Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Functionalized diketopyrrolopyrrole compounds for NIR-to-visible photon upconversion

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Molecular geometry as well as singlet and triplet state energies of the investigated compounds were modelled using quantum chemistry program package *ORCA*[1]. The DFT calculations were performed at the B3LYP/6-31G(d) level.

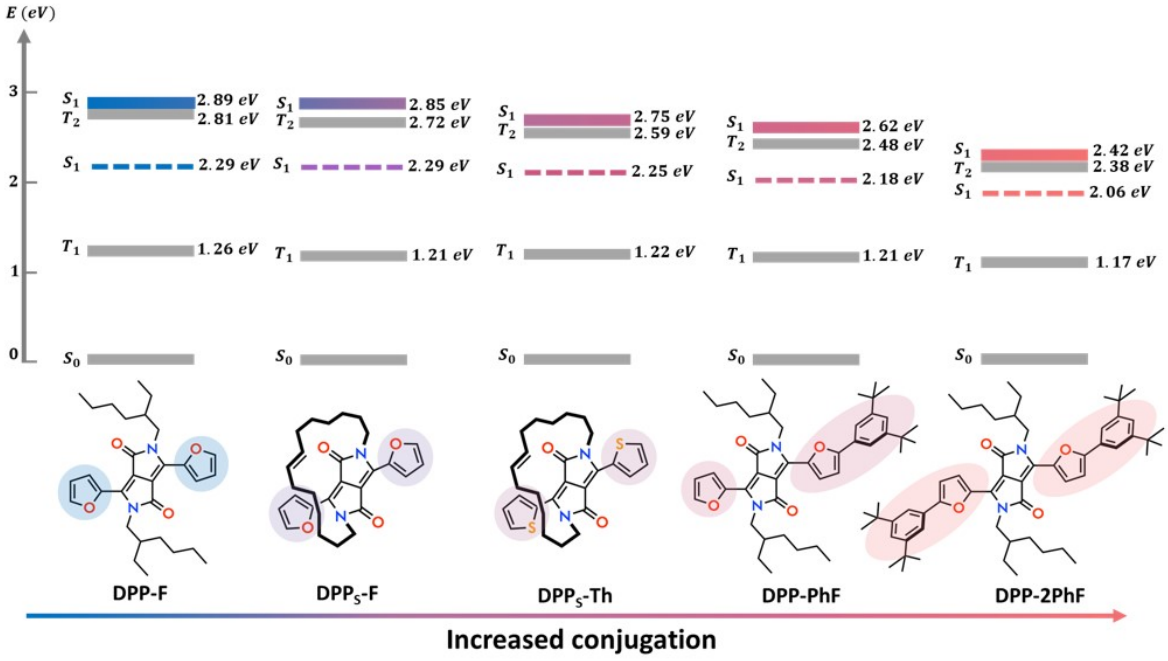


Fig. S1. Energy states of the functionalized diketopyrrolopyrrole compounds. Energy levels estimated by DFT are indicated in solid lines; experimentally determined S_1 states are shown in dashed lines.

