Supporting Information (SI)

Configurationally stable helical tetradentate Pt(II) complexes for organic light-emitting diodes with circularly polarized electroluminescence

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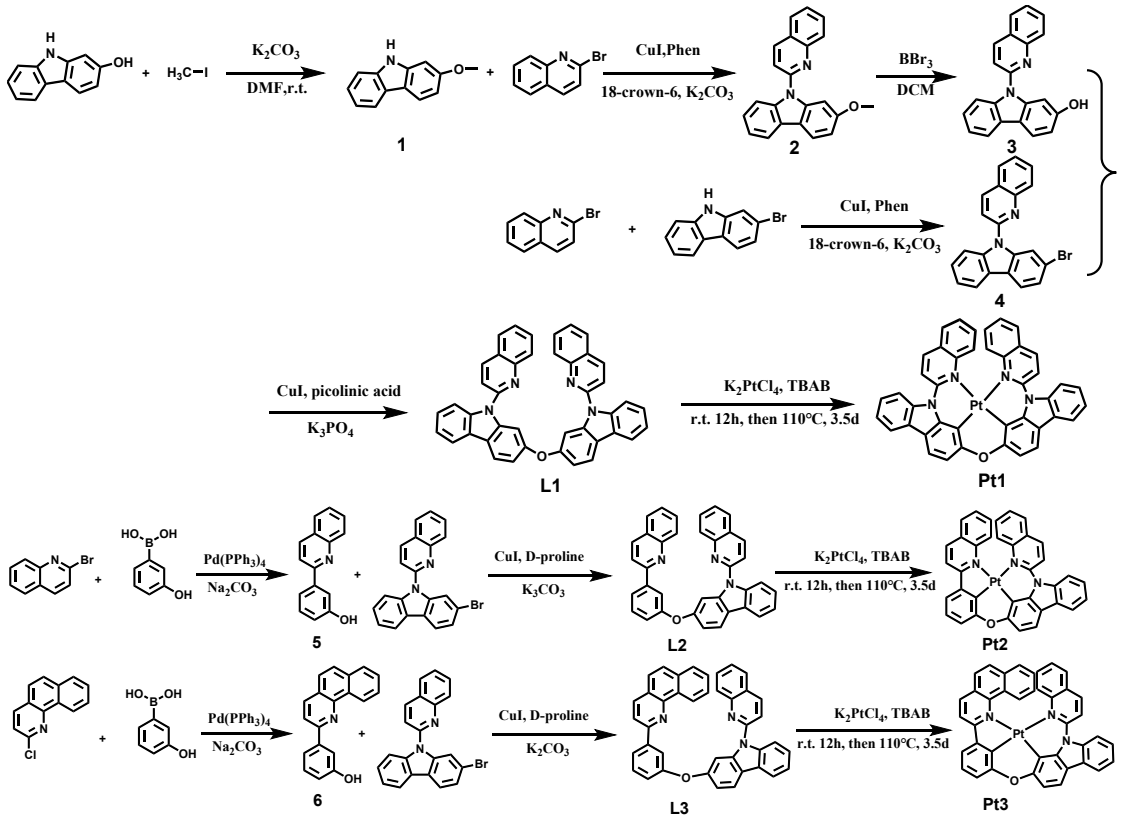
S1. General information

The starting reactants and solvents were used as commercial grade without further purification. NMR measurements were conducted on a Bruker AM 400/500 spectrometer. The mass spectra were recorded by Matrix Assisted Laser Desorption Ionization Time of Flight Mass Spectrometry (autoflex TOF/TOF, Bruker Daltonics). Absorption and photoluminescence spectra were measured on a UV-3100 spectrophotometer and a Hitachi F-4600 photoluminescence spectrophotometer, respectively. Cyclic voltammetry measurements were conducted on MPI-A multifunctional electrochemical and chemiluminescent system (Xi'an Remex Analytical Instrument Ltd. Co., China) at room temperature, with a polished Pt plate as the working electrode, a platinum thread as the counter electrode and Ag-$AgNO_3$ (0.1 M) in CH_3CN as the reference electrode, tetra-nbutylammonium perchlorate (0.1 M) was used as the supporting electrolyte, using Fc^+/Fc as the external standard, with a scan rate of 0.1 V/s. The HOMO and LUMO levels were obtained by the following equation: HOMO = -(4.8 + E_{ox}) eV, LUMO = HOMO + E_g, and E_g values were calculated from the UV-vis absorption spectra. The molecular simulations were carried out by density functional theory (DFT) B3LYP/6-31G (d,p) method with GenECP basis set specifically for the calculation of Pt(II) center. The absolute photoluminescence quantum yields (Φ) and the decay lifetimes of the compounds were measured with HORIBA FL3 fluorescence spectrometer. Thermogravimetric analysis (TGA) measurements were performed on a Pyris 1 DSC under nitrogen at a heating rate of 10 °C min^{-1}. The circular dichroism (CD) spectra were measured on a Jasco J-810 circular dichroism spectrometer with "Standard" sensitivity. The circularly polarized luminescence (CPL) and circularly polarized electroluminescence (CPEL) spectra were measured on a Jasco CPL-300 spectrophotometer with "Standard" sensitivity at 100 nm/min scan speed and respond time of 4.0 s employing "slit" mode.

S2. Experiment section

2.1 Synthesis routes and procedures for Pt1, Pt2, Pt3.



Scheme 1. Synthetic strategy to obtain the chiral tetradentate Pt(II) complexes.

2.1.1 Synthesis of 2-methoxy-9*H*-carbazole (1)

In a three-necked flask, iodomethane (1.06 g, 7.5 mmol) was slowly added to the mixture of 9*H*-carbazol-2-ol (0.96 g, 5 mmol) and K_2CO_3 (1.04 g, 7.5 mmol) in 30 mL DMF and then stirred at room temperature for 5 hours, after which the mixture was diluted with water (200 ml), and extracted with CH_2Cl_2 (3 × 40 ml). The combined organic layers were washed with saturated solution of NaCl before dried with anhydrous Na_2SO_4 and concentrated under reduced pressure to obtain the crude product. The residue was purified through column chromatography on silica gel using hexane/dichloromethane (2:1) as eluent to obtain the desired product with a yield of 95%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.7 Hz, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.35 (ddd, *J* = 11.5, 9.1, 4.4 Hz, 2H), 7.24 – 7.18 (m, 1H), 6.92 (d, *J* = 2.2 Hz, 1H), 6.86 (dd, *J* = 8.5, 2.2 Hz, 1H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.08 (s), 140.82 (s), 139.51 (s), 124.55 (s), 123.54 (s), 121.05 (s), 119.57 (s), 119.49 (s), 117.27 (s), 110.31 (s), 108.16 (s), 94.73 (s), 55.64 (s).

2.2.2 Synthesis of 2-methoxy-9-(quinolin-2-yl)-9H-carbazole (2)

A mixture of 1 (0.98 g, 5 mmol), 2-bromoquinoline (1.03 g, 5 mmol) and CuI (0.10 g, 0.5 mmol), 1,10-phenanthroline (0.18 g, 1 mmol), K_2CO_3 (1.38 g, 10 mmol), 18-crown-6 (0.26 g, 0.5 mmol) was dissolved in toluene (20 ml) filled with nitrogen. Then the tube was sealed and the mixture was stirred at 110 ℃ for about 24 h, after which the mixture was cooled down to ambient temperature. Then the mixture was filtered and the filtrate was concentrated under reduced pressure to obtain the crude product. The residue was purified through column chromatography on silica gel using hexane/dichloromethane (5:1) as eluent to obtain the desired product with a yield of 94%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.7 Hz, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 7.4 Hz, 1H), 8.00 (d, *J* = 8.5 Hz, 1H), 7.91 (t, *J* = 7.8 Hz, 2H), 7.81 (dt, *J* = 6.9, 1.5 Hz, 2H), 7.60 (q, *J* = 6.5 Hz, 2H), 7.42 – 7.37 (m, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 6.98 (dd, *J* = 8.5, 2.2 Hz, 1H), 3.90 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.30 (s), 150.90 (s), 147.66 (s), 140.88 (s), 139.57 (s), 138.76 (s), 130.34 (s), 128.69 (s), 127.63 (s), 126.45 (s), 126.35 (s), 124.98 (s), 124.78 (s), 121.31 (s), 120.83 (s), 119.43 (s), 118.34 (s), 117.60 (s), 111.20 (s), 109.54 (s), 96.33 (s), 55.63 (s).

2.2.3 Synthesis of 9-(quinolin-2-yl)-9*H*-carbazol-2-ol (3)

In a three-necked flask, 2 (1.62 g, 5 mmol) was dissolved in CH_2Cl_2 under the protection of nitrogen. After the solution was cooled down to 0 ℃, BBr_3 (15 mL, 15 mmol (1 M/L)) was slowly added to the solution. The mixture was stirred at room temperature for 2 hours and poured into excessive $NaHCO_3$ solution, and extracted with CH_2Cl_2 (3 × 40 ml). The combined organic layers were washed with saturated solution of NaCl, dried with anhydrous Na_2SO_4 and concentrated under reduced pressure to obtain the crude product. The residue was purified through column chromatography on silica gel using hexane/ ethyl acetate (6:1) as eluent to obtain the desired product with a yield of 95%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.6 Hz, 1H), 8.17 (d, *J* = 8.3 Hz, 1H), 8.00 (d, *J* = 7.5 Hz, 1H), 7.89 (t, *J* = 8.7 Hz, 3H), 7.79 (t, *J* = 8.2 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.52 (s, 1H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.31 (t, *J* = 7.4 Hz, 1H), 6.84 (d, *J* = 7.6 Hz, 1H).

2.2.4 Synthesis of 2-bromo-9-(quinolin-2-yl)-9*H*-carbazole (4)

A mixture of 2-bromo-9*H*-carbazole (1.22 g, 5 mmol), 2-bromoquinoline (1.03 g, 5 mmol) and CuI (0.10 g, 0.5 mmol), 1,10-phenanthroline (0.18 g, 1 mmol), K_2CO_3 (1.38 g, 10 mmol), 18-crown-6 (0.26 g, 1 mmol) was dissolved in toluene (20 ml) filled with nitrogen. Then the tube was sealed and the mixture was stirred at 110 ℃ for about 24 h, after which the mixture was cooled down to ambient temperature. Then the mixture was filtered and the filtrate was concentrated under reduced pressure to obtain the crude product. The residue was purified through column chromatography on silica gel using hexane/dichloromethane (5:1) as eluent to obtain the desired product with a yield of 94%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.6 Hz, 1H), 8.19 (dd, *J* = 4.8, 3.3 Hz, 2H), 8.10 (d, *J* = 7.4 Hz, 1H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.96 – 7.90 (m, 2H), 7.82 (ddd, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 1H), 7.62 (ddd, *J* = 8.1, 7.0, 1.1 Hz, 1H), 7.53 – 7.44 (m, 2H), 7.40 – 7.32 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.32 (s), 147.66 (s), 140.37 (s), 139.65 (s), 139.12 (s), 130.58 (s), 128.85 (s), 127.69 (s), 126.74 (s), 126.70 (s), 126.66 (s), 124.42 (s), 123.96 (s), 123.50 (s), 121.65 (s), 121.33 (s), 120.31 (s), 119.93 (s), 117.56 (s), 114.81 (s), 111.56 (s).

2.2.5 Synthesis of 3-(quinolin-2-yl)phenol (5)

To a dry pressure Schlenk tub, added 2-bromoquinoline (1.03 g, 5 mmol), (3-hydroxyphenyl)boronic acid (0.90 g, 6.5 mmol), $Pd(PPh_3)_4$ (0.58 g, 0.1 mmol) and Na_2CO_3 (0.79 g, 7.5 mmol). Then THF (30 ml) and water (10 ml) were added, and the tube filled with nitrogen was sealed. The mixture was stirred at 75 ℃ for 6 hours and cooled down to ambient temperature. Then the mixture was diluted with water (500 ml) and extracted with CH_2Cl_2 (3 × 40 ml). The combined organic layers were washed with saturated solution of NaCl, dried with anhydrous Na_2SO_4 and evaporated under reduced pressure to obtain the crude product. The residue was purified through column chromatography on silica gel using hexane/ethyl acetate (5:1) as eluent to obtain the desired product with a yield of 97%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (t, *J* = 8.8 Hz, 2H), 7.86 – 7.80 (m, 3H), 7.72 (ddd, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.35 (t, *J* = 7.9 Hz, 1H), 6.92 (ddd, *J* = 8.1, 2.5, 0.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.70 (s), 156.84 (s), 147.82 (s), 140.88 (s), 137.35 (s), 130.11 (s), 130.06 (s), 129.05 (s), 127.56 (s), 127.34 (s), 126.54 (s), 119.70 (s), 119.67 (s), 116.98 (s), 115.03 (s).

2.2.6 Synthesis of 3-(benzo[h]quinolin-2-yl)phenol (6)

Compound 6 was synthesized with the above process but replacing 2-bromoquinoline by 2-chlorobenzo[*h*]quinoline[1] (1.07 g, 5 mmol) with a yield of 97% .

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.48 (dd, *J* = 8.0, 0.7 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.4 Hz, 1H), 7.95 – 7.89 (m, 2H), 7.83 (d, *J* = 7.8 Hz, 1H), 7.80 (d, *J* = 8.8 Hz, 1H), 7.78 – 7.66 (m, 3H), 7.41 (t, *J* = 7.9 Hz, 1H), 7.04 – 6.90 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.14 (s), 154.90 (s), 146.07 (s), 141.30 (s), 136.68 (s), 133.91 (s), 131.65 (s), 130.07 (s), 128.26 (s), 127.82 (s), 127.64 (s), 126.95 (s), 125.36 (s), 125.05 (s), 124.74 (s), 119.93 (s), 118.97 (s), 116.35 (s), 114.38 (s).

2.2.7 Synthesis of 2,2'-oxybis(9-(quinolin-2-yl)-9*H*-carbazole) (L1)

A mixture of 3 (0.31 g, 1 mmol), 4 (0.37 g, 1 mmol) and CuI (0.02 g, 0.1 mmol), D-proline (0.02 g, 0.2 mmol) and K_2CO_3 (0.27 g, 2 mmol) was dissolved in DMSO (5 ml) filled with nitrogen in a dry pressure Schlenk tube. The tube was sealed and the mixture was stirred at

110 ℃ for about 24 h, after which the mixture was cooled down to ambient temperature. Then the mixture was filtered and the filtrate was concentrated under reduced pressure to obtain the crude product. The residue was purified through column chromatography on silica gel using hexane/dichloromethane (1:3) as eluent to obtain the desired product with a yield of 30%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.7 Hz, 1H), 8.07 (dd, *J* = 7.9, 5.4 Hz, 2H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.84 (d, *J* = 7.5 Hz, 1H), 7.78 (d, *J* = 2.1 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.67 (ddd, *J* = 8.4, 7.0, 1.4 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.46 – 7.40 (m, 1H), 7.38 – 7.31 (m, 1H), 7.11 (dd, *J* = 8.5, 2.1 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.86 (s), 149.57 (s), 146.55 (s), 139.56 (s), 138.87 (s), 137.81 (s), 129.29 (s), 127.67 (s), 126.52 (s), 125.40 (s), 125.33 (s), 124.59 (s), 123.46 (s), 120.39 (s), 120.00 (s), 119.38 (s), 118.75 (s), 116.34 (s), 112.11 (s), 110.45 (s), 101.32 (s).

