# Electronic Supplementary Information

# High Performance Cyano-Substituted Quinoxaline-Based Polymers for Both Fullerene and Nonfullerene Polymer Solar Cells

Shinta Lieviana Handoko, Mijin Jeong, Dong Ryeol Whang, Joo Hyun Kim\* and Dong Wook Chang\*

# 1. Experimental

# 1.1. Materials and instruments

1,2-bis(4-((2-ethylhexyl)oxy)phenyl)ethane-1,2-dione, <sup>[S1]</sup> 5-fluoro-4,7-di(thiophen-2vl)benzo[c][1,2,5]thiadiazole (1),<sup>[S2]</sup> and (4,8-bis(5-(2-ethylhexyl)thiophene-2-yl)benzo[1,2b:4,5-b']dithiophene-2,6-diyl)-bis(trimethylstannane) (5)<sup>[S3]</sup> and (4,8-bis(5-(2-ethylhexyl)-4fluorothiophen-2-yl)benzo-[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(trimethylstannane) (6) were synthesized according to the previously literatures. <sup>[S4]</sup> 2,2'-((2Z,2'Z)-((12,13-bis(2-butyloctyl)-12,13-dihydro-[1,2,5]thiadiazolo[3,4-e]thieno[2",3":4',5']thieno[2',3':4,5]pyrrolo[3,2g]thieno[2',3':4,5]thieno[3,2-b]indole-2,10-diyl)bis(methanylylidene))bis(5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile (Y6BO) was also synthesized according to the previous report.<sup>[S5]</sup> All other chemicals and solvents were purchased from Sigma-Aldrich Co., Inc. <sup>1</sup>H, <sup>13</sup>C, and <sup>19</sup>F nuclear magnetic resonance (NMR) measurements were carried out on JEOL JNM-ECA-600 NMR spectrometer. UV-visible spectra were measured with JASCO V-530 UV-Vis spectrometer. A Bruker Ultraflex spectrometer was used for matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) measurement. Gel Permeation Chromatography (GPC) was performed using Agilent 1200 series instrument with THF as the solvent. Cyclic voltammetry was measured with VersaSTAT3 potentiostat (Princeton Applied Research) with tetrabutylammonium hexafluorophosphate solution (0.1 M) in acetonitrile as the electrolyte. In CV measurement, a glassy carbon electrode coated with the polymers and platinum wire were used as working and counter electrode, respectively. Meanwhile silver wire was used for pseudo-reference electrode with a ferrocene/ferrocenium external standard. Photoluminescence spectra of the polymers and blended films were obtained by a Perkin-Elmer LS-55. The blend morphology was examined by the transmission electron microscope (HITACHI LTD. H-7500). Grazing-incidence wide-angle X-ray scattering (GIWAXS) spectra were obtained on the 3C beamline with 13 keV ( $\lambda = 0.123$  nm) X-ray irradiation source and the beam size of 300 µm (height) × 23 µm (width) in the Pohang Accelerator Laboratory (PAL). A two-dimensional charge-coupled device detector (Mar165 CCD) was used, and the distance from the sample to the detector was 0.2 m. The X-ray beam angle of the incidence was chosen such that the beam would penetrate the entire active layer while minimizing scattering from the substrate: ~ 0.12°. The samples were partially completed devices so that the entire exposed surface is composed of active layer on the Si wafer and were examined under ambient. The scattering vector (q) and d spacing (d) were calculated from the equation:  $q = 4\pi \sin (\phi)/\lambda$  and  $q = 2\pi/d$ .

#### 1.2. Synthesis

4,7-bis(5-bromothiophen-2-yl)benzo[c][1,2,5]thiadiazole-5-carbonitrile (2)

4,7-bis(5-bromothiophen-2-yl)-5-fluorobenzo[c][1,2,5]thiadiazole (1, 0.66 mmol), KCN (0.85 mmol), and 18-crown-6 (0.085 mmol) were added to round bottom flask and dissolved in a mixed solvent of anhydrous THF (20 mL) and DMF (5 mL). The nitrogen was then bubbled through the solution and the mixture was refluxed at 65 °C under N<sub>2</sub> protection for 48 hr. The THF was evaporated under reduced pressure and the residue was dissolved in dichloromethane to be washed using water three times. The ammonia solution was added to the water phase to destroy remaining cyanide, while the organic phase was dried over magnesium sulfate (MgSO<sub>4</sub>) and filtered. The solvents in the solution were then removed using vacuum rotary evaporator. The crude product was further purified by recrystallization using methanol and chloroform.

