Supporting Information

Tetraphenylpyrazine-based chiral deep-blue dyes with high brightness for energy delivery

Xiang He,‡[a] Canze Zheng,‡[a] Xin Deng,[a] Yingjuan Hong,[a] Miao Meng,[a] Chunxuan Qi,[b] Hai-Tao Feng,[b] Ming Chen*[a] and Ben Zhong Tang [c]

[a] College of Chemistry and Materials Science, Jinan University, Guangzhou 510632, China. E-mail: chenming@jnu.edu.cn

[b] AIE Research Center, Shaanxi Key Laboratory of Photochemistry, College of Chemistry and Chemical Engineering, Baoji University of Arts and Sciences, Baoji 721013, China.

[c] School of Science and Engineering, Shenzhen Institute of Aggregate Science and Technology, The Chinese University of Hong Kong, Shenzhen (CUHK-SZ), Guangdong, China.

‡ These authors contributed equally to this work.

Experimental Section

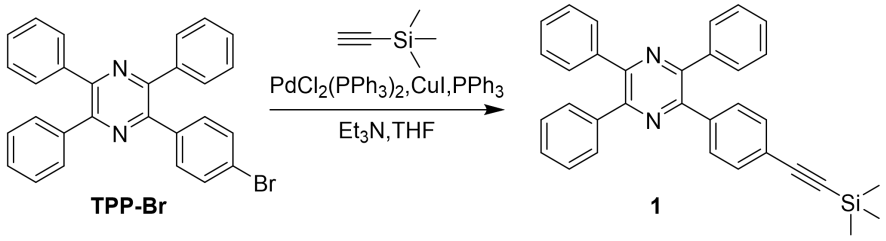
Materials and Instrumentation

All chemicals including (R)-1,1'-Bi-2-naphthol (**R1**) and (S)-1,1'-Bi-2-naphthol (**S1**) were purchased from Energy Chemical and J&K Scientific, and used directly without further purification. TPP-Br was prepared in our previous work.[1] THF was distilled from sodium benzophenone ketyl under nitrogen before use. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVIII 400 spectrometer using $CDCl_3$ as a solvent. High-resolution mass spectra (HRMS) were recorded on an LC/MS/MS consisting of a High Performance Liquid Chromatography (HPLC) system (Ultimate 3000 RSLC, Thermo Scientific, USA) and a Q Exactive Orbitrap mass spectrometer. UV-Vis spectra were measured on a TU-1810PC/SPC spectrophotometer. PL spectra were performed on a HITACHI F-47000 spectrophotometer. CD spectra were measured on a UK Applied Photophysics Ltd Chirascan spectrometer. The absolute quantum yield (Φ_F) was recorded on a Hamamatsu Quantaurus-QY C11347 spectrometer. Transient PL spectra were recorded on a Hamamatsu C11367-11 Quantaurus-Yau time resolved spectrometer. SEM images were taken using a HITACHI SU1000 scanning electron microscope. Fluorescence images were taken with a ZEISS Axio Observer 3 inverted fluorescence microscope. TGA was performed on a METTLER TG TGA2 thermogravimetric analyzer under N_2 at a heating rate of 10 ℃/min.

Synthesis of 2,3,5-triphenyl-6-(4-((trimethylsilyl)ethynyl)phenyl)pyrazine (1)

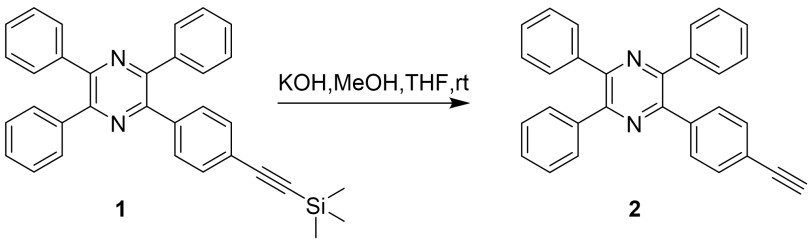
The compound **1** was synthesized base on the reference.[2] Into a 500 mL round bottom flask was added TPP-Br (9.5 g, 20.0 mmol), $PdCl_2(PPh_3)_2$ (288.0 mg, 0.4 mmol), CuI (156.2 mg, 0.8 mmol), PPh_3 (289.6 mg, 0.8 mmol), 123 mL of THF and 123 mL of triethylamine under nitrogen. Then, trimethylsilylacetylene (4.0 g, 40.0 mmol) was injected into the flask. The reaction mixture was stirred at 80 ℃ for 36 hours. After the reaction, mixture was cooled down to the room temperature, concentrated by reduced pressure, and extracted with DCM. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 2:1) as eluent. A white powder of 8.4 g was obtained in a yield of 87.9 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.67–7.56 (m,

8H), 7.42 (t, 2H), 7.39–7.28 (m, 9H), 0.25 (s, 9H).



Synthesis of 2-(4-ethynylphenyl)-3,5,6-triphenylpyrazine (2)

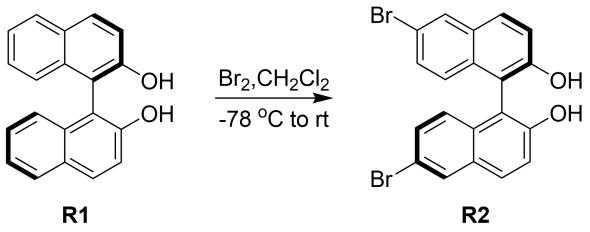
The compound **2** was synthesized base on the reference.[2] Into a 500 mL round bottom flask was added **1** (7.3 g, 15.1 mmol) and 183 mL of THF. Then, KOH dissolved in 163 mL methanol (5.1 g, 0.09 mol) was added. The mixture was stirred at room temperature overnight. After that, dilute hydrochloric acid was added to quench the reaction. The mixture was concentrated by reduced pressure and extracted with DCM. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 5:1) as eluent. A white powder of 5.1 g was obtained in a yield of 83.1 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.63 (t, 8H), 7.45 (d, 2H), 7.35 (q, 9H), 3.14 (s, 1H).



Synthesis of (R)-6,6'-dibromo-[1,1'-binaphthalene]-2,2'-diol (R2)

The compound **R2** was synthesized base on the reference.[3] Into a 500 mL round bottom flask was added **R1** (15.0 g, 52.4 mmol) and 200 mL of DCM under nitrogen. After the mixture was cooled down to -78 ℃, 69 mL of Br_2/dichloromethane solution (2 M) was added dropwise within 30 minutes. The mixture was stirred at -78 ℃ for 2 hours and then returned to room temperature for reacting for 2 hours. After that, supersaturated Na_2SO_3 aqueous solution was added to quench the reaction. Then, the mixture was concentrated by reduced pressure and extracted with DCM. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated without further purification.

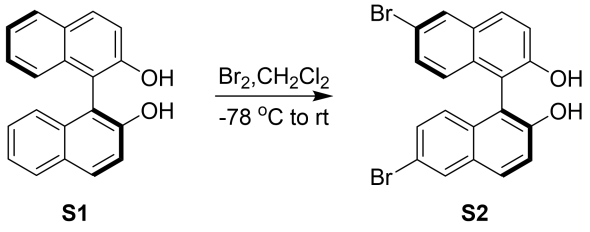
A white powder of 22.0 g was obtained in a yield of 96.3 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.06 (d, 2H), 7.90 (d, 2H), 7.43–7.34 (m, 4H), 6.96 (t, 2H).



R1 R2

Synthesis of (S)-6,6'-dibromo-[1,1'-binaphthalene]-2,2'-diol (S2)

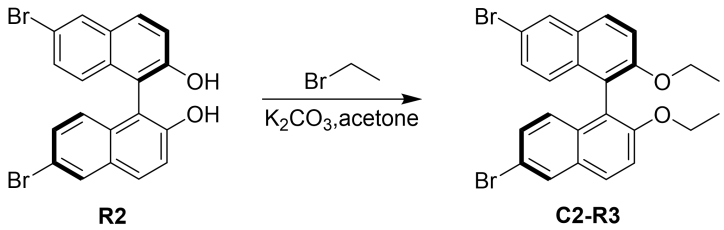
The synthetic procedure was similar to **R2**. A white powder of 21.5 g was obtained in a yield of 94.4 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.05 (d, 2H), 7.90 (d, 2H), 7.39 (d, 4H), 6.97 (t, 2H).



S1 S2

Synthesis of (R)-6,6'-dibromo-2,2'-diethoxy-4,4a-dihydro-1,1'-binaphthalene (C2-R3)

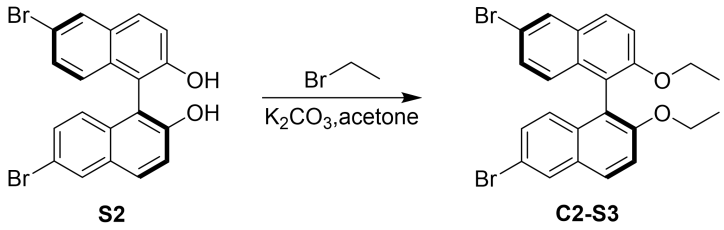
The compound **C2-R3** was synthesized base on the reference.[4] Into a 500 mL round bottom flask was added **R2** (20.0 g, 45.0 mmol), K_2CO_3 (24.9 g, 0.18 mol), 18 crown hexether (349.0 mg, 2.3 mmol) and 219 mL of acetone, followed by addition of bromohexane (29.4 g，0.27 mol) in four times. The mixture was stirred at 70 ℃ for 24 hours. After that, the mixture was cooled down to the room temperature, concentrated by reduced pressure, and extracted with DCM. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 5:1) as eluent. A white powder of 20.2 g was obtained in a yield of 90.2 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.00 (d, 2H), 7.84 (d, 2H), 7.42 (d, 2H), 7.27 (d, 1H), 7.25 (d, 1H), 6.95 (d, 2H), 4.08–3.99 (m, 4H), 1.06 (t, 6H).



R2 C2-R3

Synthesis of (S)-6,6'-dibromo-2,2'-diethoxy-4,4a-dihydro-1,1'-binaphthalene (C2-S3)

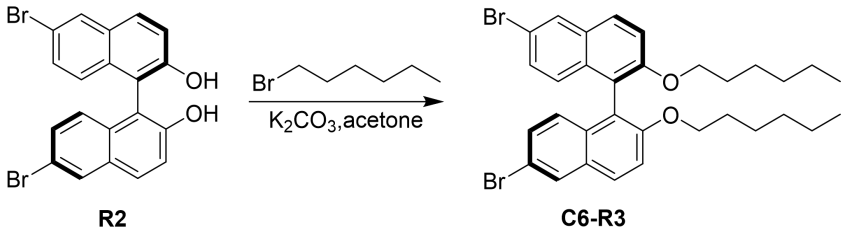
The synthetic procedure was similar to **C2-R3**. A white powder of 20.4 g was obtained in a yield of 91.1 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.00 (d, 2H), 7.84 (d, 2H), 7.41 (d, 2H), 7.26 (d, 1H), 7.24 (d, 1H), 6.94 (d, 2H), 4.09–3.97 (m, 4H), 1.05 (t, 6H).



S2 C2-S3

Synthesis of (R)-6,6'-dibromo-2,2'-bis(hexyloxy)-4,4a-dihydro-1,1'-binaphthalene (C6-R3)

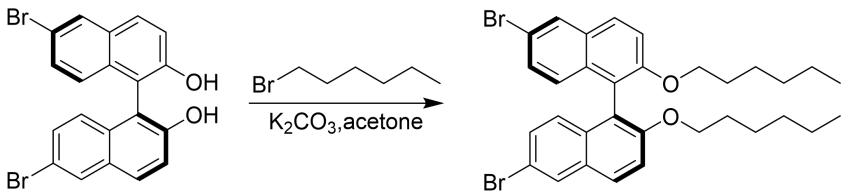
The synthetic procedure was similar to **C2-R3**. A yellow viscous liquid of 19.3 g was obtained in a yield of 93.1 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.99 (d, 2H), 7.82 (d, 2H), 7.39 (d, 2H), 7.26 (d, 1H), 7.23 (d, 1H), 6.97 (t, 2H), 4.00–3.84 (m, 4H), 1.47–1.30 (m, 4H), 1.12–0.83 (m, 12H), 0.73 (t, 6H).



