Supporting information

Enhancing photovoltaic properties of terpolymers containing benzo[1,2-*b*:4,5-*b′*]dithiophene, phenanthro[4,5-*abc*]phenazine and benzo[*c*][1,2,5]thiadiazole with a changing substituents

Qunping Fan [a], Yu Liu [a,*], Manjun Xiao [a], Wenyan Su [a], Huishan Gao [a], Jianhua Chen [a], Hua Tan [a], Yafei Wang [a], Renqiang Yang [b,*], Weiguo Zhu [a,*]

[a] *College of Chemistry, Xiangtan University, Key Lab of Environment-Friendly Chemistry and Application in Ministry of Education, Xiangtan 411105, China*

[b] *Qingdao Institute of Bioenergy and Bioprocess Technology, Chinese Academy of Sciences, Qingdao 266101, China*

Corresponding author: Prof. Yu Liu; Renqiang Yang; Weiguo Zhu

Tel: +86-731-58293377

Fax: +86-731-58292251

E-mail addresses: liuyu03b@126.com; yangrq@qibebt.ac.cn; zhuwg18@126.com

1. **DSC measurement**

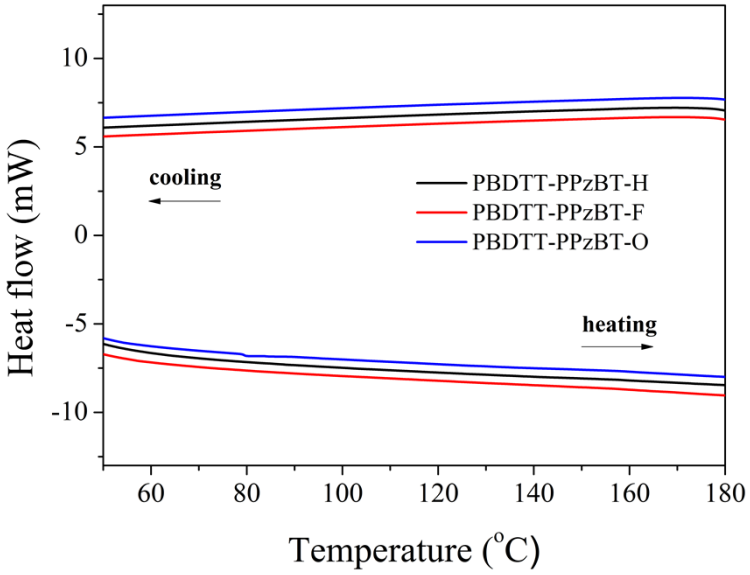

Fig. S1. DSC curves of terpolymers with a heating rate of 10 °C min^{-1} under N_2 atmosphere.