Yield: 78% (red powder). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ (ppm) = 7.98 (d, 1H, J = 4.02 Hz), 7.96 (s, 1H), 7.83 (d, 1H, J = 4.02 Hz), 7.25 (d, 1H, J = 4.02 Hz), 7.20 (d, 1H, J = 4.02 Hz). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): δ (ppm) = 152.6, 152.5, 138.4, 135.9, 131.3, 131.0, 130.5, 129.7, 128.5, 126.9, 126.1, 119.5, 118.5, 116.8, 108.5. MALDI-TOF MS: m/z calcd, 482.799; found, 482.942[M<sup>+</sup>]



(<sup>1</sup>H NMR spectrum of compound 2)



(<sup>13</sup>C NMR spectrum of compound 2)

5,8-bis(5-bromothiophen-2-yl)-2,3-bis(4-((2-ethylhexyl)oxy)phenyl)-6-fluoroquinoxaline
(3)

4,7-bis(5-bromothiophen-2-yl)-5-fluorobenzo[c][1,2,5]thiadiazole (1, 1 mmol) and zinc powder (20 mmol) were stirred in 30 mL of acetic acid for 6 hr until the color of solution was turned to white. After the reaction was completed, the mixture solution was directly filtered to remove zinc powder, meanwhile 1,2-bis(4-((2-ethylhexyl)oxy)phenyl)ethane-1,2-dione (1 mmol) was added quickly into the filtrate to be continued stirring for overnight at reflux temperature. After cooling down to room temperature, the mixture solution was poured into water and extracted with ethyl acetate. The organic phase was separated and dried over MgSO<sub>4</sub>. After removel of the solvent by vacuum rotary evaporator, the crude product was purified by column chromatography using dichloromethane/hexane (1/7, v/v) as the eluent. Yield = 43% (yellow-orange solid). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.88 (d, 1H, J = 13.56 Hz), 7.77 (d, 1H, J = 3.54 Hz), 7.68 (dd, 4H, J = 11.10, 8.58 Hz), 7.55 (d, 1H, J = 4.02 Hz), 7.16 (d, 1H, 2 J = 4.02 Hz), 7.14 (d, 1H, J = 4.02 Hz), 6.94 (dd, 4H, J = 8.58, 3.00 Hz), 3.93-3.89 (m, 4H), 1.78-1.74 (m, 2H), 1.53-1.39 (m, 8H), 1.35-1.33 (m, 8H), 0.97-0.91 (m, 12H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 160.3, 160.2, 159.1, 157.4, 151.7, 150.4, 137.9, 137.2, 137.1, 133.5, 133.1, 132.0, 131.8, 130.4, 130.3, 130.1, 130.0, 129.9, 129.8, 128.8, 128.7, 125.5, 118.1, 117.5, 115.6, 115.5, 114.6, 114.4, 114.1, 70.5, 39.4, 30.4, 29.1, 23.8, 23.1, 14.1, 11.2. MALDI-TOF MS: m/z calcd, 878.793; found, 879.308 [M<sup>+</sup>].



(<sup>1</sup>H NMR spectrum of compound 3)



(<sup>13</sup>C NMR spectrum of compound 3)

5,8-bis(5-bromothiophen-2-yl)-2,3-bis(4-((2-ethylhexyl)oxy)phenyl)quinoxaline-6carbonitrile (4)

A procedure similar to that used to prepare **3** was used to produce **4**. 4,7-bis(5-bromothiophen-2-yl)benzo[c][1,2,5]thiadiazole-5-carbonitrile (**2**, 0.42 mmol) and 1,2-bis(4-((2-ethylhexyl)oxy)phenyl)ethane-1,2-dione (0.42 mmol) were used as the reactant. The ratio