R2 C6-R3

Synthesis of (S)-6,6'-dibromo-2,2'-bis(hexyloxy)-4,4a-dihydro-1,1'-binaphthalene (C6-S3)

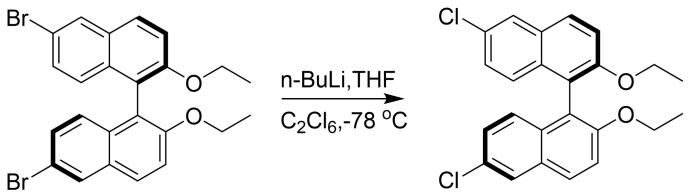
The synthetic procedure was similar to **C2-R3**. A yellow viscous liquid of 19.5 g was obtained in a yield of 94.4 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.99 (d, 2H), 7.82 (d, 2H), 7.39 (d, 2H), 7.26 (d, 1H), 7.23 (d, 1H), 6.97 (t, 2H), 3.99–3.84 (m, 4H), 1.44–1.31 (m, 4H), 1.11–0.84 (m, 12H), 0.73 (t, 6H).



S2 **C6-S3**

Synthesis of (R)-6,6'-dichloro-2,2'-diethoxy-1,1'-binaphthalene (C2-R4)

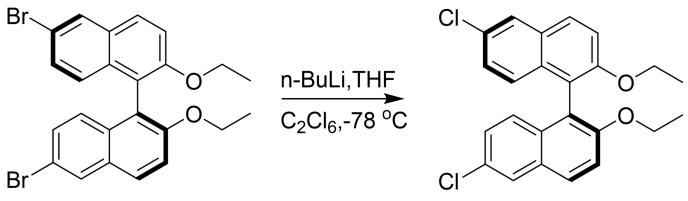
The compound **C2-R4** was synthesized base on the reference.[3] Into a 500 mL round bottom flask was added **C2-R3** (14.0 g, 28.0 mmol) and 140 mL of THF under nitrogen. After the mixture was cooled down to -78 ℃, 34 mL of n-BuLi/hexane solution (1.6 M) was dropped dropwise into the flask and the reaction proceeded at -78 ℃ for 30 minutes. Then, 28 mL of hexachloroethane/THF solution (1 M) was added to the flask at -78 ℃. After stirred for one hour, the mixture was returned to room temperature and reacted overnight. Then, the saturated NH_4Cl solution was added to quench the reaction. After that, the organic phase was separated and concentrated by reduced pressure, and extracted with ethyl acetate. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 2:1) as eluent. A white powder of 10.2 g was obtained in a yield of 89.8 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.84 (d, 4H), 7.43 (d, 2H), 7.17–7.11 (m, 2H), 7.02 (d, 2H), 4.08–3.99 (m, 4H), 1.05 (t, 6H).



C2-R3 **C2-R4**

Synthesis of (S)-6,6'-dichloro-2,2'-diethoxy-1,1'-binaphthalene (C2-S4)

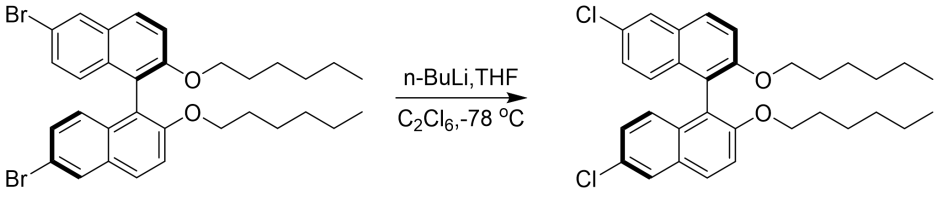
The synthetic procedure was similar to **C2-R4**. A white powder of 10.0 g was obtained in a yield of 87.5 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.84 (d, 4H), 7.42 (t, 2H), 7.17–7.10 (m, 2H), 7.05–6.99 (m, 2H), 4.08–3.99 (m, 4H), 1.06 (d, 6H).



C2-S3 **C2-S4**

Synthesis of (R)-6,6'-dichloro-2,2'-bis(hexyloxy)-1,1'-binaphthalene (C6-R4)

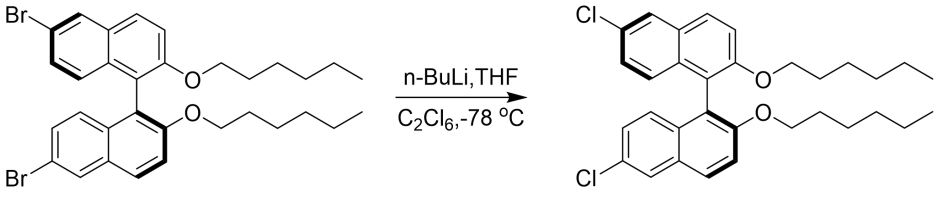
The synthetic procedure was similar to **C2-R4**. A yellow viscous liquid of 11.2 g was obtained in a yield of 88.3 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.83 (t, 4H), 7.40 (t, 2H), 7.13 (d, 2H), 7.04 (d, 2H), 3.99–3.86 (m, 4H), 1.45–1.31 (m, 4H), 1.12–0.84 (m, 12H), 0.78–0.69 (m, 6H).



C6-R3 **C6-R4**

Synthesis of (S)-6,6'-dichloro-2,2'-bis(hexyloxy)-1,1'-binaphthalene (C6-S4)

The synthetic procedure was similar to **C2-R4**. A yellow viscous liquid of 11.5 g was obtained in a yield of 90.4 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.83 (t, 2H), 7.41 (d, 1H), 7.13 (d, 3.0 Hz, 1H), 7.05 (d, 1H), 3.99–3.86 (m, 2H), 1.45–1.32 (m, 2H), 1.11–0.84 (m, 6H), 0.78–0.70 (m, 3H).

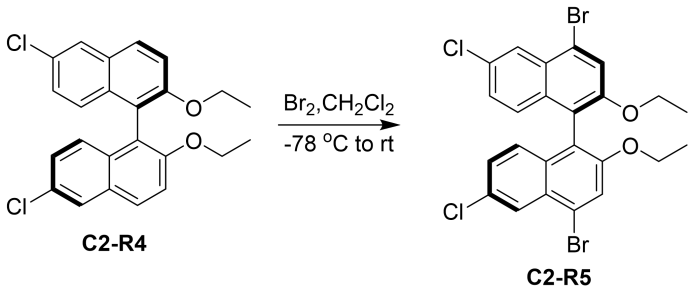


C6-S3 **C6-S4**

Synthesis of (R)-4,4'-dibromo-6,6'-dichloro-2,2'-diethoxy-1,1'-binaphthalene (C2-R5)

The compound **C2-R5** was synthesized base on the reference.[3] Into a 500 mL round bottom flask was added **C2-R4** (8.0 g，19.4 mmol) and 200 mL of DCM under nitrogen. After the mixture was cooled down to -78 ℃, 100 mL of Br_2/dichloromethane solution (3.6 M) was added dropwise within 30 minutes. The mixture was stirred at -78 ℃ for 2 hours and then returned to room temperature for reacting for 2 hours. Then, supersaturated Na_2SO_3 aqueous solution was added to quench the reaction. After that, the organic phase was separated and concentrated by reduced pressure, and extracted with DCM. The organic phase was washed

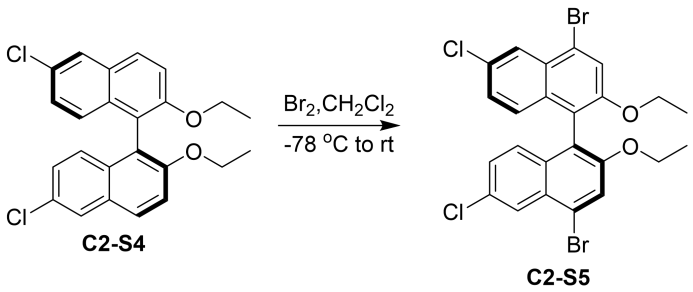
with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 10:1) as eluent. A white powder of 9.6 g was obtained in a yield of 87.7 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.22 (d, 2H), 7.72 (s, 2H), 7.17 (d, 2H), 6.99 (t, 2H), 4.07–3.98 (m, 4H), 1.11–1.04 (m, 6H).



C2-R4 C2-R5

Synthesis of (S)-4,4'-dibromo-6,6'-dichloro-2,2'-diethoxy-1,1'-binaphthalene (C2-S5)

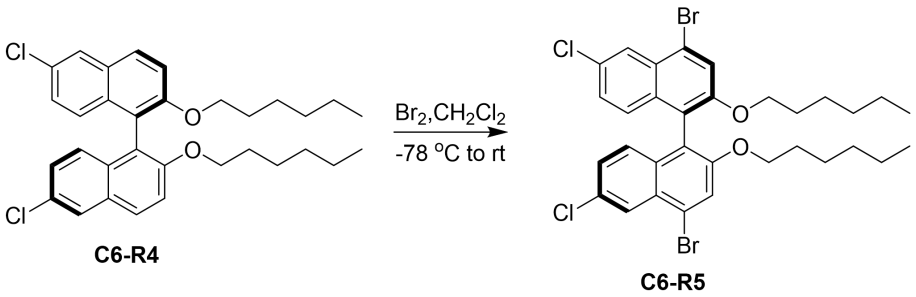
The synthetic procedure was similar to **C2-R5**. A white powder of 9.8 g was obtained in a yield of 89.1 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.21 (d, 2H), 7.72 (d, 2H), 7.19–7.13 (m, 2H), 6.99 (d, 2H), 4.06–3.97 (m, 4H), 1.10–1.03 (m, 6H).



C2-S4 C2-S5

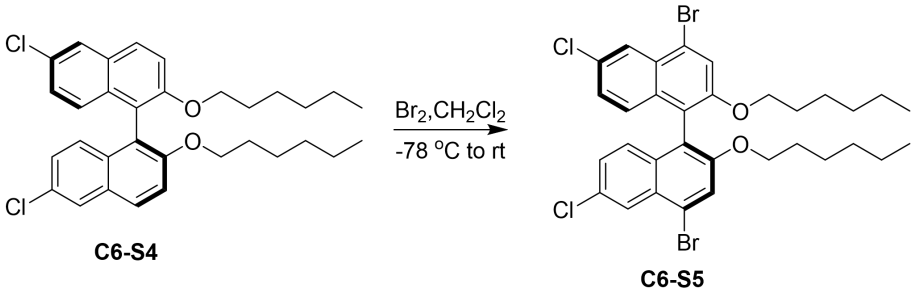
Synthesis of (R)-4,4'-dibromo-6,6'-dichloro-2,2'-bis(hexyloxy)-1,1'-binaphthalene (C6-R5)

The synthetic procedure was similar to **C2-R5**. A yellow viscous liquid of 11.1 g was obtained in a yield of 85.0 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.22 (d, 2H), 7.71 (s, 2H), 7.18 (d, 2H), 7.07–7.01 (m, 2H), 3.99–3.86 (m, 4H), 1.47–1.34 (m, 4H), 1.13–0.84 (m, 12H), 0.81–0.70 (m, 6H).



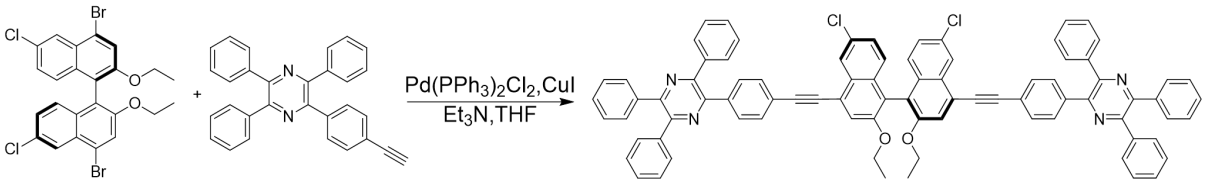
Synthesis of (S)-4,4'-dibromo-6,6'-dichloro-2,2'-bis(hexyloxy)-1,1'-binaphthalene (C6-S5)

The synthetic procedure was similar to **C2-R5**. A yellow viscous liquid of 11.5 g was obtained in a yield of 88.2 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.22 (d, 2H), 7.71 (s, 2H), 7.18 (d, 2H), 7.07–7.01 (m, 2H), 3.99–3.86 (m, 4H), 1.47–1.34 (m, 4H), 1.13–0.85 (m, 12H), 0.81–0.68 (m, 6H).



