

Supporting Information

**Isomeric thermally activated delayed fluorescence emitters based on
quinolino[3,2,1-de]acridine-5,9-dione multiple resonance core and carbazole
substituent**

*Jing-Feng Liu[#], Sheng-Nan Zou[#], Xing Chen, Sheng-Yi Yang, You-Jun Yu, Man-Keung
Fung*, Zuo-Quan Jiang*, and Liang-Sheng Liao*

Institute of Functional Nano & Soft Materials (FUNSOM), Jiangsu Key Laboratory for
Carbon-Based Functional Materials & Devices, Soochow University, 199 Ren'ai Road,
Suzhou, 215123, Jiangsu, PR China

E-mail: mkfung@suda.edu.cn; zqjiang@suda.edu.cn.

[#] These authors contributed equally.

Experimental Section

1.1 Materials and instruments

The raw reagents, catalysts and chemicals involved in the initial reaction were all from commercial companies and without further purification. Solvents used in the reaction, such as toluene, tetrahydrofuran, etc. were purified by P solvents purification system. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 spectrometer or Bruker 600 spectrometer at room temperature. Mass spectroscopy was performed using a Thermo Fisher ISQ Single Quadrupole GC-MS with direct probe system. The ultraviolet-visible (UV-vis) absorption spectra were measured by a Shimadzu UV-2600 spectrophotometer. Fluorescent as well as phosphorescent spectra were measured by a Hitachi F-4600 spectrophotometer. Thermogravimetric analysis (TGA) was measured by a METTLER TOLEDO TGA1 under high purity nitrogen atmosphere. The temperature was increased to 800 or 900 °C with a heating rate of 10 °C/minute. DFT and TD-DFT calculations were performed utilizing m062x with the 6-31g(d) atomic basis set. RDG analysis was obtained by Multiwfn (version 3.5) and plotted by VMD (version 1.9.3). Electrochemical analysis was achieved on a CHI 600D electrochemical work station, and the scan rate was 100 mV S⁻¹ at room temperature. The three-electrode configuration system in *n*-Bu₄NPF₆ (0.1 M) DMF solution. The redox potential of ferrocene/ferrocenium(Fc/Fc⁺) was measured under room temperature (for calibration). The PLQY was measured using Hamamatsu C9920-02G in nitrogen or air atmosphere. Transient spectra were obtained by using Quantaaurus-

Tau fluorescence lifetime measurement system (C11367-03, Hamamatsu Photonics Co.) in vacuum or nitrogen atmosphere. Elemental analysis was measured using Vario Micro cube.

1.2 Single crystal information

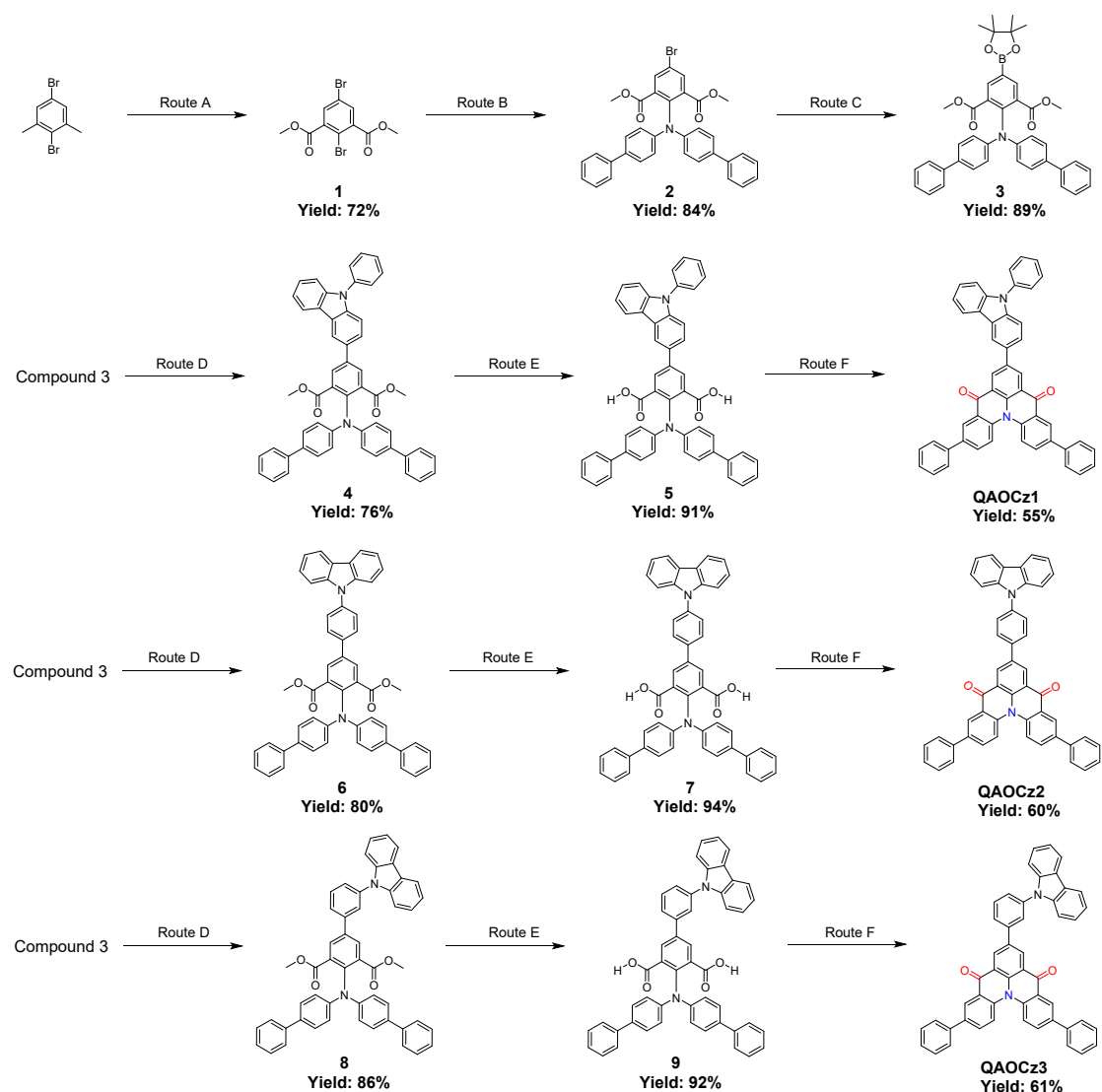
The crystal of QAOCz1, QAOCz2, and QAOCz3 was grown by slow evaporation in CHCl_3 and THF. We use Bruker D8-Venture diffractometer with a Turbo X-ray Source (Mo-K α radiation, $\lambda = 0.71073 \text{ \AA}$) adopting the direct-drive rotating anode technique and a CMOS detector to collect the single-crystal data. The structures were solved by direct methods and refined by the full-matrix least-squares on F² using the SHELXTL-2014 program. The X-ray crystallographic coordinates for structure reported in this study have been deposited at the Cambridge Crystallographic Data Centre (CCDC), under deposition number QAOCz1 (2026179), QAOCz2 (2026178), and QAOCz3 (2026181). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre “http://www.ccdc.cam.ac.uk/data_request/cif”.

1.3 Device fabrication process

OLEDs were fabricated on ITO glass substrates layer (110 nm, 15 Ω/square) under a base pressure of 3×10^{-6} Torr. The active area of each device is 0.09 cm^2 . Deposition rates and thicknesses of all materials were monitored with oscillating quartz crystals. The doping layer was deposited by utilizing two different sensors to monitor the

deposition rates of both host material and dopant material. The deposition rate of the host was controlled at 0.2 nm s^{-1} , and the deposition rate of the dopant was adjusted according to the volume ratio doped in the host materials. The electroluminescence (EL) and current density-voltage (J-V) characteristics of the devices were measured by a constant current source (Keithley 2400 SourceMeter) combined with a photometer (Photo Research SpectraScan PR655).

1.4 Syntheses of Materials



Scheme S1. Route A: Synthesis of 1: (i) KMnO_4 (2.2 equiv.), *t*-BuOH, H_2O , reflux, 24 h. (ii) MeOH, H_2SO_4 , reflux. Route B: Synthesis of 2: di([1,1'-biphenyl]-4-yl)amine (1 equiv.), Cu

(0.1 equiv.), Cu (0.1 equiv.), 2,2,6,6-tetramethylheptane-3,5-dione (0.1 equiv.), potassium carbonate (1.5 equiv.), 1-butoxybutane, reflux, 48 h. Route C: Synthesis of 3: Bpin₂ (1.4 equiv.), Pd(dppf)Cl₂ (0.05 equiv.), potassium acetate (1.4 equiv.), 1,4-dioxane, reflux, 12 h. Route D: Synthesis of 4, 6 and 8: 3-bromo-9-phenyl-9H-carbazole/9-(4-bromophenyl)-9H-carbazole/9-(3-bromophenyl)-9H-carbazole (1.2 equiv.), tetrakis(triphenylphosphine)palladium (0.05 equiv.), potassium carbonate (4 equiv.), 1,4-dioxane, 100 °C, 10 h. Route E: Synthesis of 5, 7 and 9: sodium hydroxide (5 equiv.), THF/water = 1:1, reflux, 48 h. Route F: Synthesis of QAOCz1/QAOCz2/QAOCz3: oxalyl chloride Tin(IV) (2.2 equiv.), oxalyl chloride (2.2 equiv.), DMF, DCM, reflux, 4h.

dimethyl 5-bromo-2-(di([1,1'-biphenyl]-4-yl)amino)isophthalate (2). Compound dimethyl 2,5-dibromoisophthalate (**1**) (7.04 g, 20 mmol), di([1,1'-biphenyl]-4-yl)amine (6.43 g, 20 mmol), potassium carbonate (4.15 g, 30 mmol), copper(I) iodide (0.38 g, 2 mmol), 2,2,6,6-tetramethylheptane-3,5-dione (0.37 g, 2 mmol) and activated copper powder (0.13 g, 2 mmol) were combined with 150 mL 1-butoxybutane in a roundbottom flask equipped with a reflux condenser and magnetic stir bar. The reaction mixture was heated to 142 °C for 48 h under argon. After cooled to room temperature, the reaction was filtered, the solvent removed under vacuum condition, and then the residue purified by column chromatography on silica gel using petroleum ether/dichloromethane (1/1, v/v) as eluent, yellow solid was finally obtained. Yield: 9.95 g (84%). ¹H NMR (400 MHz, Chloroform-d) δ 7.92 (s, 2H), 7.58 – 7.54 (m, 4H), 7.49 – 7.45 (m, 4H), 7.41 (t, *J* = 7.7 Hz, 4H), 7.33 – 7.28 (m, 2H), 7.09 – 7.04 (m, 4H), 3.49 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 165.90, 145.86, 143.19, 140.50, 136.61, 135.30, 134.19, 128.77, 127.48, 126.91, 126.63, 122.67, 118.31, 52.52. MS (EI) *m/z*: 591.228 [M⁺]. Calcd for C₃₄H₂₆BrNO₄: 591.10. Elemental analysis (calculated, found for C₃₄H₂₆BrNO₄): C (68.93%, 68.84%), H (4.42%, 4.50%), N (2.36%, 2.33%).

dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)isophthalate (3). Compound dimethyl 5-bromo-2-(di([1,1'-biphenyl]-4-yl)amino)isophthalate (**2**) (8.89 g, 15 mmol), 4,4,4',4',5,5,5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (5.33 g, 21.00 mmol), Pd(dppf)Cl₂ (612 mg, 0.75 mmol) and potassium acetate (5.89 g, 60 mmol) were combined with 100 mL 1,4-dioxane in a roundbottom flask equipped with a reflux condenser and magnetic stir bar. The reaction mixture was heated to 100 °C for 12 h under argon. After cooled to room temperature, the reaction was filtered, the solvent removed under vacuum condition, and then the residue purified by column chromatography on silica gel using petroleum ether/dichloromethane (3/2, v/v) as eluent, yellow solid was finally obtained. Yield: 8.54 g (89%). ¹H NMR (400 MHz, Chloroform-d) δ 8.21 (s, 2H), 7.60 – 7.53 (m, 4H), 7.49 – 7.37 (m, 8H), 7.31 (d, *J* = 7.4 Hz, 2H), 7.12 – 7.04 (m, 4H), 3.47 (s, 6H), 1.35 (s, 12H). ¹³C NMR (101 MHz, CDCl₃) δ 167.38, 146.37, 146.06, 140.59, 139.94, 135.16, 131.71, 128.73, 127.39, 126.82, 126.62, 122.92, 84.38, 52.19, 24.87. MS (EI) *m/z*: 361.12 [M⁺]. Calcd for C₃₄H₂₆BrNO₄: 591.10. MS (EI) *m/z*: 591.003 [M⁺]. Calcd for C₄₀H₃₈BNO₆: 639.28. Elemental analysis (calculated, found for C₄₀H₃₈BNO₆): C (75.12%, 75.30%), H (5.99%, 6.04%), N (2.19%, 2.25%).

dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(9-phenyl-9H-carbazol-3-yl)isophthalate (4). Compound dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-

2-yl)isophthalate (**3**) (2.24 g, 3.50 mmol), 3-bromo-9-phenyl-9H-carbazole (1.35 g, 4.20 mmol), tetrakis(triphenylphosphine)palladium (0.20 g, 0.18 mmol) and potassium carbonate (1.93 g, 14.00 mmol) were combined with 50 mL 1,4-dioxane in a roundbottom flask equipped with a reflux condenser and magnetic stir bar. The reaction mixture was heated to 100 °C for 10 h under argon. After cooled to room temperature, the reaction was filtered, the solvent removed under vacuum condition, and then the residue purified by column chromatography on silica gel using petroleum ether/dichloromethane (3/2, v/v) as eluent, yellow solid was finally obtained. Yield: 2.01 g (76%). ¹H NMR (400 MHz, Chloroform-d) δ 8.49 – 8.42 (m, 1H), 8.23 (dt, *J* = 7.8, 1.0 Hz, 1H), 8.21 (s, 2H), 7.73 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.71 – 7.57 (m, 8H), 7.57 – 7.49 (m, 6H), 7.50 – 7.41 (m, 6H), 7.39 – 7.31 (m, 3H), 7.25 – 7.15 (m, 4H), 3.59 (s, 6H). ¹³C NMR (101 MHz, Chloroform-d) δ 167.62, 146.25, 142.25, 141.47, 140.78, 140.64, 139.43, 137.47, 134.86, 132.94, 132.27, 130.56, 130.01, 128.77, 127.72, 127.44, 127.11, 126.81, 126.63, 126.43, 125.03, 124.09, 123.32, 122.56, 120.47, 120.36, 118.83, 110.34, 110.07, 52.45. MS (EI) *m/z*: 754.324 [M⁺]. Calcd for C₅₂H₃₈N₂O₄: 754.28. Elemental analysis (calculated, found for C₅₂H₃₈N₂O₄): C (82.74%, 82.83%), H (5.07%, 4.99%), N (3.71%, 3.77%).

