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Understanding the Impact of Side-chain on Photovoltaic Performance in Efficient All-polymer Solar Cells

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1. Characterization

UV-vis-NIR spectrums were recorded on a Perkin Elmer model Lambda 750. Molecular weight and its distributions were determined using a polystyrene standard through gel permeation chromatography (GPC) on a PL-GPC 50 apparatus. THF was used as an eluent at a low rate of 1.0 mL/min at 40 °C. UPS measurements were performed using an Omicron Nanotechnology system with a base pressure of 2.0×10^{-10} Torr. Density functional theory (DFT) simulations followed classical geometry optimization method at the B3LYP/6-31G(d) level without special operation. If convergence failed with total energy vibration, we would decrease the step length of optimization (maxstep = N) or other methods to obtain convergence results. GIWAXS measurements were performed at the Advanced Light Source (ALS)-Lawrence Berkeley National Laboratory on Beamline 7.3.3. Distances were estimated by the following equation: $2\pi/q$. The crystal correlation lengths (CCL) were estimated by the following equation: $CCL = 2\pi/FWHM$, where FWHM is the full-width-at-half-maximum of the fitted Gaussian. PL was tested by a FLS980 (Edinburgh Instrument, UK) using an excitation of 610 nm wavelength. Atomic force microscopy (AFM) and transmission electron microscopy (TEM) images were captured using a Veeco Multimode V instrument and Tecnai G2 F20 S-Twin transmission electron microscope, respectively. The external quantum efficiency (EQE) was performed using a certified IPCE instrument (Zolix Instruments, Inc, SolarCellScan100).

2. Sample Preparations

For the dilution solutions, all the polymers were dissolved in either chloroform or chlorobenzene at a concentration of ~0.03 mg/mL, for the concentrated solutions in chloroform at a concentration of ~0.1 mg/mL. For the thin film samples, all of the pristine polymer films were prepared by spin-coating from the chloroform solutions under identical conditions (10 mg mL^{-1}) on a quartz substrate (1*1 cm size). For the AFM measurements, it was directly performed on the solar cell devices. TEM samples were prepared by spin-casting all-polymer blend solution according to the optimal condition on the PEDOT:PSS (un-annealed) coated ITO. During the lift-off process, the spin-coated films were pre-cut into several small pieces and rinsed with water, the films were then transferred to pure copper grids without carbon membrane for testing. For the GIWAXS measurements, all the samples were prepared by spin-coating the all-polymer blend solutions using the optimal condition for device fabrication on a Si substrate. For the GIWAXS measurements, all of the pristine polymer films (20-40 nm) were prepared by spin-coating from the chloroform solutions under identical conditions (5 mg mL^{-1}) on a ITO substrate (0.5*0.5 cm size). For the PL measurements, all of the pristine and blend polymer films were prepared by spin-coating from the chloroform solutions (pristine polymer: 10 mg mL^{-1}; blend film: optimal blend solutions for solar cell fabrication) on a quartz substrate (1*1 cm size).

3. Mobility measurements by space charge limited current method

Hole-only devices were fabricated to measure the hole mobility using the space charge limited current (SCLC) method. The device structure is ITO/PEDOT:PSS/polymer or blend/MoO_3/Ag. The thickness was measured by a Profilometer. The mobility was determined by fitting the dark current to the model of a single carrier SCLC, which is described by the equation:

$$J = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_h\frac{V^2}{d^3},$$

where J is the current, ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material, μ is the zero-field mobility, d is the thickness of the polymer layer, and V is the applied voltage.

