

## Supporting Information

### Indolo[3,2-b]indole-containing donor–acceptor copolymers for high-efficiency organic solar cells

*By Jaeyoung Hwang, Jeonghun Park, Yu Jin Kim, Yeon Hee Ha, Chan Eon Park, Dae Sung Chung,\* Soon-Ki Kwon\* and Yun-Hi Kim,\**

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## Materials.

All chemicals were purchased from Sigma-Aldrich, Alfa Aesar, TCI, Strem Chemicals: methyl 2-aminobenzoate, NaH (60 % dispersion in mineral oil), Phosphorus pentachloride, Zinc, Trifluoroacetic acid, 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, bromine, Pd<sub>2</sub>(dba)<sub>3</sub>, P(o-tol)<sub>3</sub> were used without further purification. 11-(bromomethyl)tricosane (4) [1], 4,7-bis(5-bromothiophen-2-yl)benzo[c][1,2,5]thiadiazole (8) [2], 4,7-bis(5-bromothiophen-2-yl)-5-fluorobenzo[c][1,2,5]thiadiazole (9) [2] and 4,7-bis(5-bromothiophen-2-yl)-5,6-difluorobenzo[c][1,2,5]thiadiazole (10) [2] were synthesized using literature reported procedures.

**Measurement.** <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra were recorded with a Bruker Advance-300 spectrometer. A Jeol JMS-700 mass spectrometer was used to obtain the mass spectra of the samples. The thermal analysis was performed on a TA TGA 2100 thermogravimetric analyzer in a nitrogen atmosphere at a rate of 10 °C/min. Differential scanning calorimeter (DSC) was performed using a TA DSC 2010 device at a heating rate of 10 °C/min. UV-vis absorption spectra were measured by UV-1650PC spectrophotometer. Molecular weights and polydispersities of the copolymers were determined by gel permeation chromatography (GPC) analysis with polystyrene standard calibration (waters high-pressure GPC assembly Model M515 pump, u-Styragel columns of HR4, HR4E, HR5E, with 500 and 100 Å, refractive index detectors, solvent CHCl<sub>3</sub>). Cyclic voltammetry (CV) was performed using a CH instruments electrochemical analyzer. A three-electrode system was used, composing of a glassy carbon working electrode, a platinum wire counter electrode and Ag/AgCl reference electrode. Transmission electron microscopy (TEM) bulk images were measured on a HITACHI-7600 at 100 kV. The crystalline structure was investigated two-dimensional

grazing incidence wide angle X-ray scattering technique (2D-GIWAXS). For 2D-GIWAXS experiments, the active films spin-cast onto the Si substrates and their patterns were recorded MARCCD systems in 3C beam line of Pohang Accelerator Laboratory.

### **Device fabrication and characterization.**

Polymer solar cells were fabricated with the general sandwich structure through several steps. Firstly, indium-tin-oxide (ITO) patterned coating glass substrates were cleaned by ultrasonication sequentially in detergent, di-water, acetone (CMOS grade) and 2-propanol (CMOS grade). To remove residues, the cleaned ITO glass substrates were treated with UV-ozone treatments for 20 min. After that, for hole extraction layer, we chose a MoO<sub>3</sub> layer (ca. 10 nm), which is deposited via thermal evaporation. An active layer is deposited onto MoO<sub>3</sub>/ITO glass substrates with 1500 rpm for 50 s, and the thickness is ca. 92 nm. Before spin-casting active layer, the active solution is sufficiently stirred to 1:1 blend ratio with PC<sub>71</sub>BM in nitrogen-filled glove box for 12 h. Upon spin-casting active layer, the substrates with two layers were baked onto hot plate for 10 min at 80°C to remove remained solvents. Finally, the LiF/Al double cathode is thermally deposited in high vacuum condition ( $2 \times 10^{-6}$  Torr.) with 0.8/100 nm. The current-voltage ( $J$ - $V$ ) characteristics of the photovoltaic polymer solar cells were measured using a Keithley 2400  $I$ - $V$  measurement system (AM 1.5G/1 sun/100 mw cm<sup>-2</sup>). The external quantum efficiency (EQE) of the photovoltaic devices was recorded on a photomodulation spectroscopic system (Merlin model; Oriel Instruments, Irvine, CA, USA). A calibrated Si detector was used to measure the light intensity.

Charge carrier mobility measurement by the space charge limited current (SCLC) method.

Hole- and electron-only diodes were fabricated with the device structure of ITO

glass/MoO<sub>3</sub>/active layer/Au (100 nm) and Al (110 nm)/active layer/Al(110 nm), respectively. In two diodes, all metal electrodes as well as MoO<sub>3</sub> layer is thermally deposited to evaporation system in high vacuum. The active layer is spin-cast to same condition with solar cell fabrication method. Charge carrier mobility (both hole- and electron-mobilities) was determined by the Mott-Gurney equation in the SCLC region (at voltage 2-3 V, slope = 2):  $J = 9 \epsilon \epsilon_0 \mu_{h/e} V^2 / 8L^3$ , in which  $J$  is dark current density,  $\epsilon$  is the dielectric constant (polymer = assumed to be 3),  $\epsilon_0$  is the permittivity of the vacuum,  $\mu_{h/e}$  is the carrier mobility,  $V$  is internal voltage in the device, and  $L$  is film thickness of active layer [3].

