Electronic Supplementary Material (ESI) for Polymer Chemistry.

An Efficient Lactone-to-Lactam Conversion for the Synthesis of Thiophene Pechmann Lactam and Characterization of Polymers Thereof

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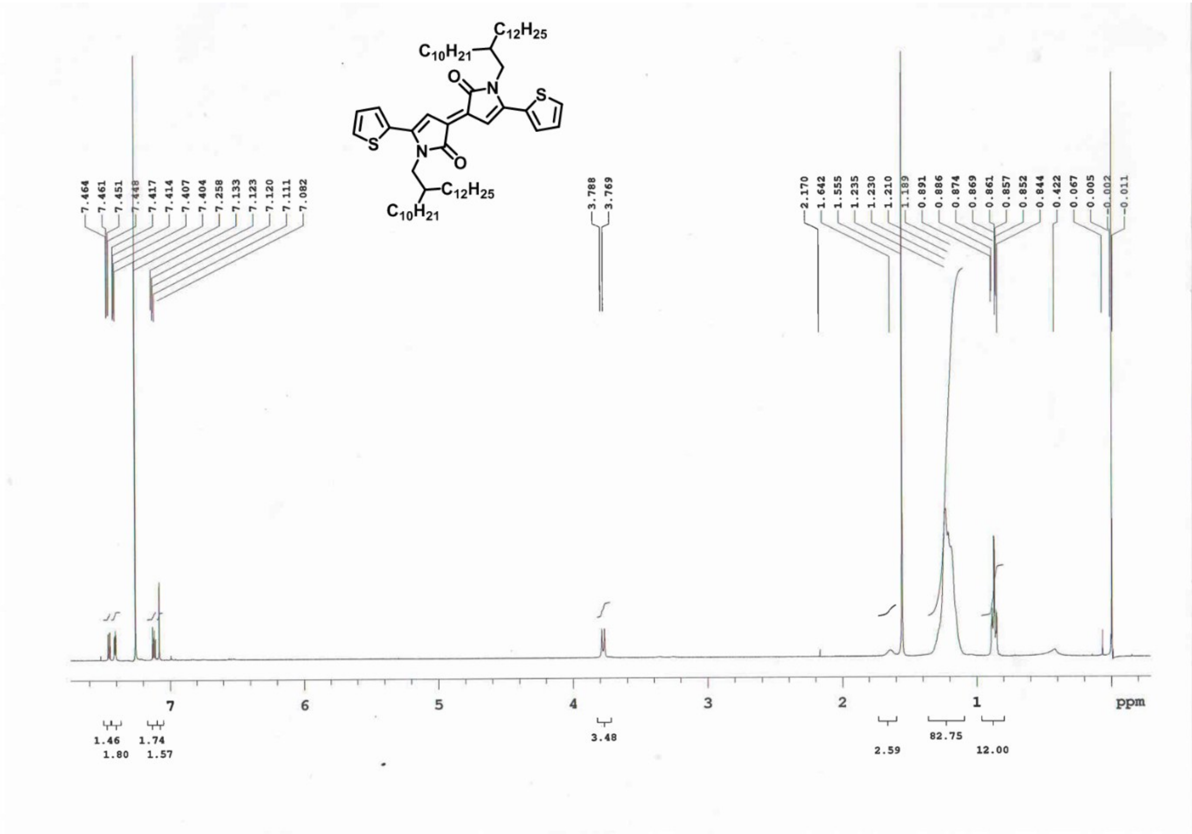

Fig. S1 ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **3**.

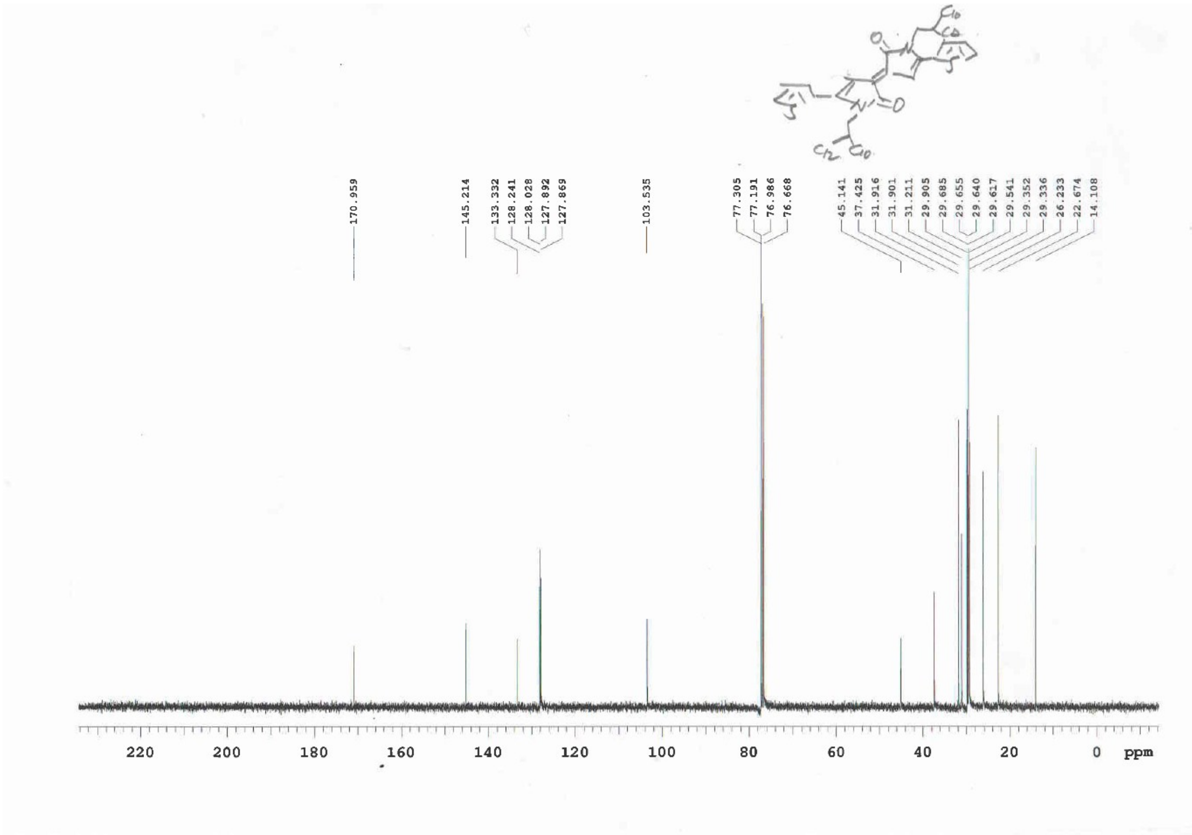

Fig. S2 ^{13}C NMR ($CDCl_3$, 400 MHz) spectrum of compound **3**.

