

Metal-Free Cascade Synthesis of Unsymmetrical 2-Aminopyrimidines from Imidazolate Enaminones†

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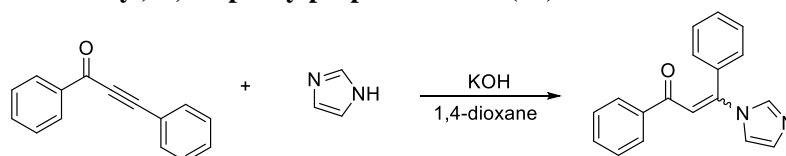
Context

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General information

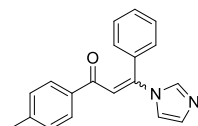
Unless otherwise stated, all reagents were used directly without further purification. Silica gel was purchased from Qing Dao Hai Yang Chemical Industry Co. All melting points were determined on a Beijing Science Instrument Dianguang Instrument Factory XT4B melting point apparatus and uncorrected. ^1H and ^{13}C NMR spectra were measured on a 400 MHz Bruker spectrometer (^1H 400 MHz, ^{13}C 100 MHz), using CDCl_3 as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. HRMS-ESI spectra were equipped with an ESI source and a TOF detector. PE is petroleum ether (60–90 °C).

Typical procedure for the preparation of (Z/E)-3-(1H-imidazol-1-yl)-1,3-diphenylprop-2-en-1-one (**1a**)¹

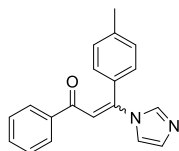


A suspension of 1,3-diphenylprop-2-yn-1-one (1.0 mmol, 206 mg), 1H-imidazole (2.0 mmol, 136 mg) and KOH (2.0 mmol, 112 mg) in 1,4-dioxane (5 mL) was stirred at rt for 5 h. After the ynone was exhausted completely (monitored by TLC), it was cooled down to room temperature and saturated aqueous brine (10 mL) was added. The mixture was stirred for 10 min and then was extracted by EtOAc (3 × 10 mL). The combined organic layers were dried over Na_2SO_4 . After filtration, removal of the solvent gave a residue, which was purified by a column chromatography (silica gel, PE/EtOAc = 6/1) to afford **1a** as yellow liquid; 247 mg, 90% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 4.0$ Hz, 1H), 7.88 (d, $J = 4.0$ Hz, 1H), 7.62–7.29 (m, 9H), 7.17–6.89 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.3, 147.6, 144.9, 138.6, 137.9, 137.5, 137.3, 135.8, 133.5, 133.3, 133.2, 131.4, 130.8, 130.7, 129.8, 129.7, 129.2, 128.8, 128.7, 128.6, 128.5, 127.9, 120.5, 118.7, 117.7, 114.5.

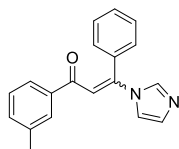
A similar procedure was used for the preparation of products **1b–1s** & **A–G**.



(Z/E)-3-(1H-imidazol-1-yl)-3-phenyl-1-(p-tolyl)prop-2-en-1-one (**1b**). 265 mg, 92% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.81 (d, $J = 4.0$ Hz, 1H), 7.79 (d, $J = 4.0$ Hz, 1H), 7.61–7.28 (m, 6H), 7.22–6.88 (m, 5H), 7.38 (s, 1.5H), 7.37 (s, 1.5H); ^{13}C NMR (100 MHz, CDCl_3) δ 189.74, 189.69, 146.9, 144.4, 144.2, 144.1, 138.4, 137.3, 135.7, 135.2, 134.6, 133.2, 131.1, 130.54, 130.48, 129.6, 129.5, 129.3, 129.2, 129.0, 128.6, 128.54, 128.50, 127.7, 120.3, 118.6, 117.8, 114.6, 21.61, 21.58.

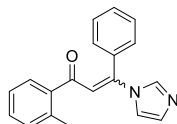


(Z/E)-3-(1H-imidazol-1-yl)-1-phenyl-3-(p-tolyl)prop-2-en-1-one (**1b'**). 262 mg, 91% yield; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.88 (d, $J = 8.0$ Hz, 1H), 7.85 (d, $J = 8.0$ Hz, 1H), 7.60–7.36 (m, 4H), 7.24–7.12 (m, 5H), 6.99–6.86 (m, 2H), 2.39 (s, 1.5H), 2.33 (s, 1.5H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.1, 190.0, 147.5, 144.9, 140.9, 138.3, 137.7, 137.3, 137.2, 133.1, 133.0, 132.7, 130.4, 130.0, 129.60, 129.56, 129.4, 129.2, 128.44, 128.39, 128.34, 128.2, 127.7, 120.3, 118.6, 116.4, 113.8, 21.28, 21.24.

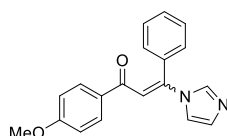


(Z/E)-3-(1H-imidazol-1-yl)-3-phenyl-1-(m-tolyl)prop-2-en-1-one (**1c**). 277 mg, 96% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.67–7.28 (m, 10H), 7.13–6.86 (m, 3H), 2.33 (s,

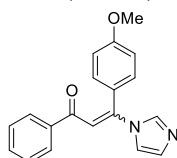
3H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.18, 190.12, 147.0, 144.3, 138.3, 138.2, 137.6, 137.2, 137.0, 135.5, 134.1, 133.8, 133.0, 131.1, 130.44, 130.39, 129.5, 129.4, 128.9, 128.7, 128.4, 128.34, 128.29, 127.6, 125.6, 125.5, 120.2, 118.5, 117.7, 114.5, 21.1.



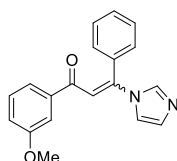
(Z/E)-3-(1H-imidazol-1-yl)-3-phenyl-1-(o-tolyl)prop-2-en-1-one (1d). 230 mg, 80% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.57–7.27 (m, 7H), 7.25–7.10 (m, 4H), 6.95–6.74 (m, 2H), 2.49 (s, 1.4H), 2.43 (s, 1.6H); ^{13}C NMR (100 MHz, CDCl_3) δ 194.0, 193.4, 147.0, 144.3, 138.5, 138.3, 138.2, 138.1, 137.3, 137.2, 135.4, 132.9, 131.8, 131.7, 131.5, 131.3, 131.2, 130.7, 130.6, 129.7, 129.6, 129.1, 129.0, 128.5, 127.6, 125.4, 120.8, 120.1, 118.5, 117.5, 20.9, 20.7.



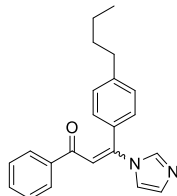
(Z/E)-3-(1H-imidazol-1-yl)-1-(4-methoxyphenyl)-3-phenylprop-2-en-1-one (1e). 280 mg, 92% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 4.0$ Hz, 1H), 7.88 (d, $J = 4.0$ Hz, 1H), 7.62–7.28 (m, 6H), 7.16–6.87 (m, 5H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 188.8, 188.7, 163.8, 163.6, 146.4, 143.7, 138.4, 137.3, 135.8, 133.3, 131.0, 130.9, 130.8, 130.7, 130.5, 130.4, 130.1, 129.6, 129.5, 129.0, 128.6, 127.7, 120.3, 118.6, 118.0, 114.8, 113.9, 113.7, 55.4.



(Z/E)-3-(1H-imidazol-1-yl)-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-one (1e'). 286 mg, 94% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.86 (t, $J = 8.0$ Hz, 2H), 7.63–7.28 (m, 5H), 7.23–6.82 (m, 6H), 3.83 (s, 1.5H), 3.78 (s, 1.5H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.3, 189.8, 162.1, 161.4, 147.4, 145.0, 138.4, 137.8, 137.5, 137.4, 133.1, 133.0, 131.5, 130.4, 129.5, 129.4, 128.5, 128.45, 128.38, 128.2, 127.8, 125.0, 120.3, 118.8, 115.3, 114.4, 113.9, 113.6, 55.4, 55.2.

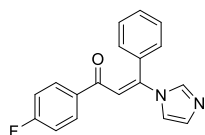


(Z/E)-3-(1H-imidazol-1-yl)-1-(3-methoxyphenyl)-3-phenylprop-2-en-1-one (1f). 268 mg, 88% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.59–7.27 (m, 9H), 7.14–6.88 (m, 4H), 3.79 (s, 1.6H), 3.77 (m, 1.4H); ^{13}C NMR (100 MHz, CDCl_3) δ 189.7, 189.6, 159.7, 159.6, 147.4, 144.7, 139.0, 138.5, 138.4, 137.2, 135.5, 133.0, 131.2, 130.6, 130.5, 129.6, 129.5, 129.4, 128.9, 128.5, 127.7, 121.0, 120.9, 120.3, 119.9, 119.7, 118.5, 117.4, 114.1, 112.4, 112.3, 55.27, 55.25.

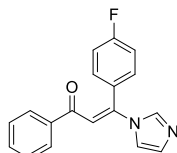


(Z/E)-3-(4-butylphenyl)-3-(1H-imidazol-1-yl)-1-phenylprop-2-en-1-one (1g). 297 mg, 90% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.87 (q, $J = 4.0$ Hz, 1H), 7.85 (q, $J = 4.0$ Hz, 1H), 7.61–7.34 (m, 4H), 7.23–6.86 (m, 7H), 2.64 (t, $J = 8.0$ Hz, 1H), 5.58 (t, $J = 8.0$ Hz, 1H), 1.60 (t, $J = 8.0$ Hz, 1H), 1.55 (t, $J = 8.0$ Hz, 1H), 1.36 (q, $J = 8.0$ Hz, 1H), 1.28 (q, $J = 8.0$ Hz, 1H), 0.92 (t, $J = 4.0$ Hz, 1.5H), 0.89 (t, $J = 4.0$ Hz, 1.5H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.5, 189.9, 147.5, 146.8, 145.9, 144.9, 138.4, 137.7, 137.34, 137.29, 133.1, 132.9, 132.8, 130.4, 130.2, 129.7,

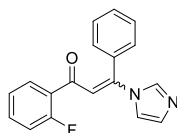
129.4, 129.0, 138.5, 128.45, 128.39, 128.3, 128.2, 127.7, 120.3, 118.6, 116.5, 114.1, 35.3, 33.1, 33.0, 22.13, 22.09, 13.75.



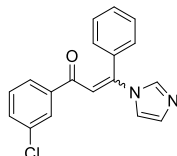
(E)-1-(4-fluorophenyl)-3-(1H-imidazol-1-yl)-3-phenylprop-2-en-1-one (1h). 237 mg, 81% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.92 (d, $J = 4.0$ Hz, 1H), 7.90 (d, $J = 8.0$ Hz, 1H), 7.61–7.28 (m, 6H), 7.17–6.90 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 188.8, 165.6 (d, $J = 254$ Hz), 147.6, 137.4, 134.2 (d, $J = 3$ Hz), 133.0, 131.2 (d, $J = 10$ Hz), 130.8 (d, $J = 3$ Hz), 129.7, 128.7, 118.5, 115.7 (d, $J = 22$ Hz), 114.0



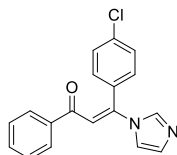
(E)-3-(4-fluorophenyl)-3-(1H-imidazol-1-yl)-1-phenylprop-2-en-1-one (1h'). 219 mg, 75% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 8.0$ Hz, 2H), 7.62–7.29 (m, 6H), 7.18–7.67 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 189.9, 163.9 (d, $J = 251$ Hz), 146.4, 137.7, 137.3, 133.3, 131.9 (d, $J = 9$ Hz), 130.8, 129.1 (d, $J = 4$ Hz), 128.5 (d, $J = 20$ Hz), 118.6, 115.9 (d, $J = 22$ Hz), 114.4.



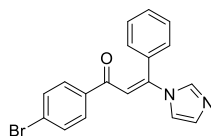
(Z/E)-1-(2-fluorophenyl)-3-(1H-imidazol-1-yl)-3-phenylprop-2-en-1-one (1i). 210 mg, 72% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.71–7.60 (m, 2H), 7.49–7.28 (m, 8H), 7.17–6.89 (m, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 187.6, 187.0, 162.1, 126.0, 159.6, 159.5, 147.7, 145.0, 135.5, 134.5, 134.4, 134.2, 134.1, 132.8, 131.3, 130.7, 130.6, 130.5, 129.8, 128.9, 128.4, 127.8, 124.5, 124.4, 124.3, 124.2, 120.1, 120.0, 116.6, 116.5, 116.4, 116.3, 116.2, 116.1,



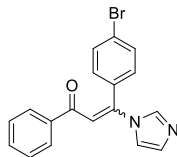
(Z/E)-1-(3-chlorophenyl)-3-(1H-imidazol-1-yl)-3-phenylprop-2-en-1-one (1j). 243 mg, 79% yield; yellow liquid. ^1H NMR (400 MHz, CDCl_3) δ 7.81 (d, $J = 4.0$ Hz, 1H), 7.74 (d, $J = 8.0$ Hz, 1H), 7.60–7.27 (m, 8H), 7.15–6.86 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 188.9, 188.7, 148.3, 145.7, 139.3, 138.7, 135.3, 134.8, 134.7, 133.1, 132.9, 132.8, 131.5, 130.8, 130.7, 129.9, 129.8, 129.6, 129.0, 128.6, 128.5, 128.2, 127.9, 126.5, 126.3, 116.7, 113.5.



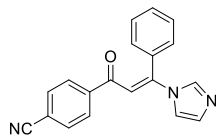
(E)-3-(4-chlorophenyl)-3-(1H-imidazol-1-yl)-1-phenylprop-2-en-1-one (1k). 231 mg, 75% yield; yellow solid, mp 119.6–1124.6 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.90 (d, $J = 4.0$ Hz, 2H), 7.26–7.34 (m, 7H), 7.24–7.00 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ 189.7, 146.3, 137.6, 137.2, 136.8, 133.3, 131.5, 131.0 (2C), 130.9, 128.9 (2C), 128.6 (2C), 128.4 (2C), 118.5, 114.5.



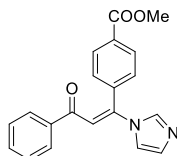
(E)-1-(3-bromophenyl)-3-(1H-imidazol-1-yl)-3-phenylprop-2-en-1-one (1l). 272 mg, 77% yield; yellow solid, mp 134.5–139.3 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.61–7.27 (m, 8H), 7.17–6.89 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 189.1, 147.9, 137.4, 136.5, 132.9, 131.8 (2C), 130.8 (2C), 129.9 (2C), 129.8 (2C), 129.8 (2C), 128.2, 118.5, 113.6,



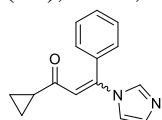
(Z/E)-3-(4-bromophenyl)-3-(1H-imidazol-1-yl)-1-phenylprop-2-en-1-one (1l'). 247 mg, 70% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.89–7.83 (m, 2H), 7.59–7.36 (m, 6H), 7.22–6.83 (m, 5H); ¹³C NMR (100 MHz, CDCl₃) δ 189.7, 189.5, 146.2, 143.4, 138.2, 137.5, 137.1, 136.8, 134.4, 133.4, 133.2, 132.2, 131.9, 131.8, 131.1, 130.7, 129.7, 129.1, 128.5, 128.3, 128.2, 125.7, 125.1, 120.0, 118.4, 117.9, 114.4.



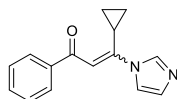
(E)-4-(3-(1H-imidazol-1-yl)-3-phenylacryloyl)benzonitrile (1m). 206 mg, 69% yield; yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.91 (d, *J* = 8.0 Hz, 2H), 7.67–7.28 (m, 8H), 7.18–6.88 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 189.0, 149.1, 141.0, 137.4, 132.6, 132.2 (2C), 131.11, 131.07, 129.8 (2C), 128.7 (2C), 118.4, 117.8, 115.9, 112.9.



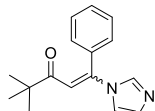
(E)-methyl 4-(1-(1H-imidazol-1-yl)-3-oxo-3-phenylprop-1-en-1-yl)benzoate (1n). 216 mg, 65% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 8.11 (d, *J* = 8.0 Hz, 2H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.58–7.41 (m, 6H), 7.04–6.87 (m, 3H), 3.95 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 190.1, 166.0, 139.7, 138.4, 136.8, 133.7, 132.5, 130.2 (2C), 130.0, 128.7 (2C), 128.4 (2C), 127.7 (2C), 120.2, 119.5, 52.5.



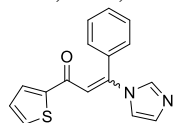
(Z/E)-1-cyclopropyl-3-(1H-imidazol-1-yl)-3-phenylprop-2-en-1-one. yellow liquid (1o). 198 mg, 83% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.61–7.34 (m, 5H), 7.30–7.27 (m, 1H), 7.18 (s, 0.5H), 7.13 (s, 0.5H), 7.06 (s, 0.5H), 6.95 (s, 0.5H), 6.49 (s, 0.5H), 6.43 (s, 0.5H), 1.67–1.53 (m, 1H), 1.10–1.00 (m, 2H), 0.84–0.69 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 200.0, 199.6, 146.1, 143.6, 138.9, 137.3, 135.4, 133.1, 131.2, 130.9, 130.7, 130.0, 129.0, 128.7, 127.6, 121.5, 120.4, 118.4, 117.9, 22.1, 21.0, 12.51, 12.48.



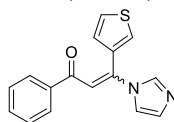
(Z/E)-1-cyclopropyl-3-(1H-imidazol-1-yl)-3-phenylprop-2-en-1-one (1o'). 157 mg, 66% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.94–7.36 (m, 6H), 7.19–6.34 (m, 3H), 2.57–2.50 (m, 0.7H), 1.81–1.74 (m, 0.3H), 1.12–1.03 (m, 2H), 0.94–0.60 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 190.7, 190.4, 151.7, 148.0, 138.2, 137.2, 137.0, 136.4, 133.23, 133.20, 130.0, 129.5, 128.7, 128.5, 128.3, 128.2, 118.8, 118.4, 117.5, 114.1, 17.2, 13.6, 8.8, 8.0.



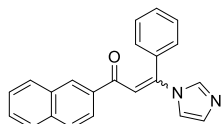
(Z/E)-1-(1H-imidazol-1-yl)-4,4-dimethyl-1-phenylpent-1-en-3-one (1p). 193 mg, 76% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.54–7.38 (m, 4H), 7.27 (s, 1H), 7.25 (d, *J* = 4.0 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 1H), 7.04 (s, 0.5H), 6.87 (s, 0.5H), 6.73 (s, 0.5H), 6.67 (s, 0.5H), 1.20 (s, 4.3H), 1.19 (s, 4.7); ¹³C NMR (100 MHz, CDCl₃) δ 203.6, 203.1, 147.2, 144.4, 138.6, 137.2, 136.3, 133.3, 131.1, 130.5, 130.3, 129.2, 128.9, 128.5, 127.7, 120.3, 118.3, 115.6, 111.7, 44.4, 44.1, 26.4, 26.3.



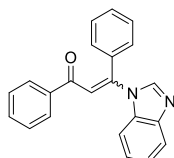
(Z/E)-3-(1H-imidazol-1-yl)-3-phenyl-1-(thiophen-2-yl)prop-2-en-1-one (1q). 204 mg, 73% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.71–7.58 (m, 3H), 7.49–7.31 (m, 5H), 7.13–6.90 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 181.3, 180.9, 147.6, 145.4, 144.9, 138.5, 137.2, 135.7, 134.6, 134.2, 134.8, 132.1, 132.0, 131.3, 130.6, 130.5, 129.5, 129.4, 128.9, 128.4, 128.1, 128.1, 127.9, 120.4, 118.4, 116.0, 112.8.



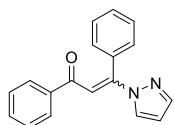
(Z/E)-3-(1H-imidazol-1-yl)-1-phenyl-3-(thiophen-2-yl)prop-2-en-1-one (1r). 190 mg, 68% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.87–7.82 (m, 2H), 7.67–7.32 (m, 6H), 7.23–6.82 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 190.3, 189.7, 141.3, 139.6, 138.0, 137.8, 137.5, 137.2, 137.1, 133.4, 133.1, 133.0, 130.4, 129.7, 129.3, 128.4, 128.3, 128.1, 127.9, 127.5, 126.2, 125.7, 120.1, 118.7, 116.3, 114.7.



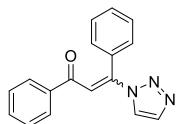
(Z/E)-3-(1H-imidazol-1-yl)-1-(naphthalen-2-yl)-3-phenylprop-2-en-1-one (1s). 285 mg, 88% yield; yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 8.44 (d, *J* = 8.0 Hz, 1H), 7.98–7.83 (m, 4H), 7.76–7.33 (m, 8H), 7.20–6.92 (m, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 190.0, 189.8, 147.3, 144.7, 138.4, 137.4, 135.7, 135.6, 135.5, 135.1, 134.6, 133.2, 132.3, 132.2, 131.3, 130.7, 130.6, 130.4, 130.3, 129.7, 129.6, 129.5, 129.4, 129.0, 128.7, 128.6, 128.5, 127.9, 127.8, 127.7, 126.9, 126.8, 123.9, 123.7, 120.3, 118.6, 117.6, 114.5.



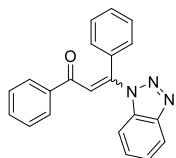
(Z/E)-3-(1H-benzo[d]imidazol-1-yl)-1,3-diphenylprop-2-en-1-one (A). 308 mg, 95% yield; yellow solid. ¹H NMR (400 MHz, CDCl₃) δ 7.94–7.72 (m, 4H), 7.51–7.27 (m, 8H), 7.24–6.81 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ 190.6, 189.5, 146.8, 144.4, 143.7, 143.5, 142.8, 137.5, 137.2, 134.8, 133.3, 133.2, 133.1, 133.0, 131.3, 130.7, 129.6, 129.0, 128.6, 128.5, 128.4, 128.3, 128.0, 127.6, 124.0, 123.4, 122.7, 120.7, 120.2, 118.2, 116.9, 112.1, 111.6.



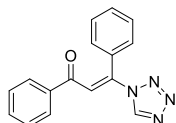
(Z/E)-1,3-diphenyl-3-(1H-pyrazol-1-yl)prop-2-en-1-one (B). 225 mg, 82% yield; yellow liquid. ¹H NMR (400 MHz, CDCl₃) δ 7.99–7.80 (m, 3H), 7.53–7.34 (m, 9H), 7.23–6.22 (m, 2H); ¹³C NMR (100 MHz, CDCl₃) δ 191.8, 189.8, 149.5, 146.7, 142.7, 141.4, 138.6, 137.4, 135.4, 133.1, 132.7, 132.6, 131.8, 130.7, 130.7, 129.8, 127.8, 127.5, 128.4, 128.38, 128.35, 128.30, 117.3, 111.3, 108.2, 107.3.



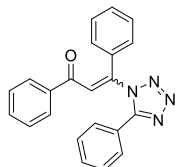
(Z/E)-1,3-diphenyl-3-(1H-1,2,3-triazol-1-yl)prop-2-en-1-one (C). 223 mg, 81% yield; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.96 (d, $J = 8.0$ Hz, 1H), 7.88 (d, $J = 8.0$ Hz, 1H), 7.84–7.69 (m, 2H), 7.56–7.32 (m, 9H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.1, 189.9, 144.9, 143.2, 137.4, 136.8, 134.3, 134.1, 133.6, 133.5, 133.4, 132.0, 131.3, 130.6, 129.5, 129.1, 128.68, 128.6, 128.57, 128.54, 127.4, 125.7, 124.3, 121.0, 116.9.



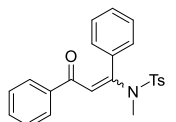
(Z/E)-3-(1H-benzo[d][1,2,3]triazol-1-yl)-1,3-diphenylprop-2-en-1-one (D). 280 mg, 86% yield; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.11–7.76 (m, 3H), 7.62–7.30 (m, 9H), 7.23–6.48 (m, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.3, 146.6, 145.7, 143.2, 137.5, 136.9, 133.8, 133.3, 133.2, 132.9, 132.5, 132.0, 131.3, 130.7, 129.6, 129.1, 128.7, 128.6, 128.5, 128.3, 128.2, 128.1, 128.0, 127.5, 124.6, 124.2, 121.0, 120.3, 120.0, 118.2, 111.7, 110.7.



(E)-1,3-diphenyl-3-(1H-tetrazol-1-yl)prop-2-en-1-one (E). 207 mg, 75% yield; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.43 (s, 1H), 7.95 (d, $J = 4.0$ Hz, 2H), 7.78 (s, 1H), 7.57 (t, $J = 8.0$ Hz, 1H), 7.51–7.41 (m, 5H), 7.35 (d, $J = 8.0$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 189.3, 142.3, 141.5, 136.8, 133.8, 131.2, 130.8, 129.3 (2C), 129.1 (2C), 128.77 (2C), 128.73 (2C), 119.2.



(Z/E)-1,3-diphenyl-3-(5-phenyl-1H-tetrazol-1-yl)prop-2-en-1-one (F). 289 mg, 82% yield; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 8.24–8.21 (m, 1H), 8.06–7.85 (m, 3H), 7.58–7.36 (m, 12H); ^{13}C NMR (100 MHz, CDCl_3) δ 190.2, 165.2, 145.0, 137.1, 133.6, 133.5, 131.4, 130.9, 130.65, 130.59, 130.54, 130.1, 129.1, 129.0, 128.8, 128.79, 128.7, 128.6, 128.4, 128.3, 127.6, 127.2, 127.1, 126.6, 122.3, 119.3.



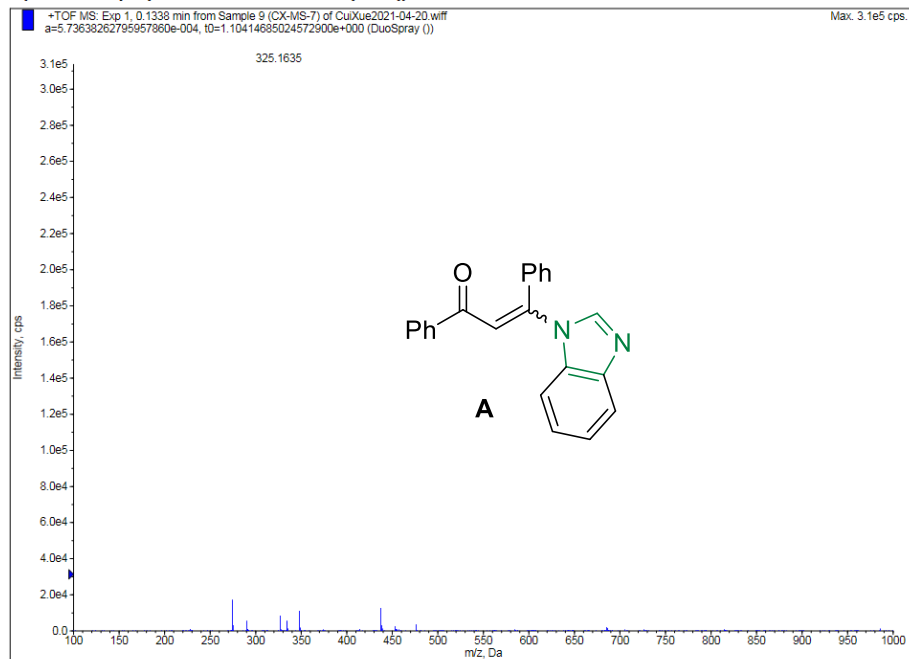
(Z/E)-N,4-dimethyl-N-(3-oxo-1,3-diphenylprop-1-en-1-yl)benzenesulfonamide (G). 332 mg, 85% yield; yellow solid. ^1H NMR (400 MHz, CDCl_3) δ 7.87 (d, $J = 4.0$ Hz, 1H), 7.79 (d, $J = 8.0$ Hz, 1H), 7.73 (d, $J = 8.0$ Hz, 1H), 7.61 (d, $J = 8.0$ Hz, 1H), 7.55–7.52 (m, 1H), 7.46–7.36 (m, 4H), 7.29 (t, $J = 8.0$ Hz, 1H), 7.24–7.11 (m, 4H), 6.97 (s, 0.5H), 6.58 (s, 0.5H), 3.19 (s, 1.5H), 3.06 (s, 1.5H), 2.48 (s, 1.5H), 2.37 (s, 1.5H); ^{13}C NMR (100 MHz, CDCl_3) δ 192.7, 189.2, 151.4, 150.3, 144.3, 143.5, 138.1, 137.6, 137.4, 136.0, 135.3, 134.8, 132.8, 132.7, 130.3, 129.8, 129.7, 129.3, 129.2, 128.8, 128.7, 128.5, 128.4, 128.24, 128.22, 127.98, 127.93, 127.77, 127.7, 120.9, 119.9, 38.5, 37.3, 21.6, 21.5.

References

[1] (a) Q. H. Teng, X. J. Peng, Z. Y. Mo, Y. L. Xu, H. T. Tang, H. S. Wang, H. B. Sun, Y. M. Pan, *Green Chem.*, 2018, **20**, 2007–2012; (b) R. Shankar, A. K. Jha, U. S. Singh, K. Hajela, *Tetrahedron lett.*, 2006, **47**, 3077–3079.

HRMS spectra of compounds B-H.

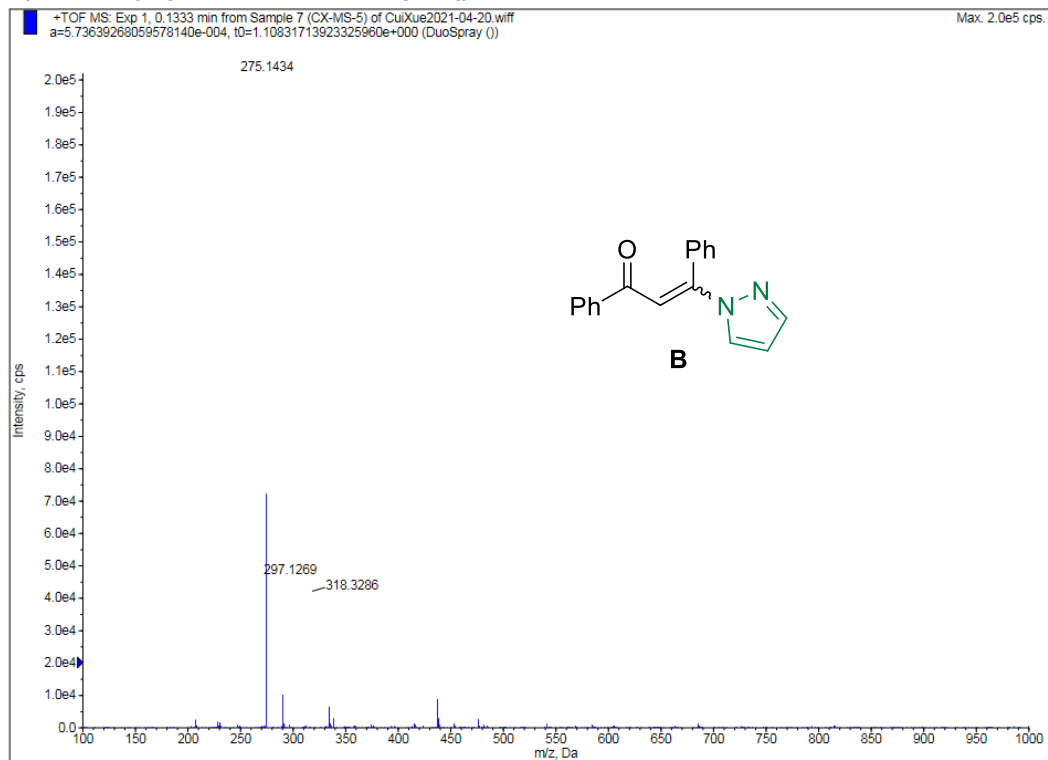
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 Acq. Date: Wednesday, May 19, 2021 Polarity/Scan Type: Positive



Analyst Version: 1.7.1

Page 1 of 1

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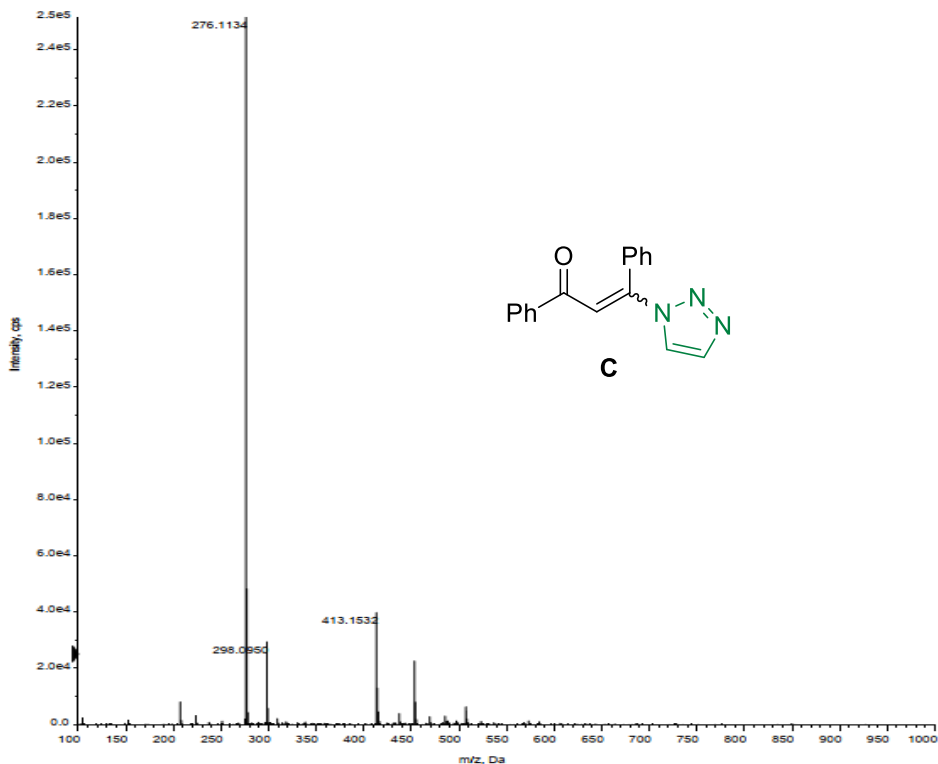


Analyst Version: 1.7.1

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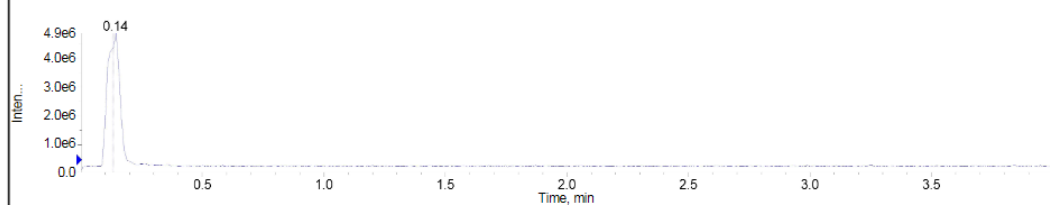
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Max. 2.5e5 cps.

