Optimize Sequence Structure by Stepwise-Feeding Terpolymerization for High-Performance Organic Solar Cells

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Experimental Procedures

General Information

All reactions and manipulations were operated under argon atmosphere and all the starting materials were purchased from commercial suppliers and used without further purification. Chloroform, Chlorobenzene, Ag (99.999%), MoO_3 (99.999%), and other materials were purchased from Alfa, Aldrich (used without further purification). Indium-tin oxide (ITO) glass was purchased from Delta Technologies Limited, whereas PEDOT:PSS (Baytron PAl4083) was obtained from Bayer Inc. F-BDT, BDD, and DTBT were purchased from SunaTech Inc. $Pd_2(dba)_3$ and $P(o\text{-Tol})_3$ were obtained from J&K.

Nuclear magnetic resonance (NMR) and gel permeation chromatography (GPC) measurement

^{1}H NMR spectra of the polymers were recorded on a Bruker AVANCE III HD 400 MHz spectrometer using deuterated $CDCl_3$ as solvent and tetramethylsilane (TMS) as an internal standard. The average number (M_n) and weight (M_w) molecular weight and PDI of the copolymer products were determined by Waters 2410 gel permeation chromatography (GPC) at 150 °C using 1,2,4-trichlorobenzene as an eluent.

Optical characterizations

UV-vis absorption spectra were recorded on a Perkin Elmer Lambda 750 spectrophotometer. All film samples were spin-cast on quartz slice substrates. Solution UV-*vis* absorption spectra at elevated temperatures also were collected on a Perkin Elmer Lambda 750 Spectrophotometer.

Electrochemical characterizations.

Cyclic voltammetry (CV) was performed by a Zahner IM6e electrochemical work station, using Ag/AgCl as the reference electrode, a Pt plate as the counter electrode, and a glassy carbon as the working electrode. Polymers were drop-cast onto the electrode from chloroform solutions to form thin films. 0.1 mol L^{-1} tetrabutylammonium hexafluorophosphate in anhydrous acetonitrile was used as the

supporting electrolyte. The scan rate was 0.05 V s^{-1}. The E_{HOMO} and E_{LUMO} are calculated as referring to the equation (1) and (2).

$$E_{HOMO} = -(E_{ox} + 4.4) \text{ eV (1)},$$

$$E_{LUMO} = -(E_{red} + 4.4) \text{ eV (2)}.$$

AFM characterizations.

The specimen for AFM measurements was prepared using the same procedures those for fabricating devices but without PDINN/Ag on top of the active layer.

GIWAXS measurement

The GIWAXS measurement was carried out at the PLS-II 6A U-SAXS beamline of the Pohang Accelerator Laboratory in Korea. The X-rays coming from the in-vacuum undulator (IVU) were monochromatic (wavelength λ=1.10994 Å) using a double crystal monochromator and focused both horizontally and vertically (450 (H) x 60 (V) um^2 in FWHM @ the sample position) using K-B type mirrors. The grazing incidence wide-angle X-ray scattering (GIWAXS) sample stage was equipped with a 7-axis motorized stage for the fine alignment of the sample, and the incidence angles of the X-ray beam were set to be 0.11°-0.13° for the neat and blend films. The GIWAXS patterns were recorded with a 2D CCD detector (Rayo nix SX165) and an X-ray irradiation time within 100 s, dependent on the saturation level of the detector. Diffraction angles were calibrated using a sucrose standard (monoclinic, P21, a=10.8631Å, b=8.7044Å, c=7.7624Å, and b=102.938Å) and the sample-to-detector distance was ~231 mm.

Device Fabrication and Characterizations

The device was fabricated with a structure of ITO/PEDOT:PSS (40 nm)/active layer/PDINN/Ag. A thin layer of PEDOT:PSS was deposited through spin-coating on precleaned ITO-coated glass from a PEDOT: PSS aqueous solution (Baytron PVP AI 4083 from H. C. Starck) at 2,000 rpm and dried subsequently at 150 C for 15 min in air, the device was transferred to a nitrogen glove box. The device processing conditions were optimized via tuning the total concentration, altering the D/A ratio, and changing the content of the solvent additive. The champion device was fabricated from the total

concentration of 13.2 mg ml^{-1} with the D/A ratio was 1:1.2 (w/w) in chloroform and a trace amount of 1-chloronaphthalene (CN) (0.5%, v/v) as solvent additive without thermal annealing and solvent vapor annealing. Subsequently, methanol solution of PDINN at a concentration of 1.0 mg ml^{-1} was deposited atop the active layer at 3,000 r.p.m. for 30 s to afford a PDINN cathode buffer layer with a thickness of about 10 nm. Finally, the top Ag electrode was deposited over the active layer by thermal evaporation under a vacuum chamber to accomplish the device fabrication. The effective area of one cell was 0.04 cm2. The current-voltage (*J-V*) characteristics were measured by a Keithley 2400 Source Meter under simulated solar light (100 mW/cm2, AM 1.5 G, Abet Solar Simulator Sun2000). The external quantum efficiency (EQE) spectra were detected on an EQE measuring system (Oriel Cornerstone 2601/4 m monochromator equipped with Oriel 70613NS QTH lamp). All the measurements were performed at room temperature under ambient atmosphere.

EQEEL measurements

EQEEL of the solar cells were determined by using a digital source meter (Keithley 2400), to inject electric current into the solar cells, and a picoammeters (Keithley 6482) collected to a Si diode, to measure emitted photons from the solar cells.

EL spectra

EL spectra of OSCs were measured by using a source meter (Keithley 2400) to inject electric current into the OSCs, and emitted photons were collected by an optical fiber and recorded by a fluorescence spectrometer (KYMERA-3281-B2, Andor), a Si EMCCD camera (DU970P-BVF, Andor), and an InGaAs camera (DU491A-1.7, Andor).

PL spectra

PL spectra of the active layers were measured with a laser (SuperK EXU-6, NKT photonics) and narrowband filters (LLTF Contrast SR-VIS-HP8, NKT photonics) as the light source. The excitation wavelength was 480 nm. Photons emitted from the thin

films were collected and recorded by the same setup used for the EL spectra measurements.

Transient photocurrent vs voltage curves

Transient photocurrent vs voltage curves of the solar cells were measured using a green LED. The V_{oc} of the solar cell under the LED illumination is close to that under the simulated AM1.5G illumination. An oscilloscope (MDO4104C, Tektronix) was used to record the transient photocurrent signals. A Keithley 2400 is used to apply voltage to the solar cell. The impact of series resistance in the electrodes of the solar cells is minimized using a "4-point" method: the sensing of the voltage applied to the active layer of the solar cell is done via connecting an additional set of anode and cathode terminals to a voltmeter.

