

Supporting Information

Synthesis, Odor Characteristics and Biological Evaluation of *N*-Substituted Pyrrolyl Chalcones

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1. General information

All reactions were carried out under air atmosphere in a dried tube. *t*-BuOK (99.9%) was purchased from Shanghai Meryer Chemical Technology Co., Ltd. All the reagents were obtained commercially and used without further purification. Silica gel was purchased from Qing Dao Hai Yang Chemical Industry Co. Analytical thin layer chromatography (TLC) was performed on precoated silica gel F₂₅₄ plates. Compounds were visualized by irradiation with UV light (254 nm).

Analytical information:

¹H NMR and ¹³C NMR spectra data were recorded by a BRUKER AVANCE III 400 MHz spectrometer (¹H 400 MHz, ¹³C 100 MHz), using CDCl₃ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. ¹H NMR spectral data are given as chemical shifts in ppm followed by multiplicity (s- singlet; d- doublet; t- triplet; q- quartet; m- multiplet), number of protons and coupling constants. ¹³C NMR chemical shifts are expressed in ppm. Infrared spectra were recorded with a Thermo Scientific Nicolet 6700 FT-IR Spectrometer. HRMS data were obtained using AB SCIEX Triple TOF 5600+ high resolution mass spectrometer (USA). The products listed below were determined by ¹H and ¹³C NMR spectra. Melting points were determined using melting point X-4 (Gongyi Kerui) apparatus.

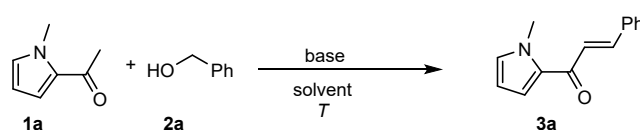
GC-MS-O analysis was carried out using an Agilent 7890B-5977A with a capillary column DB-WAX (30 m × 0.25 mm × 0.25 μm) and a sniffing port (Gerstel OP3, Germany). The analytical conditions were as follows: the oven temperature was programmed from 50°C to 280°C at a rate of 10°C/min, then held at 280°C for 5 min; carrier gas, helium; flow rate, 1.6 mL/min; electron ionization, 70 eV; ion source temperature, 230°C. The column effluent was divided (ratio 1:1) between the MSD detector and the sniffing port through one Y-shaped glass splitter. The effluent to the sniffing port was enclosed with a stream of humidified air of 16 mL/min and transferred to the glass detection cone by one length of capillary column at the temperature of 250°C. All the samples with a concentration of 5 wt.% in CH₂Cl₂, and the injection volume was 1.0 μL.

The antifungal characteristics of the target compounds were discovered using the agar well diffusion method. The medium was a mixture of filtered potato juice boiled, glucose and agar. The produced compounds were diluted in a water mixture with 20% DMSO in it. The solution of each component was added to sterilized potato dextrose agar and the final obtained concentration was 0.5 mg/mL. The mycelia of fungi were added to the test plate once the mixture had cooled, where they were cultured for 3-7

days at 25 °C. When the fungal mycelia approached the edges of the control plate, the width of the zone that inhibits bacterial growth was measured (without the additional compounds). The findings of three different investigations were averaged to get the inhibitory index.

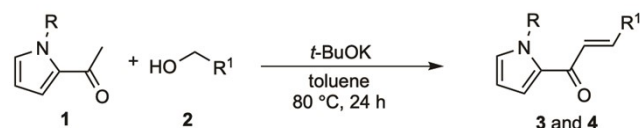
TG-DTG and differential scanning calorimeter (DSC) curves of the target compounds were detected by a simultaneous thermal analyzer (STA 449 F3, Netzsch, Germany). Every compound was preserved about 5 mg, and spectrally pure Al₂O₃ served as the standard. Each experiment was run in an air-conditioned environment at a flow rate of 60 mL min⁻¹ and heated at a rate of 10 °C min⁻¹ between 30 and 400 °C.

2. Optimization Details



Under air atmosphere, 2-acetyl-1-methylpyrrole **1a** (0.2 mmol), benzyl alcohol **2a** (2.0 equiv.) and base (1.0 equiv.) were charged into a 10 mL sealable tube equipped with a magnetic stirring bar. After the addition of toluene (1.0 mL), the resulting mixture was stirred at 80 °C for 24 h in oil bath. After cooling down, the reaction mixture was diluted with 10 mL ethyl acetate and washed with 10 mL brine. The aqueous layer was extracted twice with ethyl acetate. The combined organic phase was dried over anhydrous Na₂SO₄, filtered and concentrated in *vacuo*. The residue was purified by flash column chromatography on silica gel (eluent: petroleum ether-EtOAc) to give the pure product **3a**.

3. General procedure for the C-olefination

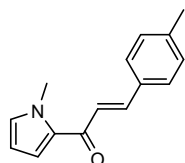


Scheme S1. Olefination of *N*-substituted-acetyl-pyrrole with alcohols

Under air atmosphere, *N*-substituted-acetyl-pyrrole **1** (0.2 mmol), corresponding alcohols **2** (0.4 mmol, 2.0 equiv.) and *t*-BuOK (0.2 mmol, 1.0 equiv.) were charged into a 10 mL sealable tube equipped with a magnetic stirring bar. After the addition of toluene (1.0 mL), the resulting mixture was stirred at 80 °C for 24 h in oil bath. After

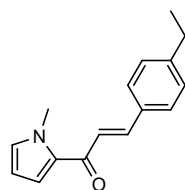
108.30, 37.83. CAS Number: 22563-50-4.

(E)-1-(1-methyl-1H-pyrrol-2-yl)-3-(p-tolyl)prop-2-en-1-one (3b)¹



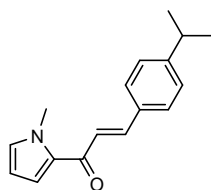
Isolated as a white solid, 39 mg, 86% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 15.6 Hz, 1H), 7.51 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 15.6 Hz, 1H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.11 (dd, *J* = 4.0, 1.4 Hz, 1H), 6.87 (s, 1H), 6.19 (dd, *J* = 4.0, 2.5 Hz, 1H), 4.03 (s, 3H), 2.38 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.93, 141.51, 140.32, 132.52, 132.08, 131.56, 129.60, 128.20, 122.63, 119.10, 108.21, 37.82, 21.49. CAS Number: 1335195-32-8.

(E)-3-(4-ethylphenyl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3c)



Isolated as a yellow liquid, 34 mg, 71% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, *J* = 15.6 Hz, 1H), 7.54 (d, *J* = 8.1 Hz, 2H), 7.37 (d, *J* = 15.6 Hz, 1H), 7.24 (t, *J* = 6.5 Hz, 2H), 7.11 (dd, *J* = 4.1, 1.6 Hz, 1H), 6.87 (s, 1H), 6.19 (dd, *J* = 4.1, 2.5 Hz, 1H), 4.03 (s, 3H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.25 (t, *J* = 7.6 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.95, 146.65, 141.54, 132.77, 132.08, 131.57, 128.41, 128.29, 122.69, 119.11, 108.21, 37.81, 28.83, 15.39. IR (KBr) ν_{\max} 3429, 3108, 2963, 2928, 1647, 1592, 1526, 1511, 987, and 736 cm⁻¹; HRMS (ESI) calcd. for C₁₆H₁₈NO: [M+H]⁺: 240.1388, found: 240.1388.

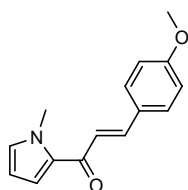
(E)-3-(4-isopropylphenyl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3d)



Isolated as a yellow liquid, 33 mg, 65% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d,

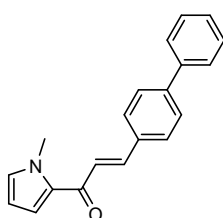
$J = 15.6$ Hz, 1H), 7.55 (d, $J = 8.2$ Hz, 2H), 7.37 (d, $J = 15.6$ Hz, 1H), 7.31 – 7.21 (m, 2H), 7.11 (dd, $J = 4.1, 1.6$ Hz, 1H), 6.87 (s, 1H), 6.19 (dd, $J = 4.1, 2.5$ Hz, 1H), 4.03 (s, 3H), 2.94 (dt, $J = 13.8, 6.9$ Hz, 1H), 1.28 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.95, 151.24, 141.53, 132.92, 132.09, 131.56, 128.31, 126.98, 122.73, 119.11, 108.21, 37.82, 34.10, 23.82. IR (KBr) ν_{max} 3419, 3116, 2959, 2926, 1648, 1593, 1526, 1064, and 735 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{17}\text{H}_{20}\text{NO}$: $[\text{M}+\text{H}]^+$: 254.1545, found: 254.1544.

(E)-3-(4-methoxyphenyl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3e)



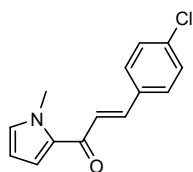
Isolated as a light yellow solid, m. p. 61 – 62 $^{\circ}\text{C}$, 40 mg, 82% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.70 (d, $J = 15.6$ Hz, 1H), 7.56 (d, $J = 8.7$ Hz, 2H), 7.29 (d, $J = 15.6$ Hz, 1H), 7.09 (dd, $J = 4.0, 1.4$ Hz, 1H), 6.92 (d, $J = 8.7$ Hz, 2H), 6.86 (s, 1H), 6.19 (dd, $J = 4.0, 2.5$ Hz, 1H), 4.02 (s, 3H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.98, 161.18, 141.23, 132.12, 131.44, 129.85, 127.99, 121.36, 118.91, 114.31, 108.16, 55.39, 37.81. IR (KBr) ν_{max} 3445, 3107, 2969, 1646, 1588, 1572, 1526, 1065, 1047, and 732 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{15}\text{H}_{16}\text{NO}_2$: $[\text{M}+\text{H}]^+$: 242.1181, found: 242.1180.

(E)-3-([1,1'-biphenyl]-4-yl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3f)



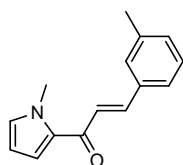
Isolated as a light yellow liquid, 26 mg, 45% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.78 (d, $J = 15.6$ Hz, 1H), 7.69 (d, $J = 8.2$ Hz, 2H), 7.66 – 7.59 (m, 4H), 7.50 – 7.41 (m, 3H), 7.37 (t, $J = 7.2$ Hz, 1H), 7.14 (d, $J = 2.9$ Hz, 1H), 6.89 (s, 1H), 6.21 (dd, $J = 3.4, 2.6$ Hz, 1H), 4.04 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.71, 142.70, 141.01, 140.32, 134.26, 132.07, 131.74, 128.90, 128.70, 127.77, 127.53, 127.06, 123.51, 119.28, 108.31, 37.85. IR (KBr) ν_{max} 3429, 2918, 1649, 1647, 1592, 1526, 1065, 987, and 740 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{18}\text{NO}$: $[\text{M}+\text{H}]^+$: 288.1388, found: 288.1387.

(E)-3-(4-chlorophenyl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3g)¹



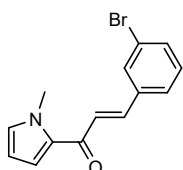
Isolated as a light yellow solid, 26 mg, 53% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.67 (d, *J* = 15.6 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 2H), 7.37 (dd, *J* = 12.0, 3.5 Hz, 3H), 7.11 (dd, *J* = 4.0, 1.4 Hz, 1H), 6.89 (s, 1H), 6.20 (dd, *J* = 4.0, 2.5 Hz, 1H), 4.03 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.36, 139.98, 135.73, 133.78, 131.92, 129.33, 129.11, 124.08, 119.41, 108.38, 37.83. CAS Number: 1335195-29-3.

(E)-1-(1-methyl-1H-pyrrol-2-yl)-3-(m-tolyl)prop-2-en-1-one (3h)¹



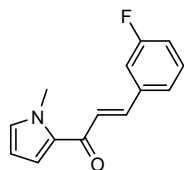
Isolated as a white solid, 34 mg, 76% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 15.6 Hz, 1H), 7.48 – 7.35 (m, 3H), 7.28 (dd, *J* = 14.9, 6.9 Hz, 1H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 2.7 Hz, 1H), 6.87 (s, 1H), 6.19 (dd, *J* = 3.8, 2.5 Hz, 1H), 4.03 (s, 3H), 2.39 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.83, 141.65, 138.49, 135.22, 132.04, 131.68, 130.80, 128.79, 128.75, 125.45, 123.42, 119.27, 108.26, 37.83, 21.38. CAS Number: 1335195-31-7.

(E)-3-(3-bromophenyl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3i)¹



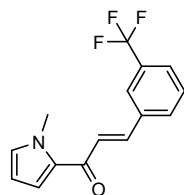
Isolated as a white solid, 36 mg, 62% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.75 (s, 1H), 7.63 (d, *J* = 15.6 Hz, 1H), 7.57 – 7.45 (m, 2H), 7.37 (d, *J* = 15.6 Hz, 1H), 7.27 (dd, *J* = 9.6, 6.1 Hz, 1H), 7.12 (d, *J* = 2.8 Hz, 1H), 6.89 (s, 1H), 6.21 (dd, *J* = 3.7, 2.5 Hz, 1H), 4.03 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.14, 139.65, 137.44, 132.64, 132.05, 131.86, 130.58, 130.36, 127.00, 124.91, 122.99, 119.63, 108.45, 37.85. CAS Number: 1610603-17-2.

(E)-3-(3-fluorophenyl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3j)



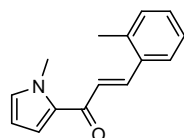
Isolated as a yellow solid, m. p. 52 – 53 °C, 23 mg, 51% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.68 (d, *J* = 15.6 Hz, 1H), 7.38 (d, *J* = 14.7 Hz, 3H), 7.31 (d, *J* = 9.6 Hz, 1H), 7.12 (d, *J* = 2.9 Hz, 1H), 7.10 – 7.02 (m, 1H), 6.89 (s, 1H), 6.26 – 6.17 (m, 1H), 4.03 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.25, 163.05 (d, *J* = 245.0 Hz), 140.01(d, *J* = 2.5Hz), 137.58(d, *J* = 7.8 Hz), 132.01, 131.88, 130.38(d, *J* = 8.2 Hz), 124.82, 124.25(d, *J* = 2.8 Hz), 119.56, 116.72(d, *J* = 21.2 Hz)114.25(d, *J* = 21.8 Hz), 108.43, 37.84. IR (KBr) ν_{\max} 3419, 3130, 2922, 1649, 1595, 1525, 1067, 988, and 748 cm⁻¹; HRMS (ESI) calcd. for C₁₄H₁₃FNO: [M+H]⁺: 230.0981, found: 230.0980.

(E)-1-(1-methyl-1H-pyrrol-2-yl)-3-(3-(trifluoromethyl)phenyl)prop-2-en-1-one (3k)



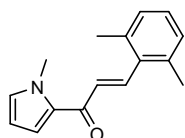
Isolated as a light yellow solid, m. p. 60 – 61 °C, 19 mg, 34% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.85 (s, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 7.6 Hz, 1H), 7.53 (t, *J* = 7.7 Hz, 1H), 7.44 (d, *J* = 15.6 Hz, 1H), 7.15 (d, *J* = 2.8 Hz, 1H), 6.91 (s, 1H), 6.28 – 6.17 (m, 1H), 4.04 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.02, 139.56, 136.10, 132.14, 131.82, 131.38(q, *J* = 32.1 Hz), 131.38, 129.39, 126.23(q, *J* = 3.7 Hz), 125.31, 124.41(q, *J* = 3.7 Hz), 123.90 (q, *J* = 270.8 Hz), 119.73, 108.49, 37.85. IR (KBr) ν_{\max} 3433, 2922, 1649, 1595, 1525, 1046, 981, 926, and 741 cm⁻¹; HRMS (ESI) calcd. for C₁₅H₁₃F₃NO: [M+H]⁺: 280.0949, found: 280.0948.

(E)-1-(1-methyl-1H-pyrrol-2-yl)-3-(o-tolyl)prop-2-en-1-one (3l) ²



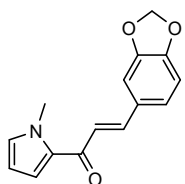
Isolated as a yellow solid, 31 mg, 69% yield; ^1H NMR (400 MHz, CDCl_3) δ 8.03 (d, $J = 15.5$ Hz, 1H), 7.66 (d, $J = 7.6$ Hz, 1H), 7.32 (d, $J = 15.5$ Hz, 1H), 7.30 – 7.19 (m, 3H), 7.11 (dd, $J = 4.0, 1.4$ Hz, 1H), 6.88 (s, 1H), 6.20 (dd, $J = 4.0, 2.5$ Hz, 1H), 4.04 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.84, 139.14, 137.99, 134.30, 132.02, 131.75, 130.81, 129.69, 126.28, 126.25, 124.75, 119.34, 108.30, 37.85, 19.88. CAS Number: 1335195-30-6.

(E)-3-(2,6-dimethylphenyl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3m)

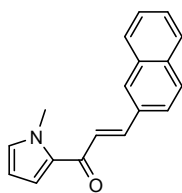


Isolated as a light yellow liquid, 19 mg, 40% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.86 (d, $J = 16.0$ Hz, 1H), 7.14 (dd, $J = 8.7, 6.0$ Hz, 1H), 7.08 (d, $J = 6.9$ Hz, 2H), 7.03 (d, $J = 16.0$ Hz, 2H), 6.89 (s, 1H), 6.18 (dd, $J = 3.9, 2.5$ Hz, 1H), 4.05 (s, 3H), 2.39 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.68, 139.93, 136.76, 135.13, 131.93, 131.82, 129.44, 128.18, 127.99, 119.46, 108.35, 37.85, 21.13. IR (KBr) ν_{max} 3429, 3130, 2924, 1648, 1602, 1526, 1065, 984, and 736 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{18}\text{NO}$: $[\text{M}+\text{H}]^+$: 240.1388, found: 240.1387.

(E)-3-(benzo[d][1,3]dioxol-5-yl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3n)³

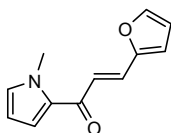


Isolated as a light yellow solid, 33 mg, 65% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.65 (d, $J = 15.5$ Hz, 1H), 7.24 (d, $J = 15.7$ Hz, 1H), 7.13 (s, 1H), 7.08 (d, $J = 5.8$ Hz, 2H), 6.86 (s, 1H), 6.83 (d, $J = 8.0$ Hz, 1H), 6.19 (s, 1H), 6.01 (s, 2H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.77, 149.35, 148.29, 141.26, 132.06, 131.54, 129.72, 124.54, 121.73, 118.99, 108.59, 108.21, 106.61, 101.51, 37.81. CAS Number: 1638512-92-1. **(E)-1-(1-methyl-1H-pyrrol-2-yl)-3-(naphthalen-2-yl)prop-2-en-1-one (3o)²**



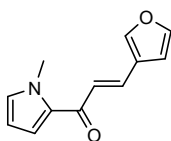
Isolated as a light yellow solid, 37 mg, 70% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.99 (s, 1H), 7.93 – 7.80 (m, 4H), 7.76 (dd, $J = 8.6, 1.4$ Hz, 1H), 7.56 – 7.46 (m, 3H), 7.16 (dd, $J = 4.1, 1.5$ Hz, 1H), 6.88 (s, 1H), 6.21 (dd, $J = 4.0, 2.5$ Hz, 1H), 4.04 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.72, 141.54, 134.14, 133.45, 132.77, 132.09, 131.76, 129.93, 128.58, 128.55, 127.79, 127.05, 126.65, 123.85, 123.81, 119.33, 108.32, 37.86. CAS Number: 1335195-34-0.

(E)-3-(furan-2-yl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3p)



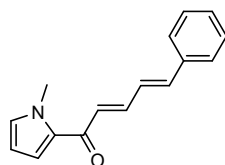
Isolated as a yellow solid, m. p. 78 – 79 °C, 32 mg, 80% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.49 (dd, $J = 8.4, 6.9$ Hz, 2H), 7.31 (d, $J = 15.4$ Hz, 1H), 7.11 (dd, $J = 4.1, 1.6$ Hz, 1H), 6.90 – 6.83 (m, 1H), 6.63 (d, $J = 3.4$ Hz, 1H), 6.48 (dd, $J = 3.4, 1.8$ Hz, 1H), 6.19 (dd, $J = 4.1, 2.5$ Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.44, 151.95, 144.27, 132.06, 131.66, 127.76, 121.41, 119.30, 114.76, 112.40, 108.29, 37.80. IR (KBr) ν_{max} 3429, 3124, 2924, 1648, 1592, 1549, 1524, 987, and 726 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{12}\text{H}_{12}\text{NO}_2$: $[\text{M}+\text{H}]^+$: 202.0868, found: 202.0867.

(E)-3-(furan-3-yl)-1-(1-methyl-1H-pyrrol-2-yl)prop-2-en-1-one (3q)



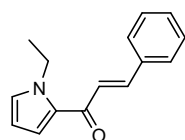
Isolated as a yellow solid, m. p. 53 – 54 °C, 16 mg, 40% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.69 (s, 1H), 7.62 (d, $J = 15.5$ Hz, 1H), 7.45 (s, 1H), 7.12 (d, $J = 15.5$ Hz, 1H), 7.07 (dd, $J = 4.1, 1.5$ Hz, 1H), 6.86 (s, 1H), 6.68 (s, 1H), 6.18 (dd, $J = 4.0, 2.5$ Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.73, 144.73, 144.25, 131.88, 131.57, 131.36, 123.53, 123.27, 119.06, 108.20, 107.58, 37.78. IR (KBr) ν_{max} 3420, 3126, 2923, 1652, 1598, 1557, 1526, 993, and 740 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{12}\text{H}_{12}\text{NO}_2$: $[\text{M}+\text{H}]^+$: 202.0868, found: 202.0867.

(2E, 4E)-1-(1-methyl-1H-pyrrol-2-yl)-5-phenylpenta-2,4-dien-1-one (3r) ²



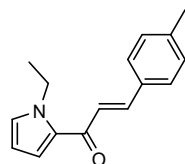
Isolated as a yellow solid, 21 mg, 45% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.58 – 7.51 (m, 1H), 7.51 – 7.46 (m, 2H), 7.36 (t, *J* = 7.4 Hz, 2H), 7.33 – 7.27 (m, 1H), 7.04 (dd, *J* = 4.0, 1.5 Hz, 1H), 7.01 – 6.91 (m, 2H), 6.86 (s, 1H), 6.18 (dd, *J* = 4.0, 2.5 Hz, 1H), 4.02 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.92, 141.47, 140.27, 136.42, 132.08, 131.55, 128.85, 128.80, 127.22, 127.12, 119.03, 108.22, 37.79. CAS Number: 1634692-31-1.

(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-phenylprop-2-en-1-one (4a)



Isolated as a light yellow liquid, 34 mg, 76% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, *J* = 15.6 Hz, 1H), 7.61 (d, *J* = 6.4 Hz, 2H), 7.40 (dd, *J* = 18.4, 10.8 Hz, 4H), 7.14 (d, *J* = 2.8 Hz, 1H), 6.95 (s, 1H), 6.28 – 6.15 (m, 1H), 4.47 (q, *J* = 7.1 Hz, 2H), 1.42 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.30, 141.35, 135.33, 131.19, 130.25, 129.88, 128.86, 128.17, 123.83, 119.82, 108.49, 44.97, 16.99. IR (KBr) ν_{\max} 3434, 2924, 2853, 1647, 1593, 1523, 1495, 1050, and 734 cm⁻¹; HRMS (ESI) calcd. for C₁₅H₁₆NO: [M+H]⁺: 226.1232, found: 226.1231.

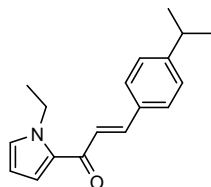
(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(p-tolyl)prop-2-en-1-one (4b)



Isolated as a light yellow liquid, 46 mg, 96% yield; ¹H NMR (400 MHz, CDCl₃) δ 7.71 (d, *J* = 15.6 Hz, 1H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.38 (d, *J* = 15.6 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.13 (dd, *J* = 4.1, 1.6 Hz, 1H), 6.99 – 6.92 (m, 1H), 6.21 (dd, *J* = 4.1, 2.5 Hz, 1H), 4.47 (q, *J* = 7.1 Hz, 2H), 2.38 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 179.49, 141.39, 140.26, 132.57, 131.25, 130.07, 129.59, 128.17,

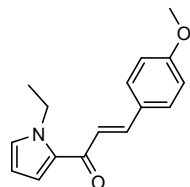
122.83, 119.62, 108.40, 44.94, 21.49, 17.00. IR (KBr) ν_{\max} 3436, 2971, 1648, 1592, 1524, 1512, 1074, 1052, and 729 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{18}\text{NO}$: $[\text{M}+\text{H}]^+$: 240.1388, found: 240.1388.

(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(4-isopropylphenyl)prop-2-en-1-one (4c)



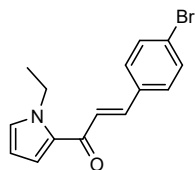
Isolated as a yellow liquid, 48 mg, 90% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.72 (d, $J = 15.6$ Hz, 1H), 7.55 (d, $J = 8.0$ Hz, 2H), 7.38 (d, $J = 15.6$ Hz, 1H), 7.26 (d, $J = 7.6$ Hz, 2H), 7.13 (d, $J = 2.7$ Hz, 1H), 6.95 (s, 1H), 6.27 – 6.17 (m, 1H), 4.47 (q, $J = 7.1$ Hz, 2H), 2.94 (dt, $J = 13.8, 7.0$ Hz, 1H), 1.43 (t, $J = 7.1$ Hz, 3H), 1.27 (d, $J = 6.8$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.51, 151.18, 141.40, 132.97, 131.26, 130.07, 128.28, 127.15, 126.97, 122.93, 119.61, 108.40, 44.94, 34.10, 23.82, 17.00. IR (KBr) ν_{\max} 3429, 3107, 2960, 2930, 2869, 1648, 1594, 1565, 1524, 1049, and 736 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{18}\text{H}_{22}\text{NO}$: $[\text{M}+\text{H}]^+$: 268.1701, found: 268.1700.

(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(4-methoxyphenyl)prop-2-en-1-one (4d)



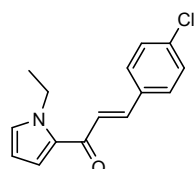
Isolated as a light yellow solid, m. p. 64 – 65 $^{\circ}\text{C}$, 45 mg, 88% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.70 (d, $J = 15.6$ Hz, 1H), 7.57 (d, $J = 8.7$ Hz, 2H), 7.31 (d, $J = 15.6$ Hz, 1H), 7.12 (dd, $J = 4.1, 1.6$ Hz, 1H), 6.93 (dd, $J = 8.9, 5.5$ Hz, 3H), 6.20 (dd, $J = 4.0, 2.5$ Hz, 1H), 4.47 (q, $J = 7.1$ Hz, 2H), 3.84 (s, 3H), 1.42 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.55, 161.14, 141.10, 131.29, 129.93, 129.81, 128.05, 121.57, 119.40, 114.30, 108.34, 55.38, 44.93, 17.01. IR (KBr) ν_{\max} 3435, 2930, 1645, 1588, 1572, 1524, 1510, 1051, and 733 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{18}\text{NO}_2$: $[\text{M}+\text{H}]^+$: 256.1338, found: 256.1337.

