Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Benzothiophene-flanked diketopyrrolopyrrole polymers: impact of isomeric frameworks on carrier mobilities

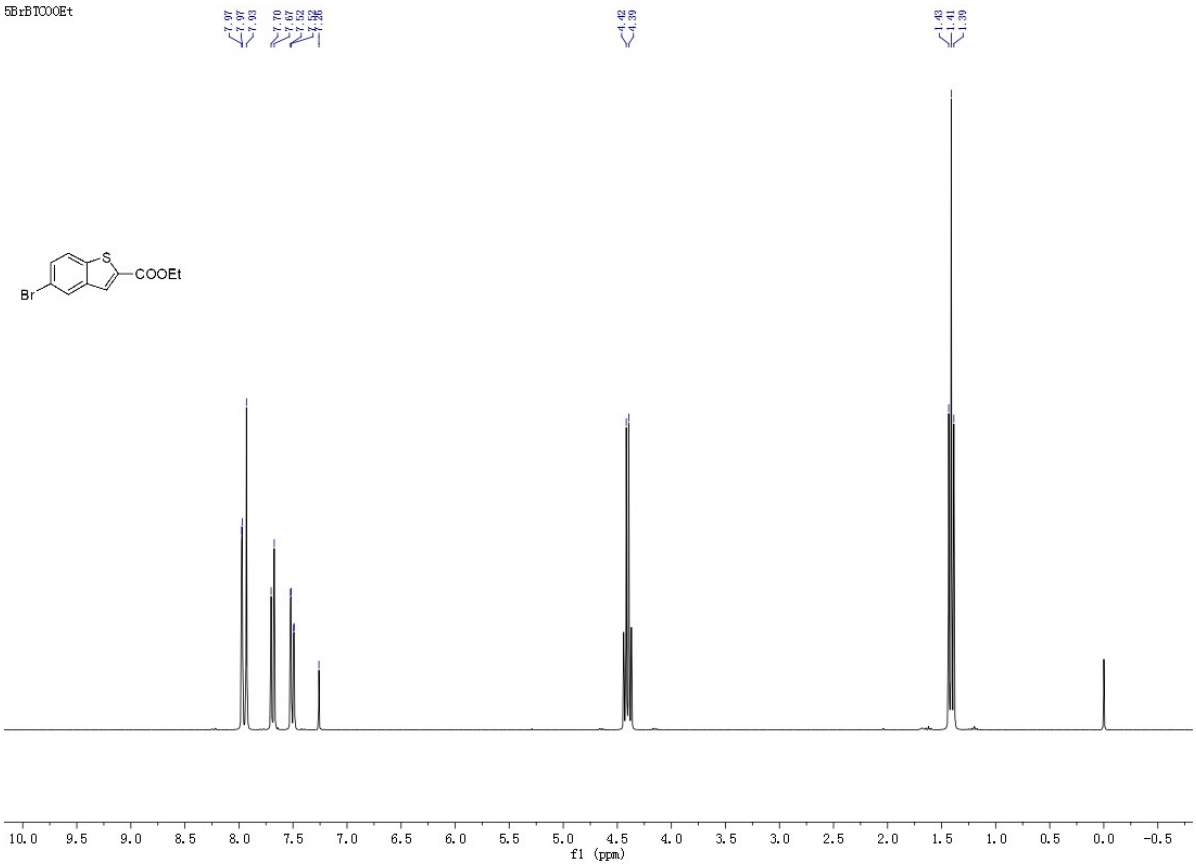
Jianyao Huang,‡[a] Xiaotong Liu,‡[a,b] Dong Gao,[a,b] Congyuan Wei,[a,b] Weifeng Zhang,[a] and Gui Yu*[a,b]

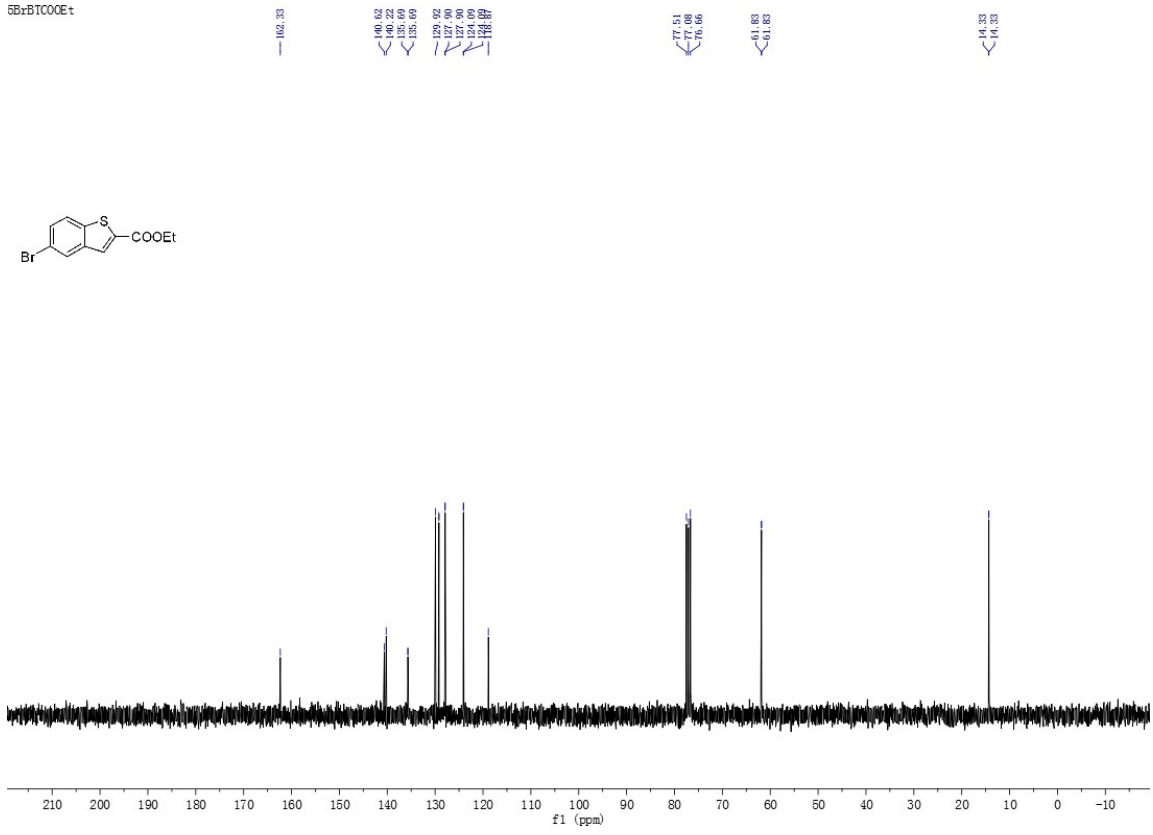
[a]Beijing National Laboratory for Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China

