Highly phosphorescent cyclometalated platinum(II) complexes based on 2-phenylbenzimidazole-containing ligands

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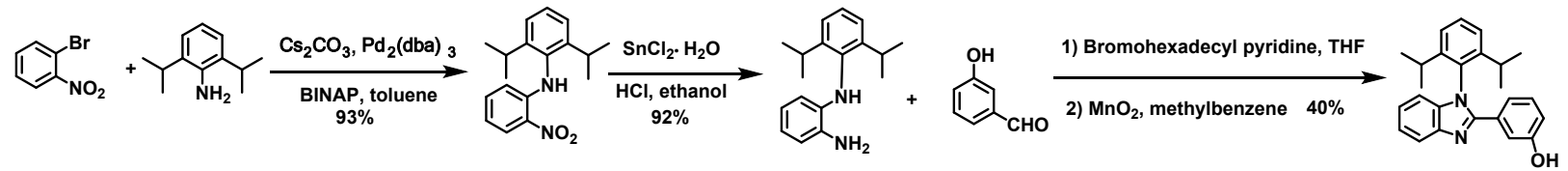
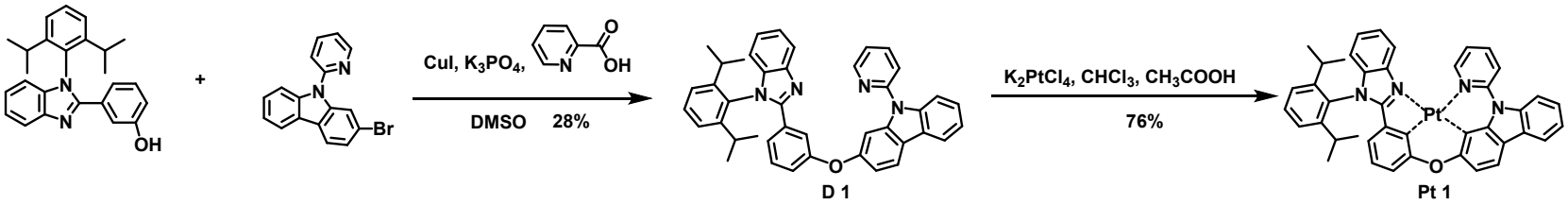
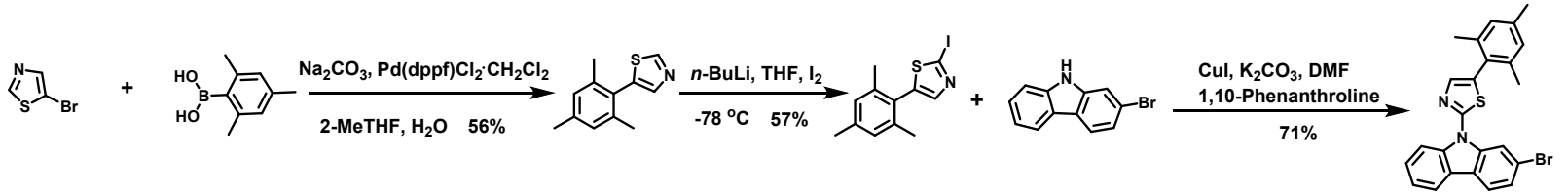
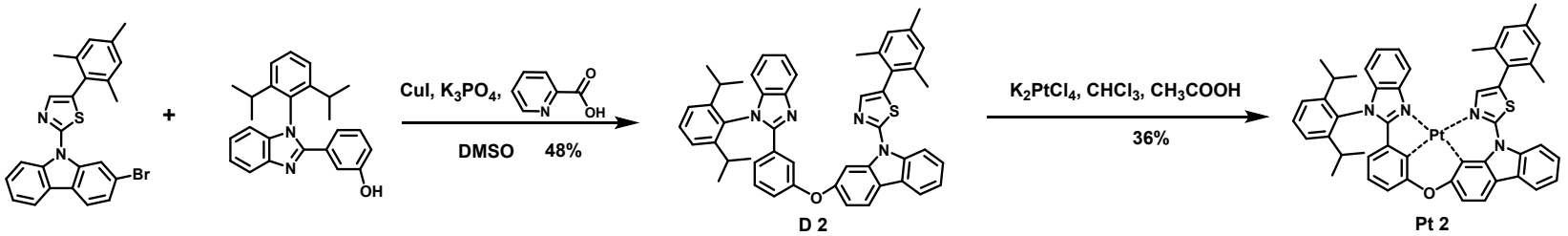

Br
NO2
NH2
Cs2CO3, Pd2(dba) 3
BINAP, toluene
93%
NH
NO2
SnCl2· H2O
HCl, ethanol
92%
NH
NH2
OH
CHO
1) Bromohexadecyl pyridine, THF
2) MnO2, methylbenzene 40%
N
N
OH


OH
Br
CuI, K3PO4,
O
N
OH
DMSO 28%
O
D 1
K2PtCl4, CHCl3, CH3COOH
76%
Pt
Pt 1


N
S
Br
HO
B
HO
Na2CO3, Pd(dppf)Cl2·CH2Cl2
2-MeTHF, H2O 56%
n-BuLi, THF, I2
-78 °C 57%
I
H
N
Br
CuI, K2CO3, DMF
1,10-Phenanthroline
71%


N
S
Br
OH
CuI, K3PO4,
O
N
OH
DMSO 48%
O
D 2
K2PtCl4, CHCl3, CH3COOH
36%
Pt
Pt 2

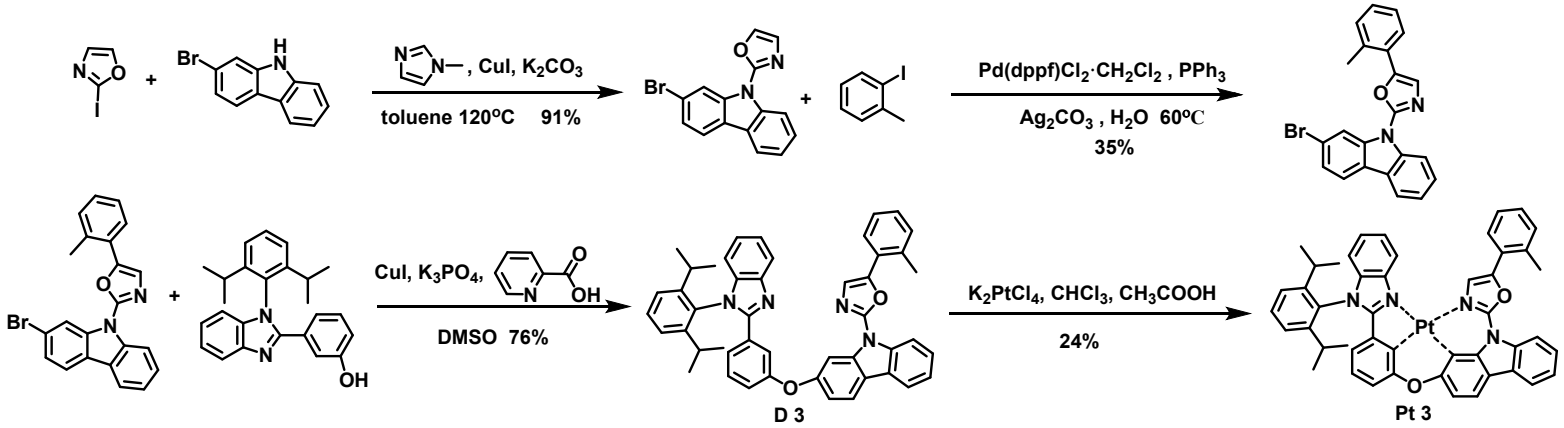
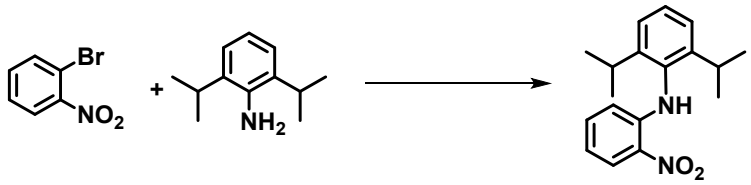
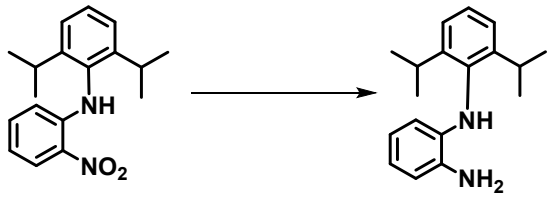


Figure S1. The synthetic routes of Pt(II) complexes **Pt 1, Pt 2** and **Pt 3**

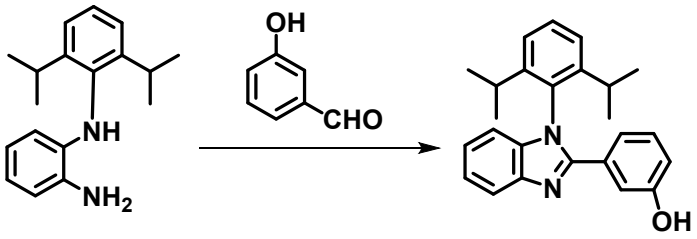


1-Bromo-2-nitrobenzene (6.4 g, 32 mmol), 2,6-diisopropylaniline (5.6 g, 32 mmol), Cs_2CO_3 (13 g, 40 mmol), $Pd_2(dba)_3$ (0.36 g, 0.4 mmol) and BINAP (0.66 g, 1mmol) were added into toluene (100 mL) under N_2. The reaction mixture was heated to reflux overnight before cooling to room temperature. The reaction mixture was washed with water. The aqueous phase was extracted with DCM (3×100 mL), and the combined organic phase was dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:1) to afford a yellow solid (8.7 g, 92%).^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.30 (s, 1H), 8.12 (d, J = 8.6 Hz, 1H), 7.40 (td, J = 7.9, 3.2 Hz, 2H), 7.30 (d, J = 7.6 Hz, 2H), 6.73 (t, J = 7.7 Hz, 1H), 6.26 (d, J = 8.6 Hz, 1H), 2.96 (m, J = 6.9 Hz, 2H), 1.14 (d, J = 6.8 Hz, 6H), 1.04 (d, J = 6.9 Hz, 6H). GC-MS: m/z calcd 298.40, found 298.17.

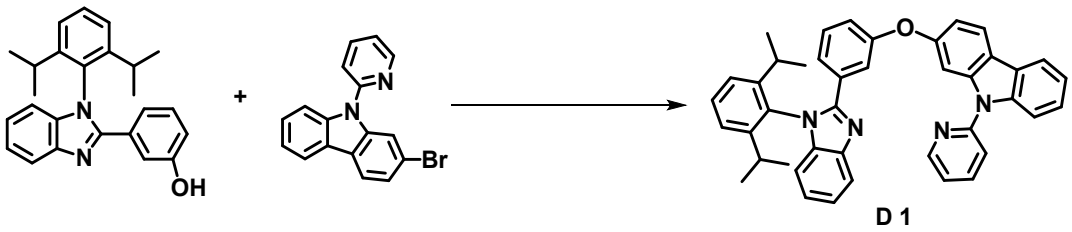


The $SnCl_2 \cdot H_2O$ (42.3 g, 0.19 mol), hydrochloric acid (40 mL) and anhydrous ethanol (30 mL) were added into a 125 mL round-bottom flask under N_2. The reaction mixture was heated to reflux for one hour, Then 2,6-diisopropyl-N-(2-nitrophenyl)aniline (7.1 g, 0.024 mol) was slowely added into this mixture, which was heated to reflux overnight. After cooling downing to room temperature, the reaction mixture was alkalified to pH = 8 with 2 M NaOH. The aqueous phase was extracted with DCM (3 × 100 mL), and the combined organic phase was dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:1) to afford a lavender solid (6 g, 85%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.20 (q, J = 5.6 Hz, 3H), 6.59 (d, J = 7.5 Hz, 1H), 6.41 (t, J = 7.4 Hz, 1H), 6.29 (t, J = 7.5 Hz, 1H), 5.95 (s, 1H), 5.77 (d, J = 7.8 Hz, 1H), 4.79 (s, 2H), 3.08 (m, J = 6.9 Hz, 2H), 1.06 (d, J

= 41.2 Hz, 12H). GC-MS: m/z calcd 268.22, found 268.19.



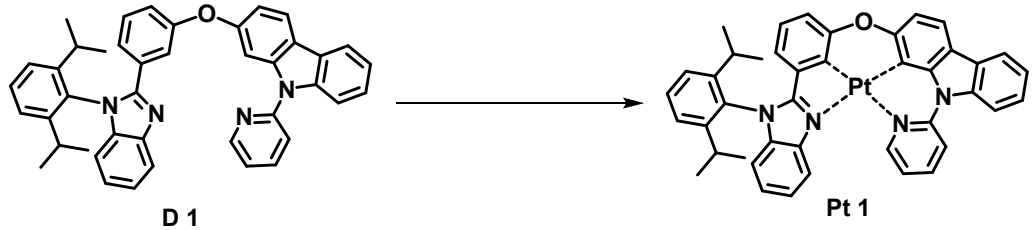
Cetyl pyridine bromide (CPB) (0.38 g, 1.0 mmol), N-(2,6-diisopropylphenyl)benzene-1,2-diamine (5.1 g, 19 mmol) and hydroxybenzaldehyde（5.3 g, 43 mmol） were dissolved in the mixture of THF (10 mL) and water (100 mL). The resulting solution was stirred at room temperature overnight. The reaction mixture was washed with water. The water phase was extracted with DCM (3 × 100 mL), and the combined organic phase was dried over $MgSO_4$. After the removal of solvent, the residue was dissolved in a small amount of toluene (50 mL), and then MnO_2 (8.9 g 0.1 mol) was added. The mixture was heated at 100 ^oC for 12 hours. The precipitate was removed by filtration. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:EA, 1:2) to afford an orange solid (2.8 g, 40%).^1H NMR (400 MHz, DMSO-*d6*) δ 9.62 (s, 1H), 7.79 (d, J = 7.9 Hz, 1H), 7.62 (t, J = 7.8 Hz, 1H), 7.45 (d, J = 7.8 Hz, 2H), 7.34 – 7.17 (m, 3H), 7.07 (t, J = 8.0 Hz, 1H), 6.91 – 6.73 (m, 3H), 0.93 (d, J = 5.8 Hz, 7H), 0.85 (d, J = 6.8 Hz, 5H). GC-MS: m/z calcd 268.22, found 268.19.



