Supporting Information

Optimizing Through-Space Charge Transfer in Thermally Activated Delayed Fluorescence Emitters for Enhanced OLED Efficiency

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1. Materials and methods

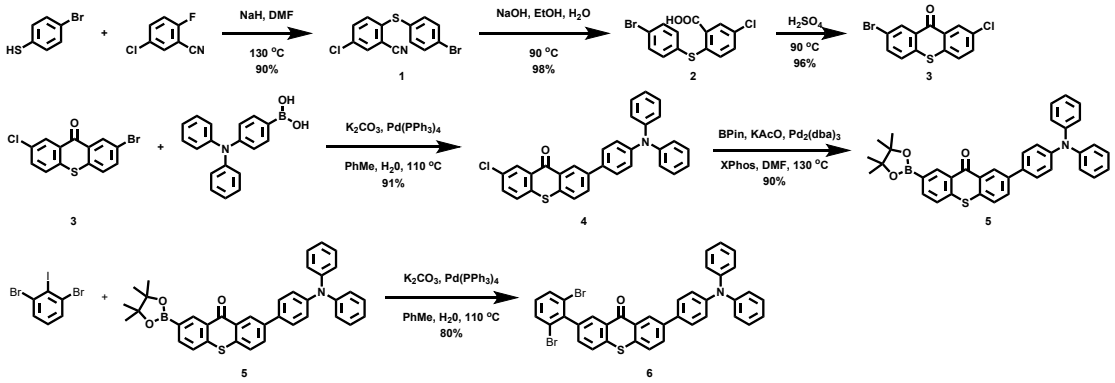
1.1 General methods.

All solvents and materials were used as received from commercial suppliers without further purification. All reactions were monitored by thin layer chromatographic analysis on a pre-coated silica gel plate, which was visualized by a UV lamp at 254 or 365 nm. Flash column chromatography was performed on glass column of silica gel (200–300 mesh) and solvent ratios were expressed in volume to volume. ^{1}H and ^{13}C NMR spectra for structural characterization were recorded on NMR spectrometer (600 MHz for ^{1}H and ^{13}C). The NMR spectra were recorded on VaRIAN-GEMINI-

300 and Bruker Avance Π-400 spectrometer at room temperature and tetramethylsilane (TMS) as an internal reference. Chemical shifts were reported as parts per million in scale using the slvent residual peak as internal standard for ^{1}H and ^{13}C NMR. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra were recorded using a ThermoFisher liquid chromatography mass spectrometer (Q-Exactive) in ESI mode. The geometric structure optimization and excited state calculation were carried out by using Gaussian 16 program[S1], 6-31G (d, p) basis set and D3 empirical dispersion correction[S2], and Multifwn and VMD were used for visualization[S3]. UV-vis spectra and fluorescence spectra were obtained with Hitachi U-3900 and F-4600 spectrophotometers, respectively. The phosphorescence spectra were measured in toluene glass matrix at 77 K using a Hitachi F-7100 fluorescence spectrometer. The absolute fluorescence quantum yields of the solid films are measured with an integrating sphere. Cyclic voltammetry was performed using a CHI600A analyzer with a scan rate of 50 mV/s at room temperature. The electrolytic cell was a conventional three-electrode cell with a glassy carbon working electrode, a platinum wire counter electrode, and a SCE (Ag/Ag^{+}) reference electrode. The measurement of oxidation potentials was performed in CH_2Cl_2 with 0.1 M of tetra-n-butylammonium hexafluorophosphate (*n*-Bu_4NPF_6) as a supporting electrolyte, and the reduction part was performed in THF with 0.1 mol/L of *n*-Bu_4NPF_6 as a supporting electrolyte. The TGA measurements were carried out using a TA Instruments TGA Q50 thermal analyzer at a heat rate of 10 °C/min**.**

1.2 Synthesis.

All solvents and materials were used as received from commercial suppliers without further purification. Synthetic routes of these compounds are shown in Scheme S1.



Scheme S1. The synthesis route of intermediate products.

Synthesis of compound 1: A mixture of 4-Bromothiophenol (12.0 g, 63.5 mmol) and NaH (60%

dispersion in mineral oil, 3.8 g, 95.2 mmol) in dry N,N-Dimethylformamide (50 mL) was stirred for 2 h at 60 ℃ under nitrogen. After cooling to room temperature, the dry N,N-Dimethylformamide (20 mL) of 5-Chloro-2-fluorobenzonitrile (10.9 g, 69.85 mmol) was added to the reaction solution through a separator and reacted for 12 h at 130 °C. After cooling to room temperature, the reaction mixture was added into water and then extracted with CH_2Cl_2. The collected organic layer was washed with water and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure. The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 5:1, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a white solid (yield =18.5 g, 90%).^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.62 (d, J = 2.3 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.40 (dd, J = 8.6, 2.3 Hz, 1H), 7.34 – 7.29 (m, 2H), 7.11 (d, J = 8.6 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 140.03, 134.88, 133.60, 133.39, 133.20, 131.86, 131.02, 123.75, 115.69, 114.86.

Synthesis of compound 2: **Compound 1** (18.5 g, 57.3 mmol) was added to the mixture of ethanol (120 mL) and potassium hydroxide aqueous solution (120 mL), and then heated to 90 ℃ for 6 h until the mixed solution became clear. After cooling to room temperature, the reaction solution was poured into ice water, and a large amount of white solid was precipitated. After suction filtration, put it into a vacuum drying oven to dry overnight to obtain white target compound (19.3 g, 98 %).^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.08 (d, J = 2.5 Hz, 1H), 7.62 – 7.55 (m, 2H), 7.45 – 7.38 (m, 2H), 7.28 (d, J = 2.4 Hz, 2H), 6.75 (d, J = 8.7 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.44, 142.51, 137.25, 133.39 (d, J = 2.3 Hz), 131.91, 131.05, 130.76, 128.78, 126.64, 124.41.

Synthesis of compound 3: Excess concentrated sulfuric acid (120 mL) was added to compound **2** (19.0 g, 55.3 mmol), and then the mixed solution was stirred at 90 ℃ for 24 h. The reaction solution was slowly poured into ice to precipitate a large amount of crude product. Dry the crude product after suction filtration, and then pass through the column to obtain the target compound (17.3 g, 96 %). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.74 (d, J = 2.3 Hz, 1H), 8.58 (d, J = 2.4 Hz, 1H), 7.74 (dd, J = 8.6, 2.3 Hz, 1H), 7.61 (dd, J = 8.6, 2.4 Hz, 1H), 7.54 (d, J = 8.6 Hz, 1H), 7.47 (d, J = 8.5 Hz, 1H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 177.93, 135.80, 135.74, 135.19, 133.20, 133.09, 132.74, 130.19, 130.06, 129.66, 127.78, 127.70, 120.79.

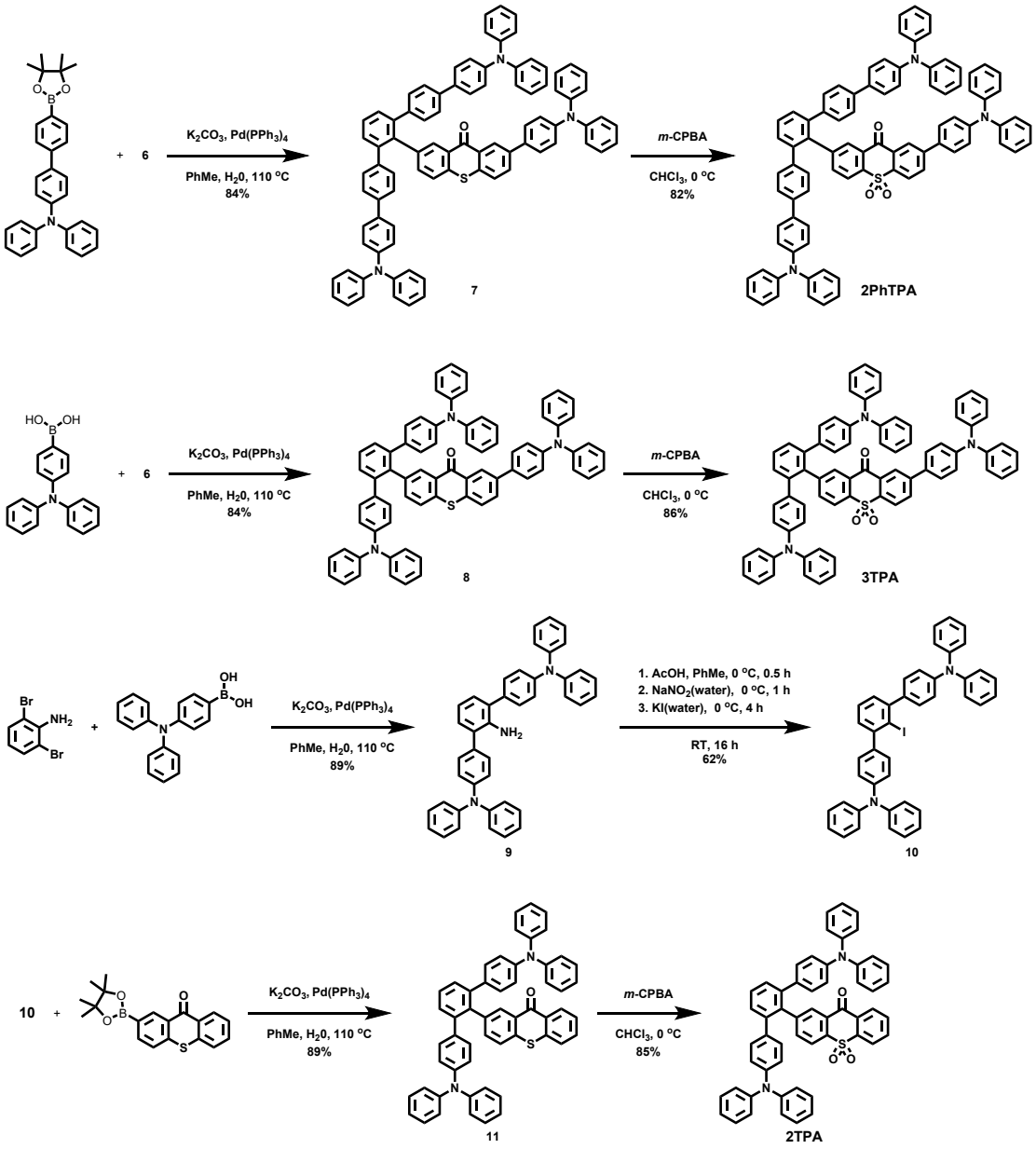
Synthesis of compound 4: A mixture of compound **3** (15.0 g, 46.1 mmol), $Pd(PPh_3)_4$ (2.7 g, 2.3 mmol), 2 M K_2CO_3 (40 mL) and [4-(N-phenylanilino)phenyl]boronic acid (13.6 g, 47.0 mmol) in

toluene (80 mL) was stirred for 24 h at 110 ℃ under nitrogen. After cooling to room temperature, the reaction mixture was added into water and then extracted with CH_2Cl_2. The collected organic layer was washed with water and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure. The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 3:1, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a white solid (yield =20.6 g, 91%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.82 (d, J = 2.1 Hz, 1H), 8.62 (dd, J = 2.3, 0.5 Hz, 1H), 7.88 (dd, J = 8.4, 2.2 Hz, 1H), 7.63 (d, J = 8.4 Hz, 1H), 7.61 – 7.51 (m, 4H), 7.35 – 7.27 (m, 4H), 7.20 – 7.12 (m, 6H), 7.11 – 7.03 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.95, 148.03, 147.59, 139.22, 135.48, 135.05, 132.84, 132.71, 132.60, 130.92, 130.30, 129.50, 129.08, 127.83, 127.62, 127.24, 126.67, 124.82, 123.66, 123.39.

Synthesis of compound 5: A mixture of compound **4** (10.0 g, 20.4 mmol), Bis(pinacolato)diborane (7.8 g, 30.6 mmol), $Pd_2(dba)_3$ (0.9 g, 1.0 mmol), XPhos (1.0 g, 2.0 mmol) and KAcO (4.0 g, 40.8 mmol) in dry N, N Dimethylformamide (20 mL) was stirred for 2 h at 130 ℃ under nitrogen. After cooling to room temperature, the reaction mixture was added into water and then extracted with CH_2Cl_2. The collected organic layer was washed with water and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure. The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2 = 1:1, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a white solid (yield =2.1 g, 90%).^{1}H NMR (600 MHz, Chloroform-*d*) δ 9.10 – 9.07 (m, 1H), 8.84 (d, J = 2.1 Hz, 1H), 7.99 (dd, J = 8.1, 1.3 Hz, 1H), 7.84 (tt, J = 7.2, 2.2 Hz, 1H), 7.64 – 7.54 (m, 4H), 7.29 (t, J = 7.8 Hz, 4H), 7.20 – 7.13 (m, 6H), 7.06 (td, J = 7.4, 1.3 Hz, 2H), 1.38 (s, 12H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 179.92, 147.85, 147.59, 140.22, 138.96, 137.58, 137.04, 135.13, 133.15, 130.59, 129.86, 129.45, 128.52, 127.85, 127.28, 126.59, 125.41, 124.71, 123.72, 123.28, 84.27, 25.02.

Synthesis of compound 6: This compound was prepared from compound **5** according to the procedure for compound **4**. The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 2:1, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a yellow solid (yield =12.1 g, 80%). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.86 (d, J = 2.1 Hz, 1H), 8.58 (d, J = 1.9 Hz, 1H), 7.88 (dd, J = 8.4, 2.2 Hz, 1H), 7.68 (dd, J = 17.0, 8.4 Hz, 2H), 7.64 – 7.52 (m, 3H), 7.45 (d, J = 8.1 Hz, 2H), 7.32

– 7.26 (m, 5H), 7.22 – 7.11 (m, 6H), 7.10 – 7.01 (m, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 179.88, 147.94, 147.62, 141.64, 139.26, 139.09, 137.21, 135.35, 133.38, 133.12, 132.12, 131.03, 130.78, 130.50, 129.57, 129.48, 129.22, 127.87, 127.30, 126.71, 126.25, 124.77, 124.65, 123.75, 123.33.



Scheme 2. The synthetic route of the final products **2TPA**, **3TPA** and **2PhTPA**.

Synthesis of compound 7: This compound was prepared from compound **6** according to the procedure for compound **4.** The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 1.2:1, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a yellow solid (yield =2.6 g, 84%). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.72 (d, J = 2.1 Hz, 1H), 8.26 (d, J = 1.9 Hz, 1H), 7.79

(dd, *J* = 8.4, 2.2 Hz, 1H), 7.61 – 7.49 (m, 6H), 7.43 – 7.36 (m, 8H), 7.28 (dd, *J* = 8.5, 7.3 Hz, 5H), 7.23 (dt, *J* = 8.6, 6.7 Hz, 9H), 7.20 – 7.12 (m, 11H), 7.10 – 7.03 (m, 13H), 7.02 – 6.98 (m, 4H). ^{13}C NMR (151 MHz, Chloroform-*d*) *δ* 179.67, 147.83, 147.74, 147.64, 147.21, 141.96, 140.06, 138.75, 138.49, 138.40, 137.70, 135.50, 135.43, 134.90, 134.56, 133.23, 132.95, 130.54, 130.45, 129.88, 129.56, 129.47, 129.35, 128.43, 128.01, 127.79, 127.67, 127.23, 126.55, 126.02, 125.32, 124.74, 124.44, 124.06, 123.76, 123.29, 122.97.

Synthesis of compound 2PhTPA: A mixture of compound **7** (2.3 g, 2.0 mmol), $CHCl_3$ (30 mL) and *m*-CPBA (1.0 g, 6.0 mmol) was ice water bath for 12 hours at 0 ℃. After returning to room temperature, the reaction mixture was added into water and then extracted with CH_2Cl_2. The collected organic layer was washed with water and dried over anhydrous Na_2SO_4, then evaporated under reduced pressure. The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 1:1.5, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as an orange red solid (yield =1.9 g, 82%). ^{1}H NMR (600 MHz, Chloroform-*d*) *δ* 8.37 (d, *J* = 1.9 Hz, 1H), 8.11 (d, *J* = 8.2 Hz, 1H), 7.99 – 7.93 (m, 2H), 7.82 (d, *J* = 8.1 Hz, 1H), 7.57 (dd, *J* = 8.5, 6.7 Hz, 1H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.49 – 7.45 (m, 2H), 7.40 (m, 9H), 7.31 – 7.26 (m, 4H), 7.25 – 7.20 (m, 9H), 7.15 – 7.04 (m, 23H), 6.99 (t, *J* = 7.3 Hz, 4H). ^{13}C NMR (151 MHz, Chloroform-*d*) *δ* ^{13}C NMR (151 MHz, Chloroform-*d*) δ 178.17, 149.08, 147.75, 147.38, 147.28, 145.89, 145.71, 141.81, 139.27, 139.11, 138.50 (d, *J* = 1.9 Hz), 137.74, 136.32, 134.33, 132.41, 131.98, 131.08, 131.05, 130.47, 130.10, 129.77, 129.60, 129.37, 128.79, 128.11, 127.76, 126.75, 126.34, 125.20, 124.48, 124.21, 124.09, 123.85, 123.01, 122.95, 122.91. HR-MS (ESI^{+}): 1202.4314 Calculated: 1201.4277. m. p.: 219 ℃.

Synthesis of compound 8: This compound was prepared from compound **6** according to the procedure for compound **4.** The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 1.5:1, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a yellow solid (yield =2.2 g, 84%). ^{1}H NMR (600 MHz, Chloroform-*d*) *δ* 8.85 (d, *J* = 2.1 Hz, 1H), 8.16 (d, *J* = 2.0 Hz, 1H), 7.88 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.61 – 7.56 (m, 2H), 7.50 (d, *J* = 1.2 Hz, 3H), 7.34 – 7.26 (m, 5H), 7.16 (m, 7H), 7.13 – 7.09 (m, 8H), 7.08 – 7.04 (m, 2H), 7.01 – 6.94 (m, 12H), 6.93 – 6.89 (m, 4H), 6.88 – 6.85 (m, 4H). ^{13}C NMR (151 MHz, Chloroform-*d*) *δ* 179.53, 147.91, 147.76, 147.64, 146.33, 141.87, 138.92, 138.50, 137.71, 136.00, 135.84, 135.49, 134.71, 133.45,

133.25, 131.11, 130.56, 129.56, 129.48, 129.34, 129.21, 128.31, 128.00, 127.83, 127.26, 126.69, 124.84, 124.76, 124.16, 123.81, 123.60, 123.31, 122.69.