(E)-3-(4-bromophenyl)-1-(1-ethyl-1H-pyrrol-2-yl)prop-2-en-1-one (4e)



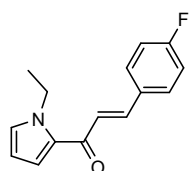
Isolated as a yellow solid, m. p. 63 – 64 °C, 37 mg, 61% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.65 (d, $J = 15.6$ Hz, 1H), 7.53 (d, $J = 8.5$ Hz, 2H), 7.47 (d, $J = 8.5$ Hz, 2H), 7.39 (d, $J = 15.6$ Hz, 1H), 7.13 (dd, $J = 4.1, 1.5$ Hz, 1H), 7.01 – 6.95 (m, 1H), 6.21 (dd, $J = 4.1, 2.5$ Hz, 1H), 4.46 (q, $J = 7.1$ Hz, 2H), 1.42 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.88, 139.92, 134.26, 132.07, 131.72, 131.47, 131.08, 130.46, 129.93, 129.55, 124.38, 123.99, 119.97, 108.59, 44.99, 16.96. IR (KBr) ν_{max} 3429, 3119, 2924, 1647, 1595, 1523, 1050, 951, and 738 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{15}\text{H}_{15}\text{BrNO}$: $[\text{M}+\text{H}]^+$: 304.0337, found: 304.0336.

(E)-3-(4-chlorophenyl)-1-(1-ethyl-1H-pyrrol-2-yl)prop-2-en-1-one (4f)



Isolated as a yellow solid, m. p. 53 – 54 °C, 49 mg, 95% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.67 (d, $J = 15.6$ Hz, 1H), 7.54 (d, $J = 8.4$ Hz, 2H), 7.38 (dd, $J = 12.0, 4.8$ Hz, 3H), 7.13 (dd, $J = 4.0, 1.5$ Hz, 1H), 7.00 – 6.94 (m, 1H), 6.22 (dd, $J = 4.0, 2.5$ Hz, 1H), 4.47 (q, $J = 7.1$ Hz, 2H), 1.42 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.89, 139.85, 135.66, 133.82, 131.08, 130.44, 129.31, 129.11, 124.28, 119.95, 108.58, 44.99, 16.97. IR (KBr) ν_{max} 3414, 3125, 1647, 1617, 1593, 1523, 1075, 1055, and 779 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{15}\text{H}_{15}\text{ClNO}$: $[\text{M}+\text{H}]^+$: 260.0842, found: 260.0840.

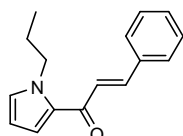
(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(4-fluorophenyl)prop-2-en-1-one (4g)



Isolated as a yellow liquid, 48 mg, 98% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.69 (d, $J = 15.6$ Hz, 1H), 7.59 (dd, $J = 8.0, 5.7$ Hz, 2H), 7.34 (d, $J = 15.6$ Hz, 1H), 7.12 (d, J

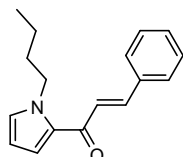
= 2.9 Hz, 1H), 7.08 (t, $J = 8.5$ Hz, 2H), 6.96 (s, 1H), 6.22 (d, $J = 2.6$ Hz, 1H), 4.46 (q, $J = 7.1$ Hz, 2H), 1.42 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.06, 163.57(d, $J = 249.1$ Hz), 140.04, 131.55(d, $J = 3.2$ Hz), 131.10, 130.32, 130.01(d, $J = 8.5$ Hz), 123.54(d, $J = 2.2$ Hz), 119.81, 115.95(d, $J = 21.8$ Hz), 108.52, 44.97, 16.97. IR (KBr) ν_{max} 3435, 2930, 1649, 1589, 1587, 1524, 1508, 996, and 731 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{15}\text{H}_{15}\text{FNO}$: $[\text{M}+\text{H}]^+$: 244.1138, found: 244.1137.

(E)-3-phenyl-1-(1-propyl-1H-pyrrol-2-yl)prop-2-en-1-one (4h)



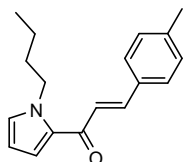
Isolated as a yellow liquid, 35 mg, 74% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, $J = 15.6$ Hz, 1H), 7.61 (d, $J = 6.4$ Hz, 2H), 7.48 – 7.34 (m, 4H), 7.14 (d, $J = 2.7$ Hz, 1H), 6.94 (s, 1H), 6.20 (s, 1H), 4.38 (t, $J = 7.1$ Hz, 2H), 1.82 (dd, $J = 14.5, 7.2$ Hz, 2H), 0.93 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.35, 141.32, 135.33, 131.27, 131.13, 129.87, 128.85, 128.16, 123.85, 119.85, 108.22, 51.67, 24.81, 11.10. IR (KBr) ν_{max} 3419, 2963, 2927, 1648, 1595, 1524, 1053, 984, and 737 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{18}\text{NO}$: $[\text{M}+\text{H}]^+$: 240.1388, found: 240.1387.

(E)-1-(1-butyl-1H-pyrrol-2-yl)-3-phenylprop-2-en-1-one (4i)



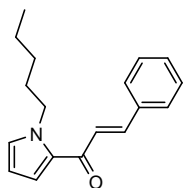
Isolated as a yellow liquid, 40 mg, 80% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, $J = 15.6$ Hz, 1H), 7.65 – 7.57 (m, 2H), 7.46 – 7.35 (m, 4H), 7.14 (dd, $J = 4.0, 1.4$ Hz, 1H), 6.93 (s, 1H), 6.20 (dd, $J = 3.9, 2.5$ Hz, 1H), 4.41 (t, $J = 7.3$ Hz, 2H), 1.85 – 1.73 (m, 2H), 1.35 (dd, $J = 15.2, 7.5$ Hz, 2H), 0.94 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.33, 141.32, 135.34, 131.27, 131.04, 129.87, 128.85, 128.46, 128.41, 128.16, 123.85, 119.83, 108.26, 49.87, 33.69, 19.88, 13.77. IR (KBr) ν_{max} 3434, 2957, 2871, 1648, 1595, 1524, 1495, 977, and 737 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{17}\text{H}_{20}\text{NO}$: $[\text{M}+\text{H}]^+$: 254.1545, found: 254.1546.

(E)-1-(1-butyl-1H-pyrrol-2-yl)-3-(p-tolyl)prop-2-en-1-one (4j)



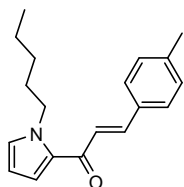
Isolated as a light yellow liquid, 43 mg, 81% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.71 (d, $J = 15.6$ Hz, 1H), 7.51 (d, $J = 8.1$ Hz, 2H), 7.38 (d, $J = 15.6$ Hz, 1H), 7.20 (d, $J = 7.9$ Hz, 2H), 7.13 (dd, $J = 4.1, 1.6$ Hz, 1H), 6.94 – 6.90 (m, 1H), 6.19 (dd, $J = 4.1, 2.5$ Hz, 1H), 4.41 (t, $J = 7.3$ Hz, 2H), 2.38 (s, 3H), 1.78 (dd, $J = 14.9, 7.4$ Hz, 2H), 1.35 (dq, $J = 14.8, 7.4$ Hz, 2H), 0.94 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.53, 141.36, 140.25, 132.58, 131.33, 130.88, 129.59, 128.17, 122.86, 119.65, 108.18, 49.85, 33.70, 21.49, 19.88, 13.77. IR (KBr) ν_{max} 3445, 3106, 2956, 2871, 1647, 1592, 1523, 1083, 1052, 979, and 728 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{18}\text{H}_{22}\text{NO}$: $[\text{M}+\text{H}]^+$: 268.1701, found: 268.1701.

(E)-1-(1-pentyl-1H-pyrrol-2-yl)-3-phenylprop-2-en-1-one (4k)



Isolated as a light yellow liquid, 44 mg, 82% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, $J = 15.6$ Hz, 1H), 7.61 (dd, $J = 7.6, 1.7$ Hz, 2H), 7.46 – 7.33 (m, 4H), 7.14 (dd, $J = 4.1, 1.6$ Hz, 1H), 6.96 – 6.91 (m, 1H), 6.20 (dd, $J = 4.1, 2.5$ Hz, 1H), 4.47 – 4.35 (m, 2H), 1.88 – 1.77 (m, 2H), 1.42 – 1.27 (m, 4H), 0.89 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.33, 141.30, 135.34, 131.25, 131.02, 129.87, 128.85, 128.16, 123.86, 119.81, 108.26, 50.10, 31.35, 28.86, 22.39, 14.04. IR (KBr) ν_{max} 3429, 3107, 2954, 2928, 2858, 1648, 1594, 1523, 1495, and 736 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{18}\text{H}_{22}\text{NO}$: $[\text{M}+\text{H}]^+$: 268.1701, found: 268.1700.

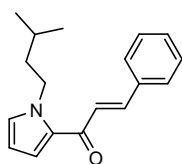
(E)-1-(1-pentyl-1H-pyrrol-2-yl)-3-(p-tolyl)prop-2-en-1-one (4l)



Isolated as a light yellow liquid, 45 mg, 80% yield; ^1H NMR (400 MHz, CDCl_3) δ

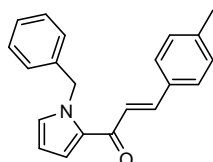
7.71 (d, $J = 15.6$ Hz, 1H), 7.51 (d, $J = 7.8$ Hz, 2H), 7.38 (d, $J = 15.6$ Hz, 1H), 7.20 (d, $J = 7.7$ Hz, 2H), 7.13 (d, $J = 2.9$ Hz, 1H), 6.92 (s, 1H), 6.19 (s, 1H), 4.40 (t, $J = 7.2$ Hz, 2H), 2.38 (s, 3H), 1.88 – 1.75 (m, 2H), 1.32 (s, 4H), 0.89 (t, $J = 6.7$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.53, 141.35, 140.24, 132.58, 131.31, 130.86, 129.59, 128.16, 122.86, 119.63, 108.17, 50.08, 31.36, 28.86, 22.39, 21.48, 14.04. IR (KBr) ν_{max} 3434, 2954, 2925, 2857, 1647, 1592, 1053, 805, and 727 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{24}\text{NO}$: $[\text{M}+\text{H}]^+$: 282.1858, found: 282.1857.

(E)-1-(1-isopentyl-1H-pyrrol-2-yl)-3-phenylprop-2-en-1-one (4m)



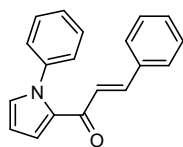
Isolated as a light yellow liquid, 38 mg, 72% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, $J = 15.6$ Hz, 1H), 7.61 (d, $J = 6.4$ Hz, 2H), 7.50 – 7.33 (m, 4H), 7.13 (d, $J = 2.8$ Hz, 1H), 6.94 (s, 1H), 6.27 – 6.16 (m, 1H), 4.50 – 4.37 (m, 2H), 1.69 (dd, $J = 14.2$, 6.6 Hz, 2H), 1.67 – 1.60 (m, 1H), 0.97 (d, $J = 6.2$ Hz, 7H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.32, 141.30, 135.34, 131.25, 130.83, 129.87, 128.85, 128.15, 123.86, 119.81, 108.35, 48.48, 40.55, 25.85, 22.52. IR (KBr) ν_{max} 3428, 2955, 2925, 1648, 1595, 1524, 1083, 1053, 974, and 734 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{18}\text{H}_{23}\text{NO}$: $[\text{M}+\text{H}]^+$: 268.1701, found: 268.1700.

(E)-1-(1-benzyl-1H-pyrrol-2-yl)-3-(p-tolyl)prop-2-en-1-one (4n)



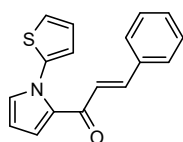
Isolated as a white solid, m. p. 132 – 133 $^{\circ}\text{C}$, 35 mg, 58% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.68 (d, $J = 15.6$ Hz, 1H), 7.49 (d, $J = 8.0$ Hz, 2H), 7.36 (d, $J = 15.6$ Hz, 1H), 7.30 (t, $J = 7.3$ Hz, 2H), 7.24 (d, $J = 7.2$ Hz, 1H), 7.22 – 7.11 (m, 5H), 6.96 (s, 1H), 6.26 (dd, $J = 3.9$, 2.6 Hz, 1H), 5.70 (s, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.74, 141.70, 140.34, 138.39, 132.49, 131.62, 131.06, 129.60, 128.63, 128.20, 127.40, 127.06, 122.63, 119.75, 108.87, 52.72, 21.49. IR (KBr) ν_{max} 3435, 3025, 2918, 1650, 1591, 1089, 1059, 992, 813, and 718 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{21}\text{H}_{20}\text{NO}$: $[\text{M}+\text{H}]^+$: 302.1545, found: 302.1544.

(E)-3-phenyl-1-(1-phenyl-1H-pyrrol-2-yl)prop-2-en-1-one (4o)



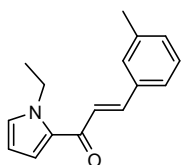
Isolated as a yellow liquid, 22 mg, 40% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.67 (d, $J = 15.7$ Hz, 1H), 7.56 (dd, $J = 7.0, 2.1$ Hz, 2H), 7.48 – 7.42 (m, 2H), 7.42 – 7.34 (m, 5H), 7.34 – 7.29 (m, 2H), 7.28 – 7.22 (m, 1H), 7.07 – 7.01 (m, 1H), 6.37 (dd, $J = 3.8, 2.7$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.84, 142.15, 140.99, 135.17, 132.73, 131.64, 130.04, 128.86, 128.73, 128.23, 127.71, 126.08, 123.44, 120.00, 109.58. IR (KBr) ν_{max} 3420, 2920, 2850, 1651, 1600, 1574, 1524, 762, and 740 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{16}\text{NO}$: $[\text{M}+\text{H}]^+$: 274.1232, found: 274.1231.

(E)-3-phenyl-1-(1-(thiophen-2-yl)-1H-pyrrol-2-yl)prop-2-en-1-one (4p)



Isolated as a yellow liquid, 22 mg, 39% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.70 (d, $J = 15.6$ Hz, 1H), 7.56 (dd, $J = 6.5, 2.9$ Hz, 2H), 7.38 (dd, $J = 5.0, 1.8$ Hz, 3H), 7.34 (d, $J = 15.6$ Hz, 1H), 7.28 – 7.24 (m, 1H), 7.22 (dd, $J = 4.0, 1.5$ Hz, 1H), 7.07 (dd, $J = 2.4, 1.7$ Hz, 1H), 7.04 – 6.93 (m, 2H), 6.37 (dd, $J = 3.9, 2.7$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.66, 142.43, 142.30, 135.09, 133.98, 132.99, 130.12, 128.87, 128.27, 125.21, 123.88, 123.76, 123.07, 119.95, 109.88. IR (KBr) ν_{max} 3426, 3124, 2875, 2712, 2563, 1698, 1587, 1502, and 845 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{17}\text{H}_{14}\text{NOS}$: $[\text{M}+\text{H}]^+$: 280.0796, found: 280.0795.

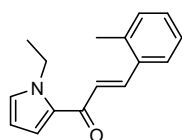
(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(m-tolyl)prop-2-en-1-one (4q)



Isolated as a light yellow liquid, 41 mg, 85% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.68 (s, 1H), 7.47 – 7.35 (m, 3H), 7.29 (t, $J = 7.9$ Hz, 1H), 7.19 (d, $J = 7.5$ Hz, 1H), 7.14 (dd, $J = 4.1, 1.6$ Hz, 1H), 7.00 – 6.89 (m, 1H), 6.21 (dd, $J = 4.0, 2.5$ Hz, 1H),

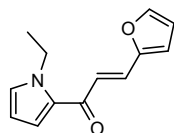
4.47 (q, $J = 7.1$ Hz, 2H), 2.39 (s, 3H), 1.42 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.39, 141.53, 138.48, 135.28, 131.23, 130.76, 130.18, 128.75, 125.44, 123.64, 119.78, 108.45, 44.95, 21.38, 17.00. IR (KBr) ν_{max} 3436, 2903, 132, 1567, 1543, 1513, 1065, 1021, and 735 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{18}\text{NO}$: $[\text{M}+\text{H}]^+$: 240.1388, found: 240.1387.

(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(o-tolyl)prop-2-en-1-one (4r)



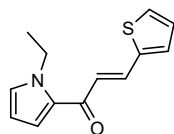
Isolated as a light yellow liquid, 38 mg, 80% yield; ^1H NMR (400 MHz, CDCl_3) δ 8.03 (d, $J = 15.5$ Hz, 1H), 7.66 (d, $J = 6.9$ Hz, 1H), 7.34 (d, $J = 15.5$ Hz, 1H), 7.24 (tt, $J = 9.7, 6.6$ Hz, 3H), 7.13 (dd, $J = 4.0, 1.5$ Hz, 1H), 6.99 – 6.90 (m, 1H), 6.25 – 6.16 (m, 1H), 4.47 (q, $J = 7.1$ Hz, 2H), 2.47 (s, 3H), 1.43 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.37, 138.99, 137.98, 134.35, 131.22, 130.82, 130.28, 129.66, 126.26, 124.95, 119.86, 108.52, 44.98, 19.91, 17.04. IR (KBr) ν_{max} 3436, 2843, 1675, 1564, 1513, 1501, 1032, 1011 and 754 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{16}\text{H}_{18}\text{NO}$: $[\text{M}+\text{H}]^+$: 240.1388, found: 240.1387.

(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(furan-2-yl)prop-2-en-1-one (4s)



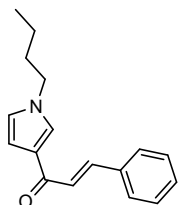
Isolated as a yellow liquid, 33 mg, 76% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.49 (dd, $J = 8.1, 7.2$ Hz, 2H), 7.33 (d, $J = 15.4$ Hz, 1H), 7.13 (dd, $J = 4.0, 1.5$ Hz, 1H), 6.98 – 6.90 (m, 1H), 6.63 (d, $J = 3.3$ Hz, 1H), 6.48 (dd, $J = 3.3, 1.8$ Hz, 1H), 6.20 (dd, $J = 4.0, 2.5$ Hz, 1H), 4.46 (q, $J = 7.1$ Hz, 2H), 1.41 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 179.00, 152.00, 144.22, 131.24, 130.14, 127.66, 121.64, 119.81, 114.65, 112.38, 108.48, 44.91, 16.97. IR (KBr) ν_{max} 3429, 3117, 2930, 1650, 1595, 1554, 1523, 1051, and 743 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{13}\text{H}_{14}\text{NO}_2$: $[\text{M}+\text{H}]^+$: 216.1025, found: 216.1024.

(E)-1-(1-ethyl-1H-pyrrol-2-yl)-3-(thiophen-2-yl)prop-2-en-1-one (4t)



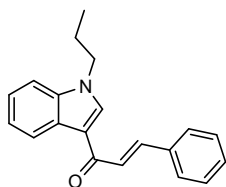
Isolated as a light yellow solid, m. p. 54 – 55 °C, 38 mg, 82% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.84 (d, $J = 15.3$ Hz, 1H), 7.35 (d, $J = 4.7$ Hz, 1H), 7.29 (d, $J = 2.7$ Hz, 1H), 7.22 (d, $J = 15.3$ Hz, 1H), 7.11 (d, $J = 2.7$ Hz, 1H), 7.09 – 6.99 (m, 1H), 6.95 (s, 1H), 6.20 (s, 1H), 4.46 (q, $J = 7.0$ Hz, 2H), 1.41 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 178.85, 140.77, 133.83, 131.09, 130.89, 130.20, 128.14, 127.72, 122.90, 119.72, 108.49, 44.93, 16.98. IR (KBr) ν_{max} 3429, 3104, 2981, 2930, 1641, 1585, 1524, 1051, and 740 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{13}\text{H}_{14}\text{NOS}$: $[\text{M}+\text{H}]^+$: 232.0796, found: 232.0795.

(E)-1-(1-butyl-1H-pyrrol-3-yl)-3-phenylprop-2-en-1-one (4u)



Isolated as a yellow liquid, 23 mg, 46% yield; ^1H NMR (400 MHz, CDCl_3) δ 7.76 (d, $J = 15.7$ Hz, 1H), 7.62 (d, $J = 6.4$ Hz, 2H), 7.40 (dd, $J = 15.9, 8.9$ Hz, 4H), 7.28 (d, $J = 16.3$ Hz, 1H), 6.73 (s, 1H), 6.67 (s, 1H), 3.92 (t, $J = 7.1$ Hz, 2H), 1.80 (dt, $J = 14.8, 7.2$ Hz, 2H), 1.34 (dq, $J = 14.7, 7.4$ Hz, 2H), 0.95 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 184.55, 141.56, 135.41, 129.85, 128.82, 128.18, 126.40, 126.06, 123.75, 122.44, 109.50, 50.01, 33.18, 19.80, 13.58. IR (KBr) ν_{max} 3420, 2958, 2928, 2872, 1651, 1593, 1527, 765 and 738 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{17}\text{H}_{20}\text{NO}$: $[\text{M}+\text{H}]^+$: 254.1545, found: 254.1544.

(E)-3-phenyl-1-(1-propyl-1H-indol-3-yl)prop-2-en-1-one (4v)



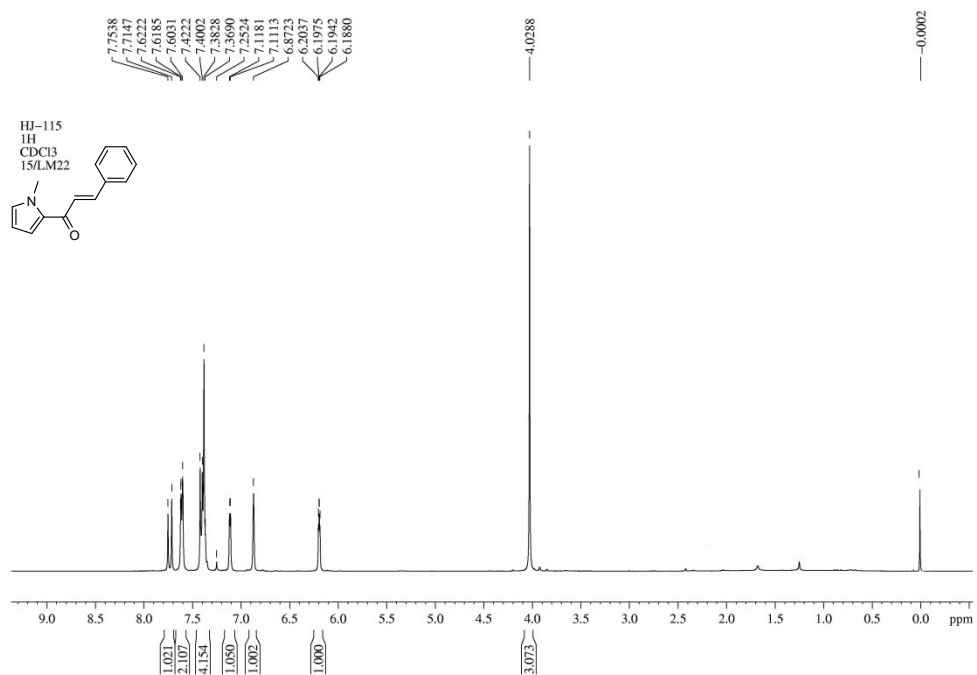
Isolated as a light yellow solid, m. p. 101 – 102 °C, 32 mg, 55% yield; ^1H NMR (400 MHz, CDCl_3) δ 8.59 – 8.49 (m, 1H), 7.89 (s, 1H), 7.82 (d, $J = 15.6$ Hz, 1H), 7.65 (d, J

= 6.6 Hz, 2H), 7.45 – 7.35 (m, 5H), 7.35 – 7.27 (m, 2H), 4.15 (t, $J = 7.1$ Hz, 2H), 2.02– 1.90 (m, 2H), 0.98 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 184.34, 140.95, 136.95, 135.42, 134.49, 129.75, 128.80, 128.10, 126.96, 123.96, 123.48, 123.09, 122.59, 117.57, 109.87, 48.82, 23.19, 11.41, 0.99. IR (KBr) ν_{max} 3012,2993,2890,2811,1645,1623,1566,1501,801, and 784 cm^{-1} ; HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{20}\text{NO}$: $[\text{M}+\text{H}]^+$: 290.1545, found: 290.1544.

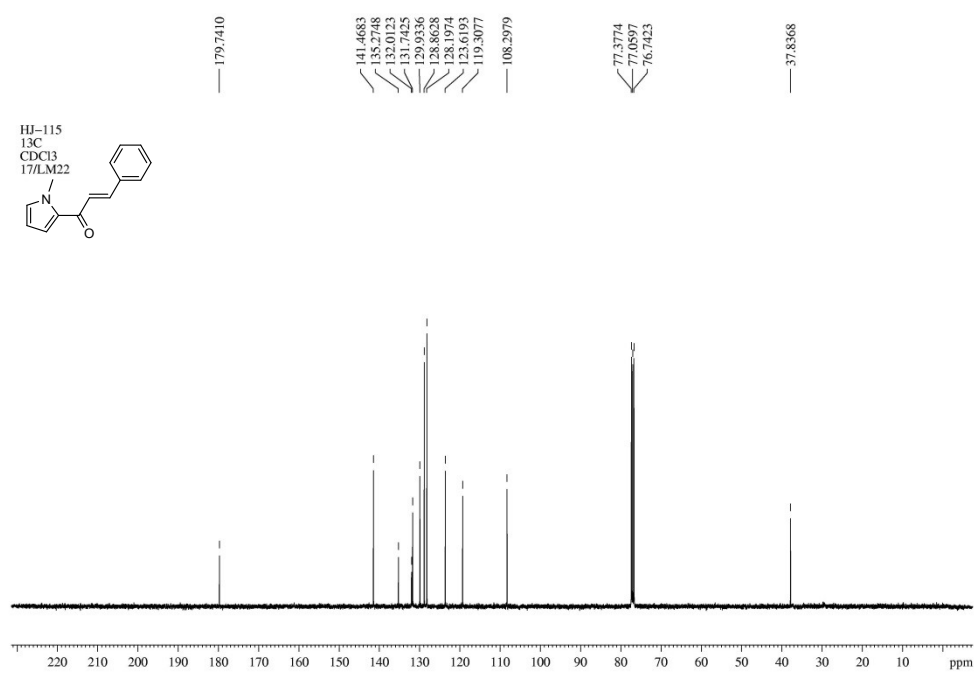
5. References

1. Thirunarayanan, G.; Vanangamudi, G.; Subramanian, M. Solvent free synthesis, spectral linearity, antimicrobial, antioxidant and insect antifeedant activities of some 1-methyl-2-pyrrolyl chalcones. *Org. Chem. An Indian J.*, **2013**, *9*, 1-16.
2. Zsolt, R.; Tamás, S.; György, K.; Áron, S.; László, D.; Péter, B. Enantioselective synthesis of heteroaromatic epoxyketones under phase-transfer catalysis using d-glucose- and d-mannose-based crown ethers. *Tetrahedron: Asymmetry*, **2011**, *22*, 1189–1196.
3. Udo, B.; B, J. E.; Ingemar, N.; Marie, B. Parallel solution phase synthesis of N-substituted 2-pyrazoline libraries. *Tetrahedron Lett.*, **2000**, *41*, 2713–2717.