Results and Discussion

Synthetic procedures

One-pot polymerization   D18 (x=0), H6 (x=0.1), H7 (x=0.2)
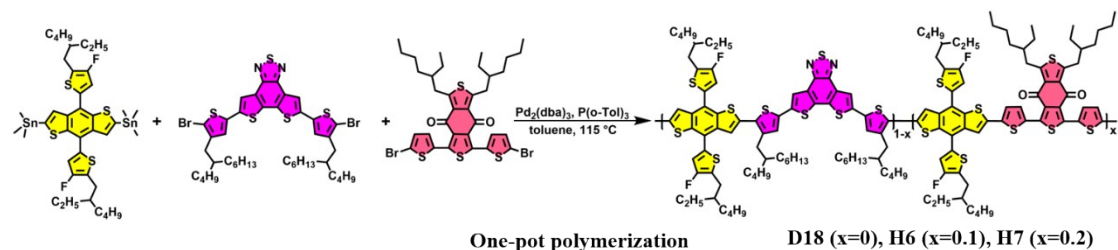
(1). copolymer D18 was synthesized as follows:

The F-BDT is 0.047g mmol (0.050 mmol), DTBT is 0.045g (0.050 mmol) and dry toluene (4 ml) were added to a 20 ml double-neck round-bottom flask. The reaction container was purged with argon for 20 min, then $Pd_2(dba)_3$ 0.00091g (0.01 mmol) and $P(o\text{-}Tol)_3$ 0.00091g (0.03 mmol) were added. After another flushing with argon for 20 min, the reactant was heated under 115 °C to reflux for 6.0h. The reactant was cooled down to room temperature and poured into methanol (50 ml), then purified by Soxhlet extraction with hexane, acetone, and chlorobenzene in sequence. The obtained D18 (yield 76%) was recovered as solid from the chlorobenzene fraction by precipitation

from methanol, and dried under vacuum 24h. Elemental analysis calculated for D18: C, 67.39; H, 7.11; S, 20.76; N:2.02. Found: C, 67.38; H, 7.06; S, 20.88; N:2.00.

(2). terpolymer H6 was synthesized as follows:

The F-BDT is 0.047g (0.050 mmol), DTBT is 0.041g (0.045 mmol), BDD is 0.0038g (0.005 mmol) and dry toluene (4 ml) were added to a 20 ml double-neck round-bottom flask. The reaction container was purged with argon for 20 min, then $Pd_2(dba)_3$ 0.00091g (0.01 mmol) and $P(o\text{-}Tol)_3$ 0.00091g (0.03 mmol) were added. After another flushing with argon for 20 min, the reactant was heated under 115 °C to reflux for 6.0h. The reactant was cooled down to room temperature and poured into methanol (50 ml), then purified by Soxhlet extraction with hexane, acetone, and chlorobenzene in sequence. The obtained terpolymer H6 (yield 75%) was recovered as solid from the chlorobenzene fraction by precipitation from methanol, and dried under vacuum 24h. Elemental analysis calculated for H6: C, 67.36; H, 7.11; S, 17.39; N:2.34 O, 0.26. Found: C, 67.28; H, 7.14; O, 0.24; S, 17.50; N:2.17.

(3). terpolymer H7 was synthesized as follows:

The synthetic method is same as terpolymer H6, except the concentration of monomers with F-BDT is 0.047g (0.050 mmol), DTBT is 0.036g (0.040 mmol), BDD is 0.0077g (0.010 mmol) and dry toluene (4 ml). Elemental analysis calculated for H7: C, 67.44; H, 7.16; O, 0.42; S, 18.17; N:1.65. Found: C, 67.42; H, 7.18; O, 0.43; S, 17.76; N:1.66.