Synthesis of TPP-C2(R)

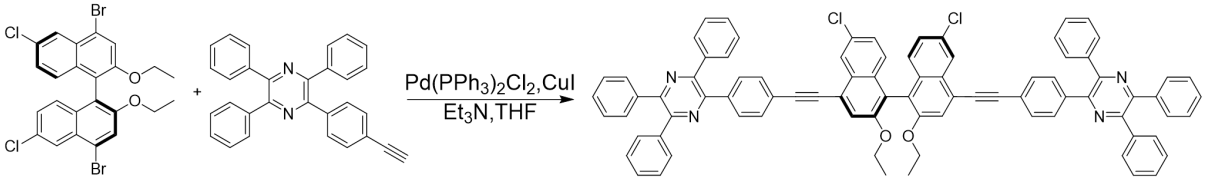
Into a 500 mL round bottom flask was added **C2-R5** (1.0 g, 1.8 mmol), **2** (1.7 g, 4.0 mmol), $Pd(PPh_3)_2Cl_2$ (123 mg, 0.18 mmol), CuI (13.4 mg, 0.07mmol), 84 mL of THF and 42 mL of triethylamine under nitrogen. Then, the mixture was stirred at 85 ℃ for 24 hours. The mixture was concentrated by reduced pressure and extracted with DCM. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 2:1) as eluent. A white powder of 968 mg was obtained in a yield of 45.3 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.41 (d, 2H), 7.84–7.49 (m, 22H), 7.38 (d, 18H), 7.28–7.17 (m, 2H), 7.08 (d, 2H), 5.71–3.04 (m, 4H), 1.11 (t, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ (ppm): 153.6, 148.4, 147.2, 138.6, 138.1, 132.99, 131.5, 130.4, 129.7, 128.6, 128.2, 127.6, 127.1, 125.0, 122.9, 121.2, 120.9, 119.8, 94.8, 88.0, 65.0, 29.5, 29.2, 14.7. HRMS (MALDI-TOF): m/z 1223.3849 ($[M]^+$), calcul for $C_{84}H_{56}Cl_2N_4O_2$ 1223.3853.



C2-R5 2 TPP-C2(R)

Synthesis of TPP-C2(S)

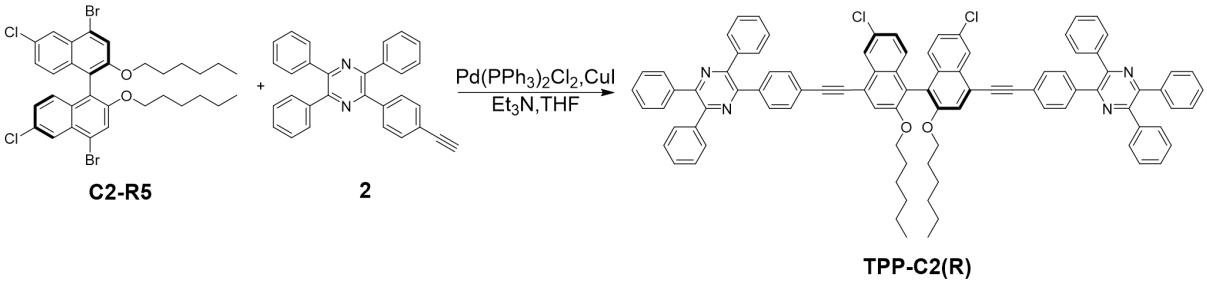
The synthetic procedure was similar to **TPP-C2(R)**. A white powder of 0.92 g was obtained in a yield of 43.0 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.41 (d, 2H), 7.91–7.55 (m, 22H), 7.55–7.30 (m, 18H), 7.22 (d, 2H), 7.08 (d, 2H), 4.15–4.02 (m, 4H), 1.11 (t, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ (ppm): 153.9, 148.7, 147.5, 138.9, 138.4, 132.3, 131.8, 130.7, 130.1, 129.0, 128.5, 128.0, 127.4, 125.3, 123.2, 121.6, 121.2, 120.1, 95.1, 88.2, 65.3, 29.8, 15.0. HRMS (MALDI-TOF): m/z 1223.3847 ([M]$^+$), calcul for $C_{84}H_{56}Cl_2N_4O_2$ 1223.3853.



C2-S5 2 TPP-C2(S)

Synthesis of TPP-C6(R)

The synthetic procedure was similar to **TPP-C2(R)**. A white powder of 0.94 g was obtained in a yield of 40.1 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.39 (d, 2H), 7.91–7.52 (m, 22H), 7.51–7.29 (m, 18H), 7.22 (d, 2H), 7.10 (d, 2H), 4.05–3.90 (m, 4H), 1.43 (d, 4H), 1.19–0.87 (m, 12H), 0.77 (t, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ (ppm): 153.9, 150.3, 149.6, 147.4, 144.8, 143.2 141.9, 140.8, 137.6, 135.6, 135.2, 127.7, 119.8, 94.8, 69.5, 31.2, 29.1, 25.3, 22.4, 13.9. HRMS (MALDI-TOF): m/z 1335.5105 ([M]$^+$), calcul for $C_{92}H_{72}Cl_2N_4O_2$ 1335.5105.

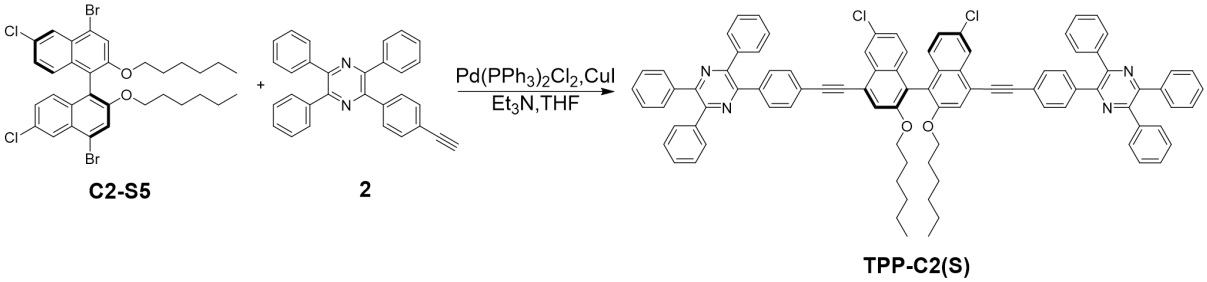


C2-R5 2 TPP-C2(R)

Synthesis of TPP-C6(S)

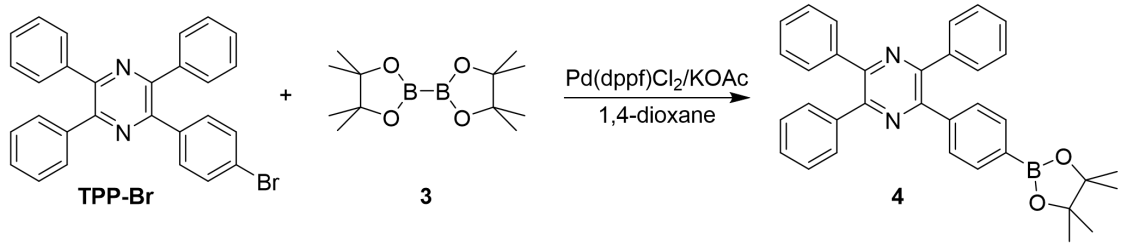
The synthetic procedure was similar to **TPP-C2(R)**. A white powder of 0.99 g was obtained in a yield of 42.4 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.39 (d, 2H), 7.70 (d, 22H),

7.45–7.30 (m, 18H), 7.22 (d, 2H), 7.10 (d, 2H), 4.04–3.91 (m, 4H), 1.44 (d, 4H), 1.18–0.87 (m, 12H), 0.77 (t, 6H). ^{13}C NMR (400 MHz, $CDCl_3$) δ (ppm): 153.9, 150.3, 149.6, 147.4, 144.8, 143.2, 141.9, 140.8, 137.6, 135.2, 127.7, 119.8, 94.8, 69.5, 31.2, 29.1, 25.3, 22.4, 13.9. HRMS (MALDI-TOF): m/z 1335.5104 ([M]$^+$), calcul for $C_{92}H_{72}Cl_2N_4O_2$ 1335.5105.



Synthesis of 2,3,5-triphenyl-6-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)pyrazine (4)

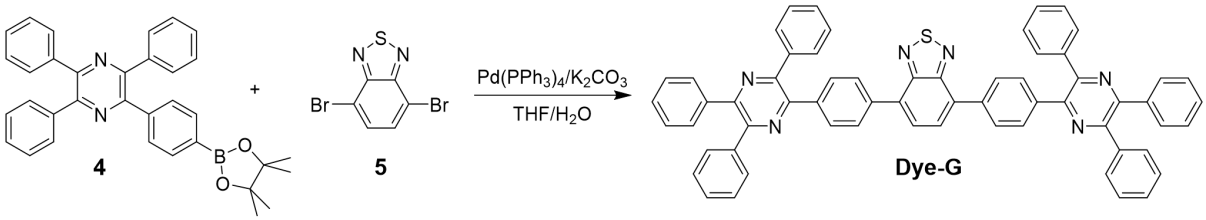
The compound **4** was synthesized base on the reference.[5] Into a 500 mL round bottom flask was added **TPP-Br** (9.85 g, 21.2 mmol), dipinacol borate (10.8 g, 42.5 mmol), $Pd(dppf)Cl_2$ (0.8 g, 1.0 mmol), potassium acetate (8.3 g, 85.0 mmol) and 163 mL of 1, 4-dioxane under nitrogen. The mixture was reacted at 110 ℃ for 10 hours. After that, the organic phase was separated and concentrated by reduced pressure, and extracted with DCM. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 2:1) as eluent. A white powder of 0.99 g was obtained in a yield of 42.2 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.75 (d, 2H), 7.67–7.60 (m, 8H), 7.38–7.28 (m, 9H), 1.26 (s, 12H).



Synthesis of Dye-G

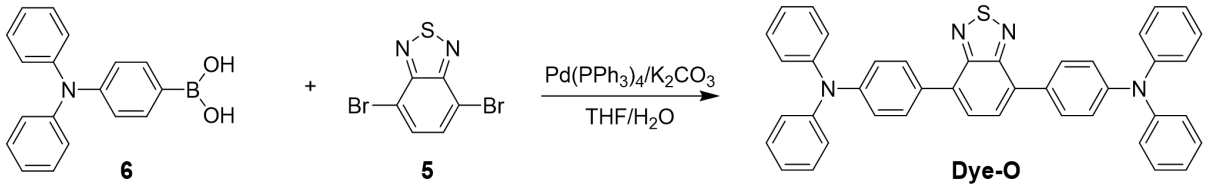
Dye-G was synthesized base on the reference.[5] Into a 500 mL round bottom flask was added **4** (1.7 g, 3.4 mmol)，dibromobenzothiadiazole (0.4 g, 1.4 mmol), $Pd(PPh_3)_4$ (157 mg, 0.1mmol), 30 mL of THF and 15 mL of K_2CO_3 aqueous solution (2 M) under nitrogen. The mixture was stirred at 80 ℃ overnight. After cooled down to room temperature, the crude product was

filtered and washed without further purification. A yellow powder of 1.8 g was obtained in a yield of 62.5 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.99 (d, 4H), 7.90–7.81 (m, 6H), 7.76 (d, 4H), 7.68 (d, 8H), 7.47–7.28 (m, 18H).