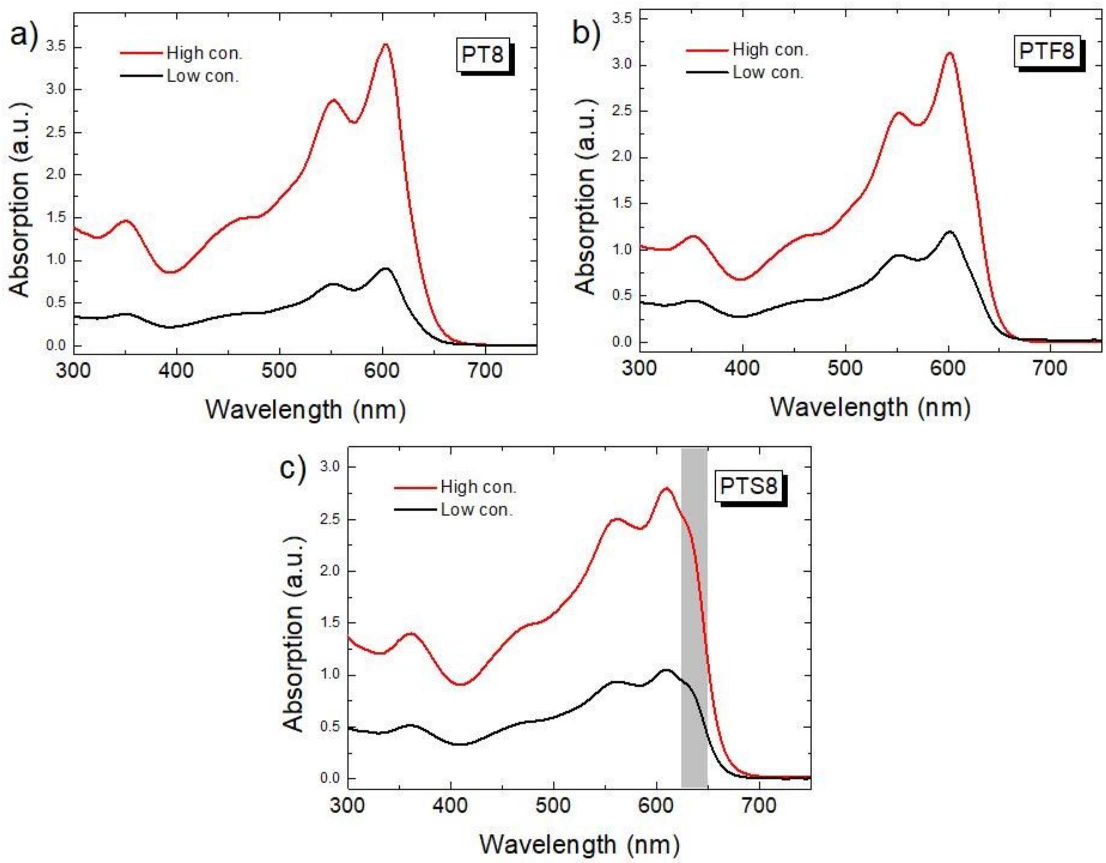

Figure S1. UV-vis absorption spectra of polymers in concentrated and diluted chloroform solutions

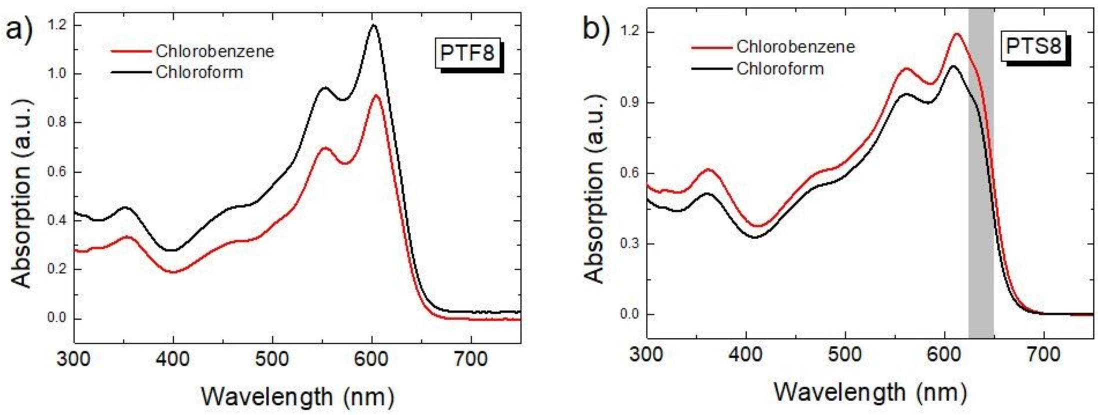

Figure S2. UV-vis absorption spectra of polymers in diluted chlorobenzene and chloroform solutions

