Electronic Supplementary Material (ESI) for RSC Advances.

Base-Mediated Regiospecific Cascade Synthesis of *N*-(2-Pyridyl)pyrroles from *N*-Propargylic β-Enaminones

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Context

General Information:

Silica gel was purchased from Qing Dao Hai Yang Chemical Industry Co. ^{1}H and ^{13}C NMR spectra were measured on a 400 MHz Bruker spectrometer (^{1}H 400 MHz, ^{13}C100 MHz), using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. HRMS-ESI spectra were obtained on Agilent 6450 spectrometer.

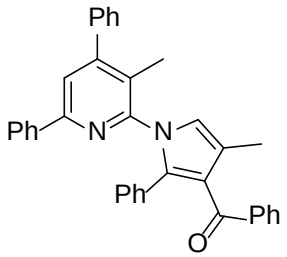
Typical Procedure for the Preparation of *N*-Propargylic Enaminones 1:

An oven-dried Schlenk tube was charged with α,β-ynones (1 mmol), propynylamine (1.2 mmol), and anhydrous MeOH (5 mL). The tube was stirred at 80 °C for 8 hours. The reaction mixture was cooled to room temperature, the solvent was evaporated and the residue was purified by silica gel, eluting with petroleum ether/ethyl acetate mixtures.

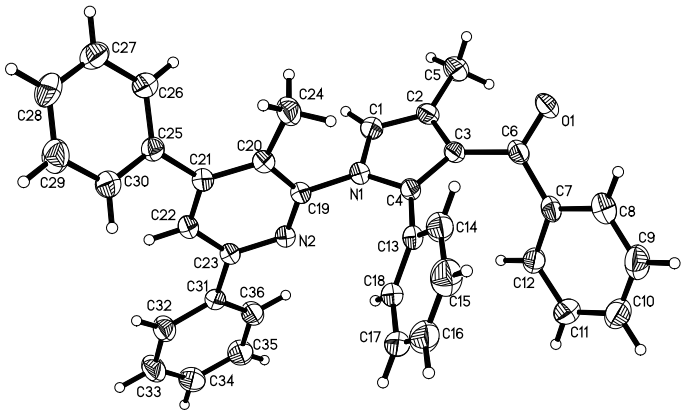
Typical Procedure for the Preparation of Polysubstituted *N*-(2-Pyridyl)pyrroles 2:

A mixture of *N*-propargylic β-enaminones **1** (0.5 mmol), KOH (56 mg, 1mmol) in CH_3CN (2 mL) was stirred under refluxing for 30 min (monitored by TLC). Then H_2O (8mL) was added and the resultant was extracted with DCM (3 x 5 mL). The combined DCM extracts were dried over Na_2SO_4 and concentrated. Then solvent was evaporated and the residue was purified by chromatography (silica gel, 10% EtOAc in PE) to give **2**.

Spectroscopic Data for Products



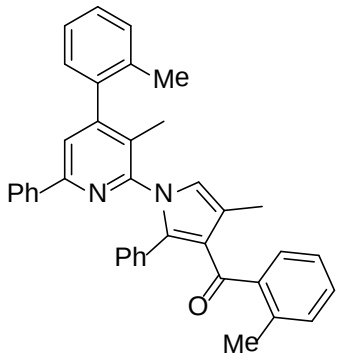
(4-Methyl-1-(3-methyl-4,6-diphenylpyridin-2-yl)-2-phenyl-1H-pyrrol-3-yl)(phenyl)methanone **2a**



CCDC 994843

White solid: mp 199-201 ^{o}C

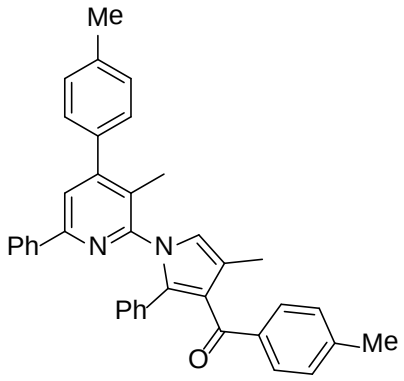
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 6.5 Hz, 2H), 7.74 – 7.59 (m, 3H), 7.46 (dd, J = 13.8, 7.2 Hz, 3H), 7.36 (s, 3H), 7.24 (dd, J = 8.3, 4.7 Hz, 1H), 7.19 – 6.86 (m, 10H), 2.31 (s, 3H), 1.58 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.7, 154.1, 153.2, 151.8, 139.3, 138.8, 138.2, 137.6, 131.6, 131.5,130.3, 129.8, 129.2, 128.8, 128.5, 128.4, 128.2, 127.5, 127.4, 127.1, 126.9, 126.6, 122.4, 121.9, 121.1, 15.0, 11.5 ; HRMS (ESI) m/z calcd for $C_{36}H_{28}N_2O$ (MH+) 505.2280, found 505.2291.



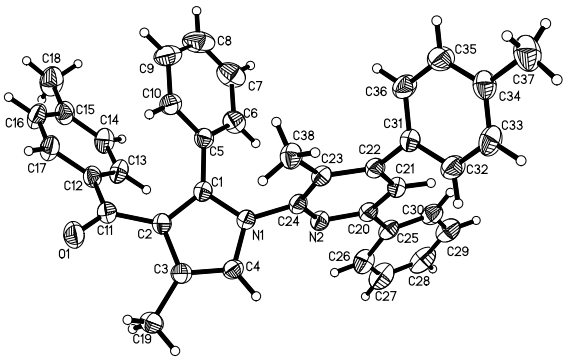
(4-Methyl-1-(3-methyl-6-phenyl-4-(o-tolyl)pyridin-2-yl)-2-phenyl-1H-pyrrol-3-yl)(o-tolyl)methanone **2b**

White solid: mp 191-193 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.4 Hz, 2H), 7.50 – 7.41 (m, 4H), 7.24 (dd, *J* = 7.9, 3.1 Hz, 2H), 7.21 – 7.13 (m, 2H), 7.03 – 6.84 (m, 9H), 6.82 (d, *J* = 7.4 Hz, 1H), 2.43 (s, 3H), 2.31 (s, 3H), 1.41 (s, 3H), 0.86 (d, *J* = 6.8 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 196.0, 154.0, 153.3, 151.3, 140.4, 139., 138.4, 138.1, 136.8, 135.0, 131.3, 130.3, 130.1, 129.8, 129.7, 129.2, 128.8, 128.2, 128.0, 127.6, 127.1, 126.8, 125.9, 124.7, 123.2, 122.2, 121.2, 121.0, 20.1, 19.0, 14.2, 12.0; HRMS (ESI) m/z calcd for $C_{38}H_{32}N_2O$ (MH+) 533.2593, found 533.2603.



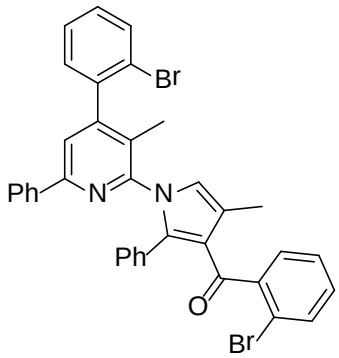
(4-Methyl-1-(3-methyl-6-phenyl-4-(p-tolyl)pyridin-2-yl)-2-phenyl-1H-pyrrol-3-yl)(p-tolyl)methanone **2c**



CCDC 994844

White crystalline solid: mp 213-216 ^{o}C

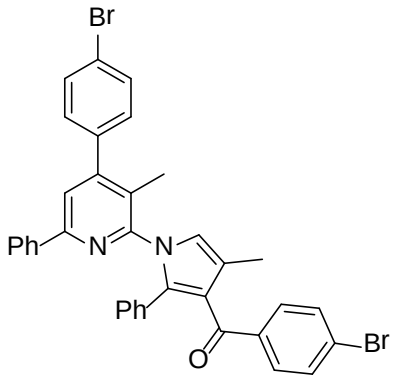
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.7 Hz, 2H), 7.60 (d, *J* = 7.5 Hz, 3H), 7.46 (dt, *J* = 14.4, 7.1 Hz, 3H), 7.17 (d, *J* = 7.9 Hz, 2H), 7.06 – 6.88 (m, 10H), 2.36 (s, 3H), 2.27 (s, 3H), 2.23 (s, 3H), 1.59 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 1945, 154.0, 1531, 1519, 142.14 (s), 1383, 138.1, 137.0, 136.6, 135.9, 131.7, 130.2, 130.0, 129.1, 128.8, 128.4, 128.3, 1275, 126.9, 126.9, 126.6, 122.6, 121.5, 121.3, 121.1, 21.4, 21.2, 15.1, 11.4; HRMS (ESI) m/z calcd for $C_{38}H_{32}N_2O$ (MH+) 533.2593, found 533.2605.



(2-Bromophenyl)(1-(4-(2-bromophenyl)-3-methyl-6-phenylpyridin-2-yl)-4-methyl-2-phenyl-1H-pyrrol-3-yl)methanone **2d**

White crystalline solid: mp 168-170 ^{o}C

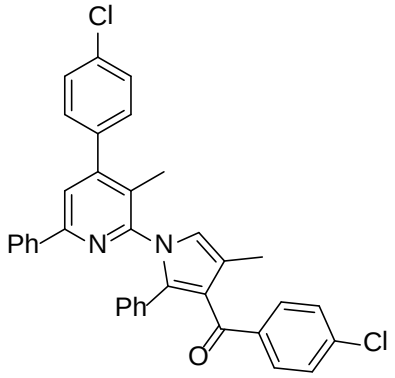
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.2 Hz, 2H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.49 – 7.39 (m, 4H), 7.32 (d, *J* = 7.4 Hz, 1H), 7.30 – 7.15 (m, 3H), 7.04 (dd, *J* = 6.2, 2.8 Hz, 3H), 6.95 – 6.84 (m, 6H), 2.40 (s, 3H), 1.54 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 192.6, 154.1, 152.3, 151.1, 142.1, 140.4, 139.6, 137.9, 132.8, 130.9, 130.7, 130.3, 130.3, 129.8, 129.6, 129.3, 128.7, 127.5, 127.3, 127.2, 126.8, 126.3, 122.9, 122.4, 121.8, 121.3, 121.0, 120.6, 14.4, 12.3; HRMS (ESI) m/z calcd for $C_{36}H_{26}Br_2N_2O$ (MH+) 663.0470, found 663.0490.



(4-Bromophenyl)(1-(4-(4-bromophenyl)-3-methyl-6-phenylpyridin-2-yl)-4-methyl-2-phenyl-1H-pyrrol-3-yl)methanone **2e**

White crystalline solid: mp 246-248 ^{o}C

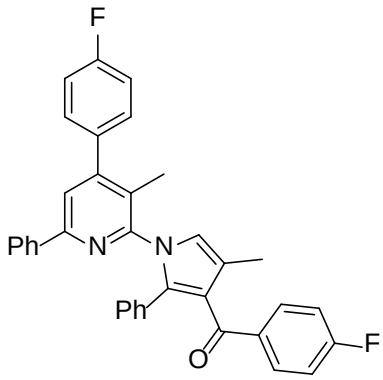
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.1 Hz, 2H), 7.57 (s, 1H), 7.55 – 7.41 (m, 7H), 7.22 (d, *J* = 8.4 Hz, 2H), 7.01 (dd, *J* = 6.0, 2.6 Hz, 1H), 6.99 – 6.88 (m, 7H), 2.31 (s, 3H), 1.56 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.3, 154.3, 152.0, 151.7, 138.1, 137.9, 137.7, 137.6, 131.7, 131.3, 131.3, 130.8, 130.3, 130.0, 129.4, 128.8, 127.6, 127.4), 126.8, 126.3, 126.3, 122.7, 122.0, 121.6, 120.8, 15.0, 11.5; HRMS (ESI) m/z calcd for $C_{36}H_{26}Br_2N_2O$ (MH+) 663.0470, found 663.0477.



(4-Chlorophenyl)(1-(4-(4-chlorophenyl)-3-methyl-6-phenylpyridin-2-yl)-4-methyl-2-phenyl-1H-pyrrol-3-yl)methanone **2f**

White crystalline solid: mp 229-230 ^{o}C

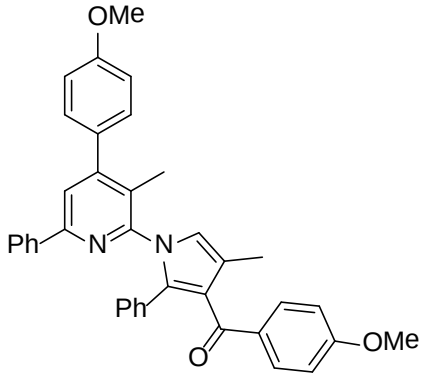
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 2H), 7.57 (s, 3H), 7.41 (dd, *J* = 50.8, 6.1 Hz, 6H), 7.06 (d, *J* = 7.0 Hz, 2H), 6.98 (d, *J* = 17.4 Hz, 7H), 2.31 (s, 3H), 1.56 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.2, 154.3, 152.0, 151.7, 137.9, 137.7, 137.6, 137.1, 134.5, 131.3, 131.2, 130.3, 129.8, 129.4, 128.9, 128.8, 127.8, 127.6, 127.4, 126.9, 126.4, 122.1, 122.0, 121.6, 120.9, 15.0, 11.5; HRMS (ESI) m/z calcd for $C_{36}H_{28}Cl_2N_2O$ (MH+) 573.1500, found 573.1510.



(4-Fluorophenyl)(1-(4-(4-fluorophenyl)-3-methyl-6-phenylpyridin-2-yl)-4-methyl-2-phenyl-1H-pyrrol-3-yl)methanone **2g**

White crystalline solid: mp 171-172 ^{o}C

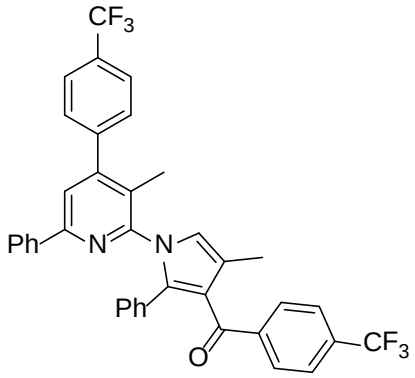
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 2H), 7.67 (s, 2H), 7.59 (s, 1H), 7.48 (d, *J* = 8.2 Hz, 3H), 7.20 – 6.84 (m, 10H), 6.76 (s, 2H), 2.32 (s, 3H), 1.56 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.0, 166.0, 163.9, 163.5, 161.4, 154.2, 152.2, 151.8, 138.0, 137.4, 135.6, 134.7, 132.3, 132..2, 131.4, 130.3, 130.6, 130.2, 129.3, 128.8, 127.6, 127.3, 126.8, 126.5, 122.2, 122.0, 121.6, 121.1, 115.6, 115.4, 114.7, 114.4, 15.0, 11.4; HRMS (ESI) m/z calcd for $C_{36}H_{28}F_2N_2O$ (MH+) 541.2091, found 41.2097.



(4-Methoxyphenyl)(1-(4-(4-methoxyphenyl)-3-methyl-6-phenylpyridin-2-yl)-4-methyl-2-phenyl-1H-pyrrol-3-yl)methanone **2h**

White crystalline solid: mp 203-204 ^{o}C

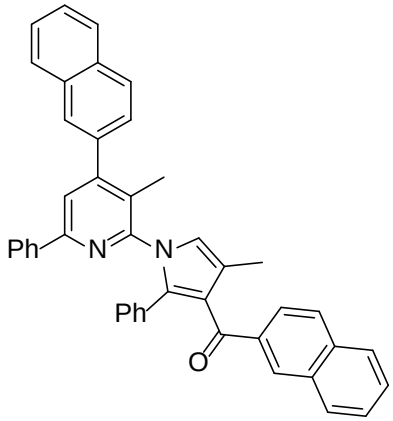
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 8.00 (m, 2H), 7.70 (d, *J* = 8.8 Hz, 2H), 7.60 (s, 1H), 7.44 (ddd, *J* = 10.9, 9.6, 5.7 Hz, 3H), 7.06 – 6.87 (m, 10H), 6.63 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 3.72 (s, 3H), 2.27 (s, 3H), 1.60 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.5, 162.5, 159.6, 154.0, 152.8, 151.9, 138.3, 136.5, 132.1, 132.1, 131.8, 131.1, 130.1, 129.8, 129.1, 128.7, 127.5, 127.0, 126.8, 126.6, 122.7, 121.4, 121.3, 121.0, 113.9, 112.9, 55.3, 55.2, 15.2, 11.3; HRMS (ESI) m/z calcd for $C_{38}H_{32}N_2O_3$ (MH+) 565.2491, found 565.2503.



(4-Methyl-1-(3-methyl-6-phenyl-4-(4-(trifluoromethyl)phenyl)pyridin-2-yl)-2-phenyl-1H-pyrrol-3-yl)(4-(trifluoromethyl)phenyl)methanone **2i**

White crystalline solid: mp 200-202 ^{o}C

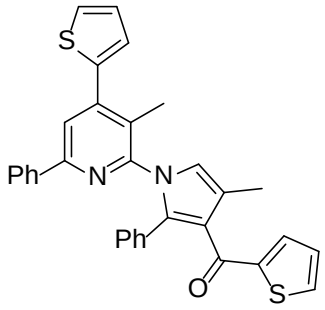
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.3 Hz, 2H), 7.66 (dd, *J* = 13.4, 8.3 Hz, 4H), 7.59 (s, 1H), 7.48 (t, *J* = 8.6 Hz, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 7.04 – 6.86 (m, 6H), 2.37 (s, 3H), 1.57 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.2, 154.5, 151.8, 151.7, 142.5, 142.3, 138.5, 137.7, 131.1, 130.5, 129.8, 129.6, 128.9, 128.8, 128.3, 127.6, 127.6, 126.9, 126.3, 125.6 (d, *J* = 3.4 Hz), 125.1, 124.43 (d, *J* = 3.6 Hz), 122.5, 122.0, 121.7, 120.9, 15.0, 11.7; HRMS (ESI) m/z calcd for $C_{38}H_{26}F_6N_2O$ (MH+) 641.2028, found 641.2044.