2.2.8 Synthesis of 9-(quinolin-2-yl)-2-(3-(quinolin-2-yl)phenoxy)-9*H*-carbazole (L2)

Ligand L2 was synthesized with similar process for L1 but replacing compound 3 by 5 with a yield of 35%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.7 Hz, 1H), 8.21 (d, *J* = 8.6 Hz, 2H), 8.10 (d, *J* = 8.3 Hz, 2H), 8.06 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 8.2 Hz, 1H), 7.91 (s, 2H), 7.86 (d, *J* = 8.1 Hz, 1H), 7.85 – 7.79 (m, 4H), 7.71 (t, *J* = 7.2 Hz, 2H), 7.59 – 7.42 (m, 4H), 7.35 (t, *J* = 7.3 Hz, 1H), 7.20 – 7.15 (m, 1H), 7.12 (dd, *J* = 8.4, 2.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.46 (s), 156.61 (s), 156.08 (s), 150.62 (s), 148.09 (s), 147.64 (s), 141.43 (s), 140.64 (s), 139.98 (s), 138.91 (s), 136.94 (s), 130.35 (s), 130.16 (s), 129.77 (s), 129.72 (s), 128.77 (s), 127.59 (s), 127.44 (s), 127.28 (s), 126.51 (s), 126.46 (s), 126.42 (s), 125.75 (s), 124.46 (s), 122.29 (s), 121.49 (s), 121.17 (s), 120.72 (s), 119.86 (s), 119.43 (s), 119.02 (s), 117.71 (s), 117.50 (s), 113.51 (s), 111.48 (s), 102.81 (s).

2.2.9 Synthesis of 2-(3-((9-(quinolin-2-yl)-9*H*-carbazol-2-yl)oxy)phenyl)benzo[h] quinoline (L3)

Ligand L3 was synthesized with similar process for L1 but replacing compound 3 by 5 with a yield of 35%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (dd, *J* = 5.7, 3.3 Hz, 1H), 8.22 (d, *J* = 8.7 Hz, 1H), 8.12 (d, *J* = 8.3 Hz, 1H), 8.01 (ddd, *J* = 11.7, 8.3, 4.6 Hz, 5H), 7.89 (t, *J* = 7.7 Hz, 2H), 7.83 – 7.78 (m, 1H), 7.77 (dd, *J* = 4.5, 2.6 Hz, 2H), 7.71 (dd, *J* = 8.7, 5.3 Hz, 2H), 7.66 – 7.56 (m, 4H), 7.44 (dd, *J* = 15.5, 7.6 Hz, 2H), 7.40 – 7.34 (m, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.09 (ddd, *J* = 6.7, 4.1, 2.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.53 (s), 156.20 (s), 154.73 (s), 150.64 (s), 147.64 (s), 146.20 (s), 141.60 (s), 140.71 (s), 139.99 (s), 138.91 (s), 136.61 (s), 133.87 (s), 131.73 (s), 130.37 (s), 130.11 (s), 128.78 (s), 128.22 (s), 127.75 (s), 127.65 (s), 127.59 (s), 126.97 (s), 126.51 (s), 126.42 (s), 125.76 (s), 125.35 (s), 125.01 (s), 124.78 (s), 124.51 (s),

122.12 (s), 121.51 (s), 121.16 (s), 120.75 (s), 119.88 (s), 119.22 (s), 118.89 (s), 117.71 (s), 117.49 (s), 113.52 (s), 111.49 (s), 102.88 (s).

2.2.10 General synthesis of Pt1-Pt3

A mixture of ligand (L1-L3) (0.5 mmol), K_2PtCl_4 (0.21 g, 0.5 mmol) and *n*-Bu_4NBr (0.02 g, 0.05 mmol) was dissolved acetic acid (30 ml) filled with nitrogen in a dry pressure Schlenk tube. The tube was sealed and the mixture was stirred at ambient temperature for 12 hours. Then the mixture was heated at 110 ℃ for 36 hours, after which the mixture was cooled down to ambient temperature. Then the mixture was diluted with water (200 ml), and extracted with CH_2Cl_2 (3 × 40 ml). The combined organic layers were washed with saturated solution of NaCl, dried with anhydrous Na_2SO_4 and evaporated under reduced pressure to obtain the crude product. The residue was purified through column chromatography on silica gel using hexane/ethyl acetate (8:1) as eluent to obtain the desired product with a yield of 16%.

Pt1: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (d, *J* = 8.7 Hz, 2H), 8.25 (d, *J* = 9.0 Hz, 2H), 8.09 (t, *J* = 7.1 Hz, 6H), 7.85 (d, *J* = 8.3 Hz, 2H), 7.47 (dd, *J* = 13.1, 6.9 Hz, 6H), 7.36 (d, *J* = 8.2 Hz, 2H), 7.24 – 7.17 (m, 2H), 7.10 (t, *J* = 7.2 Hz, 2H). MALDI-TOF-MS found: 797.176. ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.87 (s), 148.05 (s), 147.43 (s), 143.39 (s), 139.11 (s), 138.97 (s), 130.26 (s), 129.17 (s), 128.57 (s), 127.28 (s), 126.31 (s), 125.25 (s), 123.78 (s), 123.43 (s), 120.13 (s), 116.41 (s), 115.66 (s), 115.06 (s), 115.05 (s), 113.45 (s), 95.71 (s).

Pt2: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 8.7 Hz, 1H), 8.45 (d, *J* = 9.0 Hz, 1H), 8.28 (d, *J* = 8.8 Hz, 2H), 8.14 (t, *J* = 8.3 Hz, 2H), 8.05 (d, *J* = 7.3 Hz, 1H), 7.79 (d, *J* = 8.2 Hz, 3H), 7.67 (d, *J* = 7.9 Hz, 2H), 7.52 – 7.31 (m, 5H), 7.19 (t, *J* = 7.3 Hz, 1H), 7.10 (t, *J* = 7.3 Hz, 1H), 6.93 (dt, *J* = 20.9, 7.5 Hz, 2H). MALDI-TOF-MS found: 707.006. ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.30 (s), 152.62 (s), 152.49 (s), 149.19 (s), 148.61 (s), 148.20 (s), 146.89 (s), 143.49 (s), 139.44 (s), 139.21 (s), 138.35 (s), 130.29 (s), 130.03 (s), 129.56 (s), 129.15 (s), 127.81 (s), 127.69 (s), 127.26 (s), 126.47 (s), 126.07 (s), 126.00 (s), 125.90 (s), 125.40 (s), 124.49 (s), 123.95 (s), 123.47 (s), 120.33 (s), 120.21 (s), 119.24 (s), 117.58 (s), 116.81 (s), 116.26 (s), 115.33 (s), 114.67 (s), 113.88 (s), 100.24 (s).

Pt3: ^{1}H NMR (400 MHz, CD_2Cl_2) δ 10.01 (d, *J* = 8.2 Hz, 1H), 8.37 (d, *J* = 8.4 Hz, 1H), 8.30 (d, *J* = 8.5 Hz, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 8.13 (d, *J* = 9.1 Hz, 1H), 8.10 (dd, *J* = 7.6, 0.7 Hz, 1H), 8.00 (d, *J* = 8.7 Hz, 1H), 7.83 (dd, *J* = 8.3, 4.9 Hz, 3H), 7.57 – 7.52 (m, 1H), 7.48 (t, *J* = 7.5 Hz, 2H), 7.40 (dd, *J* = 12.2, 4.5 Hz, 3H), 7.36 – 7.33 (m, 2H), 7.28 (d, *J* = 7.9 Hz, 2H), 7.12 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 6.93 – 6.87 (m, 1H), 6.56 (ddd, *J* = 8.6, 7.0, 1.5 Hz, 1H). MALDI-TOF-MS found: 757.083. ^{13}C NMR (101 MHz, CD_2Cl_2) δ 163.76 (s), 152.02 (s), 151.92 (s), 148.33 (s), 148.22 (s), 147.79 (s), 146.65 (s), 144.00 (s), 139.57 (s), 138.69 (s), 138.02 (s), 133.81 (s), 129.97 (s), 128.44 (s), 128.39 (s), 128.19 (s), 128.07 (s), 127.81 (s), 127.28 (s), 126.65 (s), 126.51 (s), 126.03 (s), 125.22 (s), 124.80 (s), 124.42 (s),

124.31 (s), 124.10 (s), 123.48 (s), 123.33 (s), 123.26 (s), 120.08 (s), 119.98 (s), 118.04 (s), 117.69 (s), 116.58 (s), 115.88 (s), 115.00 (s), 114.17 (s), 113.55 (s), 98.25 (s).

2.2 NMR spectra

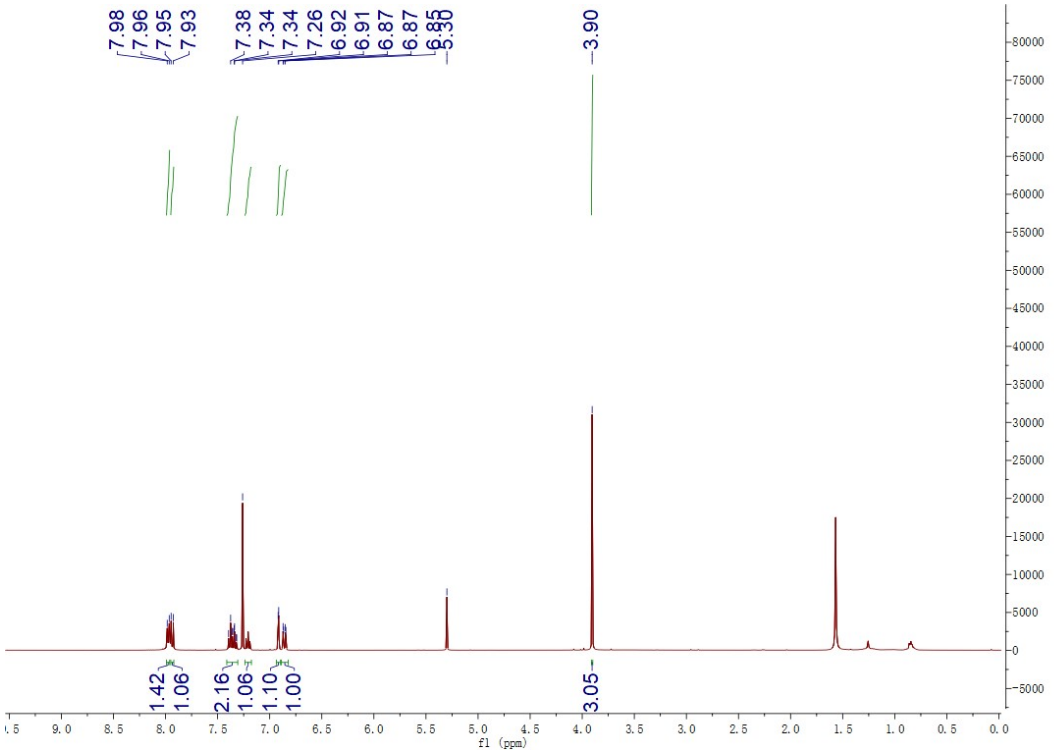


Fig. S1 The ^{1}H NMR spectrum of 1 in $CDCl_3$.

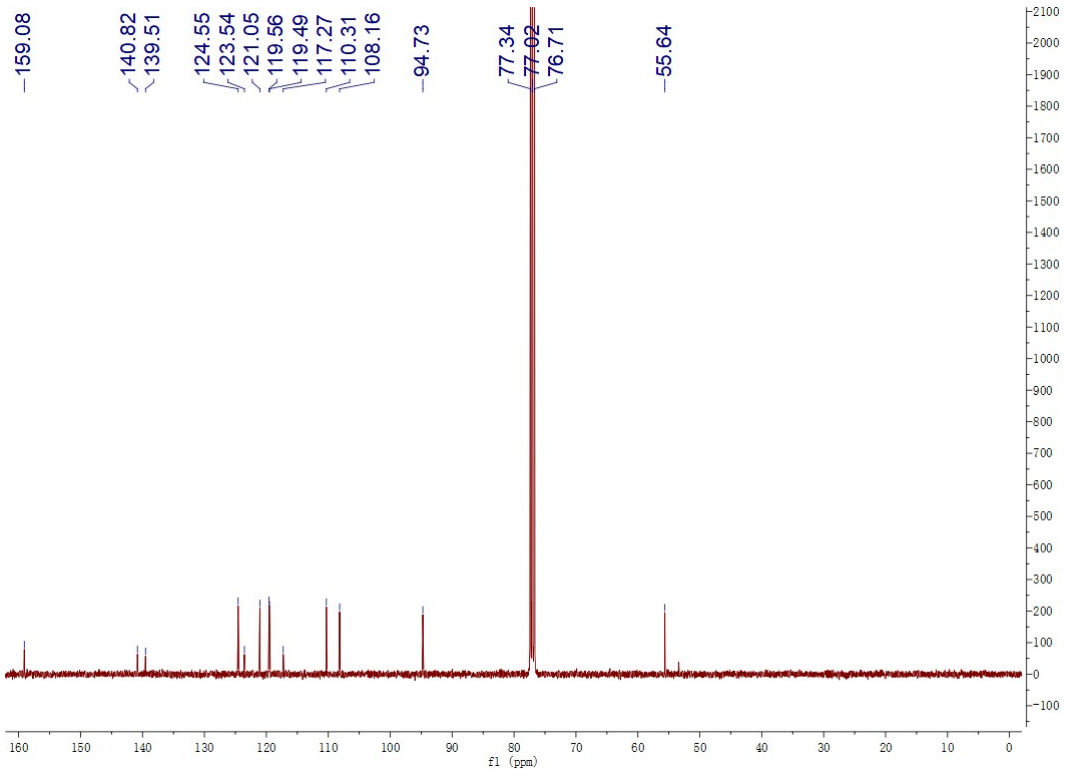


Fig. S2 The ^{13}C NMR spectrum of 1 in $CDCl_3$.

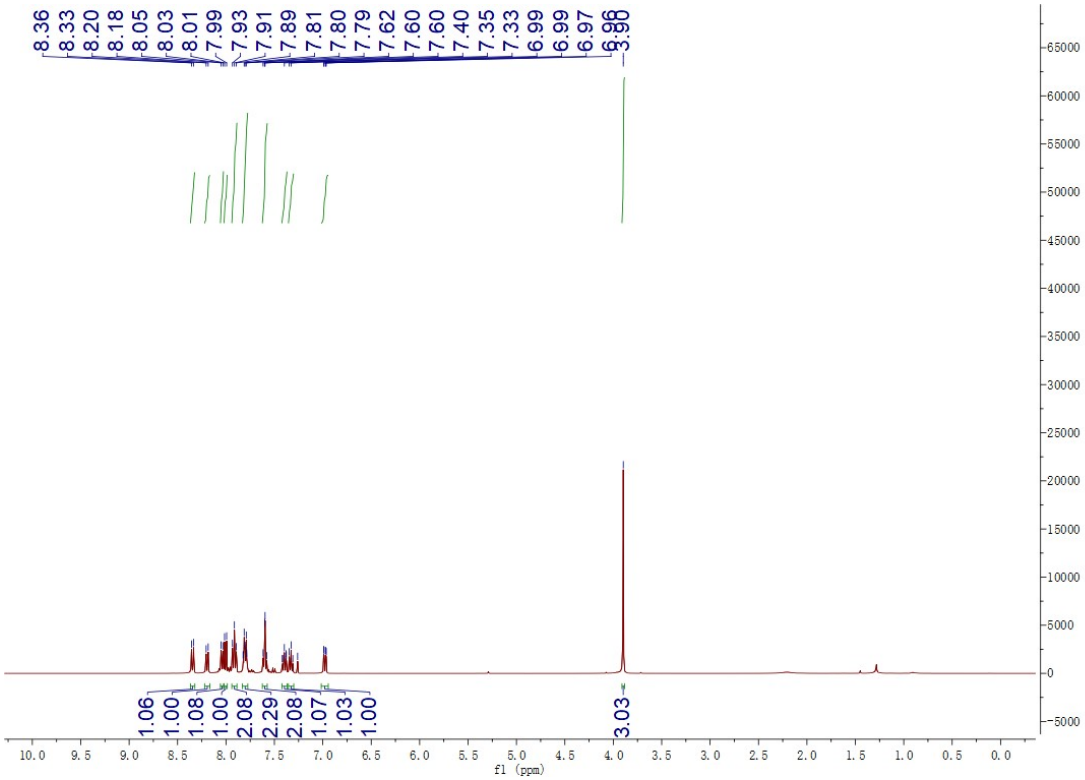


Fig. S3 The ^{1}H NMR spectrum of 2 in $CDCl_3$.