[b]University of Chinese Academy of Sciences, Beijing 100049, P. R. China

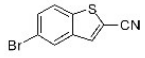
Contents

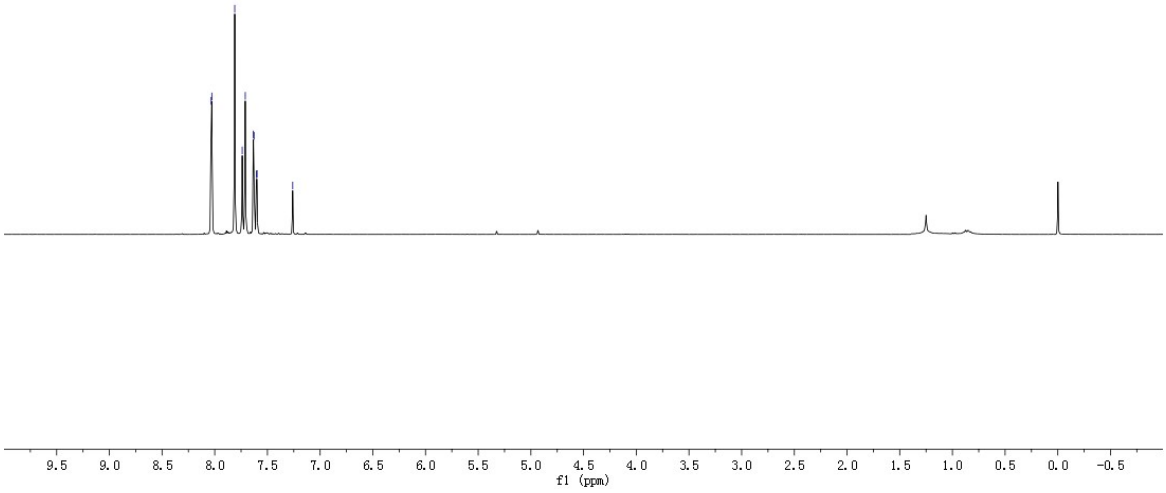
1. ^{1}H NMR and ^{13}C NMR spectra of new compounds



