Supporting Information

for

Develop Donor Polymer Using B←N Unit for Suitable LUMO/HOMO Energy Levels and Improved Photovoltaic Performance

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1. ^{1}H NMR spectra of polymers PBNCPDT and PCPDT

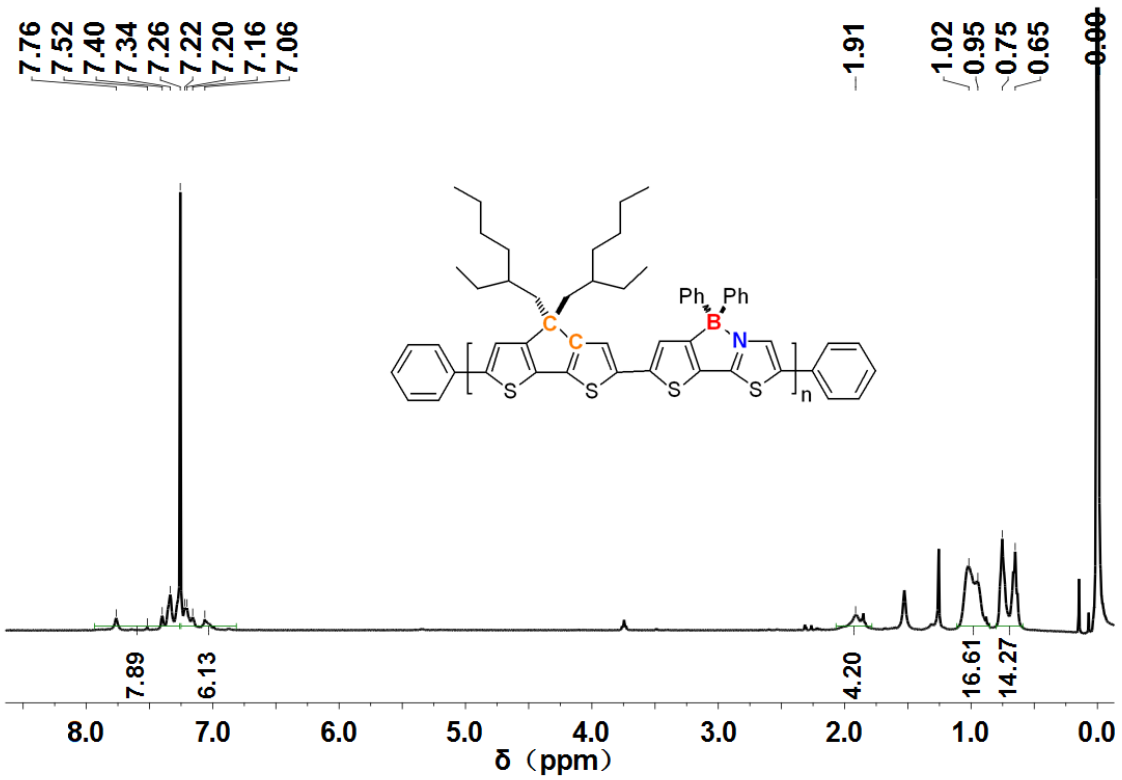

Figure S1. ^{1}H NMR spectrum of polymer **PBNCPDT** in $CDCl_3$ at 25 °C.