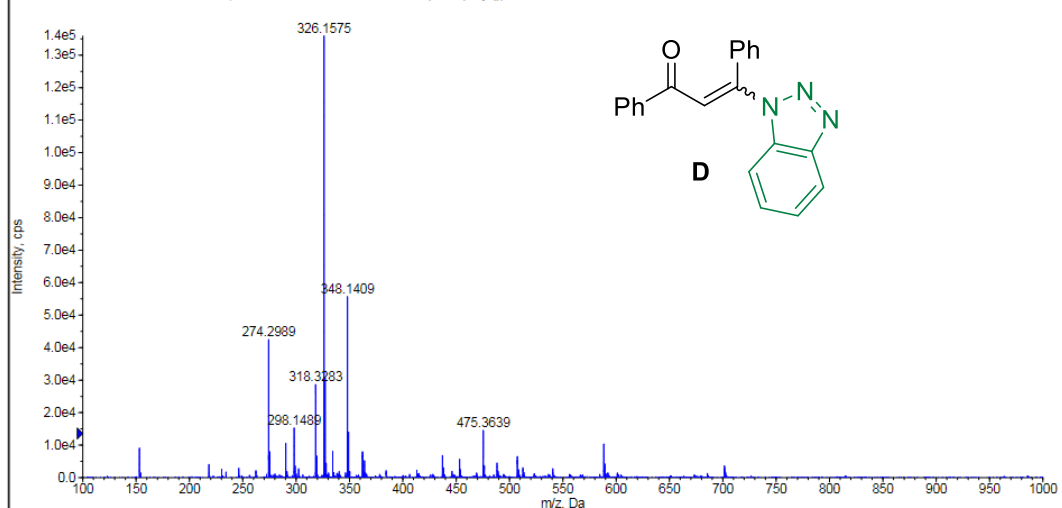


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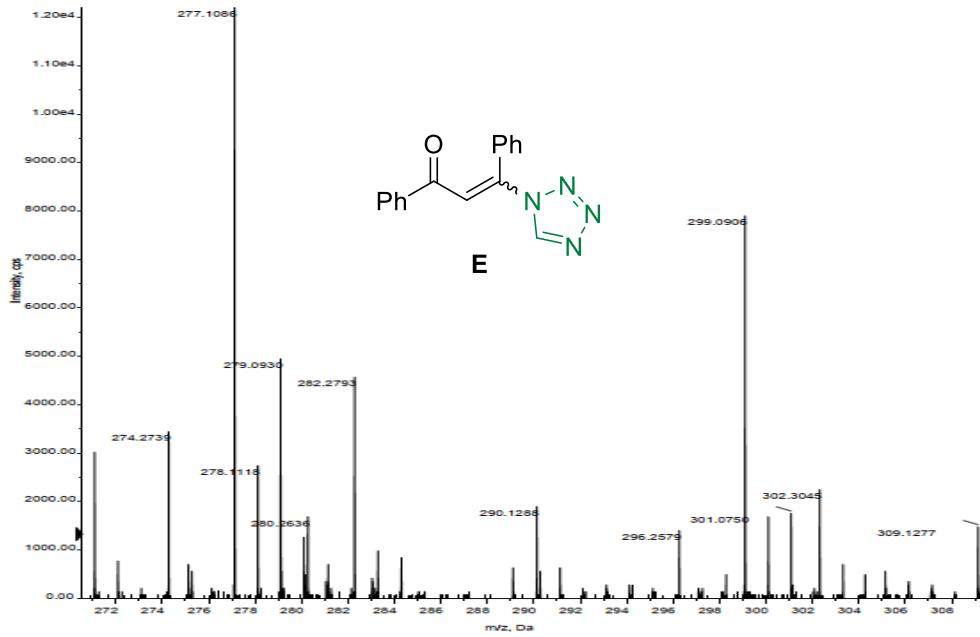


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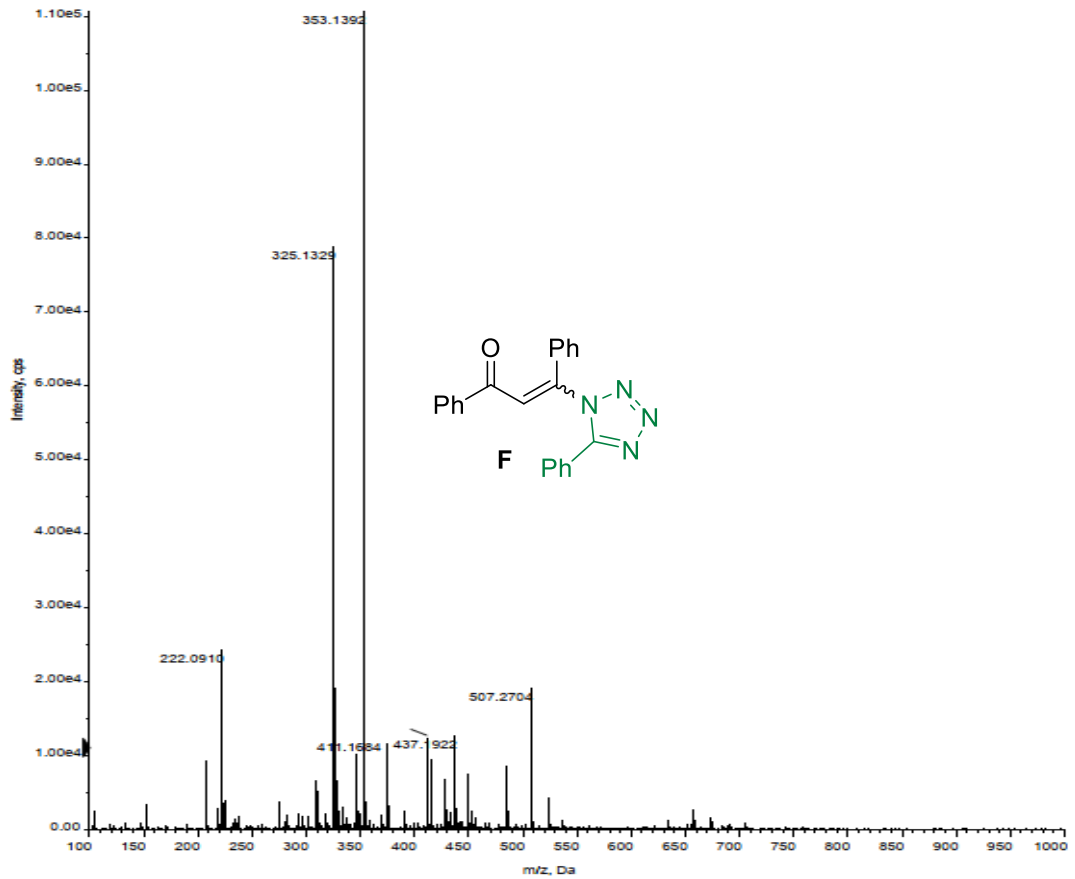
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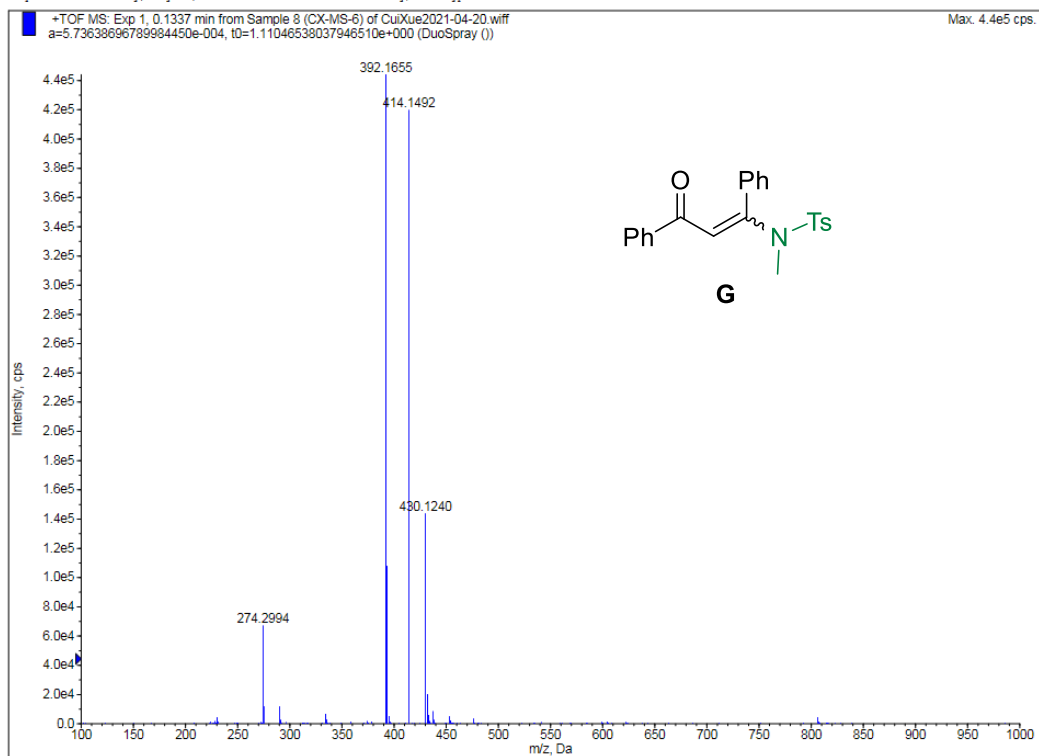
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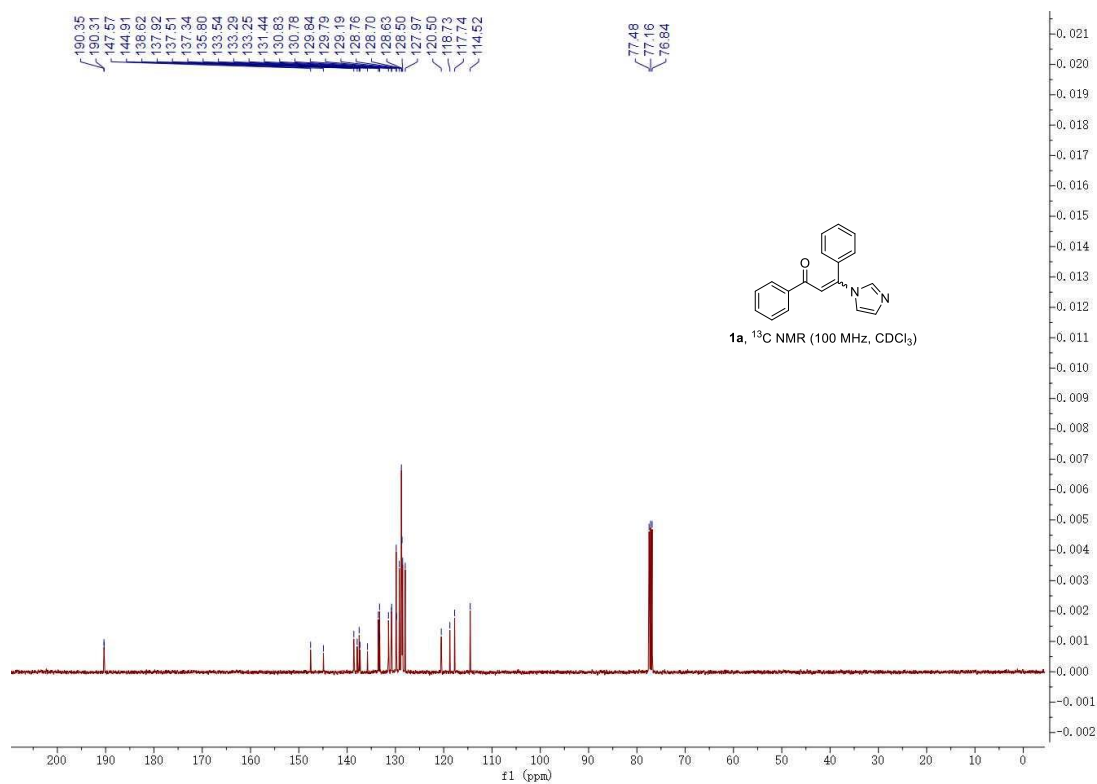
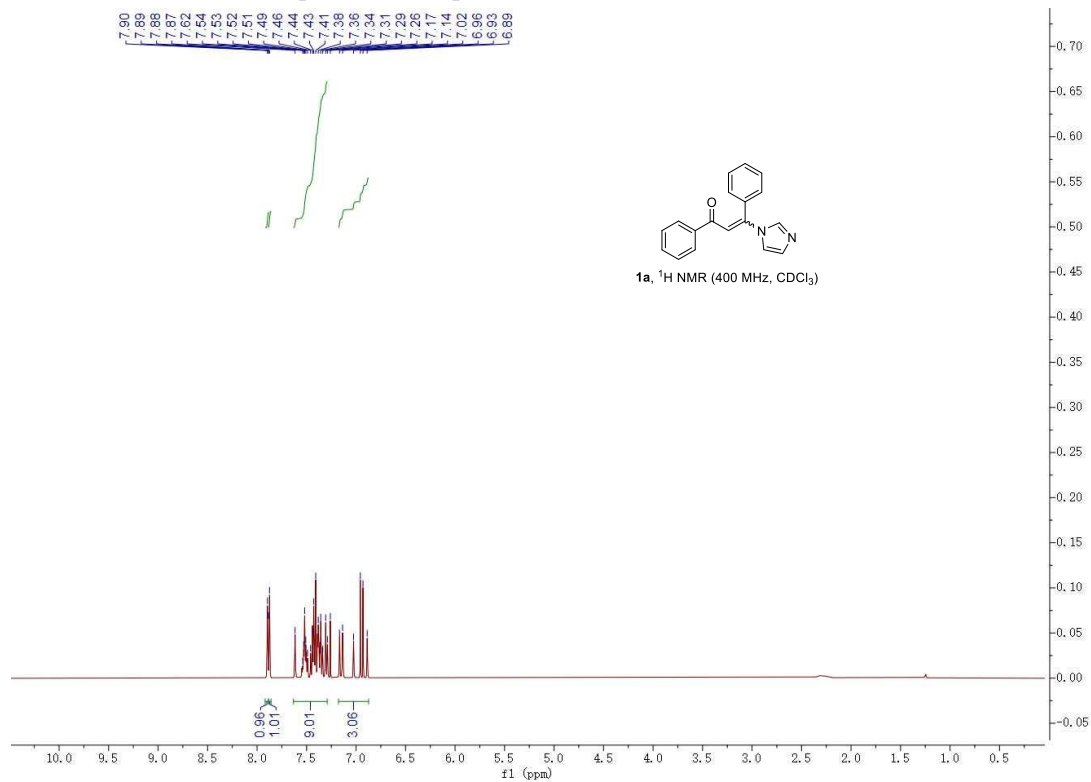
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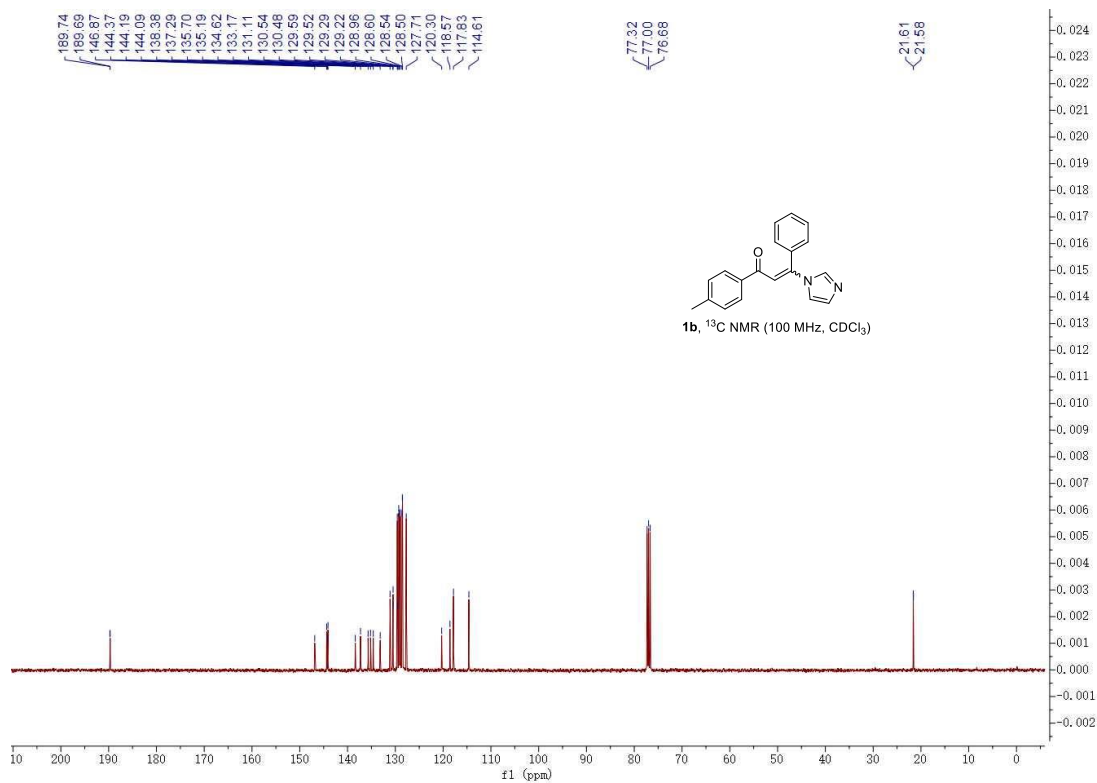
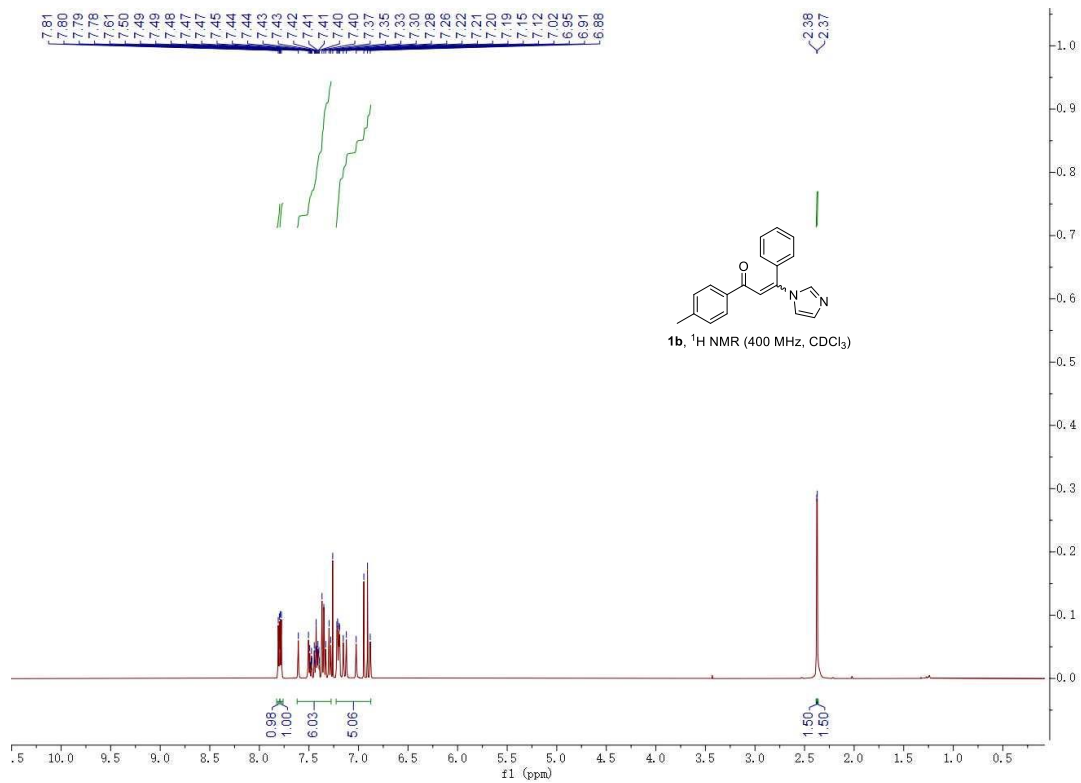
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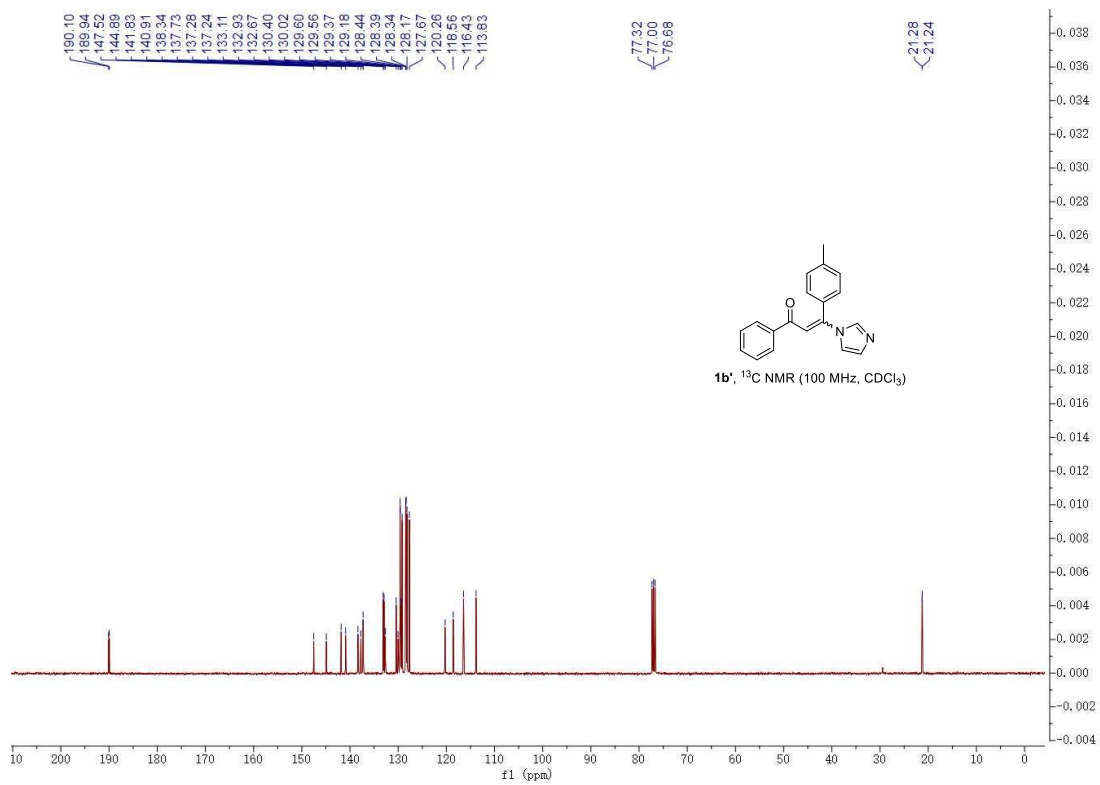
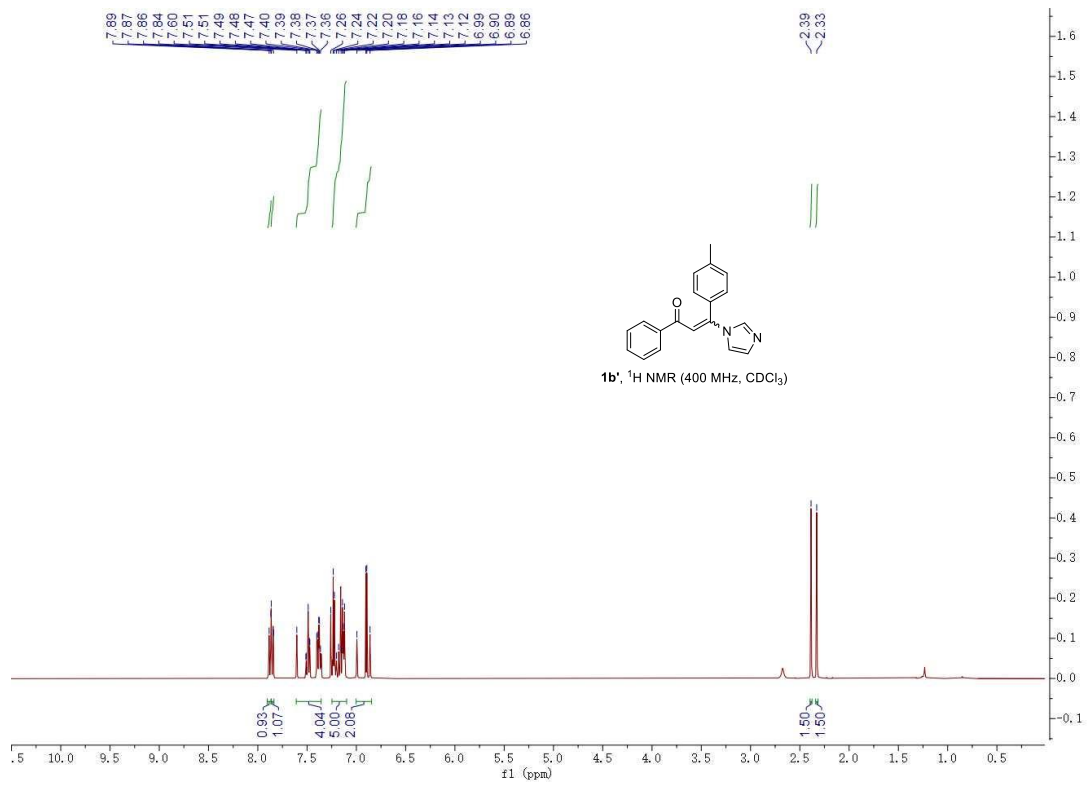
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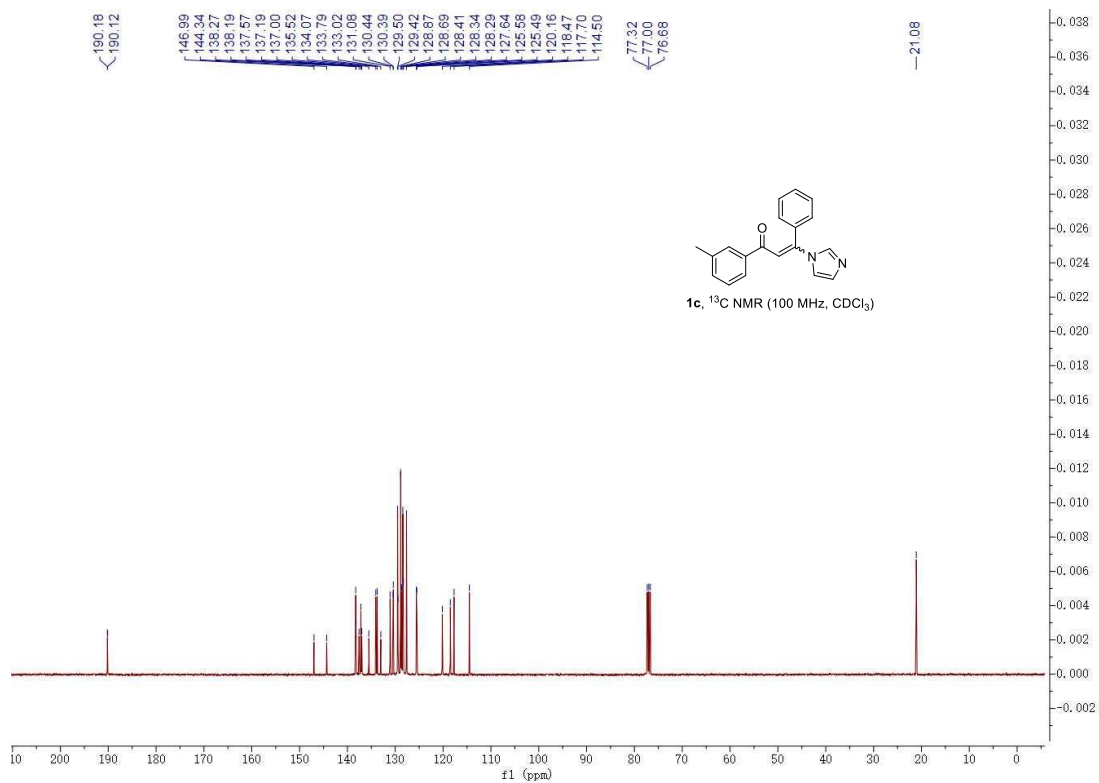
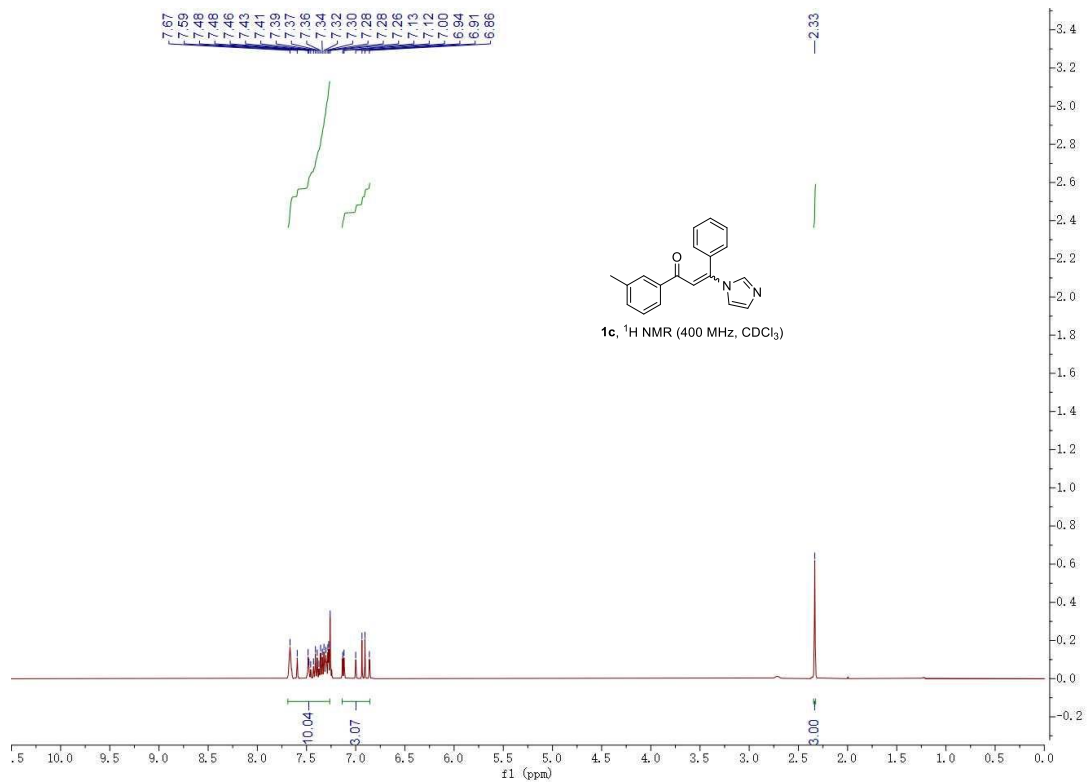


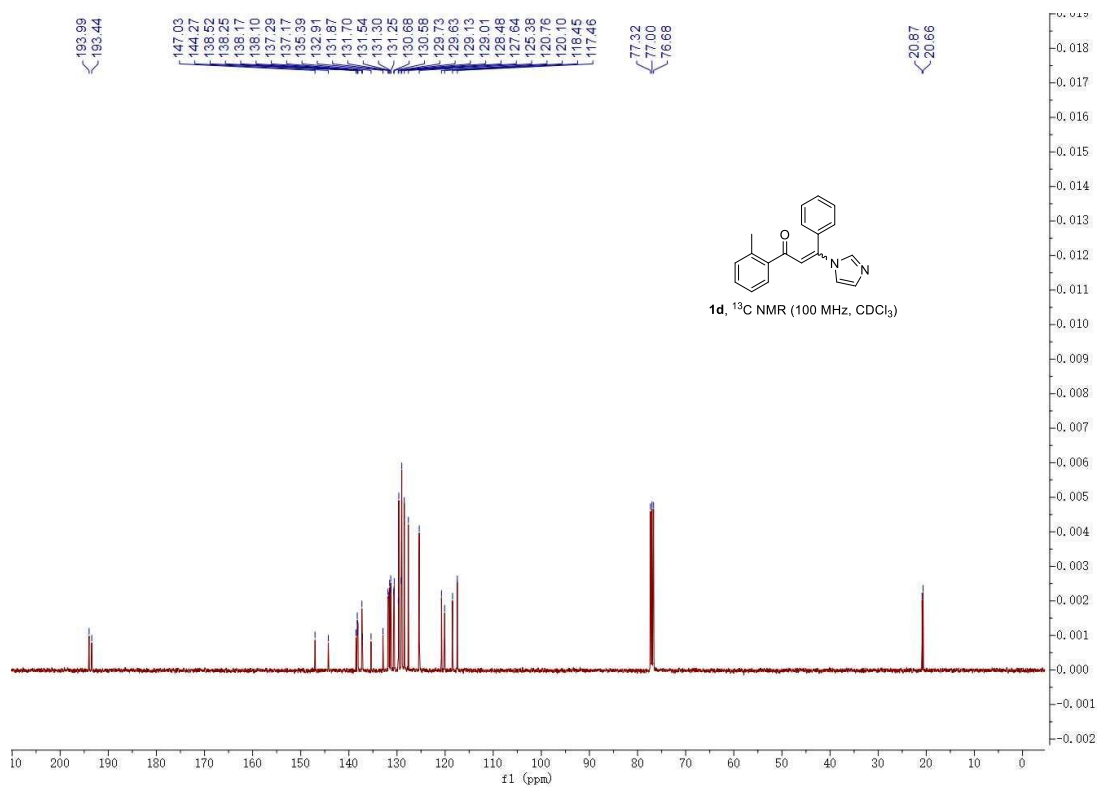
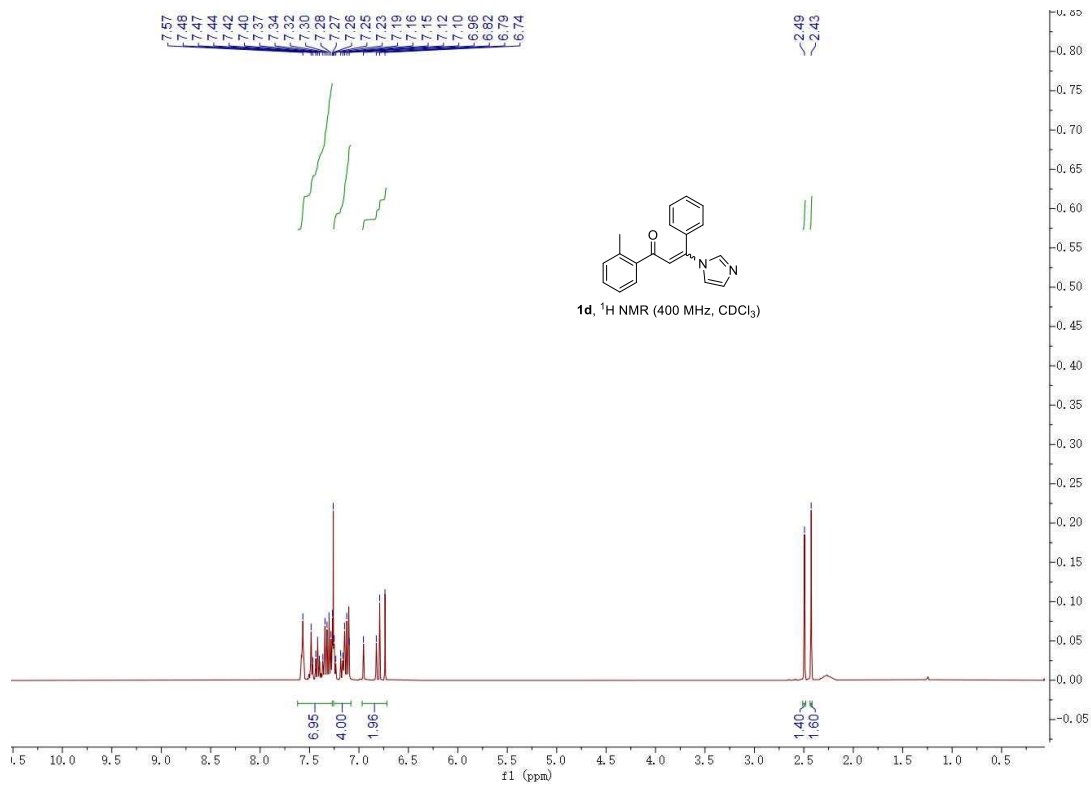
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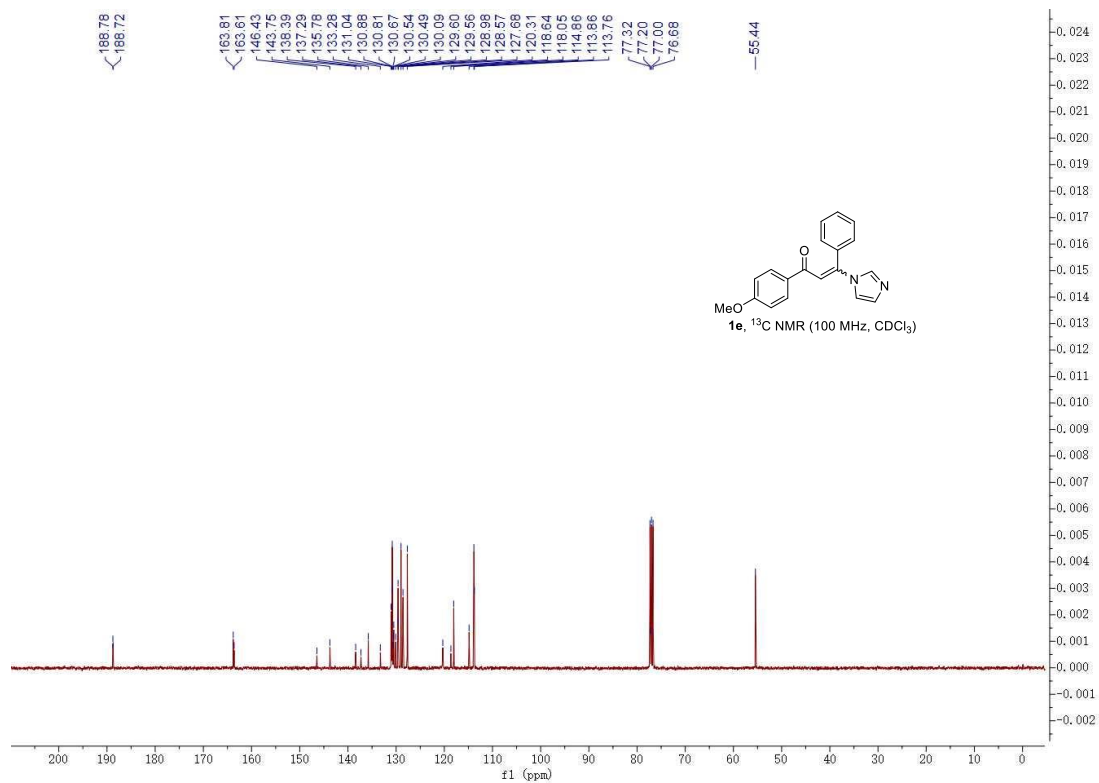
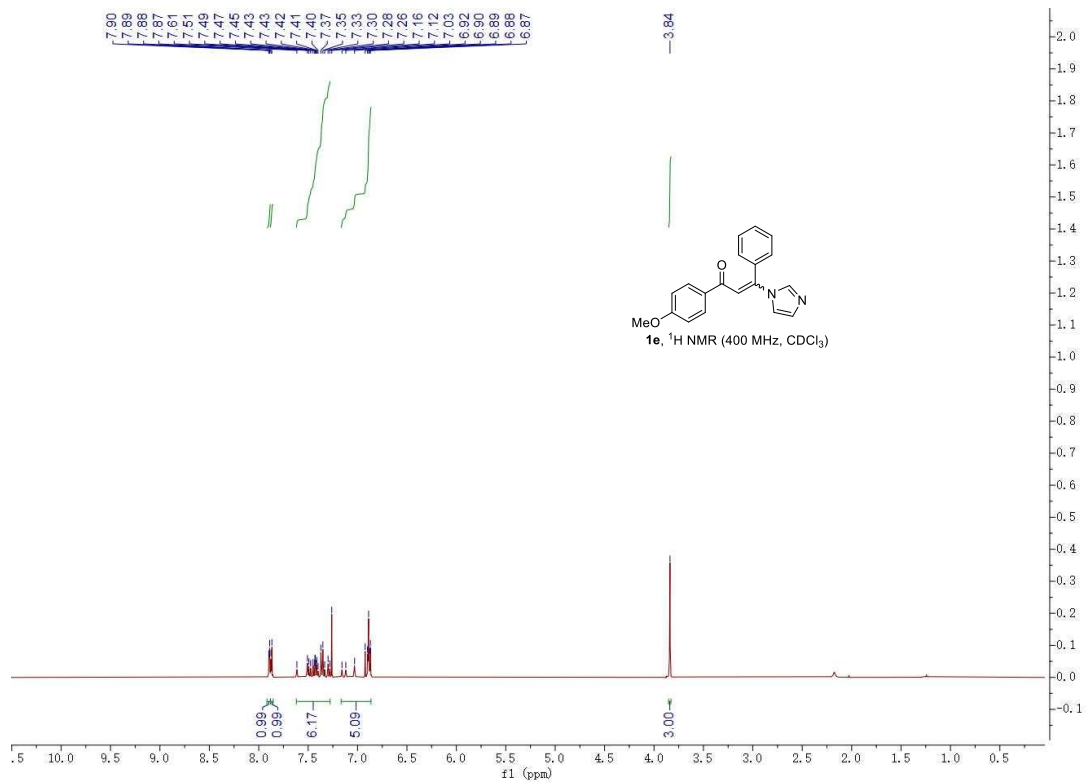


