Supporting Information

Four-Winged Propeller-Shaped Indole-Modified and Indole Substituted Tetraphenylethlenes: Greenish-Blue Emitters with Aggregation-Induced Emission Features for Conventional Organic Light-Emitting Diodes

Ferruh Lafzi,† Yunus Taskesenligil,† Betül Canımkurbeıy,‡ Selin Pıravadılı,*,§ Haydar Kılıc,† Nurullah Saracoglu*,†

†Department of Chemistry, Faculty of Sciences, Atatürk University, Erzurum, 25240, Türkiye

‡Sabuncuoglu Serefeddin Health Services Vocational School, Amasya University, Amasya, 05100, Türkiye

§Materials Technologies, Marmara Research Center (MAM), The Scientific and Technological Research Council of Turkey (TUBITAK), Gebze, Kocaeli, 41470, Türkiye
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1. Synthesis

General Information. $^1$H NMR and $^{13}$C NMR experiments were performed on either 400 MHz Varian and 400 MHz Bruker Avance II instruments using CDCl$_3$, DMSO-d$_6$, MeOD, and Acetone-d$_6$ as the solvent with tetramethylsilane (TMS) as an internal standard at room temperature, and the coupling constants $J$ are given in hertz. The multiplicity is designated as $s$ = singlet, $bs$ = broad singlet, $d$ = doublet, $t$ = triplet, $q$ = quartet, $dd$ = doublet of doublets, $m$ = multiplet. High-resolution mass spectrometry (HRMS) of all compounds was recorded on a QTOF (Quadrupole time-of-flight) spectrometry device. Column chromatography was performed using silica gel pore size 60 Å, 70-230 mesh (sigma).

General procedure for Suzuki coupling = GP1

To a stirred solution of bromo derivative (1 equiv.) and boronic acid or ester derivative (1.1 equiv.) in toluene (40 mL) and EtOH/H$_2$O (4:4 mL) was added Na$_2$CO$_3$ (10 equiv.) and then the system was purged with nitrogen several times. Then Pd(PPh$_3$)$_4$ (0.02 equiv.) was added and the reaction mixture was stirred at 85 °C for 24 h. After cooling to room temperature, the reaction mixture was mixed with water and extracted with dichloromethane (3 × 40 mL) and the organic layers were combined and dried over Na$_2$SO$_4$. After the solvent was removed under reduced pressure, the residue was purified by column chromatography (EtOAc/hexane) to give the desired compound.

General procedure for alkylation = GP2

To a solution of N-H or substituted indoles (1 equiv.) in DMSO (5 mL) sodium hydroxide (1.2 equiv.) was added and stirred for 20-30 minutes at room temperature. Then the flask was placed in an ice bath and alkyl halide (1.2 equiv.) was added slowly for 10 minutes. Removed the ice bath and stirred the reaction mixture for 5 h at room temperature. After completion, the reaction mixture was poured into ice water. Extracted the organic product with ethyl acetate (2 × 30 mL) and dried over anhydrous Na$_2$SO$_4$. Removed the solvent under vacuum and purified the product with column chromatography (EtOAc/hexane) to give the desired compound.

5-Benzyl-1H-indole (2). A reaction tube was charged with ether-imidazolium chloride (8 mg, 0.16 mmol), Pd$_2$(dba)$_3$ (3.8 mg, 0.04 mmol), and Cs$_2$CO$_3$ (540 mg, 1.6 mmol) under nitrogen atmosphere. Then, dioxane (2.0 mL) and H$_2$O (0.2 mL) were added and the mixture was stirred for 15 min at 80 °C. Benzyl chloride (105 mg, 0.8 mmol) and (1H-indol-5-yl)boronic acid (200 mg, 1.24 mmol) were added at room temperature. The reaction mixture was stirred at 90 °C for 15 h. After the reaction mixture was cooled to room temperature water and saturated Na$_2$CO$_3$ were added, and then the resulting mixture was extracted with CH$_2$Cl$_2$. The combined organic layers were dried over Na$_2$SO$_4$. Concentration and purification through silica gel column chromatography (hexane/CH$_2$Cl$_2$= 9:1) gave the 2 (160 mg, 93%) as a yellow oil. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.99 (bs, 1H), 7.45 (s, 1H), 7.35 – 7.10 (m, 7H), 7.02 (dd, $J$ = 8.3, 1.2 Hz, 1H), 6.47 (d, $J$ = 1.9 Hz, 1H), 4.07 (s, CH$_2$, 2H). $^{13}$C NMR (100 MHz, CDCl$_3$): $\delta$ 142.4, 134.5, 132.6, 129.0, 128.4, 128.1, 125.8, 124.4, 123.5, 120.6, 111.0, 102.4, 42.1.

(1H-Indol-5-yl)(phenyl)methanone (4). An oven-dried pressure tube equipped with a stir bar was charged with 1-benzoylpiperidine-2,6-dione (200 mg, 0.92 mmol), potassium carbonate (318 mg, 2.3 mmol), boric acid (114 mg, 1.84 mmol), (1H-indol-5-yl)boronic acid (178 mg, 1.1 mmol), Pd(OAc)$_2$ (6.2 mg, 0.03 mmol), and PCyHBF$_4$ (41 mg, 0.11 mmol). Tetrahydrofuran (5 mL) was added the reaction mixture was placed in a preheated oil bath at 70 °C for 12h. The reaction mixture was cooled down to room temperature, diluted with CH$_2$Cl$_2$ (10 mL), filtered, and concentrated. The residue was purified by column chromatography (EtOAc/hexane = 1:9) to give compound 4 as a white solid (145 mg, 71%, mp 154.5–155.5 °C). $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.85 (bs,
1H, 8.14 (s, 1H), 7.91 – 7.73 (m, 3H), 7.64 – 7.53 (m, 1H), 7.54 – 7.38 (m, 3H), 7.29 – 7.24 (m, 1H), 6.63 (s, 1H).

13C NMR (100 MHz, CDCl3): δ 197.7, 139.0, 138.4, 131.7, 130.0, 129.6, 128.2, 127.2, 125.9, 125.4, 124.2, 111.2, 104.2.

(1H-Indol-5-yl)(4-methoxyphenyl)methanone (5). The same procedure described for the synthesis of 4 was used. Column chromatography gave the product 5 as a white-off solid (380 mg, 74% yield; mp 145.5–146.5 °C).

1H NMR (400 MHz, CDCl3): δ 8.89 (bs, 1H), 8.11 (s, 1H), 7.58 – 7.48 (m, 2H), 7.44 (d, J = 8.6 Hz, 1H), 7.23 (d, J = 3.1 Hz, 1H), 6.62 (d, J = 3.1 Hz, 1H), 4.25 (q, J = 7.3 Hz, 2H), 1.53 (t, J = 7.3 Hz, 3H). 13C NMR (100 MHz, CDCl3): δ 196.6, 162.7, 138.2, 132.5, 131.4, 130.2, 127.1, 125.8, 124.7, 124.0, 113.4, 111.1, 104.0, 55.5.

(1-Ethyl-1H-indol-5-yl)(phenyl)methanone (6). The same procedure described for the synthesis of 4 was used. Column chromatography gave the product 6 as a white-off solid (420 mg, 73% yield). 1H NMR (400 MHz, CDCl3): δ 8.14 (s, 1H), 7.88 – 7.78 (m, 3H), 7.62 – 7.57 (m, 1H), 7.54 – 7.48 (m, 2H), 7.44 (d, J = 8.6 Hz, 1H), 7.23 (d, J = 3.1 Hz, 1H), 6.62 (d, J = 3.1 Hz, 1H), 4.25 (q, J = 7.3 Hz, 2H), 1.53 (t, J = 7.3 Hz, 3H). 13C NMR (100 MHz, CDCl3): δ 197.2, 139.2, 138.1, 131.5, 129.9, 129.1, 128.7, 128.1, 127.8, 125.6, 123.7, 109.2, 103.1, 41.3, 15.5.

(1-Ethyl-1H-indol-5-yl)(4-methoxyphenyl)methanone (7). The same procedure described for the synthesis of 4 was used. Column chromatography gave the product 7 as white-off solid (355 mg, 73% yield; mp 82–83 °C). 1H NMR (400 MHz, CDCl3): δ 8.11 (s, 1H), 7.88 – 7.85 (m, AA’ part of AA’BB’ system, 2H), 7.78 (d, J = 8.6 Hz, A part of AB system, 1H), 7.43 (d, J = 8.6 Hz, B part of AB system, 1H), 7.23 (d, J = 3.1 Hz, 1H), 7.01 – 6.98 (m, BB’ part of AA’BB’ system, 2H), 6.61 (d, J = 3.1 Hz, 1H), 4.25 (q, J = 7.3 Hz, 2H), 3.92 (s, 3H), 1.53 (t, J = 7.3 Hz, 3H). 13C NMR (100 MHz, CDCl3): δ 196.1, 162.6, 138.1, 132.4, 131.6, 129.7, 128.5, 127.8, 125.0, 123.6, 113.3, 109.0, 102.9, 55.5, 41.2, 15.5.

5-(1,2,2-Triphenylvinyl)-1H-indole (9). A 100 mL two-necked round-bottom flask with a reflux condenser was charged with zinc dust (121 mg, 1.84 mmol) and 15 mL of dry THF. The flask was evacuated under vacuum and pumped in dry nitrogen three times. The mixture was cooled to -78 °C, and TiCl4 (101 µL, 0.9 mmol) was slowly added by a syringe. The mixture was slowly warmed to room temperature, stirred for 0.5 h, and then refluxed for 2 h. Pyridine (37 µL, 0.46 mmol) was added to the mixture and refluxed for an additional 10 min. A solution of benzophenone (109 mg, 0.6 mmol) and (1H-indol-5-yl)(phenyl)methanone (102 mg, 0.46 mmol) in THF (10 mL) was added dropwise and refluxed for 18 h. The reaction was warmed to room temperature and quenched with 10% aqueous K2CO3 solution and filtrated. The filtration was extracted with dichloromethane three times, and the organic layers were combined and washed with brine twice and dried over Na2SO4. The solvent was evaporated under reduced pressure, and the crude product was purified on a silica gel column chromatography (EtOAc/hexane = 1:9) to give compound 9 as a white solid (67 mg, 39%, mp 175.0–176.0 °C). 1H NMR (400 MHz, CDCl3): δ 7.88 (bs, 1H), 7.22 (s, 1H), 7.16 (s, 1H), 7.06 – 6.91 (m, 16H), 6.82 (dd, J = 8.4, 1.4 Hz, 1H), 6.27 (s, 1H). 13C NMR (100 MHz, CDCl3): δ 194.7 (2C), 144.4 (2C), 142.1, 139.8, 135.6, 134.6, 131.53, 131.50, 131.46, 127.6 (2C), 127.5, 126.2 (2C), 126.1, 126.0, 124.2, 123.8, 110.1, 102.9. HRMS (APCI-TOF) m/z: [M + H]+ calcd for C38H22N, 372.1752; found 372.1746.

Also, 5-(1,2,2-triphenylvinyl)-1H-indole (9) was obtained in 70% yield (540 mg) from Suzuki coupling reaction (GP1).