D 1

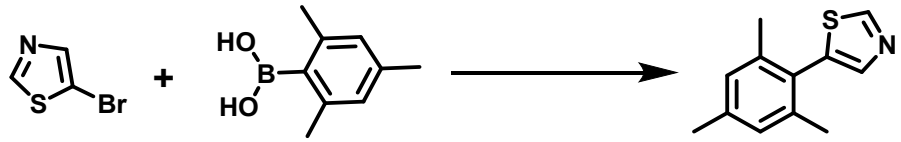
3-(1-(2,6-Diisopropylphenyl)-1H-benzimidazol-2-yl)phenol (2 g, 5.4 mmol), 2-bromo-9-(pyridin-2-yl)-9H-carbazole(1.9 g, 5.9 mmol), CuI (154 mg, 0.81 mmol), K_3PO_4 (2.7 g, 13.0 mmol) and picolinic acid (199 mg, 1.6 mmol) were added into dry DMSO (40 mL) under N_2. The reaction mixture was heated to reflux overnight before cooling to

room temperature. The solvent was removed by vacuum distillation, and the residue was washed with water. The aqueous phase was extracted with DCM (3 × 100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:2) to afford a brown solid (2.8 g, 40%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.72 (s, 1H), 8.31 (d, J = 7.8 Hz, 1H), 8.20 (d, J = 8.3 Hz, 1H), 8.10 (t, J = 7.9 Hz, 1H), 7.86 (dd, J = 23.6, 8.2 Hz, 2H), 7.71 (dd, J = 27.0, 8.0 Hz, 2H), 7.51 (t, J = 8.4 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.29 – 7.13 (m, 4H), 6.97 (d, J = 7.7 Hz, 2H), 6.82 (d, J = 8.1 Hz, 2H), 6.73 (d, J = 8.1 Hz, 1H), 6.66 (s, 1H), 1.96 (dd, J = 13.9, 7.2 Hz, 2H), 0.77 (d, J = 6.8 Hz, 6H), 0.56 (d, J = 6.8 Hz, 6H). MALDI-TOF (m/z): calculated for: 612.22, found: 612.29.

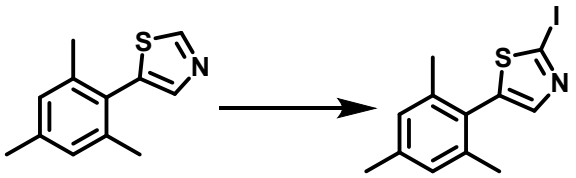


Ligand **D1** (700 mg, 1.14 mmol), K_2PtCl_4 (575 mg, 1.39 mmol) were added into a mixture of AcOH (18 mL) and chloroform (2 mL) under N_2. The reaction mixture was allowed to reflux for 4 days. After cooling to room temperature, the precipitate was collected by filtration. The crude product was purified by column chromatography (SiO_2, DCM:PE, 2:1) to afford a yellow solid (700 mg, 76%). ^{1}H NMR (600 MHz, DMSO-*d6*) δ 9.54 (dd, J = 5.9, 1.8 Hz, 1H), 8.30 – 8.20 (m, 2H), 8.13 (t, J = 8.5 Hz, 2H), 7.85 (d, J = 8.2 Hz, 1H), 7.74 (t, J = 7.9 Hz, 1H), 7.67 (d, J = 8.1 Hz, 1H), 7.58 (d, J = 7.9 Hz, 2H), 7.48 (ddd, J = 8.3, 7.2, 1.3 Hz, 1H), 7.44 – 7.34 (m, 4H), 7.15 (d, J = 8.2 Hz, 1H), 7.07 (d, J = 7.9 Hz, 1H), 7.02 (dd, J = 8.0, 1.0 Hz, 1H), 6.90 (t, J = 7.8 Hz, 1H), 6.20 (dd, J = 7.6, 1.1 Hz, 1H), 2.22 (s, 2H), 0.95 (s, 6H), 0.89 (s, 6H).^{13}C NMR (600 MHz, DMSO-*d6*) δ 154.22 , 152.42 , 152.00 , 148.66 , 146.71 , 140.89 , 139.10 , 138.41 , 137.32 , 136.81 , 132.00 , 130.06 , 128.40 , 125.90 , 124.99 , 124.85 , 124.49 ,

124.20 , 123.32 , 120.44 , 119.58 , 119.45 , 118.69 , 117.14 , 116.56 , 115.71 , 115.43 , 112.77 , 111.77 , 40.51 , 28.67 , 24.49 , 23.51 . MALDI-TOF (m/z): calculated for: 805.17, found 805.24. Anal. calcd for $C_{42}H_{34}N_4OPt$: C, 62.47; H, 4.34; N, 6.64; found: C, 62.60; H, 4.25; N, 6.95%.

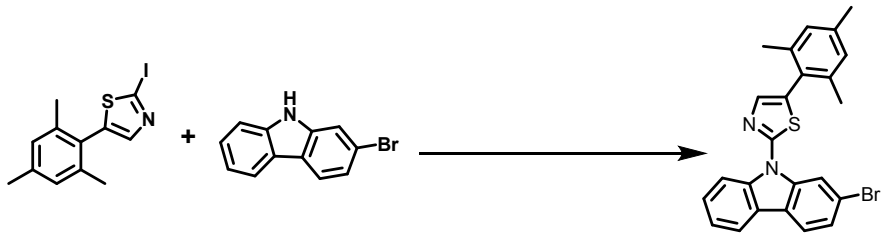


5-Bromothiazole (0.5 g, 3 mmol), mesitylboronic acid (0.55 g, 3.3 mmol), 1,1'-bis(diphenylphosphino)ferrocene-palladium(II) dichloride dichloromethane complex (124 mg, 0.15 mg) and Na_2CO_3 (0.65 g, 6 mmol) were added into the mixture of 2-MeTHF (50 mL) and water (10 mL). The reaction mixture was heated to reflux overnight before cooling to room temperature. The reaction mixture was washed with water. The aqueous phase was extracted with EA (3 × 100 mL), and the combined organic phase was dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM) to afford a white solid (0.41 g, 94.5%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 9.21 (s, 1H), 7.68 (s, 1H), 6.98 (s, 2H), 2.27 (s, 3H), 2.02 (s, 6H); MS EI (m/z): $[M]^+$calcd 203.08, found 203.10.

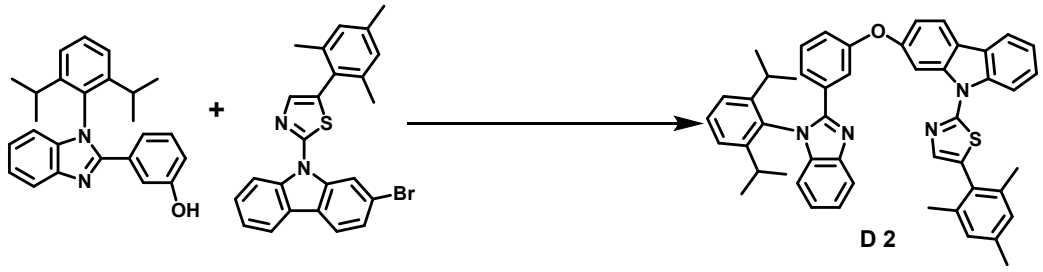


To a solution of 5-mesitylthiazole (1.5 g, 8 mmol) in dry THF (50 mL) at -78 ºC under N_2, lithium diisopropylamide (4.7 mL, 2 M in hexane, 9.5 mmol) was added slowly. The mixture was stirred for 2 hours before the addition of I_2 (3 g, 11.85 mmol). The resulting solution was stirred at room temperature overnight before quenched with $Na_2S_2O_3$ (10 mL). The product was extracted with diethyl ether. The organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM) to afford a white solid (1.7 g,

57%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 7.47 (s, 1H), 7.01 (s, 2H), 2.30 (s, 3H), 2.08 (s, 6H); GC-MS: m/z calcd 328.95, found 328.96.

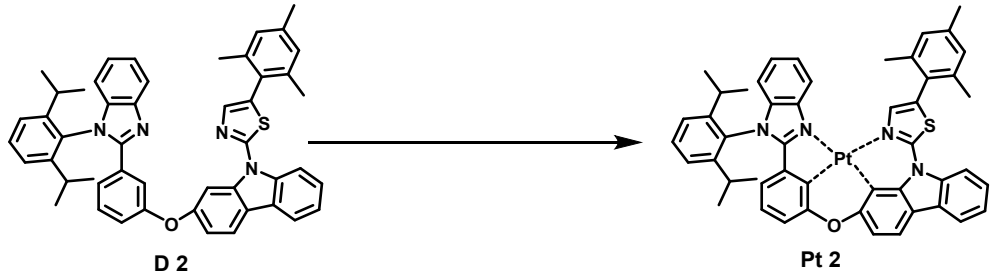


2-Bromo-9H-carbazole (0.62 g, 2.5 mmol), 2-iodo-5-mesitylthiazole (1 g, 3 mmol), CuI (240 mg, 1.2 mmol), 1,10-phenanthroline monohydrate (453 mg, 2.5 mmol) and Na_2CO_3 (0.7 g, 5 mmol) were added into dry DMF(100 mL). The reaction mixture was heated to reflux for 2 days before cooling to room temperature. The reaction mixture was washed with water. The aqueous phase was extracted with EA (3 × 100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:1) to afford a white solid (0.8 g, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 1.7 Hz, 1H), 8.22 (d, J = 8.4 Hz, 1H), 8.08 (d, J = 7.7 Hz, 1H), 7.95 (d, J = 8.3 Hz, 1H), 7.60 – 7.45 (m, 3H), 7.41 (d, J = 7.5 Hz, 1H), 7.01 (s, 2H), 2.36 (s, 3H), 2.26 (s, 6H); GC-MS: m/z calcd 446.05, found 446.07.



3-(1-(2,6-Diisopropylphenyl)-1H-benzimidazol-2-yl)phenol (0.6 g, 1.62 mmol), 2-(2-bromo-9H-carbazol-9-yl)-5-mesitylthiazole (1.09 g, 2.44 mmol), CuI (46 mg, 0.24 mmol), K_3PO_4 (0.83 g, 3.92 mmol), picolinic acid（59 mg, 0.48 mmol）were added into dry DMSO under N_2, The reaction mixture was heated to reflux overnight before cooling to room temperature. The solvent was removed by vacuum distillation, and the

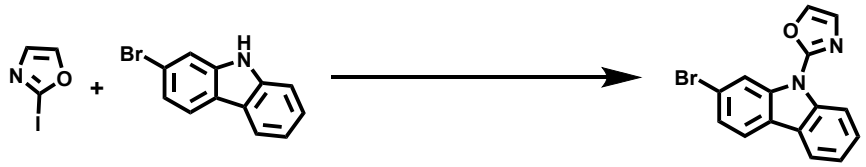
residue was washed with water. The aqueous phase was extracted with DCM (3 × 100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:2) to afford a brown solid (0.72 g, 48%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.35 (dd, J = 16.9, 8.0 Hz, 2H), 8.24 (d, J = 8.3 Hz, 1H), 7.81 – 7.72 (m, 3H), 7.63 (d, J = 10.4 Hz, 2H), 7.50 (dt, J = 15.7, 7.8 Hz, 2H), 7.26 (t, J = 7.6 Hz, 2H), 7.17 (t, J = 7.6 Hz, 1H), 7.01 (s, 2H), 6.91 (d, J = 7.6 Hz, 3H), 6.80 (t, J = 7.7 Hz, 1H), 6.72 (d, J = 8.1 Hz, 1H), 6.64 (s, 1H), 2.28 (s, 3H), 2.17 (s, 6H), 1.98 (d, J = 5.2 Hz, 2H), 0.76 (d, J = 6.8 Hz, 6H), 0.65 (d, J = 6.9 Hz, 6H); MALDI-TOF (m/z): calculated for: 736.45, found: 736.32.



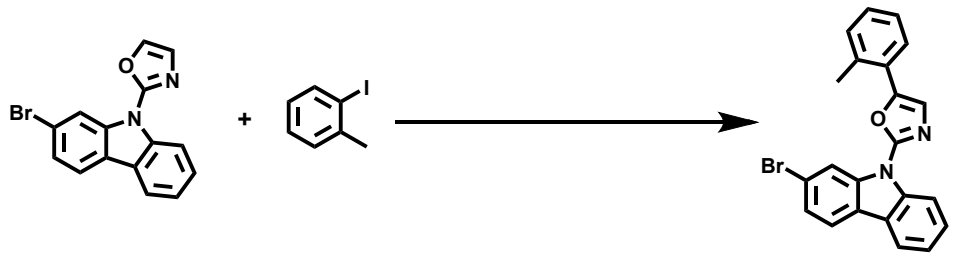
D 2 Pt 2

Ligand **D2** (700 mg, 0.75 mmol), K_2PtCl_4 (375 mg, 0.90 mmol) were added into a mixture of AcOH (18 mL) and chloroform (2 mL) under N_2. The reaction mixture was allowed to reflux for 4 days. After cooling to room temperature, the precipitate was collected by filtration. The crude product was purified by column chromatography (SiO_2, DCM:PE, 2:1) to afford a yellow solid(250 mg, 36%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 (d, J = 8.1 Hz, 1H), 8.09 (dd, J = 7.4, 1.3 Hz, 1H), 8.05 (s, 1H), 7.91 (d, J = 8.1 Hz, 1H), 7.87 (d, J = 8.2 Hz, 1H), 7.66 (t, J = 7.9 Hz, 1H), 7.49 (td, J = 7.7, 1.4 Hz, 1H), 7.46 (d, J = 7.9 Hz, 3H), 7.41 (d, J = 8.2 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.25 – 7.21 (m, 1H), 7.18 – 7.15 (m, 1H), 7.00 – 6.95 (m, 3H), 6.90 (t, J = 7.8 Hz, 1H), 6.35 – 6.31 (m, 1H), 2.36 (s, 6H), 2.32 (s, 3H), 1.56 (s, 2H), 0.97 (dd, J = 9.6, 6.8 Hz, 12H). ^{13}C NMR (600 MHz, $CDCl_3$) δ 163.03 , 156.74 , 153.57 , 151.57 , 147.18 , 141.61 , 140.66 , 139.63 , 139.57 , 139.21 , 137.80 , 137.32 , 136.54 , 131.01 , 130.41 , 128.51 ,

128.45 , 125.56 , 125.13 , 124.98 , 124.95 , 124.35 , 124.00 , 123.58 , 123.53 , 123.24 , 119.88 , 119.78 , 118.90 , 117.14 , 115.70 , 115.57 , 113.62 , 112.67 , 111.22 , 28.47 , 24.43 , 23.55 , 21.11 , 20.75. MALDI-TOF (m/z): calculated for: 929.65, found 929.27. Anal. calcd for $C_{49}H_{42}N_4OPtS$: C, 63.51; H, 4.82; N, 5.79; found: C, 63.28; H, 4.55; N, 6.02%.

