.4 (d, *J* = 21.8 Hz), 115.8, 113.2, 106.2, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{13}FN_2NaO$, 327.0904, found: 327.0914.

3-(4-chlorophenyl)-1-methacryloyl-1*H*-indole-2-carbonitrile (**4h**)
white solid, yield 57%; mp 168 – 170 °C, R_f = 0.4 (PE:EA = 10:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.67 – 7.62 (m, 2H), 7.59 – 7.52 (m, 3H), 7.43 – 7.37 (m, 1H), 5.94 (d, *J* = 1.6 Hz, 1H), 5.69 (d, *J* = 1.4 Hz, 1H), 2.27 (t, *J* = 1.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.6, 139.9, 137.3, 135.5, 134.6, 130.5, 129.5, 128.8, 128.4, 126.8, 126.7, 124.9, 121.3, 115.8, 113.1, 106.2, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{13}{}^{35}ClN_2NaO$, 343.0609, found: 343.0608.

3-(4-bromophenyl)-1-methacryloyl-1*H*-indole-2-carbonitrile (**4i**)
white solid, yield 61%; mp 167 – 169 °C, R_f = 0.4 (PE:EA = 10:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (d, *J* = 8.5 Hz, 1H), 7.73 – 7.69 (m, 3H), 7.61 – 7.52 (m, 3H), 7.40 (t, *J* = 7.6 Hz, 1H), 5.94 (d, *J* = 2.1 Hz, 1H), 5.70 (s, 1H), 2.27 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.6, 139.9, 137.3, 134.6, 132.5, 130.7, 128.9, 128.8, 126.9, 126.6, 125.0, 123.7, 121.2, 115.8, 113.1, 106.2, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{13}{}^{79}BrN_2NaO$, 387.0103, found: 387.0110.

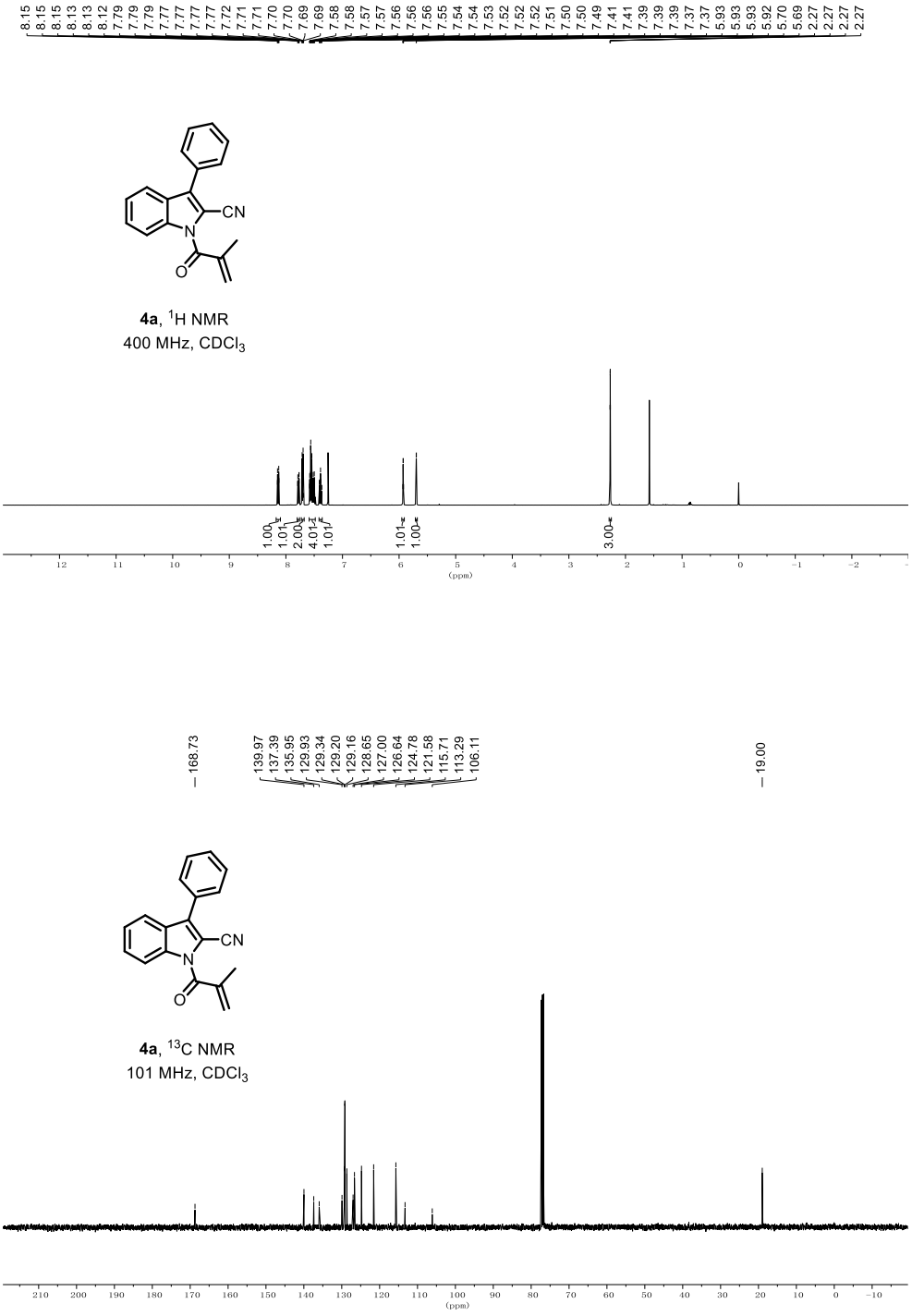
5-chloro-1-methacryloyl-3-phenyl-1*H*-indole-2-carbonitrile (**4j**)
white solid, yield 51%; mp 152 – 154 °C, R_f = 0.4 (PE:EA = 8:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.07 – 8.03 (m, 1H), 7.71 (d, *J* = 1.8 Hz, 1H), 7.67 – 7.62 (m, 2H), 7.58 – 7.52 (m, 2H), 7.52 – 7.47 (m, 1H), 7.45 (dd, *J* = 9.0, 2.1 Hz, 1H), 5.94 (q, *J* = 1.5 Hz, 1H), 5.68 (d, *J* = 1.0 Hz, 1H), 2.27 – 2.23 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.4, 139.7, 135.6, 134.9, 130.7, 129.6, 129.3, 129.1, 128.9, 128.1, 127.1, 120.9, 116.9, 112.8, 107.2, 19.0. HRMS (ESI-TOF) *m/z*: $[M + Na]^+$ calcd for $C_{19}H_{13}{}^{35}ClN_2NaO$, 343.0609, found: 343.0615.