## Synthesis and characterization.

### Synthesis of dibenzo[b,f][1,5]diazocine-6,12(5H,11H)-dione (1)

Methyl 2-aminobenzoate (30 g, 198 mmol) was dissolved in anhydrous THF (800 mL). After then was dropwise to NaH (12.8 g, 533 mmol, 60 % dispersion in mineral oil) at room temperature. The reaction mixture was refluxed for 78 h at 100 °C. The mixture was cooled to room temperature and then poured slowly into 5N HCl and ice. After the ice had melted, the precipitated product was collected by filtration, washed with distillation water (250 mL), and washed with Et<sub>2</sub>O (50 mL) to afford compound (1) as a white solid (55.7g, 79%). <sup>1</sup>H NMR (DMSO-d<sub>6</sub>,  $\delta$ ) : 10.2 (s, 1H), 7.34-7.30 (m, 4H), 7.26-7.21 (m, 2H), 7.08 (d, 2H), <sup>13</sup>C NMR (DMSO-d<sub>6</sub>,  $\delta$ ) : 169.7, 135.2, 134.0, 131.0, 128.6, 127, 7, 126.1.

### Synthesis of 6,12-dichlorodibenzo[b,f][1,5]diazocine (2)

PCl<sub>5</sub> (47 g, 226 mmol) was added to a mixed solution of compound (1) (24.0 g, 100 mmol) and anhydrous CHCl<sub>3</sub> (500 mL). The reaction mixture was refluxed for 6 h at 115 °C. After

filtration, the solid which separated on concentration of the filtrate was washed with acetone (100 mL, 3 times) to afford compound (2) as a white solid (10.4 g, 34%).  $^1\text{H}$  NMR (DMSO- $d_6$ ,  $\delta$ ) : 7.51-7.46 (m, 4H), 7.28 (t, 2H), 7.05 (d, 2H),  $^{13}\text{C}$  NMR (DMSO- $d_6$ ,  $\delta$ ) : 156.3, 145.3, 131.5, 127.0, 126.2, 125.4, 122.1.

### **Synthesis of 5,10-dihydroindolo[3,2-b]indole (3)**

The Zn power (12.0 g, 183 mL) was added to a mixed solution of the compound (2) (4.21 g, 15.3 mmol) and anhydrous THF (400 mL). After then TFA (27 mL, 367 mmol) was added dropwise at room temperature. The reaction mixture was stirred for 10 h at that temperature, then saturated aqueous  $\text{NH}_4\text{Cl}$  solution (50 mL) was added to quench the reaction. The reaction mixture was extracted with ethyl acetate and washed with water. The combined organic phase was dried with  $\text{MgSO}_4$  and concentrated under reduced pressure. The crude product was purified by recrystallization (MeOH) to afford compound (3) as white solid (1.58 g, 50 %).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ,  $\delta$ ) : 11.07 (s, 2H), 7.74 (d, 2H), 7.50 (d, 2H), 7.18-7.16 (m, 2H), 7.10-7.07 (m, 2H),  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ,  $\delta$ ) : 140.8, 125.7, 121.8, 118.4, 117.9, 115.2, 112.5,  $\text{EI}^+$  (mass):  $m/z$  = 206.

### **Synthesis of 5,10-bis(2-decyltetradecyl)-5,10-dihydroindolo[3,2-b]indole (5)**

In dry THF (50 mL), compound (3) (3.36 g, 16.3 mmol) and NaH (2.61 g, 65.2 mmol, 60 % dispersion in mineral oil) were dissolved. The reaction mixture was stirred at 70 °C for 20 min under  $\text{N}_2$  atmosphere. Then, the 11-(bromomethyl)tricosane (4) (20.42 g, 48.9 mmol) was added to the reaction mixture, and then the reaction mixture was refluxed for 24 h at same temperature. After reaction finished, the reaction mixture was poured into ice water

(500 mL), and extracted with diethyl ether. The combined organic phase was dried with  $\text{MgSO}_4$  and concentrated under reduced pressure. The crude product was purified with column chromatography with n-hexane and recrystallization (acetone) to afford compound (5) as white solid (8.74 g, 61%).  $^1\text{H}$  NMR ( $\text{CDCl}_3$ ,  $\delta$ ) : 7.86 (s, 2H), 7.14-7.46 (m, 6H), 4.38 (s, 4H), 2.21 (s, 2H), 1.42-1.19 (m, 80H), 0.91 (t, 12H).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ ,  $\delta$ ) : 141.0, 126.2, 121.3, 117.8, 114.6, 109.9, 49.97, 38.90, 31.97, 31.95, 31.76, 29.99, 29.71, 29.68, 29.62, 29.58, 29.40, 29.36, 26.57, 22.73, 14.15.  $\text{EI}^+$  (mass):  $m/z$  = 879. HRMS ( $\text{EI}^+$ ) Calcd for  $\text{C}_{62}\text{H}_{106}\text{N}_2$ : 878.8356, Found: 878.8342.