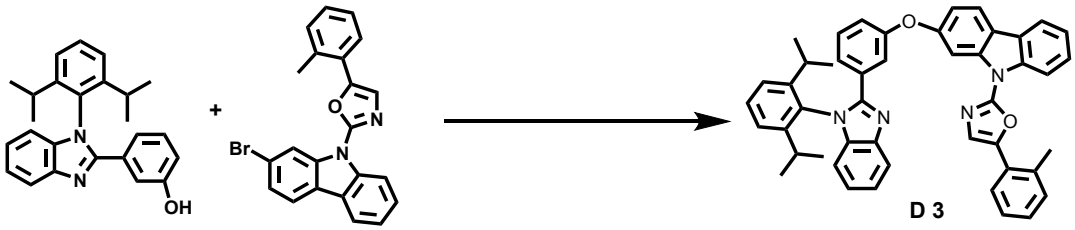


2-Bromo-9H-carbazole(5.67 g, 23 mmol), 2-iodooxazole (5.4 g, 27.7 mmol), CuI (2.18 g, 11.5 mmol), 1,10-phenanthroline monohydrate (4.15 g, 23 mmol) and Na_2CO_3 (6.36 g, 46 mmol) were added into dry DMF (100 mL) under N_2. The reaction mixture was heated to reflux for 2 days before cooling to room temperature. The reaction mixture was washed with water. The aqueous phase was extracted with EA (3 × 100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:1) to afford a white solid (6.5 g, 91.5%). ^{1}H NMR (400 MHz, DMSO-*d6*) δ 8.60 (s, 1H), 8.37 (d, J = 8.3 Hz, 1H), 8.29 (d, J = 7.6 Hz, 1H), 8.25 (d, J = 8.6 Hz, 2H), 7.67 – 7.61 (m, 2H), 7.47 (d, J = 5.8 Hz, 2H). GC-MS: m/z calcd 311.99, found 311.99.



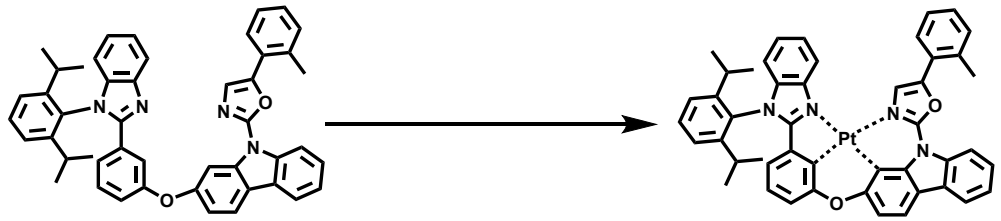
2-(2-Bromo-9H-carbazol-9-yl)oxazole (1g, 3.2 mmol), 1-iodo-2-methylbenzene (0.84 g, 3.85 mmol), 1,1'-bis(diphenylphosphino)ferrocene-palladium(II)dichloride dichloromethane complex (131 mg, 0.16 mmol) and Ag_2CO_3 (1.76 g, 6.4 mmol) were added into water (50 mL). The reaction mixture was heated to 60°C for 24 hours before

cooling to room temperature. The reaction mixture was washed with water. The aqueous phase was extracted with EA (3 × 100 mL), and the combined organic phase was dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:2) to afford a white solid (0.41 g, 94.5%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (s, 1H), 8.45 (d, J = 8.4 Hz, 1H), 8.05 (d, J = 7.8 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 7.7 Hz, 1H), 7.59 (t, J = 7.8 Hz, 1H), 7.52 (d, J = 8.2 Hz, 1H), 7.45 – 7.38 (m, 2H), 7.34 (d, J = 5.6 Hz, 3H), 2.58 (s, 3H). GC-MS: m/z calcd 402.04, found 402.04.



3-(1-(2,6-Diisopropylphenyl)-1H-benzimidazol-2-yl)phenol (0.7 g, 1.90 mmol）, 2-(2-bromo-9H-carbazol-9-yl)-5-(o-tolyl)oxazole (0.5 g, 1.24 mmol), CuI (35 mg, 0.18 mmol), K_3PO_4 (0.63 g, 2.97 mmol), picolinic acid (46 mg, 0.37 mmol) was added into dry DMSO under N_2. The reaction mixture was heated to reflux overnight before cooling to room temperature. After the removal of the solvent, the residue was washed with water. The aqueous phase was extracted with DCM (3 × 100 mL), and the combined organic phase was washed with water and dried over $MgSO_4$. After the removal of solvent, the residue was purified by column chromatography (SiO_2, DCM:PE, 1:2) to afford a brown solid (0.75 g, 76%). ^{1}H NMR (600 MHz, DMSO-*d6*) δ 8.49 (d, J = 8.3 Hz, 1H), 8.31 (d, J = 7.8 Hz, 1H), 8.22 (d, J = 8.4 Hz, 1H), 7.79 – 7.68 (m, 3H), 7.70 – 7.57 (m, 2H), 7.61 (s, 1H), 7.52 – 7.46 (m, 2H), 7.35 – 7.19 (m, 5H), 7.14 (ddd, J = 8.1, 7.1, 1.1 Hz, 1H), 6.98 (dd, J = 8.4, 2.2 Hz, 1H), 6.91 – 6.82 (m, 3H), 6.73 – 6.67 (m, 2H), 1.94 (m, J = 6.8 Hz, 2H), 0.71 (d, J = 6.8 Hz, 6H), 0.59 (d, J = 6.9 Hz, 6H) .^{13}C NMR (600MHz, DMSO-*d6*) δ 158.27 , 150.75 , 145.98 , 142.43 , 137.93 , 137.85 , 134.66 , 131.70 , 131.44 , 130.96 ,130.31 , 128.69 , 127.56 , 126.92 ,

126.70 , 126.16 , 125.52 , 124.72 , 123.99 , 123.70 , 123.28 ,122.58 , 121.53 , 120.82 , 120.61 , 119.90 , 116.29 , 115.84 , 114.22 , 110.85 , 105.54 , 40.50 , 28.19 , 24.59 , 22.80 , 21.97 . MALDI-TOF (m/z): calculated for: 692.47, found: 692.32.



D 3 Pt 3

Ligand **D3** (640 mg, 0.72 mmol), K_2PtCl_4 (360 mg, 0.87 mmol) were added into a mixture of AcOH (18 mL) and chloroform (2 mL) under N_2. The reaction mixture was allowed to reflux for 4 days. After cooling to room temperature, the precipitate was collected by filtration. The crude product was purified by column chromatography (SiO_2, DCM:PE, 1:2) to afford a yellow solid (150 mg, 24%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.37 (d, J = 8.2 Hz, 1H), 8.14 – 8.04 (m, 3H), 7.93 (d, J = 7.8 Hz, 1H), 7.89 (d, J = 8.2 Hz, 1H), 7.67 (t, J = 7.9 Hz, 1H), 7.58 – 7.53 (m, 1H), 7.49 – 7.34 (m, 8H), 7.29 (t, J = 7.6 Hz, 1H), 7.15 (d, J = 7.9 Hz, 1H), 7.02 (d, J = 8.0 Hz, 1H), 6.90 (t, J = 7.7 Hz, 1H), 6.34 (d, J = 7.5 Hz, 1H), 2.60 (s, 3H), 2.42 (p, J = 6.8 Hz, 2H), 0.99 (dd, J = 15.7, 6.8 Hz, 12H). ^{13}C NMR (600 MHz, $CDCl_3$) δ 153.77 , 151.08 , 147.18 , 137.45 , 136.36 , 135.72 , 134.87 , 131.44 , 131.04 , 130.54 , 128.97 , 127.65 , 127.47 , 126.70 , 126.38 , 125.99 , 125.20 , 124.90 , 123.83 , 123.68 , 123.62 , 123.35 , 119.72 , 119.68 , 118.89 , 117.09 , 116.06 , 113.86 , 113.84 , 111.39 , 28.49 , 24.45 , 23.60 , 22.25. MALDI-TOF (m/z): calculated for: 885.24, found: 885.26. Anal. calcd for $C_{47}H_{38}N_4O_2Pt$: C, 63.48; H, 4.50; N, 6.23; found: C, 63.72; H, 4.32; N, 6.32%.

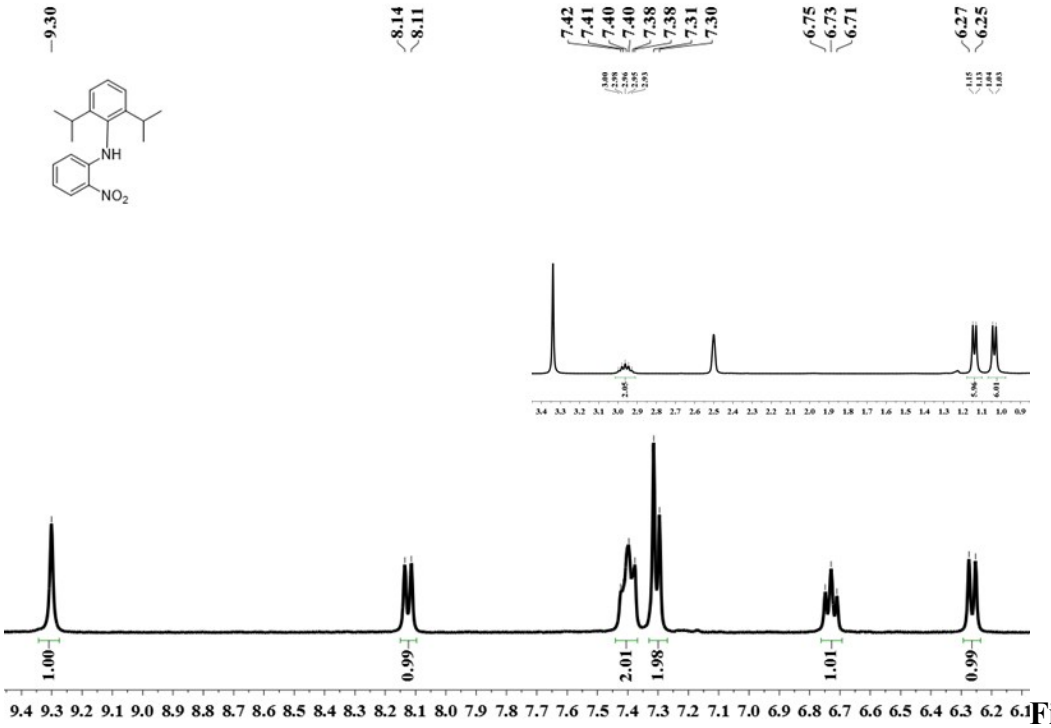


Figure S2. [1]H NMR spectrum of ligand of 2,6-diisopropyl-N-(2-nitrophenyl)aniline (DMSO-*d6*).

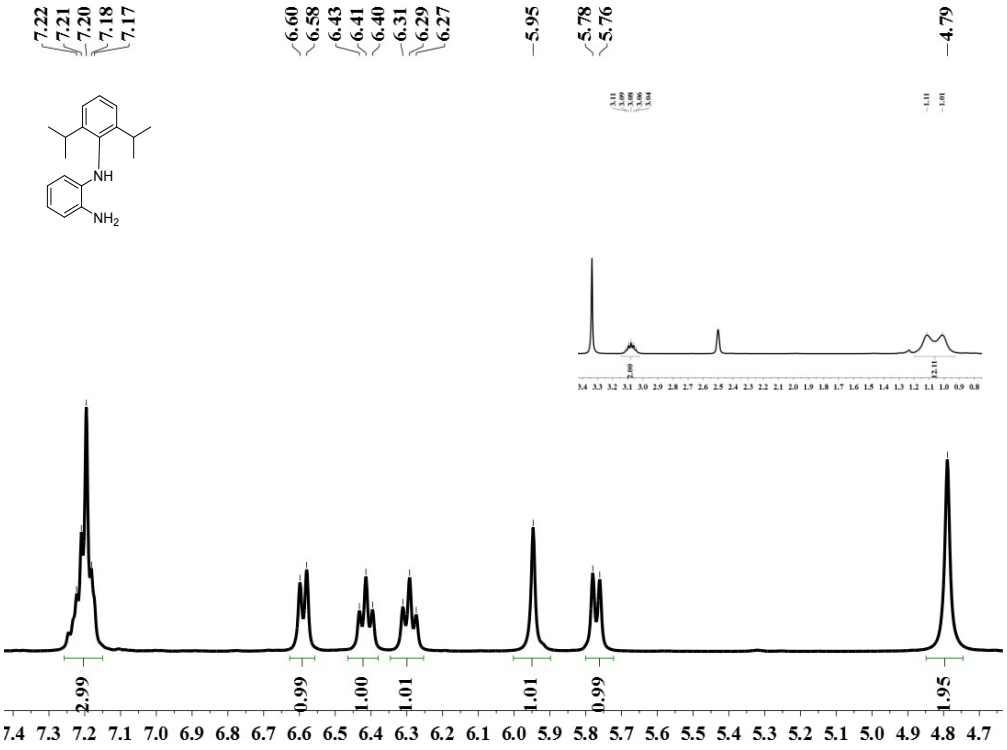


Figure S3. [1]H NMR spectrum of ligand of N1-(2,6-diisopropylphenyl)benzene-1,2-diamine (DMSO-*d6*).

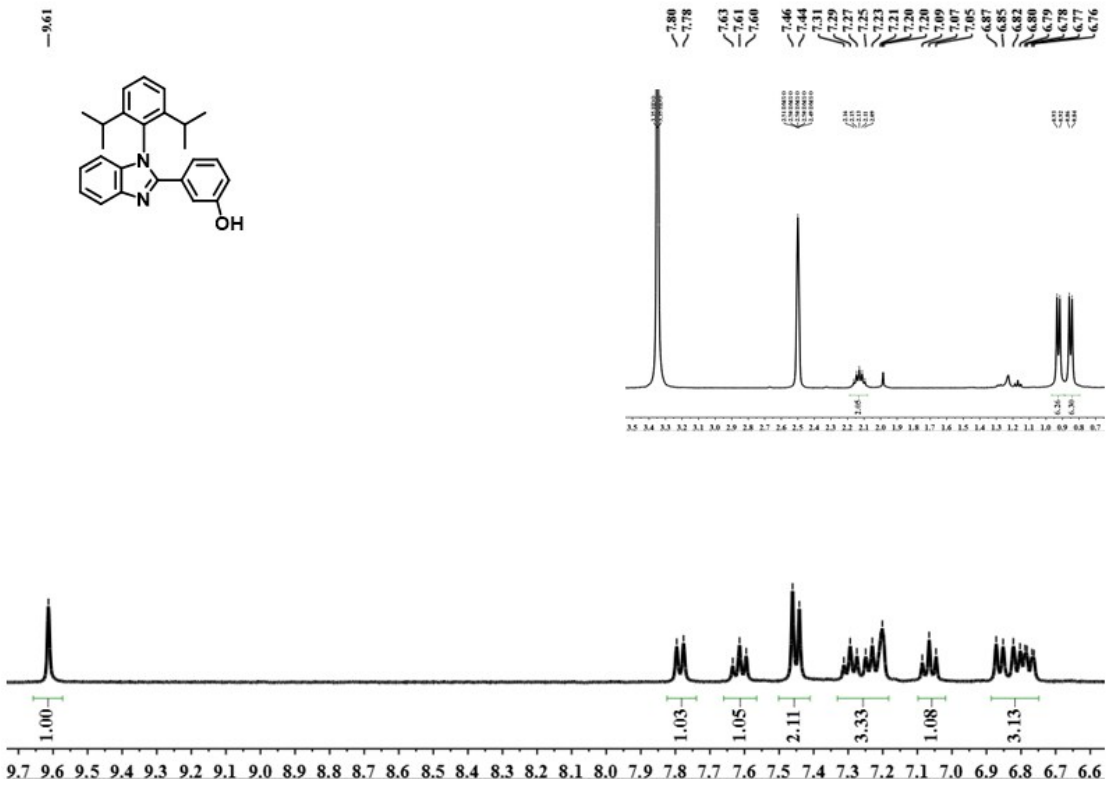


Figure S4. ^{1}H NMR spectrum of ligand of 3-(1-(2,6-diisopropylphenyl)-1H-benzo[d]imidazol-2-yl)phenol (DMSO-*d6*).