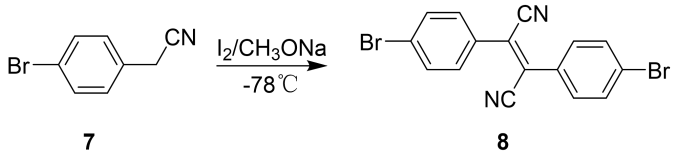
Synthesis of Dye-O

Dye-O was synthesized base on the reference.[6] The synthetic procedure was similar to Dye-G. An orange powder of 3.4 g was obtained in a yield of 63.3 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.88 (d, 4H), 7.74 (s, 2H), 7.30 (t, 8H), 7.19 (d, 12H), 7.07 (t, 4H).



Synthesis of 2,3-bis(4-bromophenyl)fumaronitrile (8)

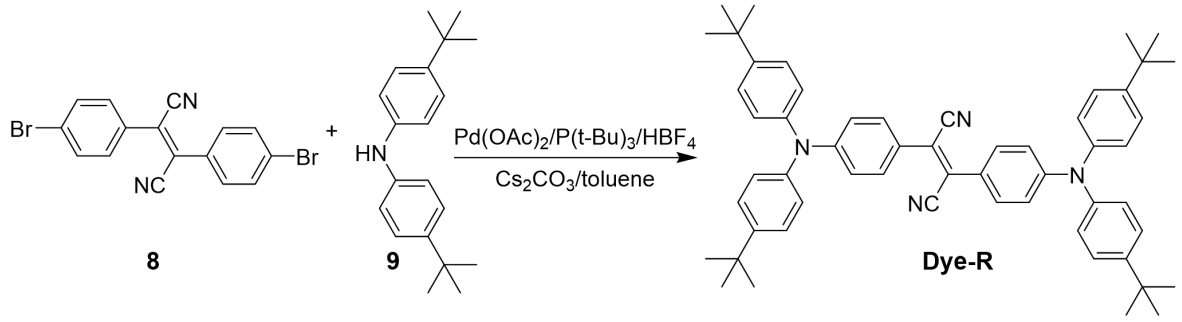
8 was synthesized base on the reference.[7] Into a 500 mL round bottom flask was added **7** (5.0 g, 22.5 mmol), iodine (6.5 g, 22.5 mmol) and 75 mL of diethyl ether under nitrogen. After the mixture was cooled down to -78 ℃, 40 mL of Sodium methanol solution (1 M) was added dropwise within 30 min. Then, the mixture was reacted at -10 ℃for 3 hours. After that, the obtained crude product was washed with water, 5% $Na_2S_2O_5$ aqueous solution, ether, petroleum ether. A light green powder of 3.0 g was obtained in a yield of 32.4 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.76–7.64 (m, 8H).



Synthesis of Dye-R

Dye-R was synthesized base on the reference.[7] Into a 500 mL round bottom flask was added **8** (2.0 g, 5.2 mmol), **9** (3.2 g, 11.3 mmol), $Pd(OAc)_2$ (27 mg, 0.12 mmol), $P(t\text{-}Bu)_3HBF_4$ (104.0 mg, 0.36 mmol), Cs_2CO_3 (1.48 g, 10.0 mmol) and 40 mL of toluene under nitrogen. The

mixture was reacted at 90 ℃ for 36 hours. The mixture was concentrated by reduced pressure and extracted with DCM. The organic phase was washed with water several times, and dried over anhydrous Na_2SO_4. The filtrate was concentrated and the crude product was purified by silica gel chromatography column with ether/dichloromethane (v/v = 2:1) as eluent. A red powder of 700 mg was obtained in a yield of 22.1 %. ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.64 (d, 4H), 7.51 (d, 8H), 7.33 (d, 8H), 6.94–6.06 (m, 4H), 1.32 (s, 36H).



Fabrication of film

The sample was weighed and added to 100 mg polymethyl methacrylate dissolved with 1 mL chloroform. After full mixing, 100 μL drops were added to 1*2 centimeters quartz sheet, which was naturally volatilized in the fume hood. After the volatilization of chloroform, the corresponding film was obtained.

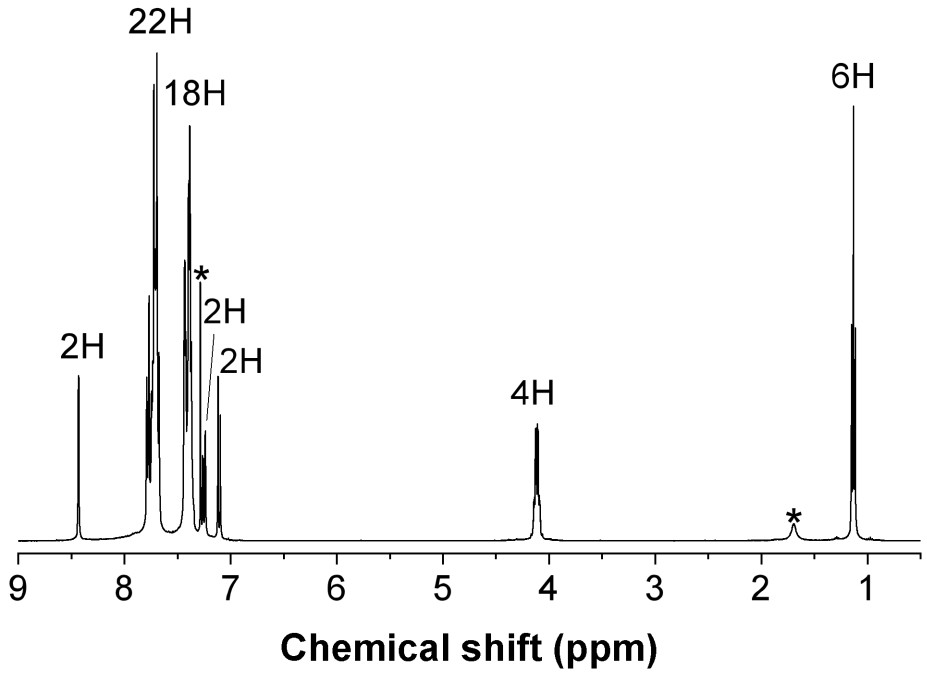


Figure S1. ^{1}H NMR spectrum of **TPP-C2(R)** in $CDCl_3$. The solvent peaks were marked with asterisks.

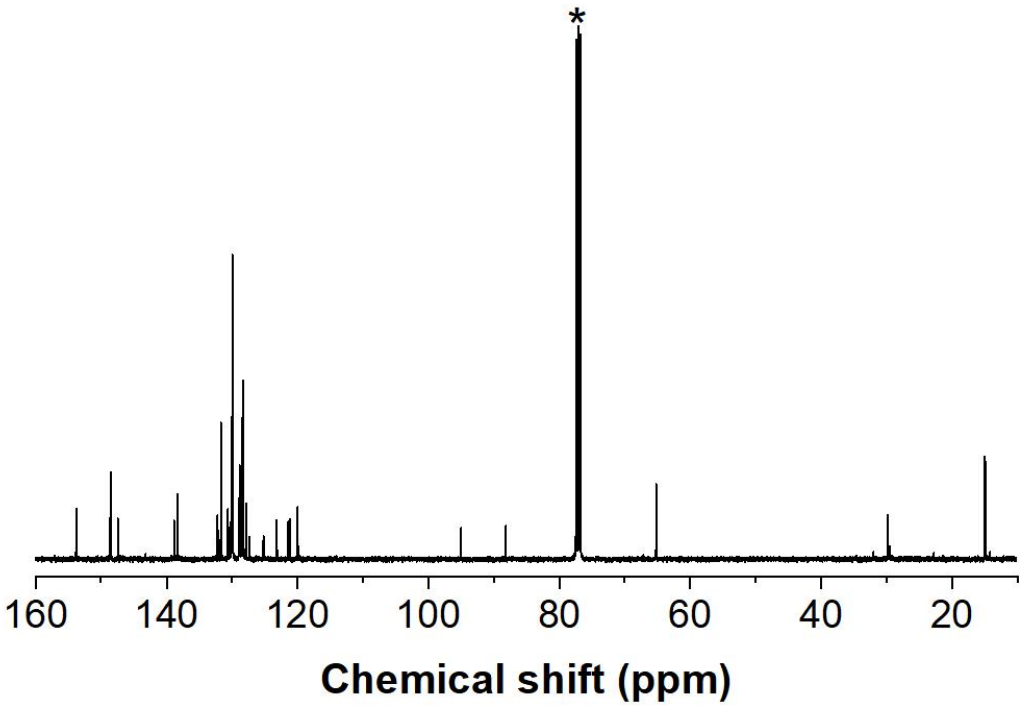


Figure S2. ^{13}C NMR spectrum of **TPP-C2(R)** in $CDCl_3$. The solvent peaks were marked with asterisk.

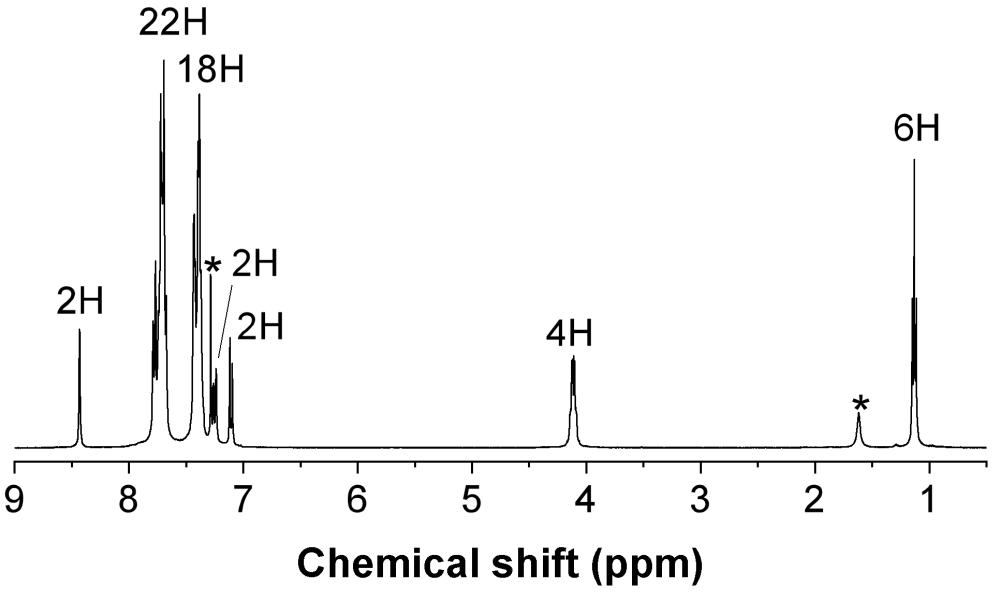


Figure S3. ^{1}H NMR spectrum of **TPP-C2(S)** in $CDCl_3$. The solvent peaks were marked with asterisks.

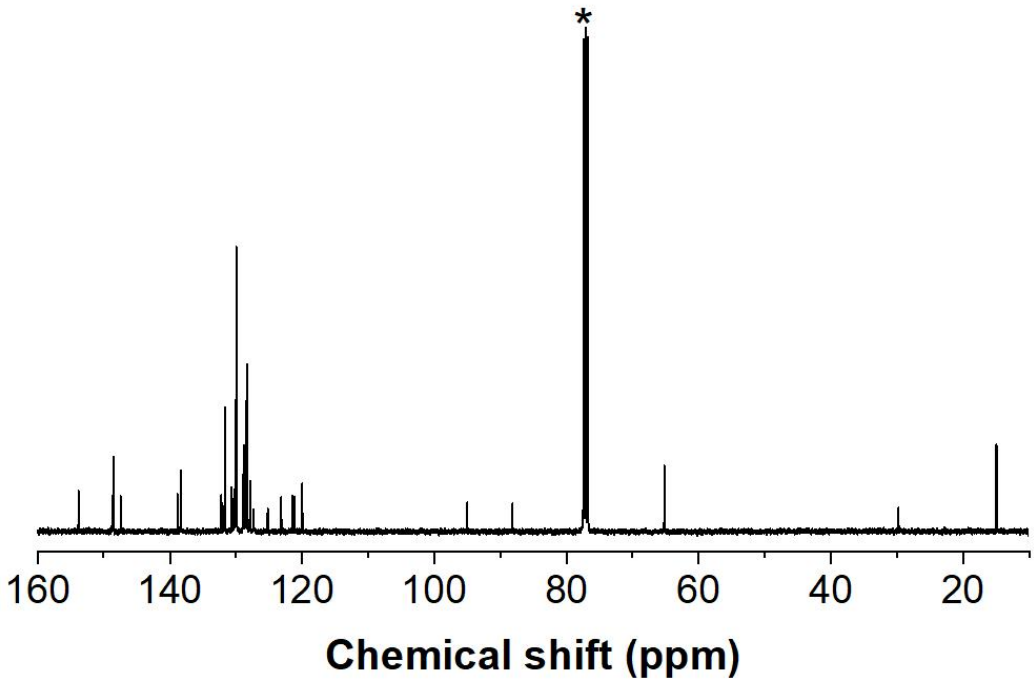


Figure S4. ^{13}C NMR spectrum of **TPP-C2(S)** in $CDCl_3$. The solvent peaks were marked with asterisk.