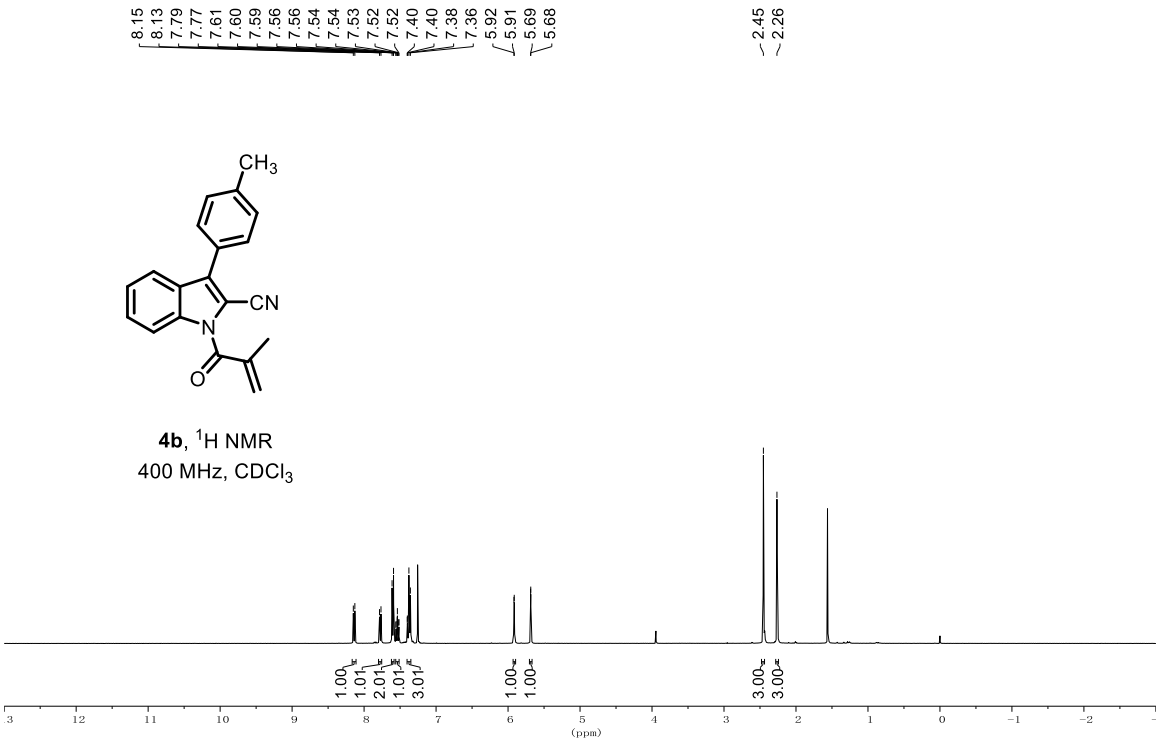
5-bromo-1-methacryloyl-3-phenyl-1*H*-indole-2-carbonitrile (**4k**)
white solid, yield 58%; mp 164 – 166 °C, R_f = 0.4 (PE:EA = 7:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 1.7 Hz, 1H), 7.67 – 7.63 (m, 2H), 7.62 – 7.50 (m, 4H), 5.95 (q, *J* = 1.5 Hz, 1H), 5.68 (d, *J* = 0.9 Hz, 1H), 2.27 – 2.24 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.4, 139.7, 136.0, 134.8, 131.6, 129.6, 129.34, 129.29, 129.1, 128.6, 127.1, 124.0, 118.2, 117.2, 112.8, 107.0, 19.0. HRMS (ESI-TOF) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{14}BrN_2O$, 365.0284, found: 365.0279.

1-methacryloyl-5-methyl-3-(m-tolyl)-1*H*-indole-2-carbonitrile (**4l**)

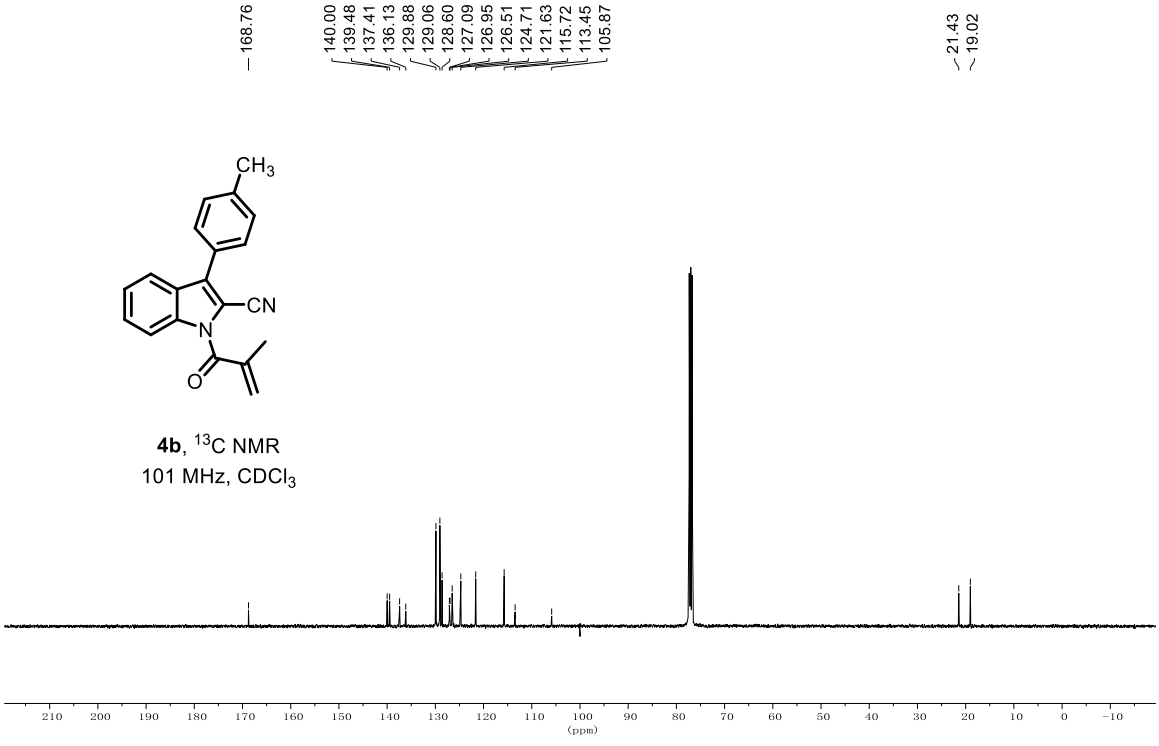
white solid, yield 81%; mp 106 – 108 °C, R_f = 0.5 (PE:EA = 8:1). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.02 (d, *J* = 8.6 Hz, 1H), 7.54 – 7.42 (m, 4H), 7.39 – 7.29 (m, 2H), 5.90 (d, *J* = 1.5 Hz, 1H), 5.67 (s, 1H), 2.47 (d, *J* = 3.2 Hz, 6H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.7, 140.0, 138.9, 136.1, 135.7, 134.6, 130.2, 130.1, 130.0, 129.8, 129.0, 127.3, 126.34, 126.27, 121.1, 115.4, 113.4, 106.0, 21.5, 21.4, 19.1. HRMS (ESI-TOF) *m/z*: [M + Na]$^+$ calcd for $C_{21}H_{18}N_2NaO$, 337.1311, found: 337.1314.

