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Structural Engineering of Pyrrolo[3,4-*f*]benzotriazole-5,7(2*H*,6*H*)-dione-based Polymers for Non-fullerene Organic Solar Cells with an Efficiency over 12%

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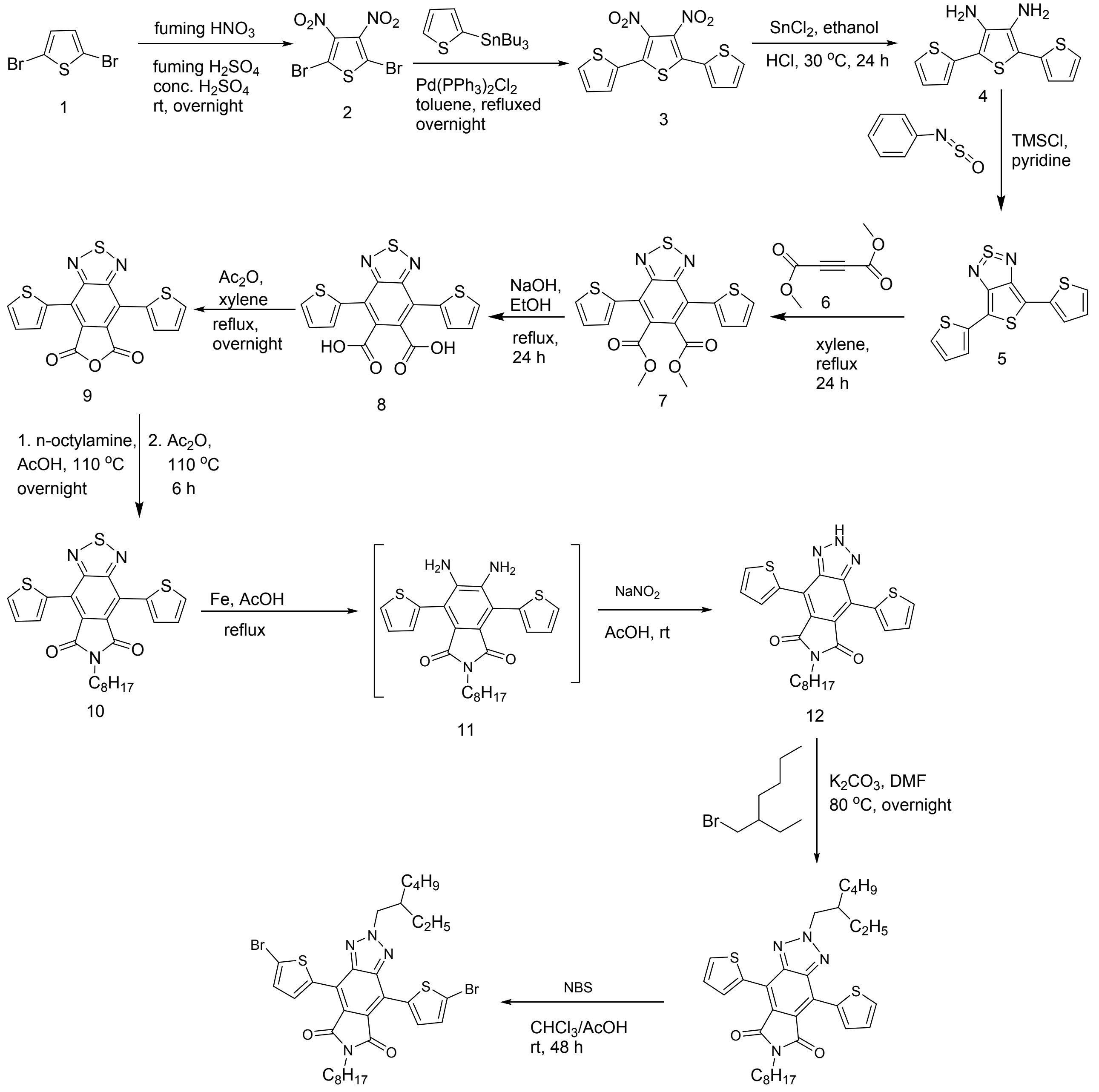
Experimental section

The TzBI-based monomer, 4,8-bis(5-bromothiophen-2-yl)-2-(2-ethylhexyl)-6-octyl-[1,2,3]triazolo[4,5-*f*]isoindole-5,7(2*H*,6*H*)-dione (**1**) was synthesized by modifying procedures reported in the literature.[1] The BDT-based monomers (4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-*b*:4,5-*b′*]dithiophene-2,6-diyl)bis(trimethylstannane) (**2**) and (4,8-bis(5-(2-ethylhexyl)-4-fluorothiophen-2-yl)benzo[1,2-*b*:4,5-*b′*]dithiophene-2,6-diyl)bis(trimethylstannane) (**3**) were purchased from Solarmer Materials and used without purification.

