Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Side Chain Modification: An Effective Approach to Modulate the Energy Level of Benzodithiophene Based Polymer for High-Performance Solar Cells

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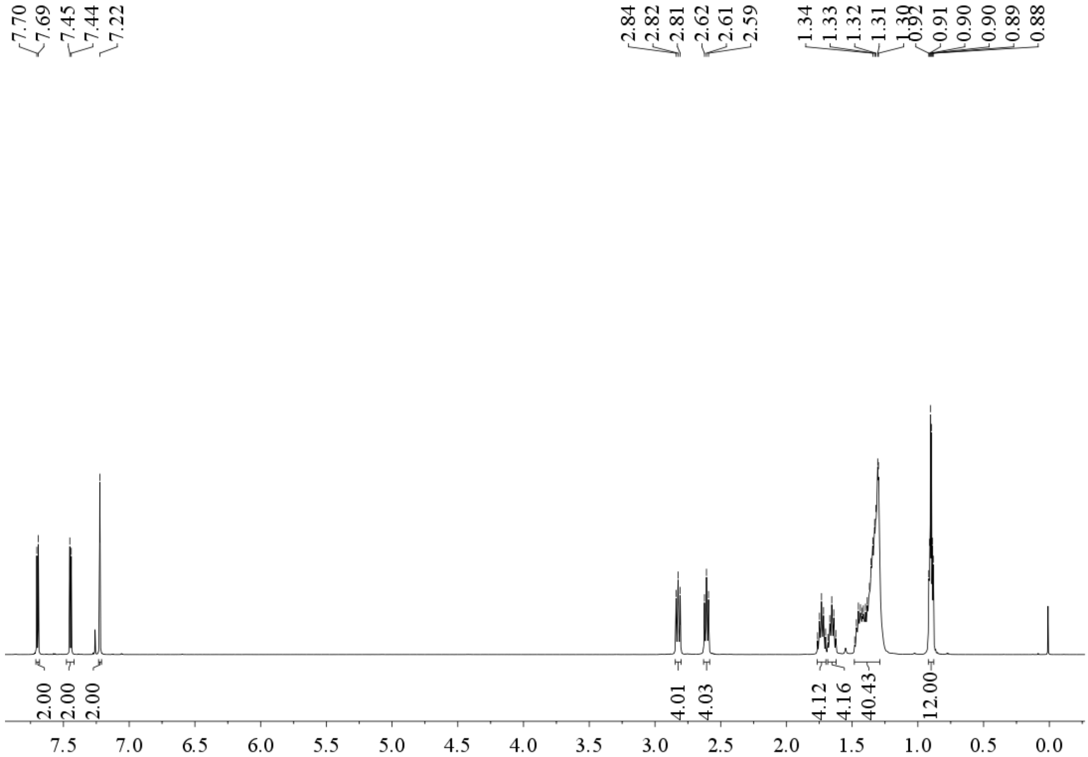


Figure S1. The ^{1}H NMR spectrum of compound 1b.

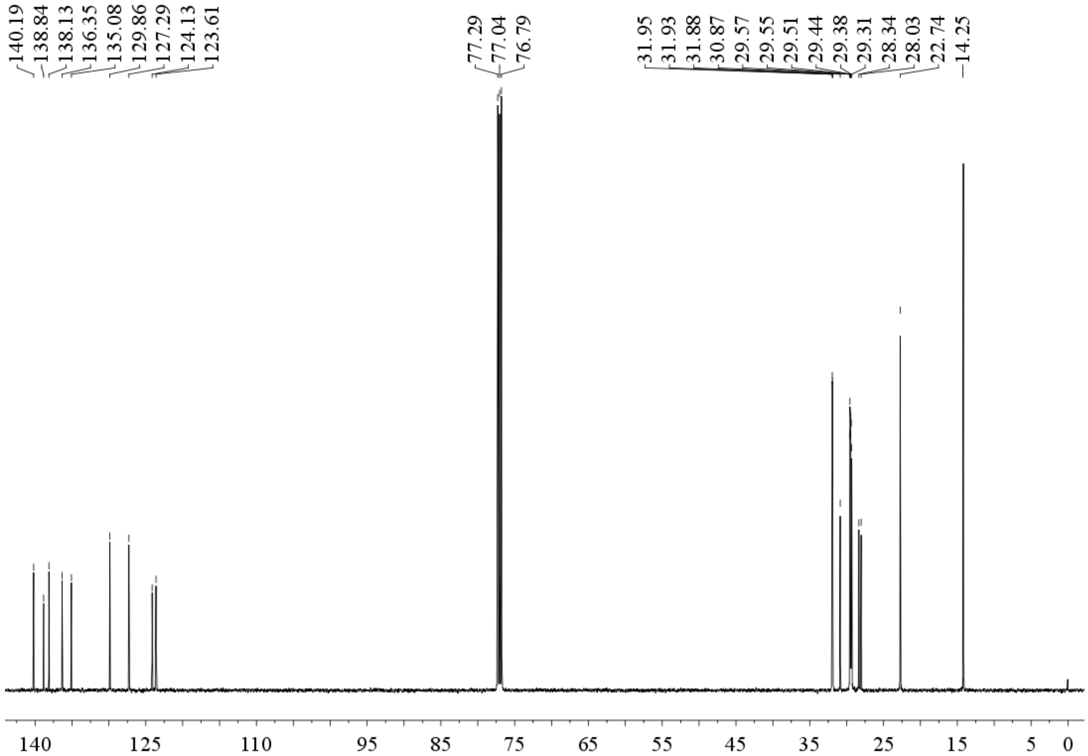


Figure S2. The ^{13}C NMR spectrum of compound 1b.