(4). terpolymer H8 was synthesized as follows:
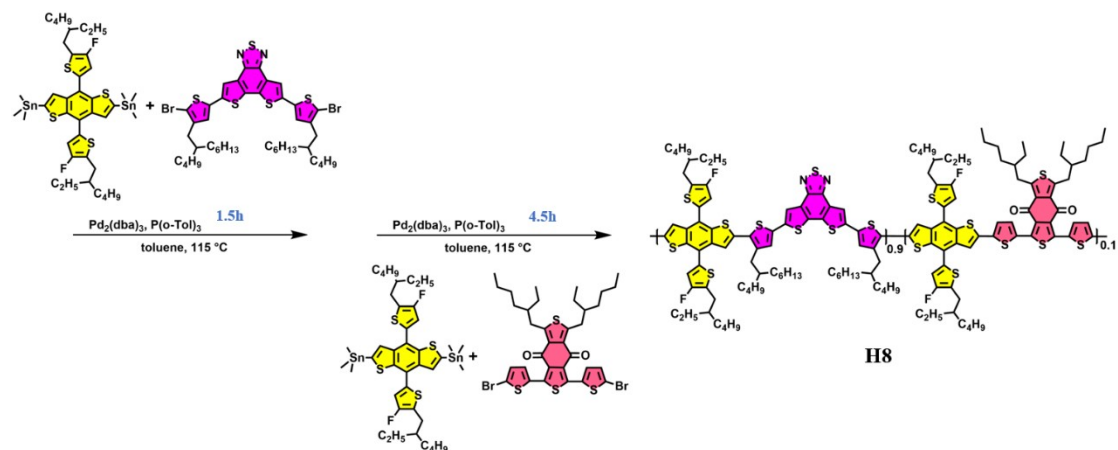
The F-BDT is 0.042g (0.045 mmol), DTBT is 0.041g (0.045) mmol and dry toluene (3.6 ml) were added to a 20 ml double-neck round-bottom flask. The reaction container was purged with argon for 20 min, then Pd$_2$(dba)$_3$ 0.00091g (0.01 mmol) and P(o-Tol)$_3$ 0.00091g (0.03 mmol) were added. After another flushing with argon for 20 min, the reactant was heated under 115 °C to reflux for 1.5h. Then the solution based on F-BDT 0.0047g (0.005 mmol) and BDD 0.0038mg (0.005 mmol) in dry toluene (0.4 ml) were injected by syringe quickly. Continue polymerization under argon atmosphere for another 4.5h. The reactant was cooled down to room temperature and poured into methanol (50 ml), purified by Soxhlet extraction with hexane, acetone, and chlorobenzene in sequence. The obtained terpolymer H8 (yield 70%) was recovered as solid from the chlorobenzene fraction by precipitation from methanol, and dried under vacuum 24h. Elemental analysis calculated for H8: C, 67.36; H, 7.11; S, 17.39; N:2.34 O, 0.26. Found: C, 67.30; H, 7.10; O, 0.25; S, 17.40; N:2.24.
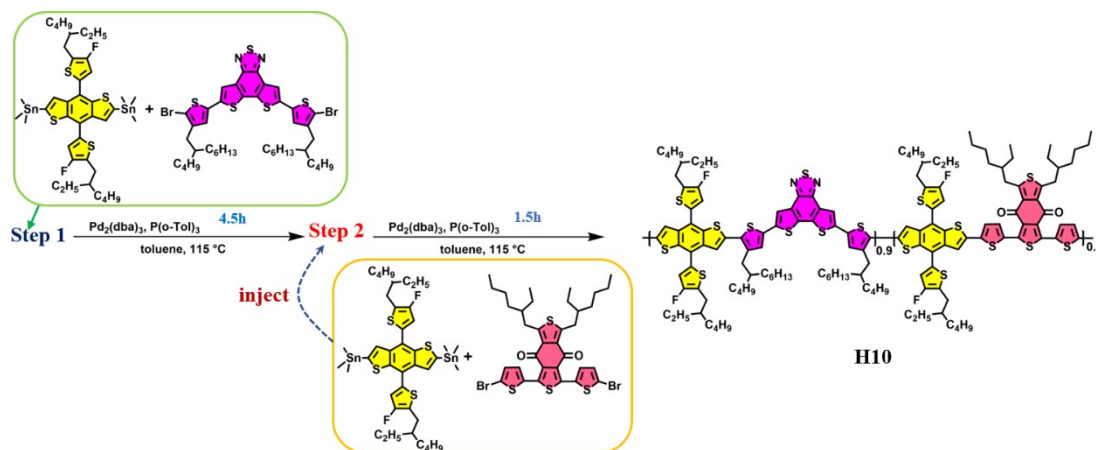
**(5). terpolymer H9 was synthesized as follows:**
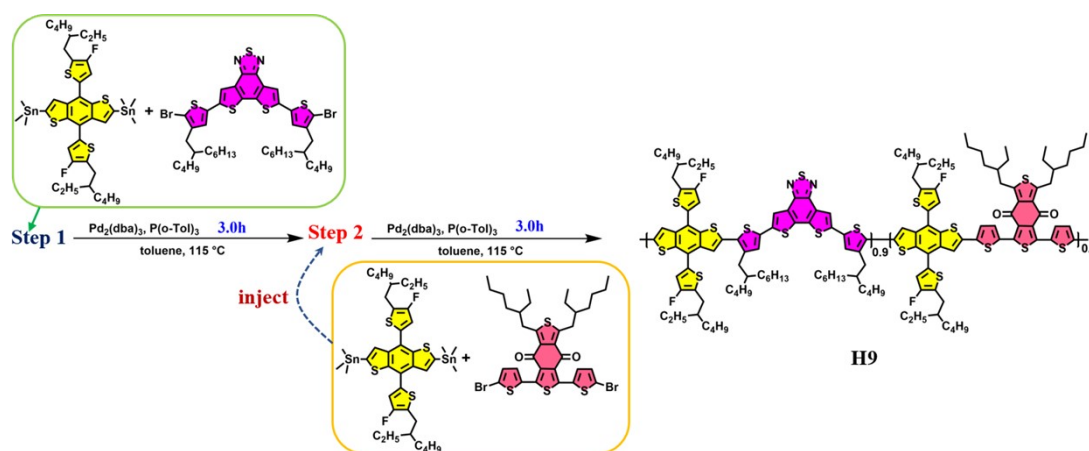
The F-BDT is 0.042g (0.045 mmol), DTBT is 0.041g (0.045) mmol and dry toluene (3.6 ml) were added to a 20 ml double-neck round-bottom flask. The reaction container was purged with argon for 20 min, then Pd$_2$(dba)$_3$ 0.00091g (0.01 mmol) and P(o-Tol)$_3$ 0.00091g (0.03 mmol) were added. After another flushing with argon for 20 min, the reactant was heated under 115 °C to reflux for 3.0h. Then the solution based on F-BDT 0.0047g (0.005 mmol) and BDD 0.0038mg (0.005 mmol) in dry toluene (0.4 ml) were injected by syringe quickly. Continue polymerization under argon atmosphere for another 3.0h. The reactant was cooled down to room temperature and poured into

methanol (50 ml), purified by Soxhlet extraction with hexane, acetone, and chlorobenzene in sequence. The obtained terpolymer H9 (yield 70%) was recovered as solid from the chlorobenzene fraction by precipitation from methanol, and dried under vacuum 24h. Elemental analysis calculated for H9: C, 67.36; H, 7.11; S, 17.39; N:2.34 O, 0.26. Found: C, 67.28; H, 7.06; O, 0.26; S, 17.42; N:2.36.

(6). terpolymer H10 was synthesized as follows:

H10

The F-BDT is 0.042g (0.045 mmol), DTBT is 0.041g (0.045) mmol and dry toluene (3.6 ml) were added to a 20 ml double-neck round-bottom flask. The reaction container was purged with argon for 20 min, then $Pd_2(dba)_3$ 0.00091g (0.01 mmol) and $P(o\text{-Tol})_3$ 0.00091g (0.03 mmol) were added. After another flushing with argon for 20 min, the reactant was heated under 115 °C to reflux for 4.5h. Then the solution based on F-BDT 0.0047g (0.005 mmol) and BDD 0.0038mg (0.005 mmol) in dry toluene (0.4 ml) were injected by syringe quickly. Continue polymerization under argon atmosphere for another 1.5h. The reactant was cooled down to room temperature and poured into methanol (50 ml), purified by Soxhlet extraction with hexane, acetone, and chlorobenzene in sequence. The obtained terpolymer H10 (yield 65%) was recovered as solid from the chlorobenzene fraction by precipitation from methanol, and dried under vacuum 24h. Elemental analysis calculated for H10: C, 67.04; H, 6.64; O, 0.11; S, 21.00; N:0.97. Found: C, 66.98; H, 7.16; S, 19.03; N:2.39, O, 0.26.

Distribution Plots
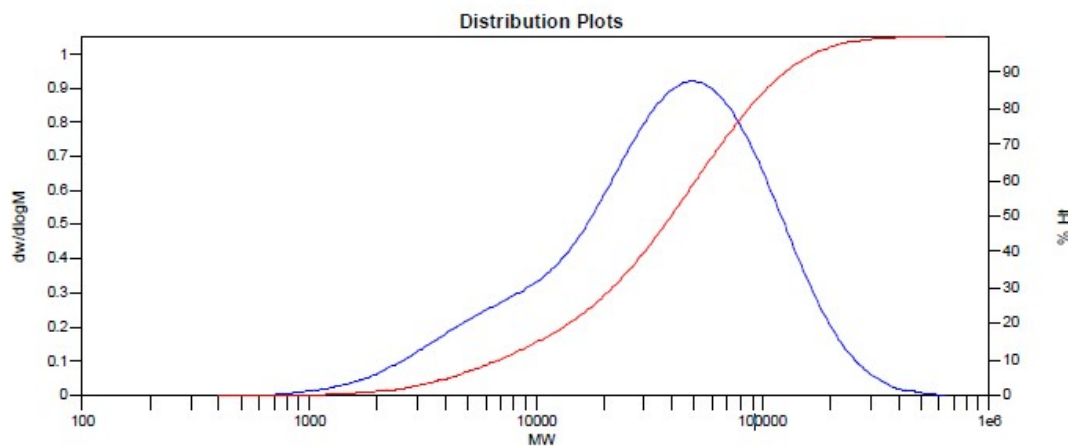
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	49362	16763	55578	111726	177593	48867	3.31552

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		12.15	13.93	17.30	-43.177	100	4530.77	100

Figure S1. GPC spectra of H8-based prepolymer.