2-(di([1,1'-biphenyl]-4-yl)amino)-5-(9-phenyl-9H-carbazol-3-yl)isophthalic acid (5). Compound **4** (1.89 g, 2.50 mmol) and sodium hydroxide (0.50 g, 12.50 mmol) in a solution of 1:1 THF/water (100 mL) heated to reflux for 48 h. Acidification with concentrated hydrochloric acid precipitated the triarylamine diacid, which was collected by vacuum filtration and oven-dried (80 °C) overnight, then employed directly without further purification. Yield: 1.65 g (91.0%).

3,11-diphenyl-7-(9-phenyl-9H-carbazol-3-yl)quinolino[3,2,1-de]acridine-5,9-dione (QAOCz1). Compound **5** (1.60 g, 2.20 mmol) was dispersed in dry dichloromethane (20 mL) in a three-neck round-bottom flask equipped with a magnetic stir bar and reflux condenser with a drying tube. Two drops of *N,N*-dimethylformamide was added followed by oxalyl chloride (0.41 mL, 4.84 mmol). The reaction was heated to reflux for 0.5 h. Tin(IV) chloride (2.0 mL, 4.84 mmol) was added and the reaction refluxed for an additional 3 h. The reaction mixture was added dropwise to an aqueous solution of sodium hydroxide (≈ 1 M) and extracted with dichloromethane. The organic layer dried over sodium sulfate and concentrated. The crude product was then purified by flash chromatography using DCM/petroleum ether (3/1, v/v) as the eluent to give a bright yellow-green solid. Yield: 0.93 g (61.0%). This compound was further purified by sublimation before used in device fabrication. ¹H NMR (400 MHz, Chloroform-d) δ 9.18 (s, 2H), 8.81 (d, *J* = 2.3 Hz, 2H), 8.63 (d, *J* = 1.8 Hz, 1H), 8.31 (t, *J* = 8.3 Hz, 3H), 8.12 (d, *J* = 6.9 Hz, 1H), 8.01 (dd, *J* = 8.8, 2.4 Hz, 2H), 7.92 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.87 – 7.73 (m, 4H), 7.73 – 7.59 (m, 4H), 7.59 – 7.44 (m, 9H), 7.38 (ddd, *J* = 8.0, 5.6, 2.5 Hz, 1H). ¹³C NMR (101 MHz, CDCl₃) δ 180.93, 139.49, 138.65, 137.96, 137.65, 136.96, 133.46, 133.43, 133.00, 132.66, 129.25, 128.87, 128.78, 128.62, 126.90, 125.63, 125.52, 122.81, 121.32, 116.45, 116.23. MS (EI) *m/z*: 690.304 [M⁺]. Calcd for C₅₀H₃₀N₂O₂: 690.23. Elemental analysis (calculated, found for C₅₀H₃₀N₂O₂): C (86.94%, 86.86%), H (4.38%, 4.29%), N (4.06%, 4.12%).

dimethyl 4'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylate (6). Compound dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(4,4,5,5-tetramethyl-

1,3,2-dioxaborolan-2-yl)isophthalate (**3**) (2.24 g, 3.50 mmol), 9-(4-bromophenyl)-9H-carbazole (1.35 g, 4.20 mmol), tetrakis(triphenylphosphine)palladium (0.20 g, 0.18 mmol) and potassium carbonate (1.93 g, 14.00 mmol) were combined with 50 mL 1,4-dioxane in a roundbottom flask equipped with a reflux condenser and magnetic stir bar. The reaction mixture was heated to 100 °C for 10 h under argon. After cooled to room temperature, the reaction was filtered, the solvent removed under vacuum condition, and then the residue purified by column chromatography on silica gel using petroleum ether/dichloromethane (3/2, v/v) as eluent, yellow solid was finally obtained. Yield: 2.11 g (80%). ¹H NMR (400 MHz, Chloroform-d) δ 8.20 (dt, *J* = 7.7, 1.0 Hz, 2H), 8.18 (s, 2H), 7.94 – 7.89 (m, 2H), 7.76 – 7.70 (m, 2H), 7.65 – 7.60 (m, 4H), 7.57 – 7.44 (m, 12H), 7.35 (ddt, *J* = 8.1, 6.7, 1.3 Hz, 4H), 7.23 – 7.17 (m, 4H), 3.59 (s, 6H). ¹³C NMR (101 MHz, Chloroform-d) δ 167.30, 146.16, 143.40, 140.73, 140.58, 137.74, 137.48, 137.42, 135.14, 133.09, 132.25, 128.79, 128.36, 127.55, 127.50, 126.89, 126.65, 126.07, 123.56, 122.72, 109.78, 52.48. MS (EI) *m/z*: 754.335 [M⁺]. Calcd for C₅₂H₃₈N₂O₄: 754.28. Elemental analysis (calculated, found for C₅₂H₃₈N₂O₄): C (82.74%, 82.83%), H (5.07%, 5.14%), N (3.71%, 3.83%).

4'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylic acid (7). Compound **6** (2.11 g, 2.80 mmol) and sodium hydroxide (0.56 g, 14.00 mmol) in a solution of 1:1 THF/water (100 mL) heated to reflux for 48 h. Acidification with concentrated hydrochloric acid precipitated the triarylamine diacid, which was collected by vacuum filtration and oven-dried (80 °C) overnight, then employed directly without further purification. Yield: 1.91 g (94.0%).

7-(4-(9H-carbazol-9-yl)phenyl)-3,11-diphenylquinolino[3,2,1-de]acridine-5,9-dione (QAOCz2). Compound **7** (1.89 g, 2.60 mmol) was dispersed in dry dichloromethane (20 mL) in a three-neck round-bottom flask equipped with a magnetic stir bar and reflux condenser with a drying tube. Two drops of N, N-dimethylformamide was added followed by oxalyl chloride (0.35 mL, 5.72 mmol). The reaction was heated to reflux for 0.5 h. Tin(IV) chloride (1.69 mL, 5.72 mmol) was added and the reaction refluxed for an additional 3 h. The reaction mixture was added dropwise to an aqueous solution of sodium hydroxide (≈ 1 M) and extracted with dichloromethane. The organic layer dried over sodium sulfate and concentrated. The crude product was then purified by flash chromatography using DCM/petroleum ether (3/1, v/v) as the eluent to give a bright yellow-green solid. Yield: 0.99 g (55.0%). This compound was further purified by sublimation before used in device fabrication. ¹H NMR (400 MHz, Chloroform-d) δ 9.13 (s, 2H), 8.79 (d, *J* = 2.3 Hz, 2H), 8.29 (d, *J* = 8.8 Hz, 2H), 8.17 (d, *J* = 7.7 Hz, 2H), 8.11 – 8.05 (m, 2H), 8.00 (dd, *J* = 8.9, 2.4 Hz, 2H), 7.86 – 7.69 (m, 6H), 7.63 – 7.39 (m, 10H), 7.36 – 7.30 (m, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 140.86, 140.80, 139.91, 139.07, 138.75, 138.40, 138.18, 137.29, 136.56, 133.38, 133.20, 129.03, 128.94, 127.94, 127.91, 127.87, 127.34, 126.38, 126.27, 125.96, 125.22, 123.90, 121.79, 120.50, 110.13. MS (EI) *m/z*: 690.298 [M⁺]. Calcd for C₅₀H₃₀N₂O₂: 690.23. Elemental analysis (calculated, found for C₅₀H₃₀N₂O₂): C (86.94%, 86.45%), H (4.38%, 4.56%), N (4.06%, 4.09%).

dimethyl 3'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylate (8). Compound dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)isophthalate (**3**) (2.24 g, 3.50 mmol), 9-(3-bromophenyl)-9H-carbazole (1.35 g, 4.20 mmol), tetrakis(triphenylphosphine)palladium (0.20 g, 0.18 mmol) and potassium carbonate (1.93 g, 14.00 mmol) were combined with 50 mL 1,4-dioxane in a roundbottom flask

equipped with a reflux condenser and magnetic stir bar. The reaction mixture was heated to 100 °C for 10 h under argon. After cooled to room temperature, the reaction was filtered, the solvent removed under vacuum condition, and then the residue purified by column chromatography on silica gel using petroleum ether/dichloromethane (3/2, v/v) as eluent, yellow solid was finally obtained. Yield: 2.27 g (86%). ¹H NMR (400 MHz, Chloroform-d) δ 8.16 (dt, *J* = 7.9, 1.1 Hz, 2H), 8.07 (s, 2H), 7.79 – 7.68 (m, 2H), 7.63 – 7.59 (m, 1H), 7.59 – 7.55 (m, 4H), 7.51 – 7.47 (m, 4H), 7.46 – 7.39 (m, 8H), 7.34 – 7.28 (m, 4H), 7.15 – 7.11 (m, 4H), 3.51 (s, 6H). ¹³C NMR (101 MHz, Chloroform-d) δ 167.15, 146.08, 143.57, 140.86, 140.55, 140.47, 138.60, 137.18, 135.14, 133.08, 132.17, 130.65, 128.76, 127.46, 126.86, 126.82, 126.62, 126.08, 125.92, 125.56, 123.47, 122.73, 120.40, 120.11, 109.71, 52.42. MS (EI) *m/z*: 754.335 [M⁺]. Calcd for C₅₂H₃₈N₂O₄: 754.28. Elemental analysis (calculated, found for C₅₂H₃₈N₂O₄): C (82.74%, 82.83%), H (5.07%, 5.16%), N (3.71%, 3.68%).

3'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylic acid (9). Compound **6** (2.36 g, 3.00 mmol) and sodium hydroxide (0.60 g, 15.00 mmol) in a solution of 1:1 THF/water (100 mL) heated to reflux for 48 h. Acidification with concentrated hydrochloric acid precipitated the triarylamine diacid, which was collected by vacuum filtration and oven-dried (80 °C) overnight, then employed directly without further purification. Yield: 2.01 g (92.0%).

7-(3-(9H-carbazol-9-yl)phenyl)-3,11-diphenylquinolino[3,2,1-de]acridine-5,9-dione (QAOCz3). Compound **9** (1.96 g, 2.70 mmol) was dispersed in dry dichloromethane (20 mL) in a three-neck round-bottom flask equipped with a magnetic stir bar and reflux condenser with a drying tube. Two drops of N, N-dimethylformamide was added followed by oxalyl chloride (0.51 mL, 5.94 mmol). The reaction was heated to reflux for 0.5 h. Tin(IV) chloride (0.68 mL, 5.94 mmol) was added and the reaction refluxed for an additional 3 h. The reaction mixture was added dropwise to an aqueous solution of sodium hydroxide (≈ 1 M) and extracted with dichloromethane. The organic layer dried over sodium sulfate and concentrated. The crude product was then purified by flash chromatography using DCM/petroleum ether (3/1, v/v) as the eluent to give a bright yellow-green solid. Yield: 1.08 g (58.0%). This compound was further purified by sublimation before used in device fabrication. ¹H NMR (400 MHz, Chloroform-d) δ 9.02 (s, 2H), 8.72 (d, *J* = 2.3 Hz, 2H), 8.23 (d, *J* = 8.8 Hz, 2H), 8.16 (dt, *J* = 7.6, 1.0 Hz, 2H), 8.00 – 7.93 (m, 3H), 7.92 – 7.88 (m, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.75 – 7.70 (m, 4H), 7.63 (ddd, *J* = 7.9, 2.0, 1.0 Hz, 1H), 7.53 – 7.47 (m, 6H), 7.46 – 7.39 (m, 4H), 7.30 (ddd, *J* = 7.9, 6.9, 1.2 Hz, 2H). ¹³C NMR (101 MHz, CDCl₃) δ 181.01, 140.74, 139.60, 139.45, 138.93, 138.74, 137.97, 133.05, 133.00, 130.94, 129.25, 129.20, 128.61, 128.58, 126.91, 126.87, 126.12, 125.81, 125.59, 125.47, 123.46, 122.88, 121.39, 120.12. MS (EI) *m/z*: 690.322 [M⁺]. Calcd for C₅₀H₃₀N₂O₂: 690.23. Elemental analysis (calculated, found for C₅₀H₃₀N₂O₂): C (86.94%, 87.05%), H (4.38%, 4.43%), N (4.06%, 3.98%).

2 Supplemental Figures

2.1 Experimental data of synthesis

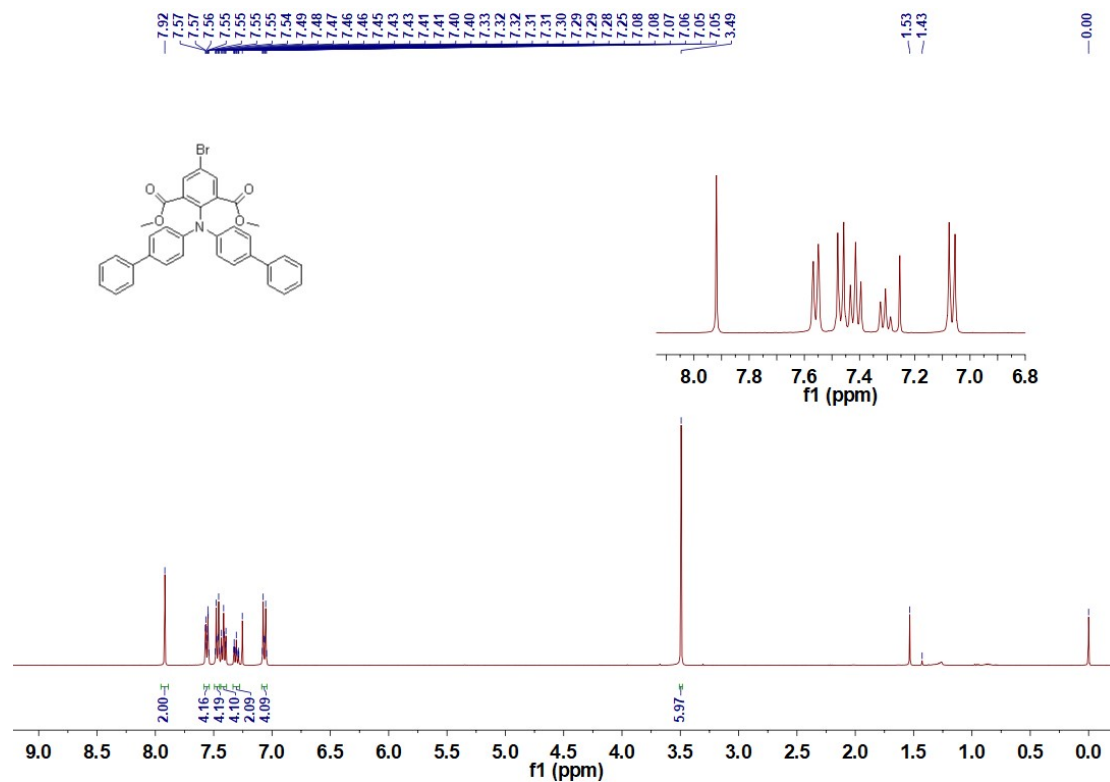


Figure S1. ¹H NMR spectrum of dimethyl 5-bromo-2-(di([1,1'-biphenyl]-4-yl)amino)isophthalate (2).

