Supporting Information for:

Synthesis and Characterization of Thieno[3,4-*b*]thiophene-based Copolymers Bearing 4-Substituted Phenyl Ester Pendants: Facile Fine-Tuning of HOMO Energy Levels

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1. Materials

Anhydrous solvents (toluene, *N*,*N*-dimethylformamide (DMF), tetrahydrofuran (THF)), common organic solvents, and phenol were purchased from Kanto (Tokyo, Japan). Trimethyltin chloride was available from Tokyo Kasei (Tokyo, Japan). Oxalyl chloride, 4-trifluoromethylphenol, zinc, tetrabutylammonium bromide, and *n*-butyllithium (1.6 M in hexane) were purchased from Wako (Osaka, Japan). 4-Methoxyphenol and chlorobenzene were obtained from Kishida (Osaka, Japan). Tetrakis(triphenylphosphine)palladium(0) and sodium hydroxide were purchased from Nacalai (Kyoto, Japan). Poly(3,4-ethylenedioxylenethiophene):poly(4-styrene sulfonic acid) (PEDOT:PSS) 1.3 wt% dispersion in water, polyoxyethylene tridecyl ether (PTE), 4-fluorophenol, anhydrous pyridine, and chlorobenzene were purchased from Sigma-Aldrich. Indium tin oxide

(ITO) glass substrates (sheet resistance = 10 Ω/sq.) and Au wire were obtained from Furuuchi Chemical Co. (Tokyo, Japan). 4,6-Dibromothieno[3,4-*b*]thiophene-2-carboxylic acid (**1**),[1] 4,8-dihydrobenzo[1,2-*b*:4,5-*b*']dithiophen-4,8-dion,[2] 1-iode-2-octyldodecane,[3] and 2,6-bis(trimethyltin)-4,8-bis(2-ethylhexyloxy)benzo[1,2-*b*:3,4-*b*′]dithiophene (**BDTa**)[4] were prepared according to literature procedures.

2. Instruments

The ^{1}H and ^{13}C NMR spectra were measured in $CDCl_3$ at room temperature and 50 ˚C with a JEOL ECA-500 spectrometer (JEOL, Tokyo, Japan). IR spectra were obtained using a JASCO FT/IR-460Plus spectrometer (JASCO, Tokyo, Japan) as a KBr pellet. Molecular weights and distributions of polymers were estimated by size exclusion chromatography equipped with a Shodex KF-805L column (Showa Denko, Tokyo, Japan), JASCO PU-2080Plus HPLC pump, JASCO UV-970 UV/VIS Detector at 650 nm, and JASCO CO-1560 column oven. THF was used as eluent and polystyrene as standards. Thermogravimetric analysis (TGA) was conducted with a TG/DTA6200 (SII NanoTechnology Inc., Chiba, Japan) at a heating rate of 10 ˚C/min under a nitrogen flow. UV-vis-NIR spectra were measured in chlorobenzene with 10 mm quartz cell using a JASCO V-570 spectrometer. Spin-coated films on glass plate substrates from chlorobenzene solution (5 mg/mL) were used for solid state UV-vis-NIR spectra measurements. HOMO levels of polymers were measured using a photoelectron spectrometer AC-2 (Riken Keiki, Tokyo, Japan) by measuring the ionization potential of polymer film in air. The ionization potential of the polymers was estimated by the plots of the photoelectron quantum yield from the polymer solid surface against the incident photon energy. That is, the threshold of the photoelectron quantum yield was correlated with the ionization potential. Space charge limited current (SCLC) measurements were carried out using an HZ-5000 electrochemical analyzer (Hokuto Denko, Japan). Atomic force microscopy (AFM) was performed using a SII SPI3800N AFM (Seiko, Japan).

3. Synthesis

4-Trifluoromethylphenyl 4,6-dibromothieno[3,4-*b*]thiophene-2-carboxylate (TT1). To 4,6-dibromo-thieno[3,4-*b*]thiophene-2-carboxylic acid (**1**) (500 mg, 1.46 mmol) in anhydrous toluene (5 mL) were added oxalyl chloride (371 mg, 2.92 mmol) and two drops of DMF at 0 °C under nitrogen atmosphere. The mixture was stirred at room temperature for 2 h and then volatile species were removed by evaporation in vacuo. To the residue were added 4-trifluoromethylphenol (355 mg, 2.19 mmol) and anhydrous pyridine (5 mL) at room temperature. After the reaction mixture was stirred at room temperature for 12 h, the solvent was removed in vacuo and the residue was extracted with dichloromethane. The organic layer was washed with brine, dried over anhydrous Na_2SO_4, and concentrated by evaporation. The crude product was purified by silica gel chromatography using hexane–dichloromethane (4/1) to yield **TT1** as a yellowish solid (483 mg, 1.08 mmol, 72%). Mp 152.6 – 152.9 ˚C. IR (KBr): 1720 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, rt): δ 7.77 (s, 1H), 7.72 (d, 2H, J = 9.0 Hz), 7.38 (d, 2H, J = 8.5 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, rt): δ 160.68, 153.13, 145.75, 140.79, 139.49, 129.46, 129.19, 128.93, 128.67, 127.39, 125.67, 125.23, 122.37, 103.93, 97.99. Anal. Calcd for $C_{14}H_5Br_2F_3O_2S_2$: C, 34.59; H, 1.04. Found: C, 34.61; H, 1.09.

4-Fluorophenyl 4,6-dibromothieno[3,4-*b*]thiophene-2-carboxylate (TT2). The title compound was prepared from **1** and 4-fluorophenol in the same way for **TT1** and obtained in 80% yield. Mp 151.4 – 151.6 ˚C. IR (KBr): 1735 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, rt): δ 7.74 (s, 1H), 7.21-7.18 (m, 2H), 7.12 (t, 2H, J = 8.3 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, rt): δ 161.59, 160.93, 159.65, 146.25, 145.54, 140.55, 139.66, 125.02, 123.04, 122.97, 116.53, 116.34, 103.36, 97.61. Anal. Calcd for $C_{13}H_5Br_2FO_2S_2$: C, 35.80; H, 1.16. Found: C, 36.07; H, 1.22.

Phenyl 4,6-dibromothieno[3,4-*b*]thiophene-2-carboxylate (TT3). The title compound was prepared from **1** and phenol in the same way for **TT1** and obtained in 79% yield. Mp 134.8 – 135.1 ˚C. IR (KBr): 1720 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, rt): δ 7.75 (s, 1H), 7.44 (t, 2H, J = 7.8 Hz), 7.30 (t, 1H, J = 7.5 Hz), 7.23 (d, 2H, J = 8.0 Hz). ^{13}C NMR (125 MHz, $CDCl_3$, rt): δ 160.95,

150.47, 145.63, 140.63, 140.08, 129.76, 126.52, 124.86, 121.54, 103.20, 97.55. Anal. Calcd for $C_{13}H_6Br_2O_2S_2$: C, 37.34; H, 1.45. Found: C, 37.33; H, 1.45.