2. **DFT calculation**

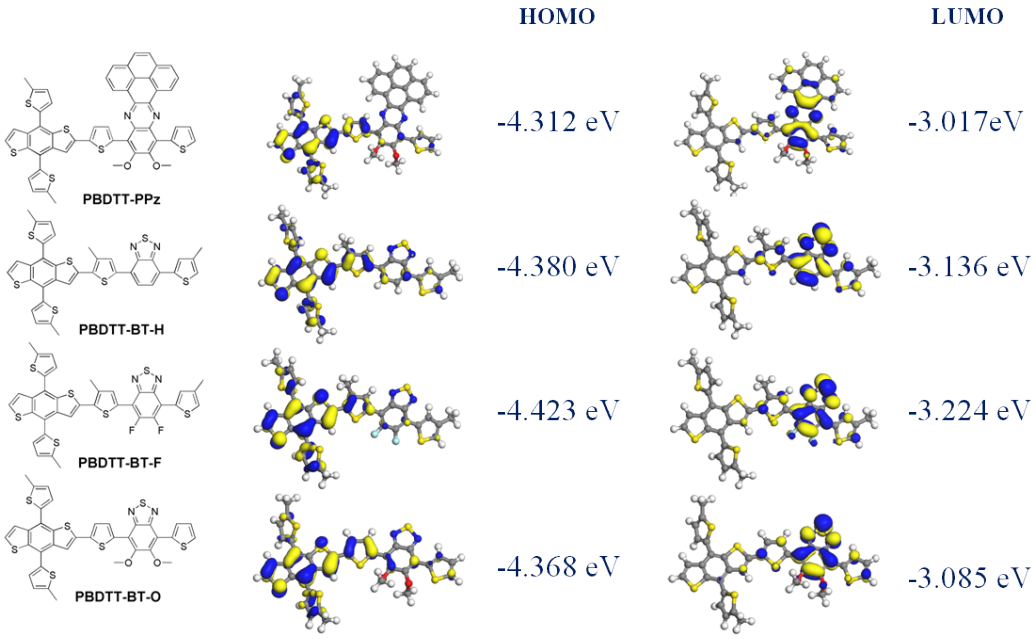

Fig. S2. HOMO and LUMO distribution mode of polymers obtained using calculated at the B3LYP/6-31G* level.

3. Photovoltaic properties of the terpolymer-based PSCs at different conditions

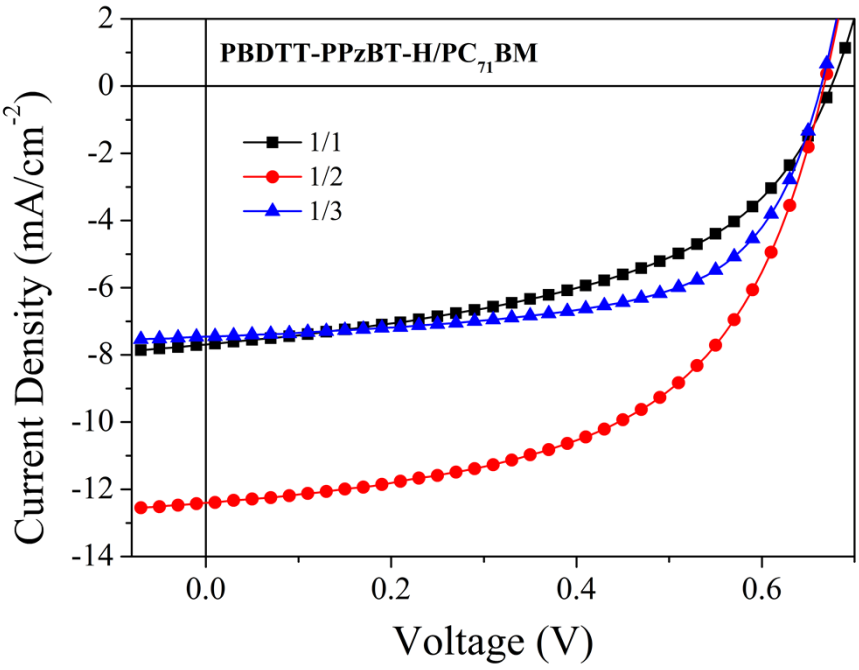

Fig. S3a. *J-V* curves of the PBDTT-PPzBT-H/$PC_{71}BM$-based PSCs with different blend ratios (*w/w*) under AM 1.5G illumination (100 mW cm^{-2}).

Table S1a. Photovoltaic properties of the PBDTT-PPzBT-H/$PC_{71}BM$-based PSCs with different blend ratios (*w/w*) under AM 1.5G illumination (100 mW cm^{-2}).

D/A Ratio	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
1/1	7.7	0.67	49.4	2.6
1/2	12.4	0.67	55.0	4.5
1/3	7.5	0.66	61.9	3.1

