Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Pyridine-bridged diketopyrrolopyrrole conjugated polymers for field-effect transistors and polymer solar cells

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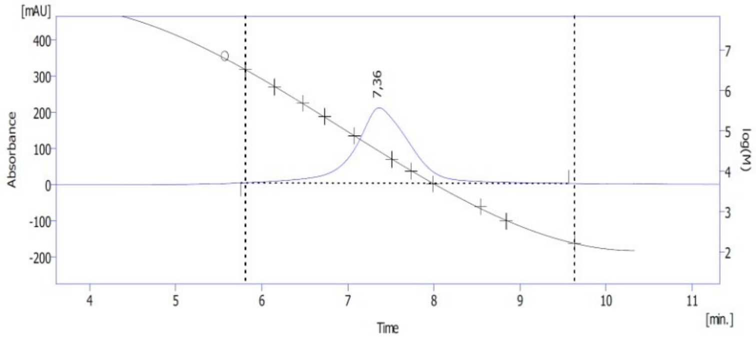
The supporting information contains GPC curves of DPP polymers (Fig. S1), absorption spectra of the polymers in chloroform (Fig. S2), Dihedral angle between the planes of pyridine-DPP and alternated aromatic units (Fig. S3), X-ray diffraction patterns and GIWAXS of the DPP polymers thin films (Fig. S4 and Fig. S5), Solar cell parameters of the DPP polymers with [70]PCBM (1:2) spin coated from chloroform with 3% vol. 1-CN (Table S1) and synthesis procedure, optical and photovoltaic properties based on OD-PDPP2PyT (Scheme S1, Fig. S6 and Table S2).

(a)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300
200
100
0
-100
-200
Absorbance
7,36
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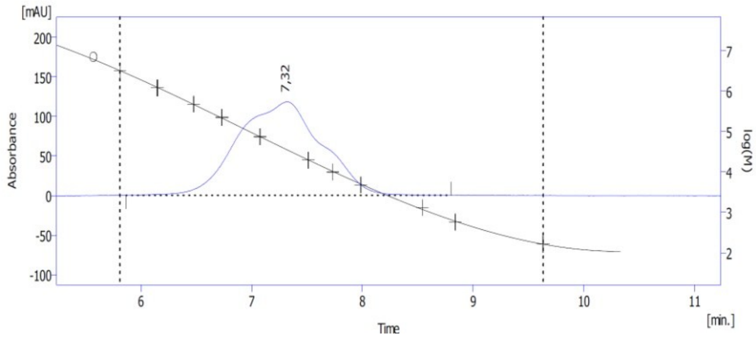
Time
[min.]
7 6 5 4 3 2
log(M)

(b)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Absorbance
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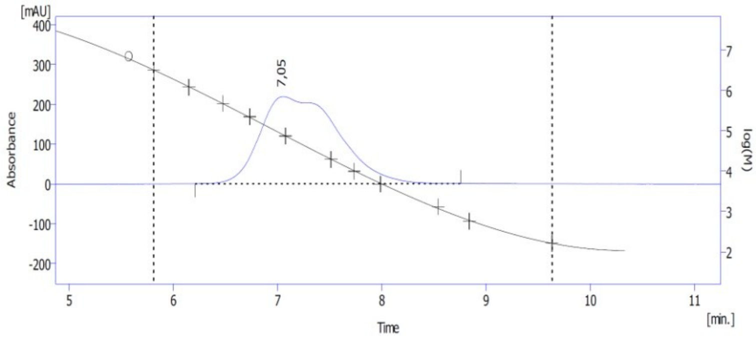
log(M)

(c)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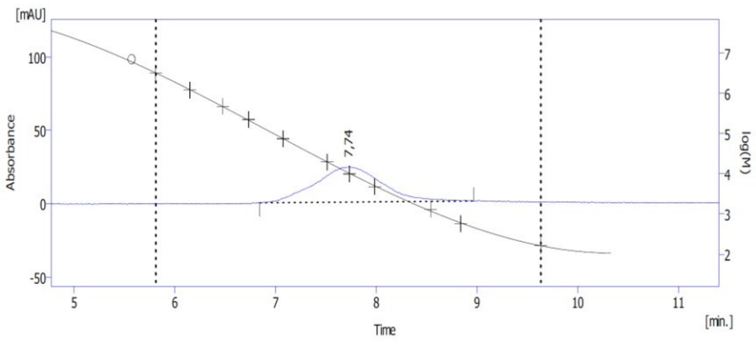
log(M)