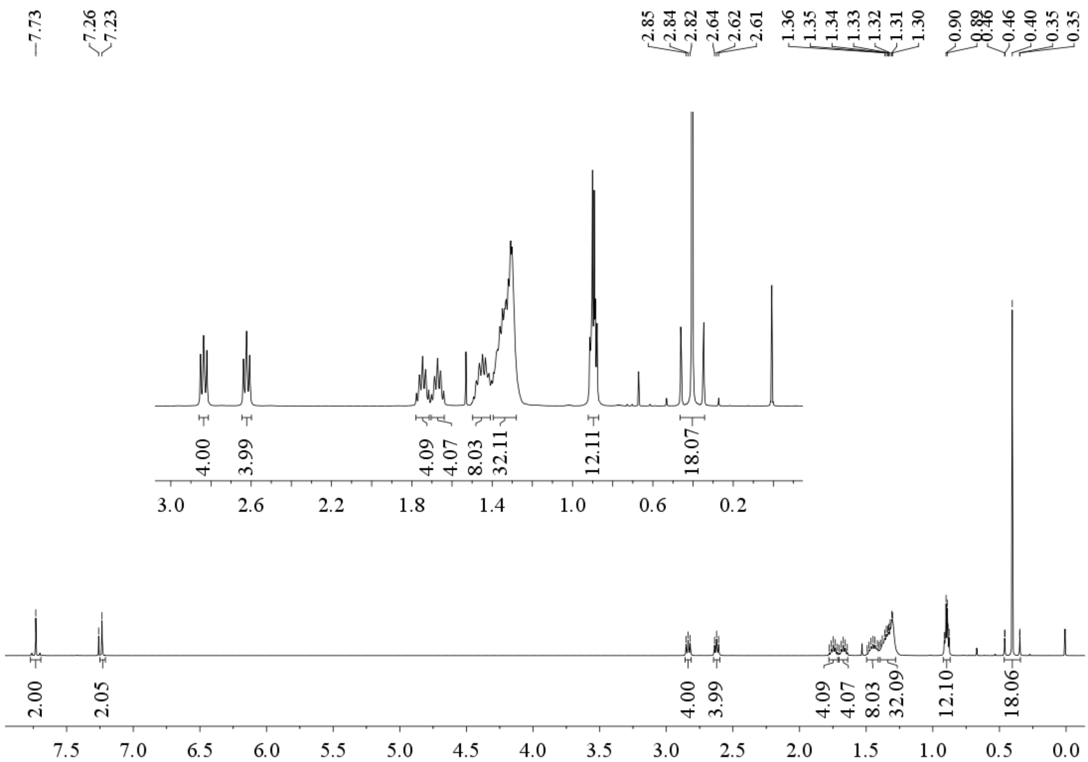


Figure S3. The ^{1}H NMR spectrum of compound 2b.

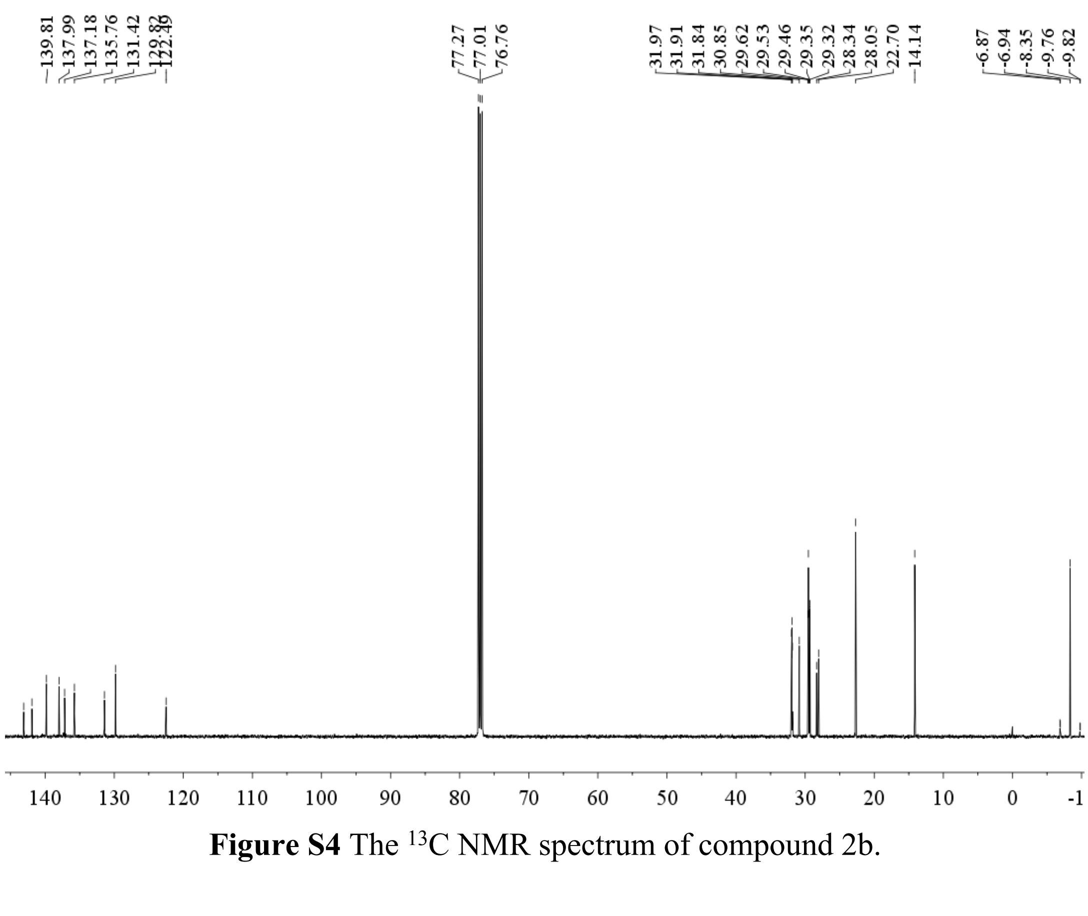


Figure S4 The ^{13}C NMR spectrum of compound 2b.