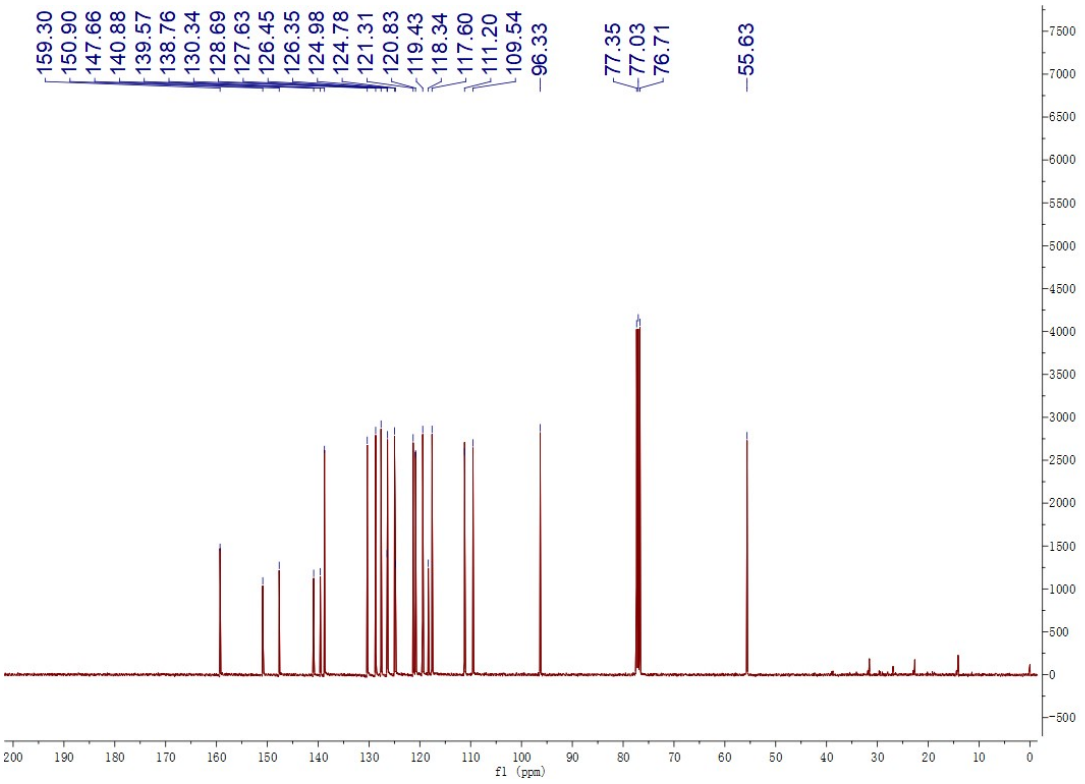


Fig. S4 The ^{13}C NMR spectrum of 2 in $CDCl_3$.

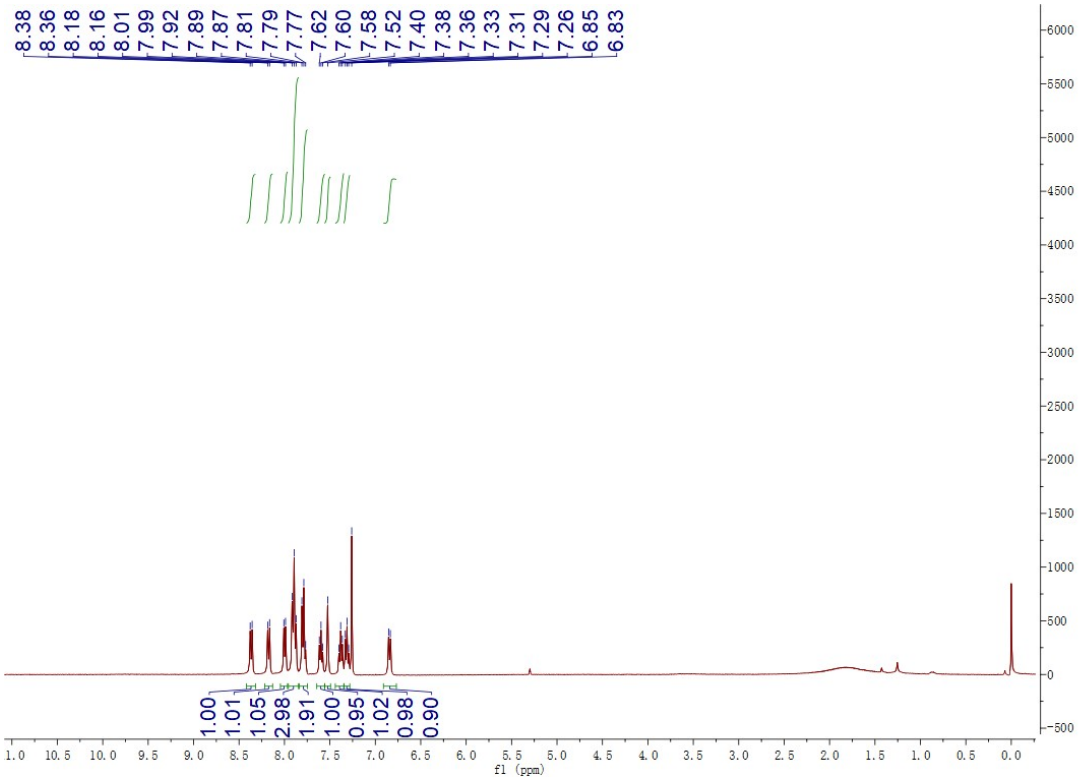


Fig. S5 The ^{1}H NMR spectrum of 3 in $CDCl_3$.

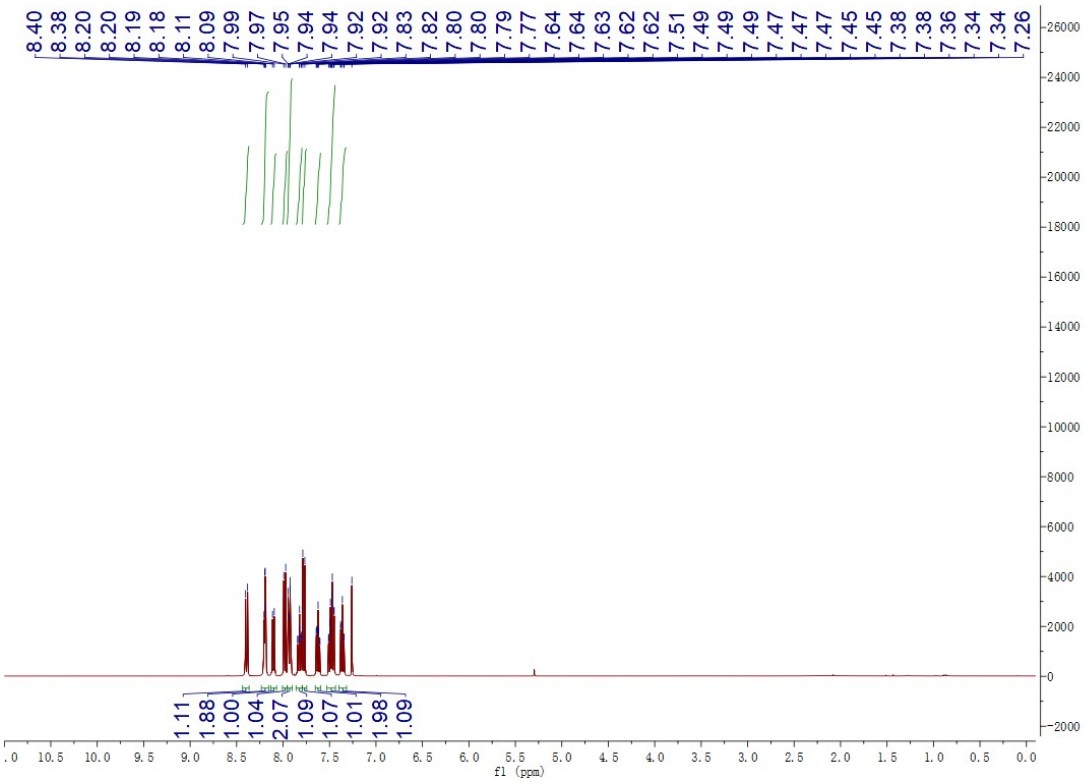


Fig. S6 The ^{1}H NMR spectrum of 4 in $CDCl_3$.

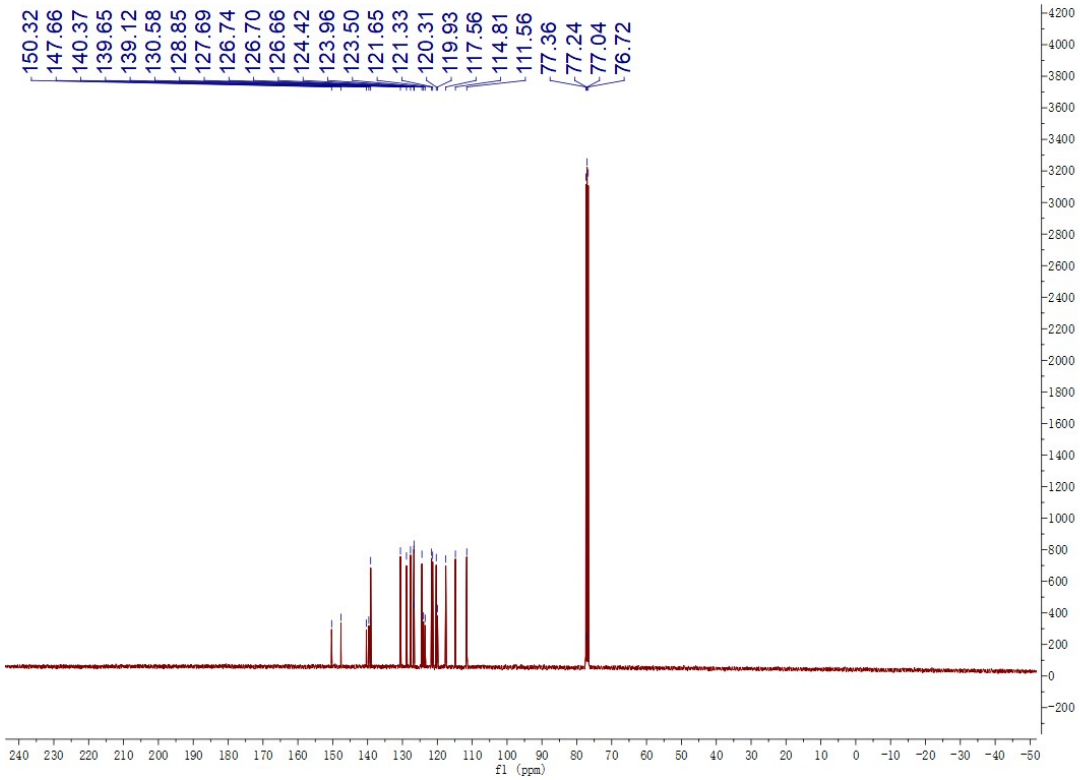


Fig. S7 The ^{13}C NMR spectrum of 4 in $CDCl_3$.

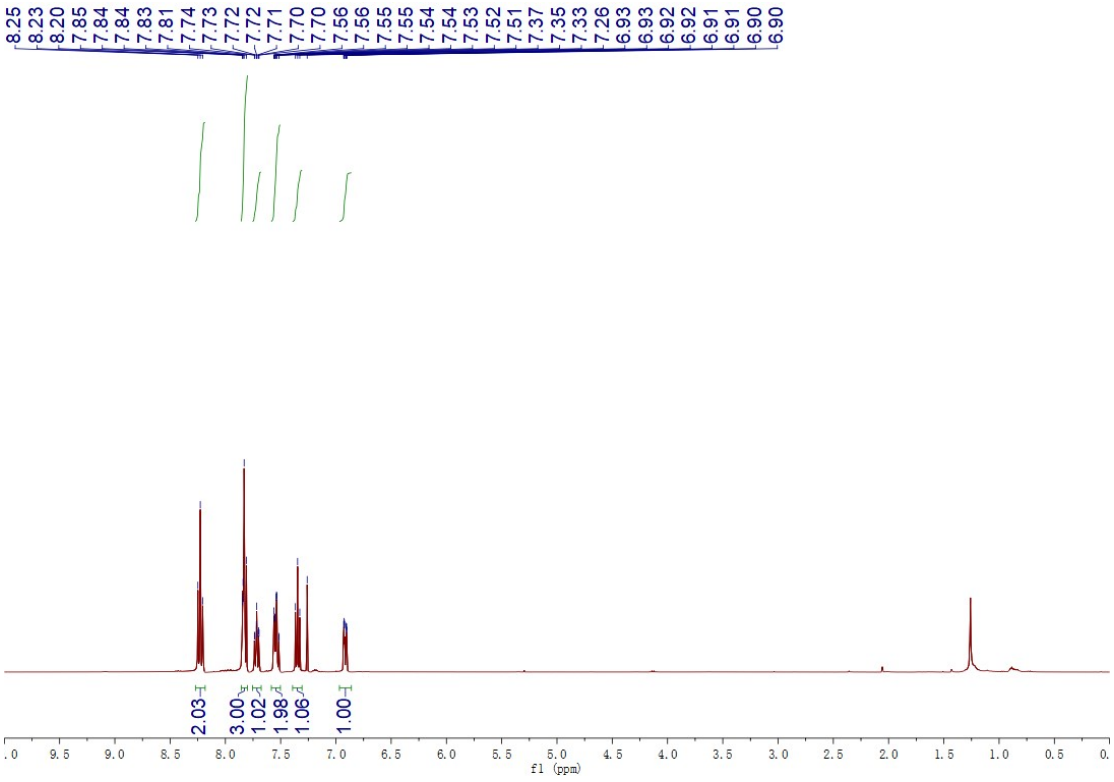


Fig. S8 The ^{1}H NMR spectrum of 5 in $CDCl_3$.