Synthesis of compound 3TPA: This compound was prepared from compound **8** according to the procedure for compound **2PhTPA**. The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 1:1.5, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as an orange red solid (yield =1.8 g, 86%). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.48 (t, J = 1.7 Hz, 1H), 8.23 – 8.19 (m, 1H), 8.04 (dd, J = 8.2, 1.9 Hz, 1H), 7.90 – 7.86 (m, 2H), 7.56 – 7.47 (m, 5H), 7.38 (dt, J = 8.2, 1.5 Hz, 1H), 7.31 (t, J = 7.8 Hz, 4H), 7.17 (t, J = 7.8 Hz, 14H), 7.10 (t, J = 7.4 Hz, 2H), 6.98 (d, J = 7.9 Hz, 8H), 6.94 (t, J = 7.4 Hz, 4H), 6.89 (s, 8H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ ^{13}C NMR (151 MHz, Chloroform-*d*) δ 178.49, 149.13, 147.59, 147.29, 146.81, 146.07, 145.84, 141.81, 138.72, 138.48, 138.06, 136.39, 134.64, 132.66, 131.98, 131.28, 131.11, 130.96, 129.77, 129.62, 129.56, 129.35, 128.75, 128.14, 126.70, 125.23, 124.47, 124.36, 123.89, 123.14, 123.04, 122.98, 122.46. HR-MS (ESI^+): 1050.3685, Calculated: 1049.3651. m. p.: 190 ℃.

Synthesis of compound 9: This compound was prepared from 2,6-Dibromoanilinea and 4-(Diphenylamino) phenylboronic acid according to the procedure for compound **4.** The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 1:2, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a yellow solid (yield = 3.2 g, 89%). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.37 (m, 4H), 7.31 – 7.24 (m, 8H), 7.18 – 7.10 (m, 14H), 7.07 – 7.00 (m, 4H), 6.87 (t, J = 7.5 Hz, 1H), 4.02 (s, 2H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.78, 147.02, 141.08, 133.67, 130.13, 129.61, 129.42, 127.71, 124.64, 123.75, 123.11, 118.29.

Synthesis of compound 10: Compound **9** (1.3 g, 5 mmol) was dissolved in a mixed solvent of AcOH and PhMe (AcOH/PhMe = 4:1, v/v) and stirred at 0 ℃ for 30 minutes. 3 mL of an aqueous solution of $NaNO_2$ (3 mmol, 1.2 g) was slowly added to the reaction mixture and stirred at 0 ℃ for 1 hour. Then, 3 mL of an aqueous solution of KI (3 mmol, 1.2 g) was slowly added, and the mixture was stirred at 0 ℃ for 4 hours. After the reaction, the mixture was allowed to reach room temperature, and 5 mL of saturated sodium thiosulfate solution was added. The reaction mixture was extracted with dichloromethane and water. The organic layer was then dried over anhydrous Na_2SO_4 and evaporated under reduced pressure. The crude product was purified by silica gel column

chromatography (eluent: PE/CH_2Cl_2 = 2:1, v/v). After evaporation of the solvent, the obtained solid was dried under vacuum to yield a white solid (2.1 g, 93%).^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.76 (t, *J* = 1.9 Hz, 1H), 7.52 (dd, *J* = 9.5, 7.4 Hz, 6H), 7.47 (dd, *J* = 8.7, 6.4 Hz, 1H), 7.28 (dd, *J* = 8.5, 7.3 Hz, 7H), 7.15 (dd, *J* = 8.3, 4.5 Hz, 12H), 7.04 (t, *J* = 7.3 Hz, 4H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 147.80, 147.40, 141.30, 135.27, 129.42, 129.27, 128.01, 125.33, 124.55, 124.04, 123.07.

Synthesis of compound 11: This compound was prepared from compound **10** according to the procedure for compound **4.** The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 1:1, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as a yellow solid (yield = 1.2 g, 56%). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.63 (dt, *J* = 8.2, 1.8 Hz, 1H), 8.14 (q, *J* = 2.1 Hz, 1H), 7.67 – 7.58 (m, 2H), 7.54 – 7.47 (m, 4H), 7.29 (dt, *J* = 8.3, 1.5 Hz, 1H), 7.15 (dq, *J* = 8.3, 1.8 Hz, 1H), 7.13 – 7.09 (m, 8H), 7.00 – 6.89 (m, 16H), 6.89 – 6.84 (m, 4H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 178.09, 147.58, 146.81, 146.19, 141.80, 141.41, 138.30, 138.11, 136.35, 134.71, 134.61, 133.29, 132.60, 130.94, 130.75, 129.54, 129.49, 129.34, 129.17, 128.76, 124.47, 123.66, 123.14, 123.03, 122.48.

Synthesis of compound 2TPA: This compound was prepared from compound **11** according to the procedure for compound **2PhTPA**. The crude product was further purified by column chromatography on silica gel (eluent: PE/CH_2Cl_2= 1:1.2, v/v). After removal of the solvents by evaporation, the resulting solid was dried under vacuum to give the desired product as an orange red solid (yield =1.8 g, 85%). ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.66 (dd, *J* = 8.1, 1.4 Hz, 1H), 8.19 (d, *J* = 2.0 Hz, 1H), 7.64 (dtd, *J* = 15.6, 8.2, 1.5 Hz, 2H), 7.54 – 7.49 (m, 4H), 7.32 (d, *J* = 8.2 Hz, 1H), 7.18 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.16 – 7.10 (m, 8H), 6.99 (td, *J* = 8.6, 1.7 Hz, 12H), 6.94 (td, *J* = 7.3, 1.2 Hz, 4H), 6.92 – 6.88 (m, 4H). ^{13}C NMR (151 MHz, Chloroform-*d*) δ 179.44, 147.73, 146.31, 141.85, 138.50, 137.69, 137.31, 136.00, 135.80, 134.75, 133.34, 132.27, 131.08, 129.95, 129.34, 129.32, 129.19, 128.34, 127.99, 126.42, 126.14, 124.75, 124.14, 123.55, 122.67. HR-MS (ESI^+): 807.2628, Calculated: 806.2603. m. p.: 152 ℃.

1.3 Transient photophysical measurement.

The transient photoluminescent decay characteristics were measured using an Edinburgh Instruments FLS1000 spectrometer. The temperature dependence experiment is conducted under

low temperature refrigeration system from Advanced Research Systems Company. The transient decay curves were fitted with the multi-exponential equation:

$$I(t) = \sum_i A_i \, exp(-\, t/\, \tau_i)$$

where A_i is the pre-exponential factor, τ_i is the decay time, and $I(t)$ is the emission intensity. The Φ_{Prompt} and Φ_{TADF} were determined by using total PL quantum efficiency and the ratio between prompt and delayed components. The intensity ratio between prompt (r_1) and delayed (r_2) components were obtained by fitting. Then, Φ_{Prompt} and Φ_{TADF} were determined using intensity ratio (r_1, r_2) and total emission quantum yield, and the rate constants are calculated as follows [2].

$$\Phi_{Prompt} = \Phi_{Total} \cdot r_1$$

$$\Phi_{TADF} = \Phi_{Total} \cdot r_2$$

$$k_p = \frac{1}{\tau_s} \quad (1)$$

$$k_d = \frac{1}{\tau_d} \quad (2)$$

$$k_F = k_p \Phi_F \quad (3)$$

$$\frac{k_r^s}{k_r^s + k_{nr}^s} = \Phi_{Total} \quad (4)$$

$$k_r^s(1 - \Phi_F) = k_{ISC} \quad (5)$$

$$k_{RISC} = \frac{k_p . k_d . \Phi_{TADF}}{k_{ISC} . \Phi_{Prompt}} \quad (6)$$

$$k_{nr}^T = k_d - (1 - \frac{k_{ISC}}{k_F + k_{ISC}}) k_{RISC} \quad (7)$$

Here, k_p and k_d the rate constants of prompt and delayed fluorescence, τ_s is the emission lifetime of the singlet excited state taken from lifetime measurements of the short range and τ_d is the emission lifetime of the delayed components. k_r^s and k_{nr}^s are the radiative and non-radiative rate constants from S_1 state, respectively, k_{ISC} is the intersystem crossing rate. The triplet formation efficiency (Φ_T) could be calculated by the intersystem crossing rate (k_{ISC}) and the emission lifetime of the prompted components (τ_s). The reverse intersystem crossing constant (k_{RISC}) was calculated by the rate constants of prompt fluorescence（k_p）, the rate constants of delayed fluorescence （

k_d), the quantum yield of the delayed components (Φ_{TADF}), the intersystem crossing rate (k_{ISC}) and the quantum yield of the prompt components (Φ_{Prompt}). The intersystem crossing constant (k_{ISC}), the radiative rate constants (k_r^S), triplet non-radiative decay (k_{nr}^T) and the singlet non-radiative rate constant (k_{nr}^S) were calculated assuming that k_{ISC} was independent of temperature.

1.4 Device fabrication.

Before device fabrication, the ITO glass substrates were sequentially cleaned with detergents, de-ionized water, acetone, ethanol, dried at 75 °C, and treated with oxygen plasma for 10 min. After that, the clean substrates were transferred into a vacuum deposition system with a pressure below 5 × 10^{-4} Pa for organic and metal deposition. The devices were fabricated by evaporating organic materials onto the substrate at a rate of 1–2 Å/s while Liq at a rate of 0.05 Å/s and Al metal through a rate of 2 Å/s. Then capped with EL luminescence spectra and CIE color coordinates were measured with a Spectrascan PR650 photometer and the current-voltage characteristics were measured with a computer-controlled Keithley 2400 Source Meter and CS-200 under ambient atmosphere.

2. Supplementary figures and tables

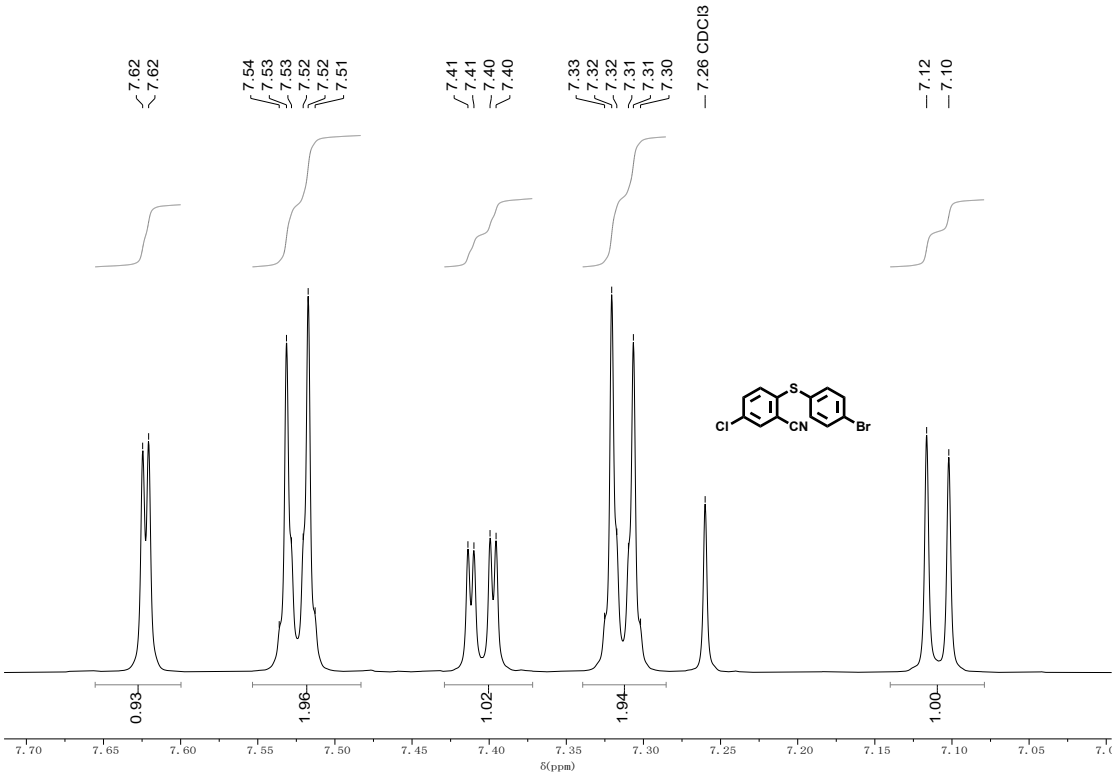


Figure S1. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

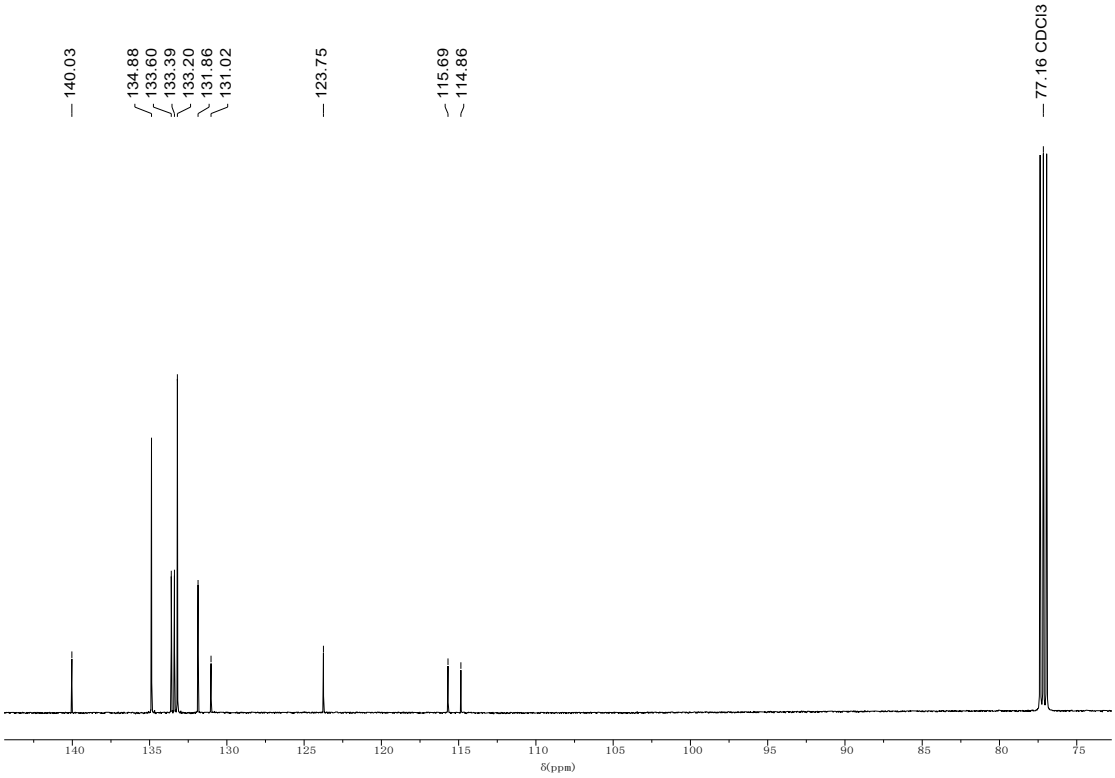


Figure S2. ^{13}C NMR spectrum of **1** in $CDCl_3$.

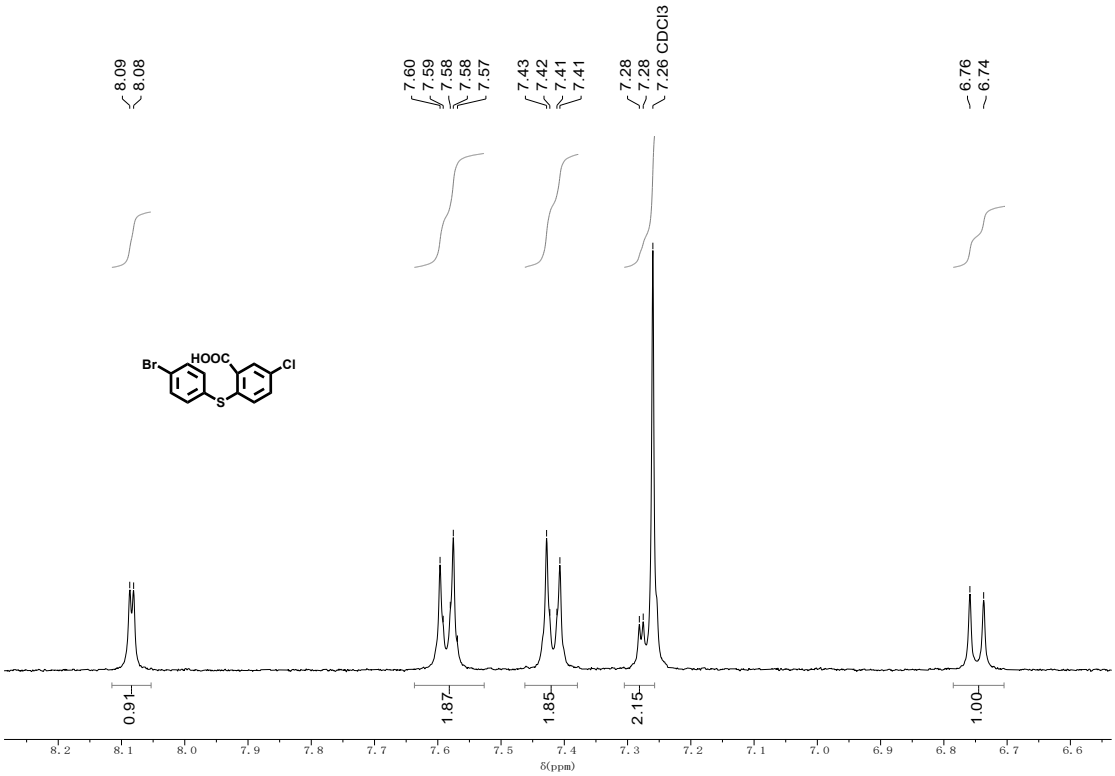


Figure S3. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

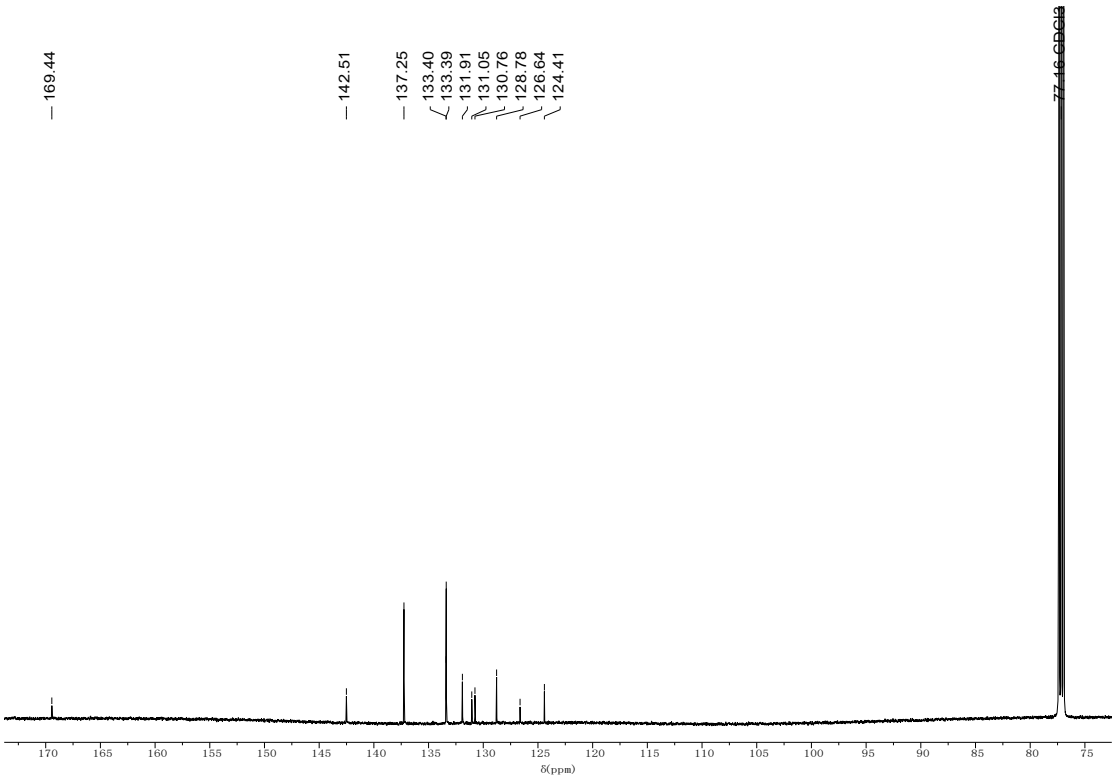


Figure S4. ^{13}C NMR spectrum of **2** in $CDCl_3$.