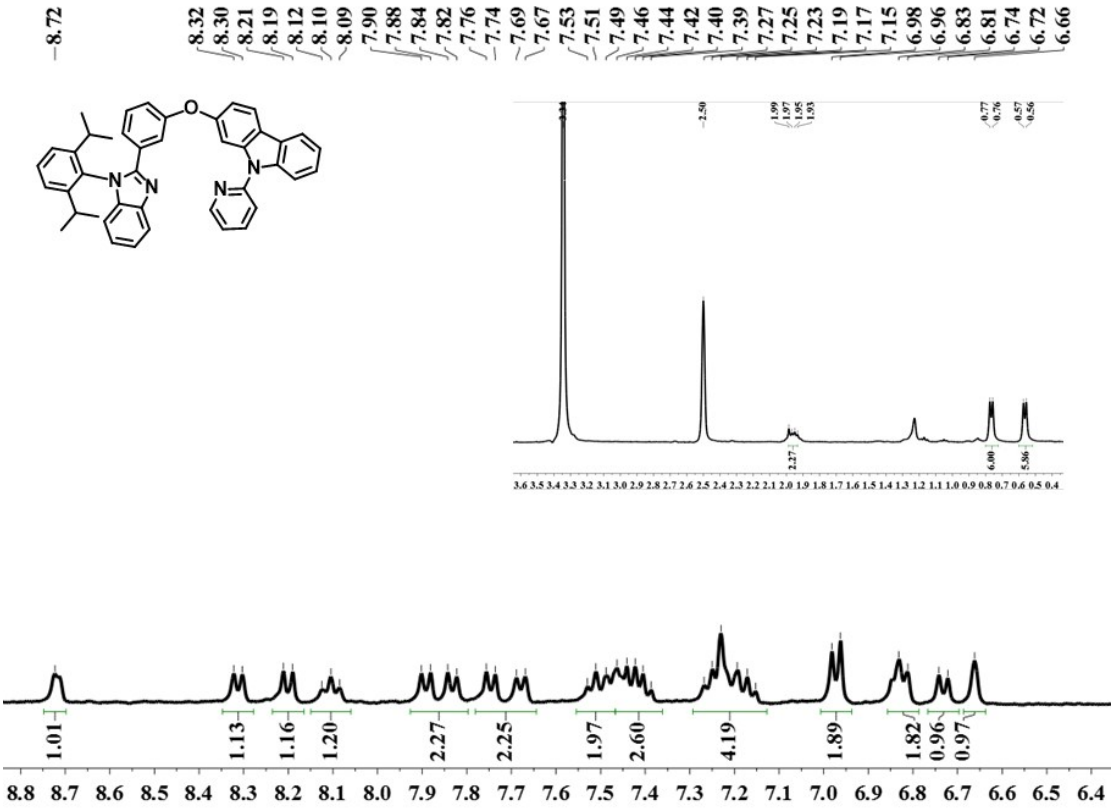


Figure S5. ^{1}H NMR spectrum of ligand of **D 1** (DMSO-*d6*).

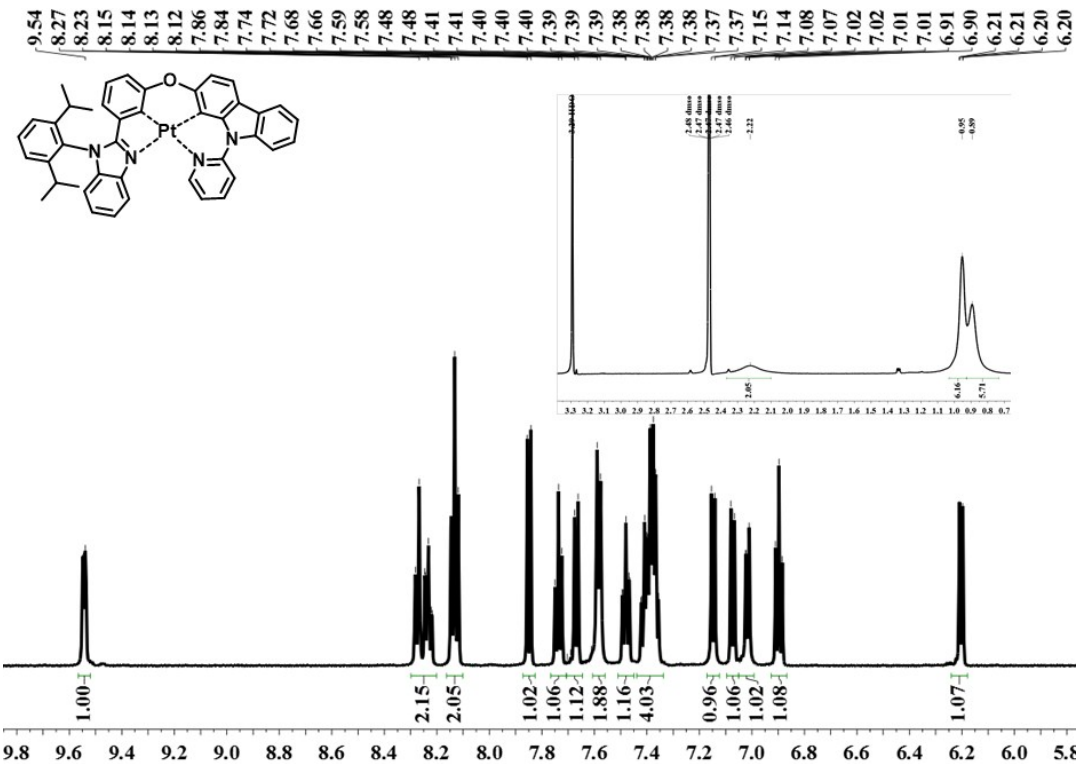


Figure S6. ^{1}H NMR spectrum of complex of **Pt 1** (DMSO-*d6*).

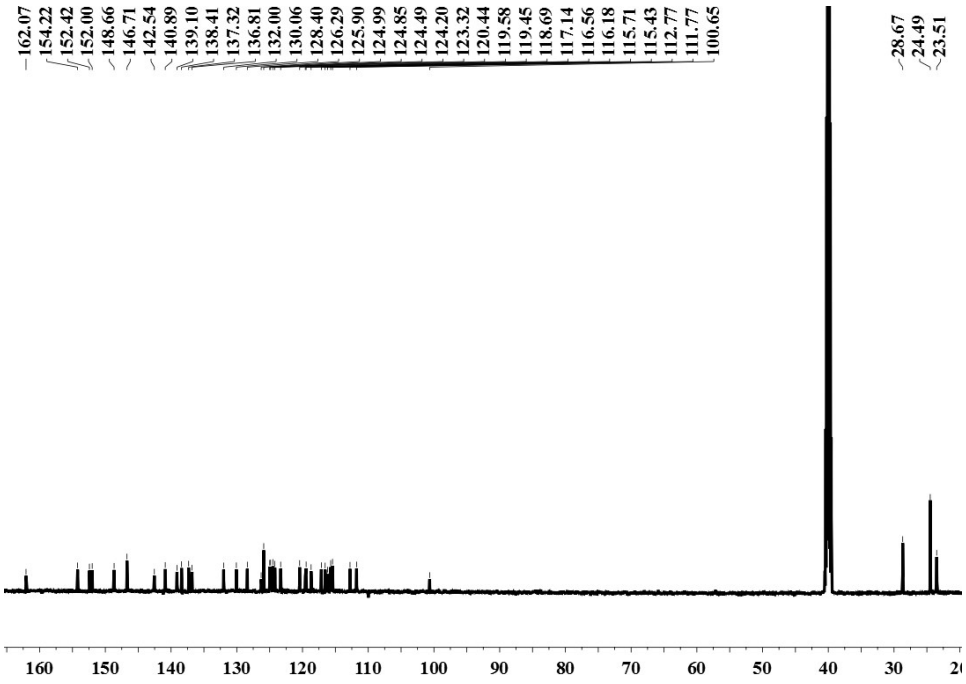


Figure S7. ^{13}C NMR spectrum of complex of **Pt 1** (DMSO-*d6*).

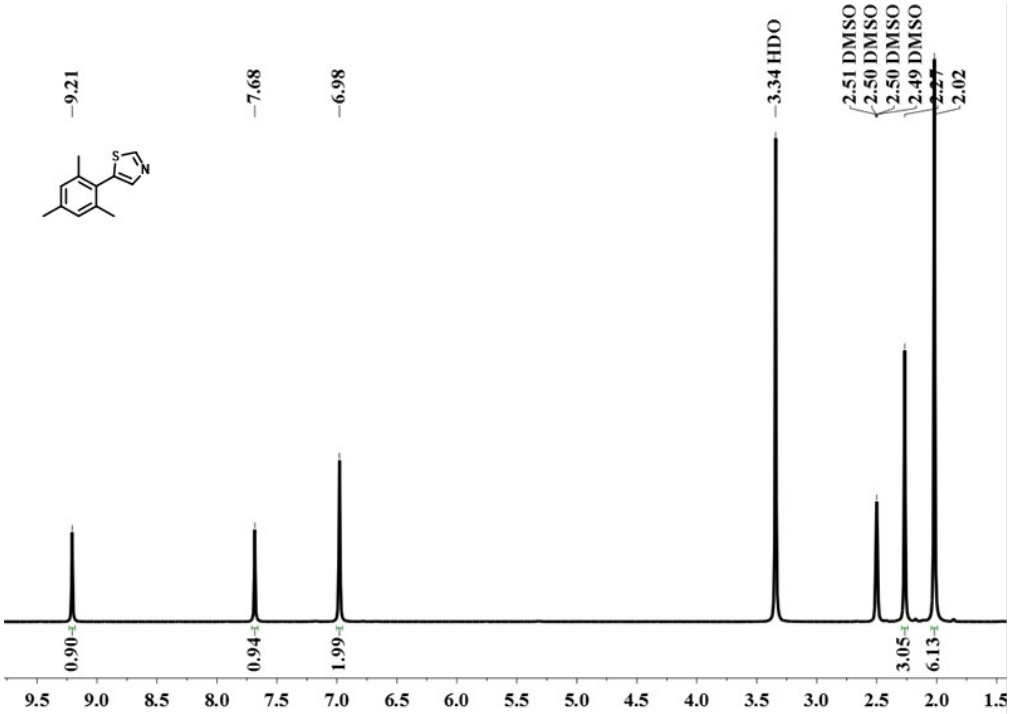


Figure S8. ^{1}H NMR spectrum of ligand of 5-mesitylthiazole (DMSO-*d6*).

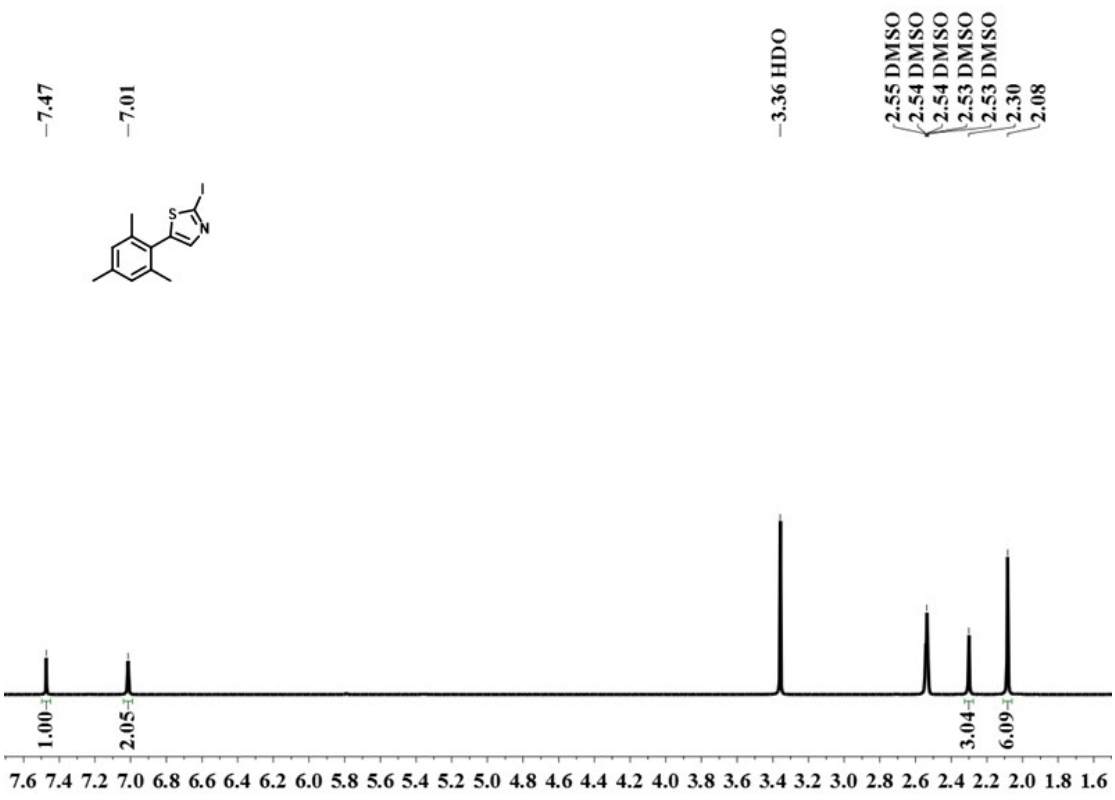


Figure S9. ^{1}H NMR spectrum of ligand of 2-iodo-5-mesitylthiazole (DMSO-*d6*).