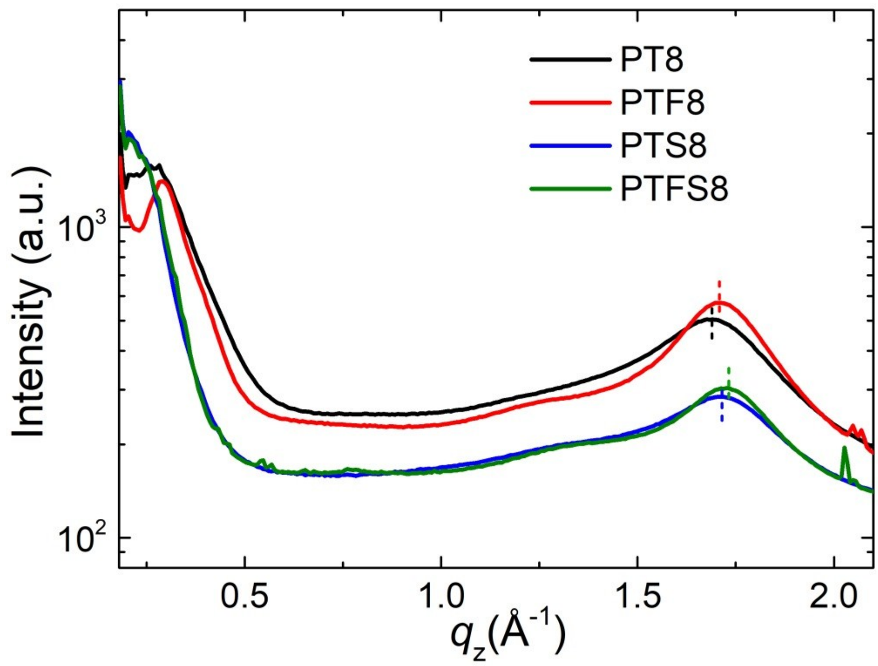

Figure S3. Out-of-plane line cuts of the corresponding 2D GIWAXS images.