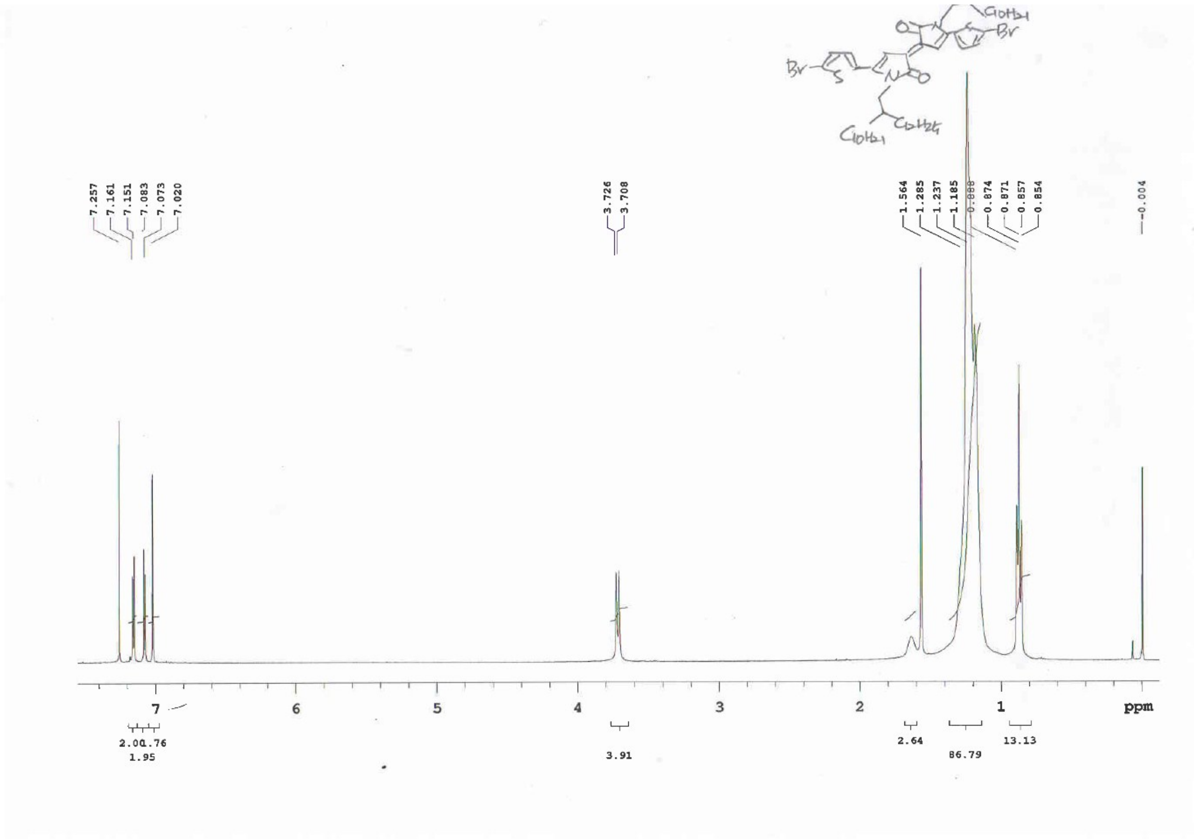

Fig. S3 ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **4**.

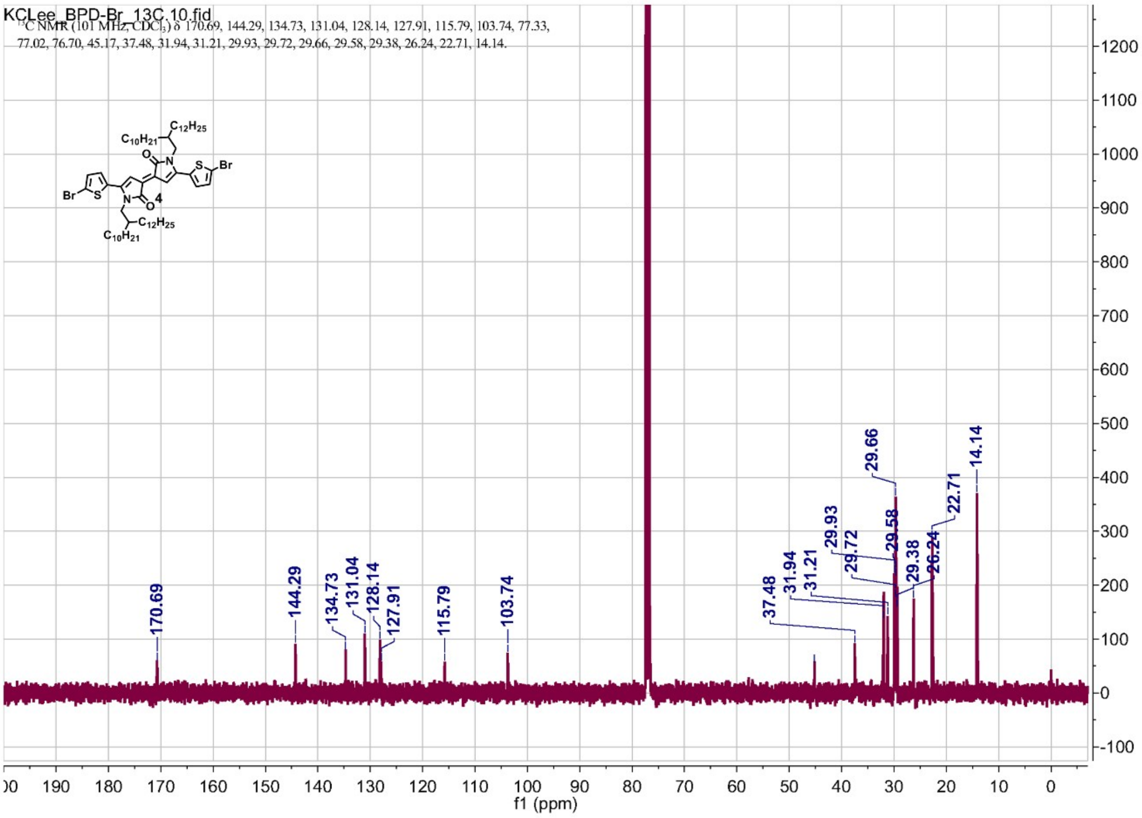

Fig. S4 ^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **4**.