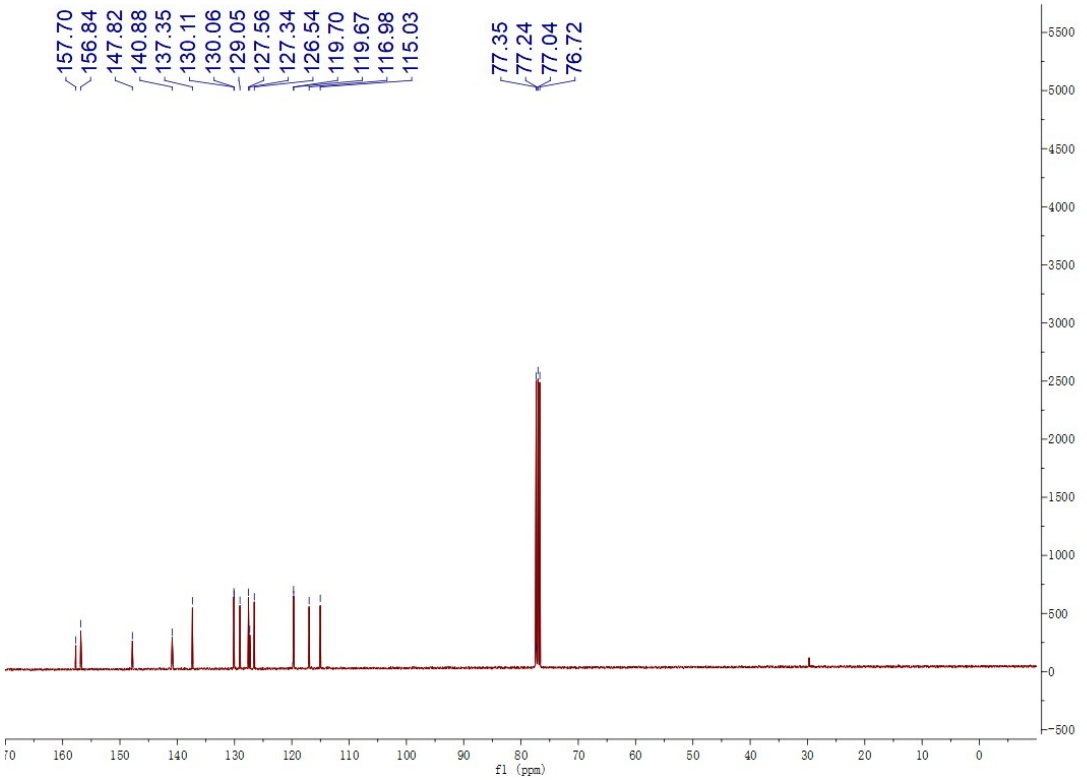


Fig. S9 The ^{13}C NMR spectrum of 5 in $CDCl_3$.

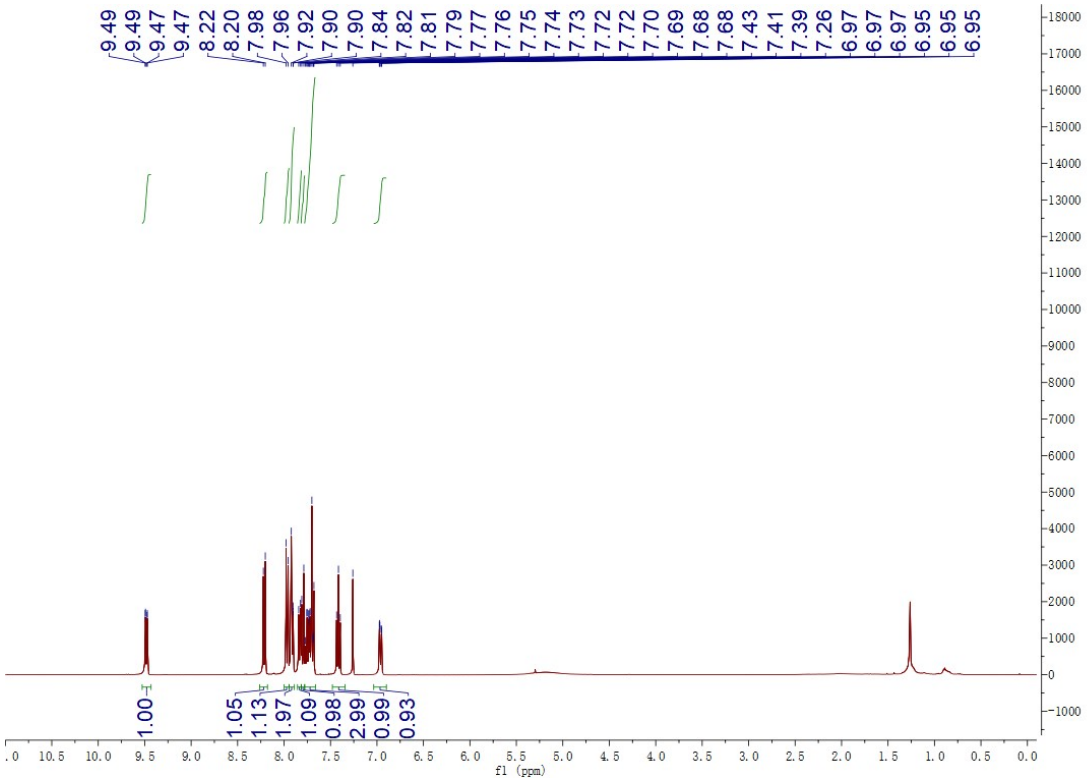


Fig. S10 The ^{1}H NMR spectrum of 6 in $CDCl_3$.

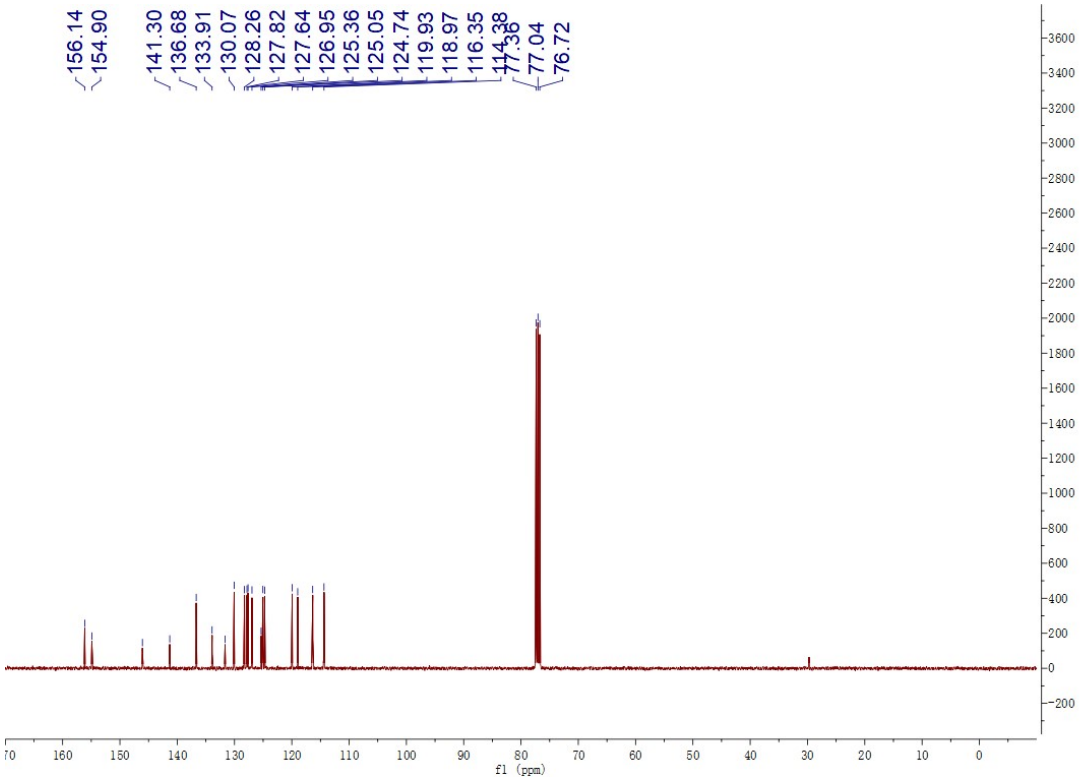


Fig. S11 The ^{13}C NMR spectrum of 6 in $CDCl_3$.

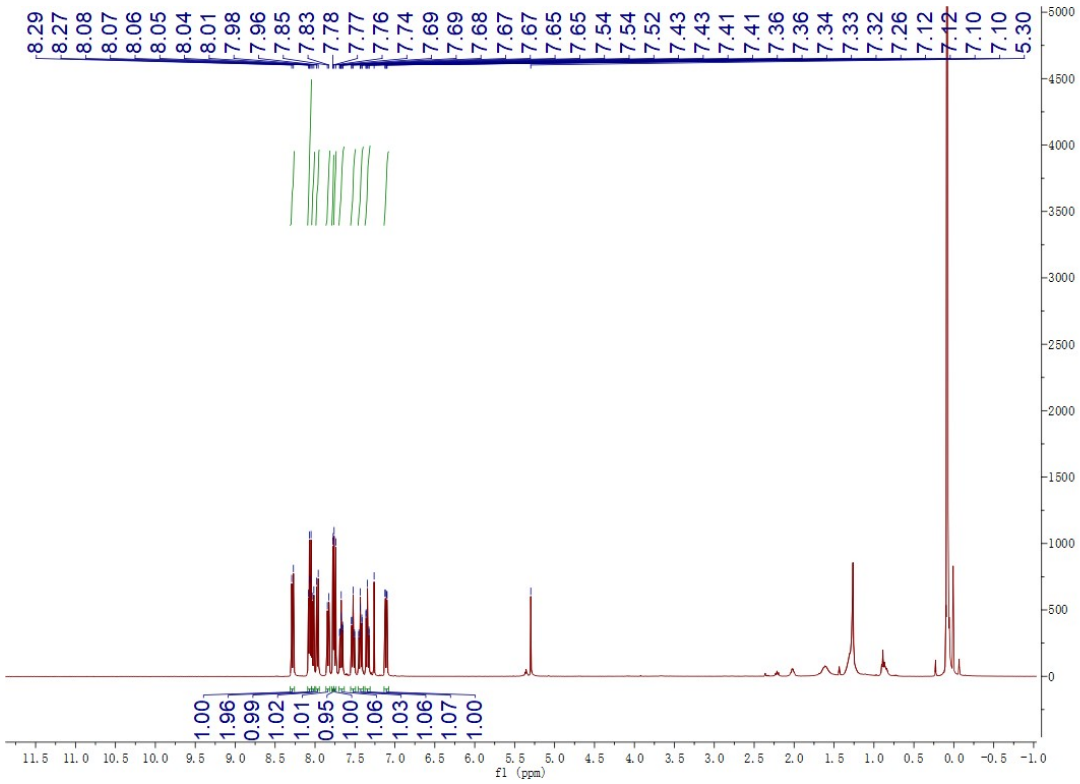


Fig. S12 The ^{1}H NMR spectrum of L1 in $CDCl_3$.

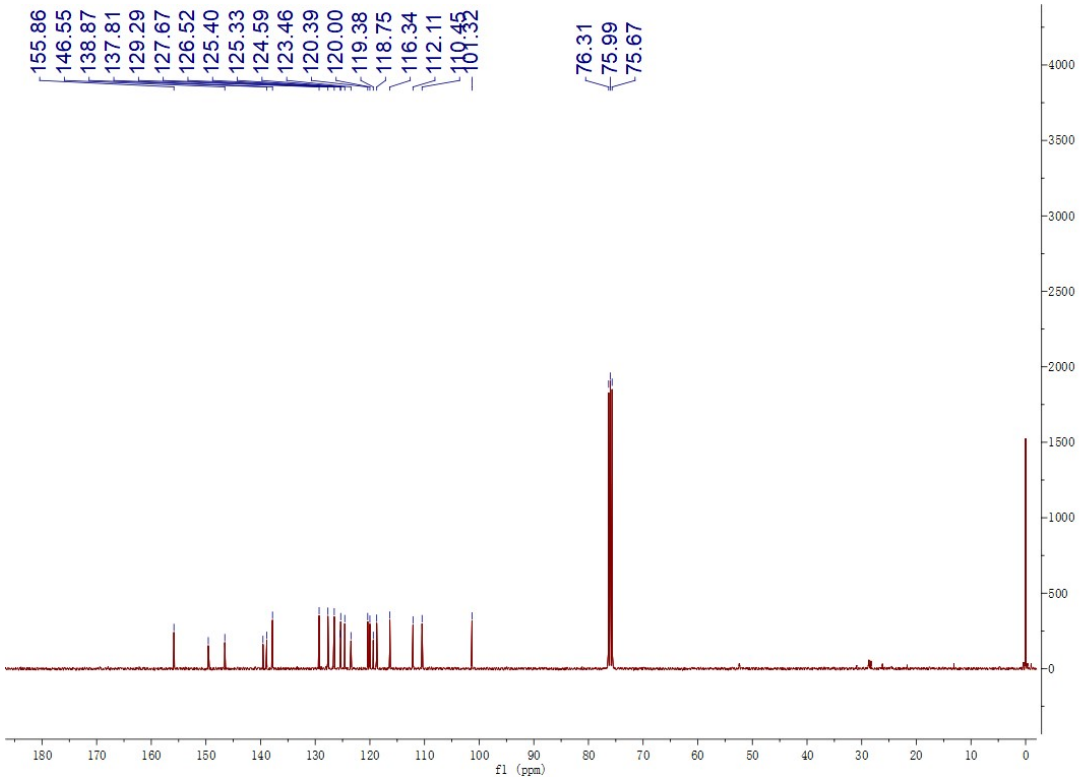


Fig. S13 The ^{13}C NMR spectrum of L1 in $CDCl_3$.

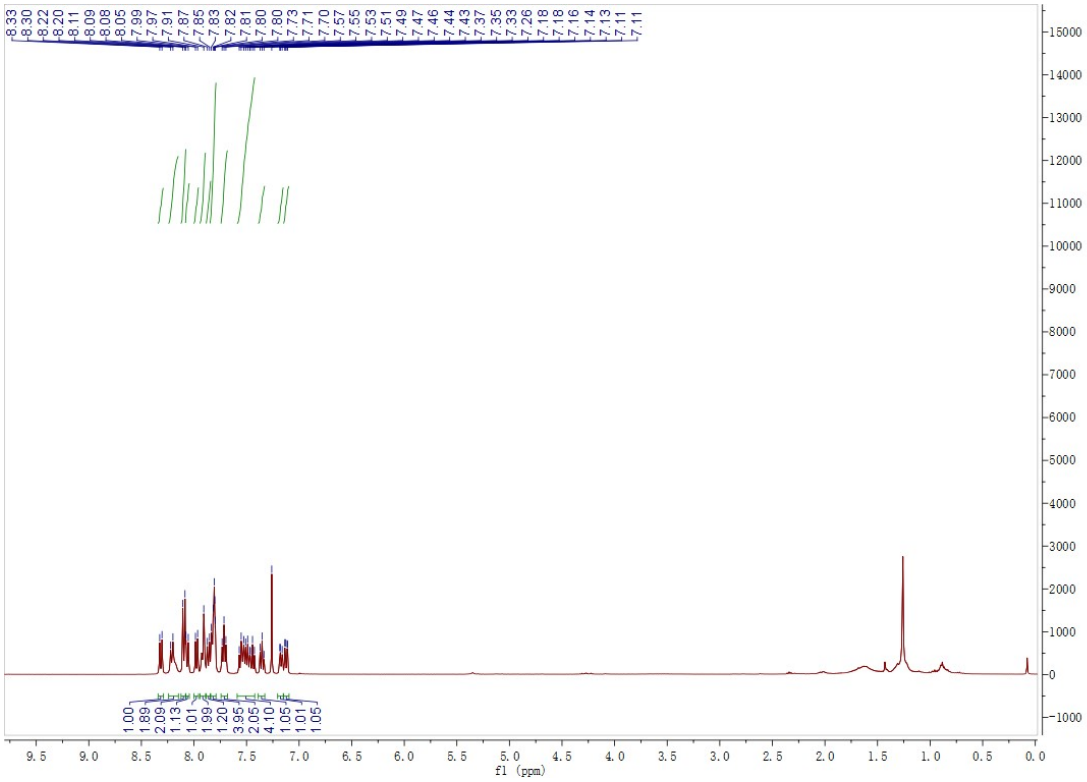


Fig. S14 The ^{1}H NMR spectrum of L2 in $CDCl_3$.