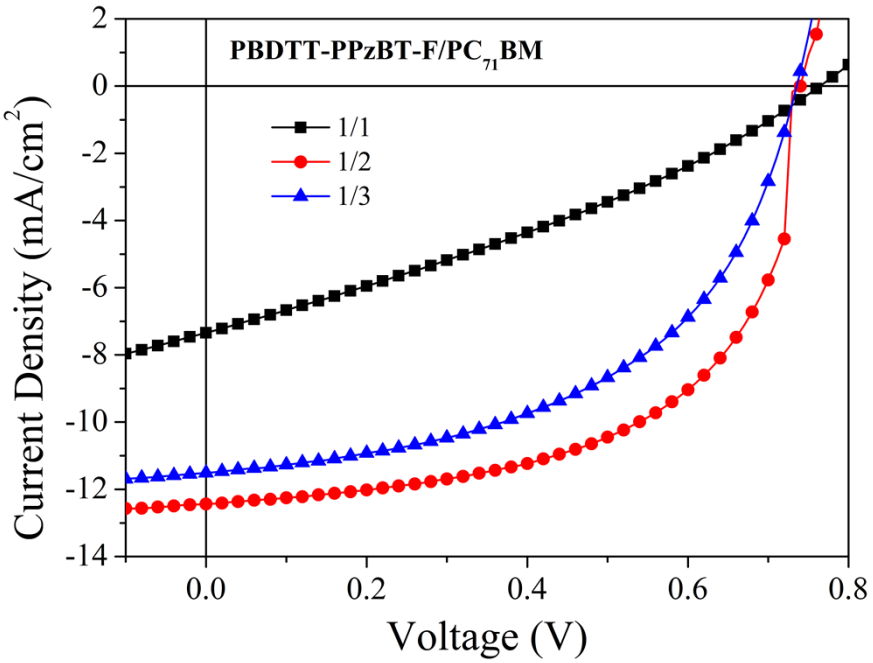

Fig. S3b. *J-V* curves of the PBDTT-PPzBT-F/$PC_{71}BM$-based PSCs with different blend ratios (*w/w*) under AM 1.5G illumination (100 mW cm^{-2}).

Table S1b. Photovoltaic properties of the PBDTT-PPzBT-F/$PC_{71}BM$-based PSCs with different blend ratios (*w/w*) under AM 1.5G illumination (100 mW cm^{-2}).

D/A Ratio	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
1/1	7.3	0.76	31.5	1.8
1/2	12.4	0.74	59.6	5.5
1/3	11.5	0.73	51.7	4.4

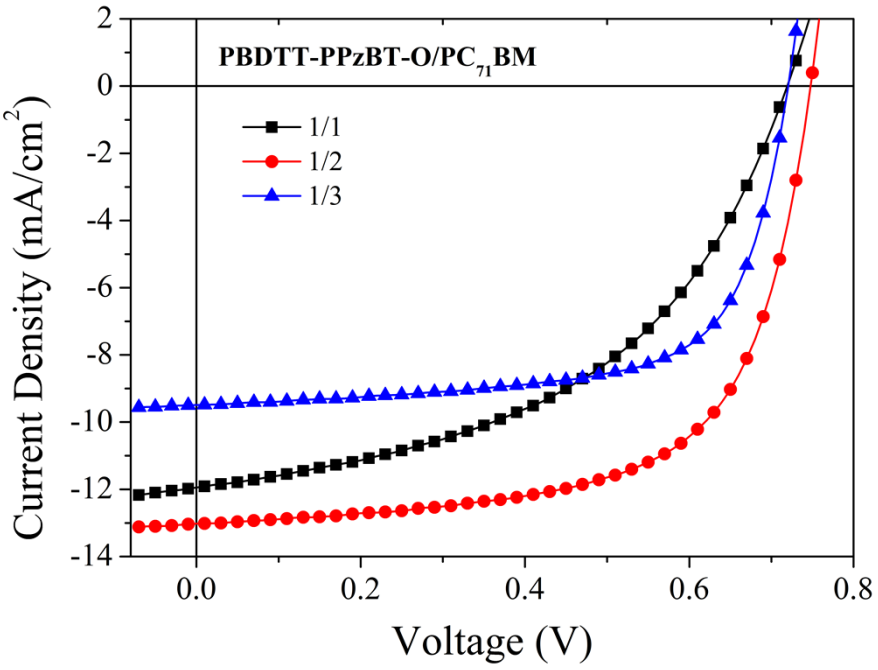

Fig S3c. *J-V* curves of the PBDTT-PPzBT-O/$PC_{71}BM$-based PSCs with different blend ratios (*w/w*) under AM 1.5G illumination (100 mW cm^{-2}).

