Supporting Information

LIQUID-ASSISTED MECHANOSYNTHESIS OF *TRANS*-2,3-DIHYDROPYRROLES FROM CHALCONES AND ENAMINONES

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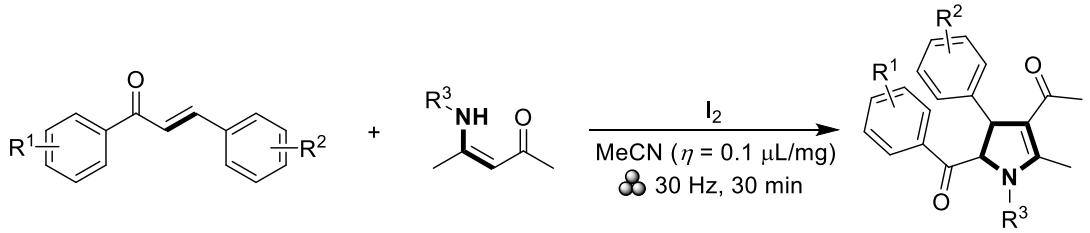
1. General Information

NMR spectra were recorded on a 400 MHz NMR spectrometer (400 MHz for ^{1}H NMR; 100 MHz for ^{13}C NMR) or 500 MHz NMR spectrometer (500 MHz for ^{1}H NMR; 125 MHz for ^{13}C NMR). ^{1}H NMR chemical shifts were determined relative to internal TMS at δ 0.0 ppm. ^{13}C NMR chemical shifts were determined relative to $CDCl_3$ at δ 77.16 ppm. Data for ^{1}H NMR and ^{13}C NMR are reported as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet). High-resolution mass spectra (HRMS) were measured with ESI-TOF in a positive mode. Ball-milling reactions were performed in a MM400 mixer mill (Retsch GmbH, Haan, Germany) at room temperature. All solvents were obtained from SCRC (Sinopharm Chemical Reagent Co., Ltd. China) in AR grade and used without further purification.

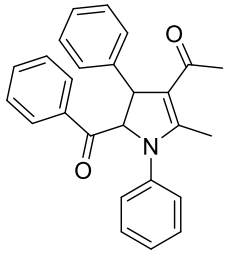
2. General Procedure for the Synthesis of Products 3



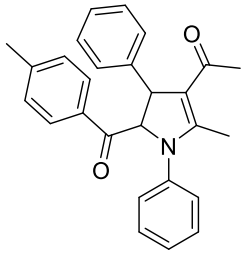
1 **2** **3**

A mixture of chalcones **1** (0.5 mmol), enaminones **2** (0.75 mmol), I_2 (253.8 mg, 1.0 mmol) and MeCN (49 μL, η = 0.1 μL/mg) together with a stainless ball (7 mm in diameter) were introduced into a stainless steel jar (5 mL). The reaction vessel along with another identical empty vessel was closed and fixed on the vibration arms of a Retsch MM400 mixer mill, and was vibrated vigorously at a rate of 1800 rounds per minute (30 Hz) at room temperature for 30 min. After completion of the reaction, the resulting mixture was extracted with ethyl acetate, and the combined solution was evaporated to remove the solvent in vacuo. The residue was separated by flash column chromatography on silica gel with ethyl acetate/petroleum ether as the eluent to afford 2,3-dihydropyrrole derivative **3**.

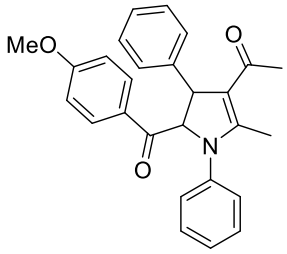
3. Characterization Data for Products 3



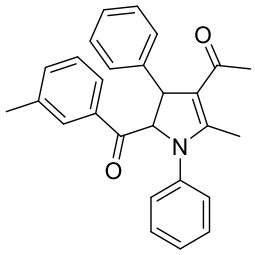
1-(*trans*-5-Benzoyl-2-methyl-1,4-diphenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3aa). Yield: 83% (158.1 mg); yellow solid, mp 146−148 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.88 (dd, J = 8.4, 1.2 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.50-7.45 (m, 2H), 7.40 (t, J = 7.3 Hz, 2H), 7.37-7.28 (m, 5H), 7.24-7.18 (m, 3H), 5.40 (d, J = 3.3 Hz, 1H), 4.15 (d, J = 3.3 Hz, 1H), 2.53 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 193.95, 192.89, 160.06, 143.57, 140.03, 133.95, 133.72, 129.37 (2C), 129.18 (2C), 129.11 (2C), 128.90 (2C), 127.56, 127.32 (2C), 126.56, 126.25 (2C), 114.07, 77.78, 51.58, 29.16, 15.17; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{24}NO_2$ $[M + H]^+$ 382.1807, found 382.1808.



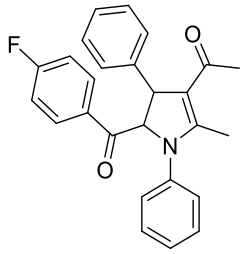
1-(*trans*-2-Methyl-5-(4-methylbenzoyl)-1,4-diphenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ba). Yield: 75% (148.4 mg); yellow solid, mp 129−131 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.78 (d, J = 8.2 Hz, 2H), 7.39 (t, J = 7.3 Hz, 2H), 7.35-7.30 (m, 3H), 7.30-7.23 (m, 4H), 7.23-7.14 (m, 3H), 5.35 (d, J = 3.2 Hz, 1H), 4.11 (d, J = 3.2 Hz, 1H), 2.51 (s, 3H), 2.43 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.70, 193.08, 160.23, 145.15, 143.70, 140.13, 131.17, 129.72 (2C), 129.45 (2C), 129.37 (2C), 129.26 (2C), 127.63, 127.45 (2C), 126.56, 126.24 (2C), 114.21, 77.75, 51.74, 29.30, 21.88, 15.35; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_2$ $[M + H]^+$ 396.1964, found 396.1966.



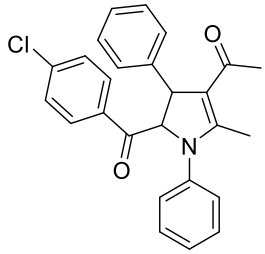
1-(*trans*-5-(4-Methoxybenzoyl)-2-methyl-1,4-diphenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ca). Yield: 72% (147.8 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84 (d, J = 8.8 Hz, 2H), 7.39 (t, J = 7.2 Hz, 2H), 7.35-7.26 (m, 5H), 7.23-7.15 (m, 3H), 6.93 (d, J = 8.9 Hz, 2H), 5.33 (d, J = 3.5 Hz, 1H), 4.12 (d, J = 3.5 Hz, 1H), 3.87 (s, 3H), 2.51 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.04, 192.71, 164.28, 160.22, 143.78, 140.15, 131.53 (2C), 129.42 (2C), 129.24 (2C), 127.59, 127.44 (2C), 126.57, 126.52, 126.21 (2C), 114.21 (3C), 77.62, 55.69, 51.94, 29.27, 15.33; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_3$ $[M + H]^+$ 412.1913, found 412.1909.



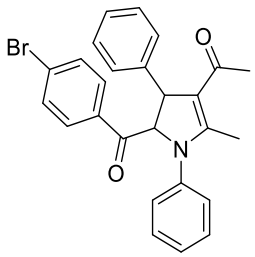
1-(*trans*-2-Methyl-5-(3-methylbenzoyl)-1,4-diphenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3da). Yield: 73% (143.9 mg); yellow solid, mp 124−126 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.68-7.63 (m, 2H), 7.45-7.30 (m, 7H), 7.27 (t, J = 8.7 Hz, 2H), 7.20 (t, J = 7.7 Hz, 3H), 5.36 (d, J = 3.4 Hz, 1H), 4.11 (d, J = 3.4 Hz, 1H), 2.51 (s, 3H), 2.36 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.17, 193.08, 160.28, 143.69, 140.15, 138.89, 134.83, 133.68, 129.94, 129.45 (2C), 129.23 (2C), 128.88, 127.66, 127.49 (2C), 126.63, 126.39, 126.35 (2C), 114.05, 77.94, 51.70, 29.30, 21.38, 15.34; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_2$ $[M + H]^+$ 396.1964, found 396.1969.



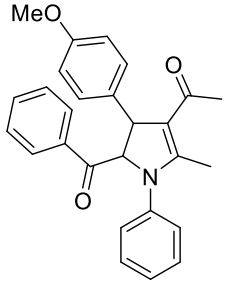
1-(*trans*-5-(4-Fluorobenzoyl)-2-methyl-1,4-diphenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ea). Yield: 78% (156.0 mg); yellow solid, mp 121−123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.88 (td, J = 7.1, 3.5 Hz, 2H), 7.43-7.31 (m, 5H), 7.27 (d, J = 7.2 Hz, 2H), 7.24-7.10 (m, 5H), 5.33 (d, J = 3.4 Hz, 1H), 4.11 (d, J = 3.4 Hz, 1H), 2.49 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.02, 192.62, 166.35 (d, J = 256.8 Hz), 160.12, 143.59, 140.06, 131.93 (d, J = 9.4 Hz, 2C), 130.18 (d, J = 3.0 Hz), 129.53 (2C), 129.36 (2C), 127.77, 127.39 (2C), 126.79, 126.43 (2C), 116.26 (d, J = 21.9 Hz, 2C), 114.22, 77.80, 51.76, 29,33, 15.30; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}FNO_2$ $[M + H]^+$ 400.1713, found 400.1713.



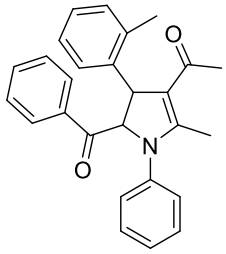
1-(*trans*-5-(4-Chlorobenzoyl)-2-methyl-1,4-diphenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3fa). Yield: 85% (176.8 mg); yellow solid, mp 138−140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.79 (d, J = 8.6 Hz, 2H), 7.47-7.30 (m, 7H), 7.29-7.15 (m, 5H), 5.32 (d, J = 3.4 Hz, 1H), 4.10 (d, J = 3.4 Hz, 1H), 2.49 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.03, 193.01, 160.12, 143.52, 140.73, 140.02, 132.10, 130.61 (2C), 129.54 (2C), 129.38 (4C), 127.80,127.39 (2C), 126.83, 126.44 (2C), 114.17, 77.83, 51.71, 29.34, 15.29; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}ClNO_2$ $[M + H]^+$ 416.1417, found 416.1424.



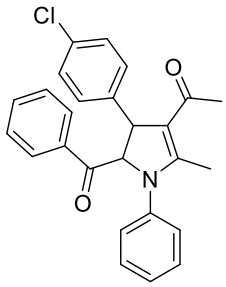
1-(*trans*-5-(4-Bromobenzoyl)-2-methyl-1,4-diphenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ga). Yield: 76% (175.1 mg); yellow solid, mp 143−145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.71 (d, J = 8.6 Hz, 2H), 7.61 (d, J = 8.6 Hz, 2H), 7.44-7.30 (m, 5H), 7.30-7.15 (m, 5H), 5.31 (d, J = 3.4 Hz, 1H), 4.09 (d, J = 3.4 Hz, 1H), 2.49 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.21, 193.04, 160.13, 143.50, 140.02, 132.51, 132.37 (2C), 130.68 (2C), 129.55 (2C), 129.53, 129.39 (2C), 127.81, 127.39 (2C), 126.84, 126.44 (2C), 114.16, 77.82, 51.69, 29.34, 15.29; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}BrNO_2$ $[M + H]^+$ 460.0912, found 460.0910.



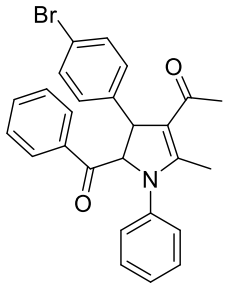
1-(*trans*-5-Benzoyl-4-(4-methoxyphenyl)-2-methyl-1-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ha). Yield: 73% (150.5 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.87 (d, J = 7.4 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.8 Hz, 2H), 7.33 (t, J = 7.8 Hz, 2H), 7.24-7.14 (m, 5H), 6.92 (d, J =8.6 Hz, 2H), 5.35 (d, J = 3.3 Hz, 1H), 4.08 (d, J = 3.3 Hz, 1H), 3.83 (s, 3H), 2.50 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.09, 193.19, 159.95, 159.07, 140.16, 135.81, 134.04, 133.79, 129.45 (2C), 129.24 (2C), 129.00 (2C), 128.45 (2C), 126.58, 126.28 (2C), 114.58 (2C), 114.28, 78.11, 55.43, 50.94, 29.26, 15.32; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_3$ $[M + H]^+$ 412.1913, found 412.1912.



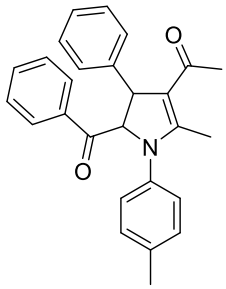
1-(*trans*-5-Benzoyl-2-methyl-1-phenyl-4-*o*-tolyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ia). Yield: 78% (154.1 mg); yellow solid, mp 122−124 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.75 (d, J = 7.6 Hz, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.43-7.30 (m, 5H), 7.29-7.15 (m, 5H), 7.12 (d, J = 7.3 Hz, 1H), 5.38 (d, J = 4.5 Hz, 1H), 4.45 (d, J = 4.5 Hz, 1H), 2.46 (s, 3H), 2.07 (s, 3H), 1.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.74, 192.85, 159.80, 142.51, 140.28, 135.18, 135.11, 134.47, 134.05, 130.71, 129.54 (2C), 129.04 (2C), 128.98 (2C), 127.40, 127.24, 126.83, 126.62 (2C), 114.55, 77.81, 51.56, 29.09, 19.45, 15.35; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_2$ $[M + H]^+$ 396.1964, found 396.1961.



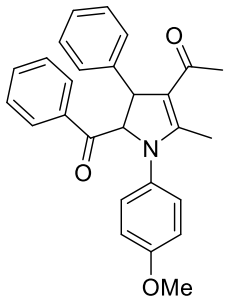
1-(*trans*-5-Benzoyl-4-(4-chlorophenyl)-2-methyl-1-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ja). Yield: 68% (141.1 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86-7.81 (m, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.8 Hz, 2H), 7.38-7.31 (m, 4H), 7.25-7.15 (m, 5H), 5.32 (d, J = 3.4 Hz, 1H), 4.12 (d, J = 3.4 Hz, 1H), 2.48 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.80, 192.56, 160.13, 142.27, 139.93, 134.21, 133.71, 133.41, 129.57 (2C), 129.44 (2C), 129.17 (2C), 129.11 (2C), 128.74 (2C), 126.89, 126.46 (2C), 114.27, 77.53, 50.94, 29.30, 15.33; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}ClNO_2$ $[M + H]^+$ 416.1417, found 416.1431.



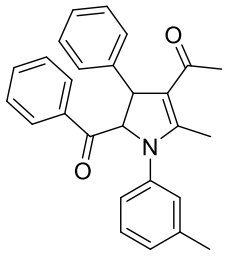
1-(*trans*-5-Benzoyl-4-(4-bromophenyl)-2-methyl-1-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ka). Yield: 65% (149.9 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86-7.81 (m, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.47 (t, J = 7.8 Hz, 2H), 7.34 (t, J = 7.8 Hz, 2H), 7.25-7.13 (m, 5H), 5.32 (d, J = 3.3 Hz, 1H), 4.11 (d, J = 3.3 Hz, 1H), 2.48 (s, 3H), 1.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.76, 192.54, 160.19, 142.78, 139.89, 134.22, 133.69, 132.39 (2C), 129.57 (2C), 129.16 (2C), 129.11 (2C), 129.10 (2C), 126.91, 126.47 (2C), 121.51, 114.22, 77.48, 50.99, 29.28, 15.33; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}BrNO_2$ $[M + H]^+$ 460.0912, found 460.0906.



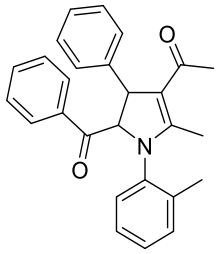
1-(*trans*-5-Benzoyl-2-methyl-4-phenyl-1-*p*-tolyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ab). Yield: 85% (168.2 mg); yellow solid, mp 121−123 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84 (d, J = 7.8 Hz, 2H), 7.60 (t, J = 7.3 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.38 (t, J = 7.3 Hz, 2H), 7.32 (d, J = 6.9 Hz, 1H), 7.27 (d, J = 7.9 Hz, 2H), 7.13 (d, J = 8.3 Hz, 2H), 7.10 (d, J = 8.3 Hz, 2H), 5.34 (d, J = 3.2 Hz, 1H), 4.12 (d, J = 3.2 Hz, 1H), 2.47 (s, 3H), 2.31 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.16, 192.86, 160.72, 143.88, 137.41, 136.87, 134.03, 133.88, 130.07 (2C), 129.27 (2C), 129.25 (2C), 128.98 (2C), 127.62, 127.46 (2C), 126.66 (2C), 113.64, 77.99, 51.66, 29.25, 21.13, 15.20; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_2$ $[M + H]^+$ 396.1964, found 396.1965.



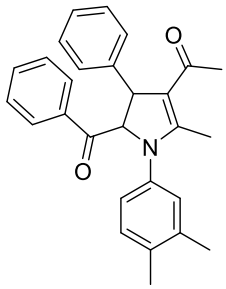
1-(*trans*-5-Benzoyl-1-(4-methoxyphenyl)-2-methyl-4-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ac). Yield: 86% (177.2 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.83 (d, J = 7.3 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 7.39 (t, J = 7.3 Hz, 2H), 7.35-7.25 (m, 3H), 7.19 (d, J = 8.9 Hz, 2H), 6.85 (d, J = 8.9 Hz, 2H), 5.31 (d, J = 3.6 Hz, 1H), 4.13 (d, J = 3.6 Hz, 1H), 3.77 (s, 3H), 2.43 (s, 3H), 1.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.24, 192.69, 161.27, 158.56, 143.98, 133.98, 133.89, 132.61, 129.23 (2C), 129.17 (2C), 128.92 (2C), 128.80 (2C), 127.56, 127.41 (2C), 114.61 (2C), 112.93, 78.17, 55.56, 51.64, 29.14, 14.95; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_3$ $[M + H]^+$ 412.1913, found 412.1918.