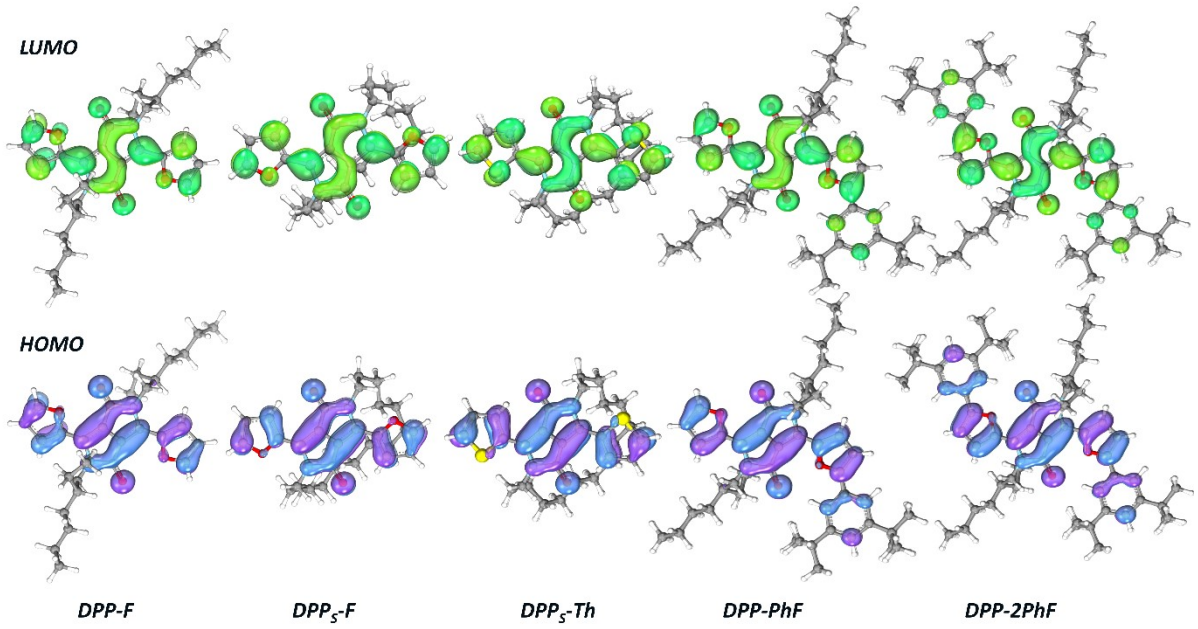


Fig. S2. Visualization of the highest occupied (HOMO) and lowest unoccupied molecular orbitals (LUMO) of DPP compounds.

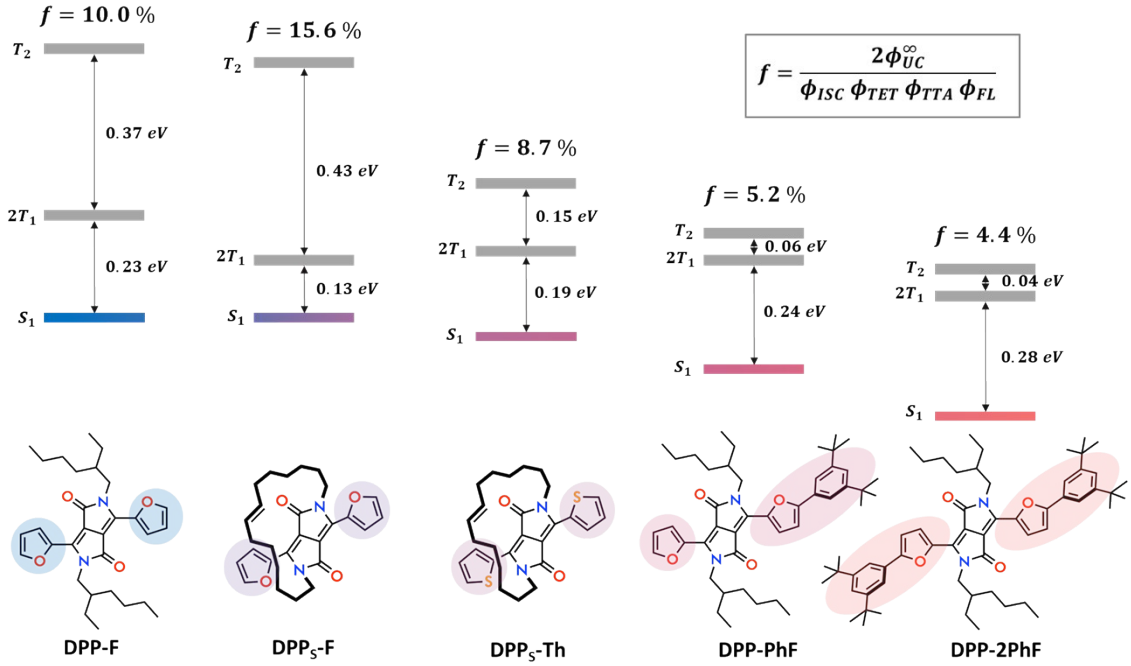


Fig. S3. Representation of energy differences $2T_1 - S_1$ and $T_2 - 2T_1$ of the functionalized DPP compounds. Statistical probability factor f, indicated.

Estimation of annihilation radius

The formula for the calculation of annihilation radius (shown below) was derived from the Eq. 5 and 6:

$$R = \frac{2(k_T)^2}{8\pi f D I_{th} \alpha(E)\, \phi_{TET}}.$$

Here, the absorption coefficient $\alpha(E)$ = 6.52 cm^{-1}. Coefficient of DPP molecule diffusion in toluene (D) was assumed to be the same as the self-diffusion coefficient of liquid toluene at room temperature (D = 2.5 × 10^{-5} cm^2 s^{-1}).[2]

Table S1. The main parameters used in the estimation of *R*.