3. NMR Copies of Products





4b, ^{1}H NMR
400 MHz, $CDCl_3$



4b, ^{13}C NMR
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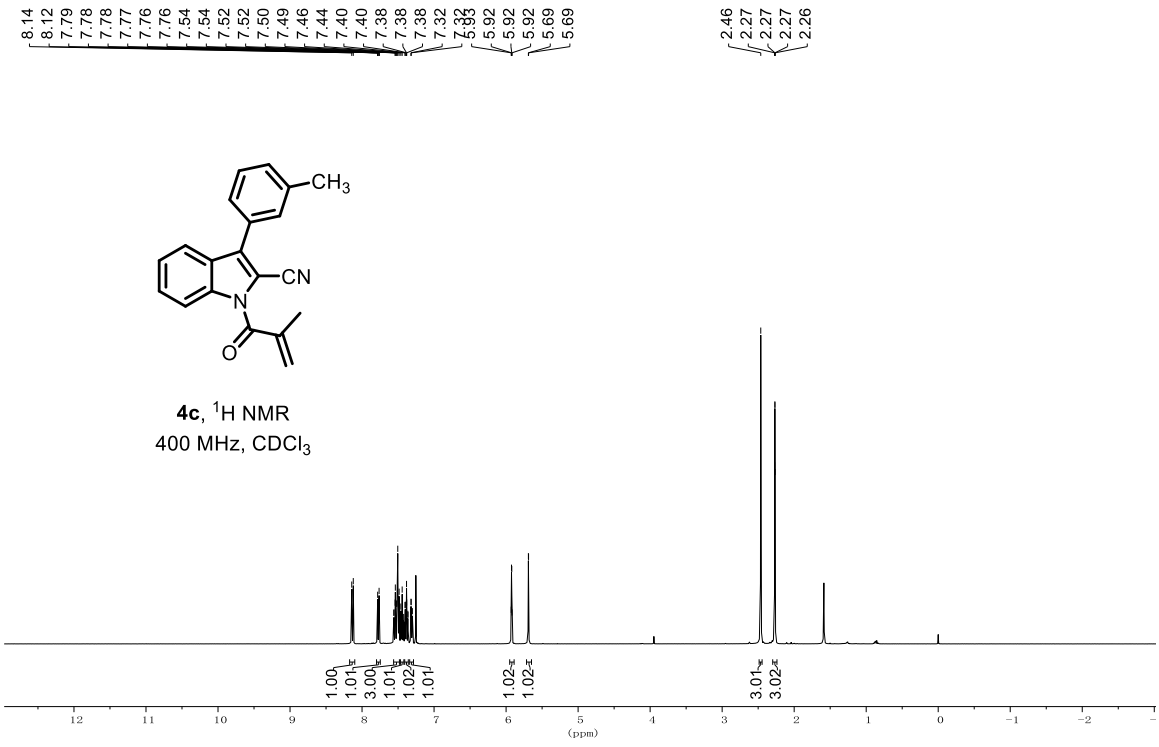
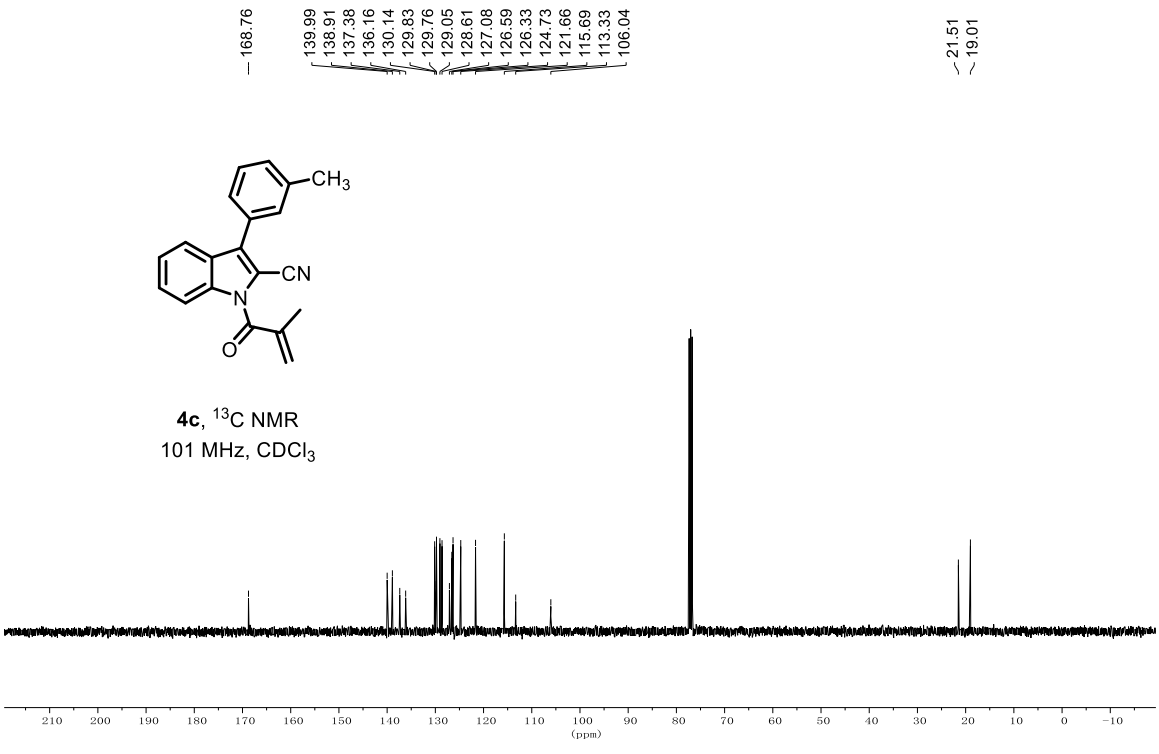
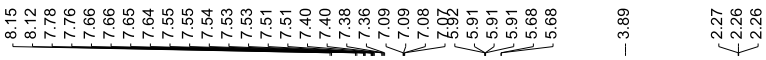
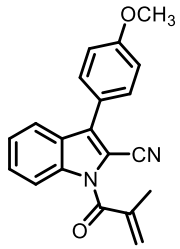