Table S1c. Photovoltaic properties of the PBDTT-PPzBT-O/$PC_{71}BM$-based PSCs with different blend ratios (*w/w*) under AM 1.5G illumination (100 mW cm^{-2}).

D/A Ratio	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
1/1	11.9	0.72	48.1	4.1
1/2	13.0	0.75	64.8	6.3
1/3	9.5	0.72	67.8	4.6

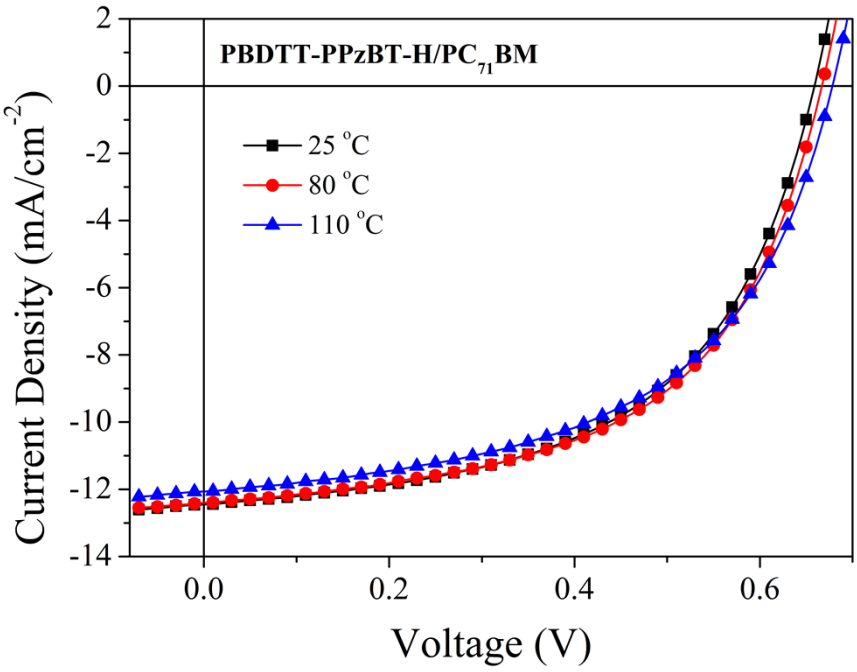

Fig. S4a. *J-V* curves of the PBDTT-PPzBT-H/$PC_{71}BM$-based PSCs with different temperature under AM 1.5G illumination (100 mW cm^{-2}).

Table S2a. Photovoltaic properties of the PBDTT-PPzBT-H/$PC_{71}BM$-based PSCs with different temperature under AM 1.5G illumination (100 mW cm^{-2}).

Temperature/ °C	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
25	12.4	0.66	54.4	4.4
80	12.4	0.67	55.0	4.5
110	12.0	0.68	53.7	4.4

