

## **Supporting Information**

Modulation of the Properties of Pyrrolo[3,4-c]pyrrole-1,4-dione Based Polymers  
Containing 2,5-Di(2-thienyl)pyrrole Derivatives With Different Substitutions on  
the Pyrrole Unit

*Rajalingam Agneeswari,<sup>a</sup> Insoo Shin,<sup>b</sup> Vellaiappillai Tamilavan,<sup>a</sup> Dal Yong Lee,<sup>b</sup> Shinuk Cho,<sup>c</sup>  
Youngup Jin,<sup>d</sup> Sung Heum Park,<sup>\*b</sup> and Myung Ho Hyun<sup>\*a</sup>*

<sup>a</sup> *Department of Chemistry, Chemistry Institute for Functional Materials, Pusan National University, Busan 690-735, Republic of Korea*

<sup>b</sup> *Department of Physics, Pukyong National University, Busan 608-737, Republic of Korea*

<sup>c</sup> *Department of Physics and EHSRC, University of Ulsan, Ulsan 680-749, Republic of Korea*

<sup>d</sup> *Department of Industrial Chemistry, Pukyong National University, Busan 608-739, Republic of Korea*

**Fig. S1.** The XRD images of the polymers such as P(DKPP-TPTH), P(DKPP-TPTE), P(DKPP-TPTA), and P(DKPP-TPTI) as a film state. ----- 4

**Fig. S2.**  $J-V$  Curves of the PSCs prepared from P(DKPP-TPTH):PC<sub>70</sub>BM blend at different ratios (a), concentrations for P(DKPP-TPTH):PC<sub>70</sub>BM (1:2 wt%)+3vol% DIO blend (b), solvents for P(DKPP-TPTH):PC<sub>70</sub>BM (1:2 wt%) blend (c) and additives for P(DKPP-TPTH):PC<sub>70</sub>BM (1:2 wt%) blend (d). Note: All PSCs were prepared with 22 mg/ml blend solution expect for that made from 11 mg/ml blend solution in dichlorobenzene (DCB) and except for that made from chlorobenzene (CB). ----- 5

**Fig. S3.**  $J-V$  Curves of the PSCs prepared from P(DKPP-TPTE):PC<sub>70</sub>BM blend at different ratios (a) and concentrations for P(DKPP-TPTE):PC<sub>70</sub>BM (1:2 wt%) (b). Note: All PSCs were prepared with 22 mg/ml blend solution expect for that made from 33 mg/ml blend solution in dichlorobenzene (DCB). ----- 7

**Fig. S4.**  $J-V$  Curves of the PSCs prepared from P(DKPP-TPTA):PC<sub>70</sub>BM blend at different ratios (a) and concentrations for P(DKPP-TPTA):PC<sub>70</sub>BM (1:3 wt%) (b). Note: All PSCs were prepared with 22 mg/ml blend solution expect for that made from 33 mg/ml blend solution in dichlorobenzene (DCB). ----- 9

**Fig. S5.**  $J-V$  Curves of the PSCs prepared from P(DKPP-TPTI):PC<sub>70</sub>BM blend at different ratios (a), concentrations for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (b), solvents for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (c), additives (2 vol%) for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (d) and thermal post annealing for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (e). Note: All

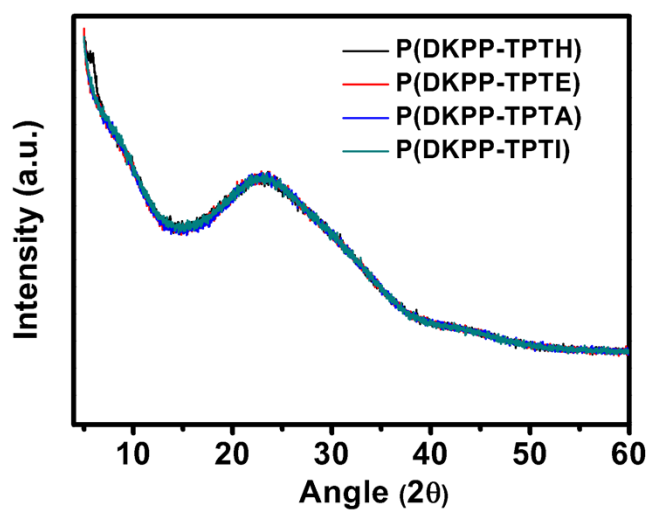
PSCs were prepared with 22 mg/ml blend solution expect for that made from 33 mg/ml blend solution in dichlorobenzene (DCB). -----11