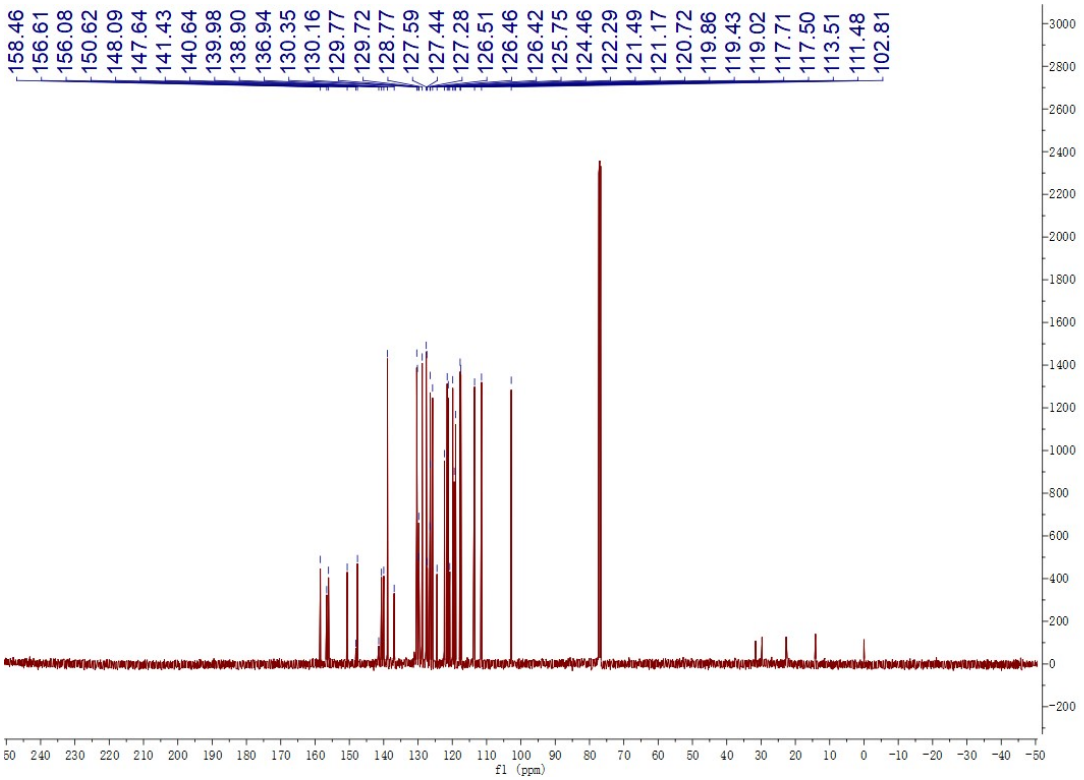


Fig. S15 The ^{13}C NMR spectrum of L2 in $CDCl_3$.

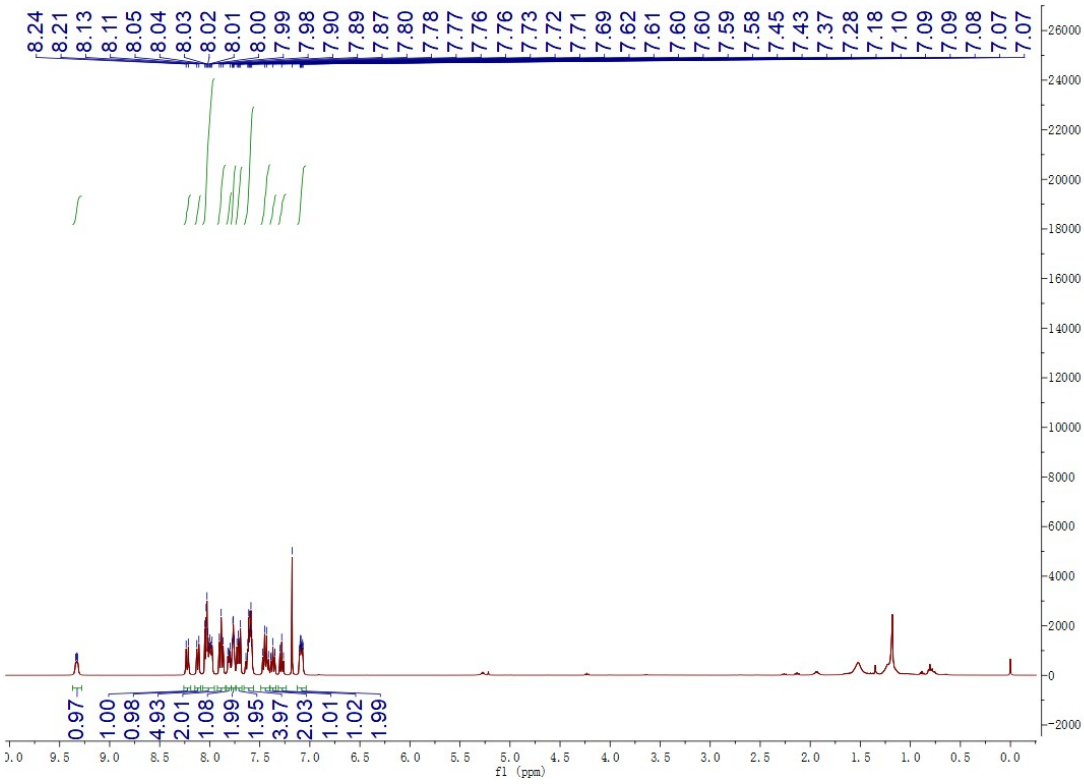


Fig. S16 The ^{1}H NMR spectrum of L3 in $CDCl_3$.

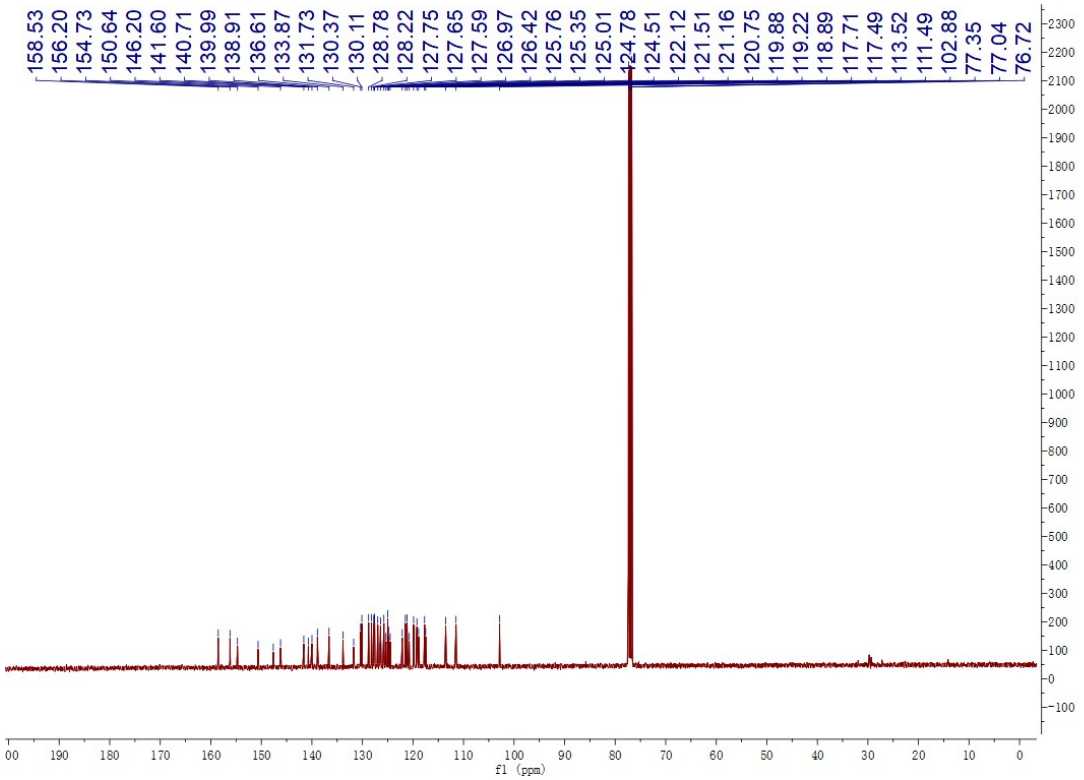


Fig. S17 The ^{13}C NMR spectrum of L3 in $CDCl_3$.

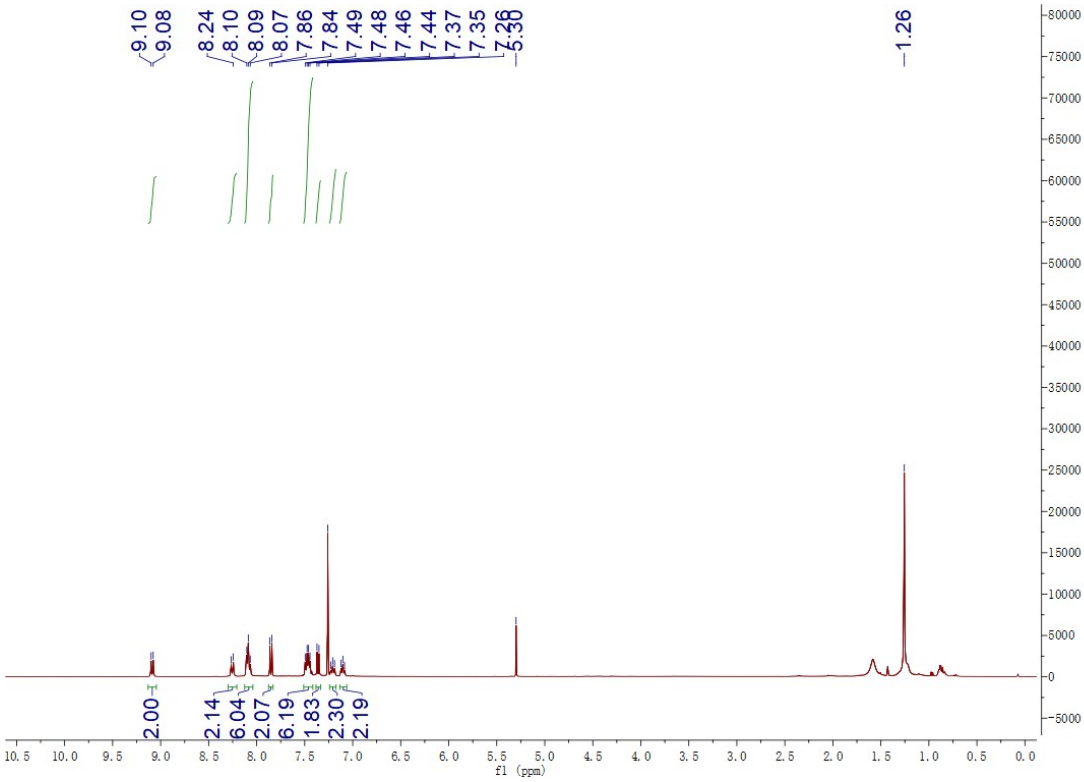


Fig. S18 The ^{1}H NMR spectrum of Pt1 in $CDCl_3$.

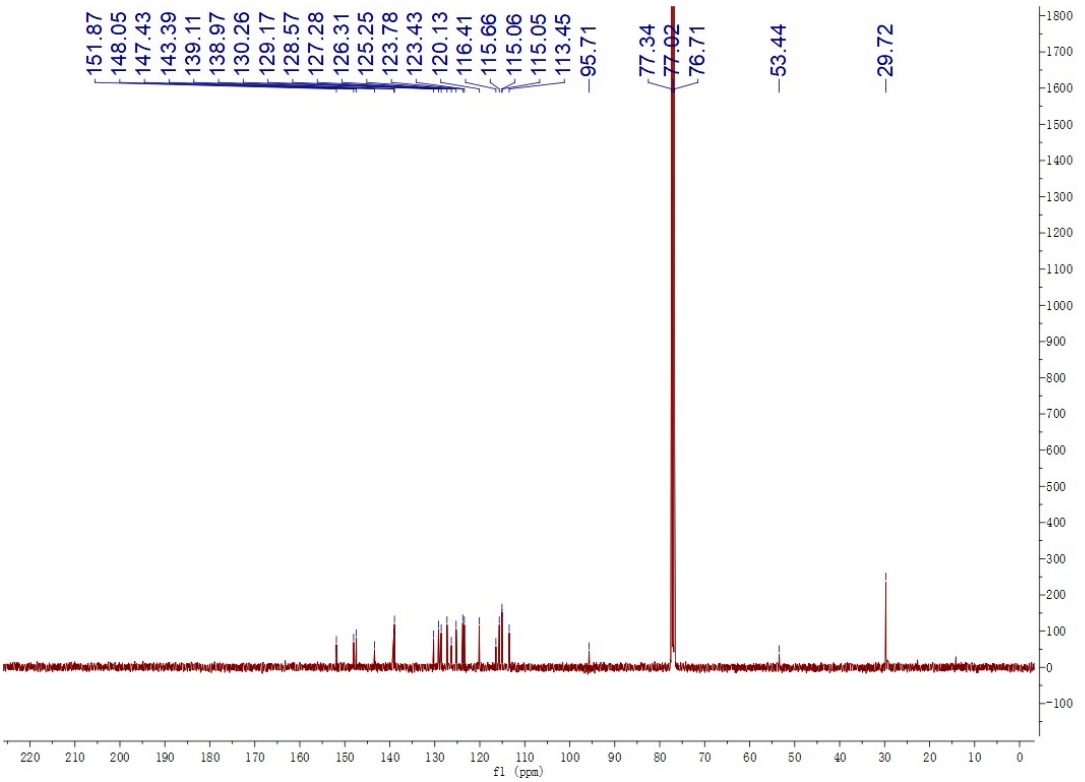


Fig. S19 The ^{13}C NMR spectrum of Pt1 in $CDCl_3$.