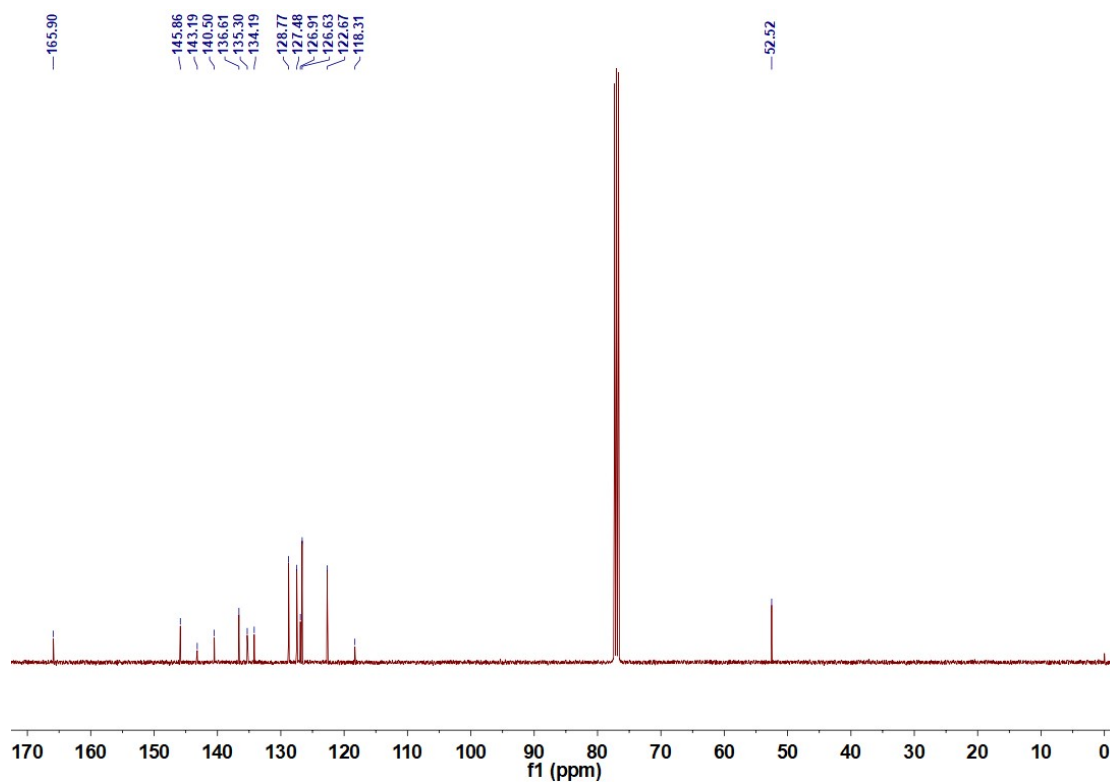


Figure S2. ^{13}C NMR spectrum of dimethyl 5-bromo-2-(di([1,1'-biphenyl]-4-yl)amino)isophthalate (2).

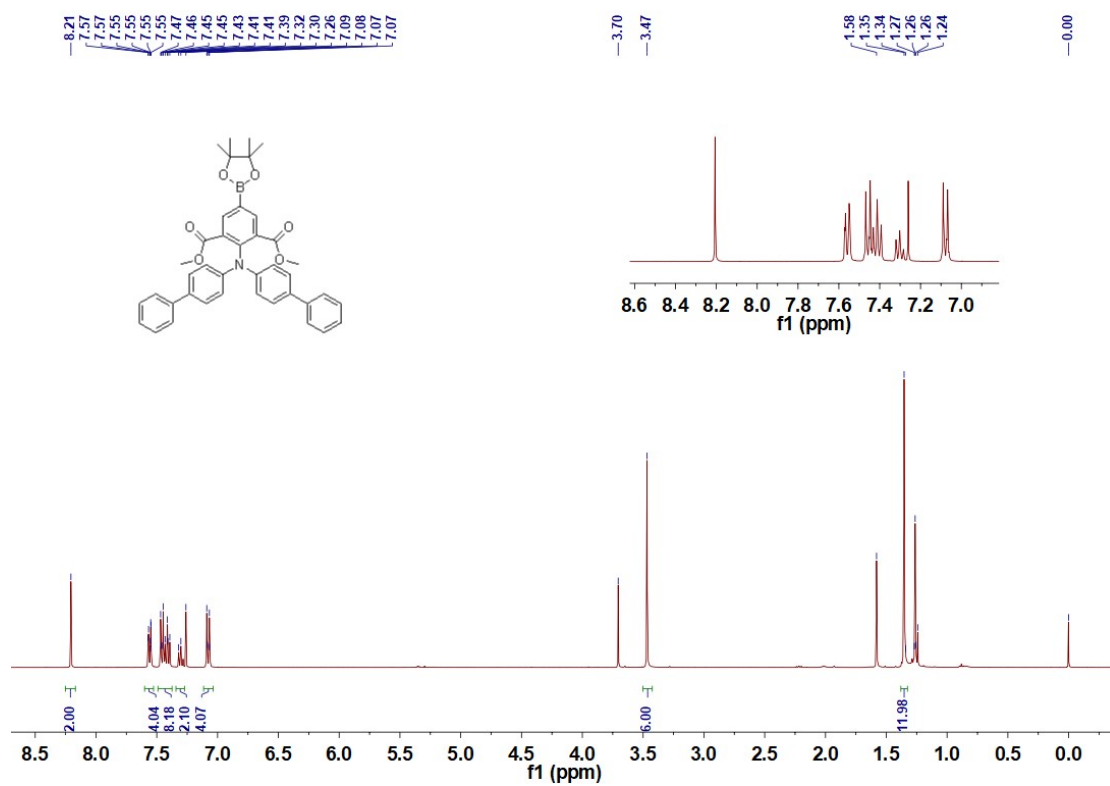


Figure S3. ^1H NMR spectrum of dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)isophthalate (3).

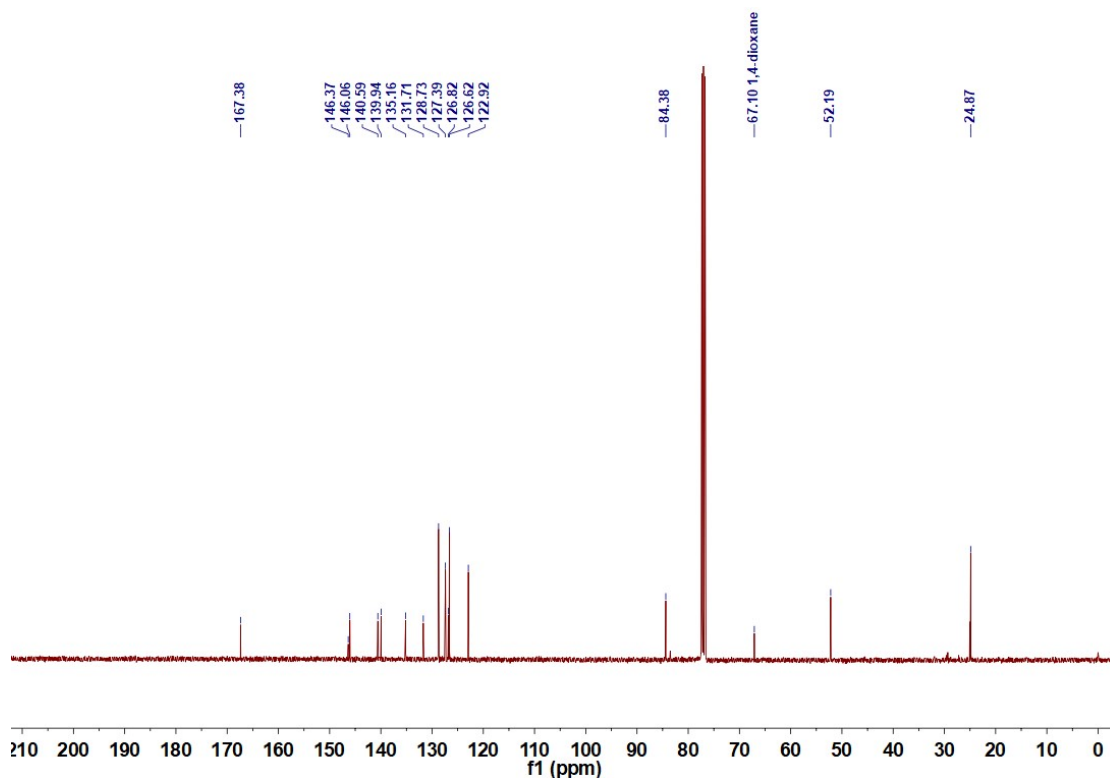


Figure S4. ^{13}C NMR spectrum of dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)isophthalate (3).

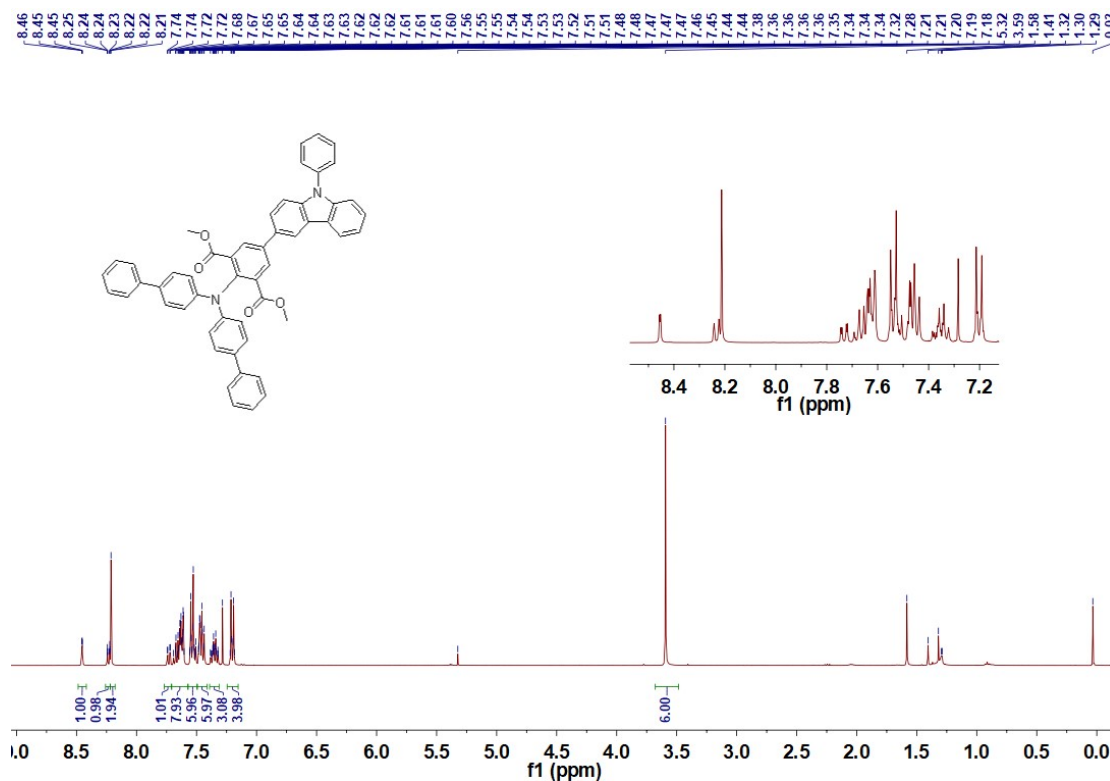


Figure S5. ^1H NMR spectrum of dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(9-phenyl-9H-carbazol-3-yl)isophthalate (4).

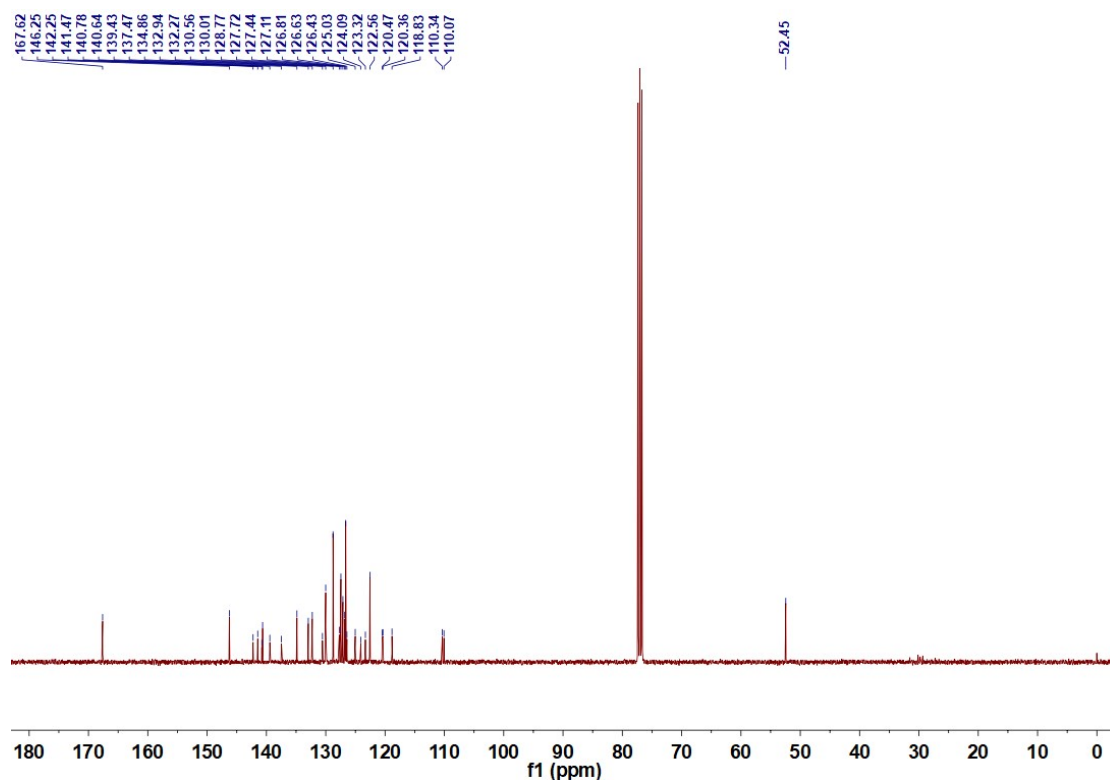


Figure S6. ^{13}C NMR spectrum of dimethyl 2-(di([1,1'-biphenyl]-4-yl)amino)-5-(9-phenyl-9H-carbazol-3-yl)isophthalate (4).