	κ_T, s^{-1}	f	I_{th}, photon s^{-1} m^{-2}	φ_{TET}	*R*, m
DPP-F	4.5 × 10^4	0.100	3.7 × 10^{24}	0.46	5.9 × 10^{-10}
DPP$_S$-F	3.6 × 10^4	0.156	1.7 × 10^{23}	0.65	3.7 × 10^{-9}
DPP$_S$-Th	5.6 × 10^4	0.087	6.7 × 10^{23}	0.54	4.8 × 10^{-9}
DPP-PhF	5.7 × 10^4	0.052	7.4 × 10^{23}	0.56	7.4 × 10^{-9}
DPP-2PhF	3.6 × 10^4	0.044	1.1 × 10^{25}	0.46	2.9× 10^{-10}

Although the estimated absolute *R* values are of the same order as Dexter energy transfer distance (typically ~1 nm), they should not be considered as true annihilation radii. They purpose here is to reveal relative changes in effective distance of various DPP derivatives at which TTA is feasible.

Evaluation of triplet lifetime and triplet transfer from PdPc sensitizer to DPP$_S$-F emitter

UC transients were obtained at low excitation densities (k_T[T] >> γ_{TTA}[T]^2), so that the dynamics of the triplet population can be simplified to the following formula:

$$\frac{d[T]}{dt} = G_T - k_T[T] - \gamma_{TTA}[T]^2 \approx G_T - k_T[T]$$

Taking into account that generation $G_T \propto e^{-\frac{t}{\tau_r}}$ and that $I_{UC} \propto$ [T]^2, we obtain:

$$I_{UC}(t) \propto [T]^2 \propto \left(a_1 \exp\left(-\frac{t}{\tau_T}\right) - a_2 \exp\left(-\frac{t}{\tau_r}\right)\right)^2$$

To prove the condition k_T[T] >> γ_{TTA}[T]^2 is met, we performed UC transient measurements at a range of excitation intensities (see Fig. S4 below). For this experiment we specifically chose **DPP$_S$-F:PdPc** with the lowest UC threshold, and therefore with potentially the highest contribution from the 2nd order term (γ_{TTA}[T]^2). Excitation intensity was varied in the range of 1-6 μJ per pulse, while excitation area was maintained rather large (20 mm^2). The same conditions (with excitation intensity of 4 μJ, which implies excitation density of 20 μJ/cm^2) were employed for measuring transients of all the studied DPP compounds displayed in Fig. 6.

As it is demonstrated in Fig. S4 below, the triplet lifetime remains unchanged (2×14 μs) at least up to 6 μJ intensity, thereby permitting to disregard TTA decay term as negligible at these experimental conditions.

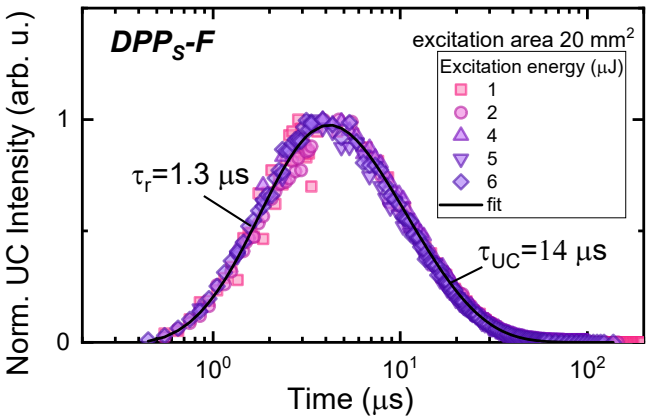


Fig. S4. UC transients of **DPP$_S$-F:PdPc** solution in toluene at the emitter and sensitizer concentrations of 8 mM and 30 μM, respectively. Excitation wavelength, 730 nm; pulse repetition rate, 1 kHz. Excitation energies and area, indicated.

UC threshold evaluation by the "classical" method

Shown below are UC thresholds (I_{th}) determined by the "classical" method from the intersection of the fitted UC slopes of 2 and 1. This method yielded similar values as those estimated by Murakami methodology (*Phys. Chem. Chem. Phys.*, 2021, 23, 18268) for **DPP$_S$-F, DPP$_S$-Th** and **DPP-PhF** (see Fig. 5)**.** Unfortunately, in contrast to Murakami approach, the limitations of the "classical" method has not permitted determination of I_{th} for the **DPP-F** and **DPP-2PhF** for which the threshold is close to or above the highest excitations used in the experiment, i.e. ≥100 W/cm^2.