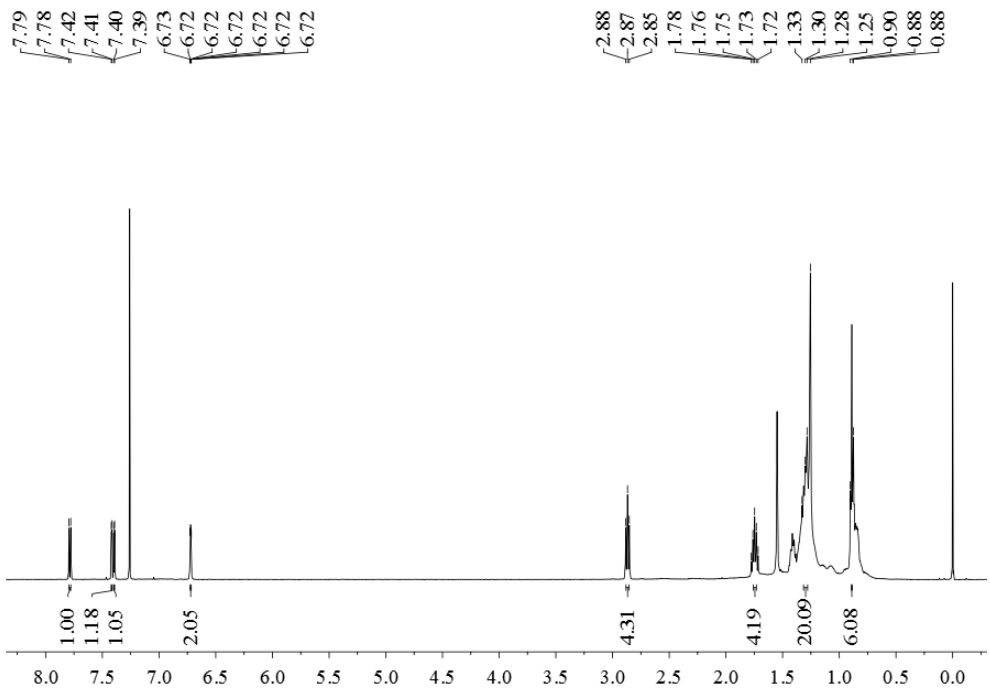


Figure S5 The [1]H NMR spectrum of compound 6.

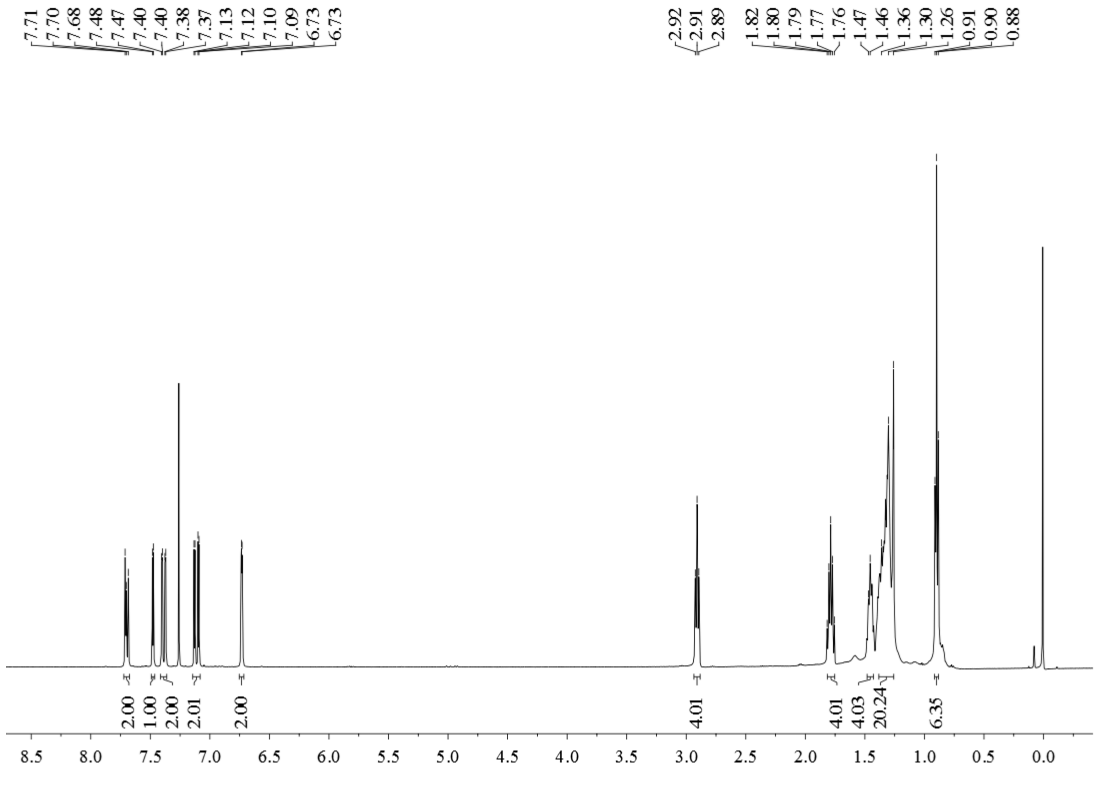


Figure S6 The [1]H NMR spectrum of compound 8.