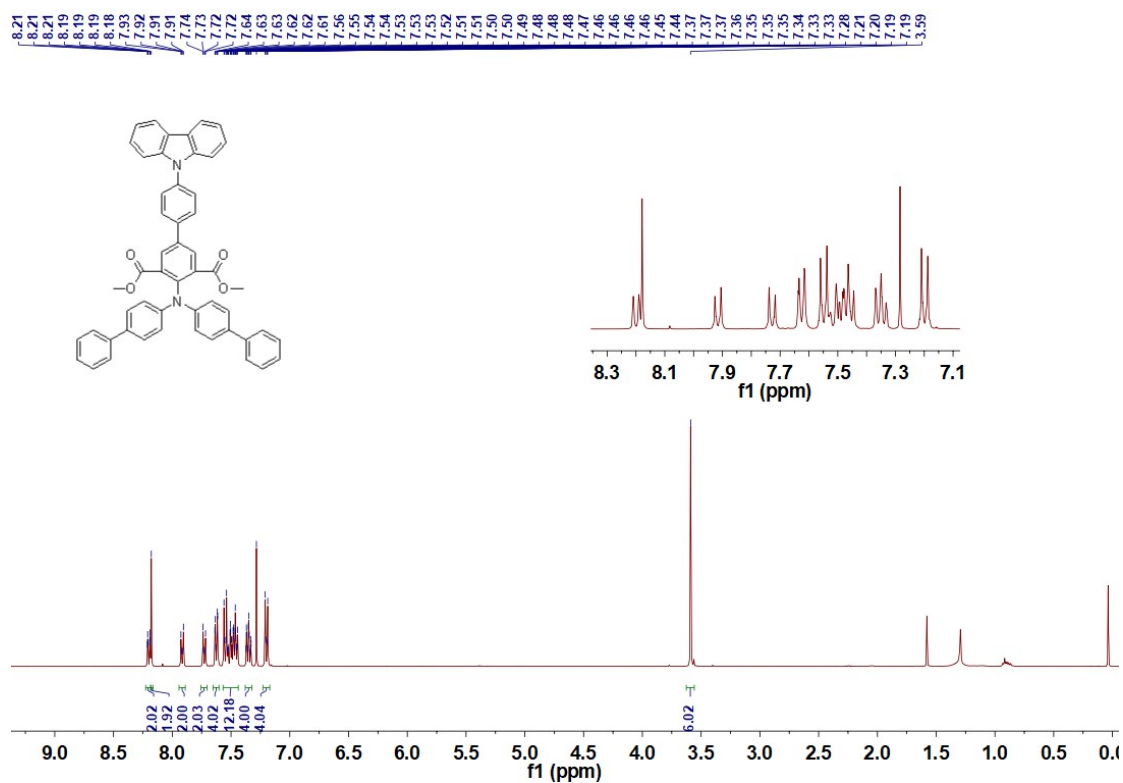


Figure S7. ^1H NMR spectrum of dimethyl 4'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylate (6).

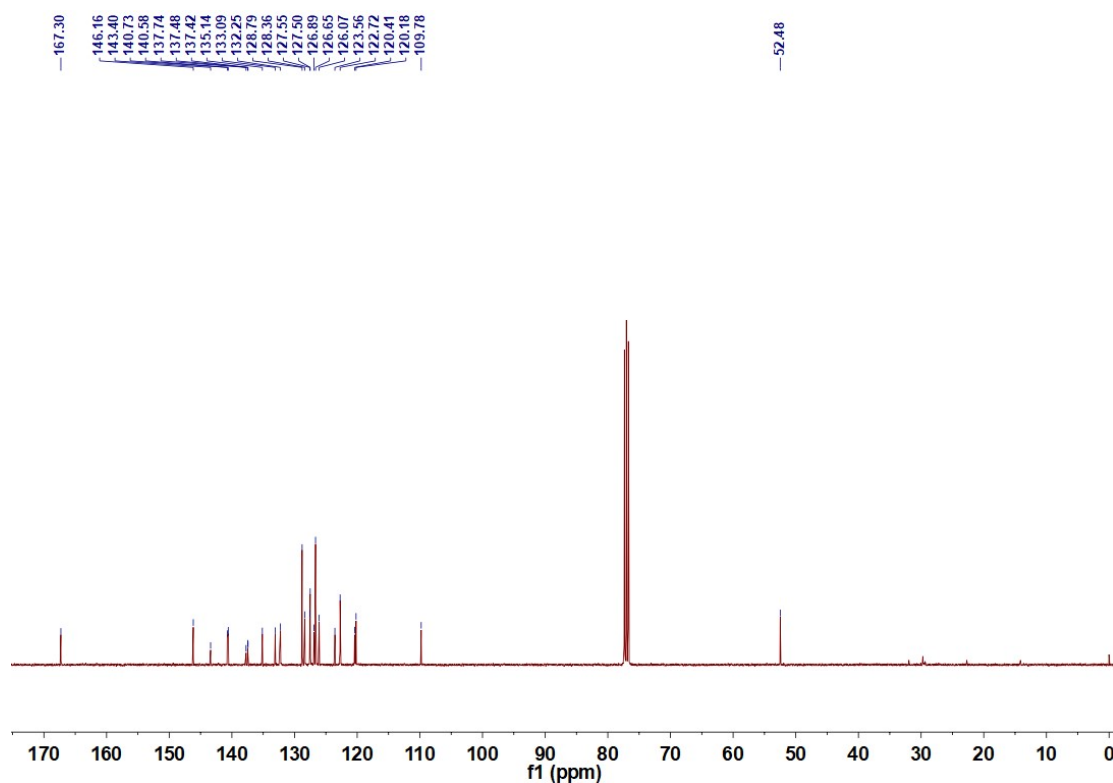


Figure S8. ^{13}C NMR spectrum of dimethyl 4'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylate (6).

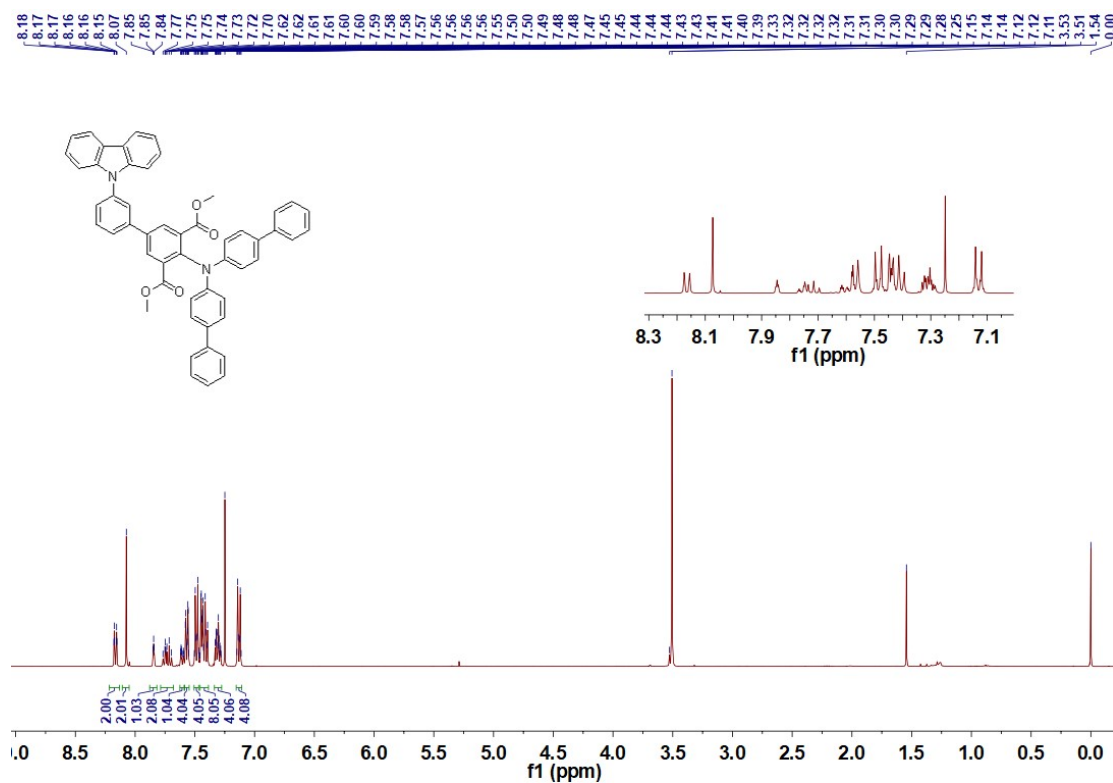


Figure S9. ^1H NMR spectrum of dimethyl 3'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylate (8).

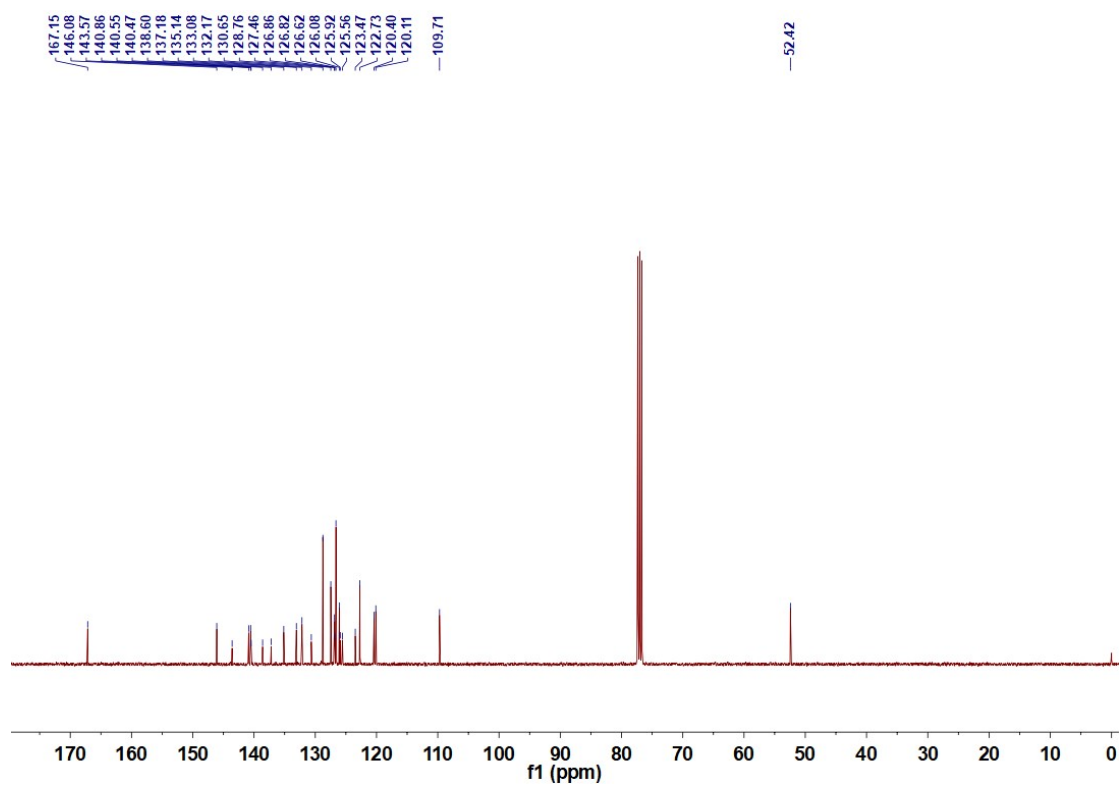


Figure S10. ^{13}C NMR spectrum of dimethyl 3'-(9H-carbazol-9-yl)-4-(di([1,1'-biphenyl]-4-yl)amino)-[1,1'-biphenyl]-3,5-dicarboxylate (8).

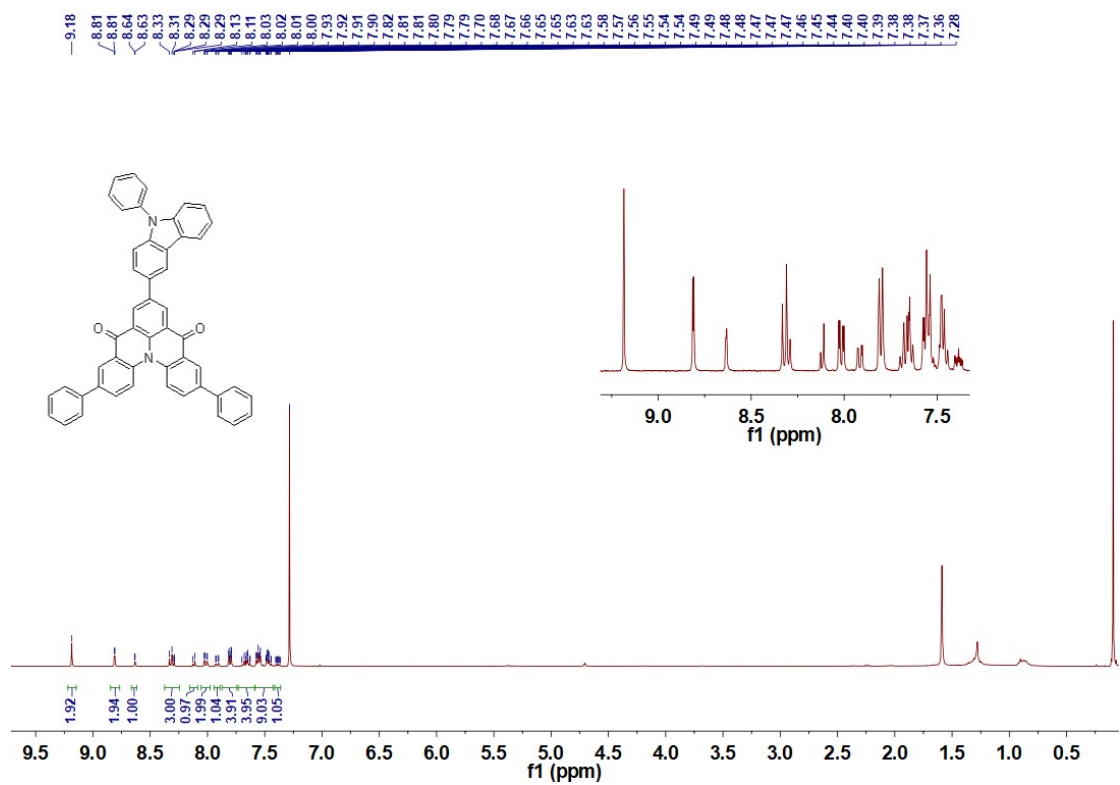


Figure S11. ^1H NMR spectrum of QAOCz1.