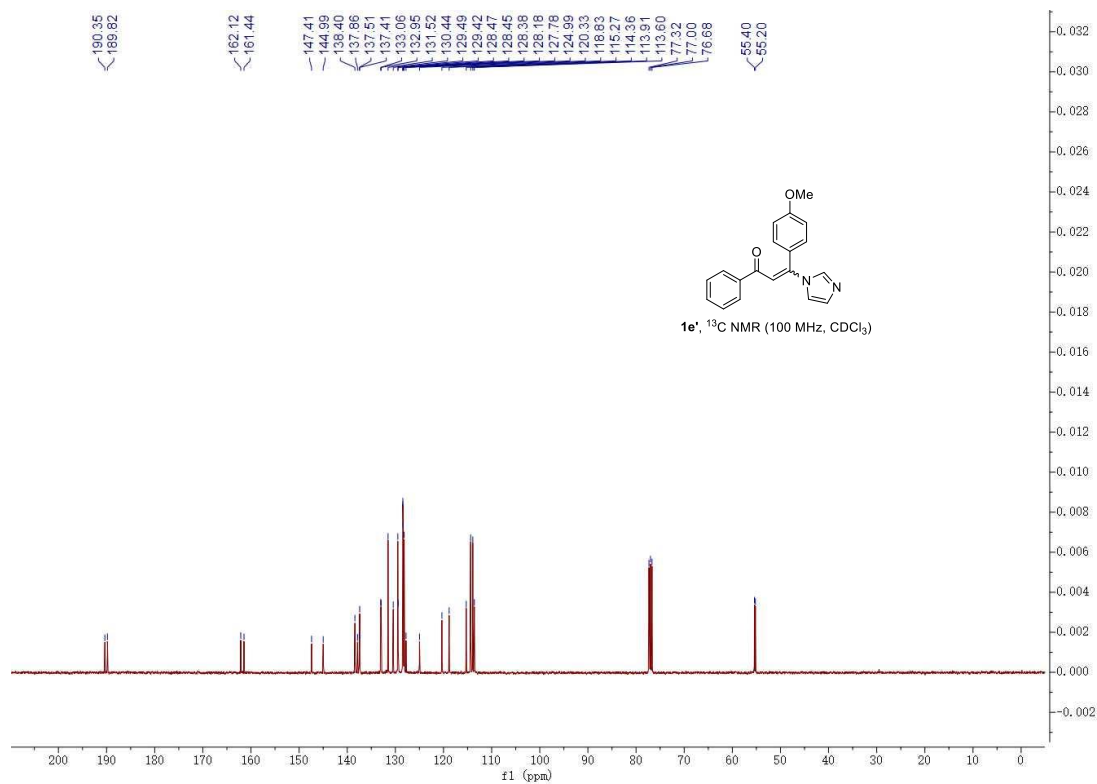
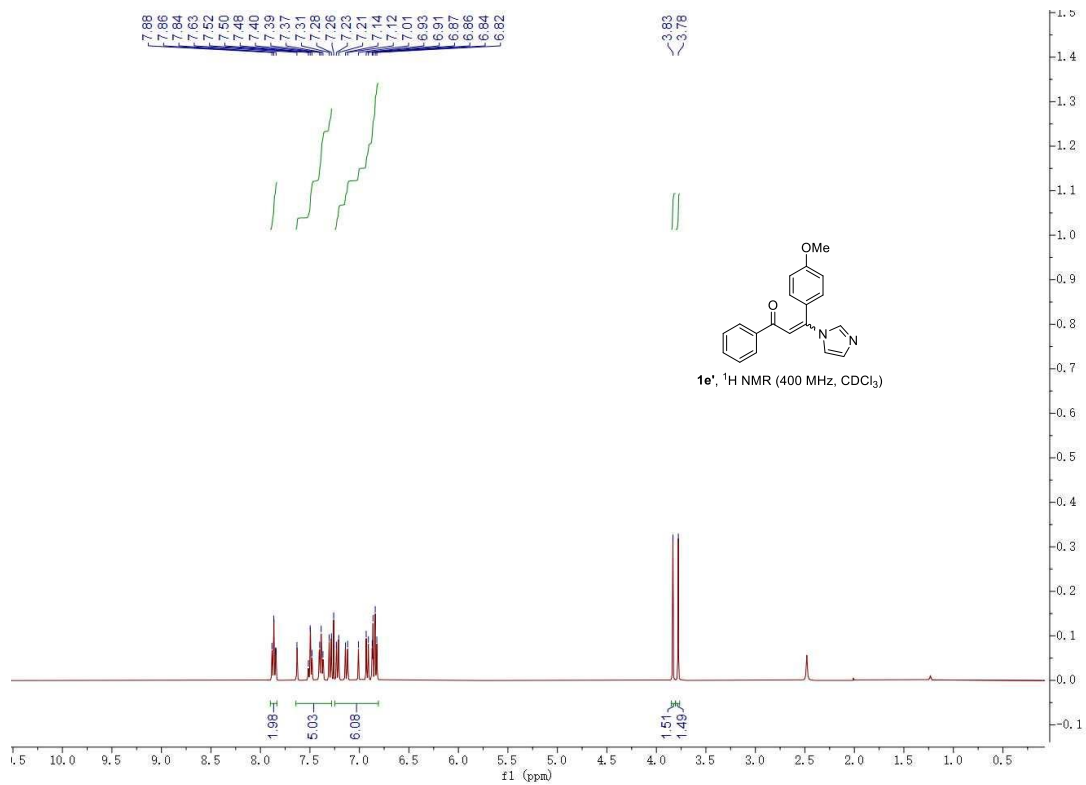


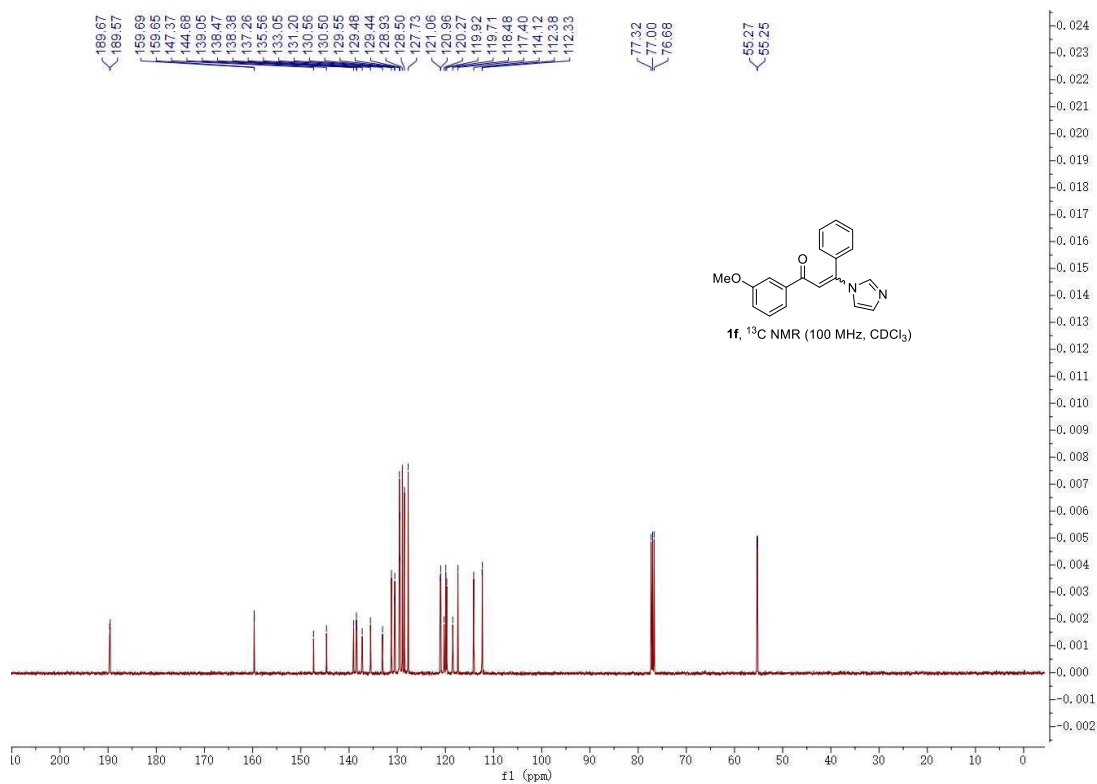
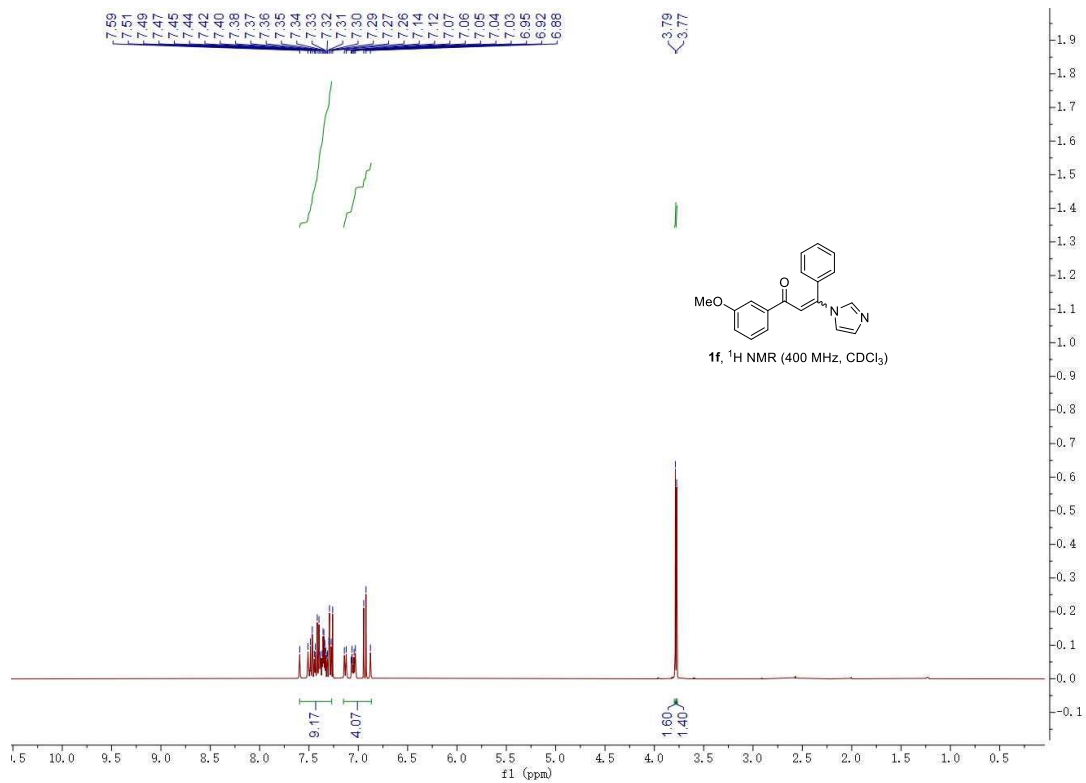


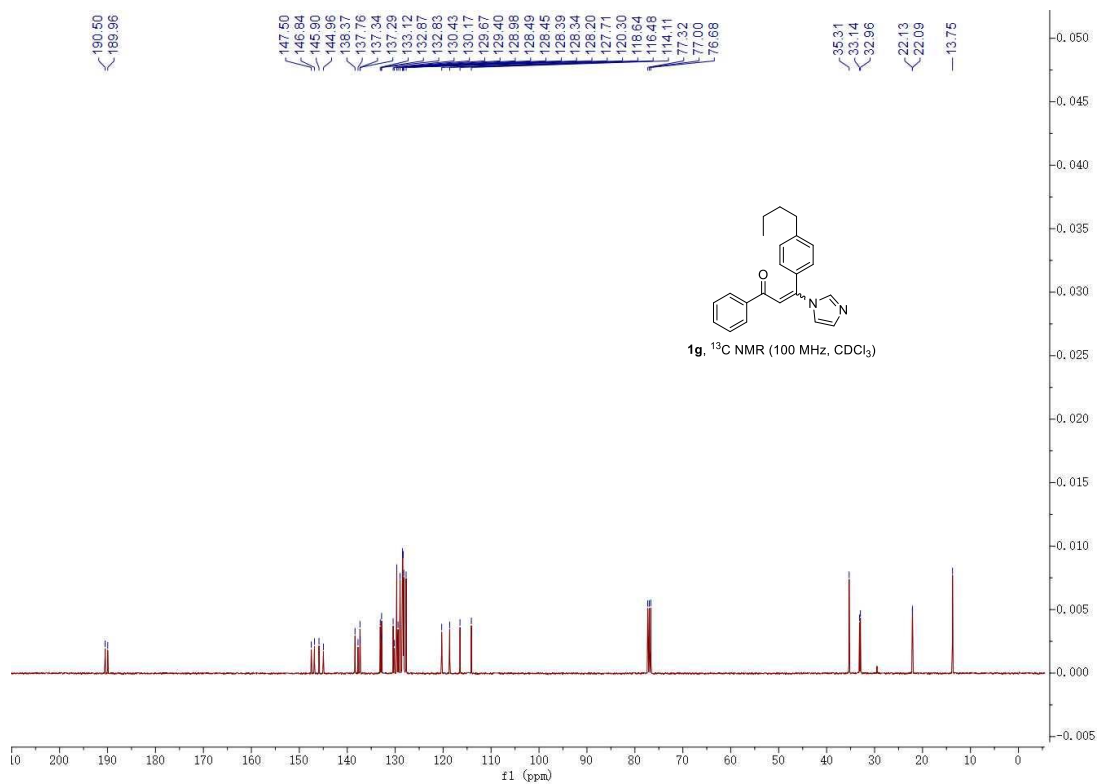
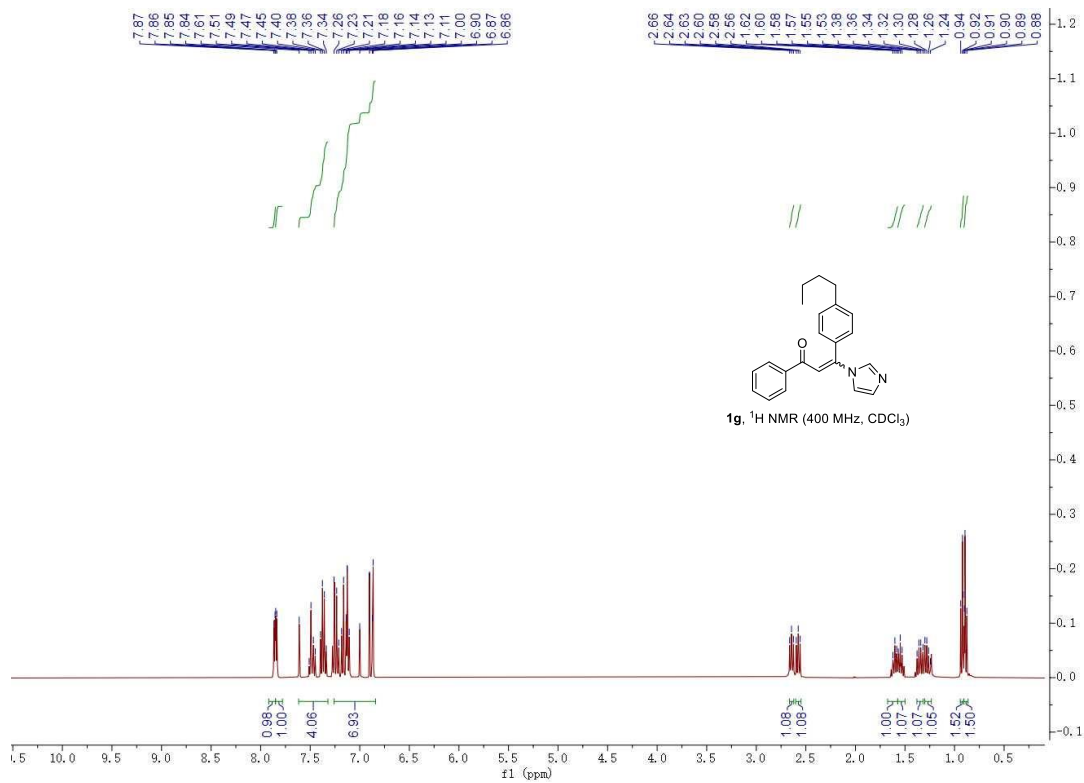


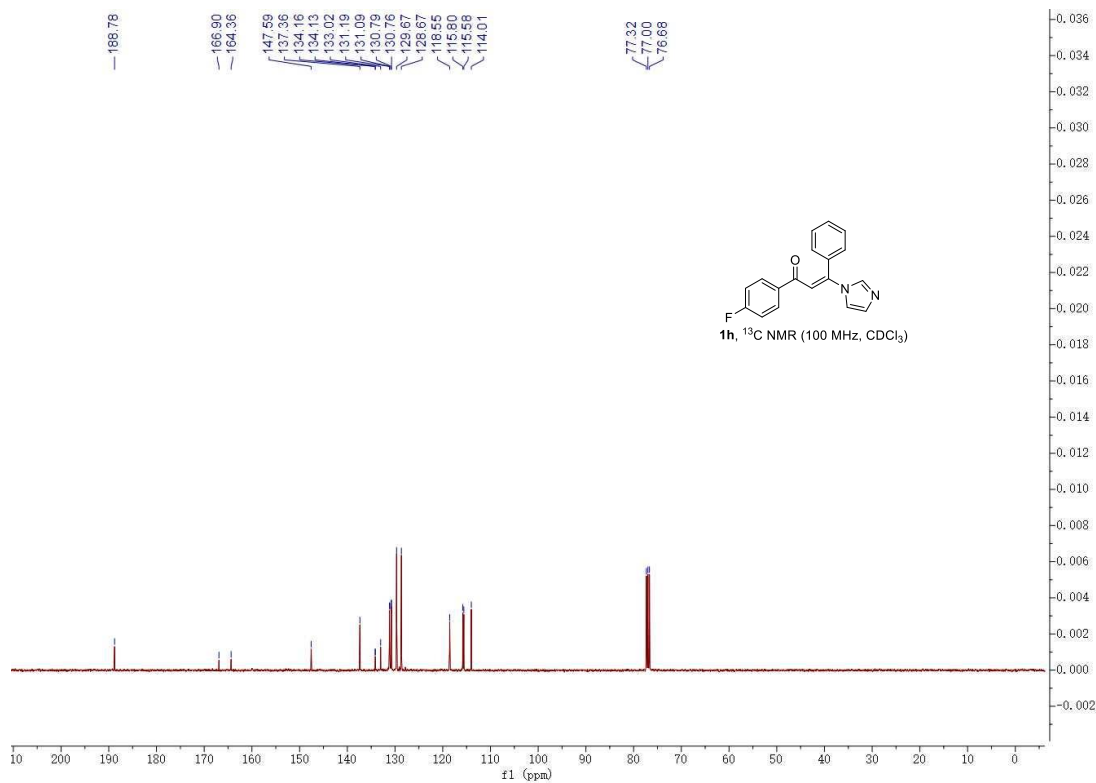
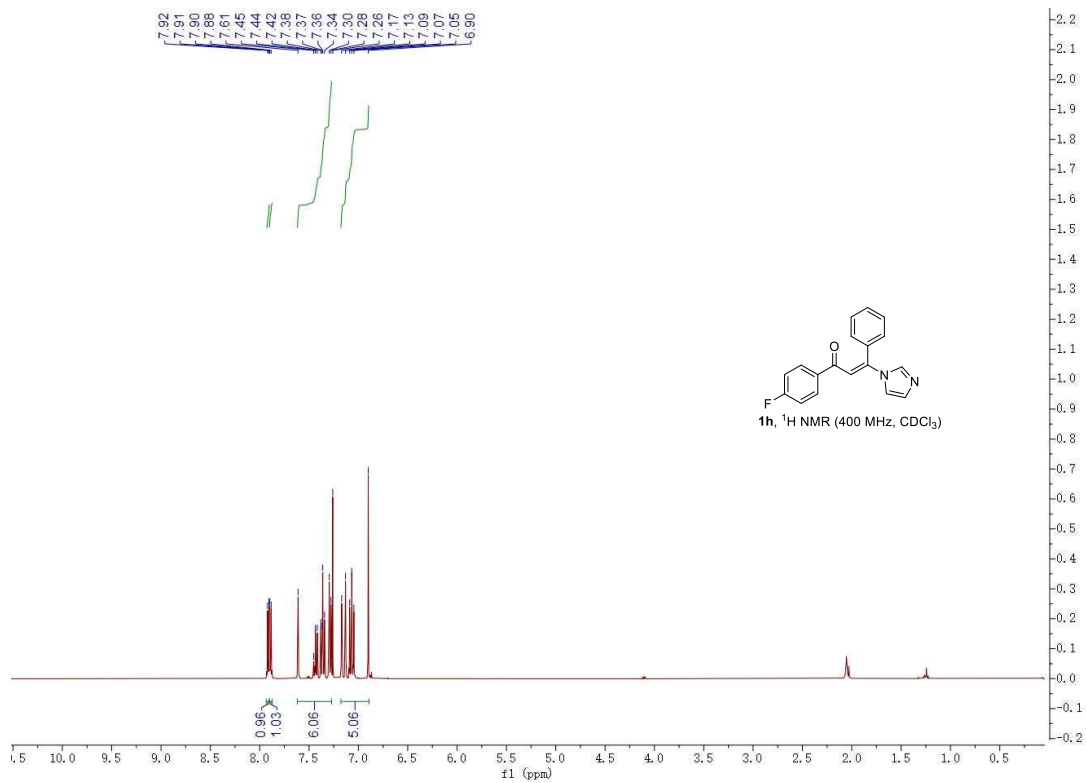


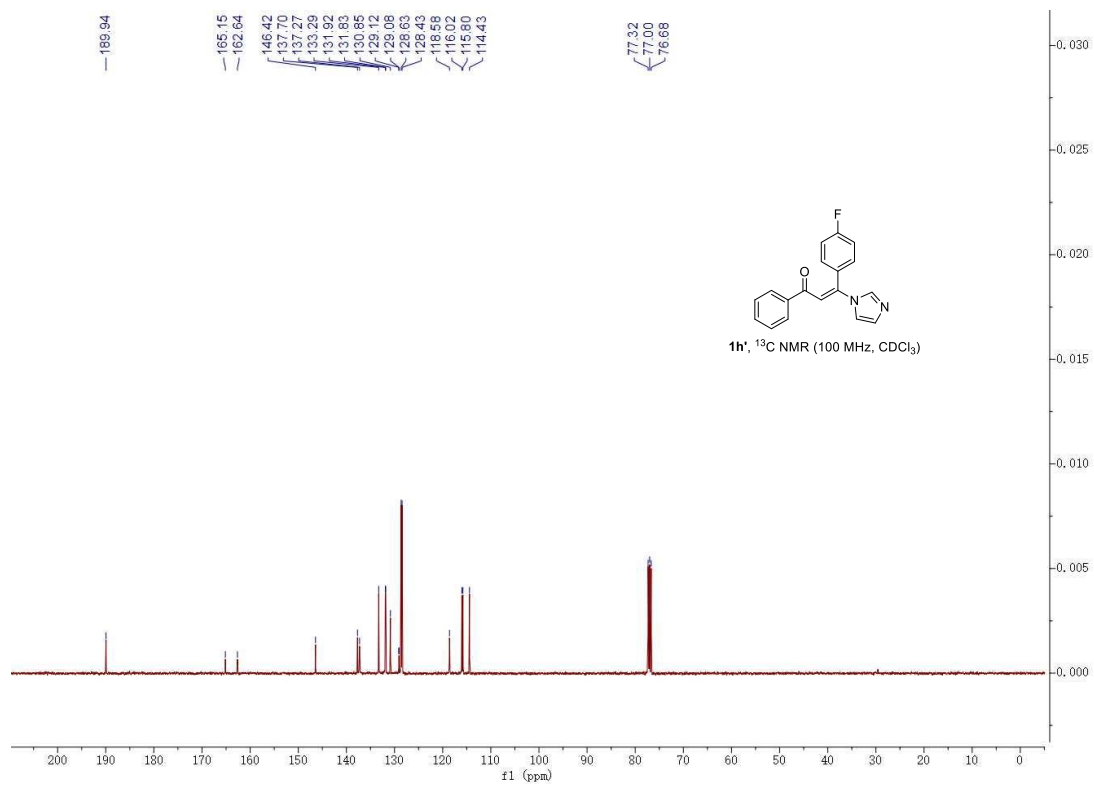
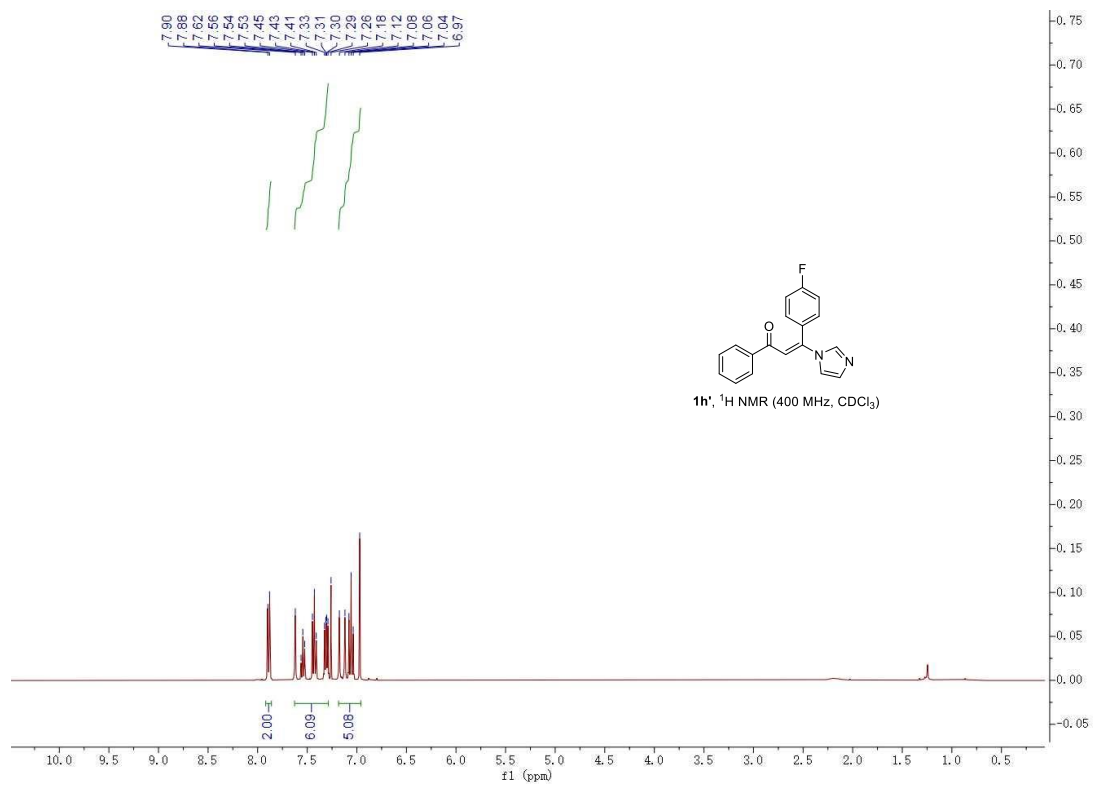


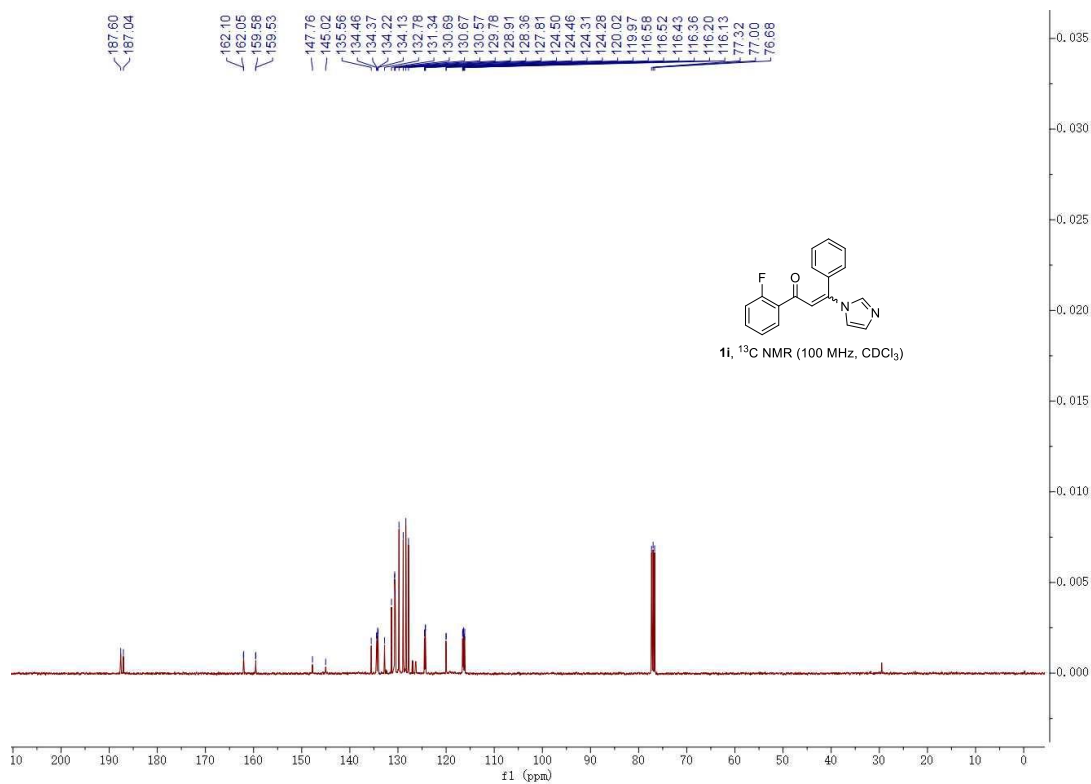
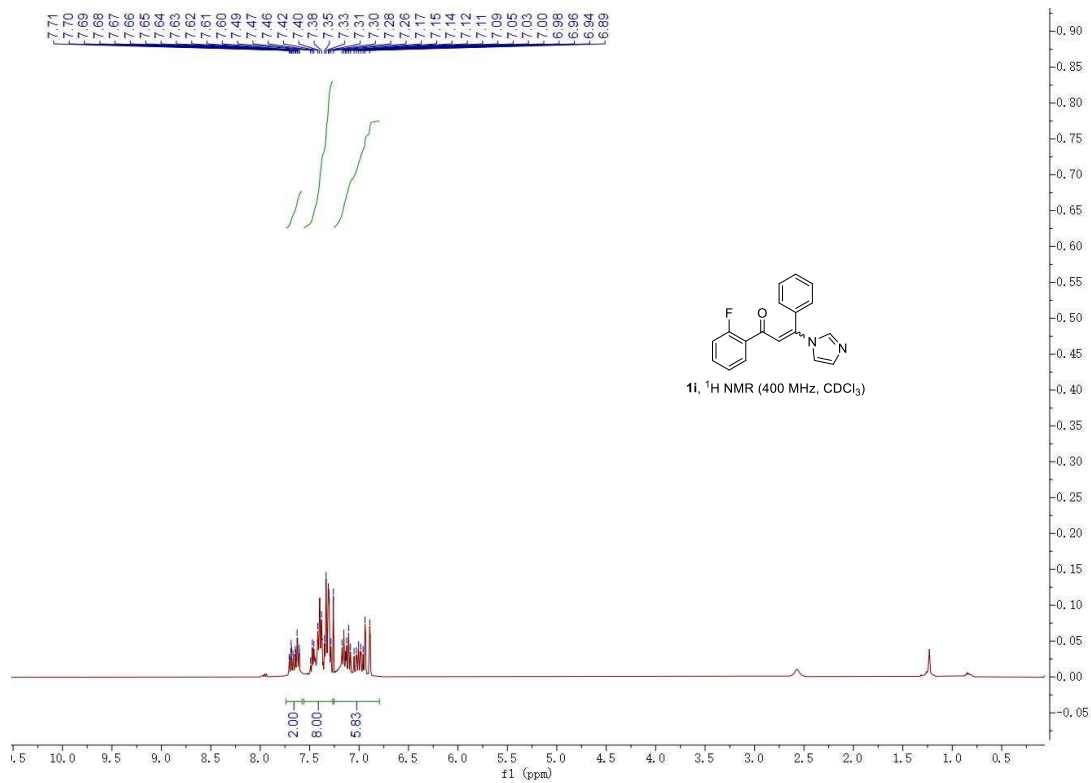


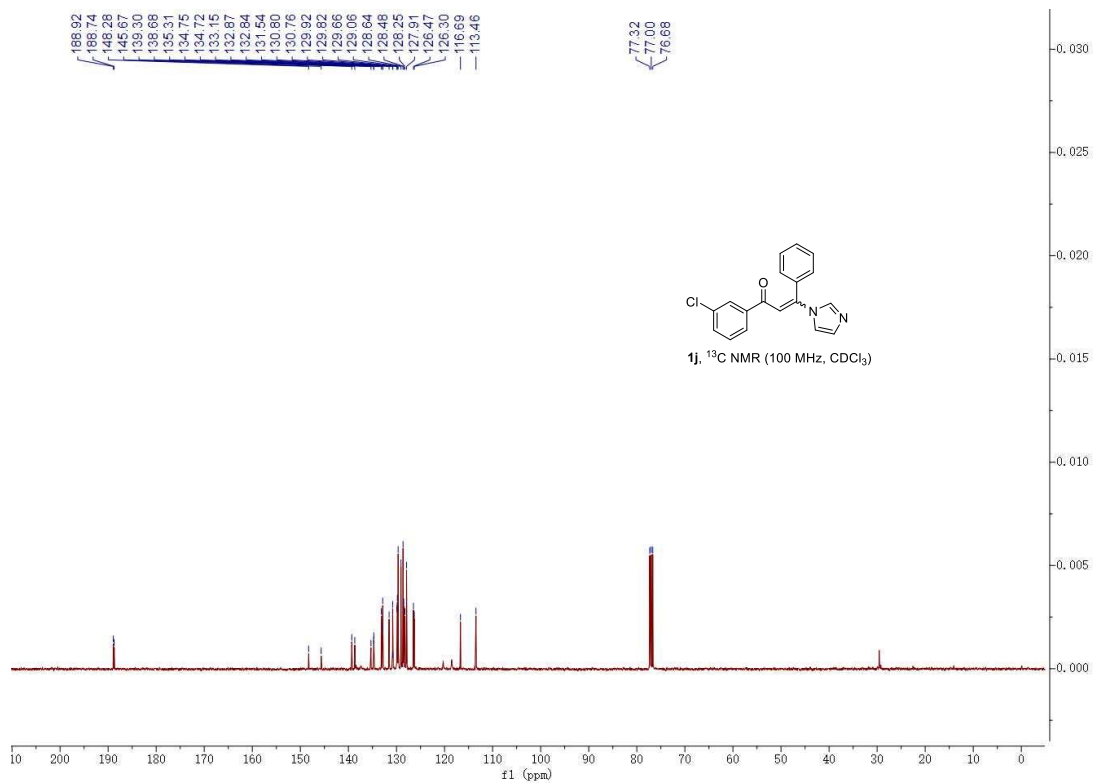
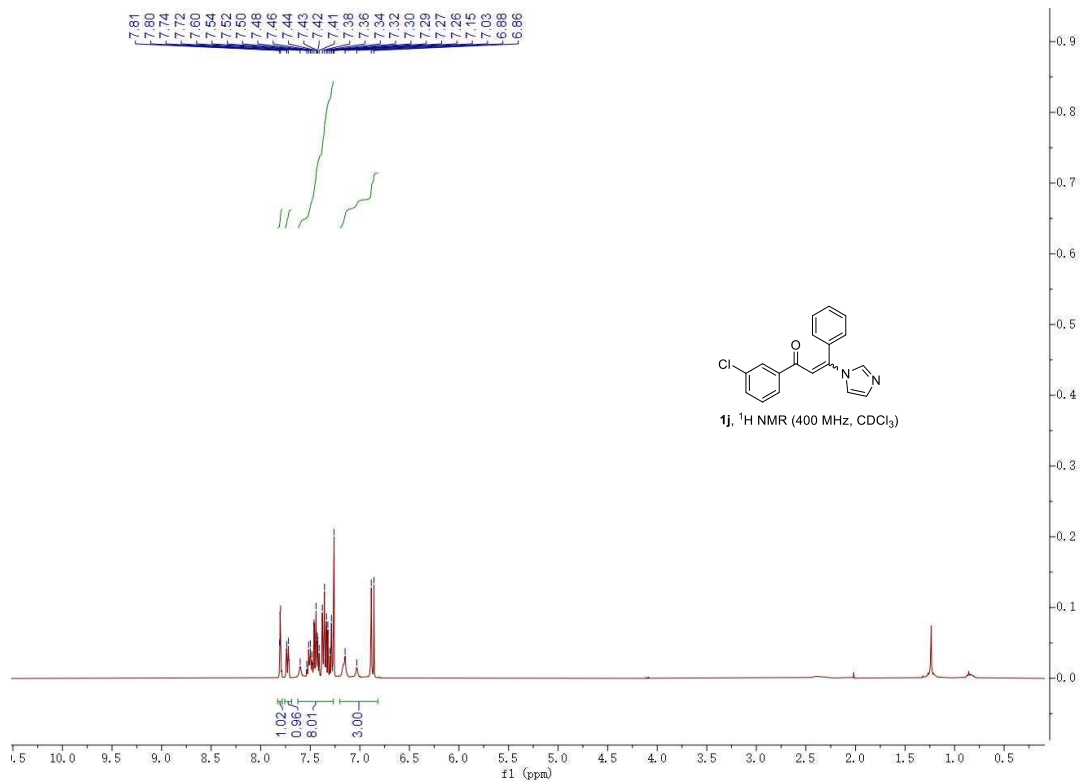


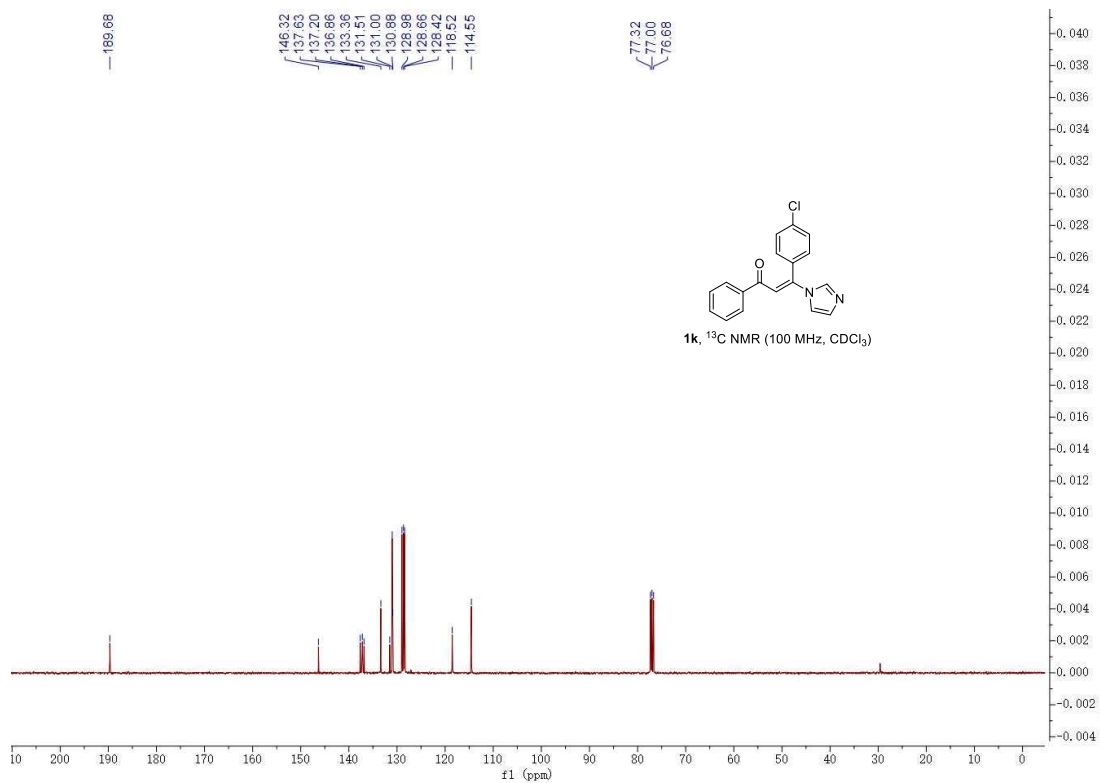
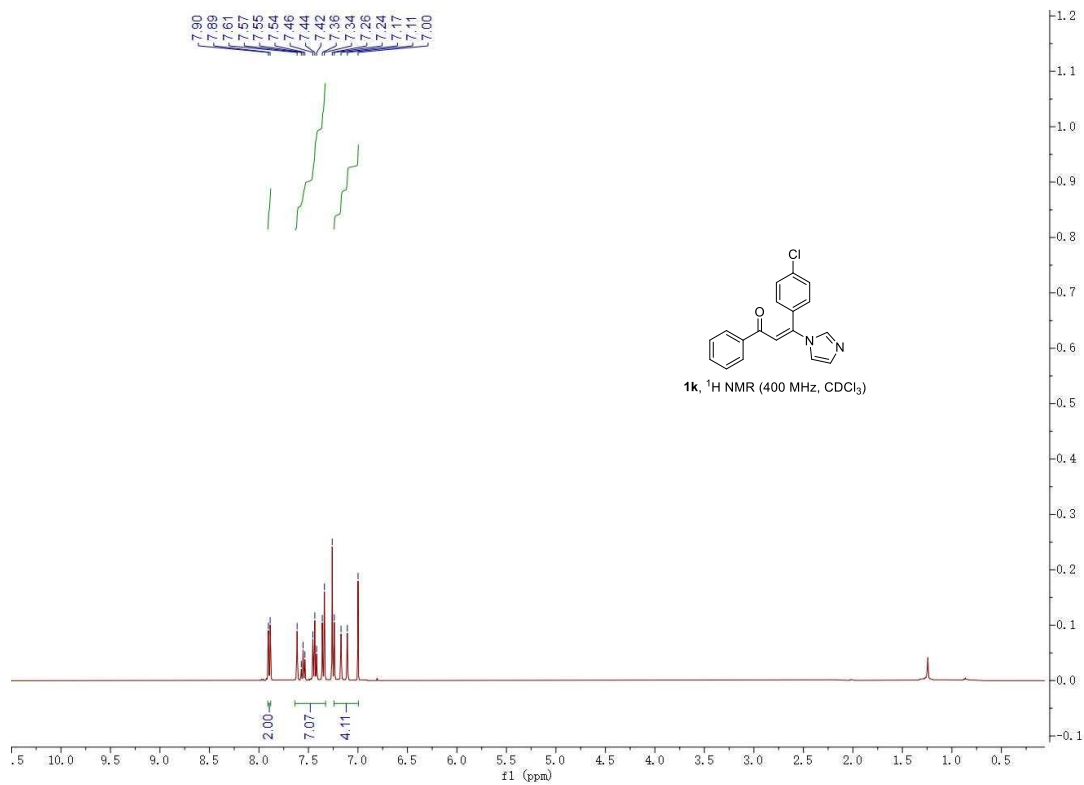