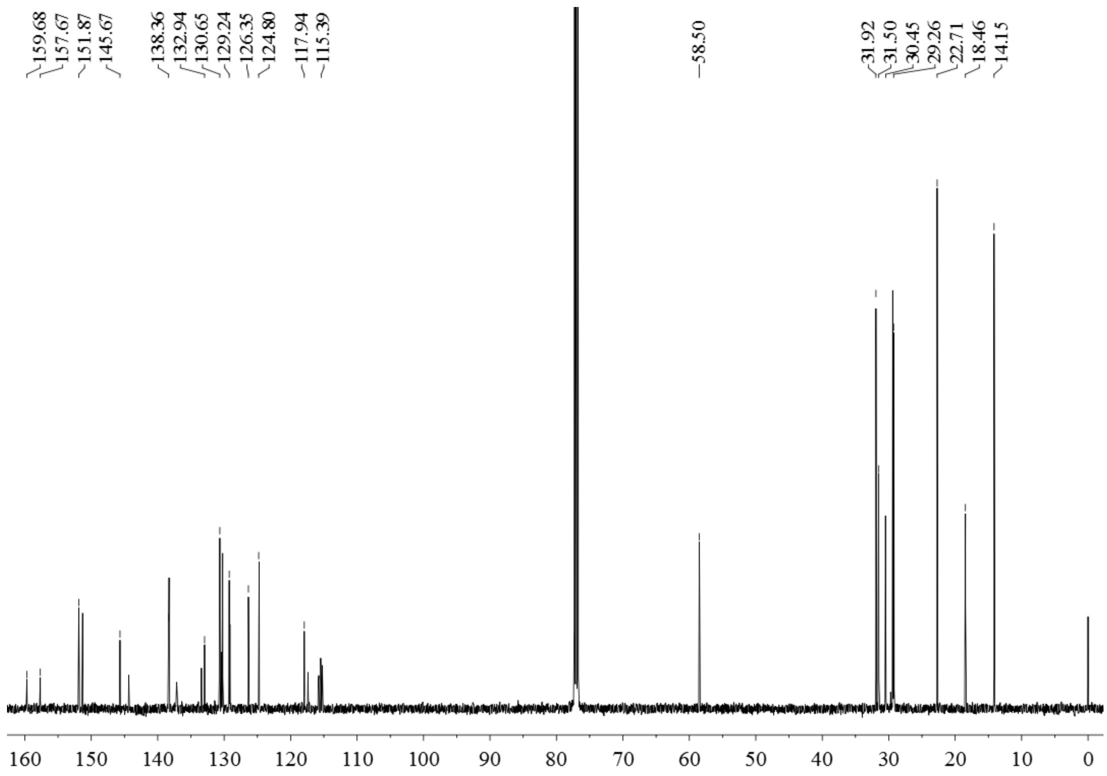


Figure S7 The ^{13}C NMR spectrum of compound 8.

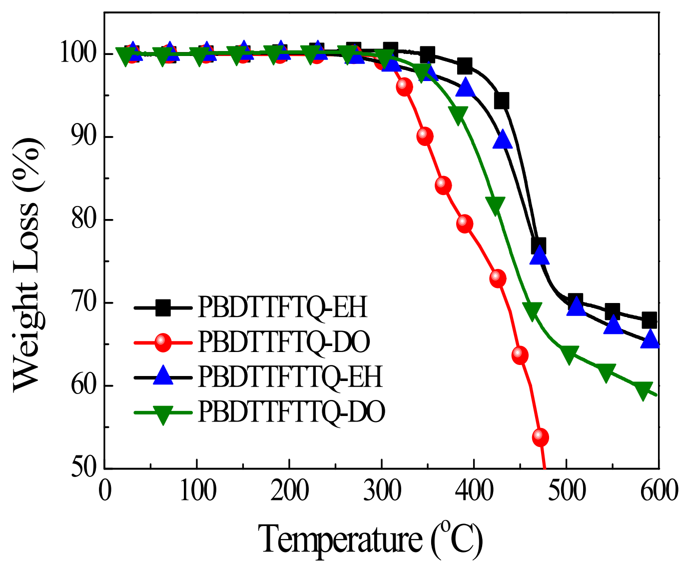


Figure S8. Thermalgravimetric analysis curves of polymers with a hearing rate of 10 °C/min in nitrogen.