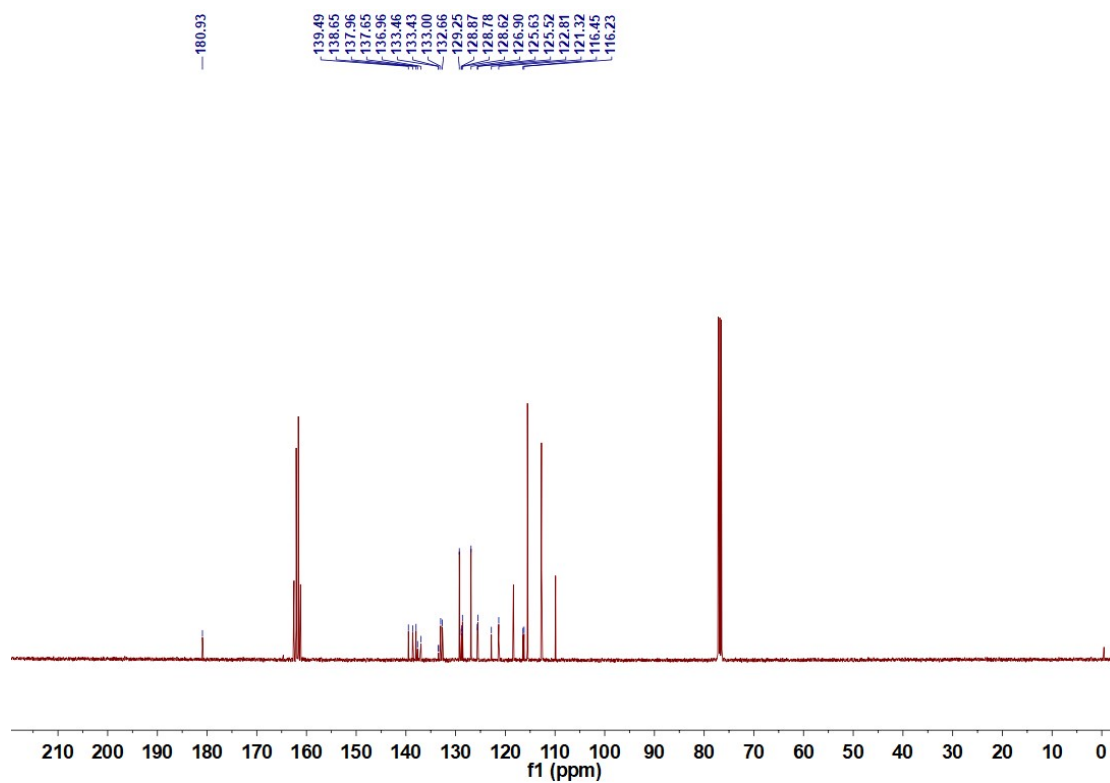


Figure S12. ^{13}C NMR spectrum of QAOCz1.

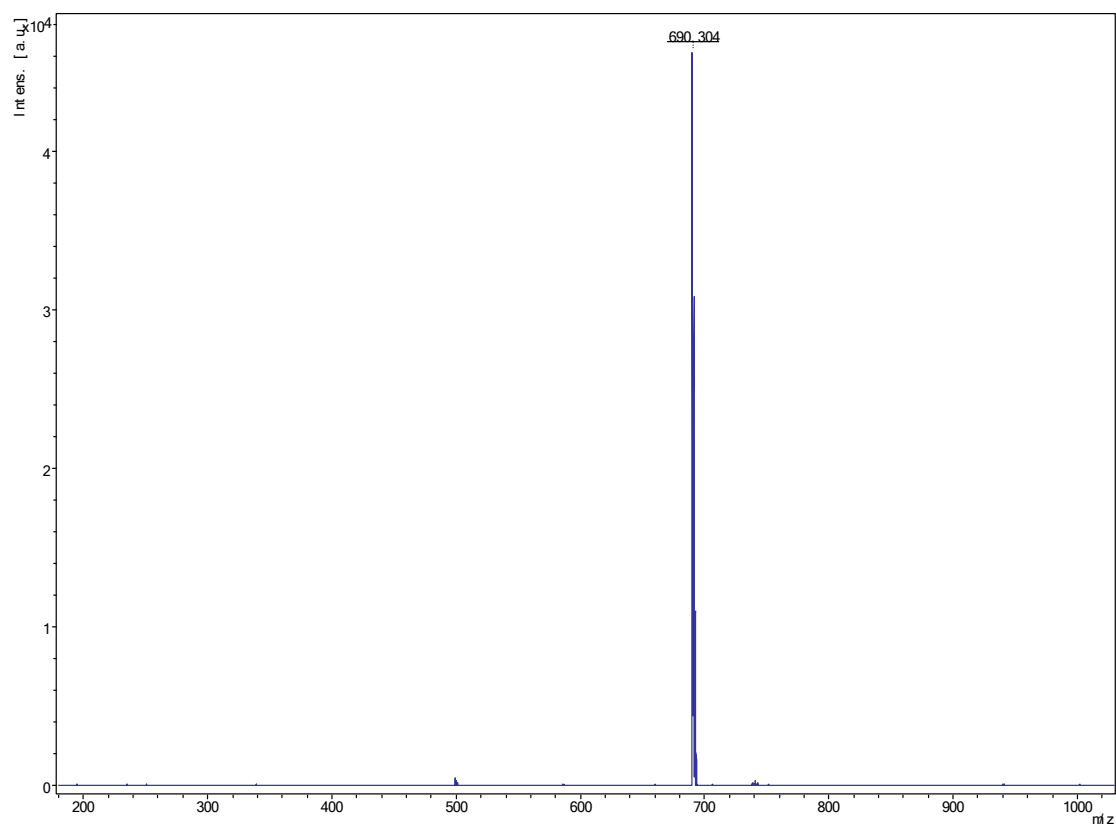


Figure S13. MALDI-TOF-MS spectrum of QAOCz1.

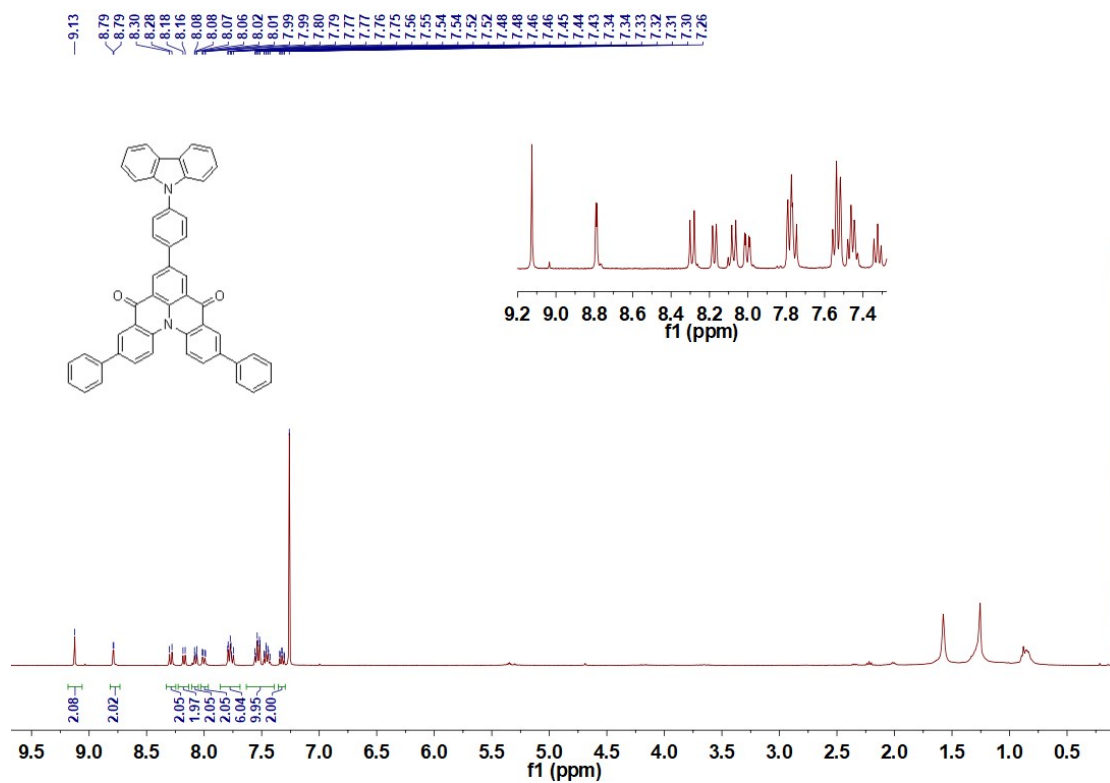


Figure S14. ¹H NMR spectrum of QAOCz2.

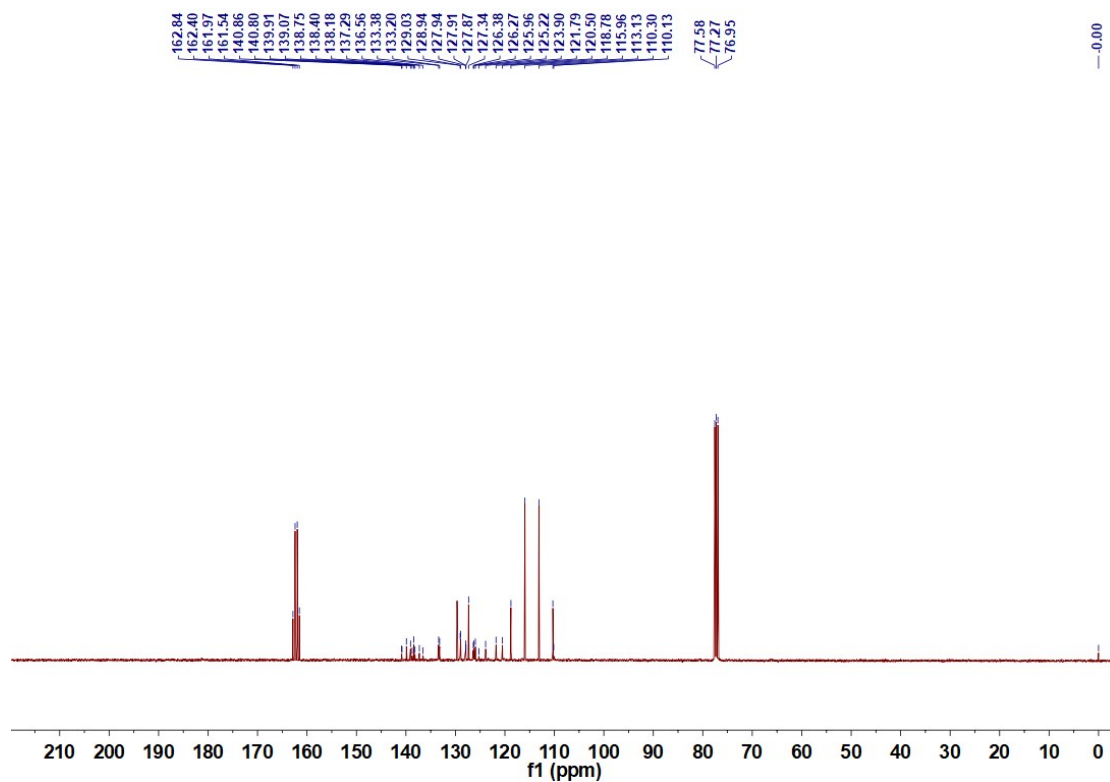


Figure S15. ¹³C NMR spectrum of QAOCz2.

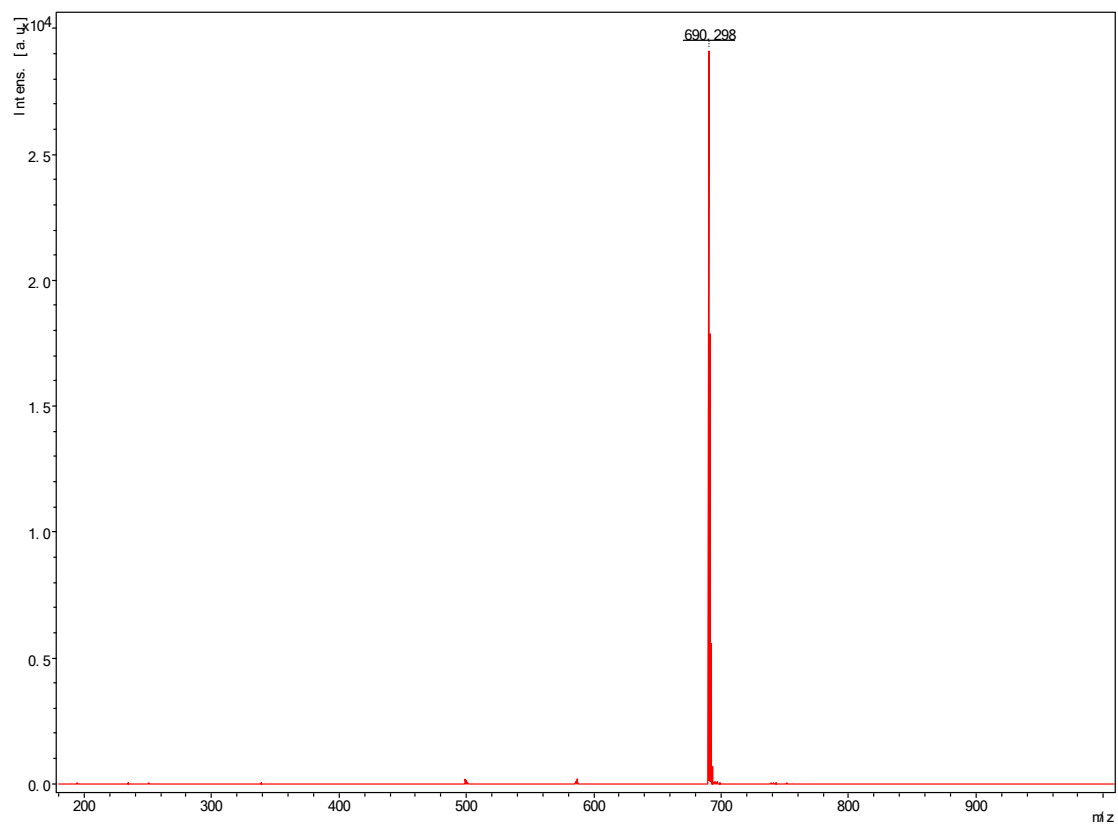


Figure S16. MALDI-TOF-MS spectrum of QAOCz2.