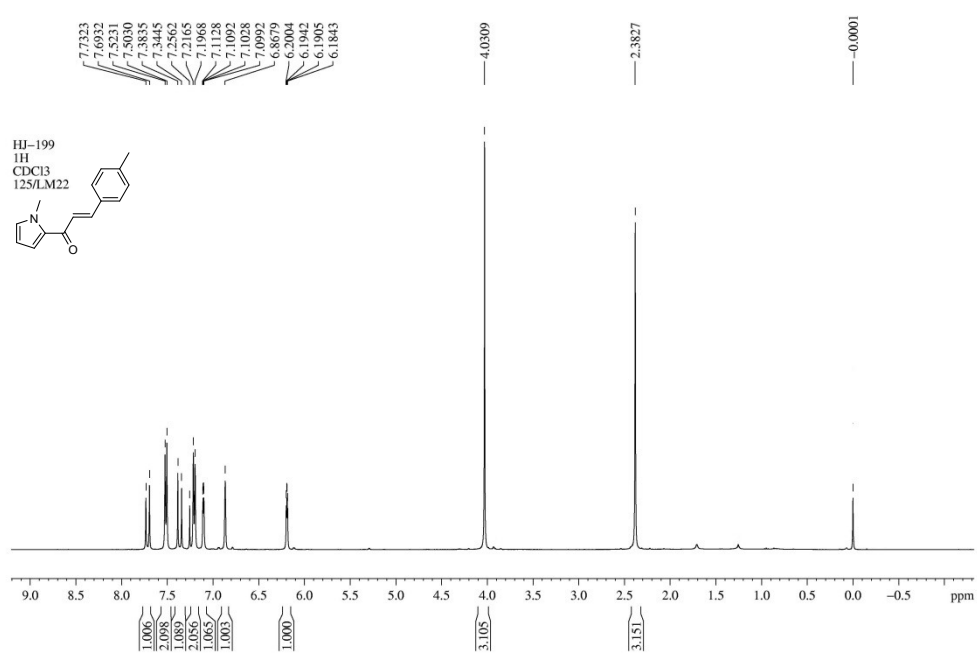
6. Copy of ¹H and ¹³C NMR Spectra



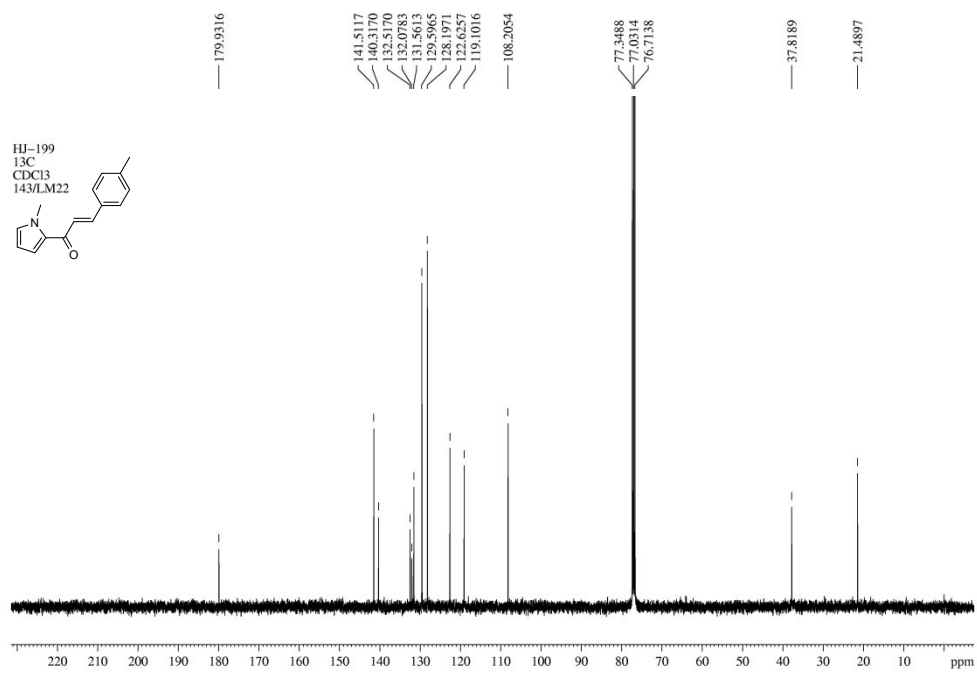
¹H NMR spectrum of compound 3a



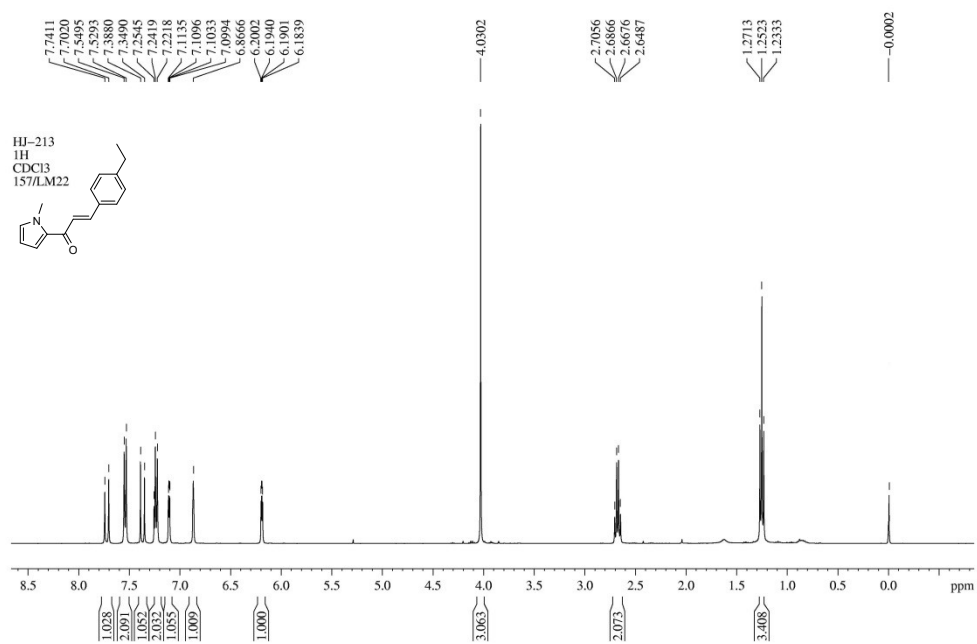
¹³C NMR spectrum of compound **3a**



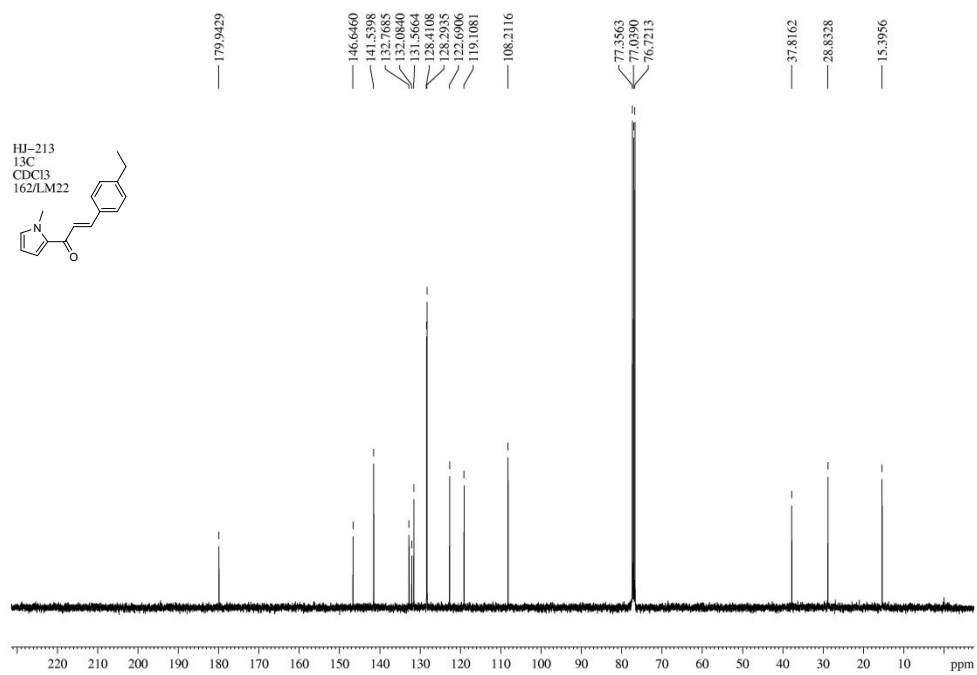
¹H NMR spectrum of compound **3b**



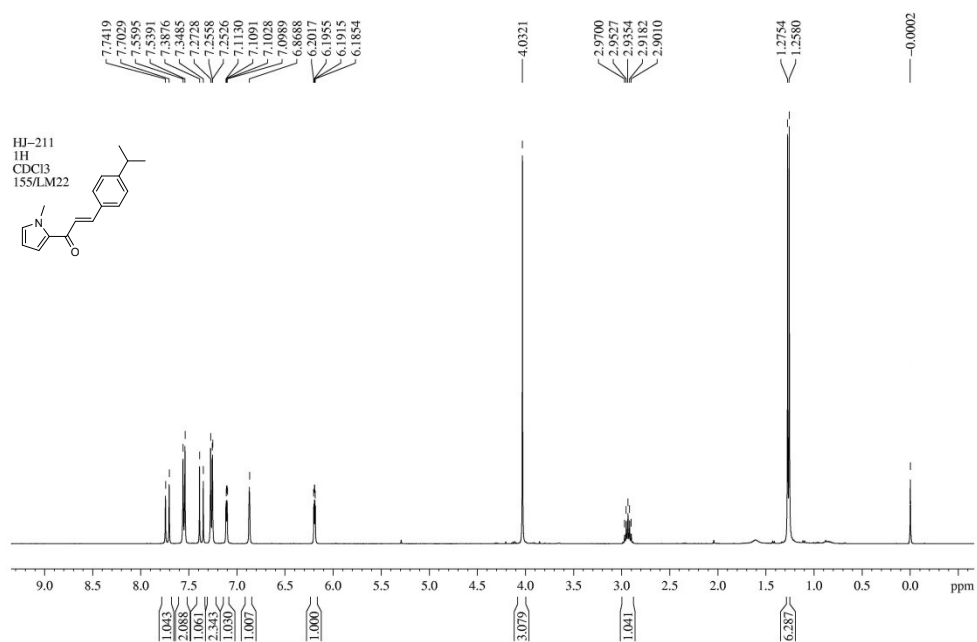
¹³C NMR spectrum of compound **3b**



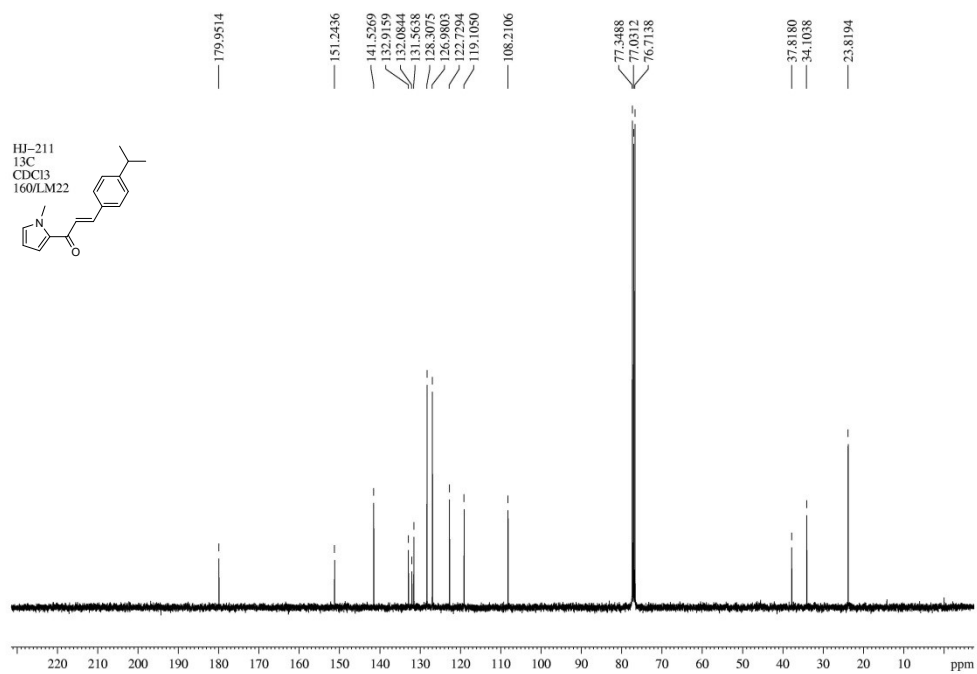
¹H NMR spectrum of compound **3c**



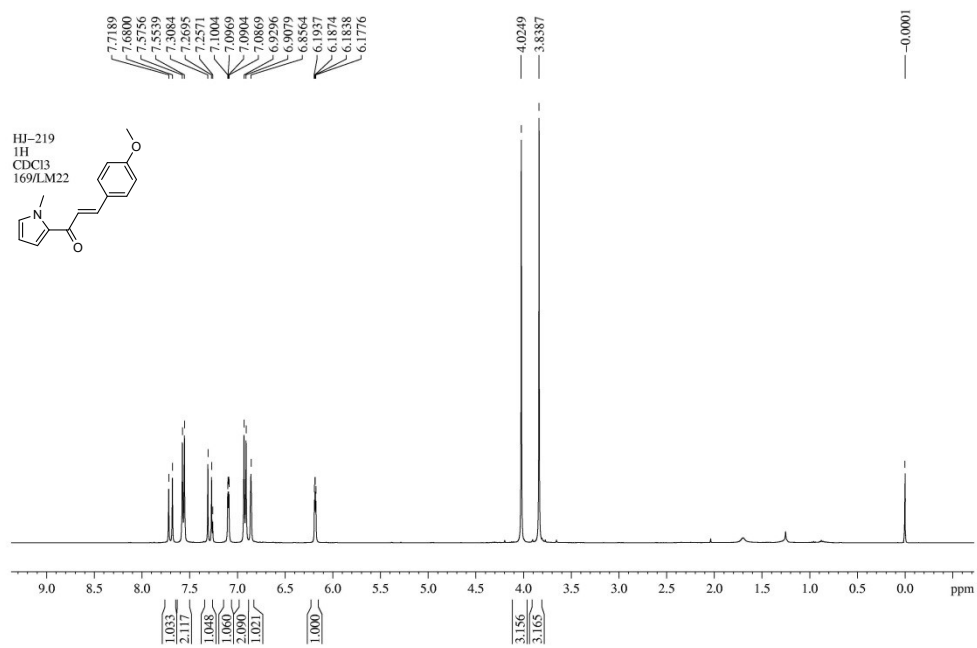
^{13}C NMR spectrum of compound **3c**



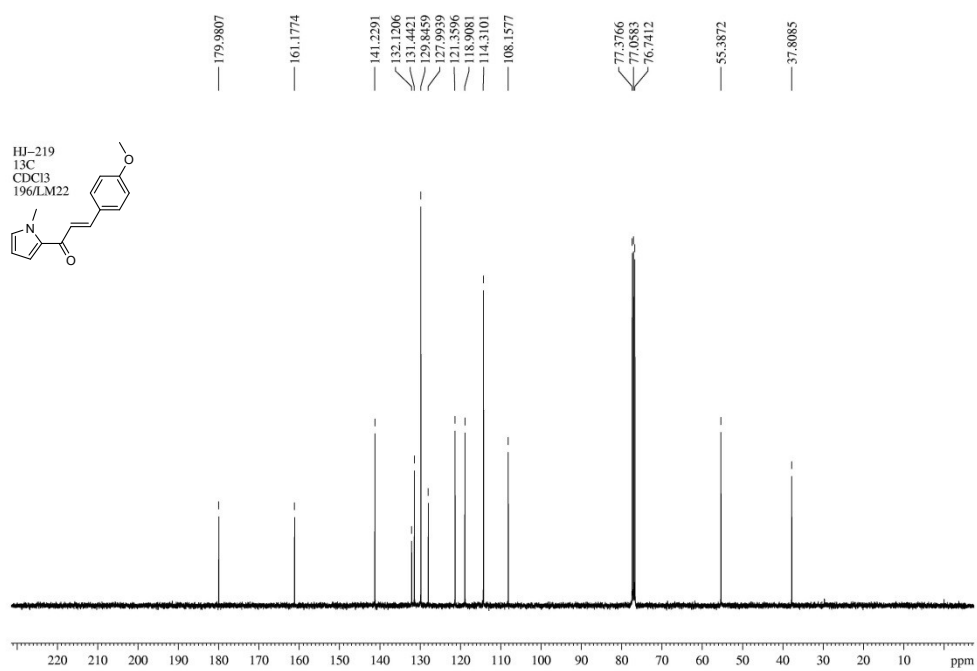
¹H NMR spectrum of compound **3d**



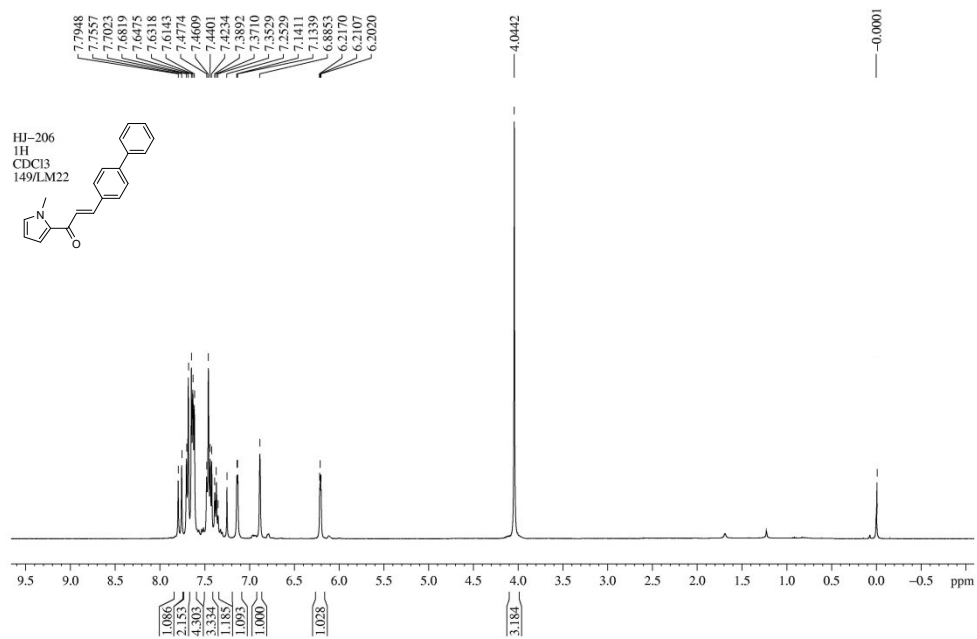
¹³C NMR spectrum of compound **3d**



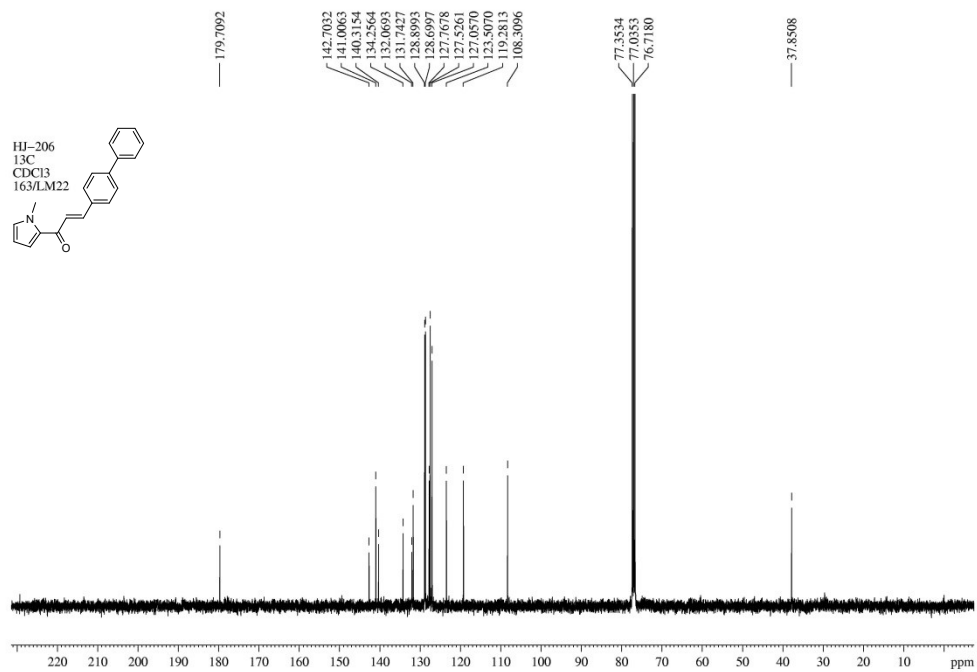
¹H NMR spectrum of compound **3e**



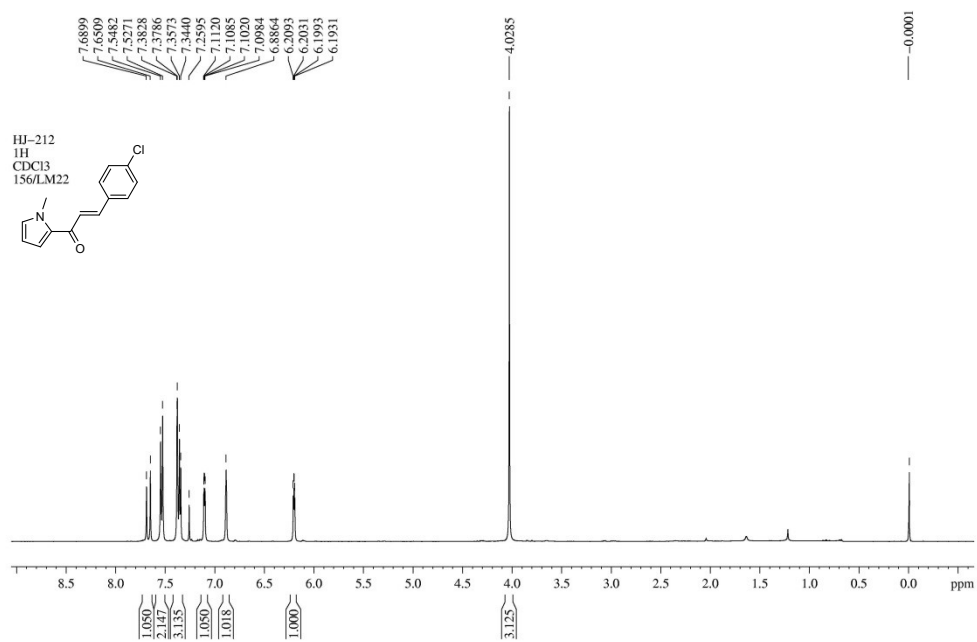
¹³C NMR spectrum of compound **3e**



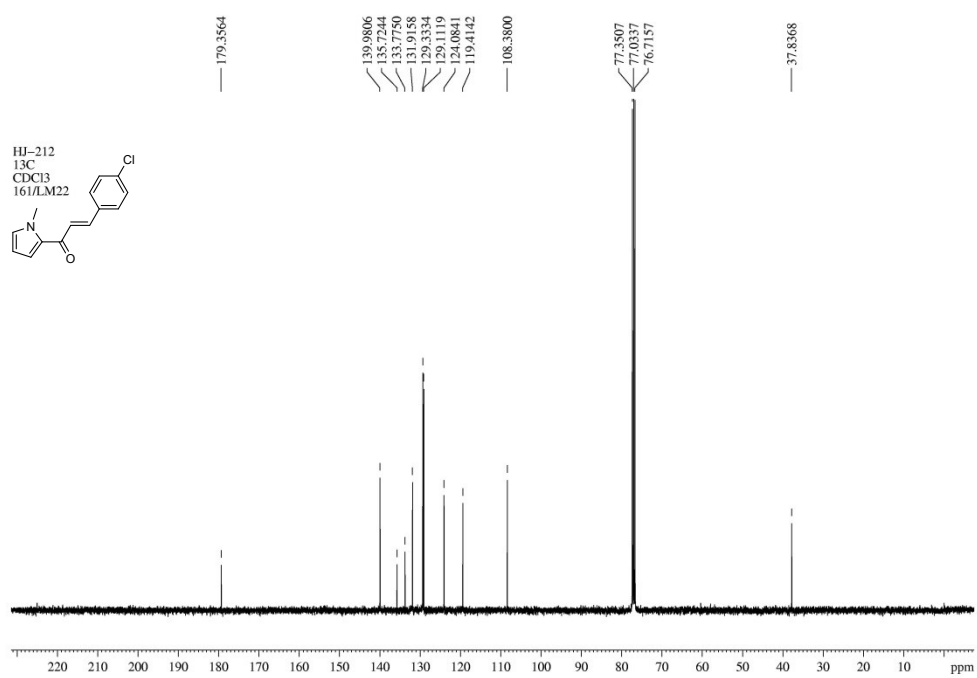
¹H NMR spectrum of compound **3f**



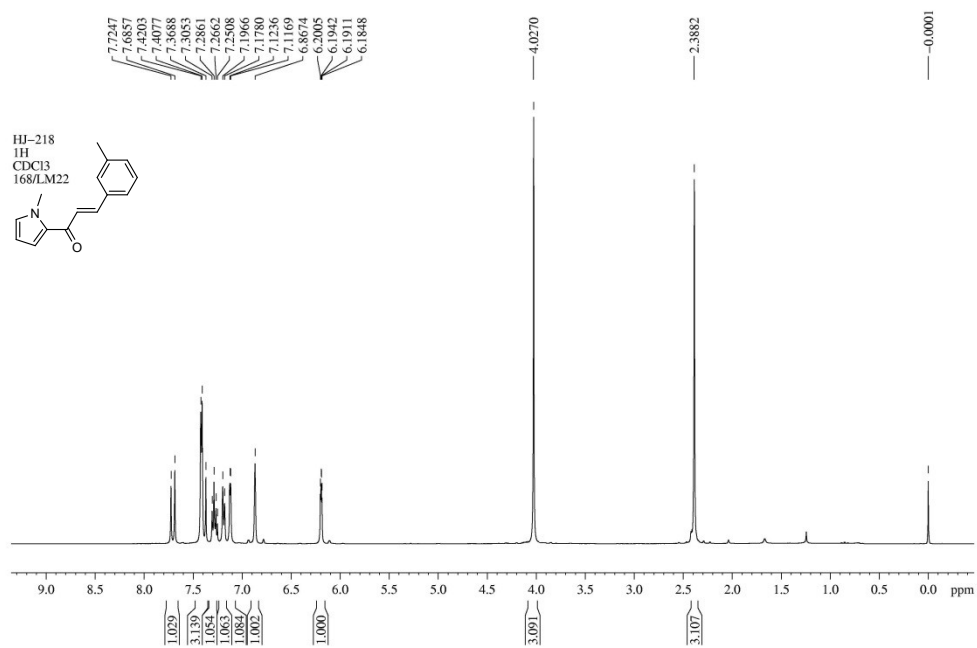
¹³C NMR spectrum of compound **3f**



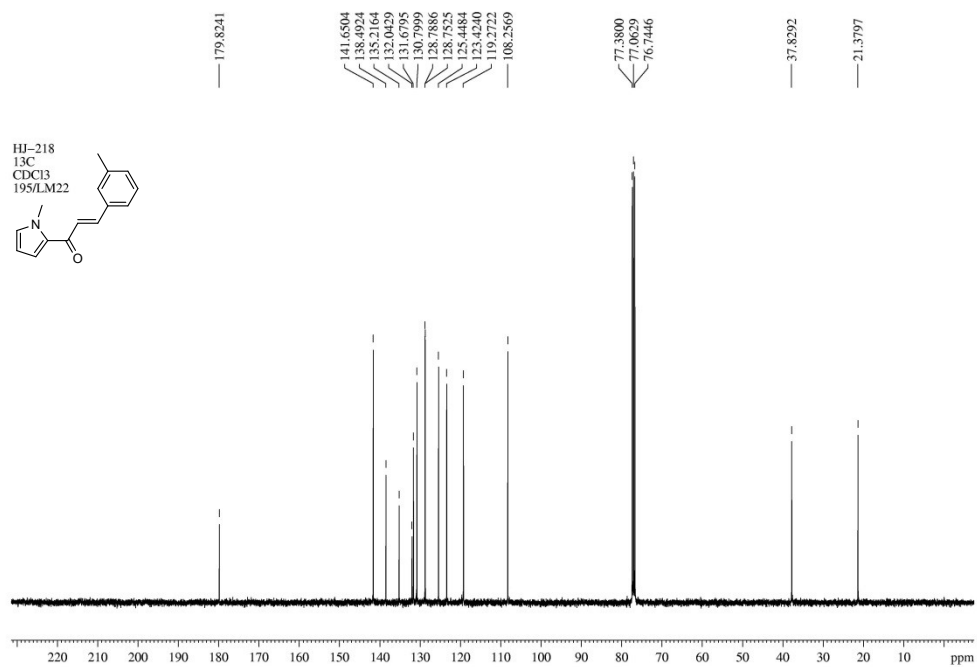