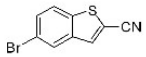


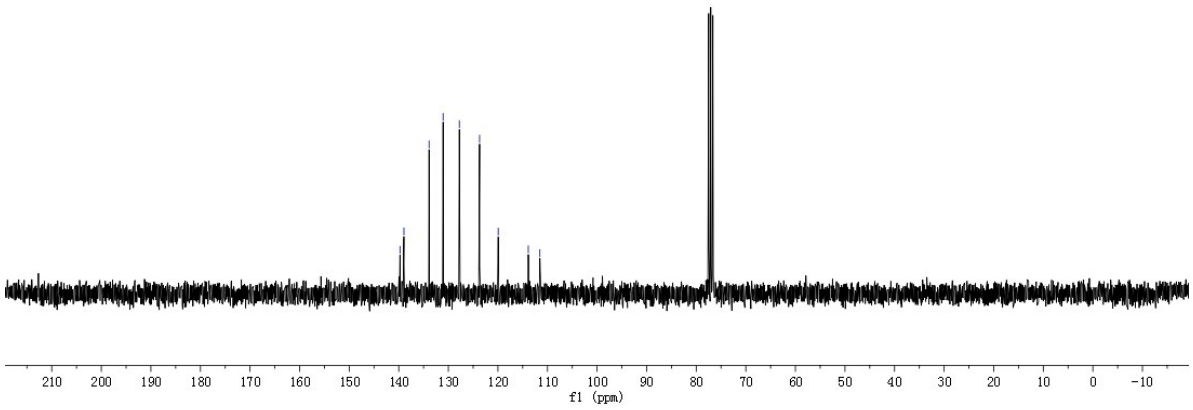
5BrBTCN

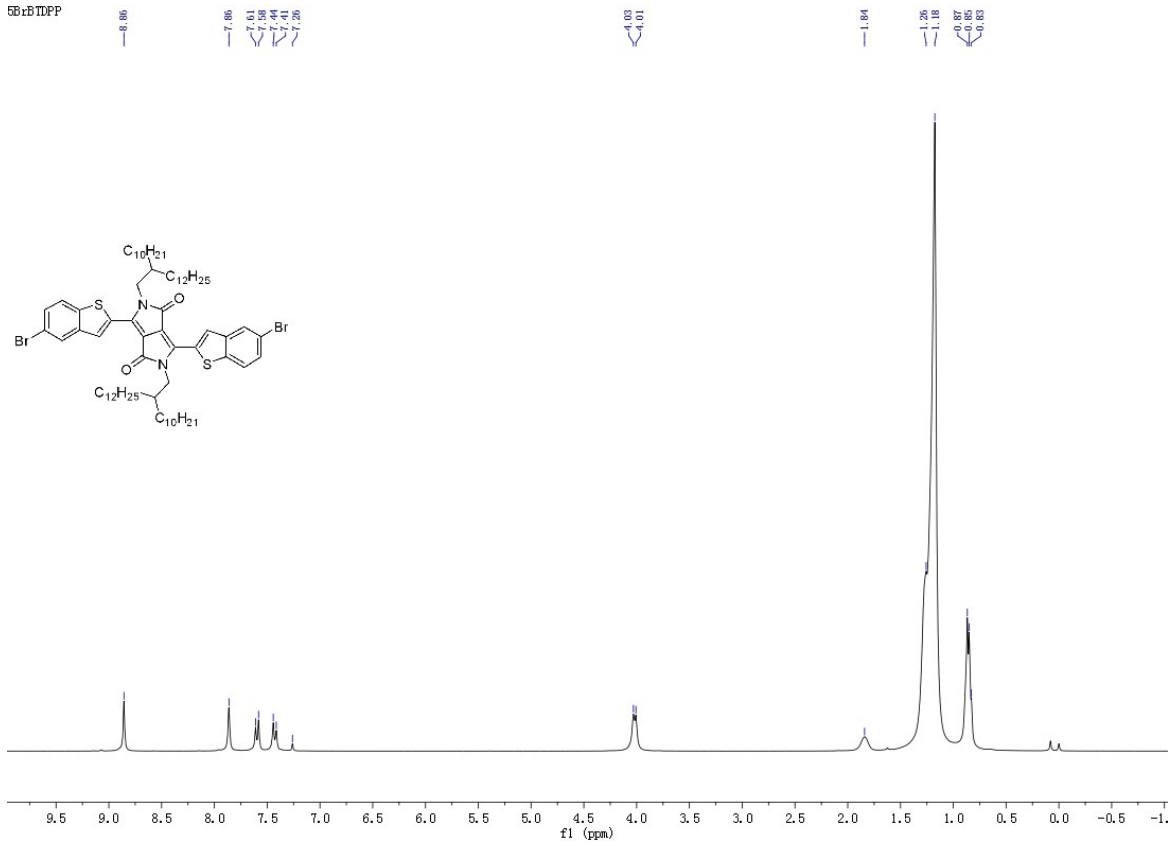


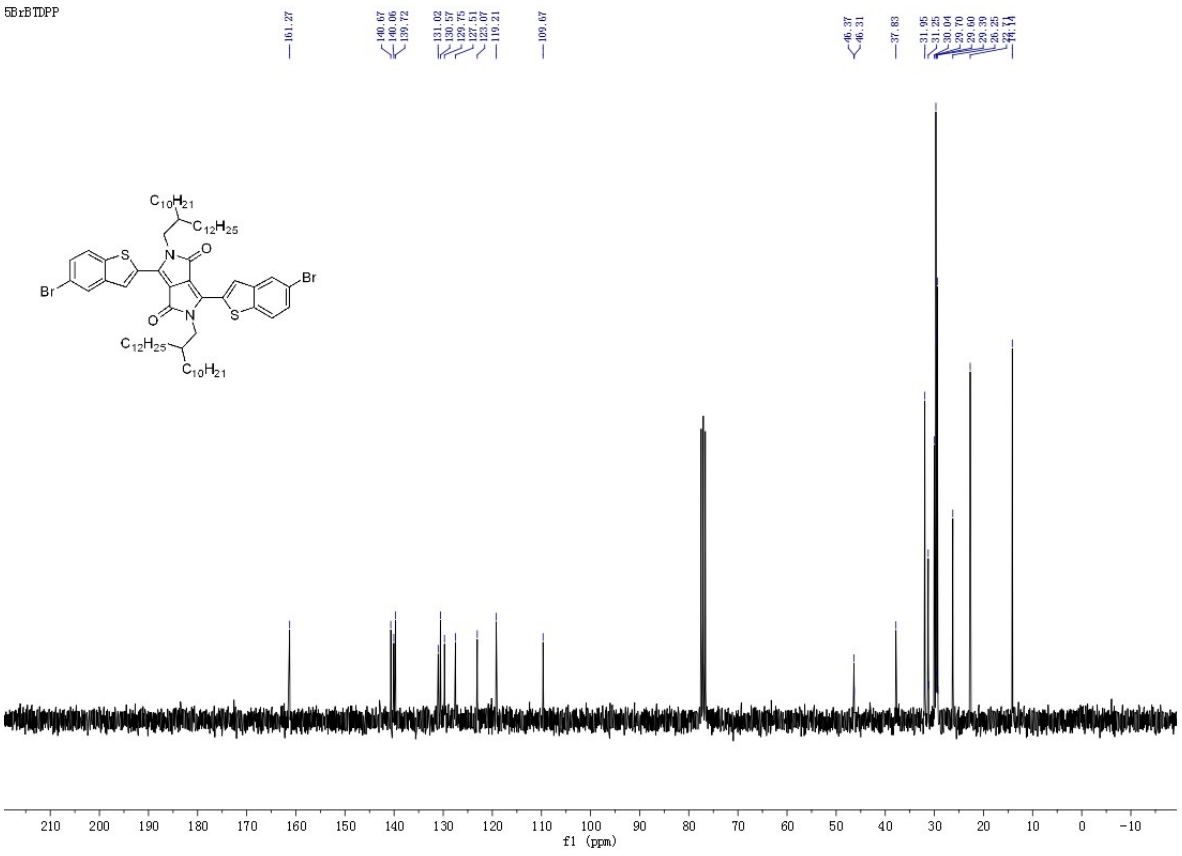


5BrBTCN

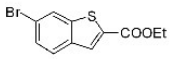


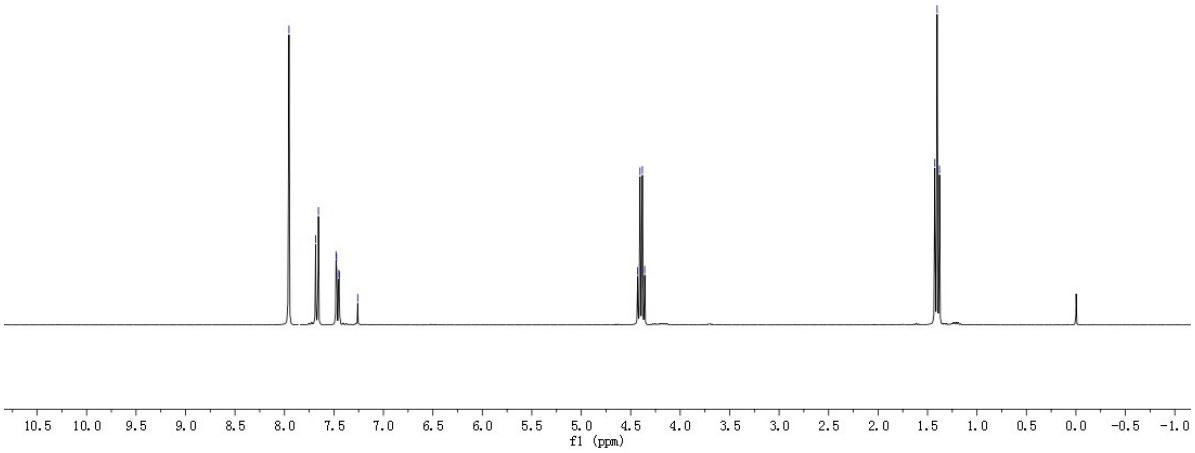



5BrBTDPP
8.86
7.61
7.58
7.44
7.41
7.26
4.03
4.01
1.84
1.26
1.18
0.87
0.85
0.83
f1 (ppm)

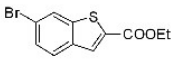

5BrBTDPP
161.27
140.67
140.06
139.72
131.02
130.57
129.75
127.51
123.07
119.21
109.67
46.37
46.31
37.83
31.95
31.25
30.04
29.70
29.60
29.39
26.25
22.74
14.14
f1 (ppm)