(4-Methyl-1-(3-methyl-4-(naphthalen-2-yl)-6-phenylpyridin-2-yl)-2-phenyl-1H-pyrrol-3-yl)(naphthalen-2-yl)methanone **2j**

White crystalline solid: mp 158-161 ^{o}C

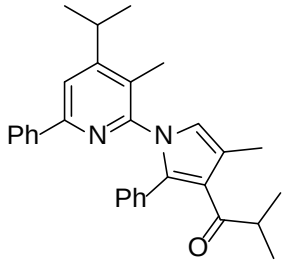
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (s, 1H), 8.07 (d, *J* = 7.7 Hz, 2H), 7.89 – 7.77 (m, 4H), 7.75 – 7.62 (m, 4H), 7.57 (s, 1H), 7.48 (dt, *J* = 14.8, 6.2 Hz, 6H), 7.37 (t, *J* = 7.4 Hz, 1H), 7.16 – 6.97 (m, 4H), 6.86 (d, *J* = 7.0 Hz, 3H), 2.34 (s, 3H), 1.65 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.5, 154.2, 153.2, 151.8, 138.2, 137.6, 136.5, 136.3, 134.8, 133.0, 132.8, 132.1, 132.0, 131.7, 130.2, 129.2, 129.2, 128.8, 128.1, 128.1, 127.7, 127.7, 127.6, 127.5, 127.4, 127.0, 126.9, 126.8, 126.6, 126.1, 126.0, 125.5, 122.7, 121.9, 121.5, 121.3, 15.2, 11.5; HRMS (ESI) m/z calcd for $C_{44}H_{32}N_2O$ (MH+) 605.2593, found 605.2606.



(4-Methyl-1-(3-methyl-6-phenyl-4-(thiophen-2-yl)pyridin-2-yl)-2-phenyl-1H-pyrrol-3-yl)(thiophe n-2-yl)methanone **2k**

White crystalline solid: mp 132-133 ^{o}C

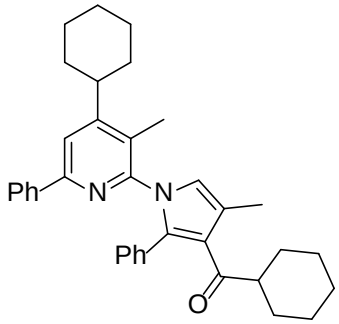
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 7.2 Hz, 2H), 7.77 (s, 1H), 7.44 (ddd, *J* = 24.2, 11.5, 5.6 Hz, 5H), 7.21 (d, *J* = 3.6 Hz, 1H), 7.12 – 7.05 (m, 3H), 6.99 (dd, *J* = 17.9, 5.1 Hz, 4H), 6.91 (s, 1H), 6.75 – 6.68 (m, 1H), 2.30 (s, 3H), 1.77 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 186.4, 154.3, 152.2, 145.6, 145.3, 139.6, 138.0, 136.3, 134.5, 132.7, 131.7, 130.0, 129.3, 128.8, 128.3, 127.8, 127.6, 127.2, 127.2, 127.2, 126.9, 126.5, 122.9, 121.5, 121.3, 121.7, 105.0, 15.5, 11.0; HRMS (ESI) m/z calcd for $C_{32}H_{24}N_2OS_2$ (MH+) 517.1408, found 517.1418.



1-(1-(4-Isopropyl-3-methyl-6-phenylpyridin-2-yl)-4-methyl-2-phenyl-1H-pyrrol-3-yl)-2-methylpr opan-1-one **2l**

White crystalline solid: mp 169-171 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.5 Hz, 2H), 7.55 (s, 1H), 7.49 – 7.40 (m, 3H), 7.16 (s, 5H), 6.76 (s, 1H), 2.96 (dt, *J* = 13.6, 6.8 Hz, 1H), 2.62 (dt, *J* = 13.5, 6.7 Hz, 1H), 2.30 (s, 3H), 1.66 (s, 3H), 0.96 (d, *J* = 6.6 Hz, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 206.0, 159.1, 154.4, 151.1, 138.8, 136.8, 132.3, 130.3, 129.0, 128.7, 127.8, 127.7, 126.9, 126.5, 123.2, 121.2, 121.2, 116.8, 38.8, 29.6, 22.3, 12.8, 11.8; HRMS (ESI) m/z calcd for $C_{30}H_{32}N_2O$ (MH+) 437.2593, found 437.2599.

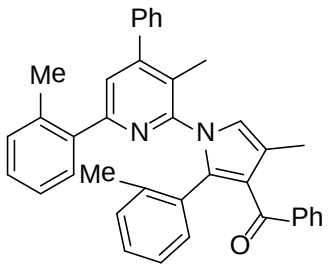


Cyclohexyl(1-(4-cyclohexyl-3-methyl-6-phenylpyridin-2-yl)-4-methyl-2-phenyl-1H-pyrrol-3-yl)m

ethanone **2m**

White crystalline solid: mp 185-186 ^{o}C

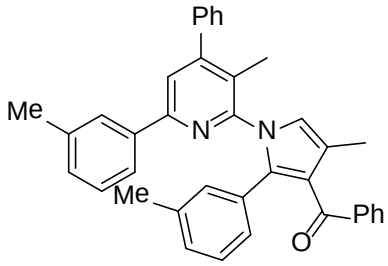
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.5 Hz, 2H), 7.52 (s, 1H), 7.43 (dt, *J* = 22.7, 7.1 Hz, 3H), 7.23 – 7.12 (m, 5H), 6.72 (s, 1H), 2.55 (s, 1H), 2.34 – 2.24 (m, 4H), 1.89 – 1.58 (m, 11H), 1.52 – 1.00 (m, 10H), 0.73 (q, *J* = 12.8 Hz, 2H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 204.8, 158.0, 154.2, 138.8, 137.1, 132.4, 130.4, 128.9, 128.7, 127.8, 127.6, 126.9, 126.5, 121.4, 121.0, 117.5, 49.1, 40.3, 32.8, 26.7, 26.0, 25.8 12.9, 12.0; HRMS (ESI) m/z calcd for $C_{36}H_{40}N_2O$ (MH+) 517.3219, found 517.3221.



(4-Methyl-1-(3-methyl-4-phenyl-6-(o-tolyl)pyridin-2-yl)-2-(o-tolyl)-1H-pyrrol-3-yl)(phenyl)methanone **2n**

Yellow oil.

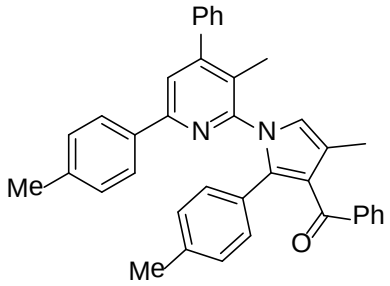
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.7 Hz, 2H), 7.37 (t, *J* = 4.9 Hz, 3H), 7.31 – 7.25 (m, 3H), 7.25 – 7.19 (m, 3H), 7.10 (t, *J* = 7.6 Hz, 4H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.98 – 6.89 (m, 2H), 6.85 (t, *J* = 6.1 Hz, 2H), 2.32 (s, 3H), 2.29 (s, 3H), 2.09 (s, 3H), 1.83 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.6, 156.6, 152.6, 151.2, 139.2, 138.7, 135.8, 132.0, 131.5, 131.3, 130.7, 129.8, 129.7, 129.5, 128.5, 128.5, 128.3, 127.8, 127.3, 125.9, 125.6, 124.6, 124.6, 121.5, 121.3, 20.4, 20.4, 15.5, 11.7; HRMS (ESI) m/z calcd for $C_{38}H_{32}N_2O$ (MH+) 533.2593, found 533.2595.



(4-Methyl-1-(3-methyl-4-phenyl-6-(m-tolyl)pyridin-2-yl)-2-(m-tolyl)-1H-pyrrol-3-yl)(phenyl)methanone **2o**

White crystalline solid: mp 163-164 ^{o}C

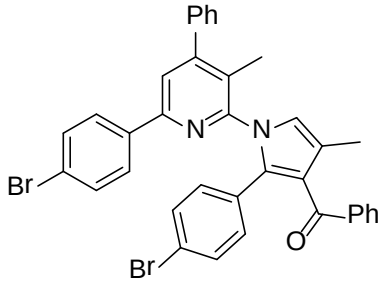
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 2H), 7.62 (d, *J* = 25.4 Hz, 3H), 7.37 (s, 4H), 7.25 (s, 2H), 7.09 (s, 4H), 6.93 (s, 1H), 6.78 (s, 4H), 2.44 (s, 3H), 2.32 (s, 3H), 1.98 (s, 3H), 1.60 (d, *J* = 3.8 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.8, 154.3, 153.1, 151.8, 139.5, 138.9, 138.5, 138.2, 138.0, 136.8, 131.5, 131.3, 129.9, 129.6, 128.7, 128.4, 128.2, 127.7, 127.6, 127.4, 127.3, 127.1, 126.4, 124.0, 122.3, 122.0, 121.4, 121.2, 21.5, 21.0, 15.0, 11.6; HRMS (ESI) m/z calcd for $C_{38}H_{32}N_2O$ (MH+) 533.2593, found 533.2600.



(4-Methyl-1-(3-methyl-4-phenyl-6-(p-tolyl)pyridin-2-yl)-2-(p-tolyl)-1H-pyrrol-3-yl)(phenyl)methanone **2p**

White crystalline solid: mp 199-201 ^{o}C

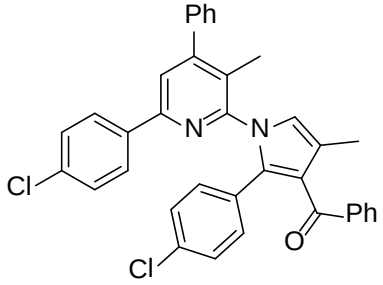
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.0 Hz, 2H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.58 (s, 1H), 7.36 (d, *J* = 4.4 Hz, 3H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.23 (s, 1H), 7.16 – 7.05 (m, 4H), 6.95 – 6.84 (m, 3H), 6.72 (d, *J* = 7.9 Hz, 2H), 2.42 (s, 3H), 2.28 (s, 3H), 2.12 (s, 3H), 1.57 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.8, 154.1, 153.0, 151.8, 139.4, 139.3, 139.0, 137.8, 136.8, 135.5, 131.3, 130.2, 129.8, 129.5, 128.6, 128.5, 128.4, 128.7, 128.1, 127.5, 126.8, 126.3, 122.1, 121.7, 121.2, 120.7, 21.3, 21.0, 14.9, 11.6; HRMS (ESI) m/z calcd for $C_{38}H_{32}N_2O$ (MH+) 533.2593, found 533.2598.



(2-(4-Bromophenyl)-1-(6-(4-bromophenyl)-3-methyl-4-phenylpyridin-2-yl)-4-methyl-1H-pyrrol-3-yl)(phenyl)methanone **2q**

White crystalline solid: mp 181-182 ^{o}C

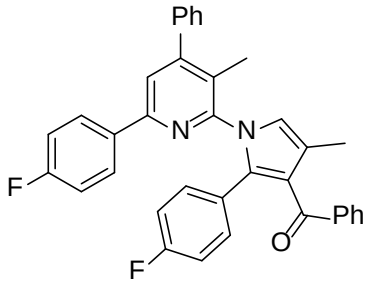
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 6.4 Hz, 2H), 7.67 (s, 2H), 7.60 (s, 3H), 7.40 (s, 3H), 7.32 (s, 1H), 7.11 (dd, *J* = 24.7, 17.8 Hz, 6H), 6.89 (d, *J* = 6.4 Hz, 3H), 2.26 (s, 3H), 1.64 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.4, 153.6, 153.0, 151.6, 139.2, 138.5, 136.8, 136.0, 132.0, 131.8, 131.7, 130.7, 130.5, 129.7, 128.6, 128.5, 128.4, 128.4, 127.8, 126.9, 123.8, 122.9, 122.0, 121.7, 121.5, 121.0, 15.0, 11.5; HRMS (ESI) m/z calcd for $C_{36}H_{26}Br_2N_2O$ (MH+) 663.0470, found 663.0491.



(2-(4-Chlorophenyl)-1-(6-(4-chlorophenyl)-3-methyl-4-phenylpyridin-2-yl)-4-methyl-1H-pyrrol-3-yl)(phenyl)methanone **2r**

White crystalline solid: mp 229-230 ^{o}C

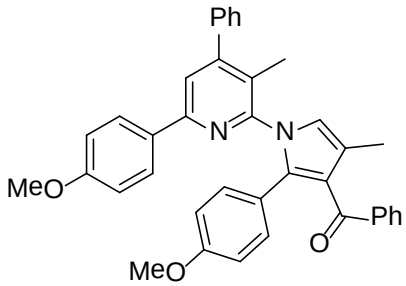
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 5.4 Hz, 2H), 7.57 (s, 3H), 7.48 (d, *J* = 8.1 Hz, 3H), 7.35 (d, *J* = 6.9 Hz, 2H), 7.16 – 6.85 (m, 10H), 2.31 (s, 3H), 1.56 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 193.2, 154.3, 152.0, 151.7, 137.9, 137.7, 137.6, 137.1, 134.5, 131.6, 131.6, 130.3, 129.8, 129.4, 128.9, 128.8, 127.8, 127.6, 127.8, 126.8, 126.4, 122.1, 122.1, 121.6, 121.0, 15.0, 11.5; HRMS (ESI) m/z calcd for $C_{36}H_{26}Cl_2N_2O$ (MH+) 573.1500, found 573.1510.



(2-(4-Fluorophenyl)-1-(6-(4-fluorophenyl)-3-methyl-4-phenylpyridin-2-yl)-4-methyl-1H-pyrrol-3-yl)(phenyl)methanone **2s**

White crystalline solid: mp 186-187 ^{o}C

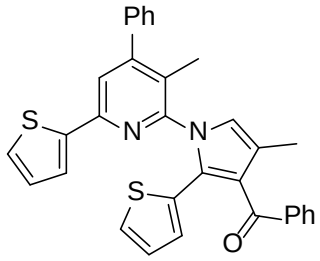
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 7.95 (m, 2H), 7.65 (d, *J* = 7.5 Hz, 2H), 7.57 (s, 1H), 7.39 (d, *J* = 4.7 Hz, 3H), 7.28 (d, *J* = 7.4 Hz, 1H), 7.21 – 7.06 (m, 6H), 7.02 – 6.93 (m, 2H), 6.91 (s, 1H), 6.64 (t, *J* = 8.3 Hz, 2H), 2.29 (s, 3H), 1.63 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.5, 164.0 (d, *J* = 189.3 Hz), 161.5 (d, *J* = 188.3 Hz), 153.5, 153.1, 151.6, 139.3, 138.6, 136.4, 134.2, 132.0 (d, *J* = 8.2 Hz), 131.7, 129.7, 128.7 (d, *J* = 8.3 Hz), 128.5, 128.4, 127.7, 126.4, 122.6, 121.9, 121.4, 120.9, 115.7 (d, *J* = 21.6 Hz), 114.6 (d, *J* = 21.7 Hz), 14.9, 11.5; HRMS (ESI) m/z calcd for $C_{36}H_{28}F_2N_2O$ (MH+) 541.2091, found 541.2102.



(2-(4-Methoxyphenyl)-1-(6-(4-methoxyphenyl)-3-methyl-4-phenylpyridin-2-yl)-4-methyl-1H-pyrrol-3-yl)(phenyl)methanone **2t**

White crystalline solid: mp 160-164 ^{o}C

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 7.2 Hz, 2H), 7.54 (s, 1H), 7.41 – 7.33 (m, 3H), 7.26 (s, 1H), 7.18 – 7.05 (m, 4H), 7.01 (d, *J* = 8.8 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 6.88 (s, 1H), 6.46 (d, *J* = 8.7 Hz, 2H), 3.88 (s, 3H), 3.63 (s, 3H), 2.29 (s, 3H), 1.56 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.7, 160.6, 158.6, 153.8, 153.0, 151.7, 139.4, 138.9, 137.6, 131.6, 131.4，130.8, 129.8, 128.5, 128.4, 128.5, 127.5, 125.8, 124.1, 121.8, 121.7, 121.0, 120.4, 114.1, 113.0, 55.4, 55.1, 14.9, 11.6; HRMS (ESI) m/z calcd for $C_{38}H_{32}N_2O_3$ (MH+) 565.2491, found 565.2500.



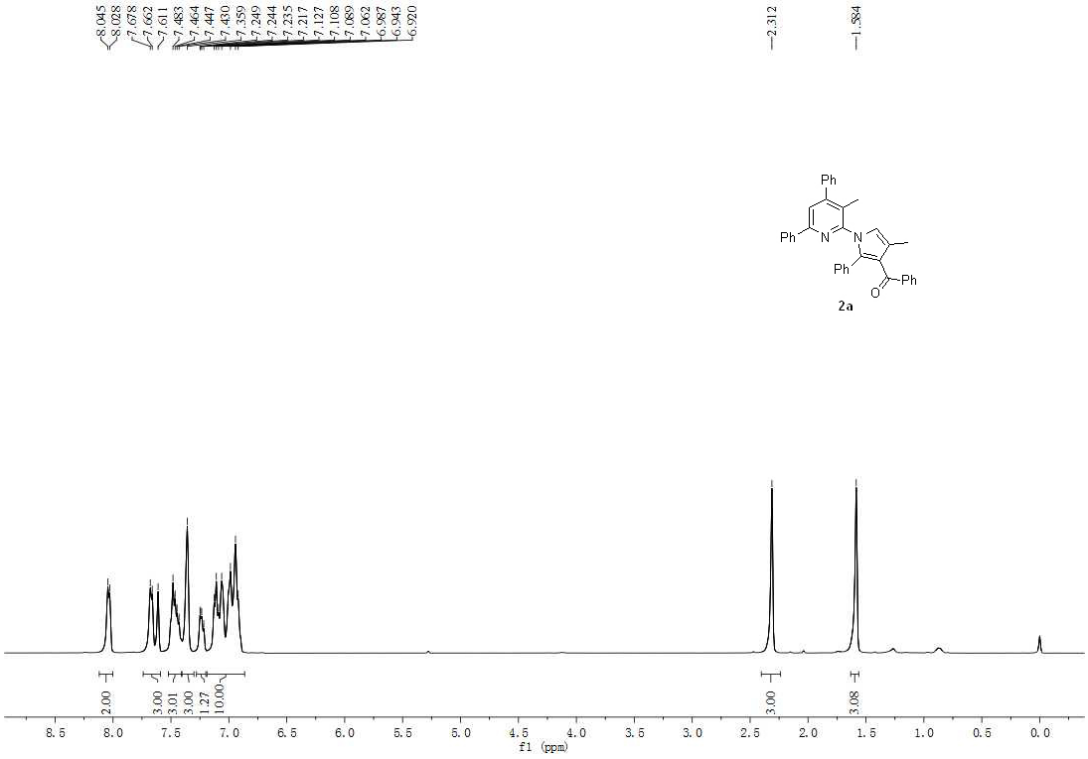
(4-Methyl-1-(3-methyl-4-phenyl-6-(thiophen-2-yl)pyridin-2-yl)-2-(thiophen-2-yl)-1H-pyrrol-3-yl)(phenyl)methanone **2u**