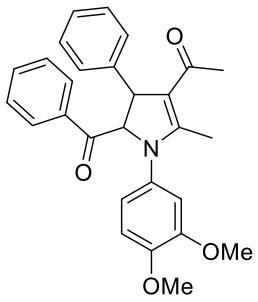
1-(*trans*-5-Benzoyl-2-methyl-4-phenyl-1-m-tolyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ad). Yield: 83% (164.2 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86 (d, J = 7.2 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.8 Hz, 2H), 7.39 (t, J = 7.5 Hz, 2H), 7.34-7.25 (m, 3H), 7.21 (t, J = 7.7 Hz, 1H), 7.01 (t, J = 7.5 Hz, 3H), 5.37 (d, J = 3.3 Hz, 1H), 4.12 (d, J = 3.3 Hz, 1H), 2.50 (s, 3H), 2.31 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.03, 192.88, 160.38, 143.69, 139.94, 139.44, 134.01, 133.77, 129.23 (2C), 129.20 (2C), 129.18, 128.96 (2C), 127.59, 127.53, 127.39 (2C), 126.88, 123.48, 113.94, 77.81, 51.59, 29.23, 21.46, 15.29; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_2$ $[M + H]^+$ 396.1964, found 396.1959.



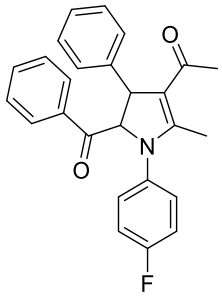
1-(*trans*-5-Benzoyl-2-methyl-4-phenyl-1-*o*-tolyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ae). Yield: 82% (162.3 mg); yellow solid, mp 33−35 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.82 (d, J = 7.7 Hz, 2H), 7.59 (t, J = 7.3 Hz, 1H), 7.44 (t, J = 7.2 Hz, 2H), 7.38 (t, J = 7.3 Hz, 2H), 7.31 (t, J = 7.2 Hz, 1H), 7.28-7.24 (m, 3H), 7.21-7.15 (m, 3H), 5.23 (d, J = 4.1 Hz, 1H), 4.27 (d, J = 4.1 Hz, 1H), 2.33 (s, 3H), 2.22 (s, 3H), 1.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.25, 193.00, 162.93, 143.66, 137.40, 136.52, 134.30, 134.01, 131.66, 131.27, 129.25 (2C), 129.20 (2C), 128.95 (2C), 128.70, 128.61, 127.89 (2C), 127.61, 127.07, 75.86, 52.36, 29.13, 18.38, 14.62; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_2$ $[M + H]^+$ 396.1964, found 396.1966.



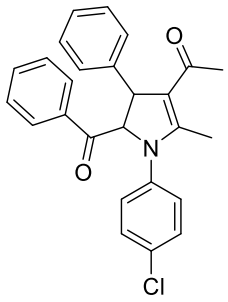
1-(*trans*-5-Benzoyl-1-(3,4-dimethylphenyl)-2-methyl-4-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3af). Yield: 79% (161.6 mg); yellow solid, mp 61−63 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.85 (d, J = 7.2 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.7 Hz, 2H), 7.39 (t, J = 7.3 Hz, 2H), 7.35-7.24 (m, 3H), 7.08 (d, J = 7.8 Hz, 1H), 6.95(d, J = 8.2 Hz, 2H), 5.33 (d, J = 3.5 Hz, 1H), 4.11 (d, J = 3.5 Hz, 1H), 2.47 (s, 3H), 2.21 (s, 6H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.18, 192.77, 160.90, 143.95, 137.89, 137.63, 135.63, 133.98, 133.93, 130.46, 129.25 (4C), 128.95 (2C), 127.78, 127.57, 127.47 (2C), 124.23, 113.47, 78.00, 51.65, 29.22, 20.01, 19.45, 15.22; HRMS (ESI-TOF) m/z calcd for $C_{28}H_{28}NO_2$ $[M + H]^+$ 410.2120, found 410.2127.



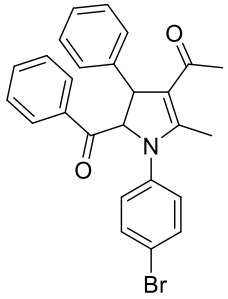
1-(*trans*-5-Benzoyl-1-(3,4-dimethoxyphenyl)-2-methyl-4-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ag). Yield: 77% (170.3 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.83 (d, J = 7.3 Hz, 2H), 7.60 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.8 Hz, 2H), 7.40 (t, J = 7.3 Hz, 2H), 7.35-7.25 (m, 3H), 6.83-6.76 (m, 3H), 5.31 (d, J = 3.7 Hz, 1H), 4.15 (d, J = 3.7 Hz, 1H), 3.84 (d, J = 7.7 Hz, 6H), 2.45 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.50, 192.82, 161.15, 149.30, 148.31, 143.97, 134.00 (2C), 132.95, 129.24 (2C), 129.17 (2C), 128.94 (2C), 127.58, 127.44 (2C), 119.79 (2C), 113.01, 111.28 (2C), 78.26, 56.12, 51.75, 29.17, 15.05; HRMS (ESI-TOF) m/z calcd for $C_{28}H_{28}NO_4$ $[M + H]^+$ 442.2018, found 442.2019.



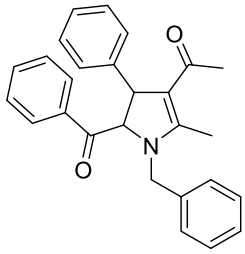
1-(*trans*-5-Benzoyl-1-(4-fluorophenyl)-2-methyl-4-phenyl-4,5-dihydro-1H-pyrrol-3-yl)ethanone (3ah). Yield: 80% (159.7 mg); yellow solid, mp 143−145 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.84 (d, J = 7.3 Hz, 2H), 7.62 (t, J = 7.4 Hz, 1H), 7.46 (t, J = 7.8 Hz, 2H), 7.40 (t, J = 7.2 Hz, 2H), 7.34 (d, J = 7.2 Hz, 1H), 7.30-7.18 (m, 4H), 7.03 (t, J = 8.5 Hz, 2H), 5.32 (d, J = 3.4 Hz, 1H), 4.13 (d, J = 3.4 Hz, 1H), 2.44 (s, 3H), 1.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.09, 193.08, 161.28 (d, J = 247.5 Hz), 160.32, 143.67, 136.02 (d, J = 3.1 Hz), 134.17, 133.75, 129.35 (2C), 129.24 (2C), 129.042 (d, J = 8.6 Hz, 2C), 129.040 (2C), 127.74, 127.41 (2C), 116.41 (d, J = 22.7 Hz, 2C), 113.71, 78.07, 51.70, 29.29, 15.02; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}FNO_2$ $[M + H]^+$ 400.1713, found 400.1720.



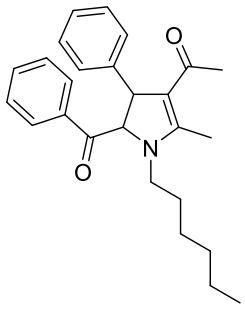
1-(*trans*-5-Benzoyl-1-(4-chlorophenyl)-2-methyl-4-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3ai). Yield: 77% (160.6 mg); yellow solid, mp 145−147 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.85 (d, J = 7.3 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.8 Hz, 2H), 7.39 (t, J = 7.2 Hz, 2H), 7.35-7.23 (m, 5H), 7.13 (d, J = 8.7 Hz, 2H), 5.34 (d, J = 3.3 Hz, 1H), 4.12 (d, J = 3.3 Hz, 1H), 2.49 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.93, 193.22, 159.54, 143.41, 138.69, 134.24, 133.61, 132.22, 129.63 (2C), 129.37 (2C), 129.25 (2C), 129.08 (2C), 127.80, 127.69 (2C), 127.38 (2C), 114.59, 77.81, 51.64, 29.36, 15.21; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}ClNO_2$ $[M + H]^+$ 416.1417, found 416.1415.



1-(*trans*-5-Benzoyl-1-(4-bromophenyl)-2-methyl-4-phenyl-4,5-dihydro-1H-pyrrol-3-yl)ethanone (3aj). Yield: 76% (174.7 mg); yellow solid, mp 152−154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.85 (d, J = 7.2 Hz, 2H), 7.63 (t, J = 7.4 Hz, 1H), 7.51-7.42 (m, 4H), 7.39 (t, J = 7.2 Hz, 2H), 7.33 (d, J = 7.2 Hz, 1H), 7.25 (d, J = 8.1 Hz, 2H), 7.06 (d, J = 8.8 Hz, 2H), 5.34 (d, J = 3.2 Hz, 1H), 4.12 (d, J = 3.2 Hz, 1H), 2.50 (s, 3H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.90, 193.26, 159.38, 143.37, 139.23, 134.25, 133.59, 132.60 (2C), 129.37 (2C), 129.26 (2C), 129.09 (2C), 127.88 (2C), 127.81, 127.38 (2C), 119.99, 114.76, 77.75, 51.64, 29.38, 15.25; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{23}BrNO_2$ $[M + H]^+$ 460.0912, found 460.0915.



1-(*trans*-5-benzoyl-1-benzyl-2-methyl-4-phenyl-4,5-dihydro-1H-pyrrol-3-yl)ethanone (3ak). Yield: 82% (162.4 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.75 (d, J = 7.3 Hz, 2H), 7.61 (t, J = 7.4 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H), 7.33-7.22 (m, 6H), 7.16 (d, J = 6.6 Hz, 2H), 7.14-7.10 (m, 2H), 4.91-4.85 (m, 2H), 4.09 (d, J = 15.8 Hz, 1H), 4.03 (d, J = 3.7 Hz, 1H), 2.67 (s, 3H), 1.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.82, 192.52, 162.46, 143.77, 136.31, 134.05, 133.89, 129.17 (2C), 129.02 (2C), 129.01 (2C), 128.95 (2C), 128.02, 127.73 (2C), 127.54 (2C), 127.43, 111.01, 74.16, 51.24, 48.96, 29.13, 13.42; HRMS (ESI-TOF) m/z calcd for $C_{27}H_{26}NO_2$ $[M + H]^+$ 396.1964, found 396.1974.



1-(*trans*-5-Benzoyl-1-hexyl-2-methyl-4-phenyl-4,5-dihydro-1*H*-pyrrol-3-yl)ethanone (3al). Yield: 79% (153.7 mg); yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90 (d, J = 7.4 Hz, 2H), 7.65 (t, J = 7.4 Hz, 1H), 7.50 (t, J = 7.8 Hz, 2H), 7.35 (t, J = 7.2 Hz, 2H), 7.30 (d, J = 7.1 Hz, 1H), 7.17 (d, J = 6.9 Hz, 2H), 5.01 (d, J = 3.5 Hz, 1H), 4.01 (d, J = 3.5 Hz, 1H), 3.62-3.51 (m, 1H), 3.01-2.90 (m, 1H), 2.59 (s, 3H), 1.71 (s, 3H), 1.52-1.43 (m, 2H), 1.32-1.24 (m, 6H), 0.86 (t, J = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 194.56, 191.91, 162.99, 144.16, 134.09, 133.85, 129.19 (2C), 129.13 (2C), 129.03 (2C), 127.46, 127.43 (2C), 110.74, 74.59, 51.22, 45.06, 31.53, 28.99, 28.58, 26.64, 22.65, 14.07, 13.24; HRMS (ESI-TOF) m/z calcd for $C_{26}H_{32}NO_2$ $[M + H]^+$ 390.2433, found 390.2437.