4c, ^{1}H NMR
400 MHz, $CDCl_3$

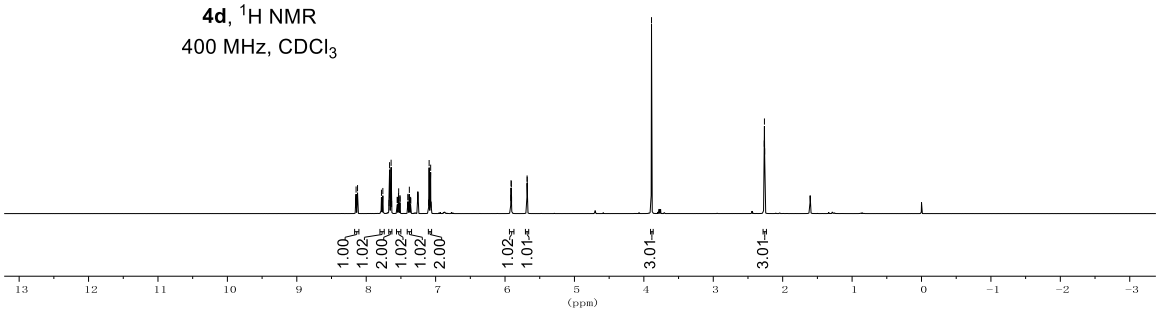


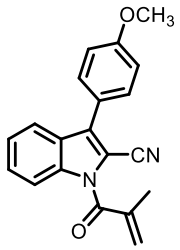
4c, ^{13}C NMR
101 MHz, $CDCl_3$



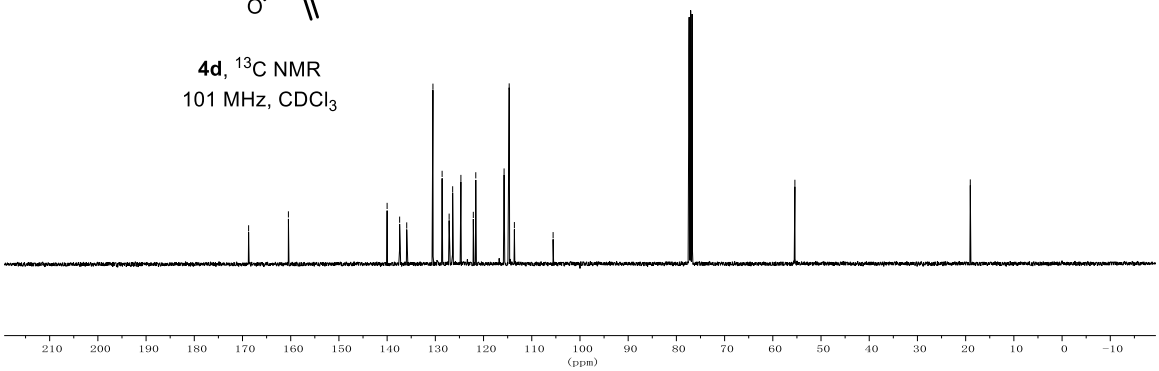


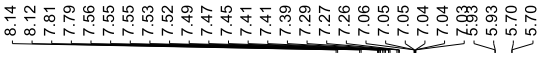
4d, ^{1}H NMR
400 MHz, $CDCl_3$

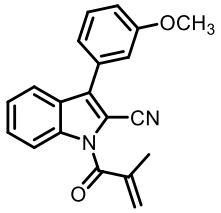




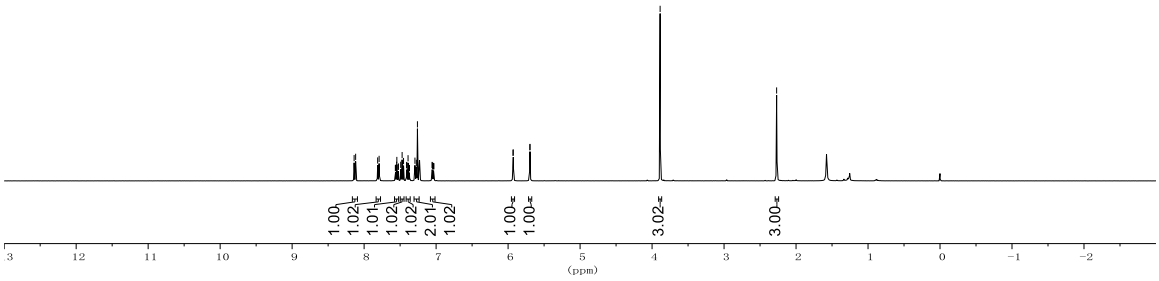
4d, ^{13}C NMR
101 MHz, $CDCl_3$

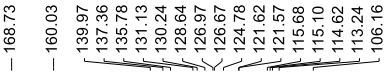


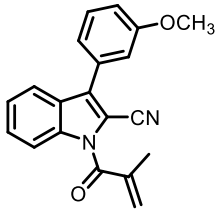