4-Methoxyphenyl 4,6-dibromothieno[3,4-*b*]thiophene-2-carboxylate (TT4). The title compound was prepared from **1** and 4-methoxyphenol in the same way for **TT1** and obtained in 92% yield. Mp 164.4 – 164.6 °C. IR (KBr): 1717 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, rt): δ 7.73 (s, 1H), 7.14 (d, 2H, J = 9.0 Hz), 6.94 (d, 2H, J = 9.0 Hz), 3.83 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$, rt): δ 161.32, 157.75, 145.65, 143.96, 140.64, 140.17, 124.73, 122.33, 114.71, 103.10, 97.52, 55.78. Anal. Calcd for $C_{14}H_8Br_2O_3S_2$: C, 37.52; H, 1.80. Found: C, 37.56; H, 1.89.

Octyl 4,6-dibromothieno[3,4-*b*]thiophene-2-carboxylate (TT5). The title compound was prepared from **1** and *n*-octanol in the same way for **TT1** and obtained in 92% yield. Mp 64.8 – 65.0 °C. IR (KBr): 1719 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, rt): δ 7.53 (s, 1H), 4.31 (t, 2H, J = 6.5 Hz), 1.75 (quit, 2H, J = 7.1 Hz), 1.47-1.25 (m, 10H), 0.89 (t, 3H, J = 7.0 Hz), ^{13}C NMR (125 MHz, $CDCl_3$, rt): δ 162.55, 145.73, 141.27, 140.57, 123.32, 102.38, 97.28, 66.35, 31.93, 29.34, 29.31, 28.71, 26.04, 22.79, 14.26. Anal. Calcd for $C_{15}H_{18}Br_2O_2S_2$: C, 39.66; H, 3.99. Found: C, 39.55; H, 3.99.

4,8-Bis(2-octyldodecyloxy)benzo[1,2-*b*:3,4-*b*]dithiophene (2b). To a mixture of 4,8-dihydrobenzo[1,2-*b*:4,5-*b*']dithiophen-4,8-dion (1.98 g, 9.00 mmol) and metallic zinc (sandy, 1.47 g, 22.5 mmol) was added 5 N NaOH aqueous solution (27 mL) and the mixture was stirred under reflux for 3 h, After 1-iode-2-octyldodecane (14.7 g, 36.0 mmol) and tetrabutylammonium bromide (585 mg, 1.80 mmol) were added to the mixture, the reaction mixture was further refluxed for 12 h. The reaction mixture was then extracted with diethyl ether, and the organic layer was washed with brine and dried over anhydrous $NaSO_4$. After evaporating the solvent, the crude product was purified by silica gel chromatography using hexane–dichloromethane (10/1) to yield **2b** as a colorless sticky oil (3.64 g, 4.64 mmol, 52%). ^1H NMR (500 MHz, $CDCl_3$, rt): δ 7.47 (d, 2H, J = 6.0 Hz), 7.36 (d, 2H, J = 5.5 Hz), 4.16 (d, 4H, J = 5.0 Hz), 1.88-1.83 (m, 2H), 1.66-1.60 (m, 4H), 1.53-1.21 (m, 60H), 0.90-0.87 (m, 12H).

2,6-Bis(trimethyltin)-4,8-bis(2-octyldodecyloxy)benzo[1,2-*b*:3,4-*b′*]dithiophene (BDTb). To a solution of **2b** (4.40 g, 5.62 mmol) in anhydrous THF (67 mL) was added dropwise *n*-butyllithium (1.6 M in hexane, 8.78 mL, 14.1 mmol) via syringe at -78 ˚C under nitrogen atmosphere. The mixture was stirred at -78 ˚C for 30 min and then at room temperature for 30 min. After the mixture was cooled to -78 ˚C again, trimethyltin chloride (3.36 g, 16.9 mmol) in anhydrous THF (17 mL) was added. The mixture was warmed to room temperature and stirred for 12 h. After quenching the reaction with water, the volatile species were evaporated in vacuo. The residue was extracted with hexane, and the organic layer was washed with brine, dried over anhydrous $NaSO_4$, and concentrated. The crude product was purified by recrystallization from 2-propanol to yield **BDTb** as a colorless crystals (4.78 g, 4.31 mmol, 77%). Mp 38.5 – 38.7 ˚C. ^{1}H NMR (500 MHz, $CDCl_3$, rt): δ 7.51 (s, 2H), 4.17 (d, 4H, J = 5.0 Hz), 1.89-1.81 (m, 2H), 1.70-1.61 (m, 4H), 1.54-1.22 (m, 60H), 0.95-0.85 (m, 12H). ^{13}C NMR (125 MHz, $CDCl_3$, rt): δ 143.40, 140.49, 134.01, 133.06, 128.13, 76.10, 39.37, 32.10, 31.59, 30.35, 29.95, 29.93, 29.89, 29.86, 29.57, 29.55, 27.25, 22.86, 14.28, -8.21. Anal. Calcd for $C_{56}H_{102}O_2S_2Sn_2$: C, 60.65; H, 9.27. Found: C, 60.69; H, 9.50.

4. Polymerization

Polymerization was carried out in a dry Schlenk flask under nitrogen atmosphere in a similar way previously reported.[4] Each monomer was purified by recrystallization just before use. A typical polymerization procedure is described below.

TT1 (100 mg, 0.206 mmol), **BDTb** (228 mg, 0.206 mmol), and $Pd(PPh_3)_4$ (9.5 mg, 9.6 μmol) was placed in a Schlenk flask under nitrogen atmosphere. Anhydrous toluene (3.3 mL) and DMF (0.82 mL) were added with a syringe and the mixture was then heated at 120 °C. After 12 h, the reaction mixture was cooled to room temperature and poured into a large amount of methanol (MeOH). The resulting polymer was collected by centrifugation, and then purified by Soxhlet extraction for 12 h with MeOH and 12 h with hexane. After the polymer was collected with chlorobenzene, the chlorobenzene solution was passed through Celite to remove the metal catalyst

and concentrated. The target polymer **PTT1BDTb** was obtained as dark red solid (142 mg, 62%) by precipitating in MeOH and drying in vacuo. IR (KBr): 1735 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, 50 °C): δ 8.40-7.00 (7H, br), 4.40-3.80 (4H, br), 2.10-0.70 (78H, br). Anal. Calcd for $(C_{64}H_{89}F_3O_4S_4)_n$: C, 69.40; H, 8.10. Found: C, 69.56; H, 8.45.

In the same way, **PTT2BDTb**, **PTT3BDTb**, **PTT4BDTb**, **PTT5BDTb**, and **PTT5BDTa** were synthesized with the corresponding monomers. The polymerization results are summarized in Table 1.

Spectroscopic data of **PTT2BDTb**. IR (KBr): 1729 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, 50 °C): δ 8.40-6.90 (7H, br), 4.40-3.80 (4H, br), 2.10-0.70 (78H, br). Anal. Calcd for $(C_{63}H_{89}FO_4S_4)_n$: C, 71.54; H, 8.48. Found: C, 71.31; H, 8.72.

Spectroscopic data of **PTT3BDTb**. IR (KBr): 1729 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, 50 °C): δ 8.40-7.00 (8H, br), 4.40-4.00 (4H, br), 2.10-0.70 (78H, br). Anal. Calcd for $(C_{63}H_{90}O_4S_4)_n$: C, 72.78; H, 8.73. Found: C, 72.63; H, 9.02.