4. Copies of NMR Spectra for Products 3

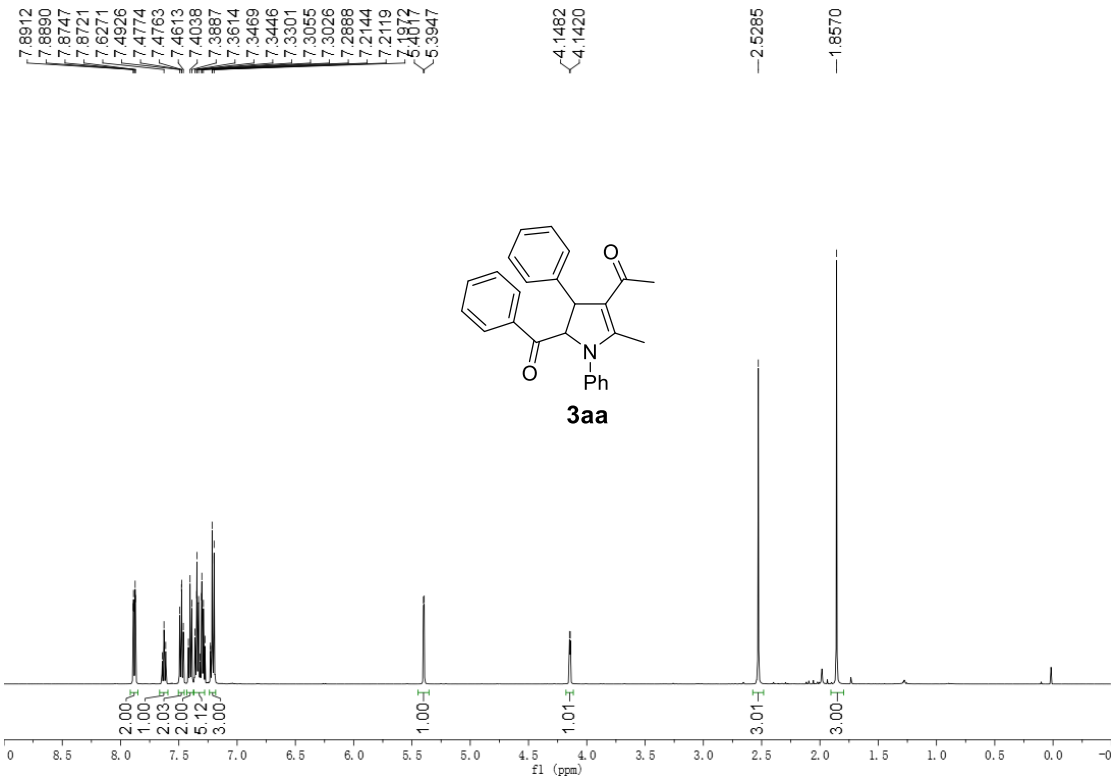


Figure S1. ^{1}H NMR (500 MHz, $CDCl_3$) of compound 3aa

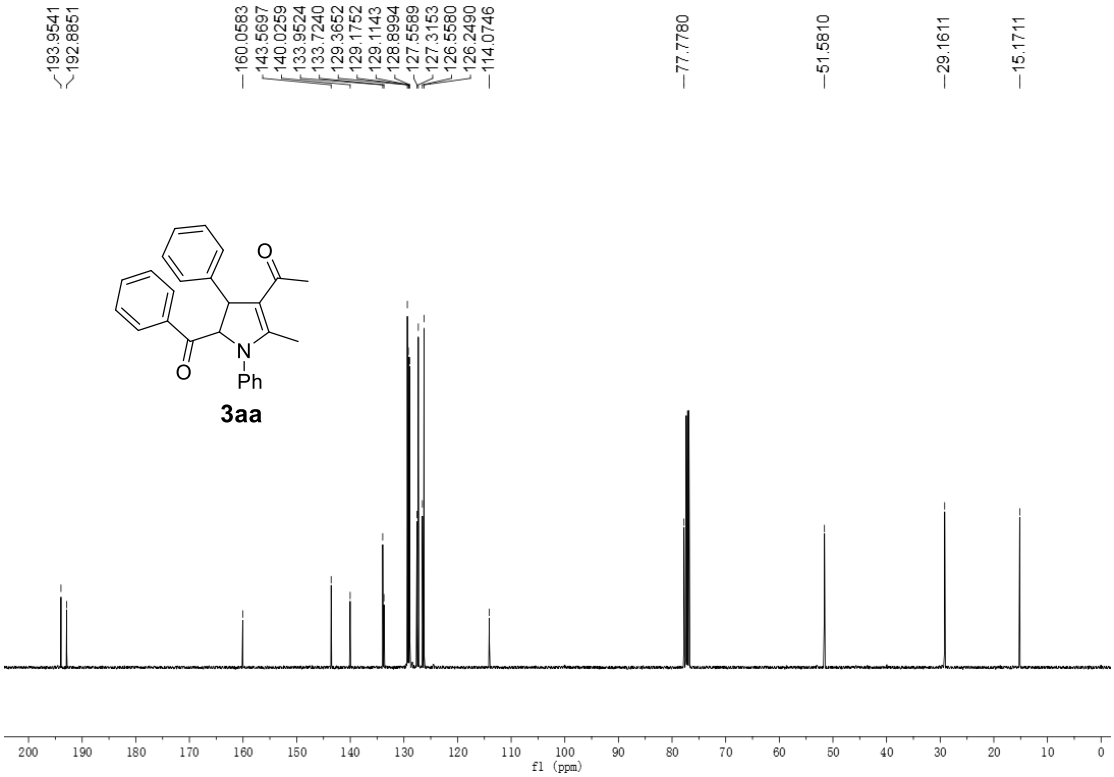


Figure S2. ^{13}C NMR (125 MHz, $CDCl_3$) of compound 3aa

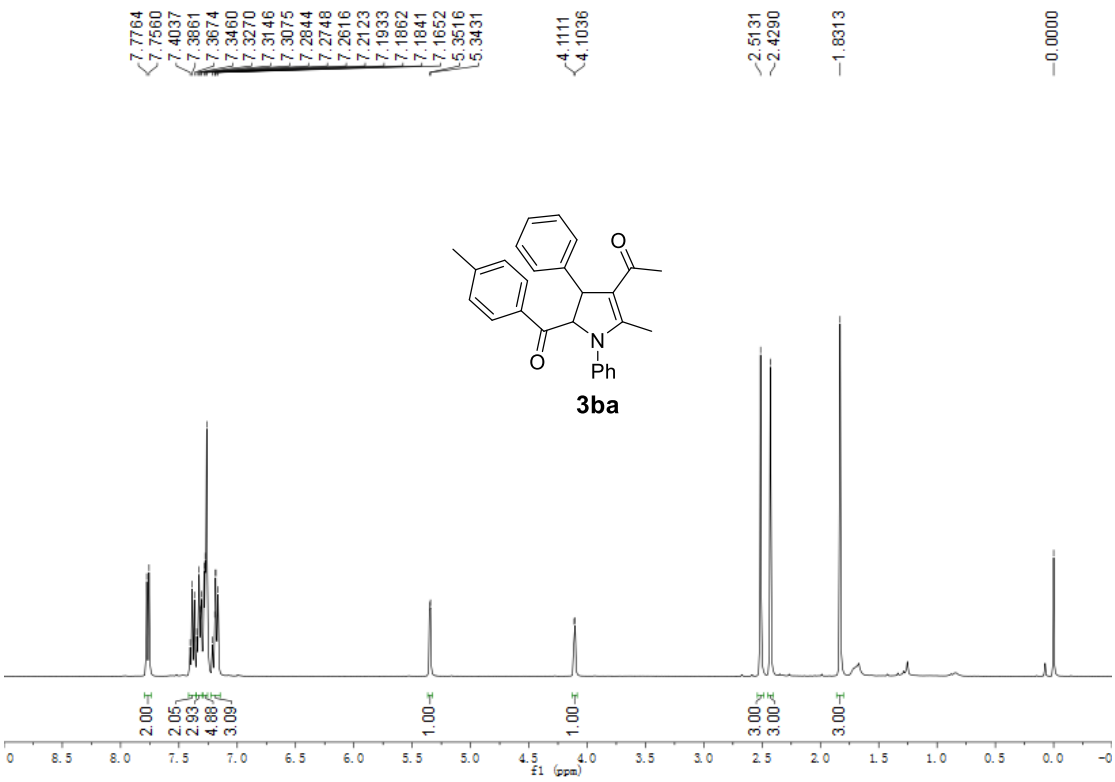


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ba

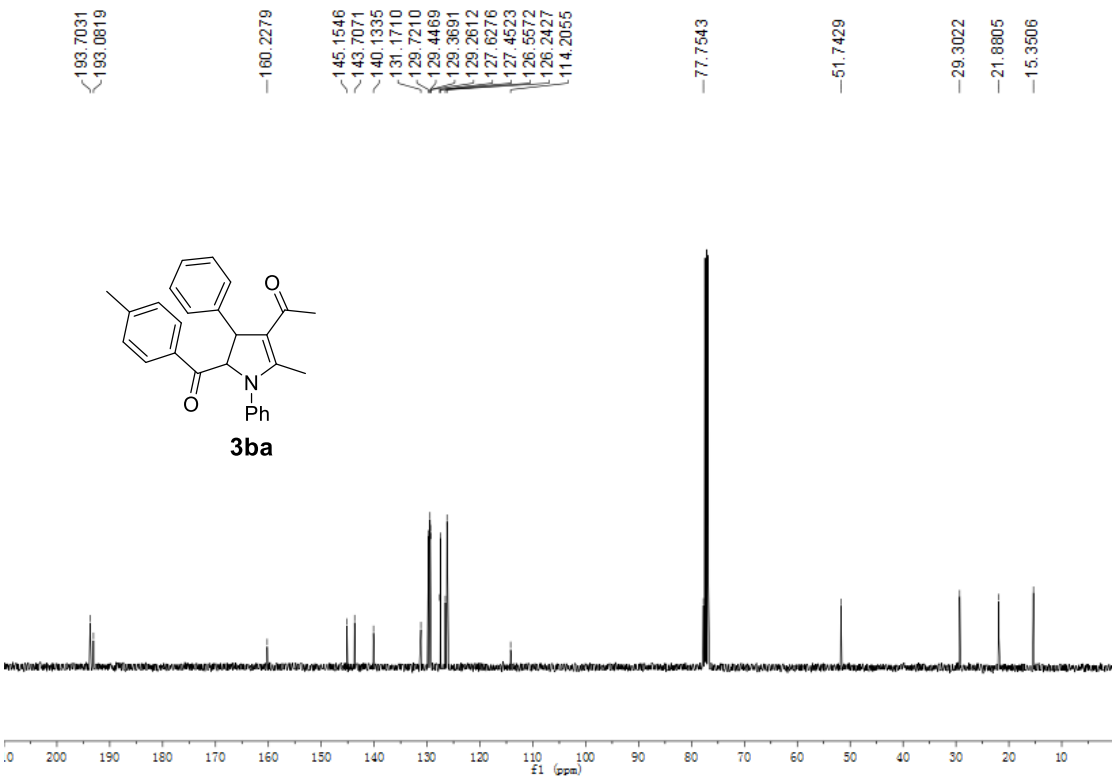


Figure S4. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ba

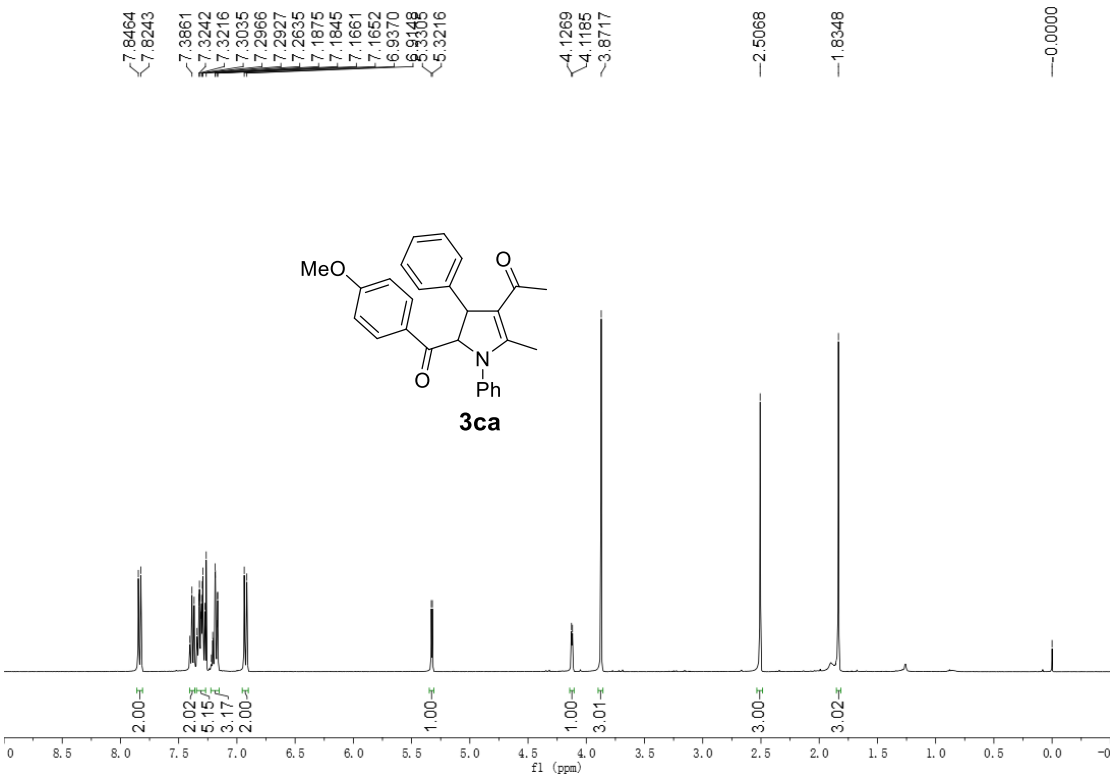


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ca

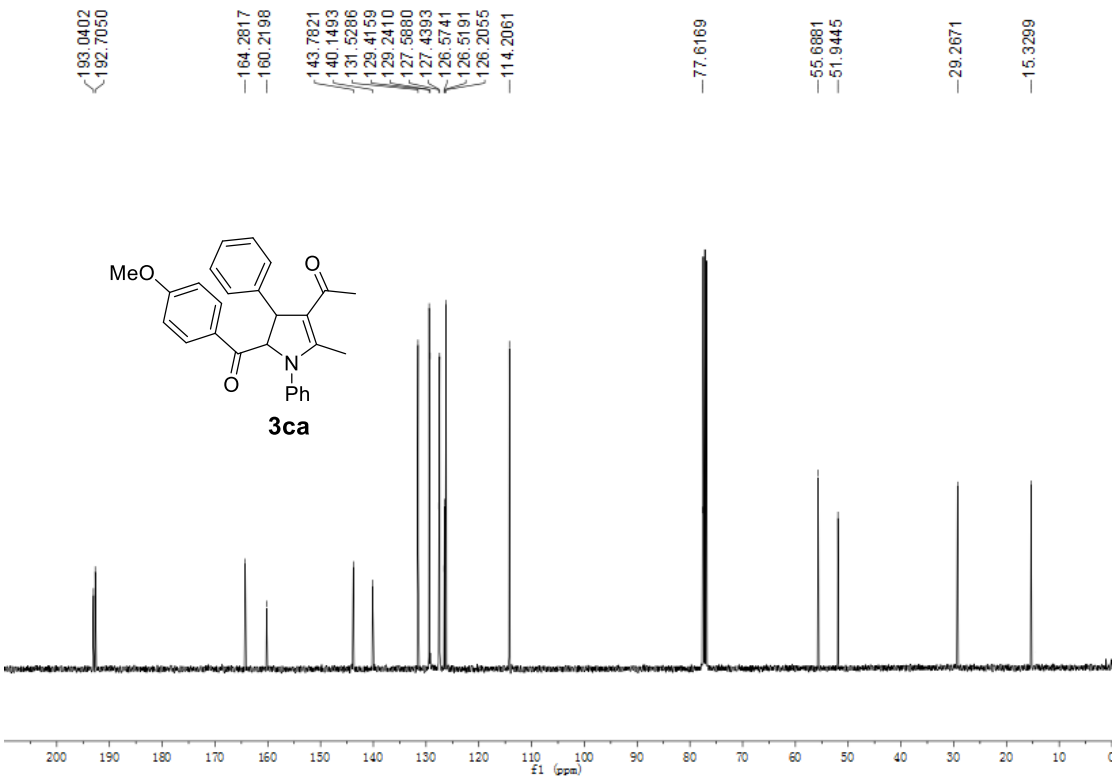


Figure S6. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ca

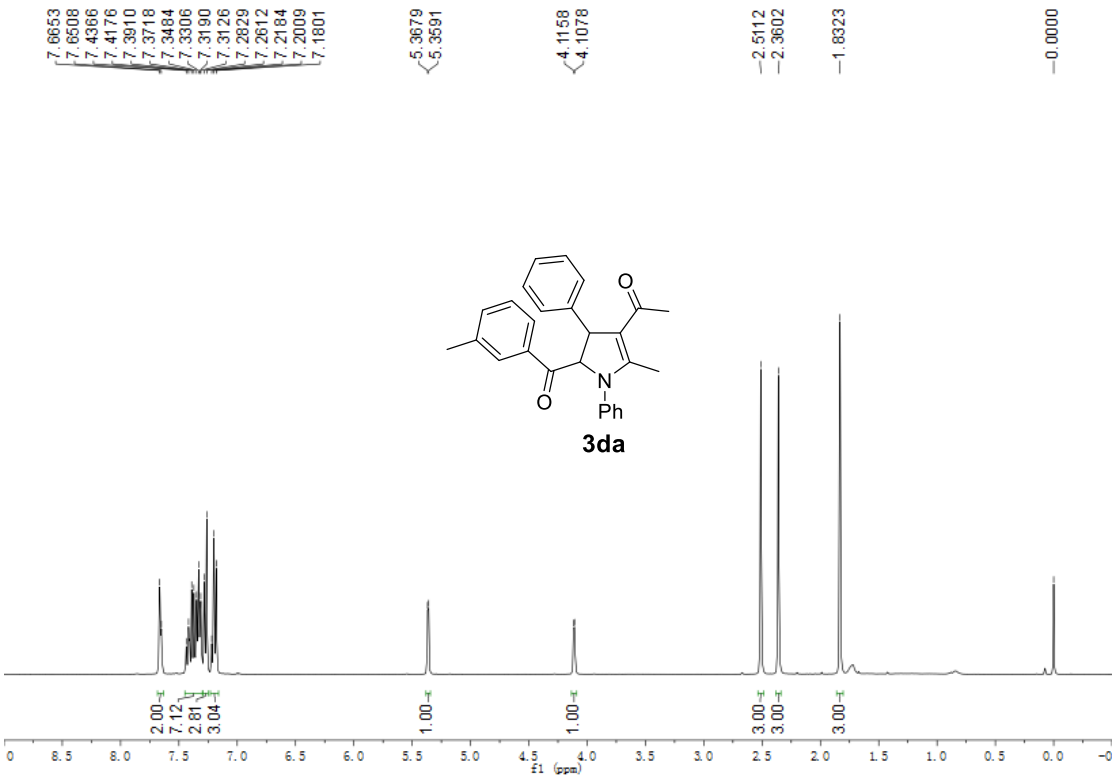


Figure S7. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3da

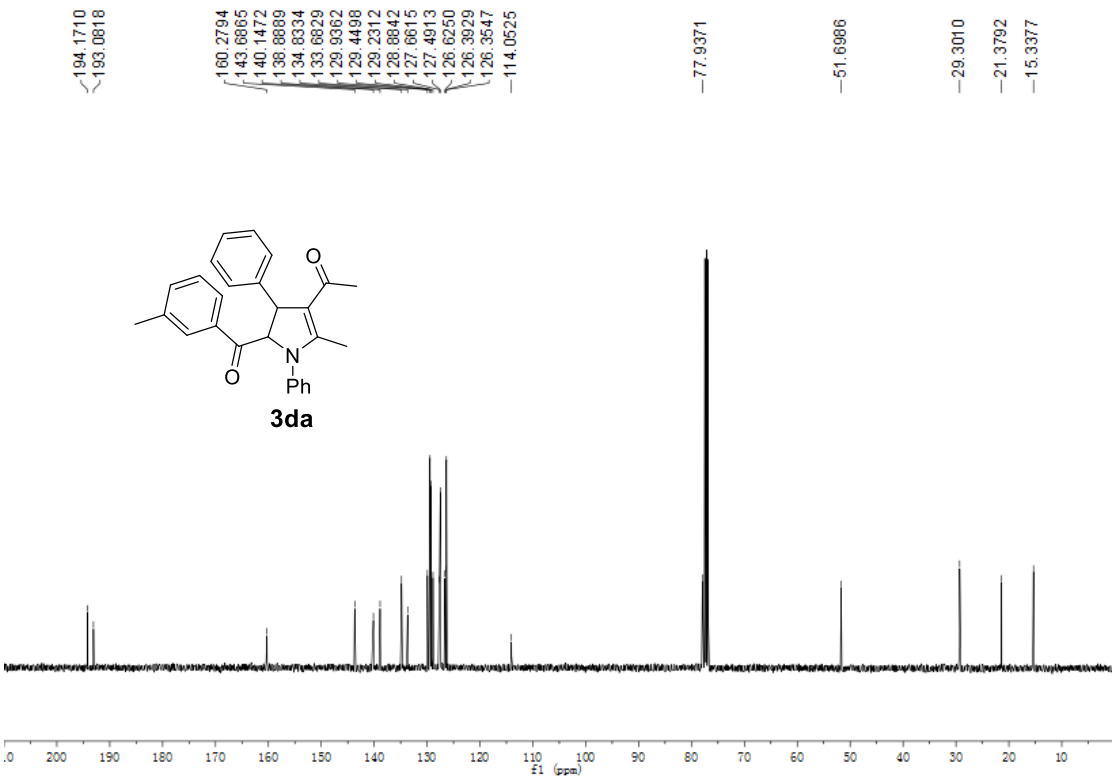