#### **Synthesis of 2,7-dibromo-5,10-bis(2-decyltetradecyl)-5,10-dihydroindolo[3,2-b]indole (6)**

Compound (5) (4.4 g, 5.0 mmol) was dissolved in  $\text{CHCl}_3$  (25 mL) and added pyridine (6 mL), then stirred for 10min at room temperature. Bromine solution (0.55mL, 10.8 mmol, in  $\text{CHCl}_3$  (10 mL)) was slowly added in reaction mixture. The reaction mixture was stirred for 2 h at room temperature and poured into 1M HCl (50 mL), the reaction mixture was extracted with ethyl acetate. The combined organic phase was dried with  $\text{MgSO}_4$  and concentrated under reduced pressure. The crude product was purified with column chromatography with n-hexane and recrystallization (acetone:n-hexane =2:1) to afford compound (6) as white solid (2.7 g, 52%).  $^1\text{H}$  NMR ( $\text{CD}_2\text{Cl}_2$ ,  $\delta$ ): 7.71 ( $J=8.48\text{Hz}$ , d, 2H), 7.62 ( $J=1.64\text{Hz}$ , d, 2H), 7.28 ( $J=8.49\text{Hz}$ , dd, 2H), 4.31 ( $J=7.64\text{Hz}$ , d, 4H), 2.20 (s, 2H), 1.36-1.20 (m, 80H), 0.91 (t, 12H).  $^{13}\text{C}$  NMR ( $\text{CD}_2\text{Cl}_2$ ,  $\delta$ ): 141.6, 126.1, 121.2, 118.9, 115.1, 113.1, 113.0, 49.97, 38.58, 3.95, 31.93, 31.59, 29.88, 29.69, 29.67 29.59, 29.48, 29.38, 29.35 26.41, 22.71, 13.90. HRMS (FAB) Calcd for  $\text{C}_{62}\text{H}_{104}\text{Br}_2\text{N}_2$  ( $\text{M}^{2+}$ ): 1034.7, Found: 1036.4.

**Synthesis of 5,10-bis(2-decyltetradecyl)-2,7-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-5,10-dihydroindolo[3,2-b]indole (7)**

n-BuLi (3.47 mL, 8.69 mmol, 2.5M solution in hexane) was added dropwise to a solution of compound (6) (4.1 g, 3.95 mmol) in anhydrous THF at -78 °C. After the reaction mixture was stirred at -78 °C for 1h. 2-Isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.56 mL, 12.55 mmol) was added to the reaction mixture at -78 °C. The reaction mixture was stirred for 30 min at -78 °C. After slowly warming to room temperature, the reaction mixture was stirred for 18 h. The reaction mixture was poured into water, extracted with ethyl acetate, and dried over MgSO<sub>4</sub>. The crude product was purified by flash column chromatography (n-hexane) and recrystallization (acetone) to afford compound (7) as white solid (1.88 g, 42%).  
<sup>1</sup>H NMR (CD<sub>2</sub>Cl<sub>2</sub>, δ): 7.94 (s, 2H), 7.88 (J=7.95Hz, s, 2H), 7.56 (J=7.98Hz, d, 2H), 4.45 (J=7.59Hz, d, 4H), 2.28 (s, 2H), 1.21-1.41 (m, 104H), 0.91 (t, 12H), HRMS (FAB) Calcd for C<sub>74</sub>H<sub>128</sub>B<sub>2</sub>N<sub>2</sub>O<sub>4</sub> : 1131.0, Found: 1131.4.

**Synthesis of poly[4-(5-(5,10-bis(2-decyltetradecyl)-5,10-dihydroindolo[3,2-b]indol-2-yl)thiophen-2-yl)-7-(thiophen-2-yl)benzo[c][1,2,5]thiadiazole] (PDHITHT)**

Compound (7) (339 mg, 0.30 mmol) and compound (8) (137 mg, 0.30 mmol) were dissolved in anhydrous toluene (10 mL) and nitrogen bubbled for 20 min in a tube-type schlenk flask. Pd<sub>2</sub>(dba)<sub>3</sub> (4.2 mg, 3 mol %, 4.5 μmol), P(o-tolyl)<sub>3</sub> (8.2 mg, 27 μmol), K<sub>3</sub>PO<sub>4</sub> (254 mg, 1.2 mmol), distilled water (3 mL), and Aliquat 336 (1 drop) were sequentially added into the flask. The reaction mixture was stirred and refluxed for 72 h before end-capping with phenylboronic acid and bromobenzene (0.03 mmol each). After it was cooled down, the mixture was poured into MeOH. The precipitate was collected and then purified by Soxhlet extraction with acetone, methanol, hexane, THF and chloroform in sequence. The chloroform

fraction was concentrated to small volume, which was followed by re-precipitation in MeOH. Finally, the precipitate was collected by suction filtration and completely dried in vacuum oven to afford deep purple polymer powder (120 mg, 25%). GPC analysis,  $M_n = 31,732 \text{ g mol}^{-1}$ ,  $M_w = 97,002 \text{ g mol}^{-1}$ , and PDI = 3.06 (against PS standard).