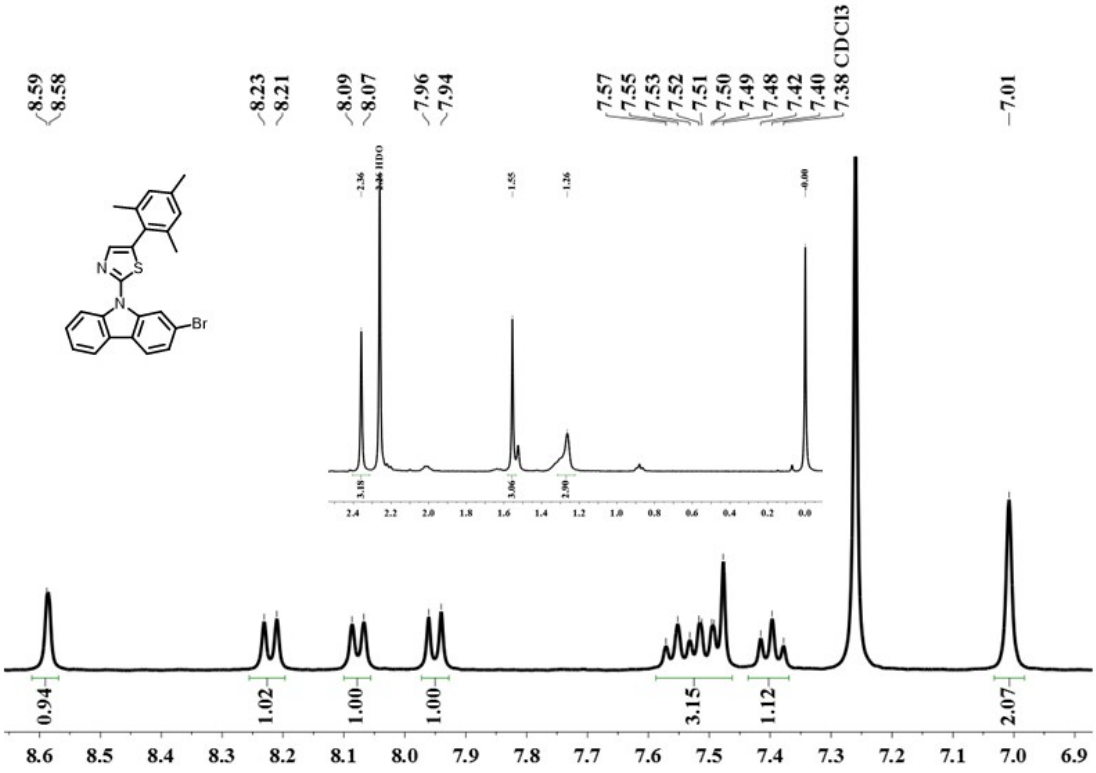


Figure S10. ^{1}H NMR spectrum of ligand of 2-(2-bromo-9H-carbazol-9-yl)-5-mesitylthiazole ($CDCl_3$).

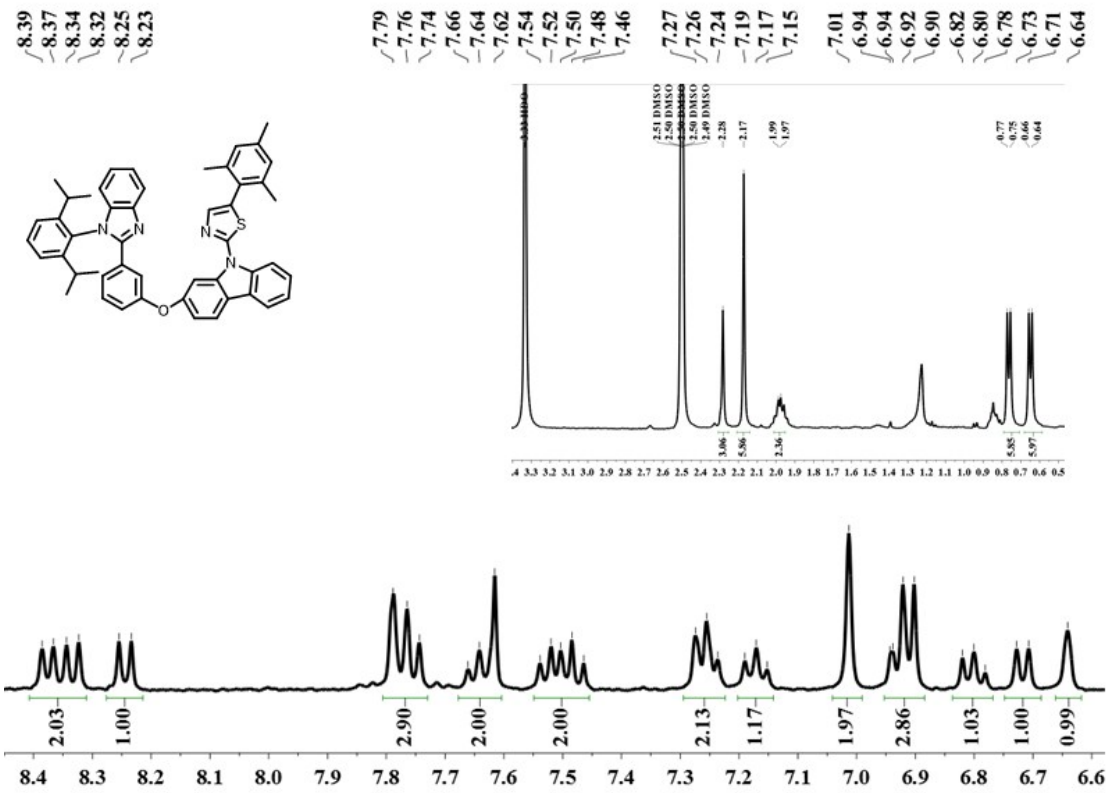


Figure S11. ^{1}H NMR spectrum of ligand of **D 2** (DMSO-*d6*).

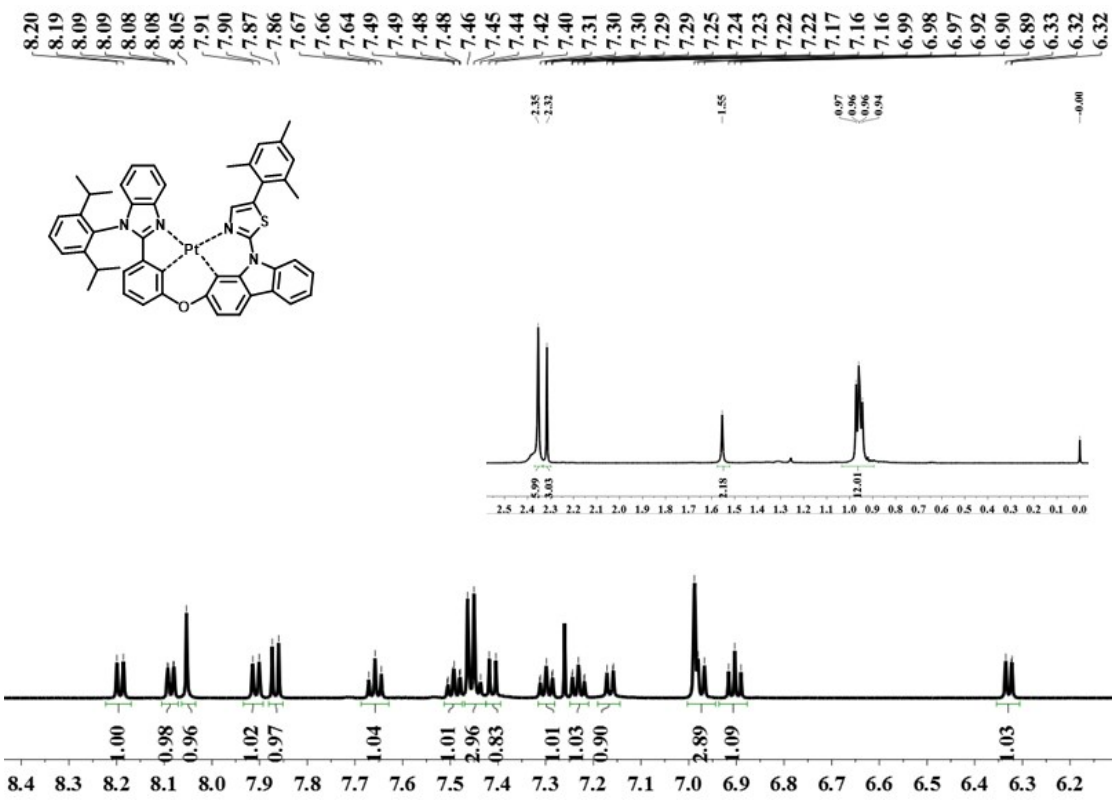


Figure S12. ^{1}H NMR spectrum of complex of **Pt 2** ($CDCl_3$).

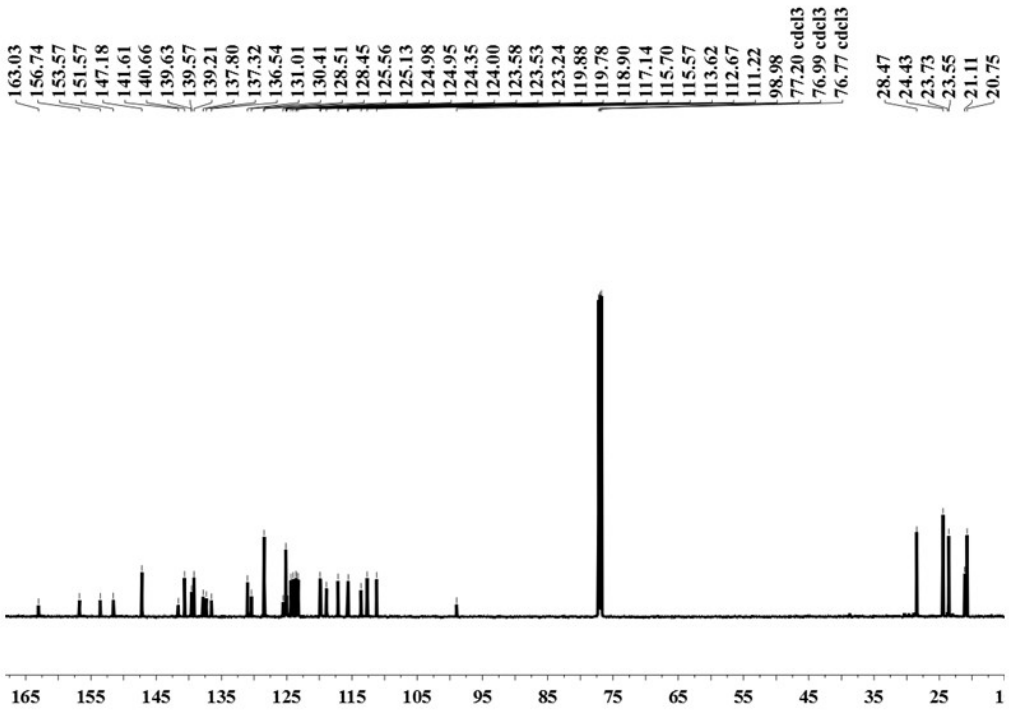


Figure S13. ^{13}C NMR spectrum of complex of **Pt 2** ($CDCl_3$).

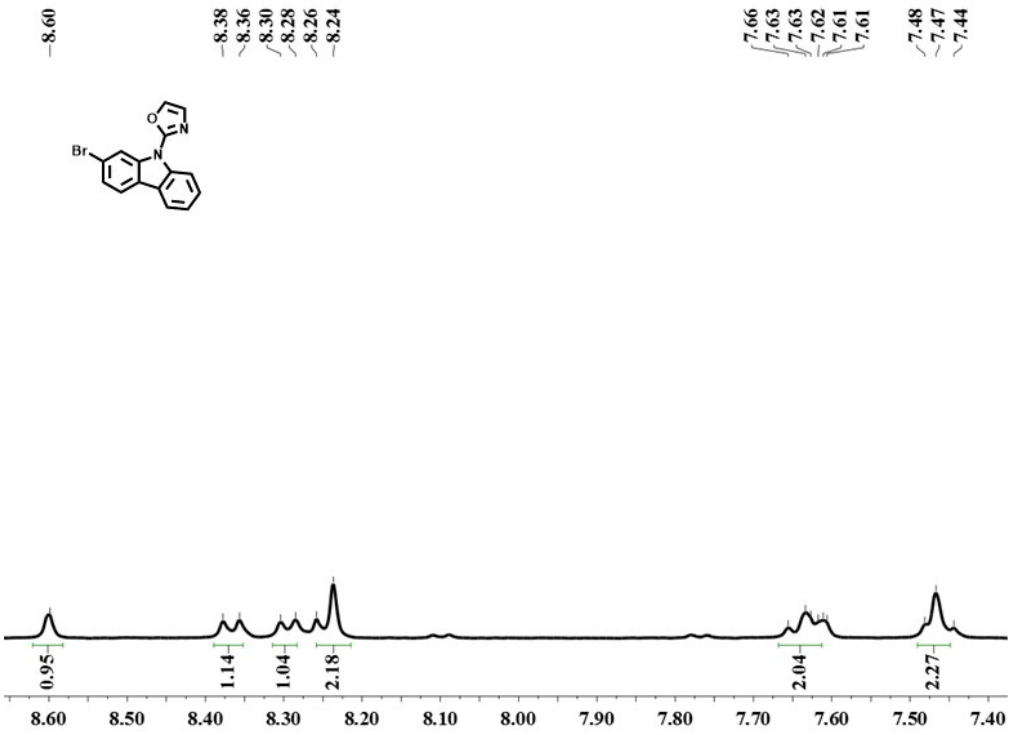


Figure S14.[1]H NMR spectrum of ligand of 2-(2-bromo-9H-carbazol-9-yl)oxazole (DMSO-*d6*).