Synthesis of monomer and polymers



Scheme S1. Syntheses route of 4,8-bis(5-bromothiophen-2-yl)-2-(2-ethylhexyl)-6-octyl-[1,2,3]triazolo[4,5-f]isoindole-5,7(2H,6H)-dione(TzBI)

Synthesis of 2,5-dibromo-3,4-dinitrothiophene (2)

2,5-Dibromothiophene (**1**) (22.4 g, 92.7 mmol) was added slowly into an ice cold solution of conc. H_2SO_4 (30 mL), fuming H_2SO_4 (66 mL) and fuming HNO_3 (41 mL) while monitoring the reaction mixture temperature not to exceed 20 ℃. After complete addition, the reaction was allowed to proceed for 20 h at room temperature. After TLC monitoring indicated complete consumption of the reactant, the reaction mixture was slowly poured into ice. The precipitate was filtered and washed with water several times to afford compound 2 (17.4 g, 56.4%) which was a pale yellow powder. ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 140.7 and 113.4.

Synthesis of 2,5-bis(2-thienyl)-3,4-dinitrothiophene (3)

Under nitrogen atmosphere, 2,5-dibromo-3,4-dinitrothiophene (**2**) (14.0 g, 42.2 mmol), Pd $(PPh_3)_2Cl_2$ (0.59 g, 0.84 mmol) and dried toluene (152 mL) were refluxed and 2-tributylstannylthiophene was added drop-wise and allowed to react overnight. After TLC monitoring (1:1 *n*-pentane/toluene) indicated complete consumption of the reactant, the cooled reaction mixture was concentrated via rotary evaporator, and the resulting brown residue was mixed with *n*-pentane, filtered and washed with *n*-pentane several times. The crude solid was further purified on silica gel with chloroform which removed the trace metal impurity. A light brown powder **3** (12.7 g, 88.8 %) was obtained. ^1H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 7.64 (*dd*, $J = 5.2, 1.2$ Hz, 2H), 7.57 (*dd*, $J = 4.0, 1.2$ Hz, 2H), 7.20 (*dd*, $J = 5.2, 4.0$ Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 136.0, 133.9, 131.3, 131.2, 128.4 and 128.1.

Synthesis of 2,5-bis(2-thienyl)-3,4-diaminothiophene (4)

Under nitrogen atmosphere, 2,5-bis(2-thienyl)-3,4-dinitrothiophene (**3**) (12.0 g, 35.5 mmol) was dissolved in a mixture of anhydrous ethanol (120 mL) and concentrated HCl (250 mL). A solution of anhydrous $SnCl_2$ (135 g, 712 mmol) in ethanol (250 mL) was added and stirred at 30 ℃ for 25 h when reaction progress monitoring by TLC (hexane: DCM, 1:1(v/v)) indicated completion of reaction. The reaction mixture was poured into 25% NaOH (860 mL) whose filtrate was extracted with toluene (1,030 mL). The organic layer was dried with Na_2SO_4 and solvent removed with rotary evaporator to give a brown cake (9.62 g, 97 %). ^{1}H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 7.30 (*dd*, *J* = 4.8, 1.2 Hz, 2H), 7.14-7.10 (*unresolved*, 4H), 3.76 (*s*, 4H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 136.0, 133.7, 127.8, 125.4, 124.0 and 123.9.

Synthesis of 4,6-di(2-thienyl)-thiano[3,4-*c*][1,2,5]-thiadiazole (5)

Under nitrogen atmosphere, *N*-thionylaniline (20.5 g, 147 mmol) was added into a stirred solution of 2,5-bis(2-thienyl)-3,4-diaminothiophene (**4**) (9.4 g, 33.8 mmol) and dry pyridine (137 mL). Then TMSCl (27.4 g, 247 mmol) was added dropwise while being cooled with ice-water bath. After 72 h the starting was completely consumed as indicated by TLC in chloroform. The reaction mixture was poured into DCM (1250 mL) and washed with 1 N HCl (860) and washed with water several times. The organic phase was dried in Na_2SO_4 and solvent removed by rotary evaporator. A fluffy royal blue compound (**5**) (10.1 g, 97%) was obtained in good purity. ^{1}H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 7.58 (*dd*, *J* = 3.6, 1.2 Hz, 2H), 7.35 (*dd*, *J* = 5.2, 1.2 Hz, 2H), 7.12 (*dd*, *J* = 5.2, 3.6 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 156.3, 135.0, 128.3, 125.5, 124.3 and 112.4.

Synthesis of dimethyl-4,7-di(2-thienyl)-2,1,3-benzothiadiazole-5,6-dicarboxylate (6)

Under nitrogen atmosphere, dimethyl acetylenedicarboxylate (**5**) (9.25 g, 65.1 mmol) was added slowly into a mixture of *o*-xylene (124 mL) and 4,6-di(2-thienyl)-thiano[3,4-*c*][1,2,5]-thiadiazole (**9**) (9.95 g, 32.4 mmol) and refluxed. TLC monitoring (chloroform) indicated complete consumption of the starting material after 5 h. The reaction mixture was concentrated using rotary evaporator and dried in vacuum oven. The crude brown solid was loaded on silica gel and eluted with chloroform and further purified by recrystallization with ethanol and then with isopropanol to furnish brown crystals (**6**) (10 g, 74.0 %). ^{1}H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 7.62 (*dd*, *J* = 1.2, 5.2 Hz, 2H), 7.45 (*dd*, *J* = 3.6, 1.2 Hz, 2H), 7.22 (*dd*, *J* = 5.2, 3.6 Hz, 2H), 3.79 (*s*, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 168.0, 153.6, 135.0, 132.0, 129.7, 128.9, 127.2, 126.2 and 53.0.