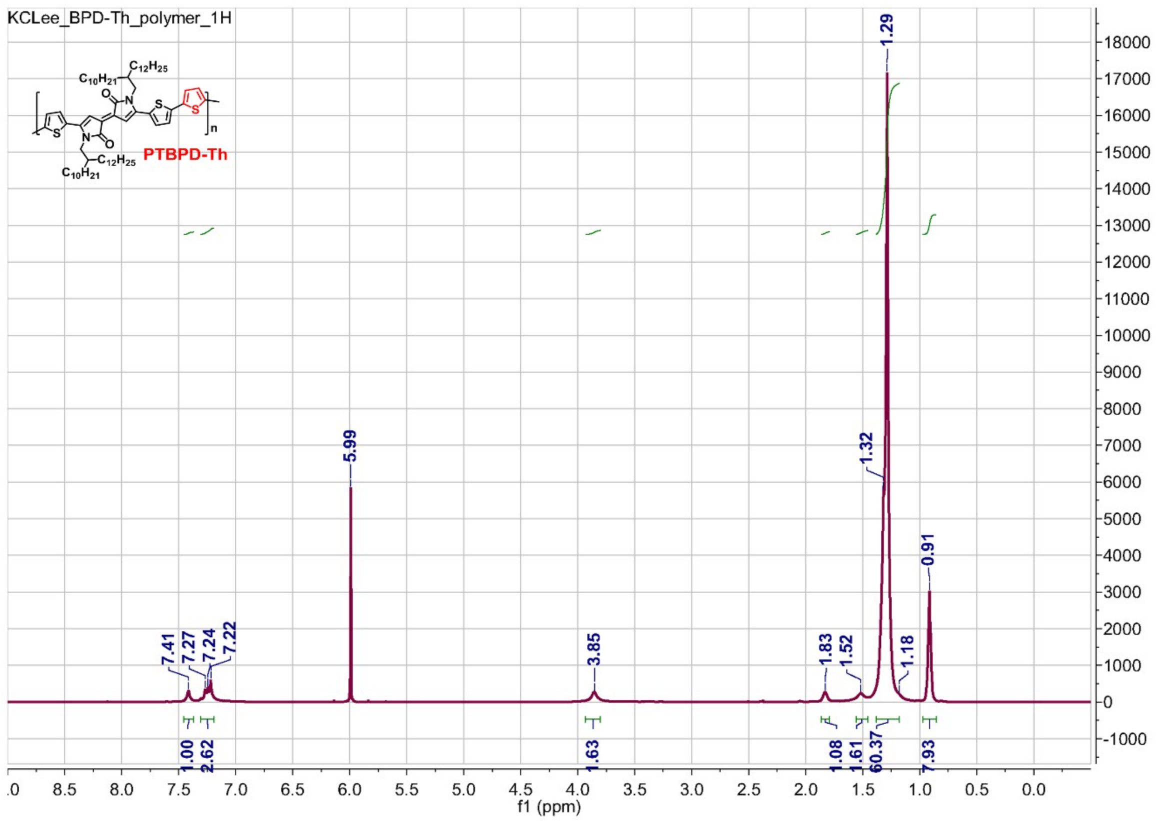

Fig. S5 ^{1}H NMR ($C_2D_2Cl_4$ at 80 ^{o}C, 600 MHz) spectrum of PTBPD-Th.

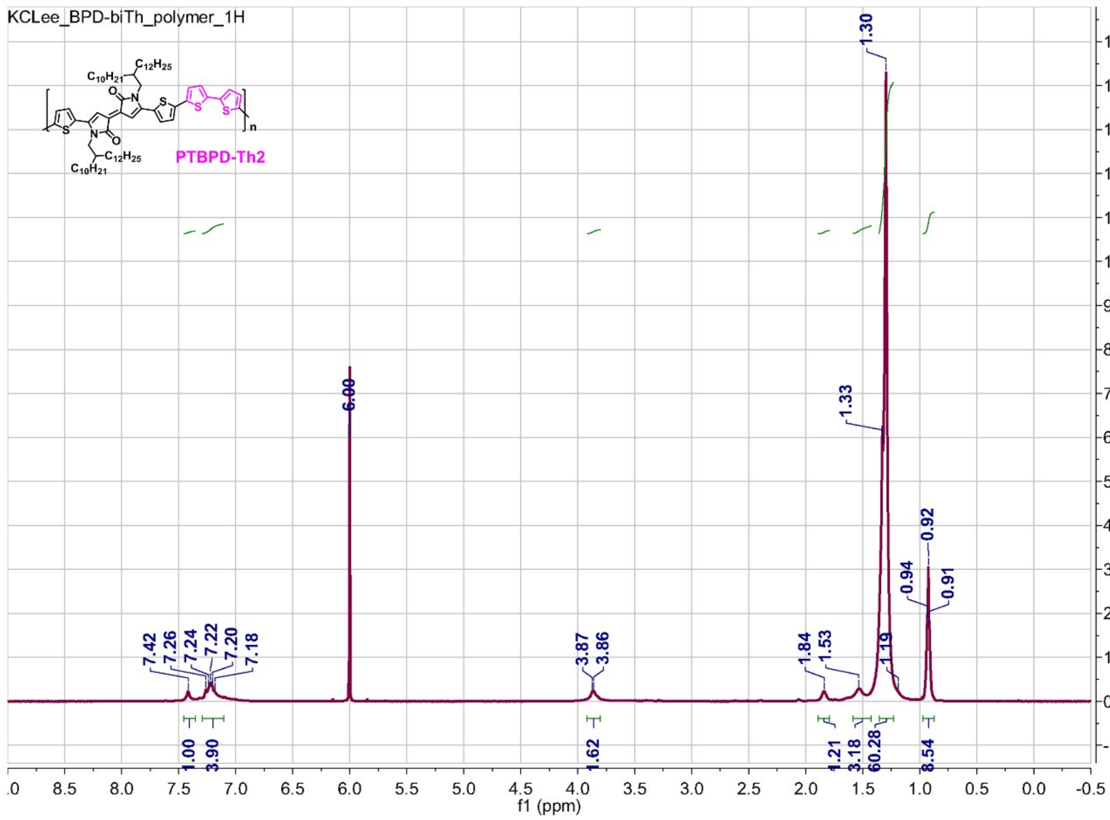

Fig. S6 ^{1}H NMR ($C_2D_2Cl_4$ at 80 ^{o}C, 600 MHz) spectrum of PTBPD-Th2.