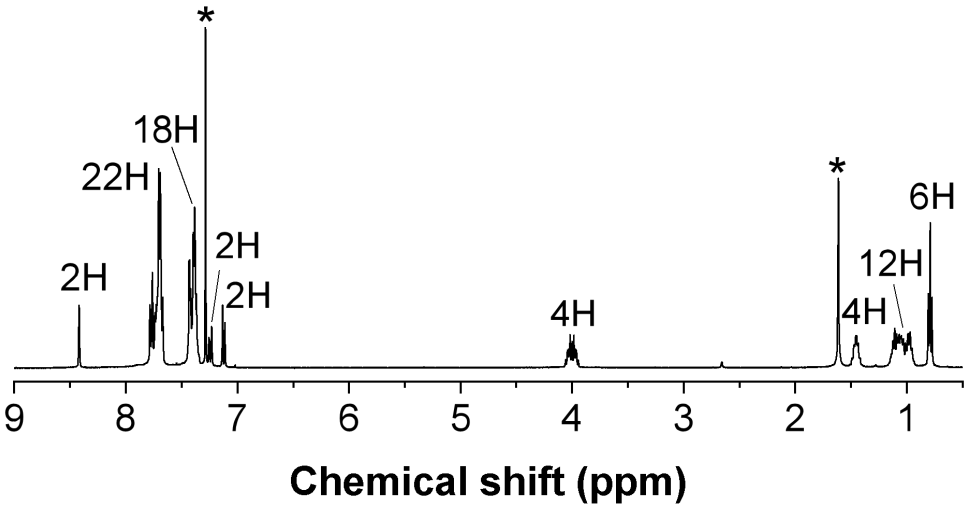


Figure S5. ^{1}H NMR spectrum of **TPP-C6(R)** in $CDCl_3$. The solvent peaks were marked with asterisks.

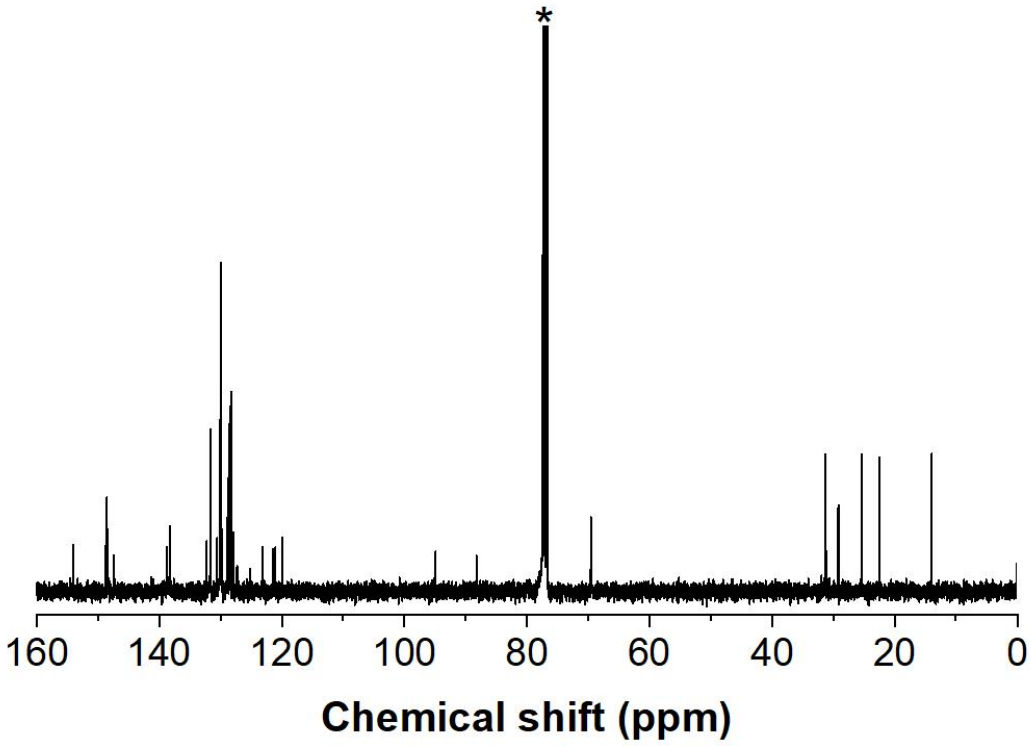


Figure S6. ^{13}C NMR spectrum of **TPP-C6(R)** in $CDCl_3$. The solvent peaks were marked with asterisk.

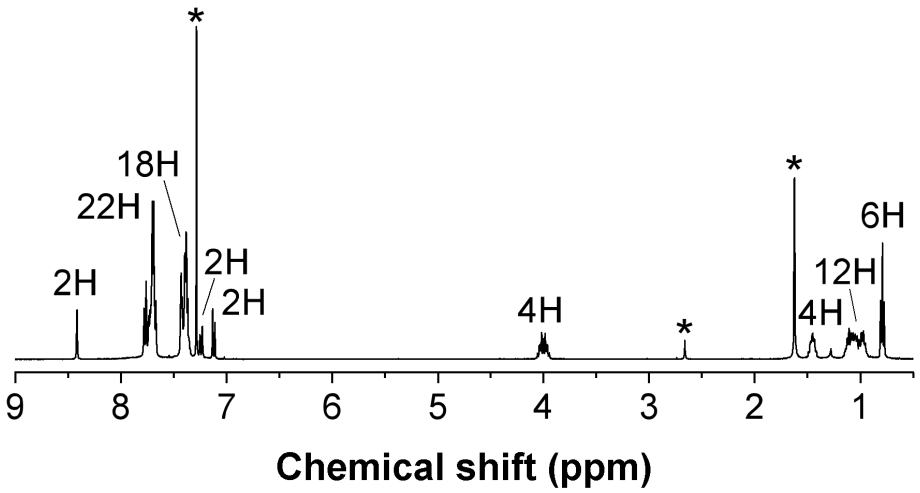


Figure S7. ^{1}H NMR spectrum of **TPP-C6(S)** in $CDCl_3$. The solvent peaks were marked with asterisks.

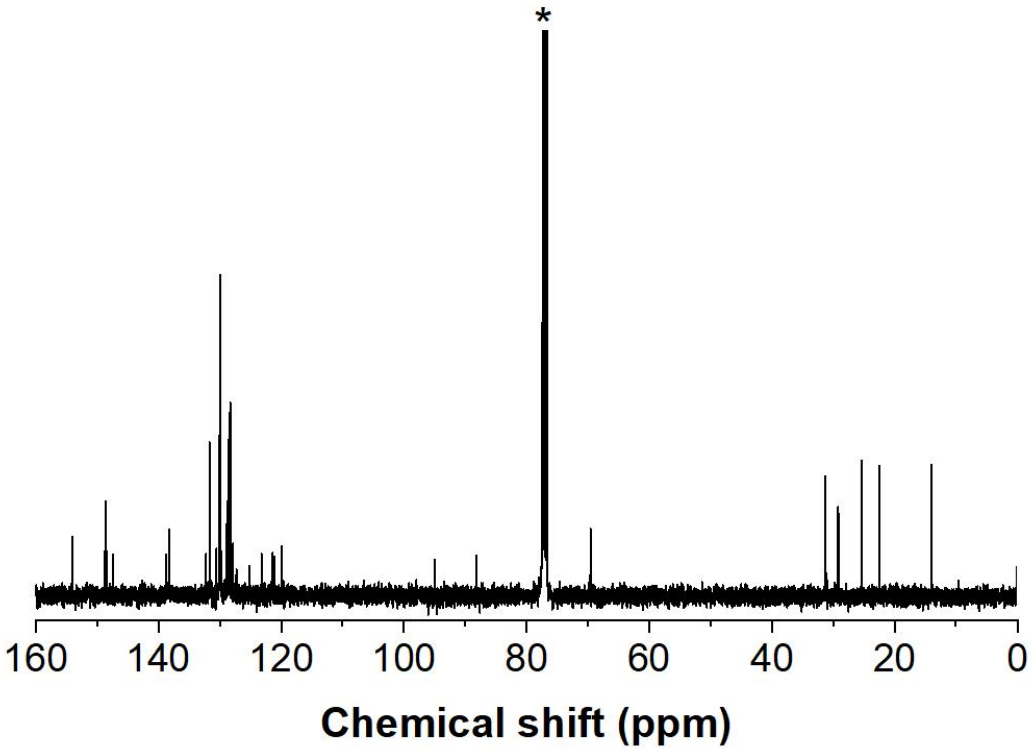


Figure S8. ^{13}C NMR spectrum of **TPP-C6(S)** in $CDCl_3$. The solvent peaks was marked with asterisk.

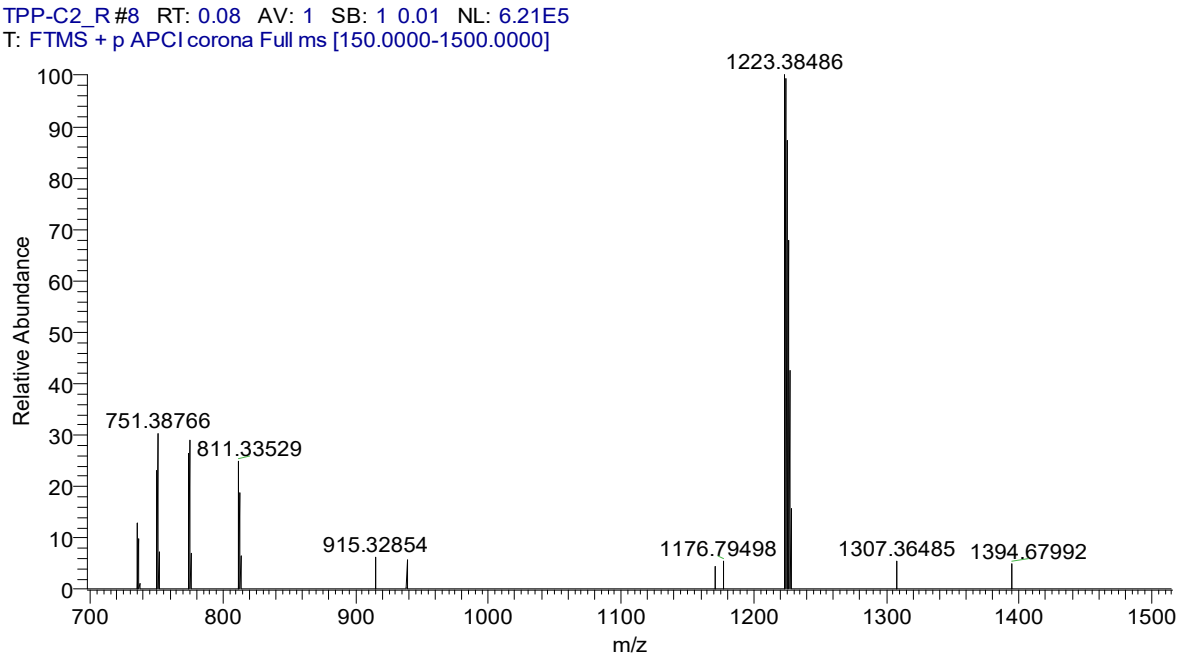


Figure S9. HRMS of **TPP-C2(R)**.

