

Supporting Information

An efficient method to achieve the balanced open circuit voltage and short circuit current density in polymers solar cells

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Fig. S1: TGA (a) and DSC (b) curves of PIDT-DTQ-TT at a heating and cooling rate of 20 °C/min under an inert atmosphere.

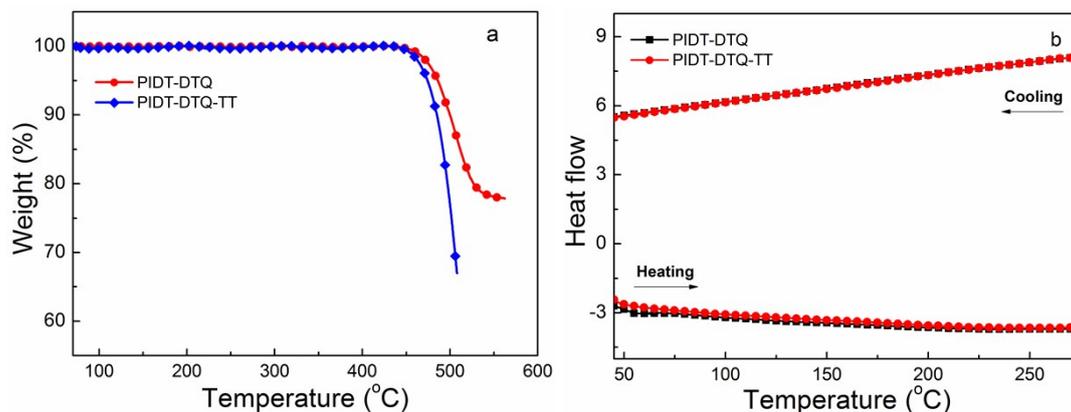


Fig. S2: Absorption coefficients of PIDT-DTQ and PIDT-DTQ-TT in thin films.

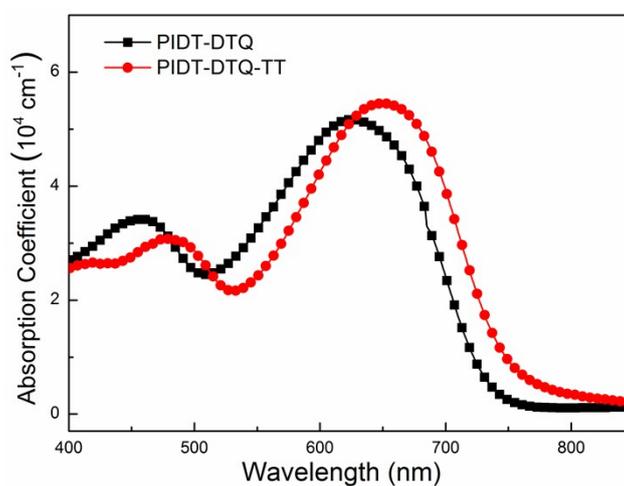
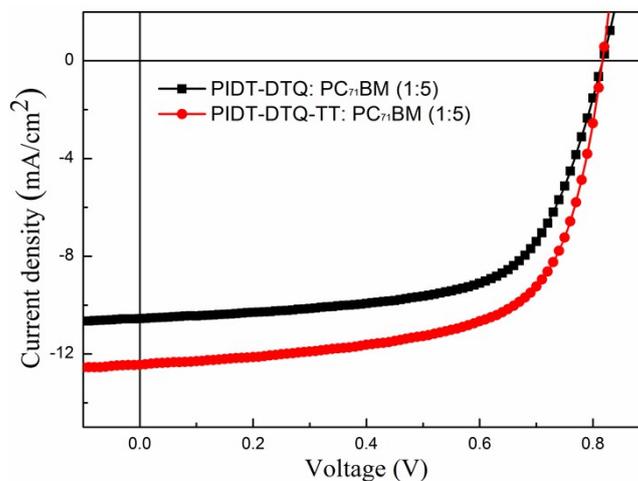
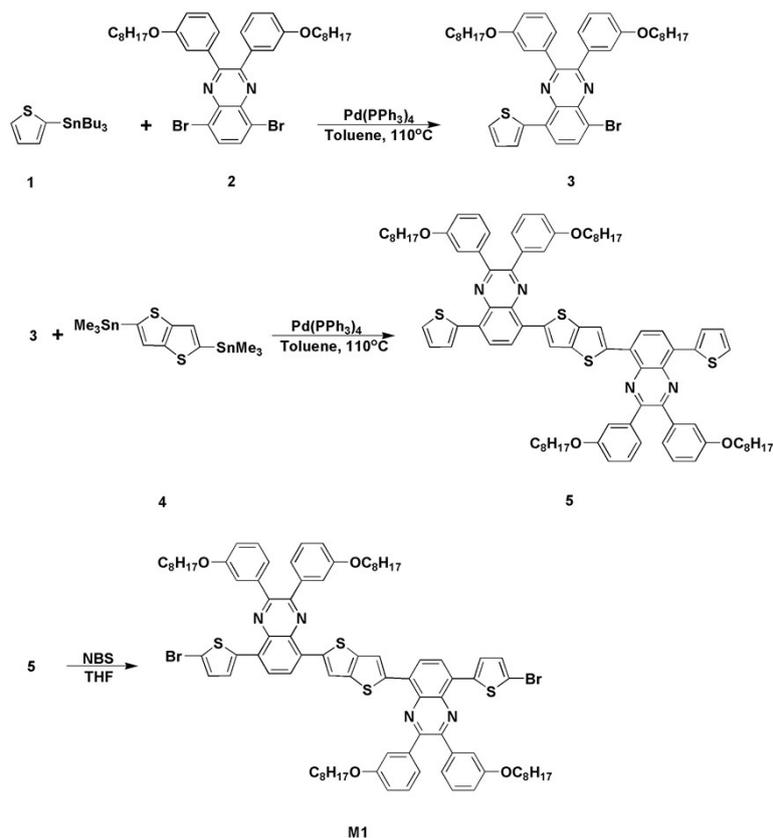