White crystalline solid: mp 76-79 ^{o}C

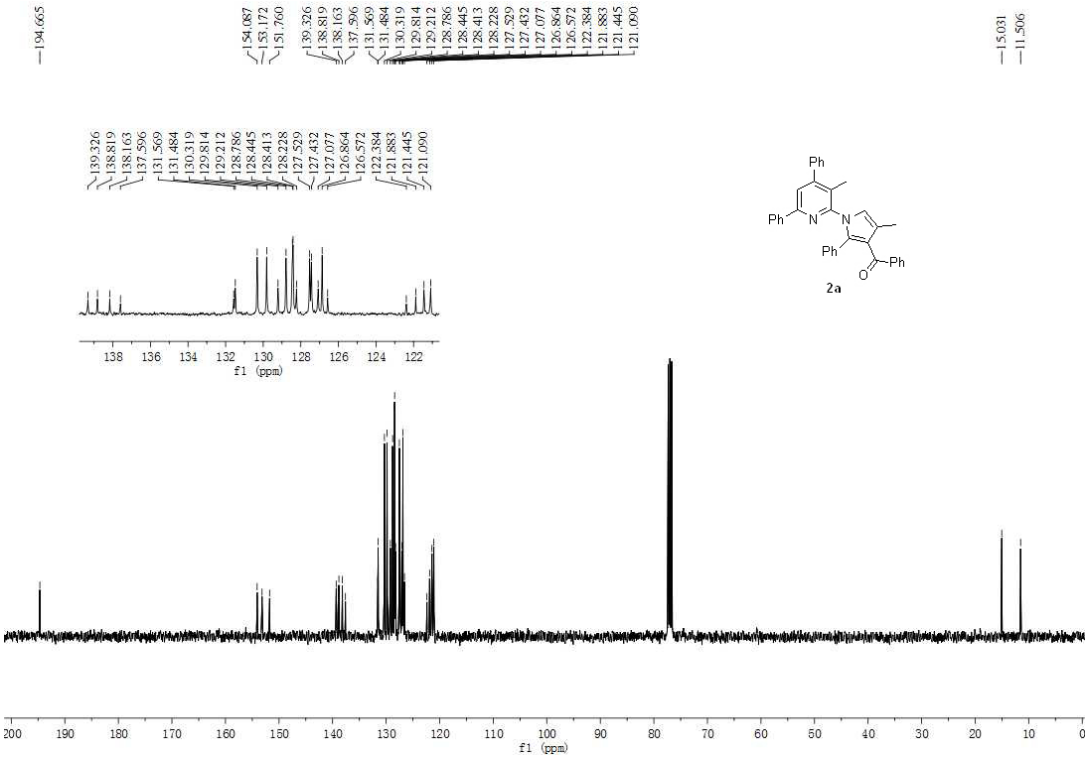
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.9 Hz, 2H), 7.65 (d, *J* = 3.6 Hz, 1H), 7.54 (s, 1H), 7.44 – 7.38 (m, 4H), 7.35 – 7.32 (m, 1H), 7.16 (ddd, *J* = 18.9, 13.8, 6.2 Hz, 5H), 6.99 (d, *J* = 5.0 Hz, 1H), 6.88 (s, 1H), 6.66 (d, *J* = 3.5 Hz, 1H), 6.62 – 6.57 (m, 1H), 2.25 (s, 3H), 1.70 (s, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 194.2, 153.1, 151.1, 149.4, 143.6, 139.2, 138.6, 132.0, 131.7, 129.8, 129.6, 129.5, 128.5, 128.4, 128.3, 128.0, 127.7, 127.1, 127.0, 126.3, 125.2, 123.4, 121.7, 120.0, 14.9, 11.5; HRMS (ESI) m/z calcd for $C_{32}H_{24}N_2OS_2$ (MH+) 517.1408, found 517.1411.