Spectroscopic data of **PTT4BDTb**. IR (KBr): 1732 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, 50 °C): δ 8.40-6.70 (7H, br), 4.40-3.70 (7H, br), 2.10-0.70 (78H, br). Anal. Calcd for $(C_{64}H_{92}O_5S_4)_n$: C, 71.86; H, 8.67. Found: C, 72.07; H, 9.07.

Spectroscopic data of **PTT5BDTb**. IR (KBr): 1717 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, 50 °C): δ 8.10-7.00 (3H, br), 4.70-4.00 (6H, br), 2.30-0.70 (93H, br). Anal. Calcd for $(C_{65}H_{102}O_4S_4 \cdot 0.5H_2O)_n$: C, 72.09; H, 9.57. Found: C, 72.10; H, 9.84.

Spectroscopic data of **PTT5BDTa**. IR (KBr): 1713 cm^{-1} ($\nu_{C=O}$). ^1H NMR (500 MHz, $CDCl_3$, 50 °C): δ 8.30-6.40 (3H, br), 4.90-3.60 (6H, br), 2.60-0.70 (45H, br). Anal. Calcd for $(C_{41}H_{54}O_4S_4)_n$: C, 66.62; H, 7.36. Found: C, 65.61; H, 7.41.

5. Computational study

All DFT calculations were performed at the B3LYP/6-31G (d,p) level[5] using the Gaussian 03 package.[6] The model compounds, which consist of one TT unit and two BDT units bearing methoxy

groups instead of octyldodecyloxy groups, were used for the computational study as simplified models.

6. Fabrication of hole-only devices

The ITO electrode was ultrasonicated in 2-propanol, cleaned in boiling 2-propanol, and then dried in air. A dispersion of PEDOT:PSS in water was spin-coated onto the clean ITO electrode at 6000 rpm, and then dried at 150 °C for 5 min. A solution of the polymers in chlorobenzene (25 mg/mL) was spin-coated onto the ITO/PEDOT:PSS substrate at 700 rpm. A dispersion of PEDOT:PSS in water containing 0.01 wt.% PTE was heated to 85 °C, and then spin-coated onto the polymer layer at 6000 rpm. The Au electrode was vacuum deposited onto the PEDOT:PSS layer under a pressure of 2×10^{-5} Torr. The structure of the hole-only device is ITO/PEDOT:PSS/polymer/PEDOT:PSS/Au, whose effective area is 0.04 cm^2.

7. Hole mobility measurements

The hole mobilities of the polymers were estimated from the SCLC *I-V* characteristics of the hole-only devices.[7] *I-V* characteristics of the hole-only devices in the dark in air are shown in Figures S17. The SCLC behavior in the trap-free region can be characterized using the Mott-Gurney square law ($J = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_h\frac{V^2}{L^3}$), where J is the current density ($A \cdot cm^{-2}$), ε_0 is the vacuum permittivity (8.85×10^{-12} $F \cdot m^{-1}$), ε_r is the dielectric constant of the organic material, μ_h is the hole mobility ($cm^2 \cdot V^{-1} \cdot s^{-1}$), L is the polymer thickness (m), and V is the applied voltage (V). The dielectric constant, ε_r, is assumed to be 3 in our analysis, which is a typical value for conjugated polymers. The thickness of the polymer films is measured by using AFM to be from 66 to 198 nm. The hole mobilities were calculated from the double-logarithmic plots of the *I-V* characteristics by fitting with a line with a slope of 2.

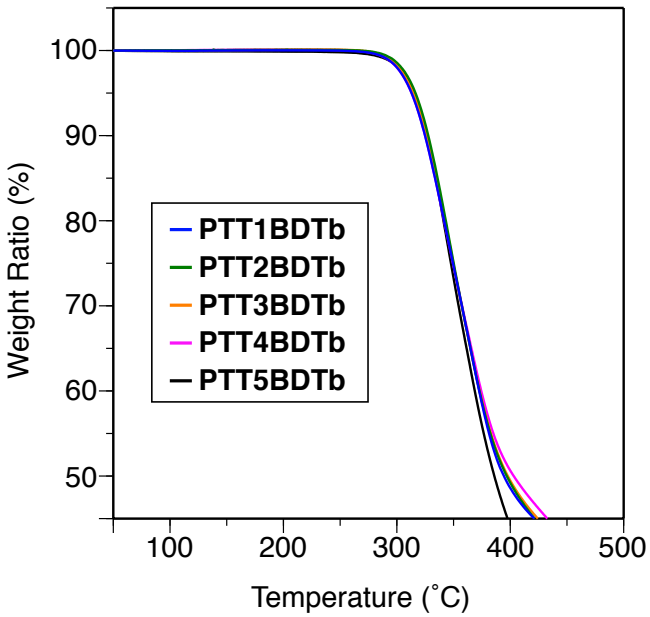

Figure S1. Thermogravimetric analysis of the polymers with a heating rate of 10 ˚C/min in N_2.

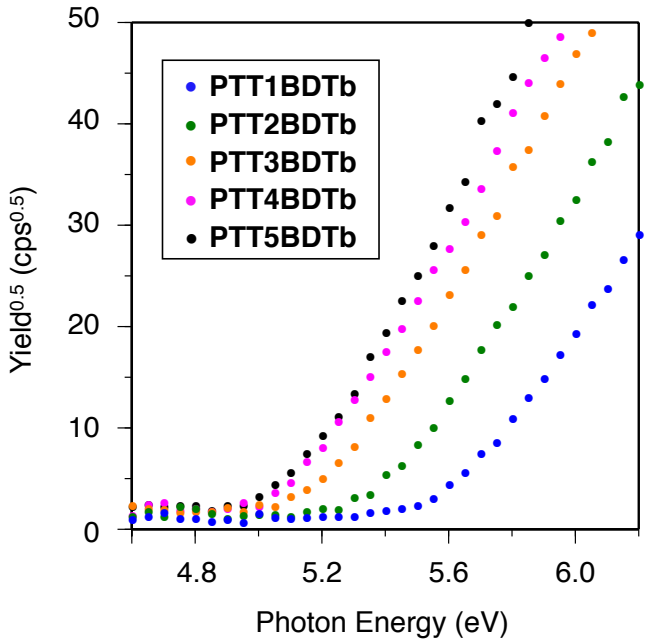

Figure S2. Photoelectron spectra of the polymers in air.