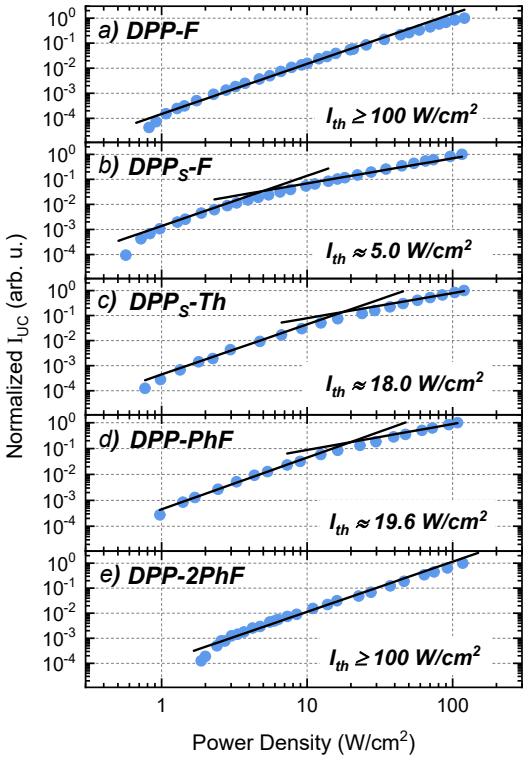


Fig. S5. Log-log plots of UC intensity *vs* excitation power density of the studied emitter:sensitizer ((a) **DPP-F:PdPc**, (b) **DPP$_S$-F:PdPc**, (c) **DPP$_S$-Th:PdPc**, (d) **DPP-PhF:PdPc** and (e**) DPP-2PhF:PdPc**) solutions

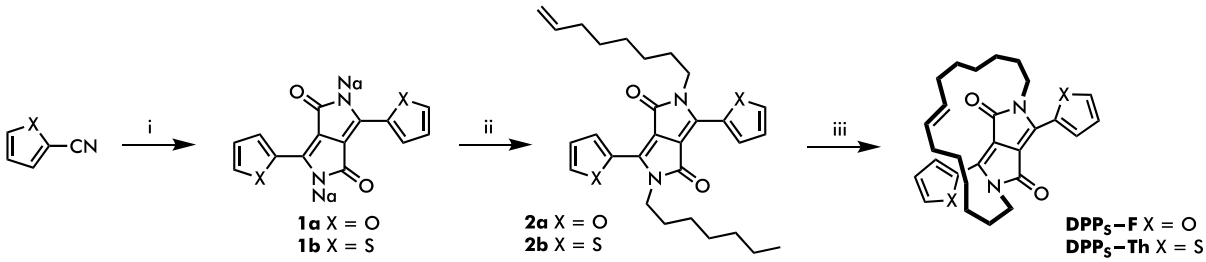
in toluene at 8 mM and 30 μM concentrations, respectively. Solutions excited with 730 nm CW laser. Black lines represent the fitted UC slopes of 2 and 1. UC thresholds (I_{th}), indicated.

Synthesis of DPP compounds

All reaction were carried out in oven-dried vessels under an inert argon atmosphere. Anhydrous solvents were prepared according with literature methods under inert argon atmosphere. All other chemicals were used as supplied. Column chromatography was carried out using Merck 60 (43.0 – 66.3 µm) silica. Reactions were monitored by thin layer chromatography using (0.25 mm Merck silica plates Kieselgel 60F-254). Components were visualized under UV light. NMR spectra were recorded on a Bruker Avance 400 spectrometer. Residual solvent peaks (δ = 7.26 ppm (H) ir δ = 77.16 ppm (C) $CDCl_3$) were used as the internal standard. ^{1}H NMR chemical shifts are quoted using the following abbreviations: s – singlet, d – doublet, t – triplet, q – quartet, qn – quintet, sxt – sextet, m – multiplet, br – broad.

DCM – dichloromethane; DMF – N,N-dimethylformamide; EA – ethylacetate; PE – petrol ether (40-60°C boiling fraction).

Synthesis of macrocyclic DPP



Scheme 1. Synthesis of macrocyclic DPP: i. Na, *t*-amyl alcohol, dimethyl succinate, 120 °C; ii. K_2CO_3, 1-bromo-8-octene, DMF, 120 °C; iii. Grubbs I, toluene (0.4 mM), 40 °C.

Compounds **1**. An oven-dried round-bottom flask equipped with a condenser was charged with a stir bar and tert-amyl alcohol (25 mL). Sodium metal pieces (0.247 g, 10.74 mmol, 3.0 equiv) were added to the warmed solution of tert-amyl alcohol (60-70 °C) in small portions. After complete addition and dissolution of sodium, the temperature was raised to 120 °C. The corresponding nitrile (for **1a** - furan-2-carbonitrile; for **1b** - thiophene-2-carbonitrile) (10,74 mmol, 3.0 equiv) was subsequently added to the above solution at 60-70 °C. Dimethyl succinate (0.47 mL, 3.58 mmol, 1.0 equiv) was then added dropwise (the reaction mixture turned dark red) and was left to stir for 1.5 h. The reaction mixture was then cooled to room temperature and the precipitate of sodium salt **1** was filtered through a glass frit filter funnel. The precipitate was washed with diethyl ether, dried under vacuum, and used without further purification. **1a** 1.08 g (96%) a dark red solid; **1b** 267 mg (25%) a dark red solid.