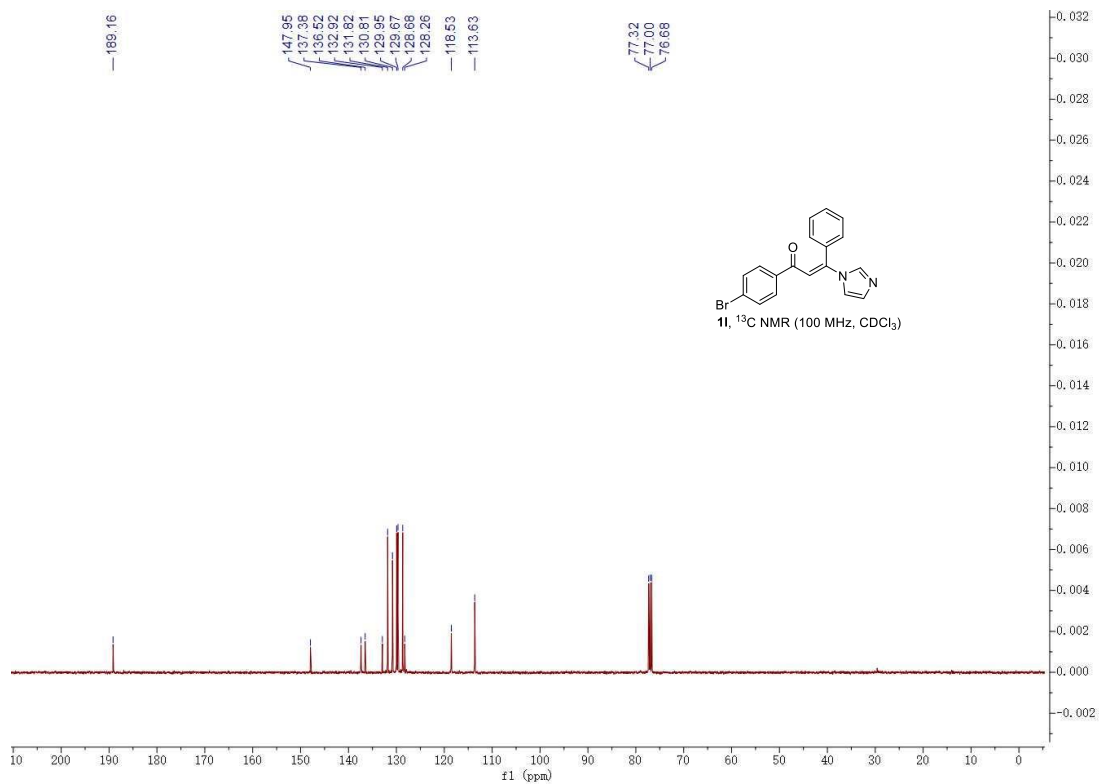
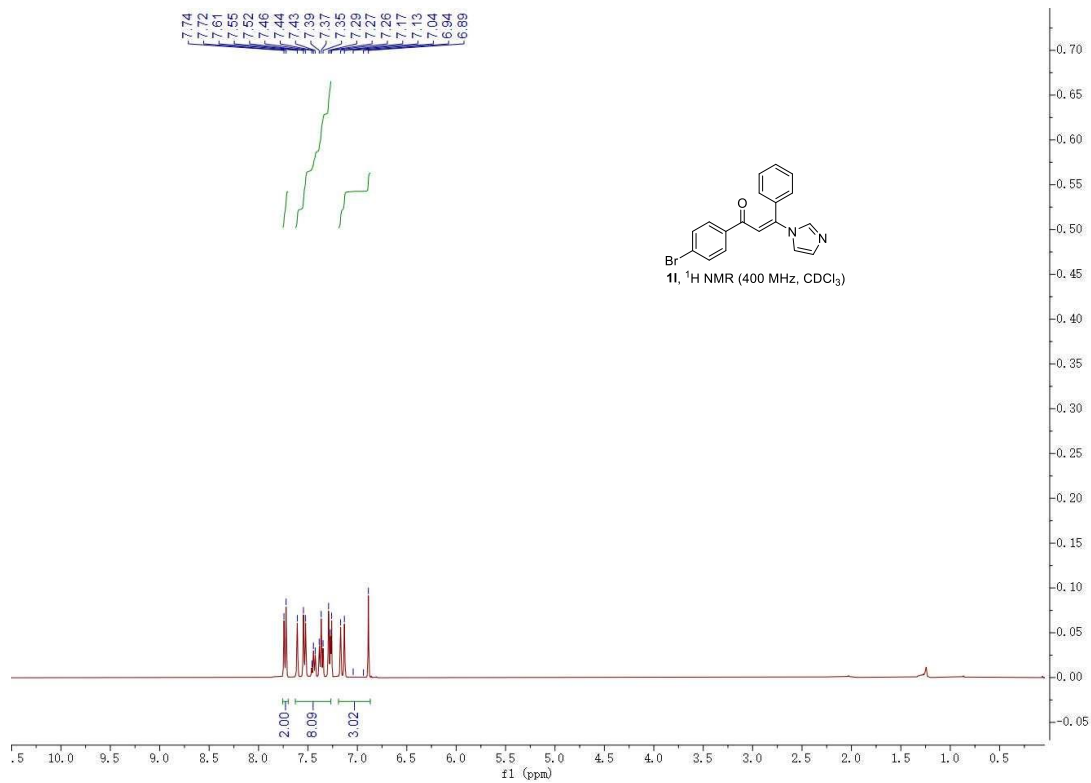


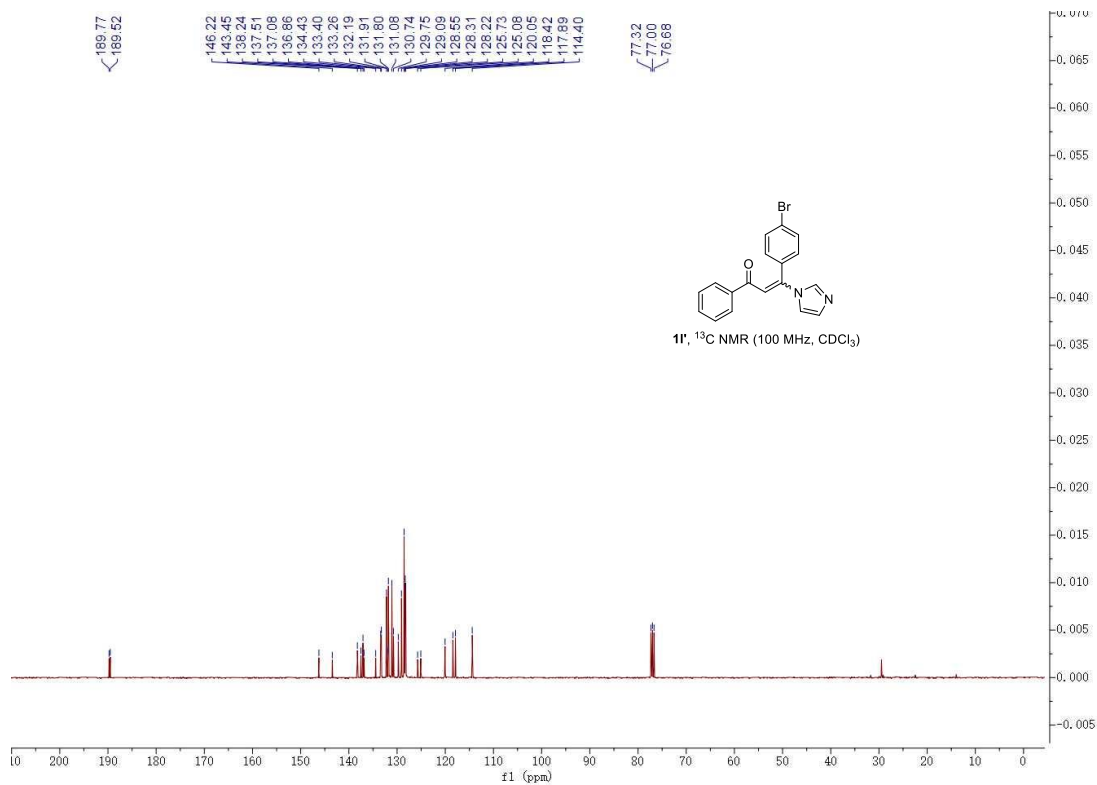
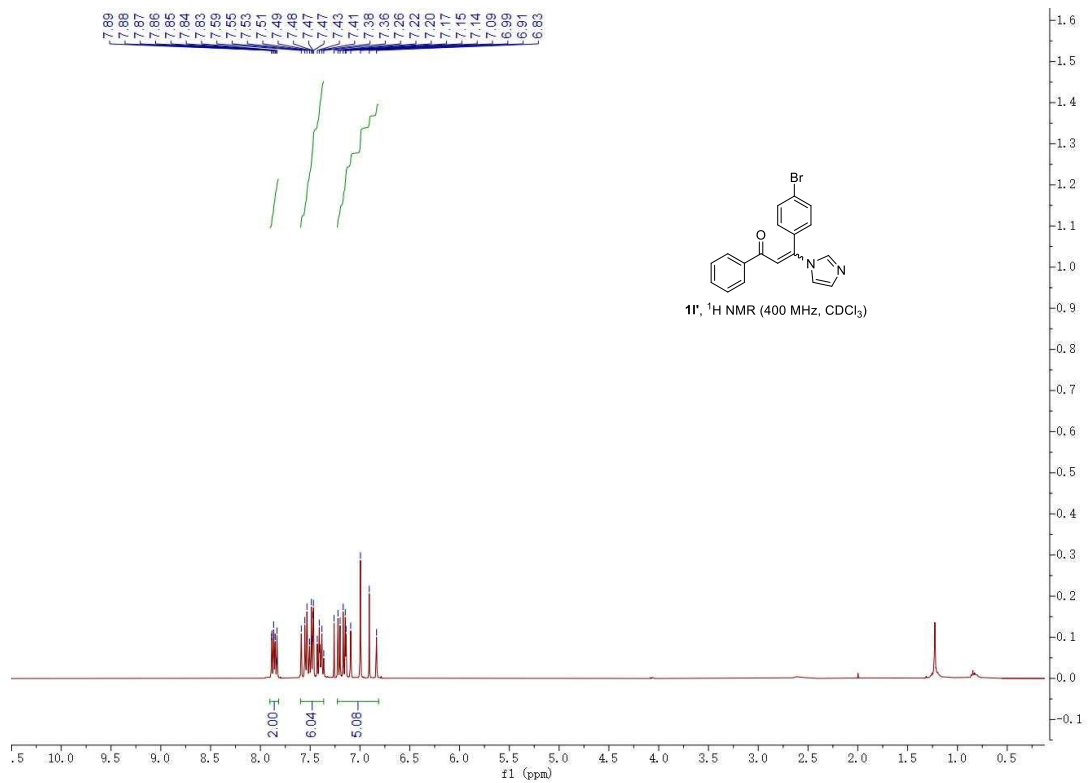


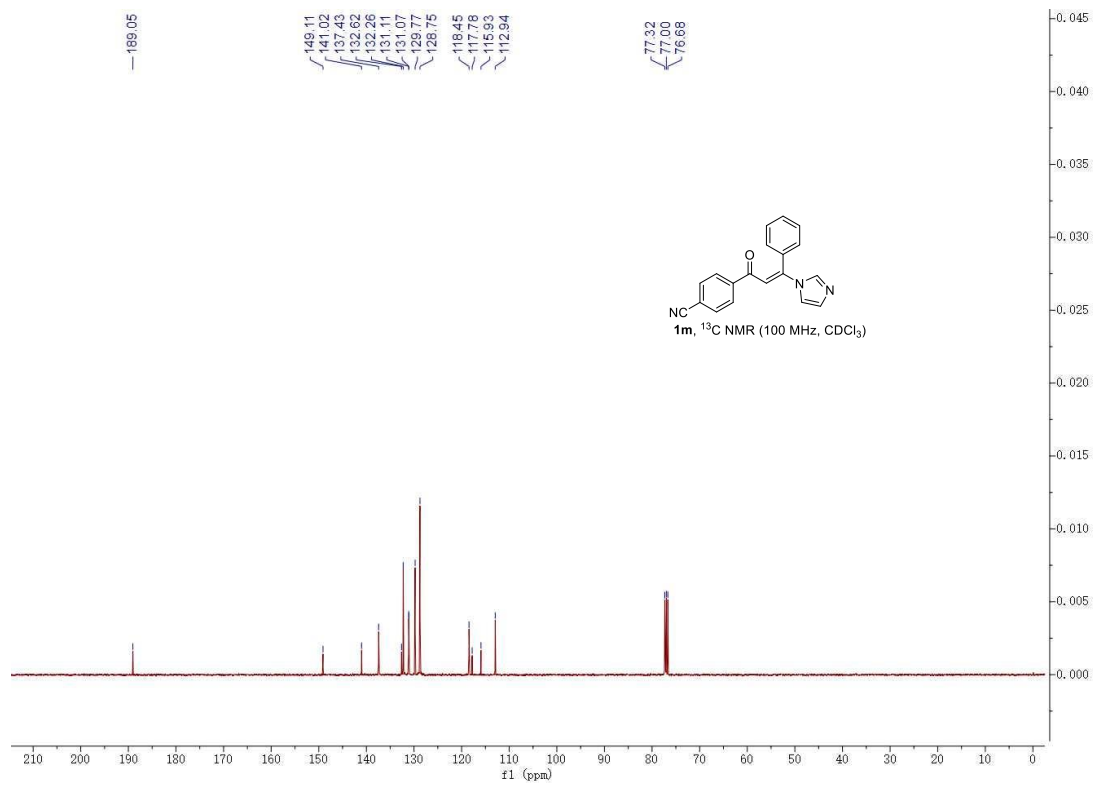
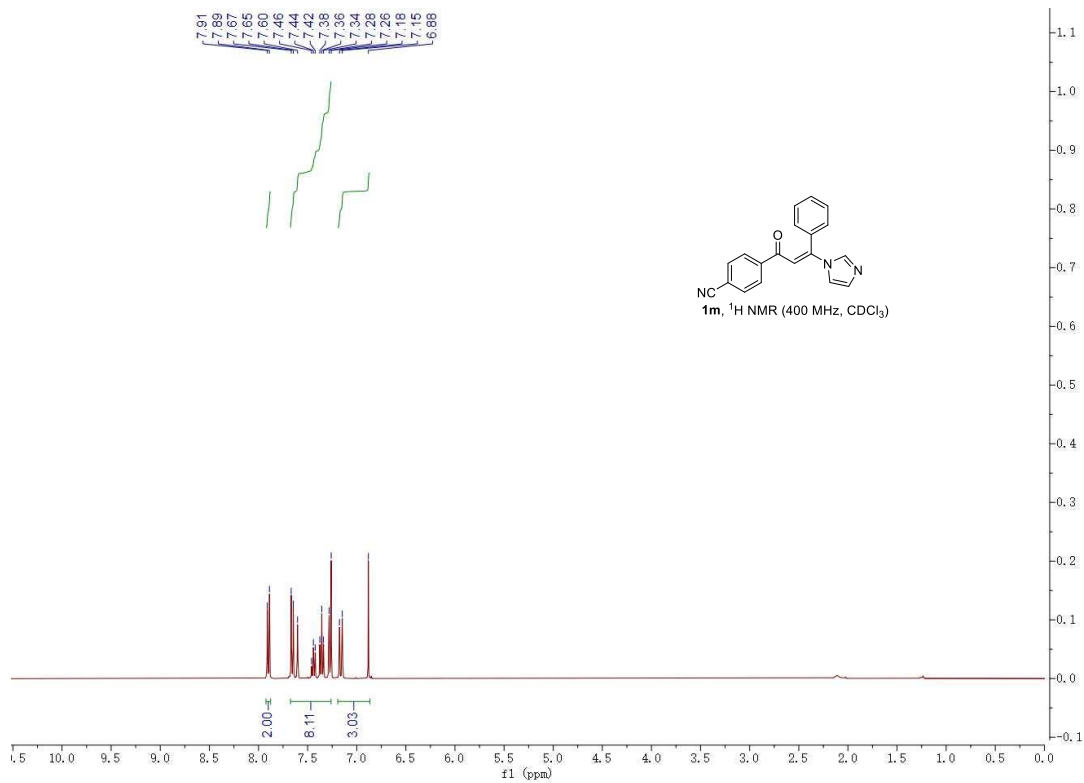


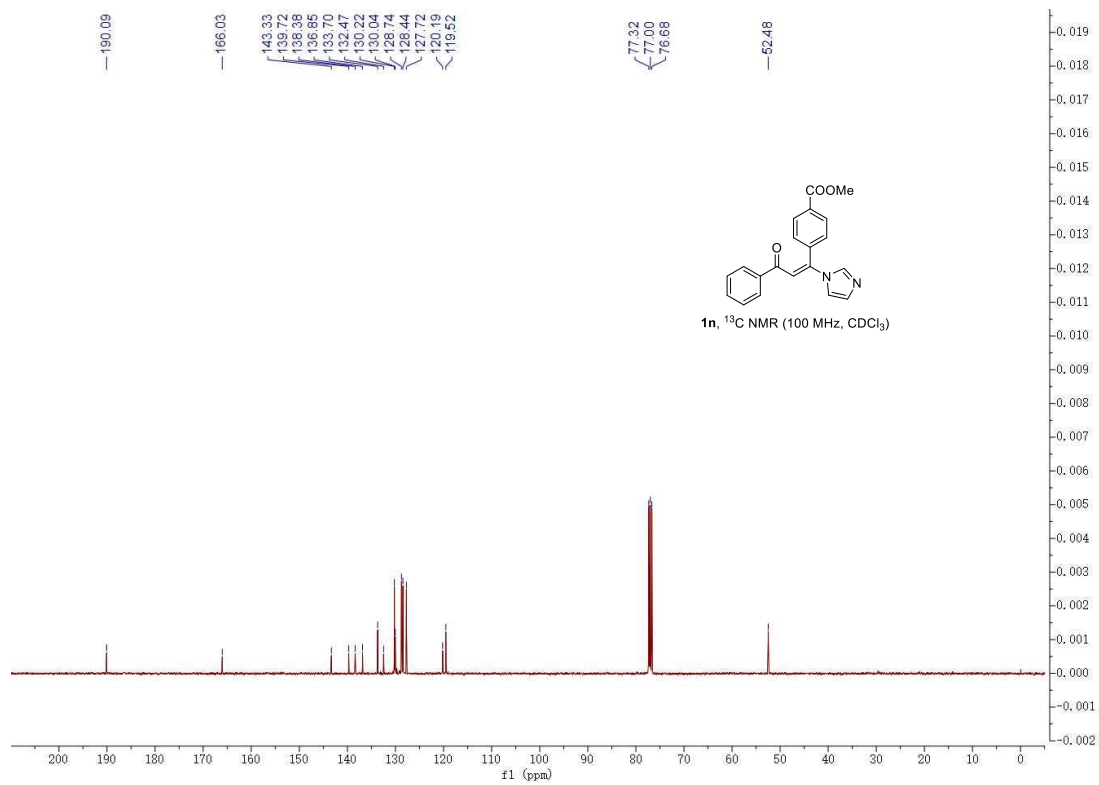
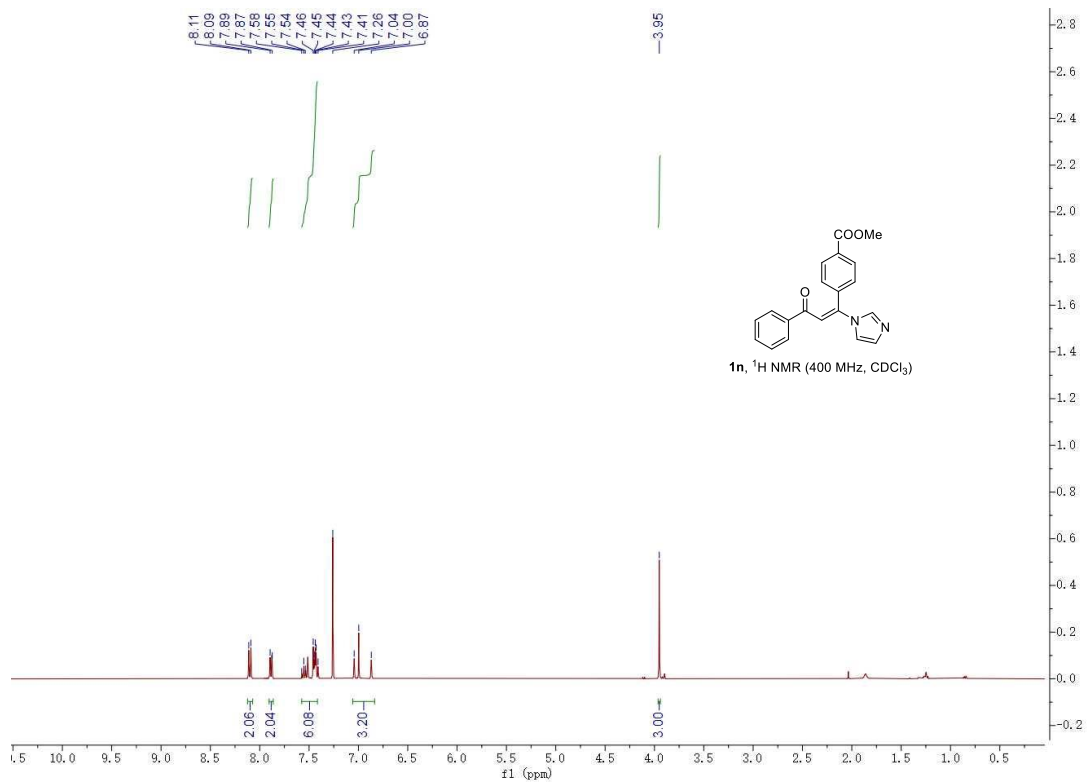


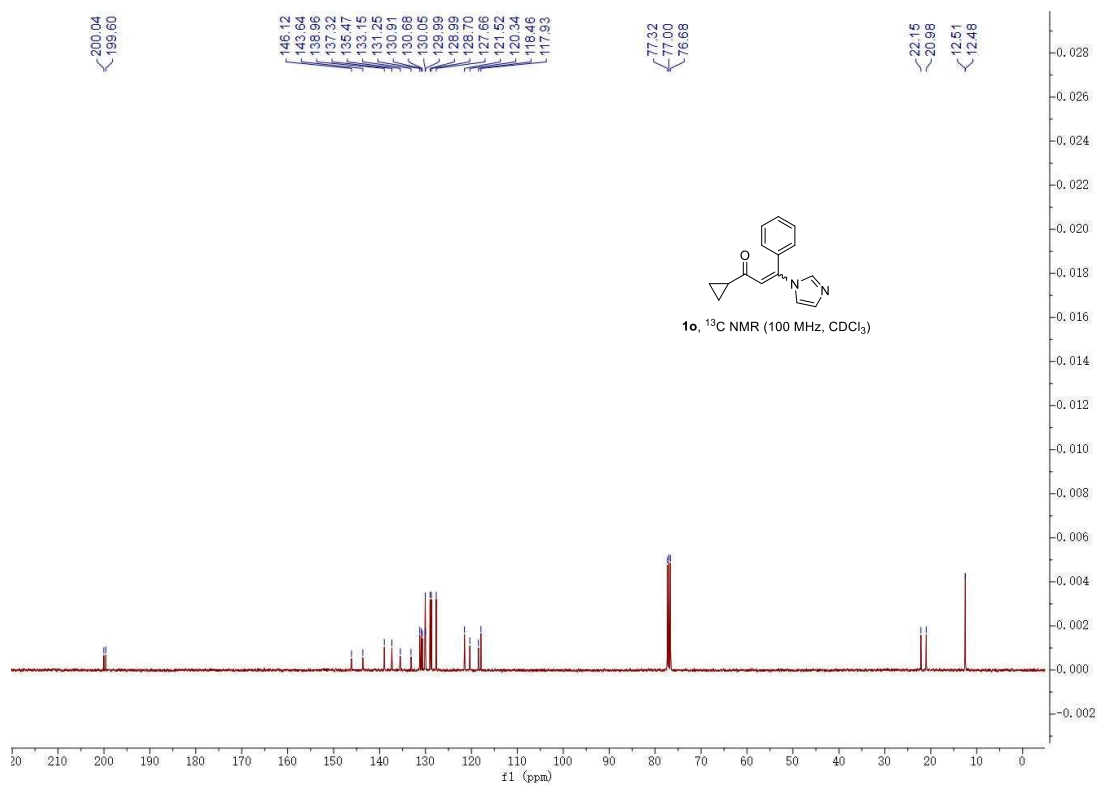
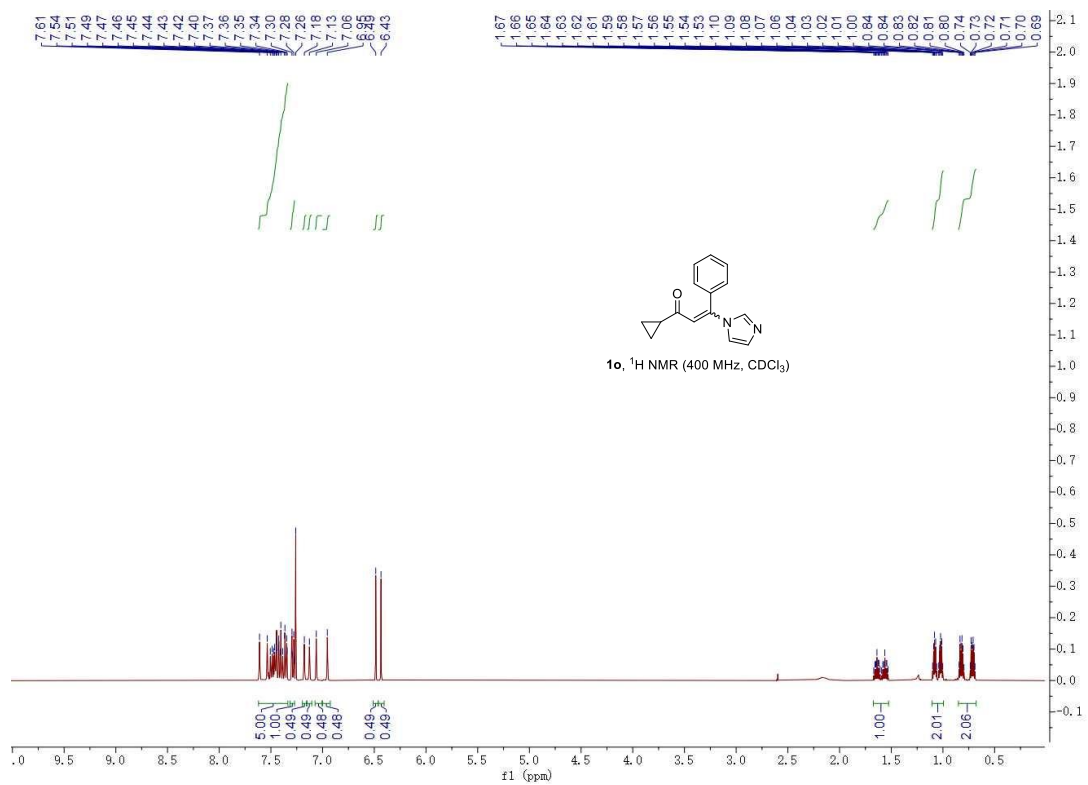


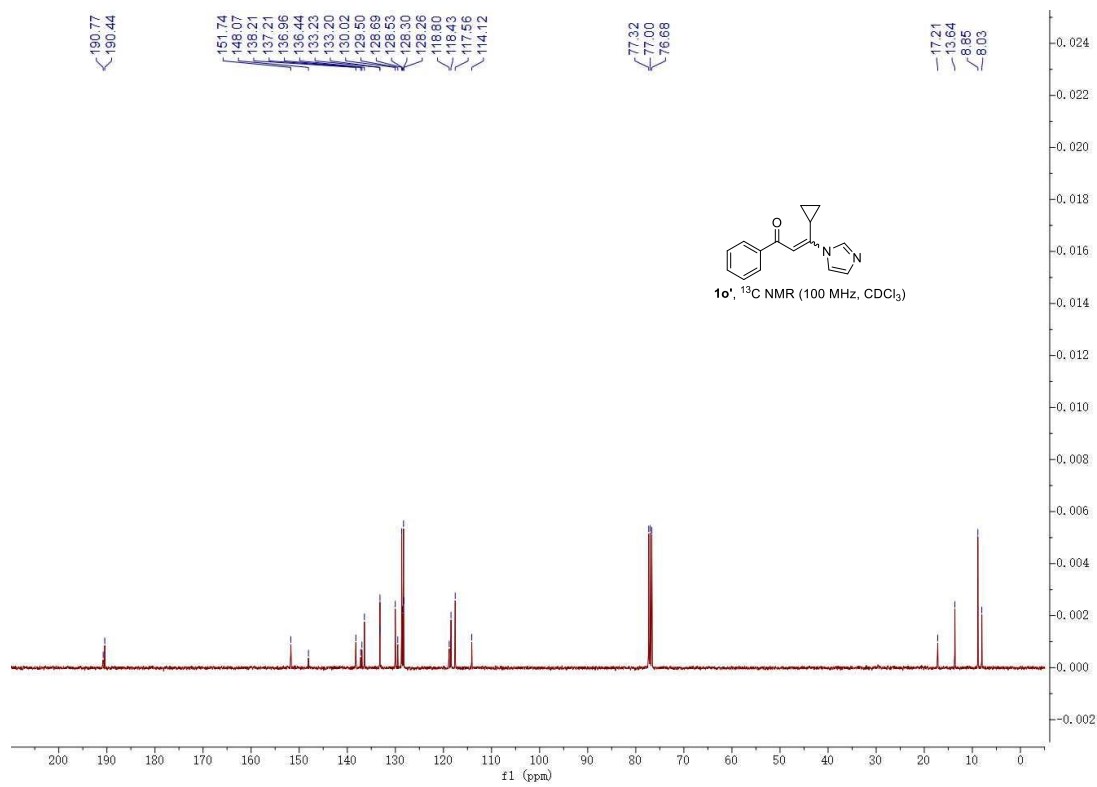
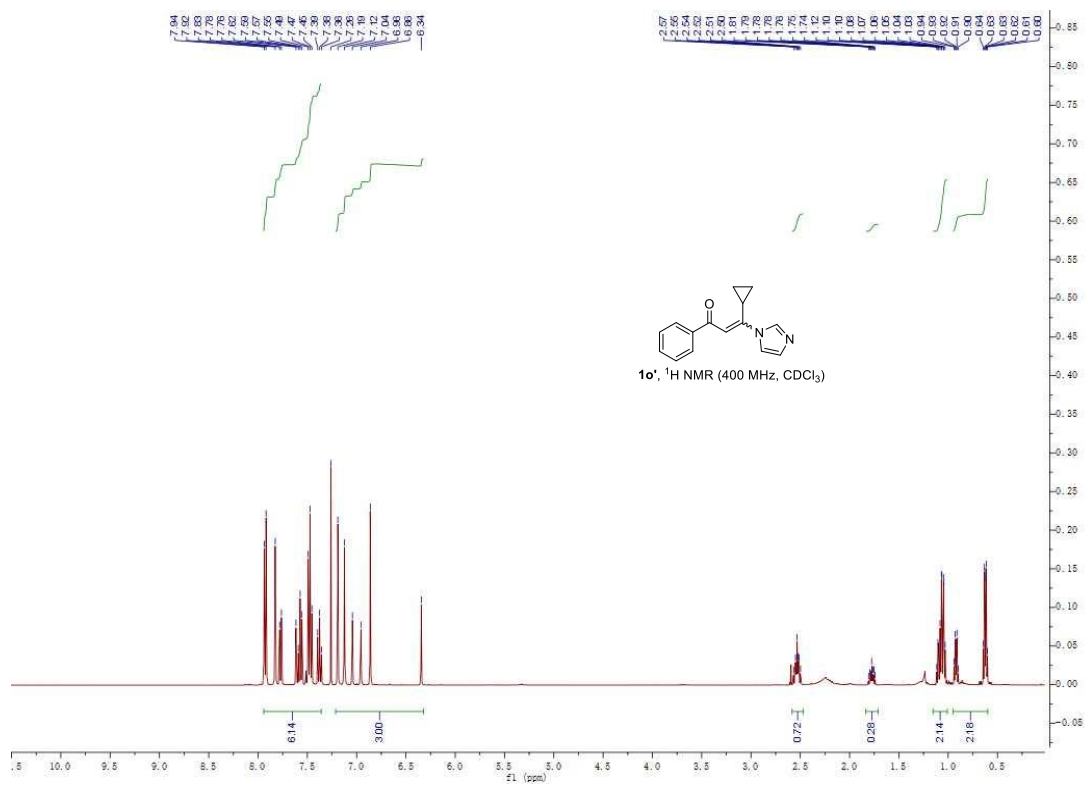


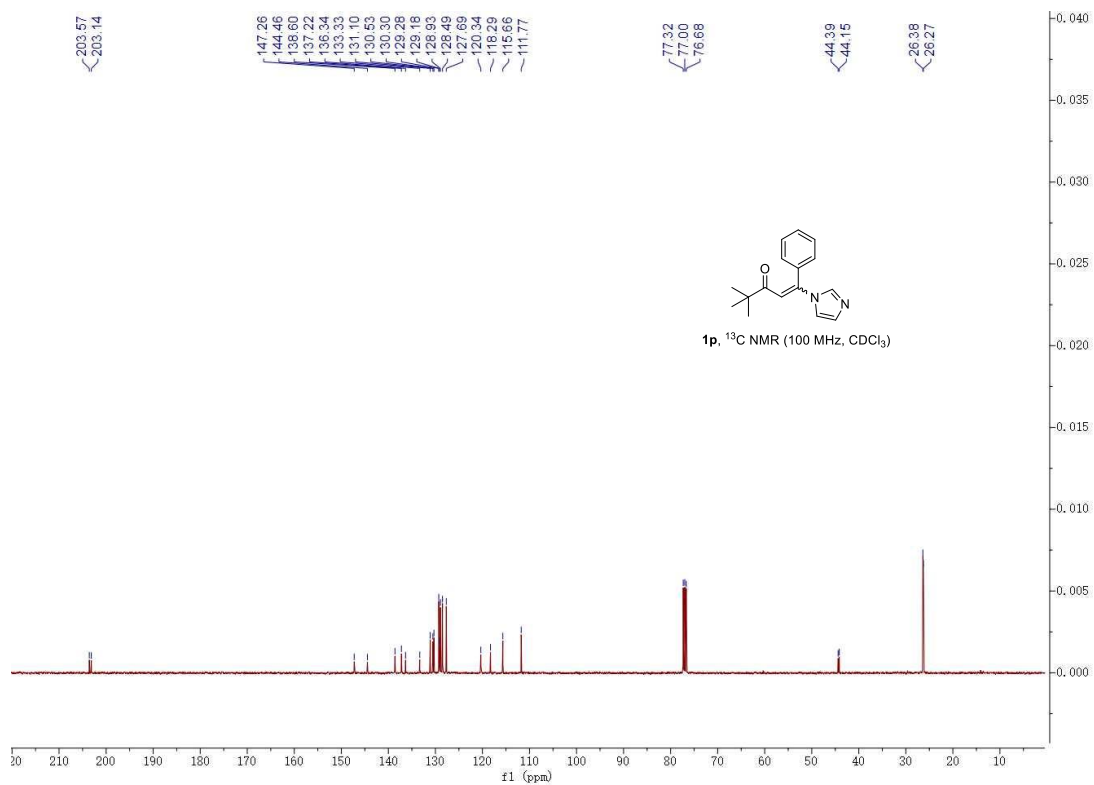
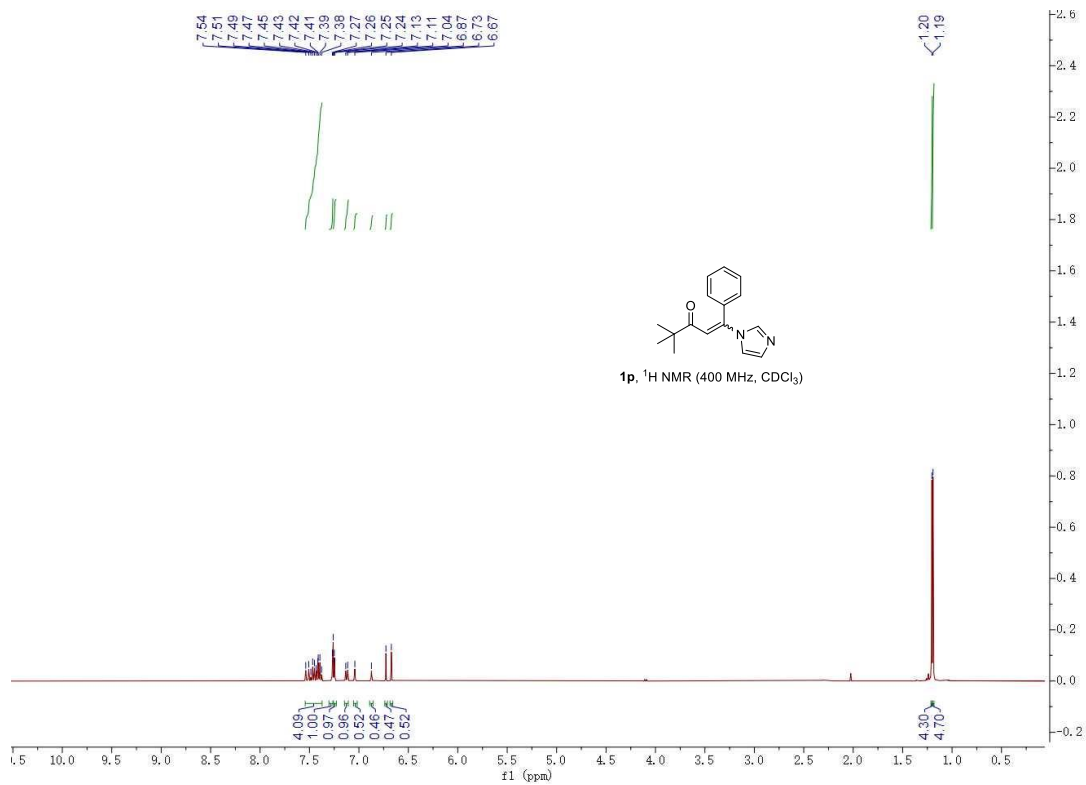