**Table S1.** Photovoltaic properties of the PSCs made from P(DKPP-TPTH) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTH):PC<sub>70</sub>BM/Al. ----- 6

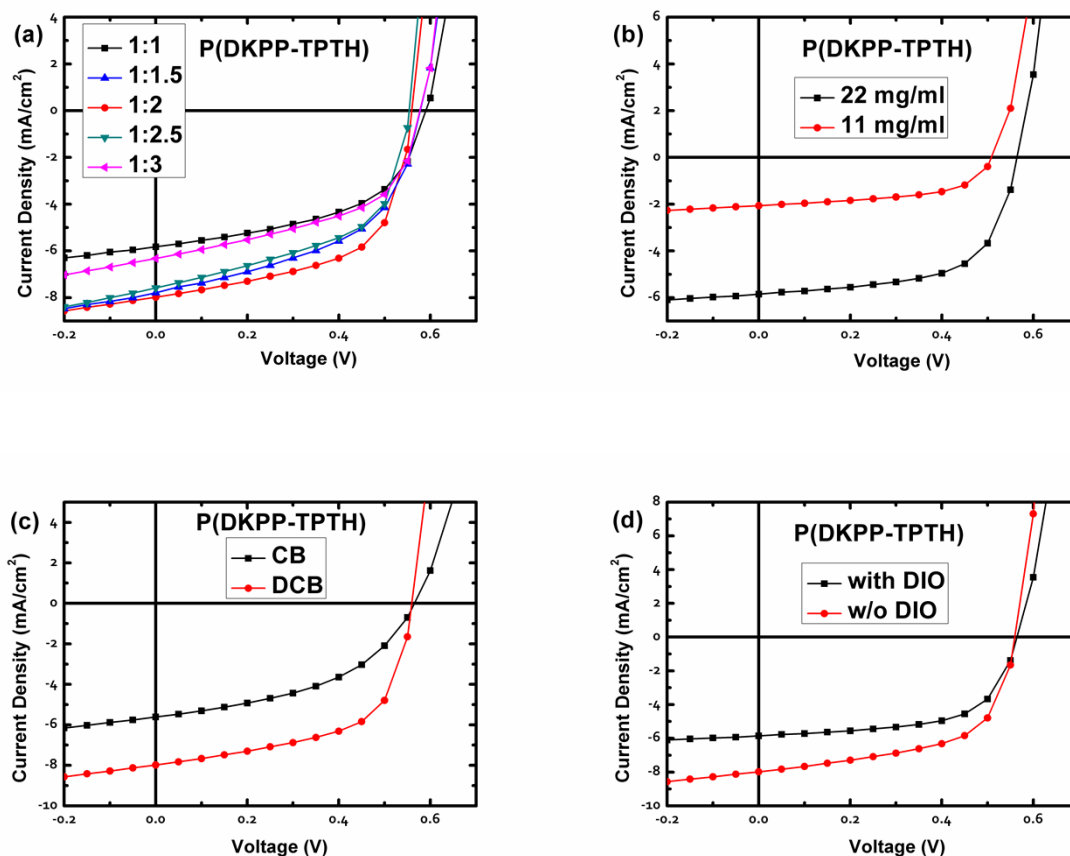
**Table S2.** Photovoltaic properties of the PSCs made from P(DKPP-TPTE) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTE):PC<sub>70</sub>BM/Al . ----- 8