5-(1-(4-Methoxyphenyl)-2,2-diphenylvinyl)-1H-indole (10). The same procedure described for the synthesis of 9 was used. Column chromatography gave the product 10 as white-off solid (25 mg, 31% yield; mp
1H NMR (400 MHz, CDCl₃): δ 7.98 (bs, 1H), 7.30 (s, 1H), 7.14 – 6.99 (m, 12H), 6.98 – 6.95 (m, AA’ part of AA‘BB’ system, 2H), 6.89 (dd, J = 8.5, 1.6 Hz, 1H), 6.66 – 6.56 (m, BB’ part of AA‘BB’ system, 2H), 6.36 (d, J = 2.1 Hz, 1H), 3.72 (s, CH₃, 3H). 13C NMR (100 MHz, CDCl₃): δ 157.9, 144.7, 144.6, 141.6, 138.9, 137.1, 135.8, 134.6, 132.7, 131.5, 131.48, 127.7, 127.5, 127.48, 126.3, 125.9, 125.8, 124.1, 123.9, 112.9, 110.0, 102.9, 55.1. HRMS (APCI-TOF) m/z: [M + H]⁺ calcd for C₂₈H₂₆NO, 402.1858; found 402.1843.

Also, 5-(1-(4-methoxyphenyl)-2,2-diphenylvinyl)-1H-indole (10) was obtained in 84% yield (690 mg) from Suzuki coupling reaction (GP1).

(2-Bromoethene-1,1,2-triyl)tribenzene (11). To a solution of ethene-1,1,2-triyltribenzene (1.0 g, 3.49 mmol) in chloroform (15 mL) was added a solution of bromine (0.49 g, 3.06 mmol) in chloroform (10 mL) slowly. After decolouration of the solution, the solvent was evaporated under reduced pressure, and the residue crystallized two times from ethanol to give 11 (0.8 mg, 62%, mp 116.0 °C) as a white solid. 1H NMR (400 MHz, CDCl₃): δ 7.32 – 7.27 (m, 4H), 7.27 – 7.18 (m, 3H), 7.12 – 7.04 (m, 3H), 7.00 – 6.96 (m, 3H), 6.94 – 6.79 (m, 2H). 13C NMR (100 MHz, CDCl₃): δ 143.8, 143.6, 141.12, 141.08, 130.4, 130.3, 129.5, 128.2, 128.0, 127.96, 127.9, 127.6, 127.0, 122.2.

(2-Bromo-2-(4-methoxyphenyl)ethene-1,1-diyl)dibenzene (12). The same procedure described for the synthesis of 11 was used. Recrystallization from ethanol gave the product as a light-brown solid (1.1 g, 90% yield; mp 124.5–125.5 °C). 1H NMR (400 MHz, CDCl₃): δ 7.41 – 7.15 (m, 8H), 7.15 – 7.04 (m, 2H), 7.01 – 6.90 (m, 2H), 6.70 (d, J = 8.8 Hz, 2H), 3.76 (s, 3H). 13C NMR (100 MHz, CDCl₃): δ 159.1, 144.1, 142.7, 141.4, 133.4, 131.8, 130.4, 129.6, 127.9, 127.5, 126.9, 122.5, 113.4, 55.2.

5-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)-1H-indole (13). To a solution of 5-bromo-1H-indole (1 g, 5.1 mmol) in dioxane were added Pd₂(dba)₃ (93 mg, 0.1 mmol), XPhos (2-dicyclopentylphosphino-2’,4’,6’-triisopropylbiphenyl) (97 mg, 0.2 mmol), KOAc (1.5 g, 15.3 mmol) and bis(pinacolato)diboron (1.42 g, 5.61 mmol). The reaction mixture was stirred on a pressure tube at 110 °C for 20 hours, then was cooled at room temperature, filtrate over Celite, and washed with ethyl acetate. To the reaction mixture was added water. The layers were separated and the aqueous phase was extracted with ethyl acetate (3 x 10). The combined organic phases were washed with brine, dried over sodium sulfate and the solvent evaporated under reduced pressure. The residue was purified by column chromatography (hexane/acetone = 0.3:9.7) to give the product as a white-off solid (1.0 g, 80% yield; mp 93.0–94.0 °C). 1H NMR (400 MHz, CDCl₃): δ 8.18 (bs, 1H), 7.64 (d, J = 8.1 Hz, 1H), 7.39 (d, J = 8.1 Hz, 1H), 7.26 (s, 1H), 7.21 – 7.18 (m, 1H), 6.58 – 6.55 (m, 1H), 1.37 (s, 12H). 13C NMR (100 MHz, CDCl₃): δ 137.9, 128.7, 128.1, 127.6, 124.2, 110.5, 103.1, 83.5, 24.9 (carbon adjacent to boron was not observed).

4-(4,4,5,5-1-Ethyl-5-(1,2,2-triphenylvinyl)-1H-indole (14). Compound 14 was obtained according to GP2. The product was obtained over column chromatography as a white-off solid (250 mg, 69% yield; mp 159.5–160.5 °C). 1H NMR (400 MHz, CDCl₃): δ 7.20 – 7.17 (m, 2H), 7.07 – 6.93 (m, 16H), 6.82 (dd, J = 8.6, 1.6 Hz, 1H), 6.22 (d, J = 3.0 Hz, 1H), 4.01 (q, J = 7.3 Hz, 2H), 1.36 (t, J = 7.3 Hz, 3H). 13C NMR (100 MHz, CDCl₃): δ 144.9, 144.5, 144.4, 142.1, 139.5, 134.9, 134.6, 131.6, 131.52, 131.50, 128.2, 127.61, 127.60, 127.5, 126.9, 126.1, 126.0, 125.6, 124.1, 108.3, 101.3, 40.9, 15.4. HRMS (APCI-TOF) m/z: [M + H]⁺ calcd for C₃₀H₂₆N, 400.2065; found 400.2067.

1-Ethyl-5-(1-(4-methoxyphenyl)-2,2-diphenylvinyl)-1H-indole (15). Compound 15 was obtained according to GP2. The product was obtained over column chromatography as a yellow solid (485 mg, 82% yield; mp 1151.3–
152.3 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 7.31 – 7.27\) (m, 2H), \(7.19 – 7.03\) (m, 11H), \(7.01 – 6.97\) (m, AA’ part of AA’BB’ system, 2H), \(6.93\) (d, \(J = 8.4\) Hz, 1H), \(6.66 – 6.62\) (m, BB’ part of AA’BB’ system, 2H), \(6.32\) (s, 1H), \(4.11\) (q, \(J = 7.3\) Hz, 2H), \(3.76\) (s, 3H), \(1.46\) (t, \(J = 7.3\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta 157.9, 144.8, 144.7, 141.7, 138.7, 137.3, 135.2, 134.6, 132.8, 131.53, 131.50, 128.1, 127.7, 127.6, 126.9, 125.9, 125.8, 125.7, 124.2, 112.9, 108.3, 101.3, 55.1, 40.9, 15.4. HRMS (APCI-TOF) \(m/z\): [M + H]\(^+\) calcd for C\(_{31}\)H\(_{28}\)NO, 430.2171; found 430.2158.

1-(2,2-Dibromoviny1)-4-nitrobenzene (17). To a solution of 4-nitrobenzaldehyde (1.0 g, 6.62 mmol) in dichloromethane (20 mL) was added CBr\(_4\) (3.29 g, 9.93 mmol) and cooled to 0 °C. Then a solution of PPh\(_3\) (5.21 g, 19.85 mmol) in dichloromethane (10 mL) was added dropwise to the reaction mixture and stirred for 2 h at room temperature. After completion, the reaction mixture was insoluble material was removed by filtration. The solvent evaporated under reduced pressure. The residue was purified by column chromatography (hexane/EtOAc = 9:5:0.5) to give the product as a yellow solid (1.75 g, 86% yield; mp 104.0–105.0 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 8.29 – 8.23\) (m, AA’ part of AA’BB’ system, 2H), \(7.76 – 7.69\) (m, BB’ part of AA’BB’ system, 2H), \(7.58\) (s, 1H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta 141.5, 134.9, 129.2, 123.7, 94.1\) (2C).

(2-(4-Nitrophenyl)ethene-1,1-diyl) dibenzene (18). Compound 18 was obtained according to GP1. Column chromatography gave the product as yellow solid (400 mg, 81% yield; mp 154.3–155.3 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 8.00\) (d, \(J = 8.8\) Hz, 2H), \(7.41 – 7.34\) (m, 8H), \(7.23 – 7.12\) (m, 4H), \(7.02\) (s, 1H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta 147.0, 145.9, 144.3, 142.4, 139.3, 130.2, 130.0, 129.0, 128.5, 128.4, 128.3, 127.9, 125.8, 123.3.

(2-Bromo-2-(4-nitrophenyl)ethene-1,1-diyl) dibenzene (19). The same procedure described for the synthesis of 11 was used. Recrystallization from ethanol gave the product as a light yellow solid (228 mg, 90% yield; mp 178.0–179.5 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 8.06\) (dd, \(J = 8.6, 1.5\) Hz, 2H), \(7.52 – 7.47\) (m, 2H), \(7.46 – 7.35\) (m, 5H), \(7.22 – 7.09\) (m, 3H), \(7.01 – 6.94\) (m, 2H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta 147.8, 146.8, 146.5, 142.8, 140.3, 131.3, 130.3, 129.4, 128.3\) (2C), \(128.1, 127.9, 123.3, 118.5. HRMS (ESI-TOF) \(m/z\): [M + H]\(^+\) calcd for C\(_{26}\)H\(_{15}\)BrNO\(_2\), 380.0281; found 380.0283.

1-Ethyl-5-(1-(4-nitrophenyl)-2,2-diphenylvinyl)-1H-indole (21). Compound 21 was obtained according to GP1. Column chromatography gave the product as yellow solid (300 mg, 85% yield; mp 169.0–170.0 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 7.96\) (d, \(J = 8.5\) Hz, 2H), \(7.31 – 7.22\) (m, 3H), \(7.19 – 7.14\) (m, 2H), \(7.15 – 7.05\) (m, 10H), \(6.89\) (d, \(J = 8.5\) Hz, 1H), \(6.35\) (d, \(J = 3.0\) Hz, 1H), \(4.13\) (q, \(J = 7.2\) Hz, 2H), \(1.48\) (t, \(J = 7.2\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta 152.3, 145.8, 143.4\) (2C), \(142.4, 140.1, 134.8, 133.7, 132.2, 131.4, 131.3, 128.4, 128.0, 127.7, 127.4, 127.0, 126.7, 125.2, 124.1, 122.9, 108.8, 101.4, 41.0, 15.4. HRMS (APCI-TOF) \(m/z\): [M + H]\(^+\) calcd for C\(_{30}\)H\(_{25}\)N\(_2\)O\(_2\), 445.1946; found 445.1954.