Synthesis of 4,7-di(2-thienyl)-2,1,3-benzothiadiazole-5,6-dicarboxylic acid (7)

Dimethyl-4,7-di(2-thienyl)-2,1,3-benzothiadiazole-5,6-dicarboxylate (**6**) (6.0 g, 14.4 mmol) was suspended in ethanol (250 mL). 20% aqueous NaOH (200 mL) was added drop-wise. After refluxing for 24 h, the reaction content was brought to room temperature and concentrated HCl was added drop-wise until pH was near 1. The reaction was allowed to continue overnight at room temperature and then filtered and washed with water. The dried compound **7** was yellow (4.86 g, 87%). ^{1}H NMR (400.13 MHz, DMSO-d_6) δ(ppm): 7.87 (*dd*, *J* = 3.6, 1.2 Hz, 2H), 7.47 (*dd*, *J* = 5.2, 1.2 Hz, 2H), 7.25 (*dd*, *J* = 5.2, 3.6 Hz, 2H); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ(ppm): 168.9, 153.1, 135.3, 133.6, 130.2, 129.8, 127.7 and 124.3.

Synthesis of 4,7-di(2-thienyl)-2,1,3-benzothiadiazole-5,6-dicarboxylic anhydride (8)

Compound **7** (4.39 g, 11.3 mmol) and acetic anhydride (37.8 g, 370 mmol) were added into xylene (110 mL), and the mixture refluxed for 36 h. After the solvent was removed by rotary evaporator, the crude solid was recrystallized in ethanol which gave red crystals **8** in very poor yield, so the filtrate was dried and combined with the precipitate in the next reaction. ^{1}H NMR (400.13 MHz, DMSO-d_6) δ(ppm): 7.78 (*dd*, 5.2, 1.2 Hz, 2H), 7.46 (*dd*, 3.2, 0.8 Hz, 2H), 7.21 (*dd*, *J* = 4.8, 3.6 Hz, 2H); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ(ppm): 168.9, 153.1, 135.3, 133.7, 130.0, 129.5, 127.5 and 124.3.

Synthesis of *N*-octyl-4,7-di(2-thienyl)-2,1,3-benzothiadiazole-5,6-dicarboxylic imide (9)

Under nitrogen atmosphere, compound **8** (4 g, 10.8 mmol) and glacial acetic acid (180 mL) were refluxed and 1-aminooctane (3.44g, 26.6 mmol) was added drop-wise. After reacting overnight acetic anhydride (80 mL) was added and refluxed overnight. After TLC analysis (chloroform) showed complete consumption of starting material, the solvent was removed via rotary evaporator. The crude solid was extracted with DCM and washed with 1 *M* HCl. The organic phase was dried in Na_2SO_4 and the solvent removed by rotary evaporator. The solid was recrystallized in isopropanol to give orange crystals **9** (4.95g, 95%). ^{1}H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 7.92 (*dd*, *J* = 3.6, 1.2 Hz, 2H), 7.73 (*dd*, *J* = 5.2, 1.2 Hz, 2H), 7.29 (*dd*, *J* = 5.2, 3.6 Hz, 2H), 3.74 (*t*, *J* = 7.2 Hz, 2H), 1.71 (*quin*, 2H), 1.34-1.28 (*unresolved,* 10H), 0.89 (*t*, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 165.8, 156.5, 133.3, 131.6, 130.3, 127.0, 126.9, 126.6, 38.9, 31.8, 29.2, 28.3, 27.0, 22.7, and 14.1.

Synthesis of N-octyl-4,7-di(5-bromo-2-thienyl)-2,1,3-benzothiadiazole-5,6-dicarboxylic imide (10)

Under inert atmosphere, compound **9** (0.9 g, 1.86 mmol) was dissolved in THF (85 mL). *N*-bromosuccinimide (0.66 g, 3.72 mmol) was added in the dark and allowed to react overnight at room temperature. TLC monitoring (petroleum ether/ethyl acetate 15:1 v/v) indicated presence of starting material in which additional NBS was added (0.066 g) in several portions until a total of 3.59 g NBS dibrominated the starting material. The reaction mixture was extracted with DCM and washed with distilled water and brine solution. The organic phase was dried in Na_2SO_4 and the solvent removed by rotary evaporator. The crude solid was passed through silica gel with 1:1 solution of chloroform/petroleum ether. Compound **10** was dark red powder (0.98 g, 82%).

^{1}H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 7.82 (*d*, *J* = 4.0 Hz, 2H), 7.23 (*d*, *J* = 4.0 Hz, 2H), 3.74 (*t*, *J* = 7.2 Hz, 2H), 1.71 (*quin*, 2H), 1.34-1.27 (*unresolved*, 10H), 0.88 (*t*, *J* = 6.8 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 165.6, 155.9, 134.1, 133.1, 129.8, 126.3, 125.9, 118.7, 39.0, 31.8, 29.2, 28.3, 27.0, 22.6 and 14.1.