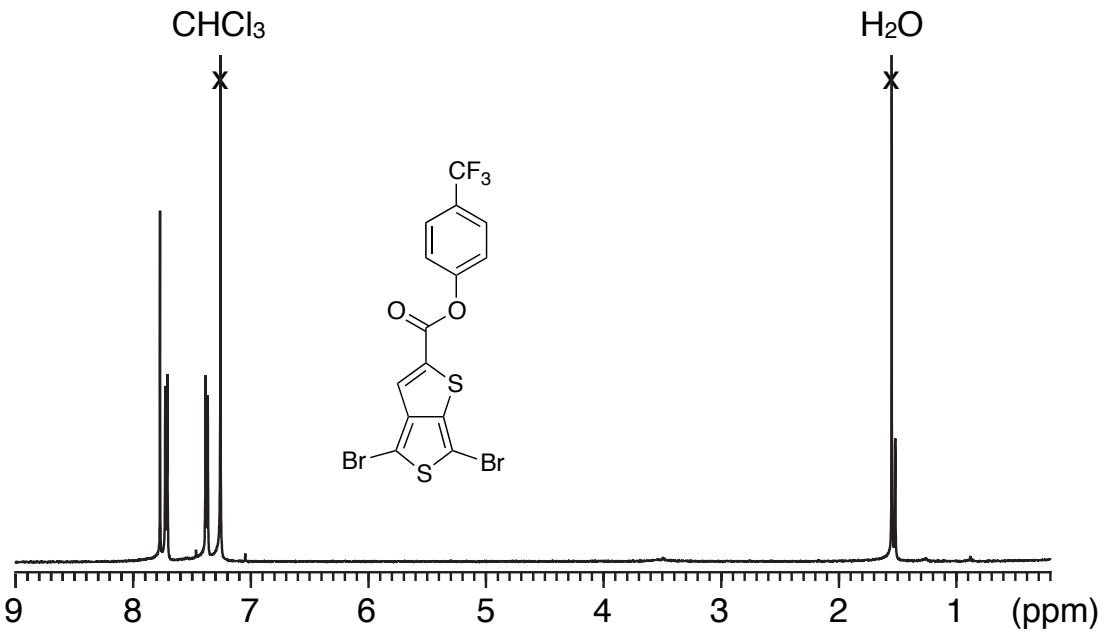

Figure S3. ^{1}H NMR spectrum of **TT1** in $CDCl_3$ at rt.

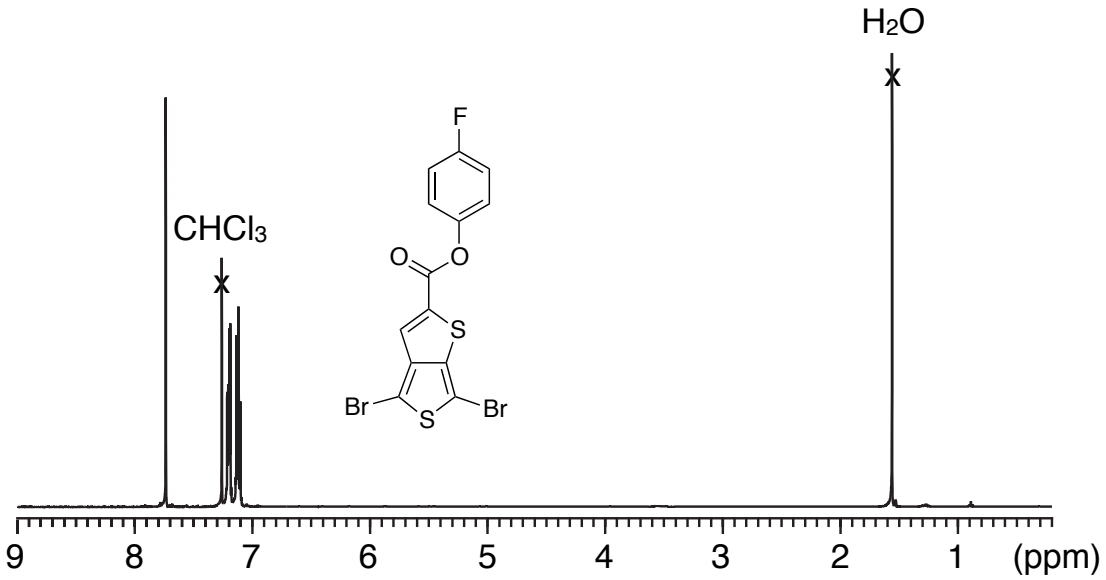

Figure S4. ^{1}H NMR spectrum of **TT2** in $CDCl_3$ at rt.

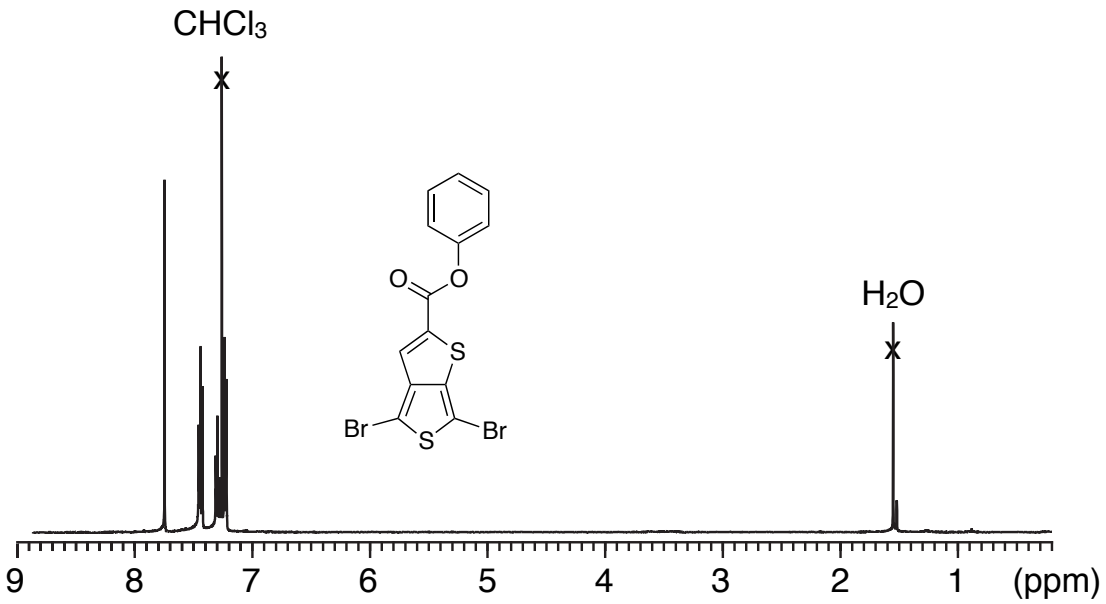

Figure S5. ^{1}H NMR spectrum of **TT3** in $CDCl_3$ at rt.

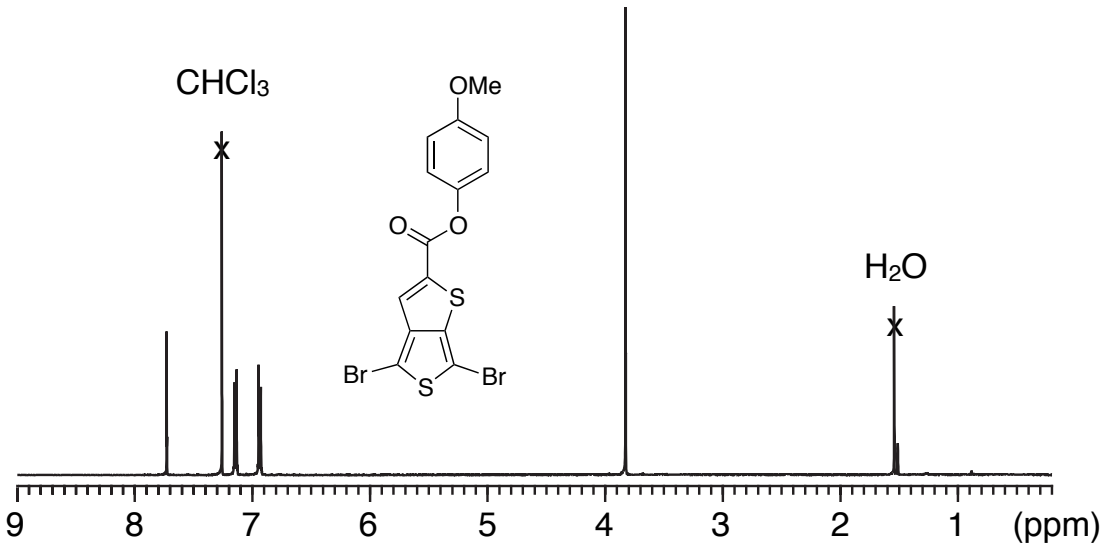

Figure S6. ^{1}H NMR spectrum of **TT4** in $CDCl_3$ at rt.