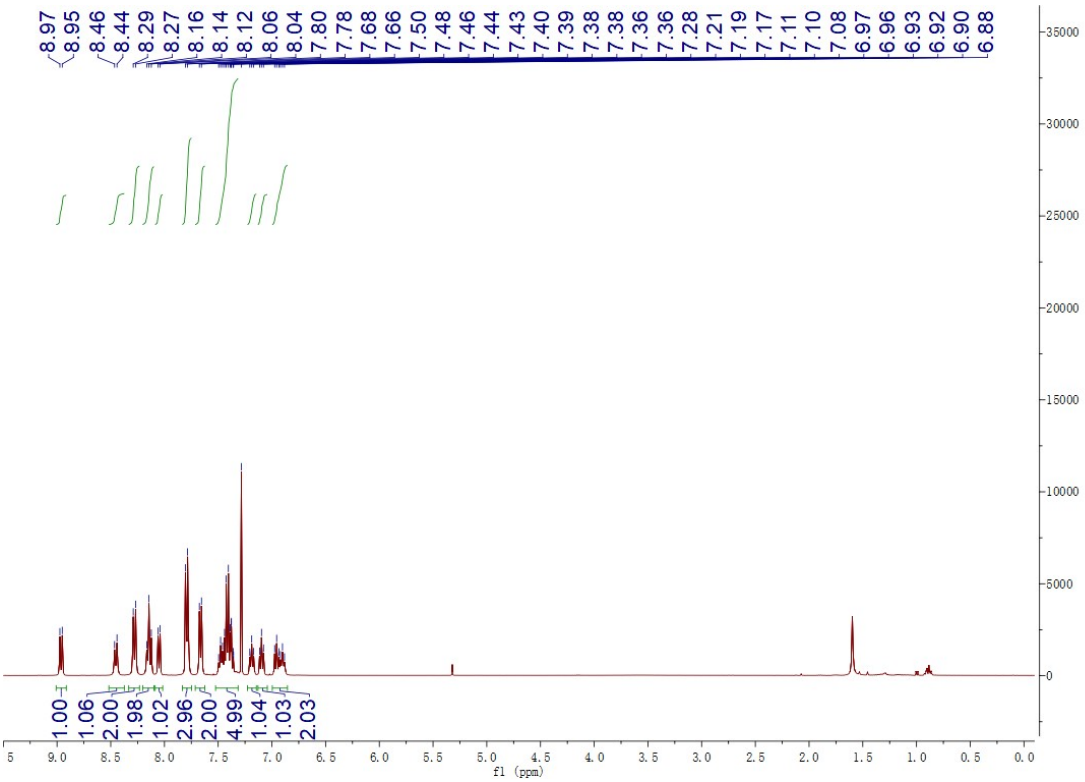


Fig. S20 The ^{1}H NMR spectrum of Pt2 in $CDCl_3$.

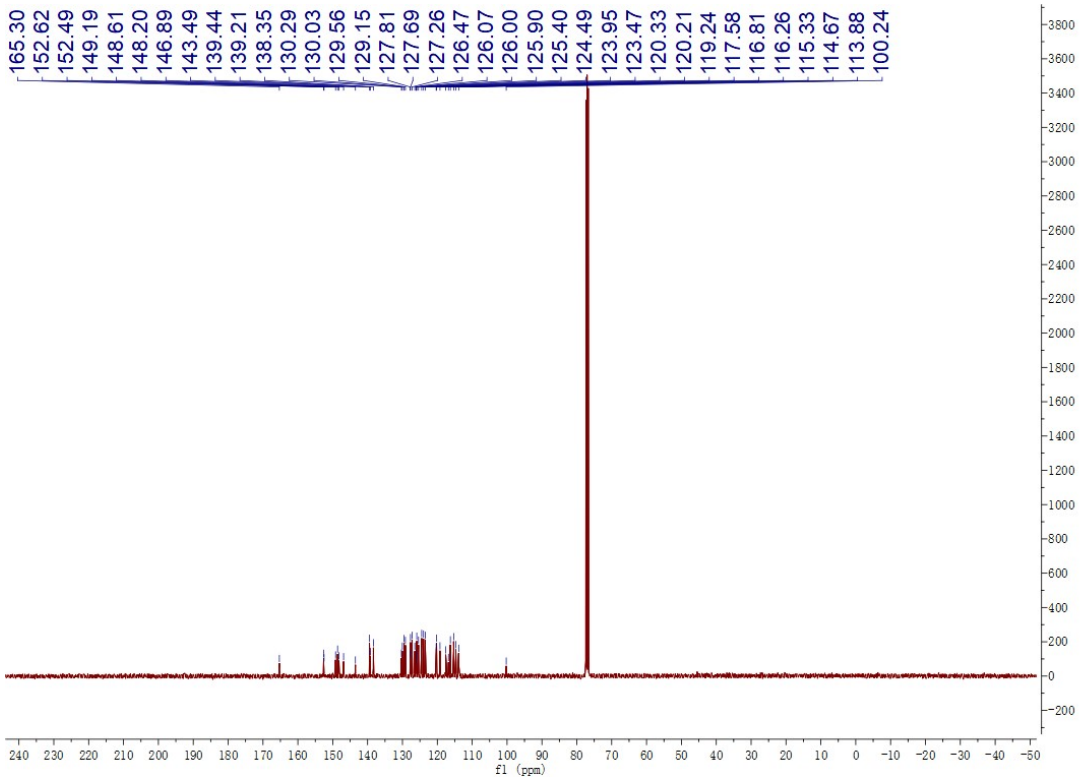


Fig. S21 The ^{13}C NMR spectrum of Pt2 in $CDCl_3$.

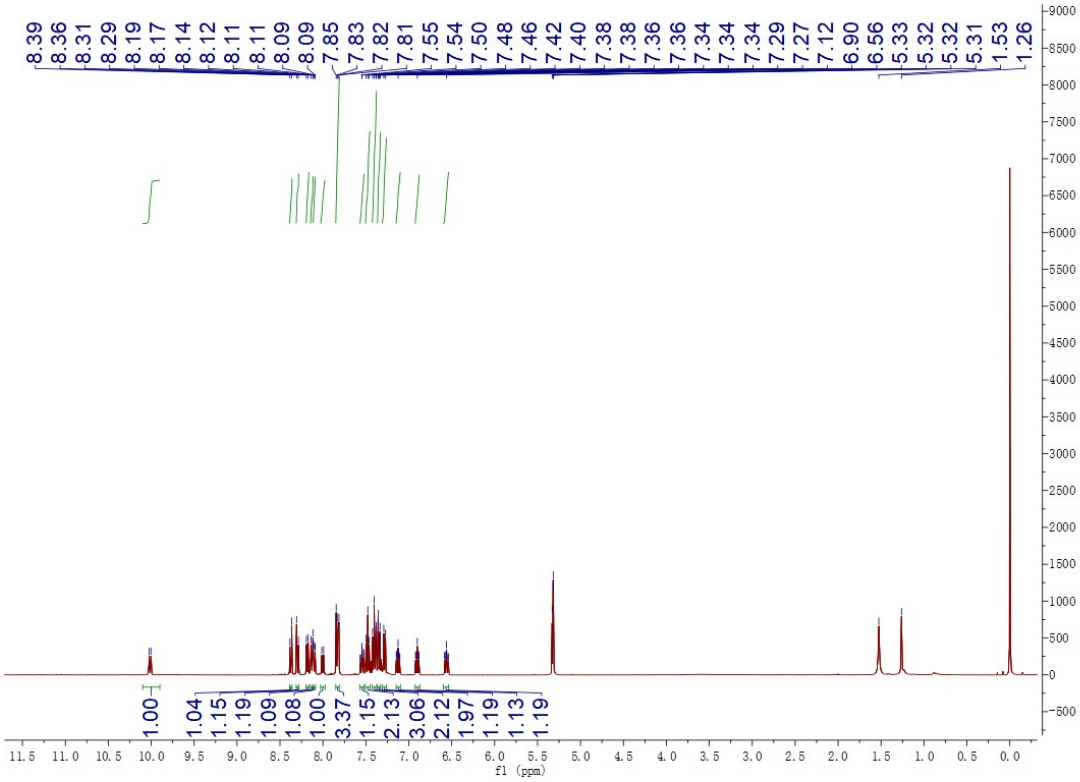


Fig. S22 The ^{1}H NMR spectrum of Pt3 in CD_2Cl_2.

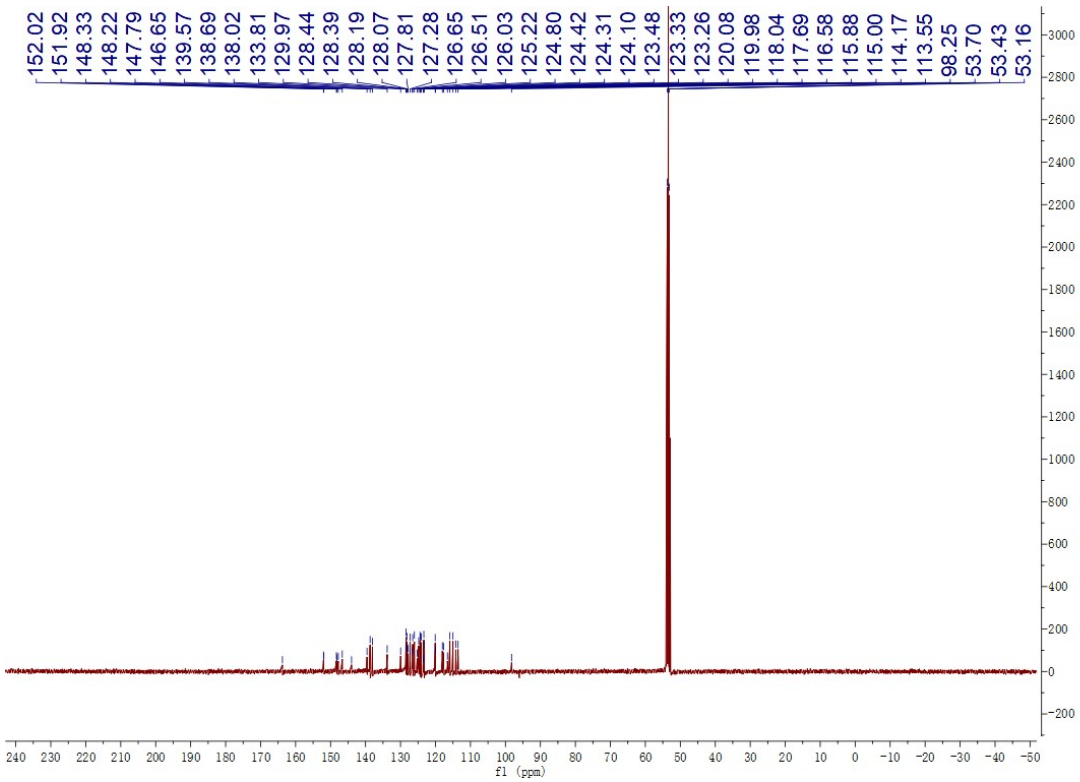


Fig. S23 The ^{13}C NMR spectrum of Pt3 in CD_2Cl_2.

2.4 X-ray crystallographic data

Table S1. Crystal data and structure refinement of Pt1, Pt2 and Pt3.

CCDC	2089099	2078055	2078039
Empirical formula	$C_{42}H_{24}N_4OPt$	$C_{36}H_{21}N_3OPt$	$C_{40}H_{23}N_3OPt$
Formula weight	795.77	706.65	756.70
Temperature/K	193.0	193.01	190.0
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	C2/c	Pbnb	$P2_12_12_1$
a/Å	26.329(5)	14.3793(5)	9.7121(5)
b/Å	9.262(2)	15.8696(6)	13.4863(7)
c/Å	15.829(3)	22.7457(8)	21.4355(10)
α/°	90.00(3)	90	90
β/°	108.70(3)	90	90
γ/°	90.00(3)	90	90
Volume/Å^3	3656.1(14)	5190.4(3)	2807.6(2)
Z	4	8	4
ρ_{calc} g/cm^3	1.754	1.809	1.790
μ/mm^{-1}	6.949	7.136	6.841
F(000)	1896.0	N/A	1480.0
Radiation	GaKα (λ = 1.34139)	GaKα (λ = 1.34139)	GaKα (λ = 1.34139)
2Θ range for data collection/°	10.142 to 110.174	6.326 to 107.768	6.736 to 107.888
Index ranges	-31 ≤ h ≤ 32, -11 ≤ k ≤ 11, -19 ≤ l ≤ 19	-17 ≤ h ≤ 16, -17 ≤ k ≤ 19, -27 ≤ l ≤ 27	-11 ≤ h ≤ 11, -12 ≤ k ≤ 16, -24 ≤ l ≤ 25
Reflections collected	13101	32148	18466
Independent reflections	3465 [R_{int} = 0.0583, R_{sigma} = 0.0445]	4749 [R_{int} = 0.0539, R_{sigma} = 0.0289]	5088 [R_{int} = 0.0566, R_{sigma} = 0.0496]
Data/restraints/parameters	3465/0/245	4749/0/370	5088/0/407
Goodness-of-fit on F^2	1.094	1.145	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0312, wR_2 = 0.0813	R_1 = 0.0369, wR_2 = 0.0801	R_1 = 0.0307, wR_2 = 0.0706
Final R indexes [all data]	R_1 = 0.0324, wR_2 = 0.0821	R_1 = 0.0515, wR_2 = 0.0843	R_1 = 0.0322, wR_2 = 0.0710
Largest diff. peak/hole / e Å^{-3}	1.01/-0.93	1.36/-0.96	1.12/-1.26
Flack parameter			0.074(17)

$R_1{}^a = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. $wR_2{}^b = [\Sigma w(F_o{}^2 - F_c{}^2)^2/\Sigma w(F_o{}^2)]^{1/2}$

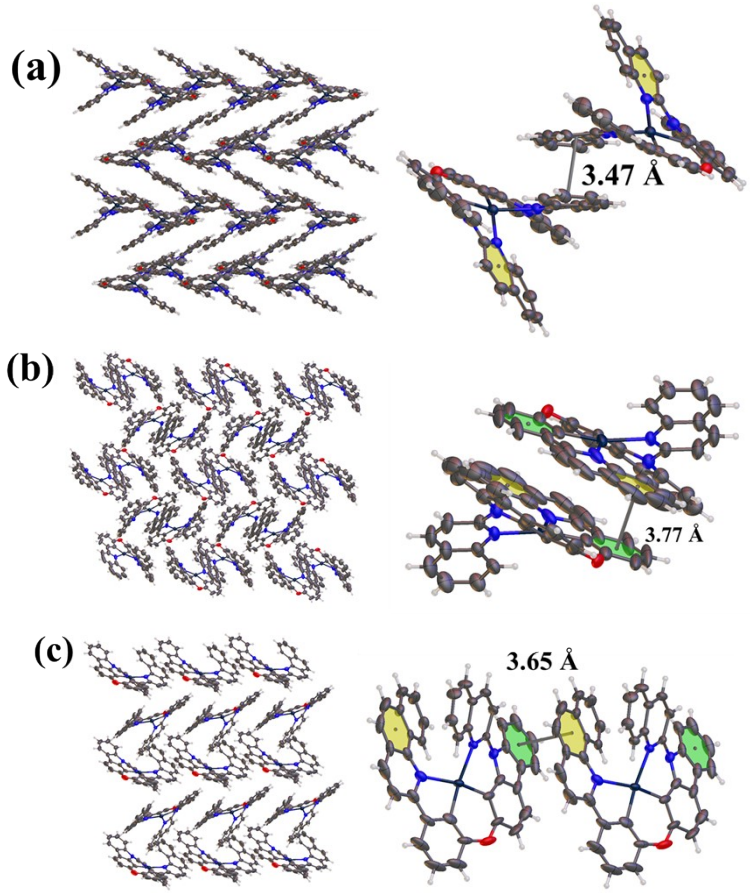


Fig. S24 (a) Crystal packing of Pt1; (b) Crystal packing of Pt2; (c) Crystal packing of Pt3.