(d)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Absorbance
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Time
[min.]
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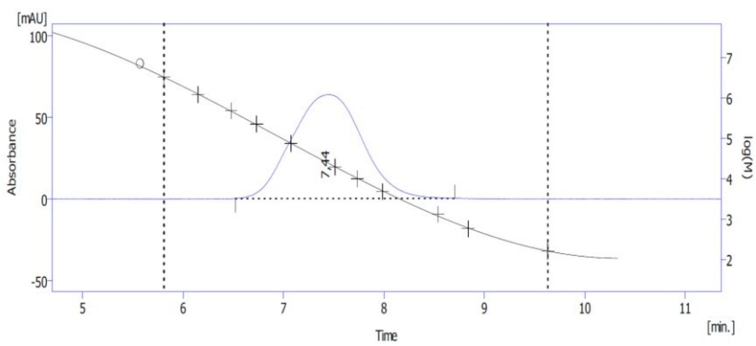
log(M)

(e)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7,44
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[min.]
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log(M)

Fig. S1 GPC recorded at 140 °C with *o*-DCB as eluent for the pyridine-bridged DPP polymers: (a) PDPP2Py2oT, (b) PDPP2PyBDT, (c) PDPP2PyT, (d) PDPP2PyBTD and (e) PDPP2PyNDI.

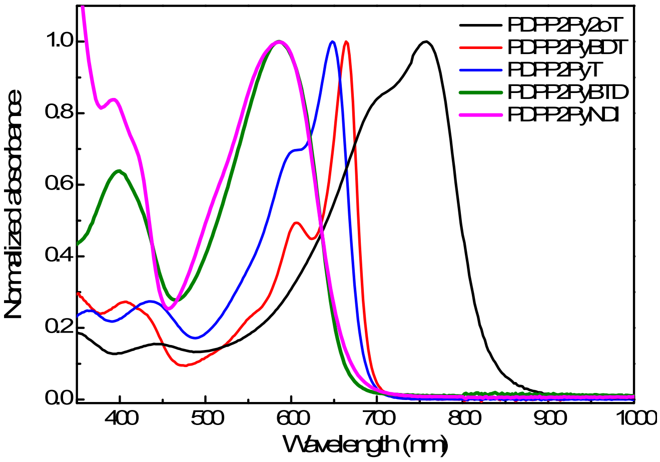


Fig. S2 Optical absorption spectra of the pyridine-bridged DPP polymers in chloroform solution.

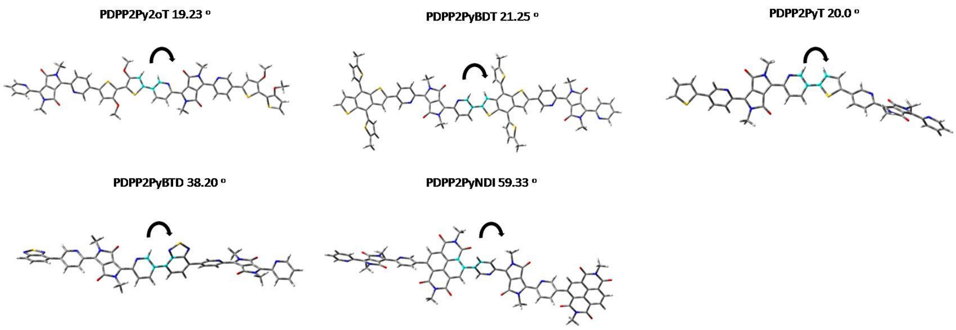


Fig. S3 Dihedral angle between the planes of pyridine-DPP and alternated aromatic units.