6BrBTCOOEt



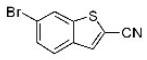


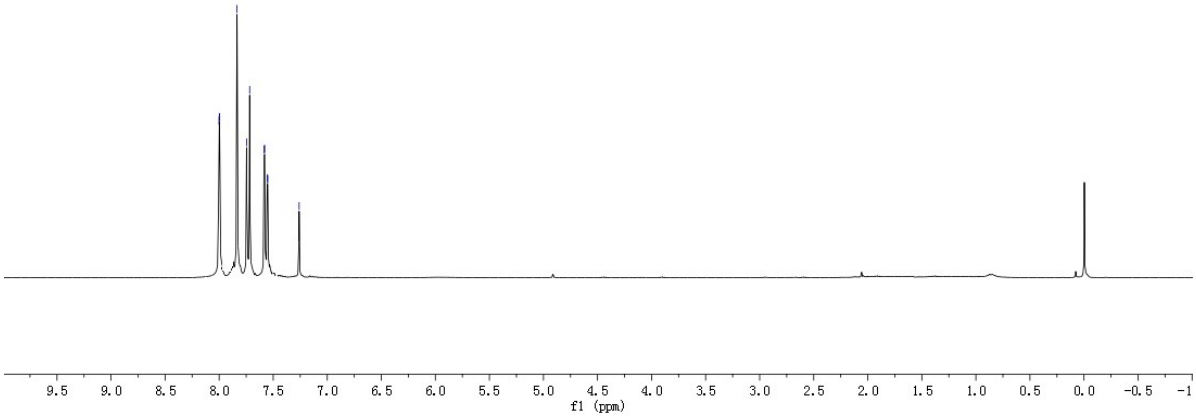
6BrBTCOOEt



6BrBTCN

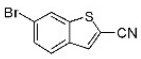
8.00
8.00
8.00
7.84
7.75
7.72
7.58
7.58
7.56
7.55
7.26