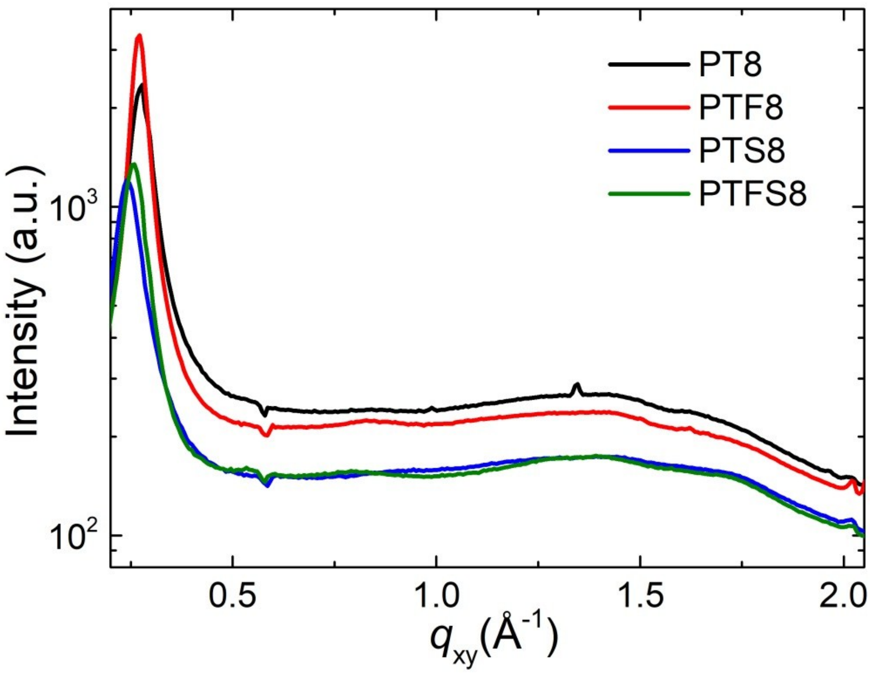

Figure S4. In-plane line cuts of the corresponding 2D GIWAXS images.

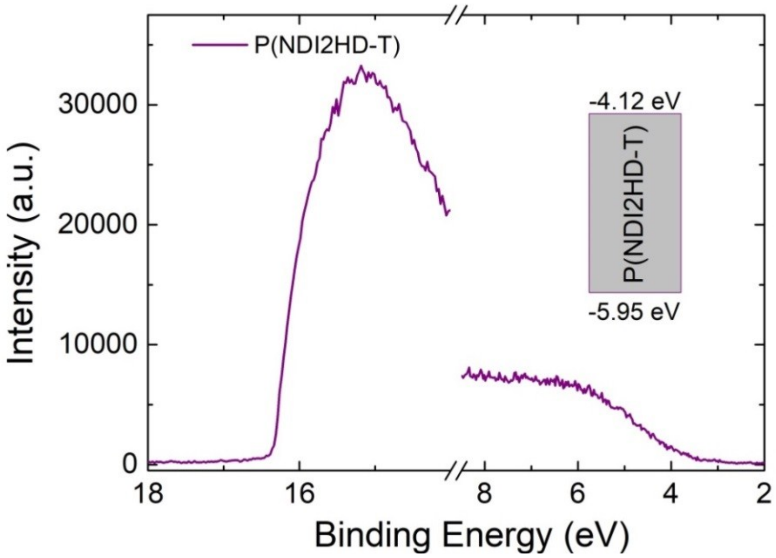

Figure S5. UPS measurement results and corresponding LUMO and HOMO energy levels of P(NDI2HD-T).

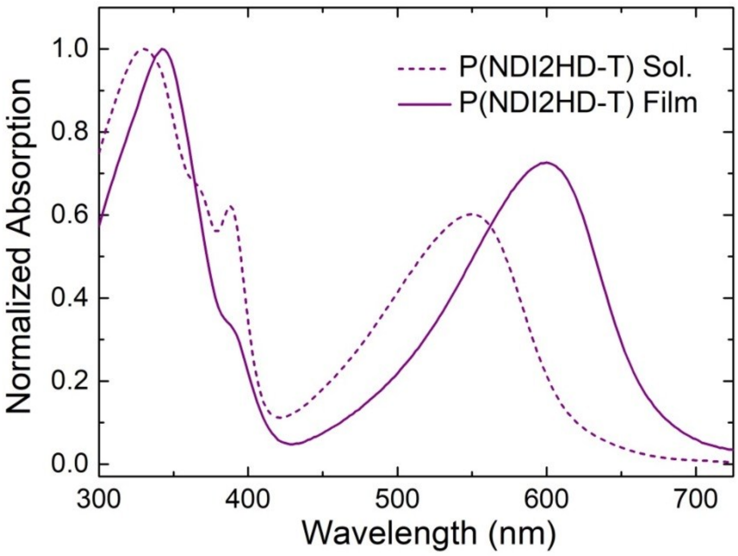

Figure S6. Normalized UV-vis absorption spectra of P(NDI2HD-T) in dilute chloroform solution and thin films spin-cast from chloroform.