Figure S8. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3da

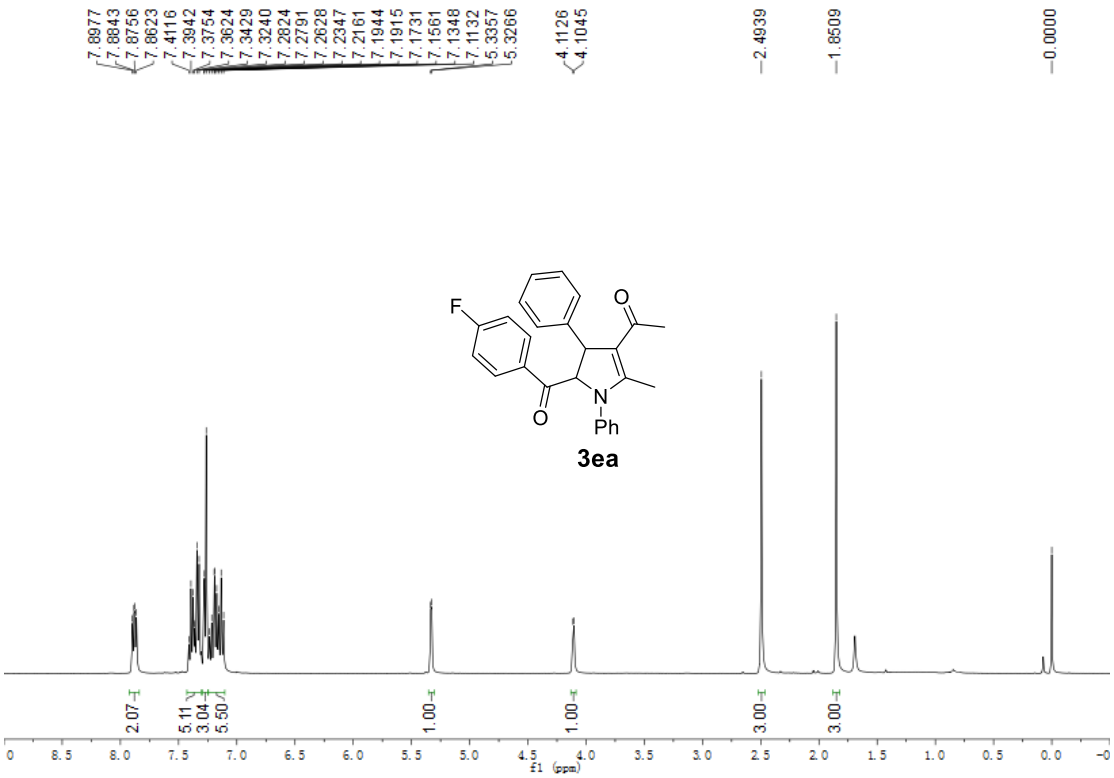


Figure S9. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ea

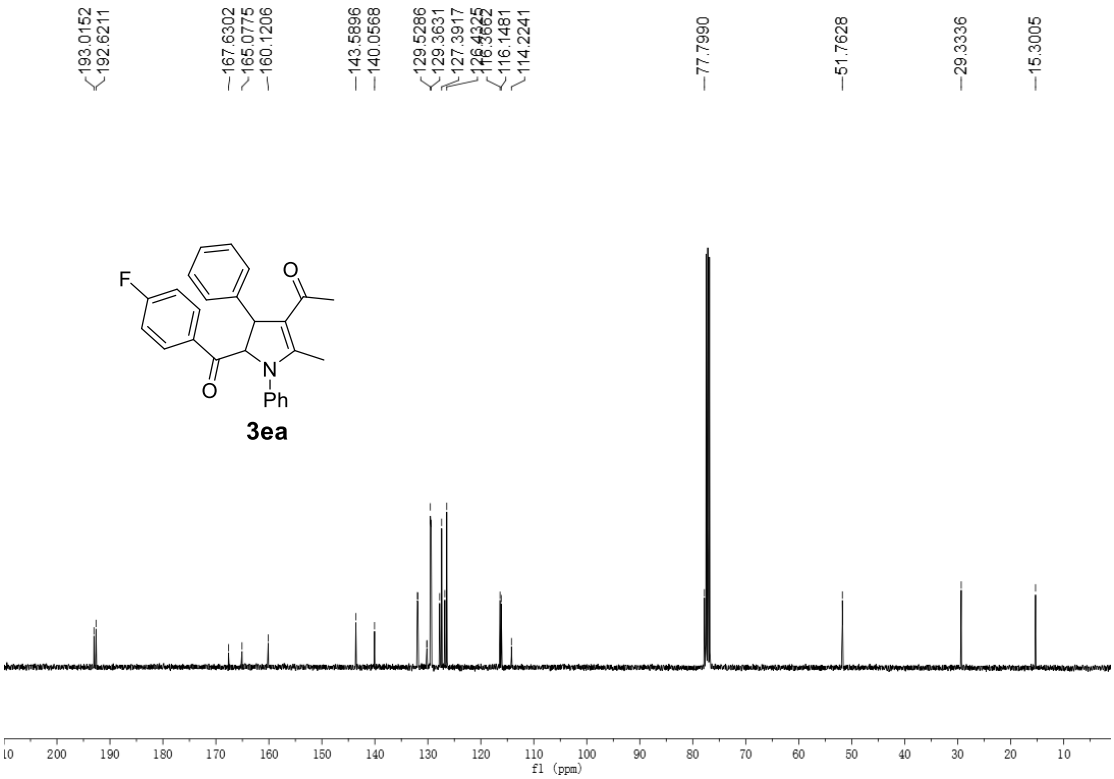


Figure S10. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ea

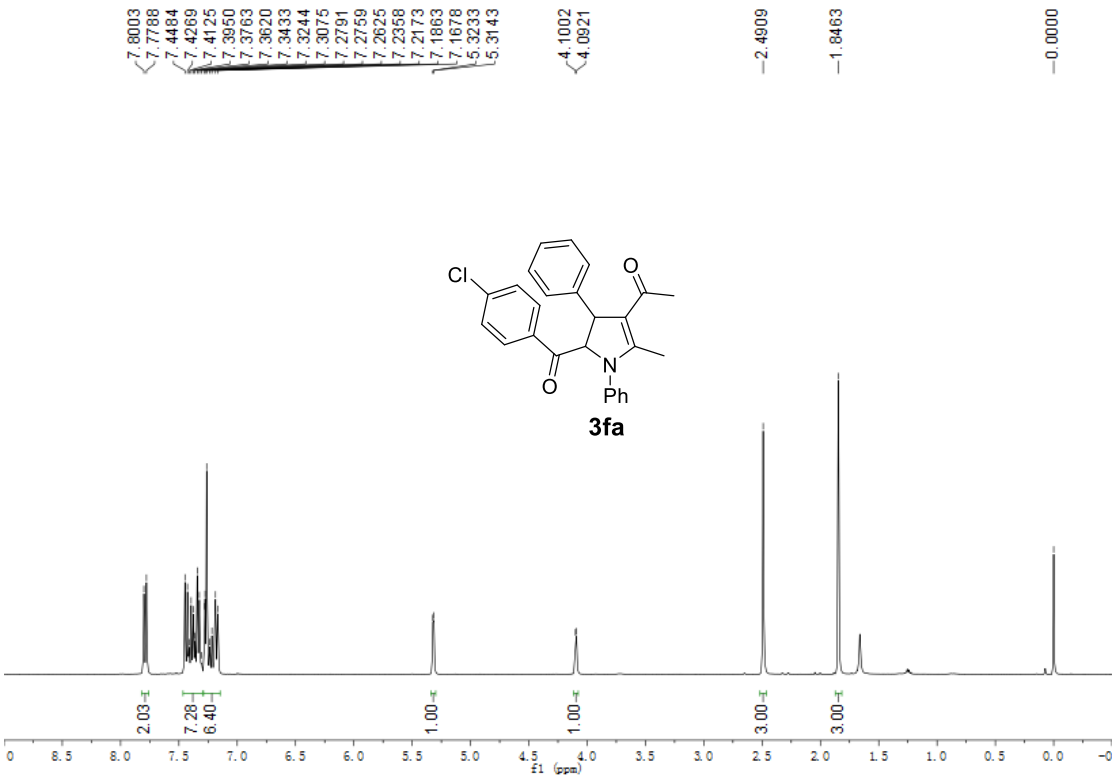


Figure S11. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3fa

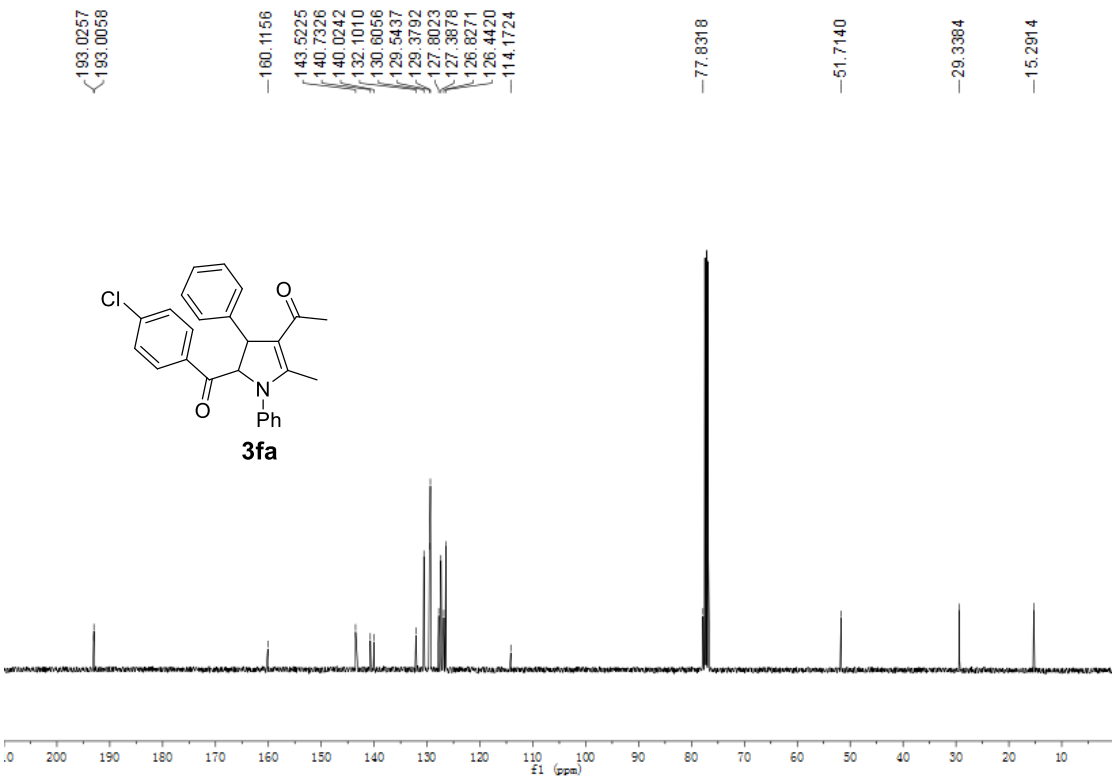


Figure S12. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3fa

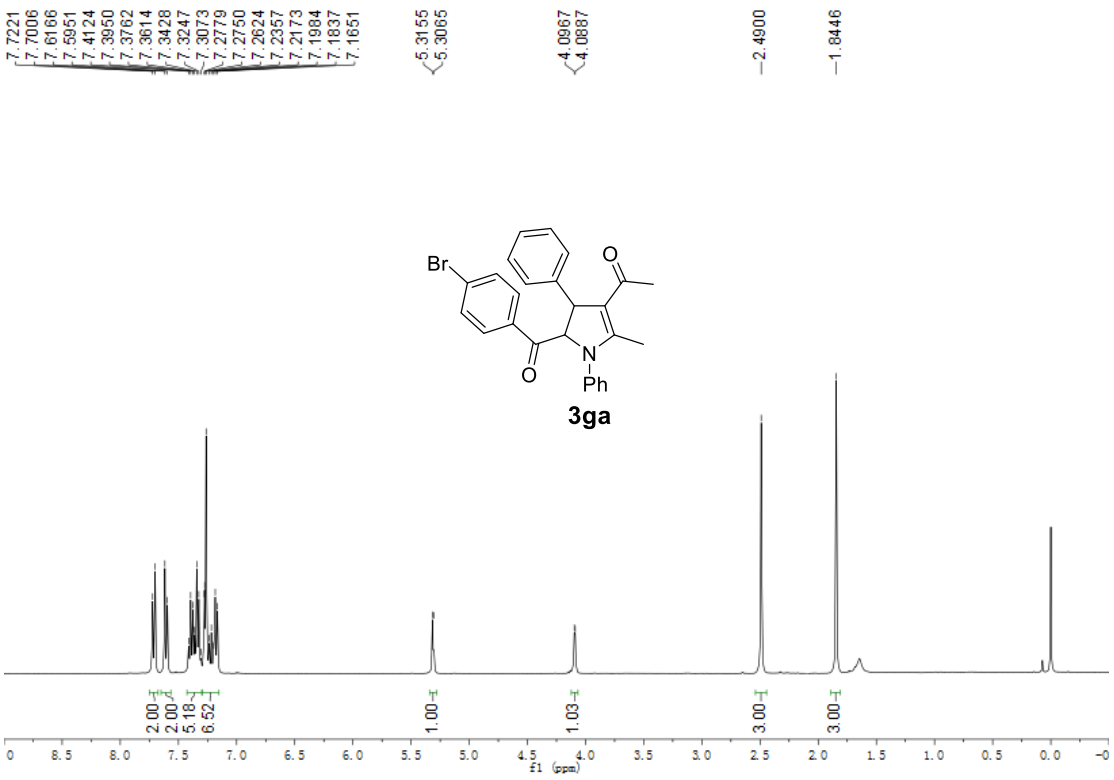


Figure S13. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ga

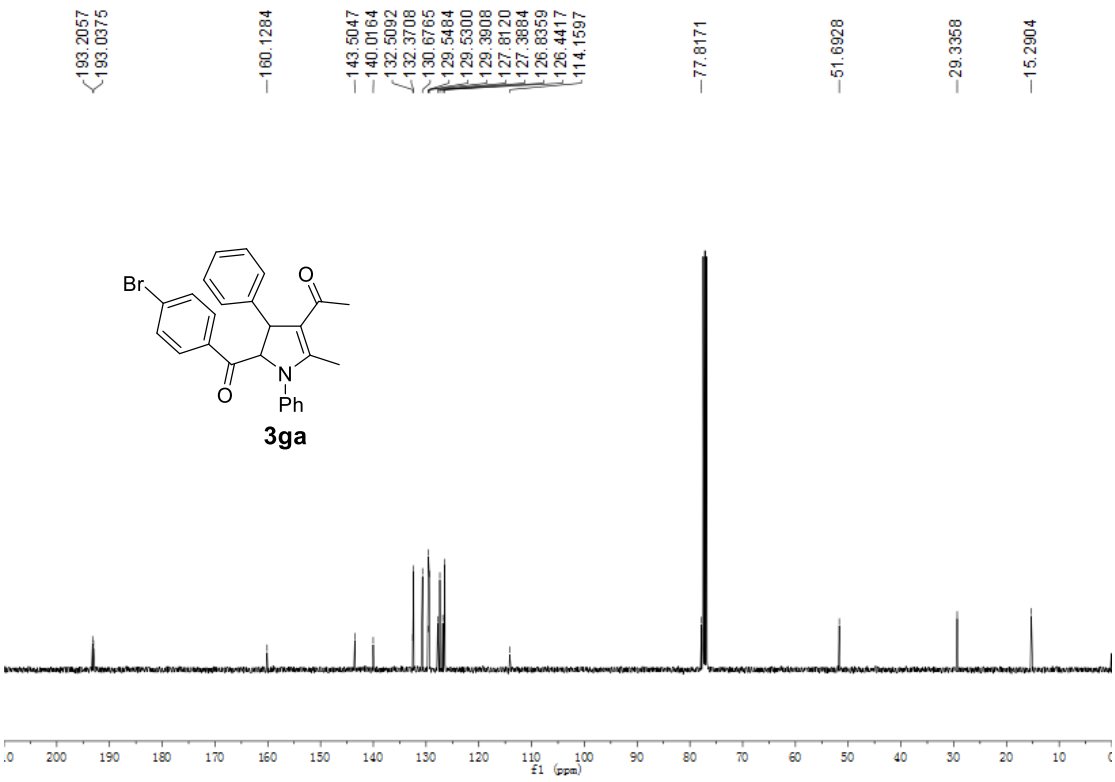


Figure S14. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ga

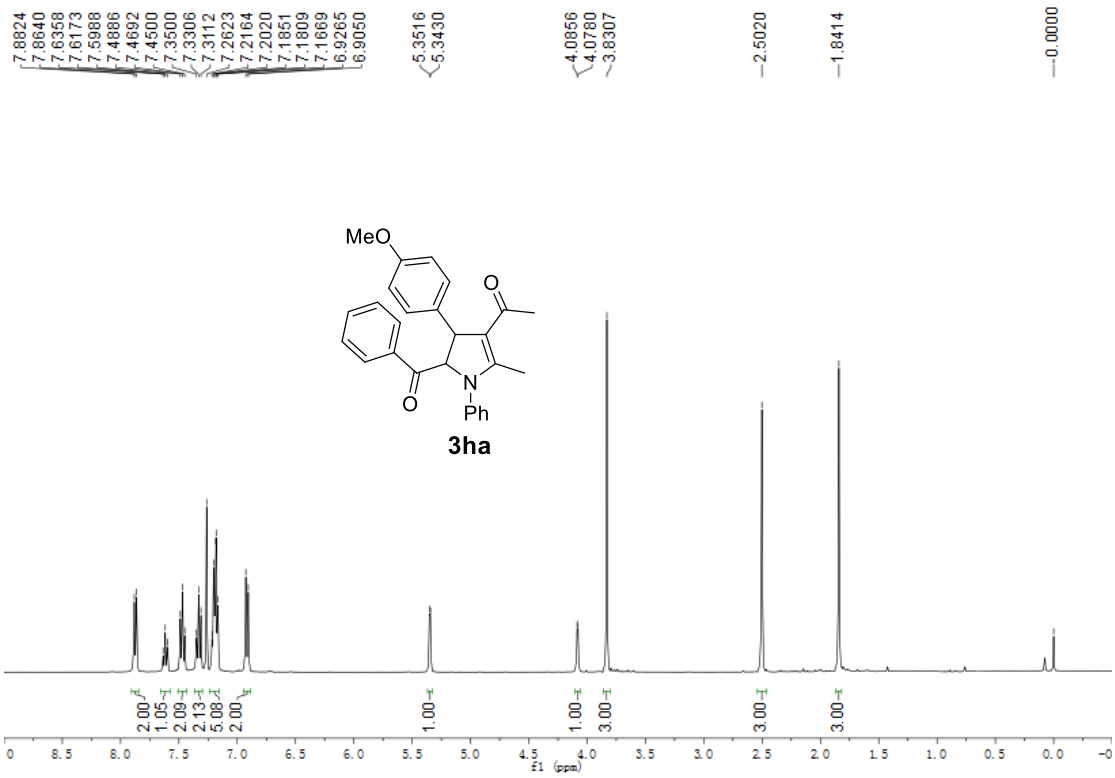