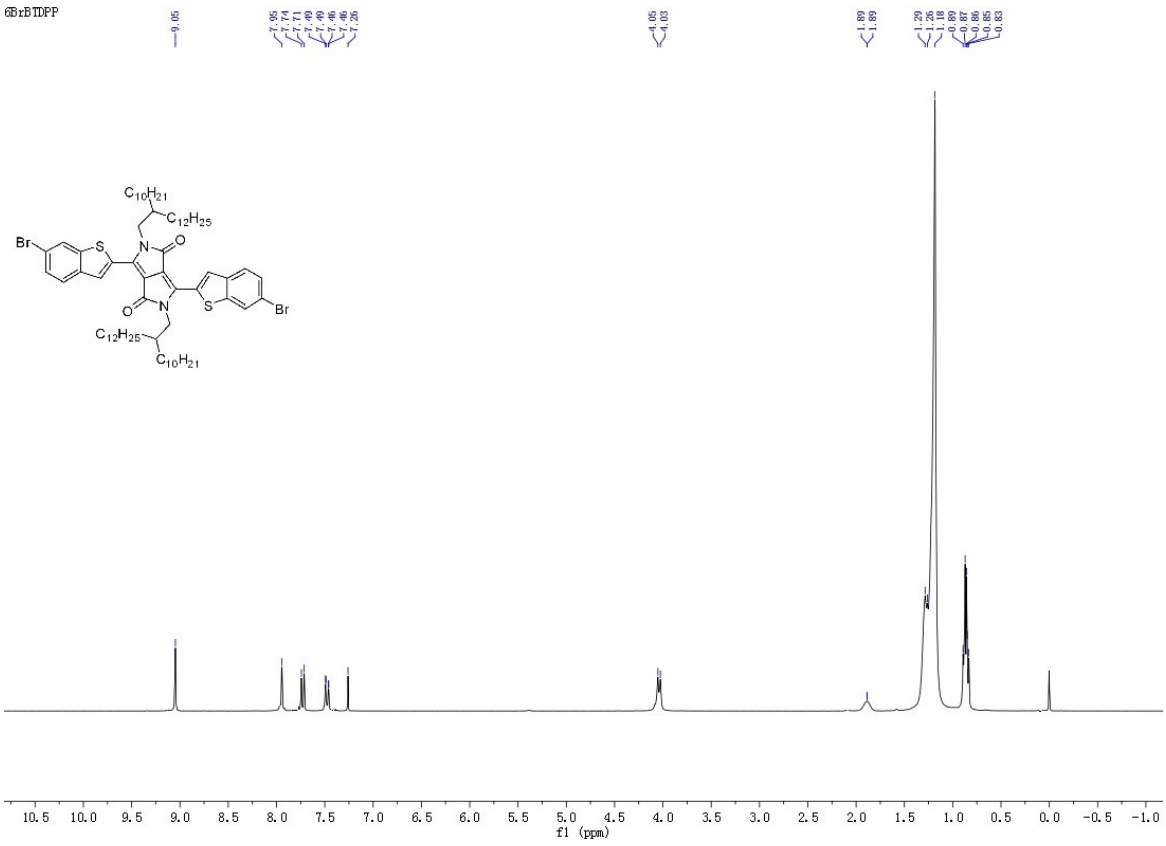


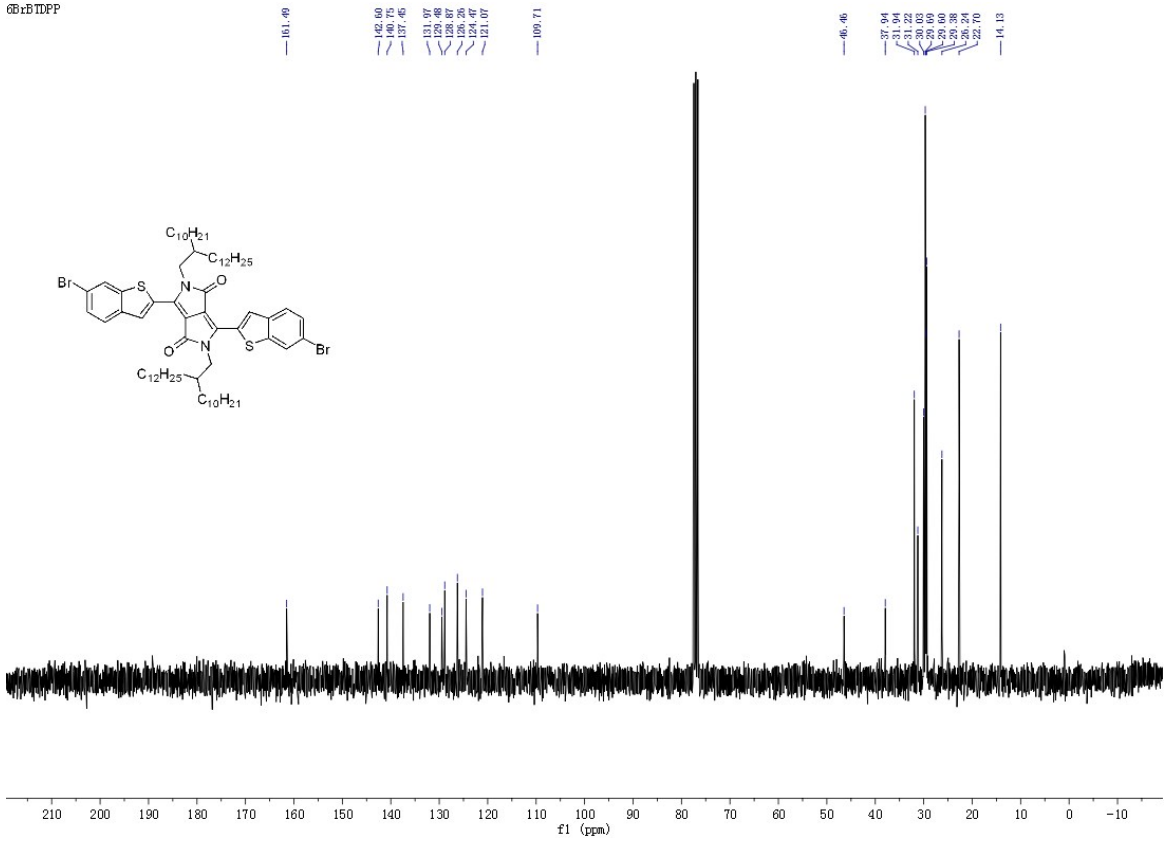


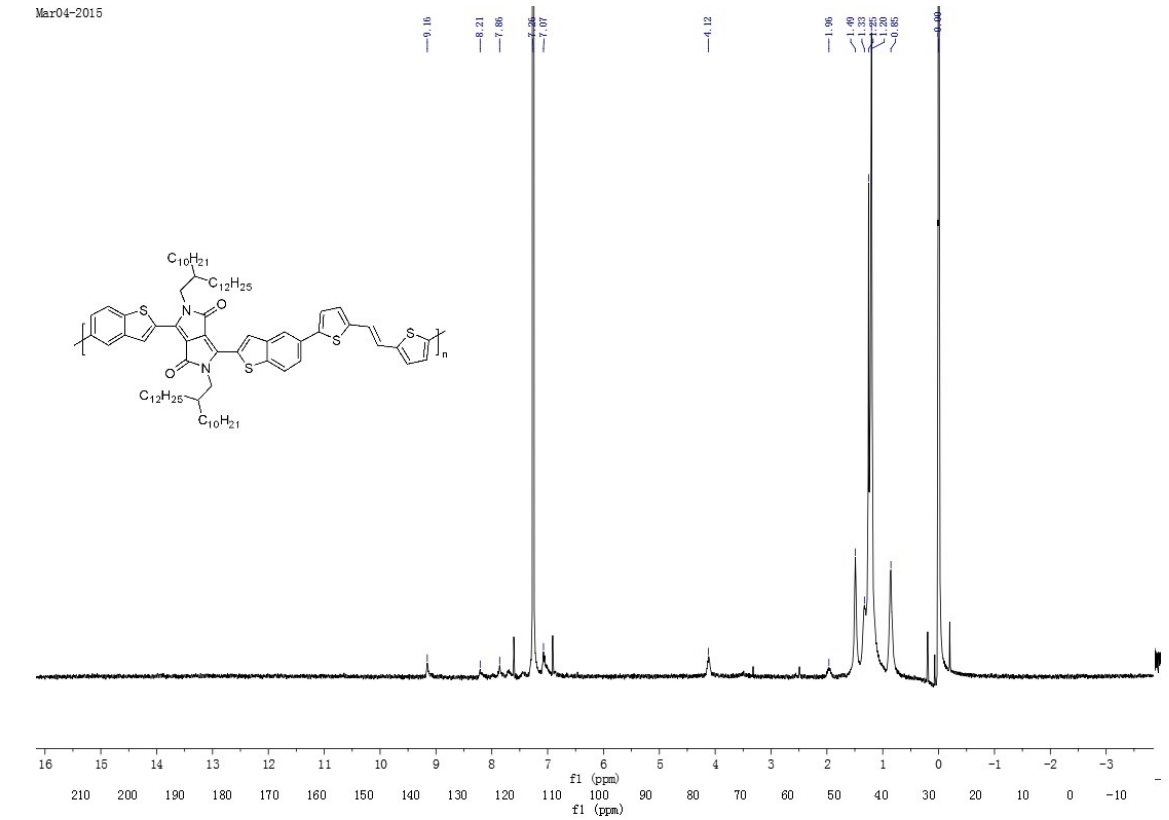
6BrBTCN

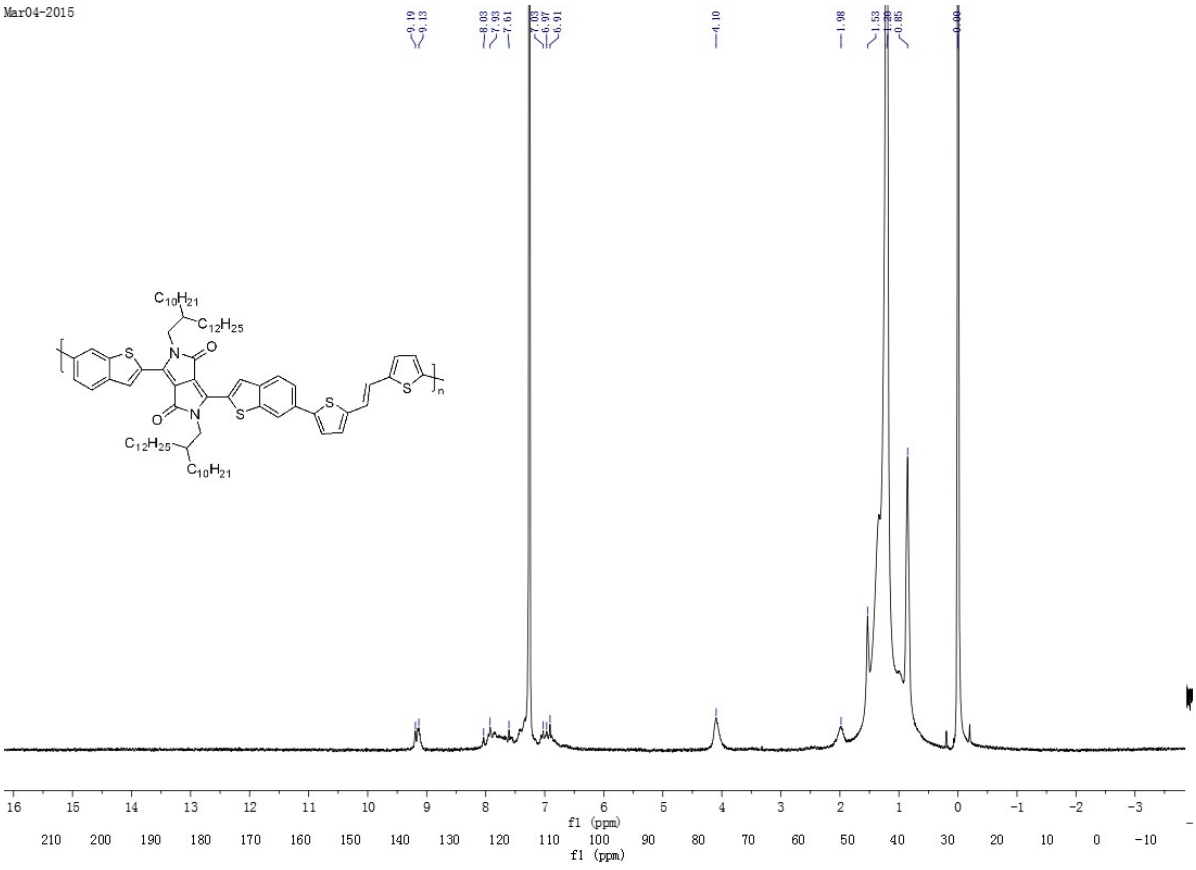
142.52
136.16
134.61
129.52
126.27
124.97
122.47
113.98
110.28
77.52
77.10
76.67