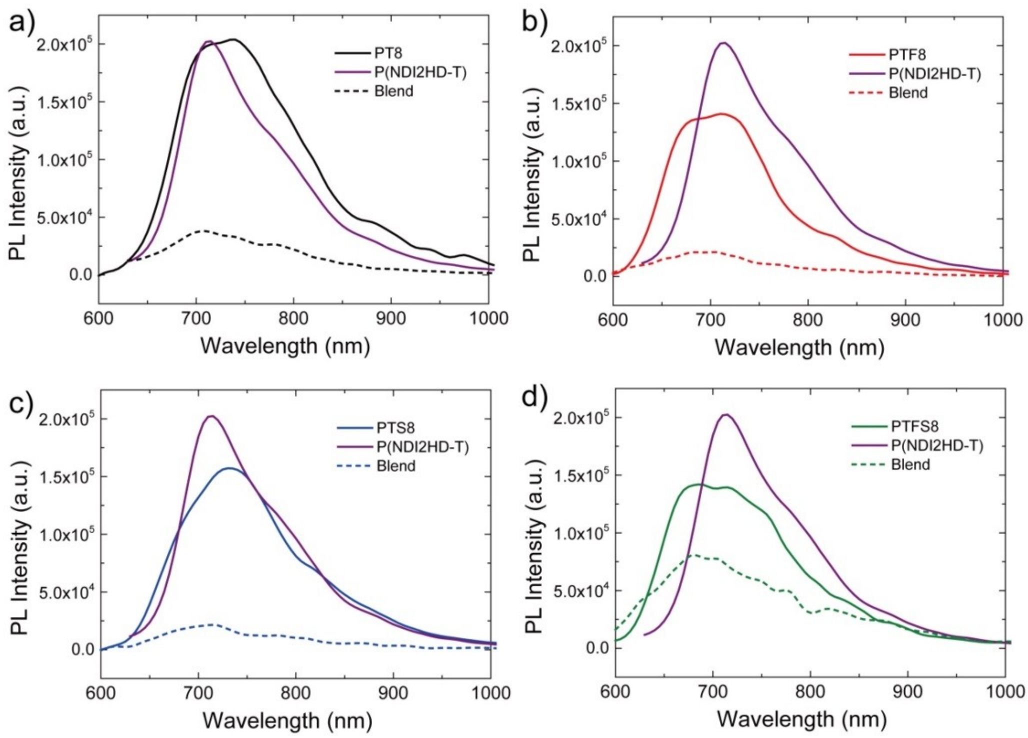

Figure S7. Photoluminescence measurements of neat polymer films and corresponding all-polymer blend prepared under optimal processing conditions. D/A ratio in the all-polymer blend is 1.3:1.

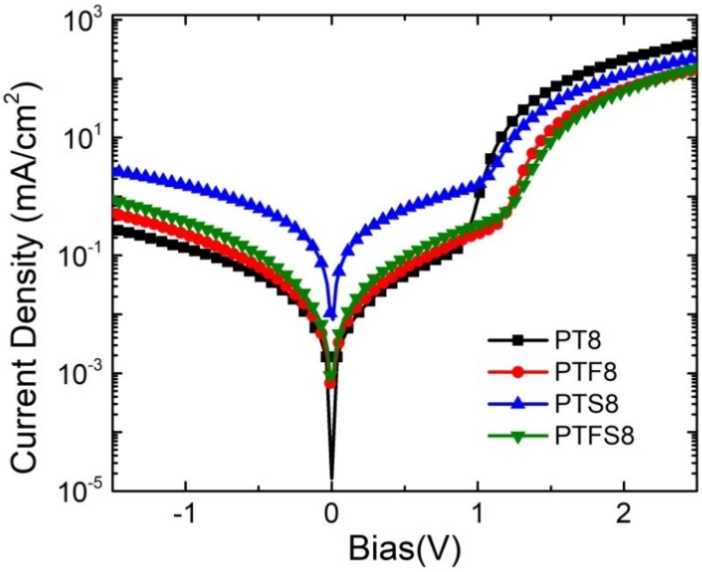

Figure S8. Corresponding dark $J-V$ characteristics of optimized all-polymer devices. D/A ratio in the all-polymer blend is 1.3:1.