Figure S15. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ha

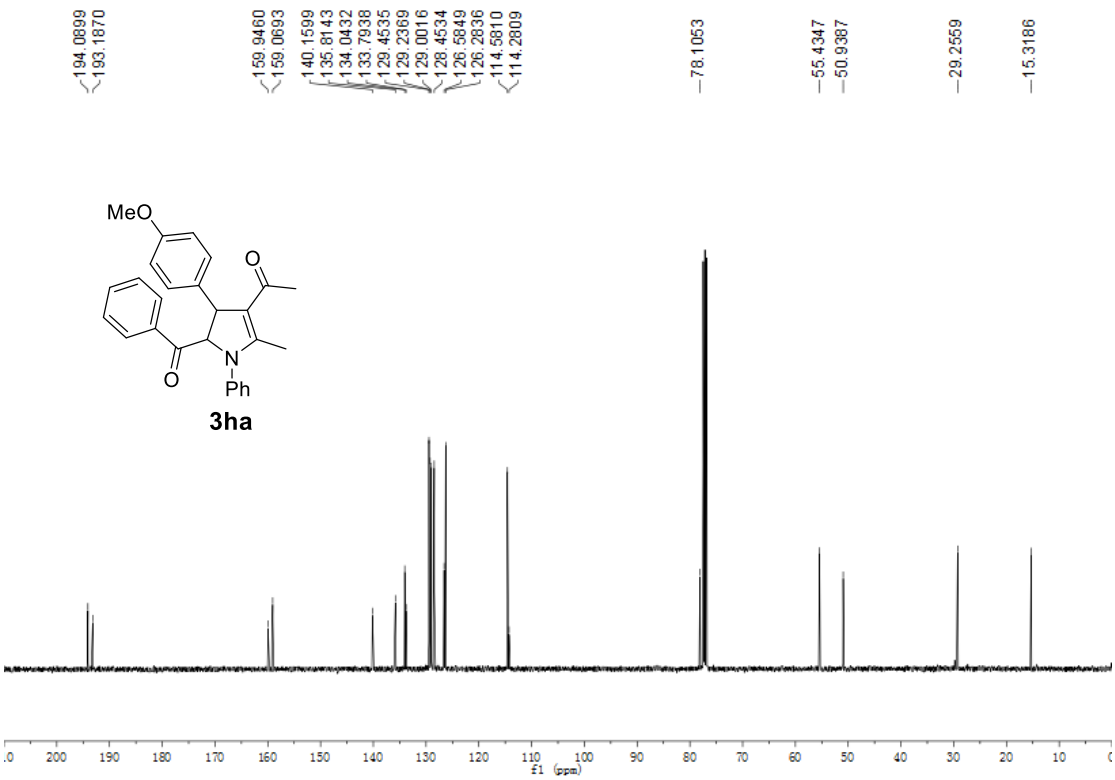


Figure S16. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ha

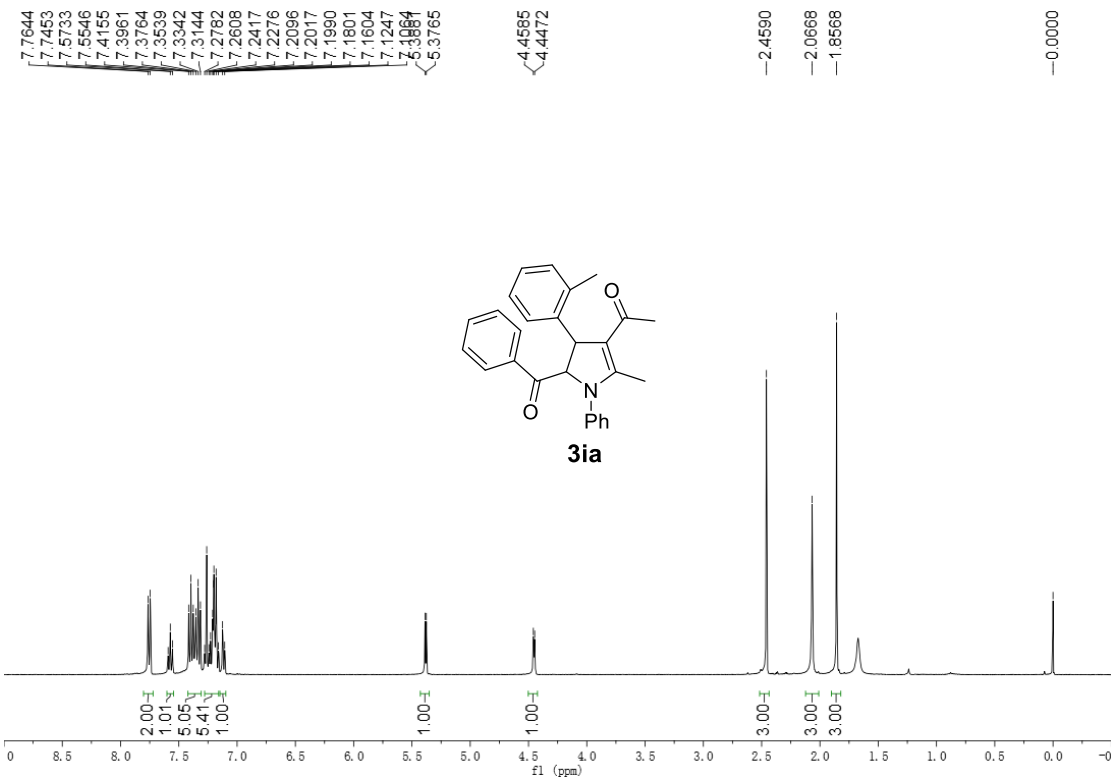


Figure S17. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ia

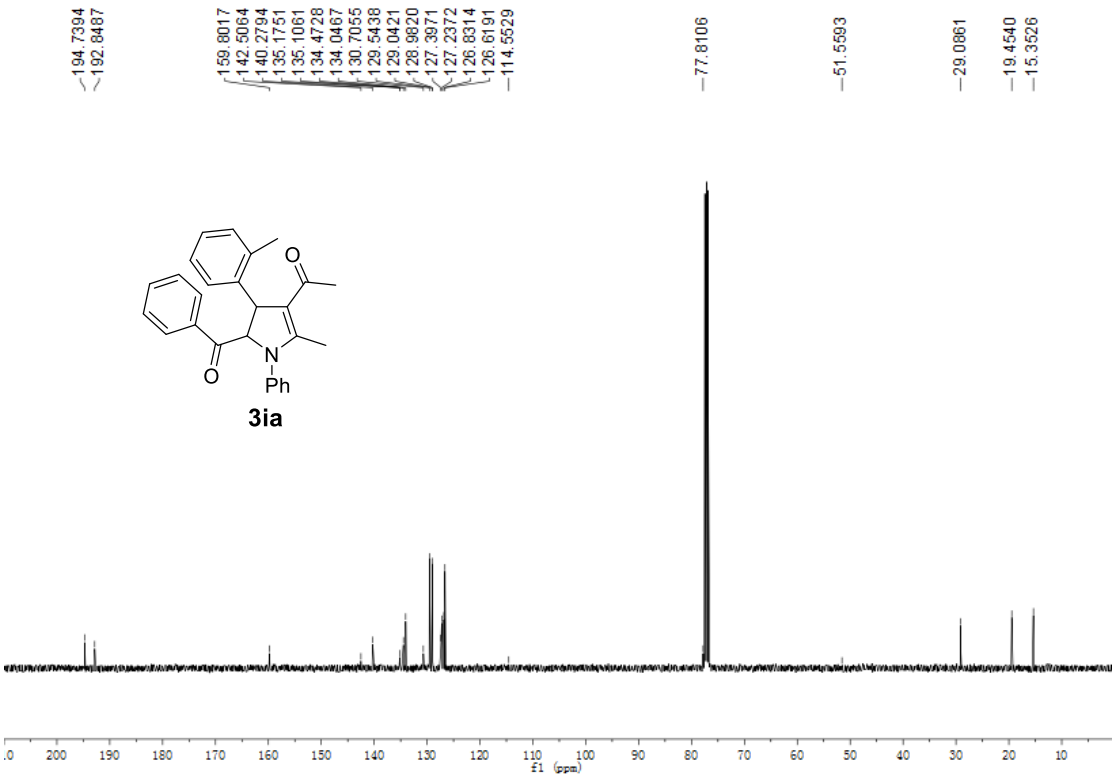


Figure S18. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ia

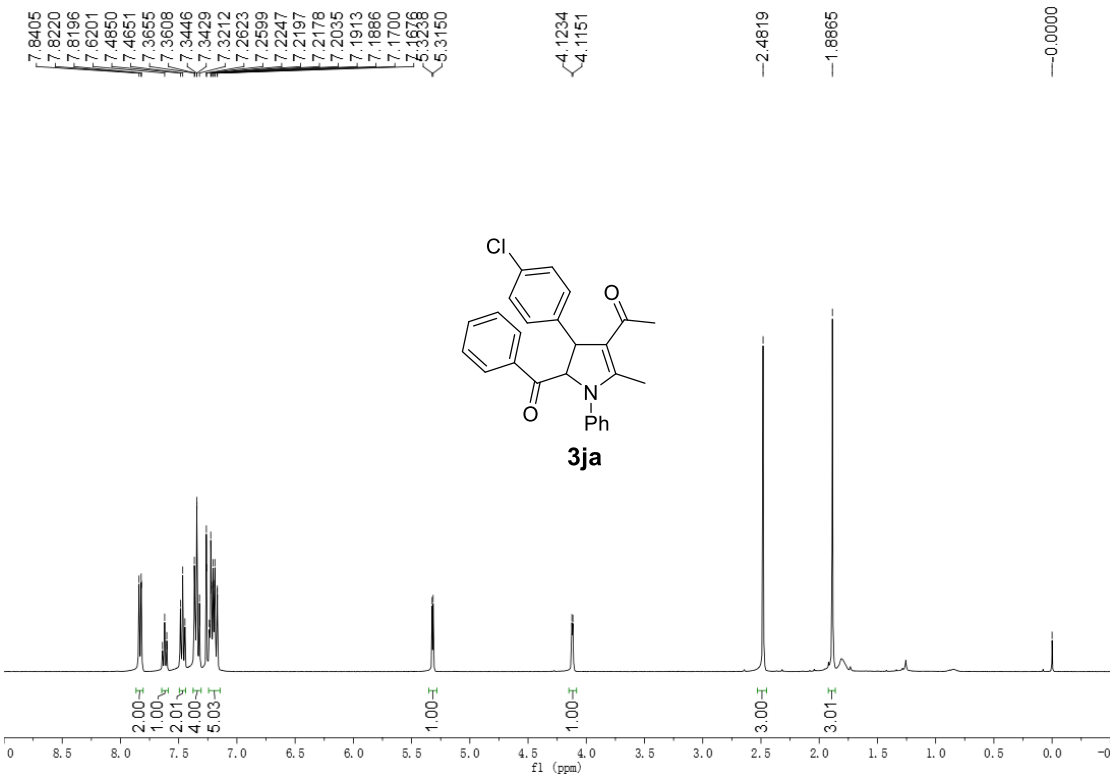


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ja

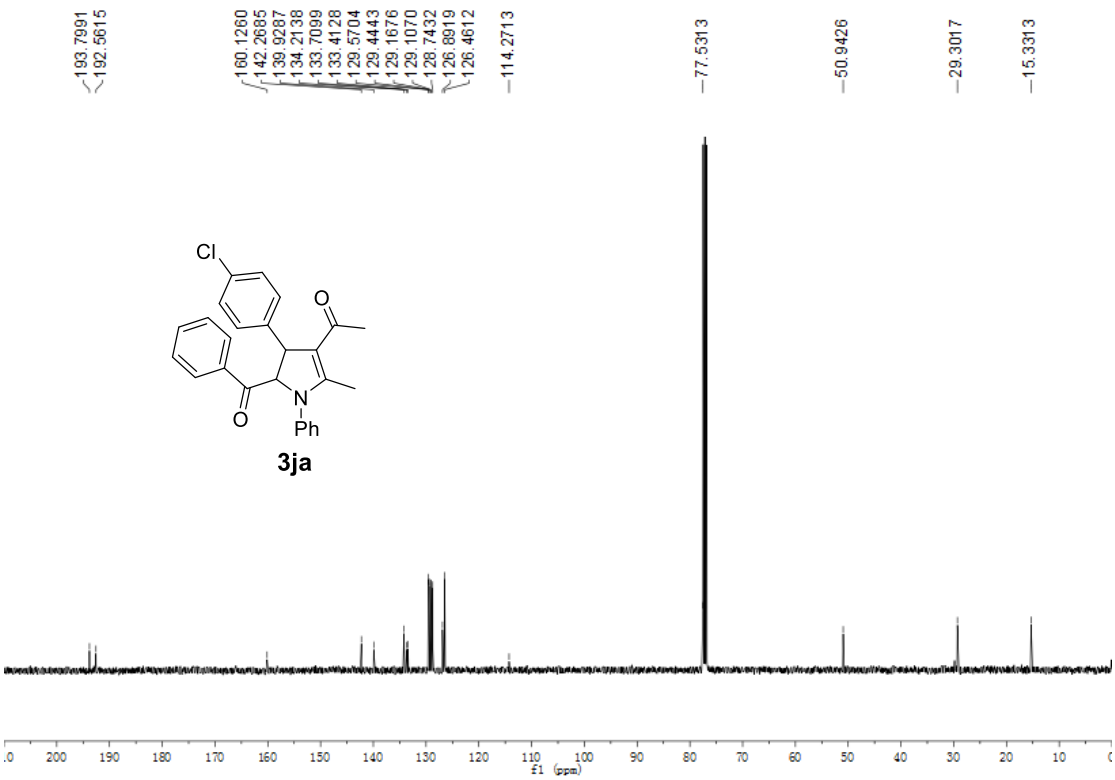


Figure S20. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ja

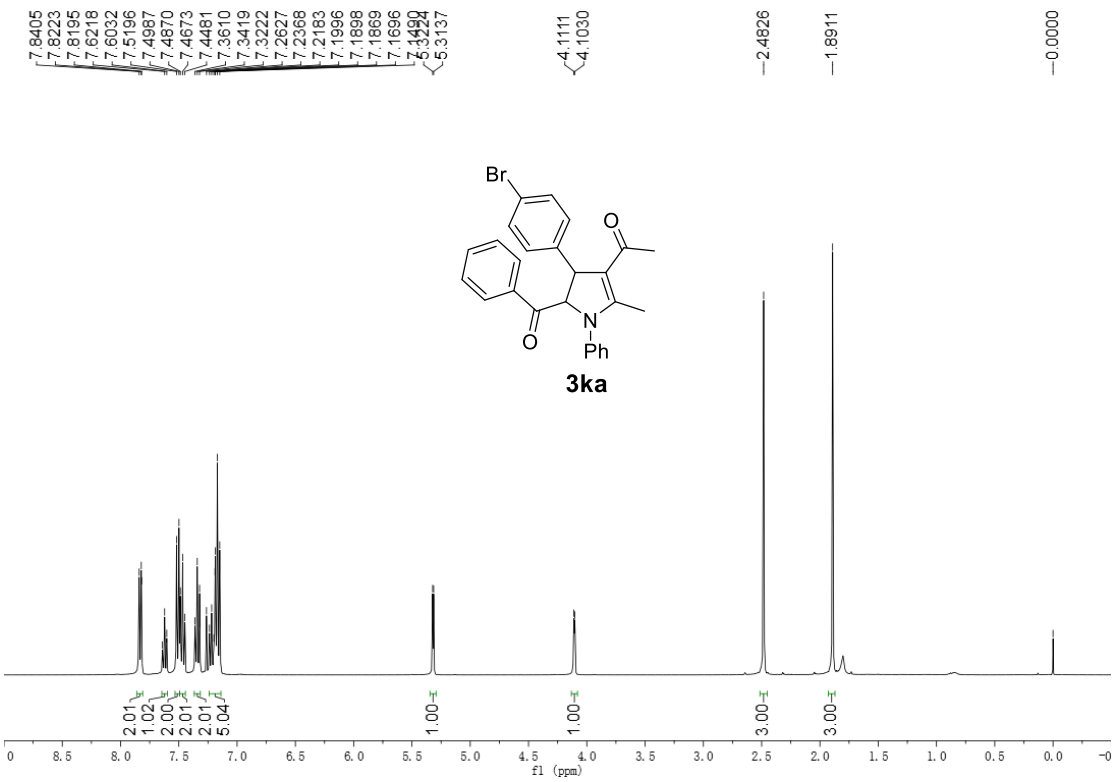


Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ka

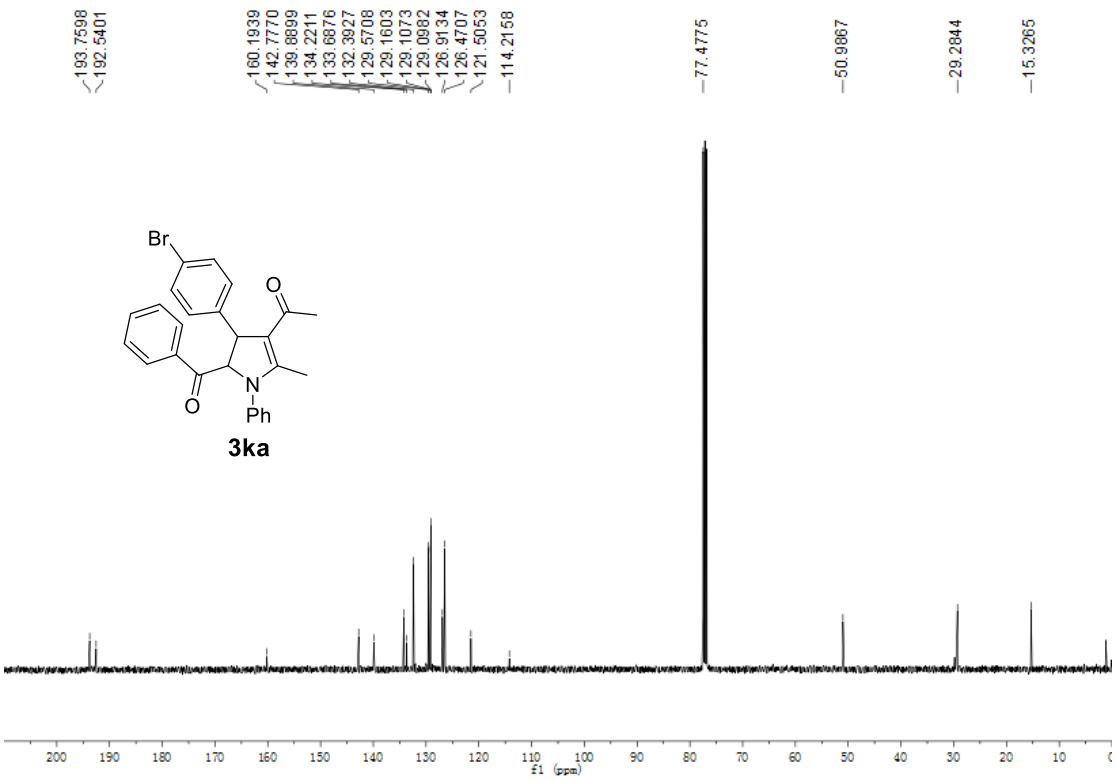


Figure S22. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ka