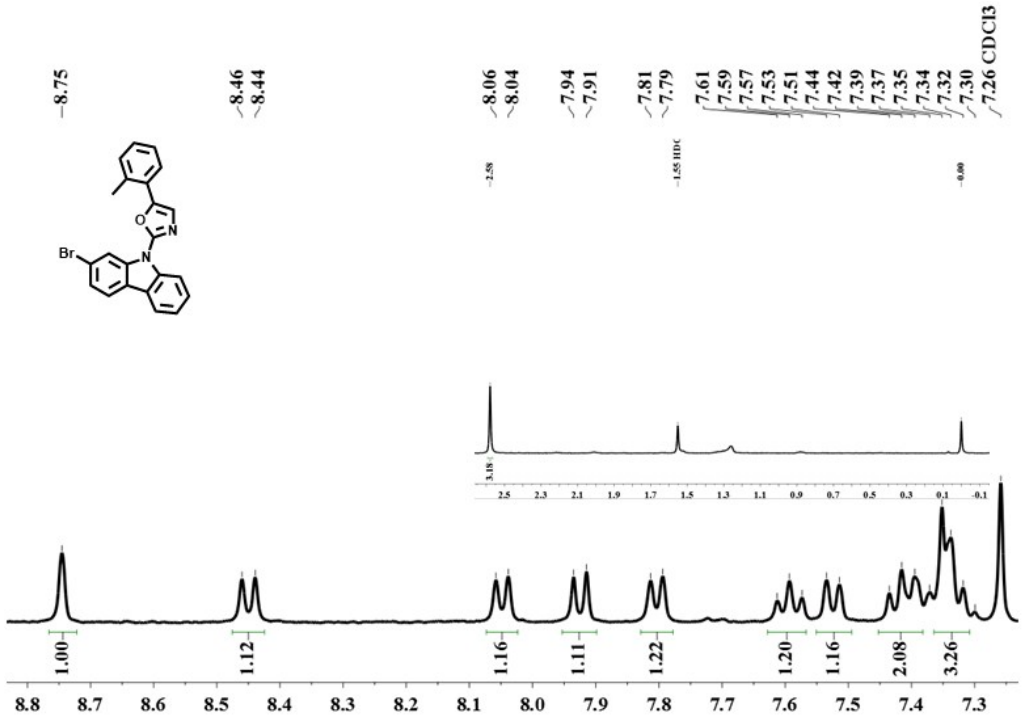


Figure S15. [1]H NMR spectrum of ligand of 2-(2-bromo-9H-carbazol-9-yl)-5-(o-tolyl)oxazole ($CDCl_3$).

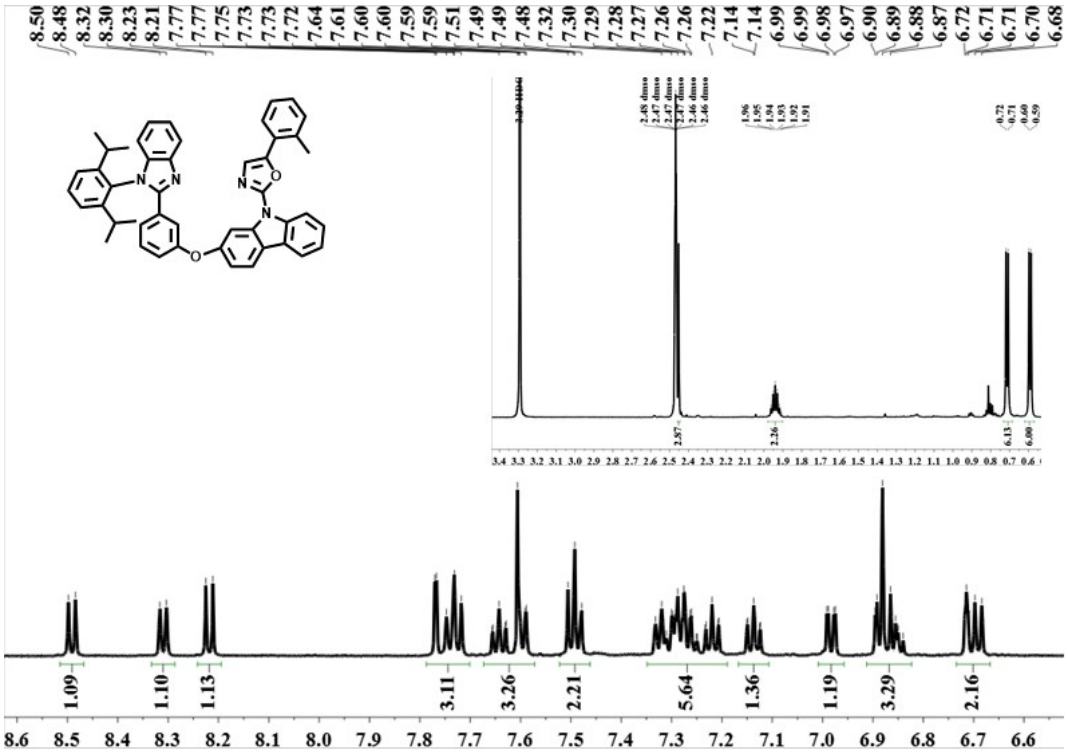


Figure S16.[1]H NMR spectrum of ligand of **D 3** (DMSO-*d6*).

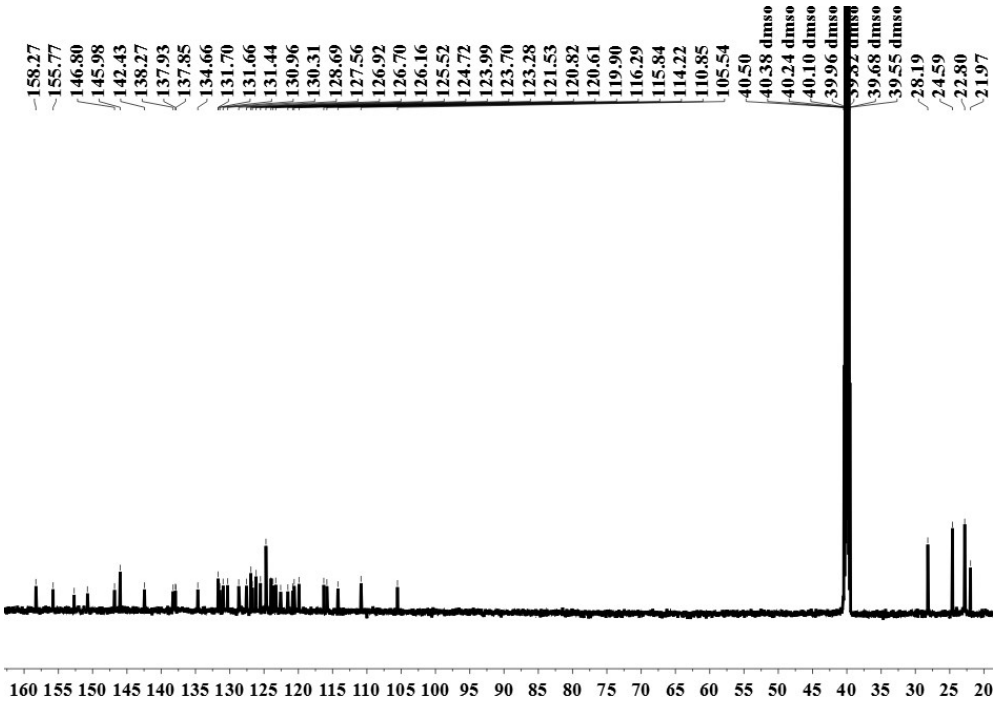


Figure S17. [13]C NMR spectrum of complex of **D 3** (DMSO-*d6*).

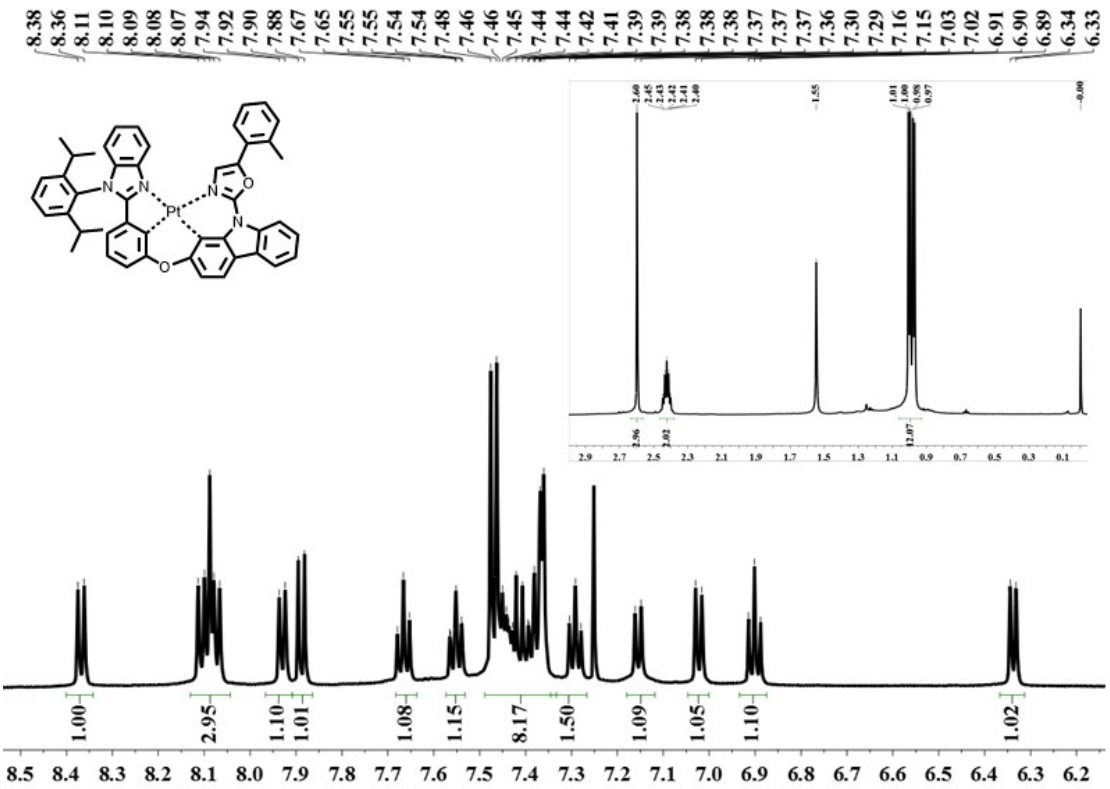


Figure S18. ^{1}H NMR spectrum of complex of **Pt 3** ($CDCl_3$).

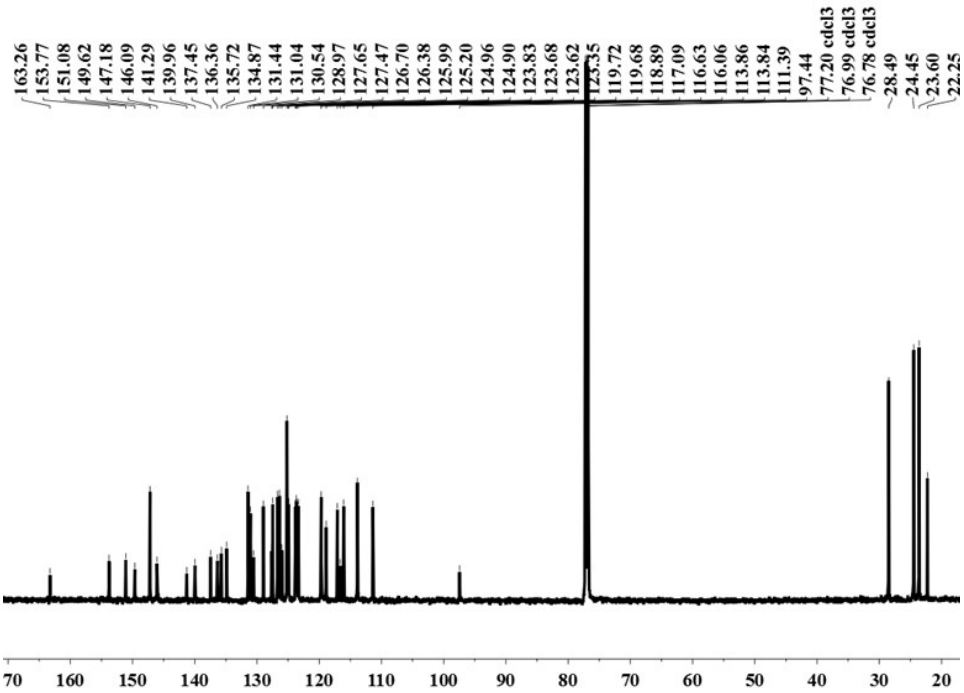


Figure S19. ^{13}C NMR spectrum of complex of **Pt 3** ($CDCl_3$).

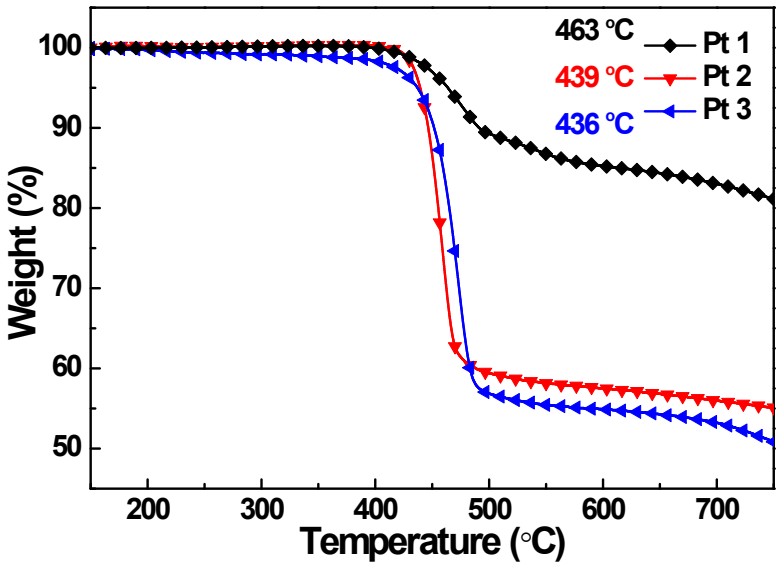


Figure S20. TGA curves of **Pt 1**, **Pt 2** and **Pt 3**.

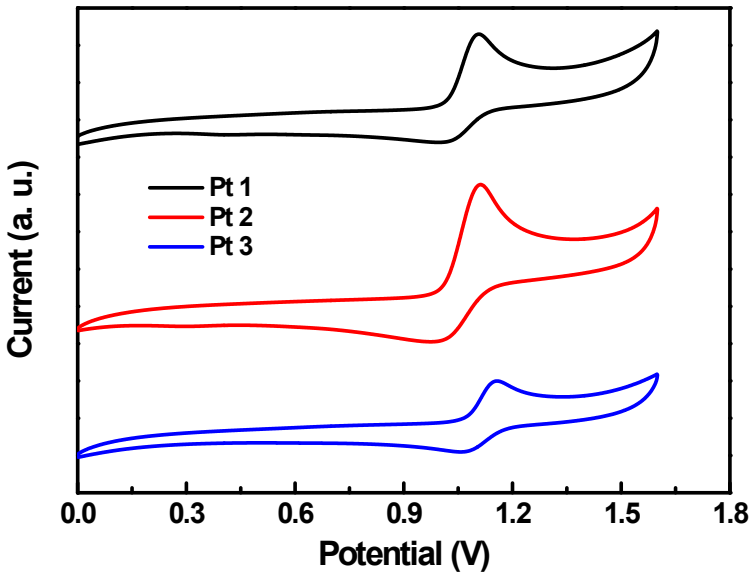


Figure S21. Cyclic voltammograms of Pt(II) complexes in DCM.