Distribution Plots
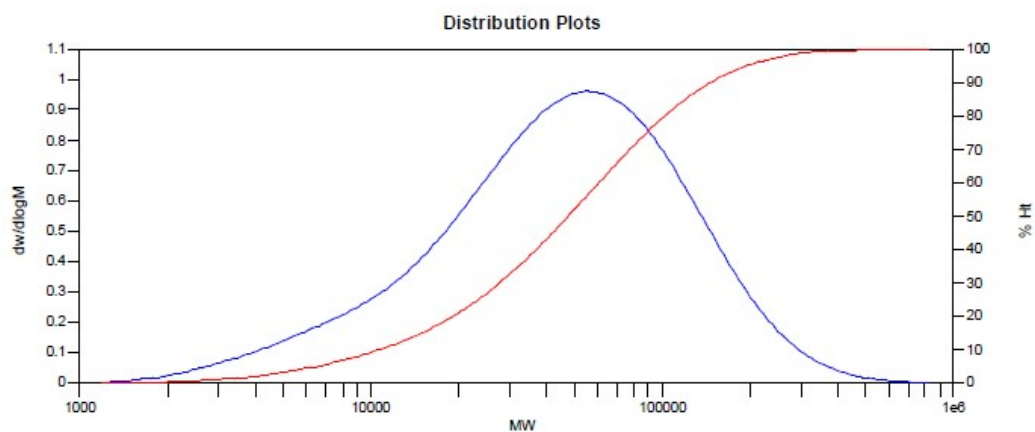
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	55619	23975	66552	131042	212860	59083	2.77589

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.97	13.85	16.53	-61.8494	100	6216.15	100

Figure S2. GPC spectra of H9-based prepolymer.

Distribution Plots
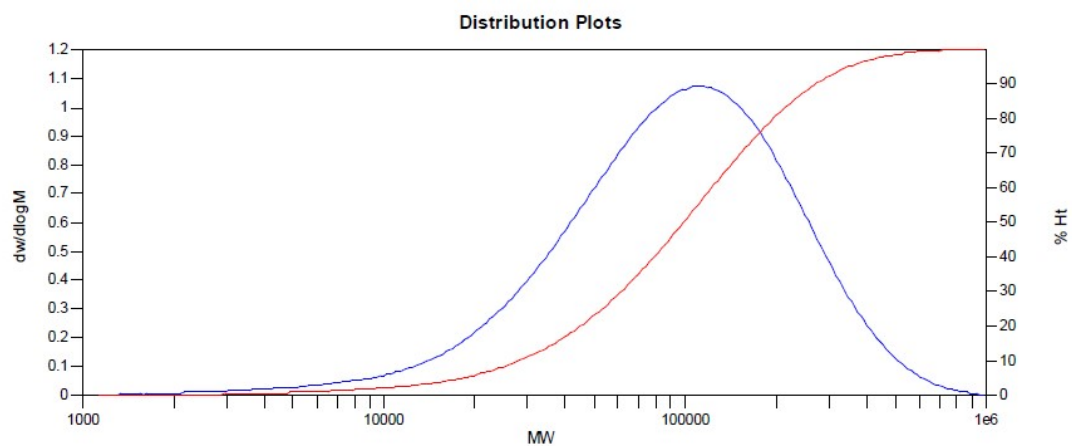
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	113811	54017	128008	219324	320022	116472	2.36977

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.85	13.35	16.57	-70.088	100	6302.45	100

Figure S3. GPC spectra of H10-based prepolymer.
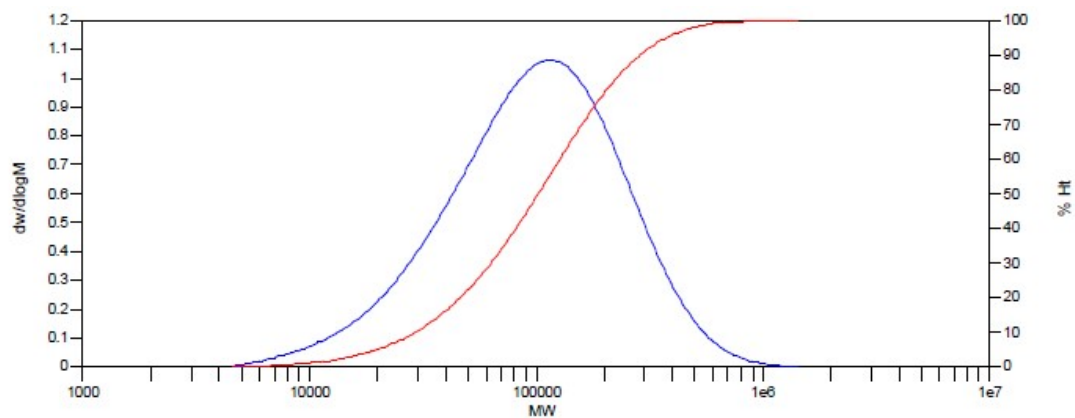
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	116560	62445	135590	242229	373604	122862	2.17135

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.58	13.35	15.60	-58.5995	100	5315.21	100

Figure S4. GPC spectra of D18.

Distribution Plots
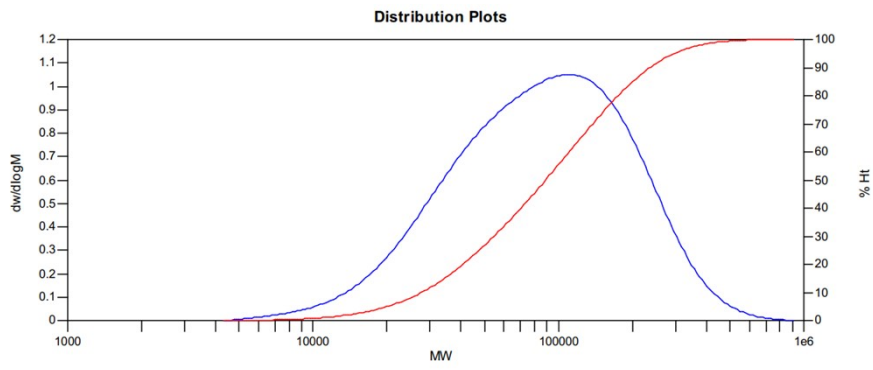
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	108506	57674	113319	187270	267675	103881	1.96482

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.90	13.38	15.63	-87.1867	100	8002.63	100