of eluent for column chromatography was dichloromethane/hexane (1/7, v/v). Yield = 73% (orange solid). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ (ppm) 8.22 (s, 1H), 7.87 (d, 1H, *J* = 4.02 Hz), 7.72 (d, 2H, *J* = 8.58 Hz), 7.66 (d, 2H, *J* = 8.58 Hz), 7.58 (d, 1H, *J* = 4.02 Hz), 7.21 (d, 1H, *J* = 4.02 Hz), 7.17 (d, 1H, *J* = 4.08 Hz), 6.96-6.92 (m, 4H), 3.92-3.89 (m, 4H), 1.78-1.73 (m, 2H), 1.52-1.40 (m, 8H), 1.35-1.33 (m, 8H), 0.97-0.91 (m, 12H). <sup>13</sup>C NMR (150 MHz, CDCl<sub>3</sub>): 161.0, 160.8, 153.3, 152.8, 137.3, 137.2, 136.4, 135.3, 133.7, 132.0, 131.9, 130.7, 130.2, 129.6, 129.5, 129.2, 129.1, 127.8, 126.1, 120.0, 119.2, 118.5, 114.4, 114.3, 108.5, 70.6, 70.5, 39.3, 30.5, 29.1, 23.8, 23.0, 14.1, 11.1. MALDI-TOF MS: m/z calcd 885.818 ; found, 886.189 [M<sup>+</sup>].



(<sup>1</sup>H NMR spectrum of compound 4)



 $(^{13}C NMR \text{ spectrum of compound 4})$ 

Synthesis of D-A type polymers by Stille coupling reaction

In a Schlenk flask, the selected BDT monomer (**5** or **6**) and dibrominated-DPQ monomer (**3** or **4**) and Pd(PPh<sub>3</sub>)<sub>4</sub> (3% mol) were mixed together in dry toluene. After nitrogen bubbling for 15 min, the solution was stirred at 90°C with nitrogen protection for 48 days. The polymerization was ended by adding two end-capping agents of 2-trimethylstannylthiophene and 2-bromothiophene at 2 hr interval. After that, the polymer solution was precipitated in methanol, and the the polymer solid was collected by filtration. Soxhlet extraction using methanol, acetone, hexane and chloroform was consecutively carried out to purify the polymer. The chloroform fraction was dried under vaccuum at 50°C.

#### PTB-FQx

4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6diyl)bis(trimethylstannane) (**5**, 0.2 mmol) and dibrominated-DPQ monomer (**3**, 0.2 mmol) were used as the reactant. Yield: 92% (deep blue solid). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 8.04-7.45 (br, 7H), 7.45-7.35 (br, 2H), 7.22-7.01 (br, 4H), 7.01-6.60 (6H), 4.31-3.78 (br, 4H), 3.20-2.80 (br, 4H), 2.27-1.99 (br, 4H), 1.52-1.40 (br, 16H), 1.40-1.25 (br, 16H), 1.10-0.90 (br. 24H). Molecular weight by GPC: number-average molecular weight (M<sub>n</sub>) = 38.40 KDa, polydispersity index (PDI) = 3.90. Elemental analysis: calcd (%) for C<sub>78</sub>H<sub>87</sub>FN<sub>2</sub>O<sub>2</sub>S<sub>6</sub> : C 72.29, H 6.77, N 2.16, S 14.85; found: C 71.83, H 6.61, N 2.07, S 13.14.



(<sup>1</sup>H NMR spectrum of PTB-FQx)



(<sup>13</sup>C NMR spectrum of PTB-FQx)

#### PTB-CNQx

4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-

diyl)bis(trimethylstannane) (**5**, 0.2 mmol) and dibrominated-DPQ monomer (**4**, 0.2 mmol) were used as the reactant. Yield = 88% (deep green solid). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.91-7.56 (br, 7H), 7.44-7.30 (br, 2H), 7.14-7.02 (br, 4H), 6.98-6.78 (br, 6H), 4.26-3.65 (br, 4H), 3.15-2.74 (br, 4H), 1.89-1.79 (br, 4H), 1.45-1.36 (br, 16H), 1.32-1.18 (br, 16H), 1.01-0.87 (br, 24H). Molecular weight by GPC: number-average molecular weight (M<sub>n</sub>) = 59.89 KDa, polydispersity index (PDI) = 3.02. Elemental analysis: calcd (%) for C<sub>79</sub>H<sub>87</sub>N<sub>3</sub>O<sub>2</sub>S<sub>6</sub> : C 72.82, H 6.73, N 3.23, S 14.77; found: C 72.19, H 6.82, N 2.91, S 14.97.