**Table S3.** Photovoltaic properties of the PSCs made from P(DKPP-TPTA) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTA):PC<sub>70</sub>BM/Al . ----- 10

**Table S1.** Photovoltaic properties of the PSCs made from P(DKPP-TPTI) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTI):PC<sub>70</sub>BM/Al . ----- 12



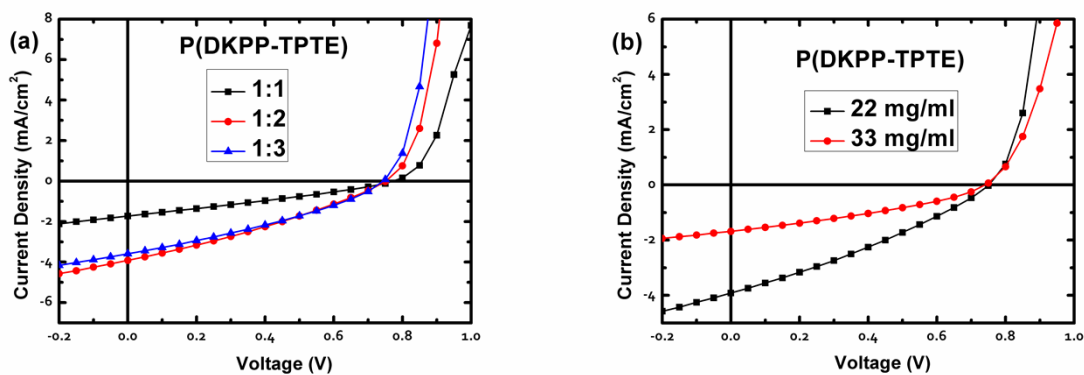
**Fig. S1.** The XRD images of the polymers such as P(DKPP-TPTH), P(DKPP-TPTE), P(DKPP-TPTA), and P(DKPP-TPTI) as a film state.



**Fig. S2.**  $J$ - $V$  Curves of the PSCs prepared from P(DKPP-TPTH):PC<sub>70</sub>BM blend at different ratios (a), concentrations for P(DKPP-TPTH):PC<sub>70</sub>BM (1:2 wt%)+3vol% DIO blend (b), solvents for P(DKPP-TPTH):PC<sub>70</sub>BM (1:2 wt%) blend (c) and additives for P(DKPP-TPTH):PC<sub>70</sub>BM (1:2 wt%) blend (d). Note: All PSCs were prepared with 22 mg/ml blend solution except for that made from 11 mg/ml blend solution in dichlorobenzene (DCB) and except for that made from chlorobenzene (CB).

**Table S1.** Photovoltaic properties of the PSCs made from P(DKPP-TPTH) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTH):PC<sub>70</sub>BM/Al.

Donor:Acceptor Ratio	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
1:1	5.82	0.59	52	1.79
1:1.5	7.79	0.59	50	2.28
1:2	7.98	0.56	59	2.63
1:2.5	7.59	0.55	53	2.23
1:3	6.32	0.59	50	1.86
Total Concentration	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
11 mg/ml	2.07	0.51	56	0.59
22 mg/ml	5.85	0.56	62	2.05
Solvent	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
CB	5.61	0.57	46	1.46
DCB	7.98	0.56	59	2.63
Additive	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
With DIO (3vol %)	5.85	0.56	62	2.05
Without DIO	7.98	0.56	59	2.63