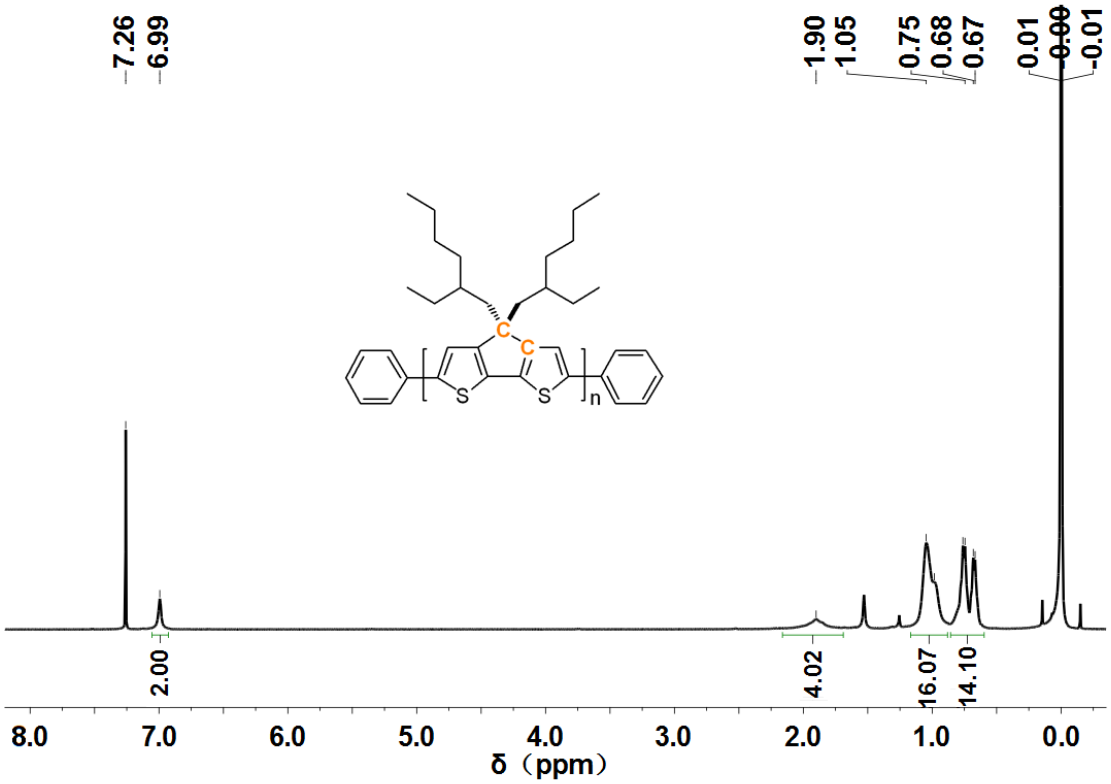

Figure S2. ^{1}H NMR spectrum of polymer **PCPDT** in $CDCl_3$ at 25 °C.

2. Thermal stability

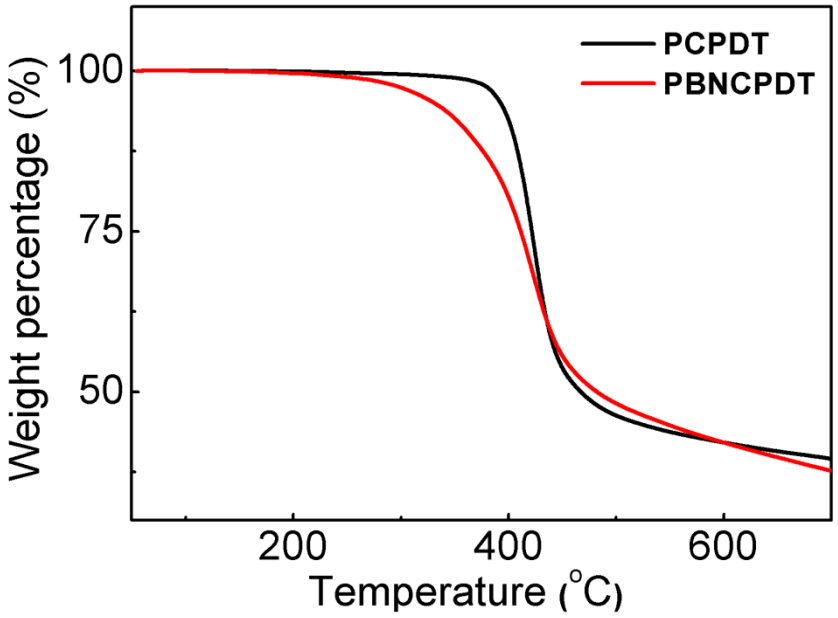

Figure S3. TGA curves of **PBNCPDT** and **PCPDT**.

3. Fluorescence spectra

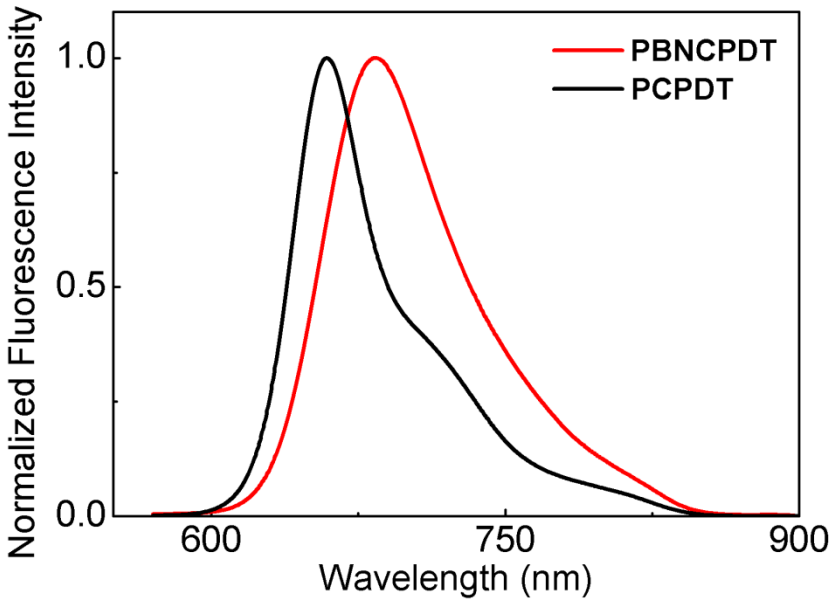

Figure S4. Normalized fluorescence spectra of **PBNCPDT** and **PCPDT** in *o*-DCB (λ_{ex} = 570 nm).