4-(1-(1-Ethyl-1H-indol-5-yl)-2,2-diphenylvinyl)aniline (22). 1-Ethyl-5-(1-(4-nitrophenyl)-2,2-diphenylvinyl)-1H-indole (21) (200 mg, 0.4 mmol) was dissolved in MeOH (10 mL), and 10% Pd/C (15 mg) was added. The mixture was stirred in an H\(_2\) atmosphere for 12 h. The Pd/C was removed by filtration and the solvent was evaporated to obtain a pure compound 22 as a yellow solid (178 mg, 95%; mp 191.0–192.0 °C). \(^1\)H NMR (400 MHz, CDCl\(_3\)): \(\delta 7.34\) (s, 1H), \(7.19 – 7.03\) (m, 12H), \(6.95\) (dd, \(J = 8.6, 1.6\) Hz, 1H), \(6.91 – 6.86\) (m, AA’ part of AA’BB’ system, 2H), \(6.50 – 6.43\) (m, BB’ part of AA’BB’ system, 2H), \(6.33\) (d, \(J = 3.1\) Hz, 1H), \(4.11\) (q, \(J = 7.3\) Hz, 2H), \(3.68\) (bs, 2H), \(1.47\) (t, \(J = 7.3\) Hz, 3H). \(^{13}\)C NMR (100 MHz, CDCl\(_3\)): \(\delta 145.1, 144.9, 144.0, 142.1, 138.1, 135.6, 135.3, 134.6, 132.7, 131.6, 131.5, 128.1, 127.6, 127.5, 126.8, 125.8, 125.7, 124.2, 114.5, 108.2, 101.3, 40.9, 15.4. HRMS (APCI-TOF) \(m/z\): [M + H]\(^+\) calcd for C\(_{30}\)H\(_{27}\)N\(_2\), 415.2169; found 415.2143.
1,2-Bis(4-(1-{1-ethyl-1H-indol-5-yl})-2,2-diphenylvinyl)phenyl)diazene (23). Solution of 4-(1-{1-Ethyl-1H-indol-5-yl})-2,2-diphenylvinylaniline (22) (510 mg, 0.12 mmol) in toluene (4 mL) was charged to a sealed tube and purged with nitrogen several times. Then t-BuOK (40.6 mg, 0.36 mmol), iodobenzene (26 µL, 0.24 mmol), Cul (0.7 mg, 0.03 mmol) and 1,10-Phenanthroline (0.7 mg, 0.03 mmol) were added to mixture and heated to 110 °C for 20h. After cooling to room temperature, the reaction solution was filtered to remove the precipitated base and washed with toluene. The solution was concentrated to obtain the crude product. Column chromatography (hexane/ EtOAc = 9.8:0.2) gave the product as red solid (70 mg, 70% yield; mp 260.0–261.0 °C). 1H NMR (400 MHz, CDCl3): δ 7.55 – 7.47 (m, AA′ part of AA′BB′ system, 4H), 7.21 (s, 2H), 7.13 – 7.06 (m, BB′ part of AA′BB′ system, 4H), 7.03 – 6.93 (m, 24H), 6.83 (dd, J = 8.6, 1.8 Hz, 2H), 6.22 (d, J = 3.1 Hz, 2H), 4.00 (q, J = 7.3 Hz, 4H), 1.35 (t, J = 7.3 Hz, 6H). 13C NMR (100 MHz, CDCl3): δ 150.9, 148.0, 144.2 (2C), 141.5, 140.7, 134.8, 134.5, 132.4, 131.6, 131.5, 128.3, 127.8, 127.7, 127.0, 126.4, 126.2, 125.6, 124.3, 122.0, 108.5, 101.4, 40.9, 15.4. HRMS (APCI-TOF) m/z: [M + H]+ calcd for C₆₀H₄₈N₄, 825.3952; found 825.3970.

(2,2-Dibromoethene-1,1-diyl)dibenzene (24). To a solution of benzophenone (0.0 g, 5.49 mmol) and CBr₄ (3.64 g, 10.98 mmol) in toluene (70 mL) was added Ph₃P (5.76 g, 21.95 mmol). The mixture was heated at 130 °C in an oil bath for 4 days. After cooling to room temperature, the solvent was removed by rotary evaporator and the residue was extracted with n-hexane. The hexane phases were combined and dried to give a residue, which was separated by column chromatography using n-hexane as the eluent to give the product. Recrystallization from ethanol gave the product as a white solid (1.6 g, 86% yield; mp 87.4–88.4 °C). 1H NMR (400 MHz, CDCl3): δ 7.31 – 7.19 (m, 10H). 13C NMR (100 MHz, CDCl3): δ 147.9, 141.4, 128.8, 128.4, 128.0, 90.3.

5-(1-Bromo-2,2-diphenylvinyl)-1H-indole (26). Under an argon atmosphere, (2,2-Dibromoethene-1,1-diyl)dibenzene (338 mg, 1.0 mmol), (1H-indol-5-yl)boronic acid (169 mg, 1.05 mmol), tri(2-furyl)-phosphine (34.8 mg, 0.15 mmol), and bis(dibenzylideneacetone)palladium (46 mg, 0.05 mmol) were placed in a 50 mL Schlenk tube. THF (5 mL), ether (2.1 mL), and a solution of cesium carbonate (652 mg, 2.0 mmol) in water (2 mL) were then added. The reaction mixture was stirred at reflux for 18 h. The product was extracted with ethyl acetate (3 x 30 mL). The combined organic layers were washed with brine (10 mL) and dried over anhydrous sodium sulfate. Evaporation followed by silica gel column chromatography (hexane/ethyl acetate = 9.5:0.5) afforded 1d as a white solid (185 mg, 46%; mp 198.7 °C).

4-(1-{1H-Indol-5-yl})-2,2-diphenylvinyl)-N,N-diphenylaniline (28). Compound 28 was obtained according to GP1. Column chromatography gave the product as a light brown solid (79 mg, 84% yield; mp 180.4–181.4 °C). 1H NMR (400 MHz, CDCl3): δ 7.83 (bs, 1H), 7.29 (s, 1H), 7.14 – 7.08 (m, 5H), 7.06 – 6.91 (m, 15H), 6.90 – 6.79 (m, 5H), 6.69 (d, J = 8.6 Hz, 2H), 6.31 – 6.28 (m, 1H). 13C NMR (100 MHz, CDCl3): δ 147.7 (2C), 145.8, 144.7, 144.4, 141.8, 139.4, 139.1, 135.4, 134.6, 132.4, 131.6, 131.5, 129.1, 127.6 (2C), 126.2, 126.1, 125.9, 124.2, 123.9, 123.0, 122.6, 110.1, 102.9. HRMS (ESI-TOF) m/z: [M + H]+ calcd for C₄₂H₂₇BrN, 539.2482; found 539.2480.

4-{1-{1-Ethyl-1H-indol-5-yl})-2,2-diphenylvinyl}-N,N-diphenylaniline (29). Compound 29 was obtained according to GP2. Column chromatography gave the product as yellow solid (60 mg, 95% yield; mp 82.3–83.3 °C). 1H NMR (400 MHz, CDCl3) δ 7.28 (d, J = 1.4 Hz, 1H), 7.17 – 7.11 (m, 5H), 7.08 – 6.94 (m, 15H), 6.91 – 6.80
The residue was purified by silica gel column chromatography. Column chromatography gave the product as a white-off solid (180 mg, 85% yield; mp 295.4–296.4 °C). $^1$H NMR (400 MHz, DMSO-$d_6$): δ 11.13 (s, 2H), 7.78 (s, 2H), 4.84 (d, $J = 7.2$ Hz, 4H), 7.43 (d, $J = 8.5$ Hz, 2H), 7.40 – 7.33 (m, 4H), 7.25 – 7.01 (m, 14H), 6.45 (s, 2H). $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 143.5, 141.1, 140.2, 140.1, 139.7, 135.5, 131.3, 130.5, 128.2, 127.9, 126.5, 125.8, 120.1, 117.9, 111.7, 101.5. HRMS (ESI-TOF) m/z: [M + H]$^+$ calcd for C$_{24}$H$_{26}$N$_4$, 448.2060; found 448.2065.

5,5’-(2,2-Diphenylethene-1,1-diyl)bis(1H-indole) (30). Compound 30 was obtained according to GP1. Column chromatography gave the product as a white-off solid (170 mg, 85% yield; mp 211.6–212.6 °C). $^1$H NMR (400 MHz, CDCl$_3$): δ 9.96 (s, 2H), 7.14 (s, 2H), 7.08 (s, 2H), 7.00 (d, $J = 8.4$ Hz, A part of AB system, 2H), 6.97 – 6.81 (m, 10H), 6.73 (d, $J = 8.4$ Hz, B part of AB system, 2H), 6.13 (s, 2H). $^{13}$C NMR (100 MHz, CDCl$_3$): δ 146.2, 144.9, 139.8, 139.6, 136.0, 132.2, 128.7, 128.4, 126.5, 126.3, 125.7, 124.2, 111.1, 102.7. HRMS (ESI-TOF) m/z: [M + H]$^+$ calcd for C$_{30}$H$_{23}$N$_2$, 567.2795; found 567.2775.

5-(4-(1,2,2-Triphenylvinyl)phenyl)-1H-indole (32). Compound 32 was obtained according to GP1. Column chromatography gave the product as a white-off solid (170 mg, 85% yield; mp 211.6–212.6 °C). $^1$H NMR (400 MHz, DMSO-$d_6$): δ 11.13 (s, 2H), 7.78 (s, 2H), 4.84 (d, $J = 7.2$ Hz, 4H), 7.43 (d, $J = 8.5$ Hz, 2H), 7.40 – 7.33 (m, 4H), 7.25 – 7.01 (m, 14H), 6.45 (s, 2H). $^{13}$C NMR (100 MHz, DMSO-$d_6$): δ 143.5, 141.1, 140.2, 140.1, 139.7, 135.5, 131.3, 130.5, 128.2, 127.9, 126.5, 125.8, 120.1, 117.9, 111.7, 101.5. HRMS (ESI-TOF) m/z: [M + H]$^+$ calcd for C$_{39}$H$_{26}$N, 567.2775.

General procedure for BIM-TPE = GP3

To a stirred solution of indole-modified (9) or indole-substituted (31) TPEs (2 equiv.) in CH$_2$Cl$_2$ (15 mL) aldehyde (1 equiv.) and a catalytic amount of Zn(CF$_3$COO)$_2$·xH$_2$O (0.01 equiv.) was added and the mixture was stirred at room temperature for 12 h. After completion of the reaction (monitored by TLC), the solvent was evaporated. The residue was purified by silica gel column chromatography (EtOAc/hexane) to give the desired compound.

3,3’-(Phenylmethylenylene)bis(5-(1,2,2-triphenylvinyl)-1H-indole) (36a). Compound 36a was obtained according to GP3. Column chromatography gave the product as yellow solid (52 mg, 93% yield; mp 163.4–163.4 °C). $^1$H NMR (400 MHz, CDCl$_3$): δ 7.50 (bs, 2H), 7.11 – 7.02 (m, 5H), 7.02 – 6.84 (m, 34H), 6.76 – 6.70 (m, 2H), 6.27 (d, $J = 1.8$ Hz, 2H), 5.20 (s, 1H). $^{13}$C NMR (100 MHz, CDCl$_3$): δ 144.5, 144.4, 144.3, 144.0, 142.2, 139.5, 135.3, 134.7, 131.44, 131.40, 131.36, 128.4, 128.0, 127.6, 127.5, 127.4, 126.6, 126.1, 125.9, 125.7, 125.6, 123.4, 123.2, 120.0, 110.1, 39.7. HRMS (ESI-TOF) m/z: [M + H]$^+$ calcd for C$_{65}$H$_{50}$N$_{5}$, 831.3734; found 831.3720.
3,3'-((4-Fluorophenyl)methylene)bis(5-(1,2,2-triphenyvinyl)-1H-indole) (36b). Compound 36b was obtained according to GP3. Column chromatography gave the product as yellow solid (51 mg, 89% yield; mp 148.9–149.9 ⁰C). ¹H NMR (400 MHz, Acetone-d₆): δ 9.86 (bs, NH, 2H), 7.15 (d, J = 8.4 Hz, 2H), 7.12 – 6.84 (m, 36H), 6.78 (dd, J = 8.4, 1.5 Hz, 2H), 6.65 (d, J = 2.0 Hz, 2H), 5.35 (s, 1H). ¹³C NMR (100 MHz, Acetone-d₆): δ 161.9 (d, J = 241.8 Hz), 145.5, 145.4, 145.3, 143.5, 141.8 (d, J = 2.4 Hz), 140.3, 136.8, 134.9, 132.1, 132.0, 131.9, 130.7 (d, J = 7.7 Hz), 128.4, 128.4, 128.3, 127.5, 127.0, 126.9, 126.8, 125.8, 124.7, 123.5, 119.9, 115.3 (d, J = 21.2 Hz), 111.4, 39.9. HRMS (ESI-TOF) m/z: [M + H]⁺ calcd for C₆₃H₄₆FN₂, 849.3640; found 849.3649.