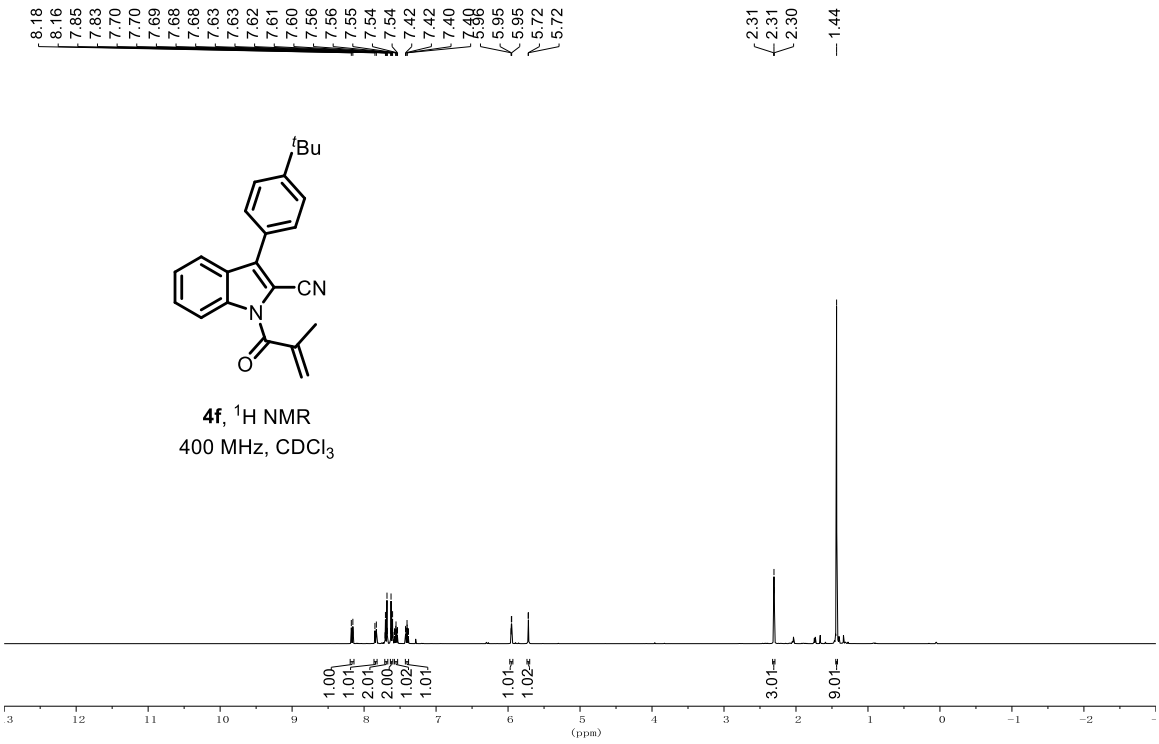
4e, ^{1}H NMR
400 MHz, $CDCl_3$



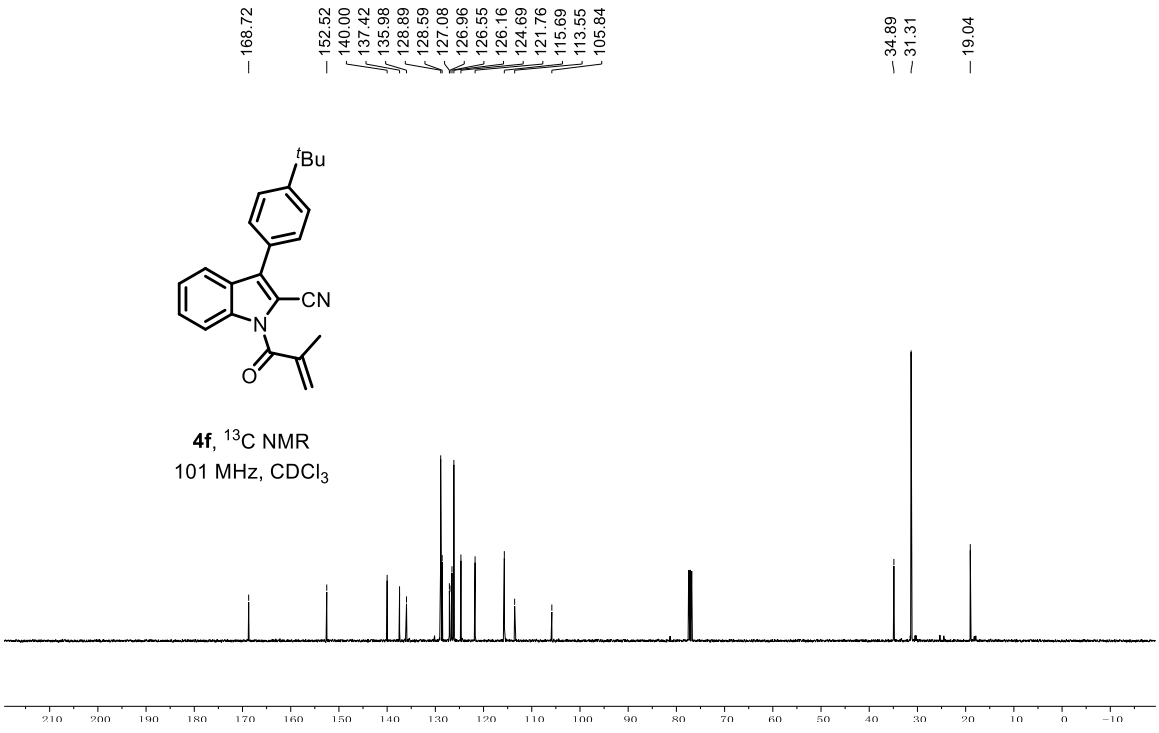




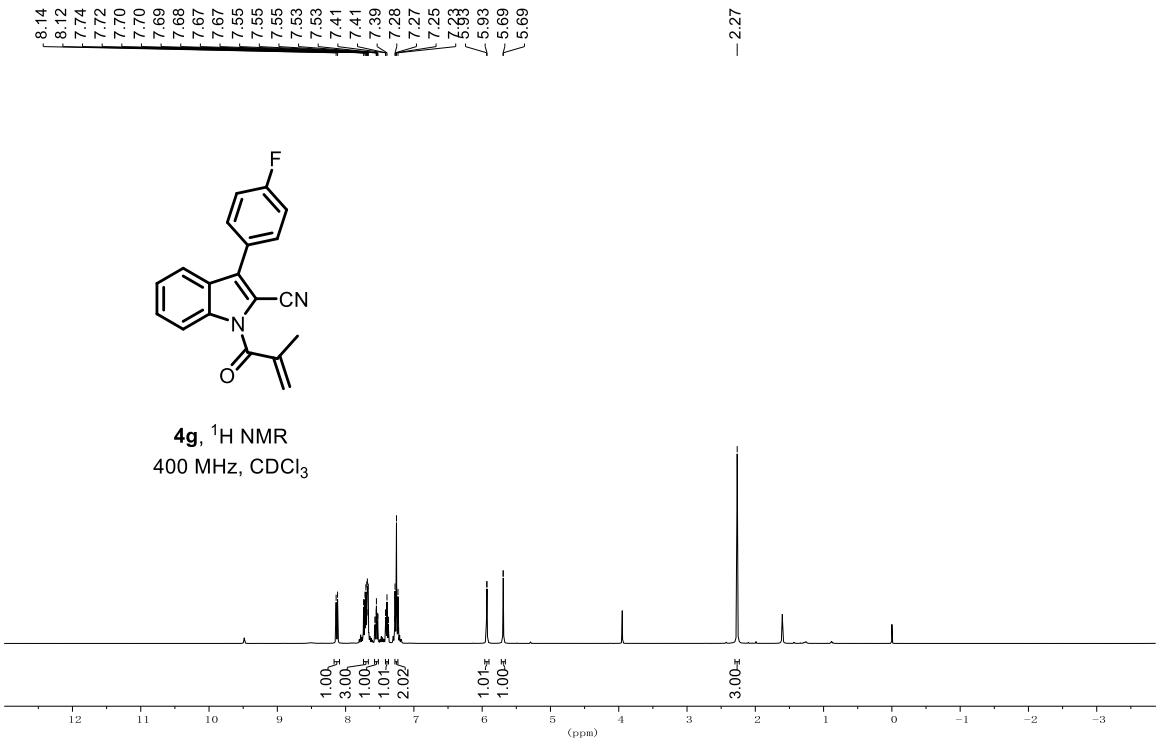
4e, ^{13}C NMR
101 MHz, $CDCl_3$



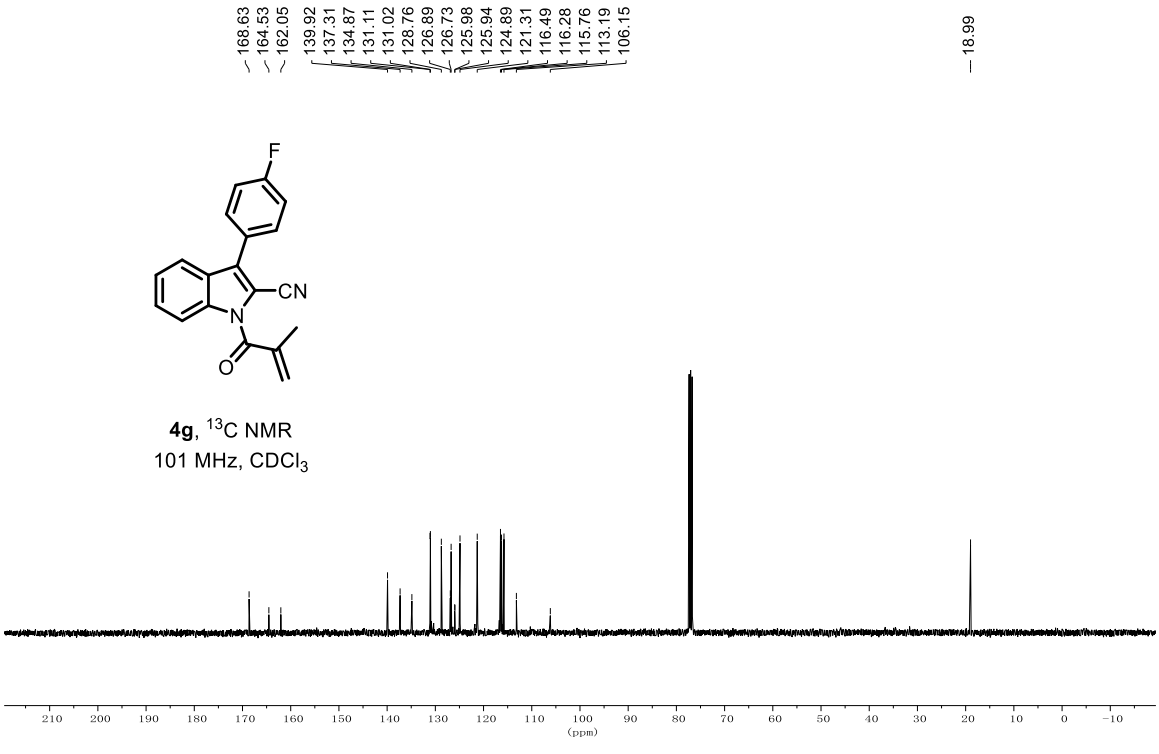
4f, ^{1}H NMR
400 MHz, $CDCl_3$



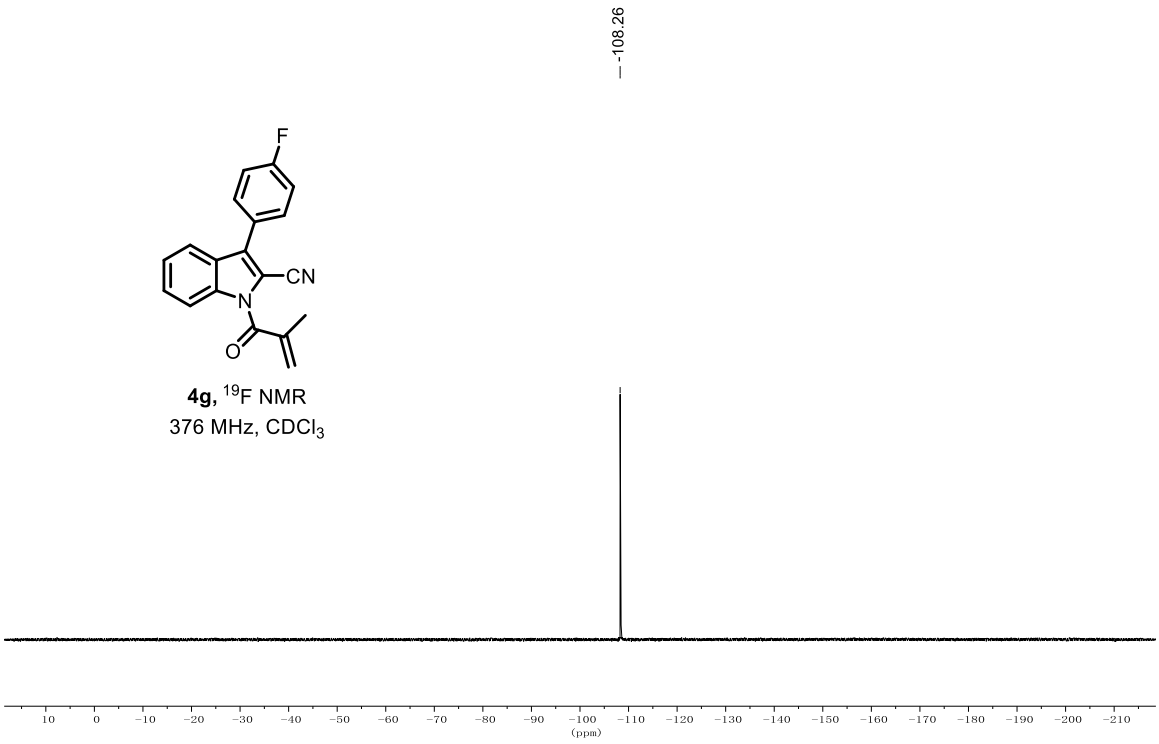
4f, ^{13}C NMR
101 MHz, $CDCl_3$



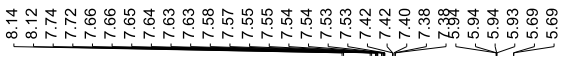
4g, ^{1}H NMR
400 MHz, $CDCl_3$

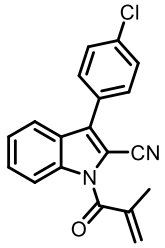


4g, ^{13}C NMR