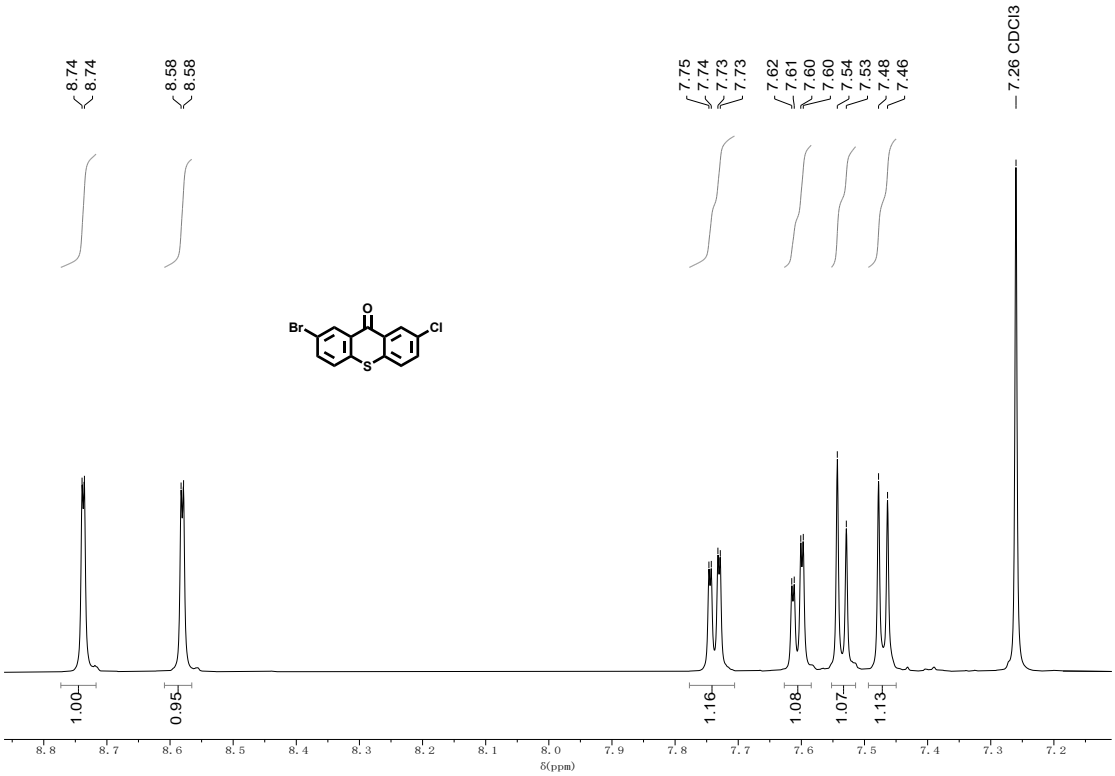


Figure S5. ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

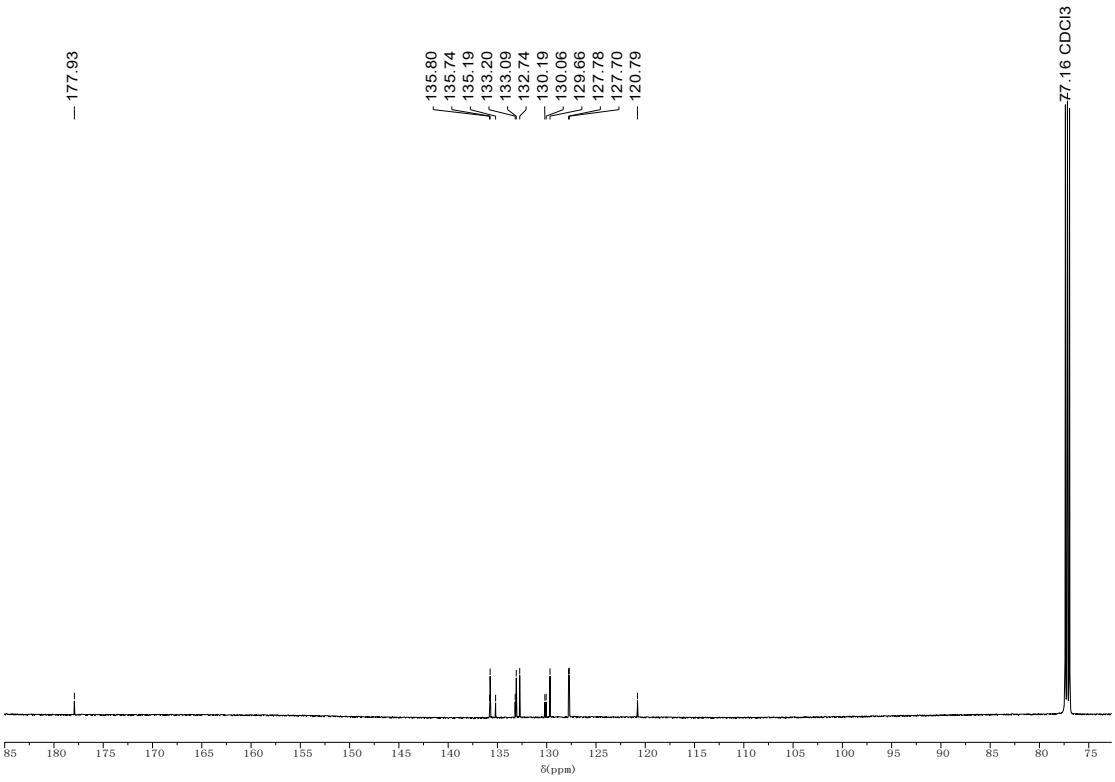


Figure S6. ^{13}C NMR spectrum of **3** in $CDCl_3$.

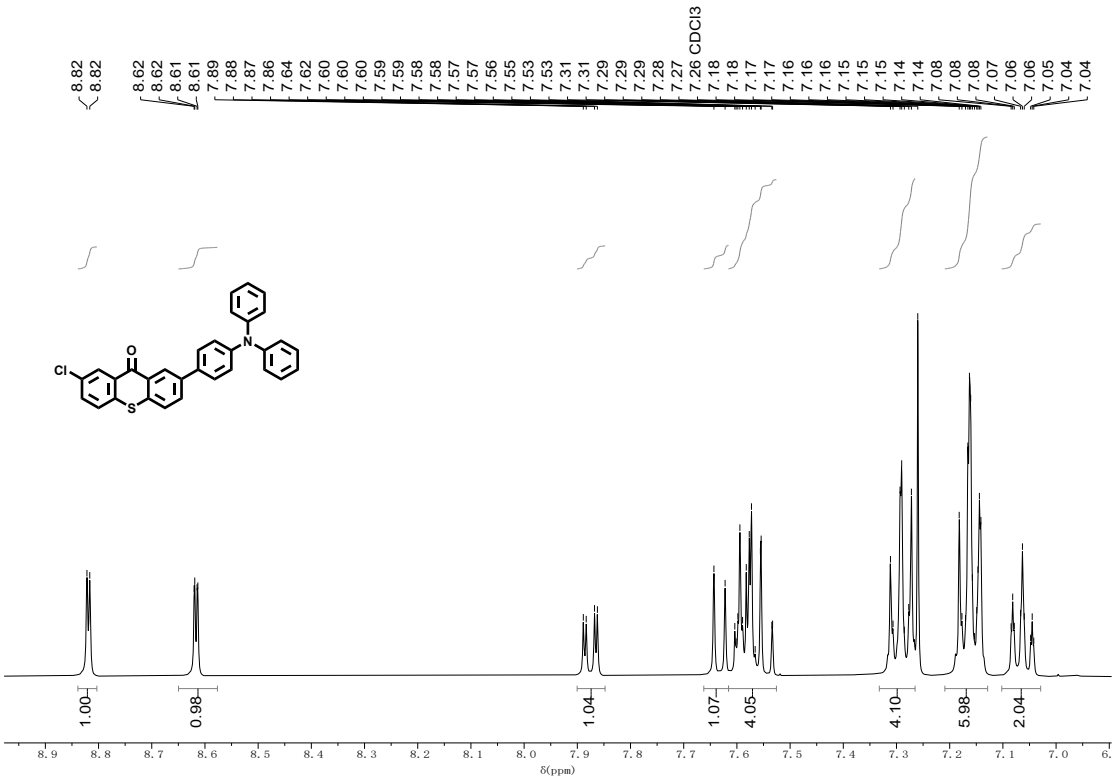


Figure S7. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

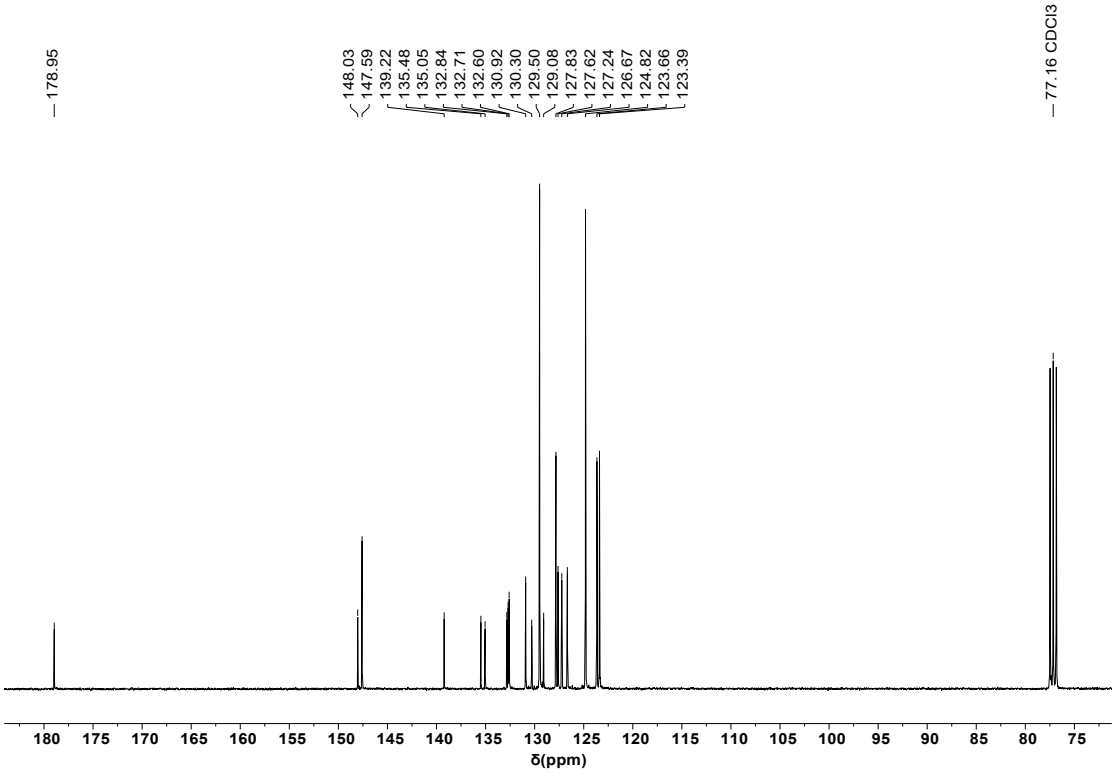


Figure S8. ^{13}C NMR spectrum of **4** in $CDCl_3$.

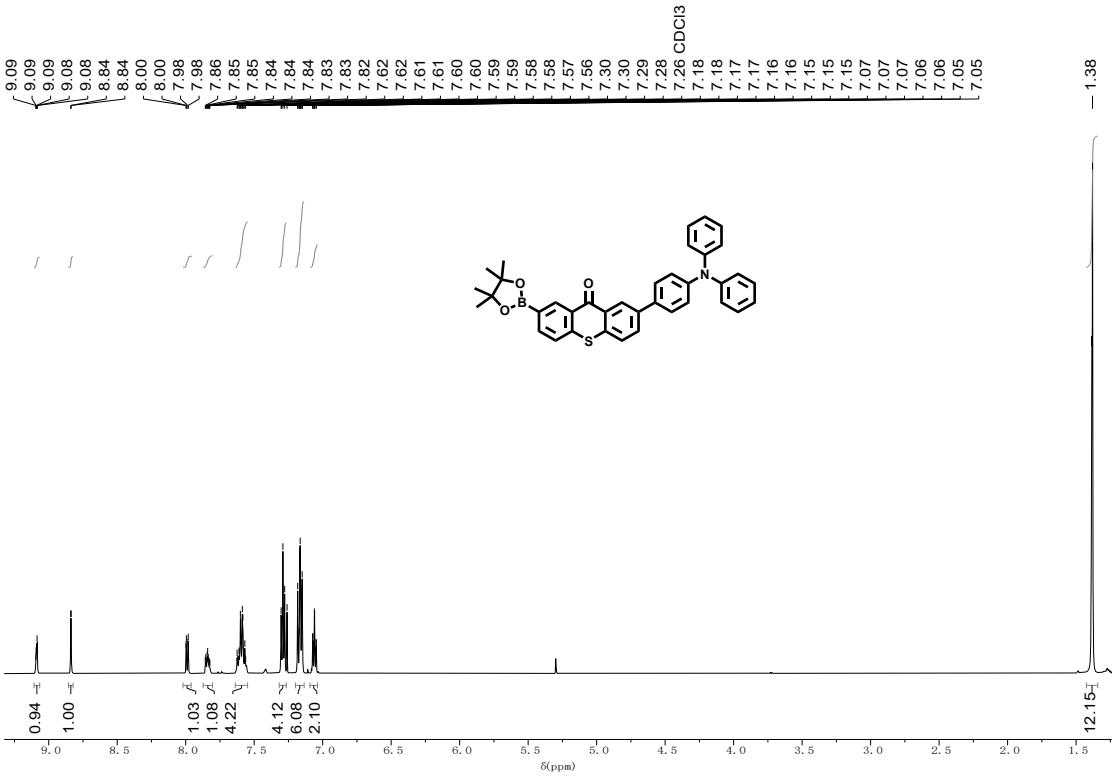


Figure S9. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

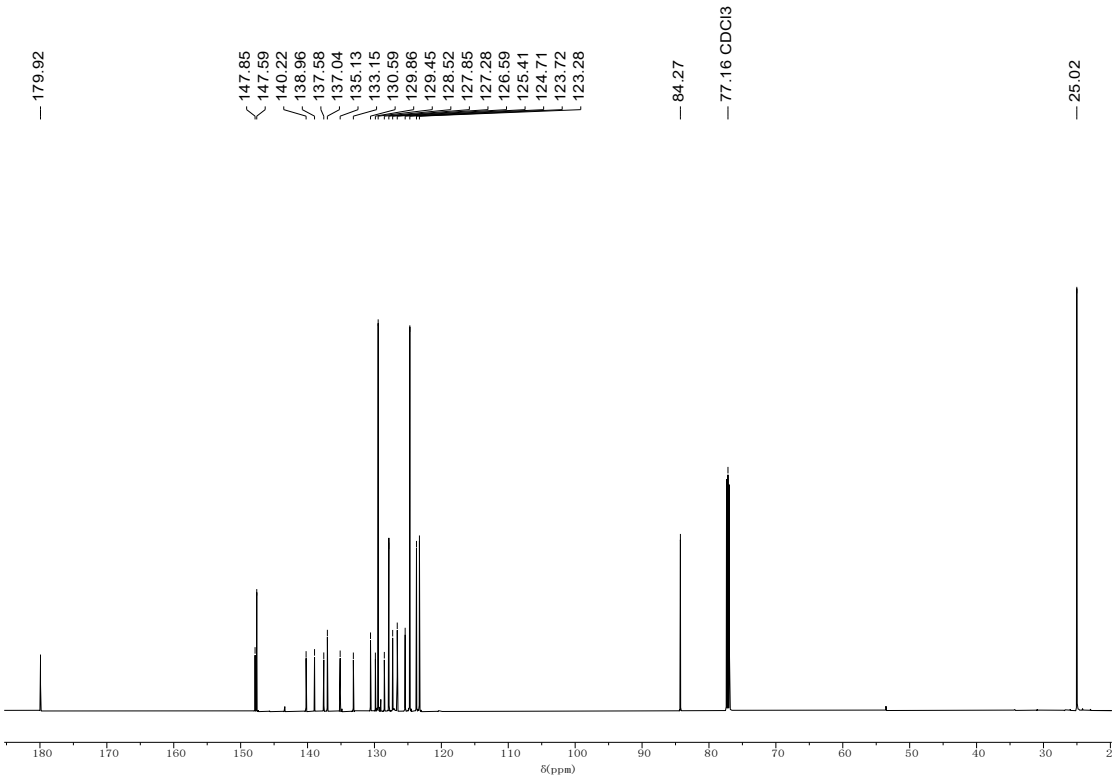


Figure S10. ^{13}C NMR spectrum of **5** in $CDCl_3$.