Copies of ^{1}H NMR, ^{13}C NMR spectra of products 2

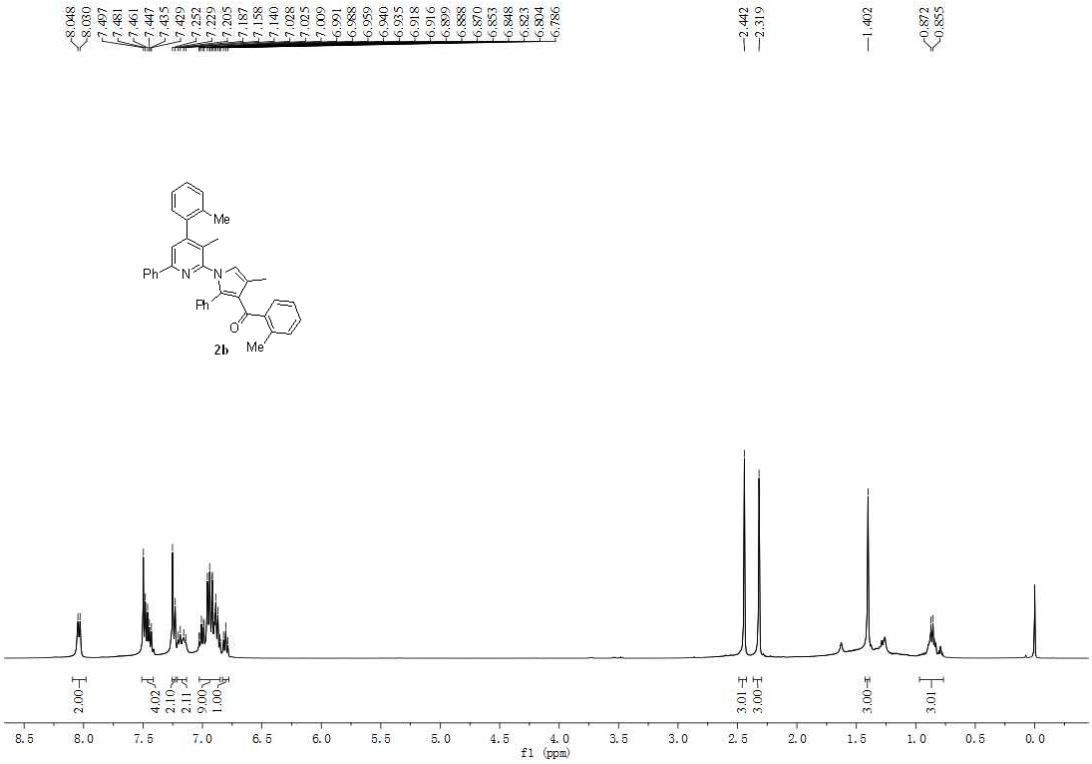
^{1}H NMR spectrum of product **2a**



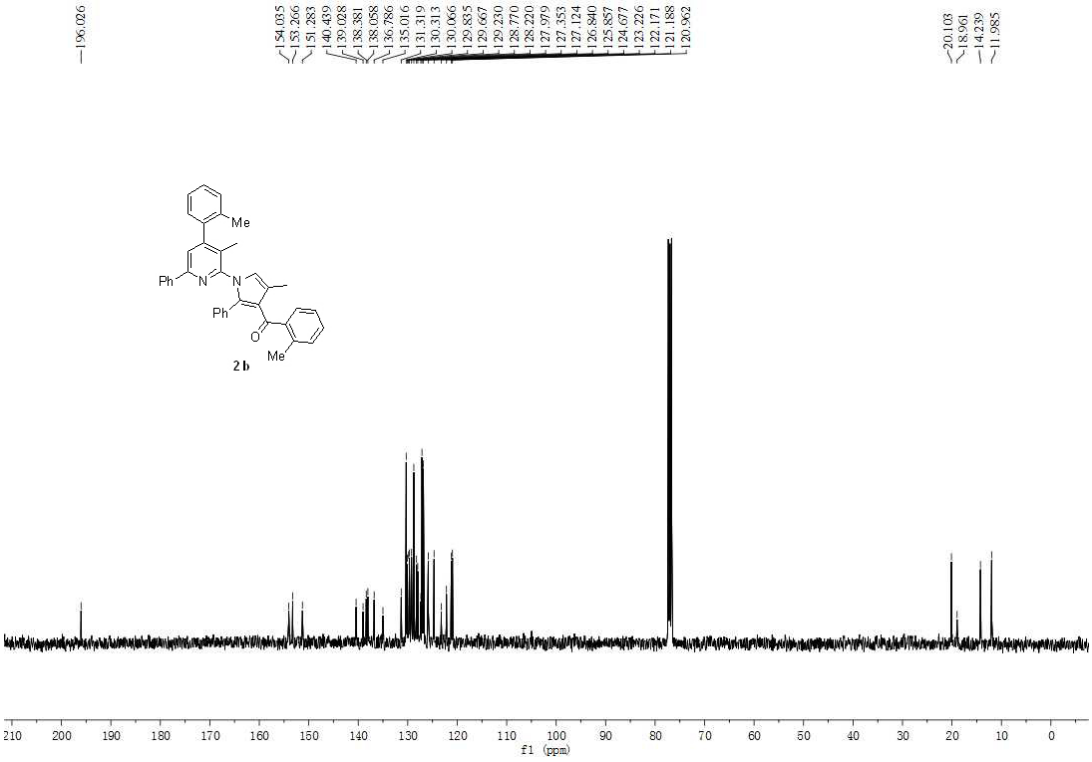
^{13}C NMR spectrum of product **2a**



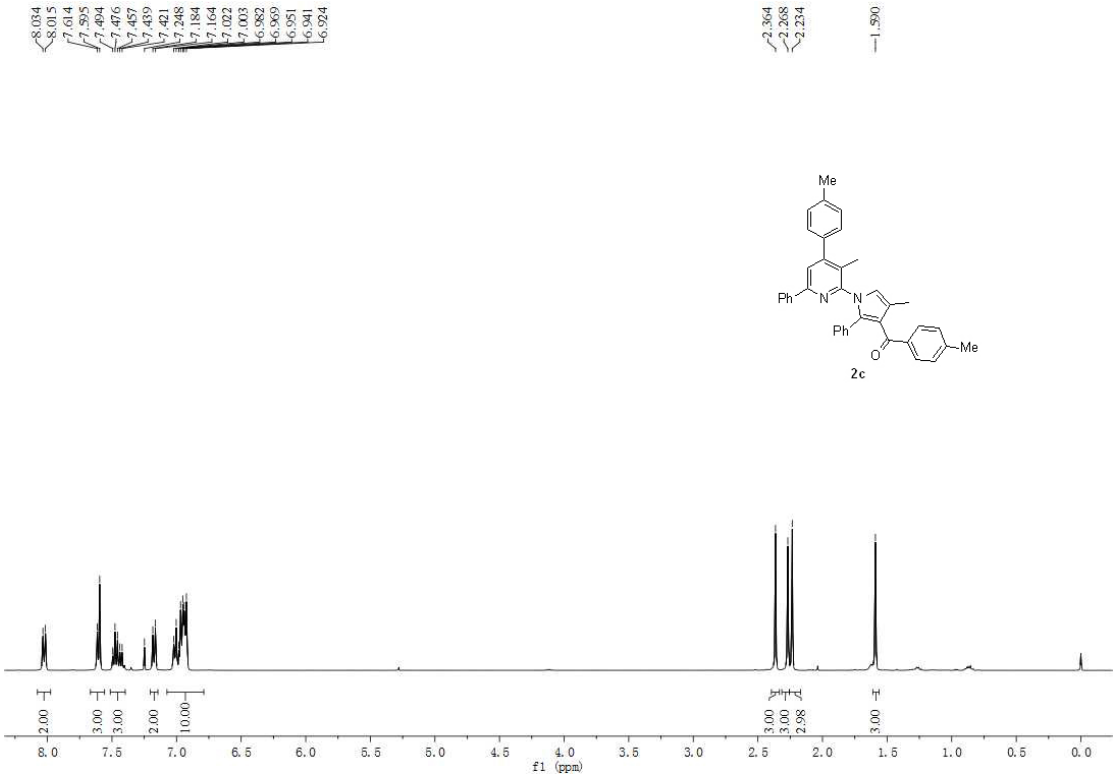
^{1}H NMR spectrum of product **2b**



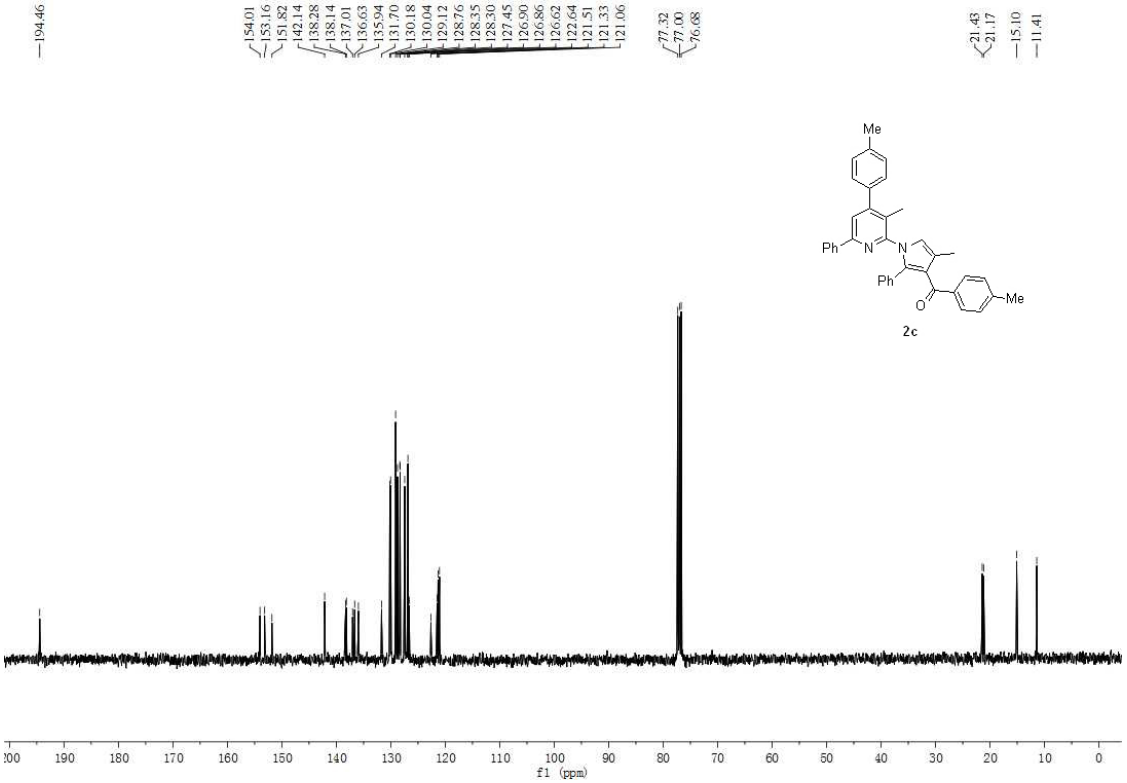
^{13}C NMR spectrum of product **2b**



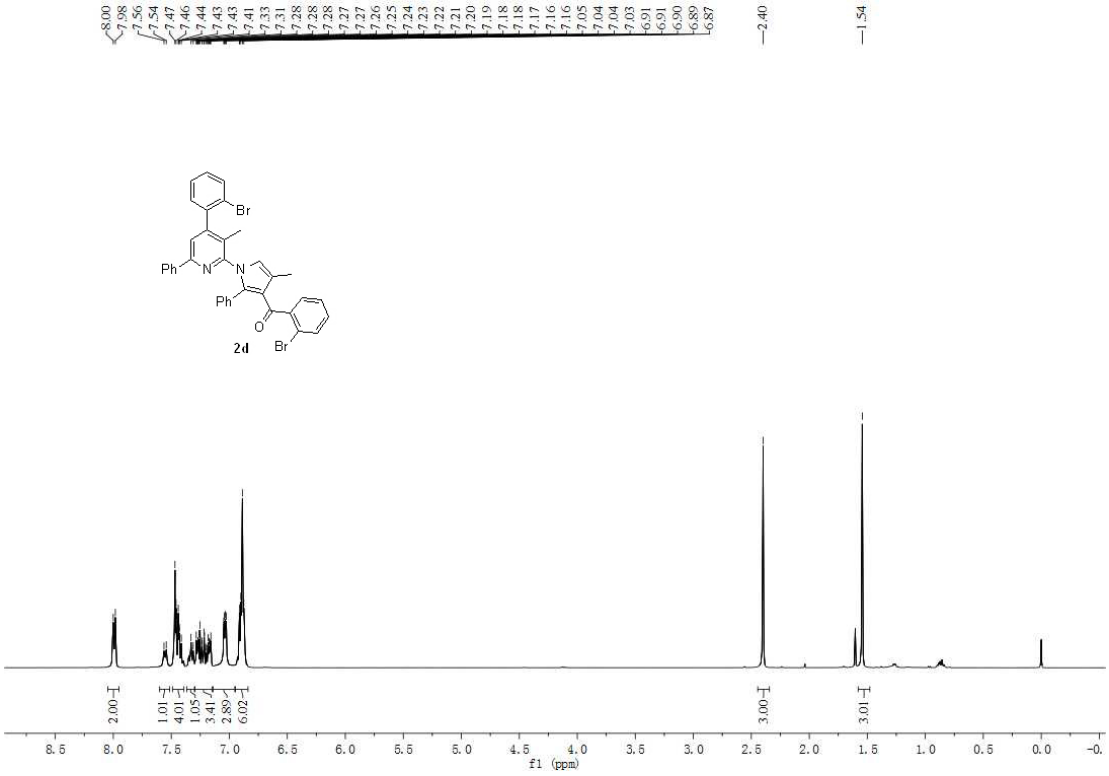
^{1}H NMR spectrum of product **2c**



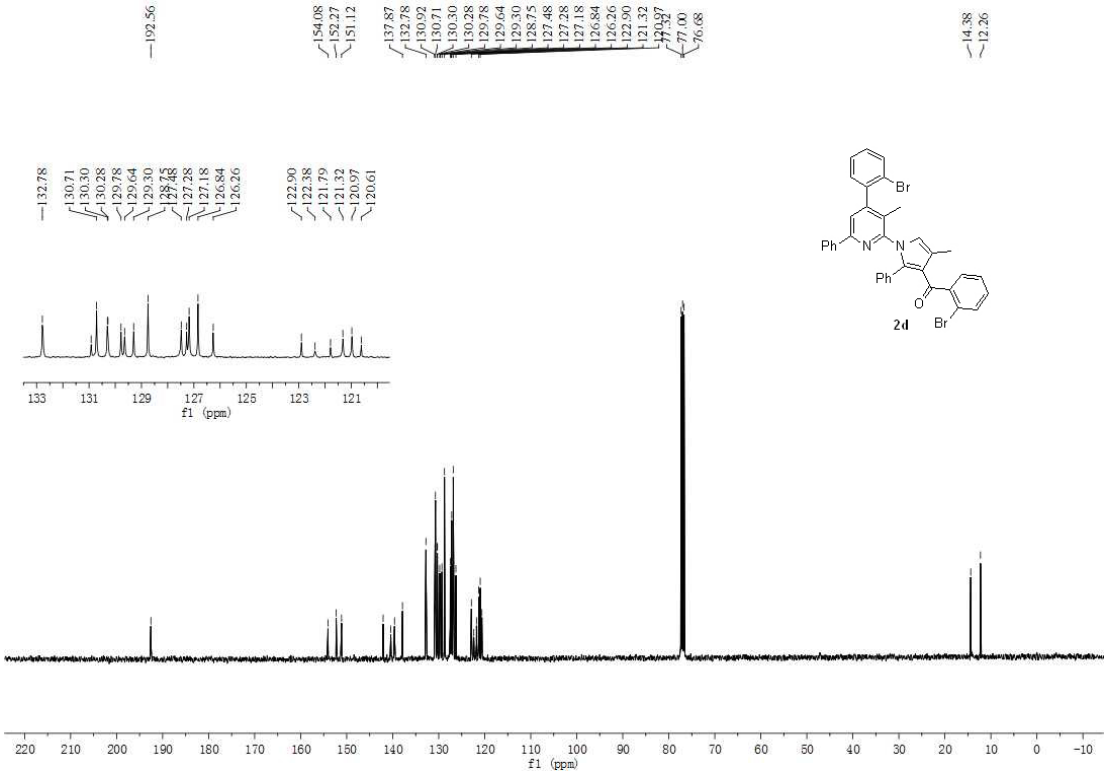
^{13}C NMR spectrum of product **2c**



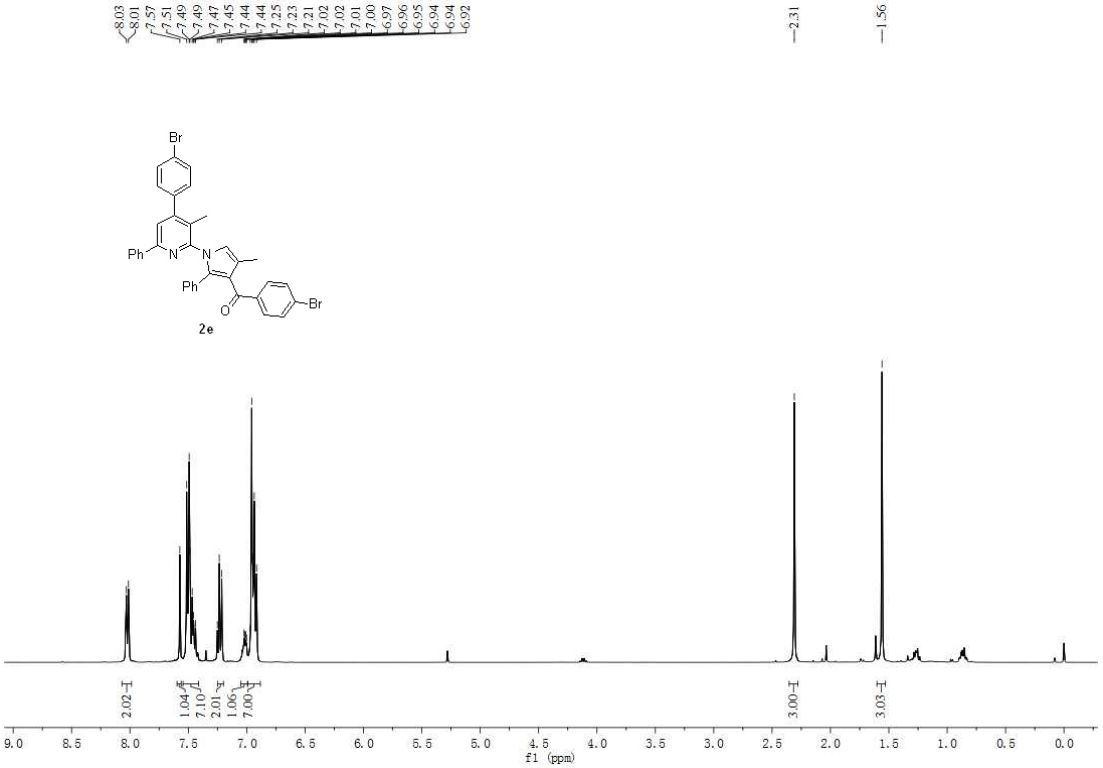
^{1}H NMR spectrum of product **2d**



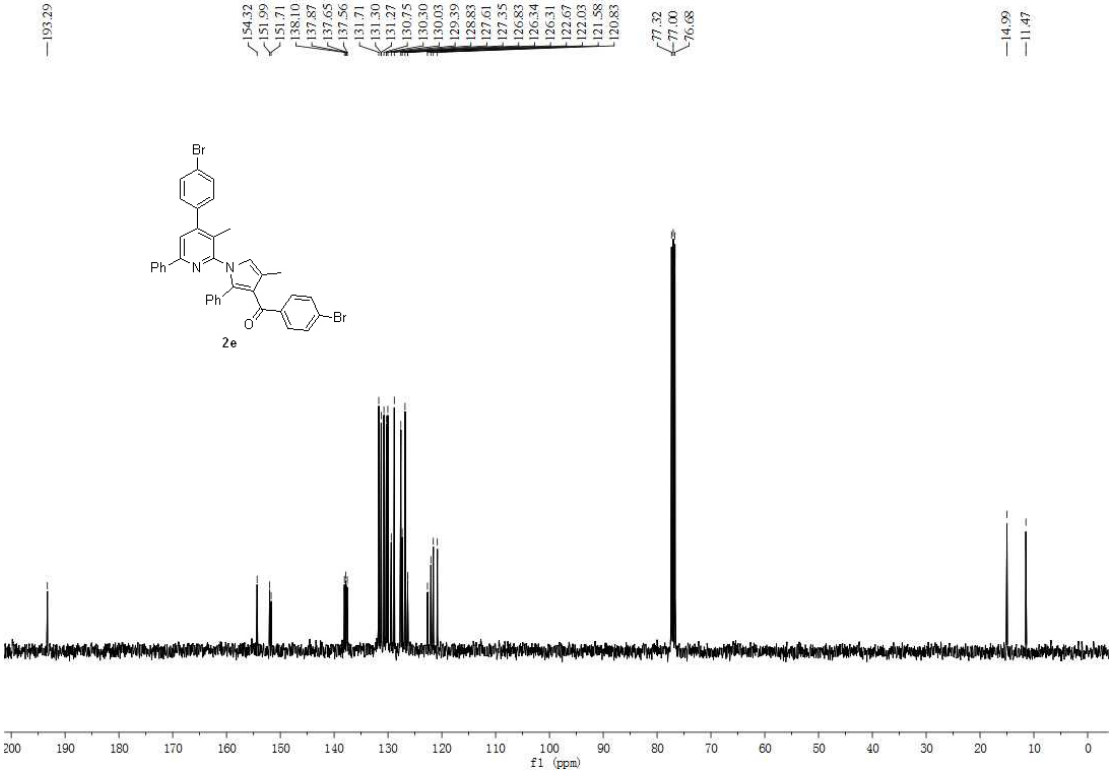