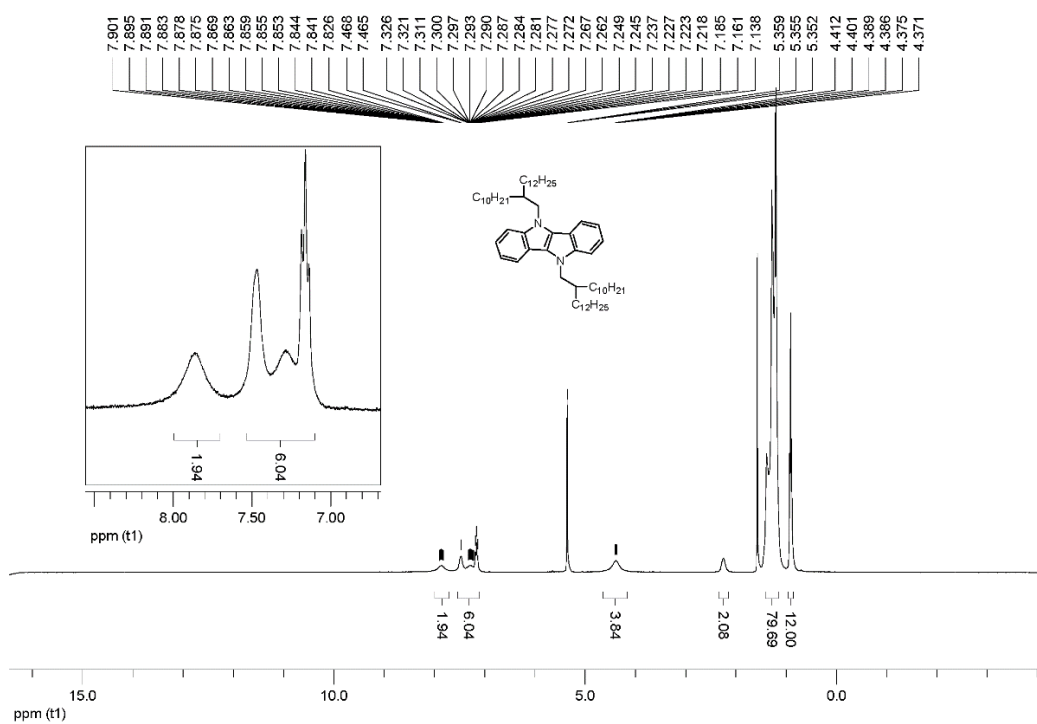
**Synthesis of poly[4-(5-(5,10-bis(2-decyltetradecyl)-5,10-dihydroindolo[3,2-b]indol-2-yl)thiophen-2-yl)-5-fluoro-7-(thiophen-2-yl)benzo[c][1,2,5]thiadiazole] (PDHITFT)**

Synthesis of PDHITFT was carried out in the same manner as PDHITHT. Compound (7) (339 mg, 0.30 mmol), compound (9) (143 mg, 0.30 mmol), anhydrous toluene (10 ml),  $\text{Pd}_2(\text{dba})_3$  (4.2 mg, 3 mol %, 4.5  $\mu\text{mol}$ ),  $\text{P}(\text{o-tolyl})_3$  (8.2 mg, 27  $\mu\text{mol}$ ),  $\text{K}_3\text{PO}_4$  (254 mg, 1.2 mmol), distilled water (3 mL), and Aliquat 336 (1 drop). PDHITFT (100 mg, 21%). GPC analysis,  $M_n = 25,777 \text{ g mol}^{-1}$ ,  $M_w = 78,610 \text{ g mol}^{-1}$ , and PDI = 3.05 (against PS standard).

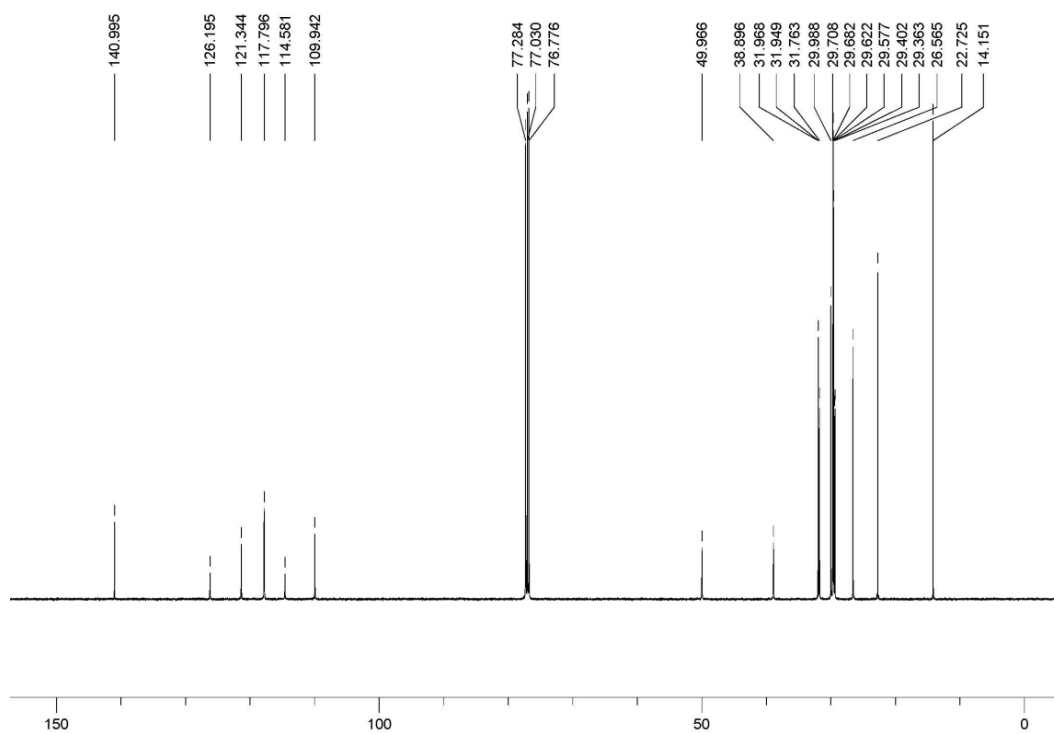
**Synthesis of poly[4-(5-(5,10-bis(2-decyltetradecyl)-5,10-dihydroindolo[3,2-b]indol-2-yl)thiophen-2-yl)-5,6-difluoro-7-(thiophen-2-yl)benzo[c][1,2,5]thiadiazole] (PDHIT2FT)**