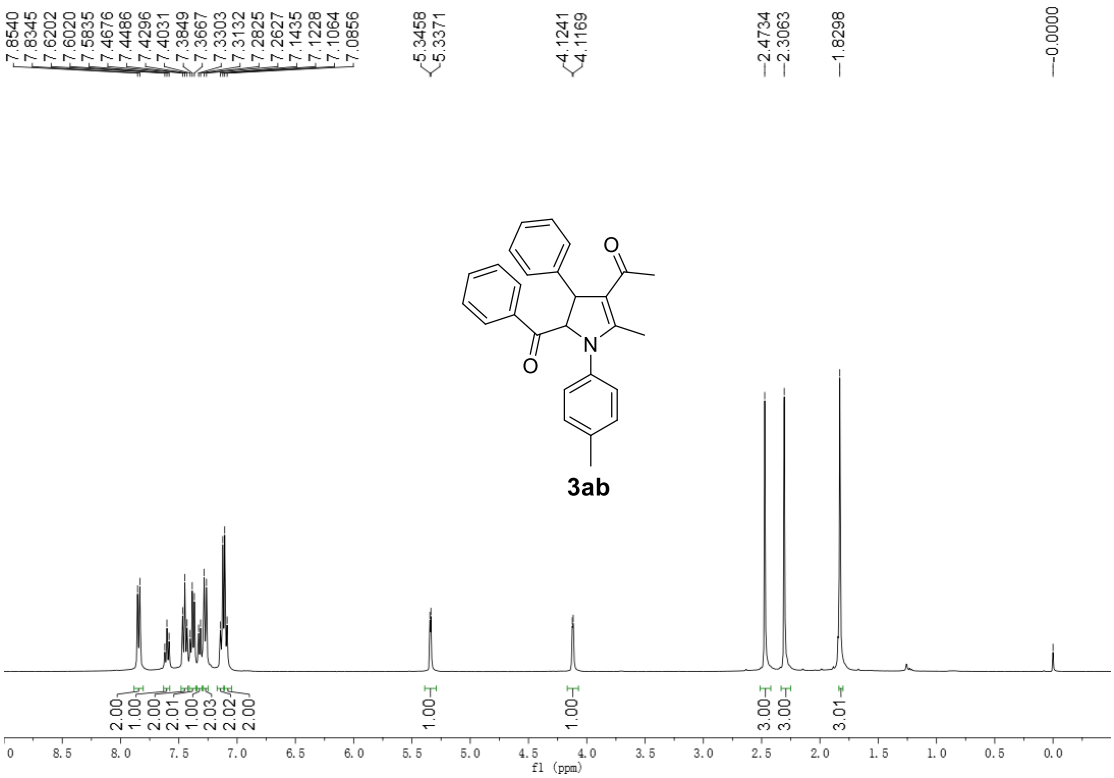


Figure S23. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ab

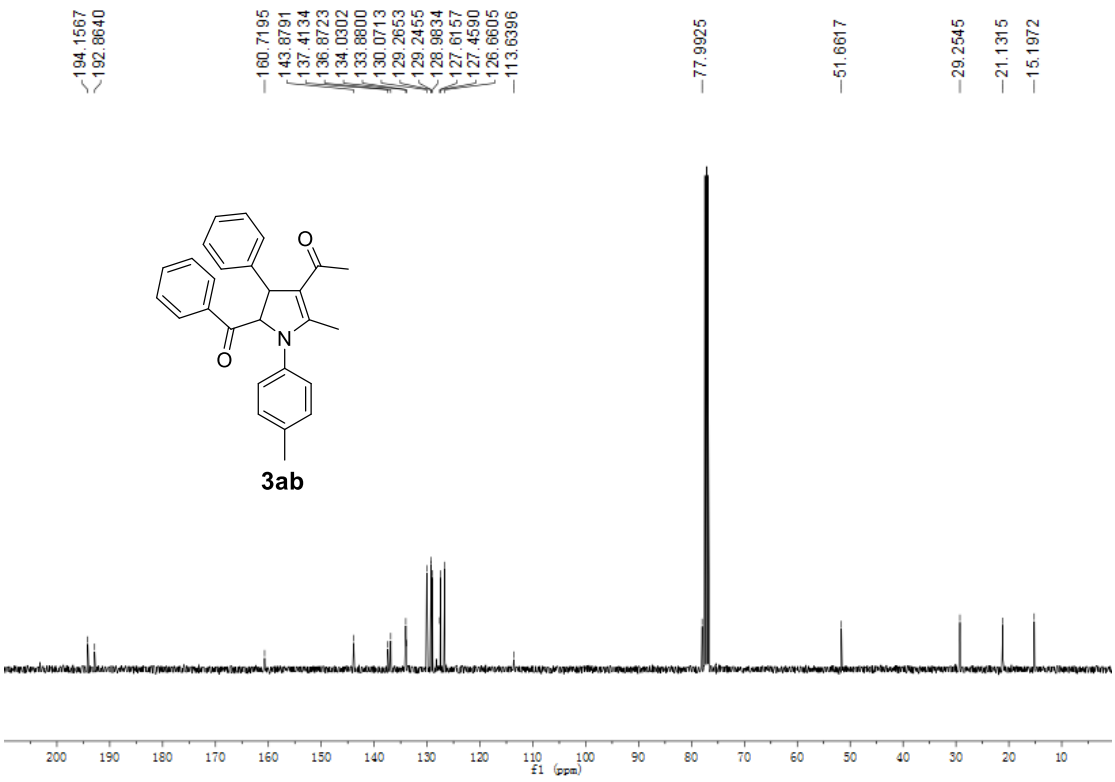


Figure S24. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ab

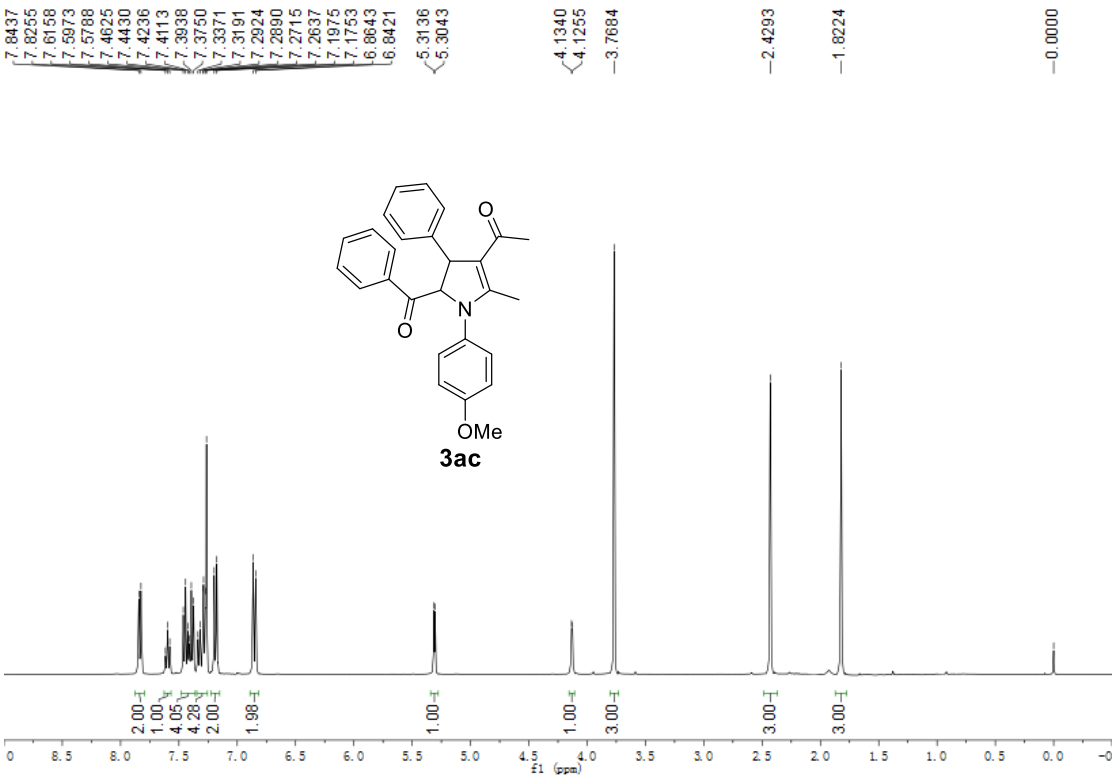


Figure S25. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ac

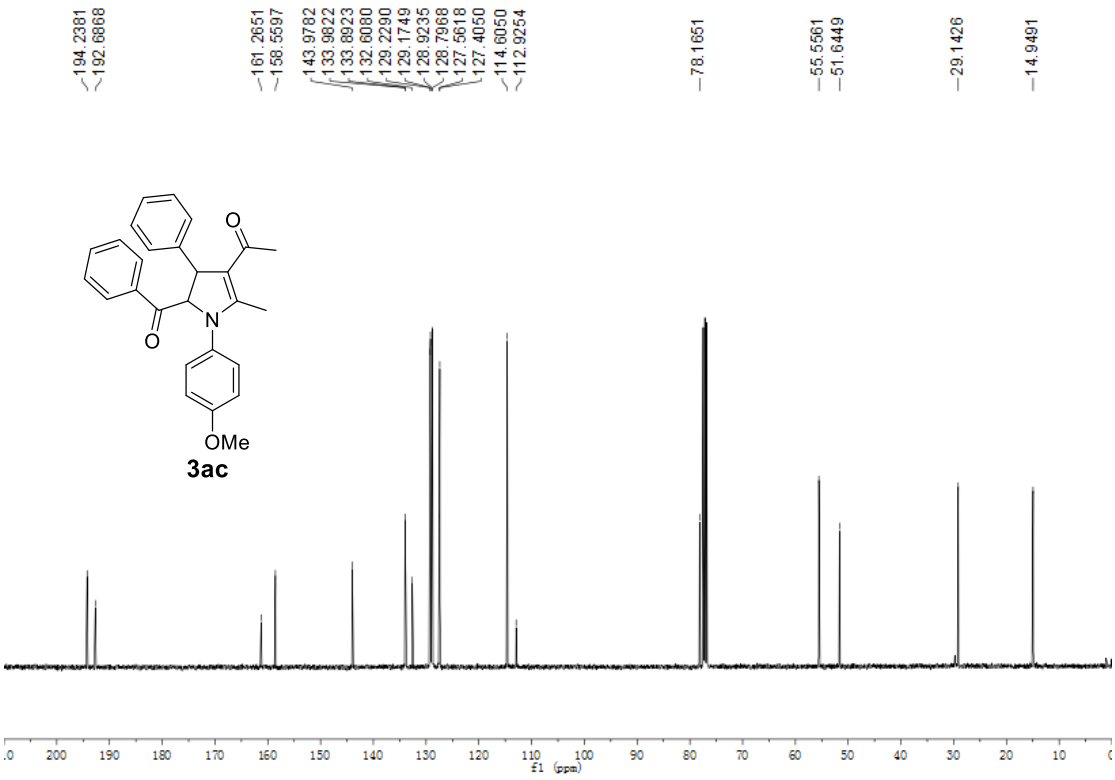


Figure S26. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ac

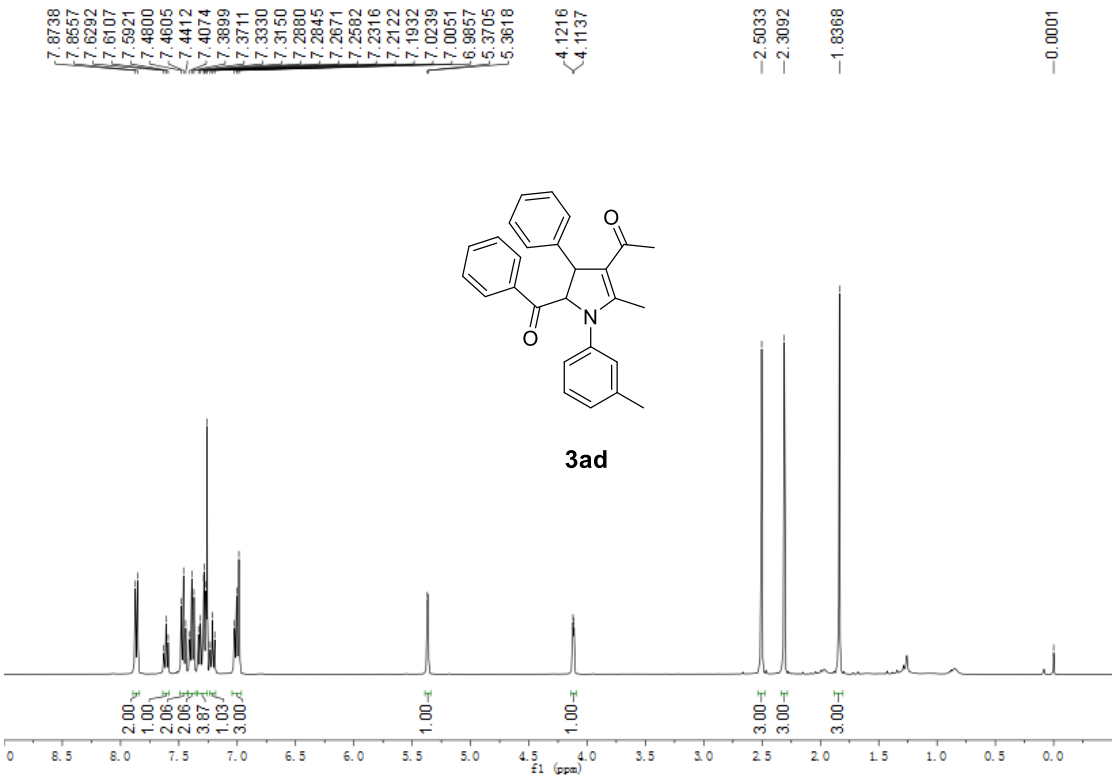


Figure S27. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ad

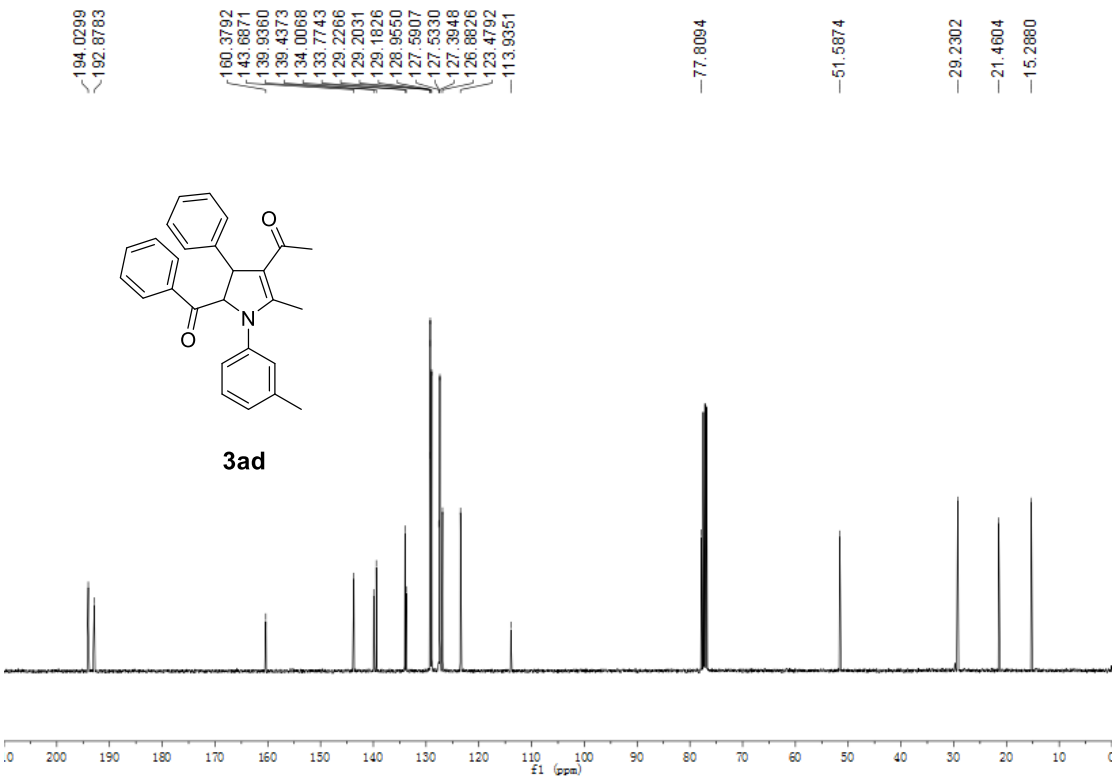


Figure S28. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ad

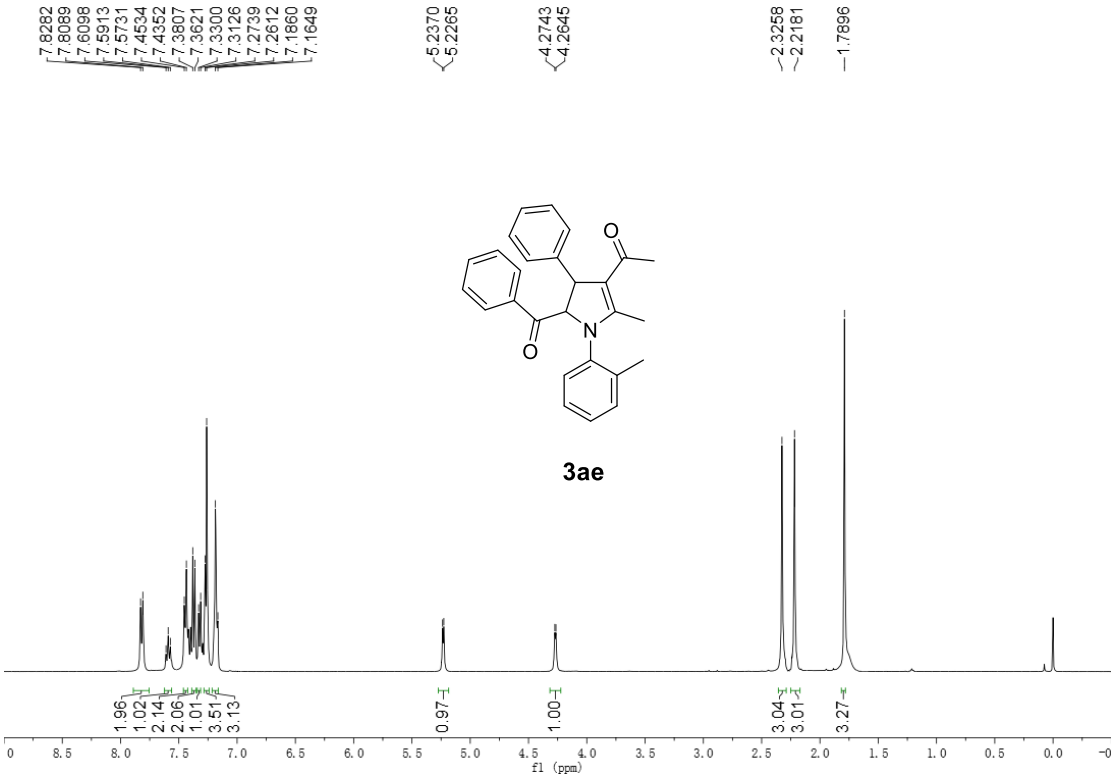


Figure S29. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ae

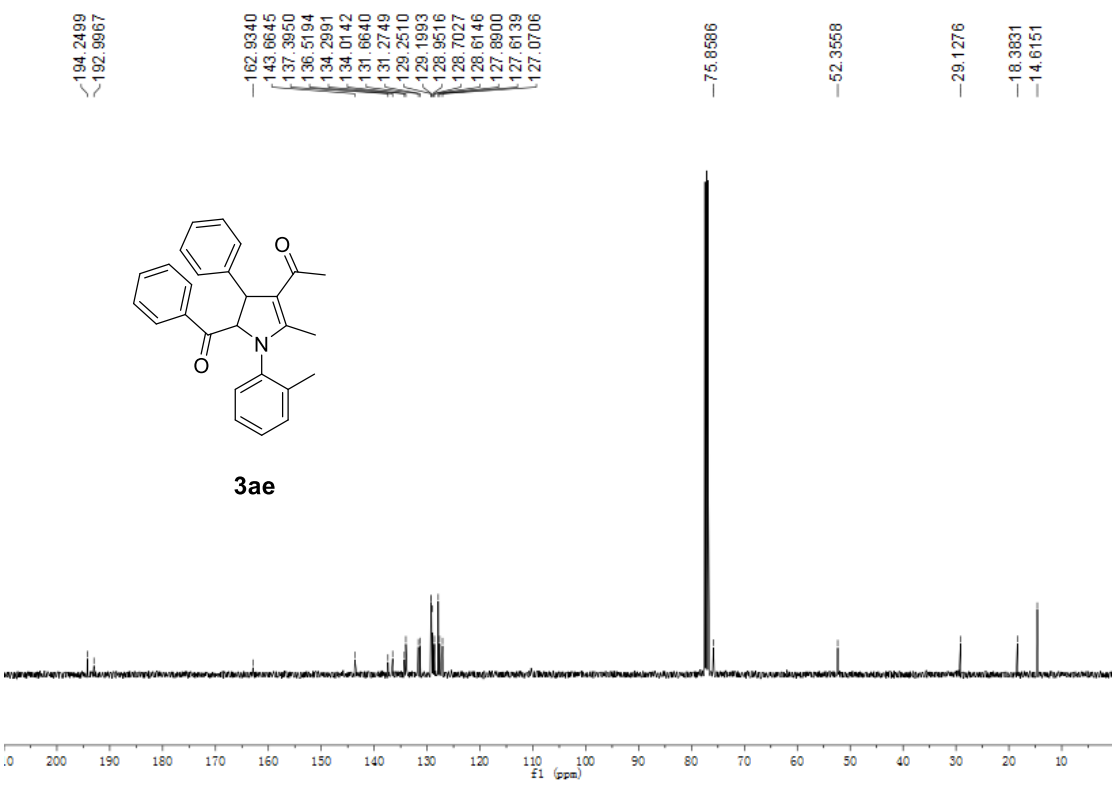