Synthesis of 4,8-di(thien-2-yl)-1*H*-6-octyl-5*H*-pyrrolo[2,4-*f*]benzotriazole-5,7-(6*H*)-dione (12)

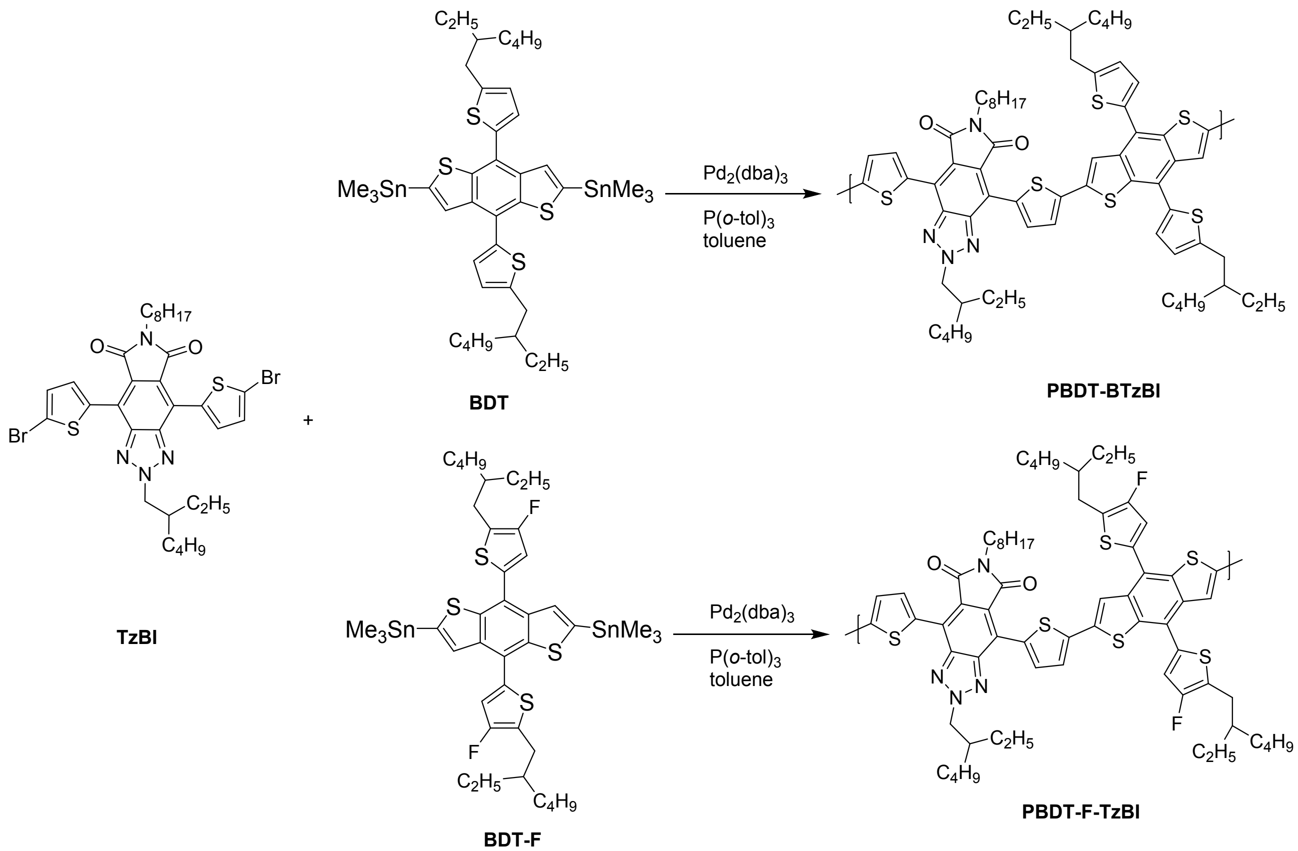
Under nitrogen atmosphere, compound **10** (4 g, 8.30 mmol) and iron powder (15.5 g, 278 mmol) and glacial acetic acid (145 mL) were refluxed overnight. When TLC monitoring (chloroform) indicated consumption of starting material after 24 h, the reaction content was cooled. The reaction content was filtered and washed with chloroform. The filtrate was concentrated to the volume of the acetic acid and the resulting solution containing the intermediate **11** was cooled in an ice bath to which a solution of $NaNO_2$ (3.28 g, 21.2 mmol) in water (30 mL) was added drop-wise. Then the reaction was allowed to continue overnight. When TLC monitoring (chloroform) showed complete reaction of starting material, the reaction content was extracted with DCM and washed with distilled water several times. The organic phase was dried with Na_2SO_4, the solvent removed with rotary evaporator and further dried in vacuum oven. The crude product containing compound **12** was pale yellow with trace colored impurities (3.66 g, 95%).

Synthesis of 2-(2-ethylhexyl)-6-octyl-4,8-di(thiophen-2-yl)[1,2,3]triazolo[4,5-*f*]isoindole-5,7-(2*H*, 6*H*)-dione (13)