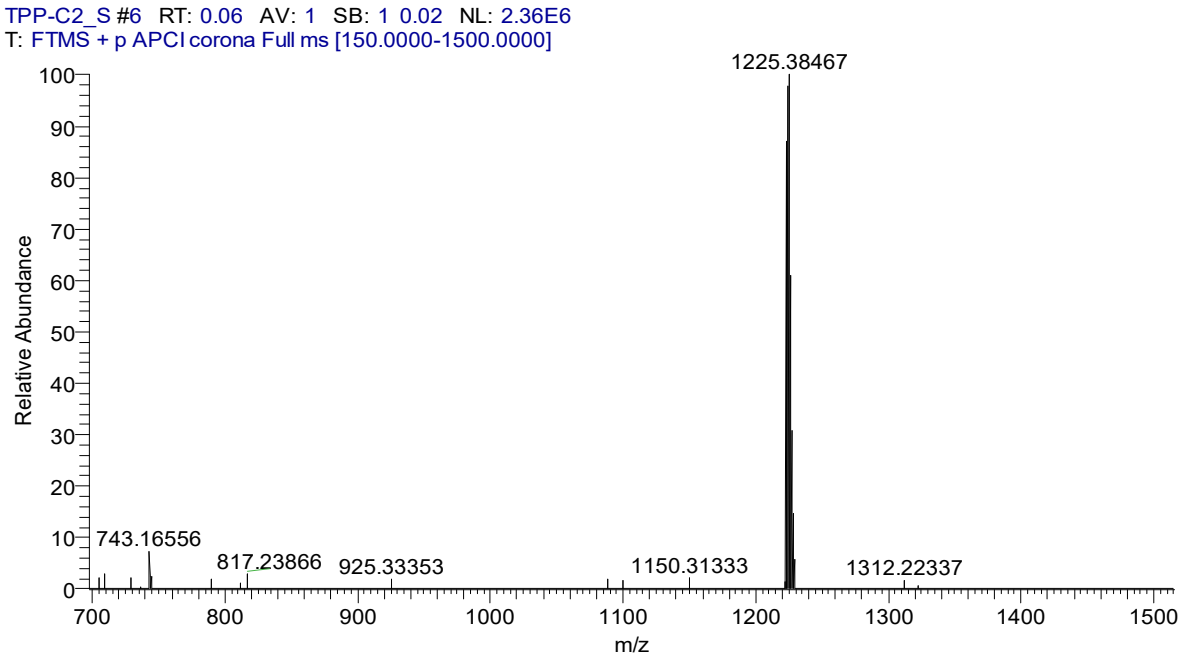


Figure S10. HRMS of **TPP-C2(S)**.

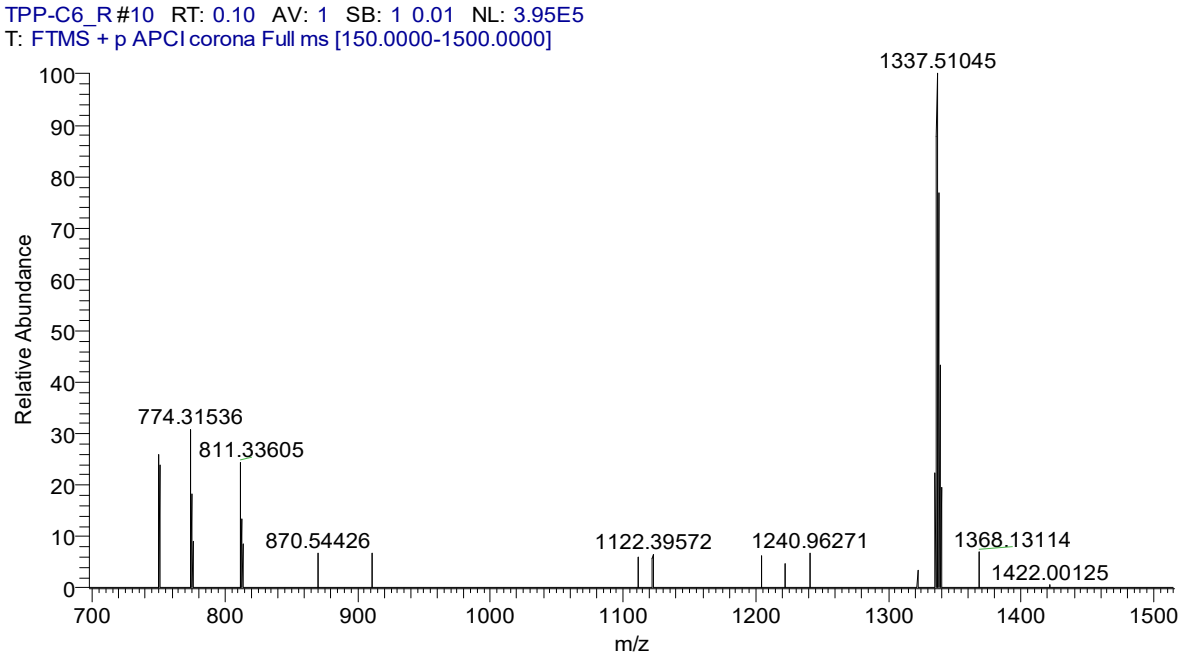


Figure S11. HRMS of **TPP-C6(R)**.

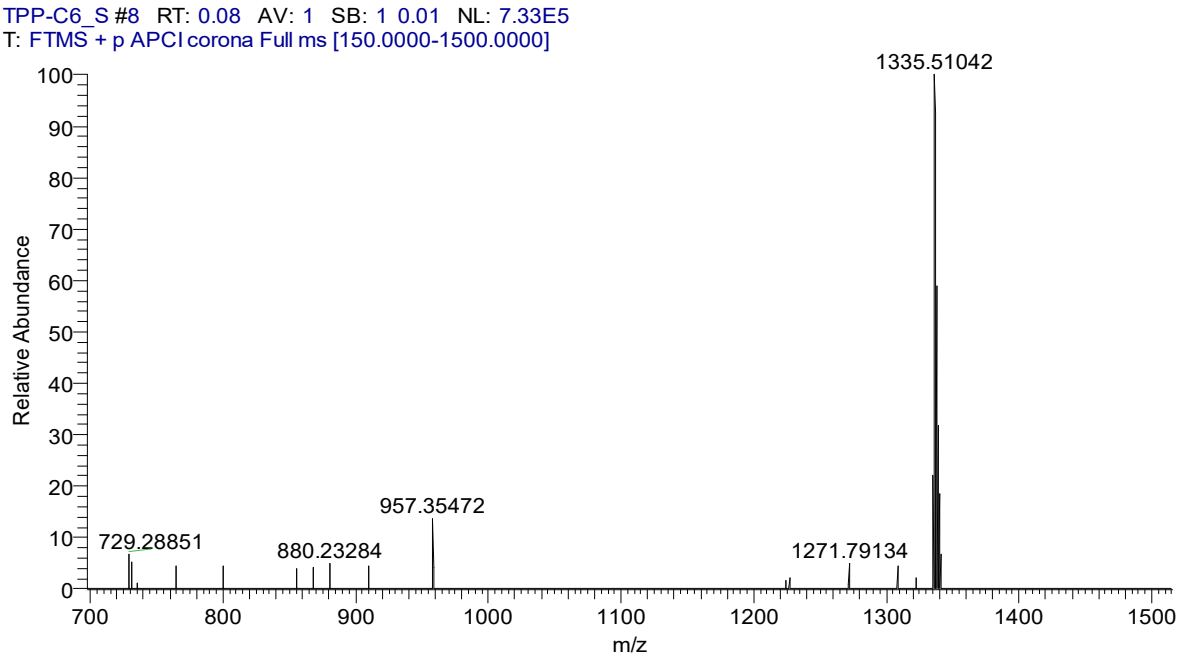


Figure S12. HRMS of **TPP-C6(S)**.

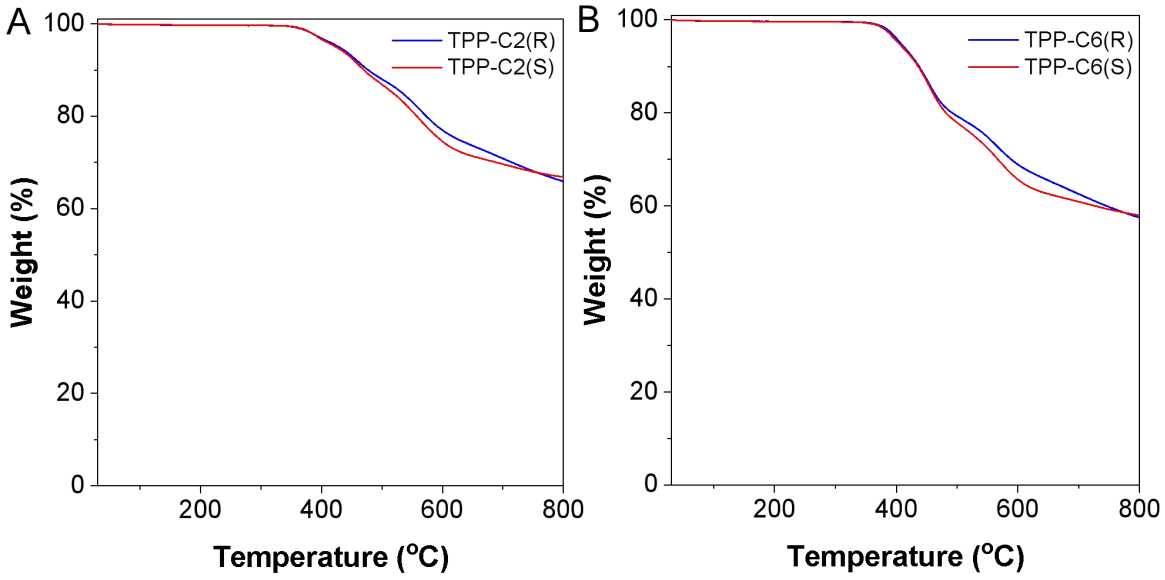


Figure S13. The thermogravimetric curves of (A) TPP-C2(R) and TPP-C2(S), (B) TPP-C6(R) and TPP-C6(S).

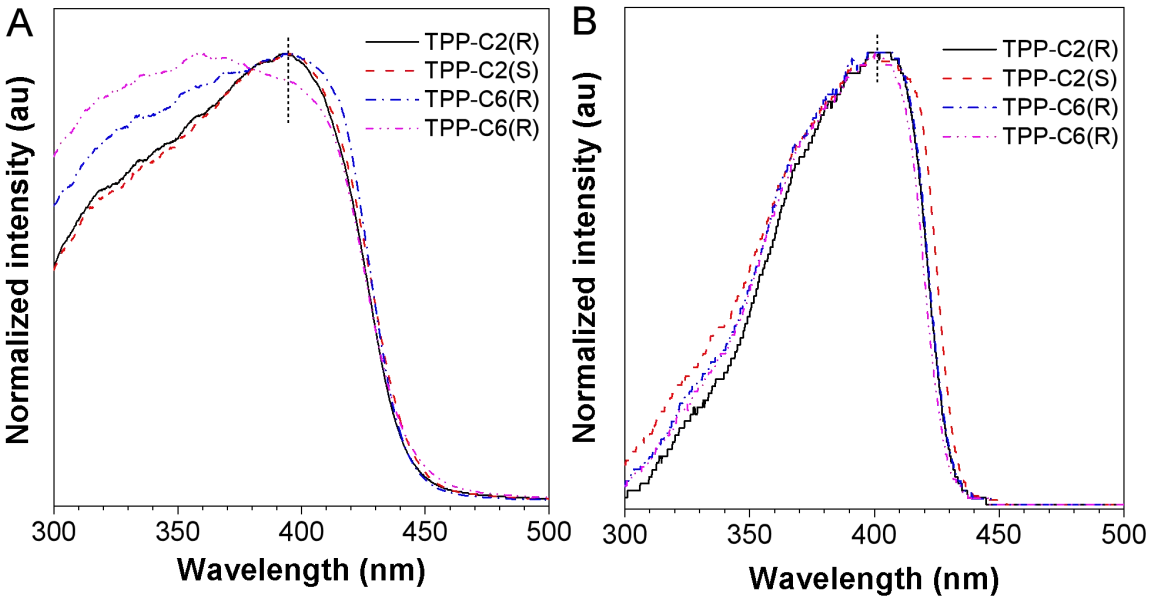


Figure S14. UV-Vis spectra of AIEgens in (A) solids and (B) films.