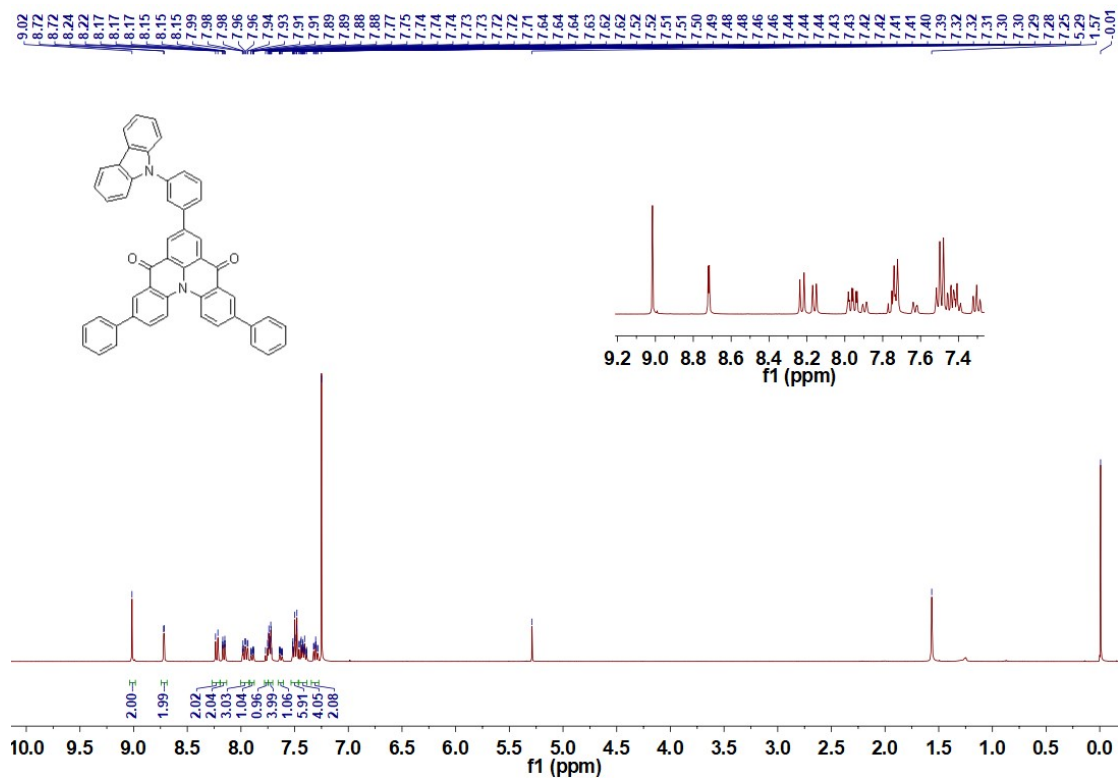


Figure S17. ¹H NMR spectrum of QAOCz3.

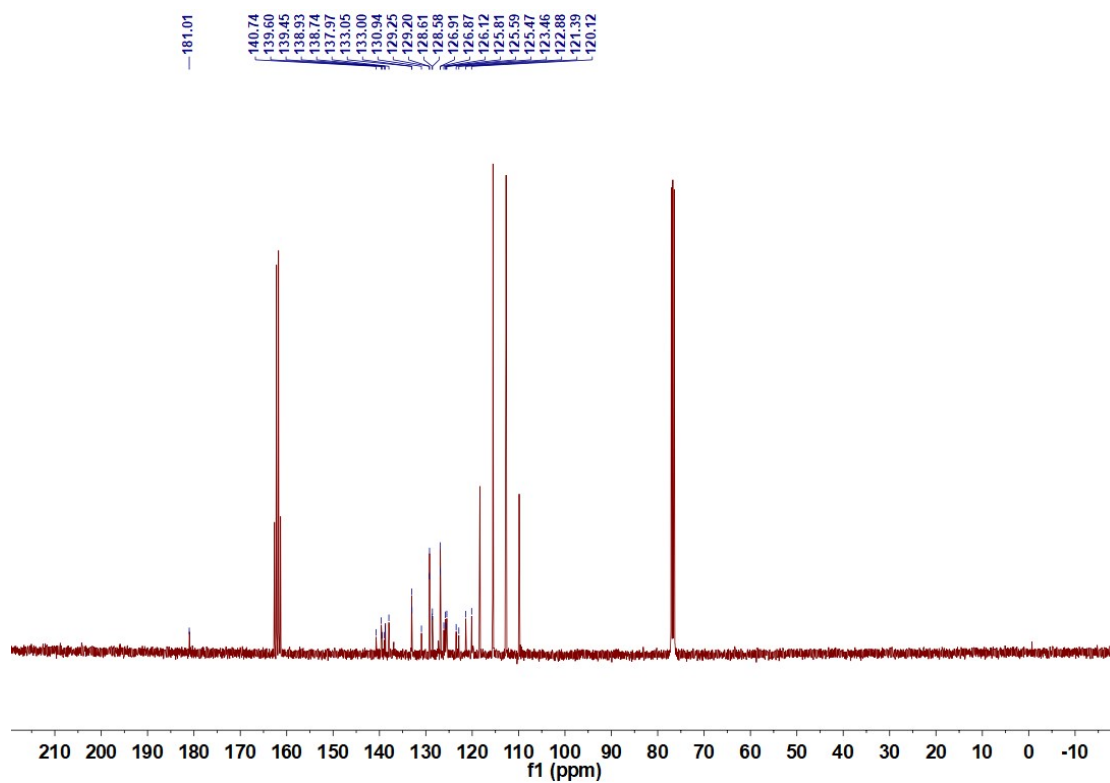


Figure S18. ^{13}C NMR spectrum of QAOCz3.

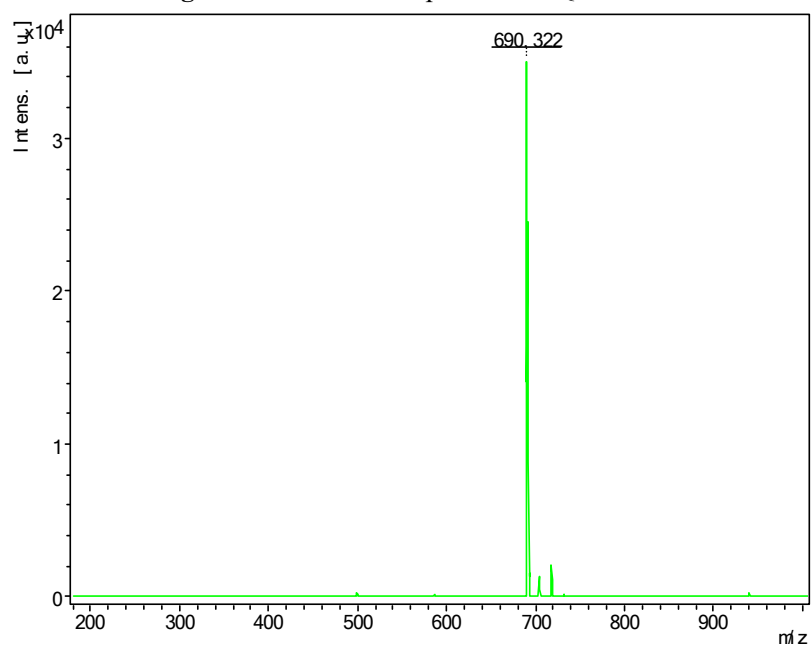


Figure S19. MALDI-TOF-MS spectrum of QAOCz3.

2.2 Photophysical properties

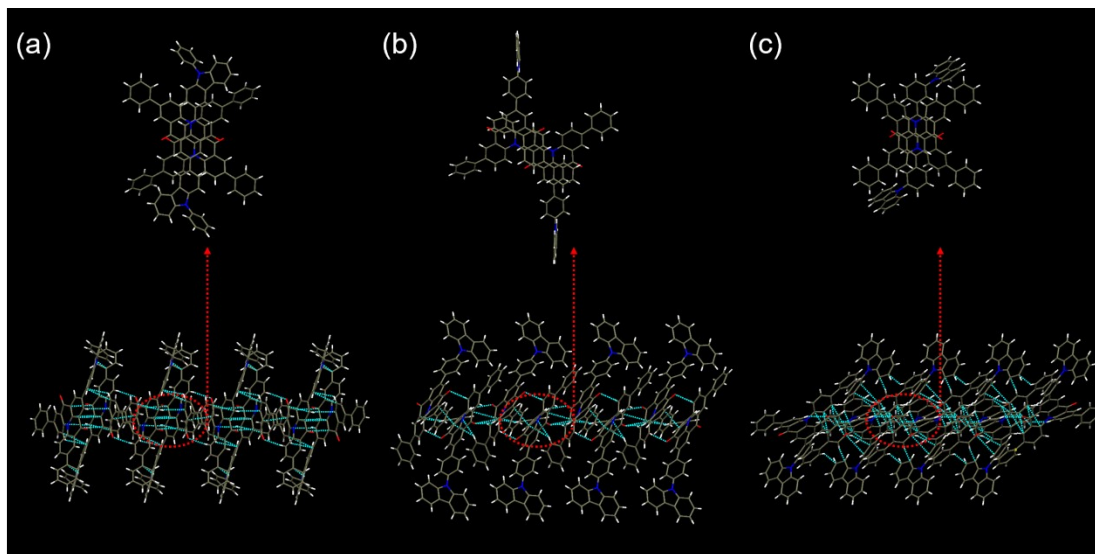


Figure S20. The packing mode of QAOCz1 (a), QAOCz2 (b), and QAOCz3 (c).

2.3 Photophysical properties

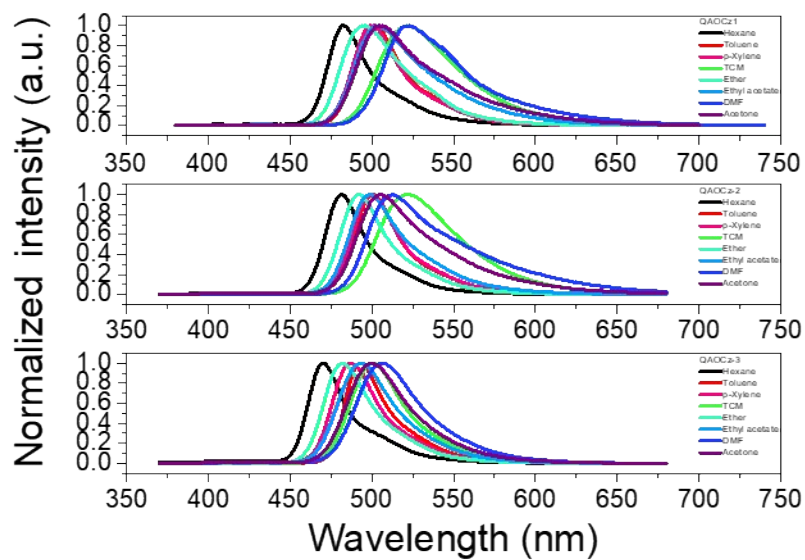


Figure S21. Solvatochromatic PL study for QAOCz1, QAOCz2, and QAOCz3.

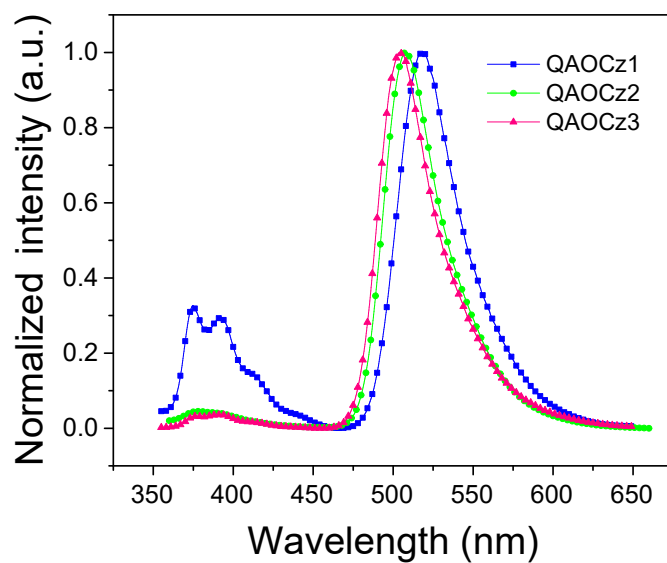


Figure S22. Emission spectra of QAOCz1, QAOCz2, and QAOCz3 in 5 wt% CBP at room temperature.

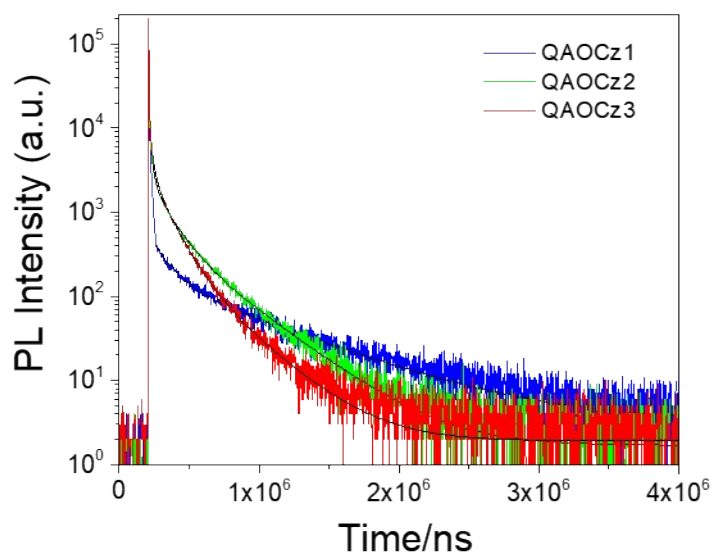


Figure S23. Transient PL decay spectrum of QAOCz1, QAOCz2 and QAOCz3 doped into CBP film (5 wt%) at room temperature.

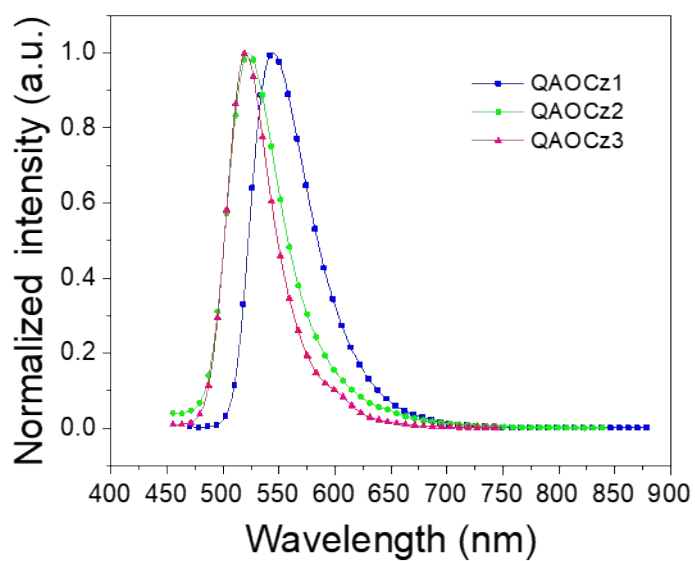


Figure S24. Emission spectra of QAOCz1, QAOCz2, and QAOCz3 in neat film at room temperature.