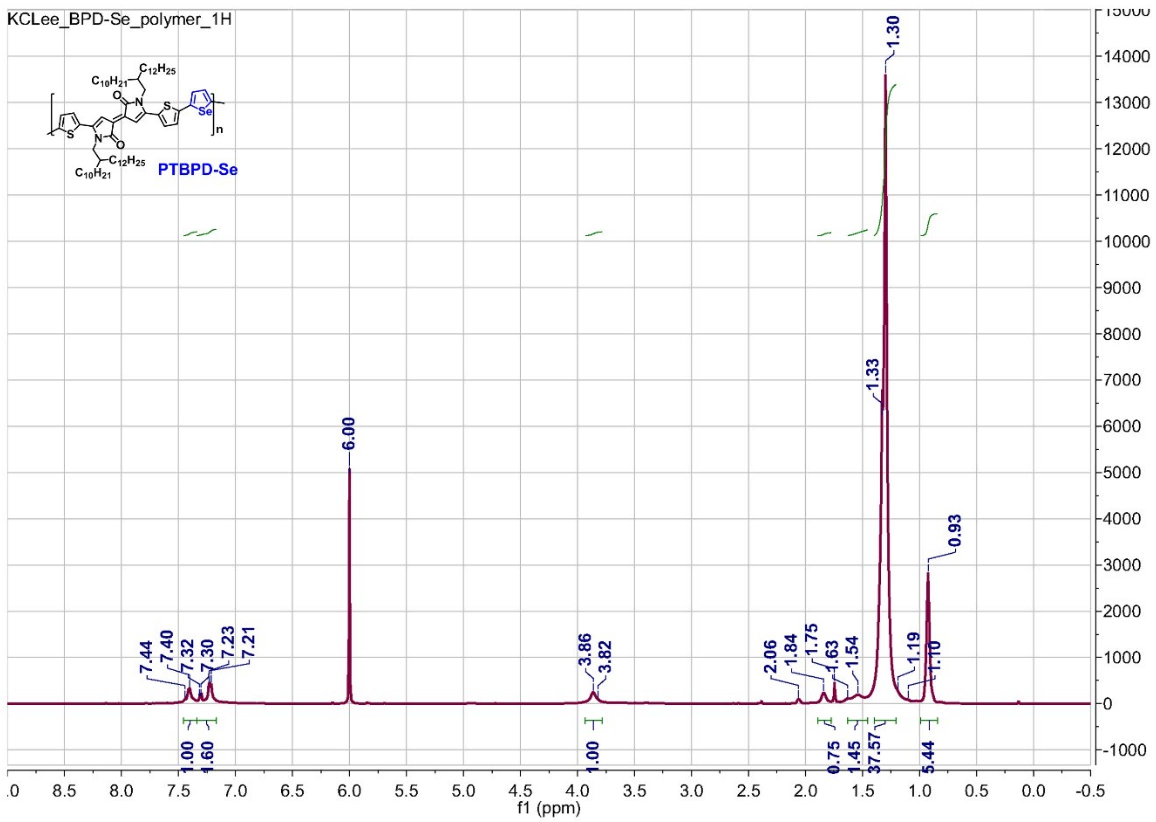

Fig. S7 ^{1}H NMR ($C_2D_2Cl_4$ at 80 ^{o}C, 600 MHz) spectrum of PTBPD-Se.

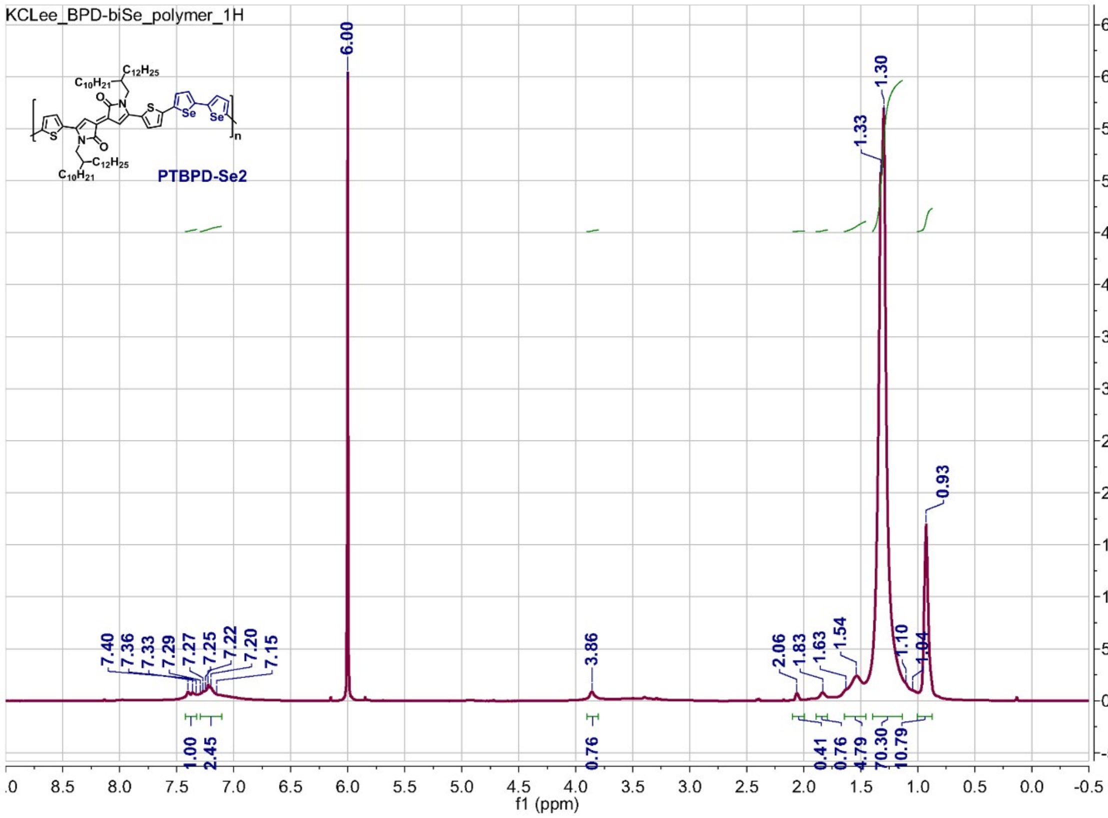

Fig. S8 ^{1}H NMR ($C_2D_2Cl_4$ at 80 ^{o}C, 600 MHz) spectrum of PTBPD-Se2.

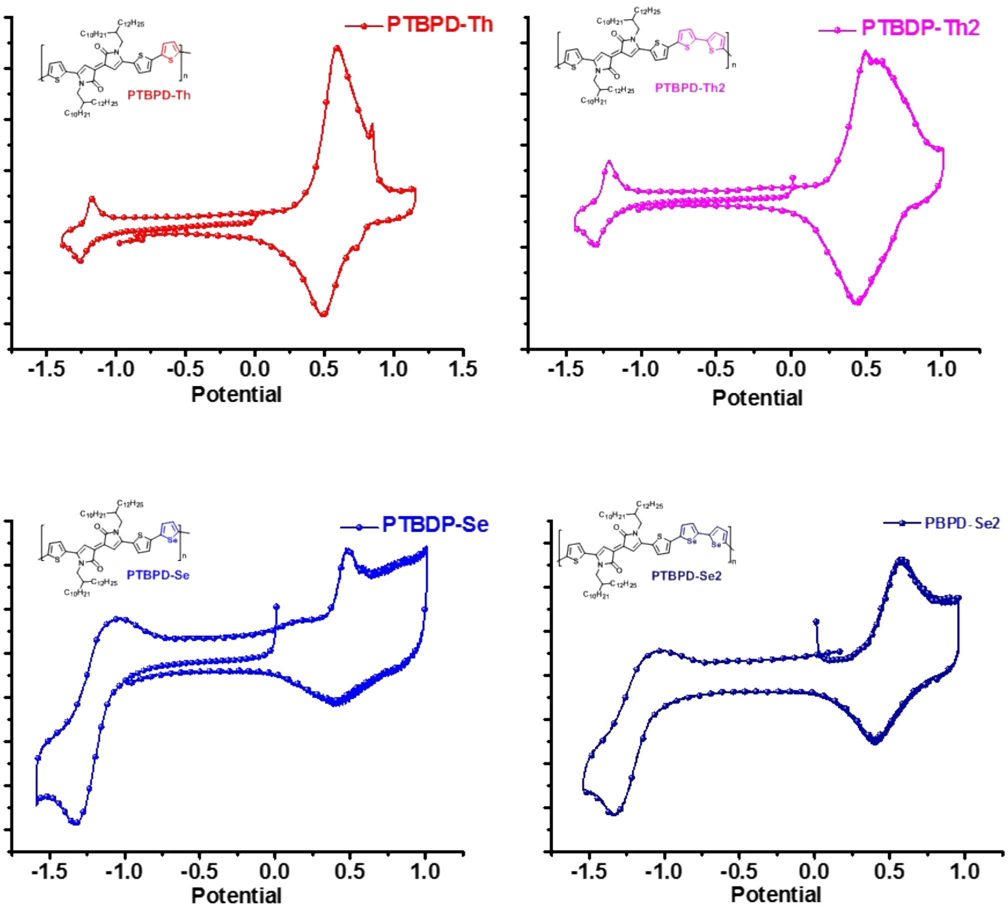

Fig. S9 Cyclic voltammetry of TBDP-based polymers.