6BrBTDPP
9.05
7.95
7.74
7.71
7.49
7.46
7.26
4.05
4.03
1.89
1.89
1.29
1.26
1.18
0.89
0.87
0.86
0.85
0.83
Br
S
N
O
O
N
S
Br
$C_{10}H_{21}$
$C_{12}H_{25}$
$C_{12}H_{25}$
$C_{10}H_{21}$
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


6BrBTDPP
161.49
142.60
140.75
137.45
131.97
129.48
128.87
126.26
124.47
121.07
109.71
46.46
37.94
31.94
31.22
30.03
29.69
29.60
29.38
26.24
22.70
14.13
Br
S
N
O
O
N
S
Br
$C_{10}H_{21}$
$C_{12}H_{25}$
$C_{12}H_{25}$
$C_{10}H_{21}$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Mar04-2015
9.16
8.21
7.86
7.26
7.07
4.12
1.96
1.49
1.33
1.25
1.20
0.85
0.00
f1 (ppm)


Mar04-2015
9.19
9.13
8.03
7.93
7.61
7.03
6.97
6.91
4.10
1.98
1.53
1.30
0.85
0.00
f1 (ppm)

2. Optical and electrochemical properties

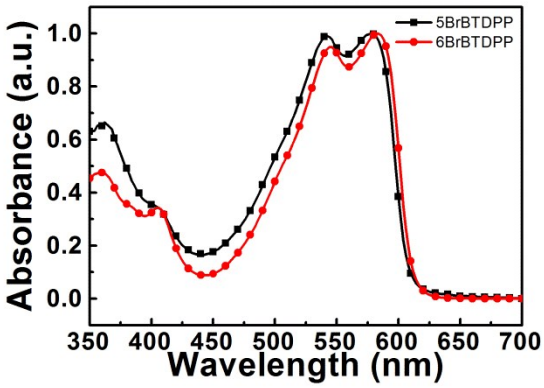


Fig. S1 UV-vis absorption spectra of the 5BrBTDPP and 6BrBTDPP monomers in dilute chloroform.

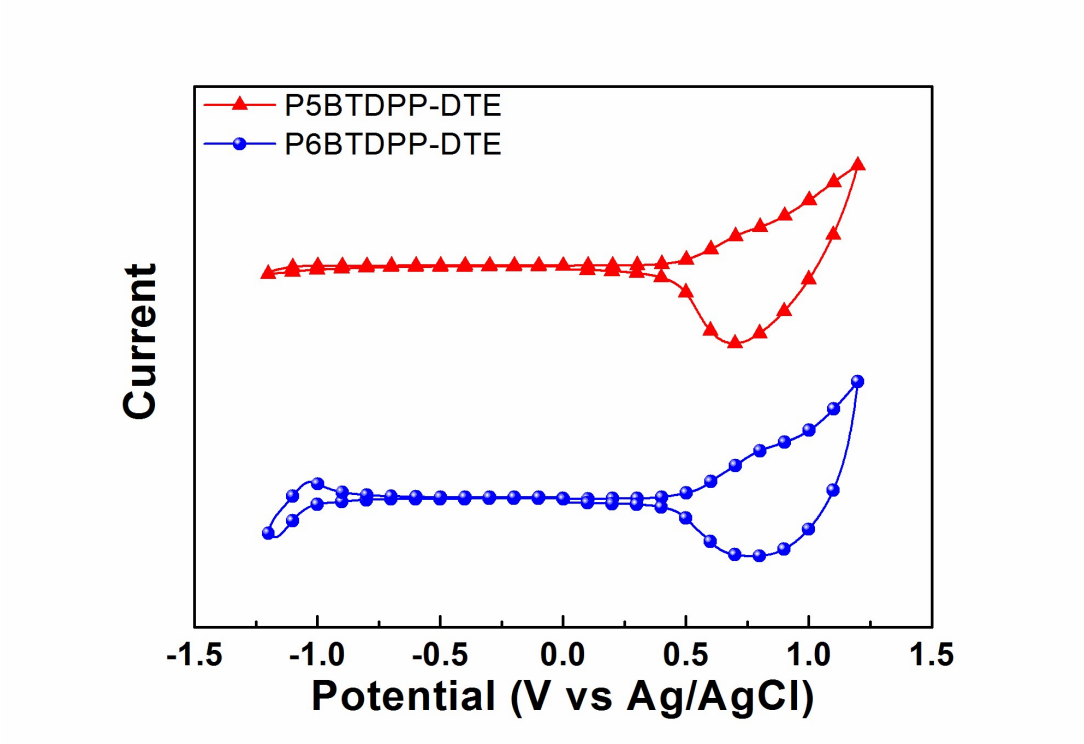


Fig. S2 Cyclic voltammograms of P5BTDPP-DTE and P6BTDPP-DTE using thin films drop-casted on a glassy carbon electrode as a working electrode in dichloromethane solution containing 0.1 M n-Bu_4NPF_6 as a supporting electrolyte.

Table S1 Summary of optical and electrochemical properties of P5BTDPP-DTE and P6BTDPP-DTE

Polymer	λ_{max} (nm)		E_g^{opt} (eV)	E_{red}^{onset} (eV)	E_{ox}^{onset} (eV)	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g^{cv} (eV)
	soln.	film						
P5BTDPP-DTE	586	582	1.60	−0.99	0.50	−4.90	−3.41	1.49
P6BTDPP-DTE	632	644	1.56	−1.02	0.48	−4.88	−3.38	1.50

3. Field-effect characteristics

Table S2 Conditions for fabricating field-effect transistors

Compounds	Solvents	Concentration (mg/mL)	Rotating speed (r/min)	Annealing conditions (°C, min)
P5BrBTDPP-DTE	*o*-DCB	10	1600, 1 min	160, 4
P6BrBTDPP-DTE		5	1000-30s 2000-30s	160, 4