Under nitrogen atmosphere, compound **12** (2.0 g, 4.30 mmol), K_2CO_3 (3.33 g, 24.1 mmol) and dry DMF (45 mL) were stirred and heated to 80 °C when 1-bromo-2-ethylhexane was added drop-wise. The reaction continued overnight and TLC analysis (10:1 petroleum ether/ethyl acetate) indicated completion of reaction, so reaction content was cooled and extracted with DCM. The organic phase was dried with Na_2SO_4 and the solvent was removed with rotary evaporator. The crude oily substance was passed through silica gel with 10:1 petroleum ether/ ethyl acetate to give a light orange gummy compound **13** (1.76 g, 71%). ^{1}H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 8.14 (*dd*, *J* = 4.0, 1.2 Hz, 2H), 7.67 (*dd*, *J* = 5.0, 1.2 Hz, 2H), 7.27 (*dd*, *J* = 5.0, 4.0 Hz, 2H), 4.69 (*d*, *J* = 6.8 Hz, 2H), 3.73 (*t*, *J* = 7.6 Hz, 2H), 2.25 (*m*, 1H), 1.71 (*m*, 2H), 1.38-1.28 (*unresolved*, 18H), 1.00 (*t*, *J* = 7.2 Hz, 3H), 0.95-0.87 (*unresolved*, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 166.6, 145.7, 133.0, 132.2, 129.7, 126.8, 125.0, 123.8, 60.3, 40.4, 38.5, 31.8, 30.6, 29.2, 29.2, 28.4, 27.1, 24.0, 23.0, 22.7, 14.1, 14.1 and 10.6

Synthesis of 4,8-bis(5-bromothiophen-2-yl)-2-(2-ethylhexyl)-6-octyl-[1,2,3]triazolo[4,5-f]isoindole-5,7(2*H*,6*H*)-dione (14)

Under nitrogen atmosphere, compound **13** (1.78 g, 3.05 mmol) was dissolved in 1:1 v/v chloroform/acetic acid (70 mL) and chilled in ice water bath in the dark. *N*-bromosuccinimide (1.09 g, 6.10 mmol) was added gradually. The reaction was allowed to proceed overnight at room temperature. A total of 1.45 g of NBS was used to complete the dibromination. The reaction content was extracted with DCM and washed with brine solution. The organic phase was dried with Na_2SO_4 and the solvent removed via rotary evaporator. The crude gummy substance was passed through silica with 12:1 petroleum ether/ethyl acetate and the relatively pure fraction was recrystallized with ethanol to give a leathery bright yellow compound **14** (1.28 g, 57%). %). ^{1}H NMR (400.13 MHz, $CDCl_3$) δ(ppm): 8.04 (*d*, *J* = 4.0 Hz, 2H), 7.21 (*d*, *J* = 4.0 Hz, 2H), 4.70 (*d*, *J* = 6.8 Hz, 2H), 3.71 (*t*, *J* = 7.6 Hz, 2H), 2.23 (*m*, 1H), 1.69 (*quin*, 2H), 1.36-1.27 (*unresolved*, 18H), 1.00 (*t*, *J* = 7.2 Hz, 3H), 0.93 (*t*, *J* = 7.2 Hz, 3H), 0.88 (*t*, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ(ppm): 166.5, 145.2, 134.0, 133.8, 129.8, 123.9, 123.5, 118.0, 60.4, 40.5, 38.6, 31.8, 30.6, 29.2, 28.4, 27.0, 24.0, 23.0, 22.6, 14.1, and 10.6.



Scheme 2. Synthesis of **PBDT-TzBI and PBDT-F-TzBI**

Synthesis of poly-4-(5-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-6-methylbenzo[1,2-*b*:4,5-*b′*]dithiophen-2-yl)thiophen-2-yl)-2-(2-ethylhexyl)-8-(5-methylthiophen-2-yl)-6-octyl-[1,2,3]triazolo[4,5-*f*]isoindole-5,7(2*H*,6*H*)dione (PBDT-TzBI)

4,8-bis(5-bromothiophen-2-yl)-2-(2-ethylhexyl)-6-octyl-[1,2,3]triazolo[4,5-*f*]isoindole-5,7(2*H*,6*H*)-dione **(86)** (147 mg, 0.2 mmol) and (4,8-bis(5-((2-ethylhexyl)thio)thiophen-2-yl)benzo[1,2-*b*:4,5-*b′*]dithiophene-2,6-diyl)bis(trimethylstannane) (**BDT)** (194 mg, 0.2 mmol), $Pd_2(dba)_3$ (3.7 mg, 0.004 mmol) and P(*o*-Tol)$_3$ (4.9 mg, 0.016 mmol) and toluene (10 mL) were added to a 25 mL two-necked round bottomed flask. The reaction flask was purged with nitrogen for 20 min. Then the reactant was heated to reflux for 2 h. Then the polymerization reaction was end cupped by adding 2-bromothiophene followed by 2-tributyl(thiophen-2-yl)stannane in 1 h difference. The reactant was cooled down to room temperature and poured into methanol, filtered through a Soxhlet thimble, and subjected to Soxhlet extraction with methanol, diethyl ether and chloroform. The chloroform fraction was passed through a column of silica gel and precipitated from methanol, dried in the oven at 40 ℃ overnight to yield **PBDT-TzBI**. (M*n* : 26.9 kDa, PDI: 3.8, 170 mg, 68%).