^1H NMR spectrum of compound **3g**



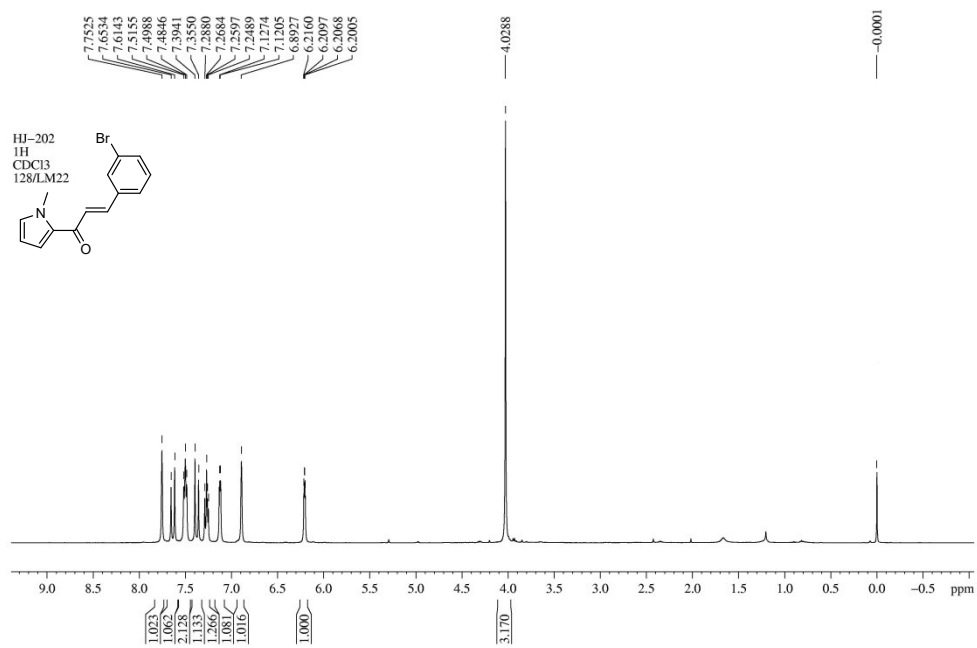
^{13}C NMR spectrum of compound **3g**



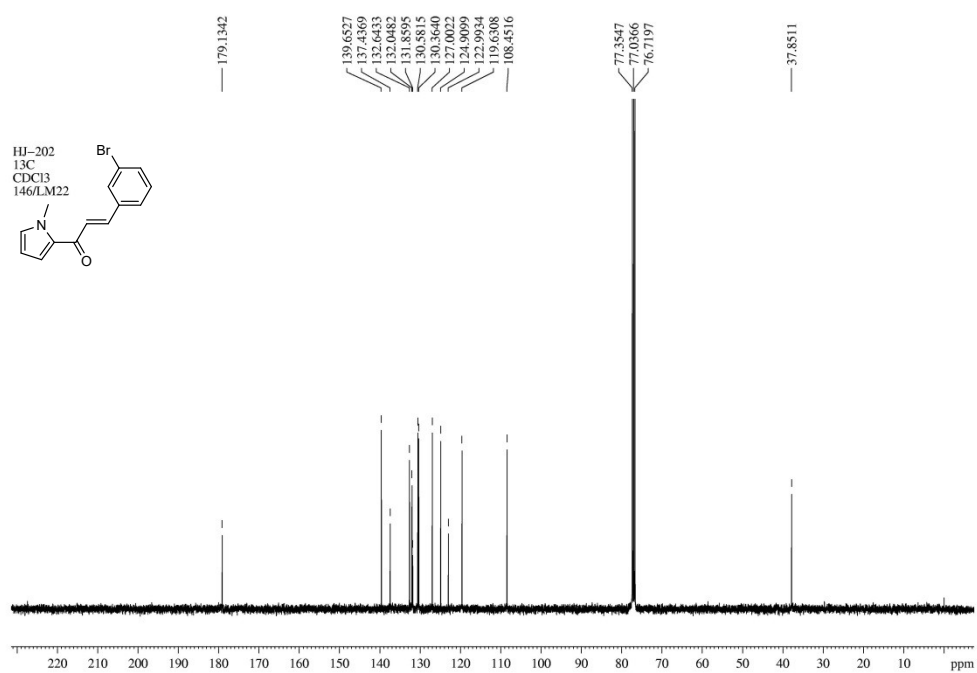
¹H NMR spectrum of compound **3h**



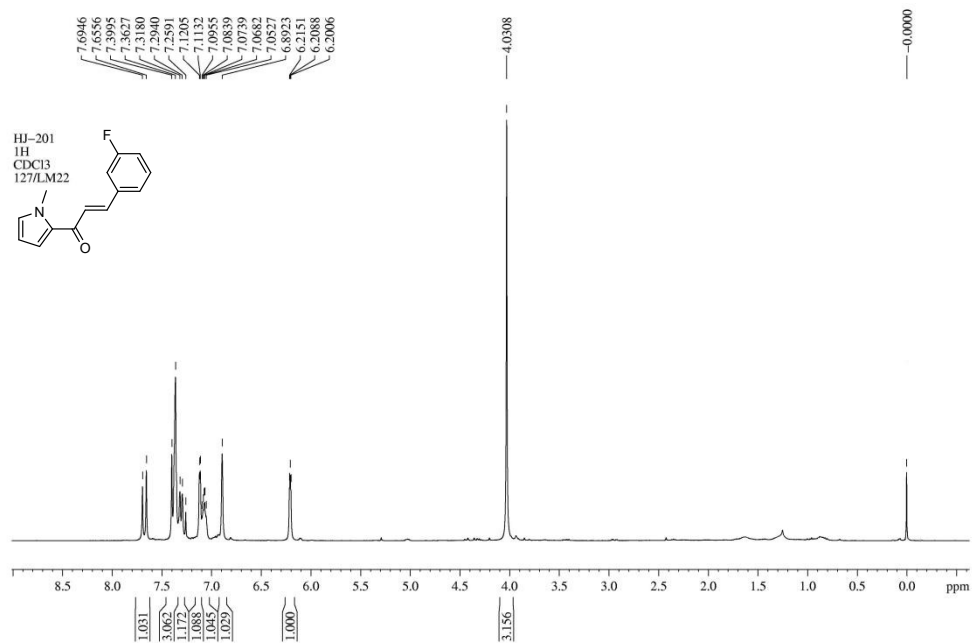
¹³C NMR spectrum of compound **3h**



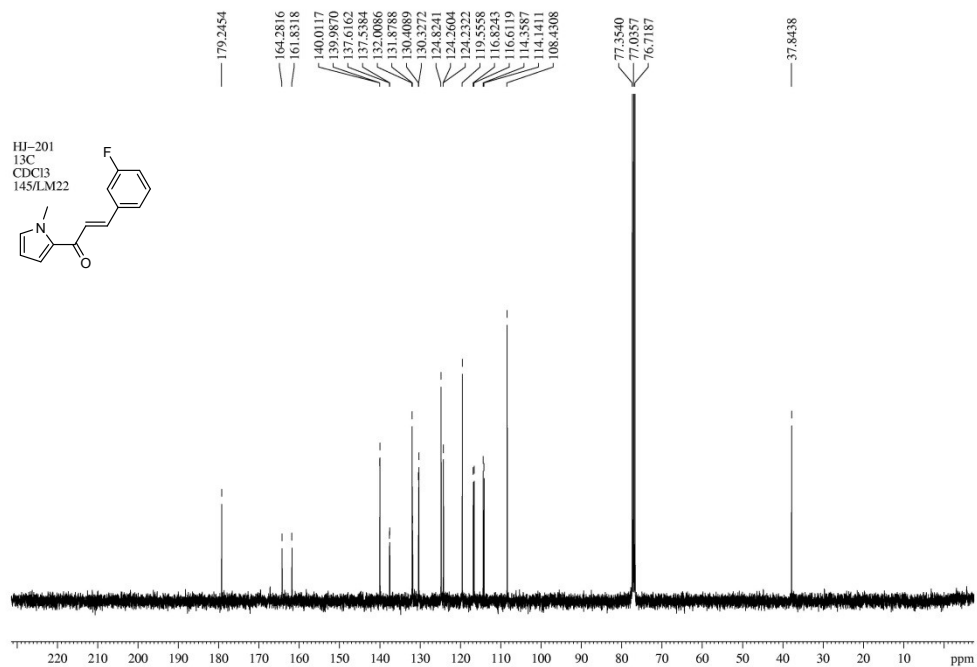
^1H NMR spectrum of compound **3i**



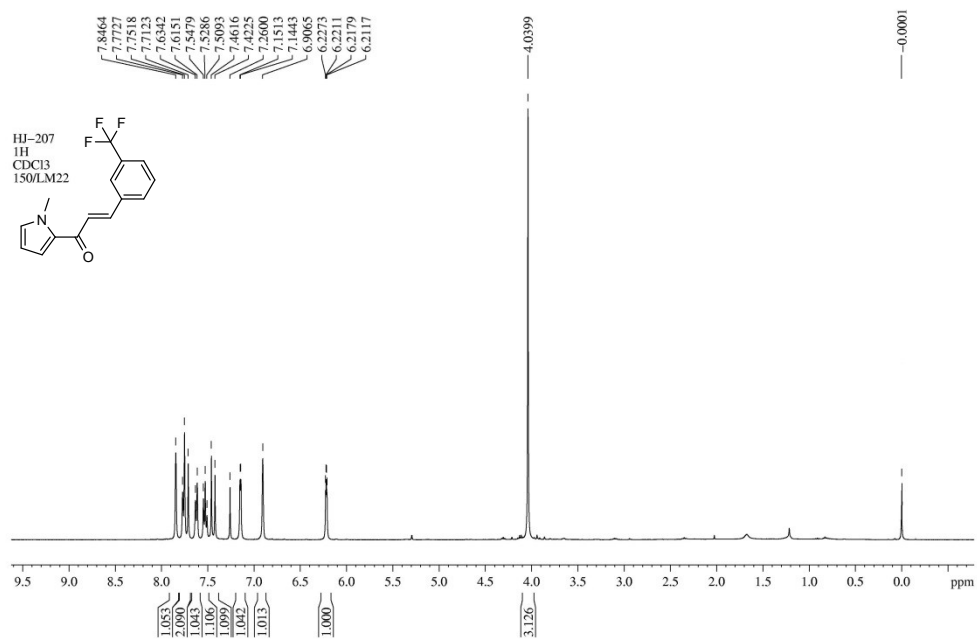
^{13}C NMR spectrum of compound **3i**



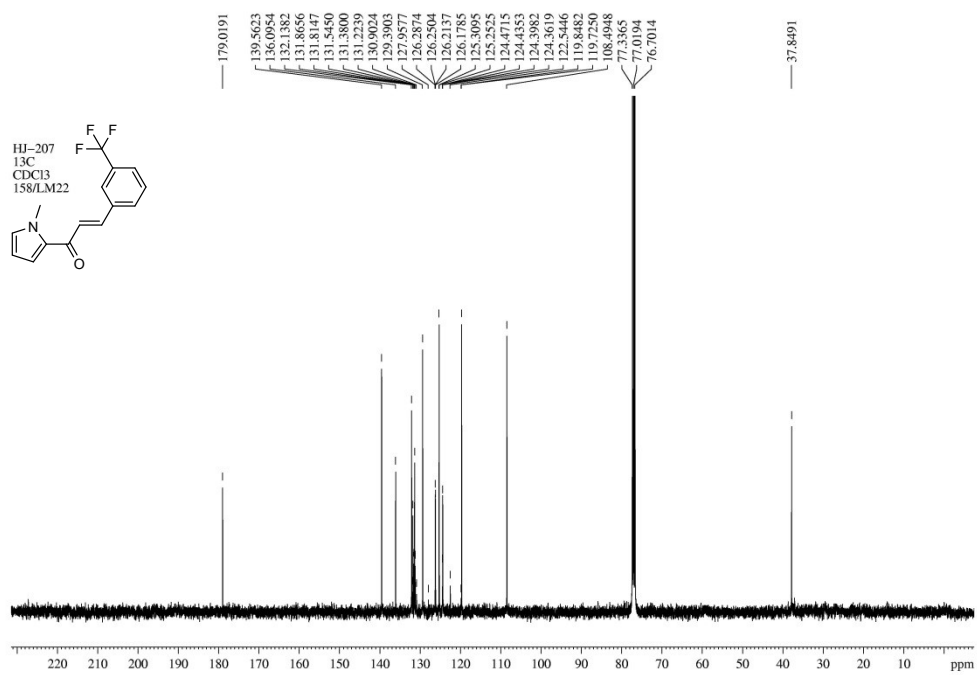
¹H NMR spectrum of compound **3j**



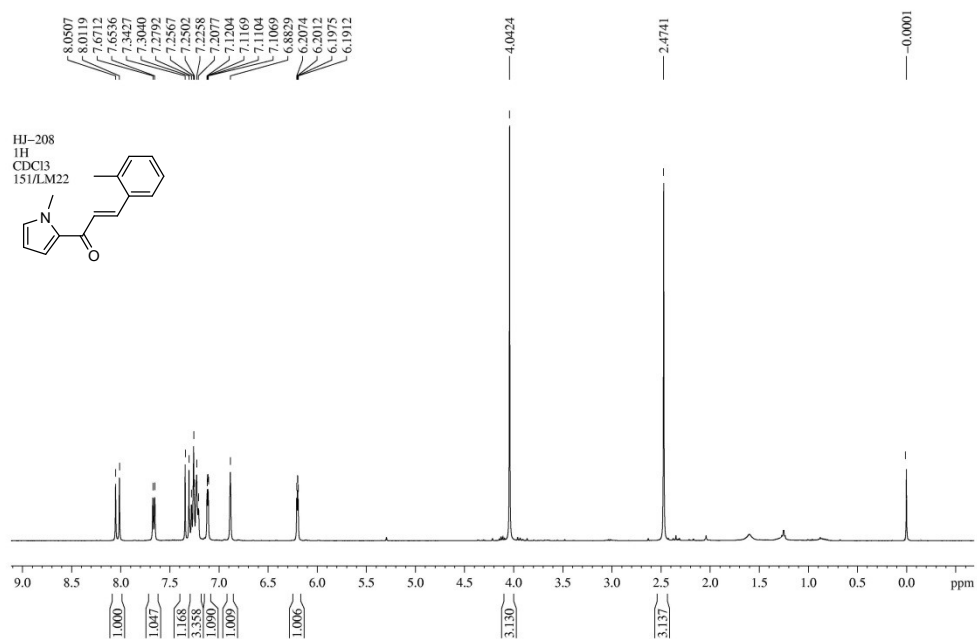
¹³C NMR spectrum of compound **3j**



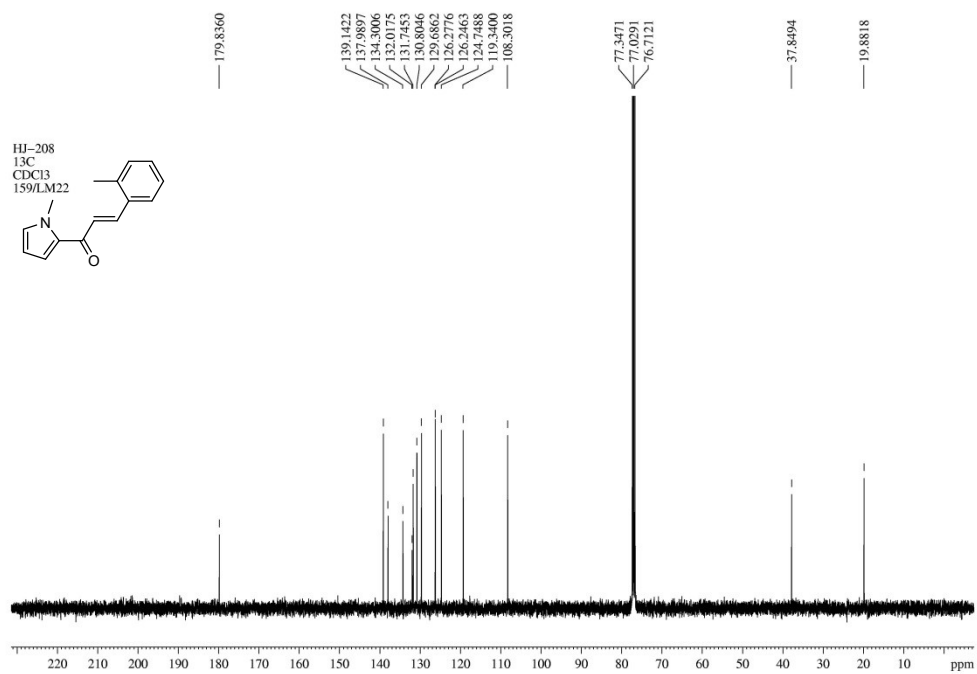
¹H NMR spectrum of compound **3k**



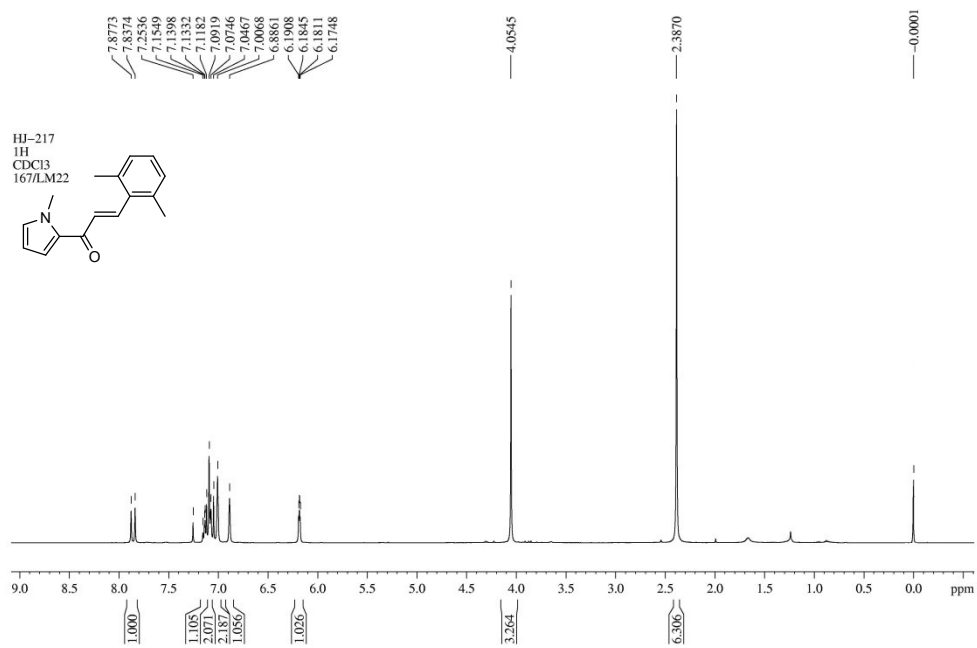
¹³C NMR spectrum of compound **3k**



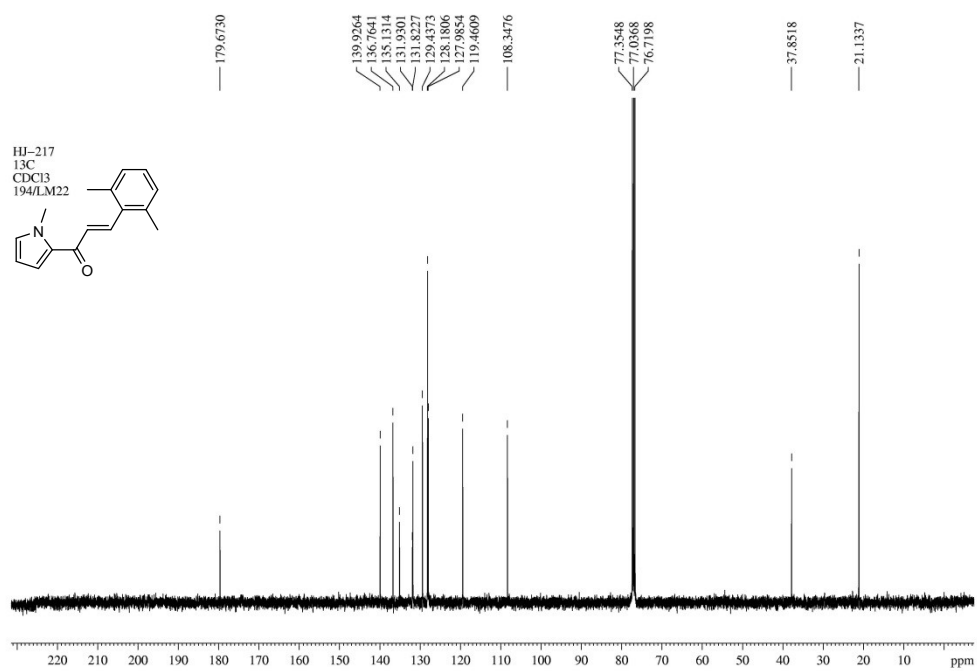
¹H NMR spectrum of compound **31**



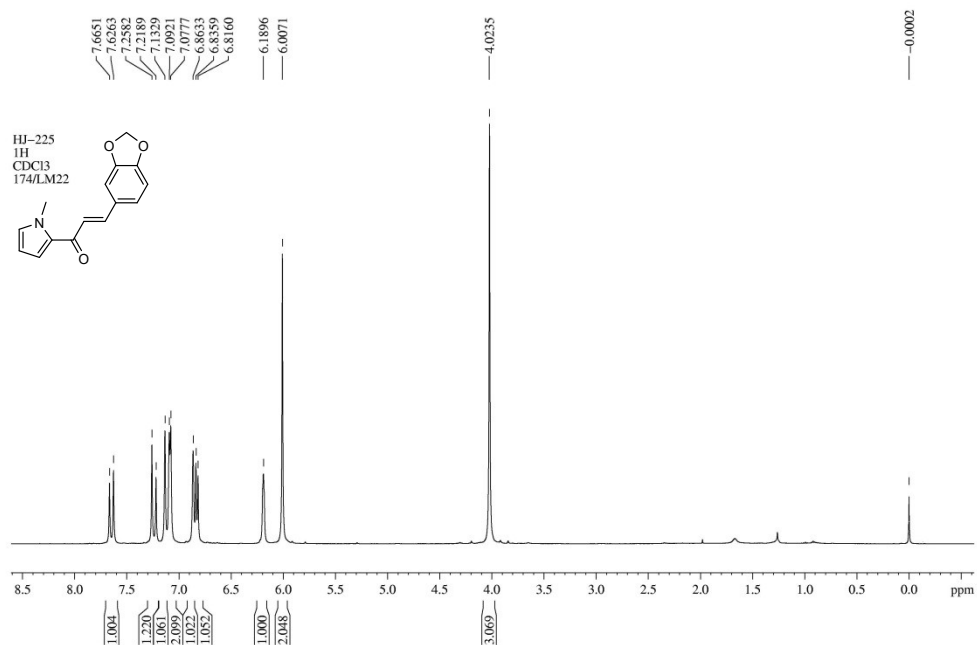
¹³C NMR spectrum of compound **31**



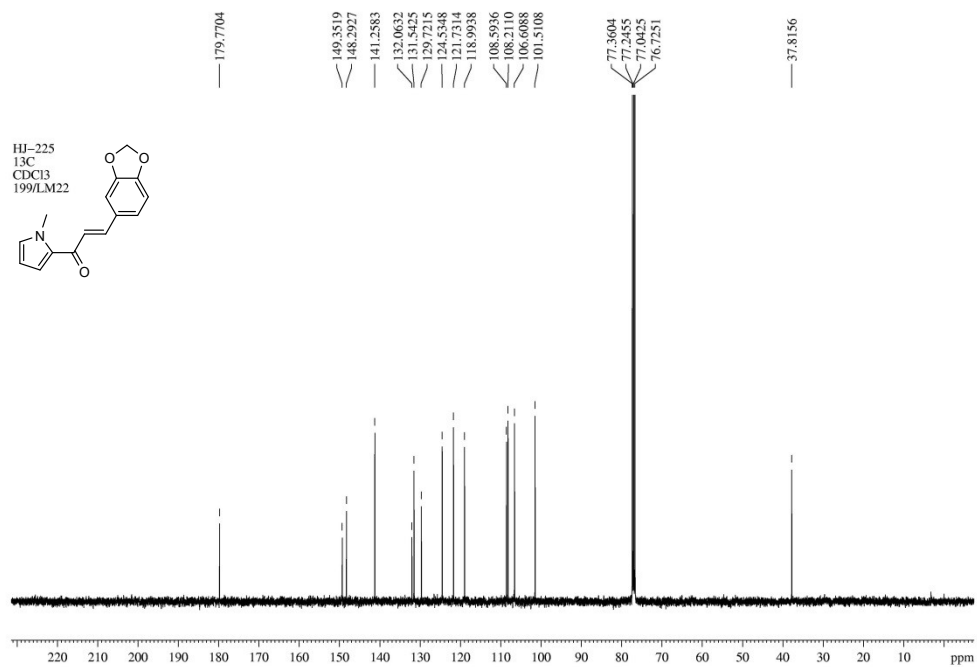
¹H NMR spectrum of compound **3m**



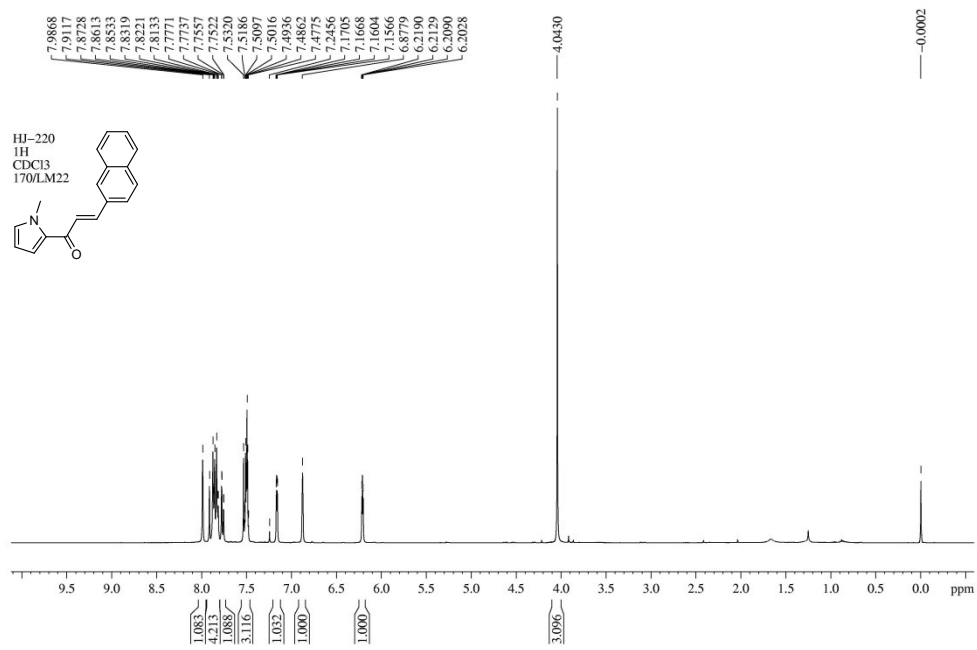