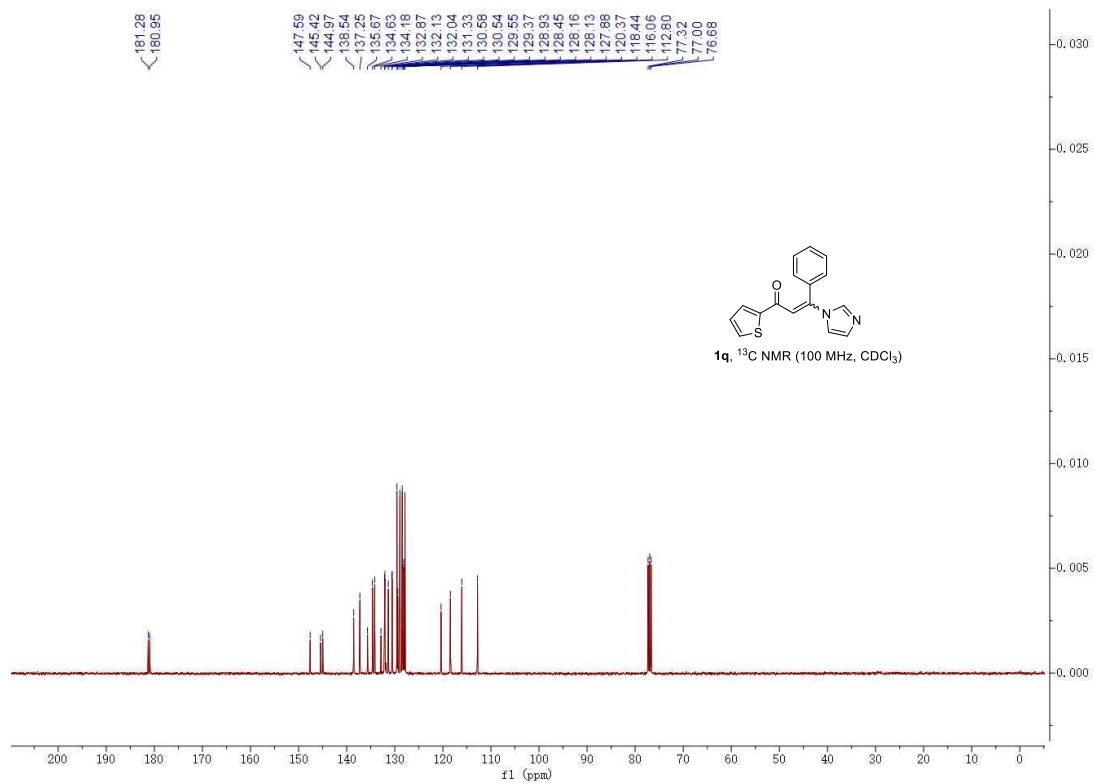
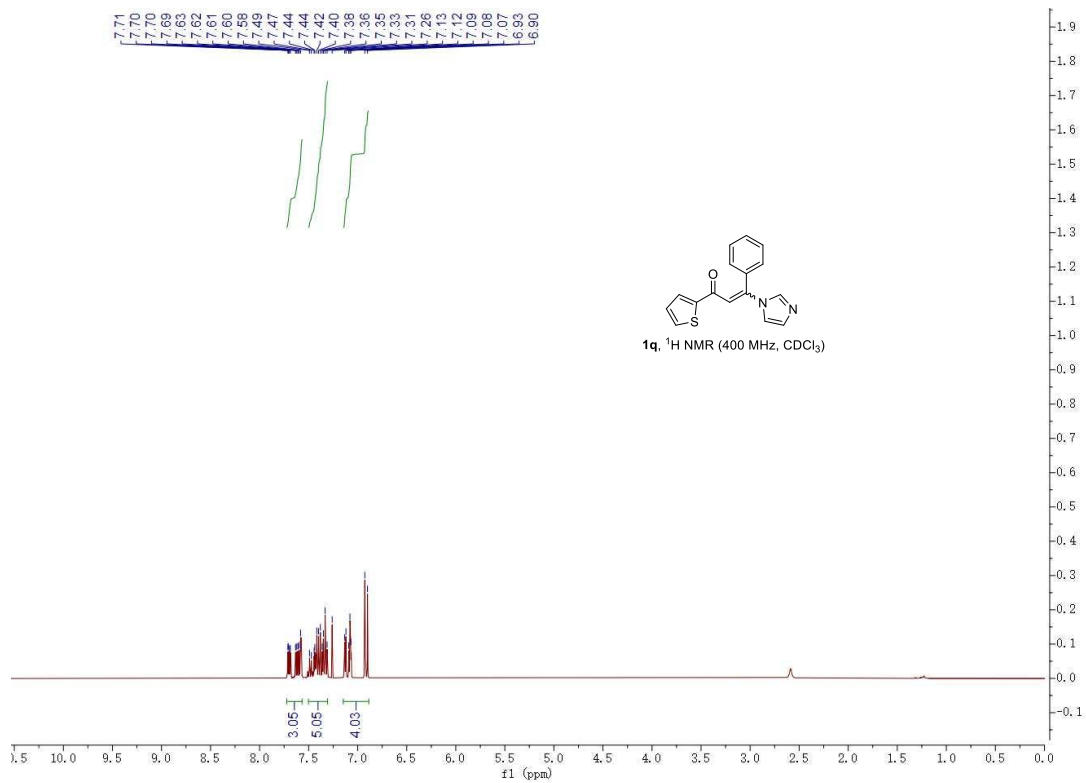


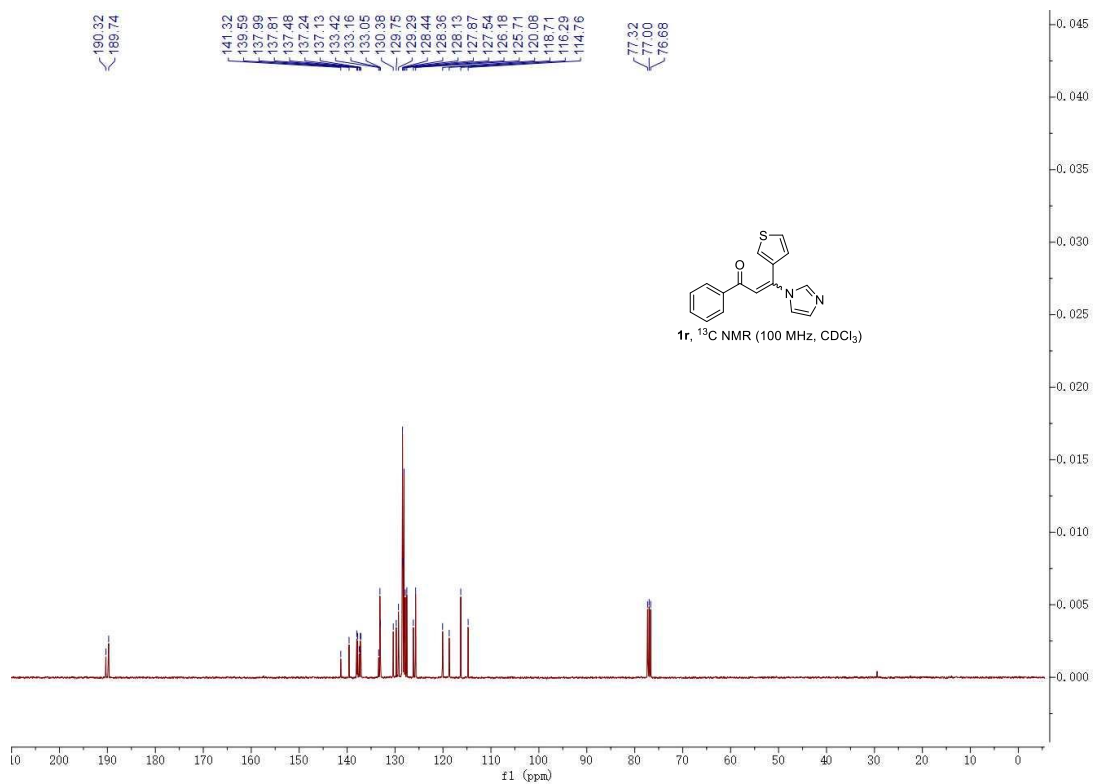
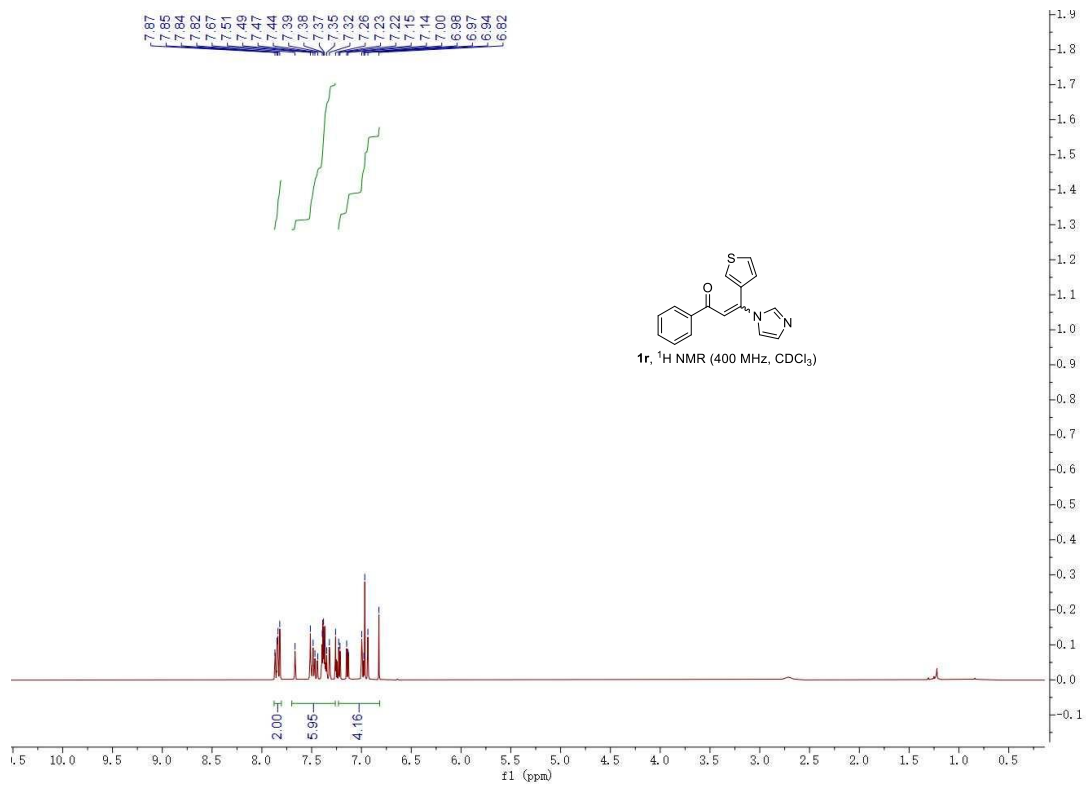


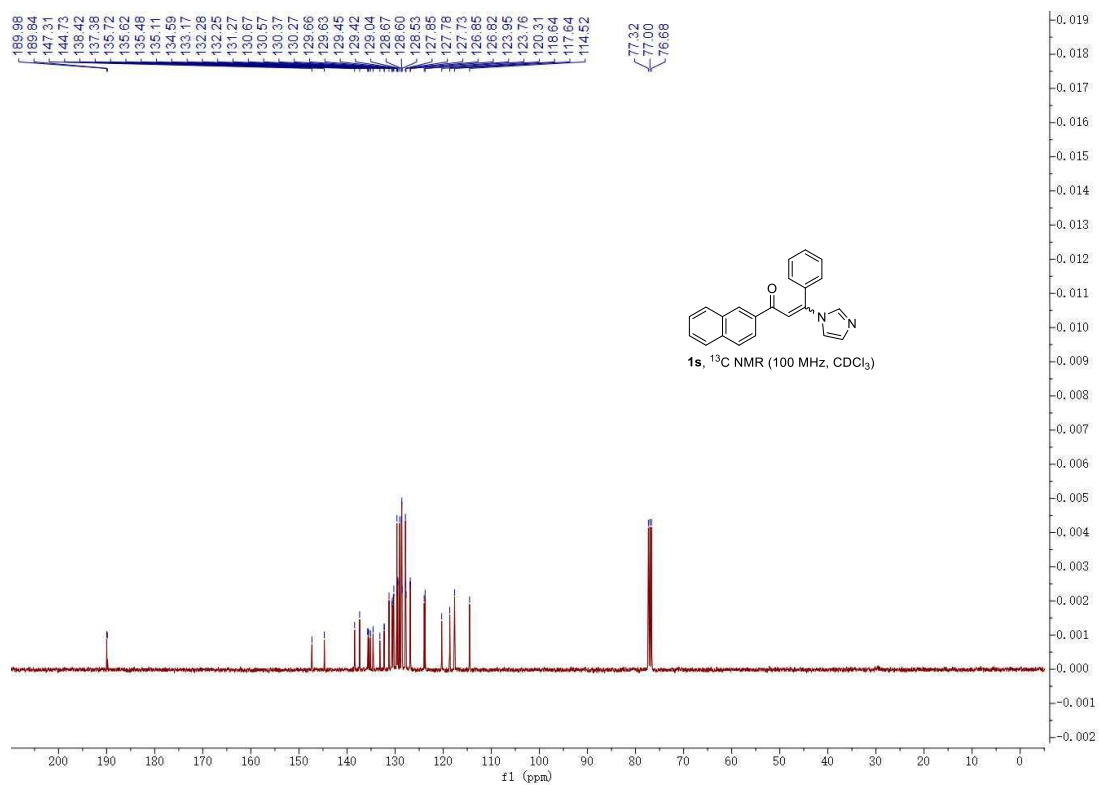
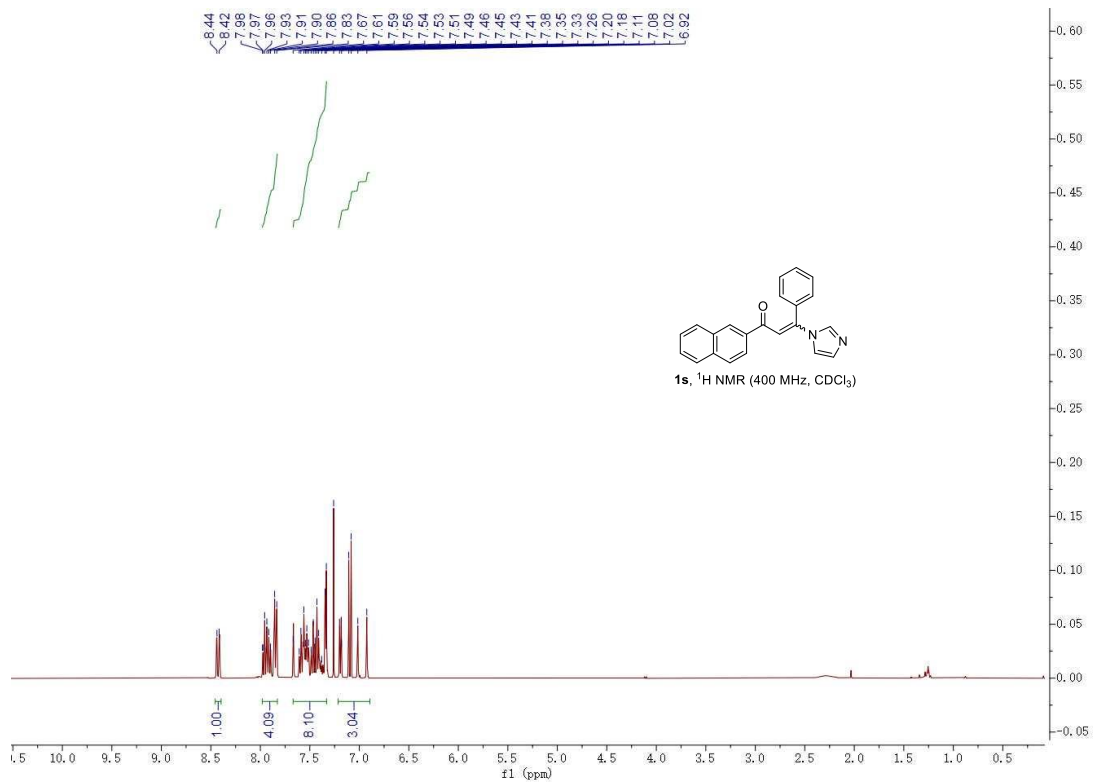


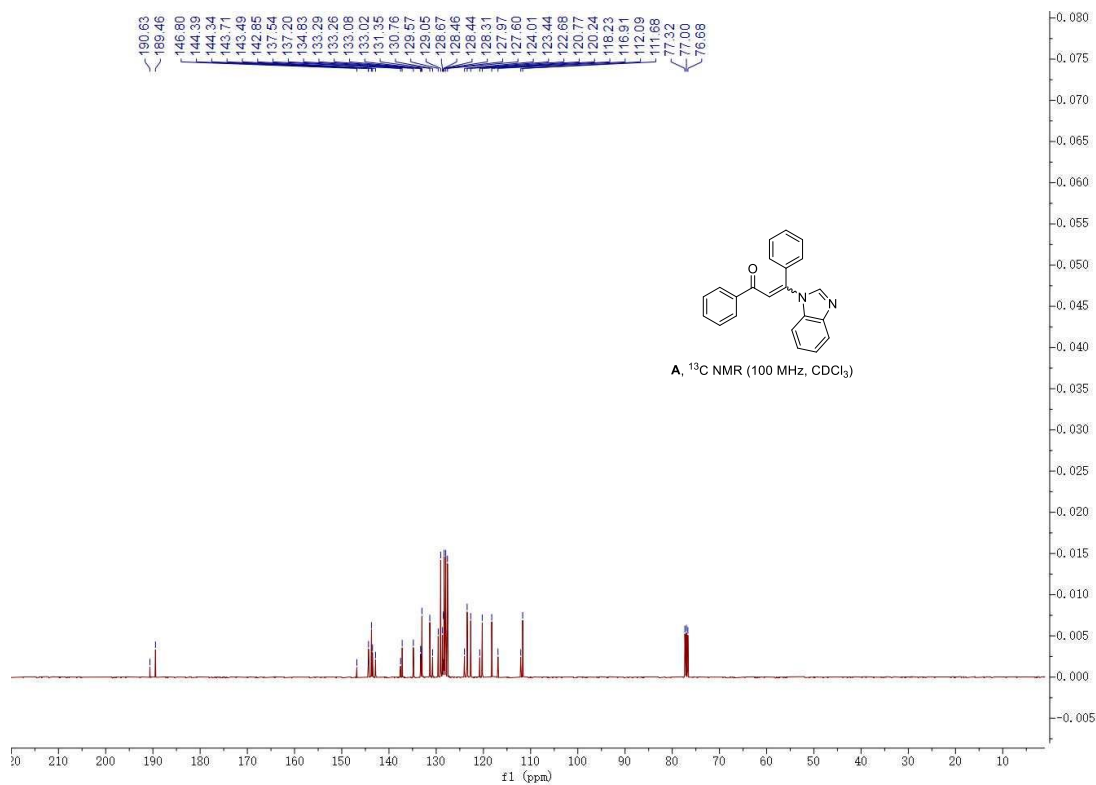
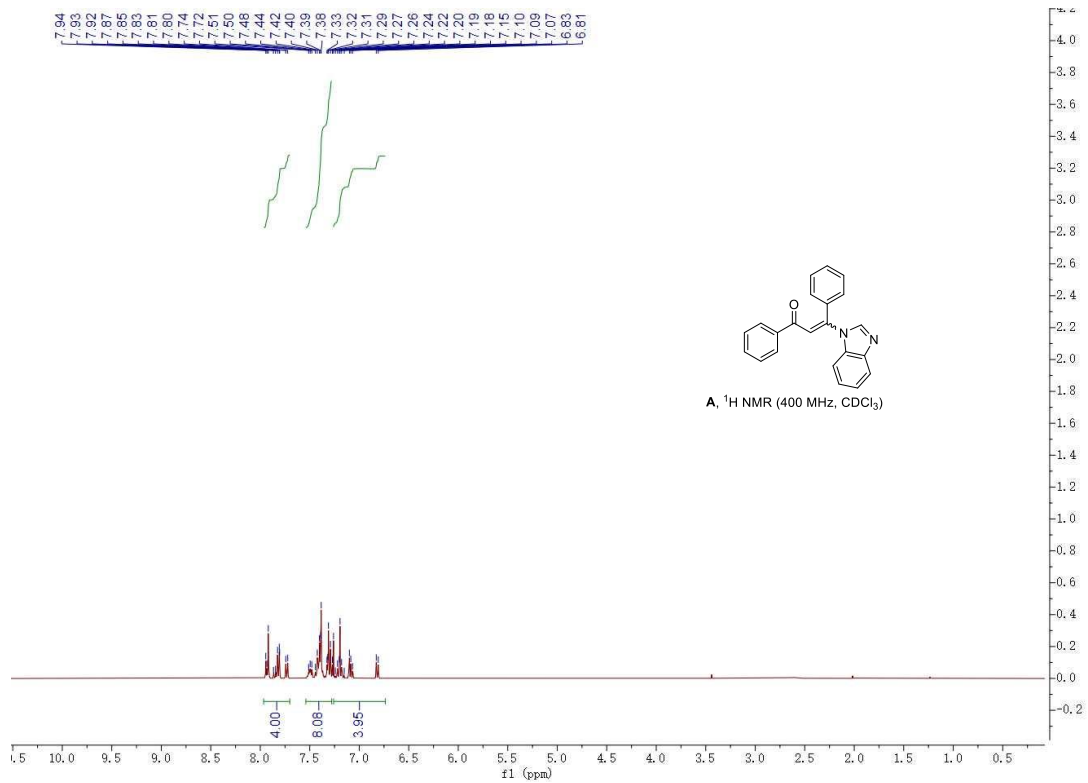


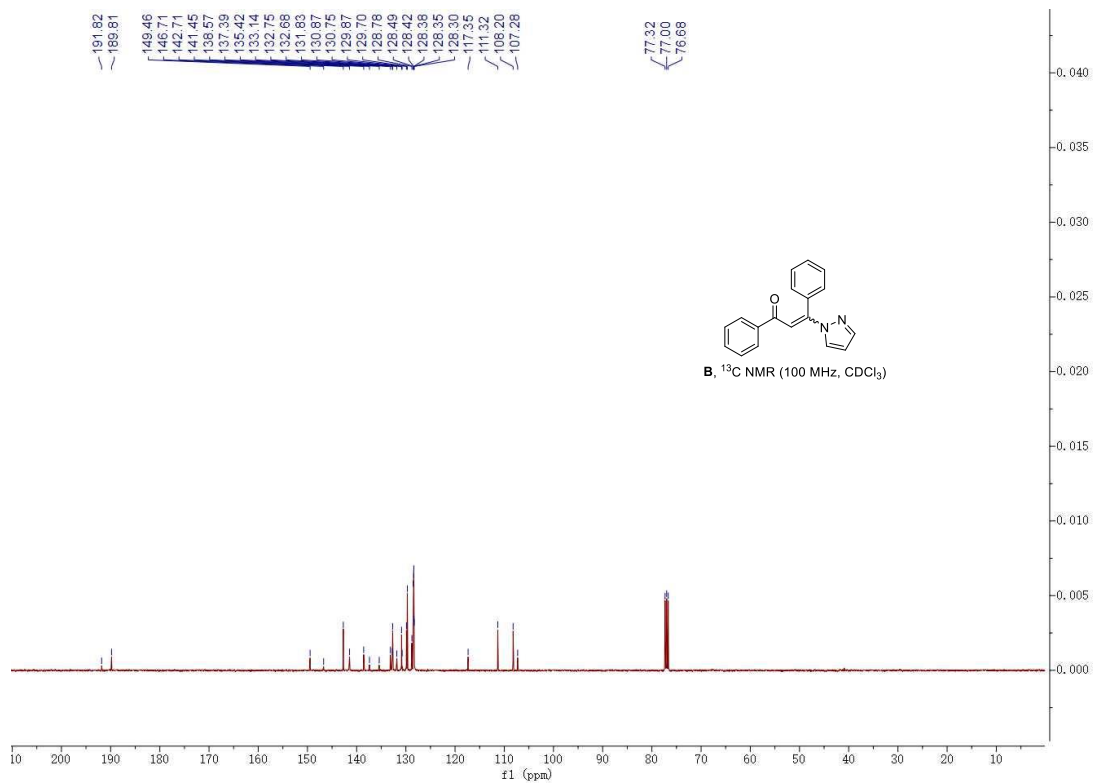
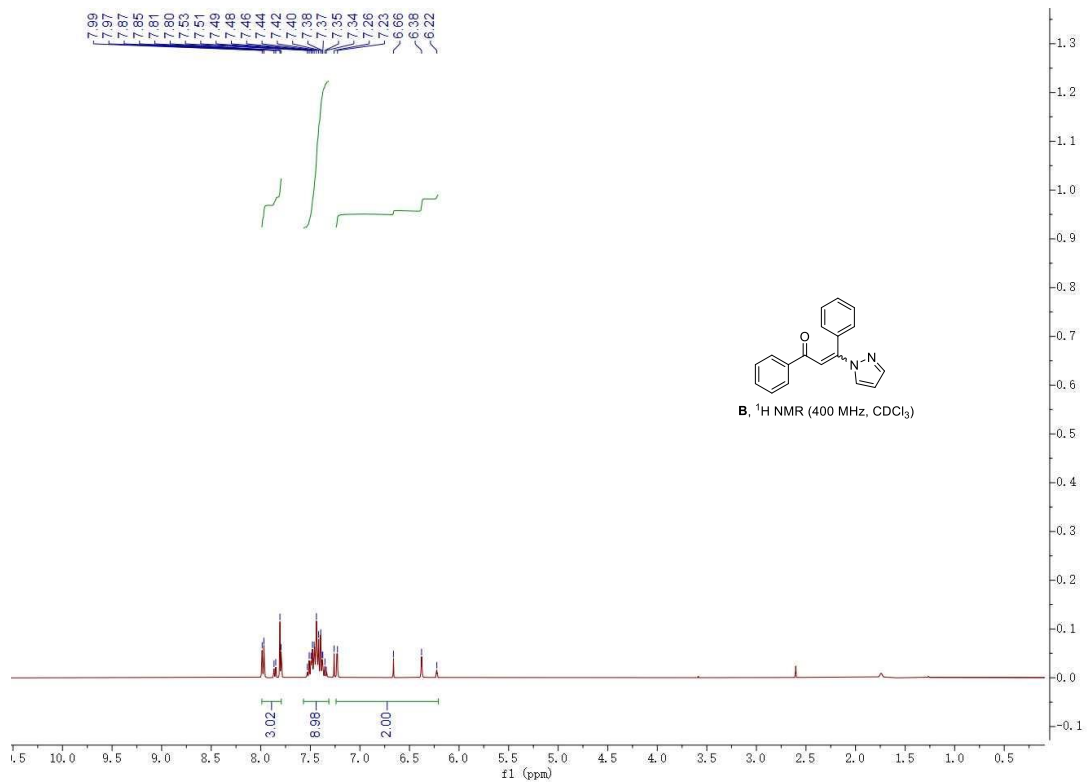


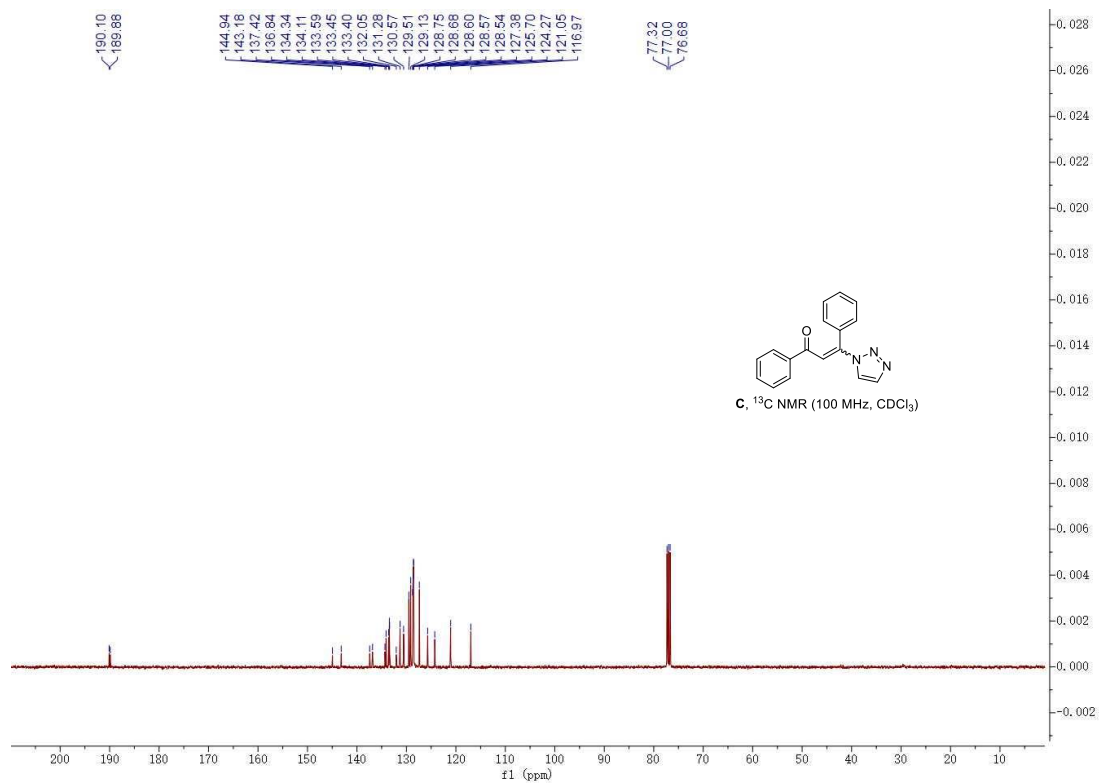
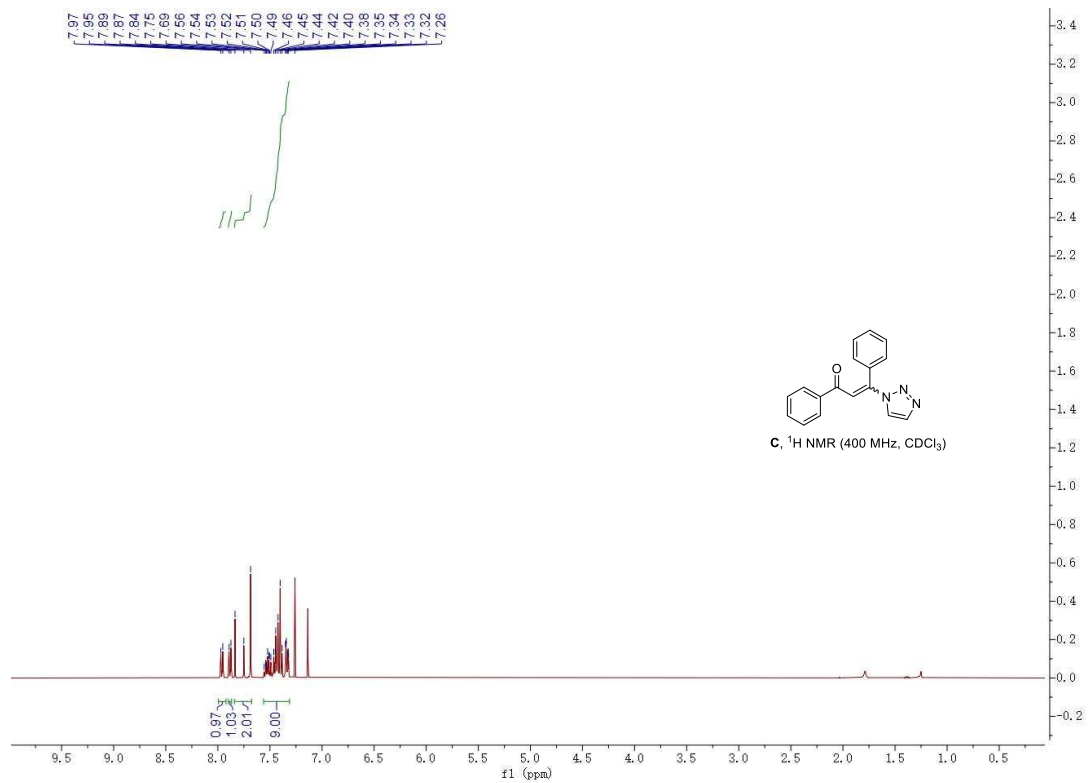


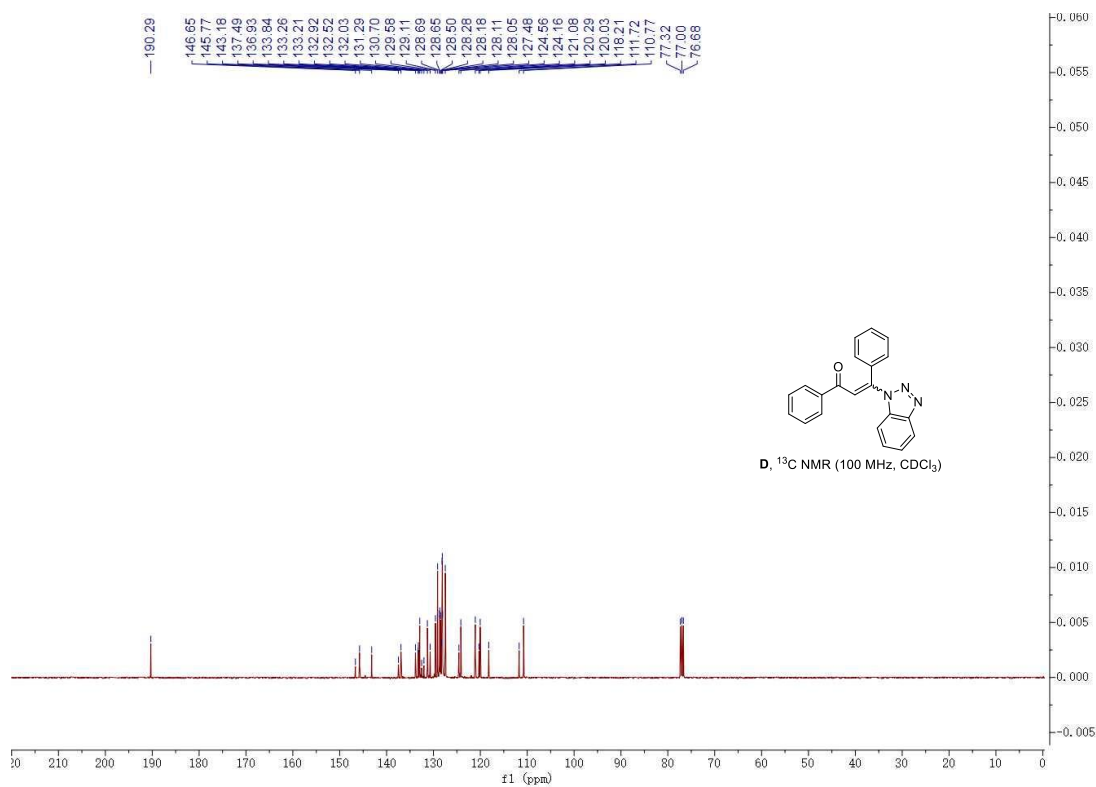
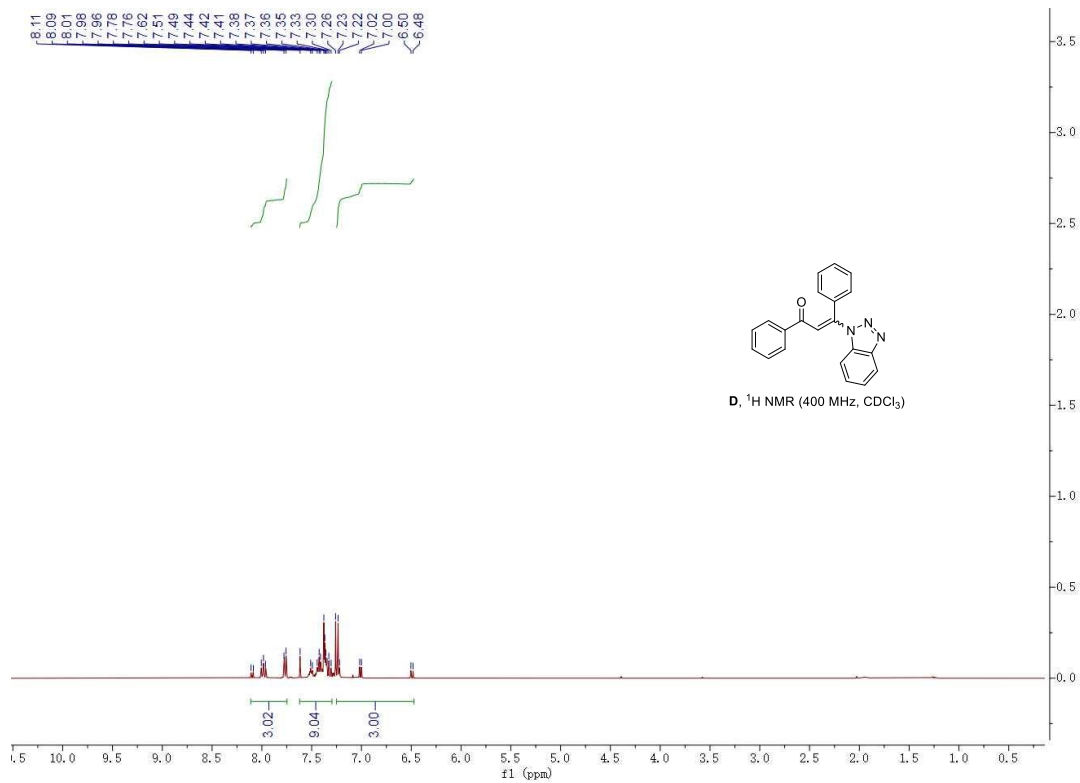