Fig. S3: Current density-voltage (J - V) characteristics of PIDT-DTQ and PIDT-DTQ-TT-based PSCs under the blending ratios of 1:5 with PC₇₁BM.





Scheme S1: Synthetic routes of monomer M1

Synthesis of compound 3:

To a solution of 5,8-dibromo-2,3-bis(3-(octyloxy)phenyl)quinoxaline (1) (1.14 g, 1.64 mmol) and 2-(tributylstannyl)thiophene (2) (0.64 g, 1.72 mmol) in toluene (50 mL) was added tetrakis(triphenylphosphine)platinum(0) [$\text{Pd}(\text{PPh}_3)_4$] (56 mg, 0.05 mmol) under nitrogen. After refluxing for 20 h, the mixture was quenched with 60 mL water and extracted with dichloromethane (DCM) three times (3×50 mL). Then the combined organic layer was washed with water and dried over anhydrous magnesium sulfate (MgSO_4). After removing the solvent, the product was purified by column chromatography on silica gel with hexane and DCM (V/V, 5:1) as the eluent and obtained as a yellow solid (0.53 g, 46.5 %). ^1H NMR (400 MHz, CDCl_3 , TMS, δ_{ppm}):

8.06 (d, $J = 8.0$ Hz, 1H), 7.98 (d, $J = 8.1$ Hz, 1H), 7.85 (s, 1H), 7.52 (d, $J = 4.6$ Hz, 1H), 7.32 (s, 1H), 7.28-7.23 (m, 5H), 7.19-7.18 (m, 1H), 6.94 (d, $J = 7.0$ Hz, 2H), 3.90-3.86 (br, 4H), 1.75-1.72 (br, 4H), 1.45-1.31 (br, 20H), 0.90-0.88 (m, 6H).

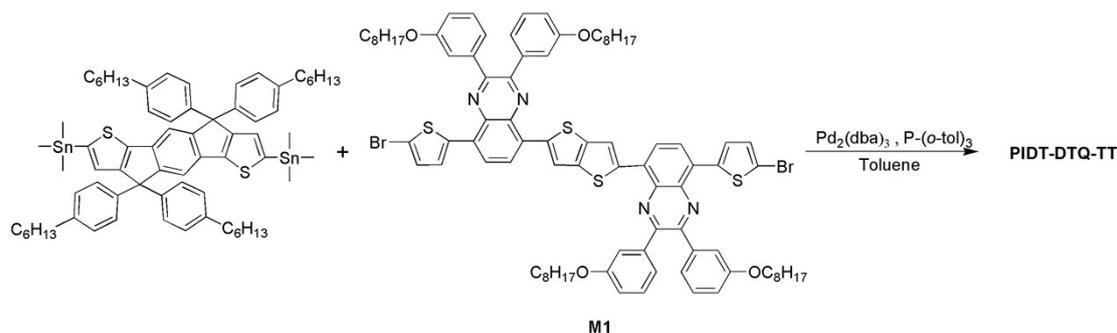
Synthesis of compound 5:

Compound 5 was synthesized according to the synthetic procedure of 3 as a dark red solid with a yield of 56.1%. ^1H NMR (400 MHz, CDCl_3 , TMS, δ_{ppm}): 8.17 (d, $J = 3.1$ Hz, 4H), 8.14 (s, 2H), 7.90 (d, $J = 3.3$ Hz, 2H), 7.52 (d, $J = 5.0$ Hz, 2H), 7.45 (s, 2H), 7.40 (s, 2H), 7.30-7.25 (m, 8H), 7.22-7.17 (m, 2H), 6.99-6.96 (m, 4H), 3.96-3.91 (m, 8H), 1.78-1.71 (m, 8H), 1.45-1.40 (m, 8H), 1.38-1.22 (m, 36H), 0.91-0.82 (m, 8H). MS (MSD, m/z): $\text{C}_{86}\text{H}_{96}\text{N}_4\text{O}_4\text{S}_4$, 1377.97, found, 1377.95.

