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

Supplementary Information

Synthesis of 6*H*-benzo[c]chromene as a new electron-rich building block of conjugated alternating copolymers and its application to polymer solar cells†

Jong Won Lee, Seunghwan Bae and Won Ho Jo*

Department of Materials Science and Engineering, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 151-744, Korea

Table S1. Photovoltaic properties of PBCTBT:$PC_{71}BM$ under standard AM 1.5G illumination cast from DCB with 2 vol% DIO.

PBCDTBT: $PC_{71}BM$ (w/w)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF	PCE (%)
1:4	0.85	4.02	0.39	1.27±0.05
1:3	0.84	6.75	0.43	2.30±0.10
1:2	0.84	9.04	0.48	3.60±0.12
1:1	0.85	6.73	0.37	2.08±0.05

Table S2. Photovoltaic properties of PBCDTBT:$PC_{71}BM$ under standard AM 1.5G illumination cast from CF and DCB mixture solvent (CF:DCB=1:2) with 2 vol% DIO.

PBCDTBT: $PC_{71}BM$ (w/w)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF	PCE (%)
1:3	0.83	8.88	0.47	3.46±0.11
1:2	0.87	11.10	0.48	4.63±0.17
1:1.5	0.87	12.51	0.52	5.56±0.14
1:1	0.84	10.68	0.45	4.04±0.13

Table S3. Photovoltaic properties of PBCDPP2T:$PC_{71}BM$ under standard AM 1.5G illumination cast from DCB with 4 vol% DIO.

PBCDTBT: $PC_{71}BM$ (w/w)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF	PCE (%)
1:4	0.78	3.36	0.43	1.11±0.09
1:3	0.78	5.79	0.45	2.01±0.15
1:2	0.79	3.89	0.47	1.46±0.12

Table S4. Calculated ground and excited state dipole moment of PFDTBT and PBCDTBT with DFT/TDDDFT B3LYP/6-31G level using Gaussian 09.

Dipole	μ_x (D)	μ_y (D)	μ_z (D)	Total (D)	$\Delta\mu_{eg}$ (D) [a]
$\mu_{g,\ PFDTBT}$	–0.7574	–0.3529	0.0736	0.8388	7.9709
$\mu_{e,\ PFDTBT}$	–7.3490	–4.8328	–0.0580	8.7959	
$\mu_{g,\ PBCDTBT}$	0.6615	–0.6416	0.2454	0.9536	9.3158
$\mu_{e,\ PBCDTBT}$	–7.4460	–5.2298	0.2063	9.1014	

[a]$\Delta\mu_{eg}$ represents the difference between the ground and excited state dipole moments, as calculated by $\Delta\mu_{eg}=[(\mu_{gx}-\mu_{ex})^2+(\mu_{gy}-\mu_{ey})^2+(\mu_{gz}-\mu_{ez})^2]^{1/2}$.

Table S5. Calculated ground and excited state dipole moment of PFDPP2T and PBCDPP2T with DFT/TDDDFT B3LYP/6-31G level using Gaussian 09.

Dipole	μ_x (D)	μ_y (D)	μ_z (D)	Total (D)	$\Delta\mu_{eg}$ (D) [a]
$\mu_{g,\ PFDPP2T}$	1.4228	0.1144	0.0806	1.4296	0.4973
$\mu_{e,\ PFDPP2T}$	0.9381	0.2200	0.0445	0.9645	
$\mu_{g,\ PBCDPP2T}$	–0.0421	–0.2382	–1.0961	1.1224	2.0865
$\mu_{e,\ PBCDPP2T}$	–0.5253	–0.3425	0.9310	1.1225	

[a]$\Delta\mu_{eg}$ represents the difference between the ground and excited state dipole moments, as calculated by $\Delta\mu_{eg}=[(\mu_{gx}-\mu_{ex})^2+(\mu_{gy}-\mu_{ey})^2+(\mu_{gz}-\mu_{ez})^2]^{1/2}$.