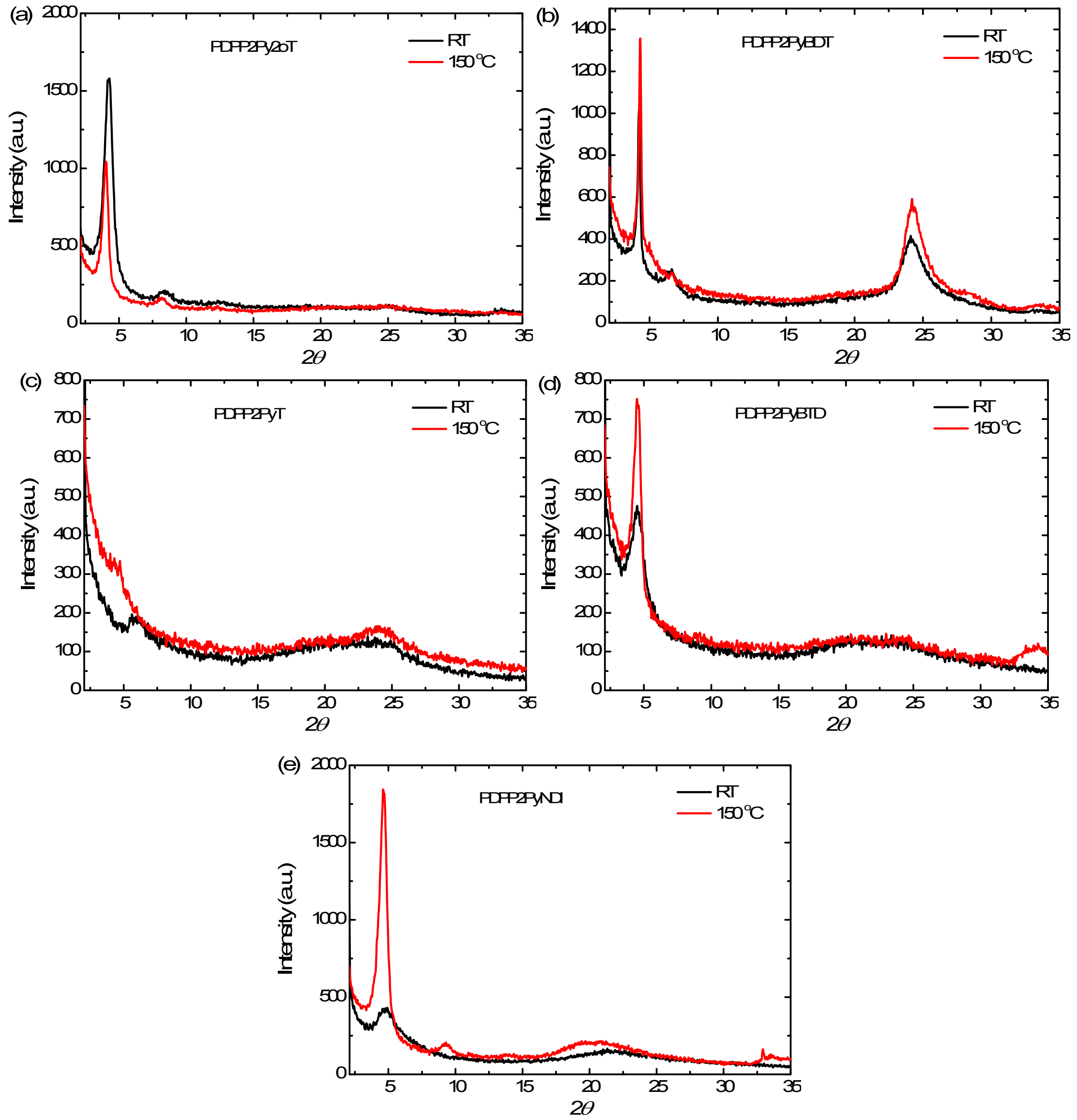


Fig. S4 X-ray diffraction patterns of thin films of the DPP polymers without thermal annealing (black line) and with thermal annealing at 150 ºC for 10 min (red line). *d*-Spacings for PDPP2Py2oT, PDPP2PyBDT, PDPP2PyT, PDPP2PyBTD and PDPP2PyNDI are 2.08 nm, 2.05 nm, 1.87 nm, 1.97 nm and 1.92 nm. Lamellar spacings for PDPP2PyBDT are 0.37 nm.

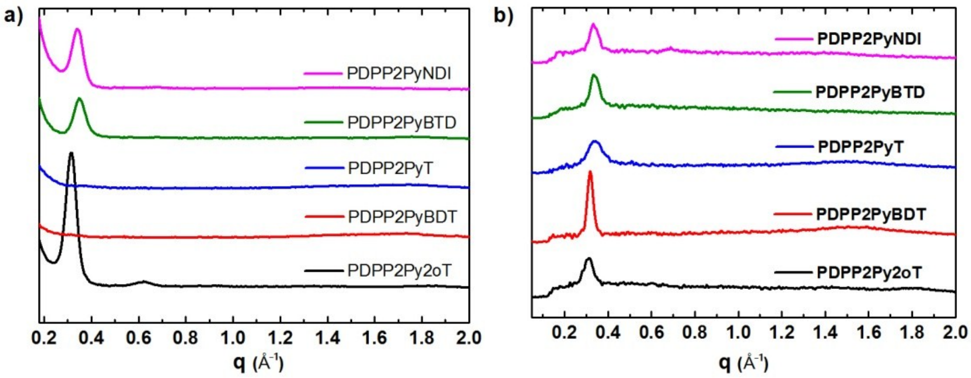
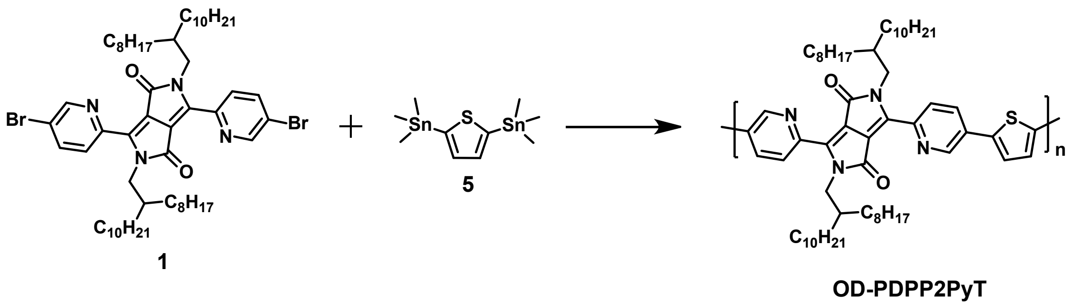