The spectral data were in accordance with literature.[3]

Compounds **2**. Compound **1** (1.60 mmol, 1.0 equiv), K_2CO_3 (884 mg, 6.40 mmol, 4.0 equiv) and 5.0 mL of dry DMF were added to a Schlenk tube with a stir bar. Then, 1-bromo-8-octene (4.0 mmol, 0.671

mL, 2.5 equiv) was added quickly. The reaction mixture was heated to 120 °C and stirred overnight. After cooling, the reaction mixture was diluted with water, the precipitate was filtered off and dissolved in chloroform. Solvent was evaporated and the resulted dark red crude product was purified by column chromatography using chloroform as eluent. **2a** dark red crystals, yield 43%, **2b** a dark red powder, yield 41%.

Compound 2a (X = O):

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (dd, *J* = 3.7, 0.7 Hz, 2H), 7.66 (dd, *J* = 1.7, 0.7 Hz, 2H), 6.72 (dd, *J* = 3.7, 1.7 Hz, 2H), 5.82 (ddt, *J* = 16.9, 10.3, 6.7 Hz, 2H), 5.05 – 4.92 (m, 4H), 4.17 – 4.07 (m, 4H), 2.10 – 2.01 (q, 6H), 1.71 (m, *J* = 7.4 Hz, 4H), 1.41 (m, *J* = 12.8 Hz, 10H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.87, 145.16, 144.67, 139.03, 133.65, 120.12, 114.26, 113.47, 106.45, 42.37, 33.69, 30.14, 28.75, 26.67

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{30}H_{37}N_2O_4$ 489.2748; Found: 489.2745.

Compound 2b (X = S):

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 3.9, 1.2 Hz, 2H), 7.64 (dd, J = 5.0, 1.2 Hz, 2H), 7.29 (dd, *J* = 5.0, 3.9 Hz, 2H), 5.79 (ddt, *J* = 17.0, 10.2, 6.7 Hz, 2H), 5.02 – 4.90 (m, 4H), 4.11 – 4.04 (m, 4H), 2.04 (q, *J* = 6.7 Hz, 6H), 1.75 (m, *J* = 7.7 Hz, 4H), 1.47 – 1.31 (m, 10H)

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.39, 140.03, 138.95, 135.26, 130.67, 129.77, 128.63, 114.32, 107.72, 42.18, 33.66, 29.91, 28.76, 28.71, 26.71.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{30}H_{37}N_2O_2S_2$ 521.2291; Found: 521.2287.

Compounds **DPP_S-F and DPP_S-Th**. **2** (0.1020 mmol) was dissolved in freshly distilled dry toluene (250 mL) in a round-bottom flask equipped with a stir bar and a condenser. The resulting solution was warmed to 40°C and 1st generation Grubbs catalyst (8.4 mg, 0.0102 mmol, 10 mol%) was added. Reaction was stirred at 40°C for 72 hours. Upon the completion of reaction, the solvent was evaporated, and the resulting crude product was purified by column chromatography using $CHCl_3$ as eluent. **DPP_S-F** a dark red solid, 57% yield; **DPP_S-Th** a dark red solid, 30% yield.

DPP_S-F (X = O):

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 3.6 Hz, 2H), 7.64 (d, J = 1.7 Hz, 2H), 6.69 (dd, J = 3.6, 1.7 Hz, 2H), 5.12 (t, J = 4.6 Hz, 2H), 4.41 – 4.26 (m, 2H), 4.17 (dt, J = 14.0, 4.4 Hz, 2H), 1.73 (s, 6H), 1.40 – 1.06 (m, 14H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.44, 145.14, 144.69, 129.72, 120.12, 113.48, 41.63, 29.70, 28.89, 28.15, 28.00, 25.75, 24.44.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{28}H_{33}N_2O_4$ 461.2435; Found: 461.2428.

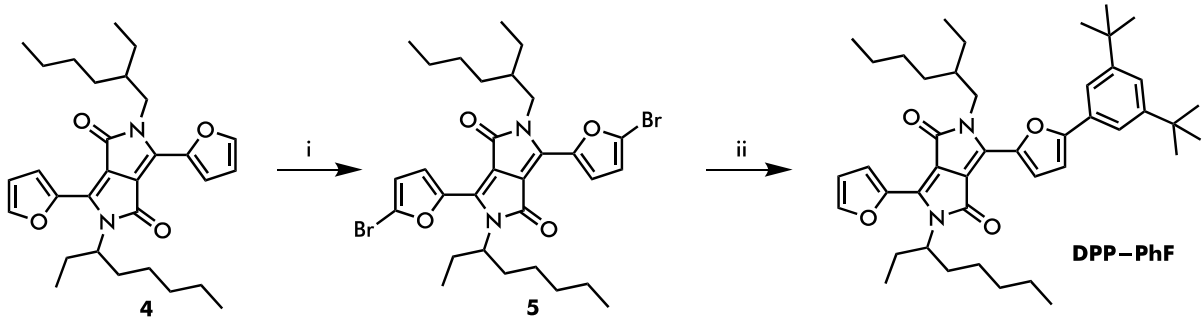
DPP_S-Th (X = S):