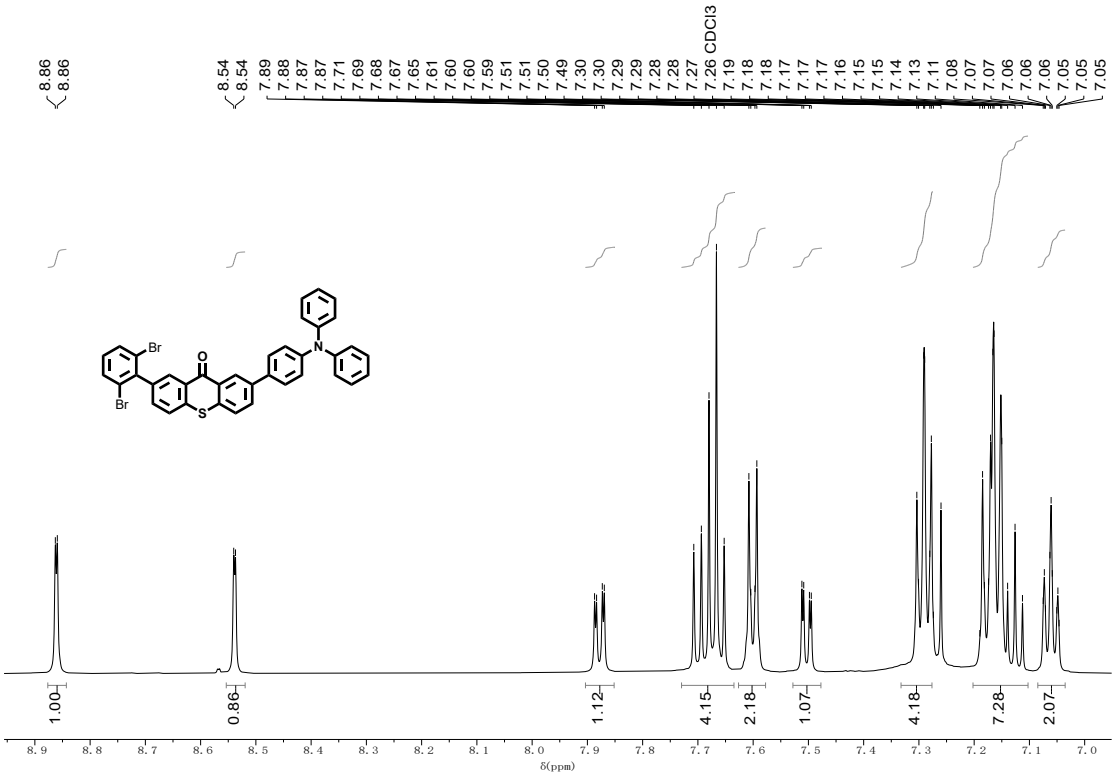


Figure S11. ^{1}H NMR spectrum of compound **6** in $CDCl_3$.

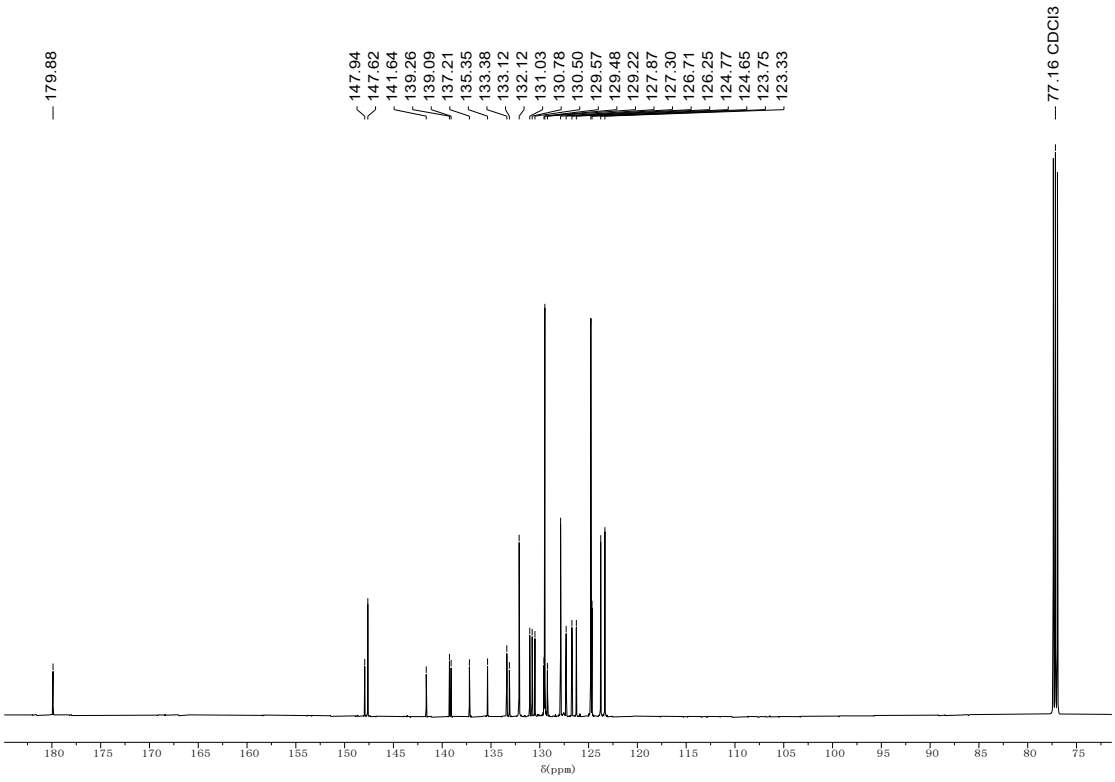


Figure S12. ^{13}C NMR spectrum of **6** in $CDCl_3$.

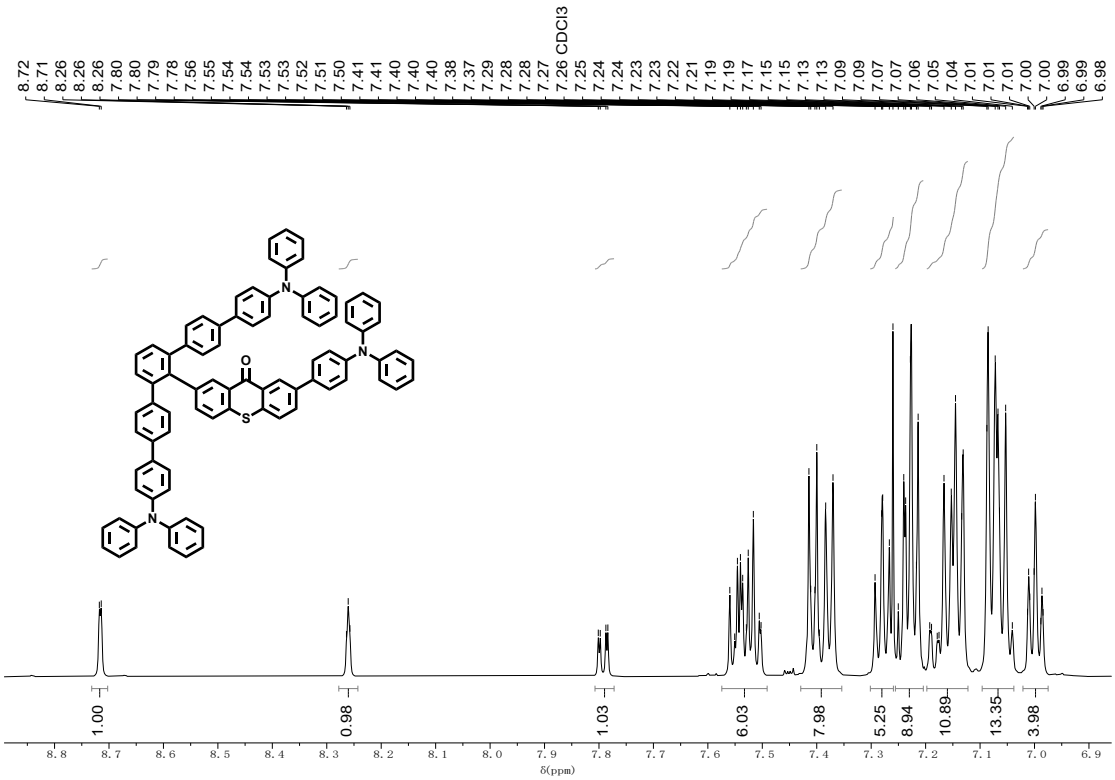


Figure S13. ^{1}H NMR spectrum of compound **7** in $CDCl_3$.

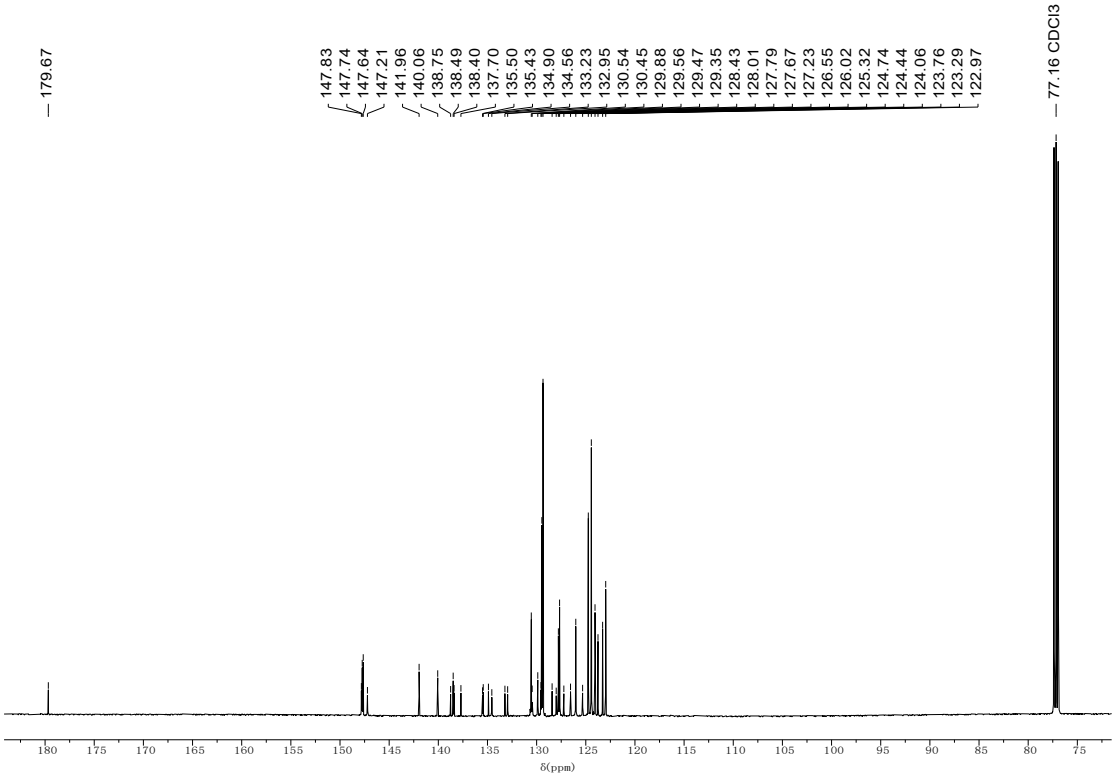


Figure S14. ^{13}C NMR spectrum of **7** in $CDCl_3$.

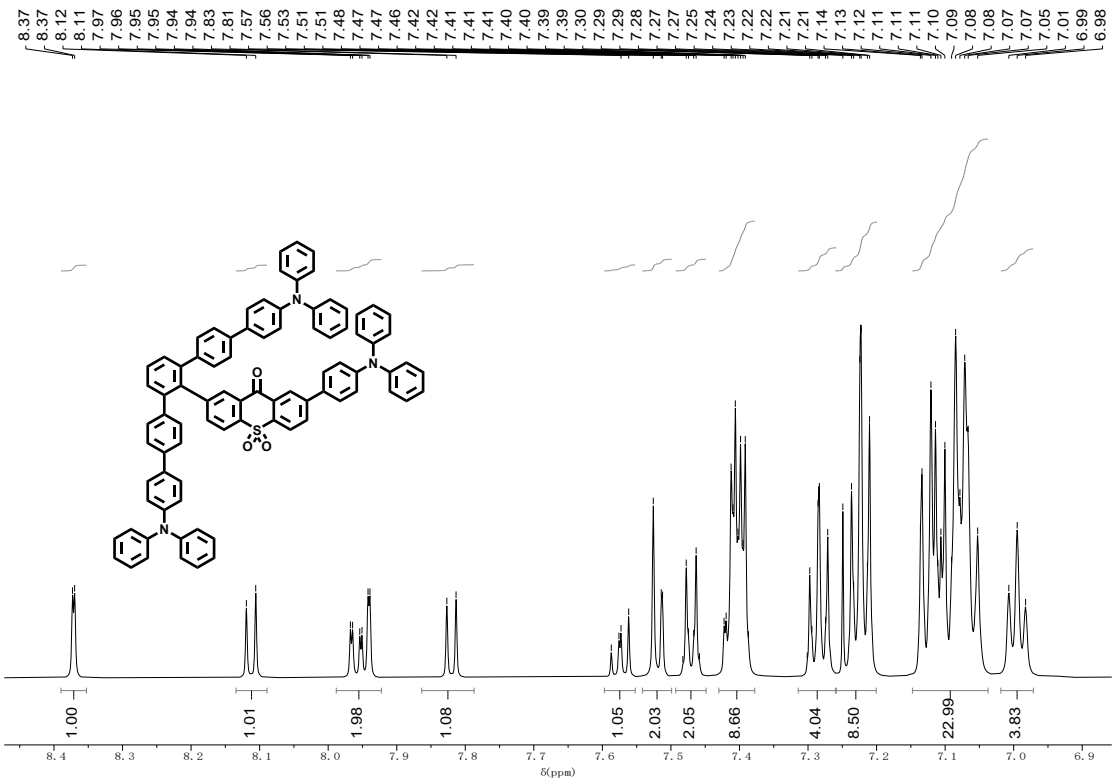


Figure S15. ^{1}H NMR spectrum of compound **2PhTPA** in $CDCl_3$.

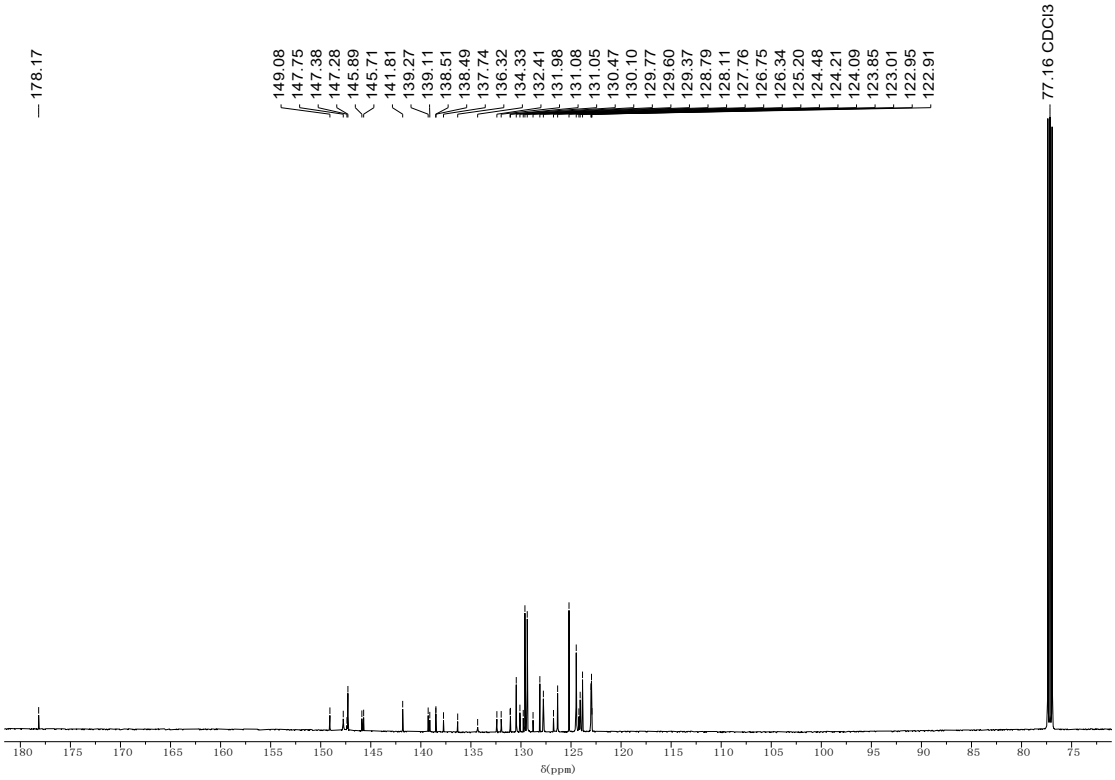


Figure S16. ^{13}C NMR spectrum of **2PhTPA** in $CDCl_3$.

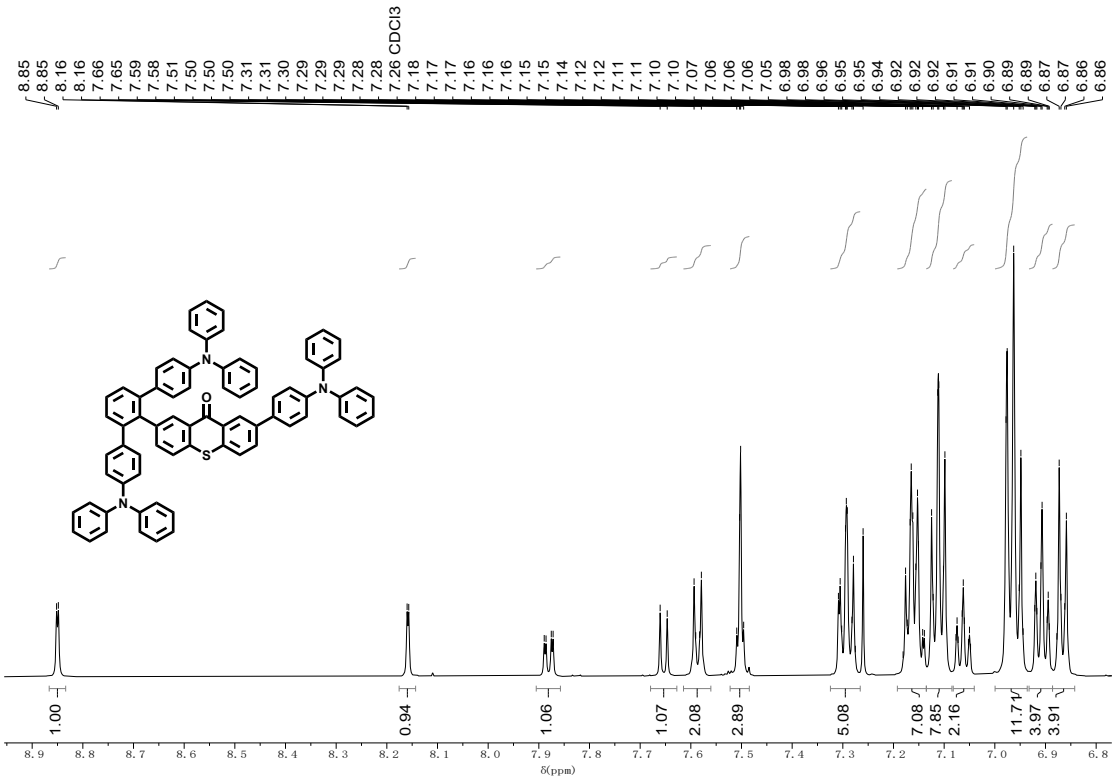


Figure S17. ^{1}H NMR spectrum of compound **8** in $CDCl_3$.