3,3'-((4-Bromophenyl)methylene)bis(5-(1,2,2-triphenyvinyl)-1H-indole) (36c). Compound 36c was obtained according to GP3. Column chromatography gave the product as yellow solid (57 mg, 93% yield; mp 213.8–214.8 ⁰C). ¹H NMR (400 MHz, CDCl₃): δ 7.60 (bs, 2H), 7.18 (s, 2H), 7.14 (d, J = 8.4 Hz, 2H), 7.09 – 6.71 (m, 36H), 6.28 (s, 2H), 5.21 (s, 1H). ¹³C NMR (100 MHz, CDCl₃): δ 144.4, 144.2, 143.1, 142.1, 139.6, 135.3, 134.9, 131.4, 131.37, 131.35, 131.1, 130.1, 127.6, 127.5, 127.4, 126.4 126.13, 126.1, 125.84, 125.77, 123.4, 120.3, 119.6, 119.3, 110.2, 104.3, 39.2. HRMS (ESI-TOF) m/z: [M + H]⁺ calcd for C₆₃H₄₆BrN₂, 909.2839; found 909.2835.

3,3'-((4-Methoxyphenyl)methylene)bis(5-(1,2,2-triphenyvinyl)-1H-indole) (36d). Compound 36d was obtained according to GP3. Column chromatography gave the product as yellow solid (55 mg, 89% yield; mp 158.0–159.0 ⁰C). ¹H NMR (400 MHz, CDCl₃): δ 7.51 (s, 2H), 7.04 – 6.83 (m, 38H), 6.73 (d, J = 8.5 Hz, 2H), 6.60 (d, J = 8.5 Hz, 2H), 6.25 (d, J = 1.5 Hz, 2H), 5.16 (s, 1H), 3.71 (s, 3H). ¹³C NMR (100 MHz, CDCl₃): δ 157.6, 144.5, 144.3, 142.2, 139.5, 136.3, 135.3, 134.7, 131.5, 131.4, 129.3, 127.6, 127.5, 126.6, 126.1, 125.7, 125.6, 123.3, 123.2, 120.3, 113.4, 110.1, 55.2, 38.9 (1C signal overlaps). HRMS (ESI-TOF) m/z: [M + H]⁺ calcd for C₆₃H₄₆O₂N₂, 861.3839; found 861.3824.

4-((Bis(5-(1,2,2-triphenyvinyl)-1H-indol-3-yl)methyl)phenyl)phenyl acetate (36e). Compound 36e was obtained according to GP3. Column chromatography gave the product as yellow solid (55 mg, 95% yield; mp 189.1–190.1 ⁰C). ¹H NMR (400 MHz, DMSO-d₆): δ 10.71 (d, J = 1.7 Hz, 2H), 7.16 – 6.82 (m, 38H), 6.77 – 6.54 (m, 4H), 5.14 (s, 1H), 2.26 (s, 3H). ¹³C NMR (100 MHz, DMSO-d₆): δ 169.1, 148.2, 144.0, 143.9, 143.7, 142.2, 142.0, 138.8, 135.0, 133.0, 130.7, 130.5, 128.5, 127.7, 127.6, 127.5, 126.2, 126.1, 125.9, 124.2, 123.6, 121.68, 121.65, 121.0, 118.1, 110.6, 38.2, 20.9. HRMS (ESI-TOF) m/z: [M + H]⁺ calcd for C₆₅H₄₉N₂O₂, 889.3789; found 889.3780.

3,3'-((4-(Trifluoromethyl)phenyl)methylene)bis(5-(1,2,2-triphenyvinyl)-1H-indole) (36f). Compound 36f was obtained according to GP3. Column chromatography gave the product as yellow solid (51 mg, 92% yield; mp 207.2–208.2 ⁰C). ¹H NMR (400 MHz, DMSO-d₆): δ 10.76 (bs, 2H), 7.43 (d, J = 7.6 Hz, 2H), 7.16 – 6.82 (m, 36H), 6.71 (s, 2H), 6.67 (d, J = 8.4 Hz, 2H), 5.31 (s, 1H). ¹³C NMR (100 MHz, DMSO-d₆): δ 149.5, 144.0, 143.9, 143.7, 142.0, 138.9, 135.1, 133.2, 130.7, 130.6, 130.5, 128.3, 127.7, 127.6, 127.5, 126.1 (q, J = 31.9 Hz), 126.1, 126.1, 125.9, 124.8 – 124.6 (m), 124.5 (q, J = 273.3 Hz), 124.3, 123.8, 121.6, 119.3, 117.2, 110.7, 38.9 (3C signal overlaps). HRMS (ESI-TOF) m/z: [M + H]⁺ calcd for C₆₅H₄₆F₂N₂, 899.3608; found 899.3617.

3,3'-((Phenylmethylene)bis(5-(4-(1,2,2-triphenyvinyl)phenyl)-1H-indole) (37a). Compound 37a was obtained according to GP3. Column chromatography gave the product as yellow solid (54 mg, 96% yield; mp 198.6–199.6 ⁰C). ¹H NMR (400 MHz, CDCl₃): δ 7.79 (d, J = 1.8 Hz, 2H), 7.53 (s, 2H), 7.40 – 7.17 (m, 14H), 7.15 – 6.96 (m, 34H), 5.89 (s, 1H). ¹³C NMR (100 MHz, CDCl₃): δ 144.0, 143.9, 143.9, 141.6, 140.8, 140.7, 140.2, 136.2, 132.3, 131.6, 131.5, 131.40, 131.36, 128.7, 128.3, 127.7, 127.63, 127.61, 127.60, 126.4, 126.3 (2C), 126.2, 124.3, 121.6, 120.1, 118.0, 111.2, 40.1 (2C signal overlaps). HRMS (ESI-TOF) m/z: [M + H]⁺ calcd for C₇₅H₅₅N₂, 983.4360; found 983.4352.
3,3’-((4-Fluorophenyl)methylene)bis(5-{4-(1,2,2-triphenylvinyl)phenyl}-1H-indole) (37b). Compound 37b was obtained according to GP3. Column chromatography gave the product as yellow solid (49 mg, 93% yield; mp 175.9–176.9 °C). 1H NMR (400 MHz, CDCl3): δ 7.69 (bs, 2H), 7.42 (s, 2H), 7.28 (dd, J = 8.5, 1.6 Hz, 2H), 7.22 (d, J = 8.5 Hz, 2H), 7.21 – 7.12 (m, 8H), 7.07 – 6.90 (m, 32H), 6.85 (t, J = 8.7 Hz, 2H), 6.49 (d, J = 1.6 Hz, 2H), 5.78 (s, 1H). 13C NMR (100 MHz, CDCl3): δ 161.5 (d, J = 243.9 Hz), 144.0, 143.90, 143.87, 141.7, 140.8, 140.1, 139.6, 139.6, 136.2, 132.4, 131.7, 131.5, 131.4, 131.4, 130.1 (d, J = 7.7 Hz), 127.8, 127.7, 127.6, 127.4, 126.4, 126.3, 124.3, 121.8, 119.9, 117.9, 115.0 (d, J = 21.2 Hz), 111.3, 39.4. HRMS (ESI-TOF) m/z: [M + H]+ calcd for C75H54FN3; 1001.4266; found 1001.4261

3,3’-((4-Bromophenyl)methylene)bis(5-{4-(1,2,2-triphenylvinyl)phenyl}-1H-indole) (37c). Compound 37c was obtained according to GP3. Column chromatography gave the product as white-off solid (52 mg, 89% yield; mp 194.1–195.1 °C). 1H NMR (400 MHz, CDCl3): δ 7.75 (bs, 2H), 7.49 (s, 2H), 7.38 – 7.32 (m, 4H), 7.28 (d, J = 8.4 Hz, 4H), 7.24 (d, J = 8.4 Hz, 4H), 7.16 (d, J = 8.4 Hz, 2H), 7.12 – 6.97 (m, 32H), 6.54 (d, J = 1.3 Hz, 2H), 5.82 (s, 1H). 13C NMR (100 MHz, CDCl3): δ 144.0, 143.91, 143.90, 143.1, 141.7, 140.8, 140.8, 140.1, 136.2, 132.5, 131.7, 131.5, 131.4, 130.5, 127.8, 127.7, 127.7, 127.3, 126.4, 126.4, 124.3, 121.8, 120.0, 119.4, 117.8, 111.4, 39.6 (3C signal overlaps). HRMS (ESI-TOF) m/z: [M + H]+ calcd for C75H54BrN3; 1061.3465; found 1061.3466

3,3’-((4-Methoxyphenyl)methylene)bis(5-{4-(1,2,2-triphenylvinyl)phenyl}-1H-indole) (37d). Compound 37d was obtained according to GP3. Column chromatography gave the product as yellow solid (52 mg, 92% yield; mp 180.0–181.0 °C). 1H NMR (400 MHz, CDCl3): δ 7.47 (bs, 2H), 7.46 (s, 2H), 7.31 – 7.22 (m, 4H), 7.21 – 7.13 (m, 6H), 7.06 – 6.88 (m, 34H), 6.72 (d, J = 8.6 Hz, 2H), 6.54 (s, 2H), 5.78 (s, 1H), 3.68 (s, 3H). 13C NMR (100 MHz, CDCl3): δ 158.0, 144.0, 143.91, 143.90, 141.6, 140.8, 140.7, 140.2, 136.3, 136.2, 132.2, 131.6, 131.6, 131.5, 131.39, 131.36, 129.6, 127.7, 127.6, 127.6, 127.5, 126.4, 126.3 (2C), 124.2, 121.6, 120.4, 118.1, 113.6, 111.2, 55.3, 39.2 (1C signal overlaps). HRMS (ESI-TOF) m/z: [M + H]+ calcd for C67H57N2O; 1013.4465; found 1013.4474

4-(Bis(5-{4-(1,2,2-triphenylvinyl)phenyl}-1H-indol-3-yl)methyl)phenyl acetate (37e). Compound 37e was obtained according to GP3. Column chromatography gave the product as yellow solid (52 mg, 95% yield; mp 201.3–202.3 °C). 1H NMR (400 MHz, CDCl3): δ 7.68 (bs, 2H), 7.43 (s, 2H), 7.27 (dd, J = 8.5, 1.4 Hz, 2H), 7.21 – 7.14 (m, 8H), 7.07 – 6.90 (m, 36H), 6.87 (d, J = 8.5 Hz, 2H), 5.78 (s, 1H), 2.18 (s, 3H). 13C NMR (100 MHz, CDCl3): δ 169.7, 149.0, 144.0, 143.91, 143.90, 141.6, 141.5, 140.8, 140.7, 140.1, 136.2, 132.3, 131.7, 131.5, 131.41, 131.40, 129.6, 127.8, 127.7, 127.6, 127.4, 126.39, 126.37, 126.3, 124.5, 121.7, 121.2, 119.7, 117.9, 111.3, 39.4, 21.2 (1C signal overlaps). HRMS (ESI-TOF) m/z: [M + H]+ calcd for C76H57N2O2; 1041.4415; found 1041.4403