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (ddd, *J* = 30.1, 3.9, 1.2 Hz, 2H), 7.63 (dt, *J* = 5.0, 1.4 Hz, 2H), 7.30 – 7.24 (m, 2H), 5.20 – 5.10 (m, 2H), 4.46 (dddd, *J* = 20.7, 14.6, 10.6, 4.1 Hz, 2H), 4.02 (ddd, *J* = 15.0, 4.4, 3.1 Hz, 2H), 1.90 – 1.75 (m, 4H), 1.37 – 1.08 (m, 10H), 0.94 – 0.78 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.05, 160.99, 139.33, 139.20, 134.00, 133.79, 129.62, 129.61, 129.07, 128.97, 128.73, 127.42, 107.48, 107.27, 40.43, 40.23, 29.81, 28.16, 27.54, 27.11, 26.85, 26.36, 26.08, 24.70, 23.51, 23.49.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{28}H_{33}N_2O_2S_2$ 493.1978; Found: 493.1977.

Synthesis of DPP-PhF



Scheme 2. Synthesis of monoarylated DPP: i. NBS, $CHCl_3$, rt; ii. 3,5-di-tert-butylphenylboronic acid, $Pd(PPh_3)_4$, K_2CO_3, toluene/EtOH/water, 110 °C.

Compound **5**. A Schlenk tube was charged with a stir bar, **4** (95 mg, 0.194 mmol, 1.0 equiv) and 5.0 mL of $CHCl_3$. The mixture was cooled to 0 °C and stirred while N-bromosuccinimide (NBS) (75.8 mg, 0.426 mmol, 2.2 equiv) was added in small portions. Upon addition of NBS, the reaction mixture was warmed to room temperature and stirred for 6 hours. The reaction was washed with water and extracted with DCM (3 x 25 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and the solvent was evaporated. The resulting dark purple crude product was purified by column chromatography using PE/DCM 1:1 as eluent to afford 42.3 mg (34%) of **5** as a dark red solid.

The spectral data were in accordance with literature.[4]