Figure S30. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ae

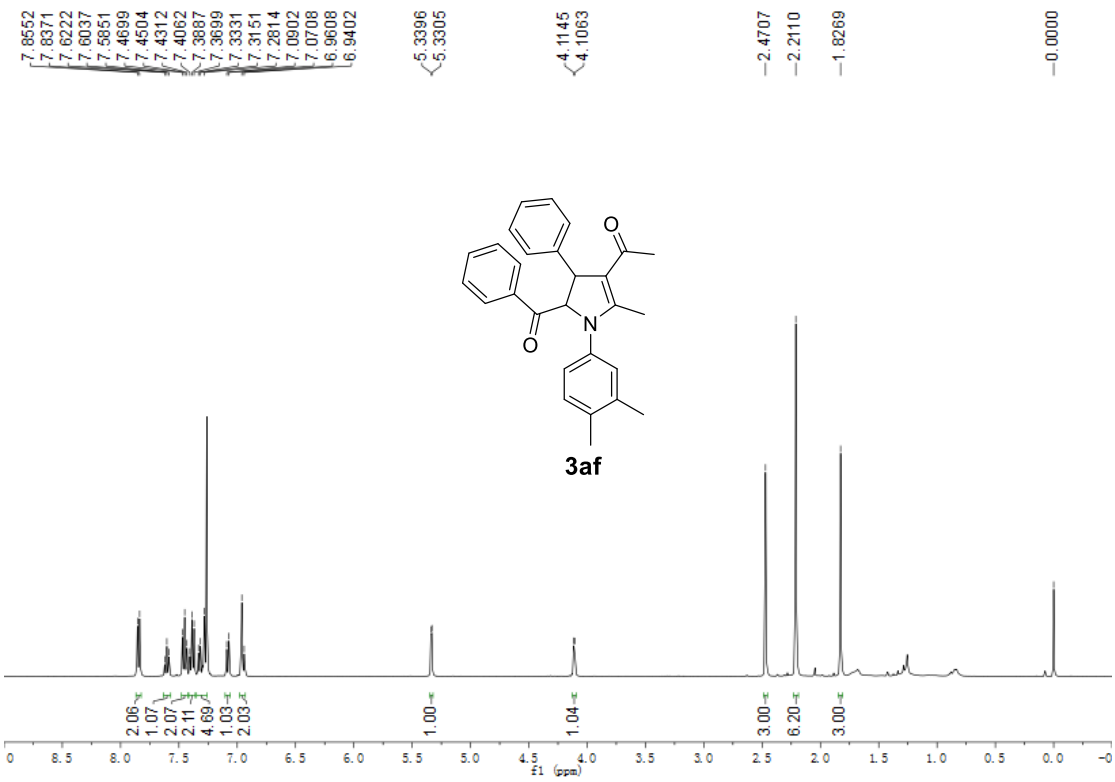


Figure S31. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3af

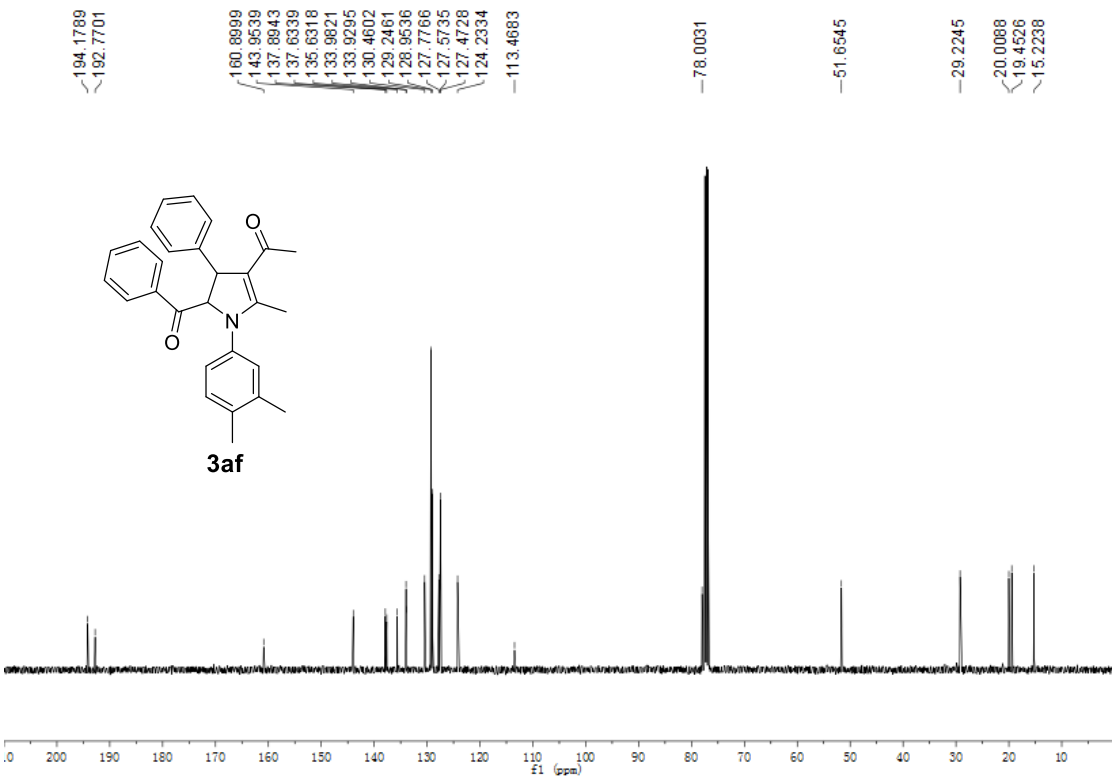


Figure S32. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3af

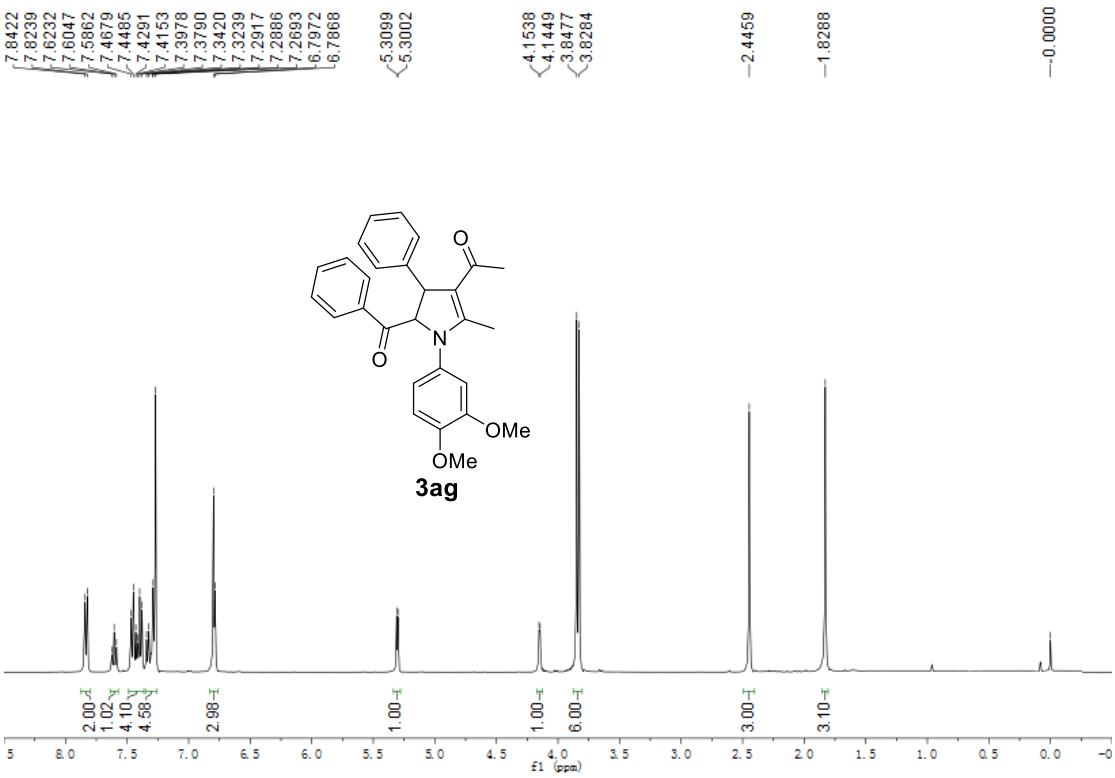


Figure S33. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ag

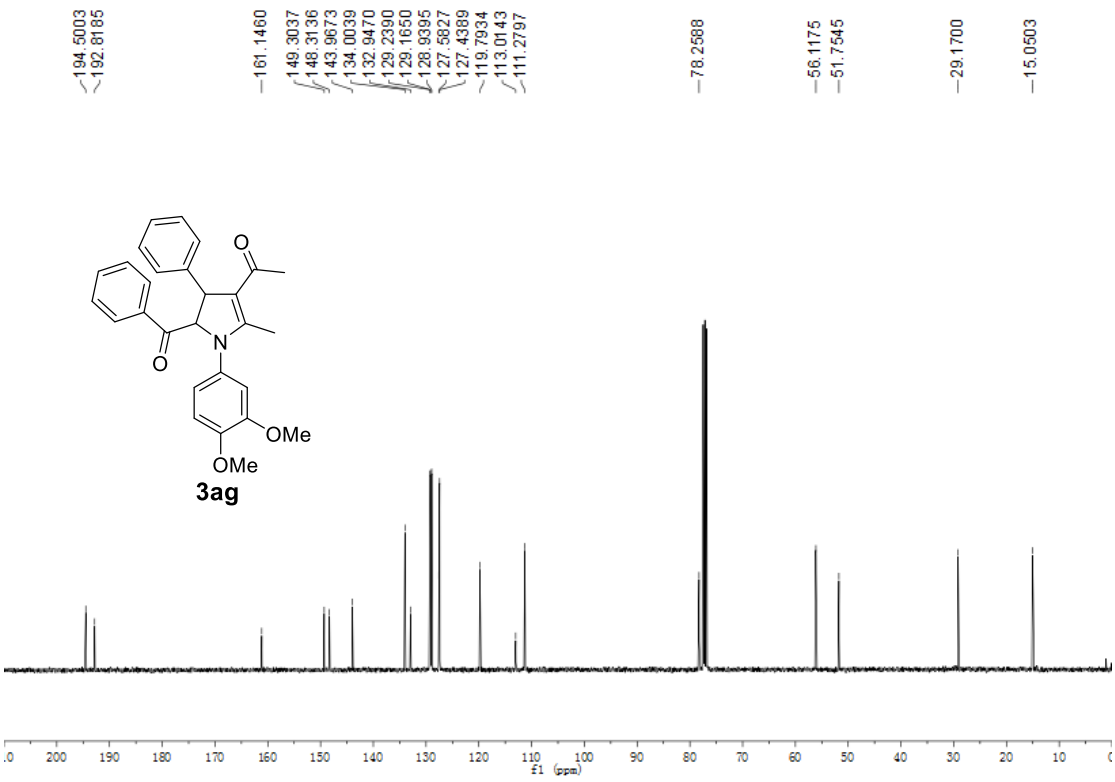


Figure S34. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ag

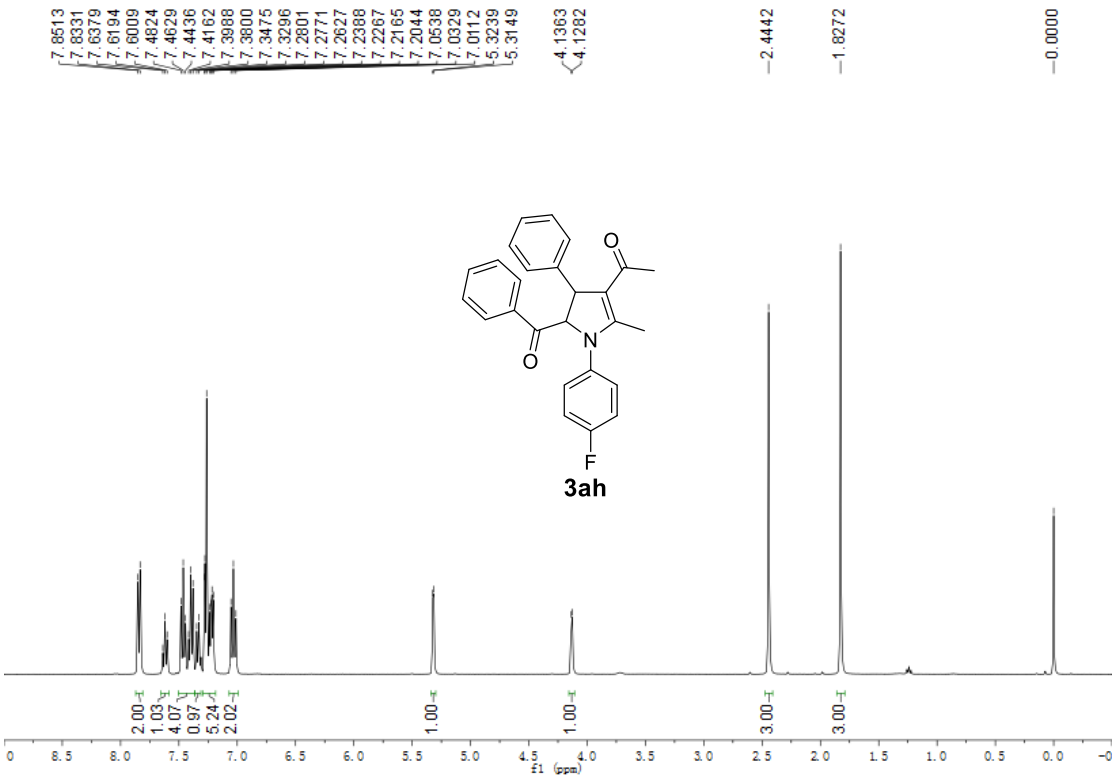


Figure S35. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ah

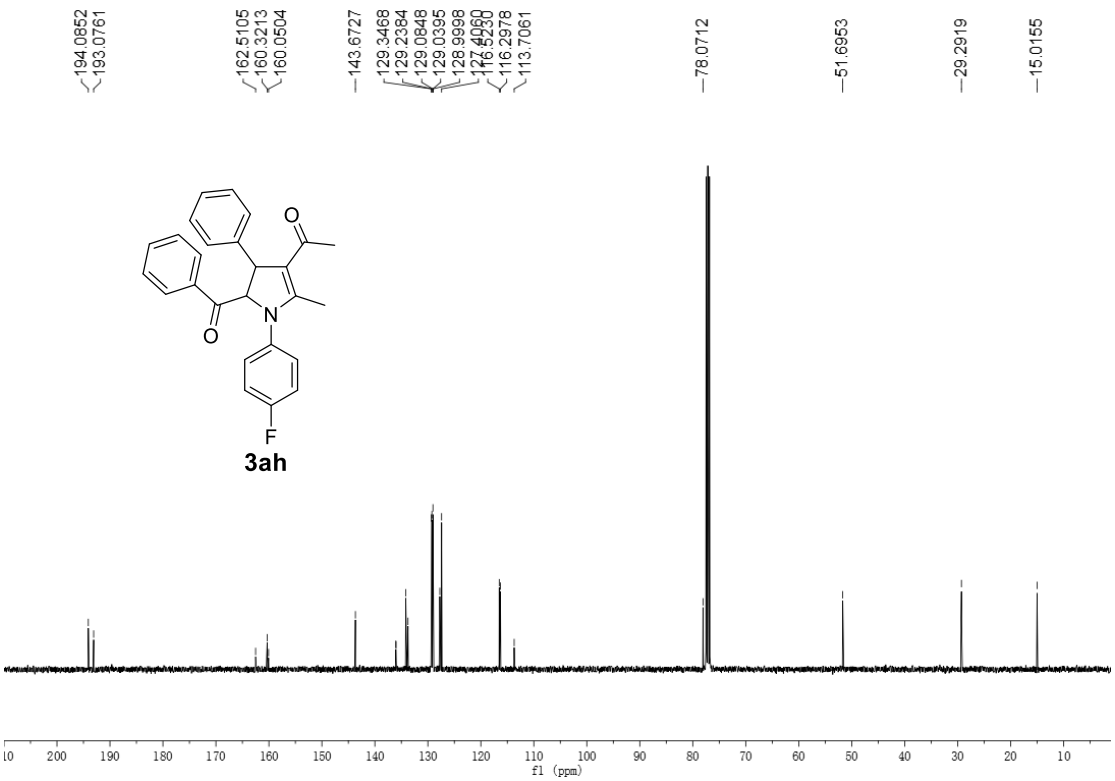


Figure S36. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ah

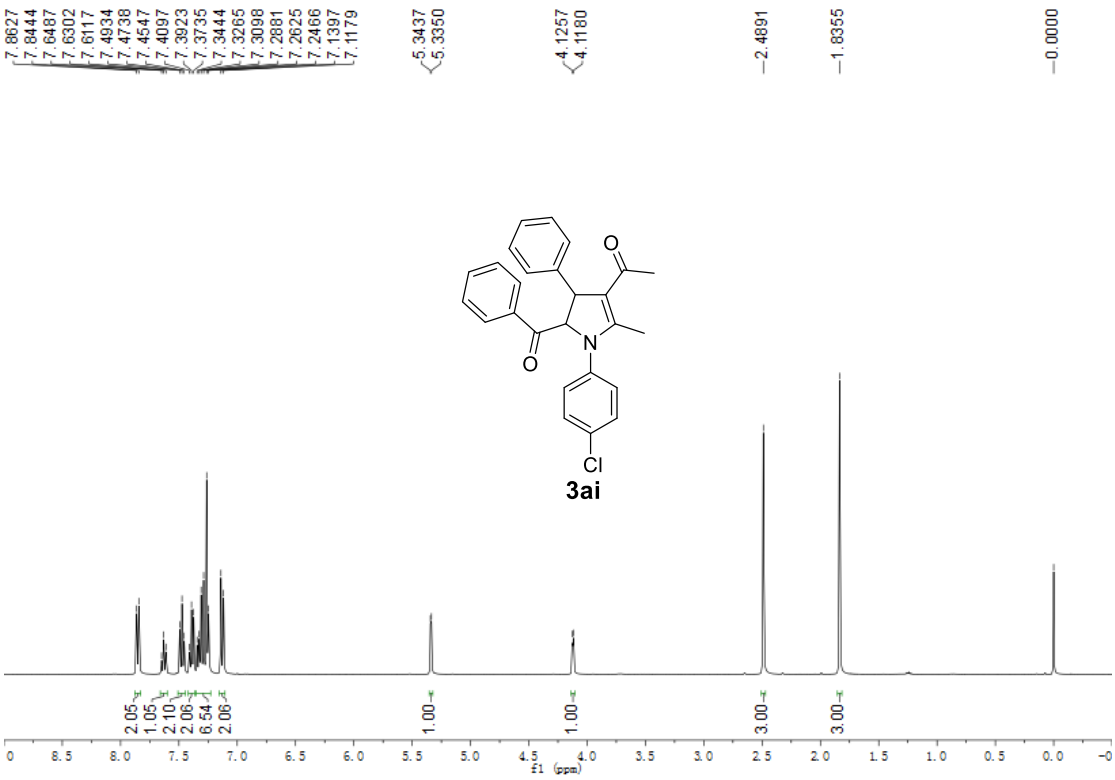