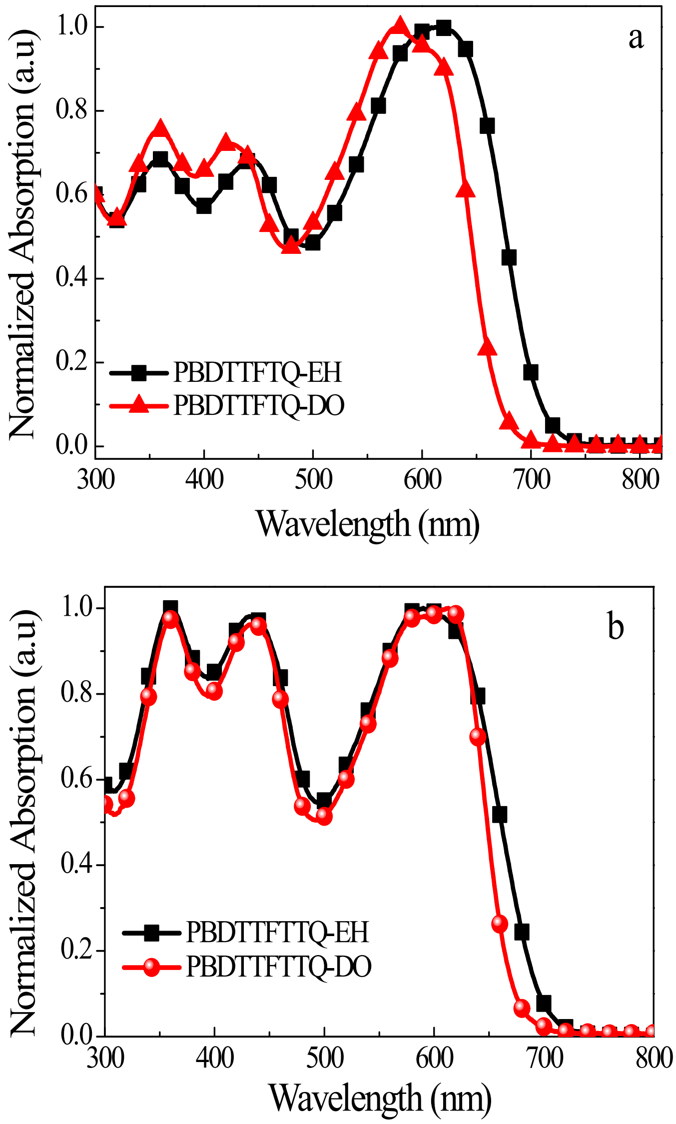
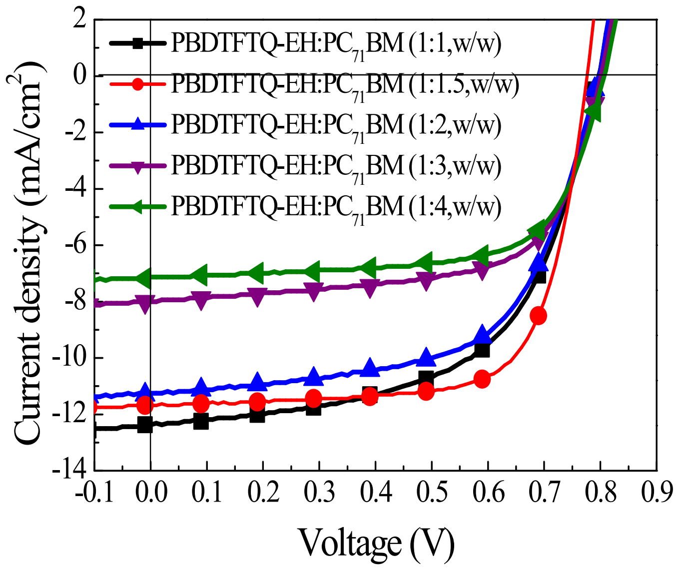
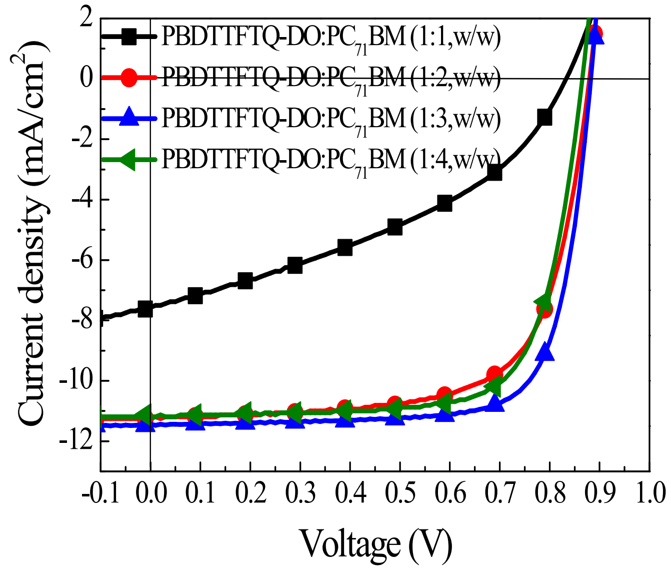


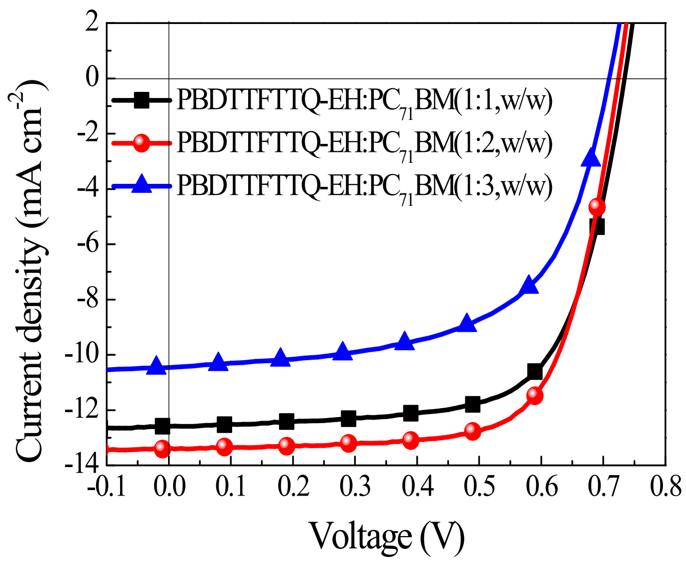
Figure S9. The UV-vis absorption spectra of polymers in $CHCl_3$, (a) PBDTTFTQ-EH and PBDTTFTQ-DO, (b) PBDTTFTTQ-EH and PBDTTFTTQ-DO



PBDTFTQ-EH:PC71BM (1:1,w/w)
PBDTFTQ-EH:PC71BM (1:1.5,w/w)
PBDTFTQ-EH:PC71BM (1:2,w/w)
PBDTFTQ-EH:PC71BM (1:3,w/w)
PBDTFTQ-EH:PC71BM (1:4,w/w)
Current density (mA/cm2)
Voltage (V)



PBDTTFTQ-DO:PC71BM (1:1,w/w)
PBDTTFTQ-DO:PC71BM (1:2,w/w)
PBDTTFTQ-DO:PC71BM (1:3,w/w)
PBDTTFTQ-DO:PC71BM (1:4,w/w)
Current density (mA/cm2)
Voltage (V)