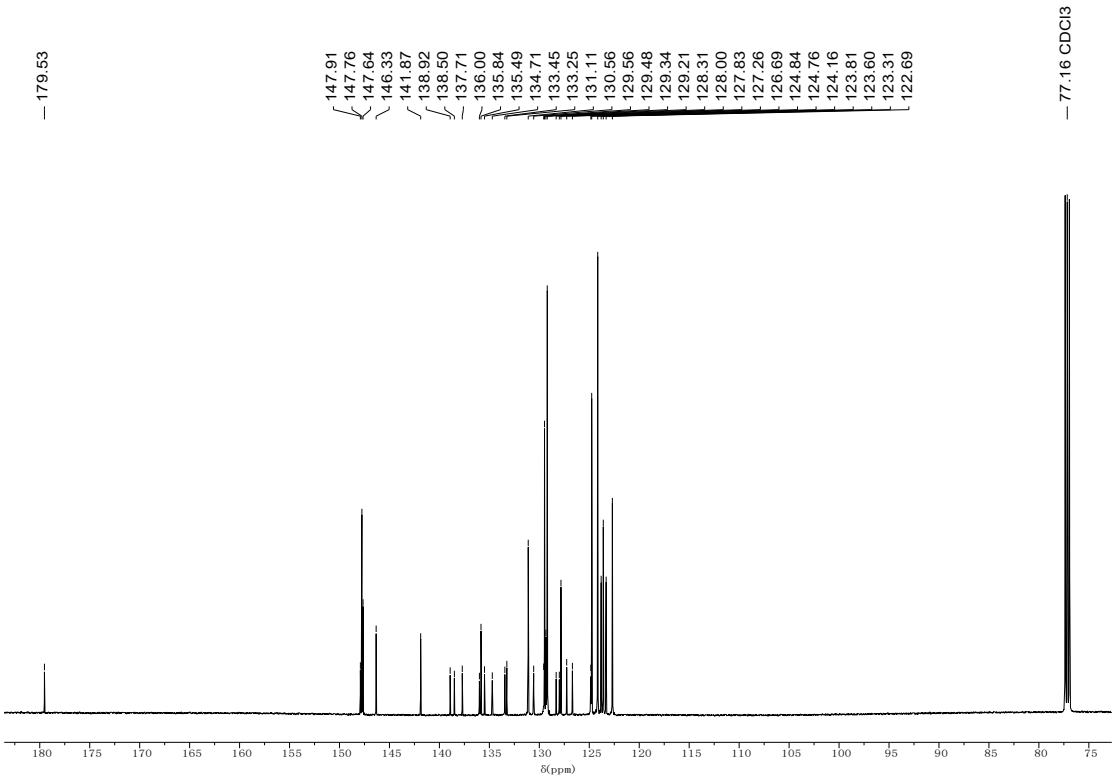


Figure S18. ^{13}C NMR spectrum of **8** in $CDCl_3$.

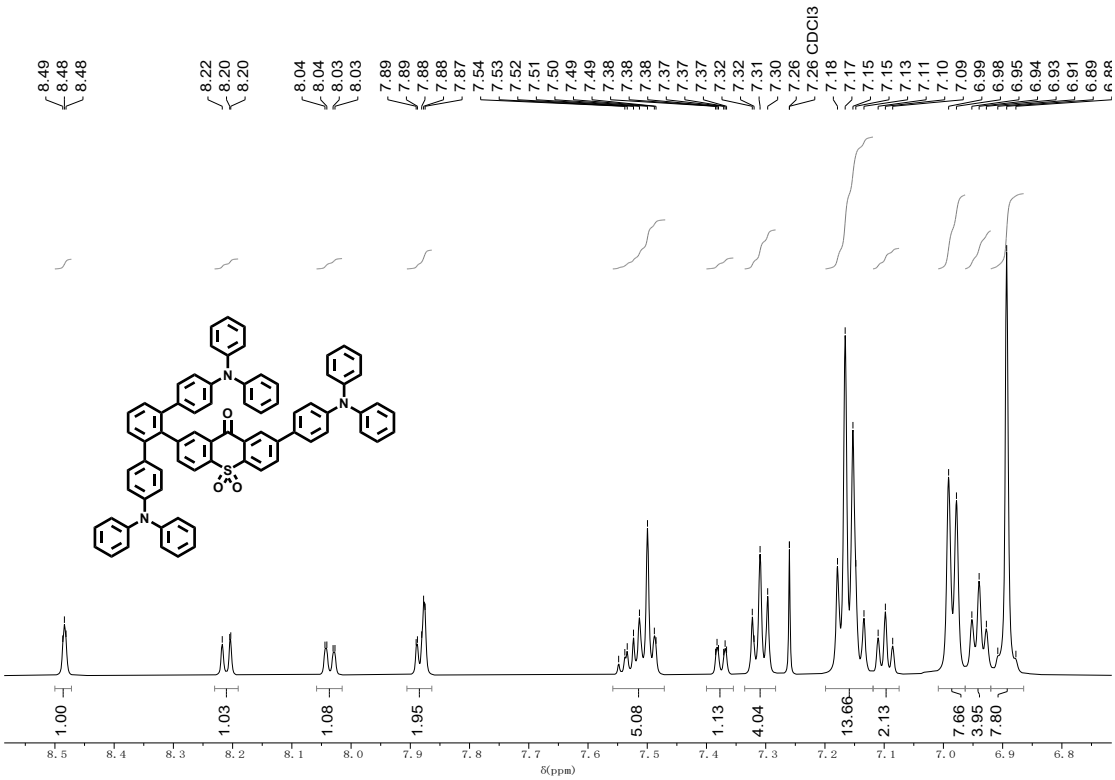


Figure S19. ^{1}H NMR spectrum of compound **3TPA** in $CDCl_3$.

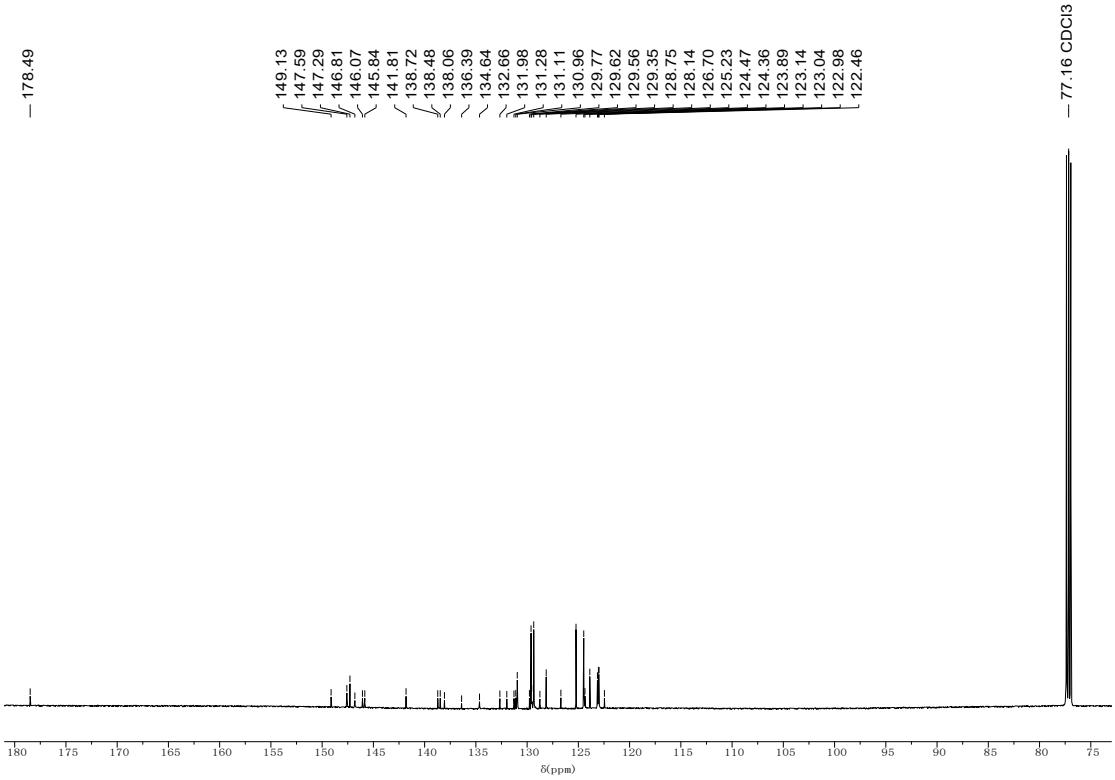


Figure S20. ^{13}C NMR spectrum of **3TPA** in $CDCl_3$.

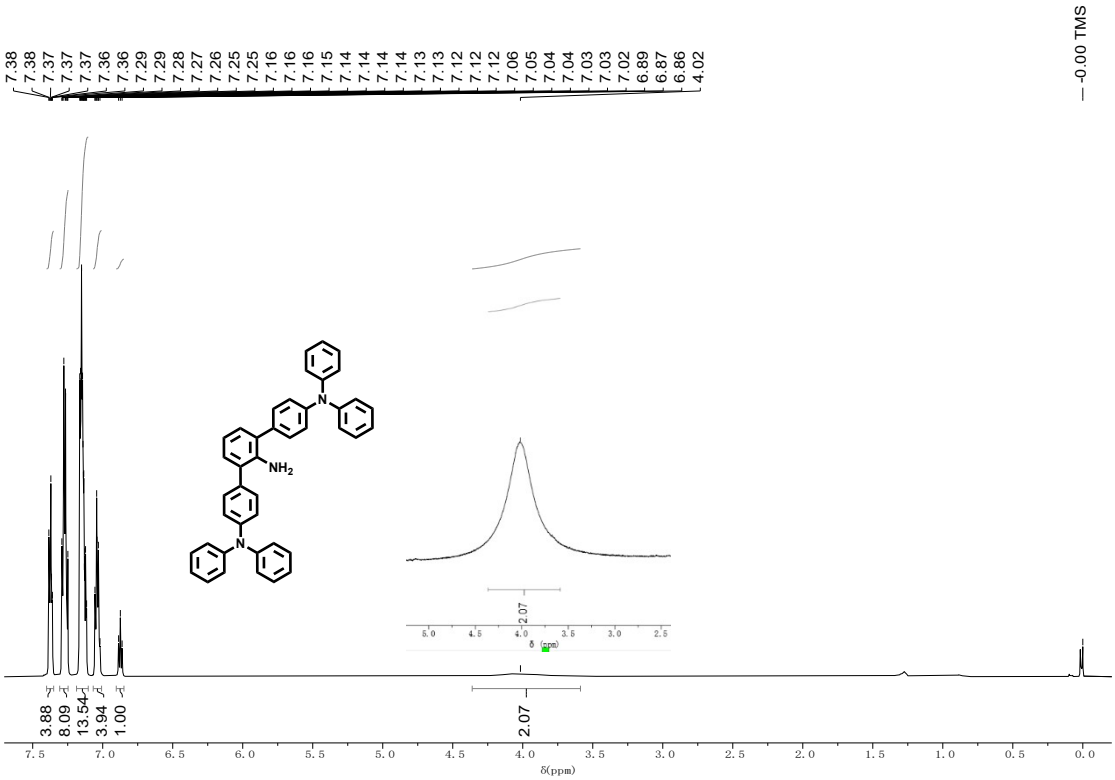


Figure S21. ^{1}H NMR spectrum of compound **9** in $CDCl_3$.

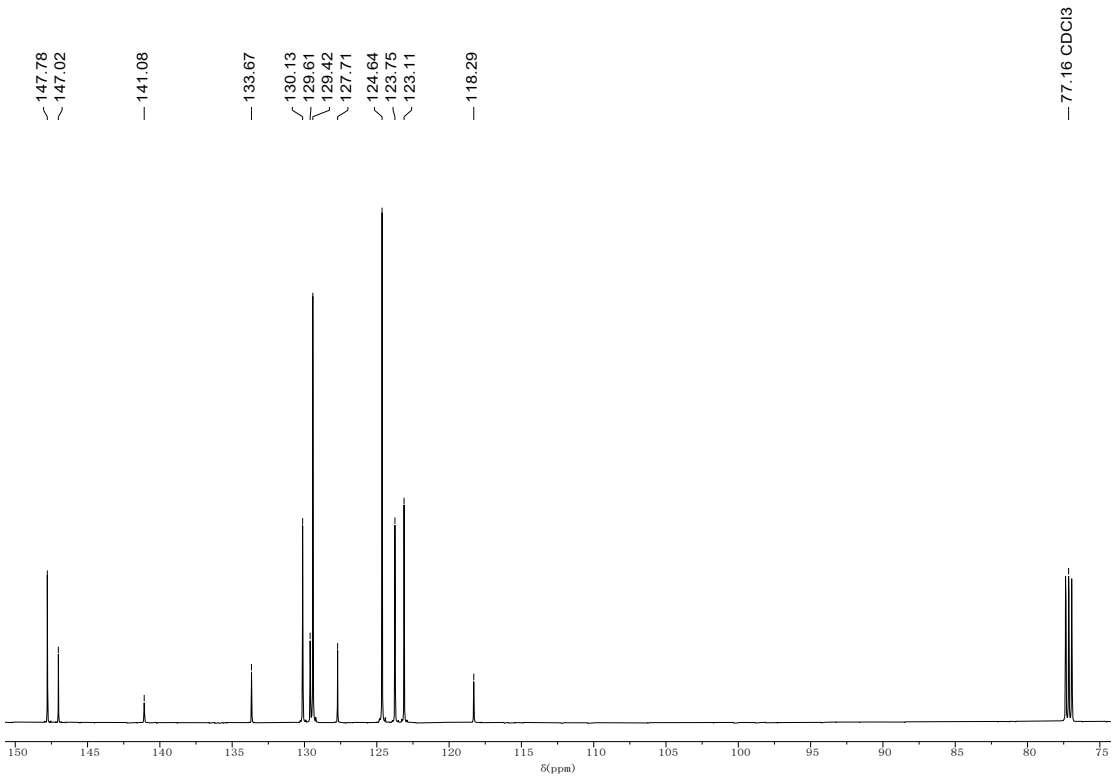


Figure S22. ^{13}C NMR spectrum of **9** in $CDCl_3$.

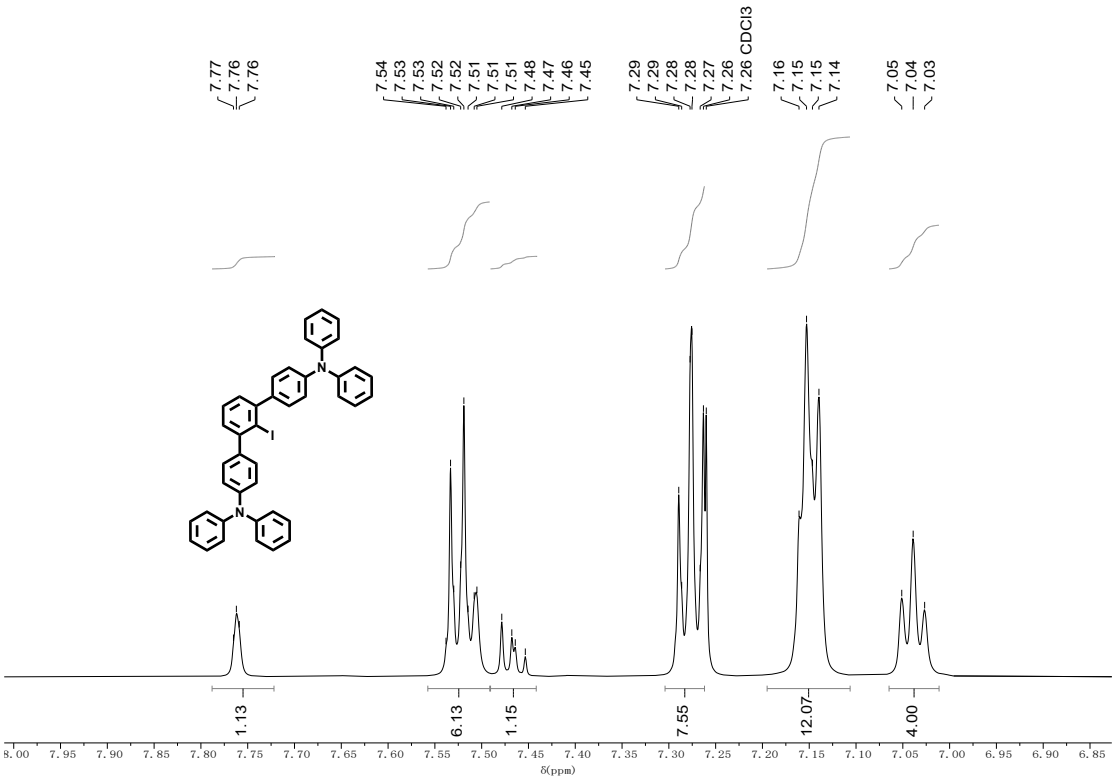


Figure S23. ^{1}H NMR spectrum of compound **10** in $CDCl_3$.