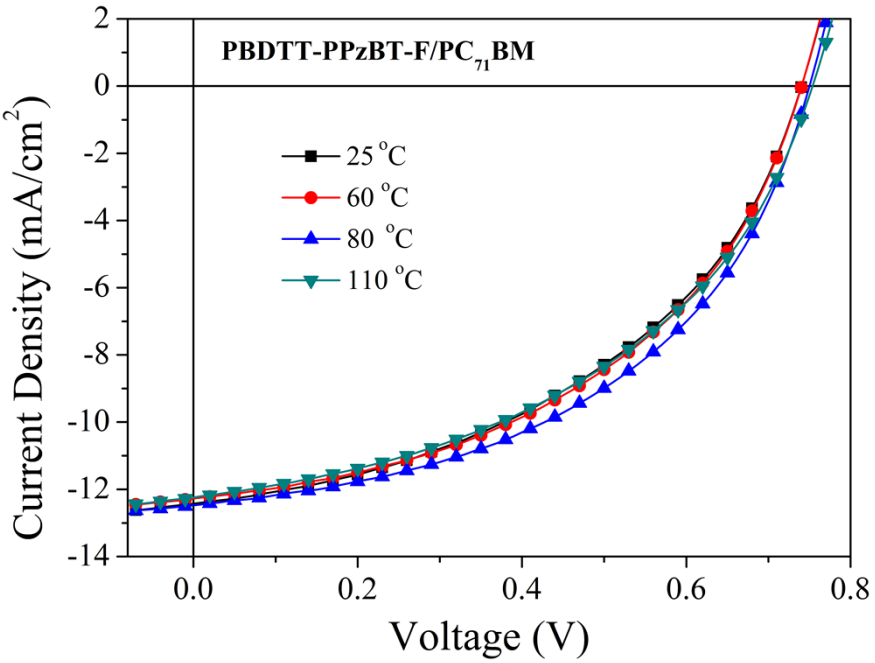

Fig. S4b. *J-V* curves of the PBDTT-PPzBT-F/$PC_{71}BM$-based PSCs with different temperature under AM 1.5G illumination (100 mW cm^{-2}).

Table S2b. Photovoltaic properties of the PBDTT-PPzBT-F/$PC_{71}BM$-based PSCs with different temperature under AM 1.5G illumination (100 mW cm^{-2}).

Temperature/ °C	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
25	12.4	0.74	45.3	4.1
60	12.3	0.74	46.6	4.2
80	12.4	0.75	48.3	4.5
110	12.2	0.75	45.4	4.2

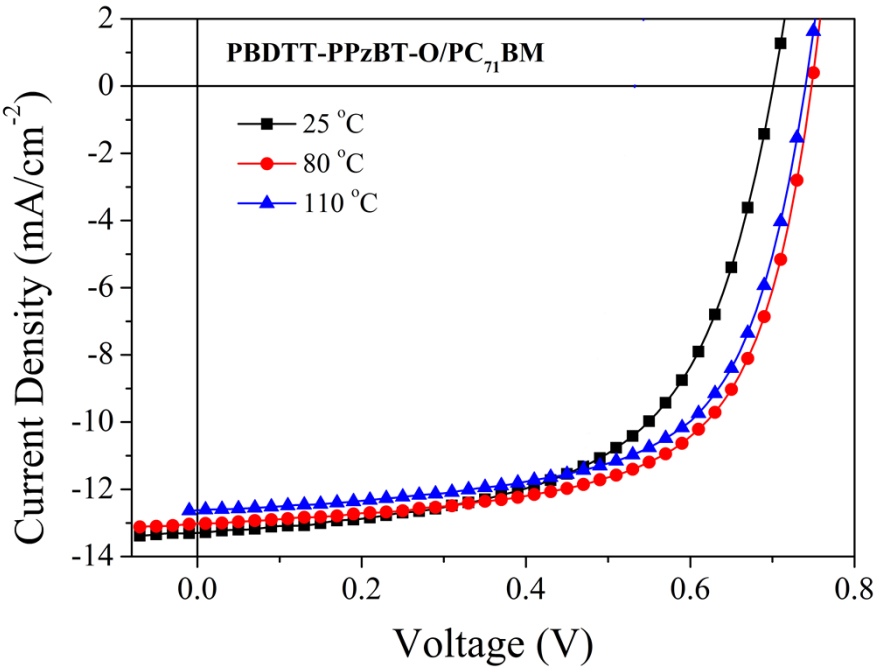

Fig. S4c. *J-V* curves of the PBDTT-PPzBT-O/$PC_{71}BM$-based PSCs with different temperature under AM 1.5G illumination (100 mW cm^{-2}).

Table S2c. Photovoltaic properties of the PBDTT-PPzBT-O/$PC_{71}BM$-based PSCs with different temperature under AM 1.5G illumination (100 mW cm^{-2}).