^{13}C NMR spectrum of product **2d**



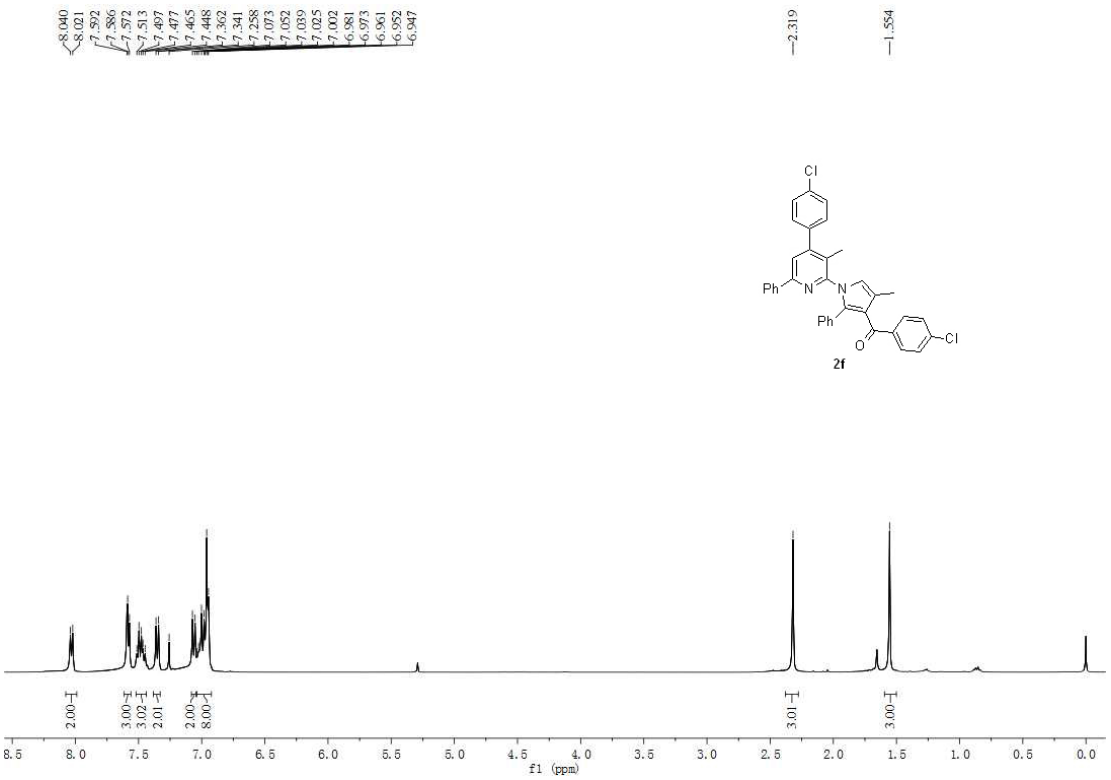
^{1}H NMR spectrum of product **2e**



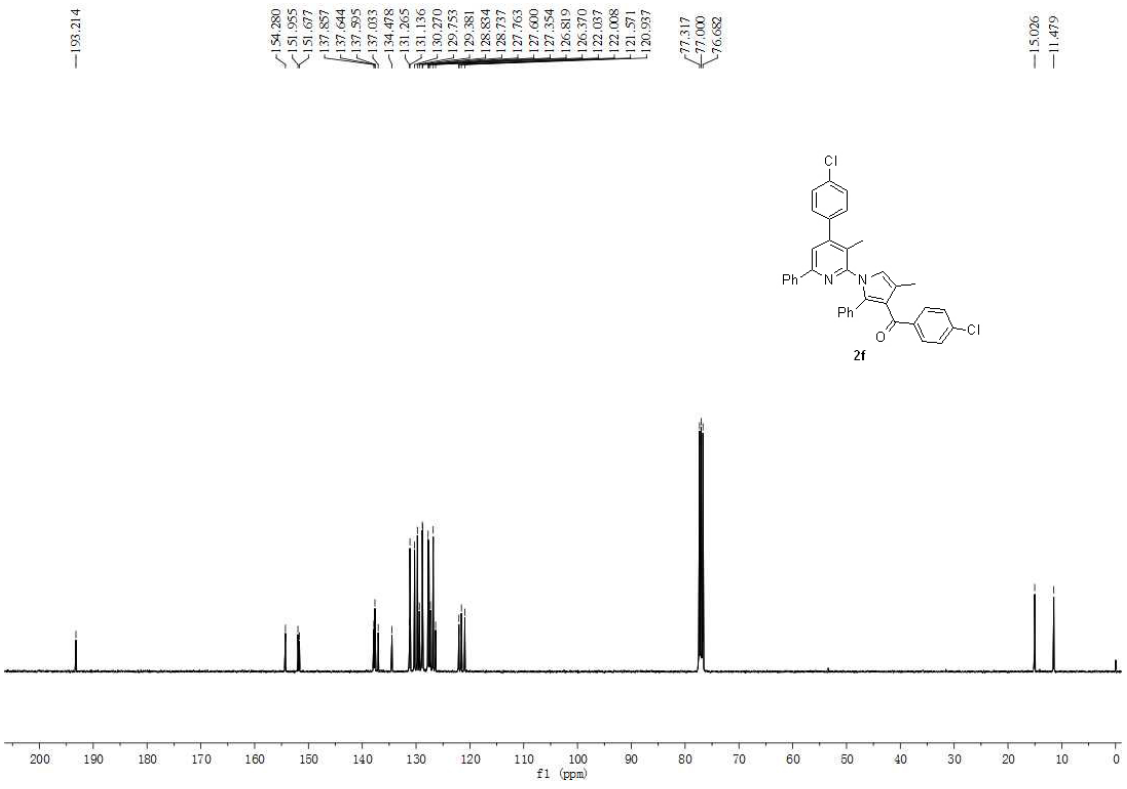
^{13}C NMR spectrum of product **2e**



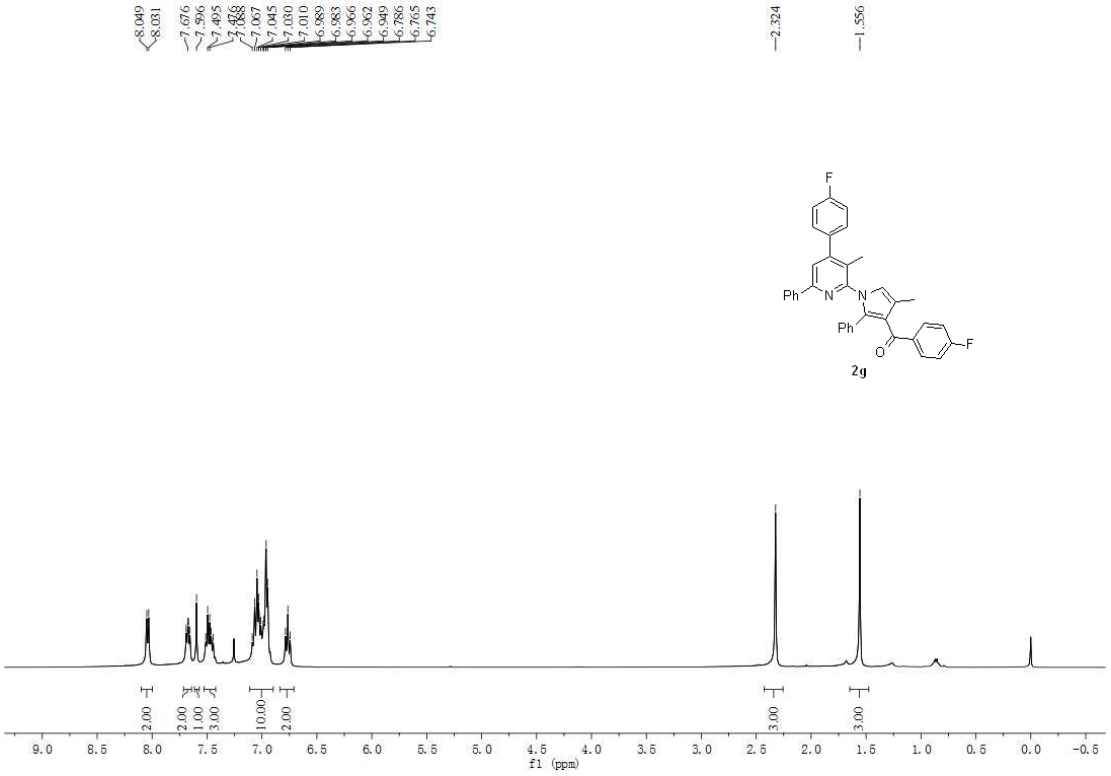
^{1}H NMR spectrum of product **2f**



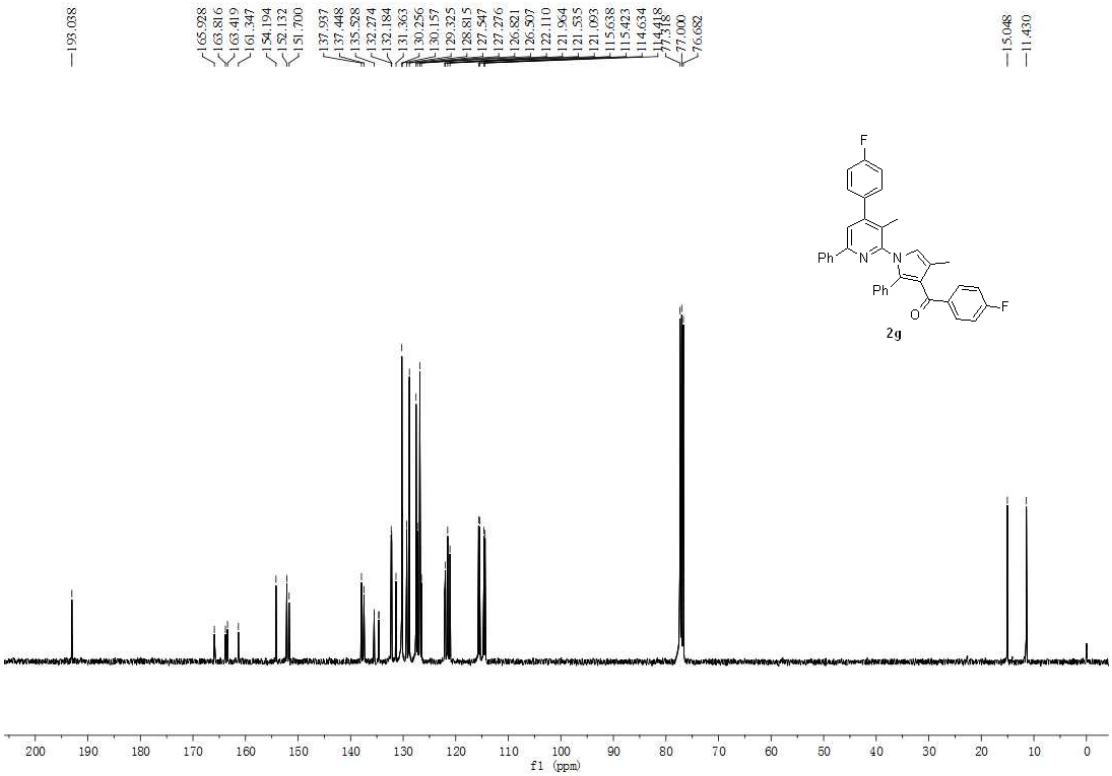
^{13}C NMR spectrum of product **2f**



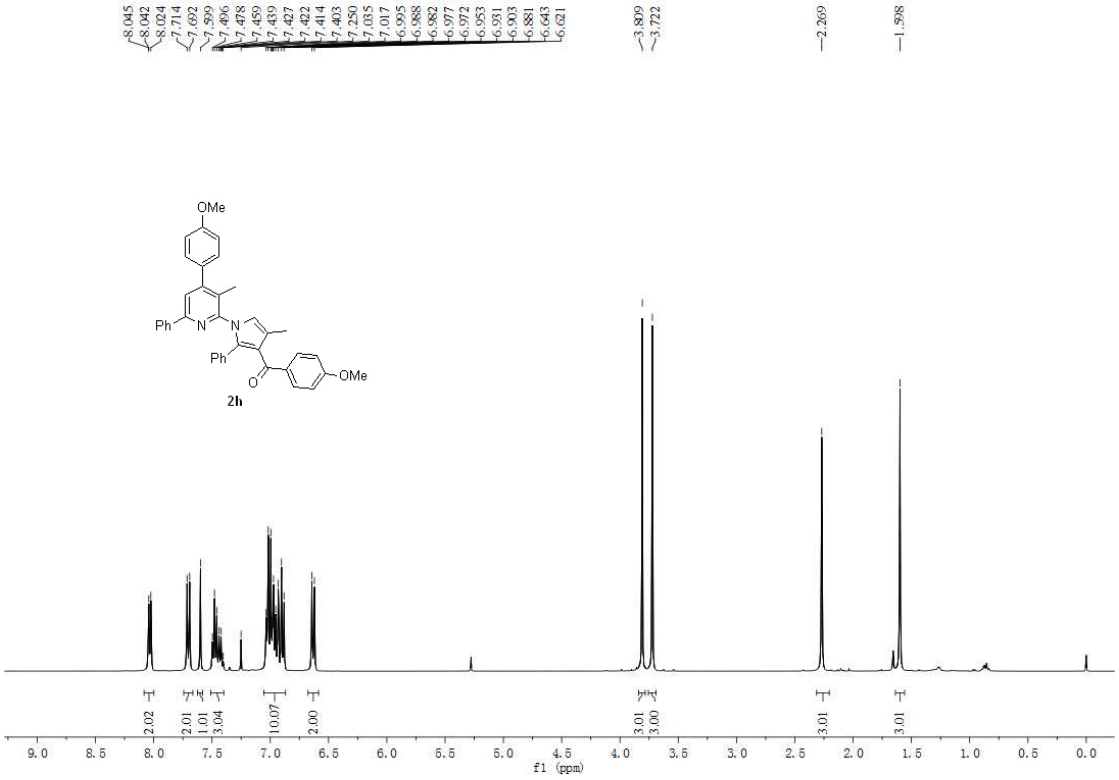
^{1}H NMR spectrum of product **2g**



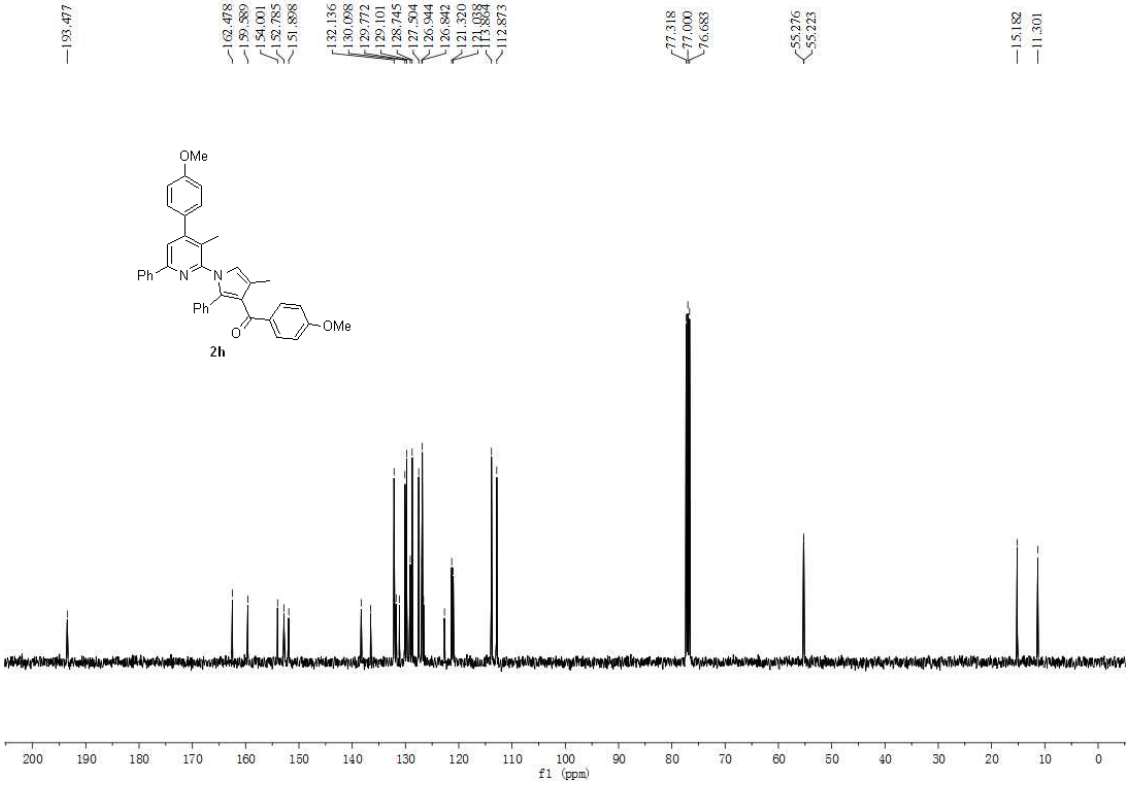
^{13}C NMR spectrum of product **2g**



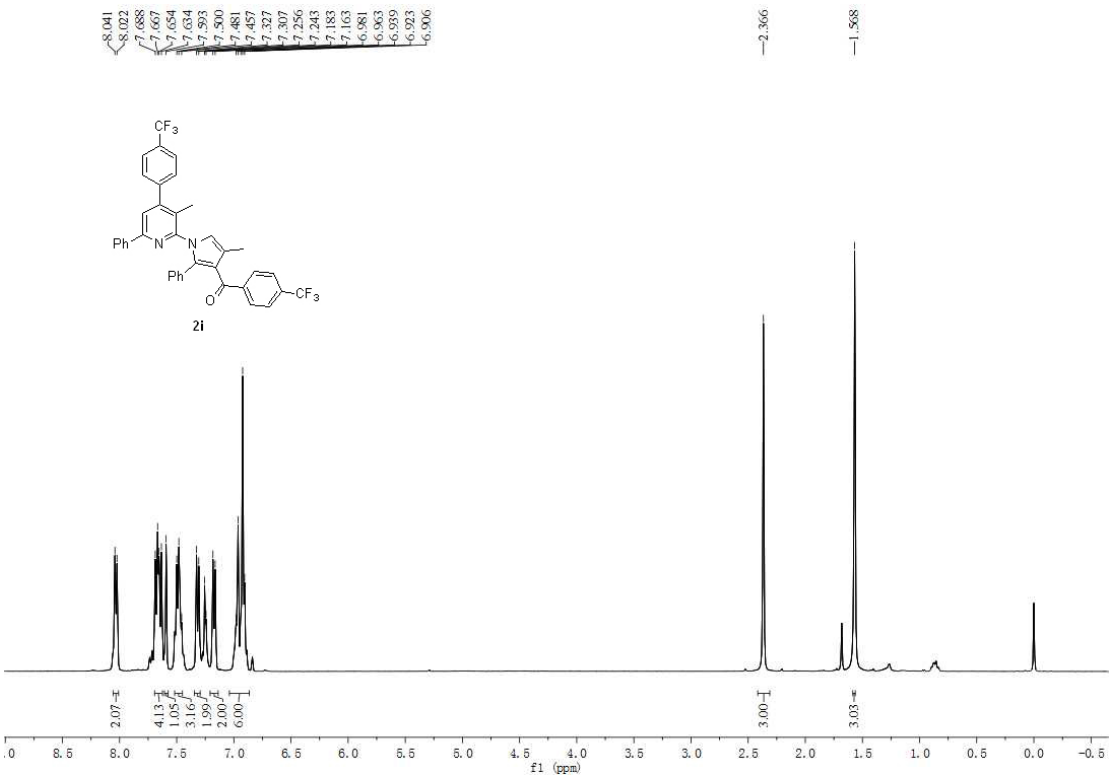
^{1}H NMR spectrum of product **2h**



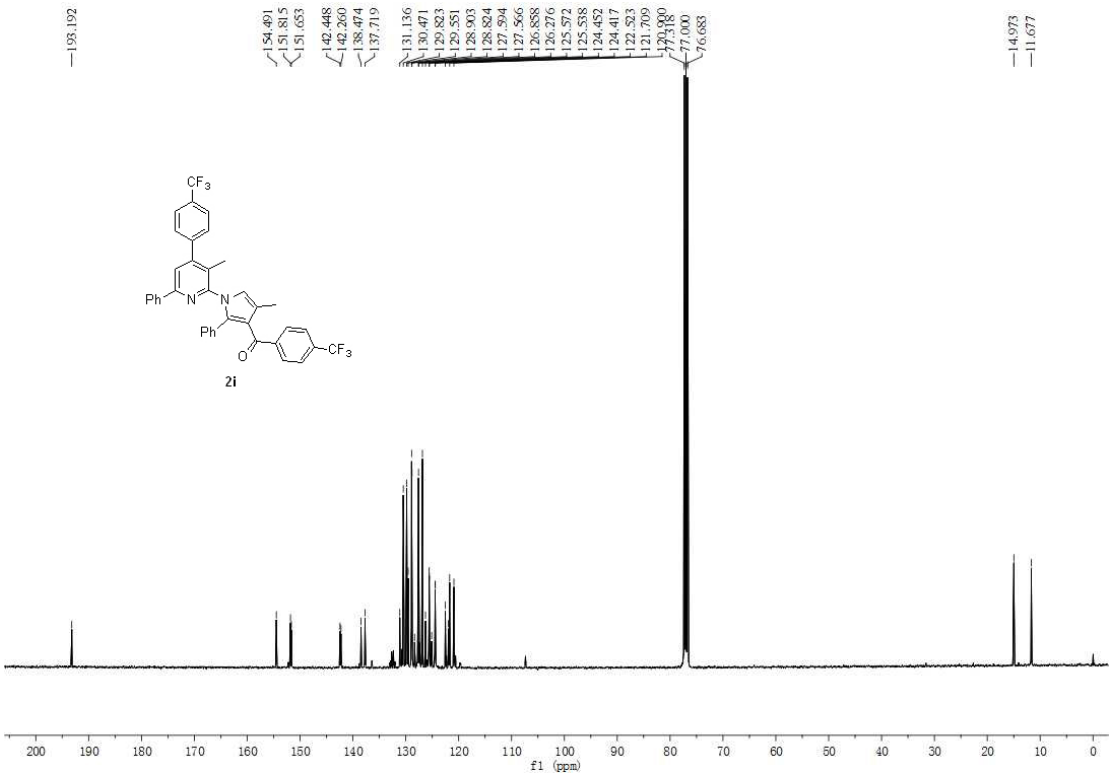
^{13}C NMR spectrum of product **2h**