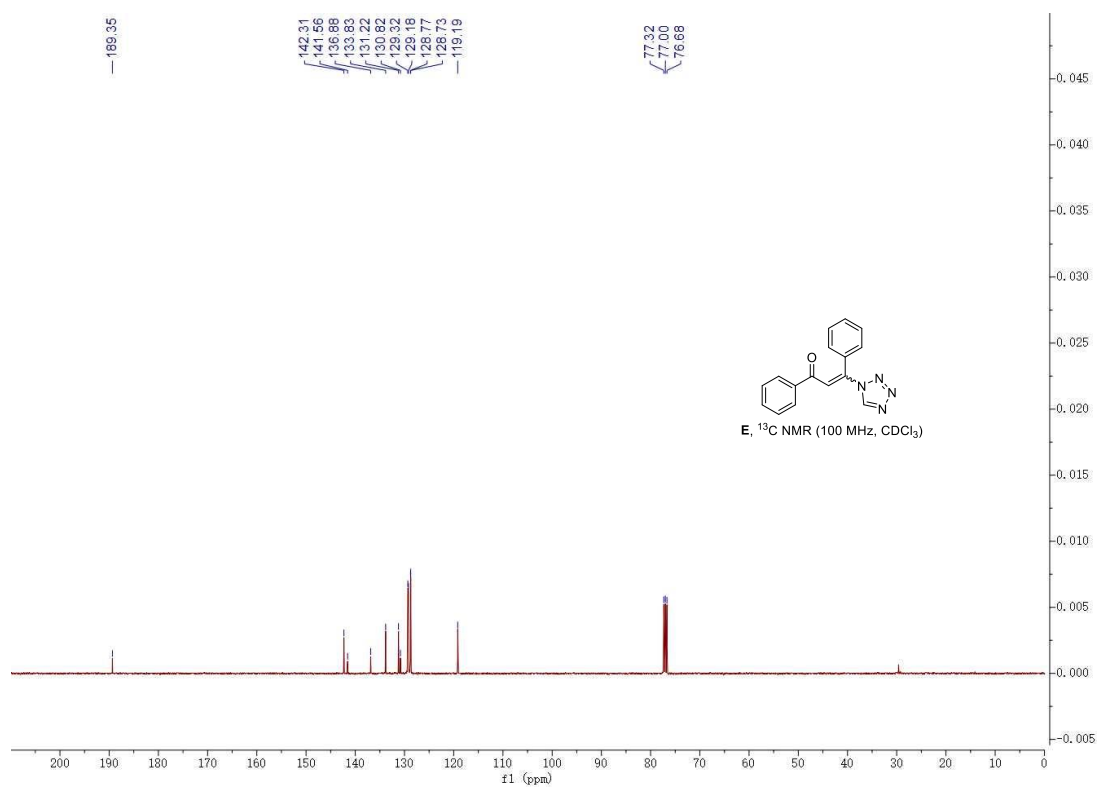
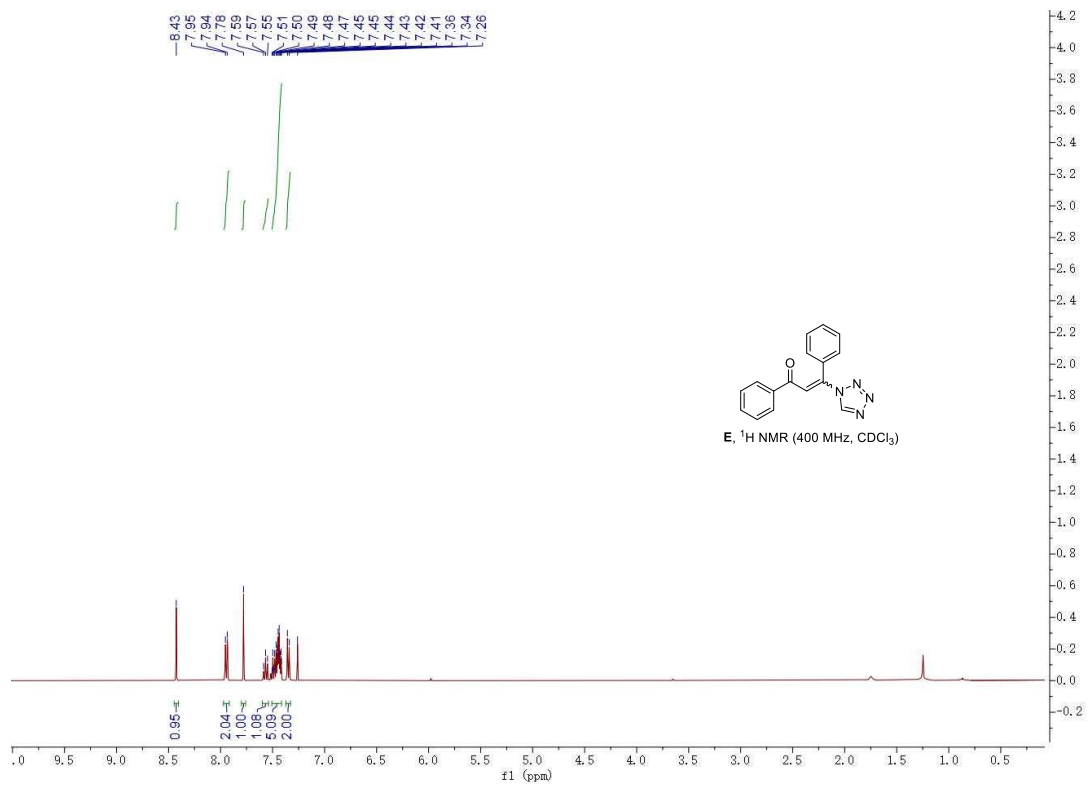


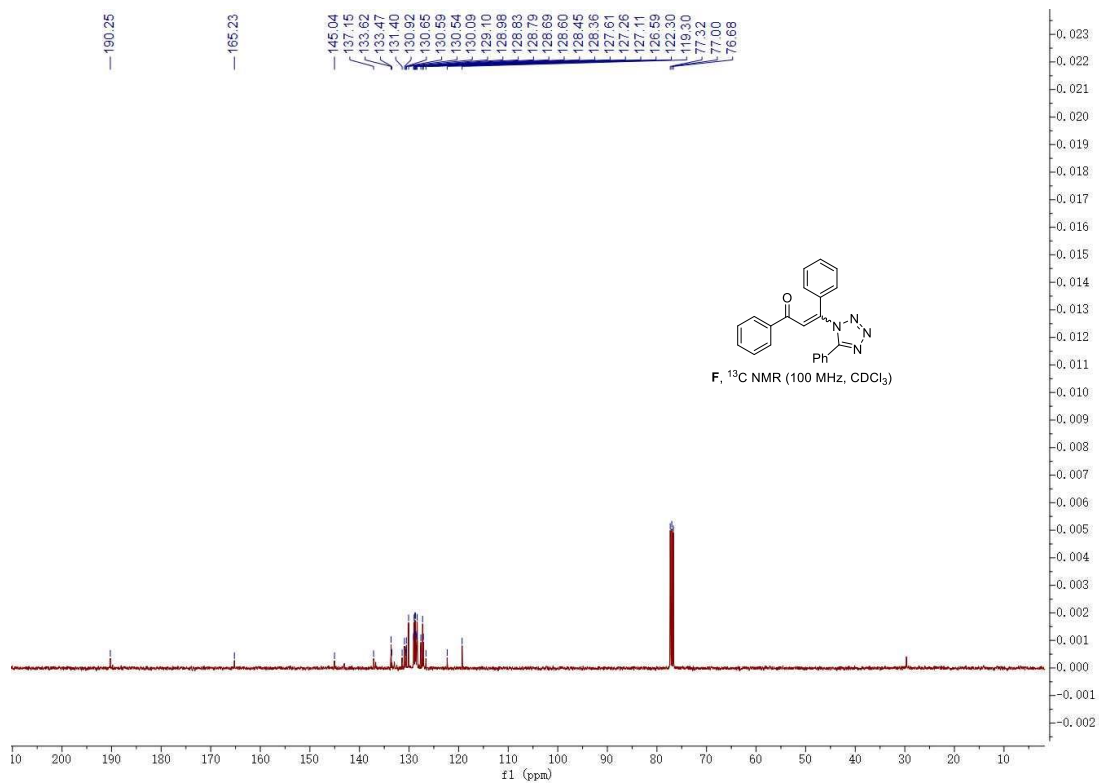
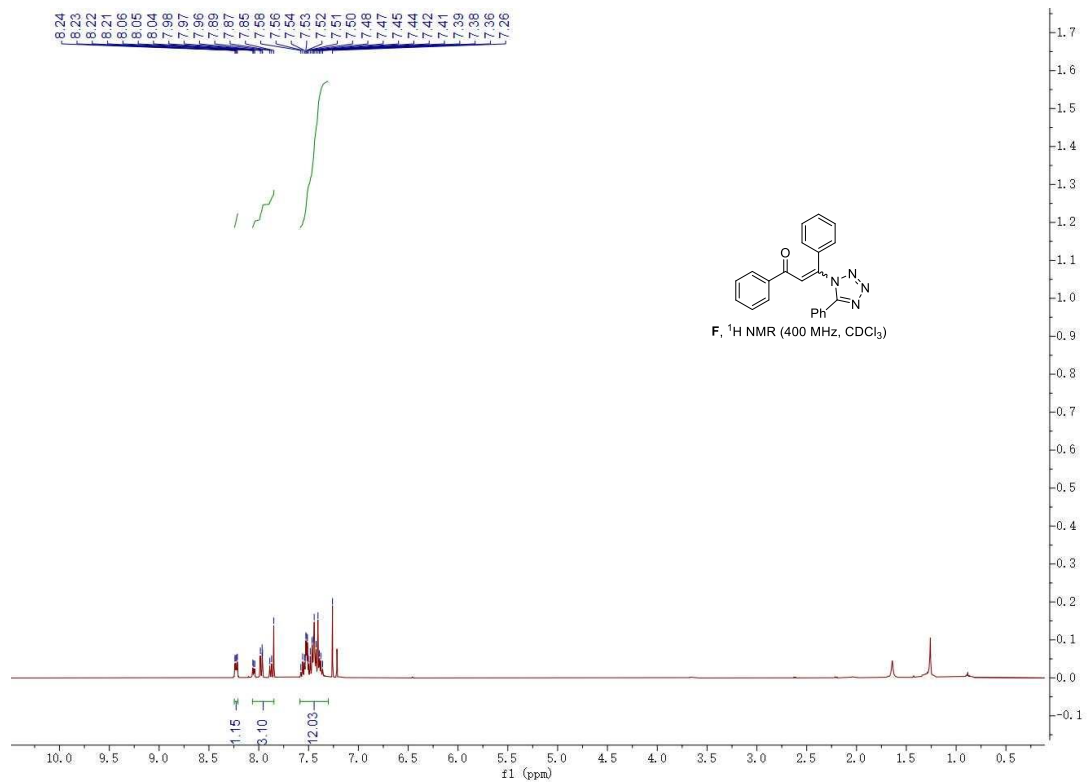


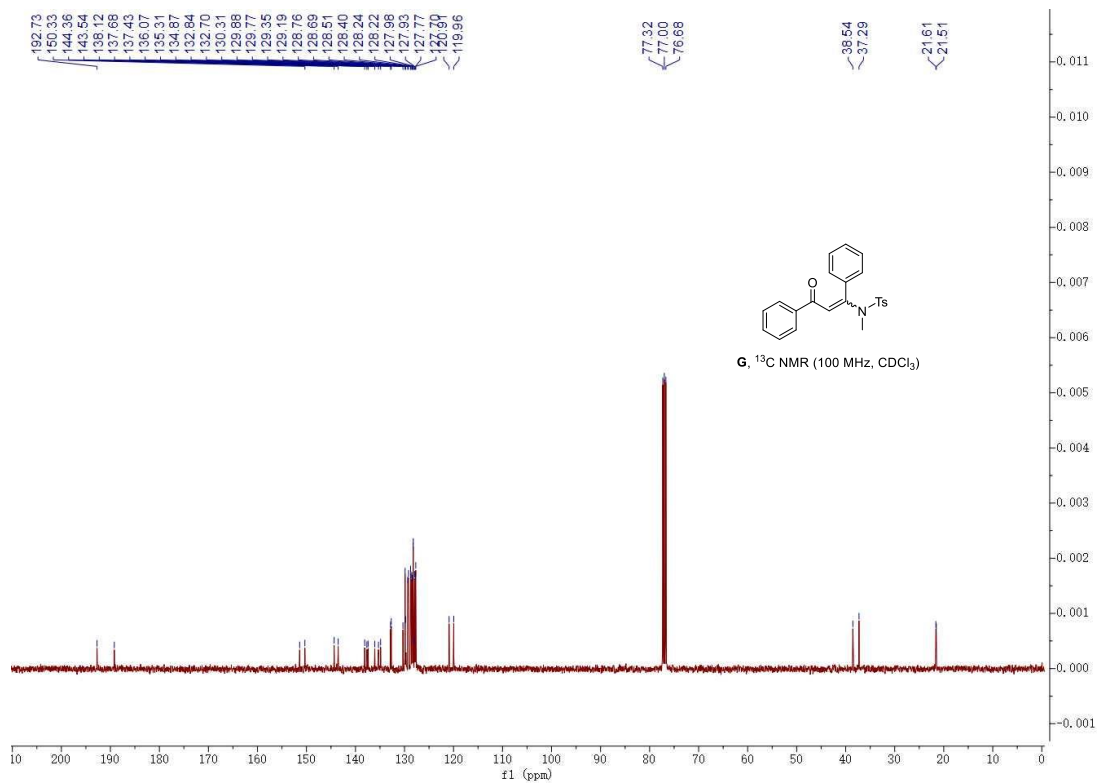
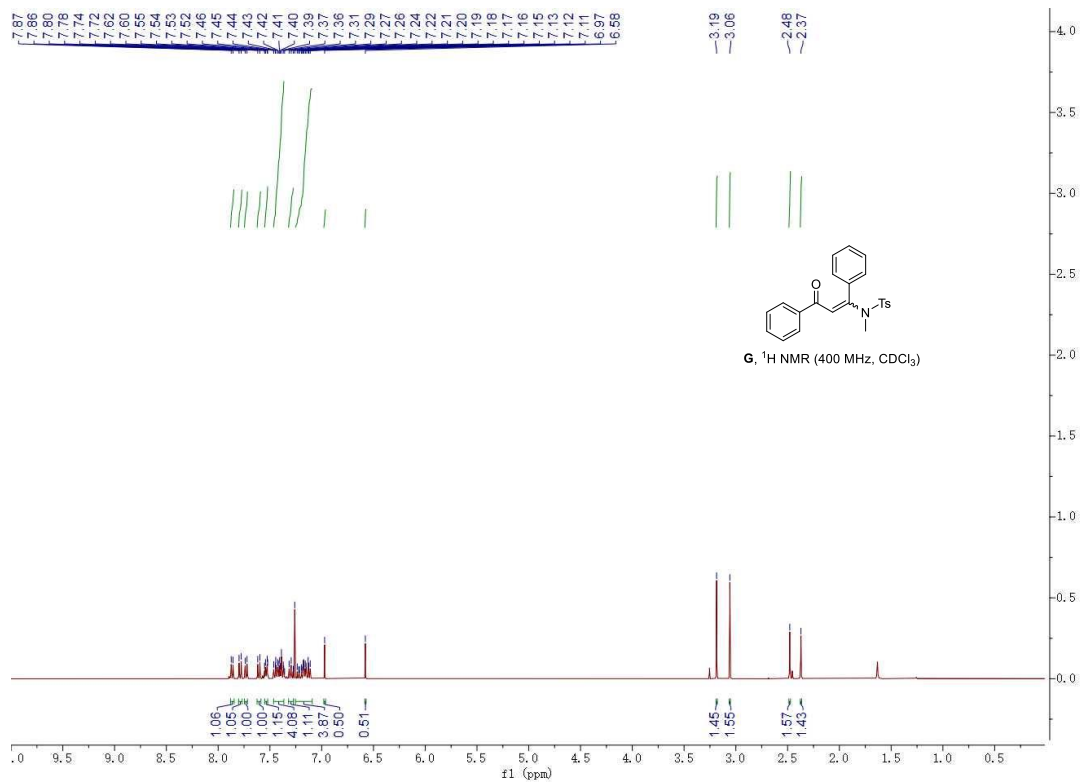




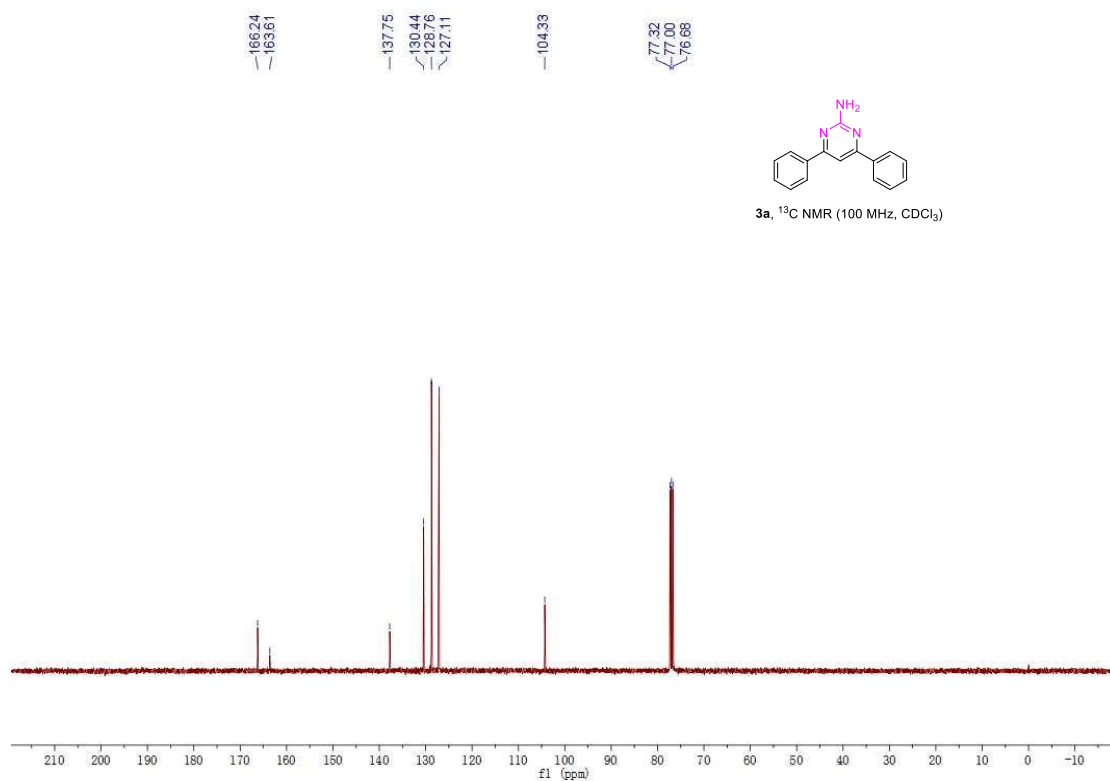
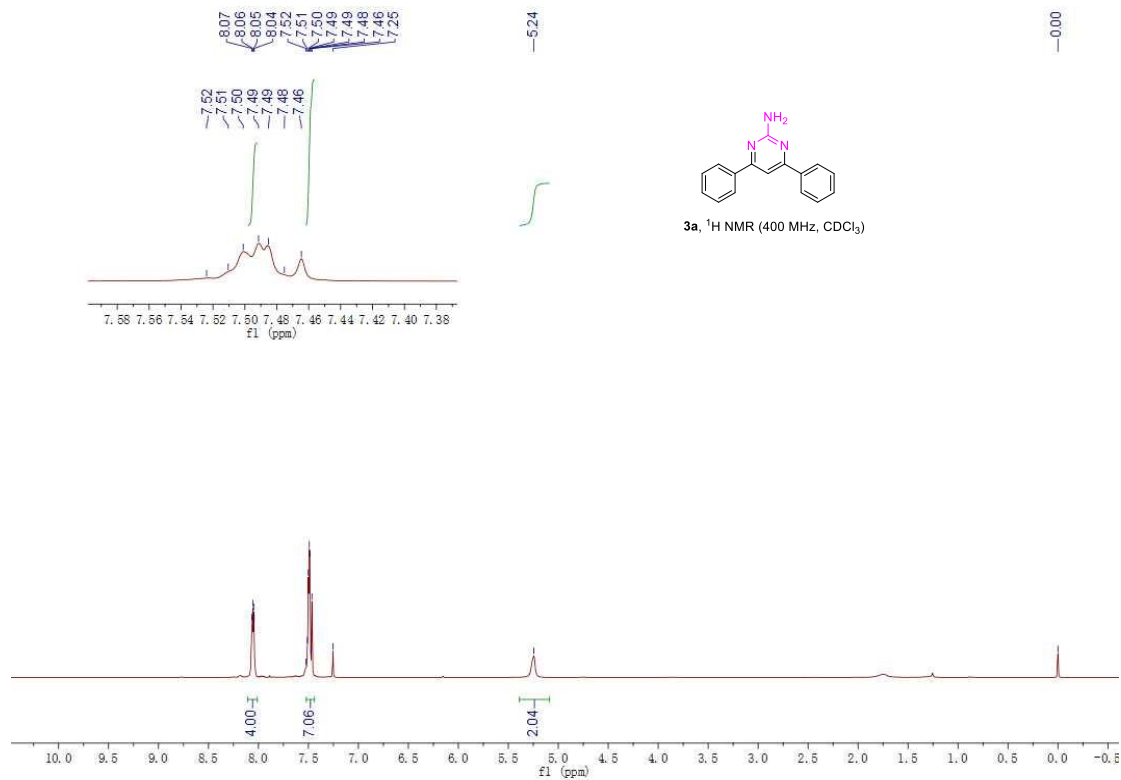


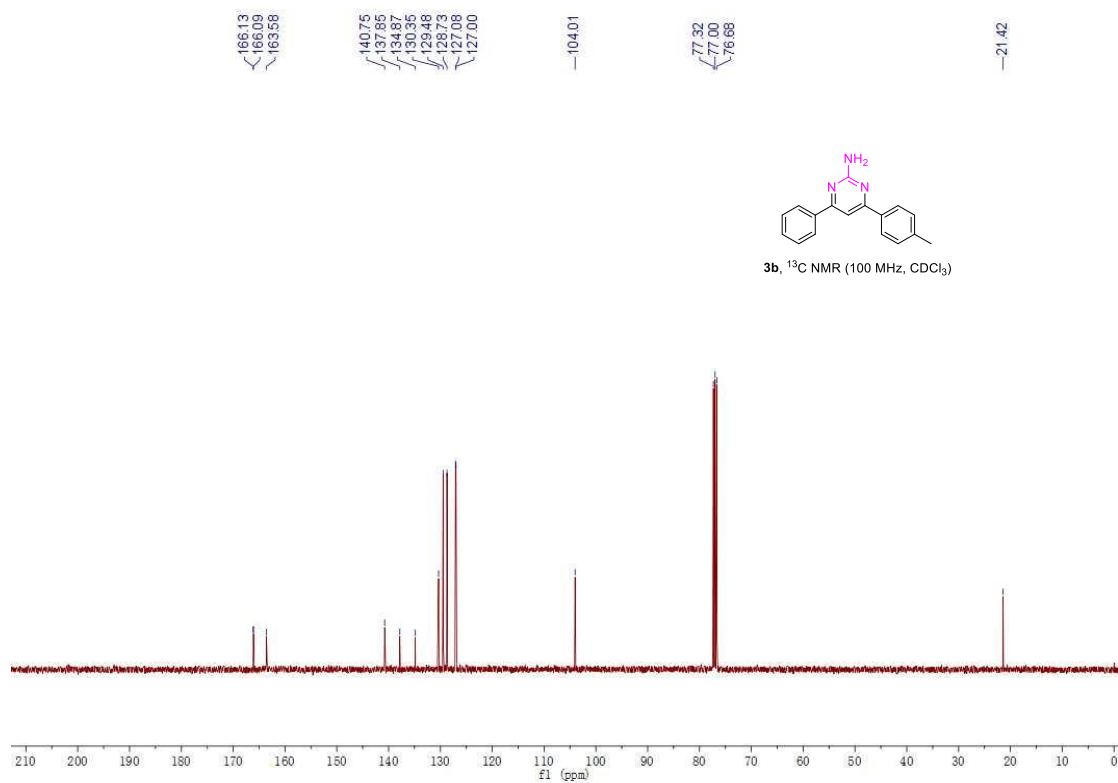
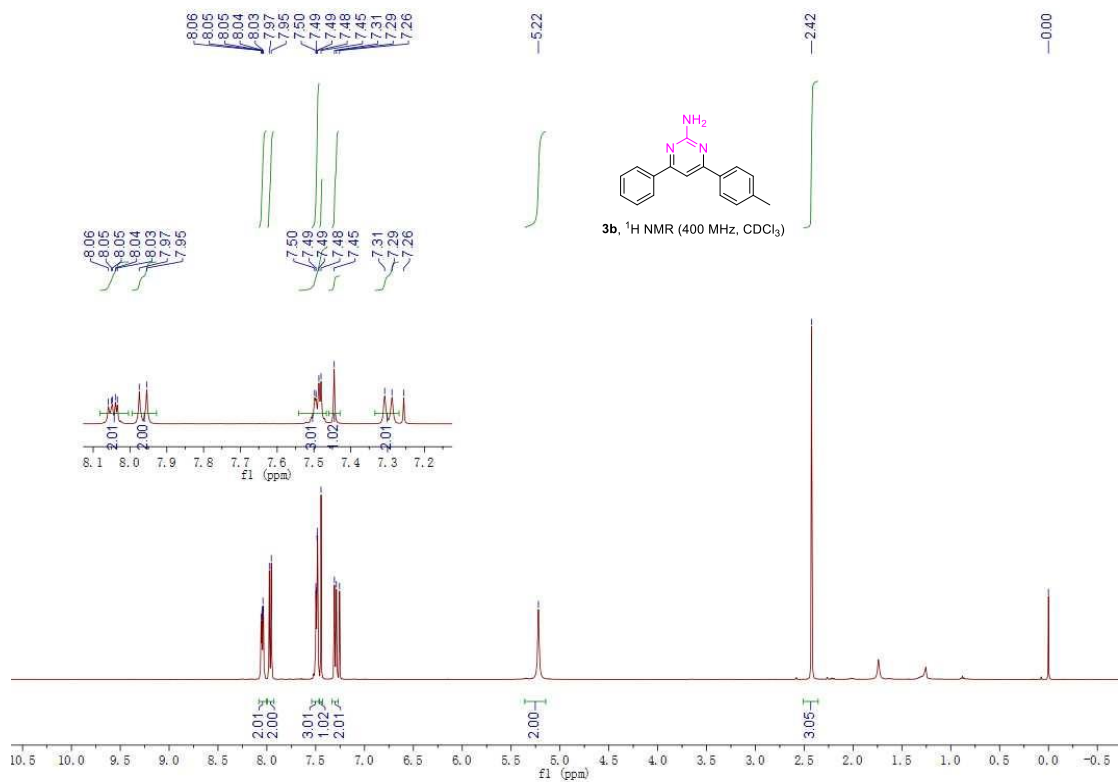


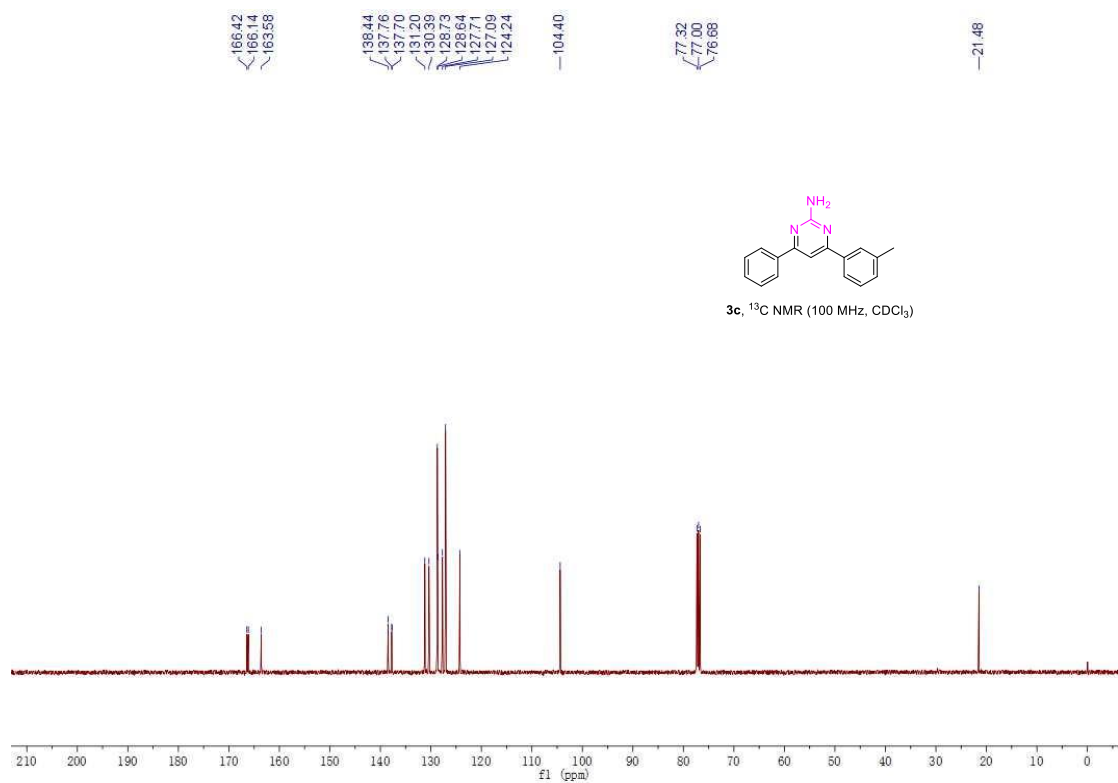
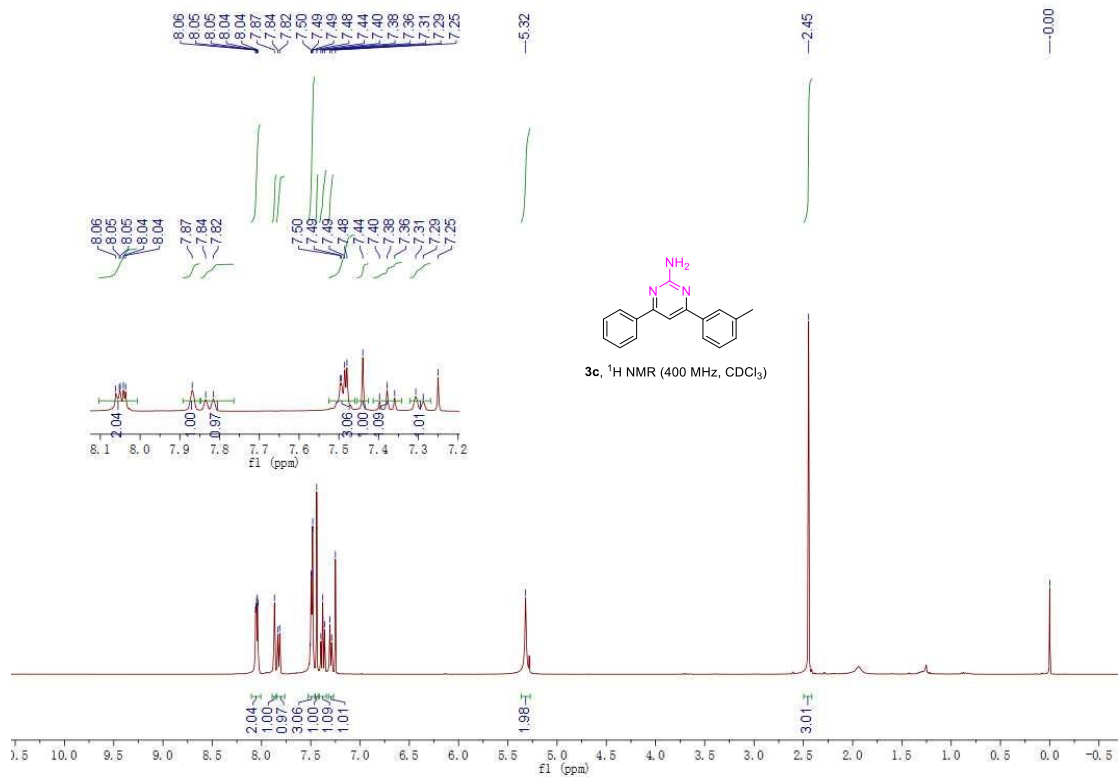


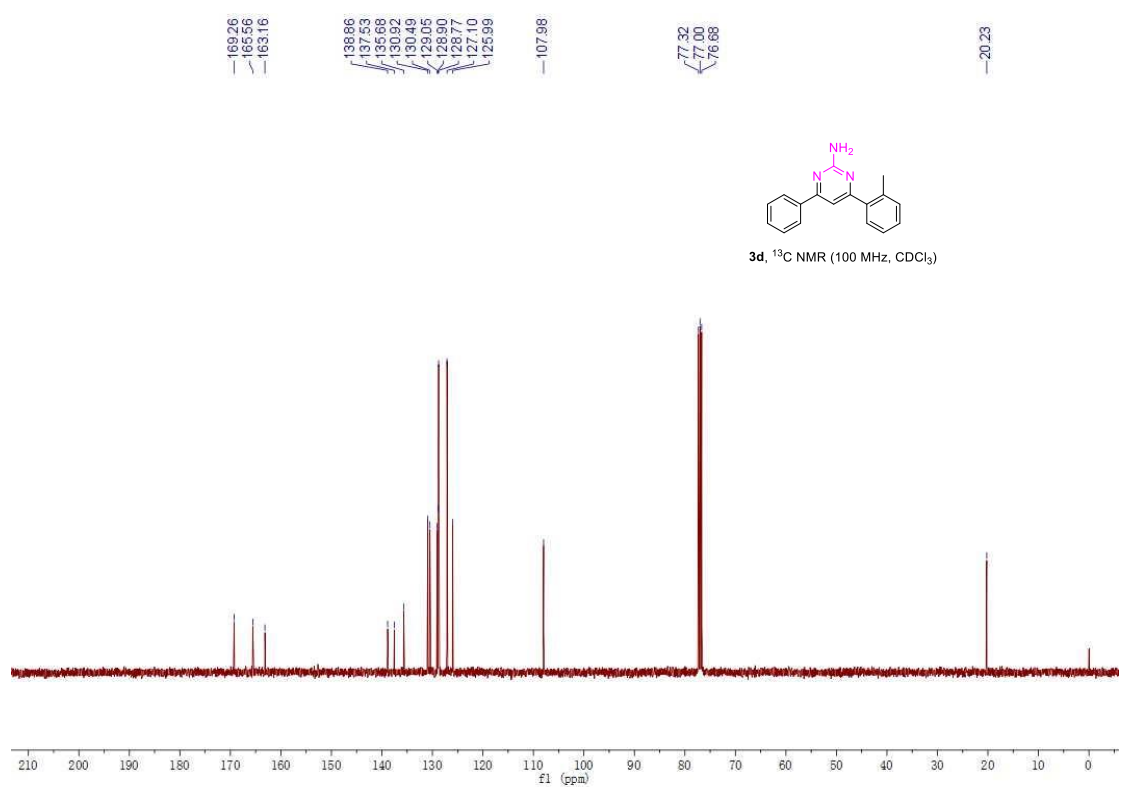
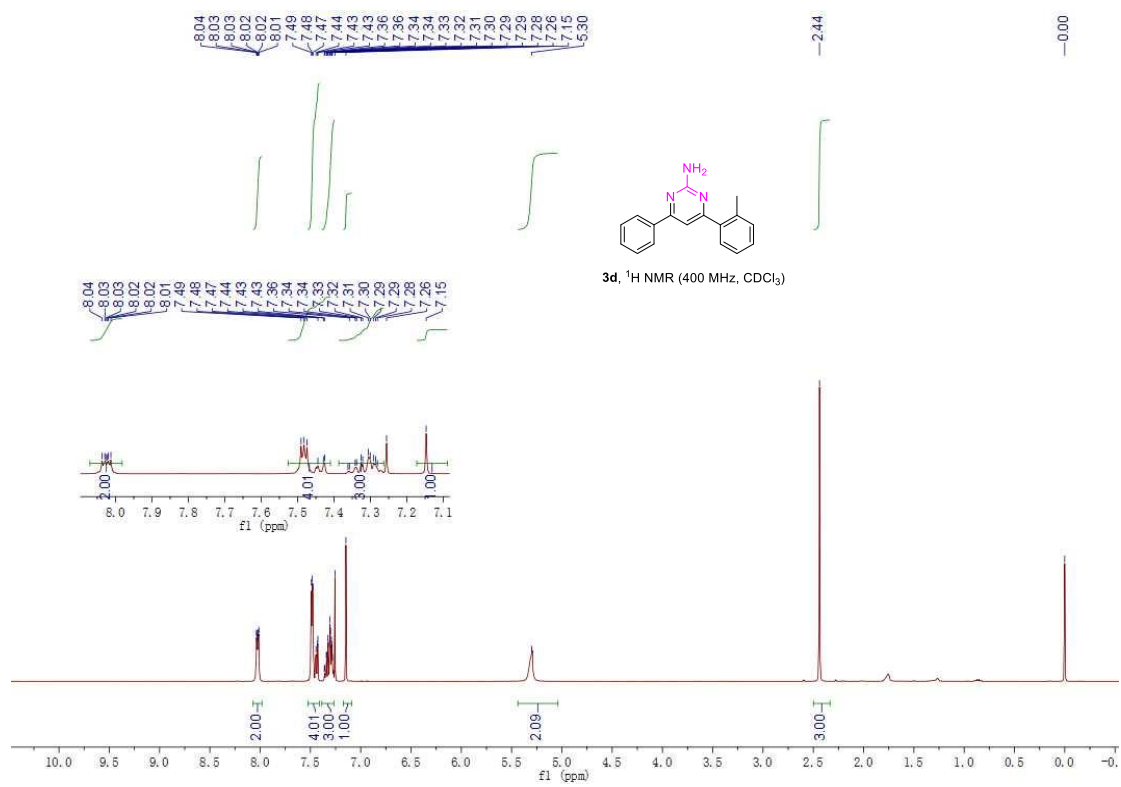


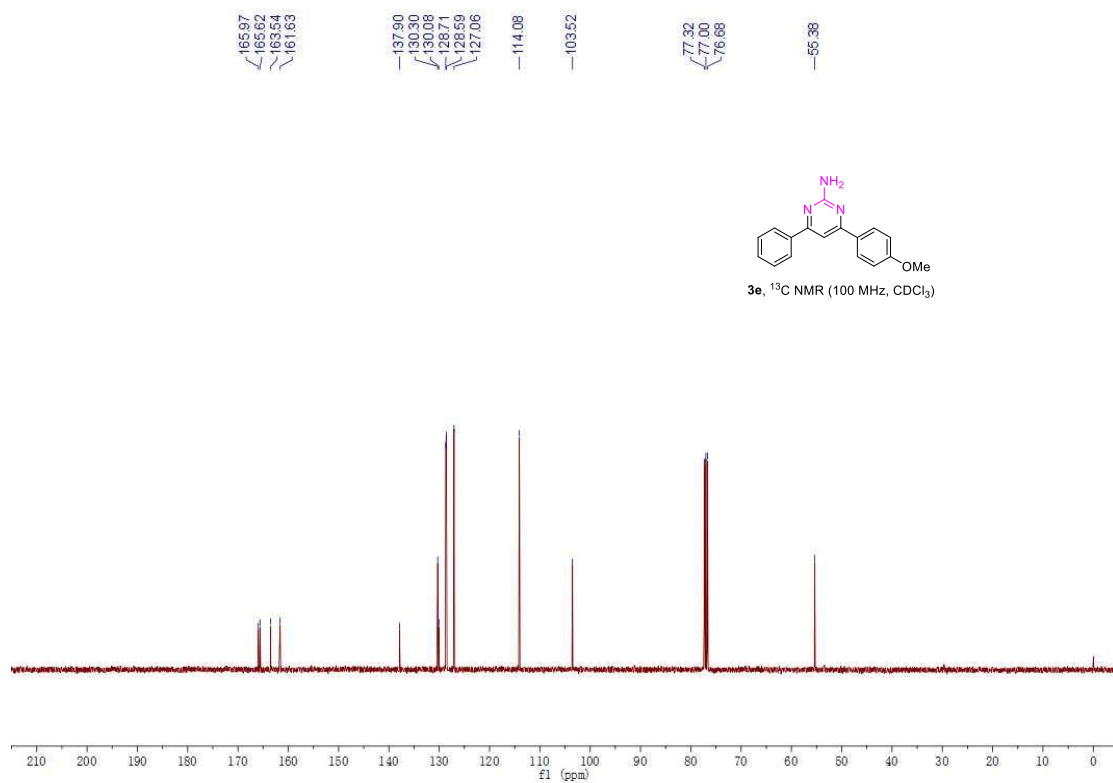
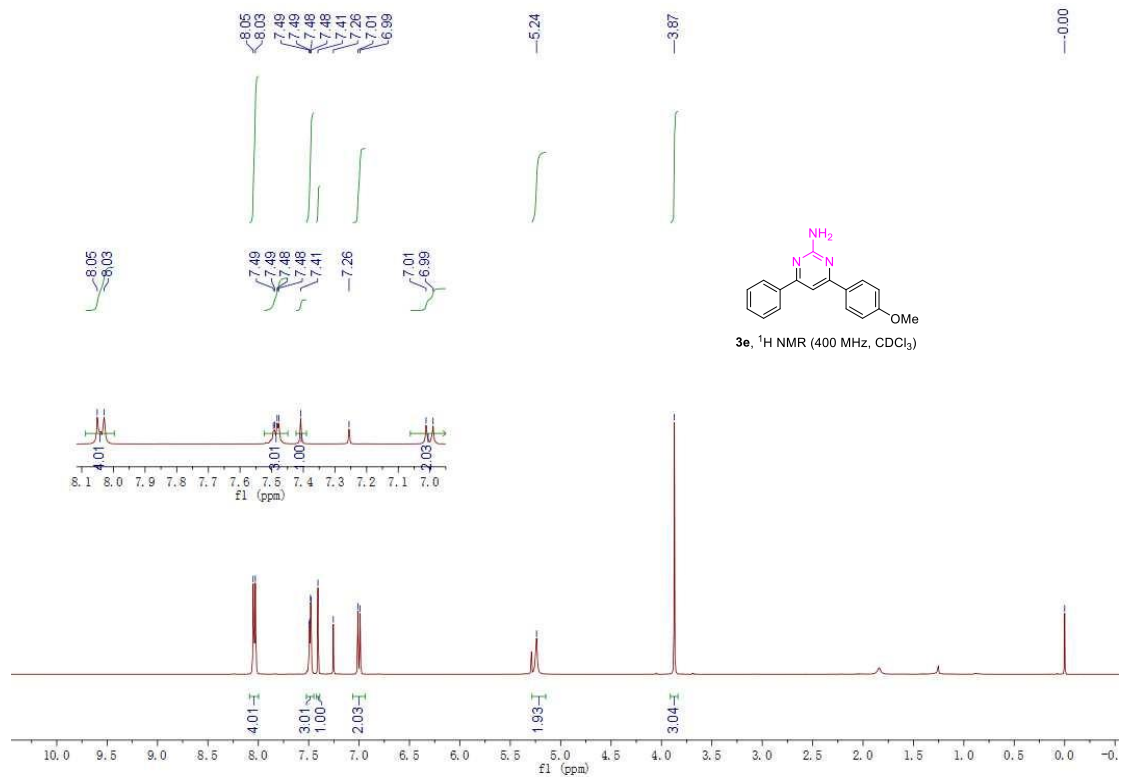
^1H NMR and ^{13}C NMR spectra of compounds **3a–3u** & **3ab–3ed**.