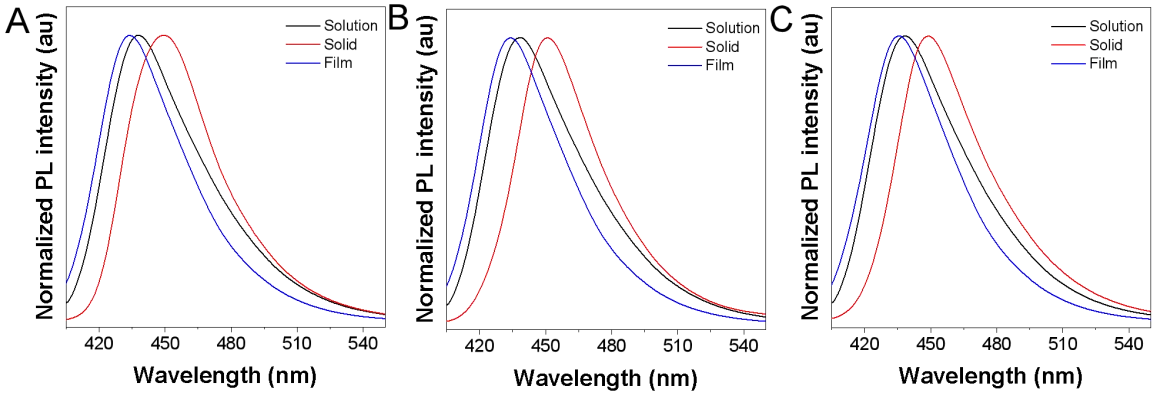


Figure S15. PL spectra of (A) TPP-C2(S), (B) TPP-C6(R) and (C) TPP-C6(S).

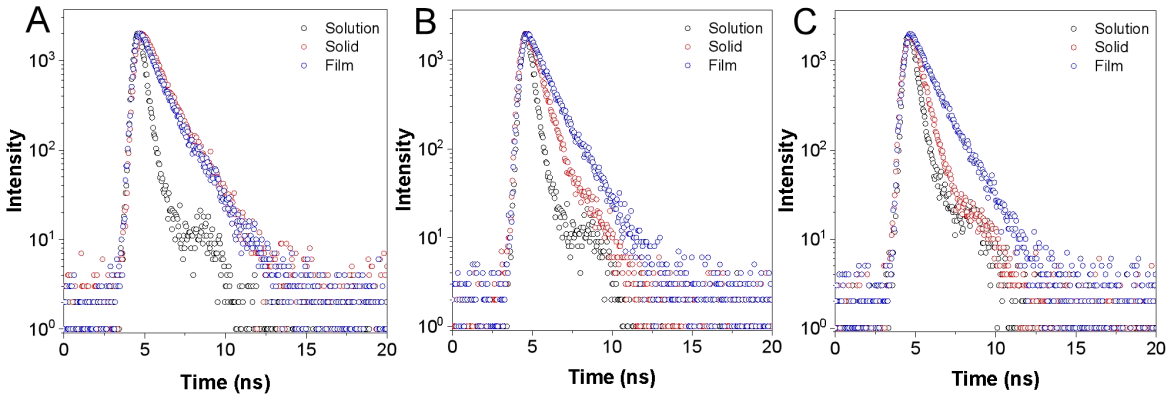


Figure S16. PL lifetime of (A) TPP-C2(S), (B) TPP-C6(R) and (C) TPP-C6(S).

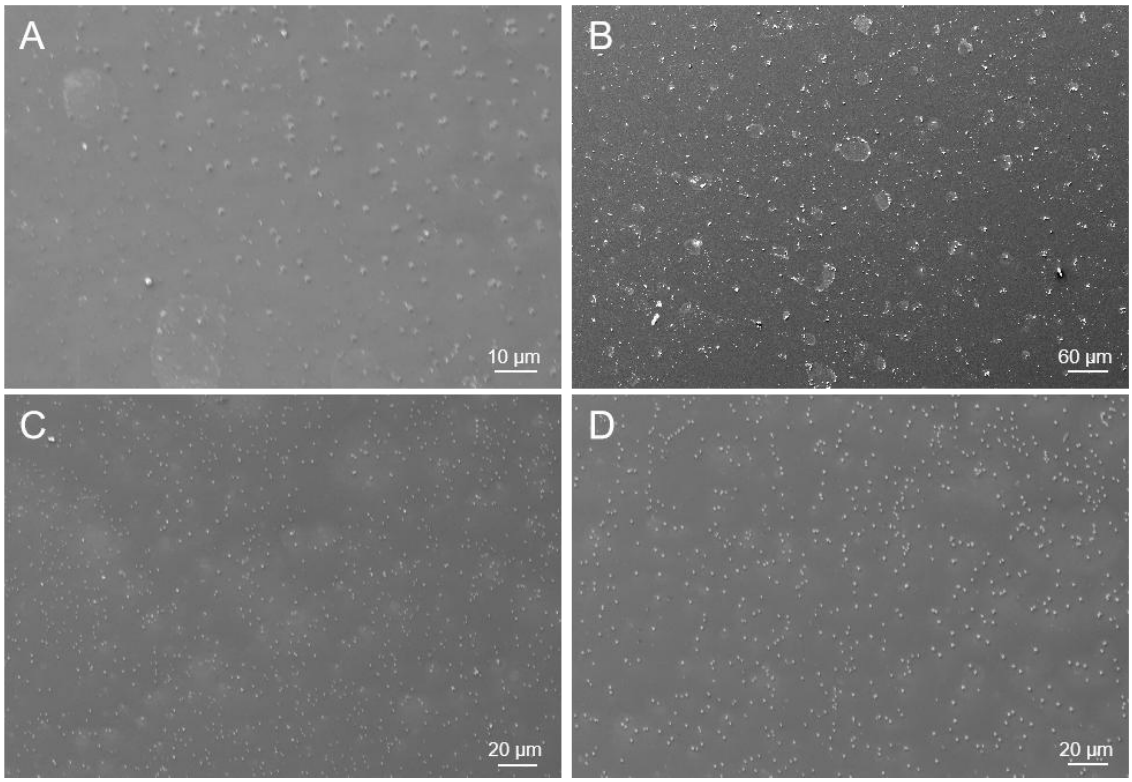


Figure S17. SEM images of (A) and (B) TPP-C2(R); (C) and (D) TPP-C2(S) assemblies in chloroform/acetonitrile (v/v = 1:1) mixture.

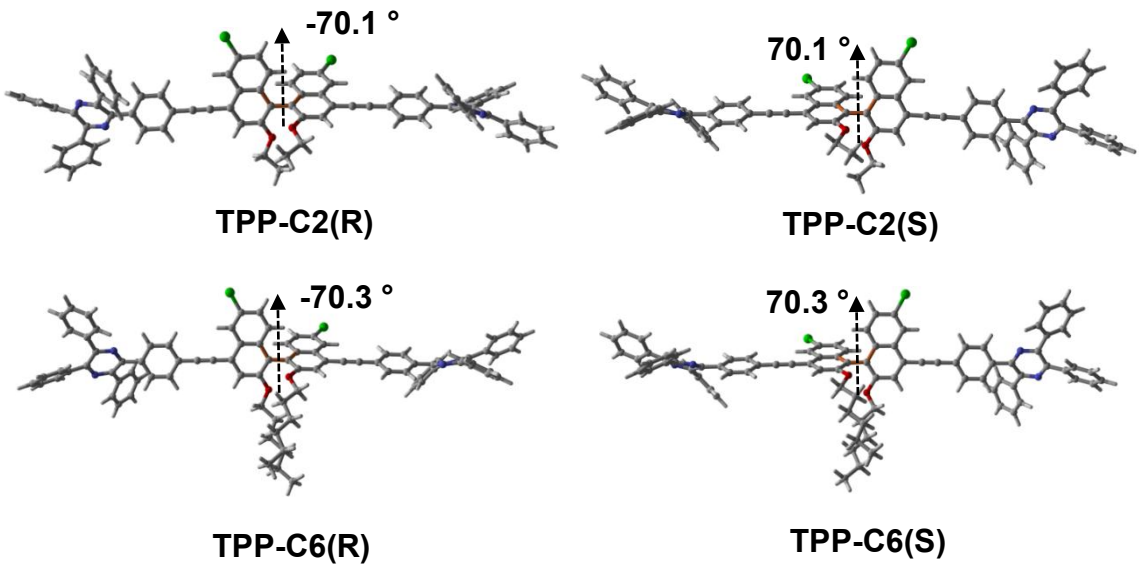


Figure S18. 3D conformations of optimized molecules.

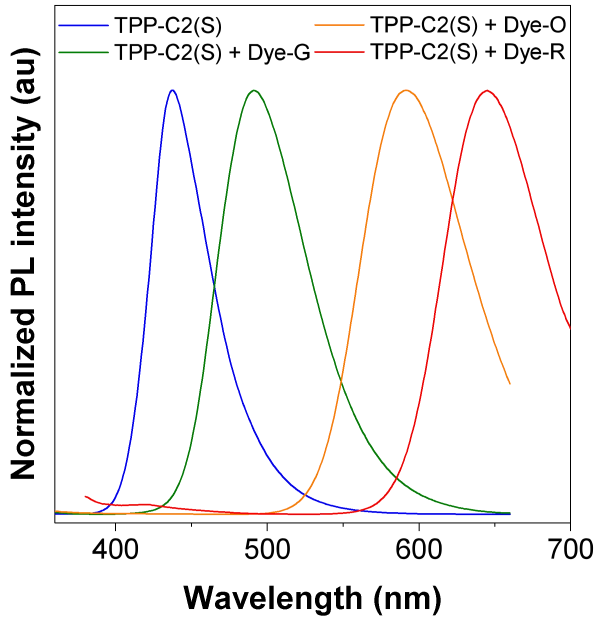


Figure S19. PL spectra of TPP-C2(S) and Dye-G/TPP-C2(S), Dye-O/TPP-C2(S), Dye-R/TPP-C2(S) in PMMA films (wt% = 1%).

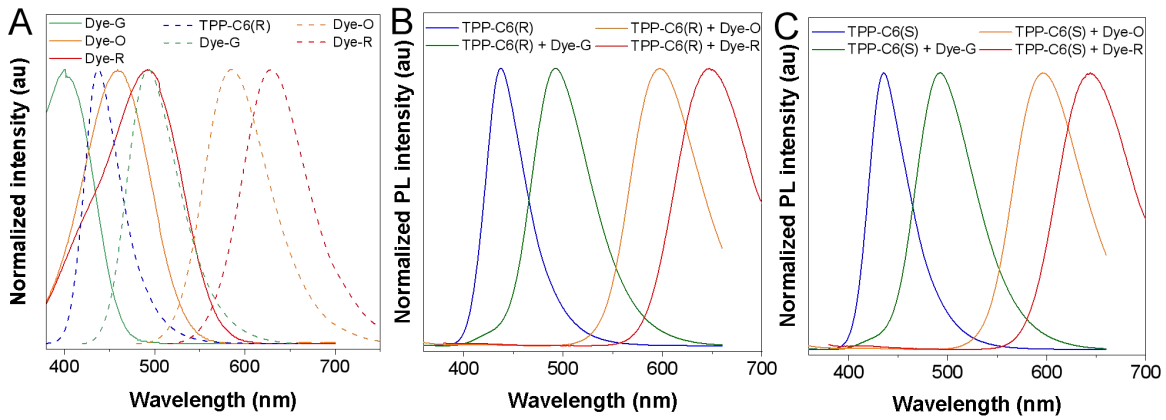


Figure S20. (A) UV-Vis or PL spectra of TPP-C6(R) and Dye-G, Dye-O, Dye-R in PMMA films. Solid line: UV-Vis spectra, dashed line: PL spectra. (B) PL spectra of TPP-C6(R) and Dye-G/TPP-C6(R), Dye-O/TPP-C6(R), Dye-R/TPP-C6(R) in PMMA films. (C) PL spectra of TPP-C6(S) and Dye-G/TPP-C6(S), Dye-O/TPP-C6(S), Dye-R/TPP-C6(S) in PMMA films.