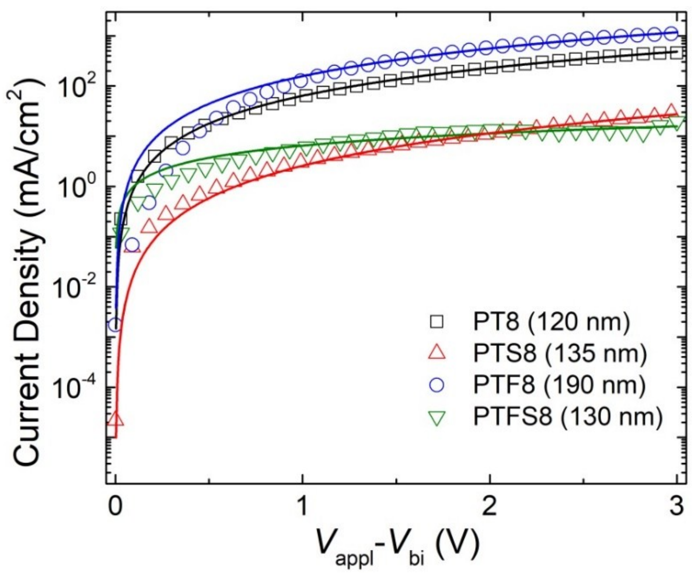

Figure S9. J-V characteristics of the hole-only devices based on PT8, PTF8, PTS8 and PTFS8. D/A ratio in the all-polymer blend is 1.3:1.

Table S1. Effect of different D:A blend ratios on photovoltaic performance of PT8:P(NDI2HD-T) solar cells with 12 mg/mL concentration in chloroform.

D:A ratio	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
1.0:1.0	0.96	6.43	0.46	2.86
1.1:1.0	0.96	6.96	0.48	3.21
1.2:1.0	0.97	6.94	0.48	3.27
1.3:1.0	0.98	7.05	0.48	3.35
1.4:1.0	0.98	6.99	0.47	3.21
1.5:1.0	0.99	6.75	0.47	3.14
1.6:1.0	0.92	7.05	0.41	2.68

Table S2. Effect of different concentration in chloroform on photovoltaic performance of PT8:P(NDI2HD-T) solar cells with D:A ratio=1.3:1.

Concentration	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
10 mg/ml	1.02	7.70	0.55	4.38
11 mg/ml	1.04	7.20	0.58	4.39
12 mg/ml	1.04	7.59	0.57	4.54
13 mg/ml	1.02	7.82	0.58	4.66
14 mg/ml	1.02	7.68	0.52	4.12
15 mg/ml	1.02	7.24	0.51	3.78
16 mg/ml	1.05	6.53	0.43	2.86

Table S3. Effect of different thermal annealing temperature on photovoltaic performance of PT8:P(NDI2HD-T) solar cells with D:A ratio=1.3:1 and 13mg/mL concentration.

Temperature	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
80 ^{o}C	1.02	9.11	0.65	6.06
100 ^{o}C	1.02	9.28	0.65	6.16
120 ^{o}C	1.02	9.16	0.68	6.39
140 ^{o}C	1.02	9.28	0.66	6.26
160 ^{o}C	1.00	8.35	0.63	5.32

Table S4. Effect of different DIO volume ratio on photovoltaic performance of PT8:P(NDI2HD-T) solar cells with D:A ratio=1.3:1 and 13mg/mL concentration.