3,3’-((4-(Trifluoromethyl)phenyl)methylene)bis(5-{4-(1,2,2-triphenylvinyl)phenyl}-1H-indole) (37f). Compound 37f was obtained according to GP3. Column chromatography gave the product as yellow solid (50 mg, 89% yield; mp 185.3–186.3 °C). 1H NMR (400 MHz, CDCl3): δ 7.85 (d, J = 1.8 Hz, 2H), 7.51 (d, J = 8.2 Hz, 2H), 7.49 (s, 2H), 7.43 (d, J = 8.2 Hz, 2H), 7.38 (dd, J = 8.5, 1.4 Hz, 2H), 7.33 (d, J = 8.5 Hz, 2H), 7.27 – 7.21 (m, 4H), 7.14 – 6.98 (m, 34H), 6.61 (d, J = 1.7 Hz, 2H), 5.95 (s, 1H). 13C NMR (100 MHz, CDCl3): δ 148.2, 148.0, 144.0, 143.9, 141.8, 140.9, 140.0, 136.2, 132.6, 131.7, 131.5, 131.43, 131.41, 129.1, 128.6 (q, J = 32.3 Hz), 127.8, 127.7, 127.69, 127.3, 126.5, 126.4, 126.38, 125.3 (q, J = 4.1 Hz), 124.5 (q, J = 272.2 Hz), 124.4, 121.9, 119.1, 117.8, 111.5, 40.0 (1C signal overlaps). HRMS (ESI-TOF) m/z: [M + H]+ calcd for C76H54F3N2; 1051.4234; found 1051.4212.
2. NMR Spectra of Compounds

Figure S1. $^1$H and $^{13}$C (APT) NMR of 2
Figure S2. $^1$H and $^{13}$C (APT) NMR of 4
Figure S3. $^1$H and $^{13}$C (APT) NMR of 5
Figure S4. $^1$H and $^{13}$C (APT) NMR of 6
Figure S5. $^1$H and $^{13}$C (APT) NMR of 7
Figure S6. $^1$H and $^{13}$C (APT) NMR of 9
Figure S7. $^1$H and $^{13}$C (APT) NMR of 10
Figure S8. $^1$H and $^{13}$C (APT) NMR of 11
Figure S9. $^1$H and $^{13}$C (APT) NMR of 12
Figure S10. $^1$H and $^{13}$C (APT) NMR of 13
Figure S11. $^1$H and $^{13}$C (APT) NMR of 14
Figure S12. $^1$H and $^{13}$C (APT) NMR of 15
Figure S13. $^1$H and $^{13}$C (APT) NMR of 17
Figure S14. \(^1\)H and \(^{13}\)C (APT) NMR of 18
Figure S15. $^1$H and $^{13}$C (APT) NMR of 19
Figure S16. $^1$H and $^{13}$C (APT) NMR of 21
Figure S17. $^1$H and $^{13}$C (APT) NMR of 22
Figure S18. $^1$H and $^{13}$C (APT) NMR of 23
Figure S19. $^1$H and $^{13}$C (APT) NMR of 24
Figure S20. $^1$H and $^{13}$C (APT) NMR of 26
Figure S21. $^1$H and $^{13}$C (APT) NMR of 28
Figure S22. $^1$H and $^{13}$C (APT) NMR of 29
Figure S23. $^1$H and $^{13}$C (APT) NMR of 30
Figure S24. $^1$H and $^{13}$C (APT) NMR of 32
Figure S25. $^1$H and $^{13}$C (APT) NMR of 33
Figure S26. $^1$H and $^{13}$C (APT) NMR of 34
Figure S27. $^1$H and $^{13}$C (APT) NMR of 36a
Figure S28. $^1$H and $^{13}$C (APT) NMR of 36b
Figure S29. $^1$H and $^{13}$C (APT) NMR of 36c
Figure S30. $^1$H and $^{13}$C (APT) NMR of 36d
Figure S31. $^1$H and $^{13}$C (APT) NMR of 36e
Figure S32. $^1$H and $^{13}$C NMR of 36f
Figure S33. $^1$H and $^{13}$C (APT) NMR of 37a
Figure S34. $^1$H and $^{13}$C (APT) NMR of 37b
Figure S35. $^1$H and $^{13}$C (APT) NMR of 37c
Figure S36. $^1$H and $^{13}$C (APT) NMR of 37d
Figure S37. $^1$H and $^{13}$C (APT) NMR of 37e
Figure S38. $^1$H and $^{13}$C NMR of 37f
3. HRMS Spectra

3.1. HRMS spectra of 9

3.2. HRMS spectra of 10

3.3. HRMS spectra of 14
3.4. HRMS spectra of 15

3.5. HRMS spectra of 19

3.6. HRMS spectra of 21
3.7. HRMS spectra of 22

3.8. HRMS spectra of 23

3.9. HRMS spectra of 26
3.10. HRMS spectra of 28

3.11. HRMS spectra of 29

3.12. HRMS spectra of 30
3.13. HRMS spectra of 32

3.14. HRMS spectra of 33

3.15. HRMS spectra of 34
3.16. HRMS spectra of 36a

3.17. HRMS spectra of 36b

3.18. HRMS spectra of 36c
3.19. HRMS spectra of 36d

3.20. HRMS spectra of 36e

3.21. HRMS spectra of 36f
3.22. HRMS spectra of 37a

3.23. HRMS spectra of 37b

3.24. HRMS spectra of 37c
3.25. HRMS spectra of 37d

3.26. HRMS spectra of 37e

3.27. HRMS spectra of 37f
4. AIE Characteristics

Figure S39. (a) Fluorescence spectra of 10 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 10 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 10 in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 10 in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 10 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S40. (a) Fluorescence spectra of 14 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 14 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 µM. Photograph of 14 in THF–water mixtures ($f_w = 0$–98%) with different water fractions (20 µM) under 365 nm UV illumination. Photograph of 14 in water–THF mixed solution ($f_w = 0$–98%) under a UV lamp. (c) DLS particle size-distribution profile of 14 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S41. (a) Fluorescence spectra of 15 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 15 in THF–water with different water fractions \(f_w\). Luminogen concentration: 20 \(\mu\)M. Photograph of 15 in THF–water mixtures \(f_w = 0–98\%\) with different water fractions (20 \(\mu\)M) under 365 nm UV illumination. Photograph of 15 in water–THF mixed solution \(f_w = 0–98\%\) under a UV lamp. (c) DLS particle size-distribution profile of 15 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S42. (a) Fluorescence spectra of 21 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 21 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 21 in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 21 in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size–distribution profile of 21 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S43. (a) Fluorescence spectra of 22 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 22 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 22 in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 22 in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 22 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S44. (a) Fluorescence spectra of 28 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 28 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 28 in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 28 in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 28 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S45. (a) Fluorescence spectra of 29 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 29 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 µM. Photograph of 29 in THF–water mixtures ($f_w = 0$–98%) with different water fractions (20 µM) under 365 nm UV illumination. Photograph of 29 in water–THF mixed solution ($f_w = 0$–98%) under a UV lamp. (c) DLS particle size-distribution profile of 29 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S46. (a) Fluorescence spectra of 30 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 30 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 30 in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 30 in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 30 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S47. (a) Fluorescence spectra of 32 in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 32 in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 32 in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 32 in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 32 in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S48. (a) Fluorescence spectra of 33 in DMSO and DMSO–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 33 in DMSO–water with different water fractions (f_w). Luminogen concentration: 20 µM. Photograph of 33 in DMSO–water mixtures (f_w = 0–98%) with different water fractions (20 µM) under 365 nm UV illumination. Photograph of 33 in water–DMSO mixed solution (f_w = 0–98%) under a UV lamp. (c) DLS particle size-distribution profile of 33 in DMSO–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S49. (a) Fluorescence spectra of 34 in DMSO and DMSO–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 34 in DMSO–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 34 in DMSO–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 34 in water–DMSO mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 34 in DMSO–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S50. (a) Fluorescence spectra of 36a in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 36a in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 36a in THF–water mixtures ($f_w = 0$–98%) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 36a in water–THF mixed solution ($f_w = 0$–98%) under a UV lamp. (c) DLS particle size-distribution profile of 36a in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S51. (a) Fluorescence spectra of 36b in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 36b in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 $\mu$M. Photograph of 36b in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 $\mu$M) under 365 nm UV illumination. Photograph of 36b in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 36b in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S52. (a) Fluorescence spectra of 36c in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 36c in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 36c in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 36c in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 36c in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S53. (a) Fluorescence spectra of 36d in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 36d in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 µM. Photograph of 36d in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 µM) under 365 nm UV illumination. Photograph of 36d in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size–distribution profile of 36d in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S54. (a) Fluorescence spectra of \(36e\) in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of \(36e\) in THF–water with different water fractions \(f_w\). Luminogen concentration: 20 \(\mu\)M. Photograph of \(36e\) in THF–water mixtures \((f_w = 0–98\%)\) with different water fractions (20 \(\mu\)M) under 365 nm UV illumination. Photograph of TFTB in water–THF mixed solution \((f_w = 0–98\%)\) under a UV lamp. (c) DLS particle size-distribution profile of \(36e\) in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S55. (a) Fluorescence spectra of 36g in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 36g in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 µM. Photograph of 36g in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 µM) under 365 nm UV illumination. Photograph of 36g in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 36g in THF–water mixture (2: 98, v: v); (d-f) SEM image.
Figure S56. (a) Fluorescence spectra of 37a in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 37a in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 $\mu$M. Photograph of 37a in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 $\mu$M) under 365 nm UV illumination. Photograph of 37a in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 37a in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S57. (a) Fluorescence spectra of 37b in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 37b in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 $\mu$M. Photograph of 37b in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 $\mu$M) under 365 nm UV illumination. Photograph of 37b in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 37b in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S58. (a) Fluorescence spectra of 37c in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 37c in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 μM. Photograph of 37c in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 37c in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 37c in THF–water mixture (10: 90, v: v); (d-f) SEM image.
Figure S59. (a) Fluorescence spectra of 37d in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 37d in THF–water with different water fractions ($f_w$). Luminogen concentration: 20 µM. Photograph of 37d in THF–water mixtures ($f_w = 0–98\%$) with different water fractions (20 µM) under 365 nm UV illumination. Photograph of 37d in water–THF mixed solution ($f_w = 0–98\%$) under a UV lamp. (c) DLS particle size-distribution profile of 37d in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S60. (a) Fluorescence spectra of 37e in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 37e in THF–water with different water fractions \( f_w \). Luminogen concentration: 20 μM. Photograph of 37e in THF–water mixtures \( f_w = 0–98\% \) with different water fractions (20 μM) under 365 nm UV illumination. Photograph of 37e in water–THF mixed solution \( f_w = 0–98\% \) under a UV lamp. (c) DLS particle size-distribution profile of 37e in THF–water mixture (5: 95, v: v); (d-f) SEM image.
Figure S61. (a) Fluorescence spectra of 37g in THF and THF–water mixtures with different water fractions; (b) Plot of peak fluorescence intensities of 37g in THF–water with different water fractions (f_w). Luminogen concentration: 20 µM. Photograph of 37g in THF–water mixtures (f_w = 0–98%) with different water fractions (20 µM) under 365 nm UV illumination. Photograph of 37g in water–THF mixed solution (f_w = 0–98%) under a UV lamp. (c) DLS particle size-distribution profile of 37g in THF–water mixture (2: 98, v: v); (d-f) SEM image.
5. Theoretical Calculations

All calculations were carried out using density functional theory (DFT) at the B3LYP (Becke 3-parameter-Lee Yang-Parr) with the basis set of 6-311G (d,p).