Synthesis of Poly-4-(5-(4,8-bis(5-(2-ethylhexyl)-4-fluorothiophen-2-yl)-6-methylbenzo[1,2-*b*:4,5-*b′*]dithiophen-2-yl)thiophen-2-yl)-2-(2-ethylhexyl)-8-(5-methylthiophen-2-yl)-6-octyl-[1,2,3]triazolo[4,5-f]isoindole-5,7(2*H*,6*H*)-dione (PBDT-F-TzBI)

4,8-Bis(5-bromothiophen-2-yl)-2-(2-ethylhexyl)-6-octyl-[1,2,3]triazolo[4,5-*f*]isoindole-5,7(2*H*,6*H*)-dione (**86)** (147 mg, 0.2 mmol) and (4,8-bis(5-(2-ethylhexyl)-4-fluorothiophen-2-yl)benzo[1,2-*b*:4,5-*b′*]dithiophene-2,6-diyl)bis(trimethylstannane) (**BDT-F**) (188.1 mg, 0.2 mmol), $Pd_2(dba)_3$ (3.7 mg, 0.004 mmol) and P(*o*-Tol)$_3$ (4.9 mg, 0.016 mmol) and toluene (10 mL) were added to a 25 mL two-necked round bottomed flask. The reaction flask was purged with nitrogen for 20 min. Then the reactant was heated to reflux for 2 h. Then the polymerization reaction was end cupped by adding 2-bromothiophene followed by 2-tributyl(thiophen-2-yl)stannane in 1 h difference. The reactant was cooled down to room temperature and poured into methanol, filtered through a Soxhlet thimble, and subjected to Soxhlet extraction with methanol, diethyl ether and chloroform. The chloroform fraction was passed through a column of silica gel and precipitated from methanol, dried in the oven at 40 ℃ overnight to yield **PBDT-F-TzBI**. (M*n*:16.5 kDa, PDI: 4.0, 170 mg, 82%).

TGA measurements

Thermogravimetric analysis (TGA) was carried out on a METTLER TOLEDO thermogravimetric analyzer TGA/DSC 3+, from 50 °C to 550 °C at a heating rate of 10 °C /min under N_2 flow.

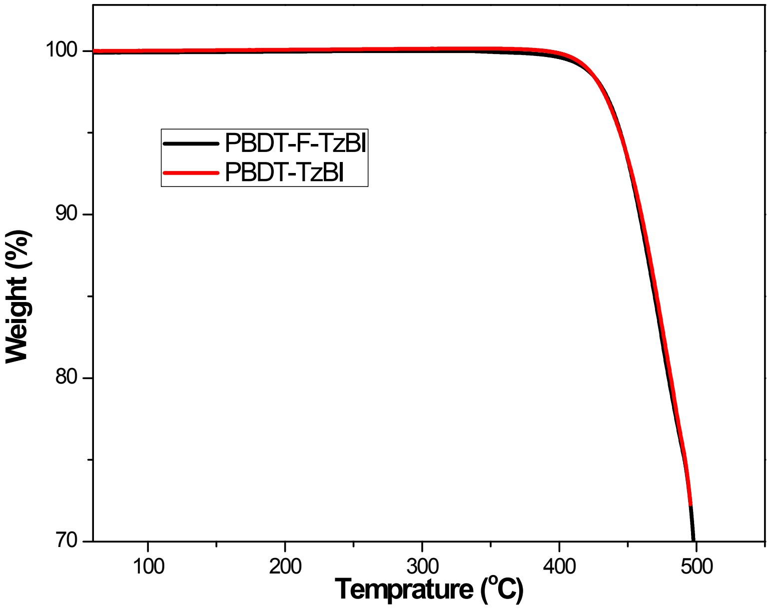


Figure S1. TGA plot of the donor polymers.

Temperature-dependent absorption measurements

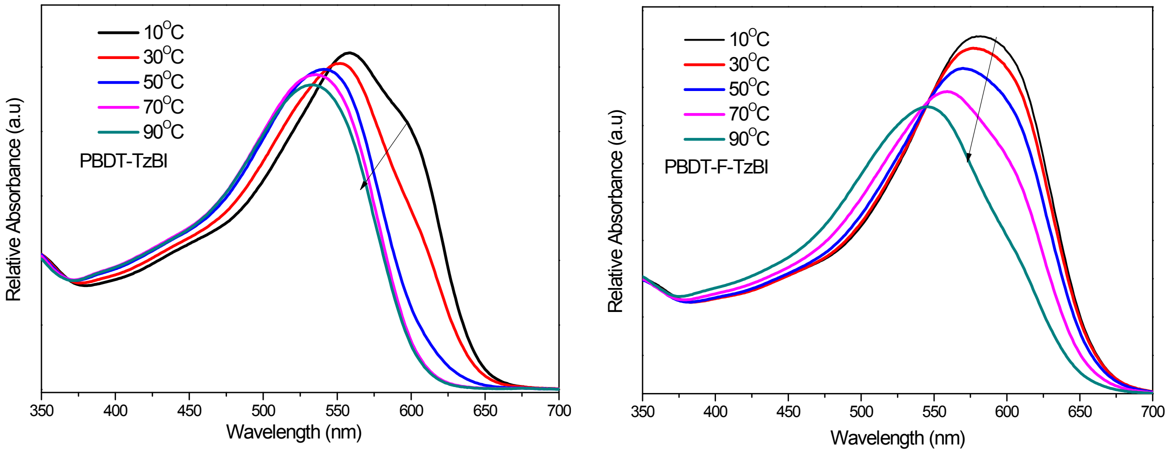


Figure S2. Temperature-dependent absorption spectra of the polymers.