Figure S5. GPC spectra of H6.
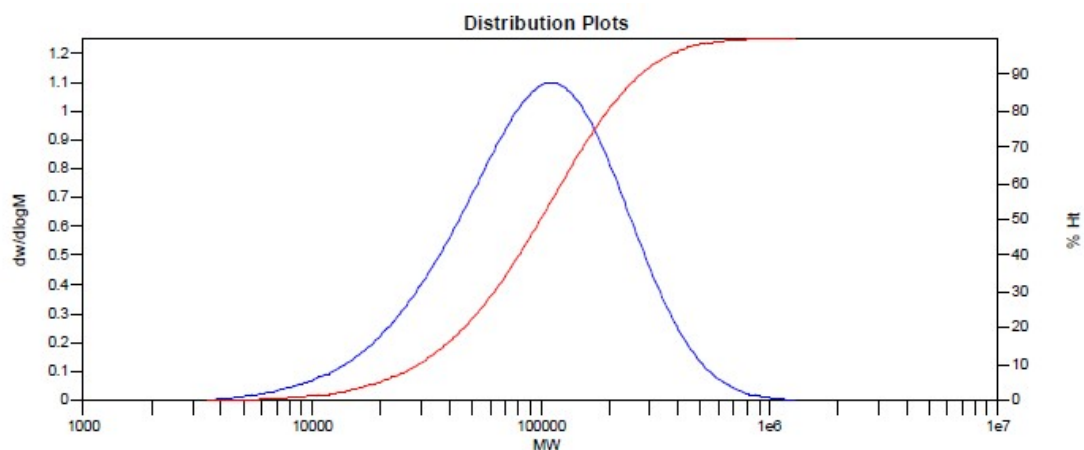
MW Averages

Peak No	Mp	Mn	Mw	Mz	Mz+1	Mv	PD
1	111126	60976	130503	229224	352056	118652	2.14024

Processed Peaks

Peak No	Name	Start RT (mins)	Max RT (mins)	End RT (mins)	Pk Height (mV)	% Height	Area (mV.secs)	% Area
1		11.65	13.37	15.78	-71.8362	100	6325.91	100

Figure S6. GPC spectra of H7.

Calibration Used: 12/11/2020 PM 7:50:17
Calibration Type: Narrow Standard   Curve Fit Used: 3
Calibration Curve: y = 22.873131 - 2.678058x^1 + 0.140444x^2 - 0.003113x^3

High Limit MW RT: 10.55 mins   Low Limit MW RT: 15.63 mins
High Limit MW: 3947531   Low Limit MW: 2740
K: 14.1000   FRM Name:
Alpha: 0.7000   Flow Marker RT: 0.00 mins
FRCF: 1.0000

MW Averages
Mp: 137403   Mn: 64310   Mv: 119642   Mw: 131341
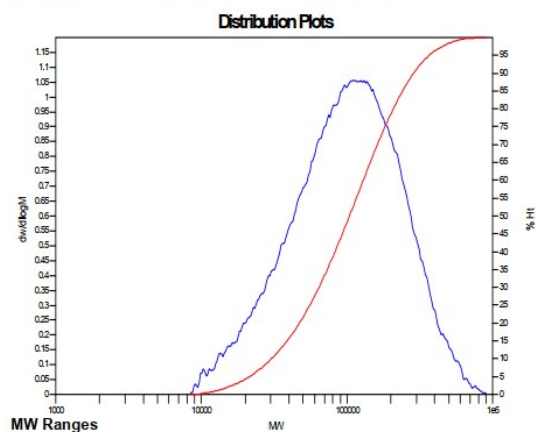Mz: 224752   Mz+1: 325346   PD: 2.0423

Figure S7. GPC spectra of H8.

Calibration Used: 12/11/2020 PM 7:50:17
Calibration Type: Narrow Standard   Curve Fit Used: 3
Calibration Curve: y = 22.873131 - 2.678058x^1 + 0.140444x^2 - 0.003113x^3

High Limit MW RT: 10.55 mins   Low Limit MW RT: 15.63 mins
High Limit MW: 3947531   Low Limit MW: 2740
K: 14.1000   FRM Name:
Alpha: 0.7000   Flow Marker RT: 0.00 mins
FRCF: 1.0000
MW Averages
Mp: 111157   Mn: 65578   Mv: 117325   Mw: 128954
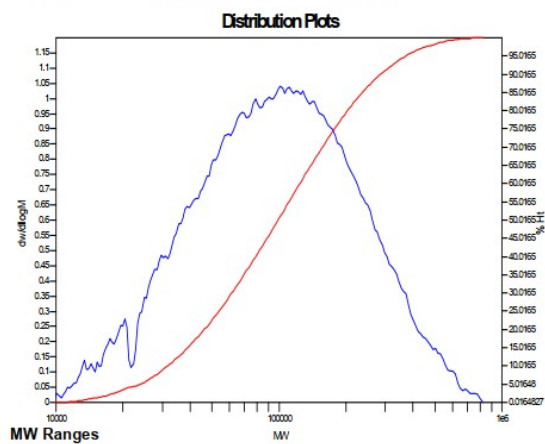Mz: 224500   Mz+1: 328225   PD: 1.9664

Figure S8. GPC spectra of H9.

Calibration Used: 12/11/2020 PM 7:50:17
Calibration Type: Narrow Standard   Curve Fit Used: 3
Calibration Curve: y = 22.873131 - 2.678058x^1 + 0.140444x^2 - 0.003113x^3

High Limit MW RT: 10.55 mins   Low Limit MW RT: 15.63 mins
High Limit MW: 3947531   Low Limit MW: 2740
K: 14.1000   FRM Name:
Alpha: 0.7000   Flow Marker RT: 0.00 mins
FRCF: 1.0000
MW Averages
Mp: 154725   Mn: 74434   Mv: 150896   Mw: 168713
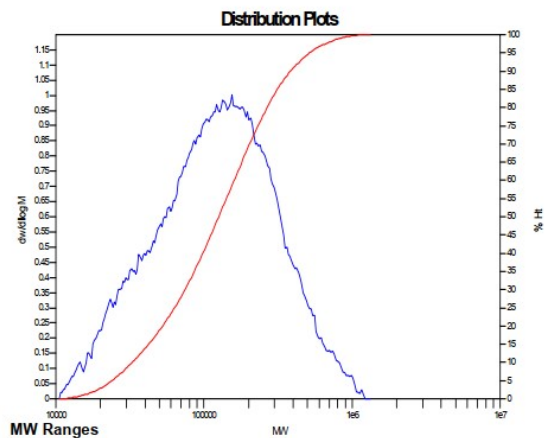Mz: 321248   Mz+1: 493947   PD: 2.2666

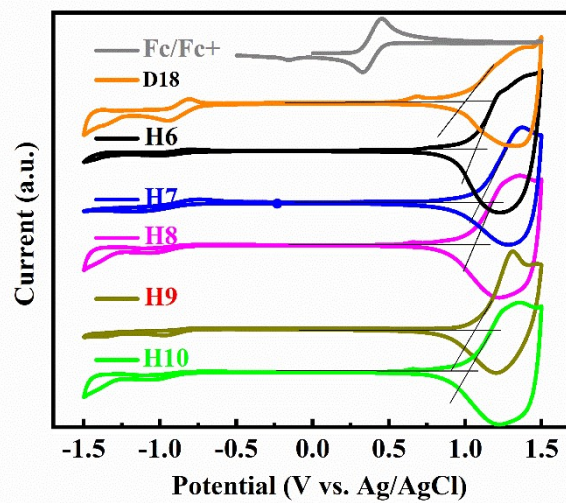**Figure S9**. GPC spectra of H10.