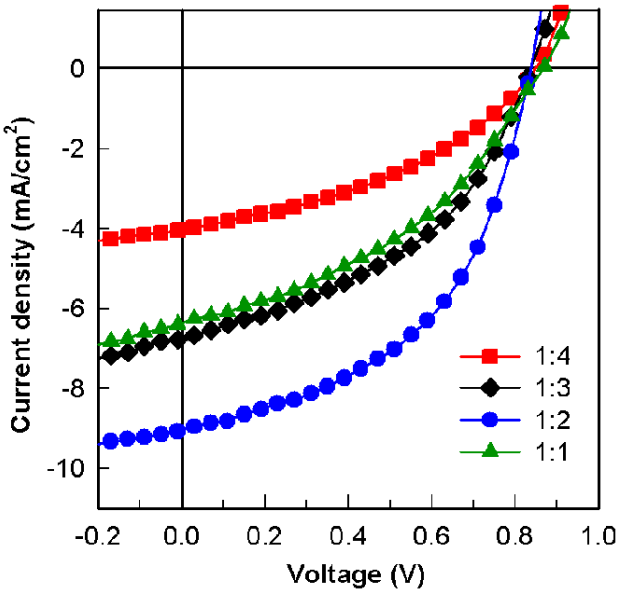

Fig. S1 *J–V* curves of PBCDTBT/$PC_{71}BM$ BHJ solar cells under AM 1.5G, 100 mW/cm^2 cast from DCB with 2 vol% DIO.

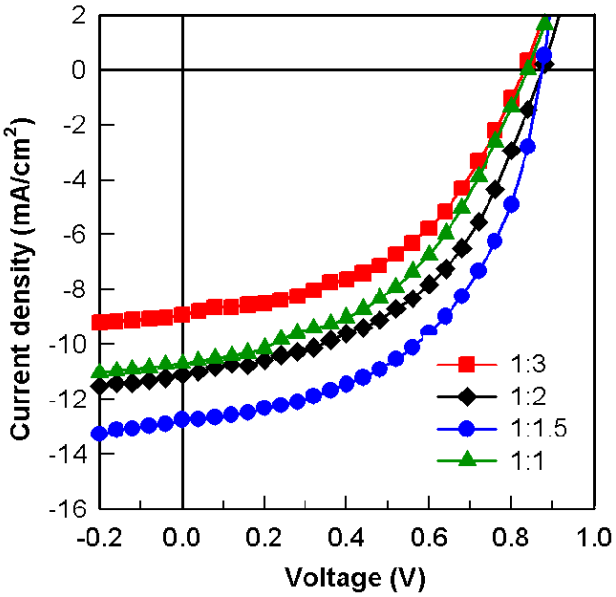

Fig. S2 *J–V* curves of PBCDTBT/$PC_{71}BM$ BHJ solar cells under AM 1.5G, 100 mW/cm^2 cast from CF and DCB mixture solvent (CF:DCB=1:2) with 2 vol% DIO.

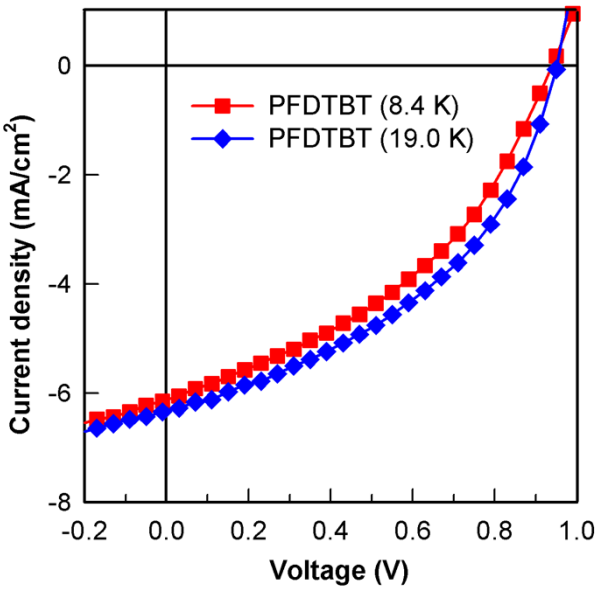

Fig. S3 *J–V* curves of BHJ solar cells fabricated from two PFDTBTs with different molecular weights blended with $PC_{71}BM$ under AM 1.5G, 100 mW/cm^2.

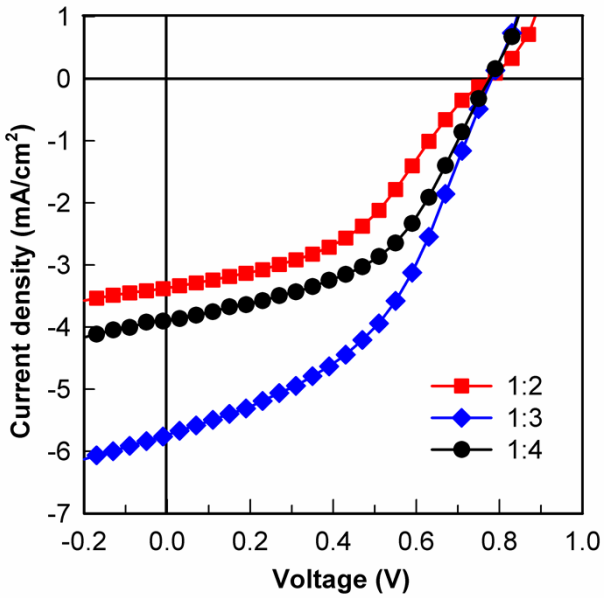

Fig. S4 *J–V* curves of PBCDPP2T/$PC_{71}BM$ BHJ solar cells under AM 1.5G, 100 mW/cm^2 cast from DCB with 4 vol% DIO.