4. PSC device performance

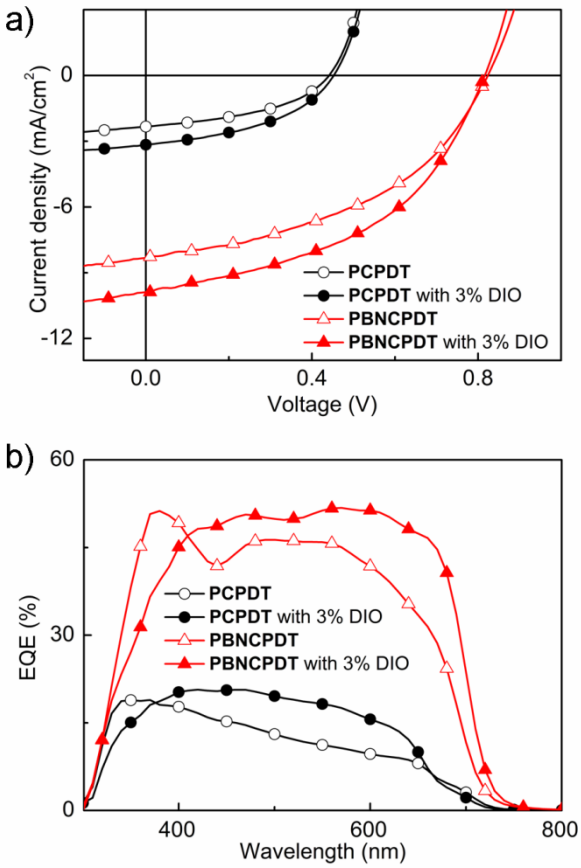

Figure S5. a) The *J-V* curves of **PBNCPDT** (red line) or **PCPDT** (black line)/$PC_{71}BM$ solar cells under AM 1.5 G (100 mW/cm^2 irradiation intensity) and b) The EQE curves of **PBNCPDT** (red line) or **PCPDT** (black line)/$PC_{71}BM$ solar cells. The performance of the device of **PBNCPDT**:$PC_{71}BM$ with DIO is significantly higher than that of the device of **PCPDT**:$PC_{71}BM$ with DIO, though their performance are both enhanced after adding DIO additive.

Table S1. Photovoltaic properties of polymer solar cells under AM 1.5 G illumination, 100 mW cm^{-2}.

Polymer/$PC_{71}BM$[a]	Voc (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
PCPDT	0.44	2.33	44.2	0.45
PCPDT[b]	0.45	3.16	44.3	0.63
PBNCPDT	0.82	8.32	44.9	3.06
PBNCPDT[b]	0.82	9.89	46.1	3.74

[a]The optimized proportion was 1:3 (Polymer:$PC_{71}BM$). [b]Processed with 3 vol % DIO (1,8-diiodooctane), relative to *o*-

DCB.

5. GI-XRD patterns of films

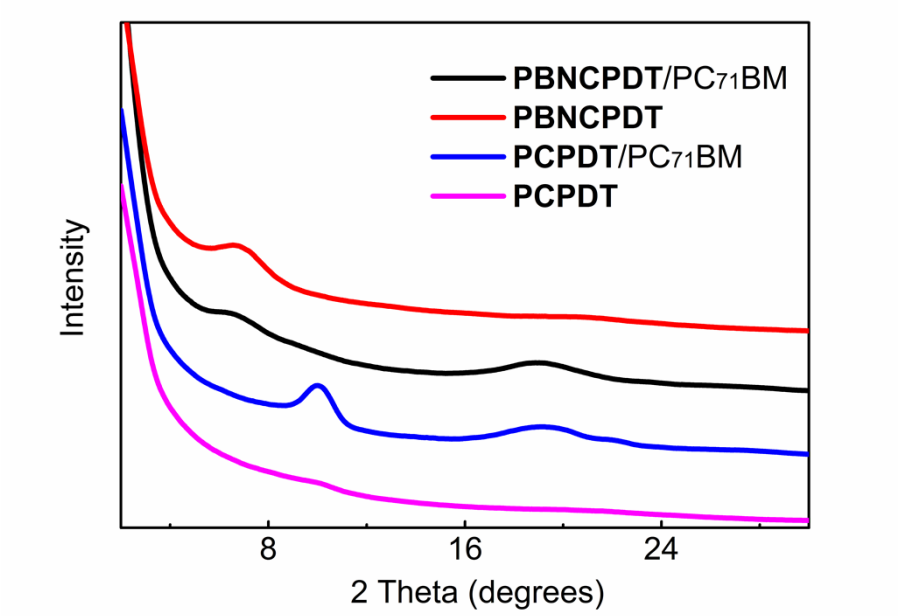

Figure S6. Out-of plane grazing incidence X-ray diffraction (GI-XRD) patterns of the prime films and blend films from *o*-DCB/DIO solutions. Compared with the **PCPDT** prime films, **PBNCPDT** shows much more ordered and crystalline packing structures with diffraction peak around 6.7 º. In the blend films, both of them show improved ordered structures.

6. Reference

Gaussian 09 (Revision A.02), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, *Gaussian, Inc*., Wallingford CT, 2009.