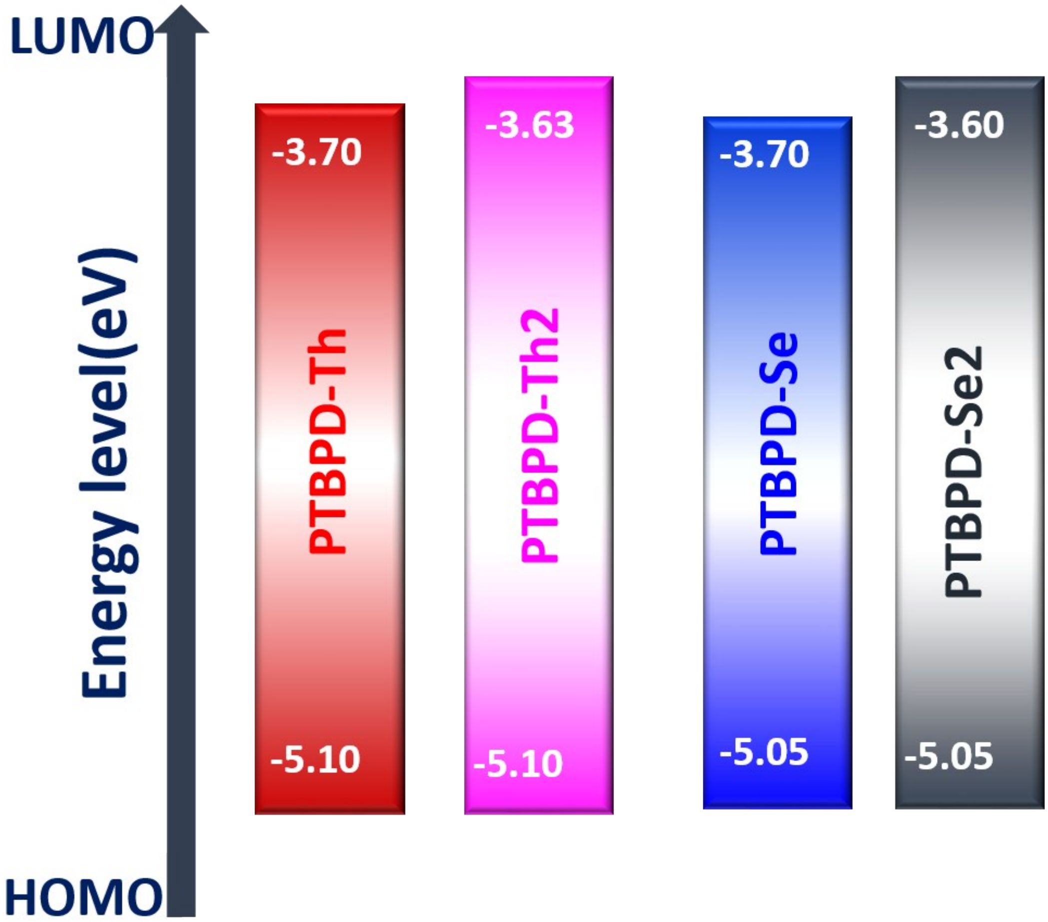

Fig. S10 Energy level diagrams of TBDP-based polymers

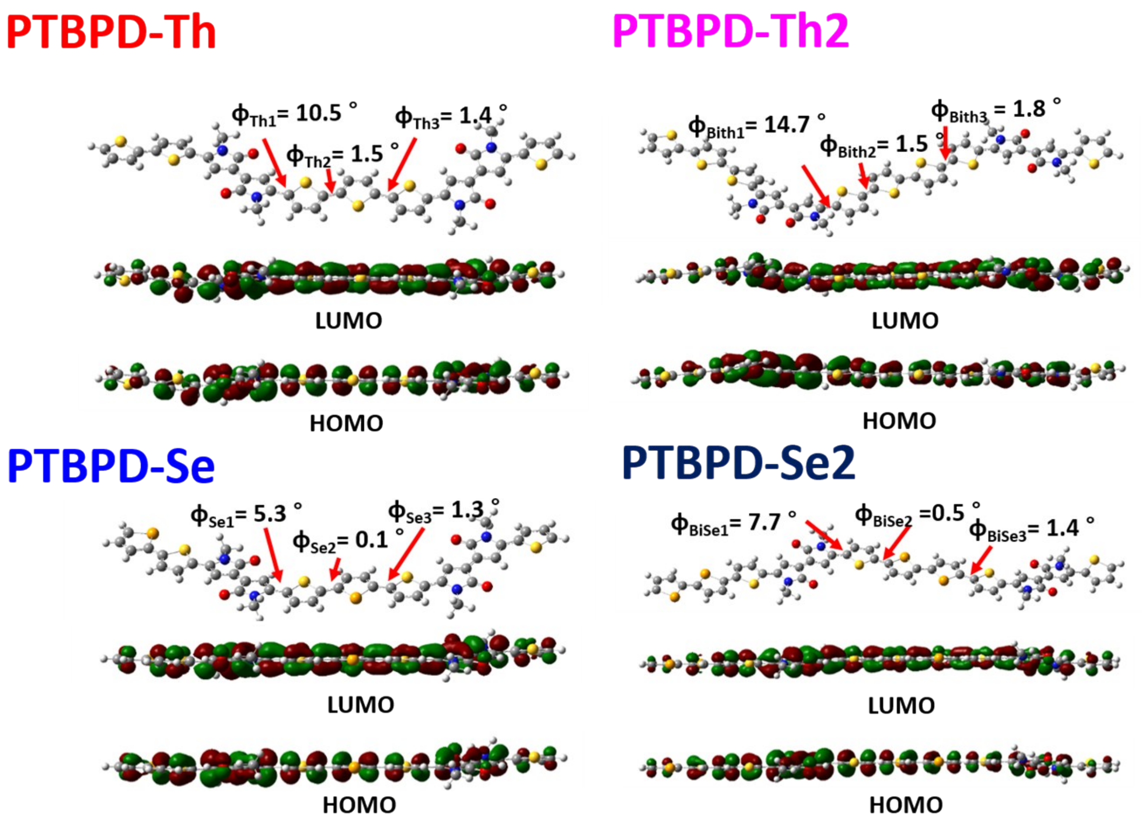

Fig. S11 DFT calculation for TBDP-based polymers with each dimer model at the B3LYP/6-31G* level.