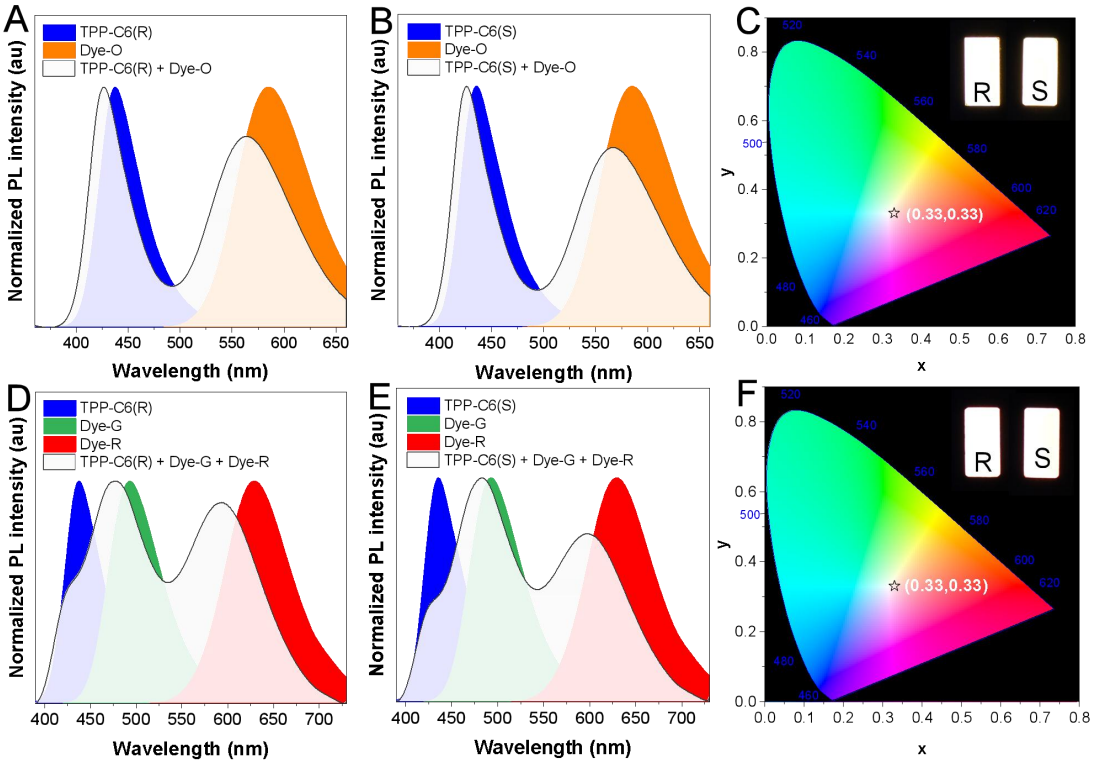


Figure S21. PL spectra of (A) TPP-C6(R) and (B) TPP-C6(S) mixed with Dye-O in the films. (C) CIE coordinates of these white light films. Inset: the photographs of these films under 365 nm UV light. PL spectra of (D) TPP-C6(R) and (E) TPP-C6(S) mixed with Dye-G and Dye-R in the

films. (C) CIE coordinates of these white light films. Inset: the photographs of these films under 365 nm UV light.

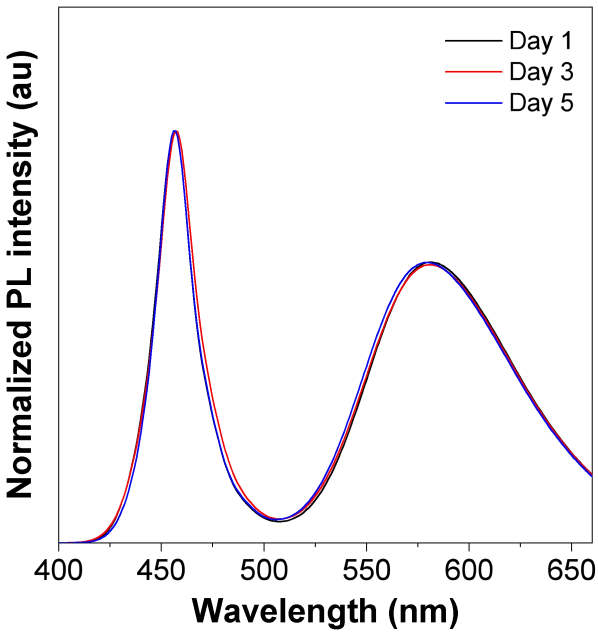


Figure S22. PL spectra of white light film coated LED in 5 days.

Table S1. Photo-physical properties of TPP-C2(R),TPP-C2(S),TPP-C6(R) and TPP-C6(S).

Compound	λ_{abs}[a] (nm)	ε[b] (10^4 L·mol^{-1}cm^{-1})	λ_{em} (nm)			Φ_F[d] (%)			$\varepsilon\Phi_F$[e] (10^4 L·mol^{-1}cm^{-1})			CIE[f]		
			Sol[a]	S[b]	Fil[c]	Sol[a]	S[b]	Fil[c]	Sol[a]	S[b]	Fil[c]	Sol[a]	S[b]	Fil[c]
TPP-C2(R)	383	8.11	438	449	434	18.3	31.3	72.2	1.48	2.54	5.86	(0.15,0.07)	(0.15,0.07)	(0.15,0.05)
TPP-C2(S)	383	8.07	438	450	434	18.7	28.0	71.9	1.51	2.26	5.80	(0.15,0.07)	(0.15,0.07)	(0.15,0.05)
TPP-C6(R)	384	8.07	438	451	434	22.0	10.0	71.8	1.78	0.81	5.79	(0.15,0.07)	(0.15,0.09)	(0.15,0.05)
TPP-C6(S)	384	8.07	438	449	436	19.5	14.6	68.6	1.57	1.18	5.54	(0.15,0.07)	(0.15,0.09)	(0.15,0.05)

[a] In THF solution (10^{-5} M); [b] In powder; [c] In Film; [d] Absolute quantum yields determined by an integrating sphere; [e] brightness = $\varepsilon\Phi_F$; [f] Commission International de L'Eclairage (CIE) coordinates.

Table S2. Fluorescence lifetime and decay rate of TPP-C2(R),TPP-C2(S),TPP-C6(R) and TPP-C6(S).

Compound	τ[d] (ns)			k_r[e] (10^9 S^{-1})			k_{nr}[f] (10^9 S^{-1})		
	Sol[a]	S[b]	Fil[c]	Sol[a]	S[b]	Fil[c]	Sol[a]	S[b]	Fil[c]
TPP-C2(R)	0.49	1.12	1.13	0.37	0.28	0.64	1.67	0.61	0.25
TPP-C2(S)	0.47	1.17	1.05	0.40	0.24	0.68	1.73	0.62	0.27
TPP-C6(R)	0.68	0.81	1.15	0.32	0.12	0.62	1.15	1.11	0.25
TPP-C6(S)	0.57	0.69	1.37	0.34	0.21	0.50	1.41	1.24	0.23

[a] In THF solution (10^{-5} M); [b] In powder; [c] In Film; [d] Fluorescence lifetime measured at room temperature in air; [e] Rate of radiative decay determined by Φ_F/τ; [f] Rate of non-radiative decay determined by $(1-\Phi_F)/\tau$.

Table S3. Photo-physical properties of doped films.

Sample	Doping ratio[a)] (wt%:wt%)	$\lambda_{em,fil}$[b)] (nm)	$\Phi_{F,fil}$[c)] (%)	η_{fil}[d)] (%)	CIE[e)]
TPP-C2(R)+Dye-G	1:2	491	74.6	93.47	(0.16,0.38)
TPP-C2(S)+Dye-G	1:2	491	74.7	93.70	(0.17,0.40)
TPP-C6(R)+Dye-G	0.9:6.3	492	59.7	97.26	(0.18,0.40)
TPP-C6(S)+Dye-G	0.9:6.3	492	59.4	97.47	(0.17,0.40)
TPP-C2(R)+Dye-O	0.9:7.3	590	99.5	99.89	(0.55,0.45)
TPP-C2(S)+Dye-O	0.9:7.3	592	98.9	99.91	(0.55,0.44)
TPP-C6(R)+Dye-O	0.9:8.5	597	99.1	99.80	(0.57,0.43)
TPP-C6(S)+Dye-O	0.9:8.5	596	98.8	99.78	(0.56,0.43)
TPP-C2(R)+Dye-R	0.8:16.5	644	54.4	97.89	(0.65,0.31)
TPP-C2(S)+Dye-R	0.8:16.5	645	54.6	98.18	(0.65,0.31)
TPP-C6(R)+Dye-R	0.8:16.5	647	53.6	99.30	(0.67,0.32)
TPP-C6(S)+Dye-R	0.8:16.5	644	56.7	99.36	(0.66,0.33)
TPP-C2(R)+Dye-O	1:0.3	430,565	99.3	-	(0.33,0.33)
TPP-C2(S)+Dye-O	1:0.3	429,566	99.5	-	(0.33,0.33)
TPP-C6(R)+Dye-O	1:0.3	427,563	99.1	-	(0.33,0.33)
TPP-C6(S)+Dye-O	1:0.3	426,566	98.9	-	(0.33,0.33)
TPP-C2(R)+Dye-G+Dye-R	1:1.2:0.2	482,597	84.1	-	(0.33,0.33)
TPP-C2(S)+Dye-G+Dye-R	1:1.2:0.2	480,597	84.7	-	(0.33,0.33)
TPP-C6(R)+Dye-G+Dye-R	1:1.2:0.2	476,595	82.5	-	(0.33,0.33)
TPP-C6(S)+Dye-G+Dye-R	1:1.2:0.2	482,597	83.4	-	(0.33,0.33)

[a)] Doping ratio in PMMA; [b)] Fluorescence emission peak of doped films; [c)] Absolute quantum yield of doped films determined by an integrating sphere ; [d)] Energy transfer efficiency of doped films determined by 1-(I_{DA}/I_D), I_{DA} is fluorescence intensity of the donor doped the receptor, I_D is fluorescence intensity of the donor without the receptor; [e)] Commission International de L'Eclairage of doped films.

Reference

1. M. Chen, L. Li, H. Nie, J. Tong, L. Yan, B. Xu, J. Z. Sun, W. Tian, Z. Zhao, A. Qin, B. Z. Tang. *Chem. Sci.*, **2015**, *6*, 1932−1937.

2. M. Chen, L. Li, H. Wu, L. Pan, S. Li, B. He, H. Zhang, J. Z. Sun, A. Qin, B. Z. Tang. *ACS Appl. Mater. Interfaces.*, **2018**, *10*, 12181−12188.

3. C. Valente, E. Choi, M. E. Belowich, C. J. Doonan, Q. Li, T. B. Gasa, Y. Y. Botros, O. M. Yaghi, J. F. Stoddart. *Chem. Commun.*, **2010**, *46*. 4911−4913.

4. H. Zhang, H. Li, J. Wang, J. Sun, A. Qin, B. Z. Tang. *J. Mater. Chem. C.*, **2015**, *3*, 5162−5166.

5. L. Pan, Y. Cai, H. Wu, F. Zhou, A. Qin, Z. Wang, B. Z. Tang. Mater. *Chem. Front.*, **2018**, *2*, 1310−1316.

6. T. Seo, N. Toyoshima, K. Kubota, H. Ito. *J. Am. Chem. Soc.*, **2021**, *143*, 6165−6175.

7. W. Qin, N. Alifu, J. W. Y. Lam, Y. Cui, H. Su, G. Liang, J. Qian, B. Z. Tang. *Adv. Mater.*, **2020**, *32*, 2000364.