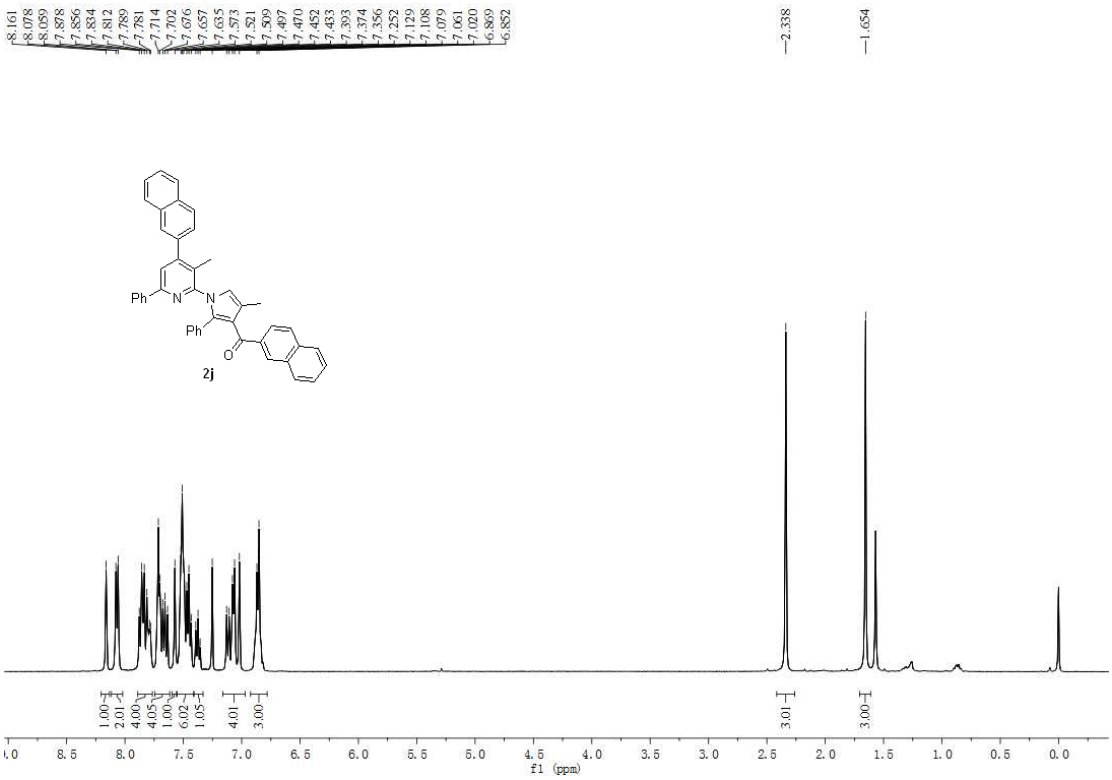
^{1}H NMR spectrum of product **2i**



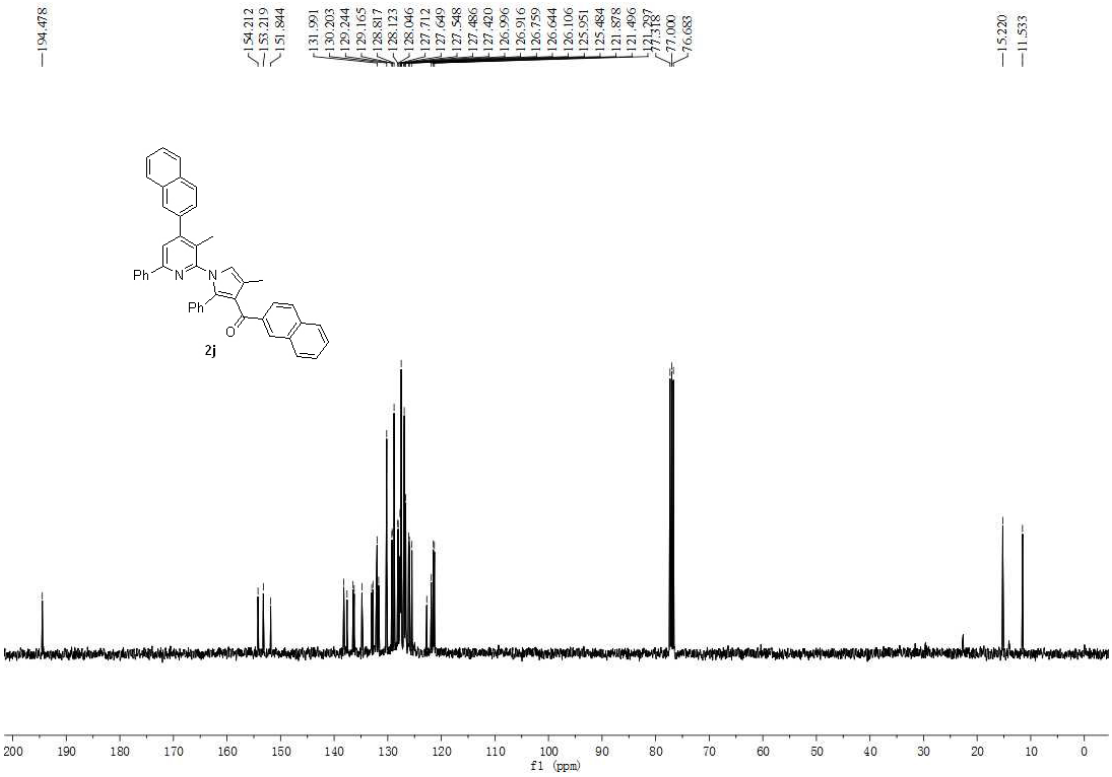
^{13}C NMR spectrum of product **2i**



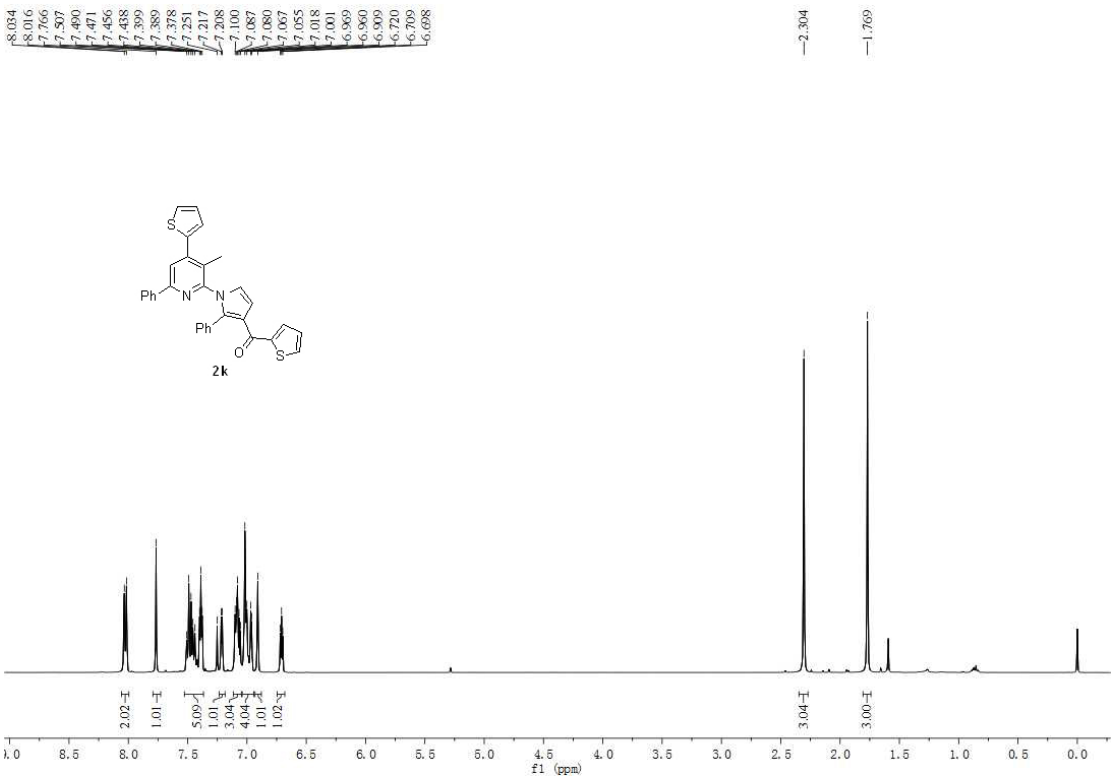
^{1}H NMR spectrum of product **2j**



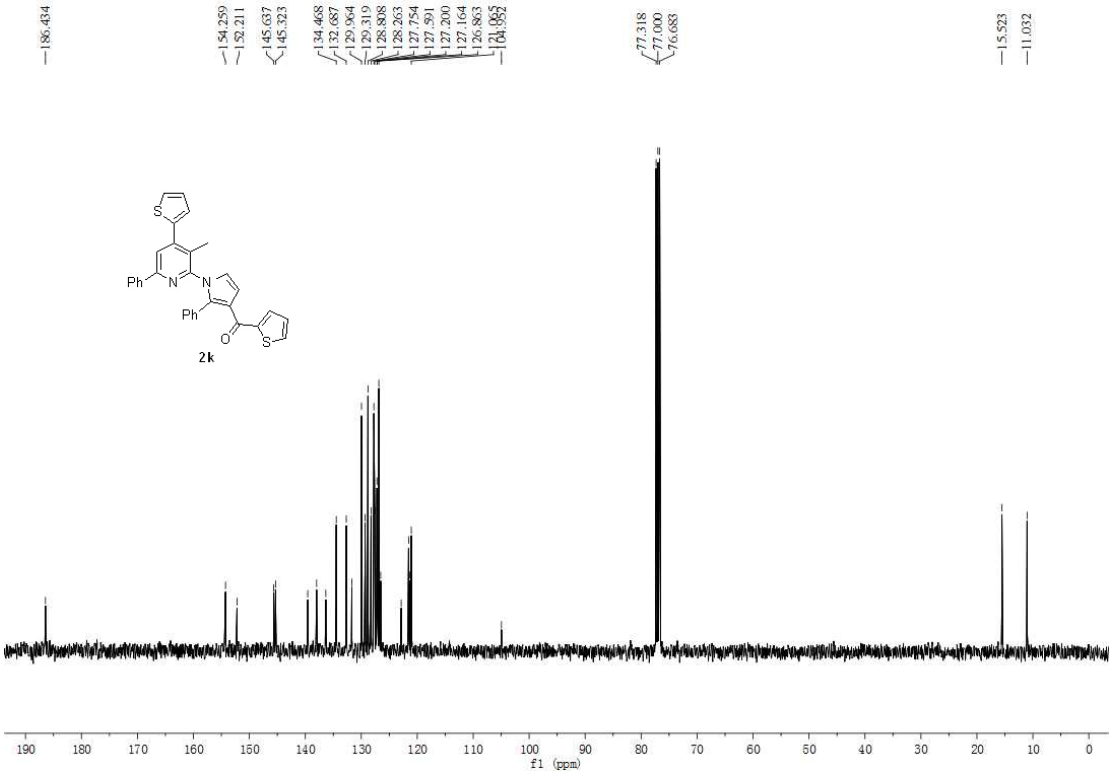
^{13}C NMR spectrum of product **2j**



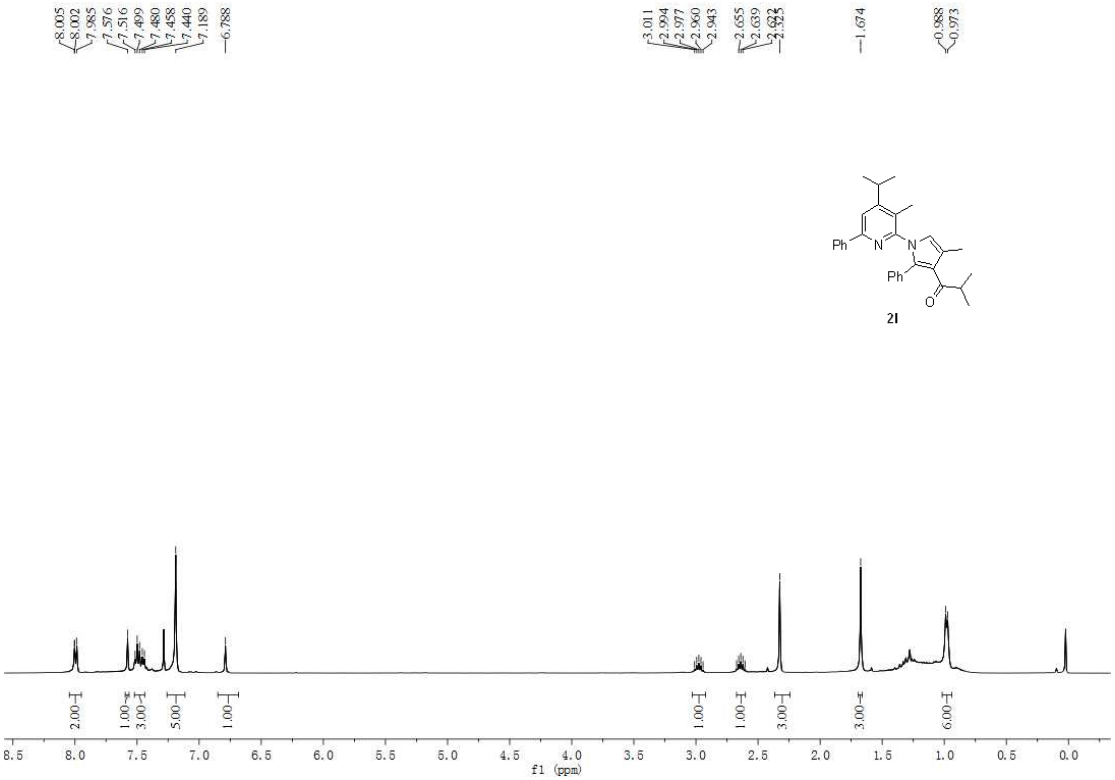
^{1}H NMR spectrum of product **2k**



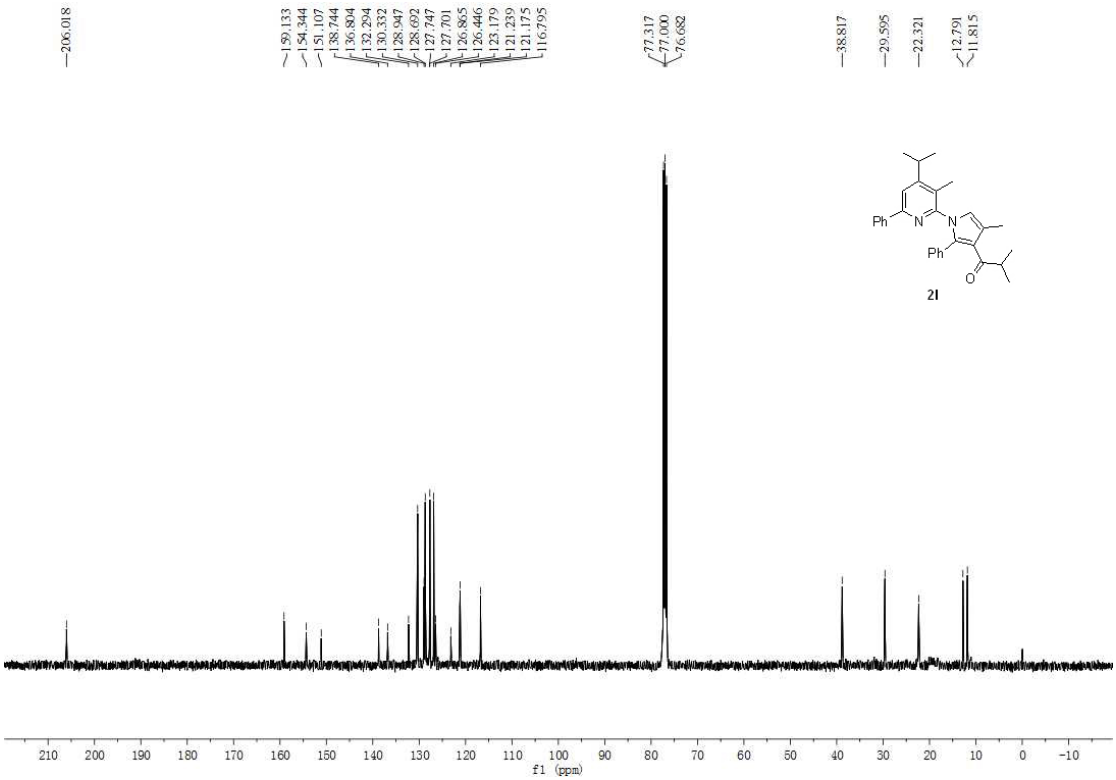
^{13}C NMR spectrum of product **2k**



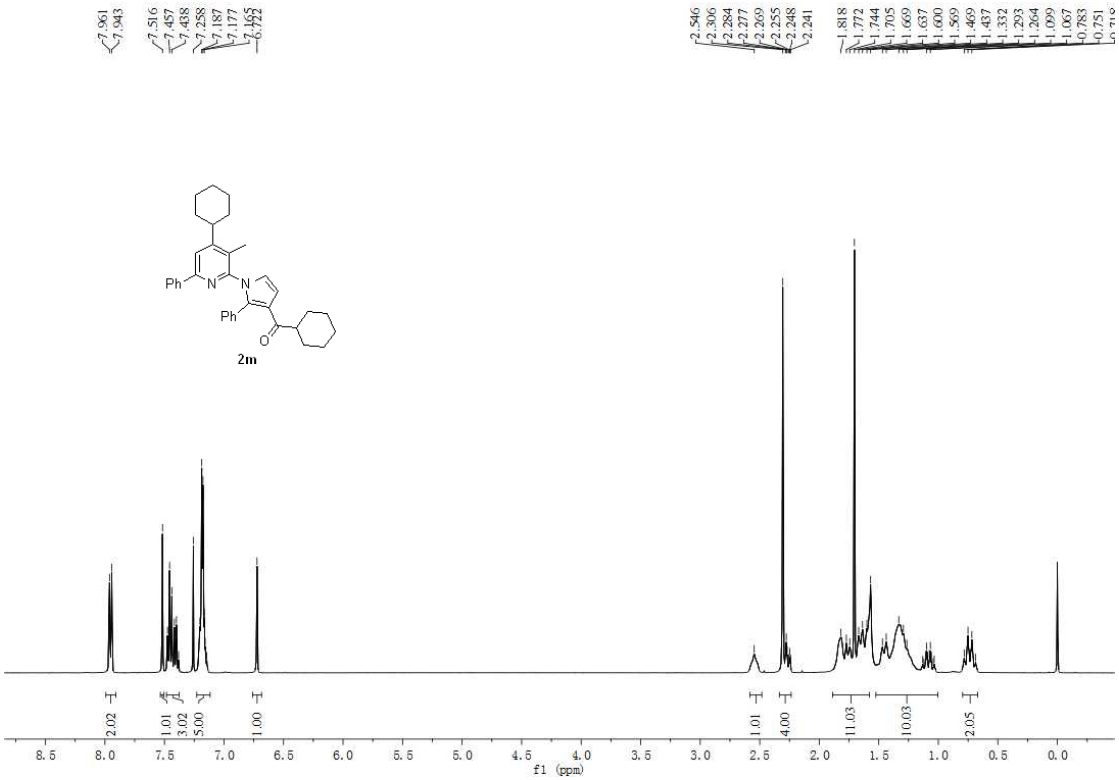
^{1}H NMR spectrum of product **2l**



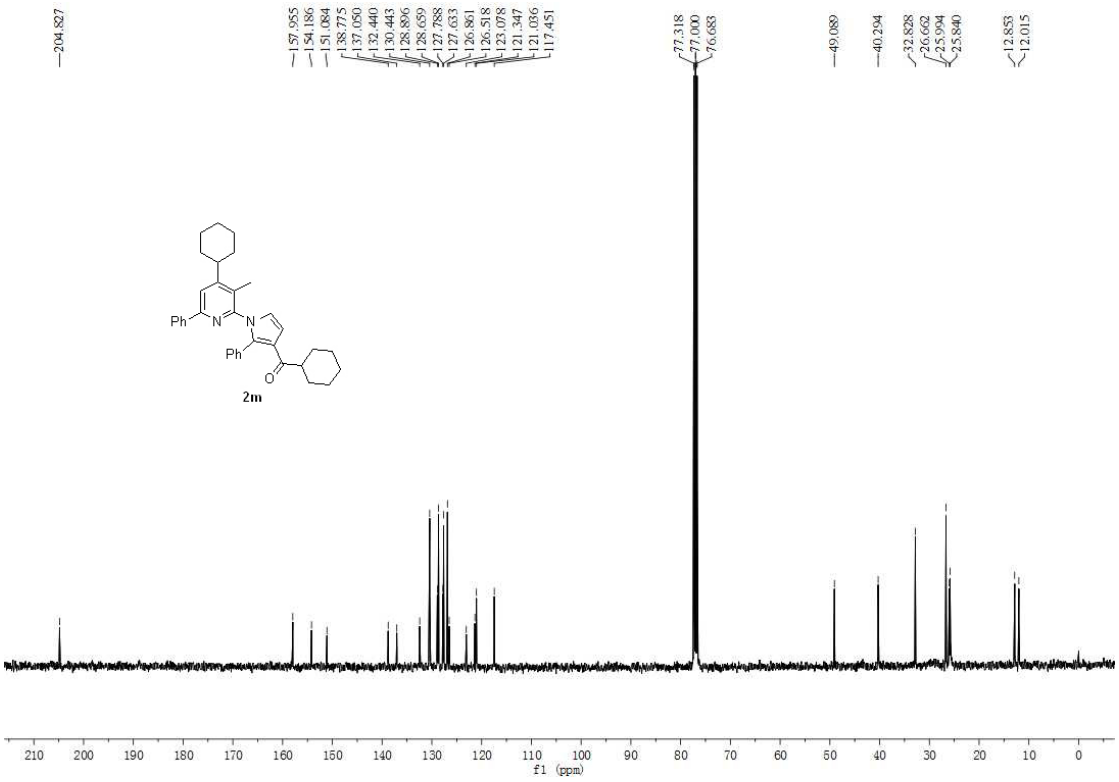
^{13}C NMR spectrum of product **2l**