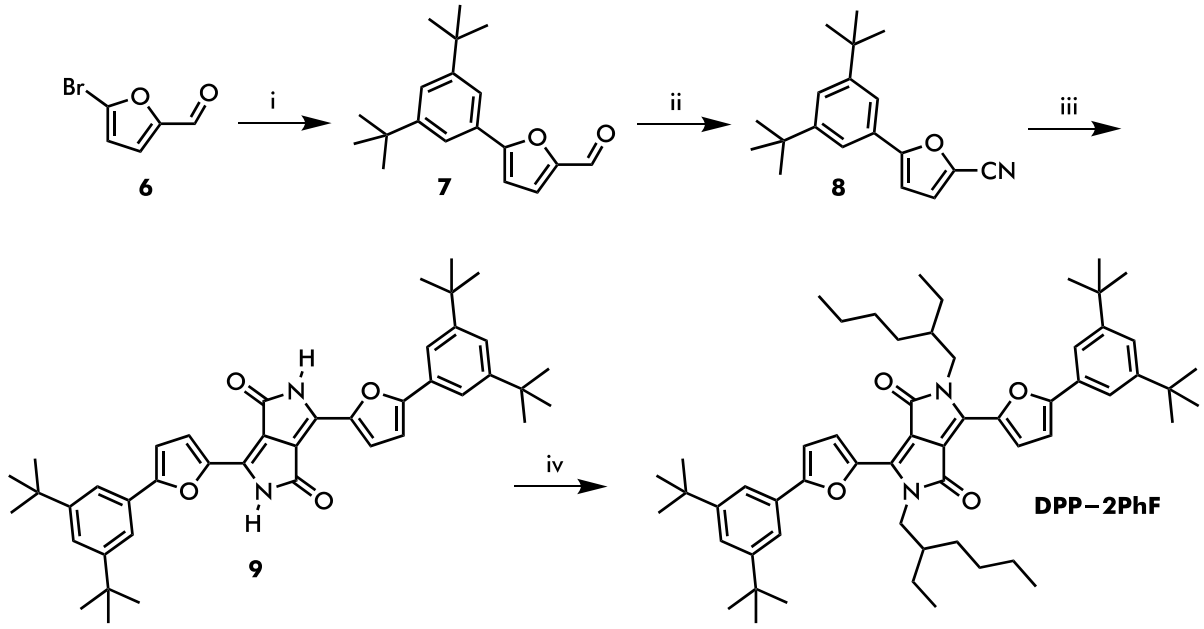
DPP-PhF. Compound **5** (39 mg, 0.06 mmol, 1.0 equiv), 3,5-di-*tert*-butylphenylboronic acid (34 mg, 0.145 mmol, 2.4 equiv) and K_2CO_3 (1.0 mg, 0,003 mmol, 0.05 equiv) were dissolved in toluene and distilled water (volume ratio 1:0.15) in a Schlenk tube with a stir bar. The resulting mixture was sparged with argon for 15 minutes. $Pd(PPh_3)_4$ (3.5 mg, 0.003 mmol, 0.05 equiv) was added and the reaction mixture was heated at 110°C for 8 days. The mixture was cooled to room temperature, washed with water and extracted with DCM (3 x 25mL). The organic phase was collected and dried with anhydrous Na_2SO_4, filtered and the solvents were evaporated. The resulting dark purple crude product was purified by column chromatography using PE:$CHCl_3$ 1:1 as eluent to afford 23 mg (39%) of **DPP**-**PhF** as a purple solid (mixture of diastereomers).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 3.9 Hz, 1H), 8.36 – 8.28 (m, 1H), 7.61 (t, *J* = 1.8 Hz, 3H), 7.45 (t, *J* = 1.8 Hz, 1H), 6.95 (d, *J* = 3.8 Hz, 1H), 6.69 (dd, *J* = 3.7, 1.7 Hz, 1H), 4.22 (d, *J* = 7.7 Hz, 2H), 4.08 – 3.98 (m, 4H), 1.38 (s, 18H), 1.35 – 1.15 (m, 16H), 0.97 – 0.82 (m, 10H), 0.78 (t, *J* = 6.9 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 161.05, 160.99, 139.33, 139.20, 134.00, 133.79, 129.62, 129.61, 129.07, 128.97, 128.73, 127.42, 107.48, 107.27, 40.43, 40.23, 29.81, 28.16, 27.54, 27.11, 26.85, 26.36, 26.08, 24.70, 23.51, 23.49.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{44}H_{61}N_2O_4$ 681.4626; Found: 681.4626.

Synthesis of DPP-2PhF



Scheme 4. Synthesis of bis-arylated DPP: i. 3,5-di-tert-butylphenylboronic acid, $Pd(PPh_3)_4$, K_2CO_3, toluene/EtOH/water, 110 °C; ii. I_2, Na_2CO_3, NH_4OAc, TBHP, 60 ºC; iii. Na, *t*-amyl alcohol, dimethyl succinate, 120 °C; iv. 2-ethylhexylbromide, K_2CO_3, DMF, 120 °C.

Compound **7**. 3,5-di-*tert*-butylphenyl boronic acid (570 mg, 2.43 mmol, 1.3 equiv), 5-bromofuran-2-carbaldehyde (327 mg, 1.87 mmol, 1.0 equiv), and Cs_2CO_3 (61 mg, 0.187 mmol, 10 mol%) were added to a Schlenk flask and dissolved in a mixture of 5.0 mL of toluene, 3.5 mL distilled water and 2.0 mL ethanol. The resulting mixture was degassed by passing a stream of argon through the solution for 20 minutes. $Pd(PPh_3)_4$ (108 mg, 0.187 mmol, 10 mol%,) was added and the reaction mixture was heated at 110 °C. After 72 hr, the reaction mixture was cooled to room temperature, washed with water and extracted with DCM (3 x 25 mL). The combined organic phase was dried with anhydrous Na_2SO_4, filtered and evaporated. The resulting crude product was purified by column chromatography using PE/EA 40:1 as eluent to afford 506 mg (95%) of **7** as a yellow viscous oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 7.65 (d, *J* = 1.8 Hz, 2H), 7.49 (t, *J* = 1.8 Hz, 1H), 7.34 (d, *J* = 3.7 Hz, 1H), 6.85 (d, *J* = 3.7 Hz, 1H), 1.37 (s, 18H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.06, 160.84, 151.75, 128.42, 124.20, 119.75, 107.49, 34.93, 31.31.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{19}H_{25}O_2$ 285.1849; Found: 285.1849.