2.4 Thermal properties

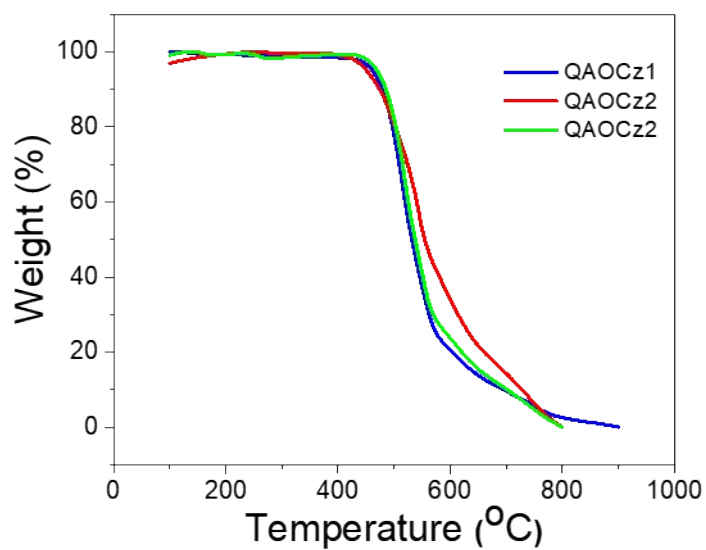


Figure S25. TGA curves of QAOCz1, QAOCz2, and QAOCz3.

2.5 Electrochemical properties

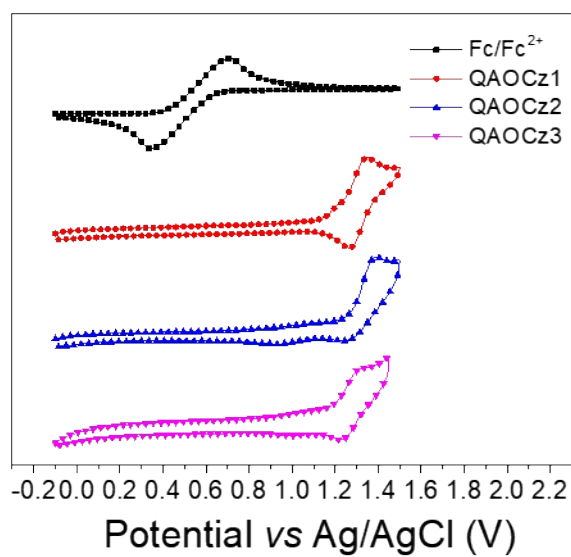


Figure S26. Cyclic voltammograms of QAOCz1, QAOCz2 and QAOCz3.

2.6 Device properties

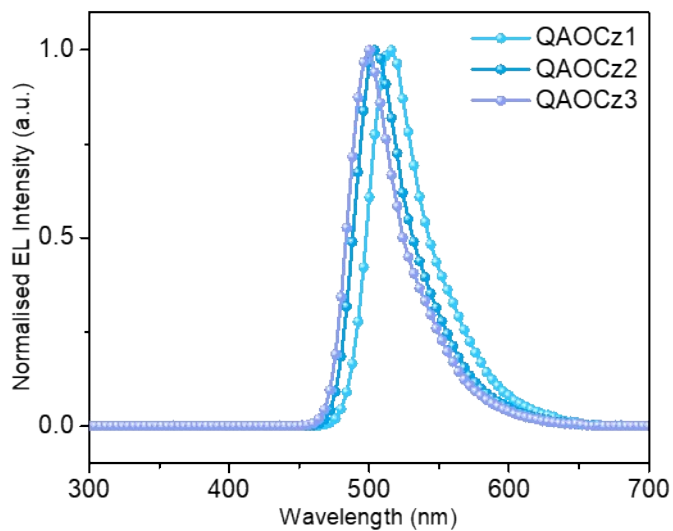
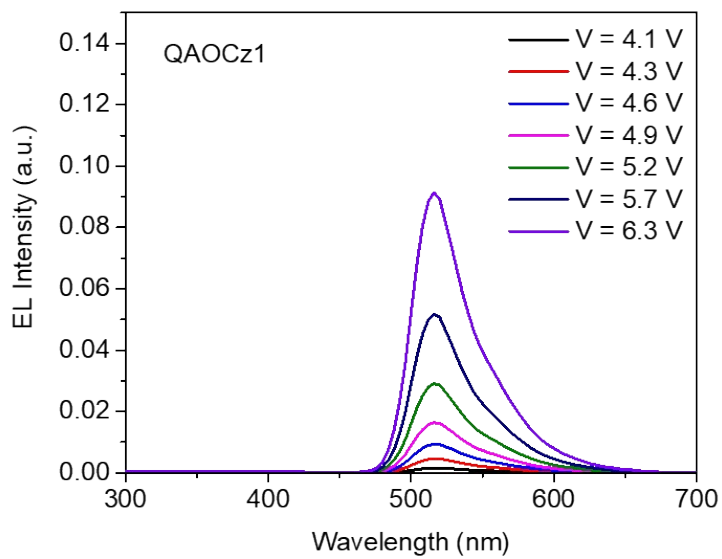


Figure S27. EL spectra of QAOCz1, QAOCz2 and QAOCz3 based devices at the current density of 5 mA/cm²



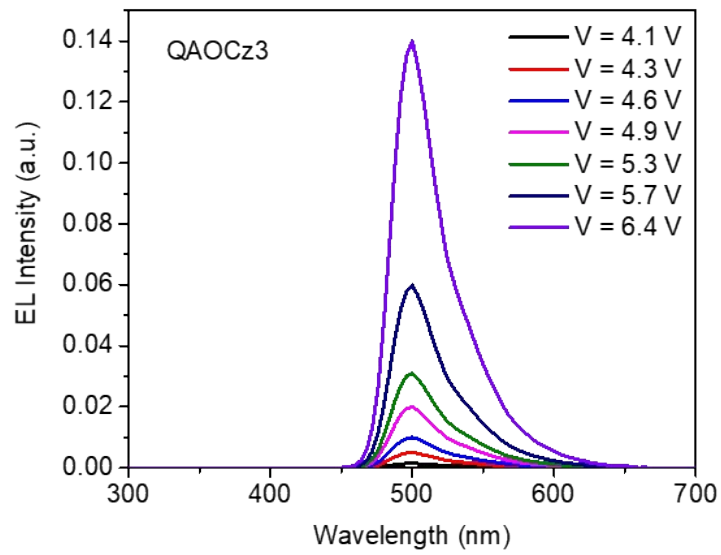
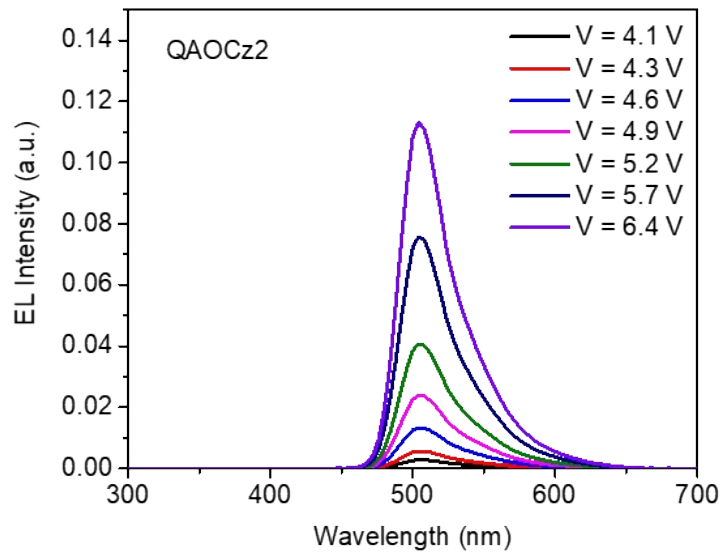


Figure S28. EL spectra of QAOCz1, QAOCz2 and QAOCz3 based devices at at different applied voltages.

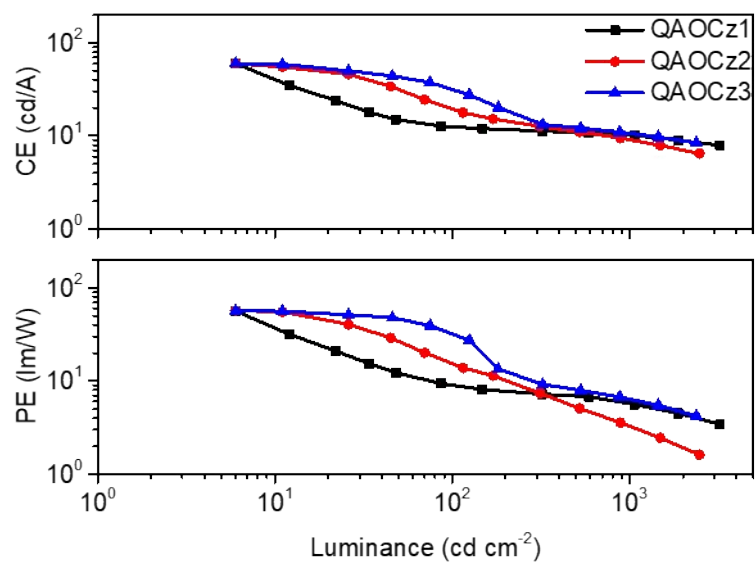


Figure S29. Power/current efficiency vs. luminance relationships of QAOCz1, QAOCz2 and QAOCz3 based devices.

3 Supplemental Tables

3.1 Crystal data and structure refinement

TableS1. Single crystal X-ray diffraction data of QAOCz1 in CHCl₃ and THF.

Compounds	QAOCz1
Empirical formula	C ₅₀ H ₃₀ N ₂ O ₂
Formula weight	690.76
Temperature/K	170.15
Crystal system	monoclinic
Space group	P21/c
a/Å	13.6522(19)
b/Å	9.9140(13)
c/Å	28.653(4)
α/°	90
β/°	98.009(5)
γ/°	90
Volume/Å ³	3840.3(9)
Z	4
ρ _{calc} /cm ³	1.195
μ/mm ⁻¹	0.073
F(000)	1440.0
Crystal size/mm ³	0.08 × 0.05 × 0.02
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.352 to 50.018
Index ranges	-16 ≤ h ≤ 16, -11 ≤ k ≤ 11, -34 ≤ l ≤ 30
Reflections collected	25861
Independent reflections	6741 [R _{int} = 0.1479, R _{sigma} = 0.1439]
Data/restraints/parameters	6741/0/487
Goodness-of-fit on F ²	0.937
Final R indexes [I >= 2σ (I)]	R1 = 0.0676, wR2 = 0.1377
Final R indexes [all data]	R1 = 0.1737, wR2 = 0.1626
Largest diff. peak/hole / e Å ⁻³	0.34/-0.29

TableS2. Single crystal X-ray diffraction data of QAOCz2 in CHCl₃ and THF.

Compounds	QAOCz2
Empirical formula	C ₅₀ H ₃₀ N ₂ O ₂
Formula weight	690.76
Temperature/K	153.0
Crystal system	monoclinic

Space group	P21/n
a/Å	9.7613(5)
b/Å	24.3715(13)
c/Å	17.4760(9)
α /°	90
β /°	104.442(2)
γ /°	90
Volume/Å ³	4026.1(4)
Z	4
ρ_{calc} /g/cm ³	1.140
μ /mm ⁻¹	0.069
F(000)	1440.0
Crystal size/mm ³	0.19 × 0.12 × 0.08
Radiation	MoK α (λ = 0.71073)
2 Θ range for data collection/°	4.118 to 52.832
Index ranges	-12 ≤ h ≤ 10, -30 ≤ k ≤ 24, -21 ≤ l ≤ 21
Reflections collected	30446
Independent reflections	8198 [R_{int} = 0.0981, R_{sigma} = 0.1077]
Data/restraints/parameters	8198/480/487
Goodness-of-fit on F ²	1.029
Final R indexes [$I \geq 2\sigma(I)$]	R1 = 0.0829, wR2 = 0.2031
Final R indexes [all data]	R1 = 0.1772, wR2 = 0.2607
Largest diff. peak/hole / e Å ⁻³	0.33/-0.24

TableS3. Single crystal X-ray diffraction data of QAOCz3 in CHCl₃ and THF.

Compounds	QAOCz3
Empirical formula	C ₅₀ H ₃₀ N ₂ O ₂
Formula weight	690.76
Temperature/K	146.0
Crystal system	monoclinic
Space group	C2/c
a/Å	36.0644(14)
b/Å	18.9834(7)
c/Å	11.1339(4)
α /°	90
β /°	103.7000(10)
γ /°	90
Volume/Å ³	7405.7(5)
Z	8
ρ_{calc} /g/cm ³	1.239
μ /mm ⁻¹	0.075
F(000)	2880.0
Crystal size/mm ³	0.19 × 0.15 × 0.12

Radiation	MoK α ($\lambda = 0.71073$)
2 Θ range for data collection/ $^{\circ}$	4.094 to 52.788
Index ranges	$-45 \leq h \leq 45, -23 \leq k \leq 23, -13 \leq l \leq 13$
Reflections collected	41225
Independent reflections	7567 [$R_{\text{int}} = 0.0496, R_{\text{sigma}} = 0.0360$]
Data/restraints/parameters	7567/0/523
Goodness-of-fit on F^2	1.020
Final R indexes [$I \geq 2\sigma(I)$]	$R1 = 0.0459, wR2 = 0.1122$
Final R indexes [all data]	$R1 = 0.0712, wR2 = 0.1300$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$	0.19/-0.19

3.2 DFT simulation

TableS4. Physical properties of QAOCz1, QAOCz2, and QAOCz3 from DFT simulation

Compound	HOMO (eV)	LUMO (eV)	S ₁ (eV)	T ₁ (eV)	E_g (eV)	ΔE_{ST} (eV)	f (eV)
QAOCz1	-5.21	-2.20	2.60	2.21	3.01	0.39	0.0535
QAOCz2	-5.25	-2.37	2.54	2.38	2.88	0.26	0.0143
QAOCz3	-5.23	-2.38	2.47	2.31	2.85	0.16	0.0018

3.3 Photophysical properties

TableS5. Physical properties of QAOCz1, QAOCz2, and QAOCz3 in films

Compound	^a λ_{em} (nm)	^a FWHM (nm)	^b λ_{em} (nm)	^b FWHM (nm)	^a PLQY (%)	τ_p (ns)	T_d (μs)
QAOCz1	501	45	544	62	86.1%	2.63	116.7 3
QAOCz2	500	41	525	57	86.8%	5.51	16.37
QAOCz3	495	42	519	49	98.9%	5.55	26.45

^a 5 wt % emitter in CBP; ^b in neat film.