Figure S37. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ai

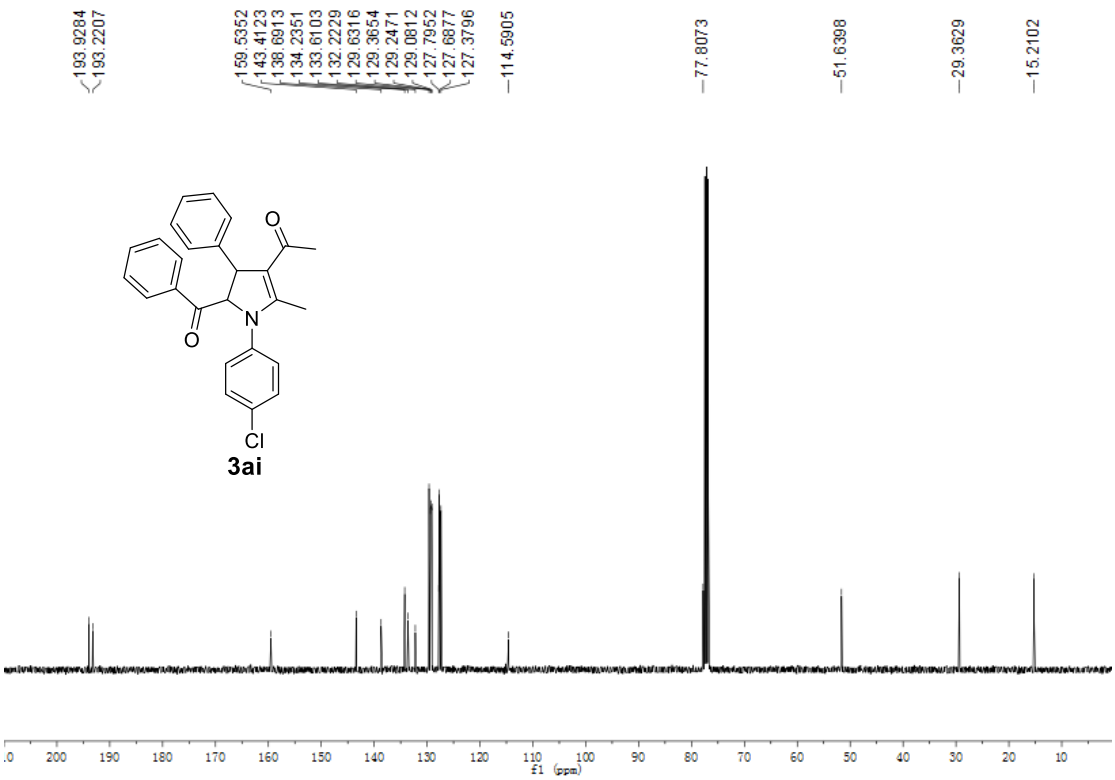


Figure S38. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ai

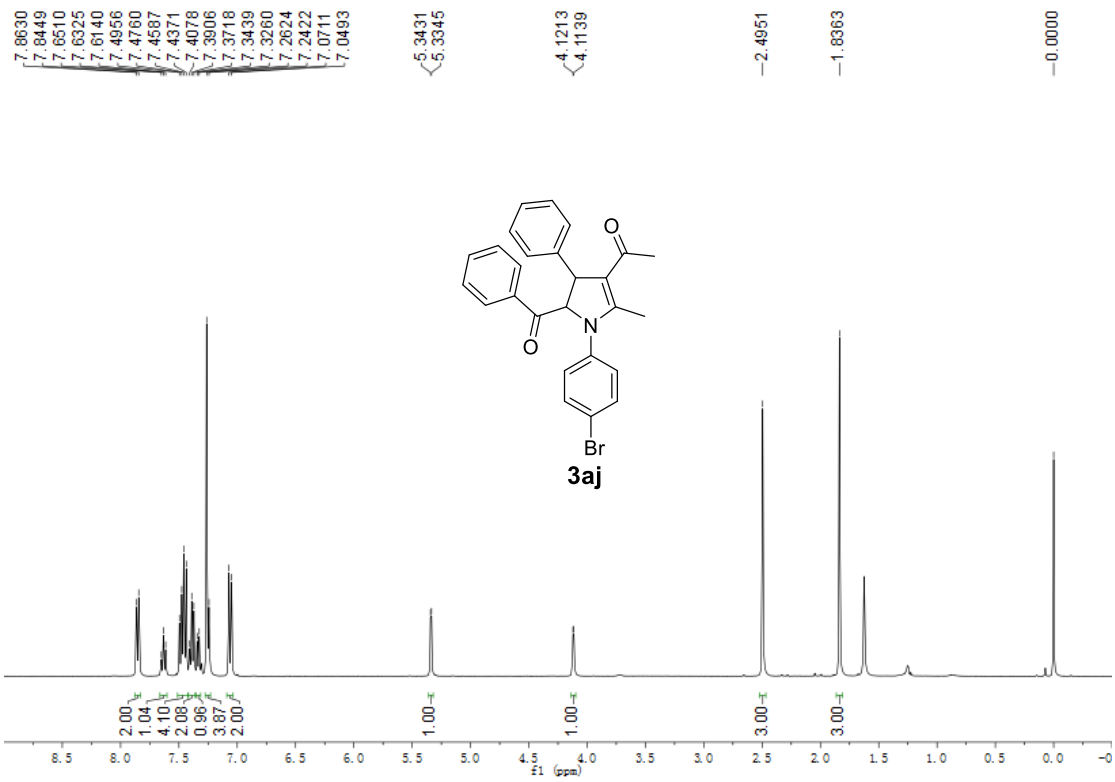


Figure S39. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3aj

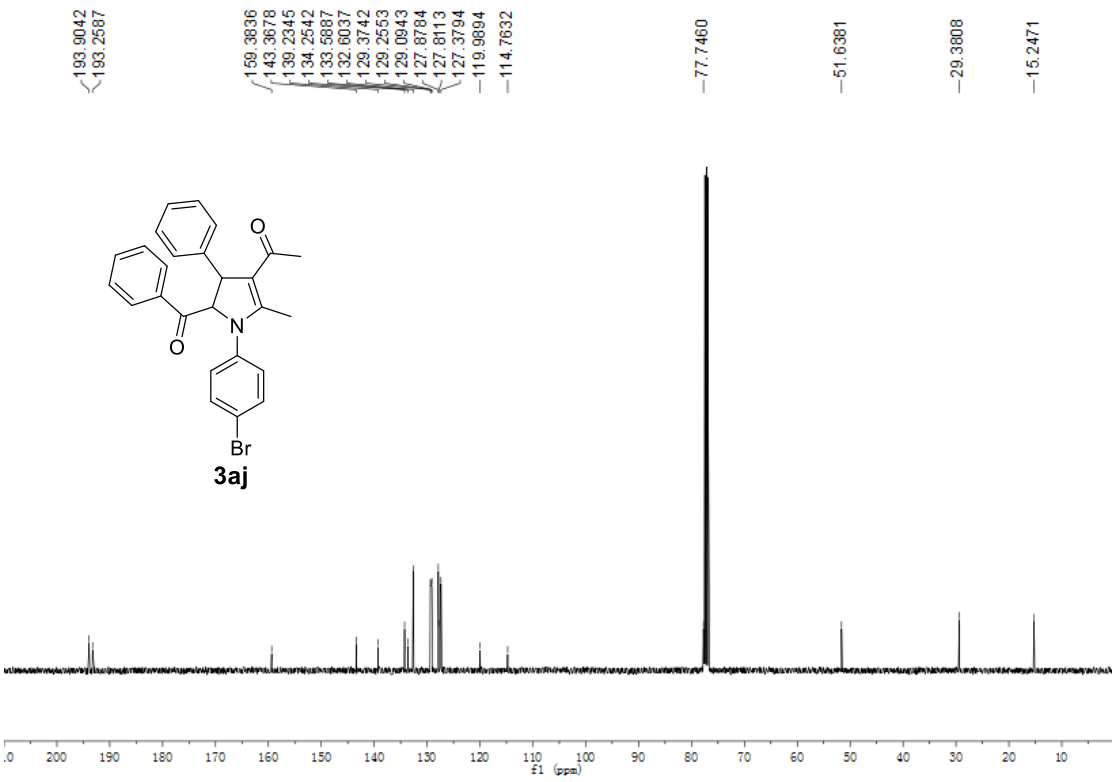


Figure S40. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3aj

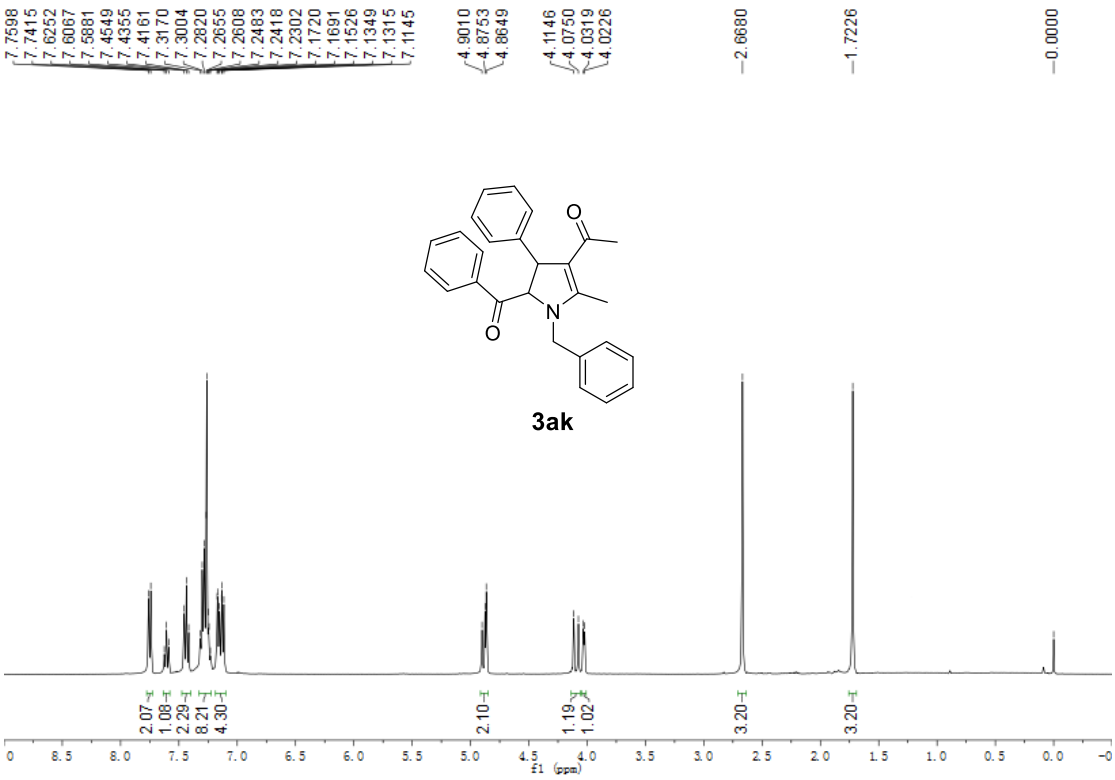


Figure S41. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3ak

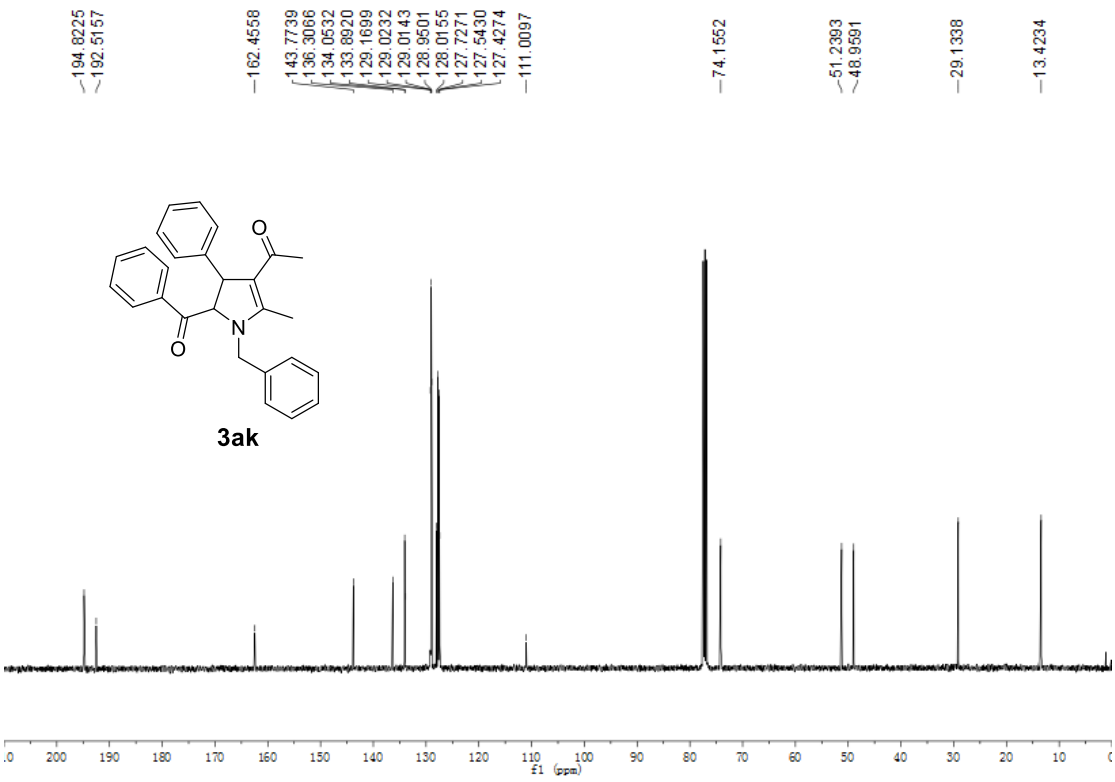


Figure S42. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3ak

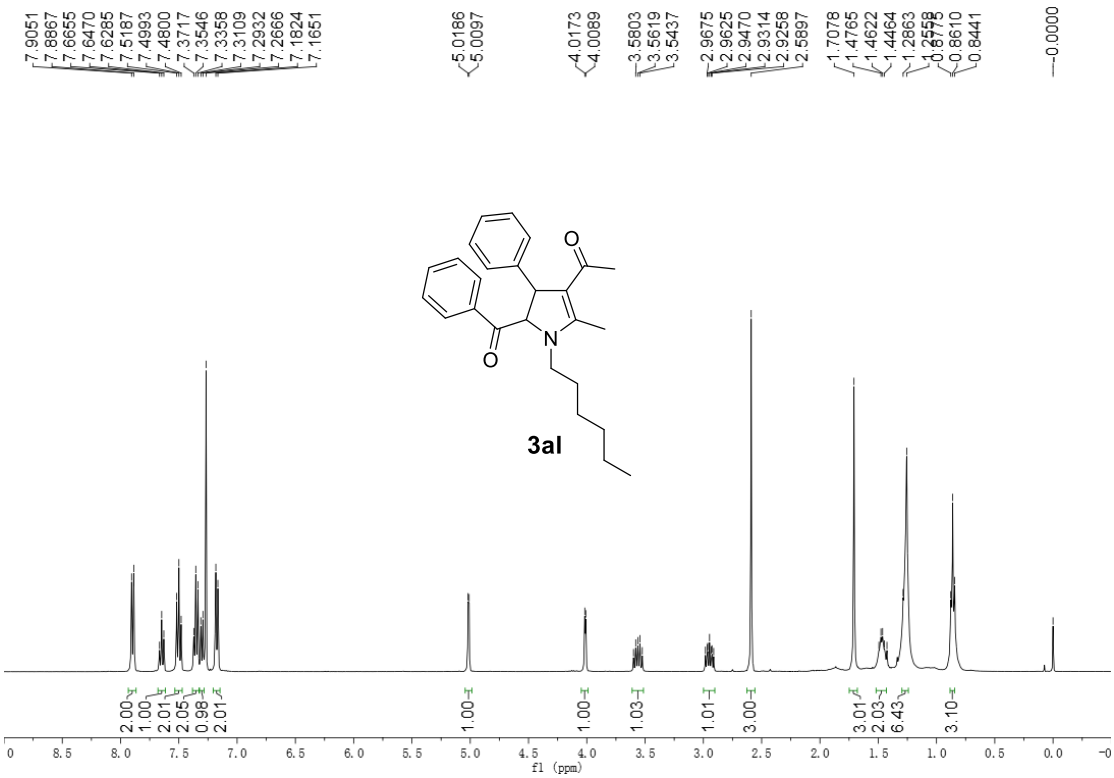


Figure S43. ^{1}H NMR (400 MHz, $CDCl_3$) of compound 3al

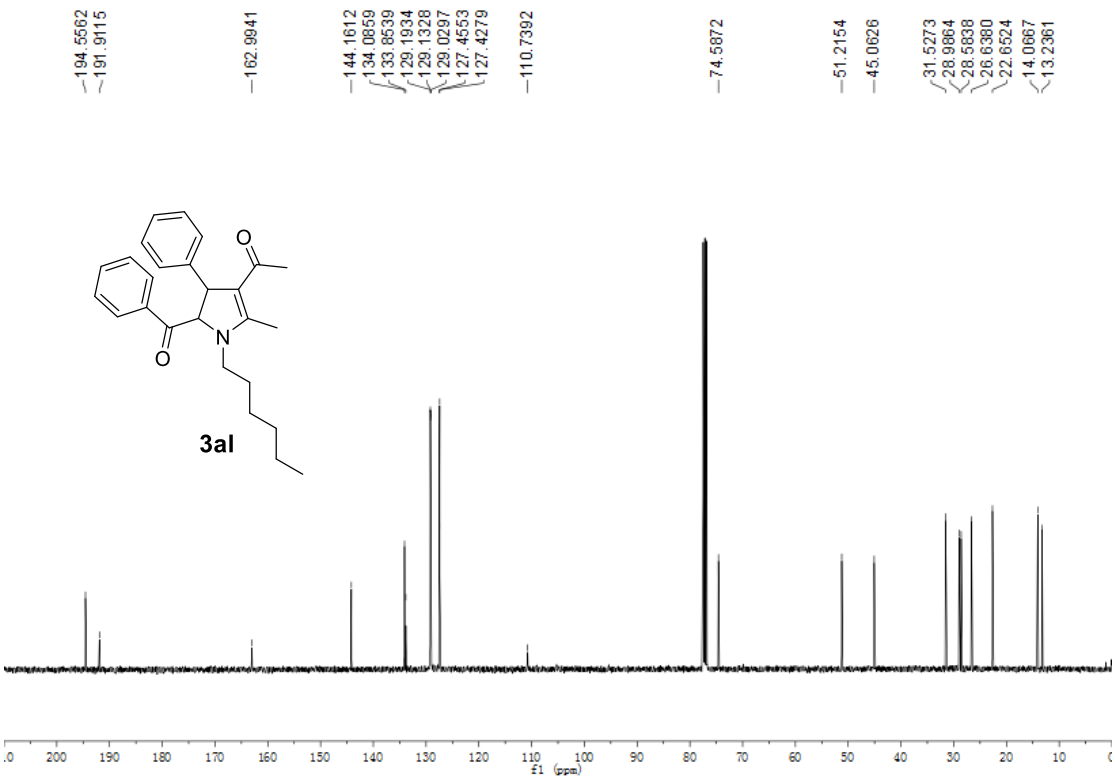


Figure S44. ^{13}C NMR (100 MHz, $CDCl_3$) of compound 3al