Synthesis of PDHIT2FT was carried out in the same manner as PDHITHT. Compound (7) (339 mg, 0.30 mmol), compound (10) (148 mg, 0.30 mmol), anhydrous toluene (10 ml),  $\text{Pd}_2(\text{dba})_3$  (4.2 mg, 3 mol %, 4.5  $\mu\text{mol}$ ),  $\text{P}(\text{o-tolyl})_3$  (8.2 mg, 27  $\mu\text{mol}$ ),  $\text{K}_3\text{PO}_4$  (254 mg, 1.2 mmol), distilled water (3 mL), and Aliquat 336 (1 drop). PDHIT2FT (120 mg, 25%). GPC analysis,  $M_n = 22,503 \text{ g mol}^{-1}$ ,  $M_w = 66,008 \text{ g mol}^{-1}$ , and PDI = 2.93 (against PS standard).

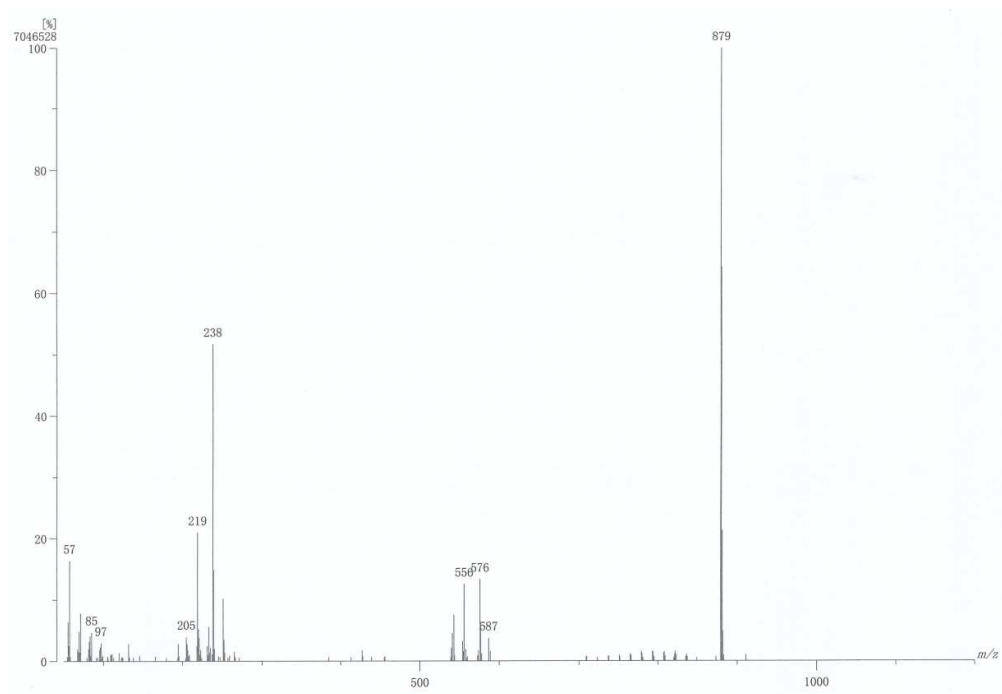




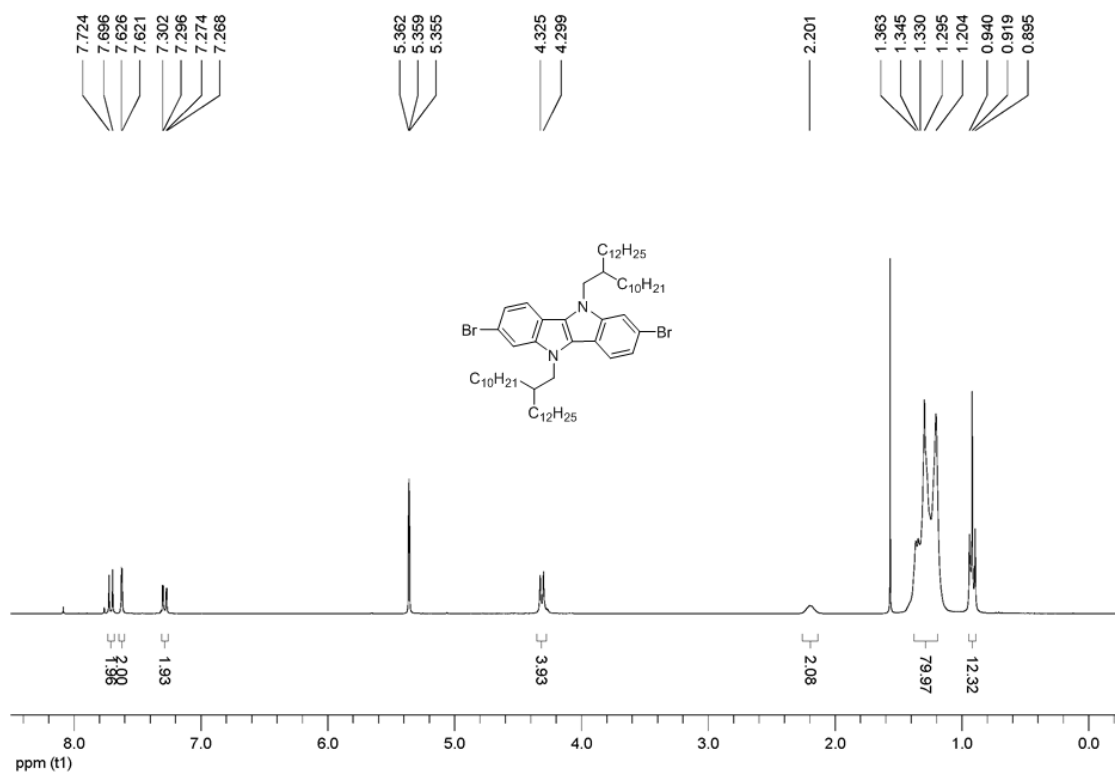
**Figure S1-1.** <sup>1</sup>H NMR spectrum of compound (5)



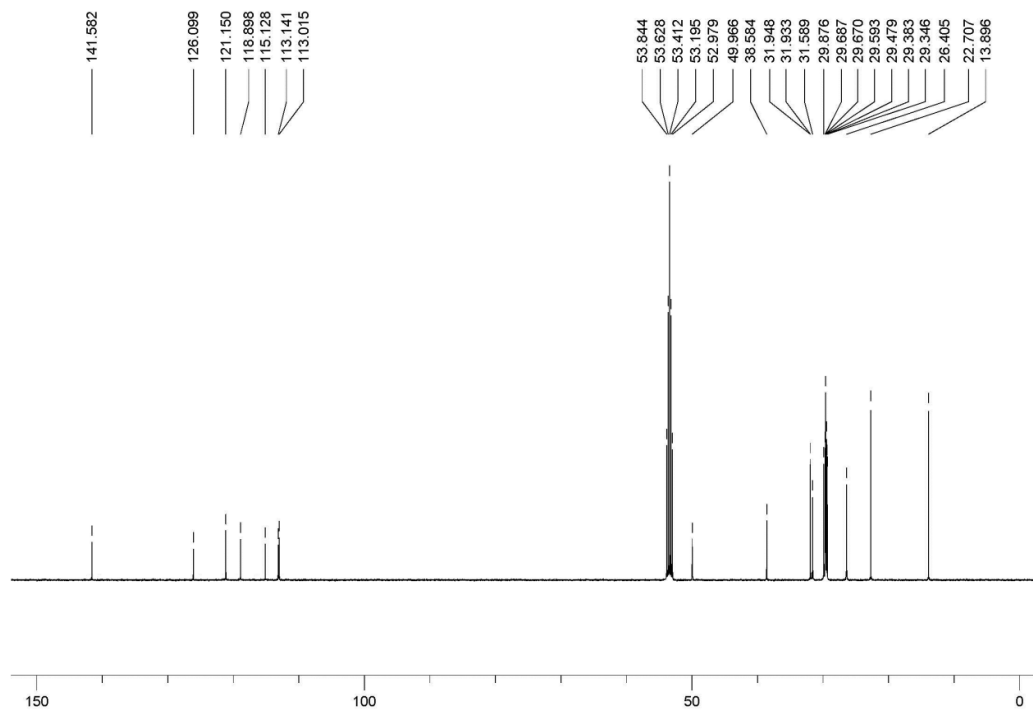
**Figure S1-2.** <sup>13</sup>C NMR spectrum of compound (5)