Figure S10. Cyclic voltammetry (CV) measurement of the related thin films (ferrocene/ferrocenium (Fc/Fc$^+$) couple used as an internal reference).

| | HOMO | LUMO | Top view | Side view |

BDD — HOMO: -5.43 eV, LUMO: -2.21 eV, Top view: 0.79636

DTBT — HOMO: -5.16 eV, LUMO: -2.32 eV, Top view: -0.02399
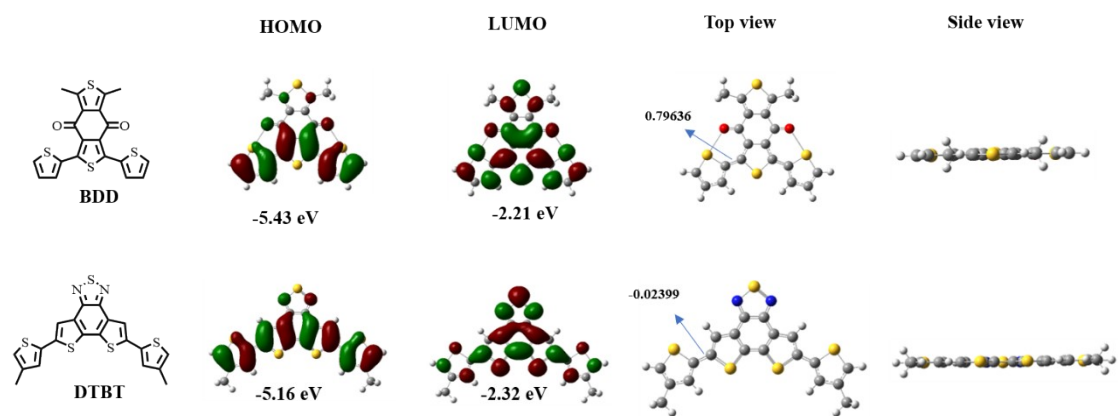
Figure S11. Density functional theory (DFT) calculations of BDD and DTBT.

	HOMO	LUMO
F-BD+BDD		
FBDT+DTBT		
F-BDT+BDD+DTBT		

Figure S12. Density functional theory (DFT) calculations of the related polymers.