^{13}C NMR spectrum of compound **3m**



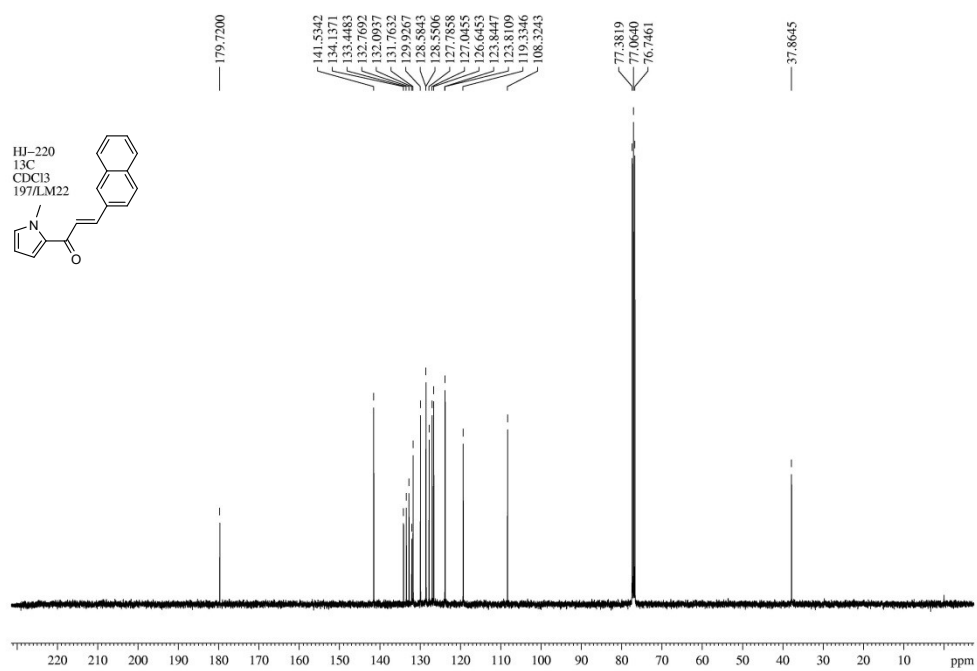
¹H NMR spectrum of compound **3n**



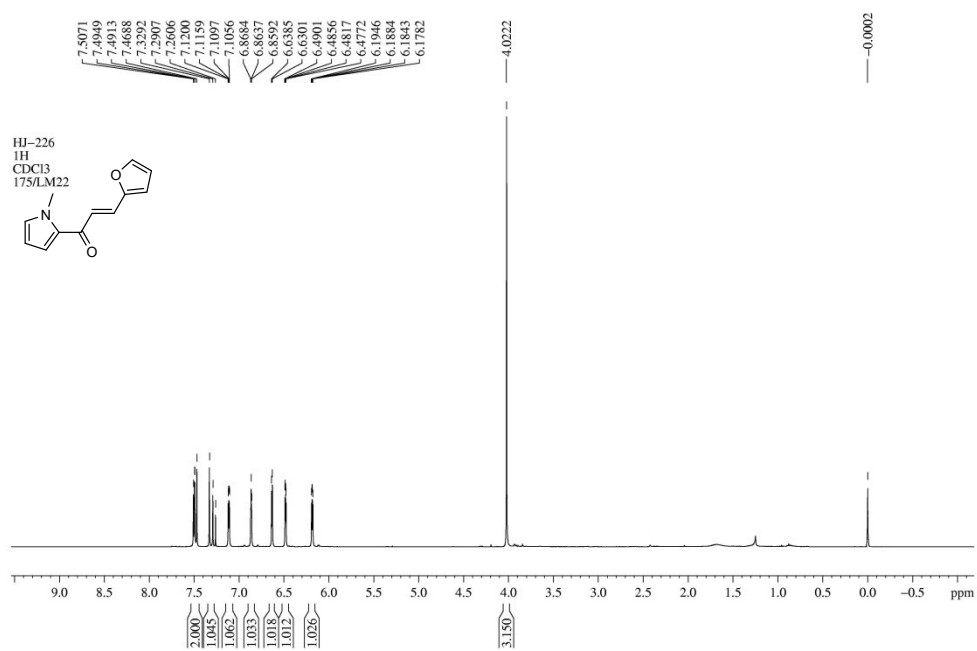
¹³C NMR spectrum of compound **3n**



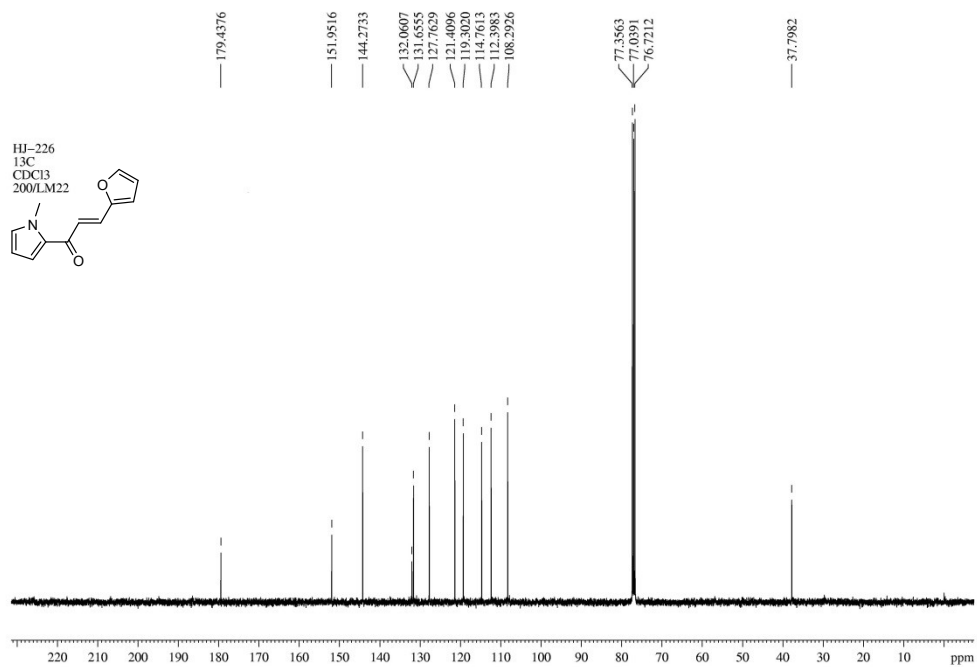
¹H NMR spectrum of compound **3o**



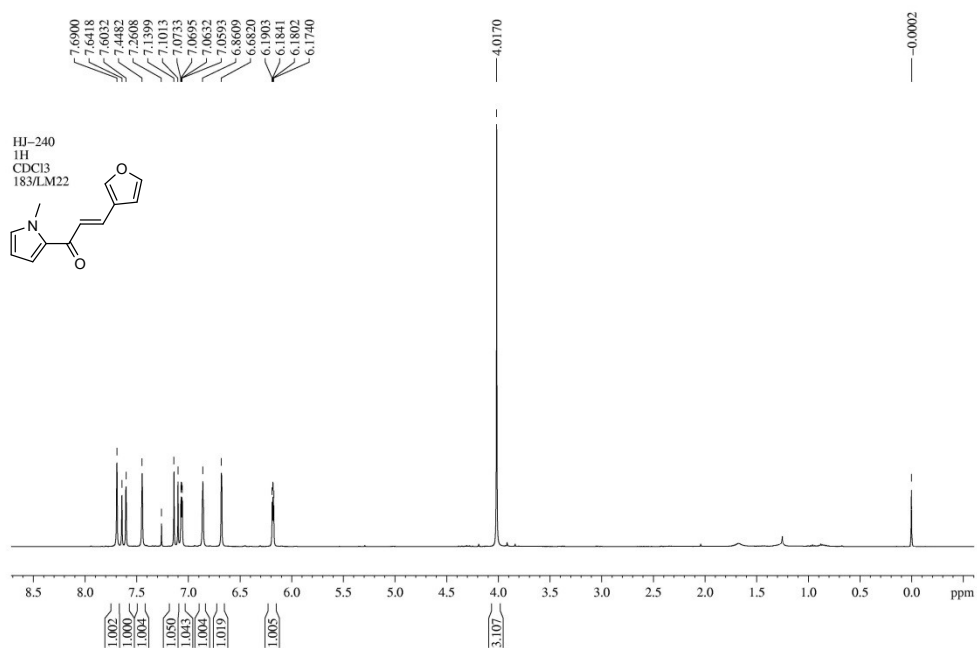
^{13}C NMR spectrum of compound **3o**



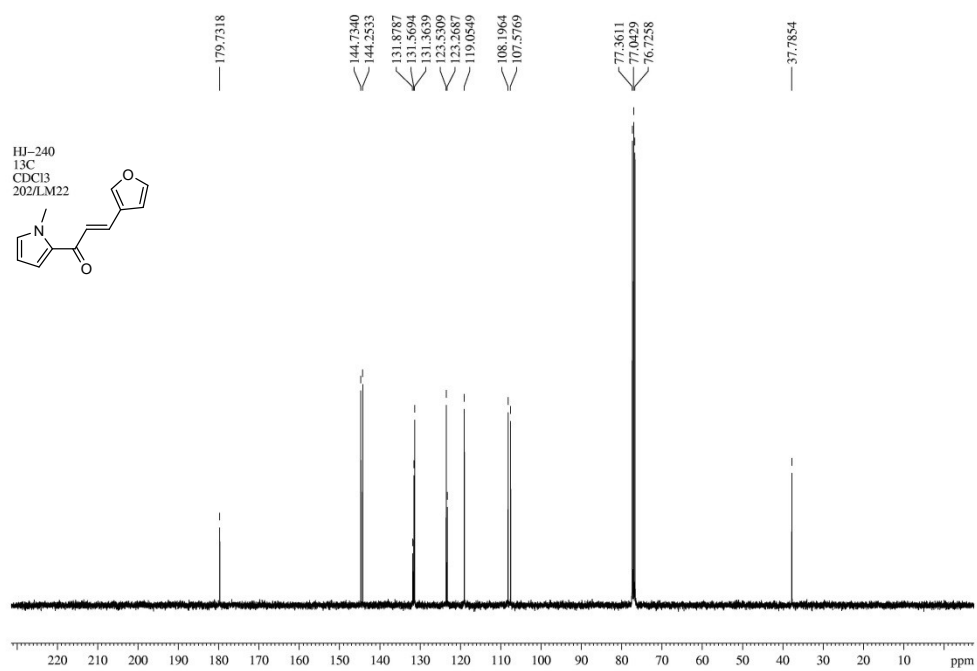
¹H NMR spectrum of compound **3p**



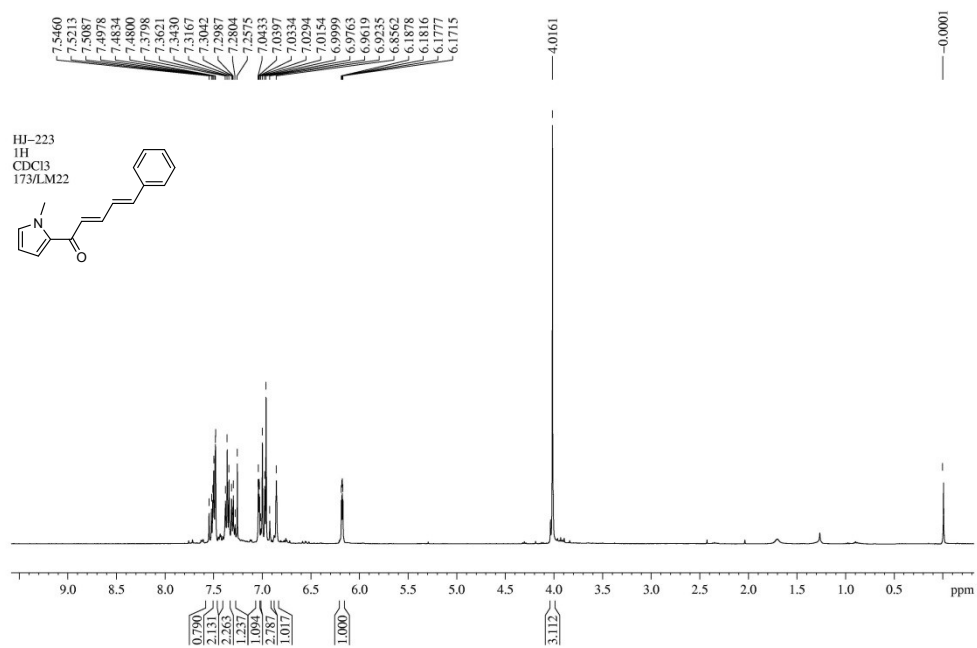
¹³C NMR spectrum of compound **3p**



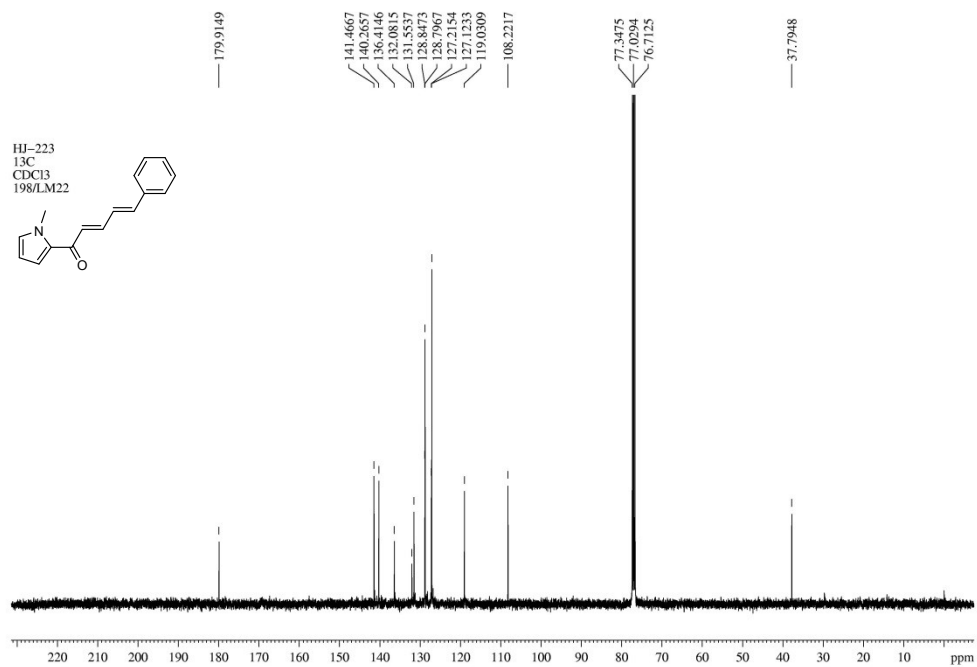
¹H NMR spectrum of compound **3q**



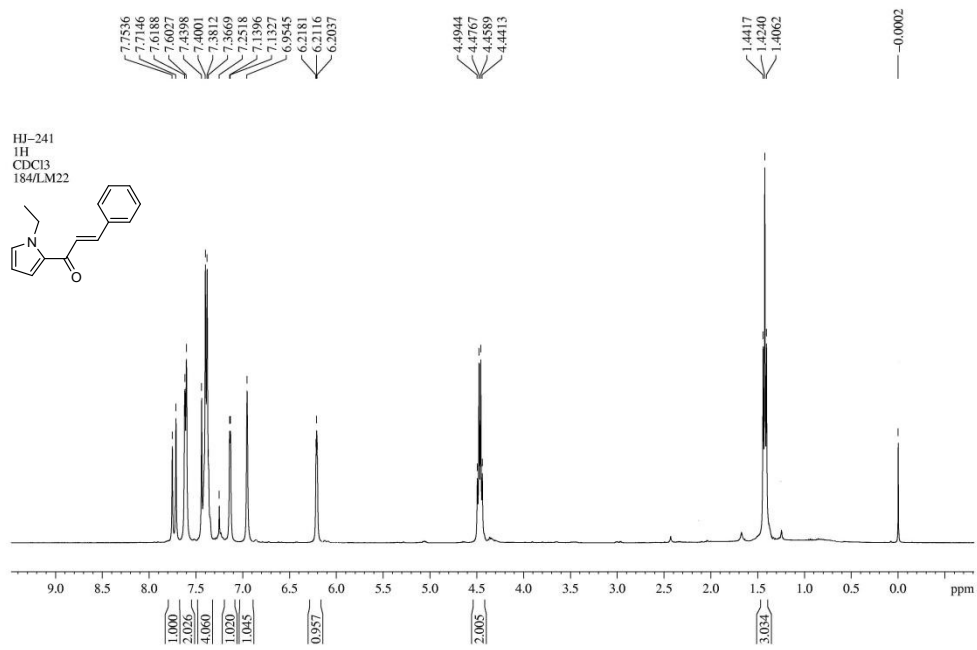
^{13}C NMR spectrum of compound **3q**



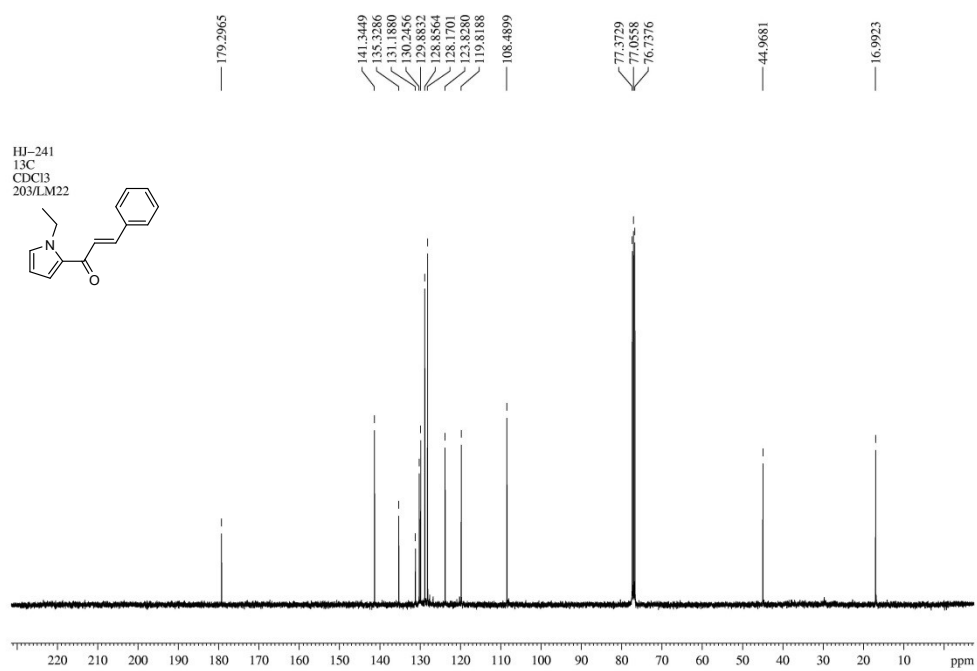
¹H NMR spectrum of compound **3r**



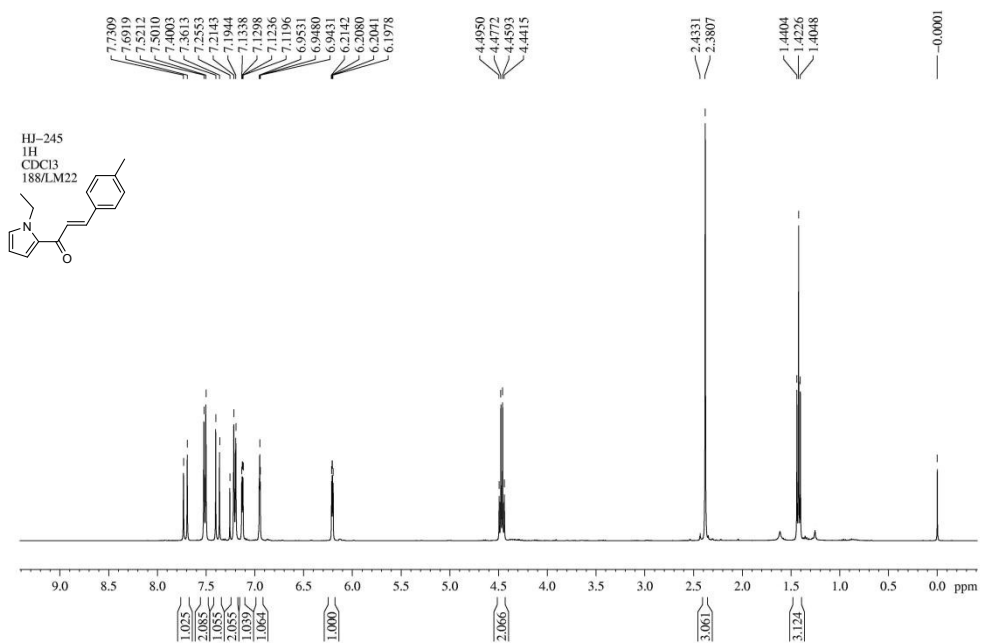
¹³C NMR spectrum of compound **3r**



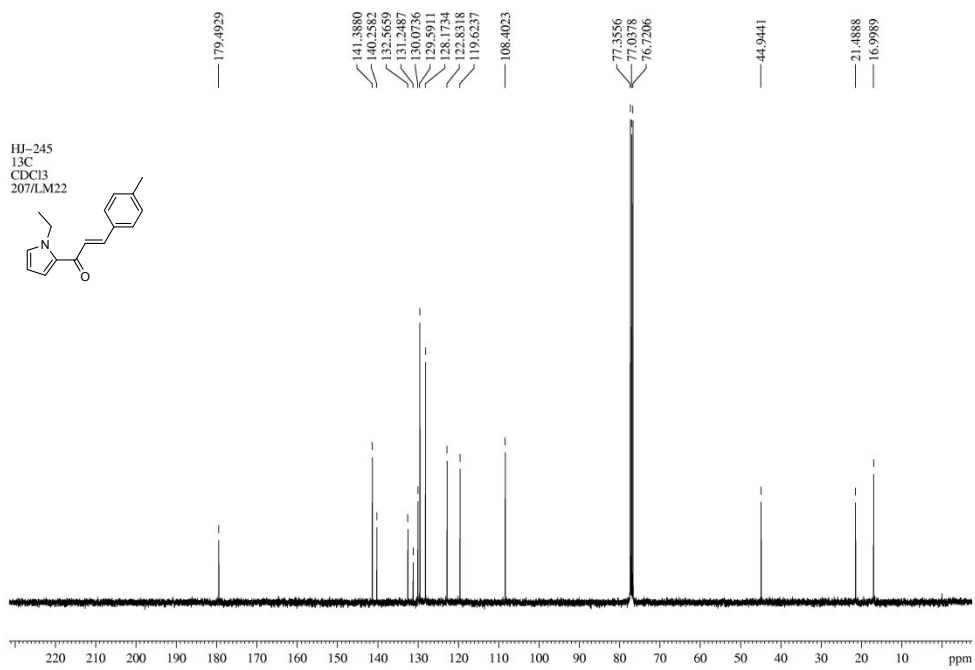
¹H NMR spectrum of compound **4a**



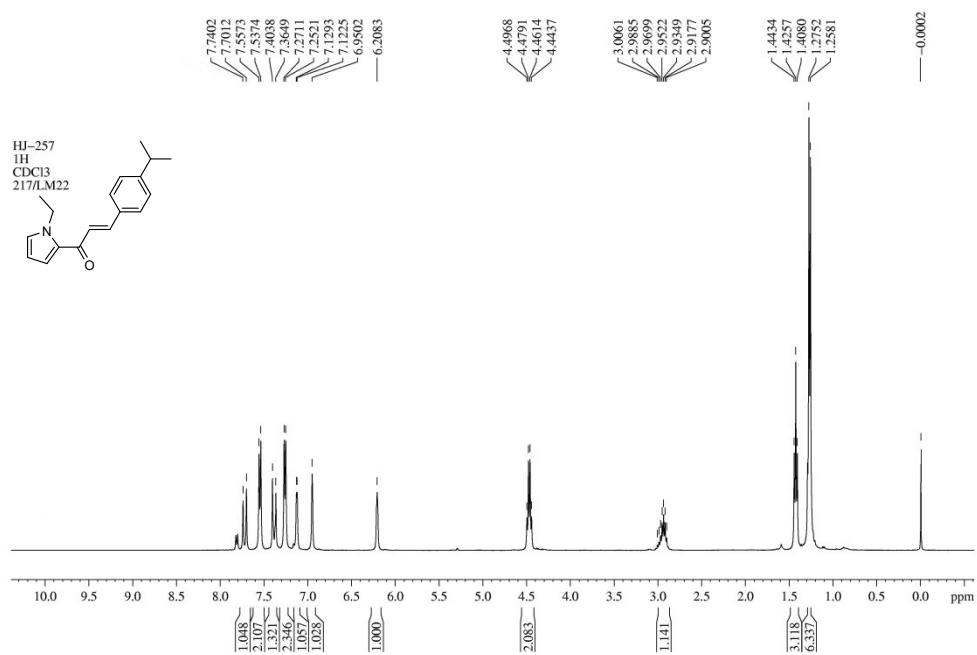
^{13}C NMR spectrum of compound **4a**



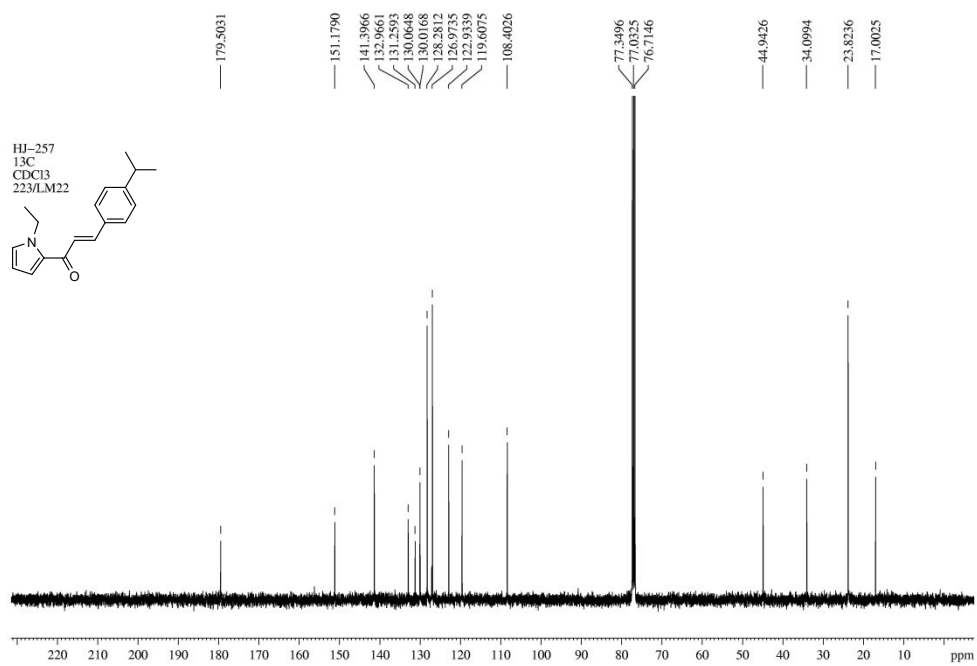
¹H NMR spectrum of compound **4b**