Temperature/ °C	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
25	13.3	0.70	59.4	5.5
80	13.0	0.75	64.8	6.3
110	12.6	0.74	64.2	6.0

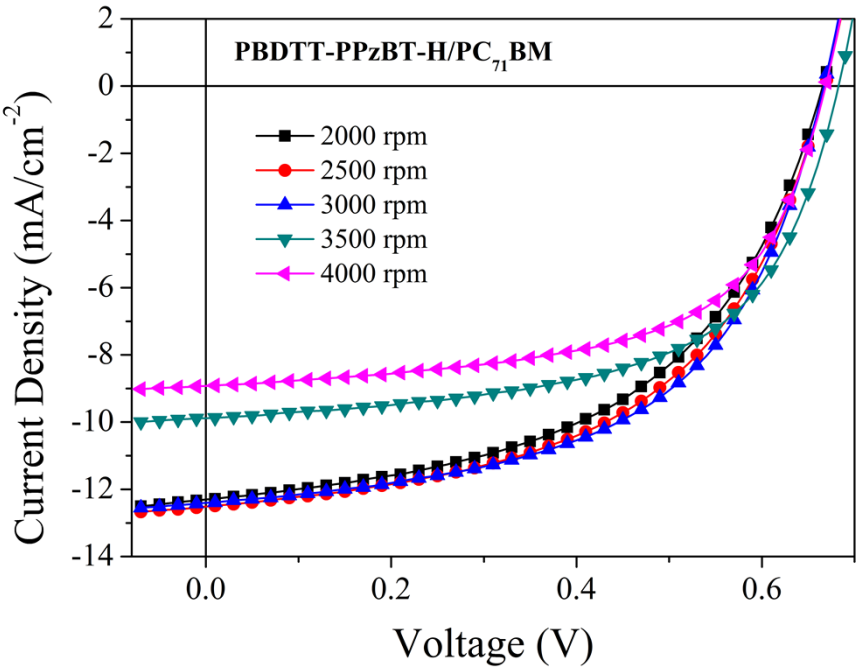

Fig. S5a. *J-V* curves of the PBDTT-PPzBT-H/$PC_{71}BM$-based PSCs with different spin-coating rate under AM 1.5G illumination (100 mW cm^{-2}).

Table S3a. Photovoltaic properties of the PBDTT-PPzBT-H/$PC_{71}BM$-based PSCs with different spin-coating rate under AM 1.5G illumination (100 mW cm^{-2}).

Spin-coating rate/ rpm	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
2000	12.3	0.66	51.5	4.2
2500	12.5	0.67	52.8	4.4
3000	12.4	0.67	55.0	4.5
3500	9.9	0.68	59.3	4.0
4000	8.9	0.67	60.0	3.6