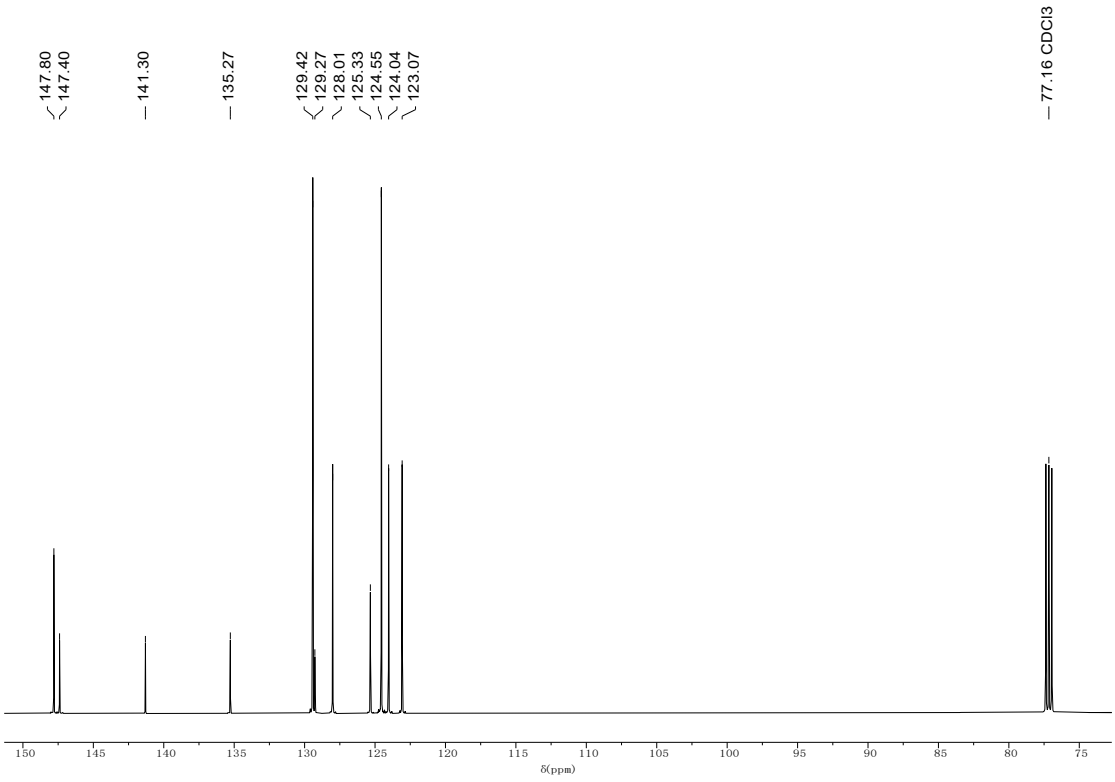


Figure S24. ^{13}C NMR spectrum of **10** in $CDCl_3$.

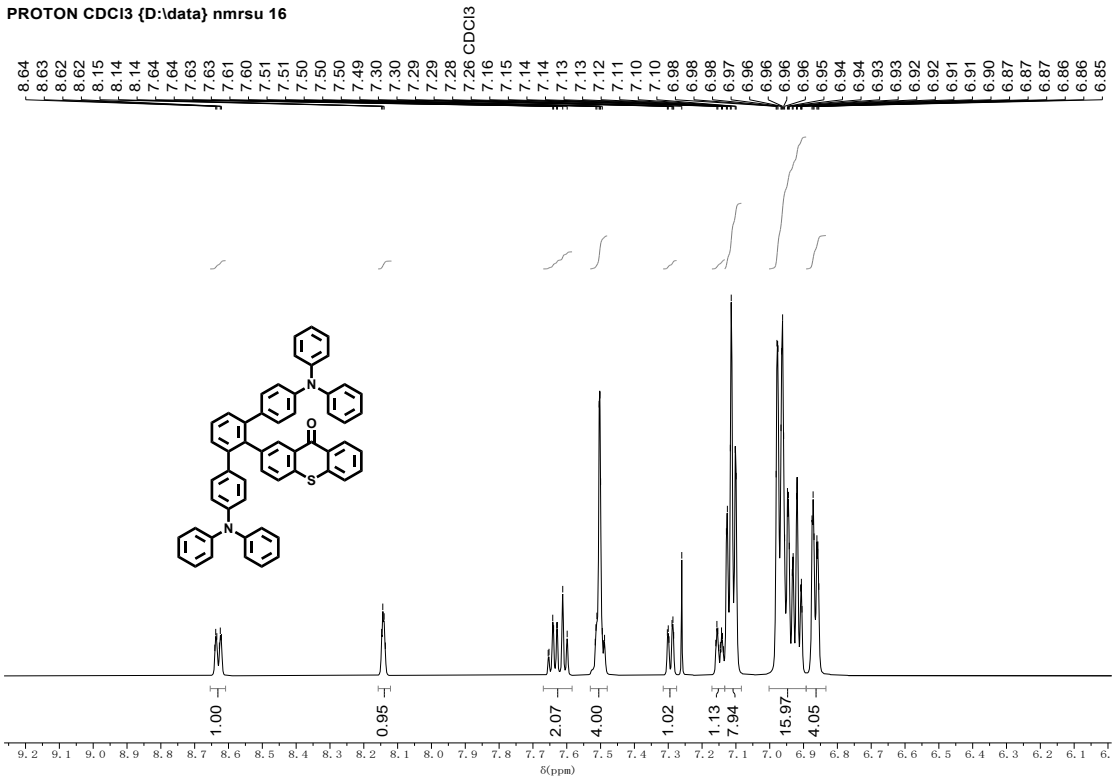


Figure S25. ^{1}H NMR spectrum of compound **11** in $CDCl_3$.

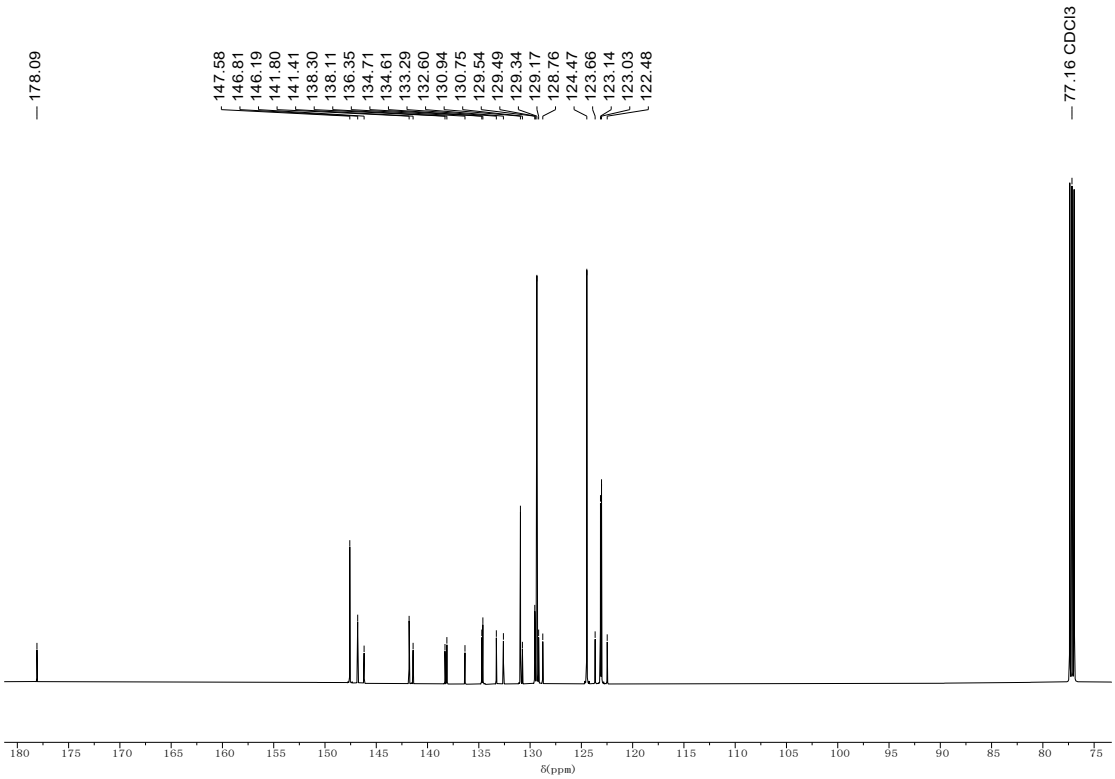


Figure S26. ^{13}C NMR spectrum of **11** in $CDCl_3$.

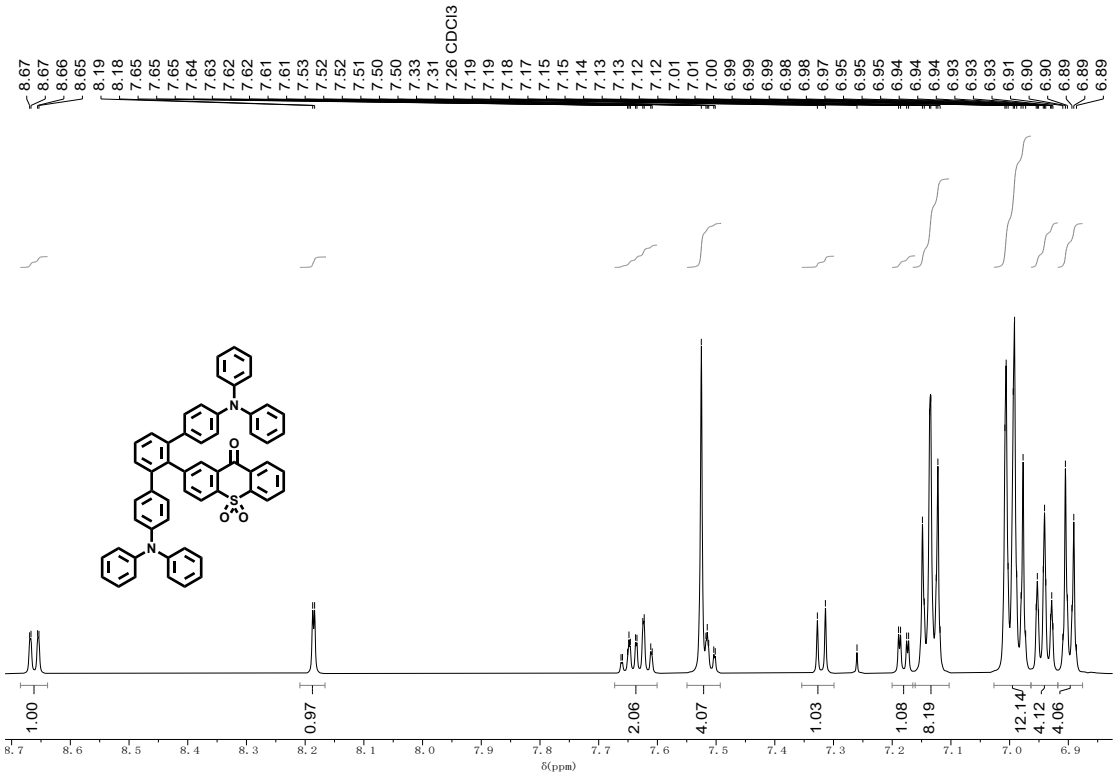


Figure S27. ^{1}H NMR spectrum of compound **2TPA** in $CDCl_3$.

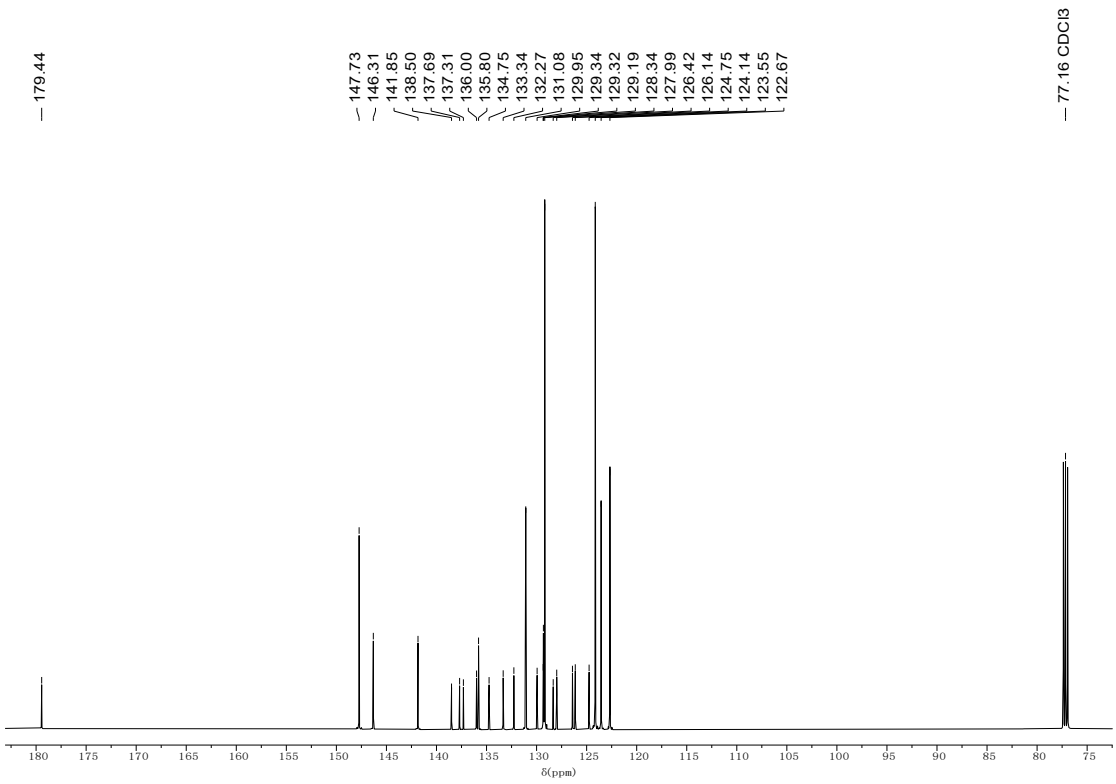


Figure S28. ^{13}C NMR spectrum of **2TPA** in $CDCl_3$.

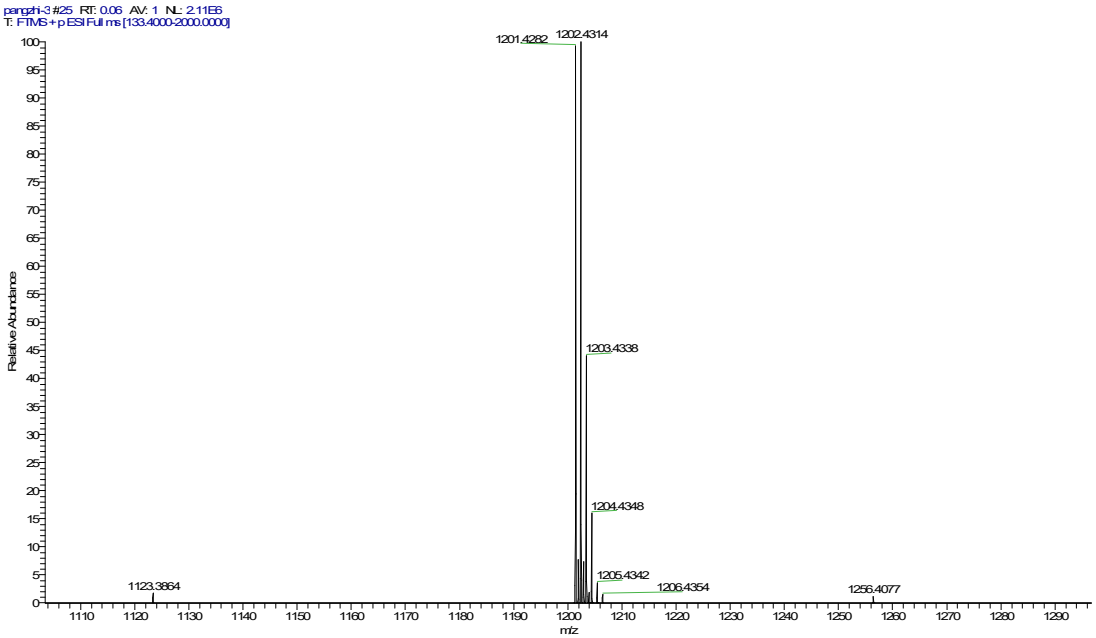


Figure S29. HR-MS spectrum of **2PhTPA**.

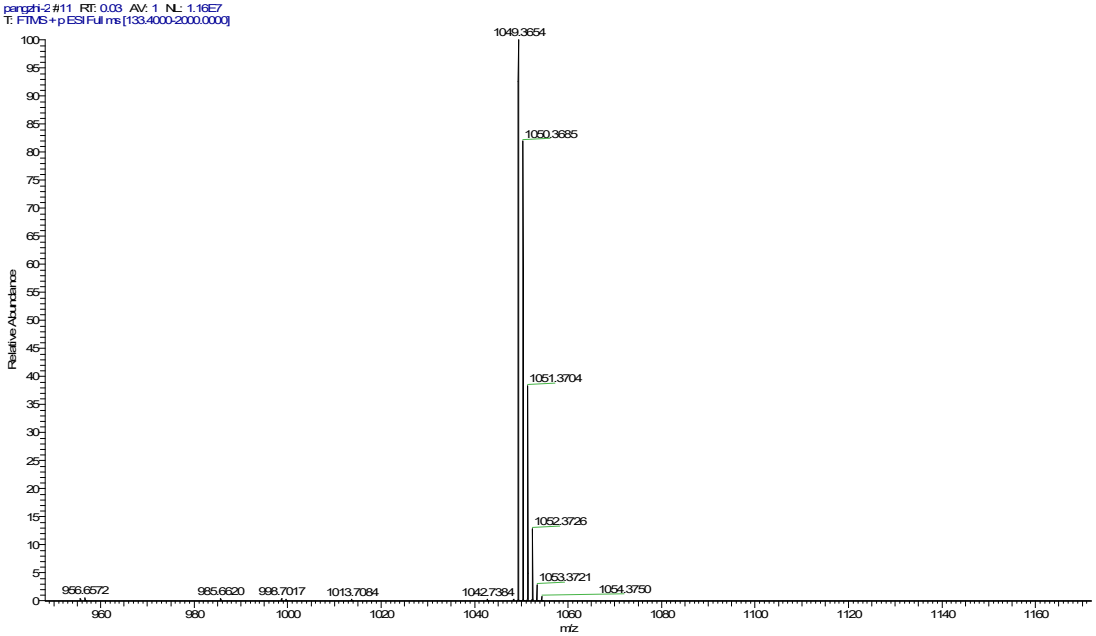


Figure S30. HR-MS spectrum of **3TPA.**

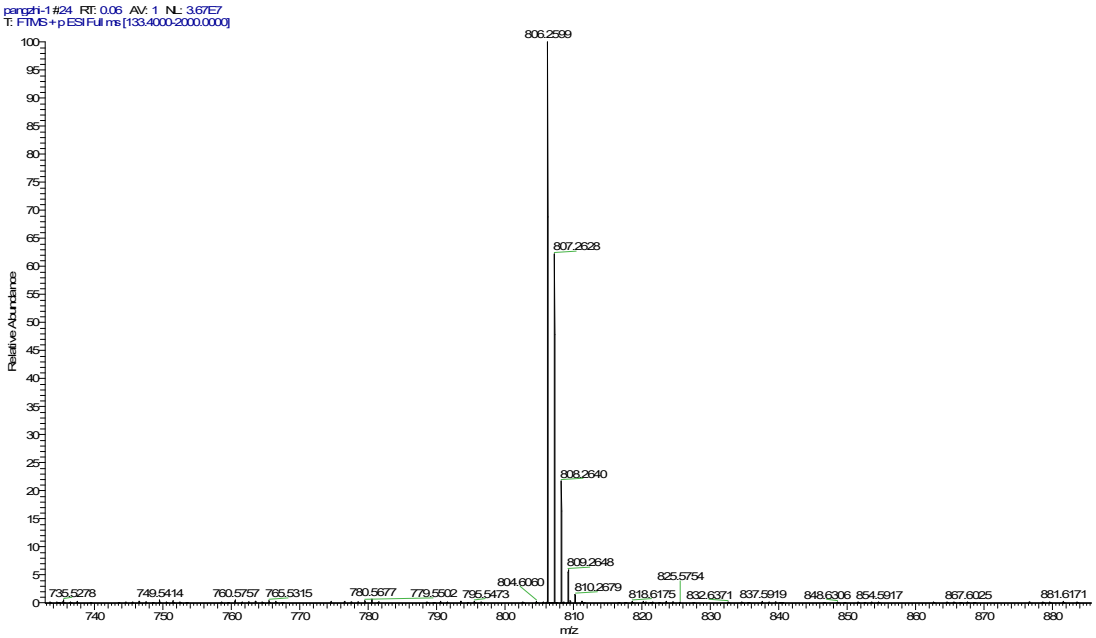


Figure S31. HR-MS spectrum of **2TPA.**

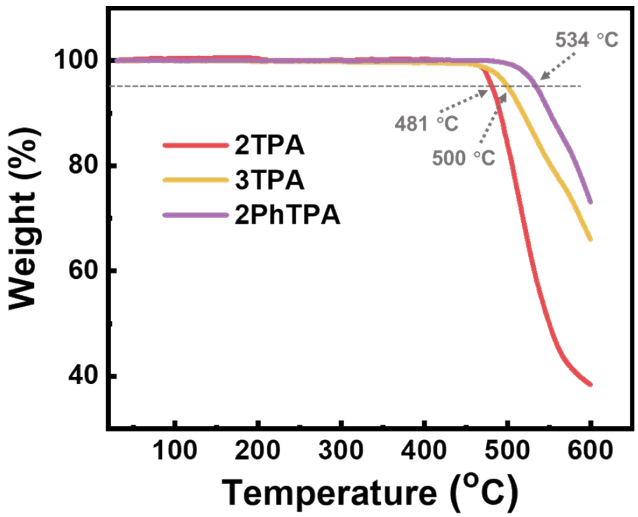


Figure S32. Thermal gravimetric analysis (TGA) curves at a heating rate of 10 ℃ min^{-1} of **2TPA**, **3TPA** and **2PhTPA**.