PBDTTFTTQ-EH:PC71BM(1:1,w/w)
PBDTTFTTQ-EH:PC71BM(1:2,w/w)
PBDTTFTTQ-EH:PC71BM(1:3,w/w)
Current density (mA cm-2)
Voltage (V)

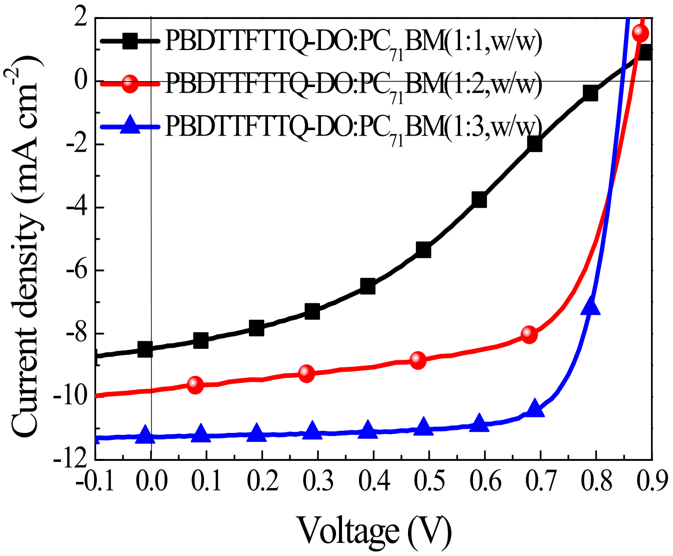


Figure S10 The J-V curves of PSCs based on the polymer:$PC_{71}BM$ with different weight ratios under the illumination of AM 1.5G, 100mW/cm^2

Table S1 The photovoltaic performances of the PSCs based on polymer:$PC_{71}BM$ with various weight ratios under the illumination of AM 1.5G, 100mW/cm^2

Polymer	D/A [w/w]	V_{oc} [V]	J_{sc} [mA cm^{-2}]	FF [%]	PCE [%]
PBDTTFTQ-EH	1:1	0.80	12.4	57.6	5.71
	1:1.5	0.80	12.3	65.4	6.47
	1:2	0.80	11.3	60.6	5.46
	1:3	0.80	7.97	64.8	4.14
	1:4	0.81	7.14	67.3	3.89
PBDTTFTQ-DO	1:1	0.83	7.54	39.1	2.45
	1:2	0.88	11.2	68.7	6.79
	1:3	0.88	11.4	75.9	7.61
	1:4	0.87	11.2	72.6	7.04
PBDTTFTTQ-EH	1:1	0.73	12.6	68.4	6.29
	1:2	0.72	13.4	70.8	6.82
	1:3	0.70	10.5	60.8	4.45

PBDTTFTTQ-DO	1:1	0.82	8.48	37.9	2.64
	1:2	0.86	9.82	65.0	5.49
	1:3	0.85	11.3	75.7	7.25

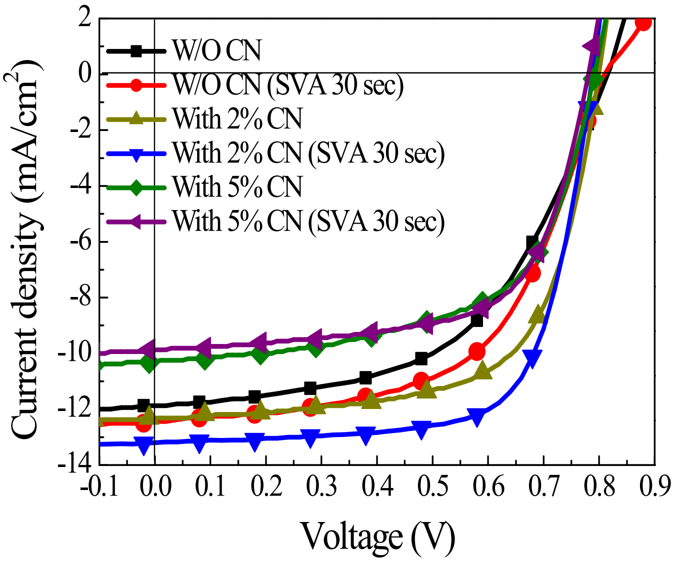


Figure S11 The J-V curves of the PSCs based on **PBDTTFTQ-EH**:$PC_{71}BM$ (1:1.5, wt/wt) with various treated processes under the illumination of AM 1.5G, 100mW/cm^2

Table S2 The photovoltaic performances of the PSCs based on **PBDTTFTQ-EH**:$PC_{71}BM$ (1:1.5, wt/wt) with various treated processes under the illumination of AM 1.5G, 100 mW cm^{-2}

Additive	Annealing process	Voc [V]	Jsc [mA cm^{-2}]	FF [%]	PCE [%]
W/O	As cast	0.82	11.9	52.9	5.15
	SVA 30 sec	0.80	12.4	57.9	5.76
2% CN	As cast	0.80	12.3	65.4	6.43
	SVA 30 sec	0.78	13.2	70.8	7.29
5% CN	As cast	0.79	10.3	59.7	4.86
	SVA 30 sec	0.78	9.89	64.7	4.99