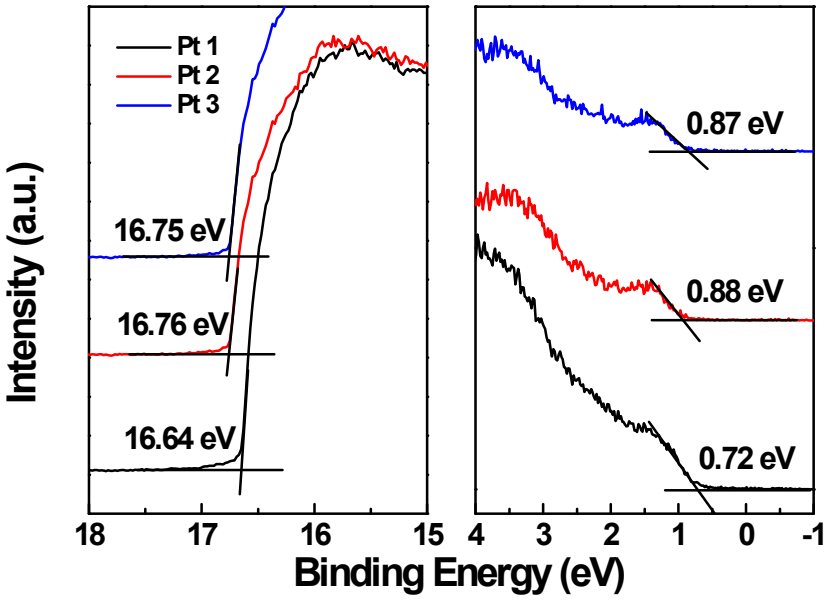


Figure S22. UPS spectra of **Pt 1**, **Pt 2** and **Pt 3**.

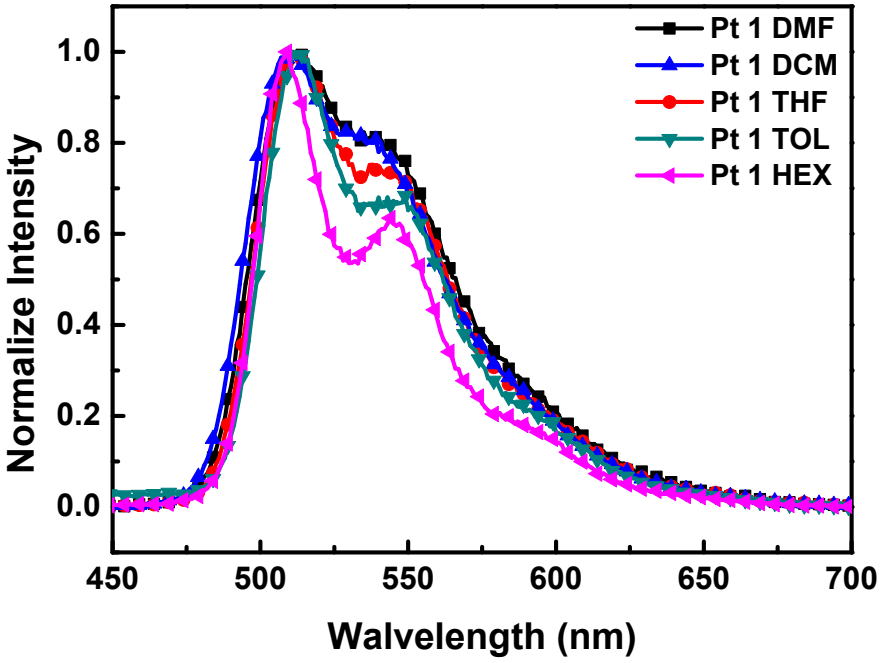


Figure S23. Photoluminescence spectra of diluted **Pt 1** in different polarity media.

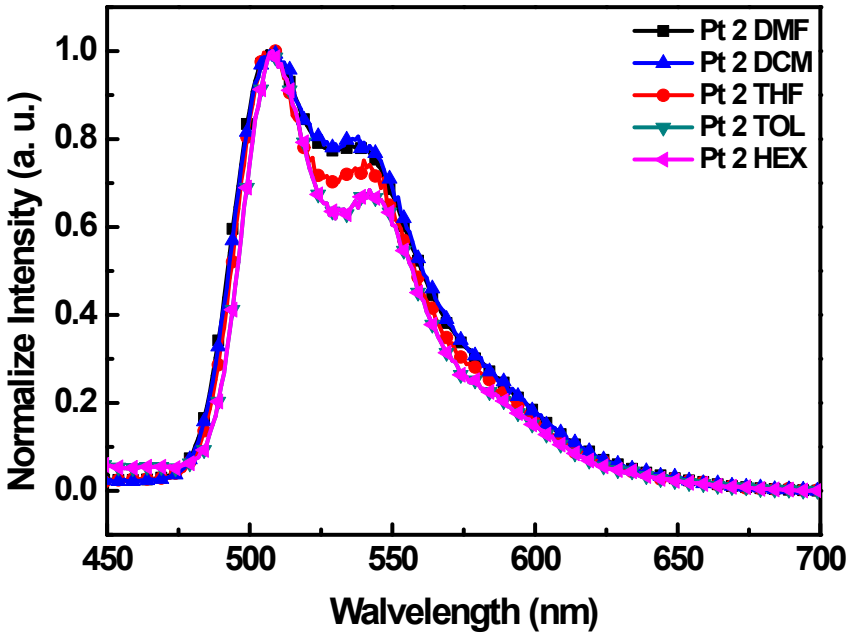


Figure S24. Photoluminescence spectra of diluted **Pt 2** in different polarity media.

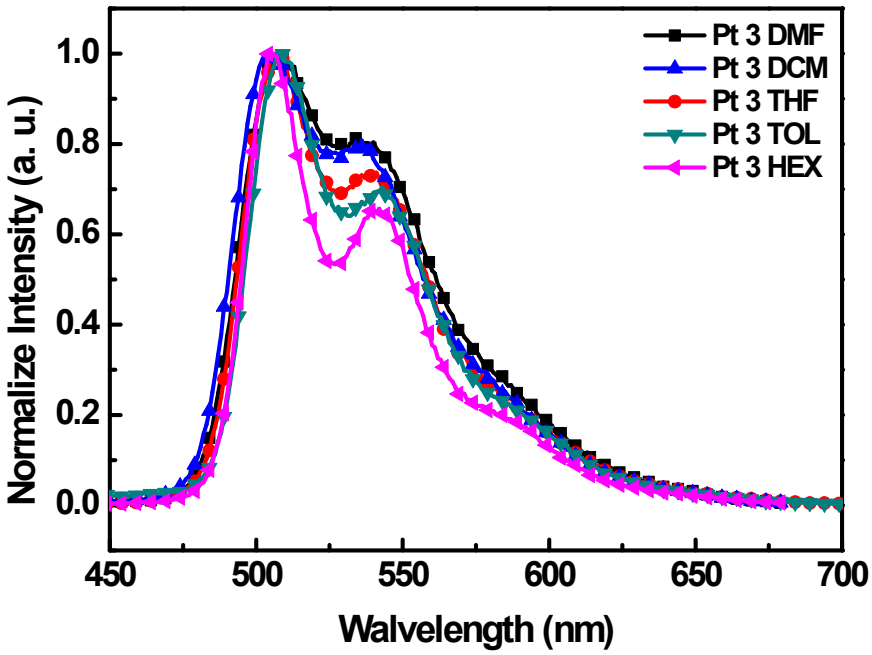


Figure S25. Photoluminescence spectra of diluted **Pt 3** in different polarity media.

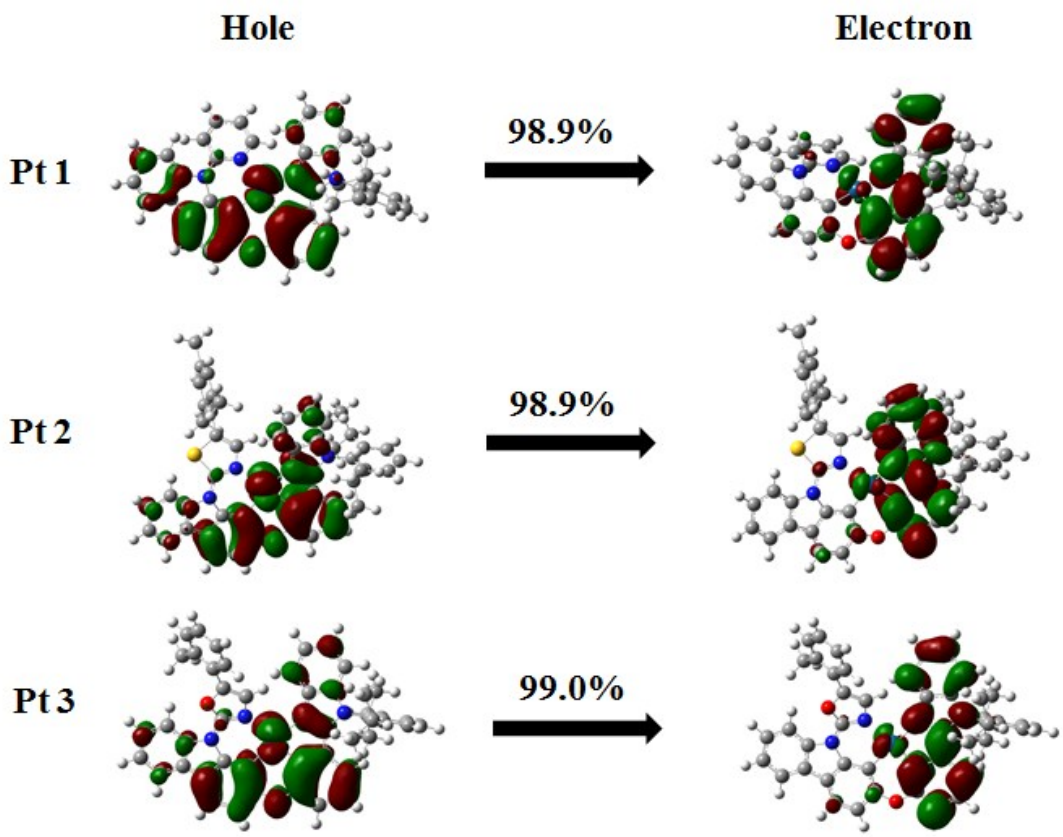


Figure S26. Natural Transition Orbitals (NTO) analyses for triplet emission of compounds **Pt 1**, **Pt 2** and **Pt 3**.

Table S1. Density functional theory (DFT) calculations for complexes **Pt 1**, **Pt 2**, and **Pt 3**.

	Pt 1	**Pt 2**	**Pt 3**
HOMO (eV)	-4.70	-4.73	-4.73
LUMO (eV)	-1.35	-1.30	-1.32
E_g (eV)	3.35	3.43	3.41
S_1 (eV)	2.76	2.83	2.82
T_1 (eV)	2.49	2.52	2.51

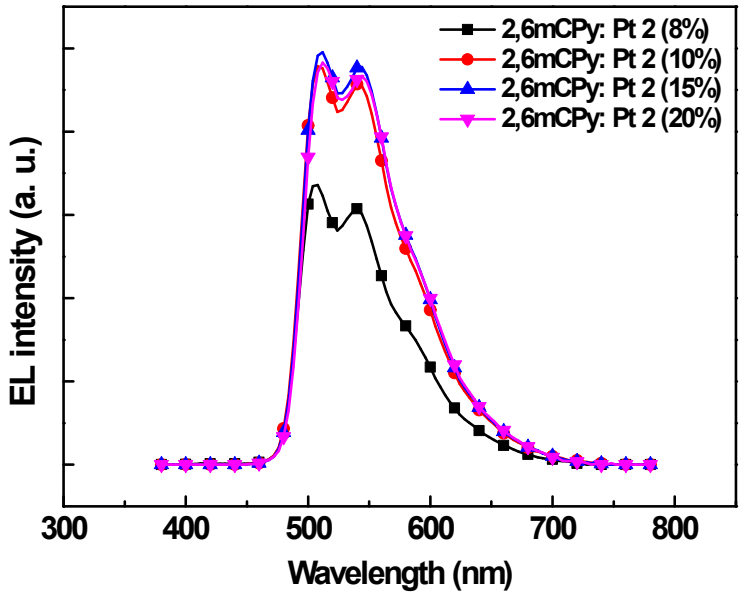


Figure S27 The EL spectra of complex **Pt 2** with different doping ratios at 5 mA/cm^2.

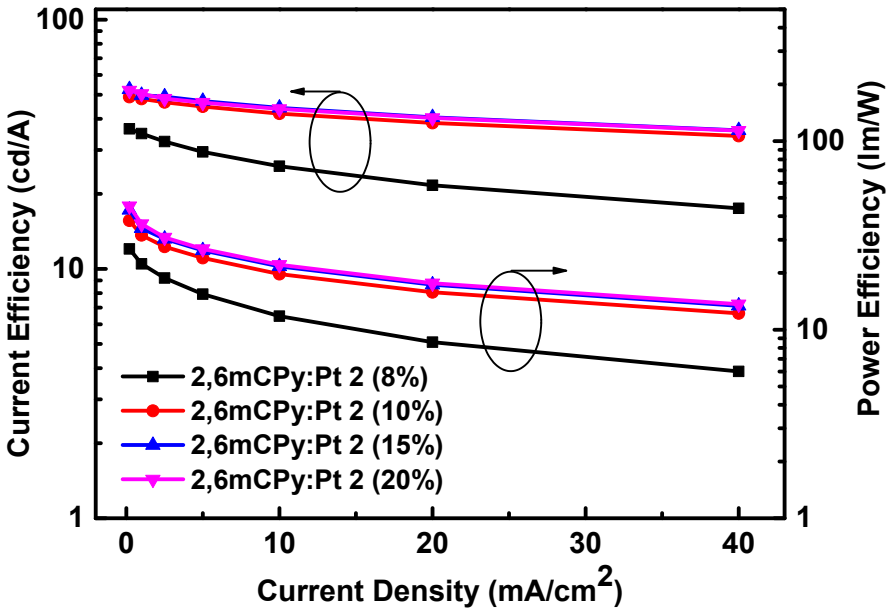


Figure S28. The power efficiency-current density-current efficiency curves for **Pt 2** in the 2,6mCPy host at different doping ratios.