(<sup>1</sup>H NMR spectrum of PTB-CNQx)



<sup>(&</sup>lt;sup>13</sup>C NMR spectrum of PTB-CNQx)

# PTBF-CNQx

(4,8-bis(5-(2-ethylhexyl)-4-fluorothiophen-2-yl)benzo-[1,2-b:4,5-b']dithiophene-2,6diyl)bis(trimethylstannane) (**6**, 0.17 mol) and dibrominated-DPQ monomer (**4**, 0.17 mmol) were used as the reactant. The polymer was also dissolved in chlorobenzene fraction. Yield = 84% (deep green solid). <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  (ppm) = 7.90-7.83 (br, 3H), 7.81-7.71 (br, 3H), 7.47-7.35 (br, 6H), 6.98-6.88 (br, 5H), 4.03-3.82 (br, 4H), 3.00-2.78 (br, 4H), 1.51-1.45 (br, 9H), 1.45-1.35 (br, 19H), 1.09-0.91 (br, 32H).. Molecular weight by GPC: number-average molecular weight (Mn) = 26.07 KDa, polydispersity index (PDI) = 3.20 Elemental analysis: calcd (%) for C<sub>79</sub>H<sub>85</sub>F<sub>2</sub>N<sub>3</sub>O<sub>2</sub>S<sub>6</sub> : C 70.76, H 6.54, N 3.13, S 14.35; found: C 69.64, H 6.66, N 3.09, S 15.61.



(<sup>1</sup>H NMR spectrum of PTBF-CNQx)



(<sup>13</sup>C NMR spectrum of PTB-CNQx)

# 2. Fabrication and analysis of PSCs

To fabricate inverted type PSCs with configuration of indium tin oxide (ITO)/ZnO/active layer(polymer:acceptor)/MoO<sub>3</sub>/Ag, a ZnO film, 25-nm-thick, was initially deposited on an ITO surface by the a sol-gel process. The partially crystalline ZnO film was prepared by thermal

curing of pre-deposited ZnO precursors at 200 °C for 10 min. The solution of ZnO precursors was prepared by dissolving zinc acetate dehydrate (0.164g) and ethanolamine (0.05 mL) in methoxyethanol (1 mL) and stirring the mixture for 30 min prior to film deposition. The active layer was fabricated using a chlorobenzene (with 3.0 vol.% of 1,8-diiodooctane as a processing addirtive) solution of the polymeric donor and PC<sub>71</sub>BM acceptor by spin-coating. Prior to spin-coating, the blended solution was filtered through a 0.2  $\mu$ m polytetrafluoroethylene membrane filter. Finally, a MoO<sub>3</sub> layer, 20-nm-thick, and Ag layer, 100-nm-thick, were consecutively deposited by thermal evaporation at 2 × 10<sup>-6</sup> Torr through a shadow mask with a device area of 0.09 cm<sup>2</sup>. The *J-V* characteristics of the device were analyzed using a KEITHLEY Model 2400 source-measure unit under AM 1.5G illumination at 100 mW/cm<sup>2</sup> from a 150 W xenon lamp. The conditions of solar simulation were calibrated prior to the measurements by using a silicon reference cell with a KG5 filter certified by the National Institute of Advanced Industrial Science and Technology.

#### 3. Fabrication of hole- and electron-only devices

Hole-only devices with the structure: [ITO/polymer: Y6BO (or  $PC_{71}BM$ )/Au (50 nm)] and electron-only devices with the structure: [ITO/ZnO (25 nm)/polymer: Y6BO (or  $PC_{71}BM$ )/Al (50 nm)], have been fabricated to investigate the hole and electron mobility.



**Scheme S1**. Synthesis of monomers and polymers (i) KCN, 18-crown-6, THF/DMF (4/1), 65 °C; (ii) zinc, acetic acid, 80 °C and then 1,2-bis(4-((2-ethylhexyl)oxy)phenyl)ethane-1,2-dione, acetic acid, reflux; (iii) Pd(PPh<sub>3</sub>)<sub>4</sub>, toluene, 90 °C, 48 h.



Figure S1. TGA thermograms of PTB-FQx, PTB-CNQx, and PTBF-CNQx



Figure S2. UV-Vis specta of PTB-FQx, PTB-CNQx, and PTBF-CNQx in film



Figure S3. CV curves of PTB-FQx, PTB-CNQx, and PTBF-CNQx



**Figure S4**. Optimized geometries and frontier molecular orbitals of two-repeating unit with theoretical HOMO/LUMO energy levels at the B3LYP/6-31G<sup>\*\*</sup> level for (a) **PTB-FQx**, (b) **PTB-CNQx**, and (c) **PTBF-CNQx** 



Figure S5. PL spectra of the polymers and their blend films with Y6BO acceptor.