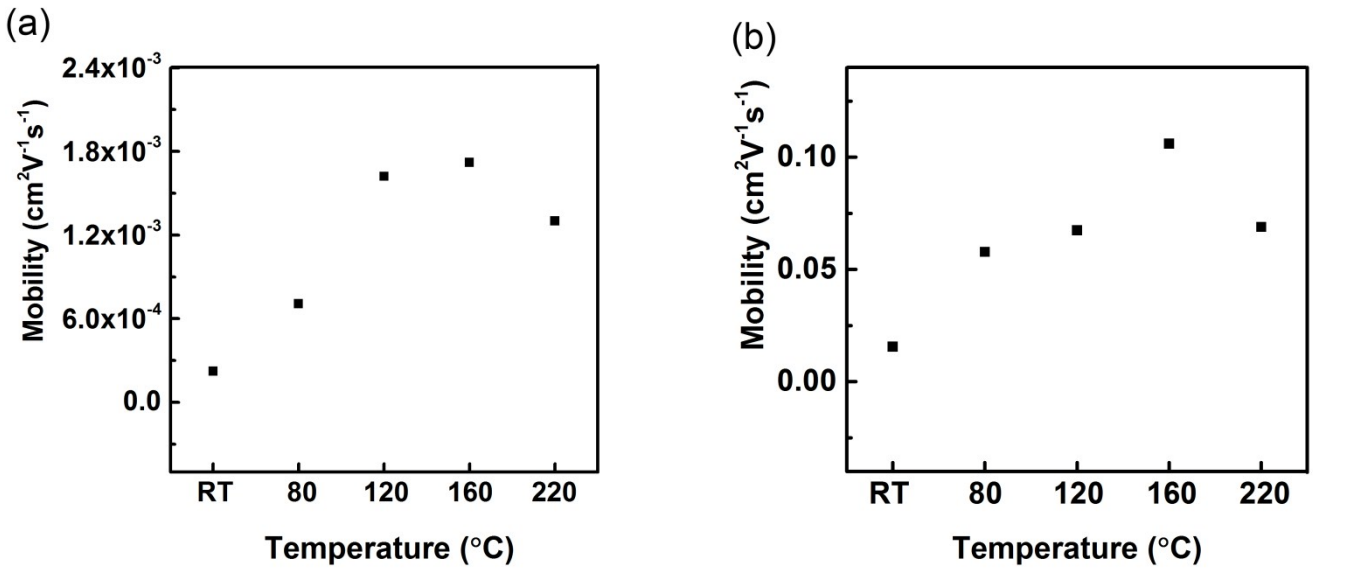


Fig. S3 A preliminary test of mobilities for each annealing temperatures. Both P5BTDPP-DTE (a) and P6BTDPP-DTE (b) tend to afford the best hole mobilities after annealing at 160°C.

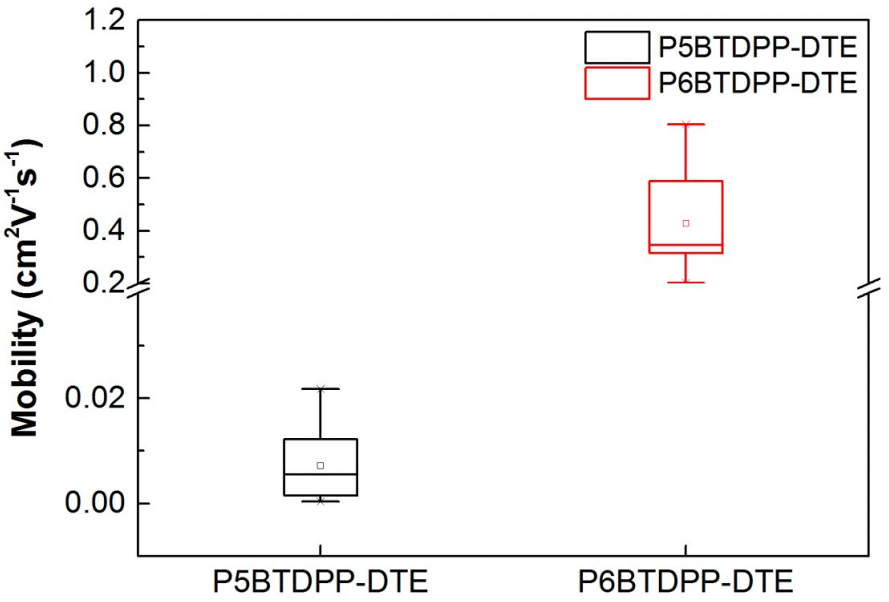


Fig. S4 Statistical display for distribution of mobilities of P5BTDPP-DTE and P6BTDPP-DTE based thin film transistors

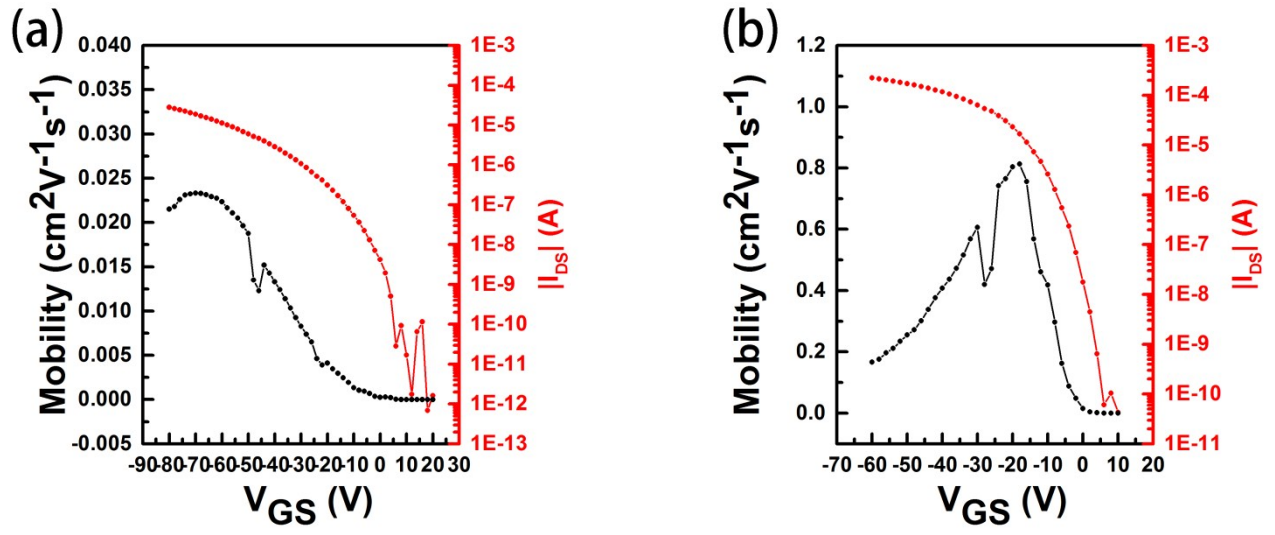


Fig. S5 Differential mobilities of two polymers: (a) P5BTDPP-DTE, (b) P6BTDPP-DTE.