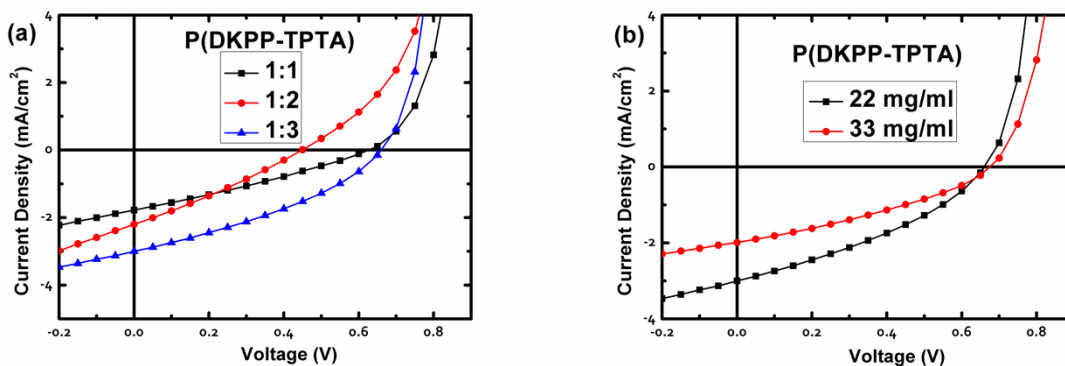


**Fig. S3.**  $J$ - $V$  Curves of the PSCs prepared from P(DKPP-TPTE):PC<sub>70</sub>BM blend at different ratios (a) and concentrations for P(DKPP-TPTE):PC<sub>70</sub>BM (1:2 wt%) (b). Note: All PSCs were prepared with 22 mg/ml blend solution expect for that made from 33 mg/ml blend solution in dichlorobenzene (DCB).

**Table S2.** Photovoltaic properties of the PSCs made from P(DKPP-TPTE) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTE):PC<sub>70</sub>BM/Al.

Donor:Acceptor				
Ratio	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
1:1	1.73	0.77	29	0.39
1:2	3.92	0.75	31	0.90
1:3	3.59	0.75	33	0.88
Total				
Concentration	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
11 mg/ml	3.92	0.75	31	0.90
22 mg/ml	1.69	0.74	33	0.42