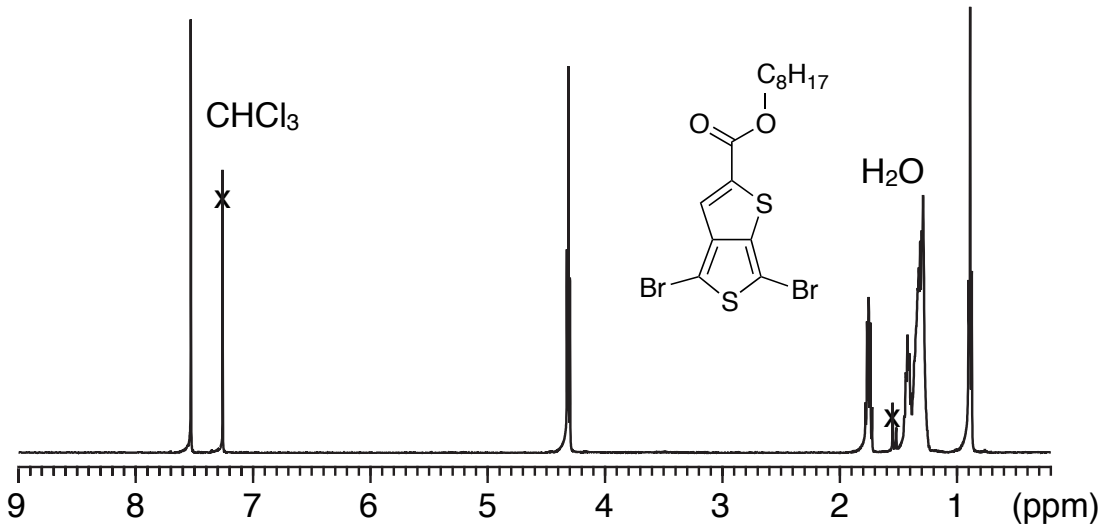

Figure S7. ^{1}H NMR spectrum of **TT5** in $CDCl_3$ at rt.

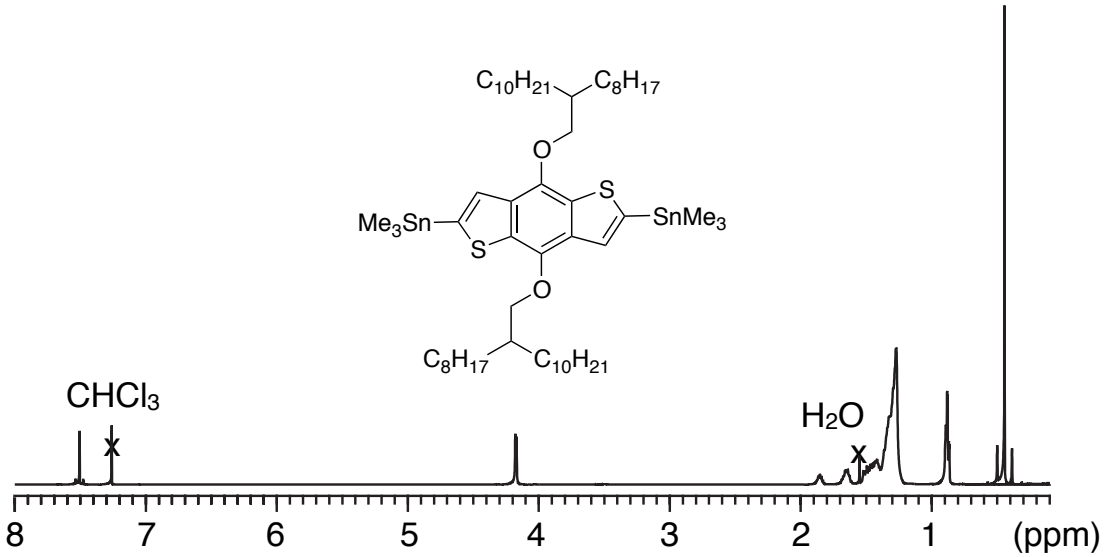

Figure S8. ^{1}H NMR spectrum of **BDTb** in $CDCl_3$ at rt.

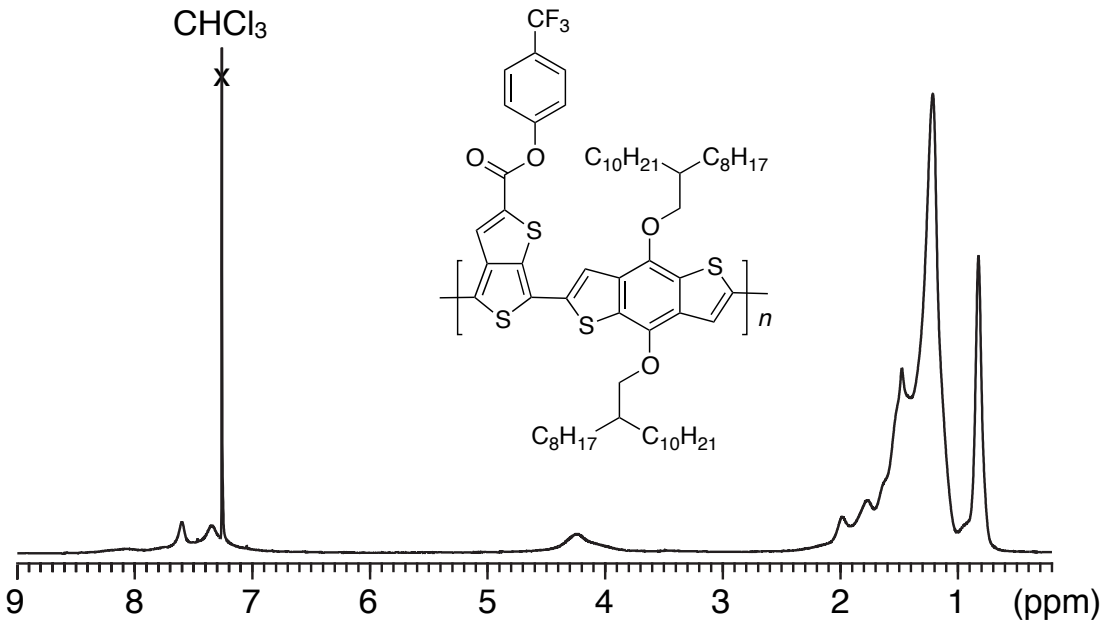

Figure S9. ^{1}H NMR spectrum of **PTT1BDTb** in $CDCl_3$ at 50 °C.