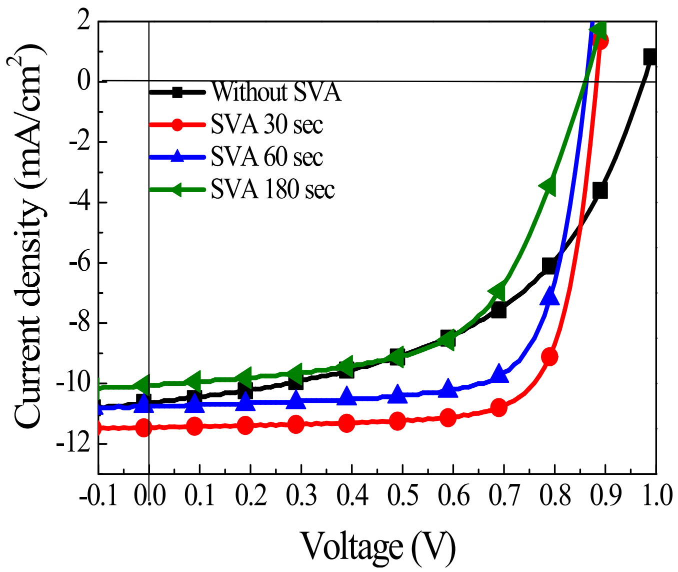


Figure S12 The J-V curves of the PSCs based on **PBDTTFTQ-DO**:$PC_{71}BM$ (1:3, wt/wt) with various THF-SVA times under the illumination of AM 1.5G, 100 mW cm^{-2}

Table S3 The photovoltaic performances of the PSCs based on **PBDTTFTQ-DO**:$PC_{71}BM$ (1:3, wt/wt) with various THF-SVA under the illumination of AM 1.5G, 100 mW cm^{-2}

Active layer	SVA time	Voc [V]	Jsc [mA cm^{-2}]	FF [%]	PCE [%]
PBDTTFTQ-DO: $PC_{71}BM$(1:3)	0 sec	0.98	10.7	49.9	5.21
	30 sec	0.88	11.4	75.9	7.61
	60 sec	0.86	10.8	73.3	6.78
	180 sec	0.86	10.1	58.9	5.09

Hole mobility measurement

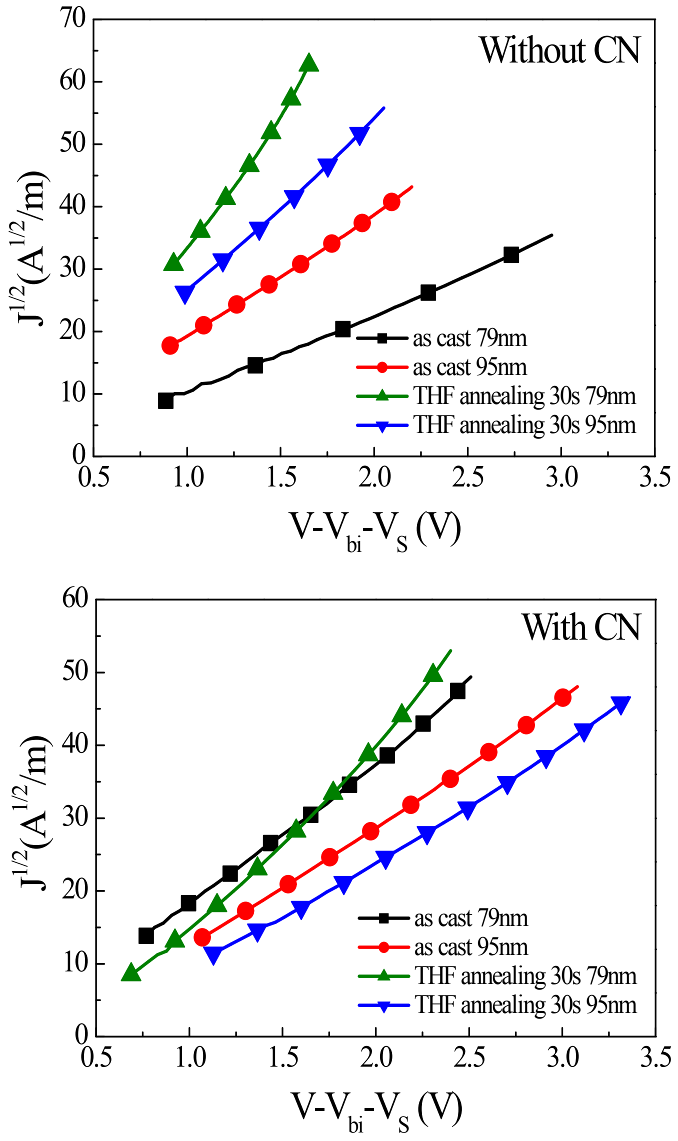


Figure S13 $J^{1/2}$~V characteristics of **PBDTTFTQ-EH** hole-only devices (without and with 2% CN) with different thicknesses measured at ambient temperature

Table S4 The SCLC mobility of **PBDTTFTQ-EH** films

Additive	Treatment	Thickness (nm)	Hole mobilities ($cm^2\ V^{-1}\ s^{-1}$)
Without CN	As cast	79	2.65×10^{-5}
Without CN	As cast	95	1.07×10^{-4}
Without CN	THF-SVA 30s	79	3.14×10^{-4}
Without CN	THF-SVA 30s	95	2.13×10^{-4}
With 2% CN	As cast	83	7.58×10^{-5}
With 2% CN	As cast	95	8.44×10^{-5}
With 2% CN	THF-SVA 30s	83	1.29×10^{-4}
With 2% CN	THF-SVA 30s	95	7.23×10^{-5}