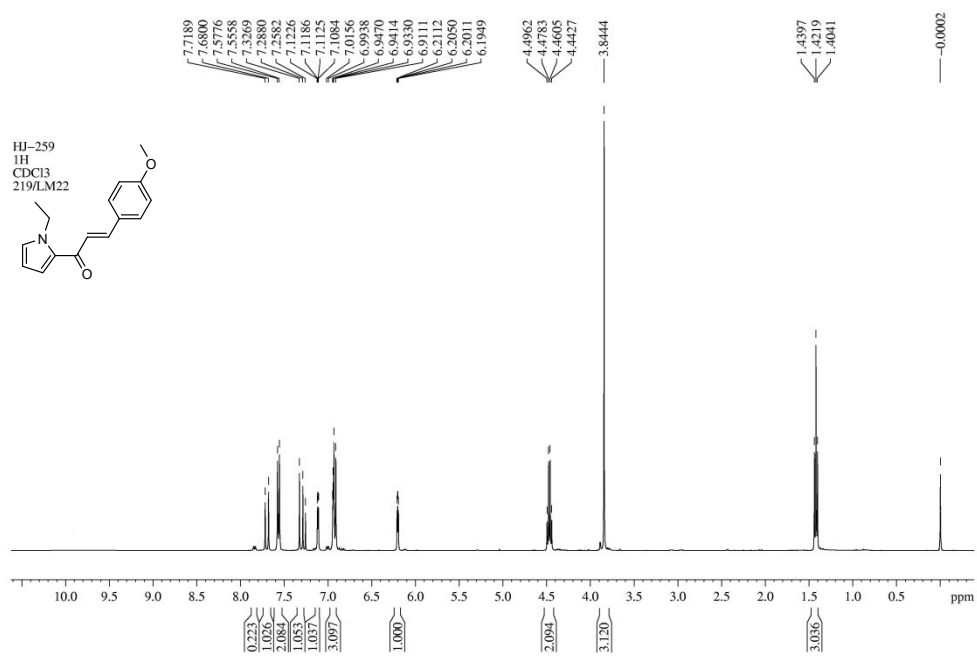
¹³C NMR spectrum of compound **4b**



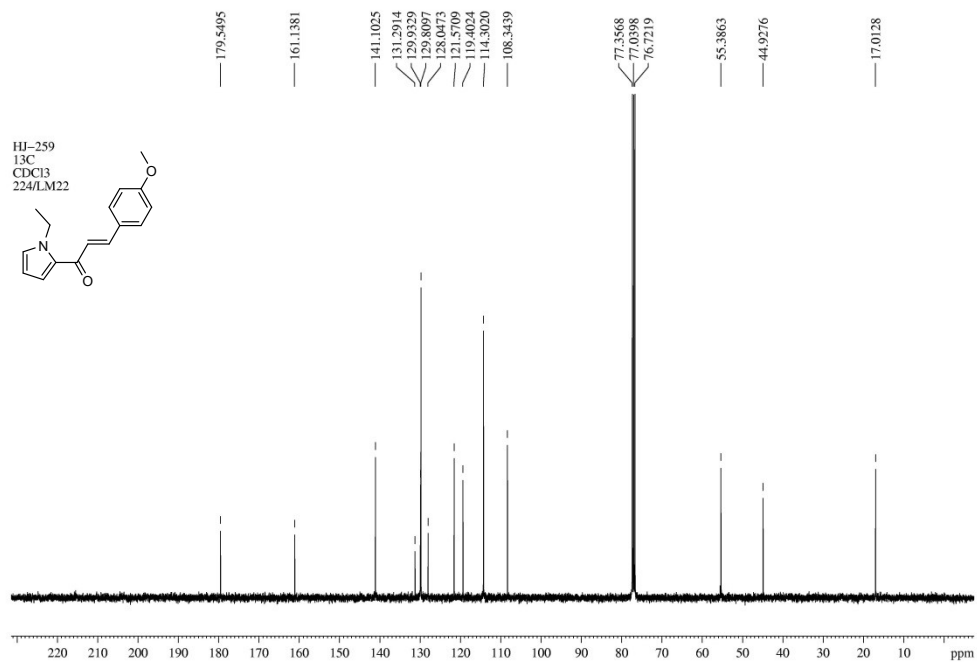
¹H NMR spectrum of compound **4c**



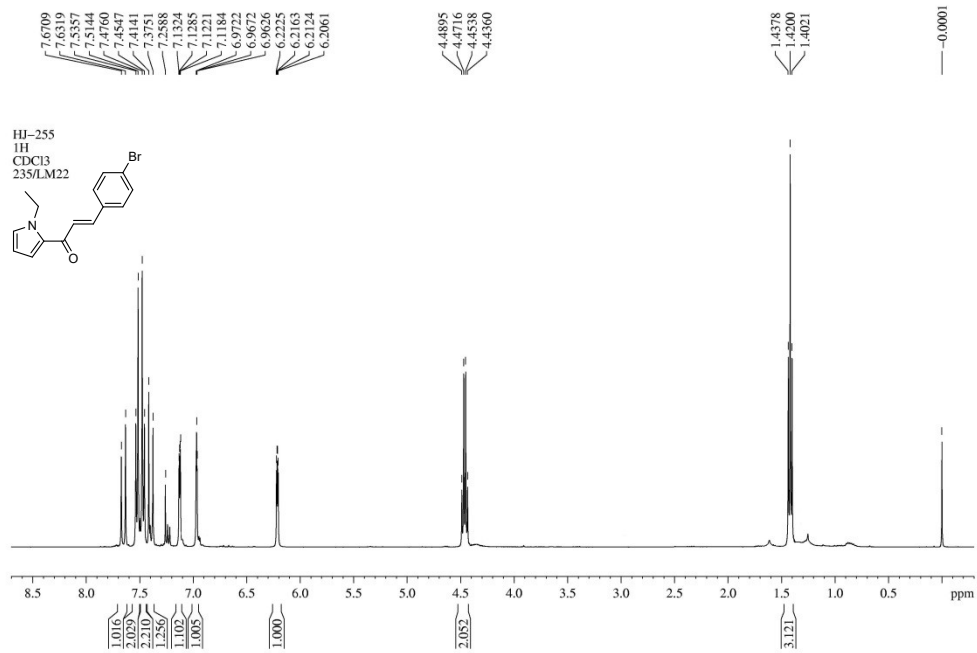
^{13}C NMR spectrum of compound **4c**



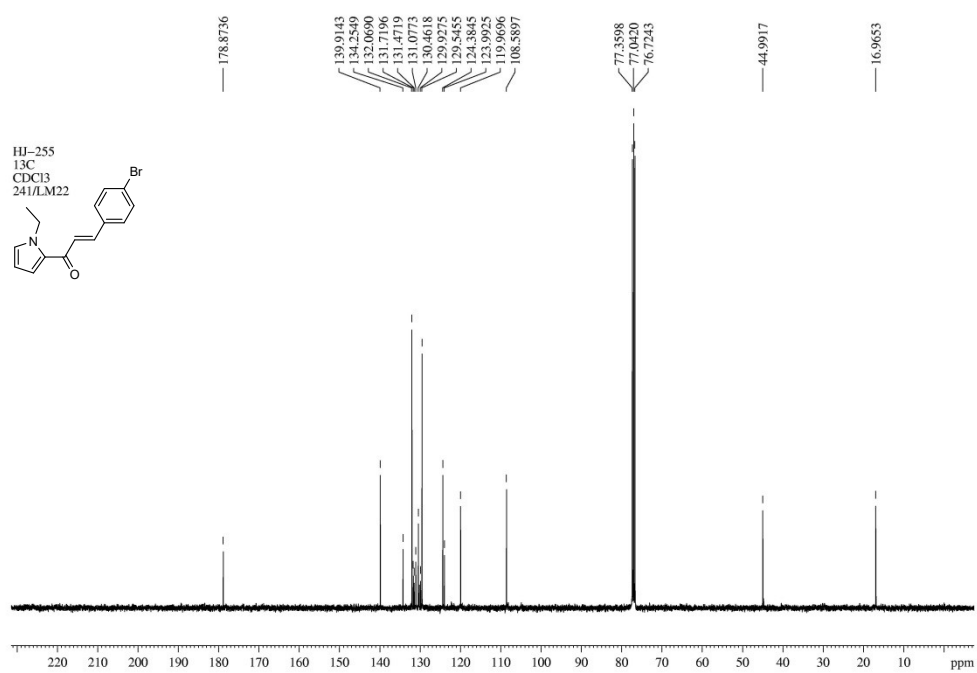
¹H NMR spectrum of compound **4d**



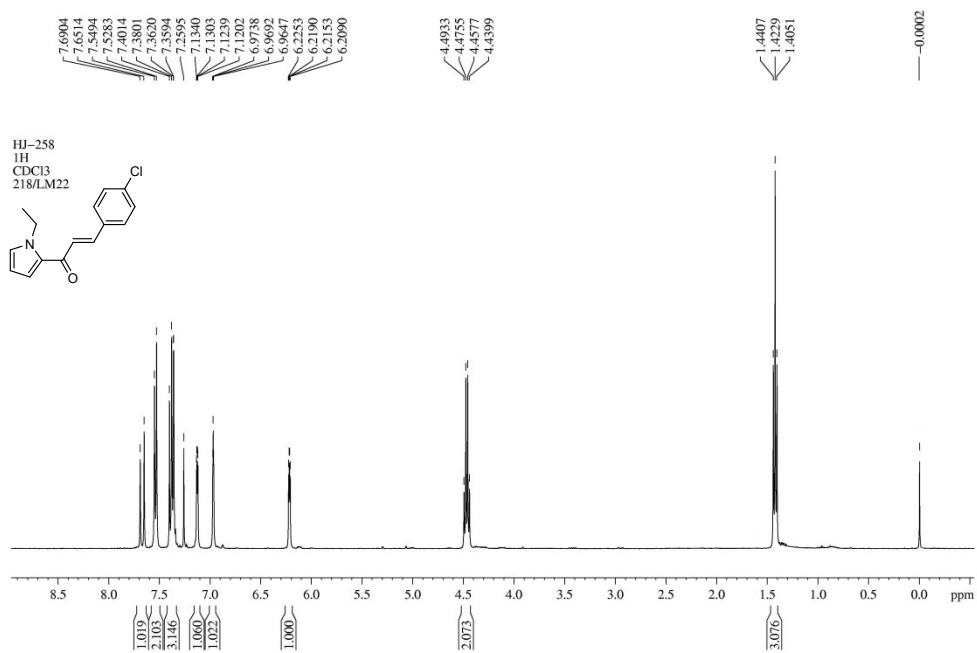
¹³C NMR spectrum of compound **4d**



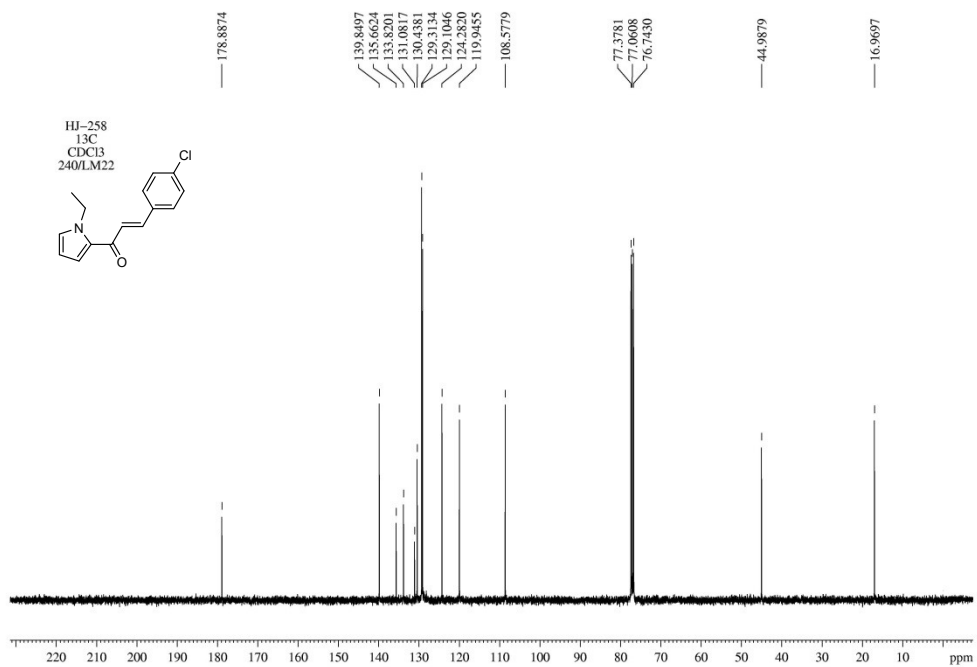
¹H NMR spectrum of compound **4e**



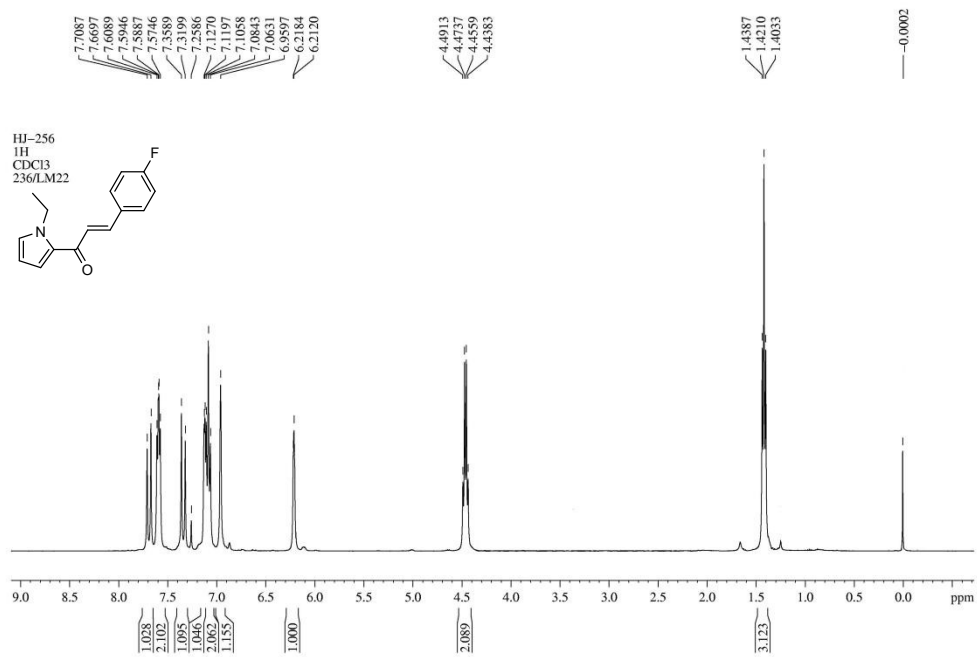
¹³C NMR spectrum of compound **4e**



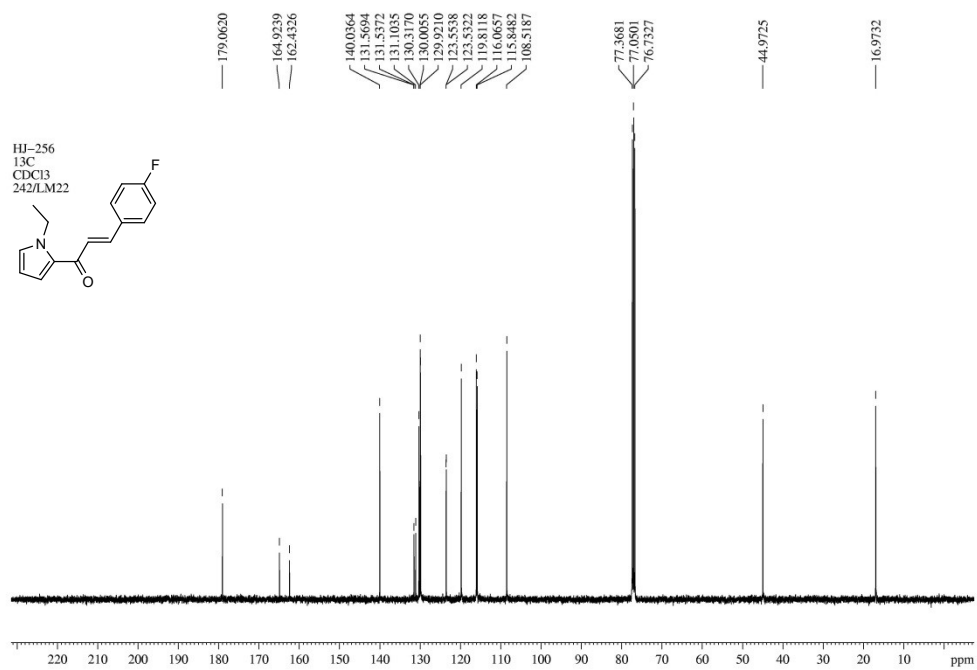
¹H NMR spectrum of compound **4f**



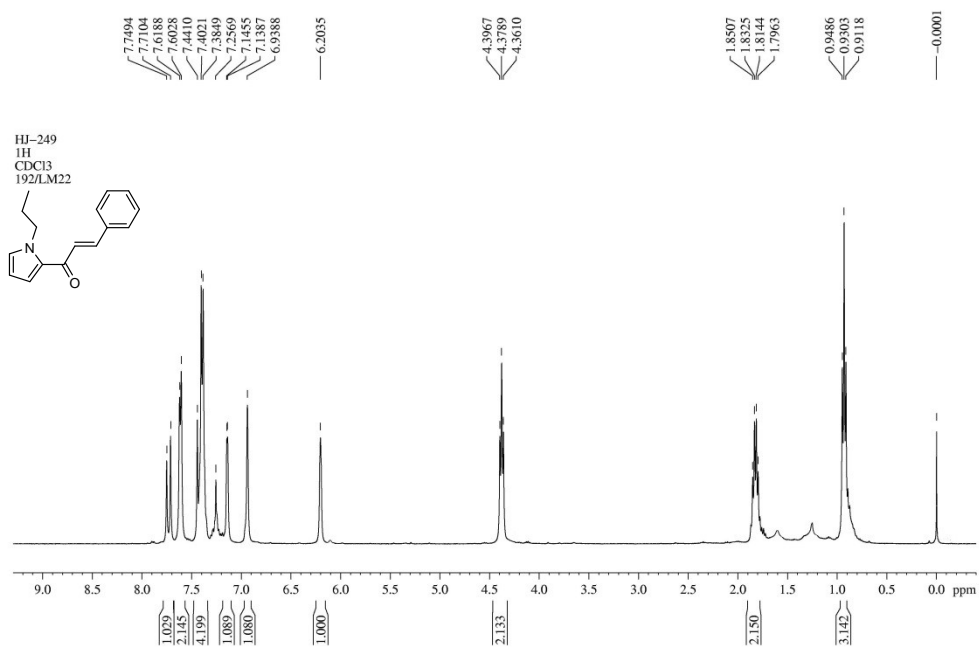
¹³C NMR spectrum of compound **4f**



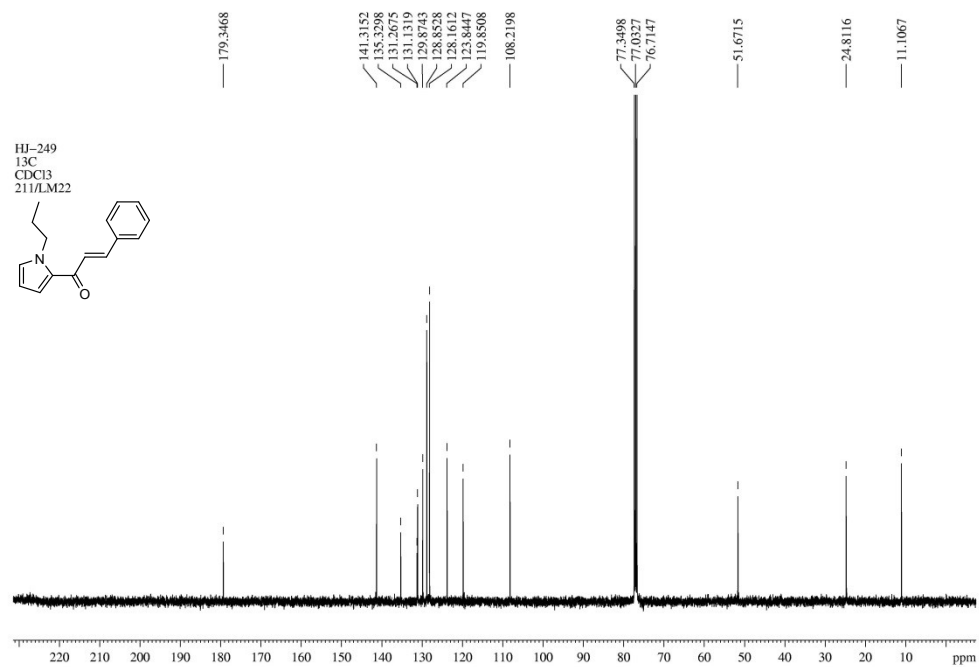
¹H NMR spectrum of compound **4g**



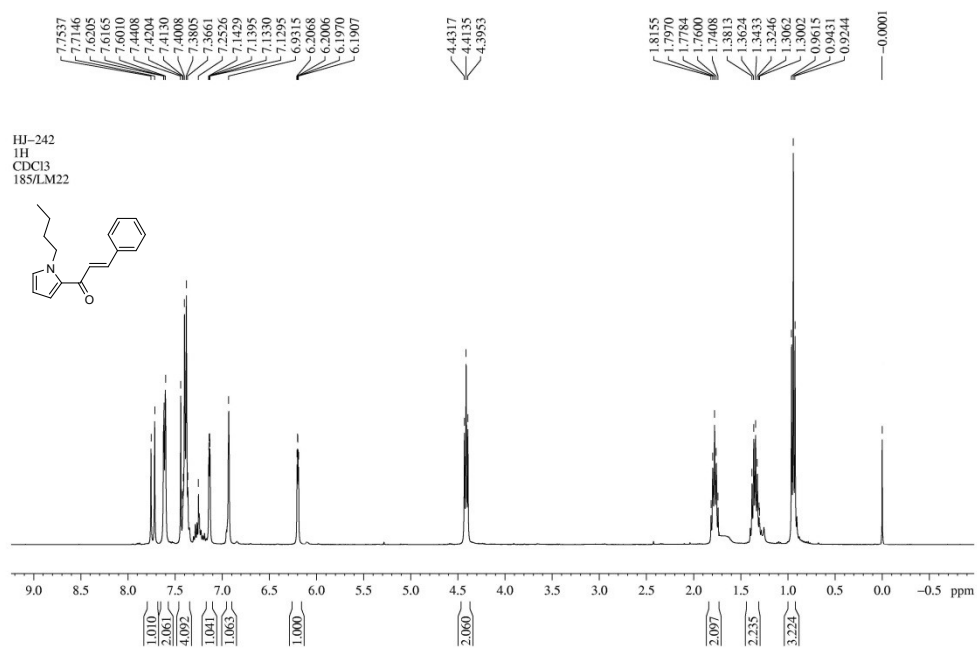
^{13}C NMR spectrum of compound **4g**



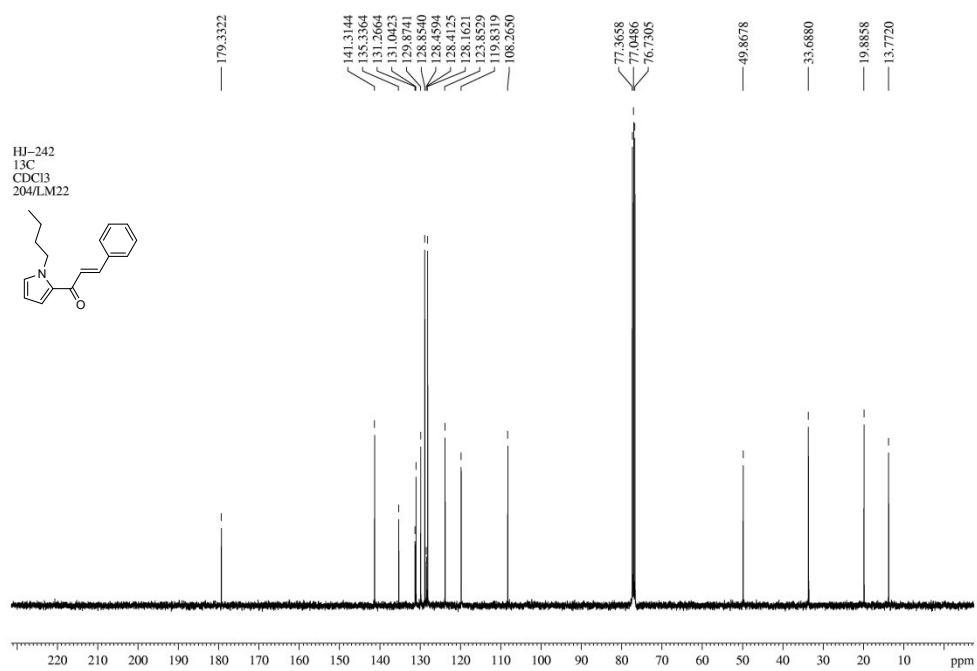
¹H NMR spectrum of compound **4h**



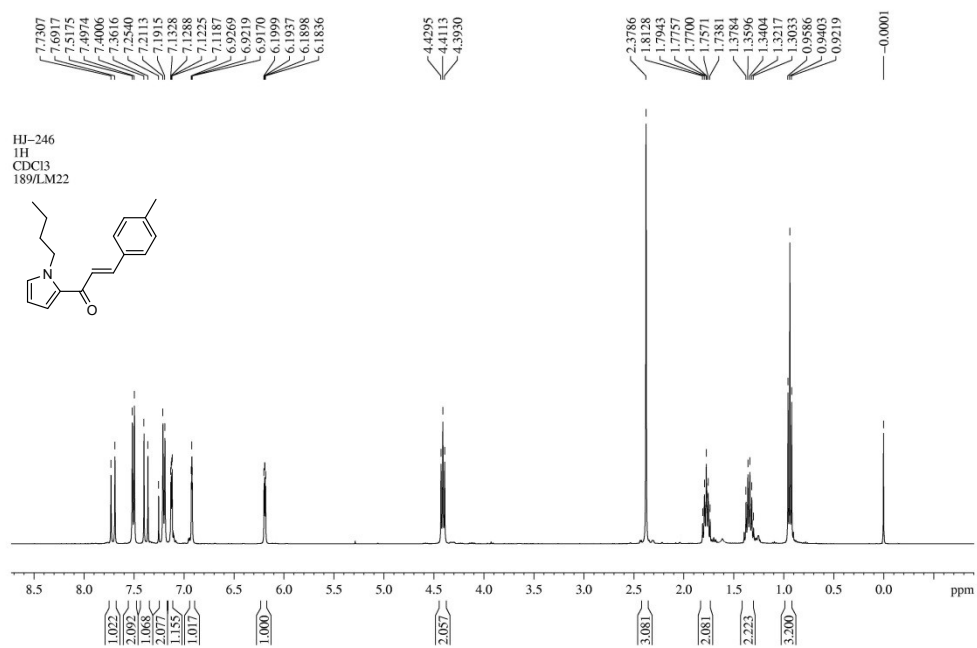
¹³C NMR spectrum of compound **4h**



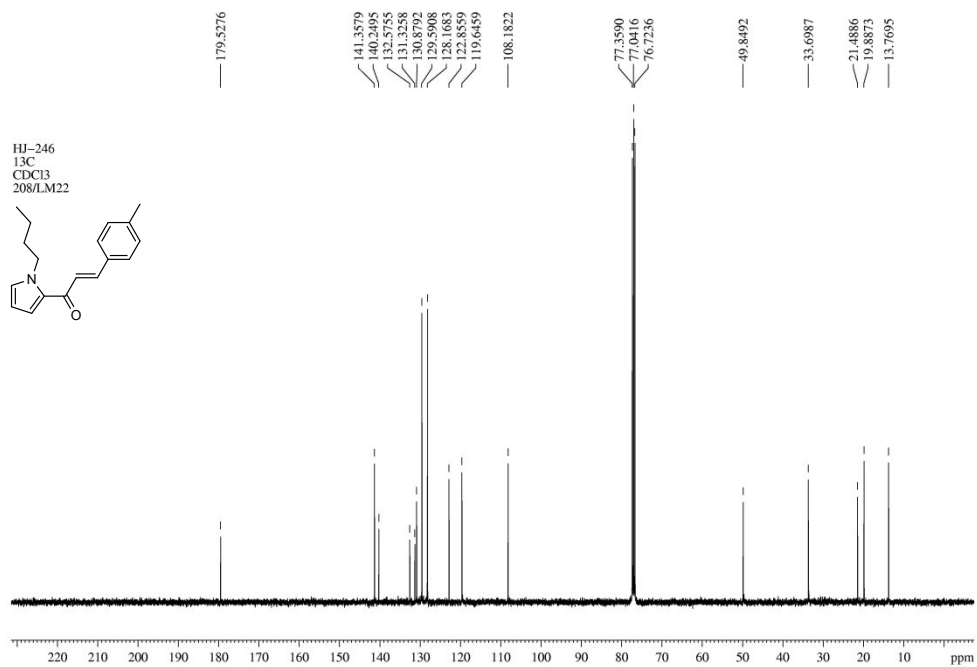