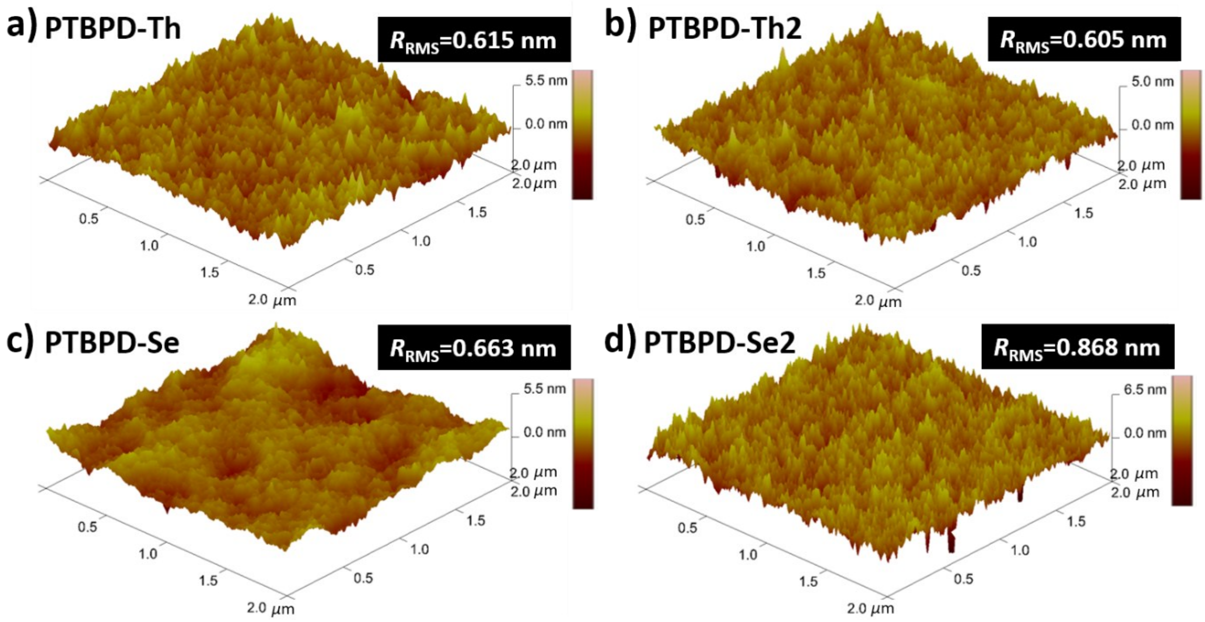

Fig. S12 AFM height images of TBPD-based polymer films annealed at 200 °C: (a) PTBPD-Th, (b) PTBPD-Th2, (c) PTBPD-Se, and (d) PTBPD-Se2.

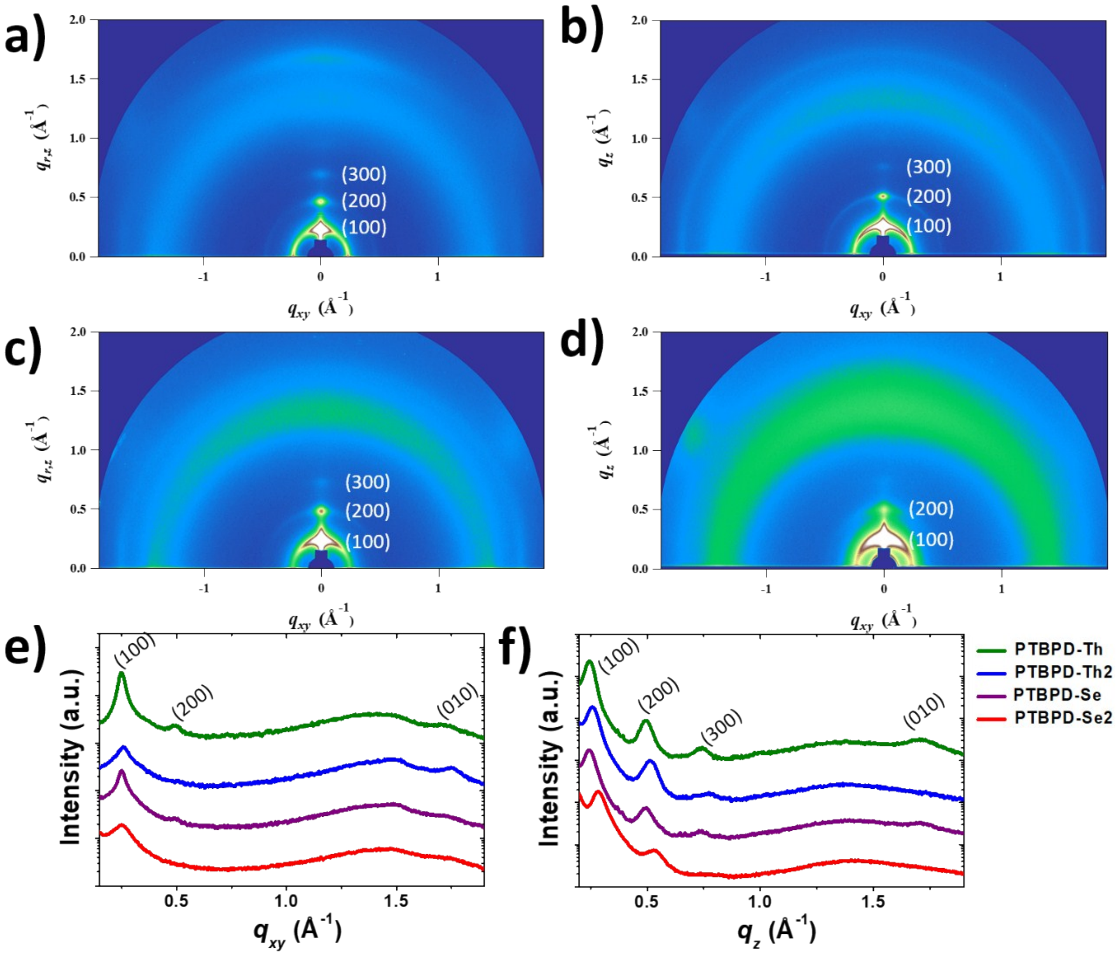

Fig. S13 2D-GIXD images of TBPD-based polymer films without thermal treatment: (a) PTBPD-Th, (b) PTBPD-Th2, (c) PTBPD-Se, and (d) PTBPD-Se2. The corresponding GIXD diffractogram profiles: (e) in-plane and (f) out-of-plane GIXD patterns.