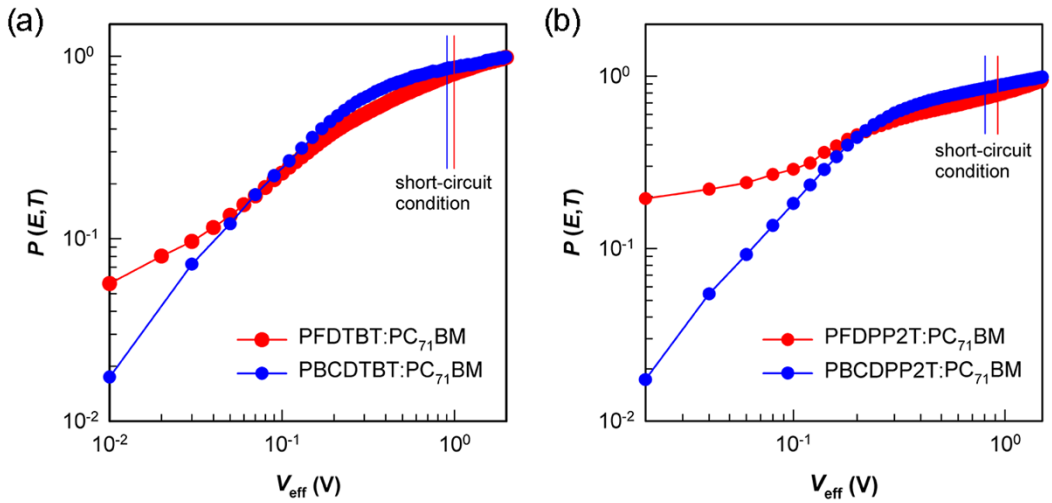

Fig. S5 Exciton dissociation probability ($P(E,T)$) plotted against effective voltage for DTBT-based polymers/$PC_{71}BM$ devices (a) and DPP-based polymers/$PC_{71}BM$ (b) under optimized condition.

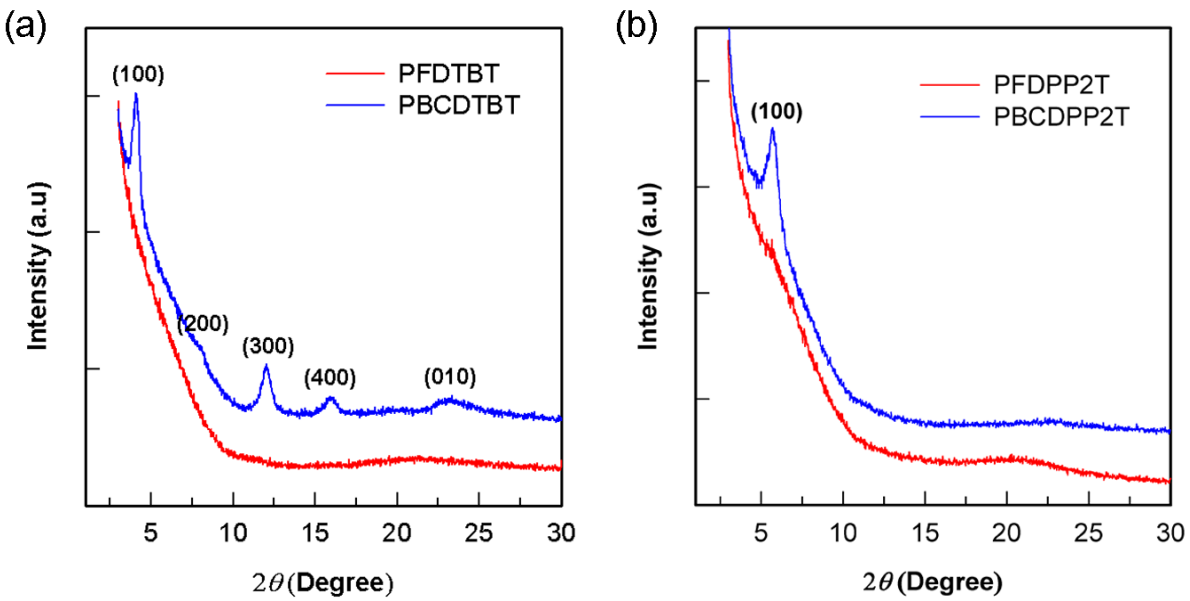

Fig. S6 XRD diffractograms of DTBT-based polymers (a) and DPP-based polymers (b) in thin film.