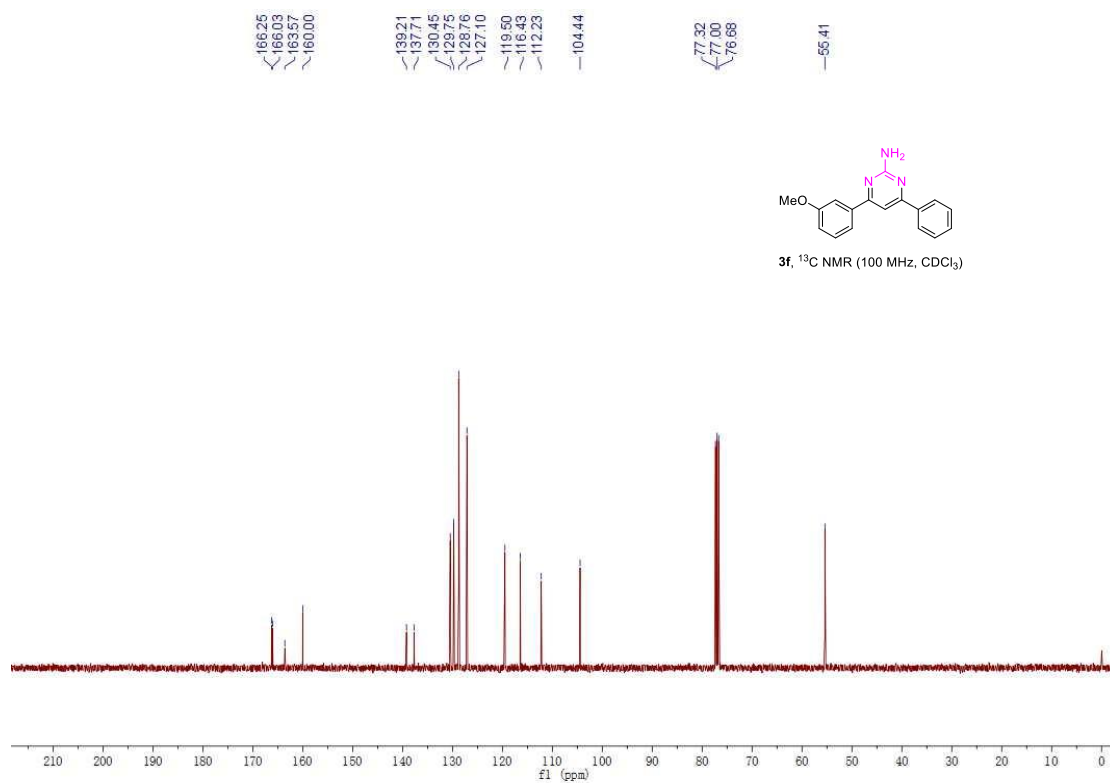
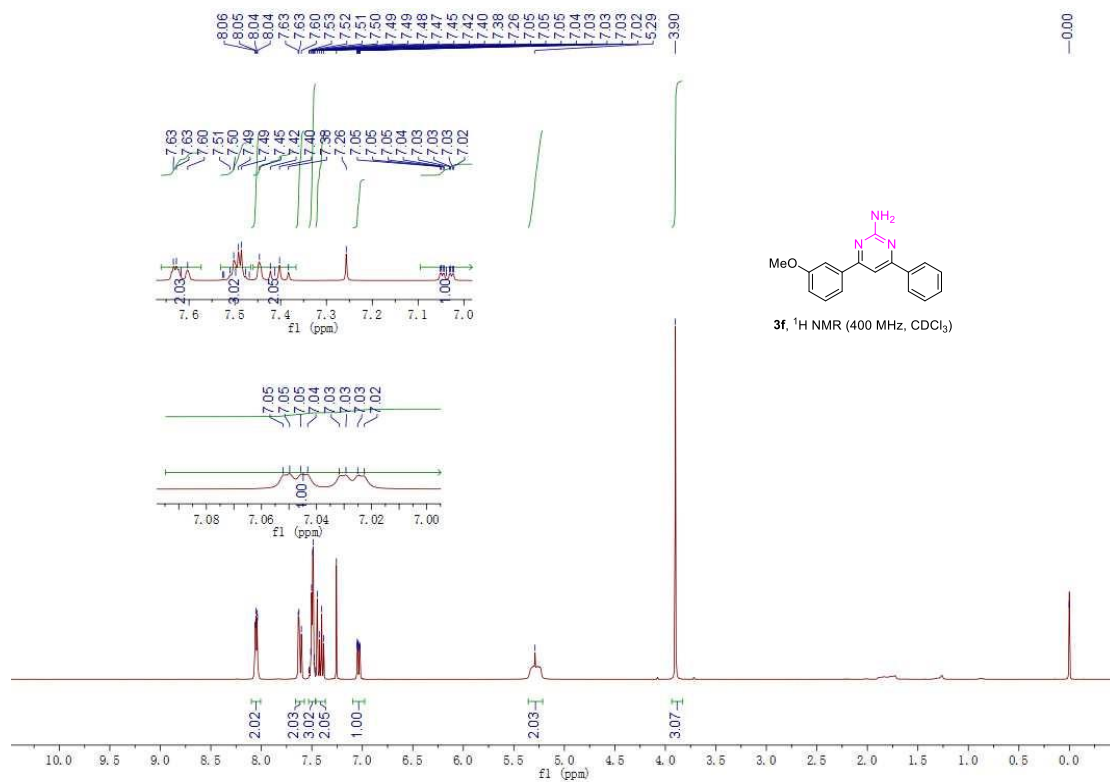


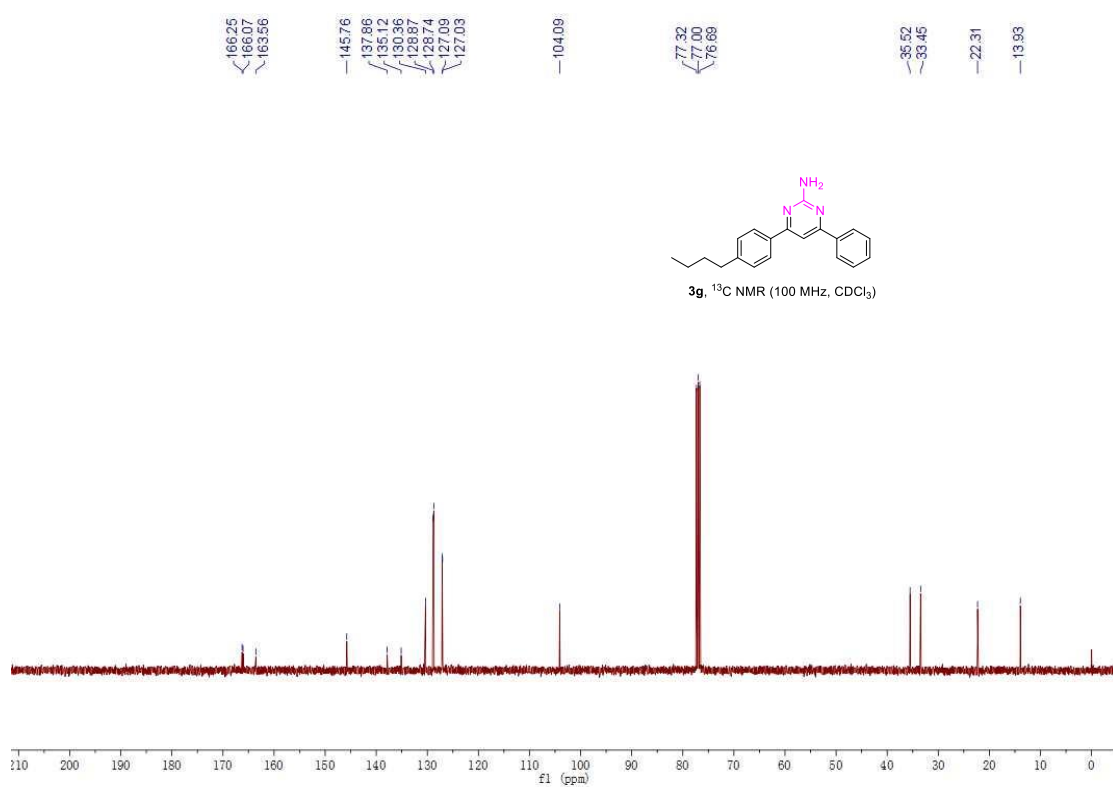
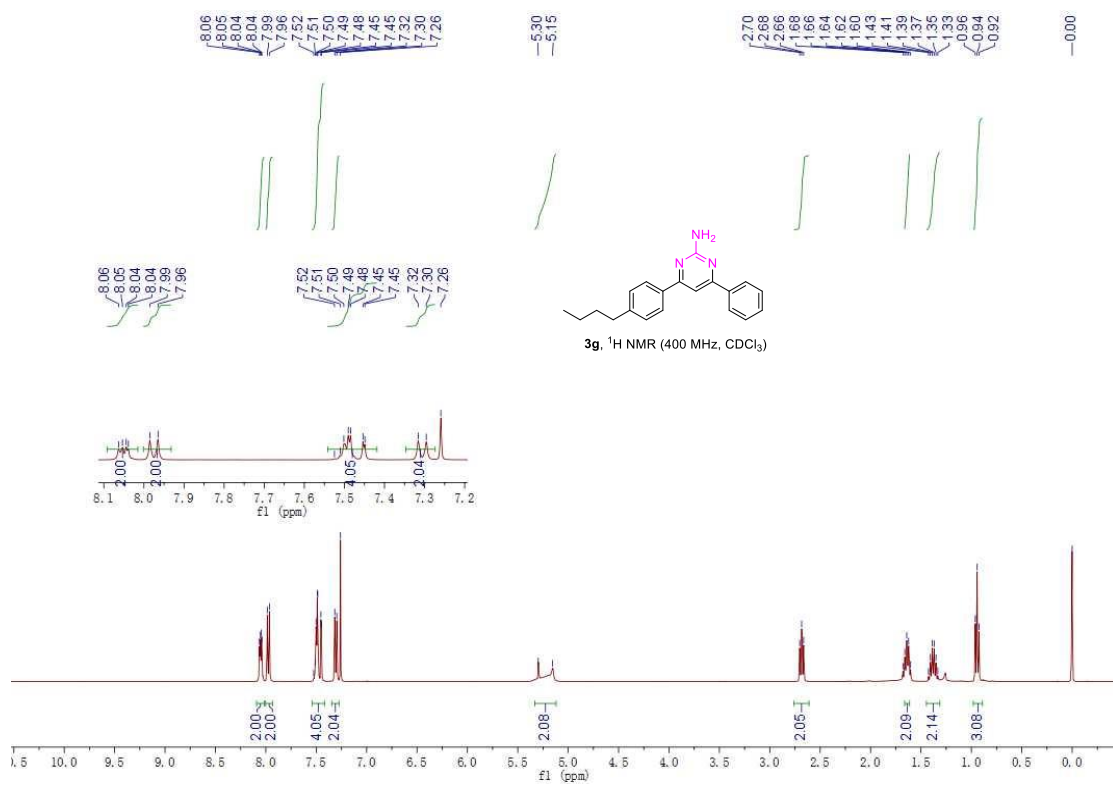


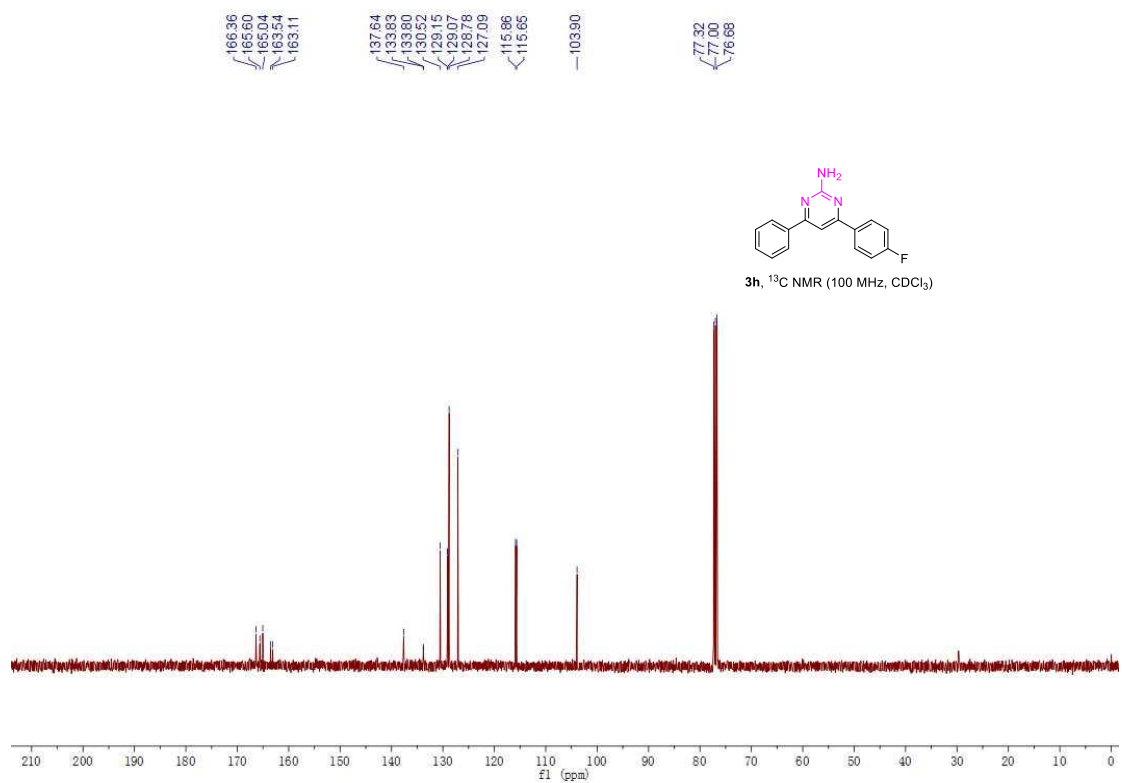
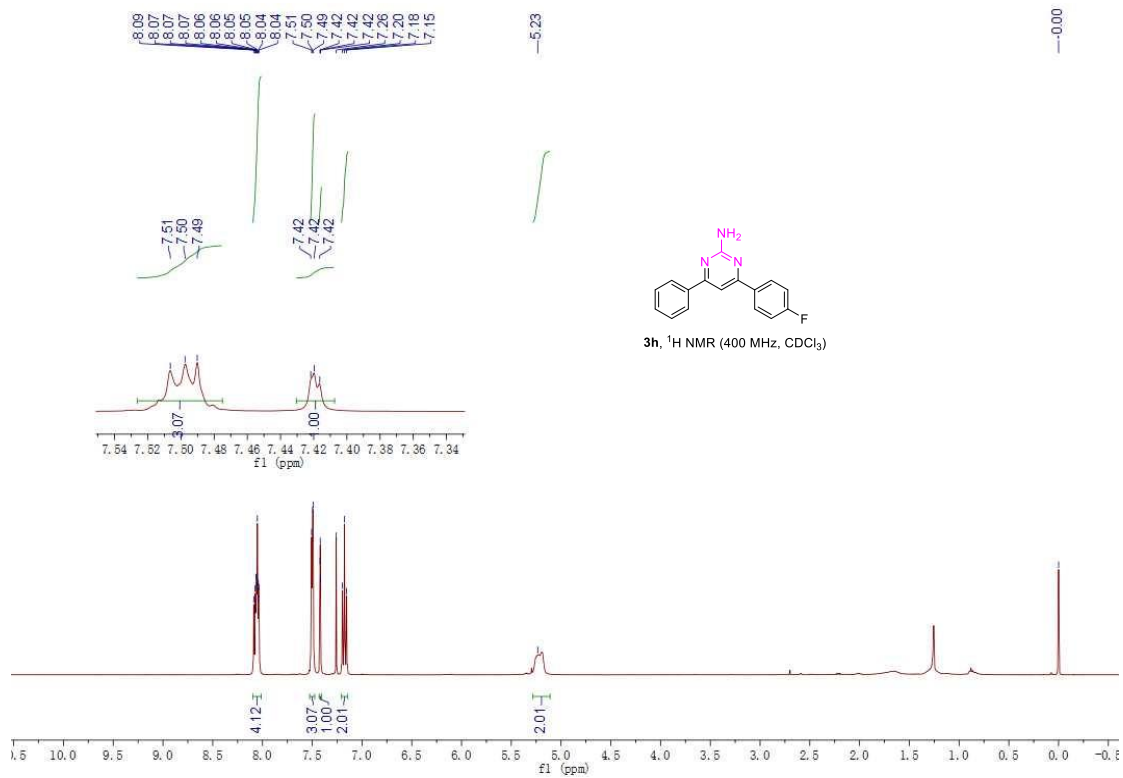


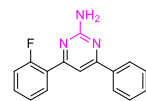
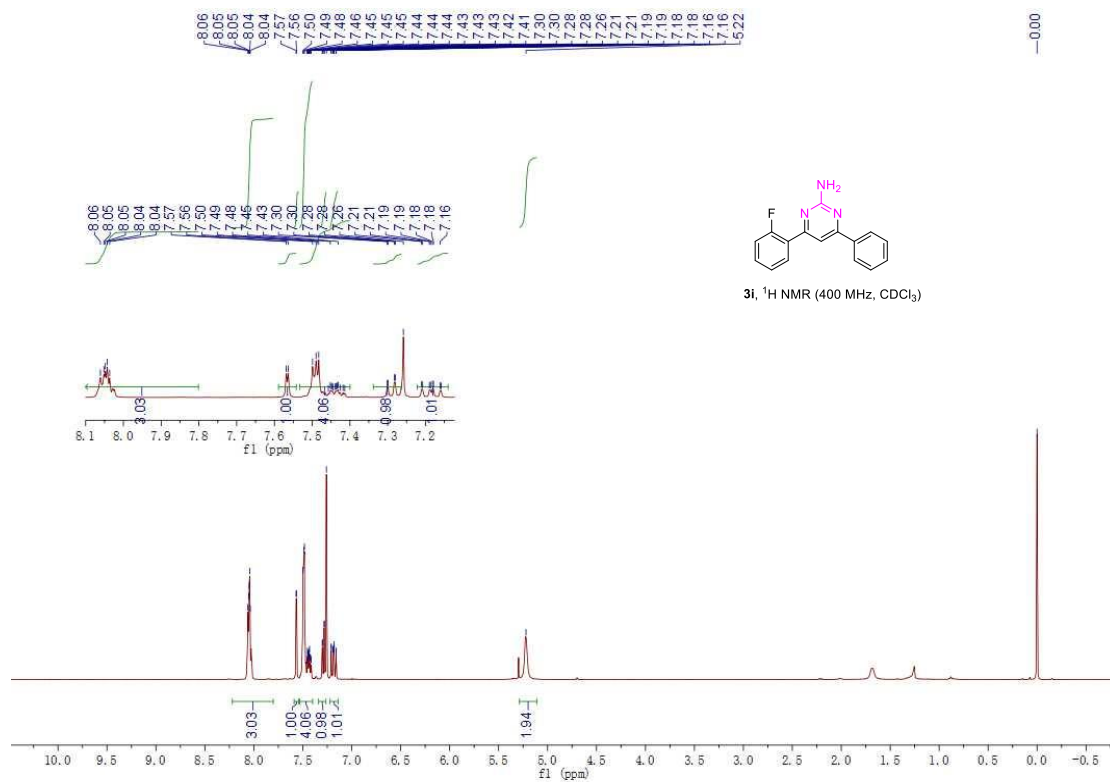




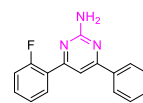
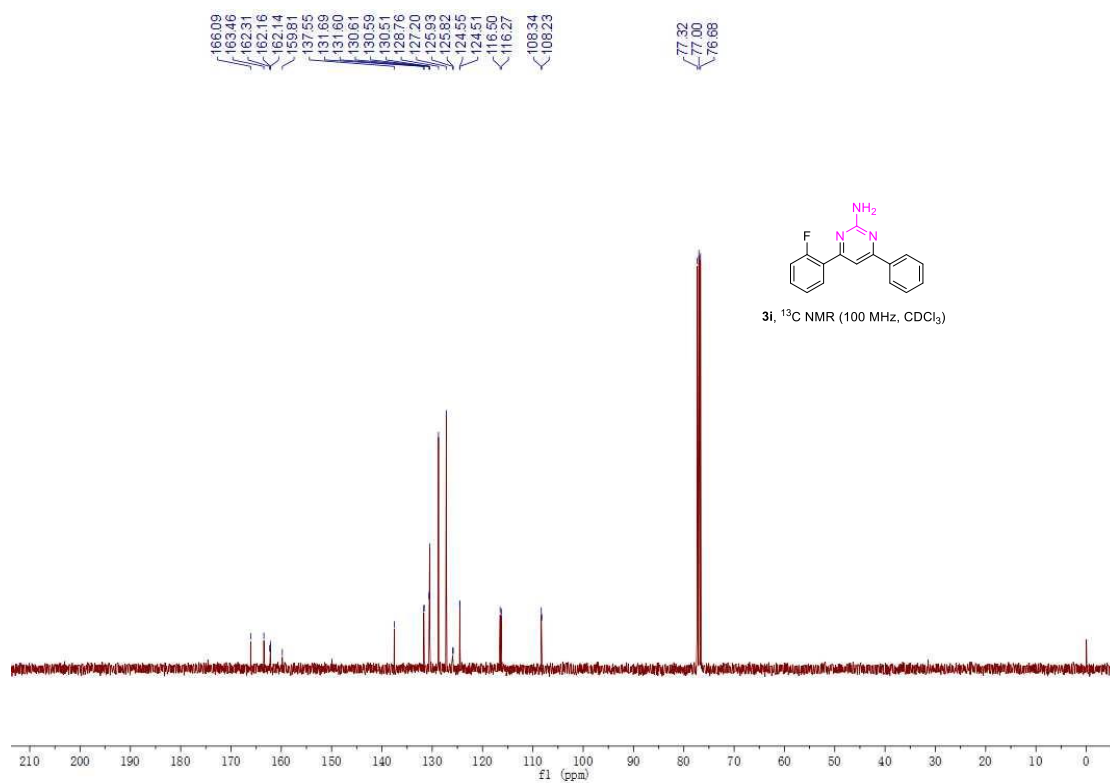




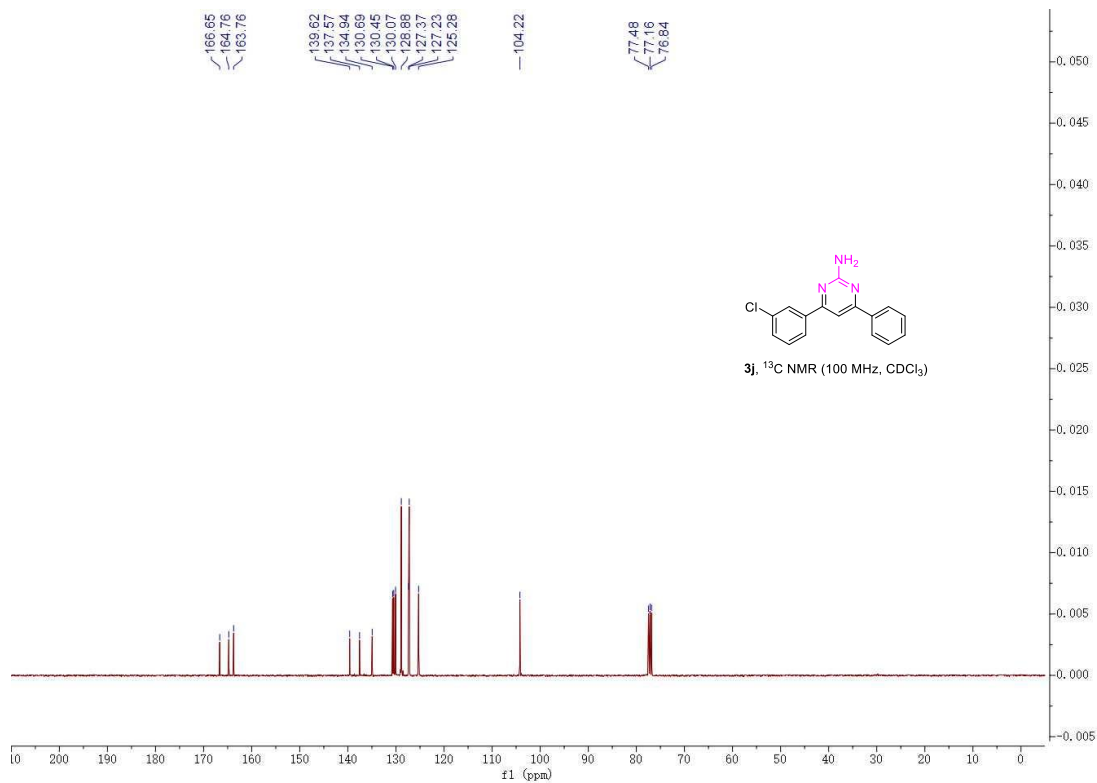
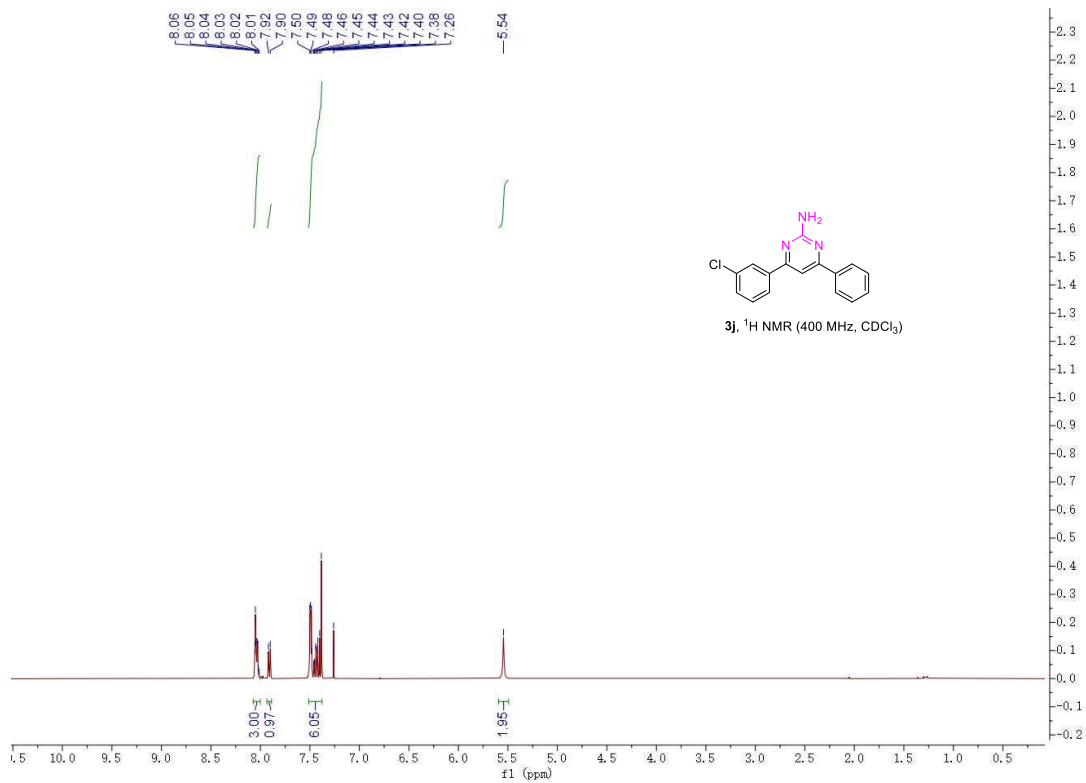


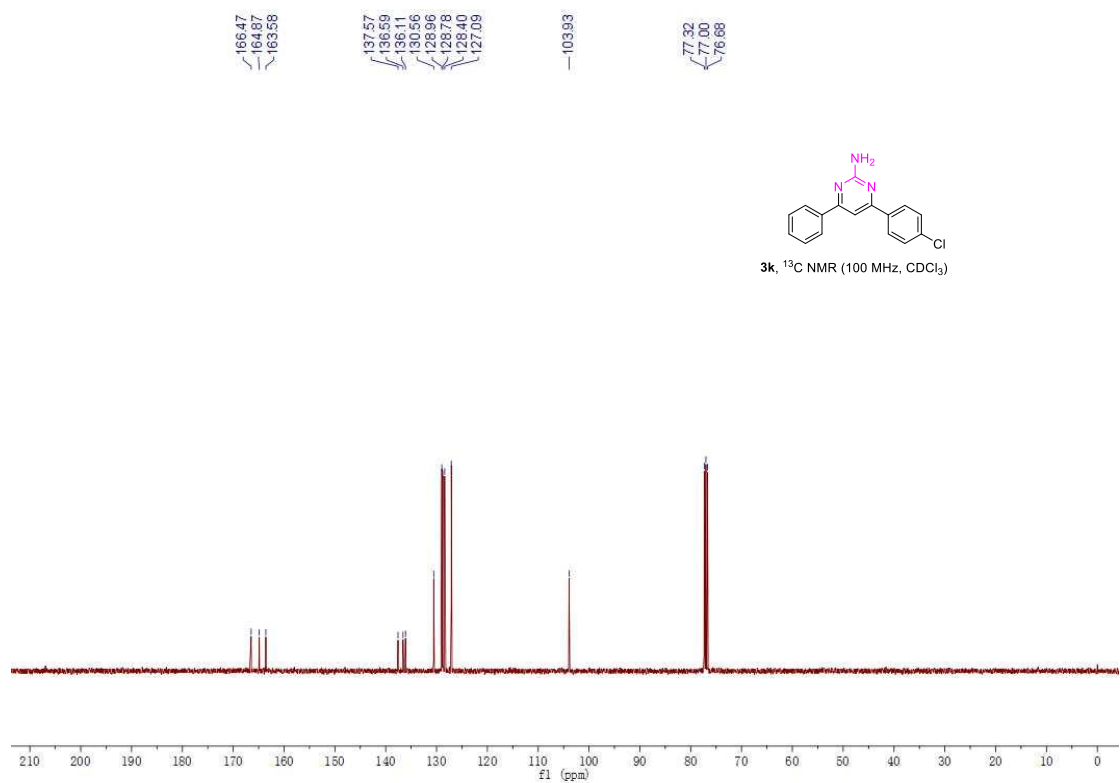
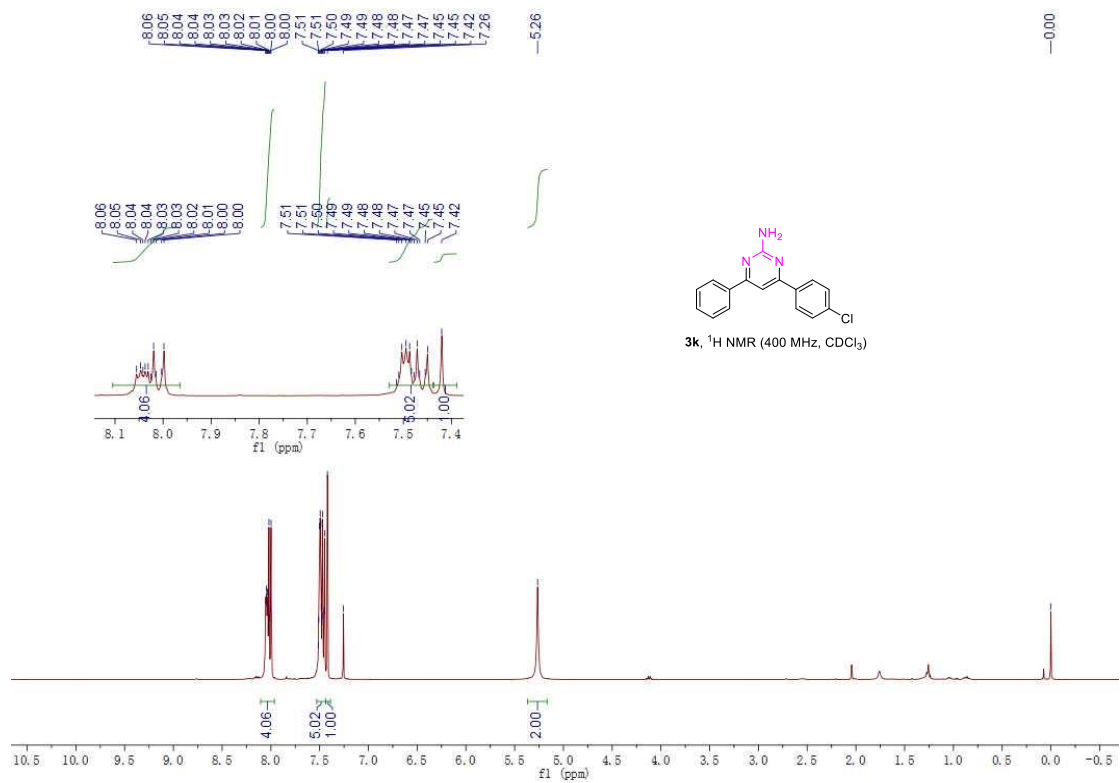


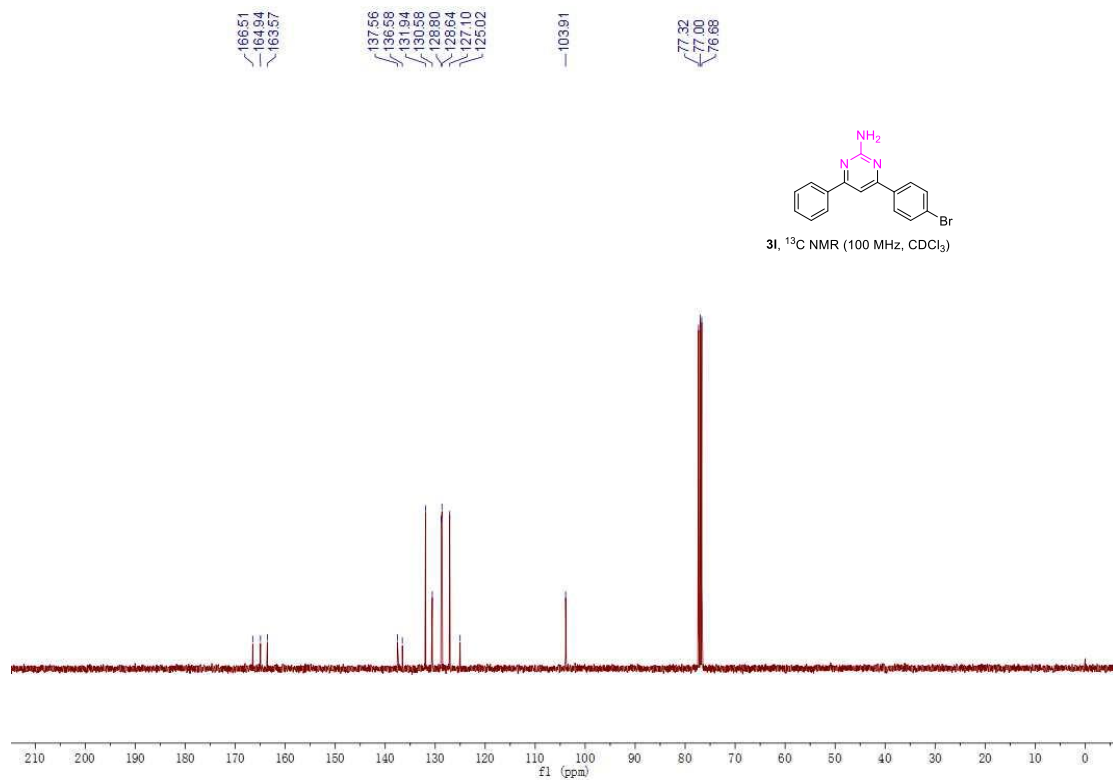
3i, ¹H NMR (400 MHz, CDCl₃)