3.4 Thermal and Electrochemical properties

TableS6. Electrochemical, thermal parameters and photophysical properties of QAOCz1, QAOCz2, and QAOCz3.

T_d	T_g	^a HOMO	^c LUMO	^b E_g
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	(°C)	(°C)	(eV)	(eV)	(eV)
QAOCz1	459	/	-5.47	-3.02	2.47
QAOCz2	450	/	-5.54	-3.06	2.48
QAOCz3	469	/	-5.47	-2.96	2.51

^a In DMF solution (in 5×10^{-3} M) using ferrocene as a reference; ^b determined from the λ of UV absorption spectra measured in toluene solution at room temperature; ^c determined from the value of HOMO and E_g .

Table S7. Color purity related parameters, FWHM and RSH of QAOCz1, QAOCz2, and QAOCz3 based devices.

	λ_1 (nm)	λ_2 (nm)	λ_3 (nm)	λ_4 (nm)	λ_{peak} (nm)	FWHM (nm)	RSH
QAOCz1	497	541	478	568	516	44	1.98
QAOCz2	488	531	472	558	504	43	1.96
QAOCz3	483	523	466	546	500	40	1.98

Computational geometry data

Summary of geometry results for QAOCz1

Calculation Method = RB3LYP

Basis Set = 6-31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = -2183.44029488 a.u.

RMS Gradient Norm = 0.00000176 a.u.

Dipole Moment = 1.7948 Debye

Point Group = C1

O	6.49390000	8.64200000	2.59390000
O	4.65520000	3.96660000	-2.46280000
N	6.76040000	7.27790000	-1.25010000
N	1.34630000	2.69560000	5.59750000
C	5.99200000	6.56510000	-0.32090000
C	6.01560000	6.65130000	-5.39810000
C	7.76290000	8.15820000	-0.75840000
C	6.84050000	8.05710000	-3.58580000
H	7.22740000	8.87930000	-3.30860000
C	5.22270000	5.45370000	-0.71330000
C	5.20900000	5.01450000	-2.11010000
C	6.50200000	7.08550000	-2.62540000
C	4.04720000	4.31460000	3.89600000
H	4.89050000	4.67550000	4.14540000
C	6.61510000	7.82510000	-4.92390000
H	6.87710000	8.48800000	-5.55170000
C	3.62130000	4.39790000	2.57550000
C	4.47000000	4.74980000	0.23070000

H	3.96180000	3.99880000	-0.05050000
C	5.81680000	5.93850000	-3.07310000
C	5.95720000	6.95170000	1.03310000
C	5.60710000	5.73430000	-4.43510000
H	5.17000000	4.93910000	-4.71650000
C	3.34840000	3.51250000	6.27170000
C	8.58970000	9.60860000	1.00160000
H	8.50170000	9.95480000	1.88190000
C	3.24380000	3.70590000	4.85130000
C	4.44700000	5.11860000	1.56820000
C	7.67520000	8.64010000	0.55360000
C	0.02170000	2.16920000	5.63870000
C	5.19420000	6.22600000	1.93450000
H	5.18460000	6.49950000	2.84420000
C	1.92610000	2.59950000	8.04560000
H	1.11120000	2.20140000	8.32890000
C	8.87430000	8.51220000	-1.52620000
H	9.01230000	8.11440000	-2.37800000
C	2.15660000	2.90980000	6.70810000
C	1.99650000	3.18140000	4.46910000
C	6.68220000	8.13540000	1.47850000
C	5.79430000	6.41730000	-6.84260000
C	4.34920000	3.77720000	7.21200000
H	5.17140000	4.16550000	6.93770000
C	9.61340000	10.07060000	0.19780000
C	5.53120000	7.48310000	-7.69940000
H	5.48070000	8.36580000	-7.35230000
C	9.77160000	9.44010000	-1.04360000
H	10.52870000	9.66050000	-1.57380000
C	2.94410000	2.89690000	8.95070000
H	2.81900000	2.70310000	9.87220000
C	2.38740000	3.82280000	2.20520000
H	2.11320000	3.85700000	1.29610000
C	4.13610000	3.47190000	8.53280000
H	4.81540000	3.65760000	9.17070000
C	1.56860000	3.21110000	3.13440000
H	0.74060000	2.82240000	2.87700000
C	10.50200000	11.19790000	0.62560000
C	5.86670000	5.13740000	-7.38620000
H	6.02760000	4.39510000	-6.81590000
C	5.34110000	7.26500000	-9.05510000
H	5.14170000	7.99640000	-9.62720000
C	10.64350000	11.54090000	1.95830000
H	10.20900000	11.01930000	2.62370000

C	5.70580000	4.93120000	-8.74610000
H	5.77800000	4.05450000	-9.10530000
C	11.13160000	11.97910000	-0.31750000
H	11.02970000	11.76670000	-1.23770000
C	-0.26530000	0.91700000	5.16540000
H	0.42540000	0.38060000	4.79430000
C	5.44190000	5.99700000	-9.57810000
H	5.32870000	5.85620000	-10.51080000
C	-0.99060000	2.94740000	6.17660000
H	-0.80540000	3.82390000	6.49360000
C	11.91990000	13.08150000	0.04710000
H	12.36980000	13.59590000	-0.61270000
C	12.02610000	13.40270000	1.38830000
H	12.53260000	14.16280000	1.65080000
C	11.41170000	12.63740000	2.33970000
H	11.50810000	12.85380000	3.25980000
C	-2.56780000	1.18370000	5.77230000
H	-3.45410000	0.84390000	5.82050000
C	-2.27690000	2.43190000	6.24640000
H	-2.96930000	2.95680000	6.63120000
C	-1.56270000	0.42830000	5.22640000
H	-1.75540000	-0.43790000	4.88650000

Summary of geometry results for QAOCz2

Calculation Method = RB3LYP

Basis Set = 6-31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = -2183.43970850 a.u.

RMS Gradient Norm = 0.00000191 a.u.

Dipole Moment = 5.6537 Debye

Point Group = C1

O	11.78520000	6.84940000	1.11500000
O	13.26240000	7.01490000	8.09220000
N	12.47380000	8.95090000	4.55730000
N	11.53290000	-0.91040000	5.25250000
C	13.06750000	9.66270000	5.63390000
C	11.81210000	9.59990000	3.48140000
C	12.44990000	7.55630000	4.60360000
C	13.75450000	9.76490000	7.95520000
H	13.86510000	9.32290000	8.78890000
C	13.28620000	9.03270000	6.86280000
C	14.06320000	11.11100000	7.86810000
C	12.15270000	6.79420000	3.45560000

C	13.52090000	10.98320000	5.49150000
H	13.49820000	11.40120000	4.63860000
C	12.72790000	6.86690000	5.79930000
C	11.29780000	10.89910000	3.60110000
H	11.39600000	11.37210000	4.41910000
C	13.08380000	7.59010000	7.01860000
C	11.86310000	7.46160000	2.17890000
C	10.45840000	10.83780000	1.31190000
C	11.57380000	8.90170000	2.29000000
C	10.92190000	9.53590000	1.22440000
H	10.79390000	9.05680000	0.41420000
C	12.10570000	5.40400000	3.53310000
H	11.90960000	4.90680000	2.74770000
C	13.99840000	11.67610000	6.58030000
H	14.29570000	12.57020000	6.45830000
C	12.65440000	5.48260000	5.84040000
H	12.82740000	5.04040000	6.66320000
C	12.33740000	4.71780000	4.72470000
C	9.73880000	11.48320000	0.18490000
C	10.65130000	11.49330000	2.54010000
H	10.32340000	12.37920000	2.64220000
C	8.68430000	12.36770000	0.41430000
H	8.42890000	12.57500000	1.30550000
C	14.42680000	11.91130000	9.07060000
C	10.08370000	11.20150000	-1.13810000
H	10.79730000	10.59960000	-1.31430000
C	10.32830000	-1.47410000	5.66090000
C	10.43340000	-2.87900000	5.58510000
C	11.75890000	-3.16970000	5.10970000
C	11.79680000	0.48520000	5.10630000
C	12.21550000	3.23860000	4.82970000
C	9.16990000	-0.84340000	6.09880000
H	9.10650000	0.10350000	6.14020000
C	9.33530000	-3.66760000	5.94560000
H	9.38180000	-4.61470000	5.88830000
C	14.75590000	11.29610000	10.27680000
H	14.79640000	10.34780000	10.31560000
C	8.00490000	12.94780000	-0.64970000
H	7.28790000	13.54770000	-0.48080000
C	12.44940000	-4.35500000	4.83030000
H	12.03460000	-5.19910000	4.96410000
C	9.40720000	11.78130000	-2.20050000
H	9.65650000	11.57850000	-3.09450000
C	12.40930000	-1.93480000	4.90460000

C	8.36450000	12.65870000	-1.94880000
H	7.89730000	13.06110000	-2.67160000
C	15.02520000	12.02660000	11.41780000
H	15.24360000	11.57880000	12.22680000
C	14.38280000	13.29690000	9.05440000
H	14.16280000	13.75110000	8.24950000
C	14.97870000	13.39350000	11.38540000
H	15.16540000	13.89920000	12.16760000
C	13.74220000	-4.27560000	4.35760000
H	14.21530000	-5.07420000	4.15520000
C	8.18520000	-3.04910000	6.38520000
H	7.43380000	-3.57570000	6.63170000
C	8.11010000	-1.65650000	6.47260000
H	7.31220000	-1.25580000	6.79690000
C	13.71060000	-1.85180000	4.43550000
H	14.13410000	-1.01230000	4.30080000
C	14.36830000	-3.03960000	4.17110000
H	15.26410000	-3.01500000	3.85570000
C	14.65760000	14.02870000	10.20540000
H	14.62330000	14.97780000	10.17740000
C	11.65460000	1.29470000	6.23280000
H	11.42270000	0.91240000	7.07070000
C	12.12310000	1.05470000	3.87900000
H	12.19960000	0.50610000	3.10720000
C	12.33670000	2.42110000	3.78060000
H	12.57790000	2.78840000	2.93780000
C	11.85330000	2.65710000	6.12030000
H	11.75450000	3.21610000	6.88180000

Summary of geometry results for QAOCz3

Calculation Method = RB3LYP

Basis Set = 6-31G(d)

Charge = 0

Spin = Singlet

E(RB3LYP) = -2183.43929311 a.u.

RMS Gradient Norm = 0.00000229 a.u.

Dipole Moment = 5.1557 Debye

Point Group = C1

O	1.50290000	15.28320000	8.22290000
O	6.40810000	10.32520000	6.64780000
N	4.95240000	13.25080000	9.12080000
C	3.58160000	17.90210000	12.16650000
C	3.47130000	15.14890000	9.54930000
C	3.13790000	16.27410000	10.32380000

H	2.30450000	16.70520000	10.17530000
C	4.29120000	12.98820000	7.91510000
C	3.98500000	16.77100000	11.29320000
C	2.59850000	14.75540000	8.42760000
C	5.89250000	11.13410000	7.43220000
C	4.66520000	14.47250000	9.80010000
C	3.16440000	13.73700000	7.54030000
C	4.74640000	11.96790000	7.07350000
C	2.51610000	13.44440000	6.33160000
H	1.74840000	13.94850000	6.08850000
N	-0.13100000	13.55400000	1.75120000
C	6.14810000	12.21640000	11.00900000
H	5.73420000	12.82140000	11.61330000
C	5.59210000	15.05330000	10.67860000
H	6.45760000	14.67300000	10.77240000
C	6.34560000	11.27600000	8.82790000
C	5.25390000	16.16710000	11.40200000
H	5.89400000	16.54350000	11.99460000
C	5.83070000	12.27520000	9.65210000
C	4.08310000	11.71850000	5.87080000
H	4.41030000	11.03180000	5.30170000
C	7.04770000	11.29900000	11.48290000
H	7.24160000	11.28390000	12.41280000
C	2.96070000	12.43830000	5.47480000
C	4.12880000	18.04120000	13.44520000
H	4.77000000	17.41080000	13.75180000
C	7.27760000	10.36060000	9.32290000
H	7.63730000	9.70490000	8.73710000
C	7.69100000	10.38300000	10.64260000
C	2.65540000	18.85210000	11.75820000
H	2.27190000	18.78530000	10.89170000
C	2.22710000	12.08040000	4.23300000
C	1.46830000	13.02100000	3.52960000
H	1.46860000	13.93190000	3.79920000
C	3.74620000	19.09230000	14.27620000
H	4.12600000	19.16970000	15.14360000
C	2.82660000	20.01490000	13.85200000
H	2.56730000	20.73020000	14.42080000
C	2.27930000	19.89450000	12.58680000
H	1.64170000	20.53100000	12.28550000
C	2.19950000	10.76020000	3.79740000
H	2.70800000	10.10810000	4.26510000
C	8.74020000	9.47310000	11.16960000
C	0.71000000	12.61560000	2.42900000

C	1.45300000	10.37210000	2.70380000
H	1.45650000	9.46410000	2.42470000
C	-0.89620000	15.36420000	0.61750000
C	0.69850000	11.30570000	2.01250000
H	0.18000000	11.04420000	1.26060000
C	-1.54260000	13.39110000	1.55140000
C	0.28760000	14.75030000	1.17530000
C	0.51730000	17.10560000	-0.17470000
H	0.62610000	17.92560000	-0.64190000
C	1.53310000	15.26570000	1.06730000
H	2.28810000	14.83160000	1.44680000
C	9.44460000	9.78490000	12.28740000
H	9.24880000	10.59100000	12.75050000
C	-2.02200000	14.50450000	0.89290000
C	-3.39210000	14.61050000	0.55040000
H	-3.73930000	15.35800000	0.07800000
C	-0.74640000	16.57930000	-0.05200000
H	-1.49930000	17.03160000	-0.41400000
C	1.65300000	16.48110000	0.36210000
H	2.50810000	16.87930000	0.24980000
C	-2.36820000	12.35310000	1.93350000
H	-2.03030000	11.58980000	2.38710000
C	9.02160000	8.26580000	10.50580000
H	8.53860000	8.01610000	9.72680000
C	10.44780000	8.94870000	12.76970000
H	10.93260000	9.19650000	13.54820000
C	10.73800000	7.79150000	12.14360000
H	11.42350000	7.22210000	12.47280000
C	-4.19030000	13.55610000	0.94800000
H	-5.11620000	13.58850000	0.73790000
C	10.02010000	7.44770000	11.01340000
H	10.21580000	6.62920000	10.57260000
C	-3.72250000	12.47790000	1.62180000
H	-4.32720000	11.79480000	1.88670000