Electrochemical measurements

The HOMO and LUMO levels were estimated from the peak oxidation and reduction potentials of the polymers using SWV by setting the oxidative peak potential of Fc/Fc$^+$ *vs.* the normal hydrogen electrode (NHE) to 0.63 V, and the NHE *vs.* the vacuum level to 4.5 V. The energy levels were calculated according to the formula

$\text{HOMO} = -(E_{\text{ox}} + 5.13)$ eV and $\text{LUMO} = -(E_{\text{red}} + 5.13)$ eV, where the E_{ox} and E_{red} were determined from the oxidation and reduction peaks, respectively.

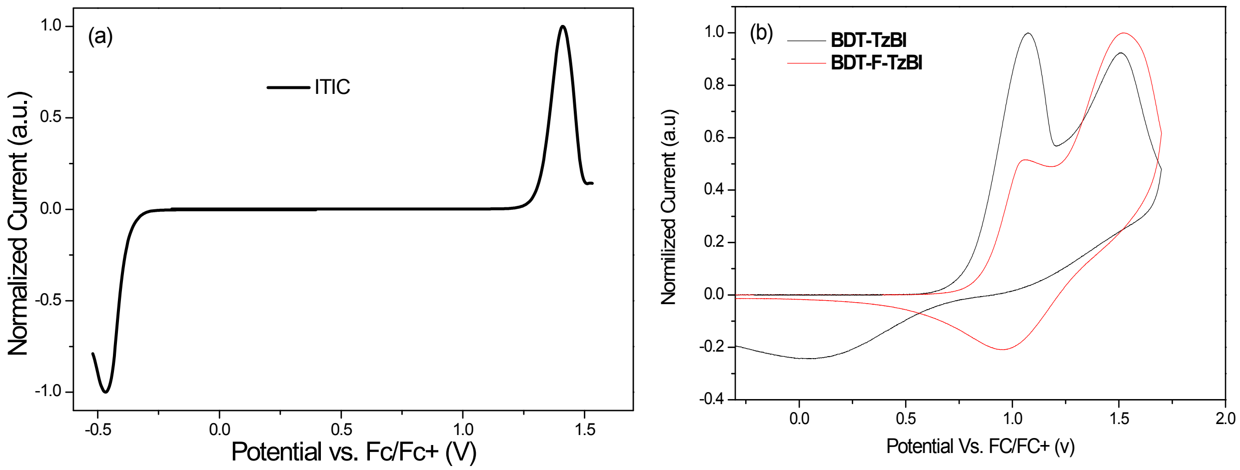


Figure S3. (a) Square wave voltammograms of **ITIC; (**b) Cyclic voltammograms of **PBDT-TzBI** and **PBDT-F-TzBI**.

Instruments and measurements

The binary polymer solar cells (PSCs) were prepared using the conventional device structure of indium tin oxides (ITO) glass/poly(3,4-ethylenedioxythiopene):poly(styrenesulfonate) (PEDOT:PSS)/Donor:Acceptors/perylene diimide functionalized with amino N-oxide (PDINO)/Al. The patterned ITO glass was sequentially cleaned in detergent, deionized water, acetone and isopropanol using the ultrasonic cleaning machine. Each step takes 13 mins. Then the

ITO substrates were treated with oxygen plasma for 6 mins. The plasma treated ITO substrates were spin coated with PEDOT:PSS (Baytron PVP Al 4083) for about 30 nm followed by annealing at 160 ℃ for 20 min. Subsequently, the substrates were transferred to a glove box filled with nitrogen.

The chlorobenzene (CB) solution of donor:acceptor with 1:1 weight ratio was stirred at room temperature overnight before spin coating. The binary solution was spin coated on PEDOT:PSS modified ITO glass to fabricate the active layer (~100 nm) at 1750 rpm for 40 seconds. The PDINO, which serves as the electron transporting layer, were spin coated onto the active layer at 3000 rpm for 30 s. Finally, the samples were transferred to a vacuum chamber, where Al (30 nm) was deposited in high vacuum (4×10^{-4} Pa) via a mask that control the active area of 0.1 cm^2. Over 16 devices were prepared in the same condition. All PSCs were measured under illumination of an AM 1.5G solar light simulator at 100 mW/cm2. The optimal active layer thickness is about 100 nm.

Fabrication and characterization of devices

Current density-voltage (*J-V*) curves of the solar cells were characterized by a Keithley 2420 source meter. A standard silicon solar cell was used to calibrate the light intensity. The external quantum efficiencies (EQEs) of devices were measured using a certified Newport incident photon conversion efficiency (IPCE) measurement system. Atomic force microscopy (AFM) was performed by tapping mode under an argon atmosphere, using an Agilent 5400 instrument. Transmission electron microscopy (TEM) were performed by a HITACHI H-7650 electron microscope at an accelerate voltage of 100 kV.