**Figure S6**. *J-V* curves of (a) hole- and (b) electron-only devices based on the polymers and  $PC_{71}BM$ , and *J-V* curves cureves cureves of (c) hole- and (d) electron-only devices absed on the polymers and Y6BO. (inset: current density vs. voltage – built-in voltage ( $V_{bi}$ ) curves with fitted lines).



**Figure S7**. Light intensity dependence of  $J_{SC}$  for the PSCs with (a) PC<sub>71</sub>BM and (b) Y6BO.



**Figure S8**. (a) GIWAX image of pristine Y6BO film and (b) the corresponding line-cuts in the in-plane and out-of-plane direction.



**Figure S9**. TEM images of the active layers based on (a) ~ (c) the polymers:PC<sub>71</sub>BM and (d) ~ (f) polymers:Y6BO blend films.



Figure S10. IQE spectra of the devices.



Figure S11. Temperature dependant absortion spectra of dilute polymer solution in chloroebnzene.

Polymer	$\lambda_{edge}(nm)^{a}$ $E_{gap}^{opt}(eV)^{b}$	$\lambda_{max}^{film} (nm)^c$	Absorption Coefficent (cm <sup>-1</sup> ) <sup>d</sup>	HOMO <sup>e</sup> /LUMO <sup>f</sup> (eV)
PTB-FQx	719 1.72	(429, 619)	6.23 x 10 <sup>4</sup> at 619 nm	-5.18/-3.46
PTB-CNQx	753 1.65	(443, 642)	6.73 x 10 <sup>4</sup> at 642 nm	-5.33/-3.68
PTBF- CNOx	743 1.67	(441, 618)	7.32 x 10 <sup>4</sup> at 618 nm	-5.48/-3.81

**Table S1**. Summary of optical and electrochemical properties of **PTB-FQx**, **PTB-CNQx**, and**PTBF-CNQx** 

<sup>a</sup>Absorption edge. <sup>b</sup>Estimated from the absorption edge. <sup>c</sup>Maximum absorption wavelength of the polymer film. <sup>d</sup>Absorption coefficient of the polymer film. <sup>e</sup>Estimated from the oxidation onset potential in CV curve. <sup>f</sup>Calculated from the HOMO and the optical band gap.

Polymer	Thickness (nm)	Blend ratio <sup>a</sup>	Solvent (additive) <sup>b</sup>	$J_{\rm sc}$ (mA/cm <sup>2</sup> )	$V_{\rm oc}$ (V)	<i>FF</i> (%)	PCE
PTR-	 PTR-		CB	14.2	0 70	57.0	5 67
FOx	75	3:5	(3% DIO)	(14.1)	(0.70)	(56.8)	(5.58)
Тұл	100	3:5	CB	16.1	0.83	56.5	7 56
			(3% DIO)	(16.1)	(0.83)	(56.3)	(7.50)
	50	3:5	CB	15.8	0.83	<u>    (30.3)</u> 60.8	7.92
			(3% DIO)	(15.7)	(0.83)	(60.0)	(7.82)
PTR-	75	3:5	CB	16.6	0.82	55.6	7.56
CNOx			(2%  DIO)	(16.4)	(0.81)	(54.6)	(7.28)
UT QA		3:5		15.5	0.82	63.3	8.04
	75		(3% DIO)	(15.2)	(0.82)	(62.5)	(7.79)
		3:5	CB	15.9	0.82	57.8	7.52
	75		(4% DIO)	(15.7)	(0.82)	(57.7)	(7.42)
		3:4	CB	15.3	0.91	60.8	8 4 5
	75		(3%  DPS)	(15.2)	(0.91)	(59.0)	(8.20)
		2.4	CB	15.0	0.92	57.2	7.87
	15	3:4	(3% DPE)	(14.9)	(0.91)	(57.0)	(7.75)
		3:4	CB	15.8	0.91	59.5	8.54
	/5		(3% CNDPE)	(15.7)	(0.91)	(58.0)	(8.31)
		3:4	СВ	14.8	0.91	56.7	7.63
	/5		(3% DIO)	(14.7)	(0.91)	(55.9)	(7.47)
	100	3:4	СВ	15.2	0.91	58.9	8.15
	100		(3% DIO)	(15.1)	(0.91)	(58.2)	(8.04)
	50	3:4	СВ	15.0	0.89	58.0	7.75
			(3% DIO)	(14.9)	(0.88)	(57.5)	(7.58)
PTBF-	75	3:4	CB	8.91	0.94	43.3	3.59
CNQx			(0% DIO)	(8.77)	(0.94)	(43.3)	(3.55)
	75	3:4	CB	15.6	0.91	60.6	8.57
			(2% DIO)	(15.5)	(0.90)	(59.9)	(8.40)
	75	3:4	CB	14.6	0.91	63.9	8.47
			(4% DIO)	(14.5)	(0.91)	(63.8)	(8.41)
	75	3:3	CB	15.2	0.78	46.1	5.45
			(3% DIO)	(15.1)	(0.73)	(44.4)	(4.89)
	75	3:3.5	CB	14.7	0.92	64.5	8.67
			(3% DIO)	(14.6)	(0.91)	(63.5)	(8.48)
	75	3:4	СВ	16.0	0.91	63.6	9.24
			(3% DIO)	(15.9)	(0.91)	(62.3)	(9.02)
	75	3:5	CB	15.1	0.88	59.0	7.77
			(3% DIO)	(14.9)	(0.88)	(58.7)	(7.68)