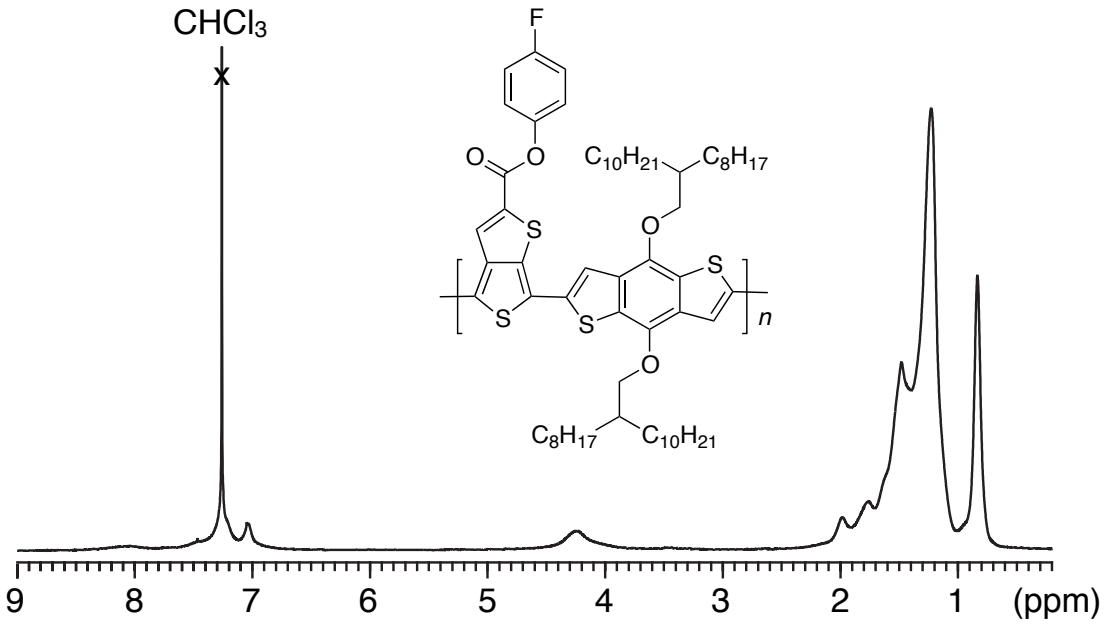

Figure S10. ^{1}H NMR spectrum of **PTT2BDTb** in $CDCl_3$ at 50 °C.

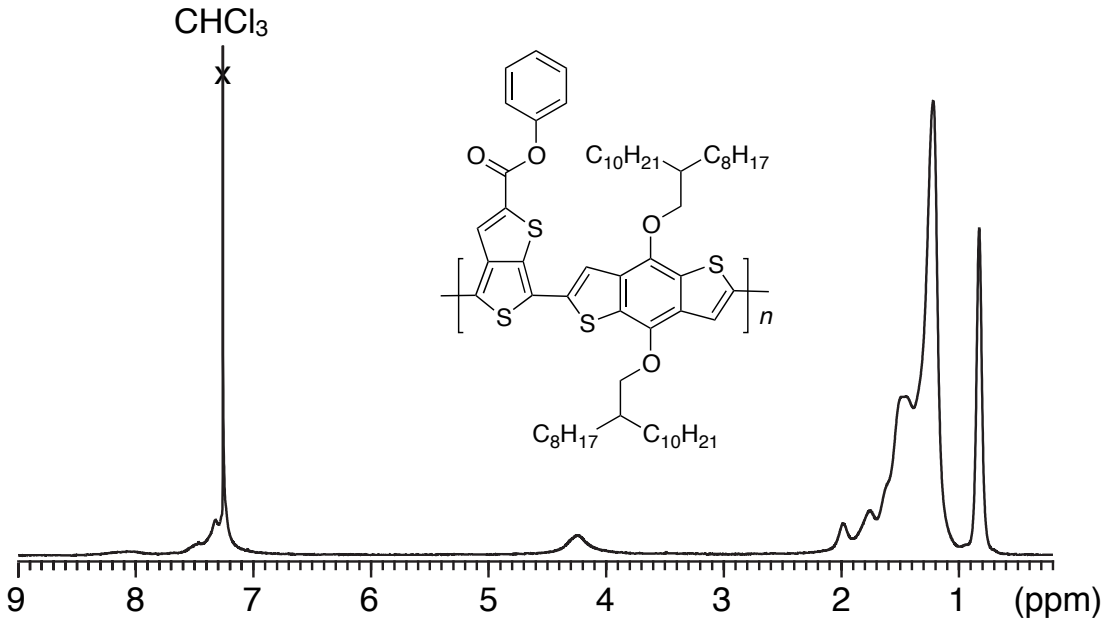

Figure S11. ^{1}H NMR spectrum of **PTT3BDTb** in $CDCl_3$ at 50 ˚C.

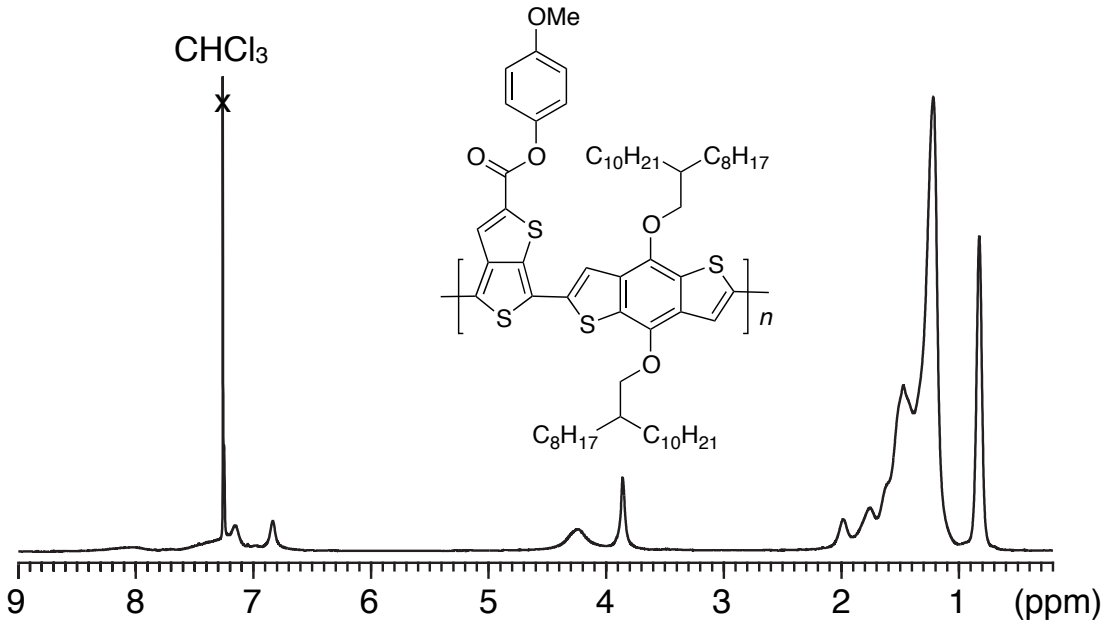

Figure S12. ^{1}H NMR spectrum of **PTT4BDTb** in $CDCl_3$ at 50 ˚C.