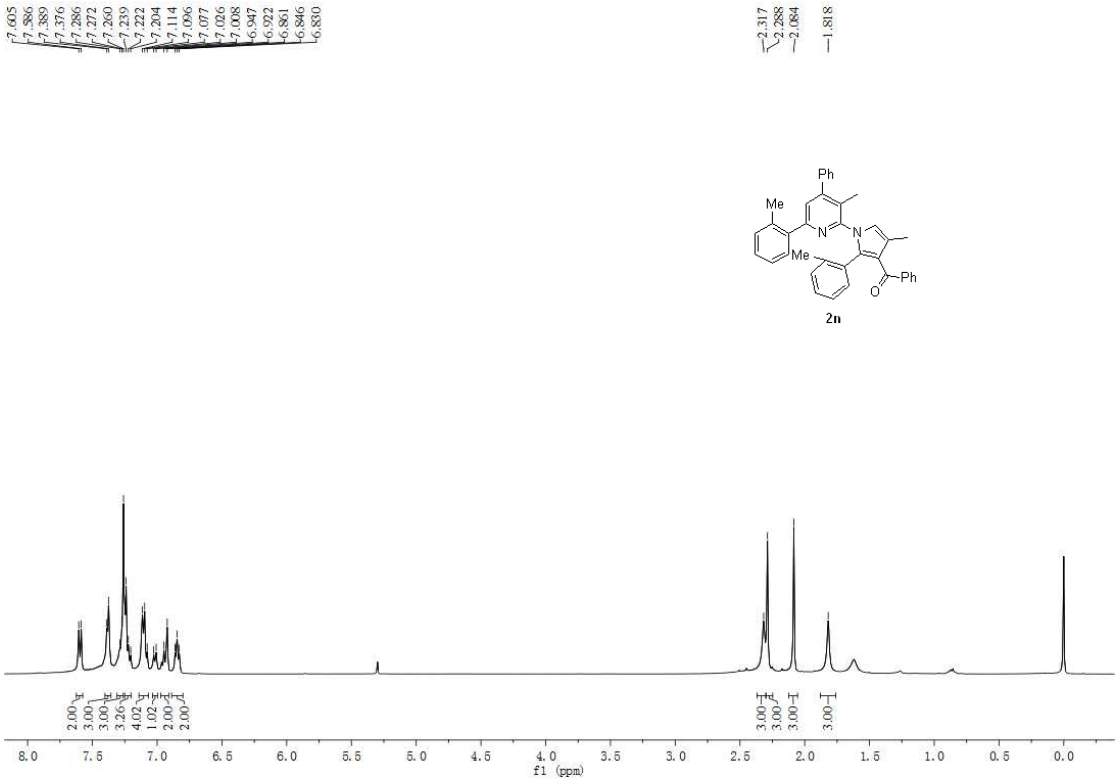
^{1}H NMR spectrum of product **2m**



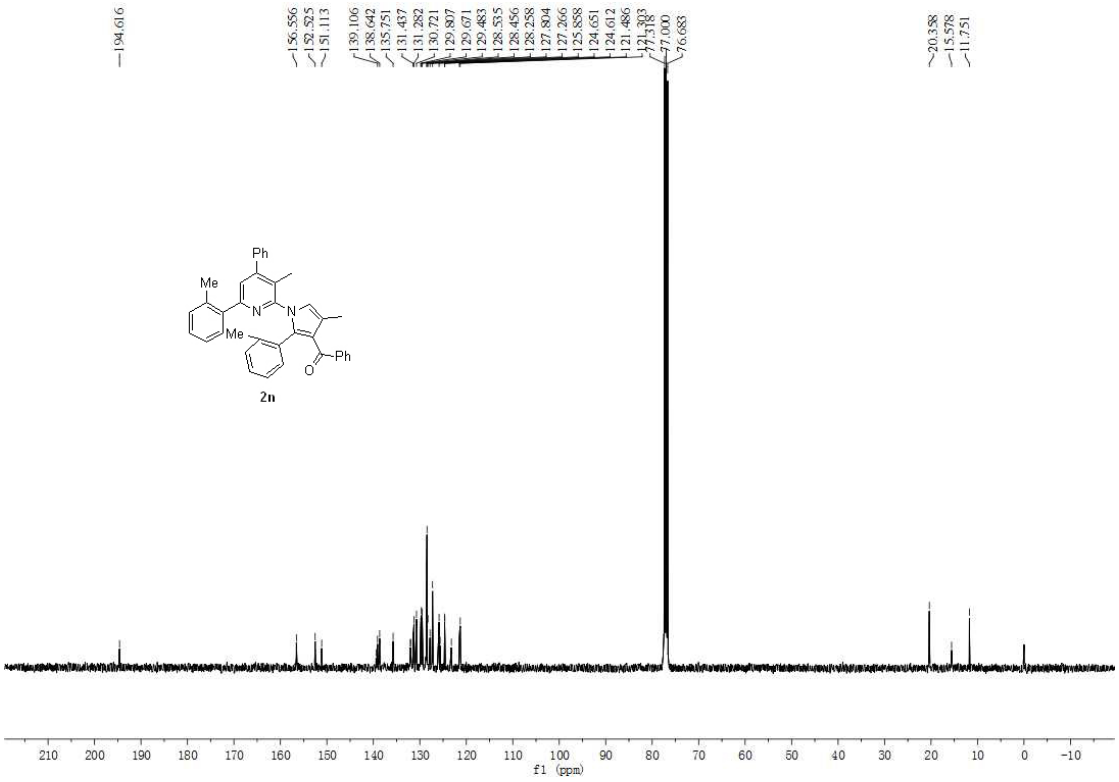
^{13}C NMR spectrum of product **2m**



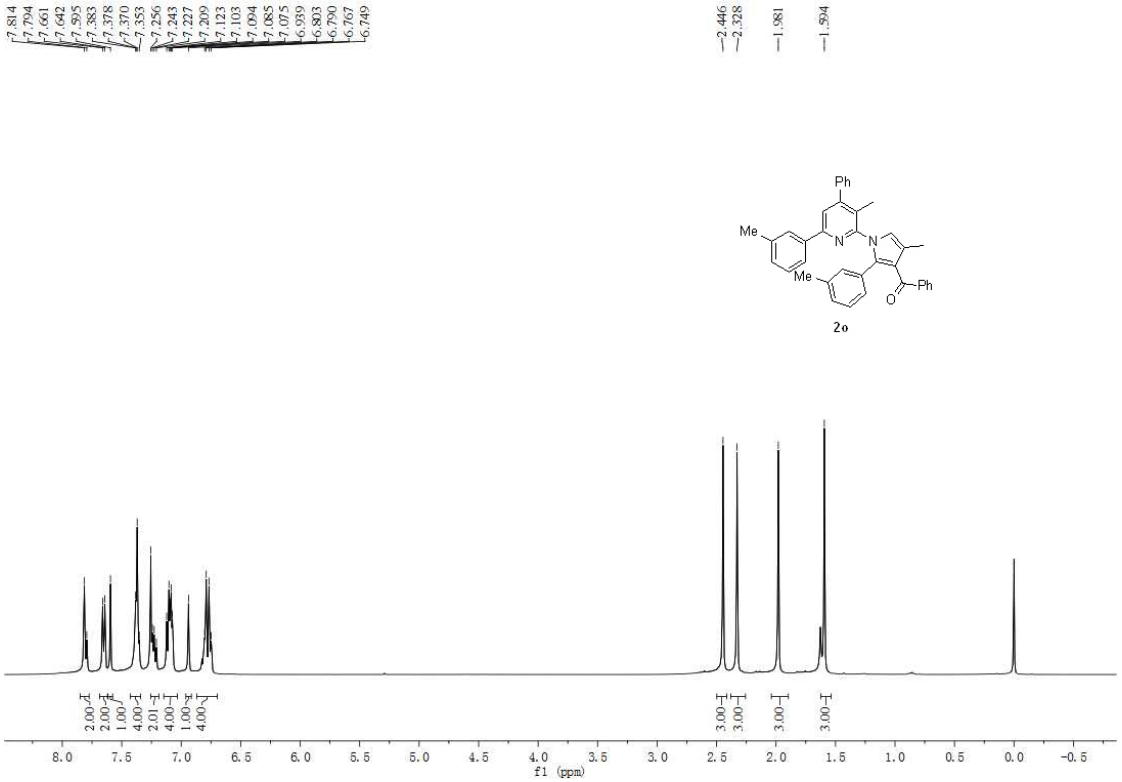
^{1}H NMR spectrum of product **2n**



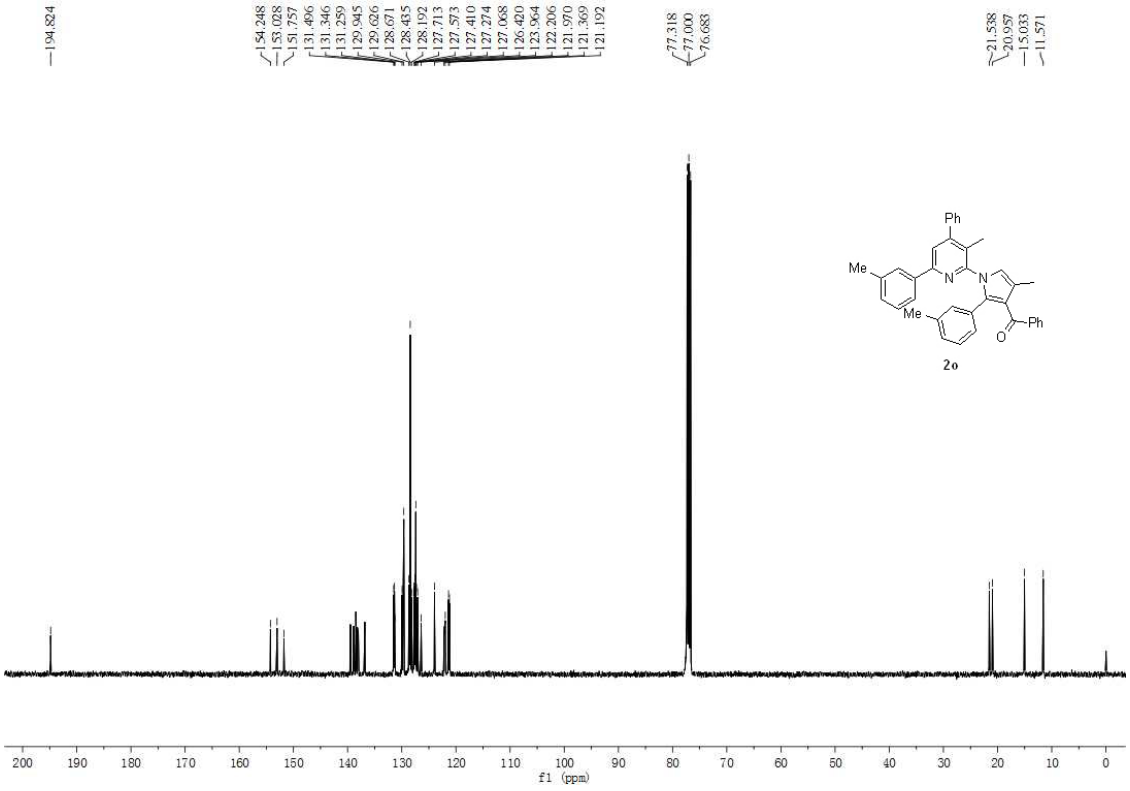
^{13}C NMR spectrum of product **2n**



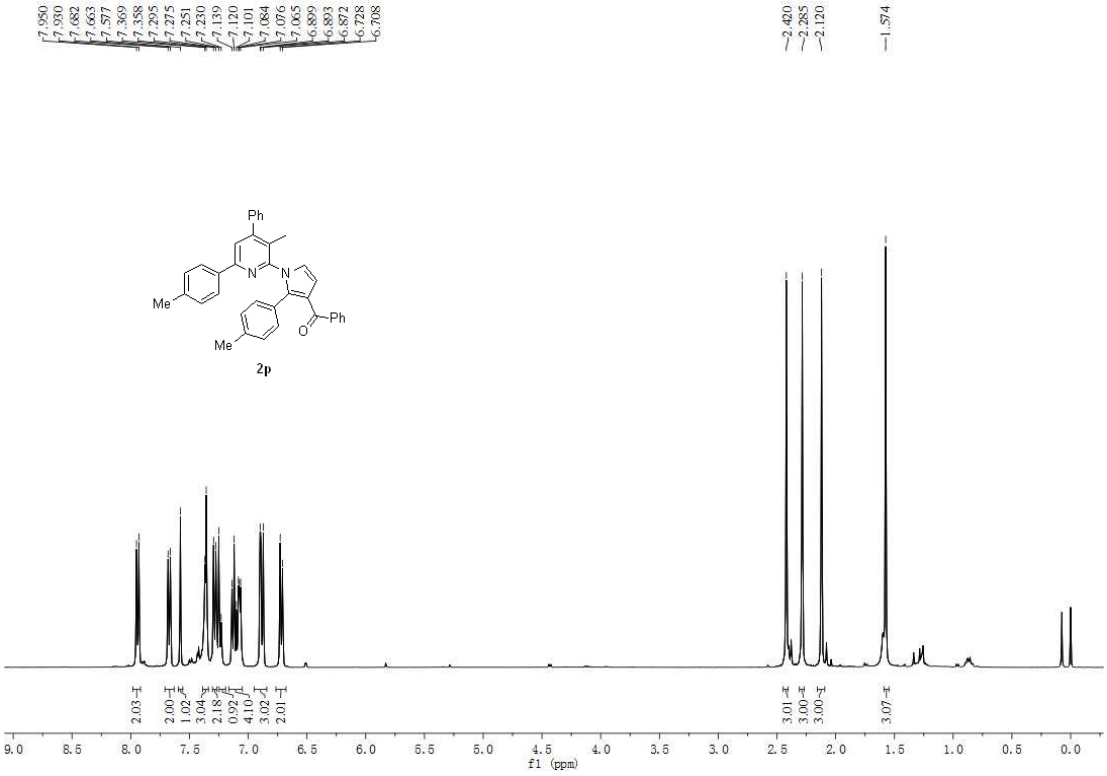
^{1}H NMR spectrum of product **2o**



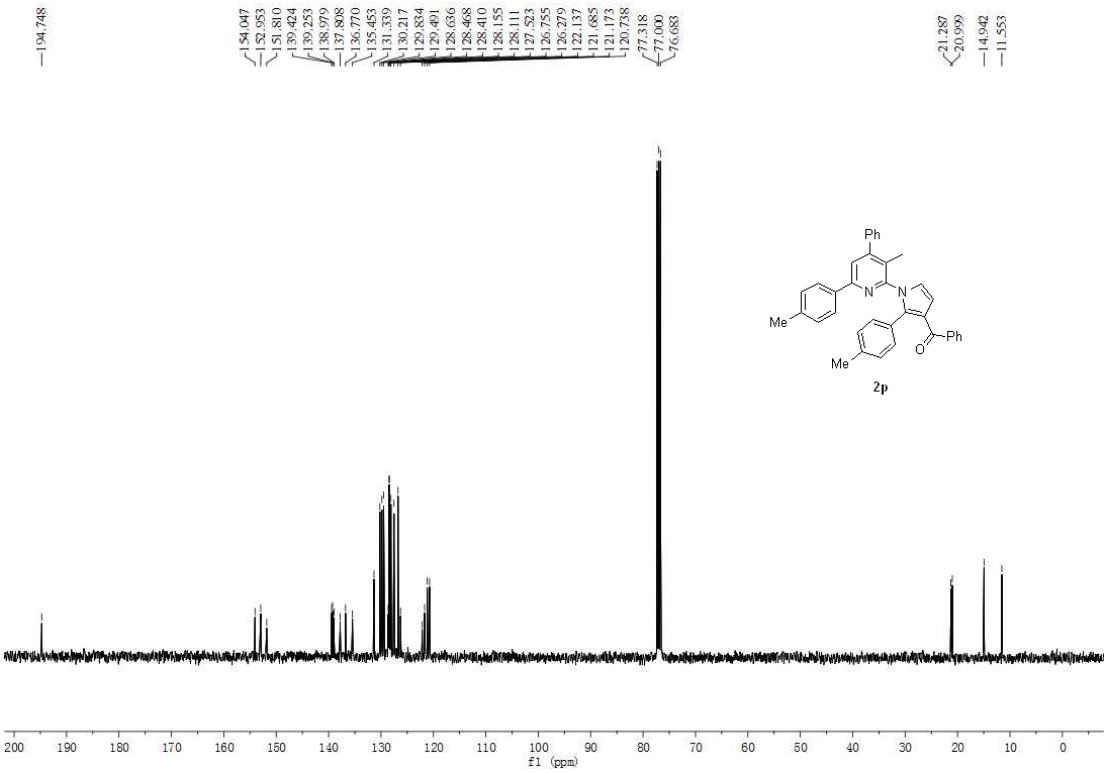
^{13}C NMR spectrum of product **2o**



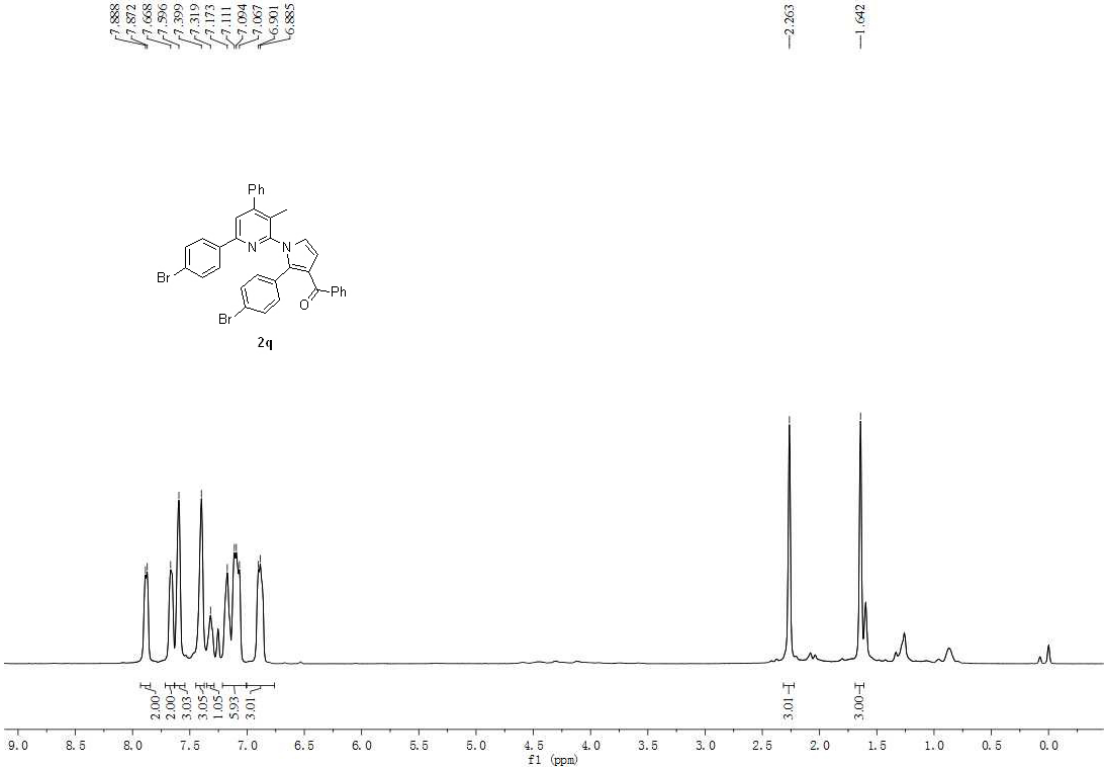
^{1}H NMR spectrum of product **2p**



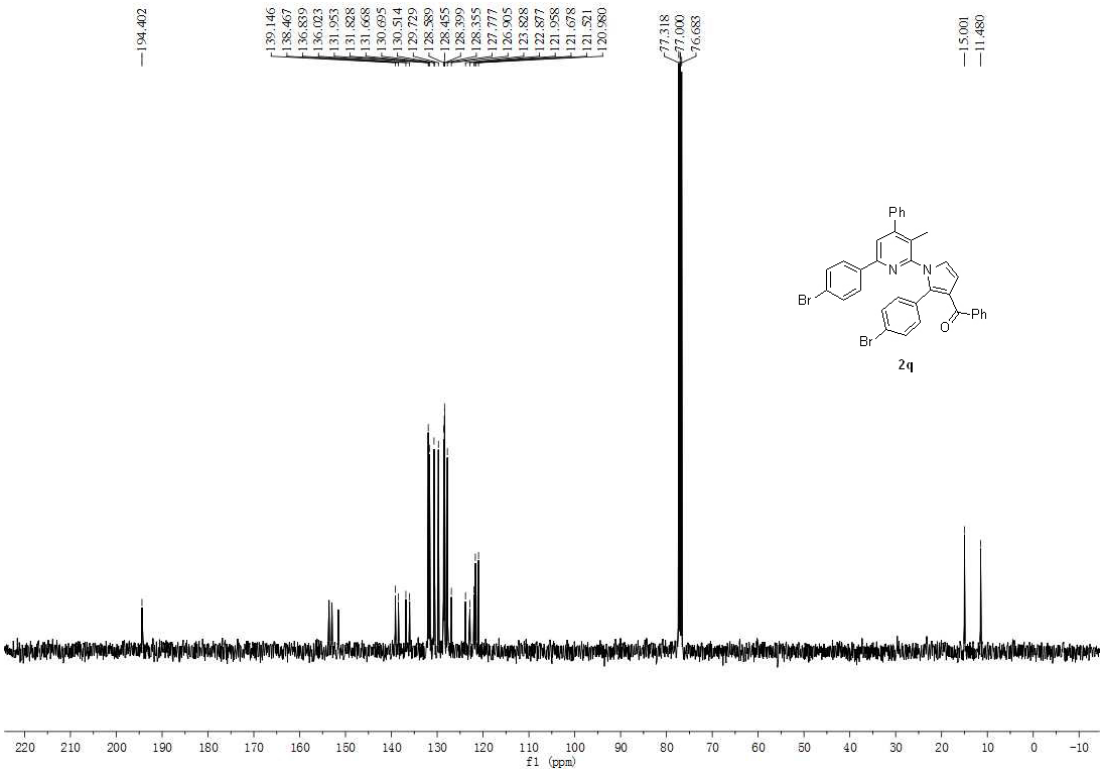
^{13}C NMR spectrum of product **2p**