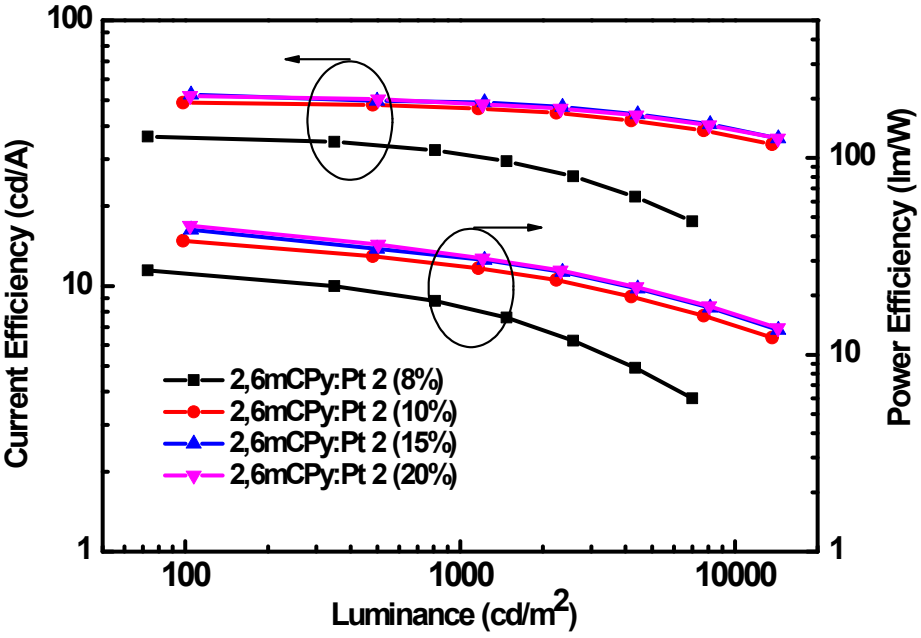


Figure S29. The power efficiency-luminance-current efficiency curves for **Pt 2** in the 2,6mCPy host at different doping ratios.

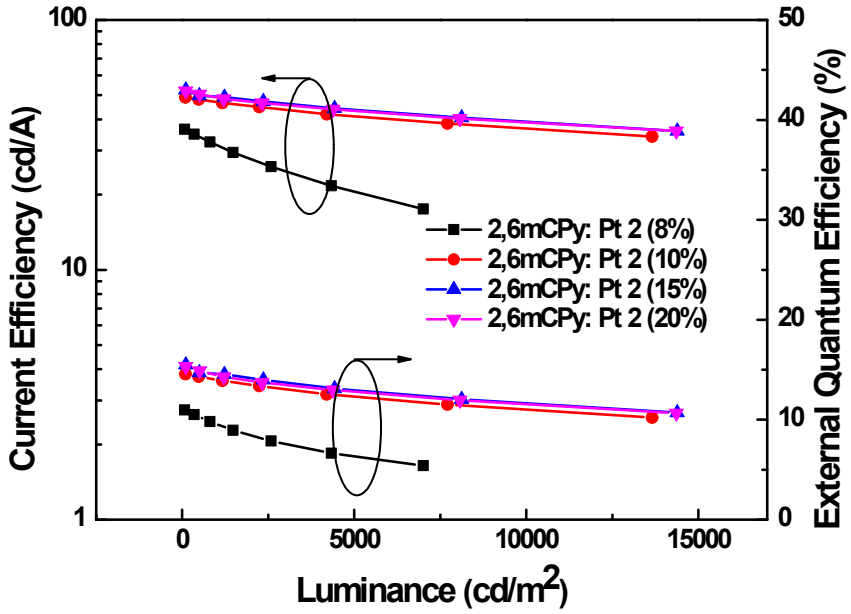


Figure S30. The EQE-luminance-current efficiency curves for **Pt 2** at different doping ratios.

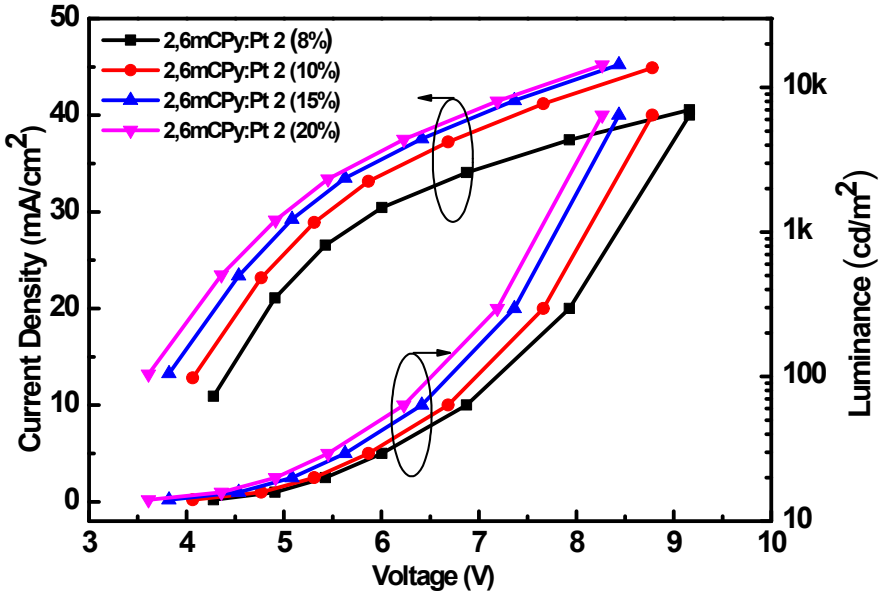


Figure S31. The current density-voltage-luminance curves for **Pt 2** in the 2,6mCPy host at different doping ratios.

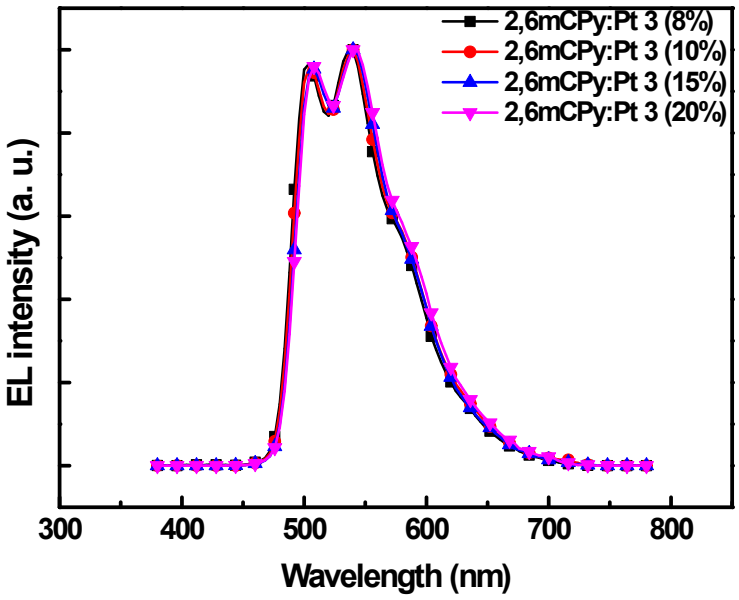


Figure S32. The EL spectra of complex **Pt 3** with different doping ratios at 5 mA/cm^2.

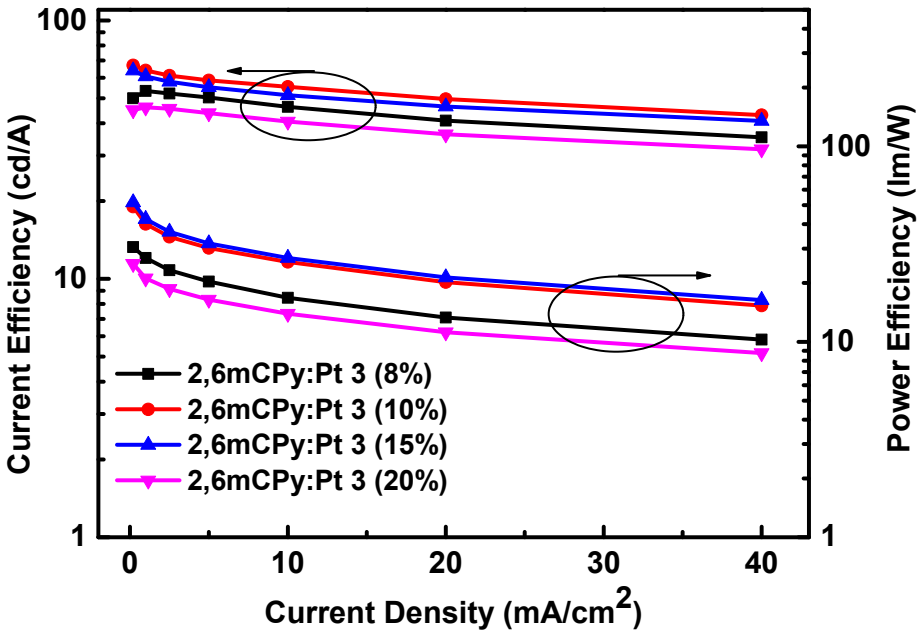


Figure S33. The power efficiency-current density-current efficiency curves for **Pt 3** in the 2,6mCPy host at different doping ratios.

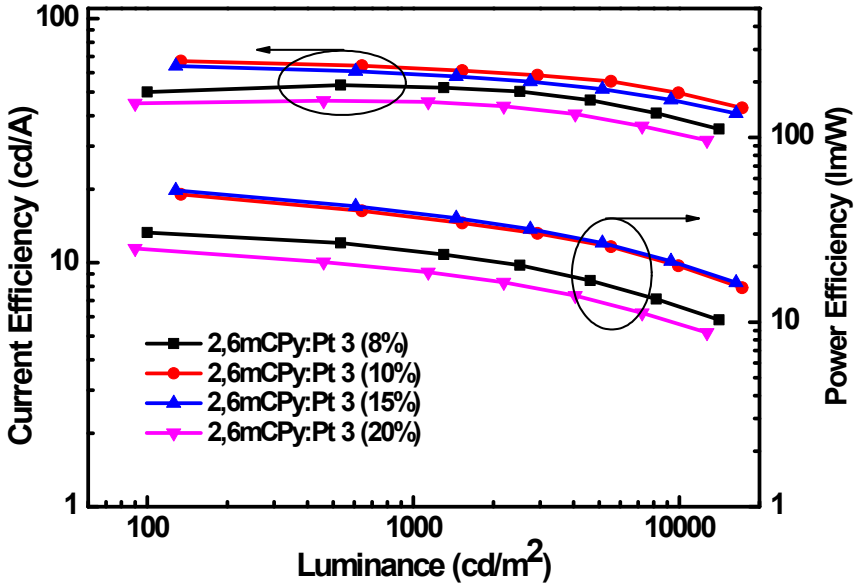


Figure S34. The power efficiency-luminance-current efficiency curves for **Pt 3** in the 2,6mCPy host at different doping ratios.

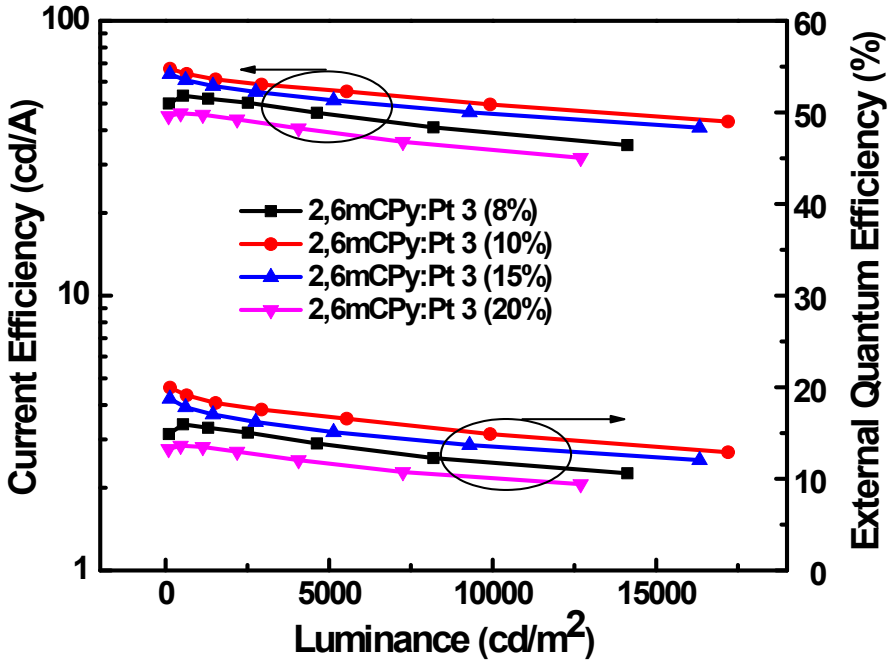


Figure S35. The EQE-luminance-current efficiency curves for **Pt 3** at different doping ratios.

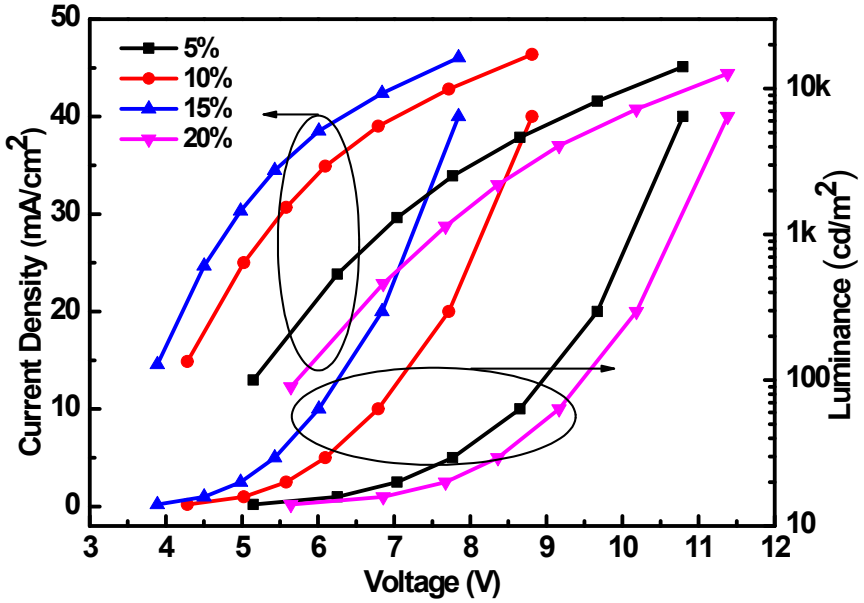


Figure S36. The current density-voltage-luminance curves for **Pt 3** in the 2,6mCPy host at different doping ratios.