S3. Thermal stability

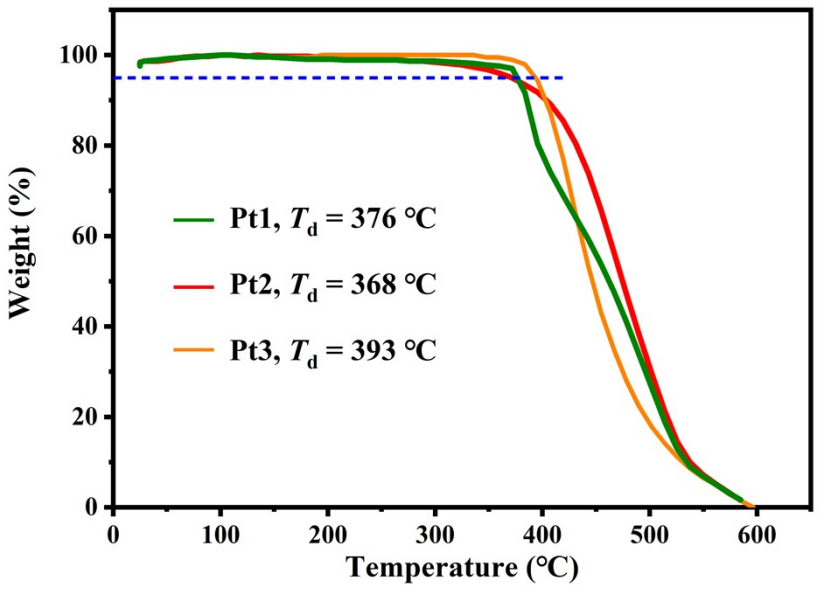


Fig. S25 The TGA curves of Pt1, Pt2 and Pt3.

S4. HPLC Data

HPLC Analysis Conditions: a) Column: Cat. No. EnantioPak®R-B, 5μm, 250 × 4.6 mm; b) Mobile phase: n-Hexane/Ethanol/dichloromethane = 80/10/10(v/v/v); c) Flow rate: 1.0 mL/min; d) Abs. detector: 254 nm.

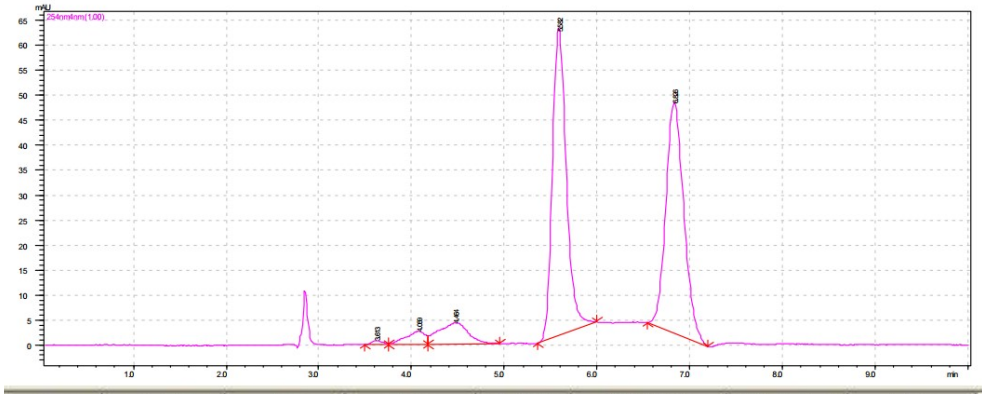


Fig. S26 HPLC profile of racemic Pt1.

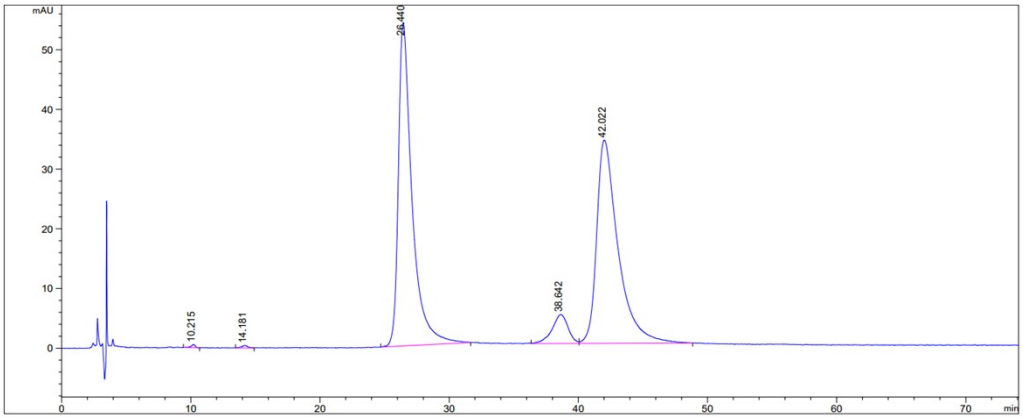


Fig. S27 HPLC profile of racemic Pt2.

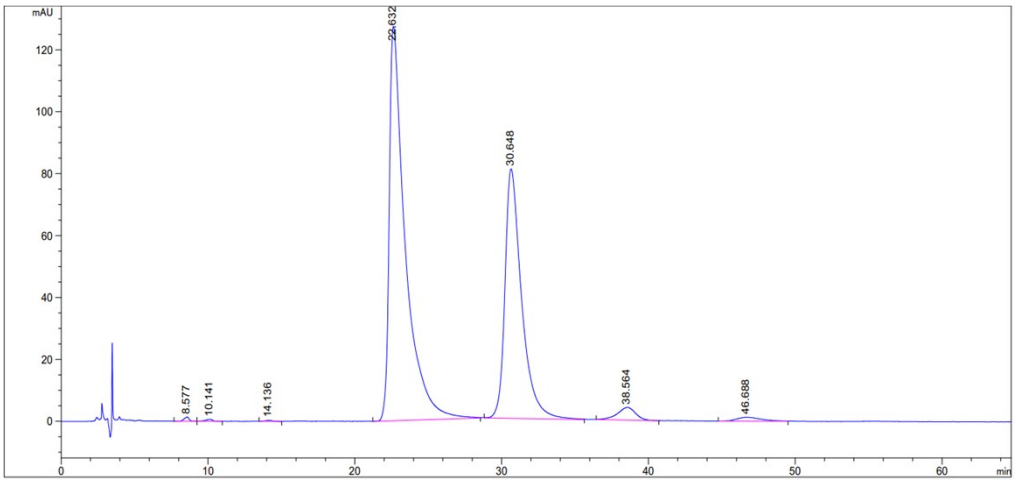


Fig. S28 HPLC profile of racemic Pt3.

S5. Photophysical measurement

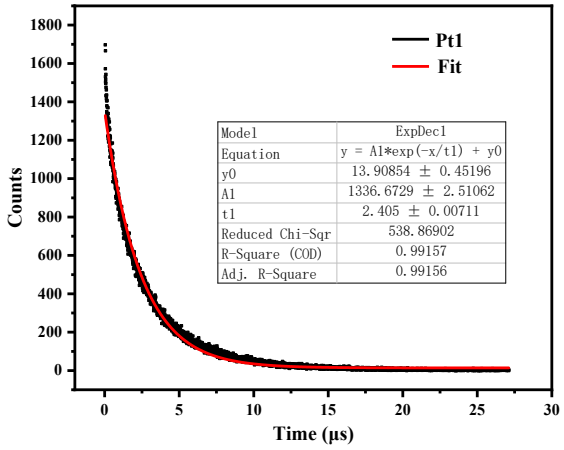


Fig. S29 The lifetime curve of Pt1 in doped film at room temperature.

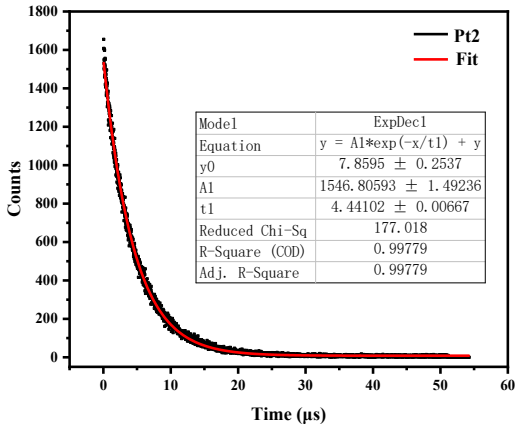


Fig. S30 The lifetime curve of Pt2 in doped film at room temperature.

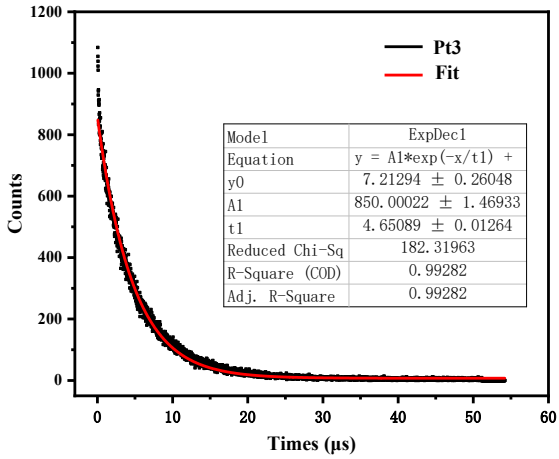


Fig. S31 The lifetime curve of Pt3 in doped film at room temperature.

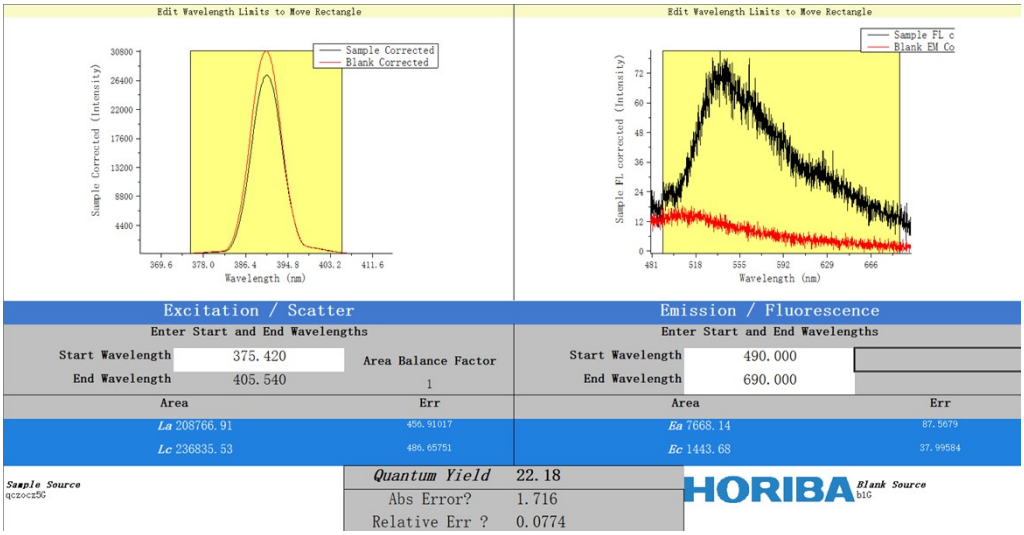


Fig. S32 The quantum yield measurement of Pt1 in CH_2Cl_2 solution at room temperature.

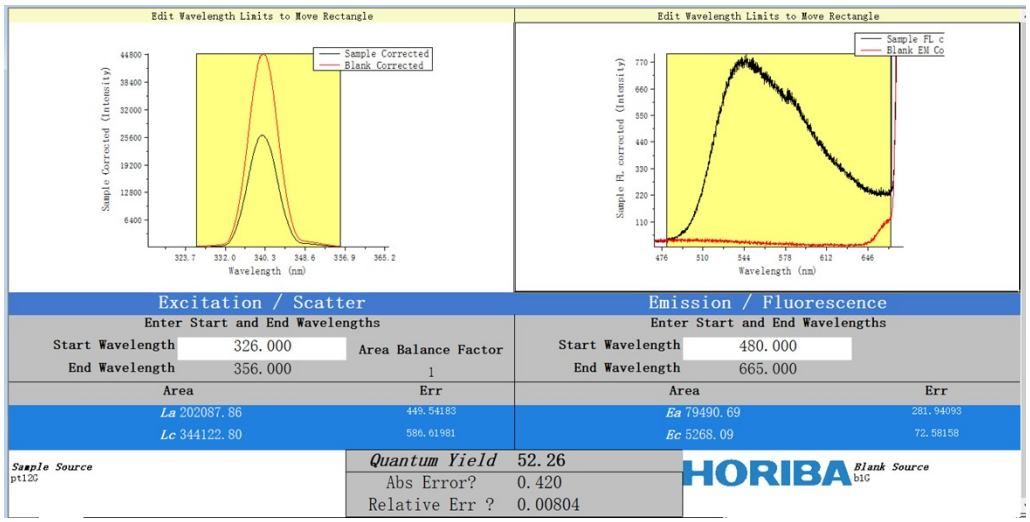


Fig. S33 The quantum yield measurement of Pt1 in doped film at room temperature.

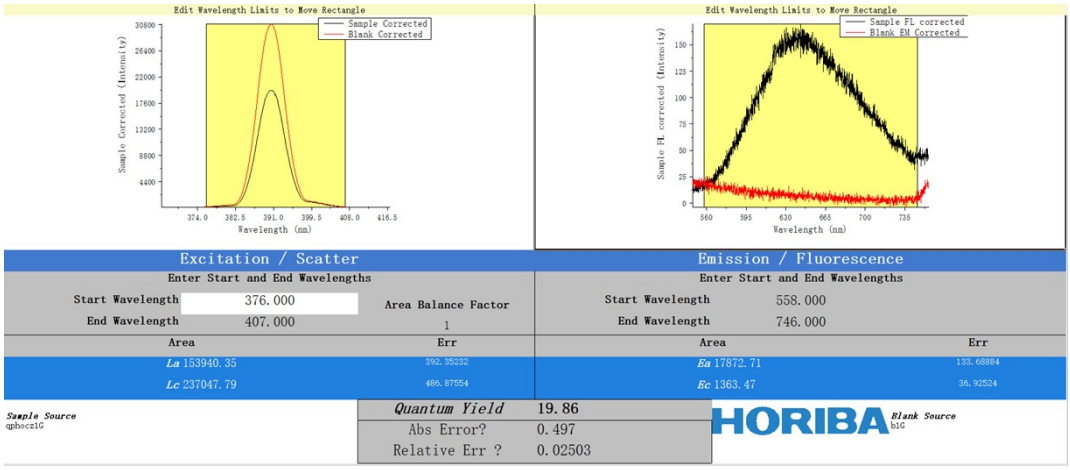


Fig. S34 The quantum yield measurement of Pt2 in CH_2Cl_2 solution at room temperature.

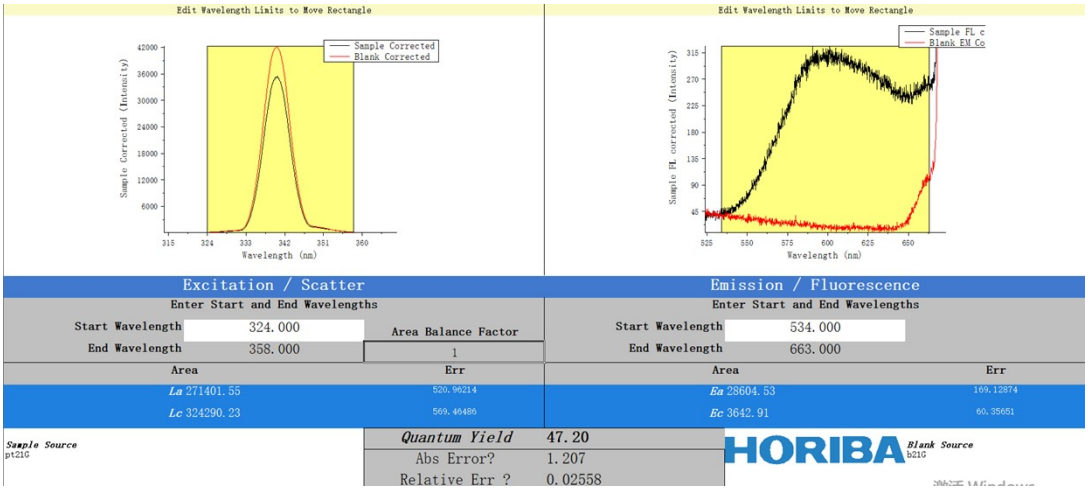


Fig. S35 The quantum yield measurement of Pt2 in doped film at room temperature.