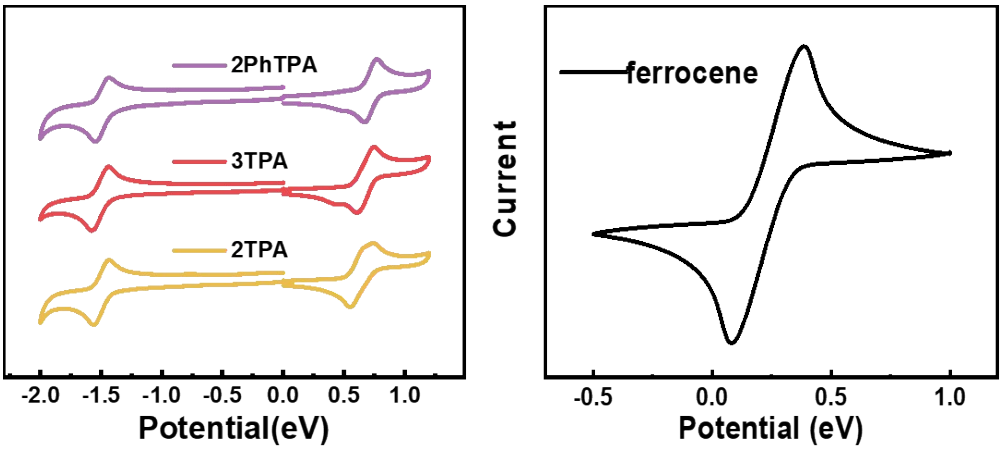


Figure S33. Cyclic voltammetry analysis of **2TPA**, **3TPA** and **2PhTPA**.

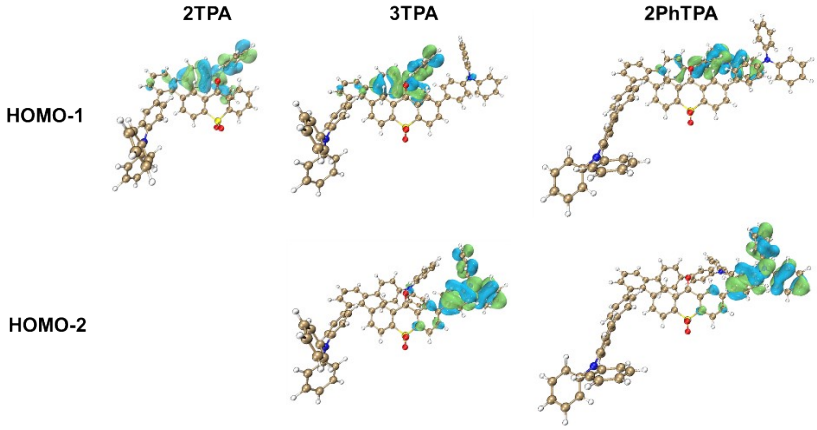


Figure S34. HOMO−1 and HOMO−2 electronic distributions of **2TPA**, **3TPA** and **2PhTPA** calculated by DFT at the b3lyp/6-31g (d, p) level.

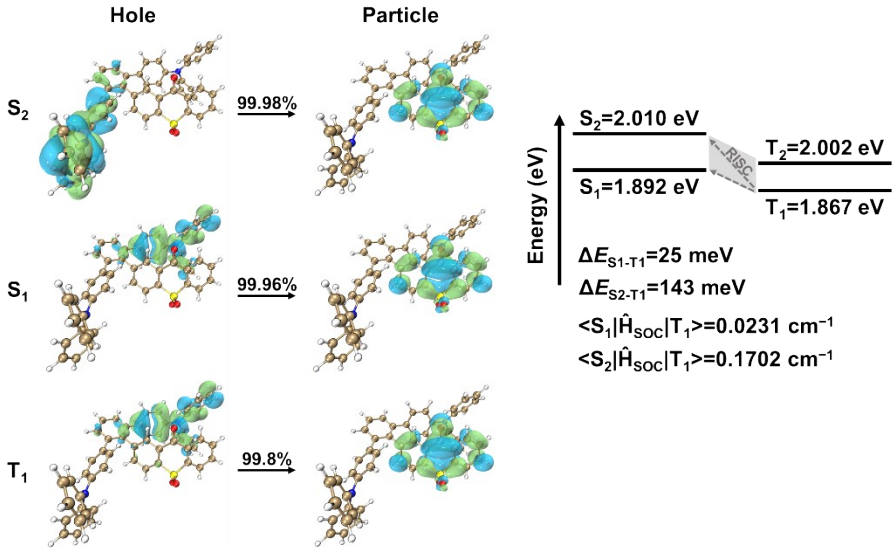


Figure S35. The natural transition orbitals (NTOs) of S_2, S_1 and T_1 for **2TPA** calculated by TD-DFT at the b3lyp/6-31g (d, p) level.

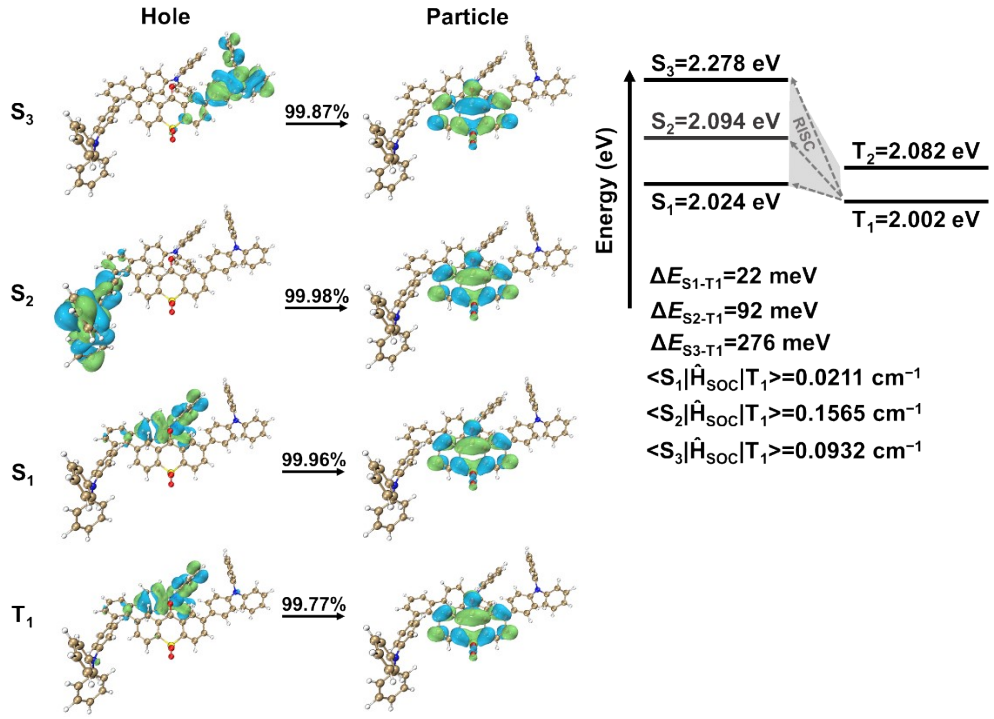


Figure S36. The natural transition orbitals (NTOs) of S_3, S_2, S_1 and T_1 for **3TPA** calculated by TD-DFT at the b3lyp/6-31g (d, p) level.

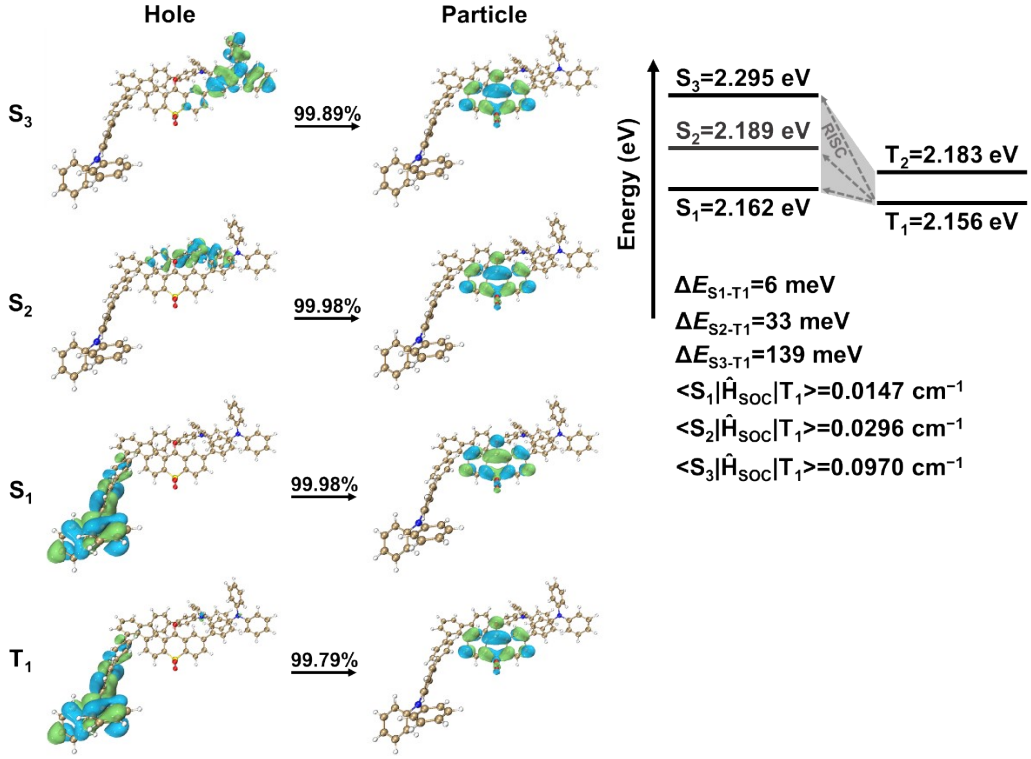


Figure S37. The natural transition orbitals (NTOs) of S_3, S_2, S_1 and T_1 for **2PhTPA** calculated by TD-DFT at the b3lyp/6-31g (d, p) level.

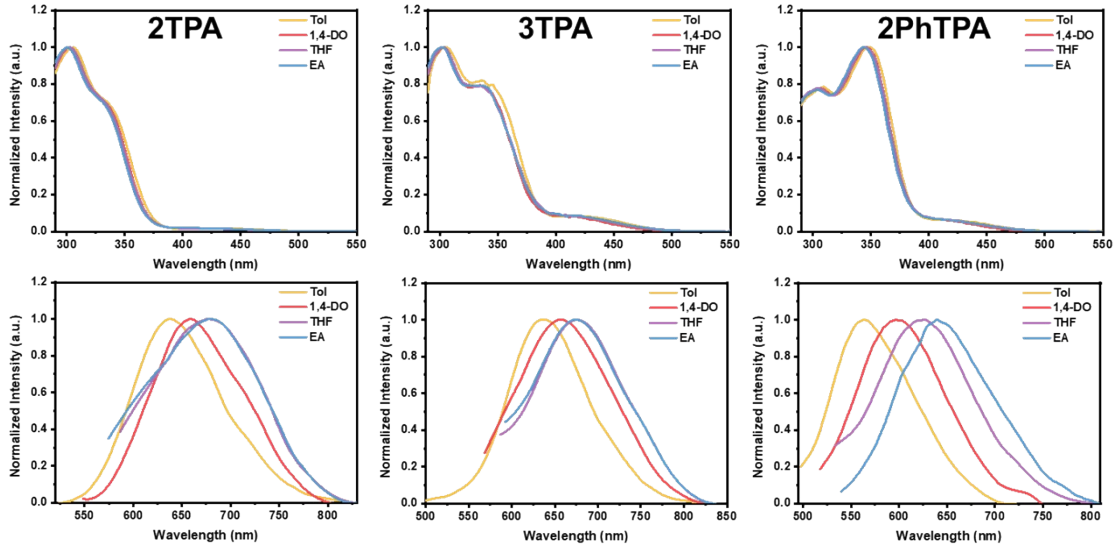


Figure S38. The normalized UV-vis absorption spectra (top) and PL spectra (bottom) for**2TPA**, **3TPA** and **2PhTPA**.

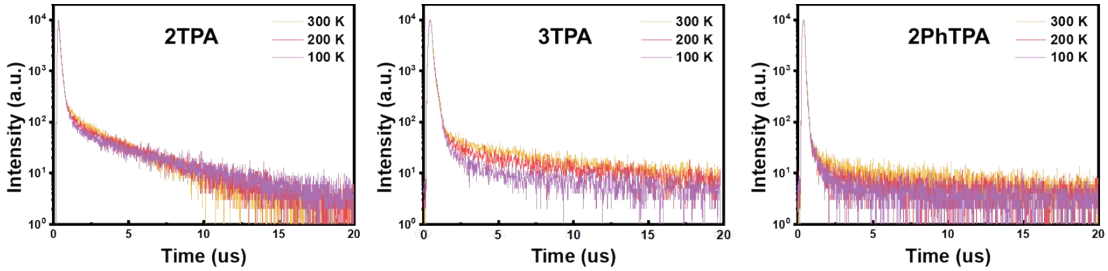


Figure S39. Transient PL decays curves of the 5 wt% emitters: 3,5DCzPPy thin films measured at varying temperatures.

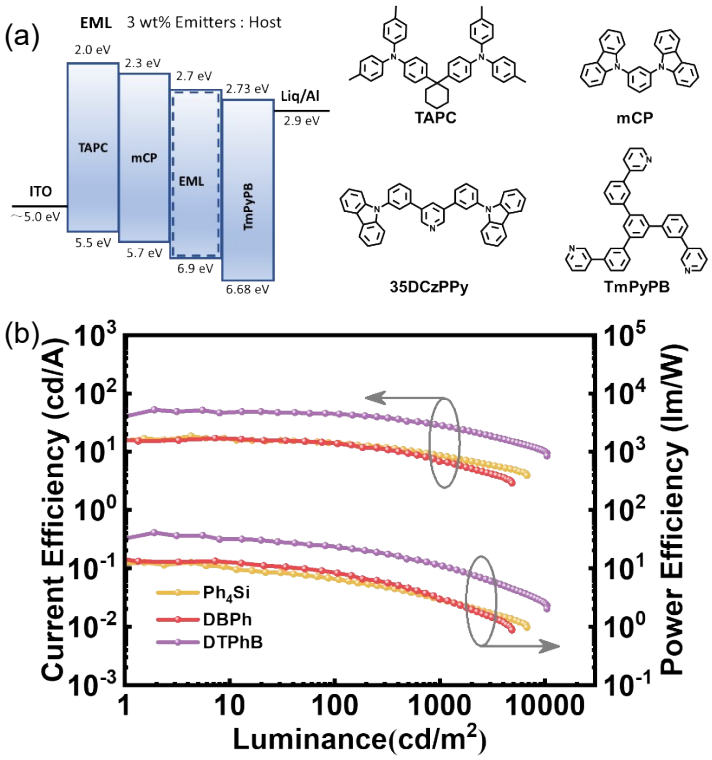


Figure S40. (a) OLED device structures, energy levels of the materials and molecular structure. (b) Current efficiency and power efficiency versus the luminance characteristic.

Table S1. Atomic coordinates for the optimized structure of **2TPA** in Gaussian 16 (gas phase).