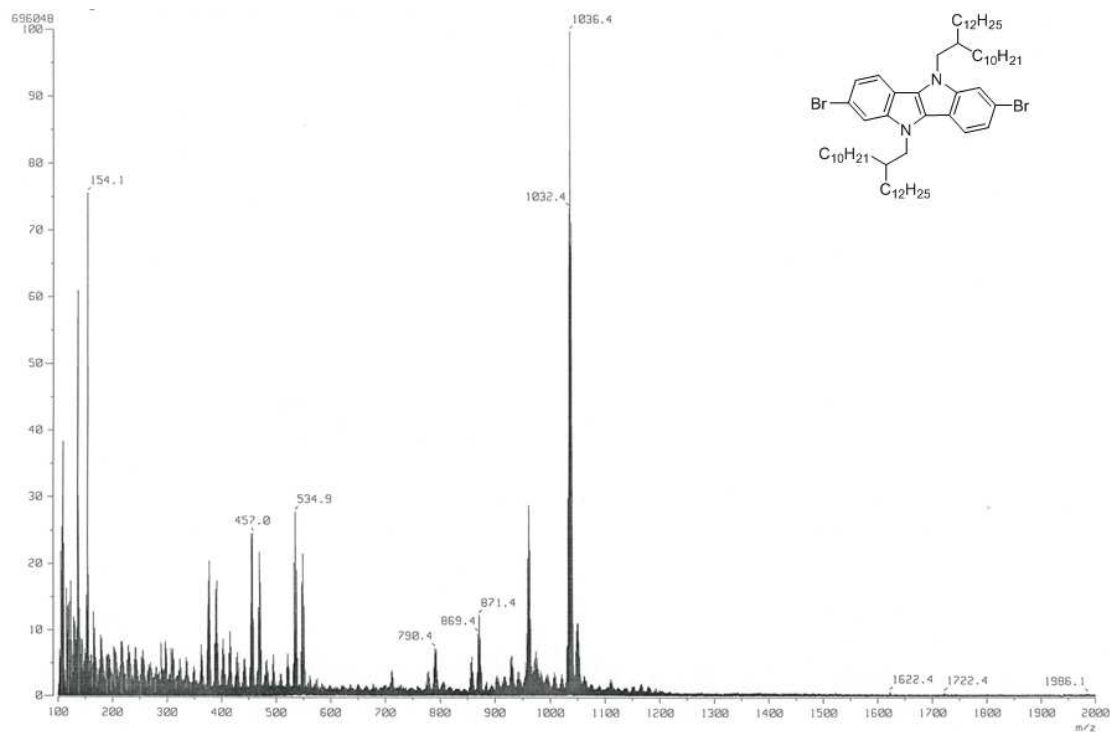
**Figure S1-3.** Mass spectrum of compound (5)



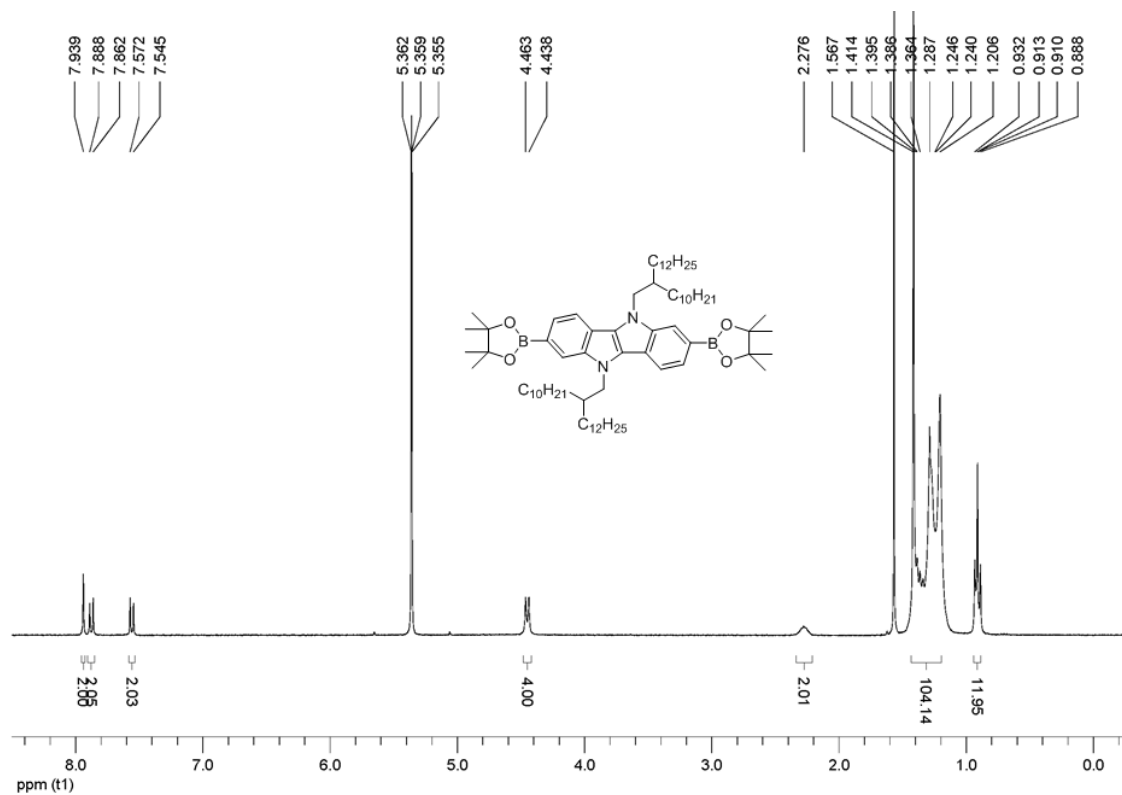
**Figure S1-4.**  $^1\text{H}$  NMR spectrum of compound (6)