101 MHz, $CDCl_3$

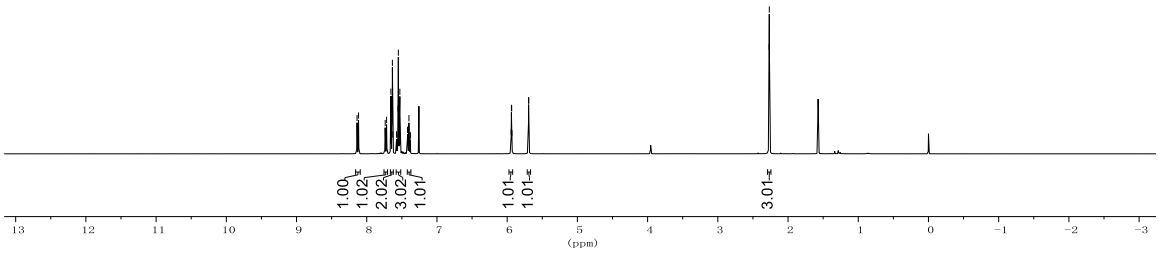


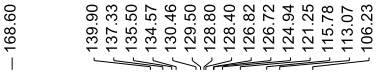
4g, ^{19}F NMR
376 MHz, $CDCl_3$

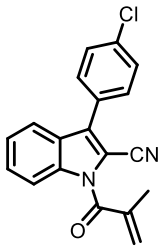




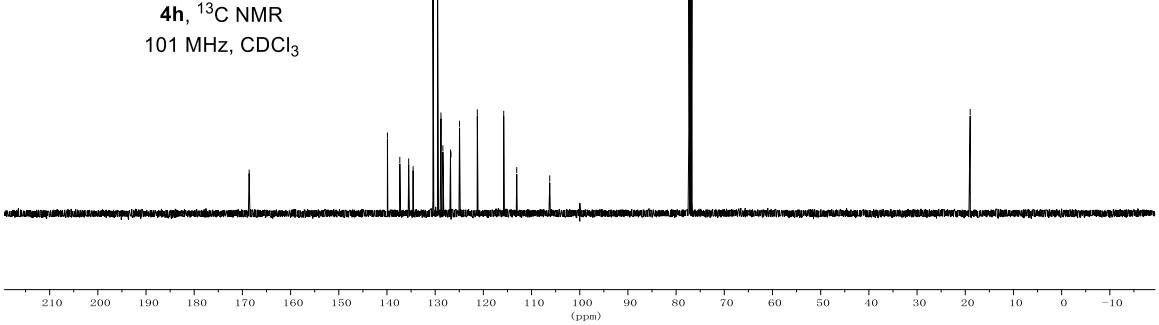
4h, ^{1}H NMR
400 MHz, $CDCl_3$

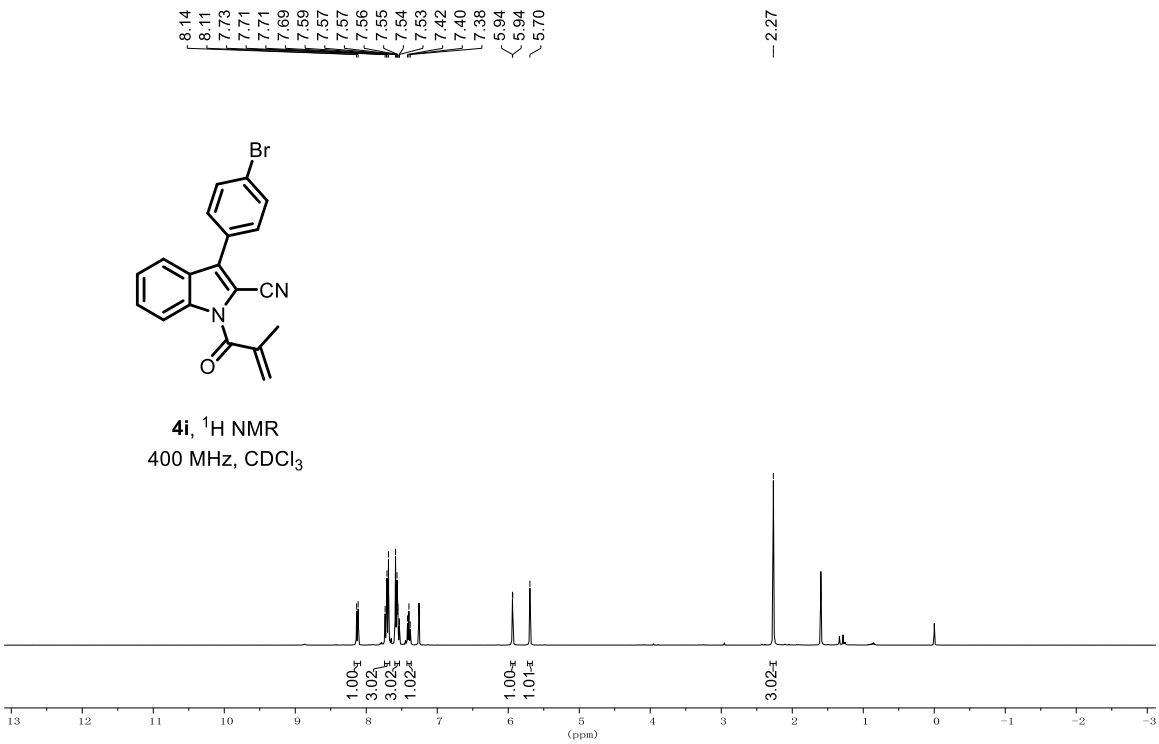




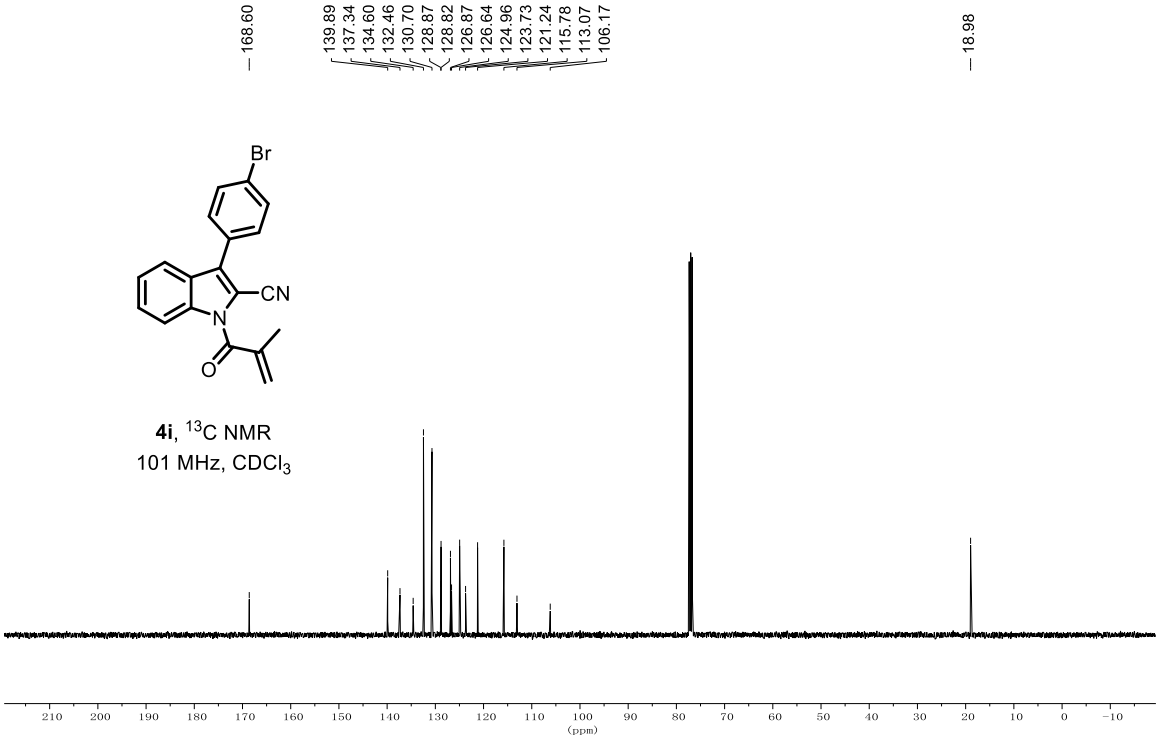


4h, ^{13}C NMR
101 MHz, $CDCl_3$

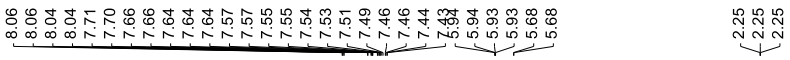


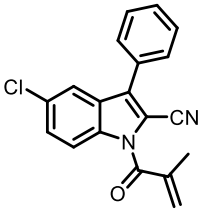


4i, ^{1}H NMR