**Table S2**. The best photovoltaic parameters of the PSCs based on  $PC_{71}BM$ . The average (10 devices are averaged) values for the photovoltaic parameters of each device are also provided in parentheses

<sup>a</sup>Mass ratio of polymer donor to PC<sub>71</sub>BM. <sup>b</sup> DIO: 1,8-diiodooctane, DPS: diphenylsulphane,

DPE: diphenyl ether, and CNDPE: 4-phenoxybenzonitrile.

Donor	Thickness (nm)	Blend ratio <sup>a,b</sup>	$J_{\rm sc}$ (mA/cm <sup>2</sup> )	$V_{\rm oc}$	FF (%)	PCE (%)
PTB- FQx	(IIII)	10110	12.4	0.66	35.5	2.9
	110	3:2	(12.3)	(0.65)	(35.5)	(2.8)
			21.9	0.62	38.3	53
	110	3:3	(21.6)	(0.61)	(37.9)	(5.1)
	90	3:3	23.8	0.63	48.1	7.2
			(23.5)	(0.62)	(45.7)	(6.8)
	85	3:3	23.5	0.63	50.2	7.4
			(22.9)	(0.62)	(49.4)	(7.1)
	70	3:3	23.2	0.63	48.9	7.1
			(23.0)	(0.62)	(46.9)	(6.8)
	110	2.2	12.4	0.66	35.7	2.9
	110	5.5	(12.3)	(0.65)	(35.5)	(2.87)
	110	3.4	20.7	0.61	39.6	5.0
-	110	J. <del>T</del>	(20.6)	(0.61)	(39.4)	(4.9)
	110	3.5	16.9	0.61	40.0	4.1
	110	5.5	(16.40)	(0.61)	(39.8)	(3.9)
	80	3.2	18.5	0.78	47.5	6.9
-		3.2	(18.2)	(0.78)	(46.8)	(6.6)
	90	3:3	25.6	0.76	57.2	11.2
DTD			(25.5)	(0.76)	(55.9)	(10.8)
PIB-	85	3:3	25.4 (25.2)	0.77	60.0 (50.6)	(11.6)
CNQX	70	3:3	(25.2)	(0.77)	<u>(59.0)</u> 50.0	10.6
-			(22.9)	(0.77)	(58.3)	(10.3)
	85	3:4	28.0	0.76	54.8	11.6
			(27.6)	(0.76)	(53.5)	(11.2)
	70	3:2	20.0	0.85	56.1	9.6
			(19.5)	(0.85)	(55.2)	(9.1)
	120	3:3	29.8	0.82	54.5	13.3
PTBF- CNQx			(29.6)	(0.82)	(53.8)	(13.1)
	105	3:3	28.9	0.83	57.6	13.8
			(29.2)	(0.82)	(56.1)	(13.4)
	<b>90</b> 80	<b>3:3</b> 3:3	27.6	0.83	61.2	14.0
			(27.4)	(0.83)	(61.0)	(13.9)
			26.0	0.82	61.6	13.1
	70	3:3	(23.3)	(0.82)	(01.0)	(12.8)
			23.9 (25.8)	(0.82)	(50.0)	12.9
	70	3:4	23.0)	0.81	62.0	12.7)
			(24.2)	(0.81)	(61.6)	(12.1)

**Table S3**. The best photovoltaic parameters of the PSCs based on Y6BO. The average (10 devices are averaged) values for the photovoltaic parameters of each device are also provided in parentheses

<sup>a</sup>Mass ratio of polymer donor to Y6BO. <sup>b</sup> 3% DIO was added as a processing additive.

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