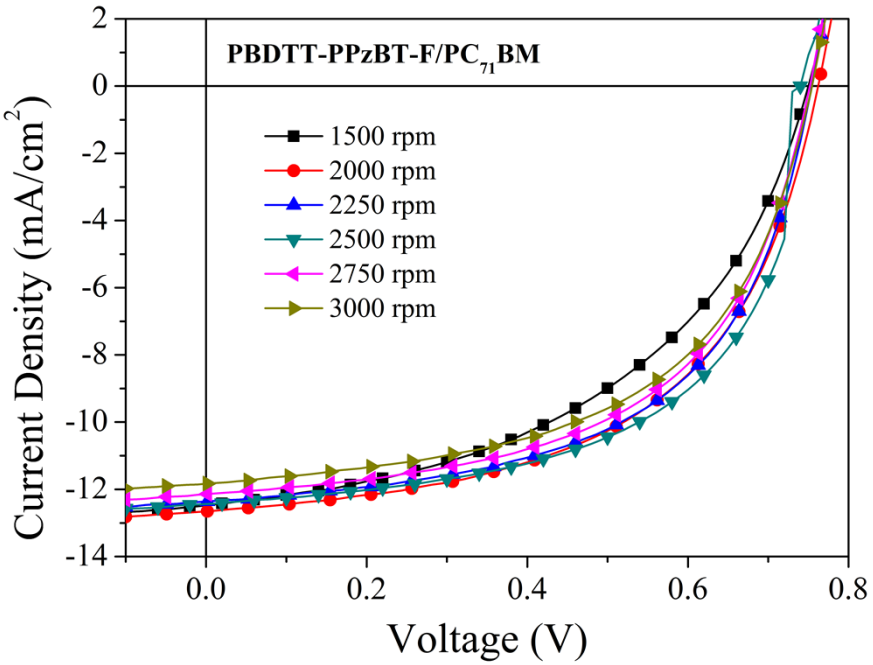

Fig. S5b. *J-V* curves of the PBDTT-PPzBT-F/$PC_{71}BM$-based PSCs with different spin-coating rate under AM 1.5G illumination (100 mW cm^{-2}).

Table S3b. Photovoltaic properties of the PBDTT-PPzBT-F/$PC_{71}BM$-based PSCs with different spin-coating rate under AM 1.5G illumination (100 mW cm^{-2}).

Spin-coating rate/ rpm	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
1500	12.4	0.75	48.3	4.5
2000	12.6	0.76	54.6	5.3
2250	12.4	0.75	56.4	5.3
2500	12.4	0.74	59.6	5.5
2750	12.1	0.75	55.7	5.1
3000	11.8	0.75	55.1	4.9

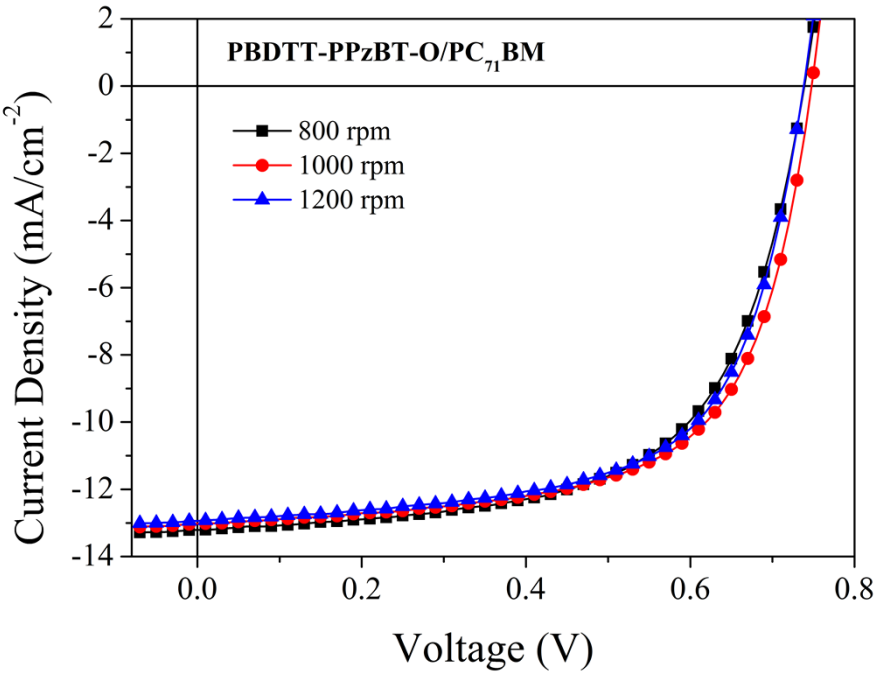

Fig S5c. *J-V* curves of the PBDTT-PPzBT-O/$PC_{71}BM$-based PSCs with different spin-coating rate under AM 1.5G illumination (100 mW cm^{-2}).

Table S3c. Photovoltaic properties of the PBDTT-PPzBT-O/$PC_{71}BM$-based PSCs with different spin-coating rate under AM 1.5G illumination (100 mW cm^{-2}).

Spin-coating rate/ rpm	J_{sc}/ mA cm^{-2}	V_{oc}/ V	*FF*/ %	PCE_{max}/ %
800	13.2	0.74	62.2	6.1
1000	13.0	0.75	64.8	6.3
1200	12.9	0.74	64.4	6.0