4. GIXRD profiles

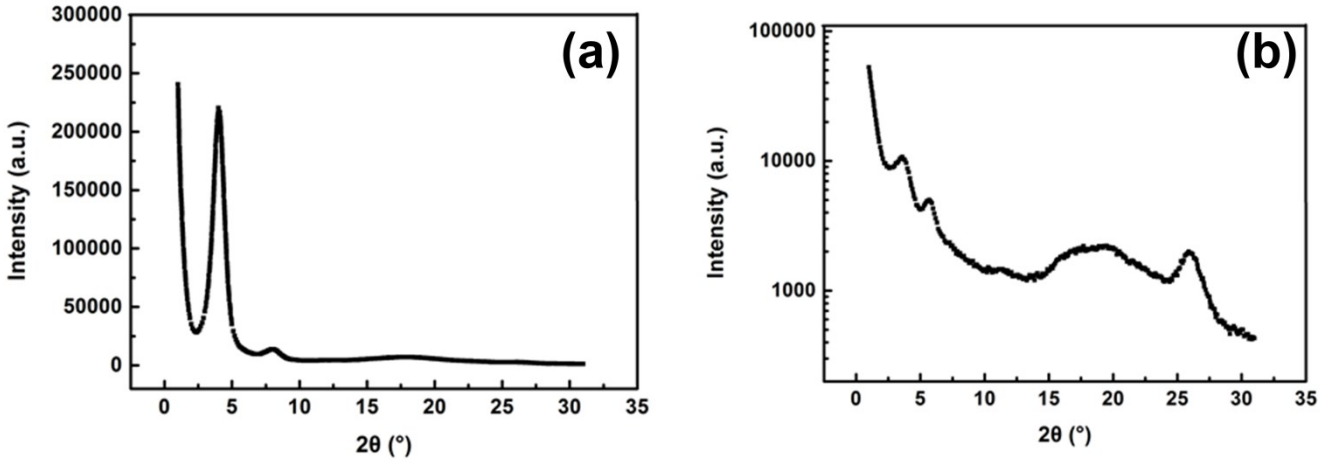


Fig. S6 One-dimensional GIXRD profiles of P5BTDPP-DTE (λ = 1.54 Å): (a) out-of-plane, (b) in-plane.

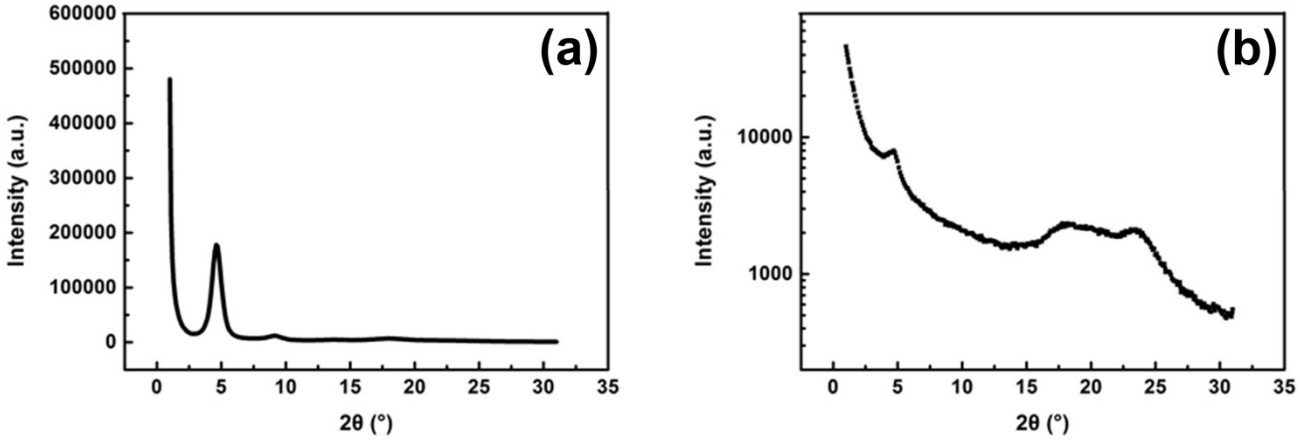


Fig. S7 One-dimensional GIXRD profiles of P6BTDPP-DTE (λ = 1.54 Å): (a) out-of-plane, (b) in-plane.

5. AFM

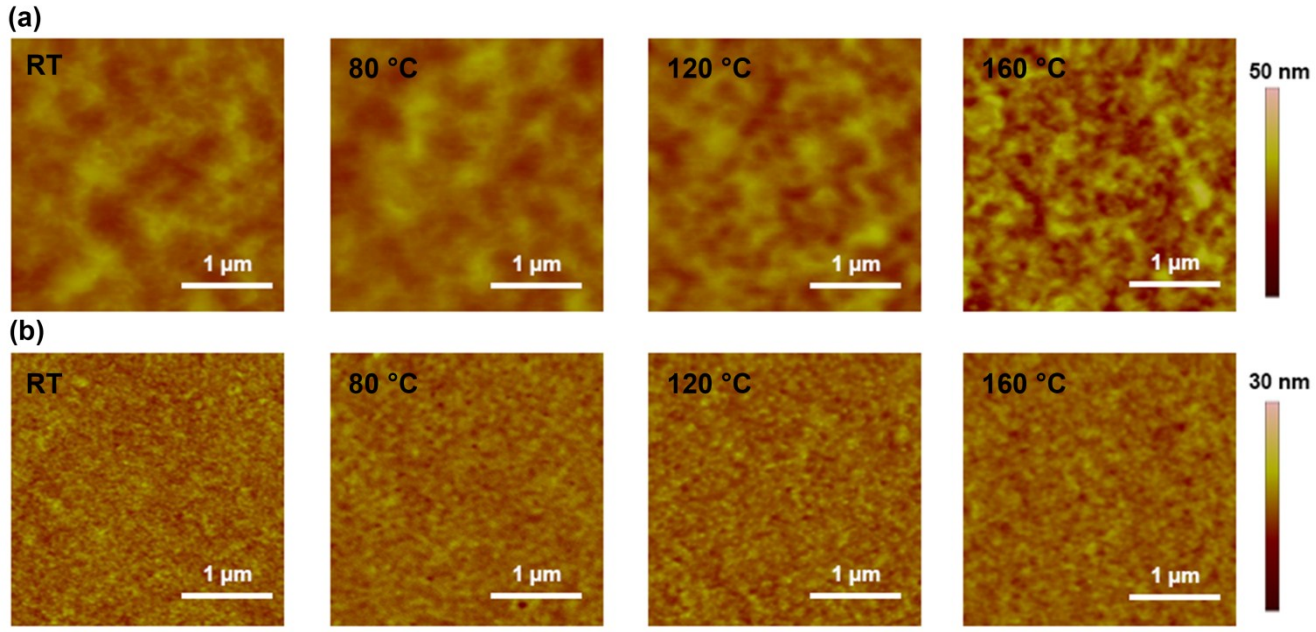


Fig. S8 AFM images of the (a) P5BTDPP-DTE and (b) P6BTDPP-DTE thin films.