Cartesian coordinates and total energy of optimized structure

![Figure S62. Optimized geometry by semi-empirical calculation using PM6 of compound 9](image)

Table S1. Atom coordinates and total energy of the optimized geometry of compound 9

Total Energy: -1134.366945 hartrees zero imaginary frequency

| Atom  | X        | Y        | Z        |
|-------|----------|----------|----------|
| C1    | 0.6777816| 5.0240045| -1.0658893|
| C2    | -0.2405919| 4.3429463| -1.8715496|
| C3    | -0.5758337| 3.0169453| -1.5884935|
| C4    | 0.0181148 | 2.3622129| -0.4981403|
| C5    | 0.9386573 | 3.0466287| 0.3106366 |
| C6    | 1.2638177 | 4.3749187| 0.0252412 |
| C7    | -0.3457479| 0.9559749| -0.1941492|
| C8    | 0.5511372 | 0.0529959| -0.2321677|
| C9    | -1.7740074| 0.7658964| 0.1552049 |
| C10   | 1.9700396 | 0.1593065| -0.6146205|
| C11   | 0.2136778 | -1.4564997| 0.1041937|
| C12   | 2.9935133 | -0.2240759| 0.2670708 |
| C13   | 4.3303101 | -0.0403291| -0.0930542|
| C14   | 4.6545163 | 0.5191890| -1.3332870|
Table S2. Atomic charges of compound 9 calculated by B3LYP/6-31G (d,p) method

| Atom Label | Natural charge | Mulliken charge | Electrostatic charge |
|------------|----------------|----------------|---------------------|
| C1         | -0.240         | -0.126         | -0.180              |
| C2         | -0.230         | -0.136         | -0.037              |
| C3         | -0.219         | -0.158         | -0.357              |
| C4         | -0.056         | +0.078         | +0.442              |
| C5         | -0.216         | -0.149         | -0.256              |
| C6         | -0.227         | -0.135         | -0.099              |
| C7         | -0.020         | -0.074         | -0.381              |
| C8         | -0.006         | -0.037         | -0.176              |
| C9         | -0.057         | +0.084         | +0.453              |
| C10        | -0.059         | +0.074         | +0.465              |
|   |   |   |   |
|---|---|---|---|
| C11 | -0.083 | +0.075 | +0.239 |
| C12 | -0.215 | -0.158 | -0.352 |
| C13 | -0.231 | -0.137 | -0.050 |
| C14 | -0.239 | -0.126 | -0.187 |
| C15 | -0.229 | -0.136 | -0.081 |
| C16 | -0.214 | -0.152 | -0.305 |
| C17 | -0.221 | -0.186 | -0.240 |
| C18 | -0.262 | -0.166 | -0.268 |
| C19 | +0.159 | +0.305 | +0.161 |
| C20 | -0.095 | +0.116 | +0.224 |
| C21 | -0.192 | -0.235 | -0.385 |
| C22 | -0.220 | -0.160 | -0.368 |
| C23 | -0.231 | -0.137 | -0.032 |
| C24 | -0.240 | -0.126 | -0.186 |
| C25 | -0.228 | -0.135 | -0.090 |
| C26 | -0.213 | -0.149 | -0.264 |
| C28 | -0.036 | +0.043 | -0.095 |
| C29 | -0.304 | -0.219 | -0.369 |
| H30 | +0.235 | +0.125 | +0.125 |
| H31 | +0.235 | +0.127 | +0.111 |
| H32 | +0.240 | +0.133 | +0.149 |
| H33 | +0.243 | +0.134 | +0.135 |
| H34 | +0.236 | +0.127 | +0.121 |
| H35 | +0.242 | +0.136 | +0.149 |
| H36 | +0.235 | +0.126 | +0.114 |
| H37 | +0.234 | +0.125 | +0.128 |
| H38 | +0.235 | +0.127 | +0.119 |
| H39 | +0.243 | +0.136 | +0.150 |
| H40 | +0.243 | +0.133 | +0.132 |
Figure S63. Optimized geometry by semi-empirical calculation using PM6 of compound 32

Table S3. Atom coordinates and total energy of the optimized geometry of compound 32

Total Energy: -1365.423022 hartrees | zero imaginary frequency

| Atom | X    | Y    | Z    |
|------|------|------|------|
| H41  | +0.235 | +0.123 | +0.164 |
| H42  | +0.245 | +0.137 | +0.191 |
| H43  | +0.241 | +0.134 | +0.152 |
| H44  | +0.235 | +0.126 | +0.110 |
| H45  | +0.234 | +0.125 | +0.126 |
| H46  | +0.235 | +0.127 | +0.118 |
| H47  | +0.243 | +0.136 | +0.147 |
| H48  | +0.430 | +0.328 | +0.343 |
| H49  | +0.232 | +0.151 | +0.168 |
| H50  | +0.243 | +0.131 | +0.188 |
| N27  | -0.572 | -0.687 | -0.365 |
| 1  | C  | C1   | 0.8814618 | 6.4703347 | -1.5904399 |
|----|----|------|-----------|-----------|-------------|
| 2  | C  | C2   | 0.5157586 | 6.1826560 | -0.2714090 |
| 3  | C  | C3   | 0.2239661 | 4.8701473 | 0.1064726  |
| 4  | C  | C4   | 0.3046678 | 3.8340826 | -0.8380097 |
| 5  | C  | C5   | 0.6710689 | 4.1243504 | -2.1615342 |
| 6  | C  | C6   | 0.9575126 | 5.4402691 | -2.5331987 |
| 7  | C  | C7   | -0.0188495 | 2.4437710 | -0.4347585 |
| 8  | C  | C8   | -1.3833211 | 2.2733120 | 0.1213379  |
| 9  | C  | C9   | 0.8537592 | 1.4217018 | -0.5633688 |
| 10 | C  | C10  | 0.5203782 | 0.0265522 | -0.1878677 |
| 11 | C  | C11  | 2.2281437 | 1.5969836 | -1.0931775 |
| 12 | C  | C12  | -1.5663460 | 1.7547025 | 1.4128978  |
| 13 | C  | C13  | -2.8556975 | 1.6150417 | 1.9323095  |
| 14 | C  | C14  | -3.9661587 | 1.9888736 | 1.1690459  |
| 15 | C  | C15  | -3.7854424 | 2.5057498 | -0.1180556 |
| 16 | C  | C16  | -2.4992570 | 2.6519090 | -0.6424500 |
| 17 | C  | C17  | 1.2930092 | -0.6410361 | 0.7759142  |
| 18 | C  | C18  | 0.9924554 | -1.9573711 | 1.1261890  |
| 19 | C  | C19  | -0.0812723 | -2.6245964 | 0.5144041  |
| 20 | C  | C20  | -0.8502195 | -1.9571965 | -0.4524641 |
| 21 | C  | C21  | -0.5516105 | -0.6397909 | -0.8017832 |
| 22 | C  | C22  | 2.6354760 | 0.8724632 | -2.2250754 |
| 23 | C  | C23  | 3.9321054 | 1.0247709 | -2.7212869 |
| 24 | C  | C24  | 4.8297613 | 1.8911915 | -2.0896938 |
| 25 | C  | C25  | 4.4268433 | 2.6105729 | -0.9579453 |
| 26 | C  | C26  | 3.1298553 | 2.4669683 | -0.4605912 |
| 27 | C  | C27  | -0.4026109 | -0.0419891 | 0.8875632  |
| 28 | C  | C28  | 0.6141410 | -5.0129721 | 0.7754174  |
| 29 | C  | C29  | 0.3774419 | -6.3334998 | 1.1066166  |
| 30 | C  | C30  | -0.9134971 | -6.6640250 | 1.5650697  |
| 31 | C  | C31  | -1.9520506 | -5.6781959 | 1.6857026  |
| 32 | C  | C32  | -1.6767281 | -4.3444441 | 1.3373338  |
| 33 | C  | C33  | -1.4520031 | -7.8962916 | 1.9727069  |
| 34 | C  | C34  | -2.7900571 | -7.6902887 | 2.3413568  |
| 35 | C  | C35  | -3.1239947 | -6.3564200 | 2.1763057  |
| 36 | H  | H36  | 1.1066353 | 7.4938444 | -1.8823393 |
| 37 | H  | H37  | 0.4558533 | 6.9837975 | 0.4631832  |
| 38 | H  | H38  | -0.0703699 | 4.6471864 | 1.1311035  |
| 39 | H  | H39  | 0.7403575 | 3.3207176 | -2.8935565 |
| 40 | H  | H40  | 1.2435689 | 5.6622968 | -3.5599273 |
| 41 | H  | H41  | -0.7023389 | 1.4527409 | 2.0035782  |
| 42 | H  | H42  | -2.9945931 | 1.2110044 | 2.9338128  |
| 43 | H  | H43  | -4.9691032 | 1.8777063 | 1.5755966  |
| 44 | H  | H44  | -4.6493151 | 2.7967935 | -0.7132124 |
| 45 | H  | H45  | -2.3580501 | 3.0622205 | -1.6415032 |
| 46 | H  | H46  | 2.1296877 | -0.1274709 | 1.2486729  |
| 47 | H  | H47  | 1.5877227 | -2.4686860 | 1.8814923  |
| 48 | H  | H48  | -1.6808265 | -2.4723143 | -0.9336497 |
| 49 | H  | H49  | -1.1554948 | -0.1225028 | -1.5468713 |
| 50 | H  | H50  | 1.9390524 | 0.1900856 | -2.7107095 |
| 51 | H  | H51  | 4.2447443 | 0.4646115 | -3.6008426 |
| 52 | H  | H52  | 5.8396651 | 2.0068597 | -2.4768059 |
| 53 | H  | H53  | 5.1238765 | 3.2870751 | -0.4680950 |
| 54 | H  | H54  | 2.8128139 | 3.0351442 | 0.4129985  |
| 55 | H  | H55  | 1.5963965 | -4.7110967 | 0.4112710 |
| 56 | H  | H56  | 1.1497774 | -7.0901360 | 1.0181726  |
| 57 | H  | H57  | -2.4537700 | -3.5878733 | 1.4284187  |
| 58 | H  | H58  | -0.9650576 | -8.7690343 | 1.9973929  |
| 59 | H  | H59  | -3.4122027 | -8.5033551 | 2.6888915  |
| 60 | H  | H60  | -4.0688642 | -5.8911790 | 2.3711939  |

Table S4. Atomic charges of compound 32 calculated by B3LYP/6-31G (d,p) method
| Atom Label | Natural charge | Mulliken charge | Electrostatic charge |
|------------|----------------|----------------|---------------------|
| C1         | -0.239         | -0.126         | -0.181              |
| C2         | -0.230         | -0.136         | -0.039              |
| C3         | -0.217         | -0.159         | -0.357              |
| C4         | -0.059         | +0.078         | +0.450              |
| C5         | -0.214         | -0.150         | -0.267              |
| C6         | -0.228         | -0.136         | -0.094              |
| C7         | -0.014         | -0.054         | -0.333              |
| C8         | -0.059         | +0.080         | +0.477              |
| C9         | -0.010         | -0.060         | -0.266              |
| C10        | -0.066         | +0.085         | +0.339              |
| C11        | -0.059         | +0.080         | +0.418              |
| C12        | -0.213         | -0.151         | -0.289              |
| C13        | -0.229         | -0.137         | -0.086              |
| C14        | -0.239         | -0.126         | -0.187              |
| C15        | -0.231         | -0.137         | -0.033              |
| C16        | -0.217         | -0.158         | -0.373              |
| C17        | -0.211         | -0.167         | -0.308              |
| C18        | -0.219         | -0.172         | -0.151              |
| C19        | -0.047         | +0.069         | +0.122              |
| C20        | -0.215         | -0.171         | -0.243              |
| C21        | -0.208         | -0.159         | -0.187              |
| C22        | -0.217         | -0.159         | -0.345              |
| C23        | -0.230         | -0.136         | -0.042              |
| C24        | -0.239         | -0.126         | -0.181              |
| C25        | -0.228         | -0.136         | -0.095              |
| C26        | -0.214         | -0.151         | -0.264              |
| C27        | -0.071         | +0.060         | +0.110              |
|    |    |    |    |
|----|----|----|----|
| C28 | -0.227 | -0.188 | -0.185 |
| C29 | -0.260 | -0.164 | -0.290 |
| C30 | +0.157 | +0.304 | +0.191 |
| C31 | -0.094 | +0.120 | +0.259 |
| C32 | -0.204 | -0.246 | -0.393 |
| C34 | -0.034 | +0.045 | -0.058 |
| C35 | -0.307 | -0.221 | -0.418 |
| C36 |    |    |    |
| C37 |    |    |    |
| C38 |    |    |    |
| C39 |    |    |    |
| C40 |    |    |    |
| C41 |    |    |    |
| C42 |    |    |    |
| C43 |    |    |    |
| C44 |    |    |    |
| C45 |    |    |    |
| C46 |    |    |    |
| C47 |    |    |    |
| C48 |    |    |    |
| C49 |    |    |    |
| C50 |    |    |    |
| C51 |    |    |    |
| C52 |    |    |    |
| C53 |    |    |    |
| C54 |    |    |    |
| C55 |    |    |    |
| C56 |    |    |    |
| C57 |    |    |    |
**Figure S64.** Optimized geometry by semi-empirical calculation using PM6 of compound 33