400 MHz, $CDCl_3$

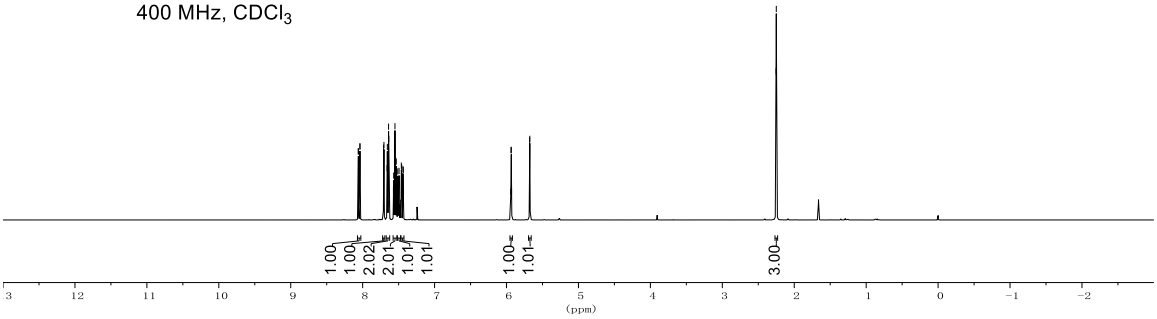


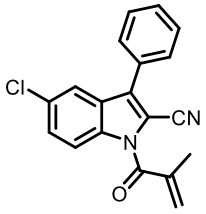
4i, ^{13}C NMR
101 MHz, $CDCl_3$



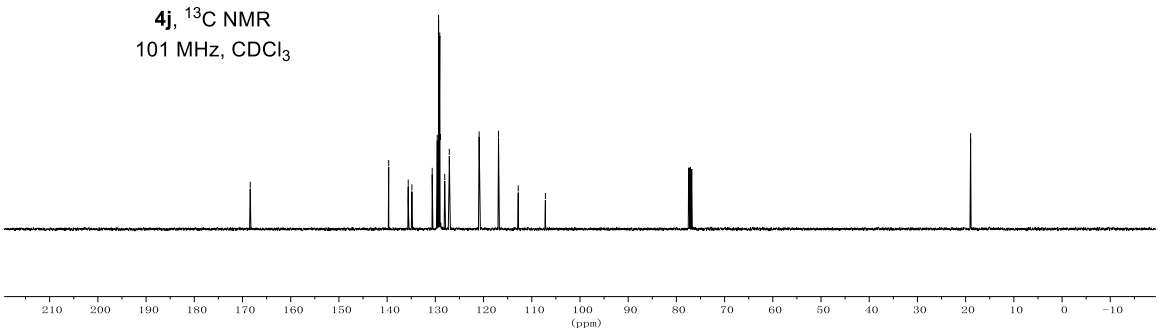


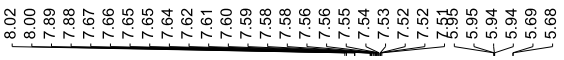
4j, ^{1}H NMR
400 MHz, $CDCl_3$

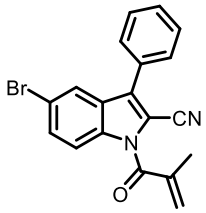




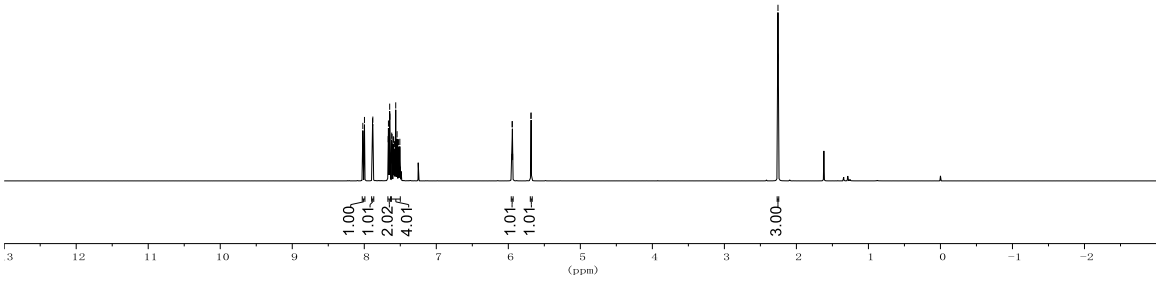
4j, ^{13}C NMR
101 MHz, $CDCl_3$

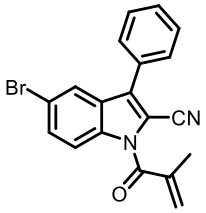




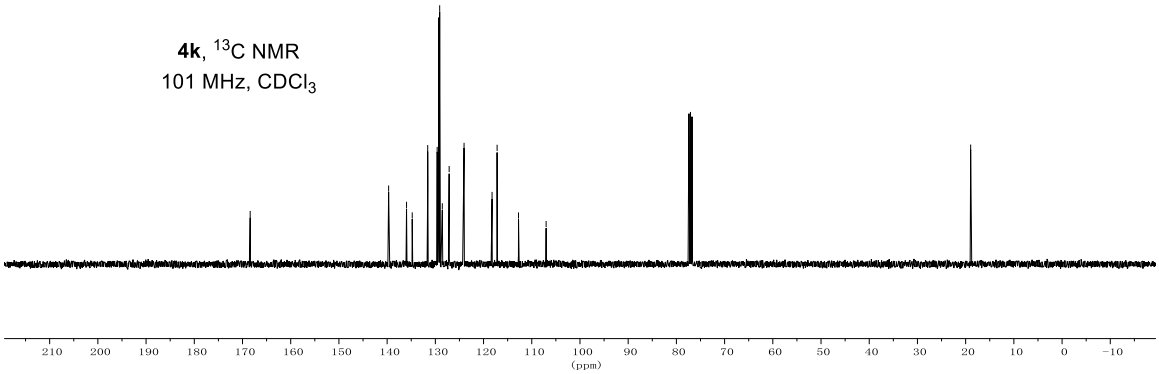


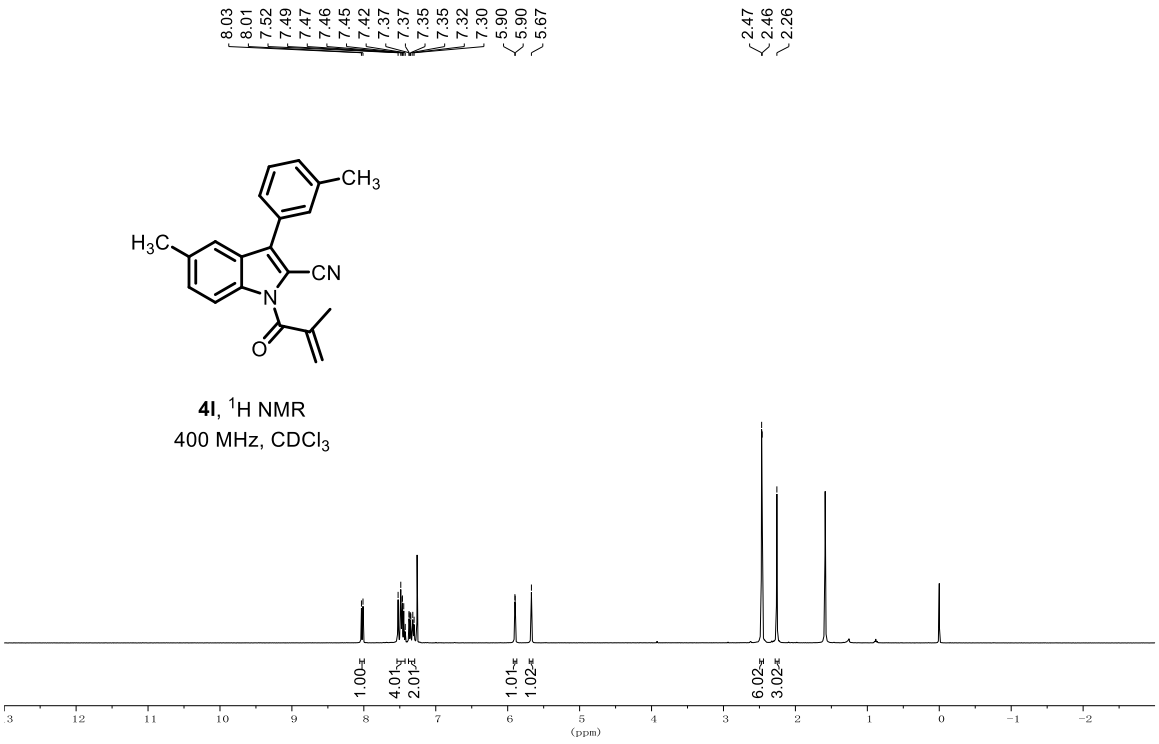