Figure S13. (a) $J^{0.5}$-V plots of hole-only devices with active layer. (b) $J^{0.5}$-V plots of electron-only devices with active layer.
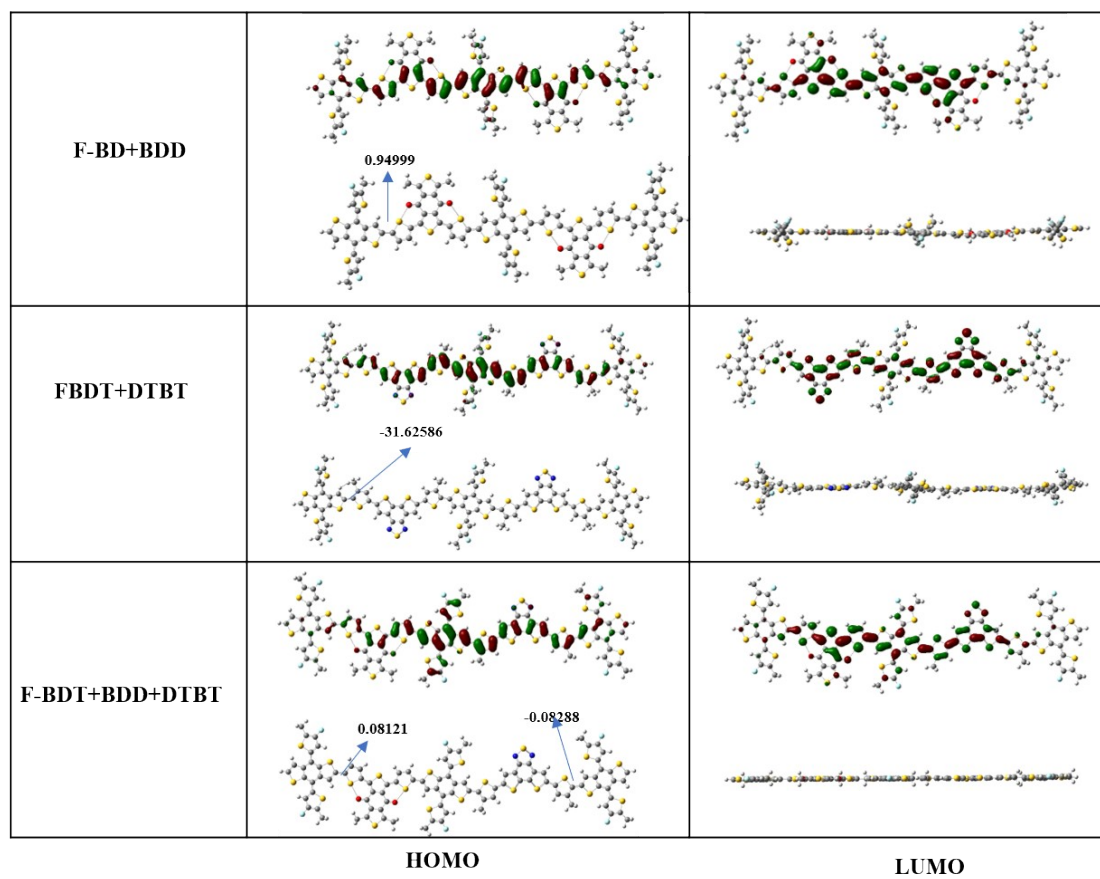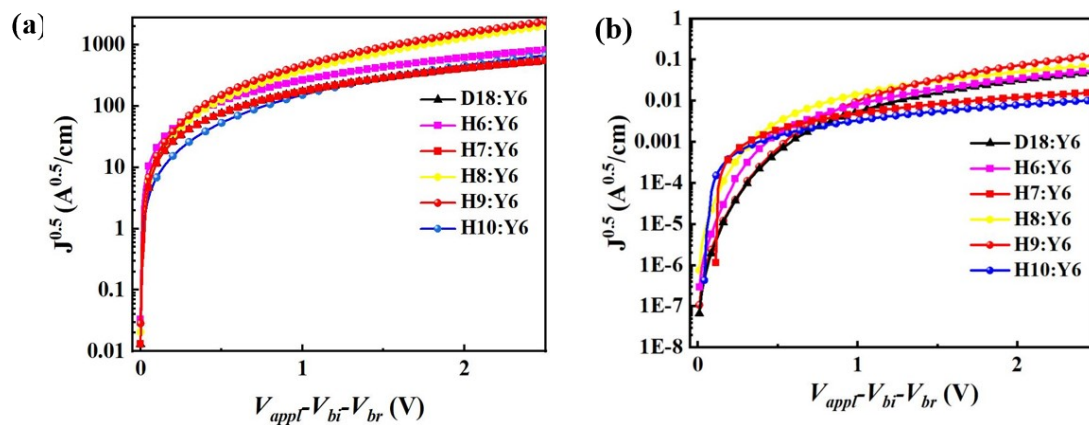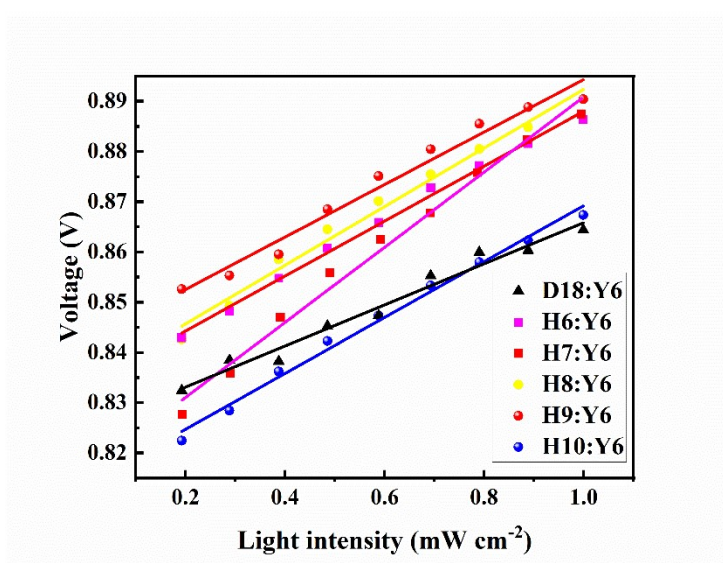
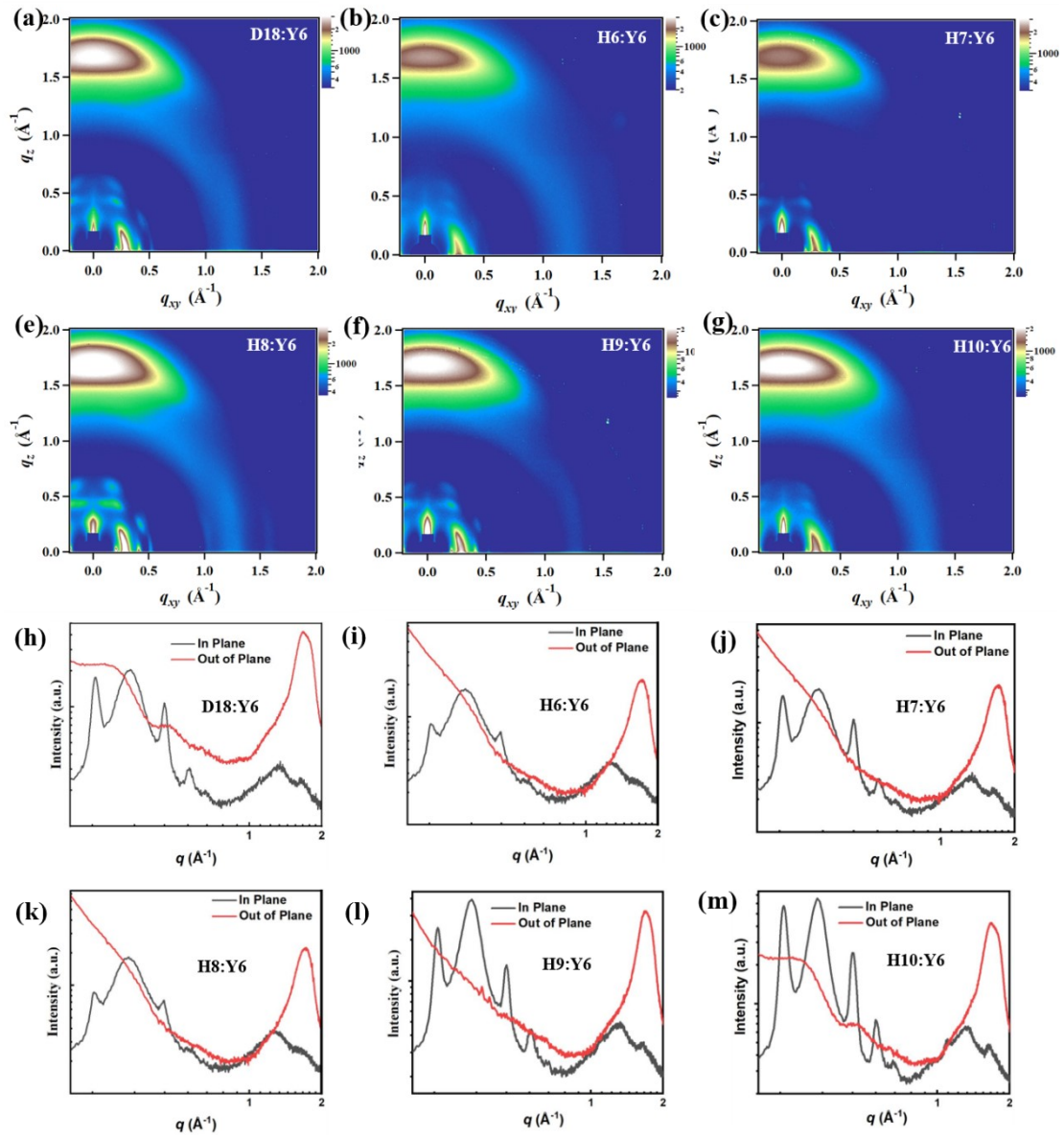**Figure S14.** The dependence of light intensity on V_{oc}.