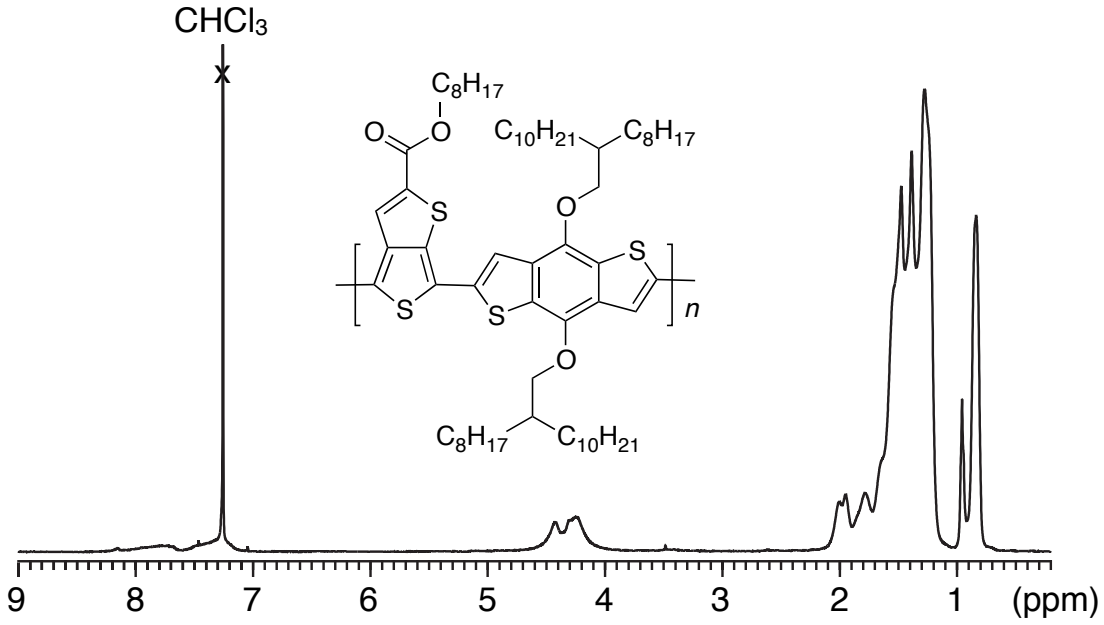

Figure S13. ^{1}H NMR spectrum of **PTT5BDTb** in $CDCl_3$ at 50 ˚C.

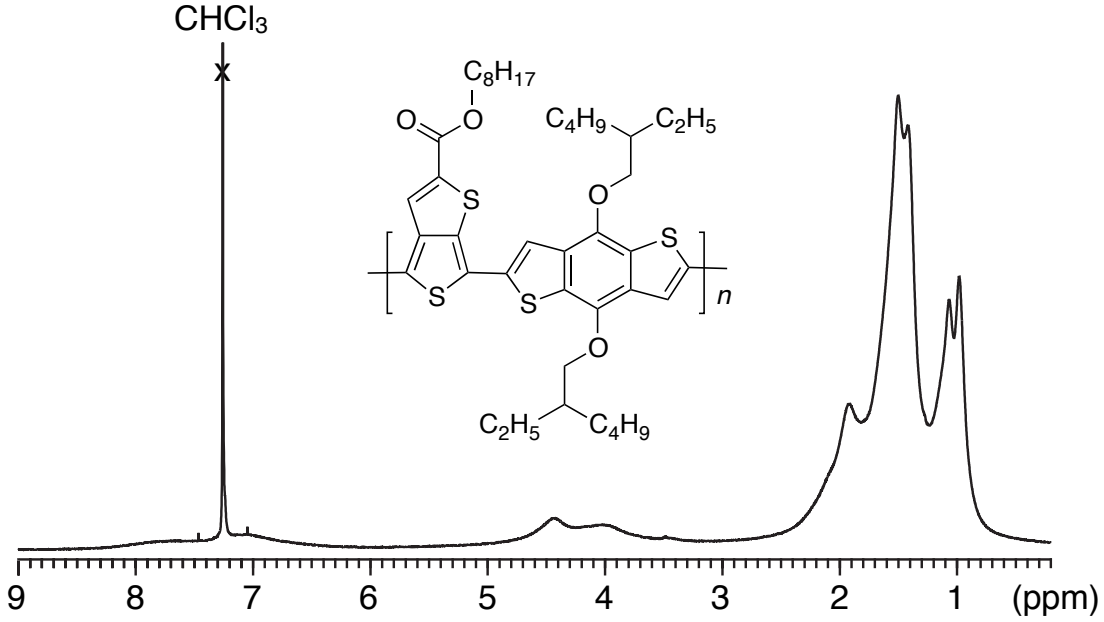

Figure S14. ^{1}H NMR spectrum of **PTT5BDTa** in $CDCl_3$ at 50 ˚C.