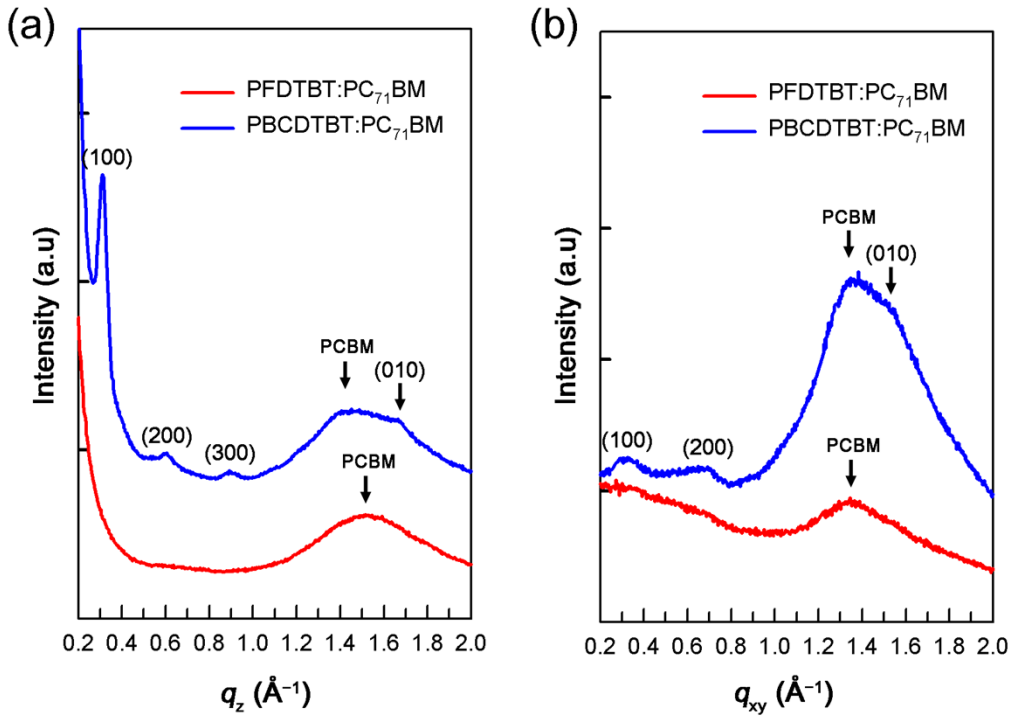

Fig. S7 GIWAXS patterns of blend thin film under optimized condition: out-of-plane (a) and in-plane scan (b).

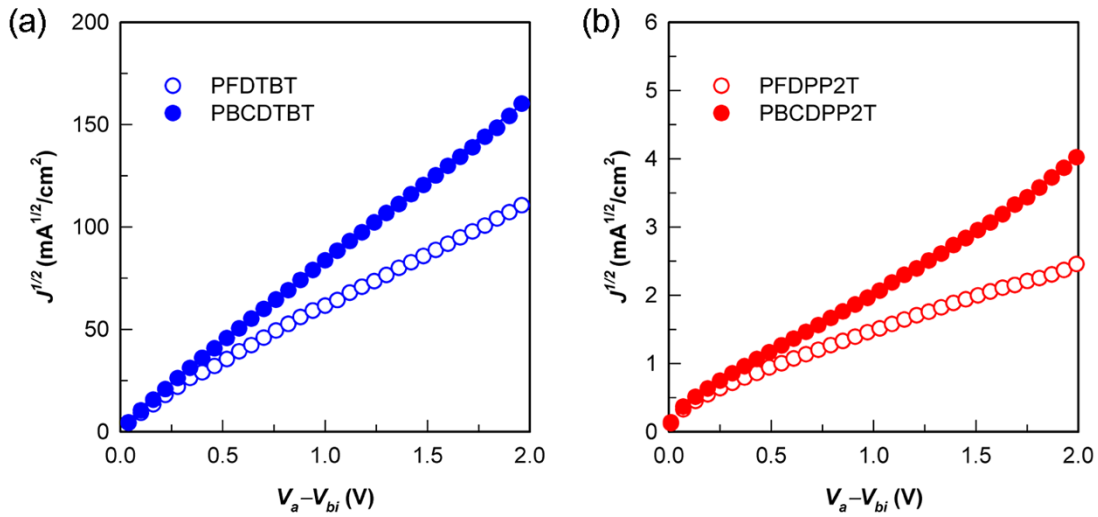

Fig. S8 Dark *J*–*V* characteristics of pristine DTBP-based polymers (a) and DPP-based polymers (b) with hole-only device.