Table S1 Crystallographic parameters of as-cast TBPD-based polymer films

Polymer	**Lamellar spacing**				***π–π* spacing**	
	q_z [Å^{-1}]	d [Å]	L_c [Å]	L_c/d	q_{xy} [Å^{-1}]	d [Å]
PTBPD-Th	0.246	25.6	142.0	5.55	1.72	3.66
PTBPD-Th2	0.260	24.2	128.8	5.32	1.75	3.59
PTBPD-Se	0.245	25.6	142.3	5.55	—[a]	—[a]
PTBPD-Se2	0.285	22.0	121.8	5.53	—[a]	—[a]

[a]Not detected

Table S2 Summary of FET performance of solution sheared non-annealed TBPD polymer films.

Polymer[a]	$\mu_{h,max}{}^{b}$ [cm^2 V^{-1} s^{-1}]	$\mu_{h,avg}{}^{c}$ [cm^2 V^{-1} s^{-1}]	$I_{on}/I_{off}{}^{d}$	$V_T{}^{e}$ [V]
PTBPD-Th	0.25	0.13 (±0.093)[f]	> 10^4	18.1
PTBPD-Th2	0.022	0.010 (±0.047)	> 10^5	14.2
PTBPD-Se	0.040	0.027 (±0.012)	> 10^4	19.7
PTBPD-Se2	0.083	0.049 (±0.015)	> 10^5	18.9

[a]The FET performance of solution sheared non-annealed polymer films fabricated with 3 mg mL^{-1} of 1,2-dichlorobenzene solution; [b]The maximum and [c]average mobility of the FET devices (L = 50 μm and W = 1000 μm); [d]The on- and off-current ratio; [e]The average threshold voltage; [f]The standard deviation.

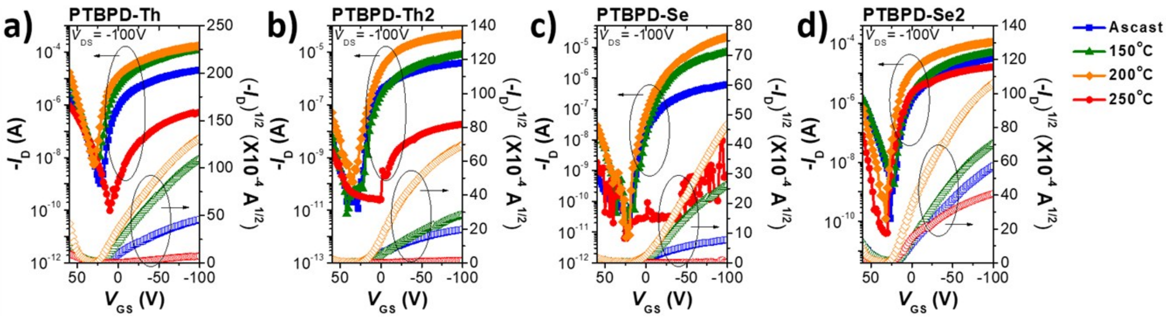

Fig. S14 Transfer characteristics obtained from TBPD-based polymer films before (blue) and after thermal treatment at various annealing temperature of 150 °C (green), 200 °C (orange), and 250 °C (red): (a) PTBPD-Th, (b) PTBPD-Th2, (c) PTBPD-Se, and (d) PTBPD-Se2.

Table S3 FET performance of TBPD polymer films fabricated using various solvents.

Condition		*p*-channel			
Polymer[a]	Solvent[b]	$\mu_{h,\max}{}^{c}$ [cm^2 V^{-1} s^{-1}]	$\mu_{h,\mathrm{avg}}{}^{d}$ [cm^2 V^{-1} s^{-1}]	$I_{on}/I_{off}{}^{e}$	$V_T{}^{f}$ [V]
PTBPD-Th	CB	0.30	0.25 (±0.034)[g]	> 10^3	15.7
	DCB	0.46	0.37 (±0.066)	> 10^4	14.7
PTBPD-Th2	CB	0.030	0.026 (±0.0031)	> 10^6	15.0
	DCB	0.12	0.10 (±0.012)	> 10^5	11.2
PTBPD-Se	CB	0.015	0.010 (±0.0021)	> 10^5	-1.3
	DCB	0.11	0.066 (±0.029)	> 10^5	25.5
PTBPD-Se2	CB	0.087	0.070 (±0.012)	> 10^5	8.6
	DCB	0.28	0.22 (±0.044)	> 10^5	17.5

[a]The FET performance of solution sheared polymer films annealed at 200 °C was tested in a nitrogen atmosphere; [b]The polymer films were fabricated with 3 mg mL^{-1} chlorobenzene and 1, 2-dichlorobezene solution; [c]The maximum and [d]average mobility of the FET devices (L = 50 μm and W = 1000 μm); [e]The on- and off-current ratio; [f]The average threshold voltage; [g]The standard deviation.

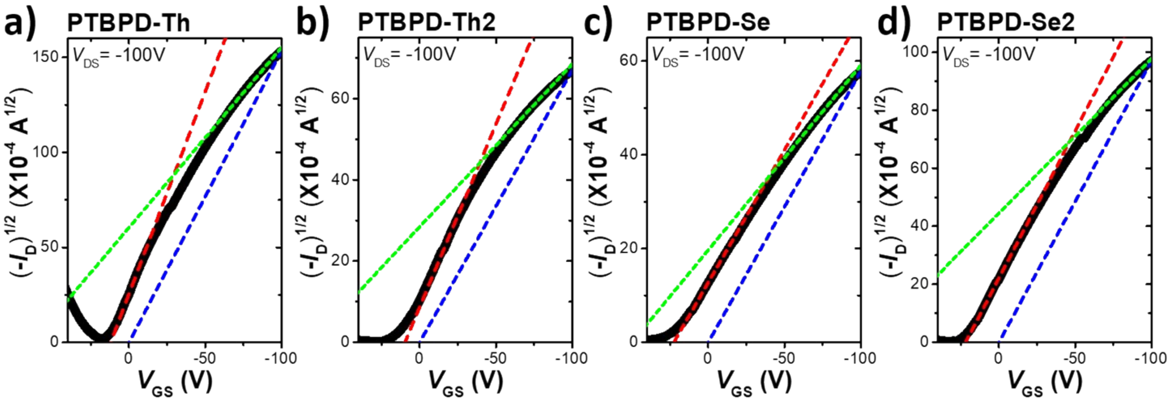

Fig. S15 Transfer curves with three fitting lines obtained from TBPD-based polymer films after thermal treatment at 200 °C: (a) PTBPD-Th, (b) PTBPD-Th2, (c) PTBPD-Se, and (d) PTBPD-Se2. The red line represents the fitting line of the maximum mobility. The green line represents the fitting line at a high gate voltage above the kink. The blue line represents the ideal FET characteristics which satisfy the ideal Shockley equations.

Table S4 Summary of the calculated mobilities of TBPD polymer-based OFETs.