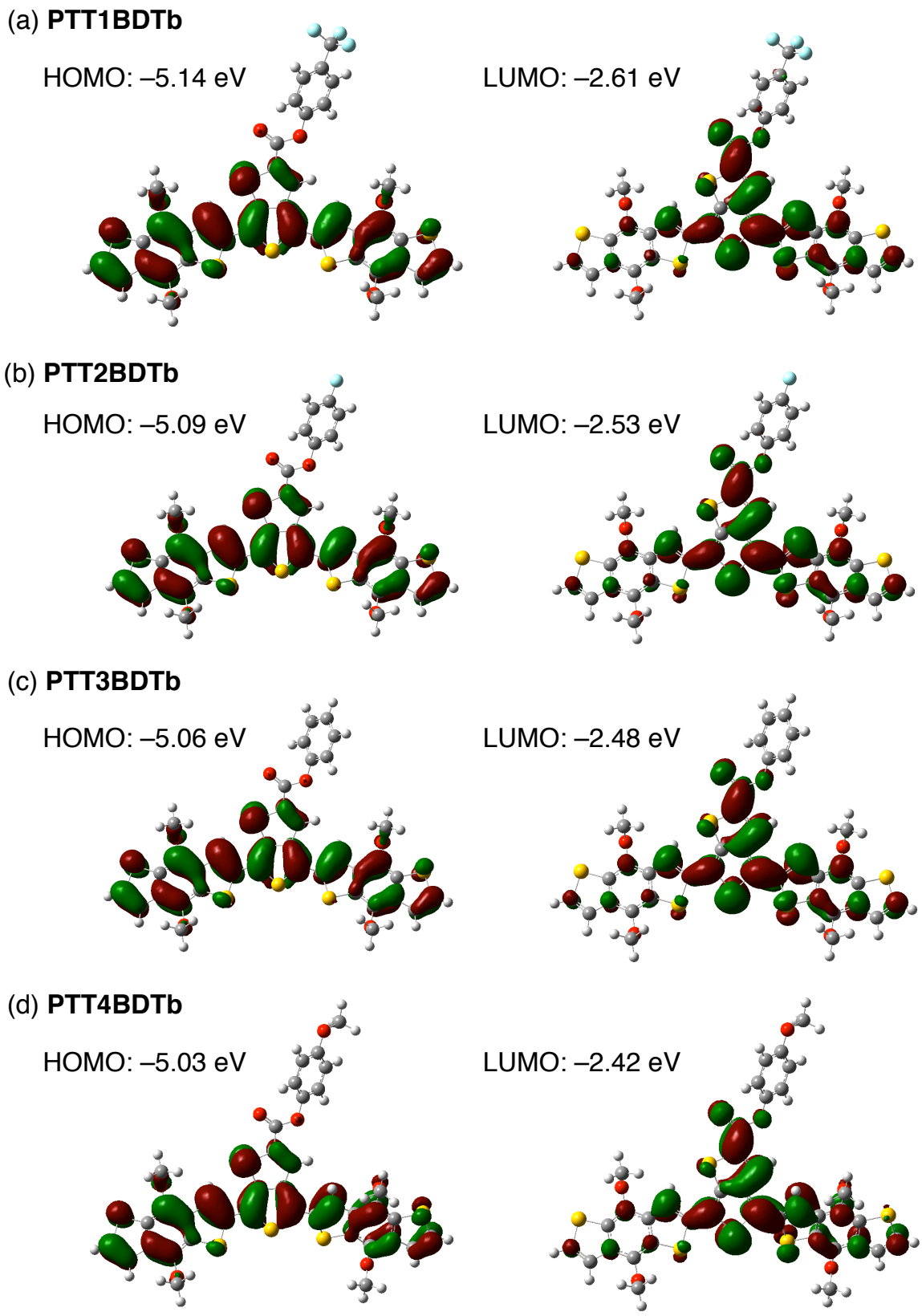

Figure S15. HOMO and LUMO energy levels and the frontier molecular orbital obtained from DFT calculations on the model compounds of (a) **PTT1BDTb**, (b) **PTT2BDTb**, (c) **PTT3BDTb**, and (d) **PTT4BDTb**.

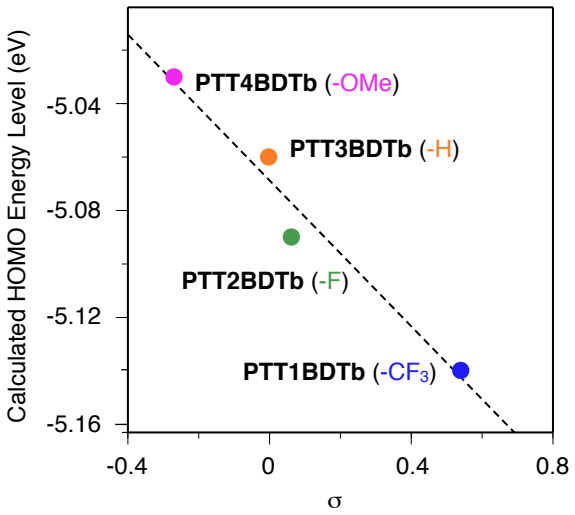

Figure S16. Plots of calculated HOMO energy levels of the polymers against the Hammett constants σ of the substituents.

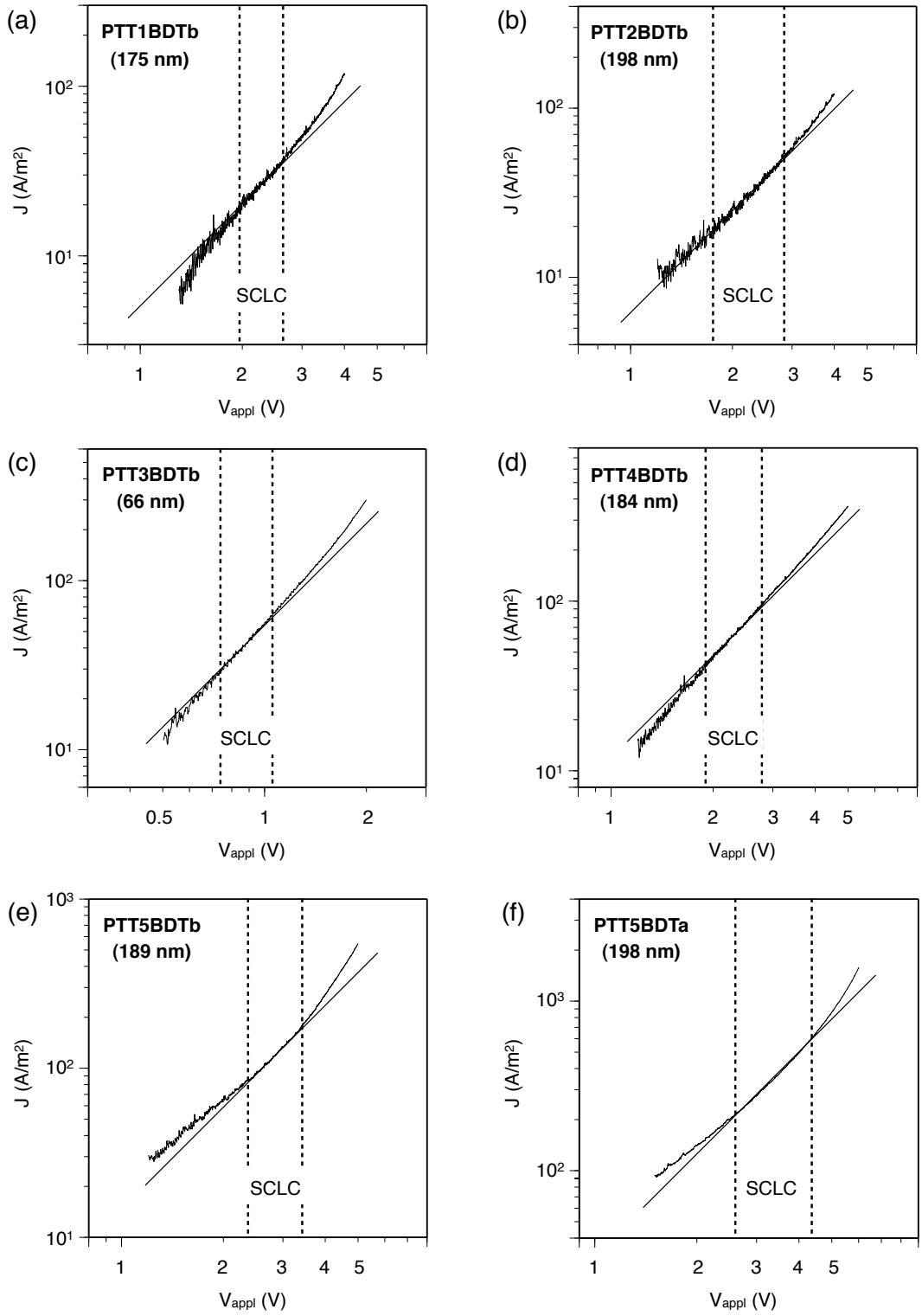

Figure S17. Double-logarithmic plots of *I-V* curves obtained for hole-only devices (ITO/PEDOT:PSS/PTB-based polymer/PEDOT:PSS/Au) in the dark in air: (a) **PTT1BDTb**, (b) **PTT2BDTb**, (c) **PTT3BDTb**, (d) **PTT4BDTb**, (e) **PTT5BDTb**, and (f) **PTT5BDTa**. The thickness (L) of the organic films determined by AFM is shown in the parentheses.

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