**Table S5.** Atom coordinates and total energy of the optimized geometry of compound 33

Total Energy -1728.04409 hartrees zero imaginary frequency

| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| C1   | -1.3073512 | 3.4849104 | 0.2300982 |
| C2   | -1.5960414 | 2.0723415 | 0.5783037 |
| C3   | -2.8791515 | 1.8726350 | 1.2947749 |
| C4   | -0.7626883 | 1.0565680 | 0.2681826 |
| C5   | -1.0388566 | -0.3529492 | 0.636763 |
| C6   | 0.5063039  | 1.2542624 | -0.4728420 |
| C7   | -1.1928935 | -0.7230376 | 1.9816060 |
| C8   | -1.4375006 | -2.0549500 | 2.3183705 |
| C9   | -1.5316721 | -3.0327340 | 1.3153416 |
| C10  | -1.3755909 | -2.6612957 | -0.0301719 |
| C11  | -1.1287370 | -1.3305549 | -0.3673311 |
| C12  | 1.7204522  | 0.8399182 | 0.0976385 |
| C13  | 2.9170726  | 1.0116259 | -0.5986221 |
| C14  | 2.9147024  | 1.5933900 | -1.8767914 |
| C15  | 1.6991581  | 2.0028391 | -2.4482406 |
| C16  | 0.5026977  | 1.8357851 | -1.7504379 |
| C17  | 4.1832273  | 1.7718867 | -2.6166322 |
| C18  | -1.7940656 | -4.4439367 | 1.6730001 |
| C19  | -0.8772986 | -5.4451580 | 1.2366273 |
| C20  | -1.0647680 | -6.7808401 | 1.5370547 |
| C21  | -2.2050135 | -7.1199173 | 2.2926184 |
Table S6. Atomic charges of compound 33 calculated by B3LYP/6-31G (d,p) method

| Atom Label | Natural charge | Mulliken charge | Electrostatic charge |
|------------|----------------|-----------------|----------------------|
| C1         | -0.058         | +0.080          | +0.506               |
| C2         | -0.016         | -0.061          | -0.368               |
|   |   |   |   |
|---|---|---|---|
| C3 | -0.058 | +0.081 | +0.450 |
| C4 | -0.008 | -0.058 | -0.240 |
| C5 | -0.065 | +0.087 | +0.387 |
| C6 | -0.066 | +0.088 | +0.359 |
| C7 | -0.208 | -0.160 | -0.230 |
| C8 | -0.215 | -0.170 | -0.219 |
| C9 | -0.048 | +0.068 | +0.112 |
| C10| -0.219 | -0.172 | -0.135 |
| C11| -0.210 | -0.168 | -0.339 |
| C12| -0.210 | -0.169 | -0.298 |
| C13| -0.218 | -0.172 | -0.168 |
| C14| -0.048 | +0.069 | +0.119 |
| C15| -0.217 | -0.172 | -0.201 |
| C16| -0.207 | -0.160 | -0.236 |
| C17| -0.071 | +0.060 | +0.096 |
| C18| -0.071 | +0.060 | +0.088 |
| C19| -0.227 | -0.188 | -0.178 |
| C20| -0.260 | -0.164 | -0.283 |
| C21| +0.157 | +0.305 | +0.186 |
| C22| -0.094 | +0.119 | +0.240 |
| C23| -0.204 | -0.245 | -0.367 |
| C24| -0.204 | -0.245 | -0.385 |
| C25| -0.094 | +0.120 | +0.253 |
| C26| +0.157 | +0.305 | +0.199 |
| C27| -0.261 | -0.164 | -0.299 |
| C28| -0.227 | -0.189 | -0.176 |
| C30| -0.034 | +0.044 | -0.065 |
| C31| -0.307 | -0.221 | -0.405 |
| C32| -0.307 | -0.221 | -0.403 |
|   |   |   |   |
|---|---|---|---|
| C33 | -0.034 | +0.045 | -0.074 |
| C35 | -0.217 | -0.158 | -0.364 |
| C36 | -0.230 | -0.136 | -0.034 |
| C37 | -0.239 | -0.126 | -0.185 |
| C38 | -0.228 | -0.136 | -0.093 |
| C39 | -0.214 | -0.150 | -0.269 |
| C40 | -0.218 | -0.158 | -0.391 |
| C41 | -0.230 | -0.136 | -0.027 |
| C42 | -0.239 | -0.126 | -0.184 |
| C43 | -0.228 | -0.136 | -0.097 |
| C44 | -0.214 | -0.150 | -0.285 |
| H45 | +0.243 | +0.135 | +0.144 |
| H46 | +0.241 | +0.132 | +0.145 |
| H47 | +0.240 | +0.131 | +0.127 |
| H48 | +0.241 | +0.134 | +0.151 |
| H49 | +0.241 | +0.134 | +0.140 |
| H50 | +0.240 | +0.131 | +0.137 |
| H51 | +0.240 | +0.131 | +0.137 |
| H52 | +0.243 | +0.135 | +0.144 |
| H53 | +0.241 | +0.130 | +0.129 |
| H54 | +0.235 | +0.123 | +0.161 |
| H55 | +0.241 | +0.132 | +0.177 |
| H56 | +0.241 | +0.131 | +0.176 |
| H57 | +0.235 | +0.123 | +0.164 |
| H58 | +0.241 | +0.131 | +0.133 |
| H59 | +0.430 | +0.328 | +0.352 |
| H60 | +0.233 | +0.151 | +0.163 |
| H61 | +0.242 | +0.130 | +0.197 |
| H62 | +0.242 | +0.130 | +0.196 |
|   |   |   |   |
|---|---|---|---|
| H63 | +0.233 | +0.151 | +0.166 |
| H64 | +0.430 | +0.328 | +0.355 |
| H65 | +0.241 | +0.134 | +0.148 |
| H66 | +0.235 | +0.127 | +0.111 |
| H67 | +0.235 | +0.126 | +0.126 |
| H68 | +0.236 | +0.128 | +0.119 |
| H69 | +0.244 | +0.137 | +0.147 |
| H70 | +0.241 | +0.135 | +0.153 |
| H71 | +0.235 | +0.127 | +0.111 |
| H72 | +0.234 | +0.125 | +0.126 |
| H73 | +0.236 | +0.128 | +0.122 |
| H74 | +0.244 | +0.137 | +0.145 |
| N29 | -0.572 | -0.686 | -0.396 |
| N34 | -0.572 | -0.687 | -0.404 |

Figure S65. Optimized geometry by semi-empirical calculation using PM6 of compound 34
Table S7. Atom coordinates and total energy of the optimized geometry of compound 34

Total Energy -2453.286868 hartrees; zero imaginary frequency

Cartesian Coordinates (Angstroms)