Atom	X	Y	Z
C	2.75434700	2.22158300	−1.10863100
C	3.95273500	2.42490000	−1.80450700
C	3.34389300	4.06557100	0.37853400
C	2.46208900	3.06900900	−0.02951400
S	0.85115800	3.03418700	0.74540300
C	0.38592000	1.32678200	0.54503900
C	0.85581700	0.57462200	−0.54240400
C	0.41608700	−0.74475300	−0.67176000
C	−0.44464400	−1.32276200	0.26649200
C	−0.93952900	−0.52502900	1.30842900
C	−0.52685300	0.79631600	1.45212900
C	1.90256000	1.05392200	−1.49335900
O	2.13207100	0.43679000	−2.52733800
C	−2.22324200	−4.68492800	0.20110200
C	−1.14416500	−5.56005000	0.27208900
C	0.15379900	−5.05971300	0.33480000
C	0.38836700	−3.68031000	0.33521900
C	−0.71086600	−2.79010600	0.24177400
C	−2.02629400	−3.29654300	0.17738100
C	−3.20521700	−2.39976900	0.07295400
C	−3.27780600	−1.38275900	−0.89152400
C	−4.37880800	−0.54093000	−0.97067700
C	−5.45940700	−0.69909200	−0.08866300
C	−5.40630000	−1.72566200	0.86604200
C	−4.29366300	−2.55546400	0.94385600

N	−6.57834200	0.16043500	−0.15715700
C	1.77636600	−3.15419200	0.42361900
C	2.13554200	−2.20343400	1.38916700
C	3.34886700	−1.53418300	1.33390200
C	4.27205000	−1.82109700	0.31345300
C	3.97474100	−2.86517300	−0.57925700
C	2.74033300	−3.50352400	−0.53191100
N	5.46072100	−1.07422500	0.19154800
C	−7.20553600	0.60512400	1.03477000
C	6.03280100	−0.76825100	−1.07065100
C	−7.05989600	0.60630800	−1.41454500
C	5.90606700	−0.31578800	1.31830000
C	−8.60358300	0.67278500	1.11503700
C	−9.21560200	1.12122000	2.28258500
C	−8.44882600	1.48961900	3.38940600
C	−7.05697400	1.41511500	3.31225000
C	−6.43513400	0.98634300	2.14259100
C	−7.45979100	1.93880400	−1.58792300
C	−7.94237400	2.36847200	−2.82130500
C	−8.01592900	1.48695500	−3.90113000
C	−7.60932100	0.16244700	−3.73104400
C	−7.14389400	−0.28189800	−2.49630300
C	6.34386400	−0.96974500	2.47352100
C	6.74252500	−0.22570100	3.58300000
C	6.71675000	1.16973300	3.54159100
C	6.28334100	1.81970800	2.38426700
C	5.87327400	1.08189300	1.27681100
C	7.41223600	−0.52070500	−1.14810100
C	7.99797200	−0.17114000	−2.36137800
C	7.22750900	−0.07934500	−3.52210000
C	5.85774500	−0.33532900	−3.44805600
C	5.25728500	−0.66800800	−2.23544300
O	1.00665200	3.32119600	2.17995300
O	−0.05182600	3.86895400	−0.06365400
H	4.18306400	1.76694400	−2.63141500
H	3.08787500	4.68728500	1.22912100
H	0.82105700	−1.33556900	−1.48366900
H	−1.61821200	−0.96087500	2.03325700
H	−0.87228000	1.40423600	2.28072900
H	−3.23558200	−5.06994400	0.13289900
H	−1.31454900	−6.63224100	0.27935400
H	1.00013600	−5.73493100	0.41167700
H	−2.45402000	−1.24170700	−1.58234500
H	−4.40973300	0.24565000	−1.71569300
H	−6.23638100	−1.85936700	1.55031600
H	−4.26171400	−3.33503100	1.69909400
H	1.42501500	−1.93383600	2.16235900
H	3.56874900	−0.76274100	2.06087800
H	4.69425000	−3.13812300	−1.34172000
H	2.50219800	−4.25631000	−1.27759000
H	−9.19873500	0.37657200	0.25843500
H	−10.29929500	1.16953900	2.33067100
H	−8.92966900	1.83213100	4.29991700
H	−6.44806000	1.70838700	4.16208600
H	−5.35369100	0.94341500	2.07667800
H	−7.38976900	2.62705000	−0.75313900
H	−8.24782400	3.40344000	−2.94152900

H	−8.38474100	1.82793700	−4.86302600
H	−7.66742400	−0.53585800	−4.56052300
H	−6.84006000	−1.31393800	−2.36079200
H	6.35890200	−2.05439200	2.49232000
H	7.08103800	−0.73727400	4.47870300
H	7.02944600	1.74598400	4.40652600
H	6.24631200	2.90413500	2.34638200
H	5.52189700	1.57638400	0.37982500
H	8.01459900	−0.59658600	−0.24979400
H	9.06638600	0.01917100	−2.39973400
H	7.68793100	0.18471600	−4.46861600
H	5.23693300	−0.25915900	−4.33591000
H	4.18754200	−0.82784000	−2.19619900
C	4.54076100	4.23870800	−0.31648600
H	5.23878500	5.00795000	−0.00213800
C	4.83676700	3.42739000	−1.41491000
H	5.76672500	3.56114300	−1.95742200

Table S2. Atomic coordinates for the optimized structure of **3TPA** in Gaussian 16 (gas phase).

Atom	X	Y	Z
C	0.49722800	−1.61432200	0.08477600
C	1.86659600	−1.57445400	0.34552600
C	2.77436100	−2.37410800	−0.36530800
C	2.26617000	−3.25839900	−1.33265700
C	0.90123800	−3.32610700	−1.59800600
C	0.02829800	−2.49616000	−0.90175000
S	−1.72053100	−2.65077000	−1.21190800
C	−2.26864100	−0.98594300	−0.87765700
C	−1.66542900	−0.24094200	0.14710200
C	−2.20302500	1.00588900	0.46999800
C	−3.28226500	1.53999500	−0.24234600
C	−3.85278800	0.77326300	−1.27045200
C	−3.36258600	−0.49307000	−1.57949800
C	−0.37876000	−0.63186600	0.79550100
O	0.01064700	−0.06538300	1.81025300
N	8.36997100	−1.69585600	0.57190200
C	8.76738700	−0.66089200	1.46248700
C	9.36078100	−2.44438700	−0.11188300
C	6.99822200	−1.88468300	0.30854900
C	9.78052800	0.23602400	1.10078200
C	10.14640900	1.26302700	1.96827300
C	9.50041600	1.41757000	3.19613700
C	8.49157900	0.52149600	3.55723800
C	8.13129200	−0.51745500	2.70346600
C	6.47436600	−3.15377800	0.00831500
C	5.11297500	−3.31488600	−0.22276500
C	4.22427500	−2.23154800	−0.13169900
C	4.76032100	−0.97123300	0.17698600
C	6.11984600	−0.79261900	0.36806200
C	9.21740600	−2.75094400	−1.47259300
C	10.19938700	−3.48805000	−2.12968900
C	11.34336900	−3.91067100	−1.45085200

C	11.49219800	−3.59406900	−0.09938200
C	10.50713700	−2.87452400	0.57141200
C	−5.58507500	4.47874800	0.46014000
C	−4.68946400	5.54273000	0.45754200
C	−3.33381300	5.30352600	0.25550600
C	−2.85638300	4.00577600	0.03261600
C	−3.76843500	2.92194800	0.03128600
C	−5.14267700	3.16396100	0.26164800
C	−6.13407600	2.05936300	0.33124600
C	−5.94479400	0.95470100	1.17585400
C	−6.86479900	−0.08347200	1.22193700
C	−8.02113200	−0.04301800	0.42690600
C	−8.23221100	1.06830100	−0.40259100
C	−7.29888400	2.09797600	−0.44824900
N	−8.95396600	−1.10351400	0.45559200
C	−1.39635200	3.80808500	−0.17621000
C	−0.88252100	3.13513300	−1.29472900
C	0.47488400	2.86484600	−1.41141100
C	1.36965100	3.28152800	−0.41383900
C	0.87444100	4.01036500	0.67599800
C	−0.48841800	4.25943600	0.79241400
N	2.74583600	2.95990200	−0.50138900
C	−9.56049800	−1.54485600	−0.74809300
C	3.44644600	2.50118600	0.64005400
C	−9.25361400	−1.75703500	1.67797000
C	3.38739500	3.01536000	−1.76812000
C	−10.92236100	−1.87676600	−0.77332000
C	−11.51144300	−2.32084800	−1.95425300
C	−10.76109800	−2.42279100	−3.12701400
C	−9.40673500	−2.08527200	−3.10375500
C	−8.80418200	−1.65855200	−1.92332300
C	−9.38697000	−3.15195100	1.72251500
C	−9.69178300	−3.78633200	2.92390900
C	−9.84899700	−3.04708100	4.09748300
C	−9.70716200	−1.65905600	4.05494200
C	−9.42194800	−1.01338900	2.85480300
C	3.18960700	4.12727200	−2.59822600
C	3.79592600	4.18326400	−3.85048300
C	4.62153700	3.14447300	−4.28399800
C	4.82521300	2.04086500	−3.45407300
C	4.20692900	1.96687300	−2.20841100
C	4.81897700	2.76383200	0.78598000
C	5.51244100	2.28382800	1.89506500
C	4.85354600	1.55074300	2.88361500
C	3.48626400	1.30571200	2.74976700
C	2.78433900	1.76757900	1.63869700
O	−1.92804400	−2.94596700	−2.63871400
O	−2.30403400	−3.54245900	−0.19612000
H	2.21640200	−0.89094000	1.10880000

H	2.95222600	−3.86537100	−1.91396600
H	0.51101400	−3.98715100	−2.36377200
H	−1.72056300	1.57494400	1.25412100
H	−4.68393900	1.17877900	−1.83565800
H	−3.79858700	−1.08682200	−2.37494200
H	10.27011300	0.12350200	0.13977500
H	10.93053700	1.95434800	1.67509600
H	9.78274700	2.22313800	3.86610700
H	7.99134400	0.62238200	4.51569500
H	7.34748100	−1.21310300	2.98110000
H	7.13657300	−4.01098400	−0.02935900
H	4.72903900	−4.30924000	−0.42969700
H	4.10970800	−0.10918100	0.24787500
H	6.49996300	0.19747600	0.57720300
H	8.33687100	−2.40973700	−2.00520200
H	10.07496100	−3.71922000	−3.18329200
H	12.10942200	−4.47873800	−1.96844500
H	12.37476800	−3.92046200	0.44229600
H	10.61654000	−2.63809800	1.62399100
H	−6.63973300	4.65101300	0.64909400
H	−5.04566800	6.55527700	0.62000400
H	−2.62784700	6.12769800	0.24352900
H	−5.05332700	0.90030100	1.79116800
H	−6.69292600	−0.93517900	1.86982600
H	−9.12445800	1.11142400	−1.01681400
H	−7.46866400	2.94378600	−1.10786000
H	−1.56125900	2.78221600	−2.06365500
H	0.85014800	2.31676200	−2.26815100
H	1.55939300	4.34985700	1.44457900
H	−0.86231100	4.78912900	1.66322700
H	−11.50667800	−1.78751400	0.13572400
H	−12.56695800	−2.57563800	−1.95945500
H	−11.22533200	−2.76298600	−4.04696900
H	−8.80871200	−2.17048700	−4.00602500
H	−7.74841900	−1.41240100	−1.90049600
H	−9.25050900	−3.72794000	0.81422800
H	−9.79083600	−4.86738700	2.94398800
H	−10.07805200	−3.54632900	5.03333600
H	−9.83305600	−1.07077400	4.95890000
H	−9.32435300	0.06598100	2.81930900
H	2.55654900	4.93780700	−2.25401900
H	3.63252900	5.04995300	−4.48378800
H	5.09894900	3.19394700	−5.25728900
H	5.45767400	1.22123600	−3.78140100
H	4.35798300	1.09968400	−1.57761900
H	5.33594900	3.33525100	0.02371100
H	6.57613200	2.48218100	1.98862200
H	5.40280200	1.17325000	3.73922000
H	2.95301200	0.73092000	3.50076300

H	1.72801000	1.54768300	1.54582300

Table S3. Atomic coordinates for the optimized structure of **2PhTPA** in Gaussian 16 (gas phase).

Atom	X	Y	Z
C	−0.64111900	0.97432900	−0.13860900
C	−1.94980500	1.33172900	0.19409600
C	−2.66443400	2.27625700	−0.55136800
C	−2.04073500	2.85305500	−1.67232500
C	−0.74400400	2.50269500	−2.03068400
C	−0.05058600	1.56968100	−1.26320400
S	1.66118000	1.28728400	−1.67606100
C	1.95602900	−0.31800700	−0.96093300
C	1.26206800	−0.72902000	0.18682200
C	1.65767300	−1.91225000	0.81025500
C	2.67410500	−2.71493800	0.28463300
C	3.33153100	−2.28721200	−0.87895600
C	2.98811900	−1.08549900	−1.49274500
C	0.03306800	−0.05857400	0.70562900
O	−0.47058400	−0.41494100	1.76411300
N	−7.96881100	3.77046600	0.95695300
C	−8.66087400	3.07517700	1.98210100
C	−8.60339100	4.85762700	0.30107600
C	−6.65506600	3.39735900	0.59851700
C	−10.03400700	2.81881600	1.85931100
C	−10.71363300	2.13918300	2.86601800
C	−10.03683200	1.68991500	4.00110600
C	−8.67037100	1.94468200	4.12466700
C	−7.98629200	2.64194600	3.13203700
C	−5.72897000	4.36798600	0.18410700
C	−4.44900000	3.99848700	−0.20575600
C	−4.03544100	2.65862400	−0.16163000
C	−4.96076500	1.69681400	0.27302800
C	−6.25277400	2.05235500	0.63321400
C	−8.47833600	5.02568400	−1.08630300
C	−9.10752000	6.09216100	−1.72324800
C	−9.88160900	6.99682100	−0.99493100
C	−10.00889500	6.82925700	0.38491700
C	−9.36888700	5.77605300	1.03318100
C	4.55876600	−5.63069600	1.84114700
C	3.52289600	−6.52678600	2.08247000
C	2.21662800	−6.18013200	1.74777600
C	1.93684900	−4.94452800	1.15565400
C	2.98764700	−4.02690200	0.91723500
C	4.31111800	−4.37358900	1.27156100
C	5.45137100	−3.43841800	1.08812300
C	5.40762000	−2.12056900	1.56740300
C	6.48214200	−1.25925200	1.38750900
C	7.64921400	−1.67909300	0.72658600
C	7.69588700	−3.00299800	0.26150900
C	6.61863700	−3.86515100	0.43926400
C	0.53304400	−4.61329200	0.78184000
C	0.17027300	−4.39035500	−0.55310600
C	−1.11872200	−3.98744100	−0.88224500
C	−2.08569800	−3.78033900	0.11409000
C	−1.72455500	−4.02127100	1.44775500
C	−0.44022800	−4.44550500	1.77464400
O	1.78881400	1.19468400	−3.13919300

O	2.48010000	2.26940000	−0.94561800
H	−2.38912500	0.87144800	1.07113800
H	−2.59196600	3.56218600	−2.28097600
H	−0.26999200	2.93161200	−2.90655900
H	1.11208300	−2.21418600	1.69359300
H	4.11659600	−2.90192000	−1.30432500
H	3.49714600	−0.74923000	−2.38898400
H	−10.56054000	3.15988200	0.97582500
H	−11.77696100	1.94913100	2.75479100
H	−10.56762400	1.15216000	4.77983000
H	−8.13198600	1.61268500	5.00714500
H	−6.92759400	2.84901500	3.23830600
H	−6.01917800	5.41184700	0.17108100
H	−3.74288900	4.76710600	−0.50460400
H	−4.68139900	0.64843800	0.26932600
H	−6.96929800	1.28923100	0.91086600
H	−7.87736400	4.32501100	−1.65380700
H	−9.00022300	6.20785900	−2.79748100
H	−10.37684000	7.82237700	−1.49544600
H	−10.59929400	7.53086800	0.96630600
H	−9.46127900	5.65333700	2.10631100
H	5.57535200	−5.88236500	2.12540600
H	3.73203800	−7.49076700	2.53571700
H	1.40046500	−6.87400800	1.92188000
H	4.51729700	−1.76627600	2.07508000
H	6.40675300	−0.23567700	1.73935400
H	8.59415700	−3.36533200	−0.22796800
H	6.67443000	−4.88194000	0.06196300
H	0.91648700	−4.50505900	−1.33265000
H	−1.37537700	−3.79889400	−1.92009400
H	−2.46382200	−3.88789900	2.23094800
H	−0.17271600	−4.61319100	2.81359400
C	−3.46274900	−3.36095100	−0.22876600
C	−4.13741600	−2.37827800	0.51402200
C	−4.15153000	−3.97945700	−1.28359700
C	−5.46471000	−2.05766900	0.24209800
H	−3.61335100	−1.86953200	1.31789700
C	−5.47298700	−3.65903800	−1.56615200
H	−3.65029500	−4.74395100	−1.86888400
C	−6.15343000	−2.71058500	−0.79029300
H	−5.98761600	−1.32073600	0.84258600
H	−6.00094200	−4.16234600	−2.36851100
C	8.78632200	−0.75733200	0.52609900
C	9.11250800	0.21712900	1.48378200
C	9.57937500	−0.81972900	−0.63159400
C	10.18210300	1.08347900	1.30170900
H	8.54267800	0.27093900	2.40584700
C	10.64100000	0.05257100	−0.83190100
H	9.33238800	−1.53525700	−1.40944600
C	10.96059900	1.01706200	0.13600400
H	10.42725400	1.81437100	2.06382100
H	11.22384000	0.00143000	−1.74448800
N	−7.52502600	−2.44948300	−1.02581400
N	12.04172800	1.90539900	−0.05958200
C	−7.99520300	−1.11613500	−1.12773000
C	−9.19154900	−0.74635600	−0.49550400
C	−7.29298100	−0.16638600	−1.88104700

C	−9.69408200	0.54134600	−0.65062300
H	−9.72424700	−1.48030500	0.09886700
C	−7.79787600	1.12537900	−2.01713900
H	−6.36172400	−0.45013100	−2.35903700
C	−9.00488000	1.48347200	−1.41652600
H	−10.61917200	0.81416300	−0.15518800
H	−7.24196500	1.85307100	−2.60035700
H	−9.39689400	2.48776400	−1.52896700
C	−8.41927800	−3.53025700	−1.22101400
C	−9.46049900	−3.43593500	−2.15681200
C	−8.27336000	−4.71204200	−0.47838400
C	−10.34017100	−4.50044400	−2.33446500
H	−9.57371400	−2.52734800	−2.73703800
C	−9.14734300	−5.77698700	−0.67794400
H	−7.47349900	−4.78683700	0.24960600
C	−10.18901000	−5.67896400	−1.60206200
H	−11.14082200	−4.41109100	−3.06263600
H	−9.02022100	−6.68437600	−0.09509100
H	−10.87272900	−6.50864900	−1.74911300
C	11.93443100	3.25749800	0.35643500
C	13.01719900	3.89346700	0.98013600
C	10.74664300	3.97244200	0.14632100
C	12.91201100	5.22395600	1.37710600
H	13.93441500	3.33934500	1.14550500
C	10.64468800	5.29656700	0.56472400
H	9.91086700	3.48315900	−0.34119000
C	11.72585300	5.93237100	1.17759200
H	13.75871200	5.70419500	1.85831800
H	9.71841900	5.83746000	0.39638700
H	11.64501600	6.96681200	1.49537900
C	13.23341700	1.45255000	−0.67973800
C	13.89768000	2.26121900	−1.61322200
C	13.76348500	0.19295800	−0.36441100
C	15.07409900	1.81734400	−2.21123700
H	13.48673700	3.23366900	−1.86011700
C	14.92996900	−0.24969900	−0.98240100
H	13.25418700	−0.43026100	0.36209700
C	15.59555100	0.55916000	−1.90515300
H	15.57756200	2.45469300	−2.93192100
H	15.32826800	−1.22747700	−0.72852400
H	16.50865600	0.21378200	−2.37900900

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