DIO(%,v/v)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
As cast	1.02	9.17	0.65	6.07
0.5% DIO	1.04	10.90	0.61	6.99
1% DIO	1.04	11.04	0.65	7.51
1.5% DIO	1.01	10.56	0.63	6.78
2% DIO	1.04	9.18	0.67	6.45
3% DIO	1.04	9.13	0.67	6.40
5% DIO	1.00	8.98	0.67	6.08

Table S5. Effect of different thermal annealing (TA) time on photovoltaic performance of PT8:P(NDI2HD-T) solar cells with 120 ^{o}C, D:A ratio=1.3:1， 13mg/mL concentration and 1% DIO.

TA time	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
As cast	1.01	10.56	0.63	6.78
5 min	1.04	10.75	0.68	7.63
10 min	1.04	10.81	0.69	7.72
15 min	1.05	11.10	0.69	8.00
20 min	1.03	10.73	0.69	7.62
30 min	1.03	10.47	0.69	7.51

Table S6. Effect of different DIO volume ratio on Photovoltaic performance of PTF8:P(NDI2HD-T) withD:A ratio=1.3:1, 13mg/mL concentration and thermal annealing at 120 ^{o}C for 15 min.

DIO(%,v/v)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
As cast	1.20	5.44	0.43	2.83
0.5% DIO	1.22	5.62	0.57	3.92
1% DIO	1.22	5.70	0.57	4.01
2% DIO	1.21	5.30	0.56	3.68

Table S7. Effect of different concentration in chloroform on Photovoltaic performance of PTF8:P(NDI2HD-T) solar cells with D:A ratio 1.3:1, 1% DIO and thermal annealing at 120 ^{o}C for 15 min.

Concentration	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
8 mg/ml	1.12	3.54	0.34	1.38
10 mg/ml	1.21	3.63	0.45	2.02
12 mg/ml	1.21	5.44	0.53	3.47
13 mg/ml	1.22	5.70	0.57	4.01
14 mg/ml	1.22	5.48	0.55	3.71
16 mg/ml	1.22	5,55	0.53	3.63

Table S8. Effect of different DIO volume ratio on photovoltaic performance of PTS8:P(NDI2HD-T) with D:A ratio=1.3:1, 13mg/ml concentration and thermal annealing at 120 ^{o}C for 15 min.

DIO(%,v/v)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
As cast	1.00	5.36	0.43	2.31
0.5% DIO	1.03	6.27	0.47	3.07
1% DIO	1.03	6.30	0.56	3.65
2% DIO	1.05	6.25	0.47	3.13

Table S9. Effect of different concentration in chloroform on photovoltaic performance of PTS8:P(NDI2HD-T) solar cells with D:A ratio 1.3:1, 1% DIO and thermal annealing at 120 ^{o}C for 15 min.

Concentration	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
8 mg/ml	1.01	3.47	0.39	1.41
10 mg/ml	1.03	5.05	0.43	2.23
12 mg/ml	1.03	6.67	0.45	3.14
13 mg/ml	1.03	6.30	0.56	3.65
14 mg/ml	1.01	5.39	0.38	1.94
16 mg/ml	0.99	5.11	0.38	1.94

Table S10. Photovoltaic performance of PTFS8:P(NDI2HD-T) solar cells with 13 mg/mL concentration in chloroform.

Condition	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
As Cast	1.00	1.62	0.31	0.50

Table S11. Effect of different concentration in chloroform on photovoltaic performance of PTFS8:P(NDI2HD-T) solar cells with D:A ratio 1.3:1, 1% DIO and thermal annealing at 120 °C for 15 min.

Concentration	V_{oc} (V)	J_{sc} (mA/cm^2)	FF	PCE (%)
8 mg/ml	0.54	1.73	0.28	0.26
10 mg/ml	0.70	1.80	0.29	0.36
12 mg/ml	1.04	1.64	0.31	0.54
13 mg/ml	1.09	1.80	0.32	0.63
14 mg/ml	1.06	1.74	0.31	0.57
16 mg/ml	1.02	1.79	0.30	0.56