Synthesis of compound M1:

N-bromosuccinimide (NBS) (89 mg, 0.50 mmol) was added in several portions to a solution of compound 5 (0.30 g, 0.22 mmol) in 90 mL tetrahydrofuran (THF) at 0 °C under N_2 atmosphere and the exclusion of light, then stirred and monitored by TLC. After that 80 mL water was added to quench the reaction and the mixture was extracted with DCM. The combined organic layer was washed with water, dried over anhydrous MgSO_4 . After filtration, the solvent was removed off by distillation and the residue was purified by a silica gel column using hexane and DCM (V/V, 2:1) as the eluent to obtain M1 as a purple solid (0.22 g, 65.1 %). ^1H NMR (400 MHz, CDCl_3 , TMS, δ_{ppm}): 7.99-7.95 (m, 4H), 7.55 (s, 2H), 7.46 (d, $J = 2.8$ Hz, 2H), 7.42 (s, 2H), 7.32-7.28 (m, 8H), 7.24-7.20 (m, 2H), 7.15-7.04 (m, 2H), 7.00-6.97 (m, 2H), 4.05-4.03 (t, $J = 6.2$ Hz, 4H), 3.95-3.93 (t, $J = 6.4$ Hz, 4H), 1.89-1.78 (m, 4H), 1.78-1.66 (m, 4H), 1.37-1.20 (m, 36H), 0.91-0.79 (m, 8H).

MS (MSD, m/z): C₈₆H₉₄Br₂N₄O₄S₄, 1535.76, found, 1536.48. ¹³C NMR (101 MHz, CDCl₃) δ 159.45, 159.08, 151.22, 142.90, 141.20, 139.71, 139.43, 139.37, 136.76, 136.18, 131.20, 129.90, 129.11, 128.83, 126.32, 125.17, 125.02, 123.01, 122.89, 118.75, 117.20, 117.09, 116.82, 115.59, 115.12, 68.38, 68.27, 31.90, 31.86, 29.70, 29.50, 29.45, 29.32, 29.28, 26.26, 26.16, 22.70, 22.65, 14.11, 14.04, 1.01.



Scheme S2: Synthetic routes of polymer

Synthesis of polymer PIDT-DTQ-TT

In a dry 25 mL flask, to a solution of 4,4,9,9-tetrakis(4-hexylphenyl)-4,9-dihydro-indaceno[1,2-*b*:5,6-*b'*]dithiophene-2,7-diylbis(trimethylstannane) (95 mg, 0.077 mmol) and 5-(5-bromothiophen-2-yl)-8-(5-(8-(5-bromothiophen-2-yl)-2,3-bis(3-(octyloxy)phenyl)quinoxalin-5-yl)thieno[3,2-*b*]thiophen-2-yl)-2,3-bis(3-(octyloxy)phenyl)quinoxaline (**M1**) (118.9 mg, 0.077 mmol) in dry toluene (8 mL) was added tris(dibenzylideneacetone)dipalladium(0) [Pd₂(dba)₃] (5.0 mg) and tri(*o*-tolyl)-phosphine [P(*o*-Tol)₃] (10.0 mg) under nitrogen, then stirred vigorously at 100 °C for 5 h. After cooled down to room temperature (RT), the mixture was poured into acetone (100 mL) to form the precipitation. After filtration, the crude product was Soxhlet-extracted successively with methanol, diethyl ether and chloroform each for 12 h. The collected chloroform part was concentrated and precipitated with acetone to

get the dark solid **PIDT-DTQ-TT** (151 mg, 85.1%). ¹H NMR (400 MHz, CDCl₃, TMS, δ_{ppm}): 8.47-8.45 (br, 4H), 8.15-8.13 (br, 2H), 7.46-7.42 (br, 8H), 7.39-7.37 (br, 4H), 7.31-7.25 (br, 12H), 7.12-7.08 (br, 8H), 7.02-6.95 (br, 8H), 4.07-4.03 (br, 4H), 3.97-3.94 (br, 4H), 2.59-2.56 (br, 8H), 1.75-1.71 (br, 8H), 1.31-1.10 (br, 88H), 0.91-0.81 (br, 24H).

NMR and TOFF Spectra