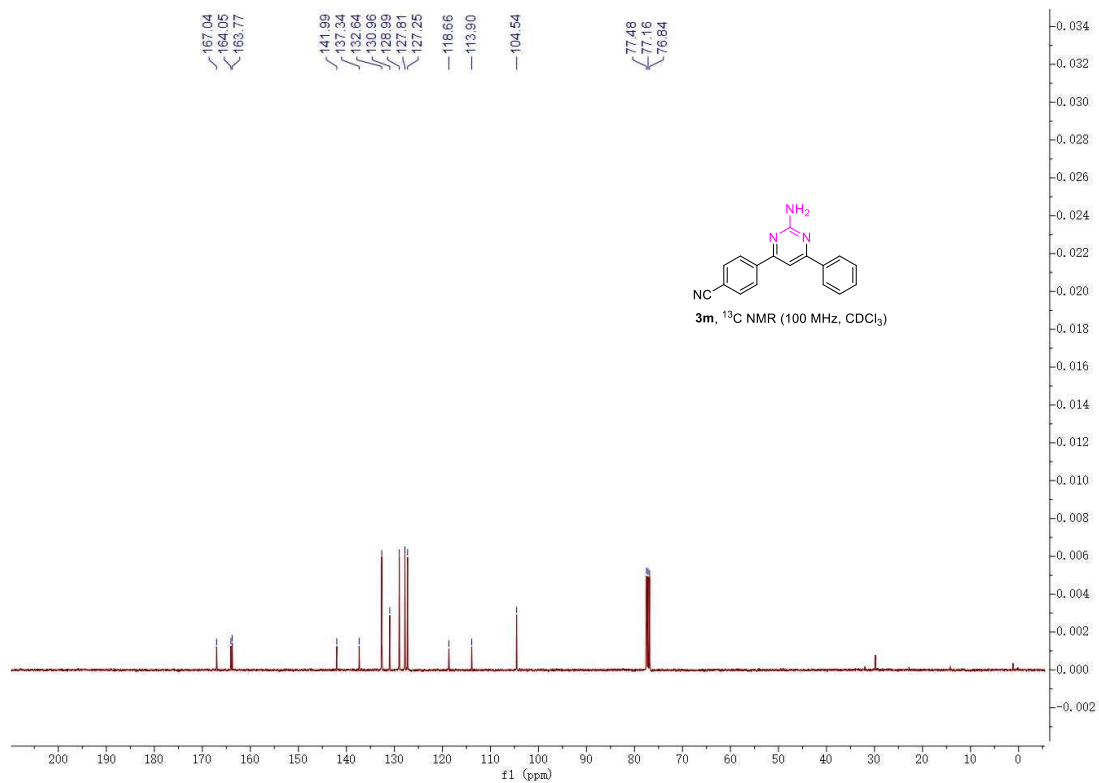
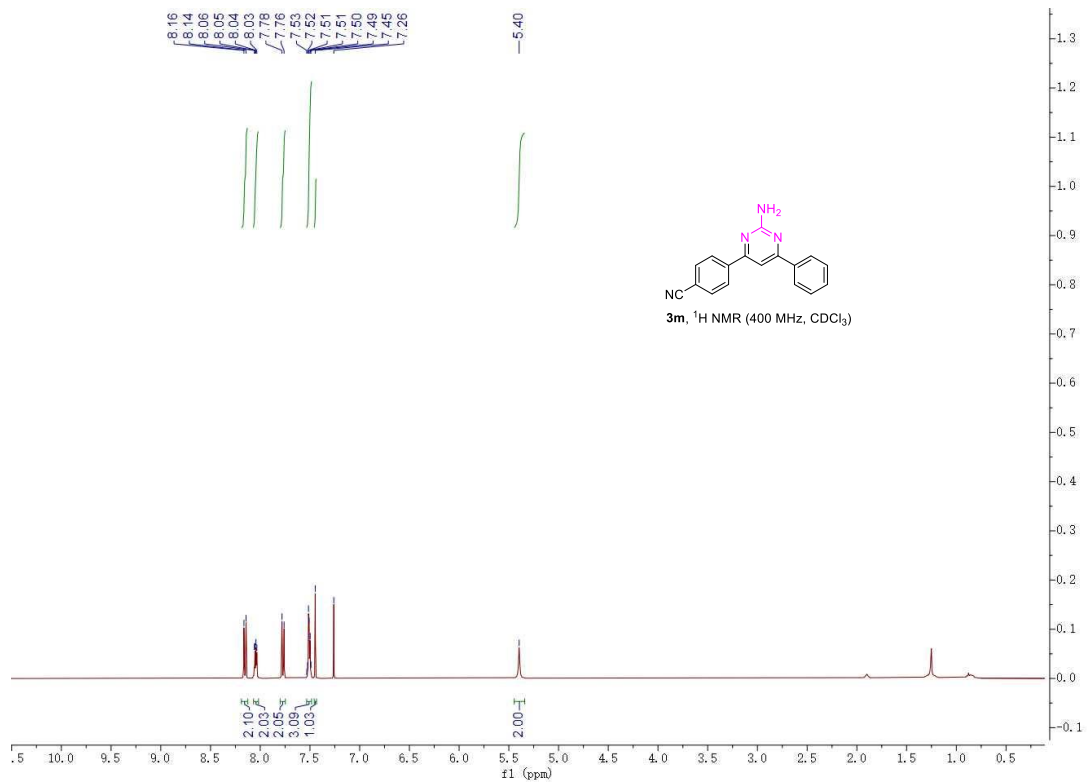


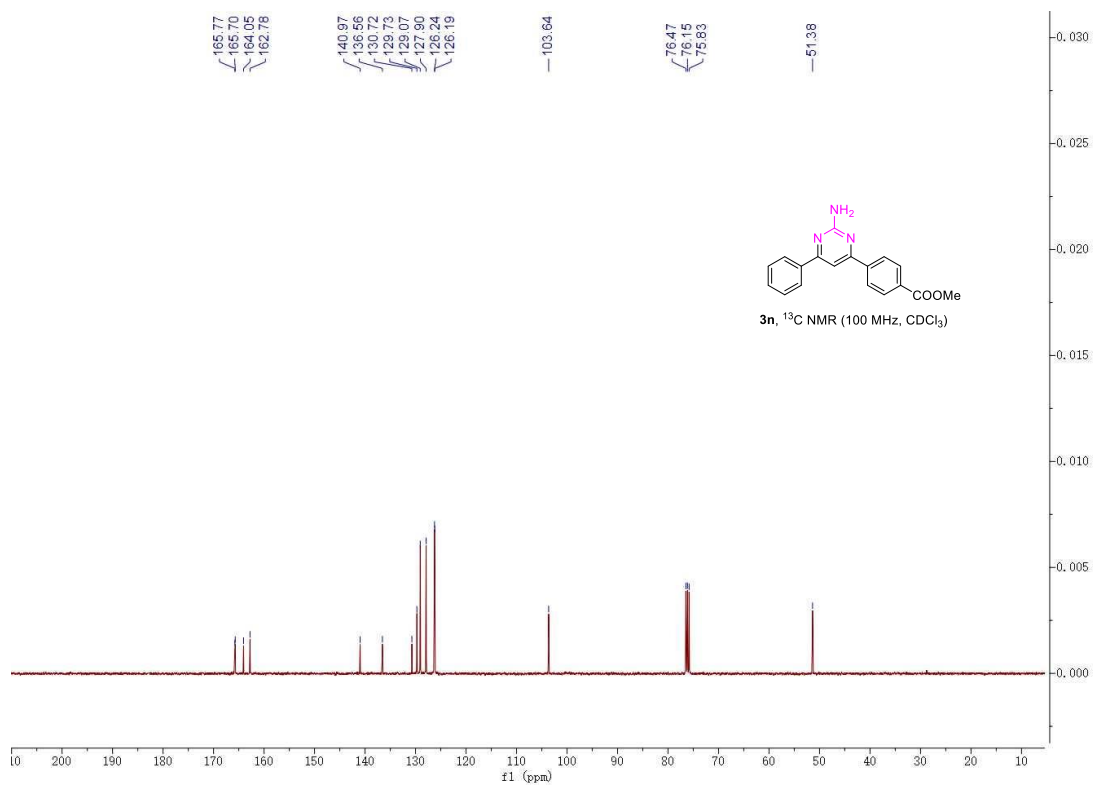
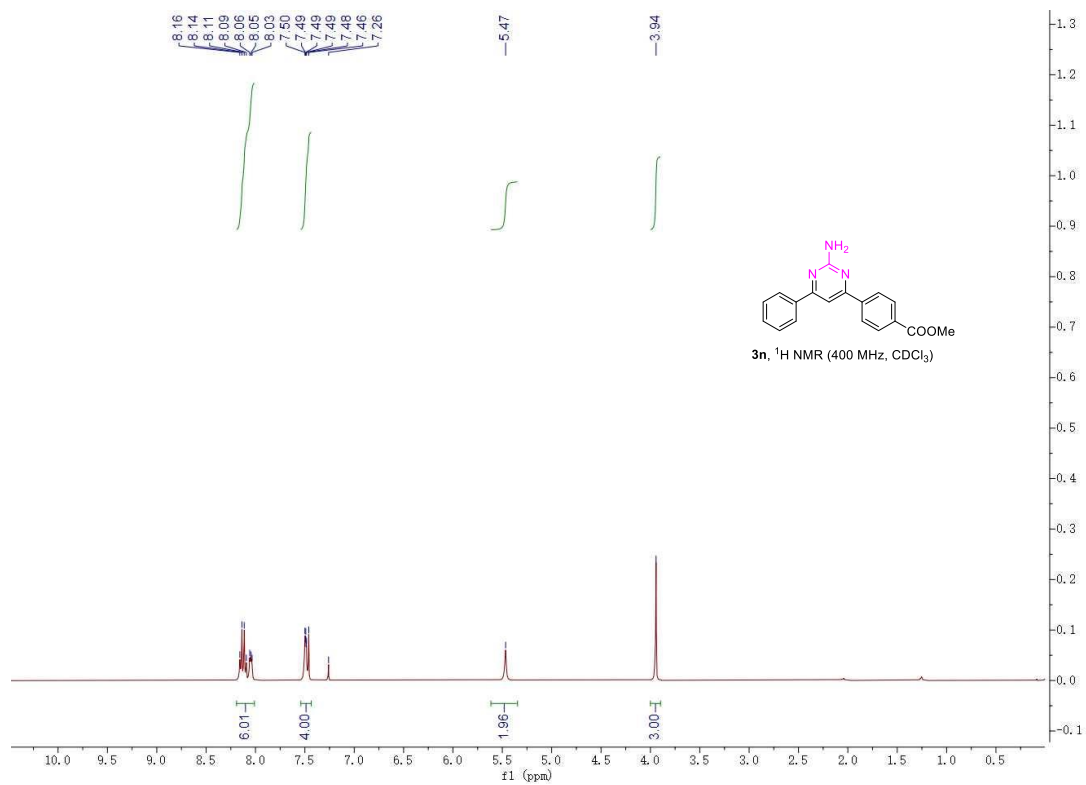
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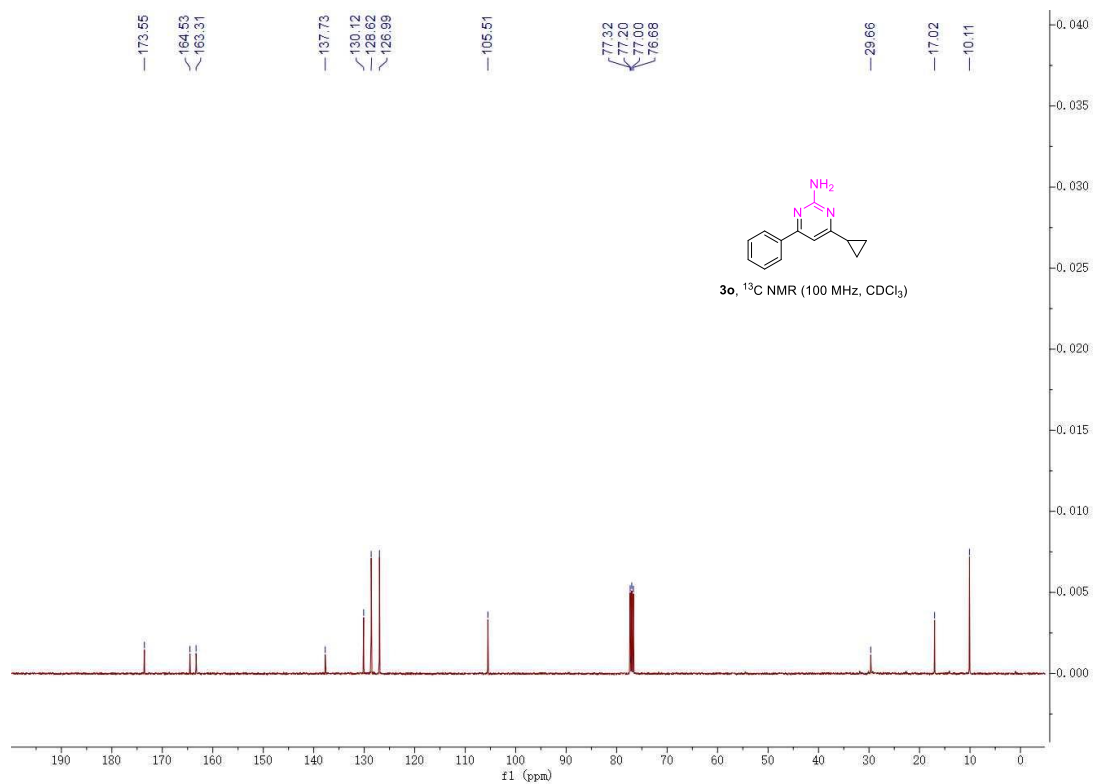
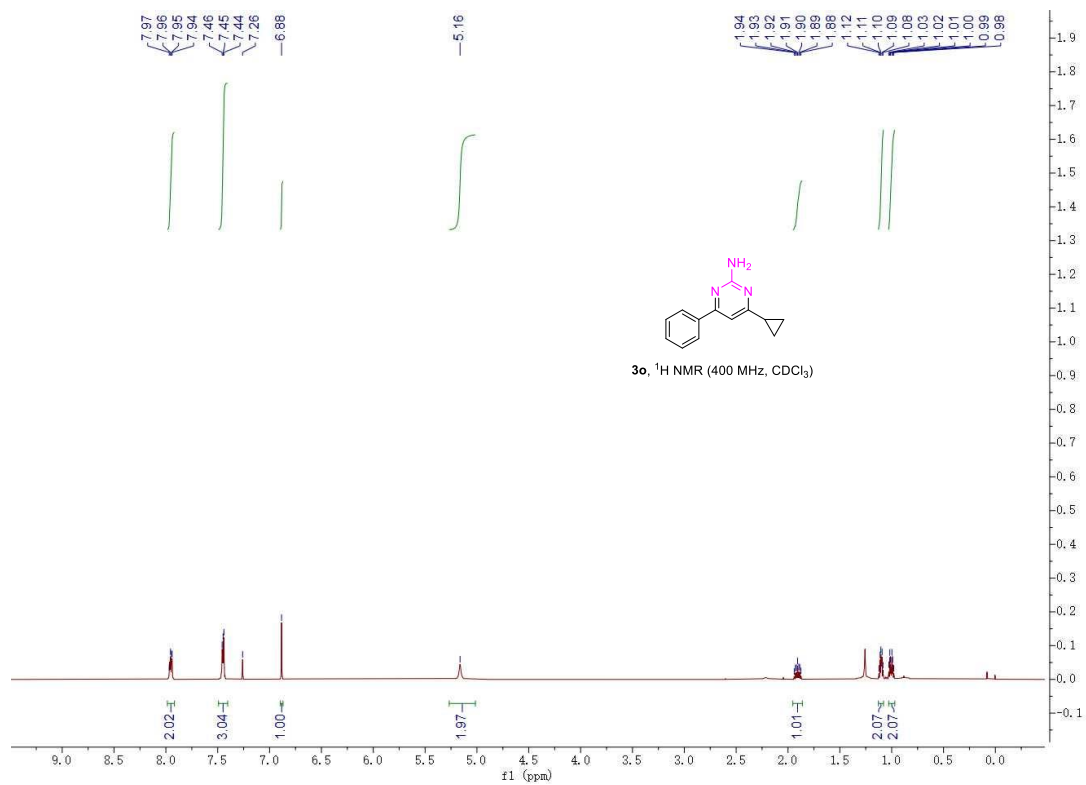


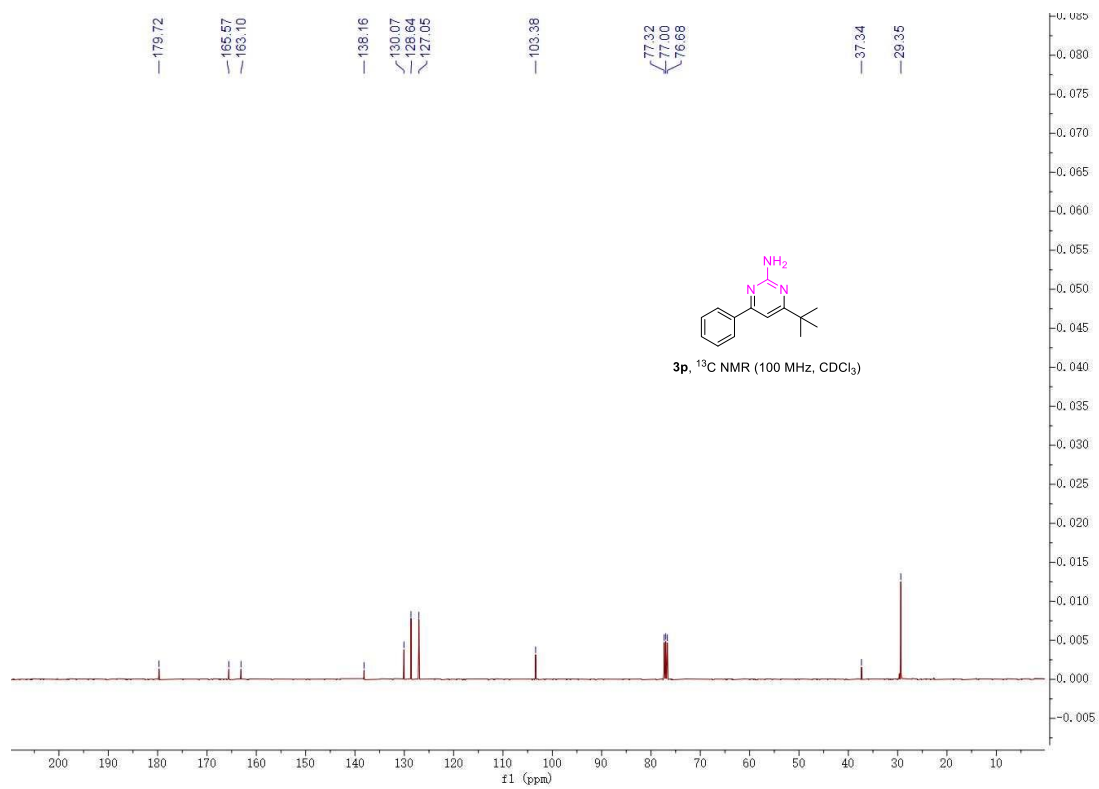
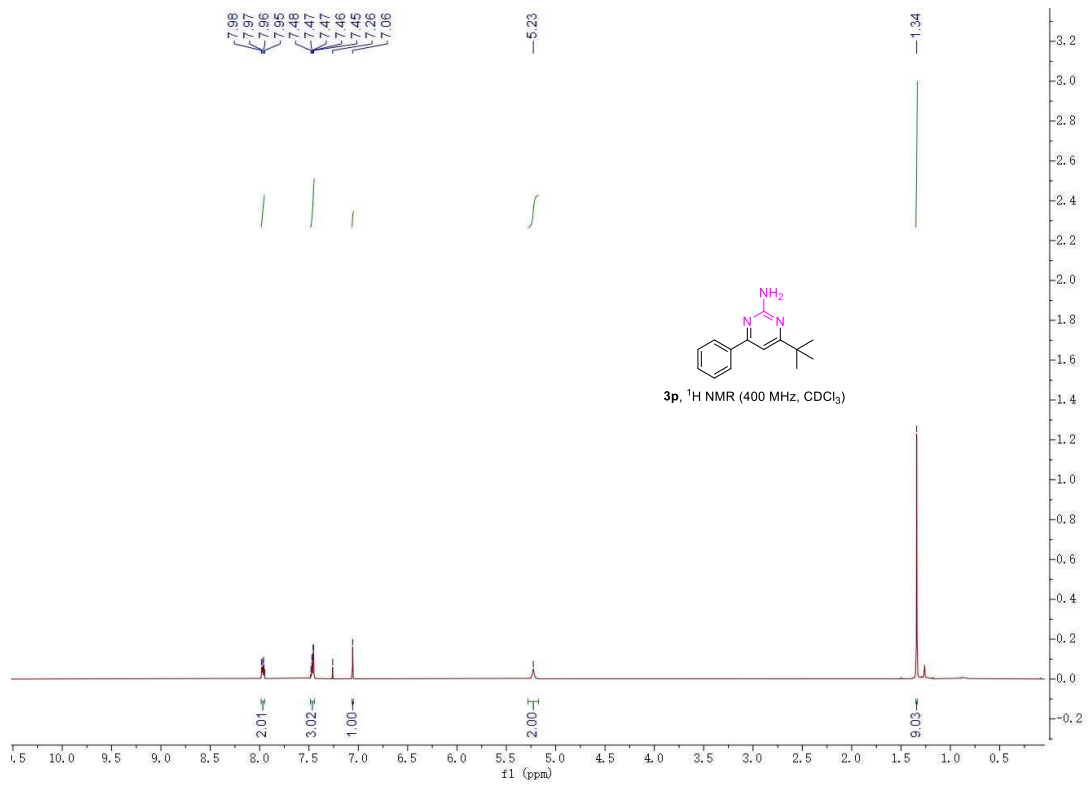


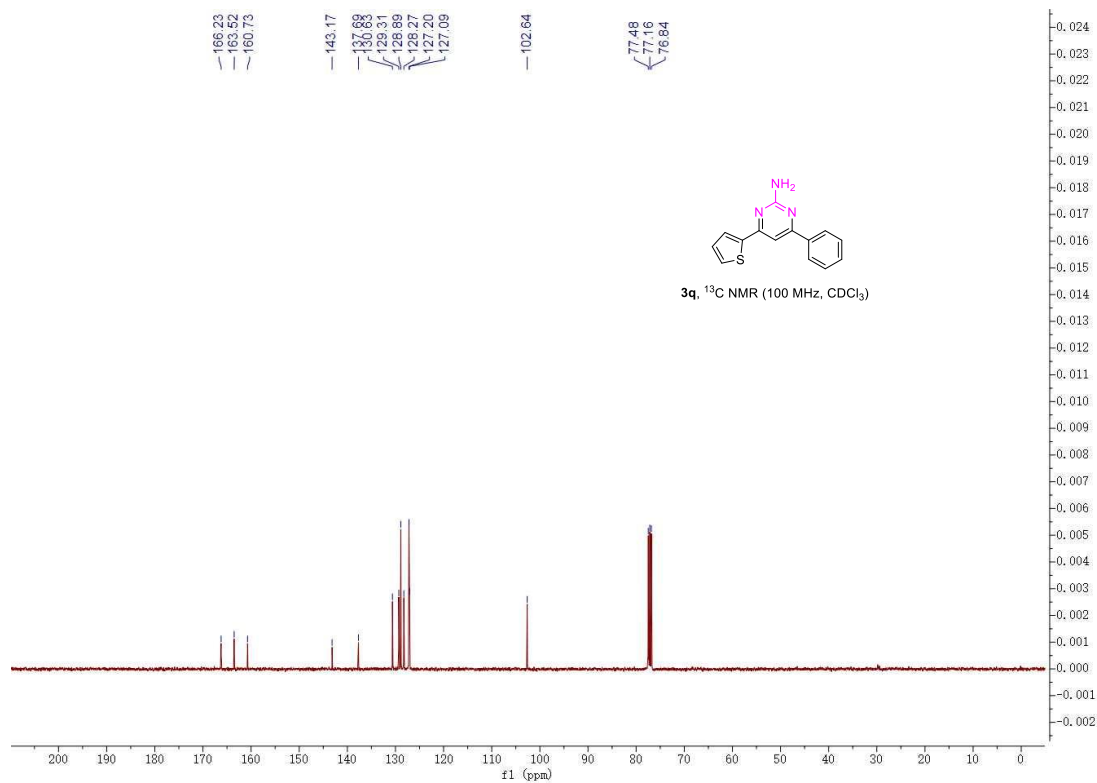
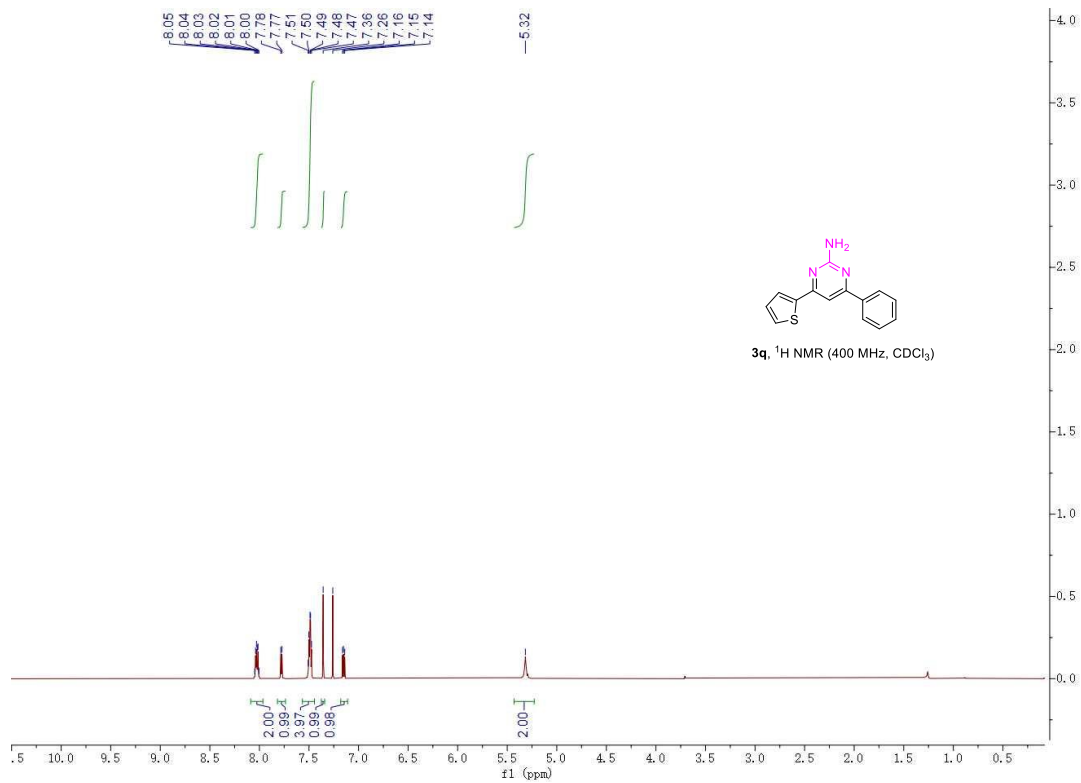


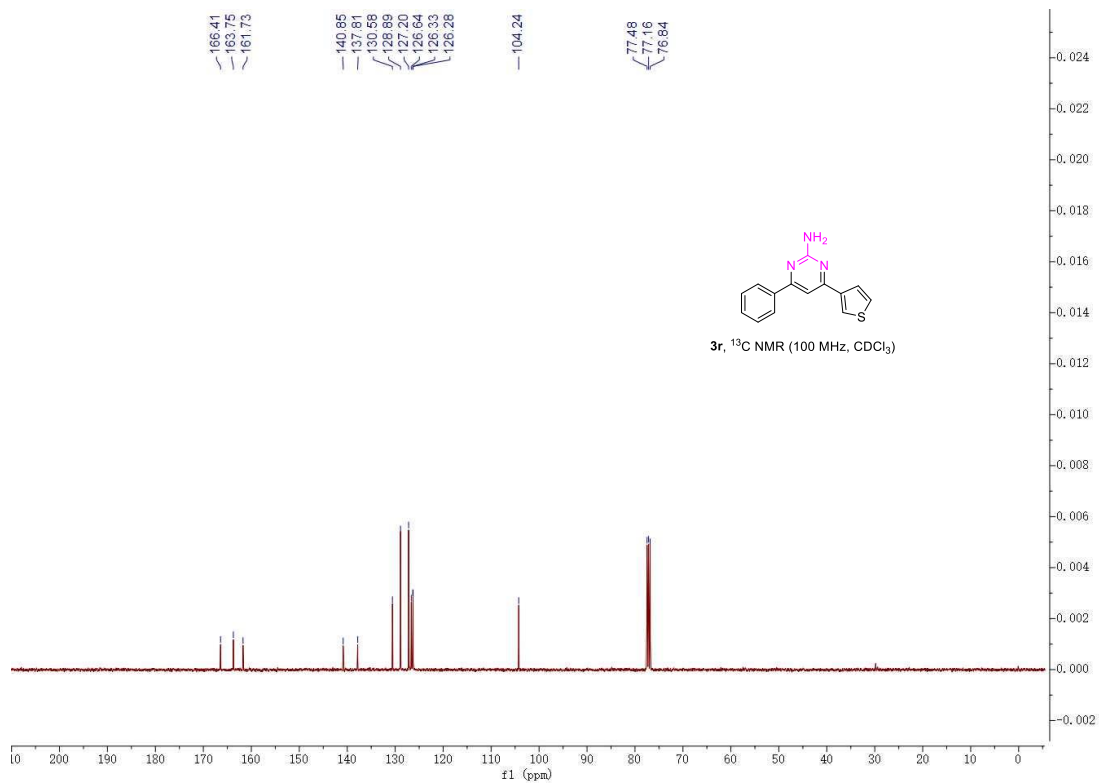
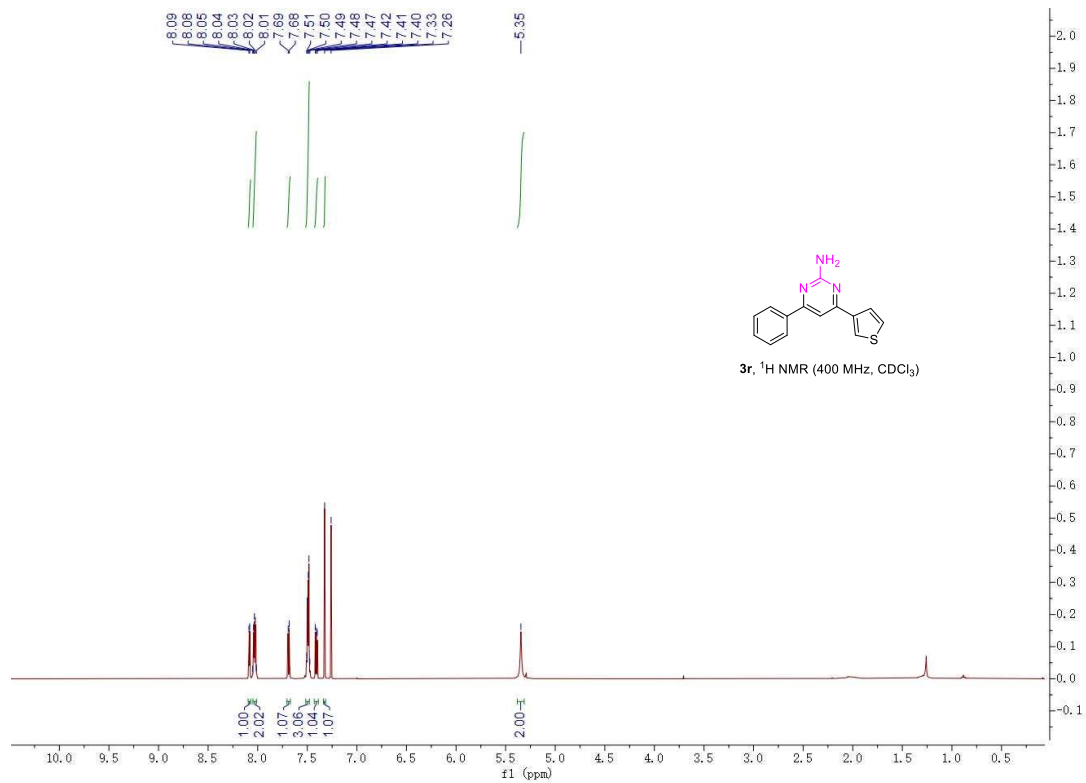


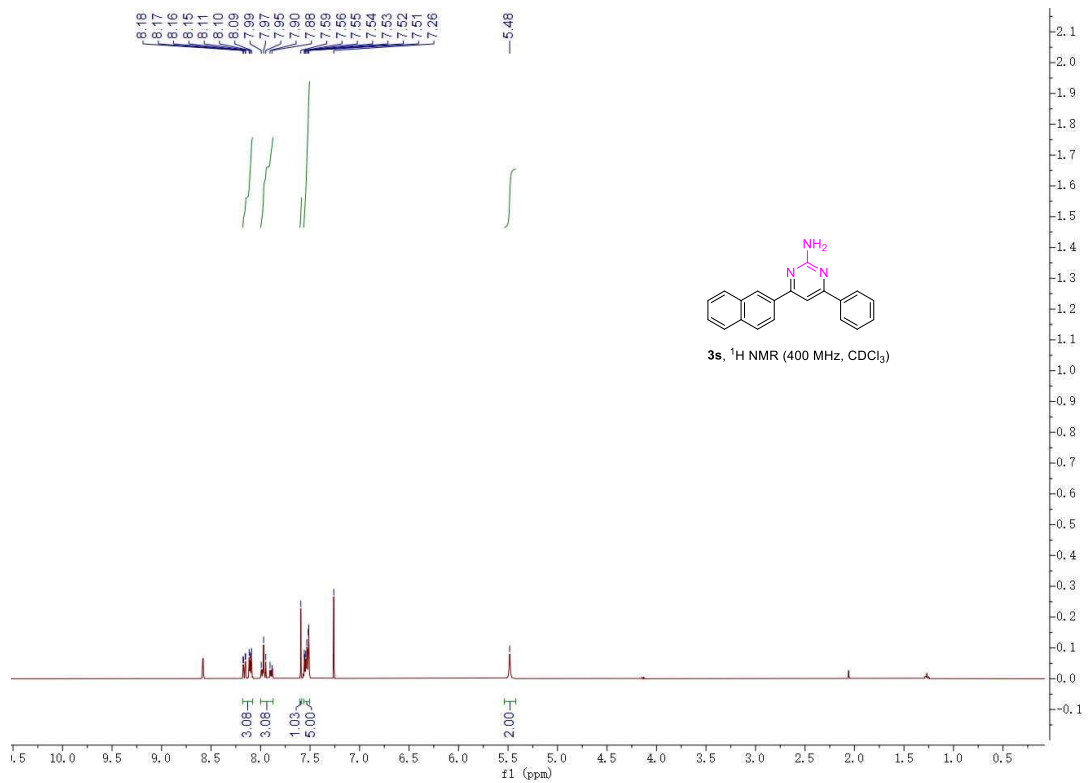


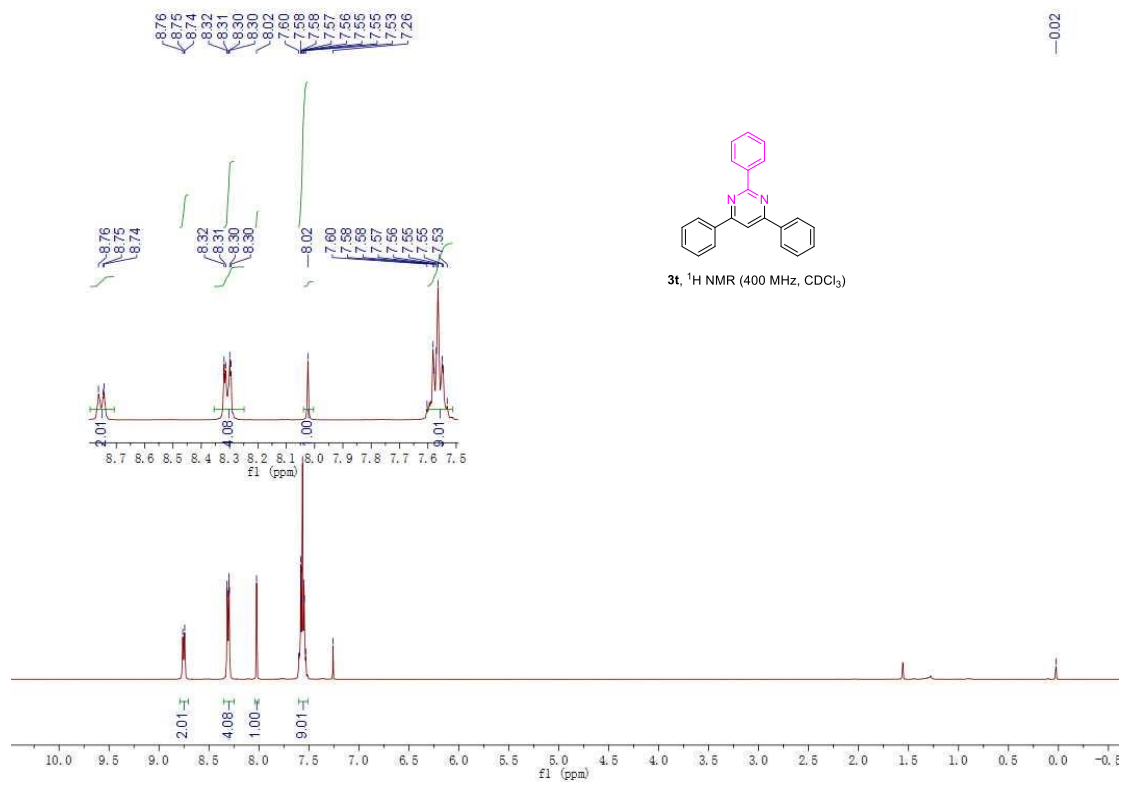












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