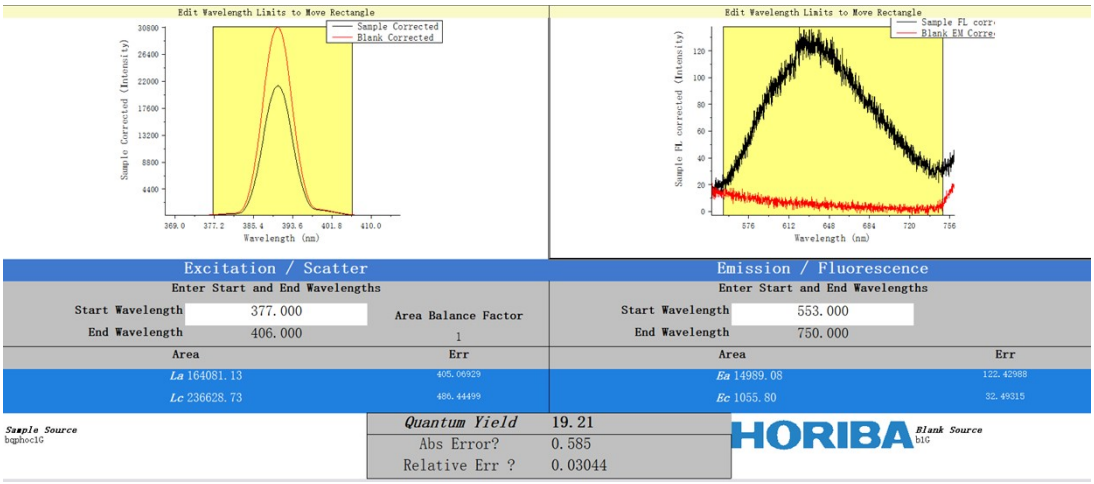


Fig. S36 The quantum yield measurement of Pt3 in CH_2Cl_2 solution at room temperature.

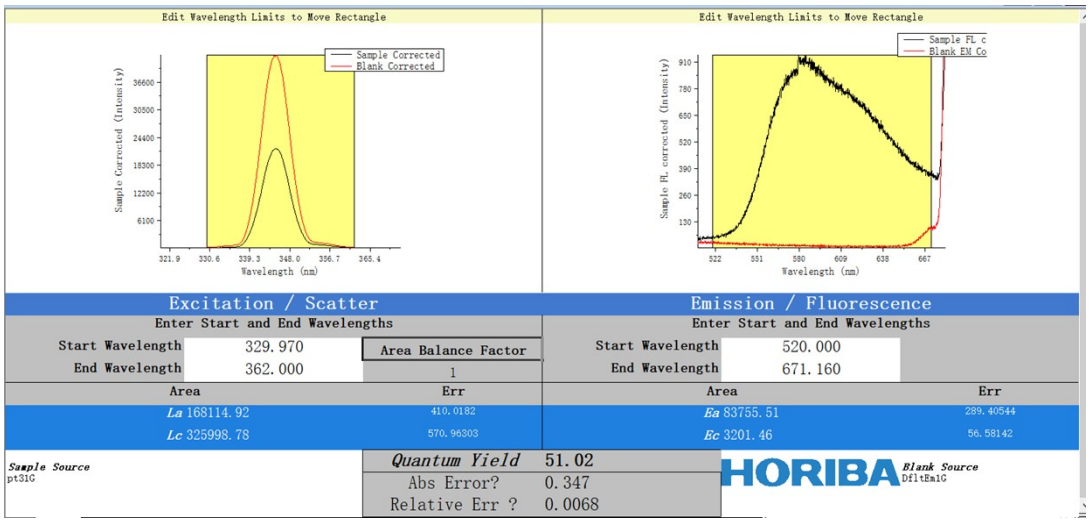


Fig. S37 The quantum yield measurement of Pt3 in doped film at room temperature.

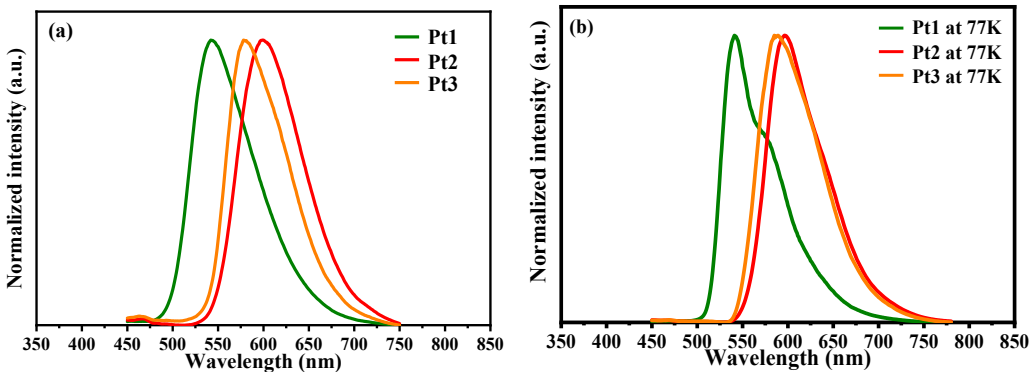


Fig. S38 (a) Normalized emission spectra in doped films and (b) emission spectra in CH_2Cl_2 solution at 77K of Pt1, Pt2 and Pt3.

S6. Electrochemical measurement and theoretical calculation

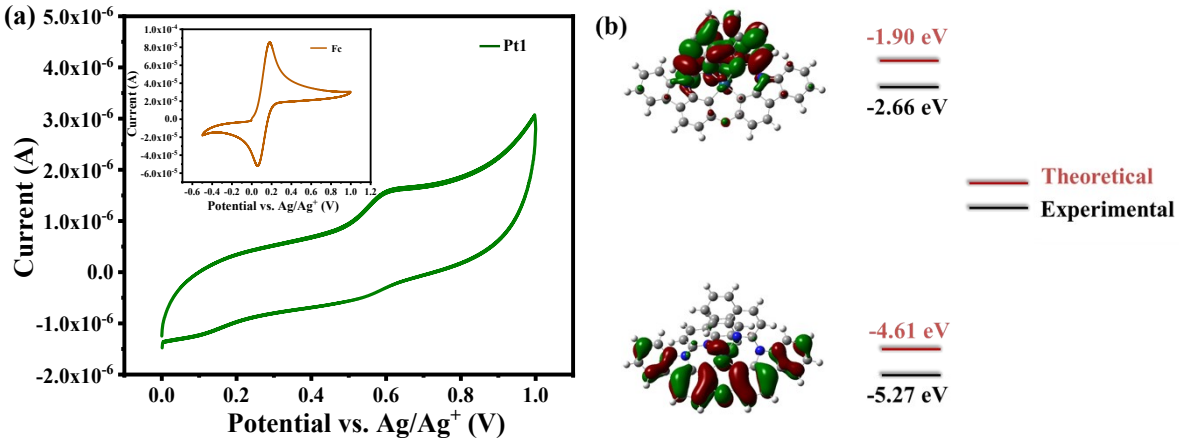


Fig. S39 (a) The cyclic voltammogram curve of Pt1; (b) Energy levels and electronic clouds distribution of Pt1.

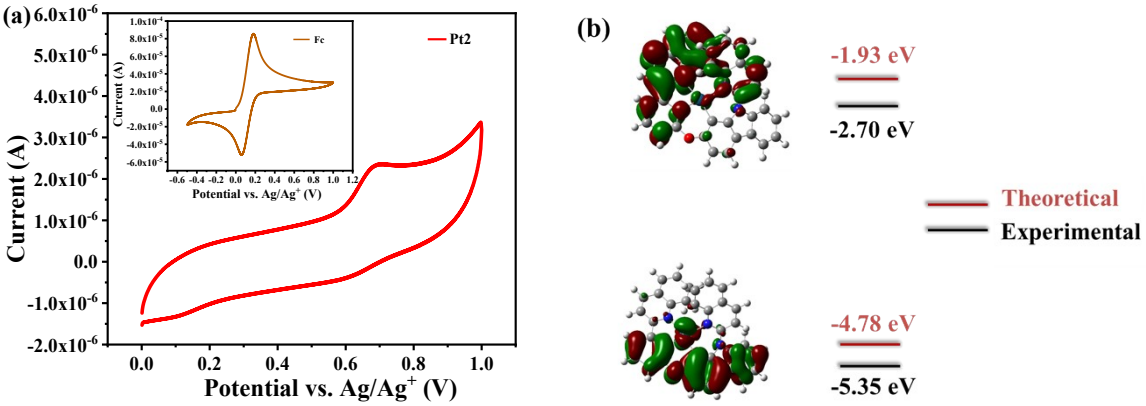


Fig. S40 (a) The cyclic voltammogram curve of Pt2; (b) Energy levels and electronic clouds distribution of Pt2.

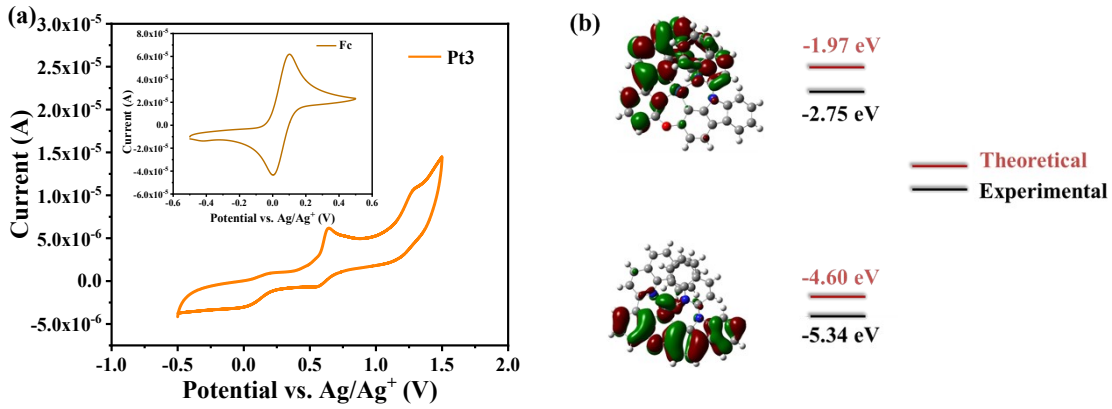


Fig. S41 (a) The cyclic voltammogram curve of Pt3; (b) Energy levels and electronic clouds distribution of Pt3.

S7. Device fabrication of D1-D3

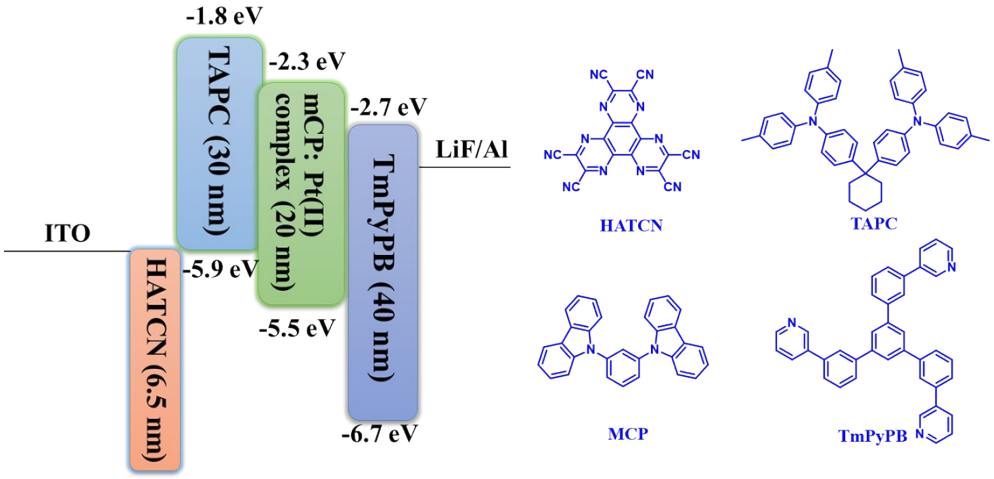
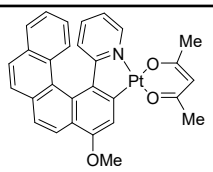
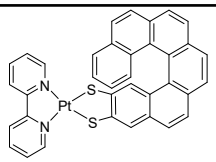
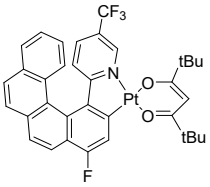
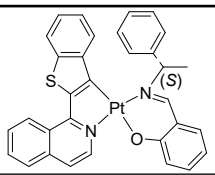
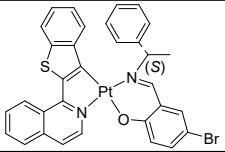
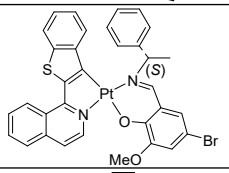
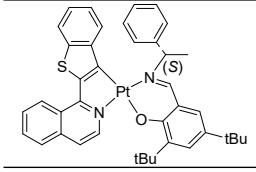
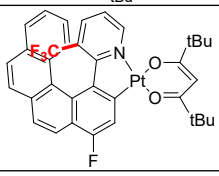
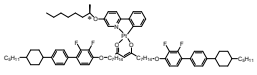
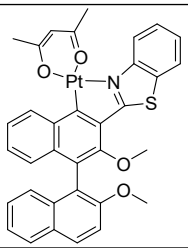
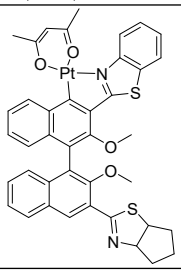


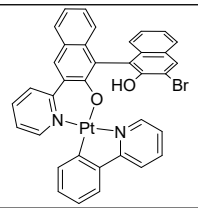
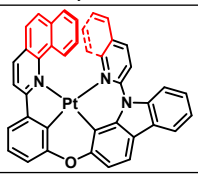
Fig. S42 Device energy level diagrams and molecular structures of each layer.

S8. Reference device performance

Table S2. The reported devices performances of chiral Pt(II) complexes.

Molecular structure	L_{max} (cd/m^2)	$\eta_{c,max}$ (cd/A)	EQE$_{max}$ (%)	$\|g_{lum}\|$ ($\times10^{-3}$)	$\|g_{EL}\|$ ($\times10^{-3}$)	Reference
	222	0.25	-	220	380	*J. Am. Chem. Soc.* 2016, **138**, 9743−9746.

	-	-	-	0.3	-	*Chem. Commun.*, 2017, **53**, 9210-9213.
	11590	22.5	18.8	3.7	5.1	*Chem. Eur. J.*, 2019, **25**, 5672-5676.
	2110	23.3	0.87-0.93	-2.1	-2.2	*J. Mater. Chem. C*, 2019, **7**, 13743-13747.
	-	-		-2.1	-1.8	
	-	-		-1.8	-1.9	
	-	-		-2.8	-2.7	
	2156	2.14	4.17	6.0	1.1	*Front. Chem.* 2020. **8** 501.
	7150	37.1	11.3	20	60 (after annealing)	*Adv. Opt. Mater.*, 2020, **8**, 2000775.
	1062	1.43	1.32	1.3	1.0	*ACS Appl. Mater. Interfaces*, 2020, **12**, 9520-9527.
	3500	2.83	2.15	1.0	-	

	-	-	1.2	-	0.11	*Chem. Sci.*, 2021, **12**, 8668-8681.
	36400	33.4	12.6	6.83	0.68	This work

S9. Reference

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