Fig. S5 (a) Out-of-plane and (b) In-plane profile of the pyridine-bridged DPP polymers thin films annealed at 150 °C for 10 min.

Table S1. Solar cell parameters of the DPP polymers with [70]PCBM (1:2) spin coated from chloroform with 3% vol. 1-CN or 10% vol. *o*-DCB.

Polymer	Solvent	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
PDPP2Py2oT	$CHCl_3$:3% 1-CN	4.5	0.53	0.45	1.1
PDPP2Py2oT	$CHCl_3$:10% *o*-DCB	3	0.53	0.29	0.46
PDPP2PyBDT	$CHCl_3$:3% 1-CN	3.5	0.88	0.47	1.4
PDPP2PyBDT	$CHCl_3$:10% *o*-DCB	2.8	0.72	0.59	1.18
PDPP2PyT	$CHCl_3$:3% 1-CN	1.3	0.88	0.45	0.5
PDPP2PyT	$CHCl_3$:10% *o*-DCB	2.1	0.74	0.52	0.81

Synthesis of OD-PDPP2PyT and their optical and photovoltaic properties



Scheme S1 Synthetic procedure for the polymer OD-PDPP2PyT.

Same procedure as for **PDPP2Py2oT** was used, but now **1** (98.68 mg, 0.098 mmol) and 2, 5-bis(trimethylstannyl)thiophene (**5**) (40.07 mg, 0.098 mmol) were used as the monomers. Yield: 55 mg (60%). GPC (*o*-DCB, 140 °C): M_n = 39.9 kg mol^{-1}, PDI = 3.76. Anal. Calcd. for $C_{60}H_{90}N_4O_2S$: C, 77.37; H, 9.74; N, 6.02. Found: C, 76.31; H, 9.61; N, 5.79.

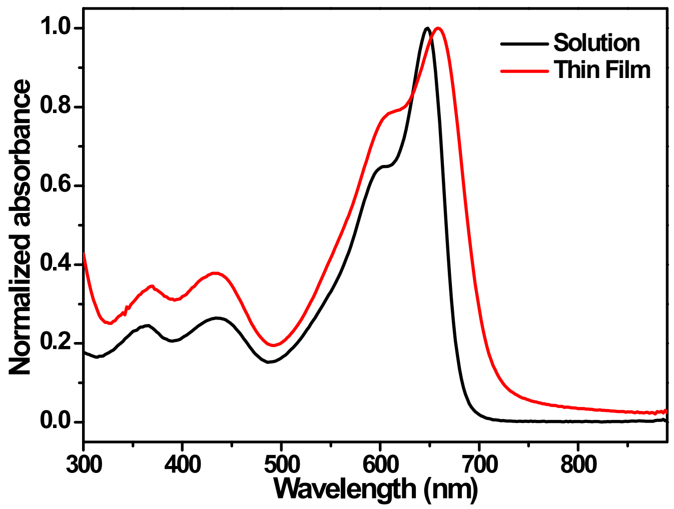


Fig. S6 Optical absorption spectra of OD-PDPP2PyT in chloroform solution and thin films. The absorption onset in thin film is 709 nm and E_g^{film} = 1.75 eV.

Table S2. Solar cell parameters of OD-PDPP2PyT:[70]PCBM (1:2) spin coated from chloroform with 5% vol. DIO, 3% vol. 1-CN or 10% vol. *o*-DCB. The thickness of the active layers is around 90 nm

Solvent	J_{sc} (mA/cm^2)	V_{oc} (V)	FF	PCE (%)
$CHCl_3$:5% DIO	1.9	0.81	0.29	0.43
$CHCl_3$:3% 1-CN	0.9	0.66	0.44	0.26
$CHCl_3$:10% *o*-DCB	0.8	0.6	0.39	0.19