¹H NMR spectrum of compound **4i**



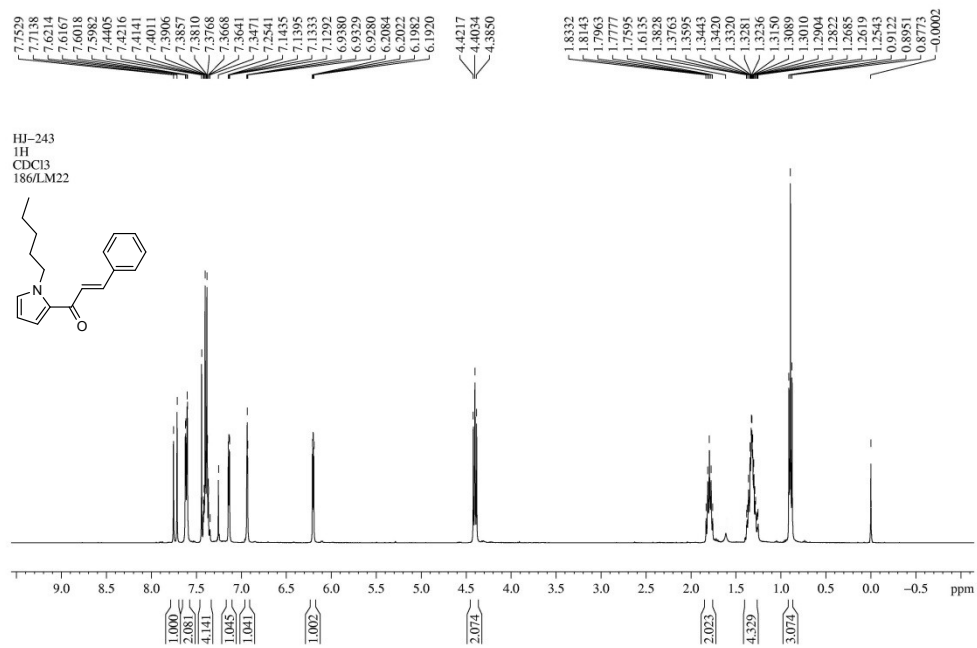
^{13}C NMR spectrum of compound **4i**



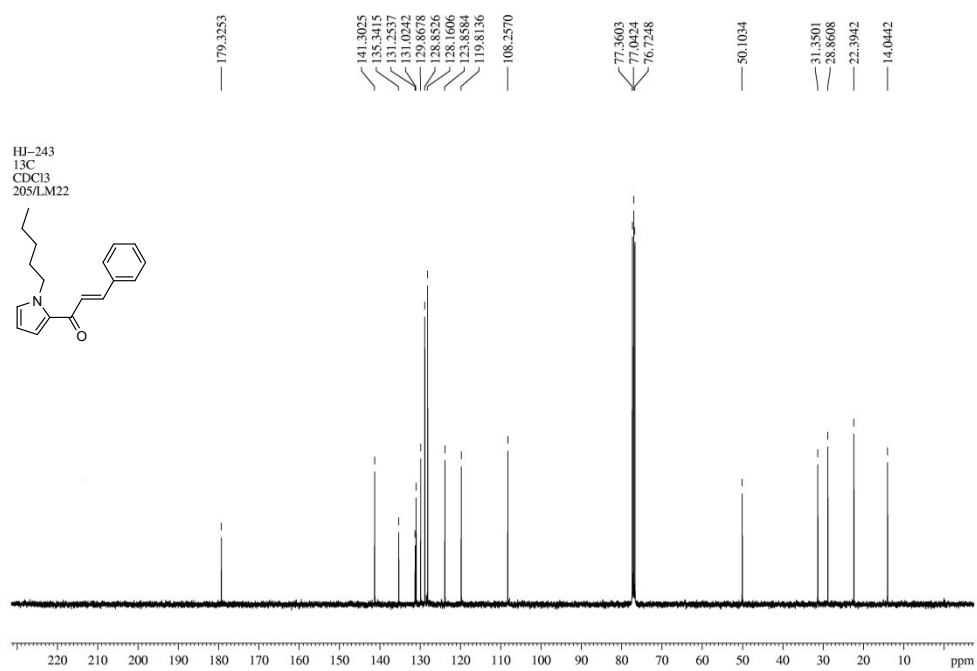
¹H NMR spectrum of compound **4j**



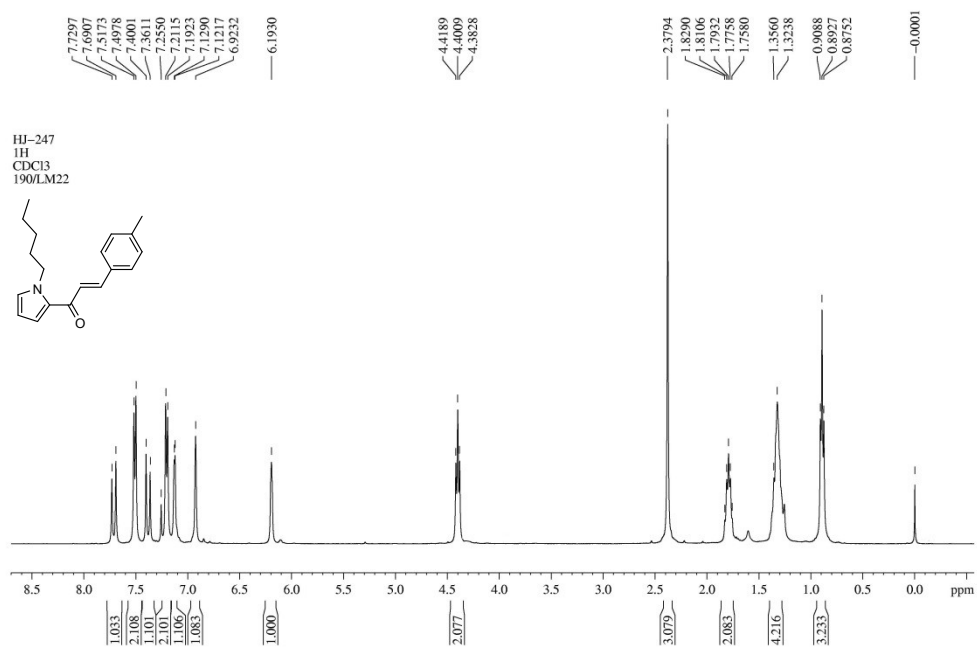
¹³C NMR spectrum of compound **4j**



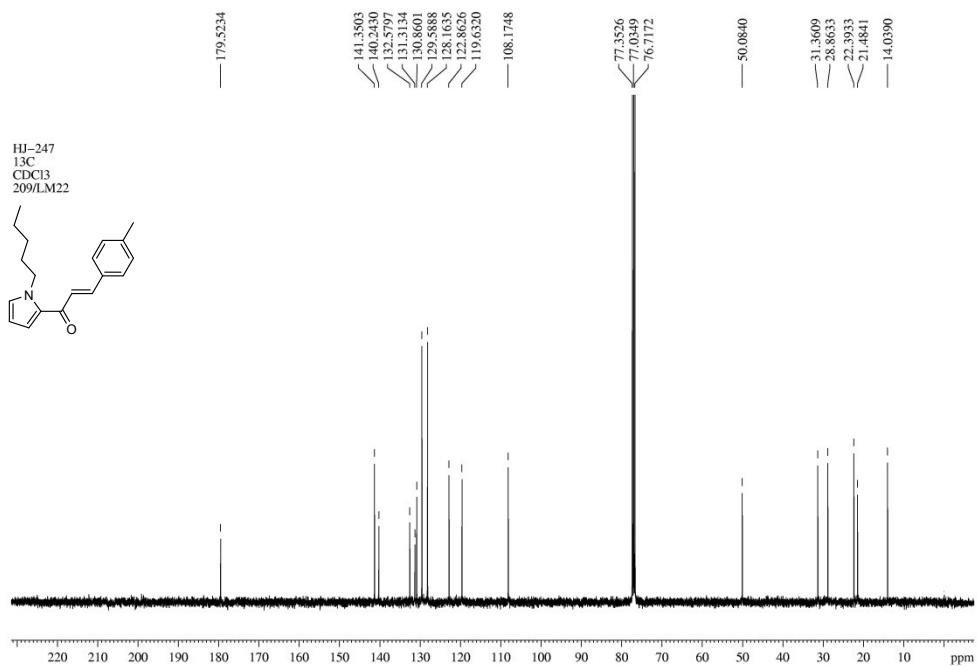
¹H NMR spectrum of compound **4k**



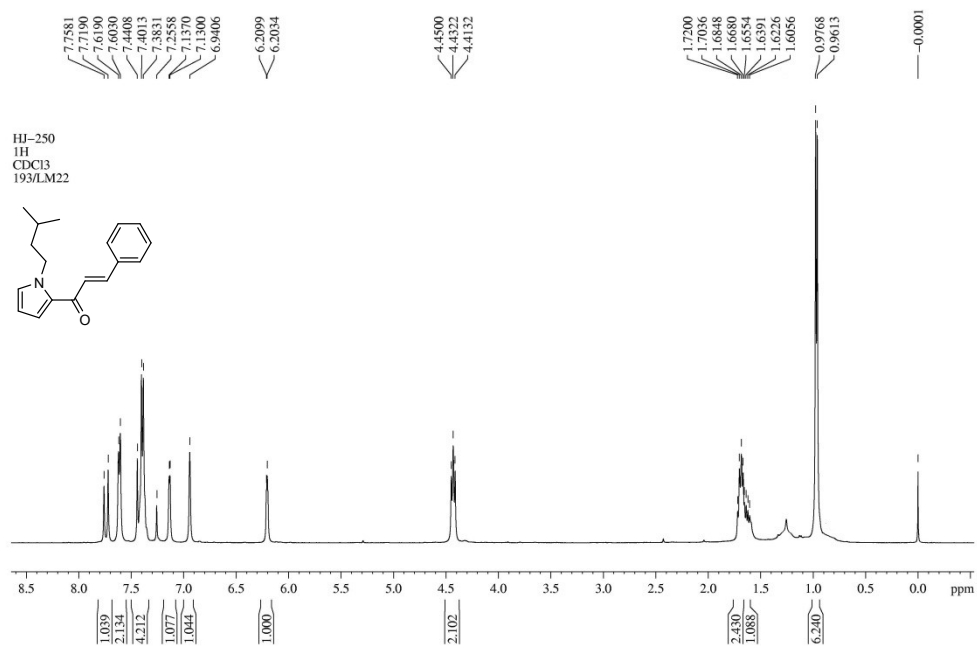
^{13}C NMR spectrum of compound **4k**



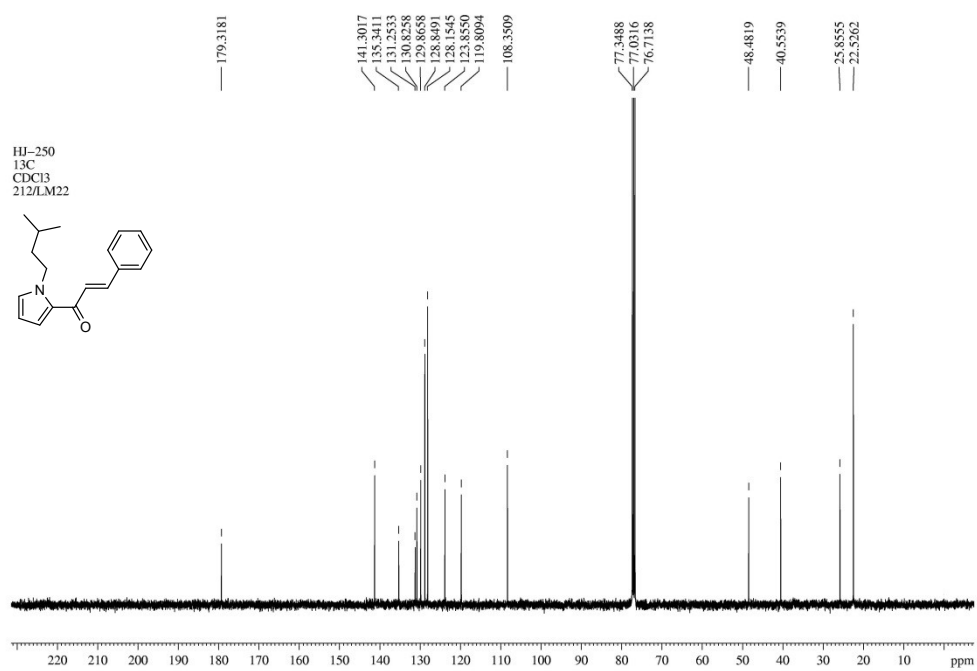
¹H NMR spectrum of compound **41**



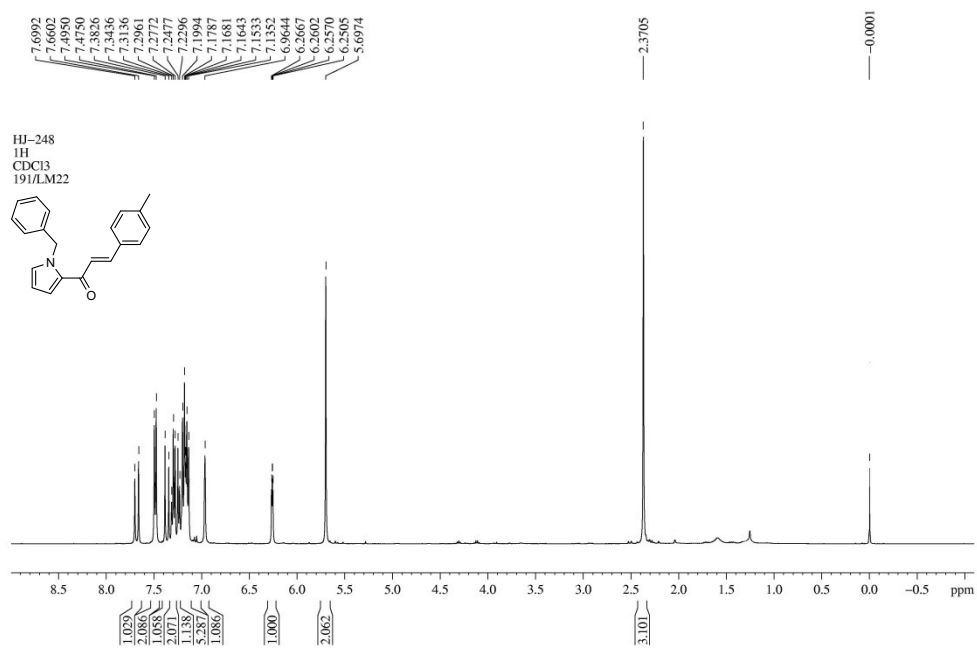
¹³C NMR spectrum of compound **41**



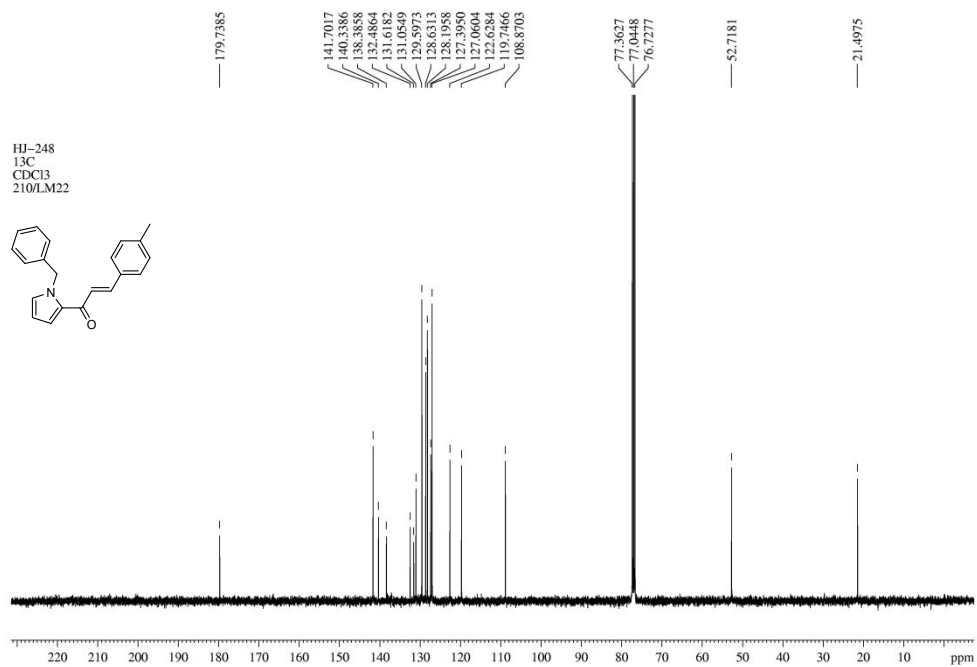
¹H NMR spectrum of compound **4m**



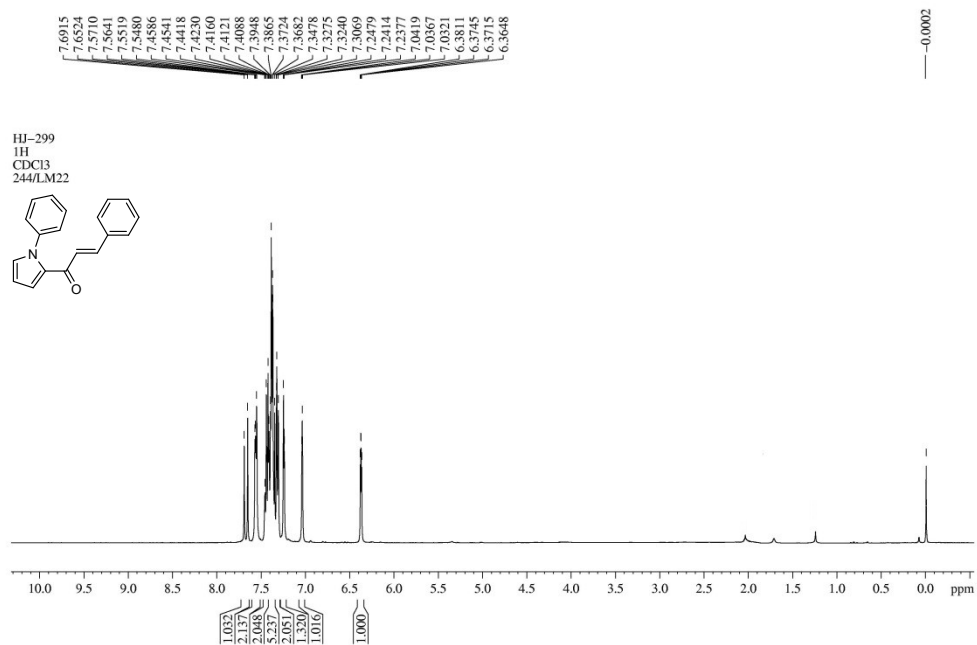
^{13}C NMR spectrum of compound **4m**



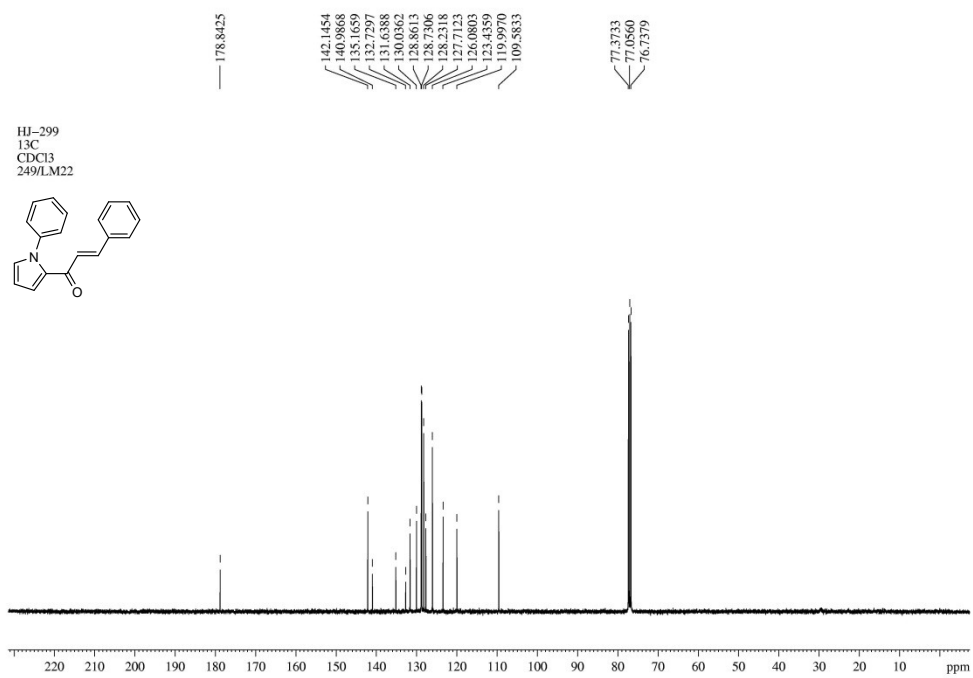
¹H NMR spectrum of compound **4n**



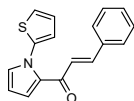
¹³C NMR spectrum of compound **4n**

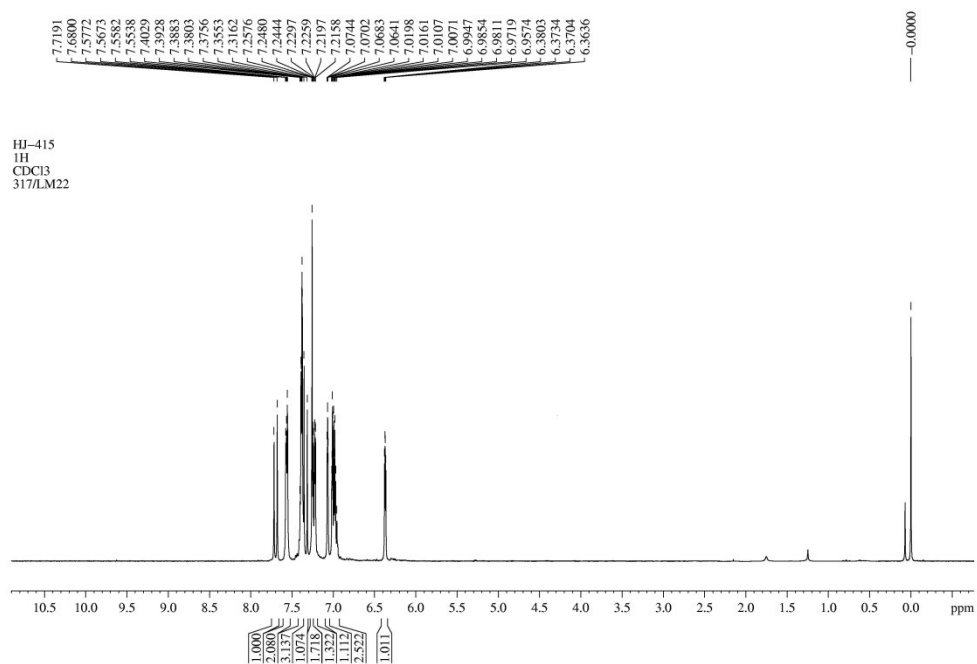


¹H NMR spectrum of compound **40**

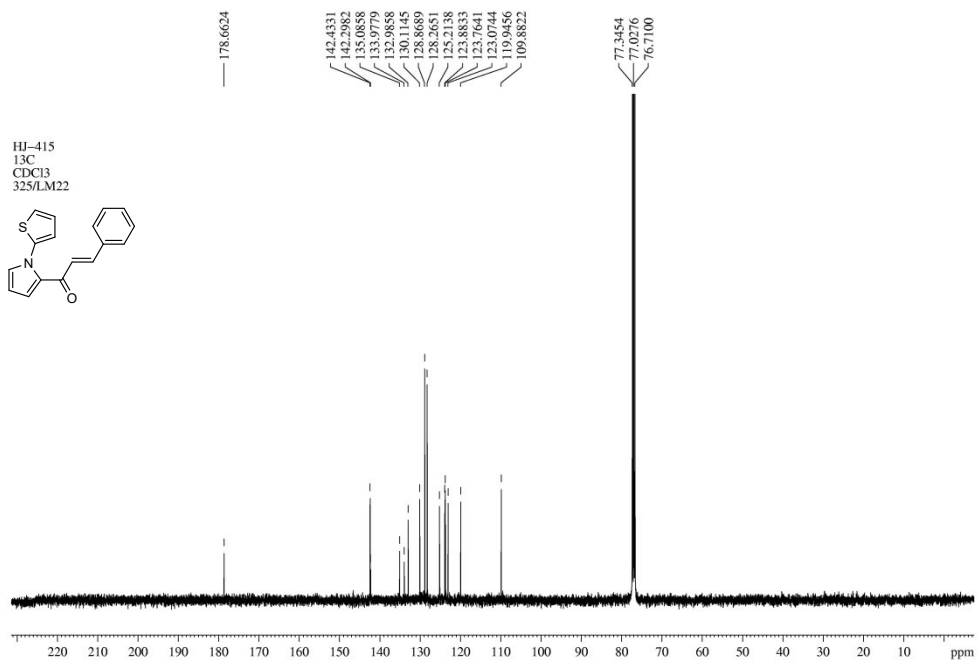