5-(3,5-di-*tert*-butylphenyl)furan-2-carbonitrile (8)

7 (530 mg, 1.86 mmol, 1.0 eq), iodine (24 mg, 0.0932 mmol, 5 mol%), Na_2CO_3 (296 mg, 2.80 mmol, 1.5 eq) and NH_4OAc (288 mg, 3.73 mmol, 2.0 eq.) were added to a round-bottom flask and were dissolved in 5.0 mL of ethanol. 2.05 mmol of TBHP (1.1 eq, 0.28 mL of 70% aqueous solution) was added to the mixture dropwise. Reaction mixture was heated at 60°C for 4h. The reaction mixture was quenched with saturated aqueous solution of $Na_2S_2O_3$, washed with distilled water and extracted with chloroform (3 x 15 mL). The organic phase was then collected and dried with anhydrous Na_2SO_4, filtered and the solvents were evaporated. The resulting crude product was purified by column chromatography using PE:EA 30:1 as eluent to afford 398 mg (76%) of **8** as dark red crystals.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (d, *J* = 1.8 Hz, 2H), 7.47 (t, *J* = 1.8 Hz, 1H), 7.17 (d, *J* = 3.7 Hz, 1H), 6.72 (d, *J* = 3.7 Hz, 1H), 1.37 (s, 18H).

^{13}C NMR ($CDCl_3$): δ 159.81, 151.92, 132.17, 132.07, 131.95, 128.57, 128.44, 128.10, 124.01, 119.24, 105.65, 35.06, 31.36.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{19}H_{24}NO$ 282.1852; Found: 282.1868.

3,6-bis(5-(3,5-di-*tert*-butylphenyl)furan-2-yl)pyrrolo[3,4-c]pyrrolo-1,4(2H, 5H)-dione (9)

An oven-dried round-bottom flask equipped with a condenser was charged with a stir bar and tert-amyl alcohol (5.0 mL). Sodium metal pieces (32 mg, 1.38 mmol, 3.1 eq.) were added to the warmed solution of tert-amyl alcohol (60-70°C) in small portions. After complete addition and dissolution of sodium, the temperature was raised to 120°C. **8** (377 mg, 1.34 mmol, 3 eq.) was subsequently added to the hot solution of sodium alkoxide. Dimethyl succinate (0.06 mL, 0.447 mmol, 1.0 eq.) was then added dropwise to the reaction mixture (the reaction mixture turned dark red) and was stirred for 2 h. The reaction mixture was cooled to room temperature, solvent was evaporated and the product was precipitated in MeOH with a few drops of conc. HCl. The precipitate was filtered over a glass frit filter funnel and was washed with MeOH. The resulting product was dried under vacuum and used without further purification. Product was isolated as a dark purple solid, 53 mg (18%).

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (s, 2H), 7.91 (d, *J* = 3.8 Hz, 2H), 7.59 (d, *J* = 1.8 Hz, 4H), 7.47 (s, 2H), 6.95 (d, *J* = 3.8 Hz, 2H), 1.39 (s, 34H).

^{13}C NMR spectrum was not acquired due to poor solubility.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{42}H_{49}N_2O_4$ ($[M+1]^+$) 645.3687, found 645.3681.

DPP-2PhF

Compound **10** (50 mg, 0.076 mmol, 1.0 eq), K_2CO_3 (42 mg, 0.304 mmol, 4.0 eq) and 3.0 mL of dry DMF were added to a Schlenk tube with a stir bar. Then, 2-ethylhexyl bromide (0.190 mmol, 0.038 mL, 2.5 eq) was added quickly. The reaction mixture was heated to 120°C and stirred for 48h. The reaction mixture was cooled to room temperature, washed with water and extracted with $CHCl_3$ (3 x 25mL). The organic phase was then collected and dried with anhydrous Na_2SO_4, filtered and the solvents were evaporated. Resulting crude product was purified by column chromatography using PE:DCM 1:1 as eluent to affoprd 42 mg (63%) of **DPP-2PhF** as a dark purple solid.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.45 (d, *J* = 3.8 Hz, 2H), 7.61 (d, *J* = 1.8 Hz, 4H), 7.45 (t, *J* = 1.7 Hz, 2H), 6.95 (d, *J* = 3.8 Hz, 2H), 4.24 (d, *J* = 7.6 Hz, 4H), 1.48 – 1.30 (m, 42H), 1.29 – 1.17 (m, 12H), 0.83 (dt, *J* = 39.7, 7.1 Hz, 12H).

^{13}C NMR ($CDCl_3$): δ 161.39, 158.06, 151.60, 143.94, 133.25, 128.92, 123.46, 122.67, 119.02, 108.94, 106.84, 46.86, 39.38, 34.98, 31.42, 30.52, 28.54, 23.86, 23.03, 13.91, 10.81.

HRMS (ESI) calcd. for ($[M+H]^+$): $C_{58}H_{81}N_2O_4$ 869.6191; Found: 869.6192.

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