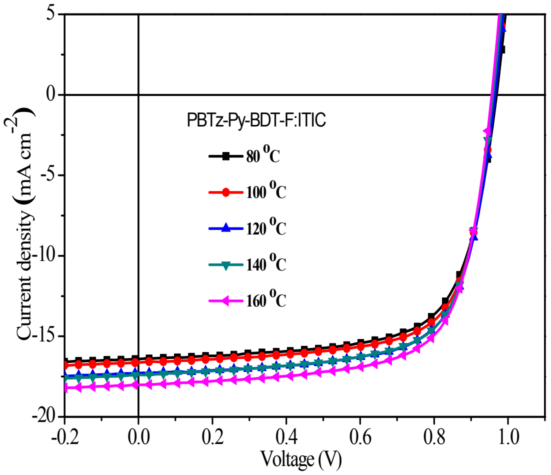
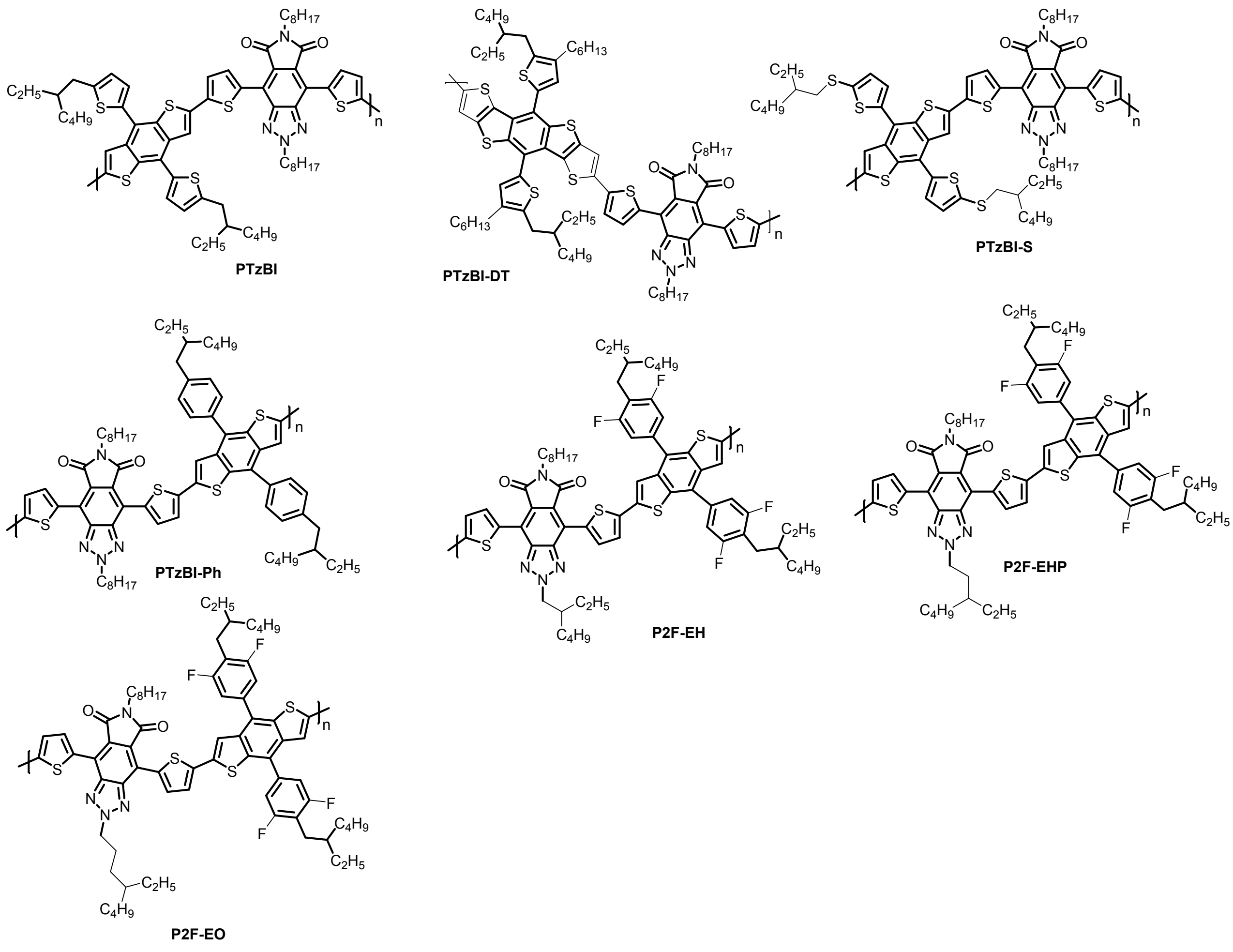


Figure S4. Current density–voltage characteristics of the PBDT-F-TzBI: ITIC upon temperature annealing

Table S1- Photovoltaic properties of TzBI-based polymers with ITIC

Donor:acceptor	V_{oc} /V	J_{sc} /mA/cm^2	FF	PCE /%	Ref
PTzBI :ITIC	0.87	18.29	0.64	10.24	[2]
PTzBI-DT :ITIC	0.91	16.84	0.62	9.43	[2]
PTzBI-S:ITIC	0.92	16.62	0.60	9.12	[3]
PTzBI-Ph:ITIC	0.92	16.39	0.68	10.19	[3]
P2F-EH:ITIC	0.98	12.40	0.51	6.13	[4]
P2F-EHP:ITIC	1.02	13.02	0.55	7.28	[4]
P2F-EO:ITIC	1.01	12.65	0.53	6.73	[4]
P2F-EHP:IT-2F	0.92	19.20	0.69	12.25	[4]
PBDT-TzBI-:ITIC	0.84	17.78	0.69	10.24	This work
PBDT-F-TzBI:ITIC	0.93	18.10	0.72	12.10	This work



Scheme S3. Chemical structure of PTzBI-based polymers

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