^{13}C NMR spectrum of compound **40**

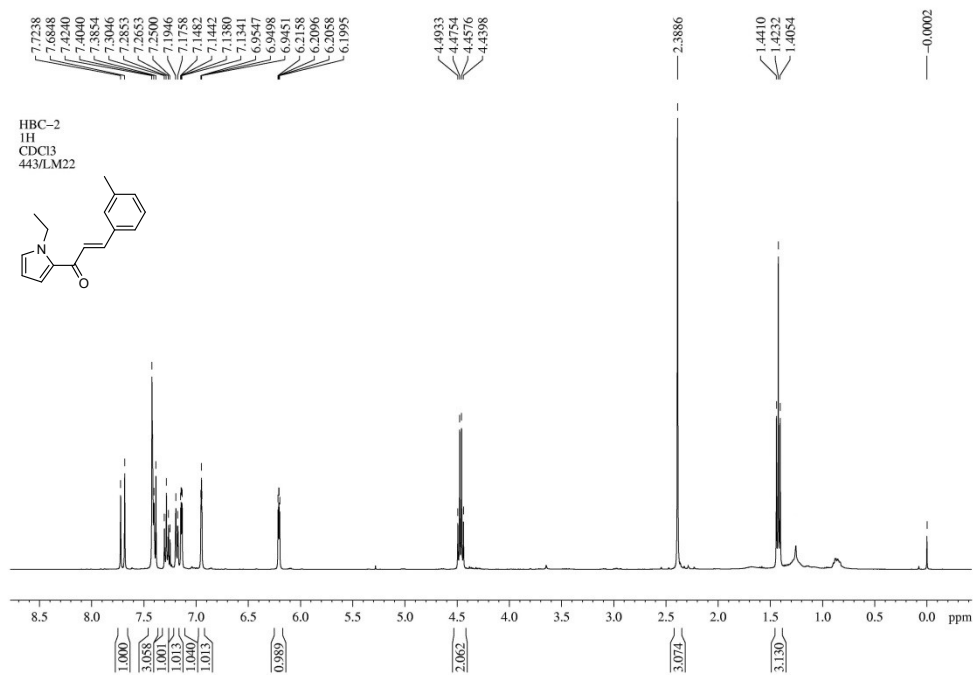




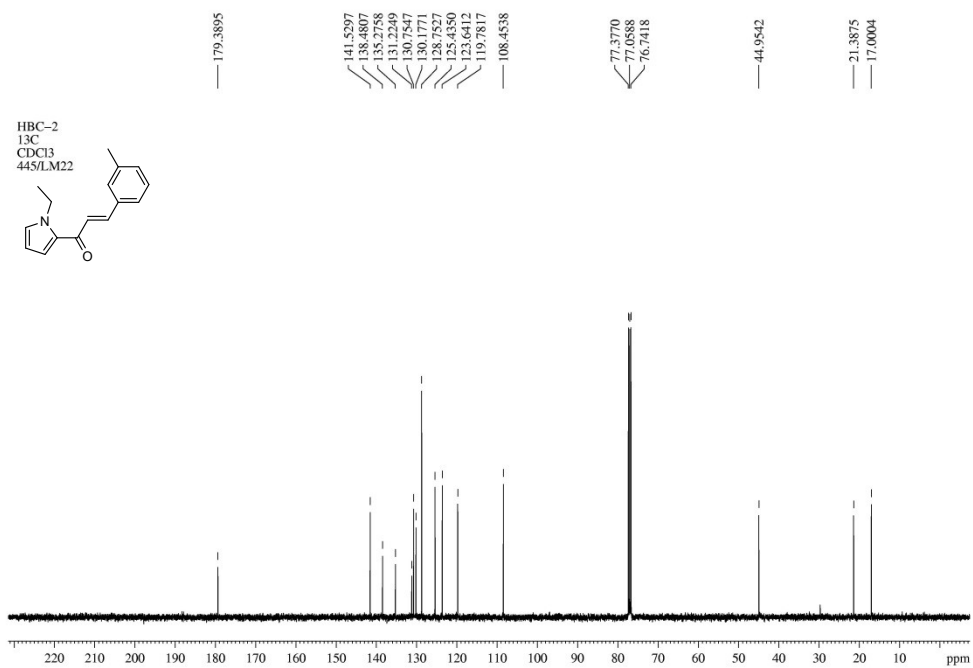
¹H NMR spectrum of compound **4p**



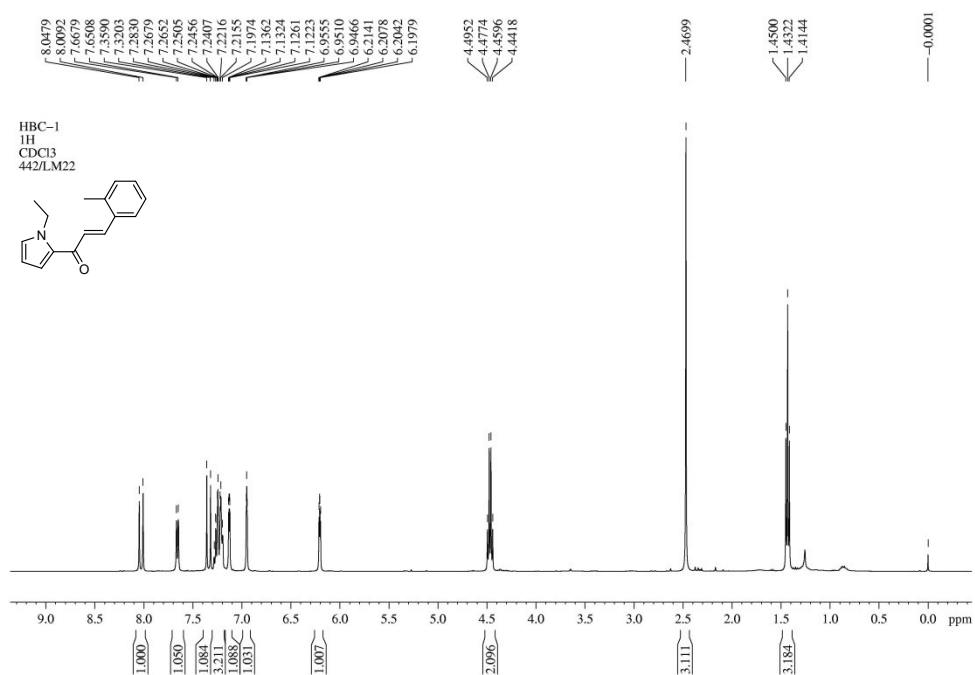
¹³C NMR spectrum of compound **4p**



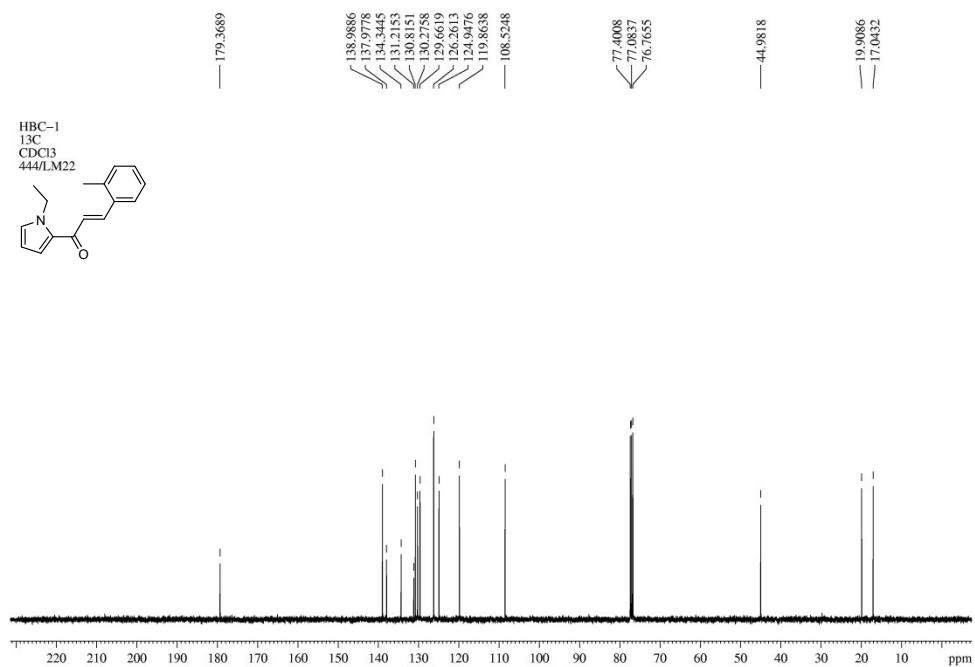
¹H NMR spectrum of compound **4q**



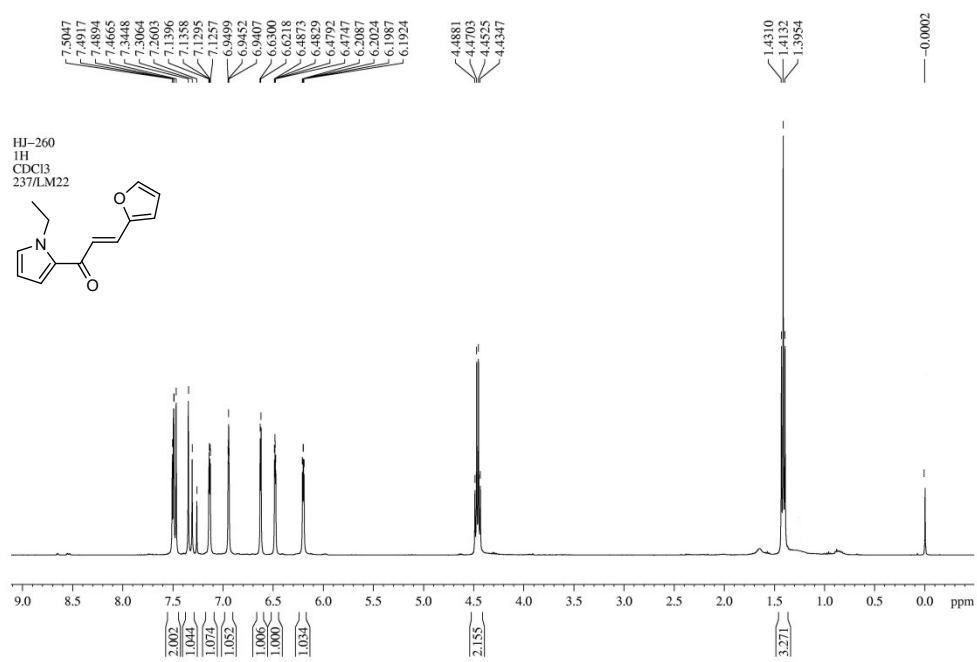
^{13}C NMR spectrum of compound **4q**



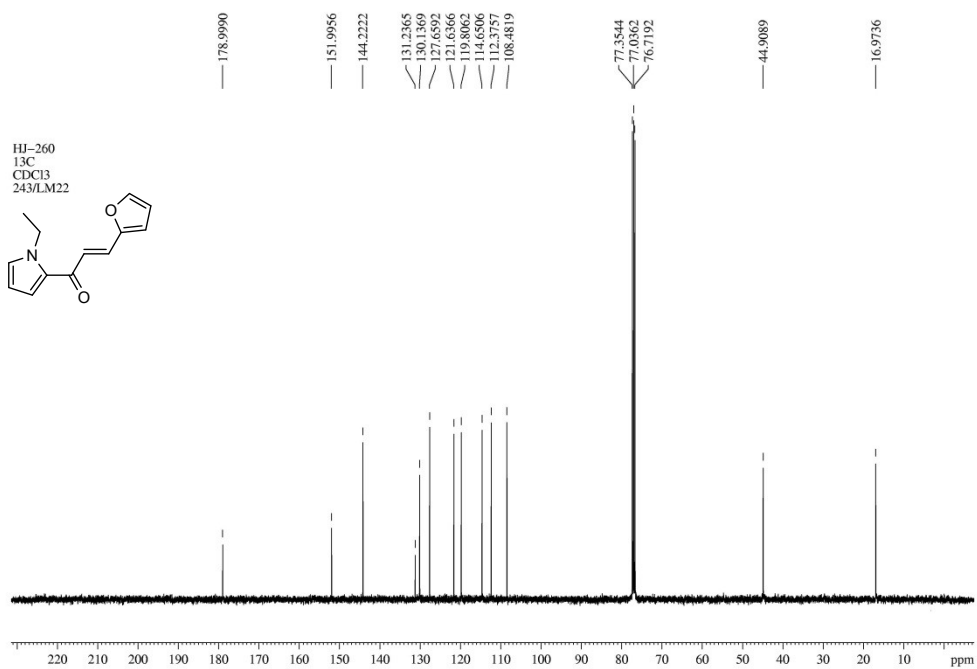
¹H NMR spectrum of compound **4r**



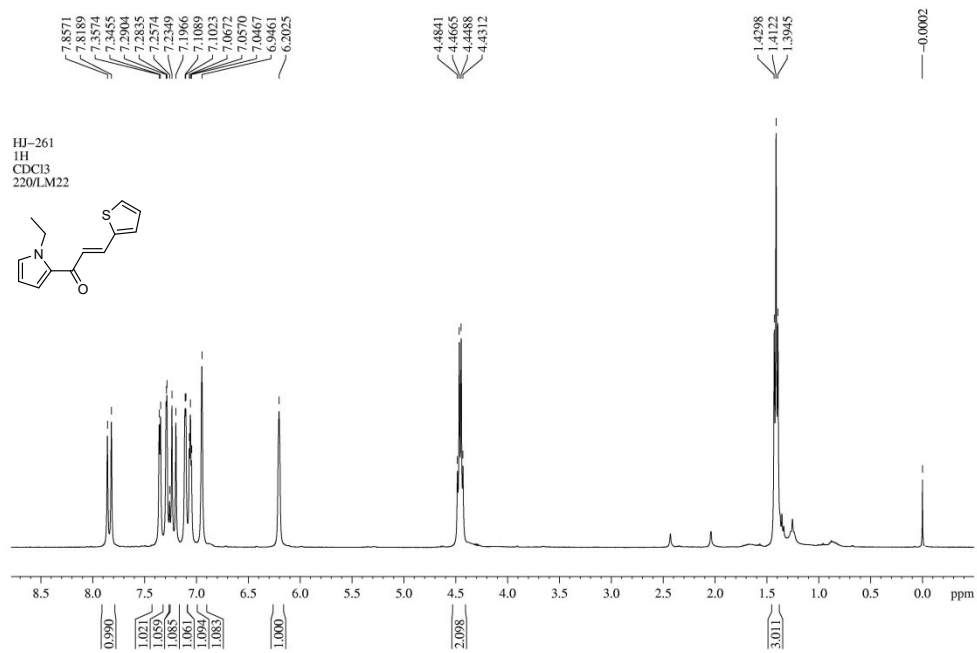
¹³C NMR spectrum of compound **4r**



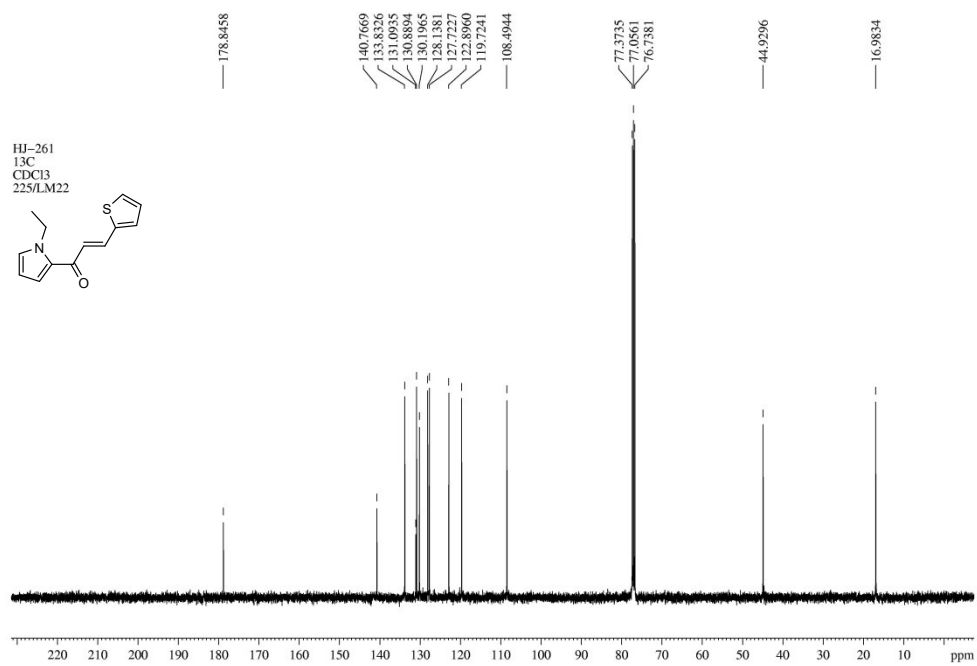
¹H NMR spectrum of compound **4s**



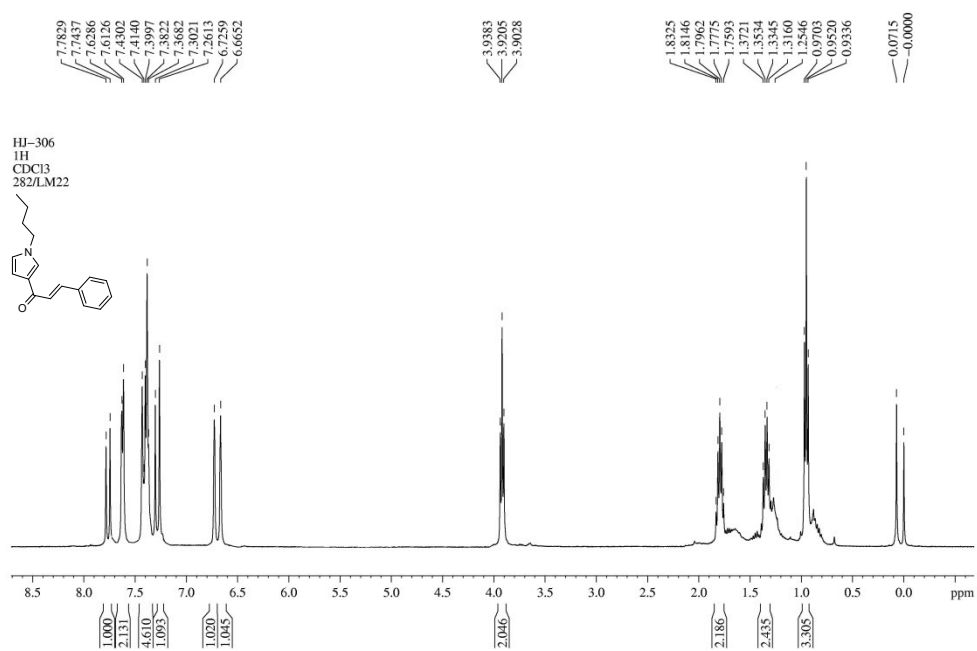
¹³C NMR spectrum of compound **4s**



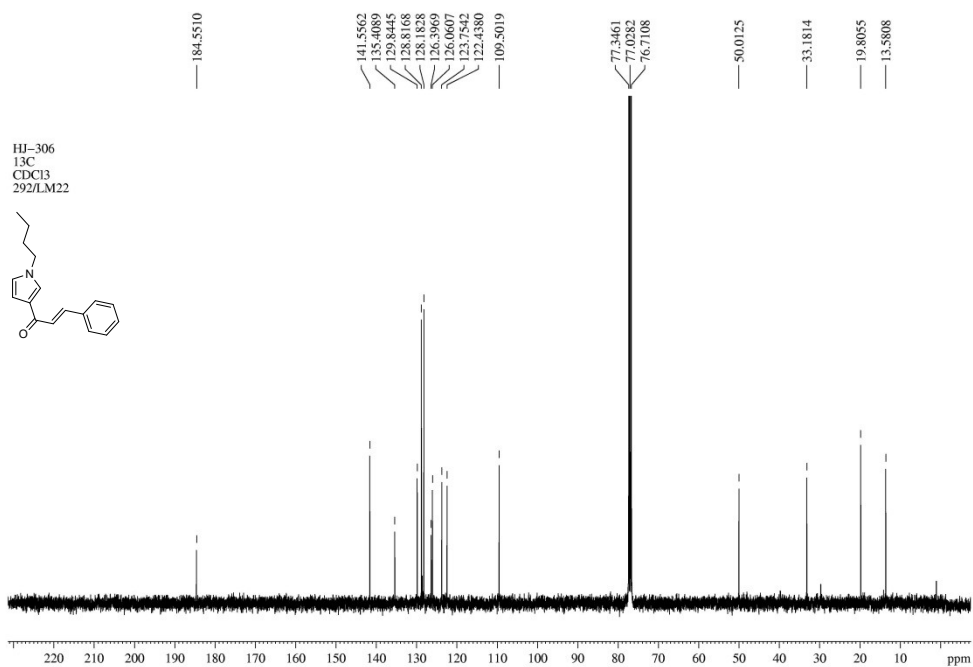
¹H NMR spectrum of compound **4t**



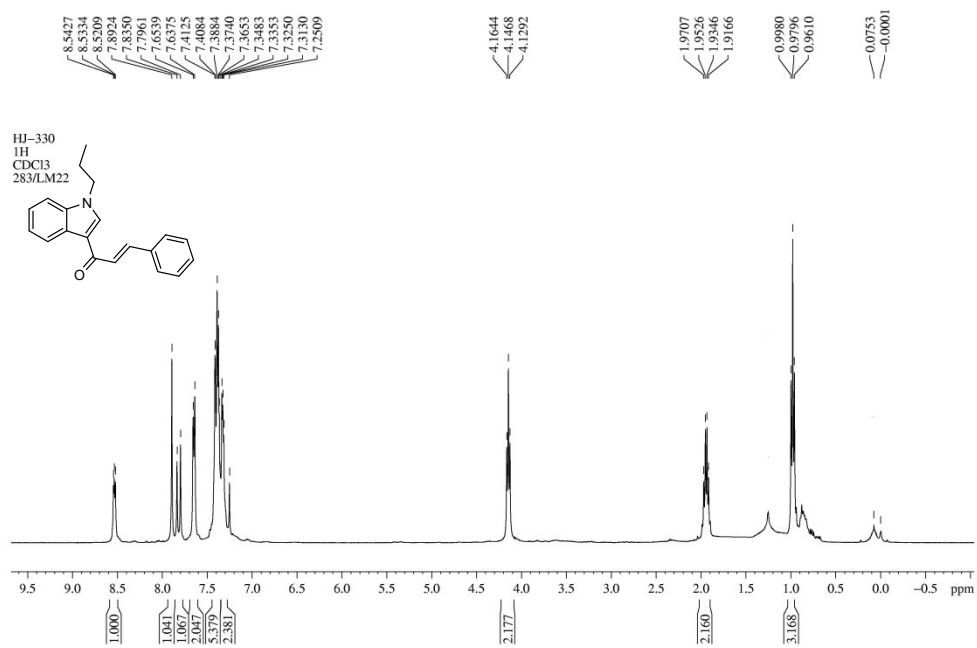
^{13}C NMR spectrum of compound **4t**



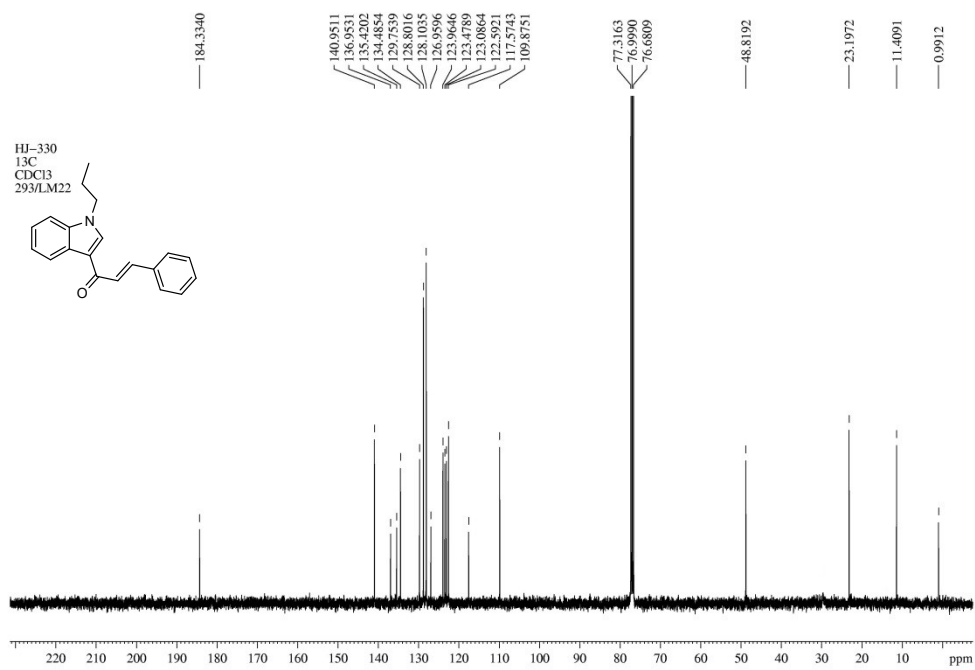
¹H NMR spectrum of compound **4u**



¹³C NMR spectrum of compound **4u**



¹H NMR spectrum of compound **4v**



^{13}C NMR spectrum of compound **4v**