4k, ^{1}H NMR
400 MHz, $CDCl_3$



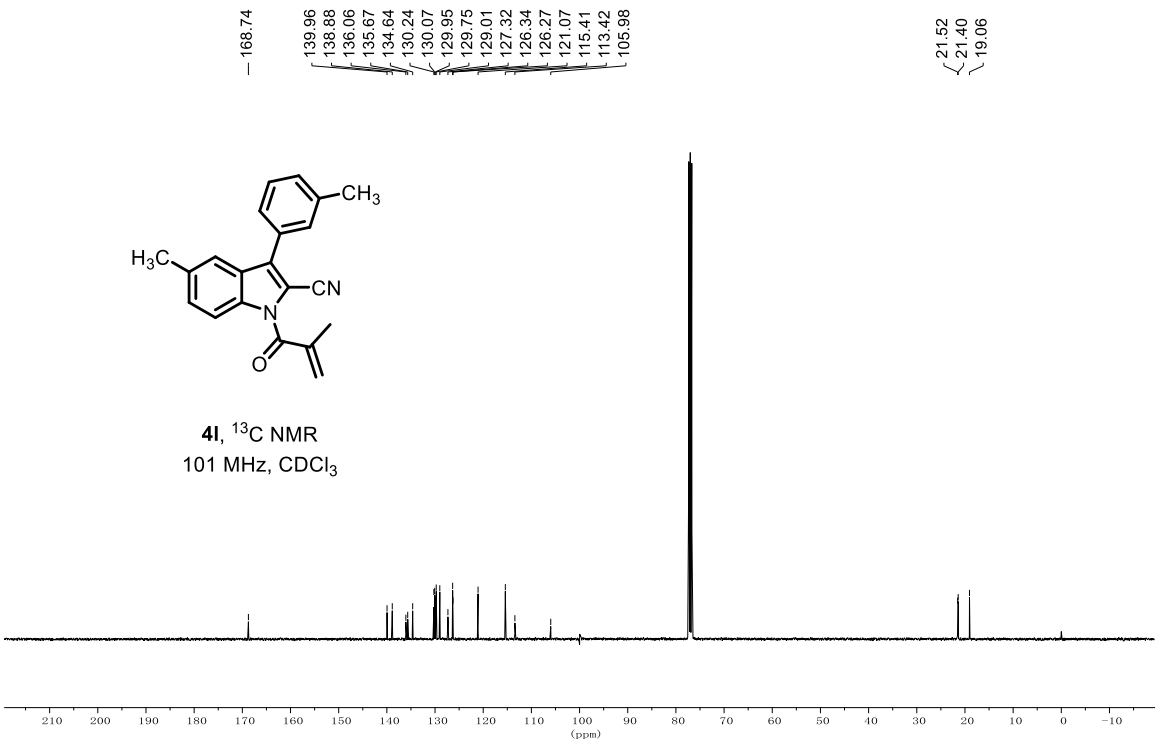


4k, ^{13}C NMR
101 MHz, $CDCl_3$

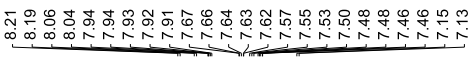


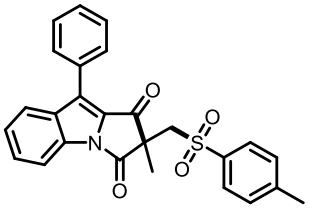


4l, ^{1}H NMR
400 MHz, $CDCl_3$

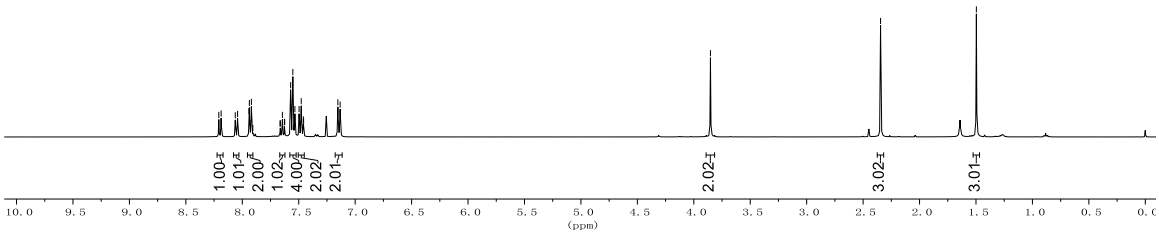


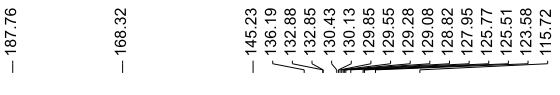
4l, ^{13}C NMR
101 MHz, $CDCl_3$

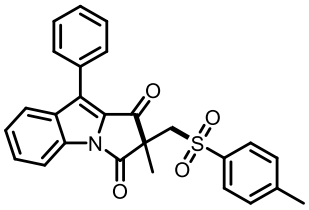




5a, ^{1}H NMR
400 MHz, $CDCl_3$







5a, ^{13}C NMR
101 MHz, $CDCl_3$