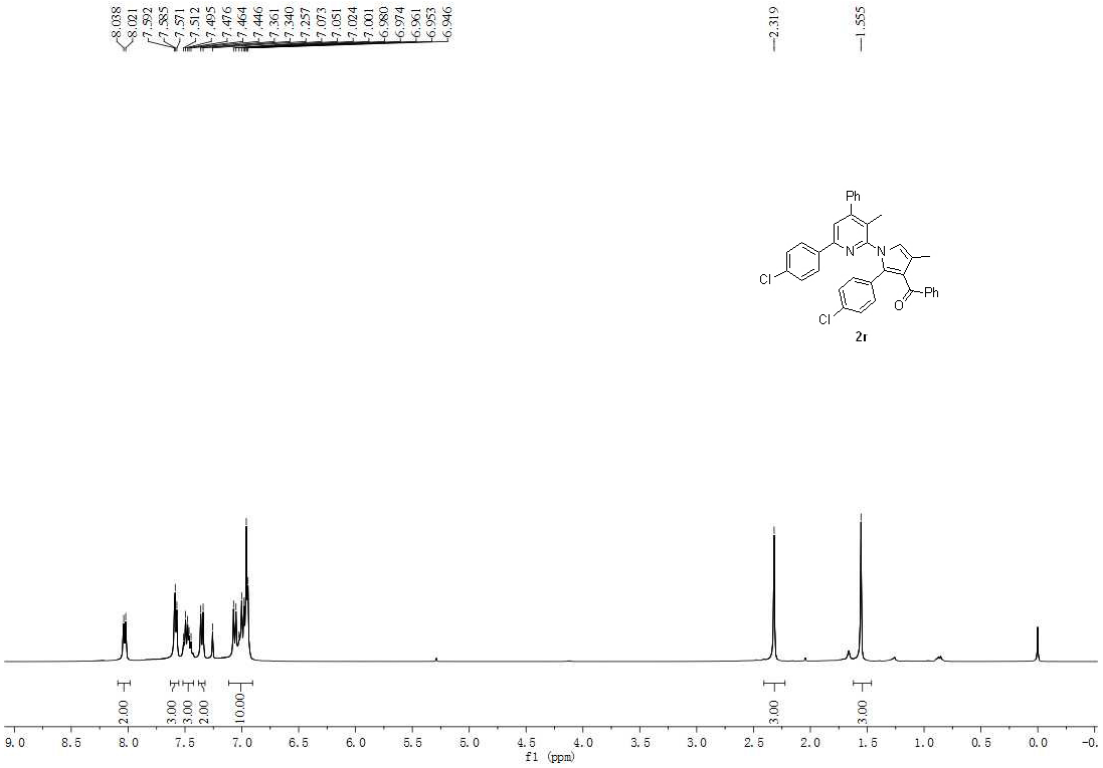
^{1}H NMR spectrum of product **2q**



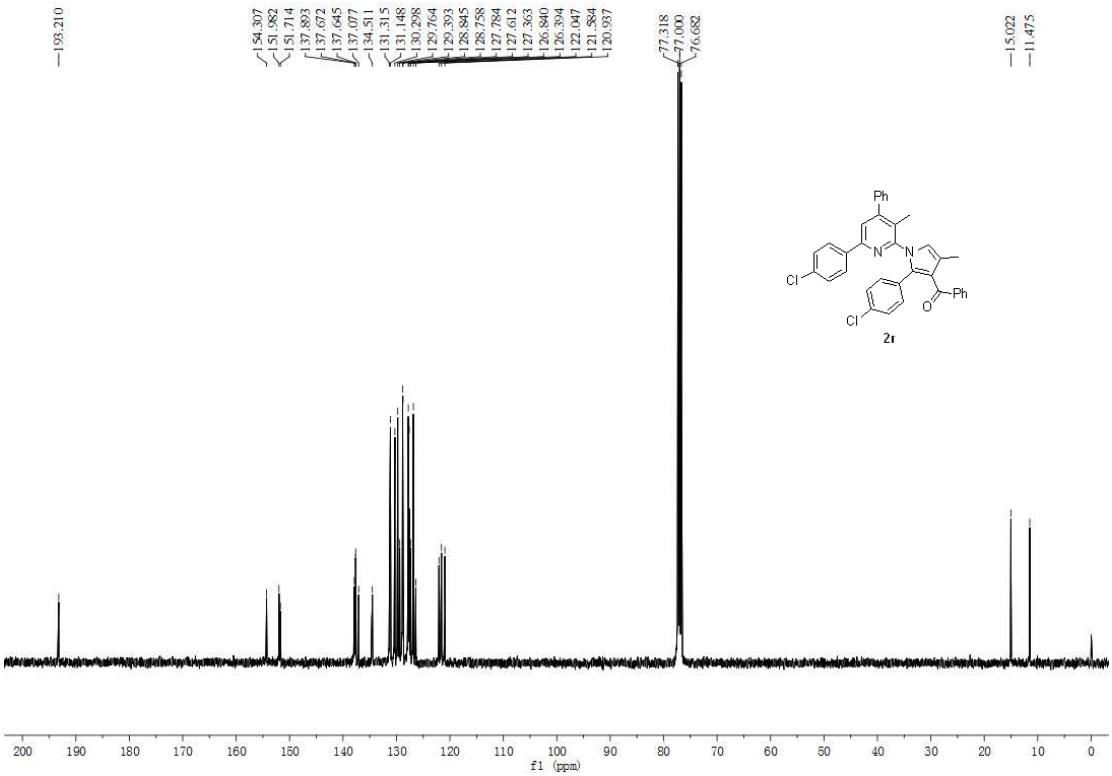
^{13}C NMR spectrum of product **2q**



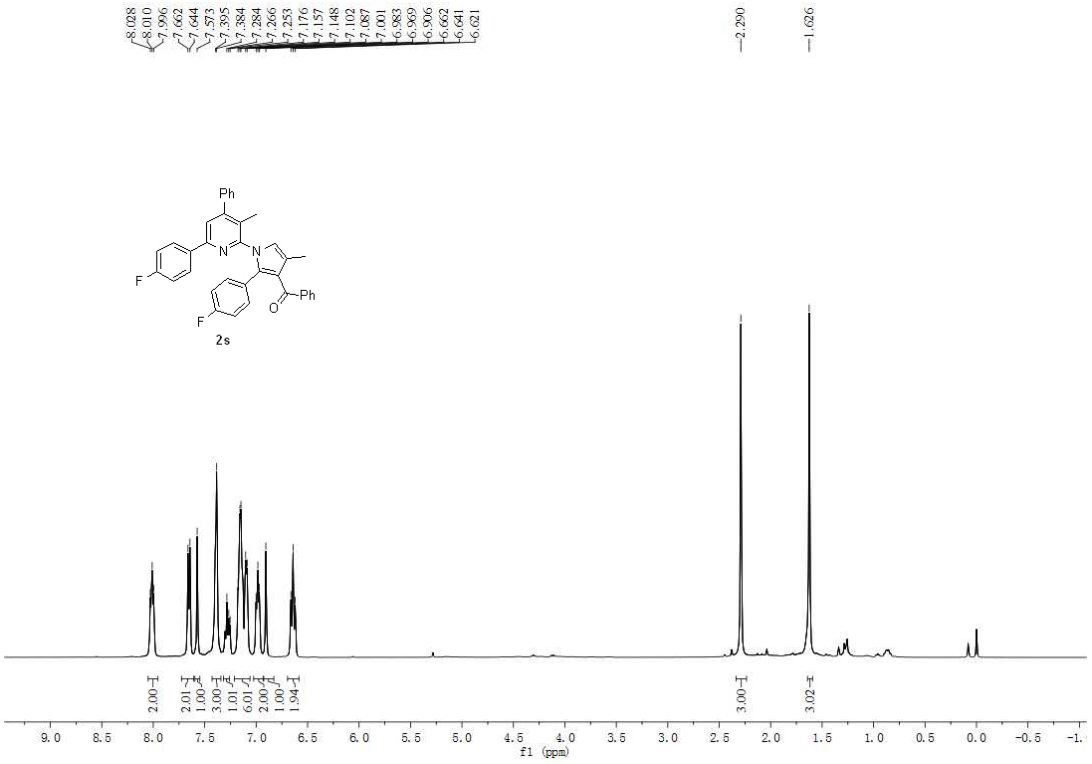
^{1}H NMR spectrum of product **2r**



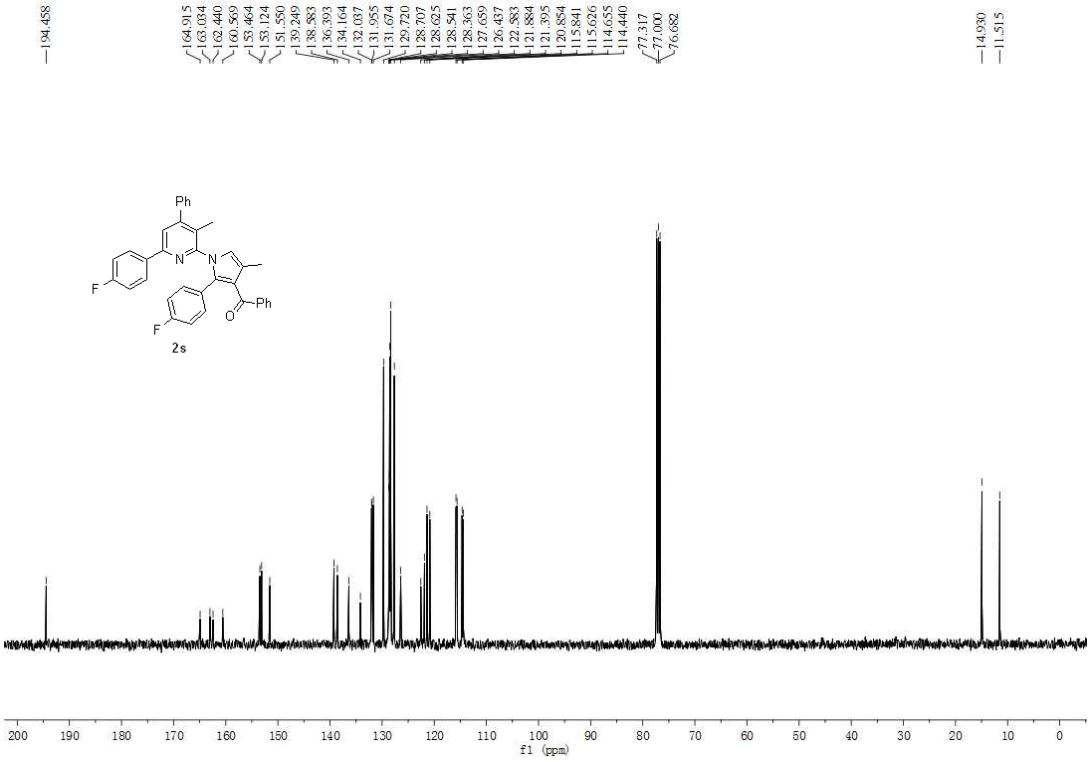
^{13}C NMR spectrum of product **2r**



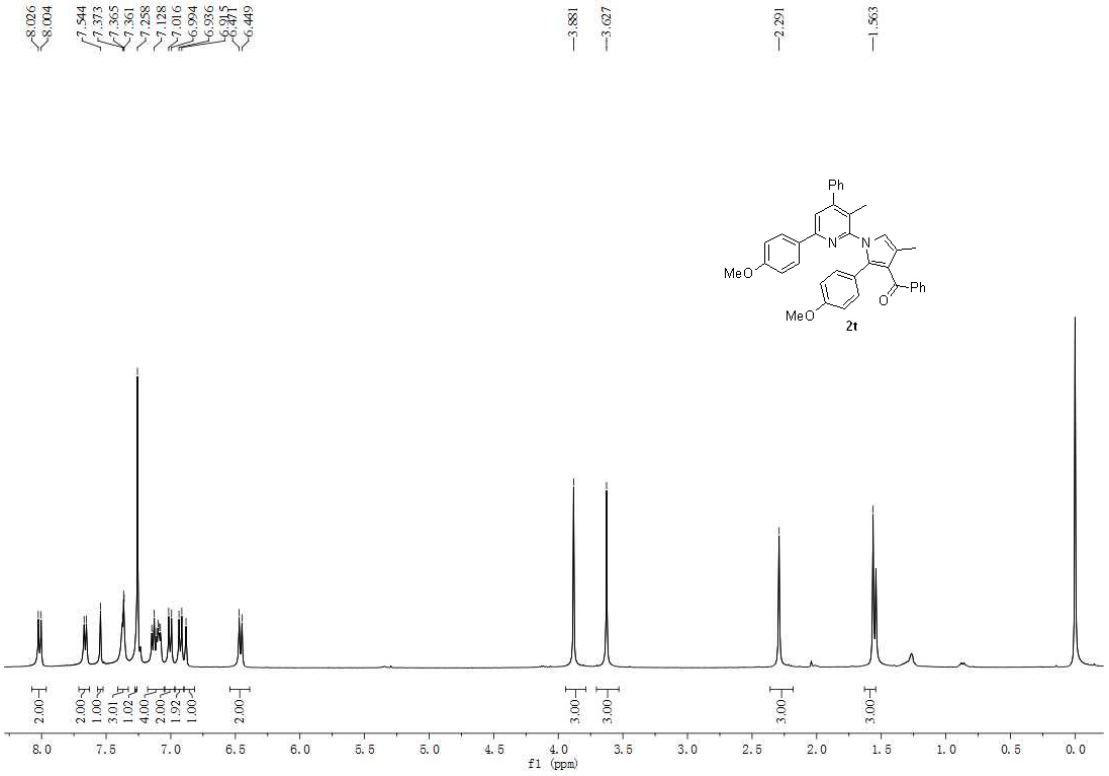
^{1}H NMR spectrum of product **2s**



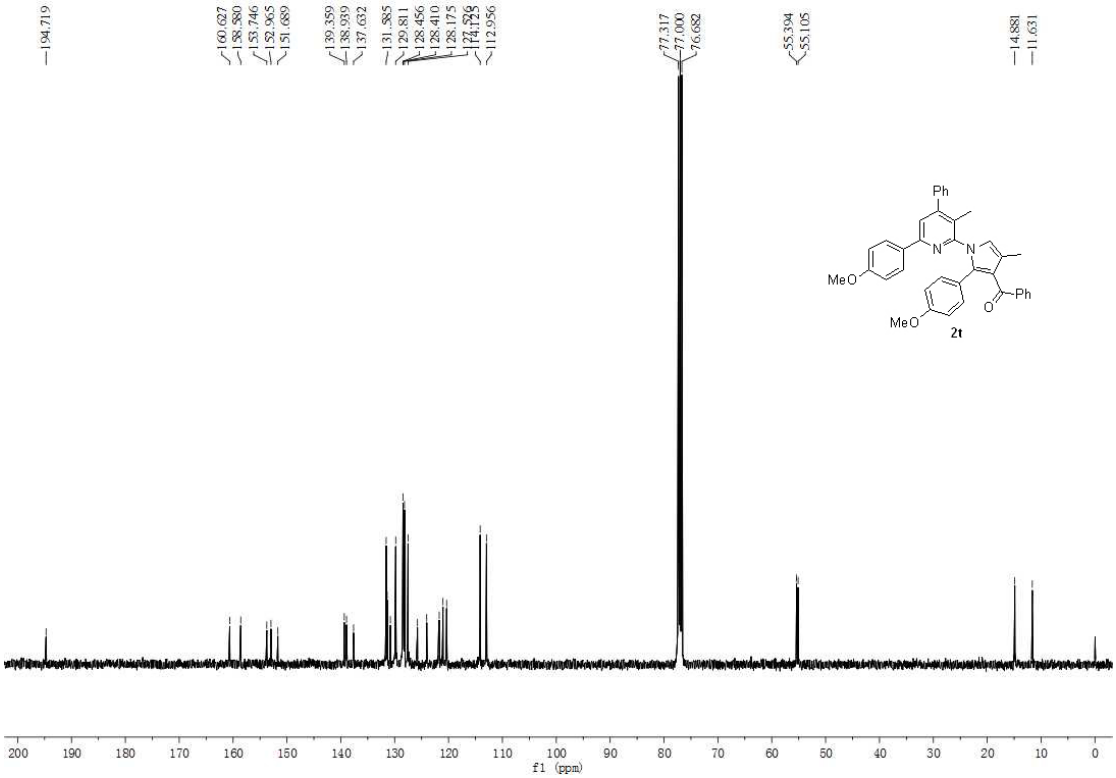
^{13}C NMR spectrum of product **2s**



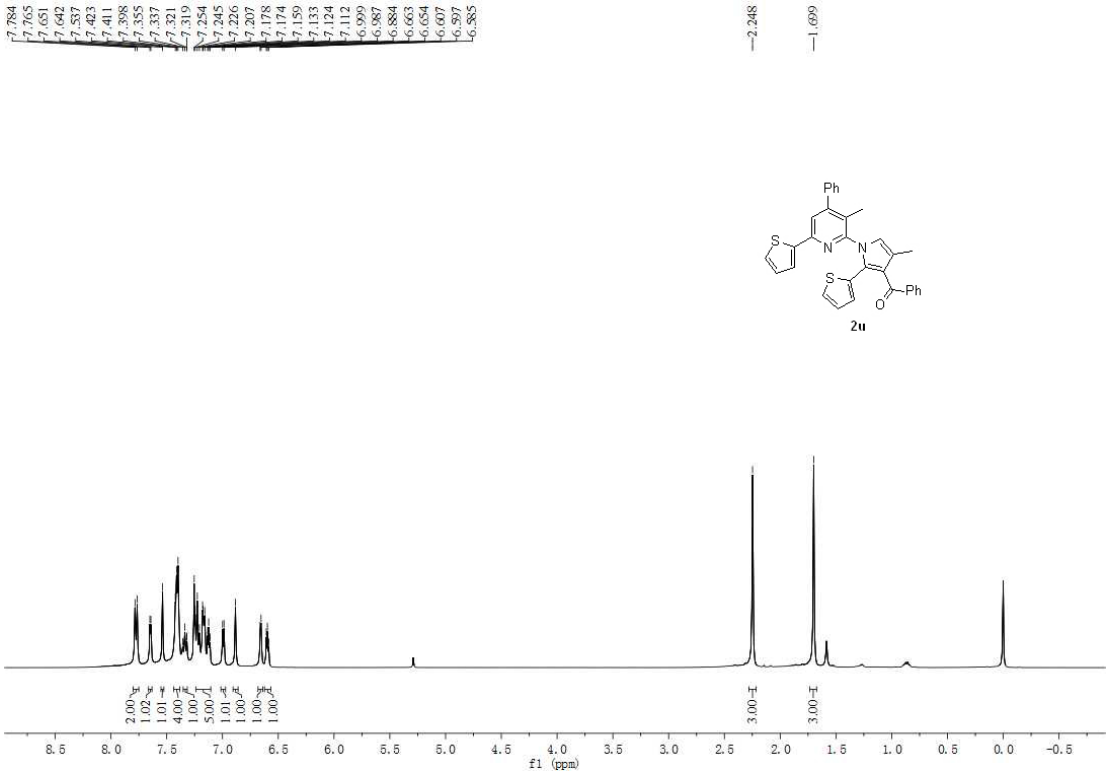
^{1}H NMR spectrum of product **2t**



^{13}C NMR spectrum of product **2t**



^{1}H NMR spectrum of product **2u**



^{13}C NMR spectrum of product **2u**