Figure S15. 2D GIWAXS patterns of the blend films (a-g). In-plane and out-of-plane line cuts of the related blend films (h-m).
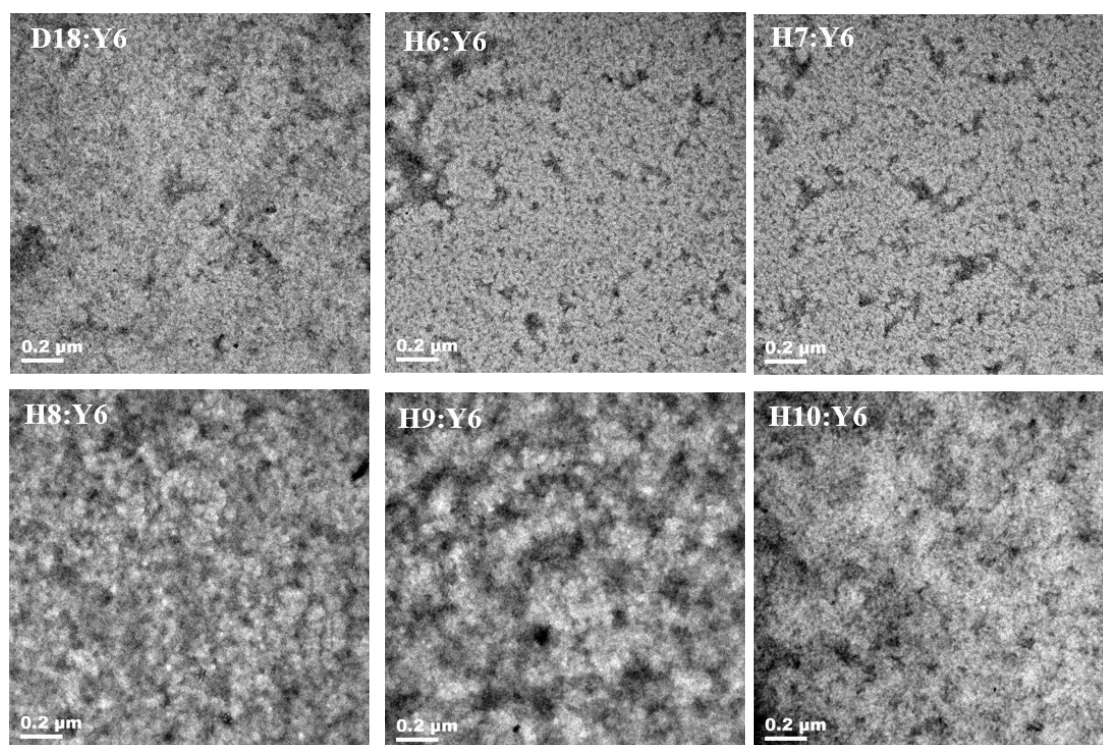
Figure S16. Transmission electron microscopy (TEM) of the blend films.

Table S1. the device performance with Y6 as the acceptor under 100 mW cm^{-2} AM 1.5G solar illumination (all the active layer blends were prepared with annealing free and CN (0.5%, v/v) as solvent additive).

Total concentration (mg/ml)	Active layer	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
12.7	H6:Y6	0.887	25.76	75.19	17.18
13.2		0.888	26.51	76.98	18.12
14.3		0.888	26.72	74.29	17.63
12.7	H7:Y6	0.889	24.97	72.35	16.06
13.2		0.889	25.79	73.80	16.92
14.3		0.887	25.81	71.64	16.40
12.7	H8:Y6	0.890	25.98	76.59	17.71
13.2		0.890	26.65	77.09	18.28
14.3		0.888	26.72	76.48	18.14
12.7	H9:Y6	0.890	25.81	77.42	17.78
13.2		0.890	26.68	77.89	18.50
14.3		0.888	25.71	75.29	17.19
12.7	H10:Y6	0.889	25.07	73.55	16.39
13.2		0.890	25.26	73.74	16.58
14.3		0.889	25.46	72.64	16.44

Table S2. the device performance with Y6 as the acceptor under 100 mW cm^{-2} AM 1.5G solar illumination (all the active layer blends were prepared with annealing free and the total concentration is 13.2 mg/ml).

CN (v/v)	Active layer	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
0	H6:Y6	0.872	25.63	72.57	16.22
0.5%		0.888	26.51	76.98	18.12
1.0%		0.888	26.05	74.95	17.33
0	H7:Y6	0.872	24.62	71.59	15.37
0.5%		0.889	25.79	73.80	16.92
1.0%		0.889	25.08	73.21	16.32
0	H8:Y6	0.887	25.68	75.82	17.27
0.5%		0.890	26.65	77.09	18.28
1.0%		0.889	25.73	74.56	17.05
0	H9:Y6	0.884	25.18	74.69	16.63
0.5%		0.890	26.68	77.89	18.50
1.0%		0.890	25.38	76.57	17.30
0	H10:Y6	0.885	24.63	72.37	15.77
0.5%		0.890	25.26	73.74	16.58
1.0%		0.890	25.04	72.58	16.17

Table S3. the device performance with Y6 as the acceptor under 100 mW cm^{-2} AM 1.5G solar illumination (CN (0.5%, v/v) as solvent additive and the total concentration is 13.2 mg/ml).

SVA	Active layer	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
CS2		0.863	25.59	75.00	16.56
/	H6:Y6	0.888	26.51	76.98	18.12
CF		0.862	26.02	74.27	16.66
CS2		0.881	24.52	72.27	15.61
/	H7:Y6	0.889	25.79	73.80	16.92
CF		0.880	25.54	71.05	15.97
CS2		0.881	25.09	75.68	16.73
/	H8:Y6	0.890	26.65	77.09	18.28
CF		0.883	26.41	76.65	17.87
CS2		0.880	25.18	76.28	16.90
/	H9:Y6	0.890	26.68	77.89	18.50
CF		0.857	25.12	75.28	16.21
CS2		0.881	24.65	73.06	15.87
/	H10:Y6	0.890	25.26	73.74	16.58
CF		0.880	25.31	70.83	15.78

Table S4. The effect of M_n on photovoltaic properties.

Active layer	M_n (kDA)	PCE (%)
	40.65	16.07
	44.32	16.84
D18:Y6	47.23	17.06
	51.85	16.85
	62.44	17.26
	40.01	17.02
	46.22	17.47
H6:Y6	51.75	17.63
	57.67	18.12
	74.43	18.02
	52.14	18.01
	56.47	18.24
H9:Y6	65.12	18.41
	65.58	18.50
	79.66	18.32

Table S5. The related parameters of the GIWAXS measurements on the neat polymer films and the blend films.

Samples	Out-of-Plane				In-Plane			
	π-π stacking cell axis (010)				Unit cell long axis (100)			
	q (Å⁻¹)	d-spacing (Å)	FWHM (Å⁻¹)	Coherence length (Å)	q (Å⁻¹)	d-spacing (Å)	FWHM (Å⁻¹)	Coherence length (Å)
D18	1.645	3.820	0.263	21.732	0.293	21.468	0.122	46.430
H6	1.636	3.841	0.274	20.855	0.304	20.668	0.096	58.925
H7	1.636	3.841	0.286	19.994	0.309	20.367	0.100	56.863
H8	1.636	3.841	0.270	21.163	0.310	20.277	0.095	59.727
H9	1.639	3.835	0.259	22.087	0.297	21.187	0.093	60.935
H10	1.643	3.824	0.261	21.896	0.291	21.592	0.125	45.253
D18:Y6	1.698	3.700	0.261	21.897	0.317	19.829	0.052	108.536
H6:Y6	1.694	3.709	0.263	21.744	0.318	19.760	0.053	106.737
H7:Y6	1.692	3.714	0.274	20.829	0.318	19.760	0.055	102.221
H8:Y6	1.720	3.653	0.246	23.267	0.319	19.697	0.084	67.160
H9:Y6	1.699	3.698	0.230	24.882	0.318	19.769	0.112	50.458
H10:Y6	1.697	3.703	0.265	21.581	0.316	19.883	0.052	106.34

The related parameters of the GIWAXS measurements on the neat polymer