Polymer[a]	$\mu_{h,\text{max}}$[b] [cm^2 V^{-1} s^{-1}]	μ_{highV}[c] [cm^2 V^{-1} s^{-1}]	μ_{eff}[d] [cm^2 V^{-1} s^{-1}]	R_{sat}[e] [%]
PTBPD-Th	0.46	0.16	0.15	33.1
PTBPD-Th2	0.12	0.032	0.048	39.5
PTBPD-Se	0.11	0.061	0.067	63.4
PTBPD-Se2	0.31	0.14	0.15	48.4

[a]The FET performance of solution sheared polymer films fabricated with 3 mg mL^{-1} of 1,2-dichlorobenzene solution was tested in a nitrogen atmosphere; [b]The maximum mobility of the FET devices; [c]The mobility obtained from the high gate voltage region; [d]The effective mobility ($\mu_{\text{eff}} = \mu_{\text{max}} \times R_{\text{sat}}$); [e]The reliability factor.

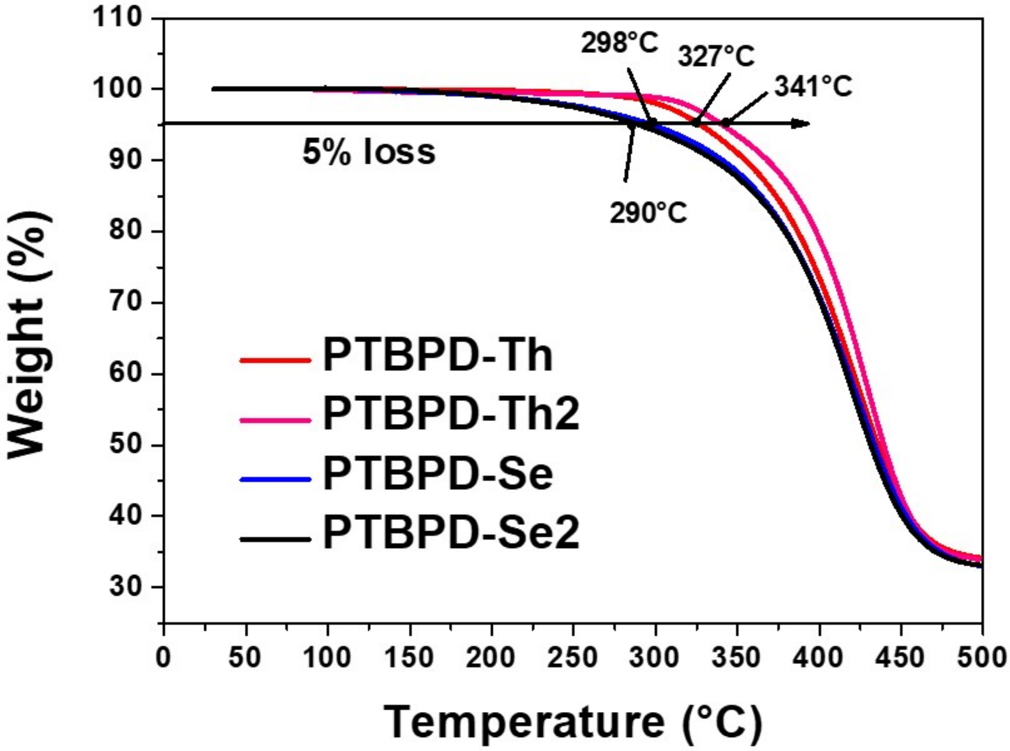

Fig. S16. Thermogravimetric analysis (TGA) of all polymers.

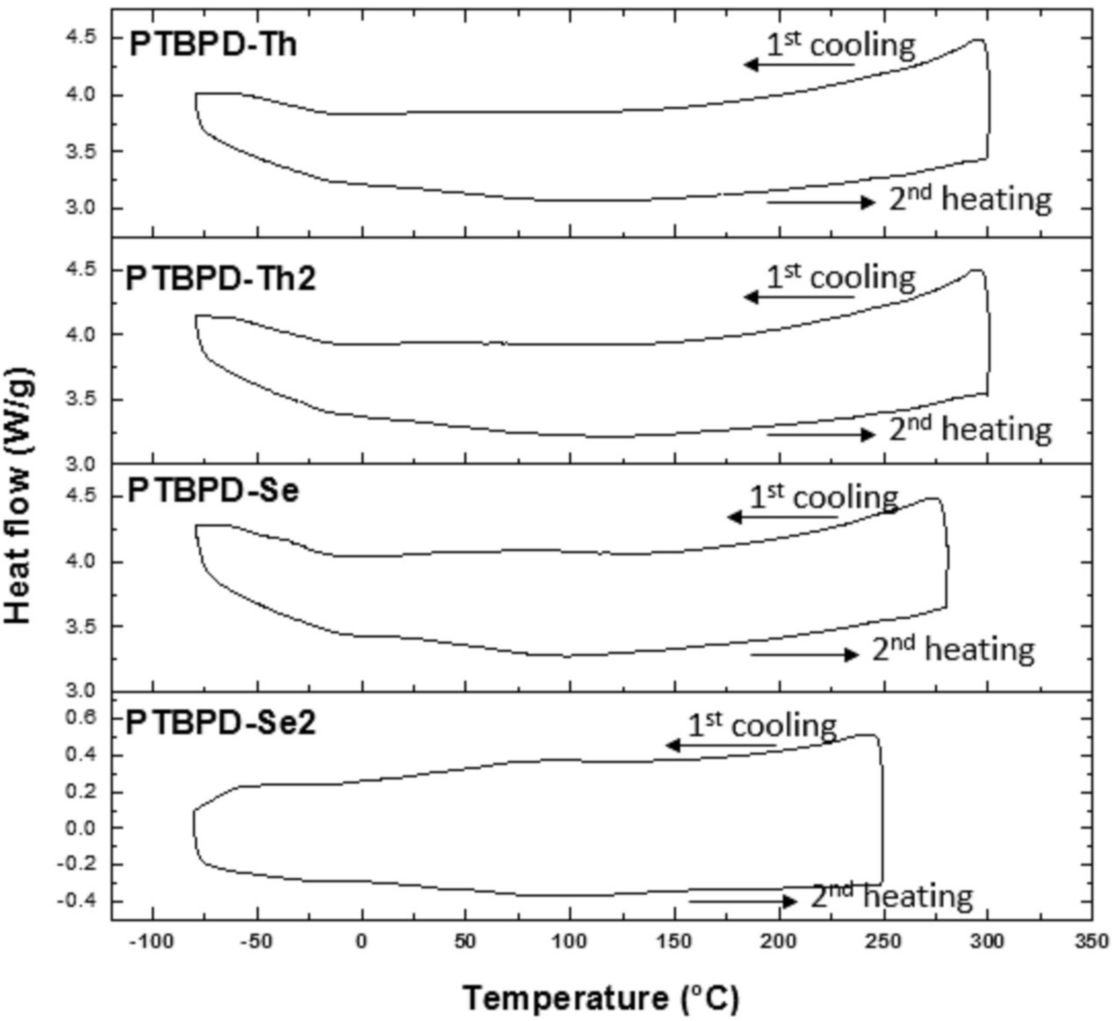

Fig. S17 The differential scanning calorimetry (DSC) data of all polymers.