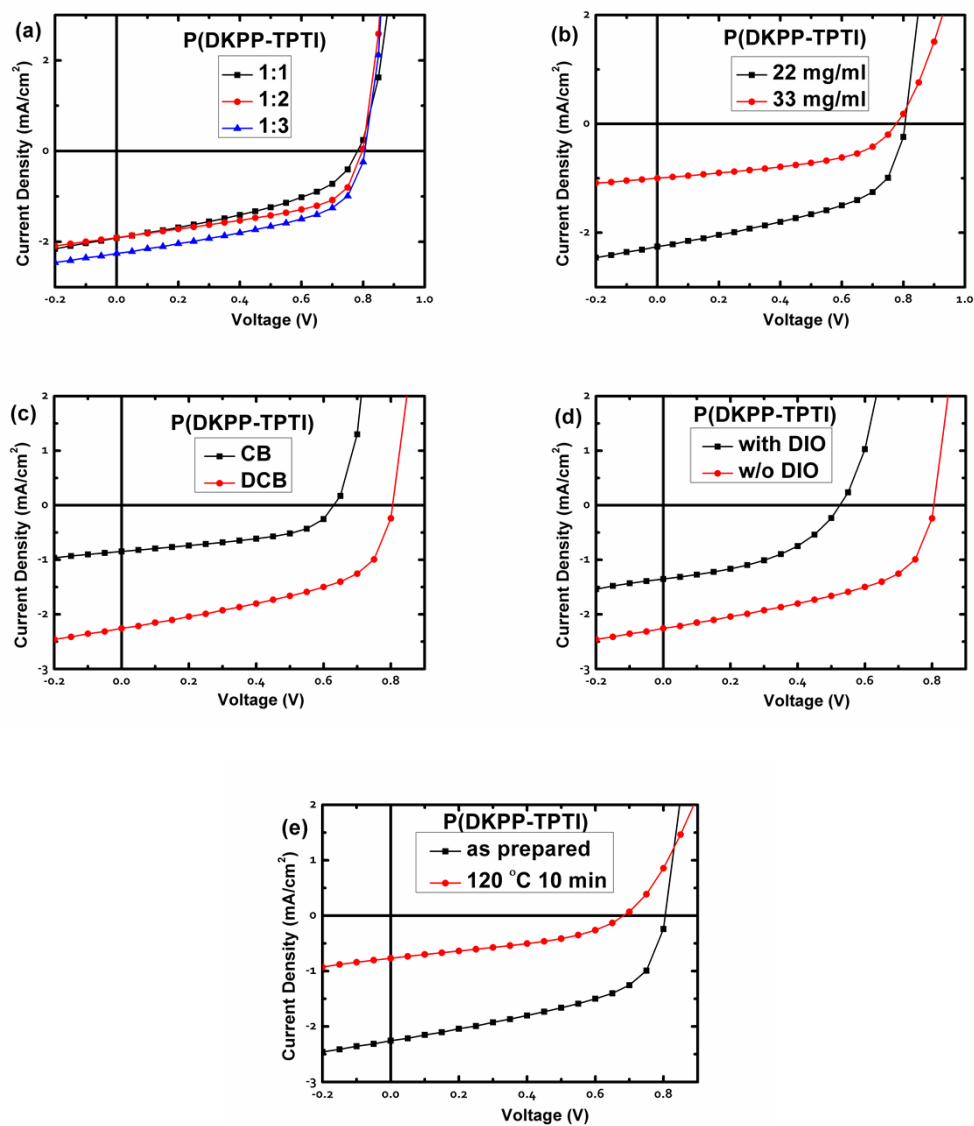




**Fig. S4.**  $J$ - $V$  Curves of the PSCs prepared from P(DKPP-TPTA):PC<sub>70</sub>BM blend at different ratios (a) and concentrations for P(DKPP-TPTA):PC<sub>70</sub>BM (1:3 wt%) (b). Note: All PSCs were prepared with 22 mg/ml blend solution expect for that made from 33 mg/ml blend solution in dichlorobenzene (DCB).

**Table S3.** Photovoltaic properties of the PSCs made from P(DKPP-TPTA) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTA):PC<sub>70</sub>BM/Al.

Donor:Acceptor Ratio	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
1:1	1.78	0.64	29	0.32
1:2	2.20	0.45	28	0.28
1:3	3.00	0.66	35	0.70
Total Concentration	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
22mg/ml	3.00	0.66	35	0.70
33mg/ml	1.99	0.67	34	0.45



**Fig. S5.**  $J$ - $V$  Curves of the PSCs prepared from P(DKPP-TPTI):PC<sub>70</sub>BM blend at different ratios (a), concentrations for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (b), solvents for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (c), additives (2 vol%) for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (d) and thermal post annealing for P(DKPP-TPTI):PC<sub>70</sub>BM (1:3 wt%) blend (e). Note: All PSCs were prepared with 22 mg/ml blend solution except for that made from 33 mg/ml blend solution in dichlorobenzene (DCB).

**Table S4.** Photovoltaic properties of the PSCs made from P(DKPP-TPTI) by using the configuration of ITO/PEDOT:PSS/P(DKPP-TPTI):PC<sub>70</sub>BM/Al.

Donor:Acceptor Ratio	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
1:1	1.92	0.79	41	0.63
1:2	1.91	0.80	51	0.78
1:3	2.26	0.81	50	0.91
Total Concentration	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
22mg/ml	2.26	0.81	50	0.91
33mg/ml	1.00	0.78	47	0.37
Solvent	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
CB	0.85	0.64	48	0.26
DCB	2.26	0.81	50	0.91
Additive	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
Without DIO	2.26	0.81	50	0.91
With DIO (3 vol%)	1.35	0.52	44	0.31
Post Annealing	J <sub>sc</sub> (mA/cm <sup>2</sup> )	V <sub>oc</sub> (V)	FF (%)	PCE (%)
As Prepared	2.26	0.81	50	0.91
Post annealing (120 °C)	0.77	0.69	39	0.21