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| 1 C  | -0.0147141 | 1.8426653 | -0.4240910 |
| 2 C  | -0.3599736  | 0.4790826  | 0.0197733  |
| 3 C  | -1.6225481  | 0.3929331  | 0.7768836  |
| 4 C  | 0.4101999   | -0.5905077  | -0.2453572 |
| 5 C  | 0.0663977   | -1.9561468  | 0.1925972  |
| 6 C  | 1.6724243   | -0.4980444  | -1.0029479 |
| 7 C  | 0.6308348   | -2.4808482  | 1.3558773  |
| 8 C  | 0.3222005   | -3.7747886  | 1.7564355  |
| 9 C  | -0.5474492  | -4.5596594  | 0.9947094  |
| 10 C | -1.1080964  | -4.0318869  | -0.1713839 |
| 11 C | -0.8048590  | -2.7360463  | -0.5694275 |
| 12 C | 2.8847926   | -0.3512500  | -0.3275173 |
| 13 C | 4.0747251   | -0.2827037  | -1.0410385 |
| 14 C | 4.0655934   | -0.3659076  | -2.4359177 |
| 15 C | 2.8498162   | -0.5160381  | -3.1083559 |
| 16 C | 1.6588580   | -0.5805233  | -2.3960606 |
| 17 C | 5.3255573   | -0.2934673  | -3.1886774 |
| 18 C | -0.8716755  | -5.9288117  | 1.4186767  |
| 19 C | -0.7969401  | -6.9772703  | 0.4726684  |
| 20 C | -1.0928750  | -8.2814292  | 0.8128746  |
| 21 C | -1.4727644  | -8.5318337  | 2.1374510  |
| 22 C | -1.5466836  | -7.4911578  | 3.0999742  |
| 23 C | -1.2450116  | -6.1767745  | 2.7321955  |
| 24 C | 6.2455163   | 0.7058589   | -2.9039338 |
| 25 C | 7.4340771   | 0.7435737   | -3.6386579 |
| 26 C | 7.6726152   | -0.2216507  | -4.6518291 |
| 27 C | 6.7448908   | -1.2314347  | -4.9371550 |
| 28 C | 5.5802236   | -1.2514548  | -4.1974644 |
| 29 N | -1.9007421  | -9.7247033  | 2.7692353  |
| 30 C | -2.1126475  | -9.4337665  | 4.1421186  |
| Atom | Symbol | X | Y | Z |
|------|--------|---|---|---|
| 31 C | C      | -1.9517755 | -8.0846330 | 4.3493471 |
| 32 C | C      | 8.5775218 | 1.6197707 | -3.5972494 |
| 33 C | C      | 9.4704400 | 1.1922030 | -4.5507984 |
| 34 N | N      | 8.9039326 | 0.1071353 | -5.2687209 |
| 35 C | C      | -1.6393966 | 0.6833300 | 2.1416463 |
| 36 C | C      | -2.8326530 | 0.6243876 | 2.8505234 |
| 37 C | C      | -4.0217787 | 0.2810110 | 2.2017455 |
| 38 C | C      | -4.0095015 | -0.0066068 | 0.8343937 |
| 39 C | C      | -2.8075299 | 0.0474992 | 0.1255735 |
| 40 C | C      | -0.4686730 | 2.3096972 | -1.6583700 |
| 41 C | C      | -0.1637697 | 3.6016464 | -2.0678714 |
| 42 C | C      | 0.6005876 | 4.4377180 | -1.2497022 |
| 43 C | C      | 1.0527067 | 3.9665563 | -0.0144219 |
| 44 C | C      | 0.7438456 | 2.6765479 | 0.3984707 |
| 45 C | C      | -5.2833566 | 0.2225978 | 2.9530380 |
| 46 C | C      | 0.9241439 | 5.8031922 | -1.6859179 |
| 47 C | C      | 2.2628805 | 6.2514680 | -1.6044771 |
| 48 C | C      | 2.6264867 | 7.5204722 | -2.0063314 |
| 49 C | C      | 1.6142610 | 8.3577896 | -2.4920875 |
| 50 C | C      | 0.2645457 | 7.9253985 | -2.5711758 |
| 51 C | C      | -0.0788085 | 6.6310323 | -2.1704069 |
| 52 C | C      | -5.3355972 | -0.4457989 | 4.1683595 |
| 53 C | C      | -6.5513829 | -0.4774302 | 4.8573875 |
| 54 C | C      | -7.6954454 | 0.1576049 | 4.3071424 |
| 55 C | C      | -7.6420695 | 0.8327935 | 3.0811451 |
| 56 C | C      | -6.4307308 | 0.8554198 | 2.4206837 |
| 57 C | C      | -6.9428120 | -1.0602496 | 6.1160607 |
| 58 C | C      | -8.2743296 | -0.7819817 | 6.3130109 |
| 59 N | N      | -8.7828513 | -0.1009300 | 5.1764570 |
| 60 N | N      | 1.6725873 | 9.6652969 | -3.0325398 |
| 61 C | C      | 0.3442590 | 10.0728568 | -3.3209018 |
| 62 C | C      | -0.5112450 | 9.0209692 | -3.0953854 |
| 63 H | H      | 1.3209184 | -1.8699022 | 1.9485518 |
| 64 H | H      | 0.7633721 | -4.1848189 | 2.6719802 |
| 65 H | H      | -1.7932795 | -4.6423479 | -0.7705245 |
66 H H66  -1.2524872  -2.3186378  -1.4783850
67 H H67  2.8937836  -0.2929216  0.7667696
68 H H68  5.0259796  -0.1643105  -0.5097963
69 H H69  2.8372187  -0.5785008  -4.2024939
70 H H70  0.7055955  -0.6931477  -2.9242031
71 H H71  -0.4930063  -6.7390148  -0.5533966
72 H H72  -1.0310448  -9.0894985  0.0779053
73 H H73  -1.3068390  -5.3681263  3.4682195
74 H H74  6.0523860  1.4518519  -2.1257040
75 H H75  6.9383585  -1.9763643  -5.7147180
76 H H76  4.8291380  -2.0271565  -4.3876805
77 H H77  -1.6351568  -10.6203157  2.4477862
78 H H78  -2.4069045  -10.2036184  4.8556723
79 H H79  -2.0996861  -7.5415263  5.2790803
80 H H80  8.6915969  2.4654216  -2.9239974
81 H H81  10.446898  1.6047403  -4.8052468
82 H H82  9.4511184  -0.5587887  -5.7515017
83 H H83  -0.7091203  0.9625820  2.6489194
84 H H84  -2.8443281  0.8505572  3.9228367
85 H H85  -4.9299011  -0.2799312  0.3211779
86 H H86  -2.7897705  -0.1854766  -0.9450986
87 H H87  -1.0647593  1.6528907  -2.3015708
88 H H88  -0.5210068  3.9685712  -3.0368152
89 H H89  1.6507310  4.6195503  0.6312662
90 H H90  1.0920815  2.3099615  1.3706192
91 H H91  3.0241900  5.5653770  -1.2151052
92 H H92  3.6645583  7.8607196  -1.9469601
93 H H93  -1.1164474  6.2873357  -2.2386058
94 H H94  -4.4516156  -0.9415352  4.5835227
95 H H95  -8.5261660  1.3254736  2.6657446
96 H H96  -6.3458240  1.3773275  1.4602701
97 H H97  -6.2847150  -1.6192058  6.7763889
98 H H98  -8.9117184  -1.0559729  7.1539036
99 H H99  -9.5824186  0.4780611  5.2137669
100 H H100 2.3894249  10.3043595  -2.8009514
Table S8. Atomic charges of compound 34 calculated by the B3LYP/6-31G (d,p) method

| Atom Label | Natural charge | Mulliken charge | Electrostatic charge |
|------------|----------------|-----------------|---------------------|
| C1         | -0.064         | +0.086          | +0.356              |
| C2         | -0.012         | -0.065          | -0.275              |
| C3         | -0.064         | +0.090          | +0.319              |
| C4         | -0.013         | -0.054          | -0.244              |
| C5         | -0.065         | +0.086          | +0.348              |
| C6         | -0.064         | +0.089          | +0.323              |
| C7         | -0.207         | -0.159          | -0.193              |
| C8         | -0.216         | -0.170          | -0.238              |
| C9         | -0.048         | +0.067          | +0.116              |
| C10        | -0.219         | -0.171          | -0.157              |
| C11        | -0.210         | -0.168          | -0.306              |
| C12        | -0.210         | -0.168          | -0.267              |
| C13        | -0.218         | -0.172          | -0.191              |
| C14        | -0.049         | +0.067          | +0.134              |
| C15        | -0.218         | -0.173          | -0.221              |
| C16        | -0.206         | -0.160          | -0.211              |
| C17        | -0.069         | +0.059          | +0.112              |
| C18        | -0.071         | +0.057          | +0.120              |
| C19        | -0.227         | -0.187          | -0.197              |
| C20        | -0.261         | -0.164          | -0.288              |
| C21        | +0.156         | +0.304          | +0.195              |
| C22        | -0.094         | +0.119          | +0.247              |
| C23        | -0.204         | -0.245          | -0.389              |
| C24        | -0.204         | -0.244          | -0.389              |
|   | C25 | C26 | C27 | C28 | C29 | C30 | C31 | C32 | C33 | C34 | C35 | C36 | C37 | C38 | C39 | C40 | C41 | C42 | C43 | C44 | C45 | C46 | C47 | C48 | C49 | C50 | C51 | C52 | C53 | C54 | C55 |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|     |       |       |       |
|-----|-------|-------|-------|
| C56 | -0.226 | -0.186 | -0.201 |
| C57 | -0.307 | -0.222 | -0.413 |
| C58 | -0.035 | +0.044 | -0.060 |
| C61 | -0.035 | +0.044 | -0.065 |
| C62 | -0.307 | -0.221 | -0.411 |
| H63 | +0.243 | +0.135 | +0.137 |
| H64 | +0.240 | +0.131 | +0.146 |
| H65 | +0.239 | +0.130 | +0.130 |
| H66 | +0.241 | +0.133 | +0.145 |
| H67 | +0.241 | +0.134 | +0.135 |
| H68 | +0.240 | +0.131 | +0.139 |
| H69 | +0.240 | +0.131 | +0.139 |
| H70 | +0.244 | +0.136 | +0.143 |
| H71 | +0.241 | +0.130 | +0.134 |
| H72 | +0.235 | +0.122 | +0.163 |
| H73 | +0.242 | +0.135 | +0.184 |
| H74 | +0.240 | +0.130 | +0.178 |
| H75 | +0.235 | +0.122 | +0.161 |
| H76 | +0.241 | +0.129 | +0.136 |
| H77 | +0.430 | +0.327 | +0.351 |
| H78 | +0.232 | +0.150 | +0.162 |
| H79 | +0.243 | +0.131 | +0.198 |
| H80 | +0.242 | +0.130 | +0.195 |
| H81 | +0.232 | +0.150 | +0.163 |
| H82 | +0.430 | +0.327 | +0.351 |
| H83 | +0.241 | +0.134 | +0.140 |
| H84 | +0.240 | +0.131 | +0.140 |
| H85 | +0.240 | +0.131 | +0.139 |
| H86 | +0.243 | +0.135 | +0.143 |
### 6. Electrochemical Measurements

The cyclic voltammetry (CV) technique was realized by CH Instruments 617D electrochemical workstation for electrochemical characterization. All CV measurements were performed under an argon (Ar) atmosphere and the electrochemical cell included an Ag wire as a reference electrode (RE), Pt wire as a counter electrode, and glassy carbon as a working electrode (WE) in a supporting electrolyte solution containing 0.1 M TBAPF₆ in acetonitrile. Molecules were drop-casted on the glassy carbon working carbon-working electrode before the potential was scanned in the monomer-free electrolyte solution.

Thermogravimetric analyses were realized by utilizing a Perkin Elmer Thermogravimetric Analyzer Pyris 1 TGA under a nitrogen (N₂) atmosphere at a heating rate of 10 °C/min. Thermal transitions were done via differential scanning calorimetry by using a Perkin Elmer, Jade DSC under a nitrogen atmosphere at a heating rate of 10 °C/min.

|     |     |     |     |
|-----|-----|-----|-----|
| H87 | +0.240 | +0.132 | +0.143 |
| H88 | +0.240 | +0.130 | +0.137 |
| H89 | +0.240 | +0.130 | +0.138 |
| H90 | +0.243 | +0.134 | +0.137 |
| H91 | +0.242 | +0.134 | +0.139 |
| H92 | +0.235 | +0.123 | +0.163 |
| H93 | +0.241 | +0.131 | +0.178 |
| H94 | +0.240 | +0.130 | +0.179 |
| H95 | +0.235 | +0.122 | +0.159 |
| H96 | +0.241 | +0.129 | +0.134 |
| H97 | +0.242 | +0.130 | +0.197 |
| H98 | +0.232 | +0.150 | +0.160 |
| H99 | +0.430 | +0.327 | +0.349 |
| H100| +0.430 | +0.327 | +0.354 |
| H101| +0.232 | +0.150 | +0.163 |
| H102| +0.242 | +0.130 | +0.198 |
| N29 | -0.573 | -0.687 | -0.402 |
| N34 | -0.572 | -0.686 | -0.395 |
| N59 | -0.572 | -0.687 | -0.388 |
| N60 | -0.572 | -0.686 | -0.406 |
The dielectric properties of ITO/TPE 33/Al devices were analyzed using HP 4194A Impedance Analyzer within the frequency range of 100 Hz–15 MHz at room temperature.

7. OLED Application

Device Fabrication and Characterization. The patterned ITO-coated glass substrates (120 nm, 5-10Ω/sq.) were supplied from Kintec Company. PEDOT: PSS was obtained from Heraeus Clevios GmbH. 0.45 µm PTFE and PVDF membrane filter (Millipore) was used to filter solution form molecules and PEDOT: PSS, respectively. For the fabrication of OLEDs, patterned ITO-coated glass substrates were cleaned ultrasonically in acetone, deionized water, and alcohol, in turn. Then, ozone treatments were applied for cleaning the substrates. PEDOT: PSS (~70 nm) as the hole injection layer (HIL) was spin-coated onto the pre-cleaned ITO-coated glass at 3000 rpm for 40 s and then baked at 120°C for 20 min. The TPEs 9, 32, 33, and 34 were prepared by dissolving in 1,2-dichlorobenzene (20 mg/mL) and growing on top of the HIL by spin casting at 1000 rpm for 40 s then baked at 50°C for 10 min in the glove box. TPBi (~40 nm) as the electron transport layer (ETL) was grown in a thermal vacuum chamber before Lithiumfloride (LiF) as an EIL (~0.5 nm) and cathode layer of aluminum (~110 nm) was deposited by vacuum evaporation (5x10^-6 mbar) method. The devices with ITO/PEDOT: PSS/TPE 9-32-33-34 (~ 40 nm)/TPBi/LiF/Al structure were fabricated. For the characterization of OLEDs, the Hamamatsu PMA-12 C10027 Photonic Multichannel analyzer and a digital multimeter (2427-C 3A Keithley) were used in a dark sample chamber after UV epoxy encapsulation of the devices. A stylus profiler (KLA Tencor P-6) was utilized to measure the thickness of organic layers.

Photophysical Measurements: The optical transmission spectra were measured and recorded using an FS5 spectrofluorometer (Edinburg Inst).