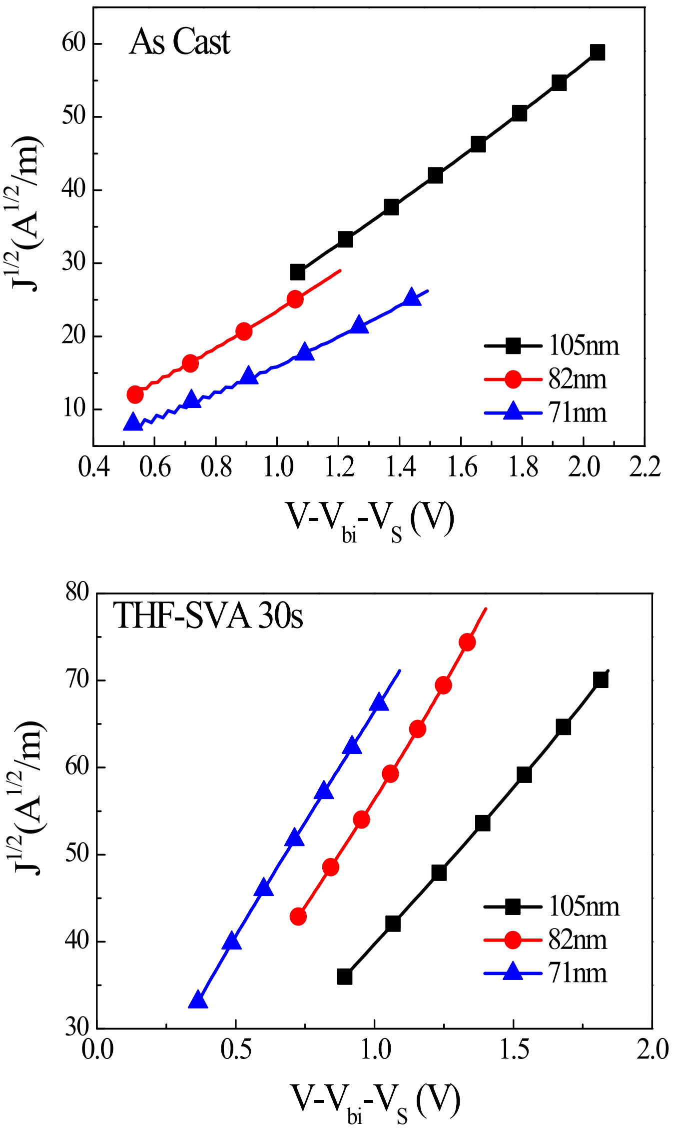
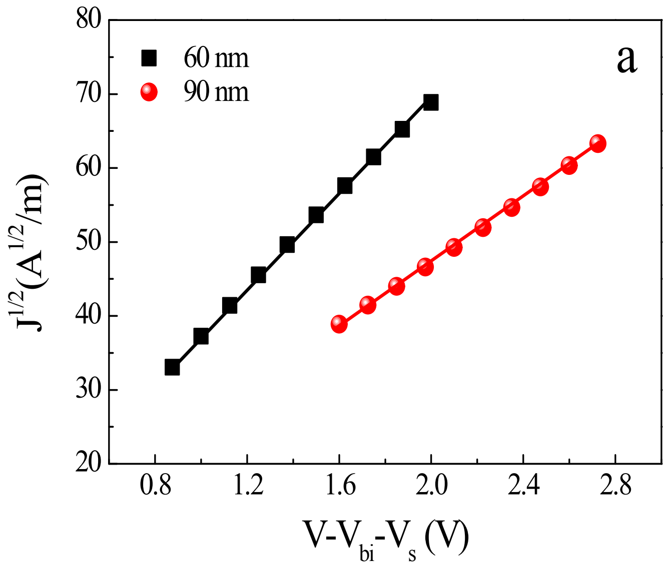


Figure S14 $J^{1/2}$~V characteristics of **PBDTTFTQ-DO** hole-only devices with different thicknesses measured at ambient temperature.

Table S5 The SCLC mobility of **PBDTTFTQ-DO** films

Treatment	Thickness (nm)	Hole mobilities (cm^2 V^{-1} s^{-1})
As cast	105	1.45×10^{-4}
	82	1.16×10^{-4}
	71	1.13×10^{-4}
THF-SVA 30s	105	5.28×10^{-4}
	82	5.03×10^{-4}
	71	3.23×10^{-4}



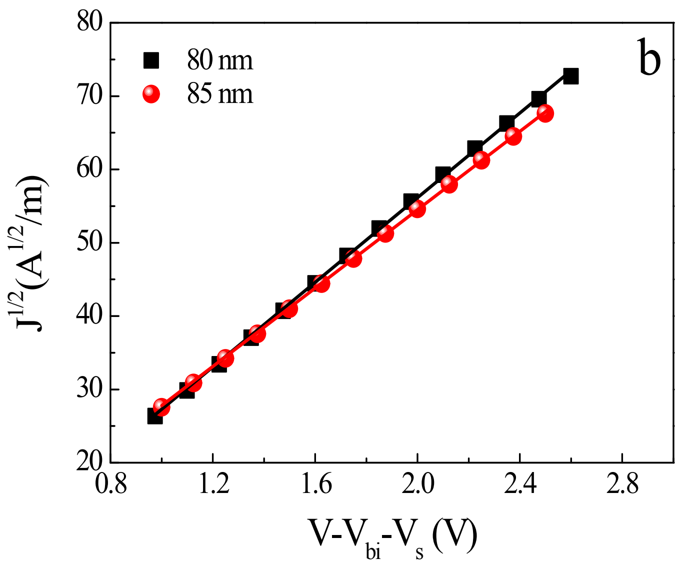


Figure S15 $J^{1/2}\sim V$ characteristics of **PBDTTFTTQ-EH** (a) and **PBDTTFTTQ-DO** (b) hole-only devices with different thicknesses measured at ambient temperature.

Table S6 The SCLC mobility of **PBDTTFTTQ-EH and PBDTTFTTQ-DO** films after THF SVA 30sec

Treatment	Thickness (nm)	Hole mobilities ($cm^2\ V^{-1}\ s^{-1}$)
PBDTTFTTQ-EH	60	7.12×10^{-5}
	90	1.14×10^{-4}
PBDTTFTTQ-EO	80	1.44×10^{-4}
	85	1.49×10^{-4}