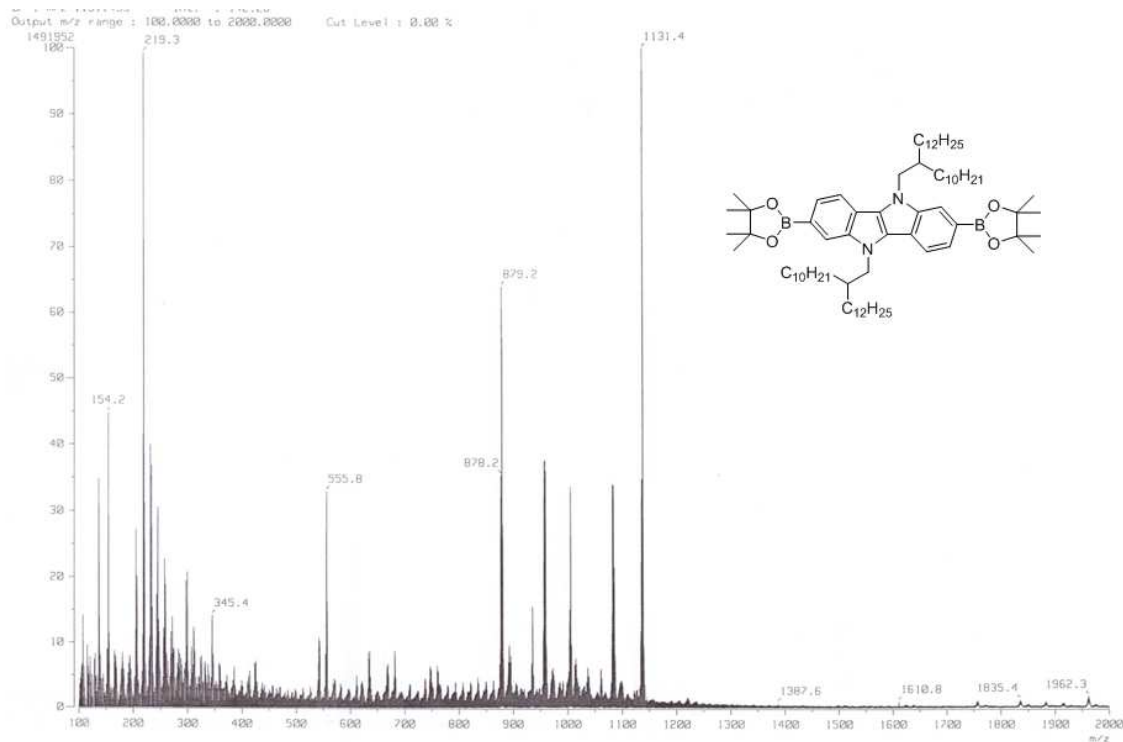
**Figure S1-5.** <sup>13</sup>C NMR spectrum of compound (6)



**Figure S1-6.** Mass spectrum of compound (6)



**Figure S1-7.** <sup>1</sup>H NMR spectrum of compound (7)



**Figure S1-8.** Mass spectrum of compound (7)

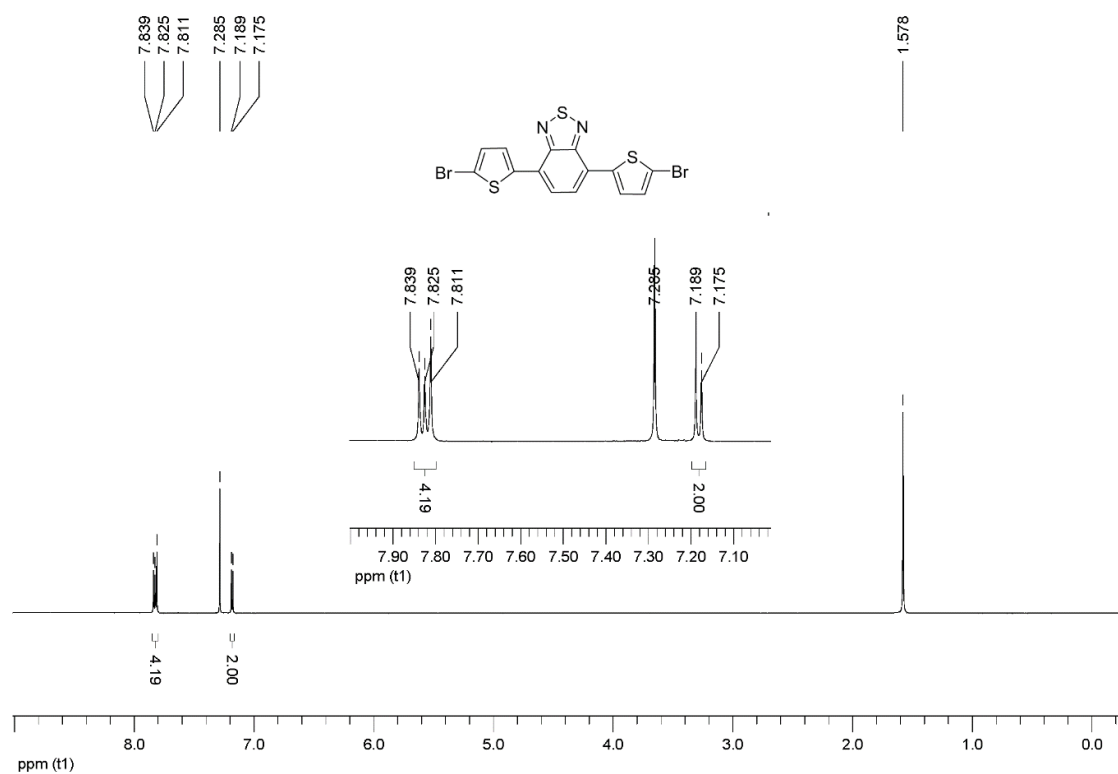


Figure S1-9. <sup>1</sup>H NMR spectrum of compound (8)

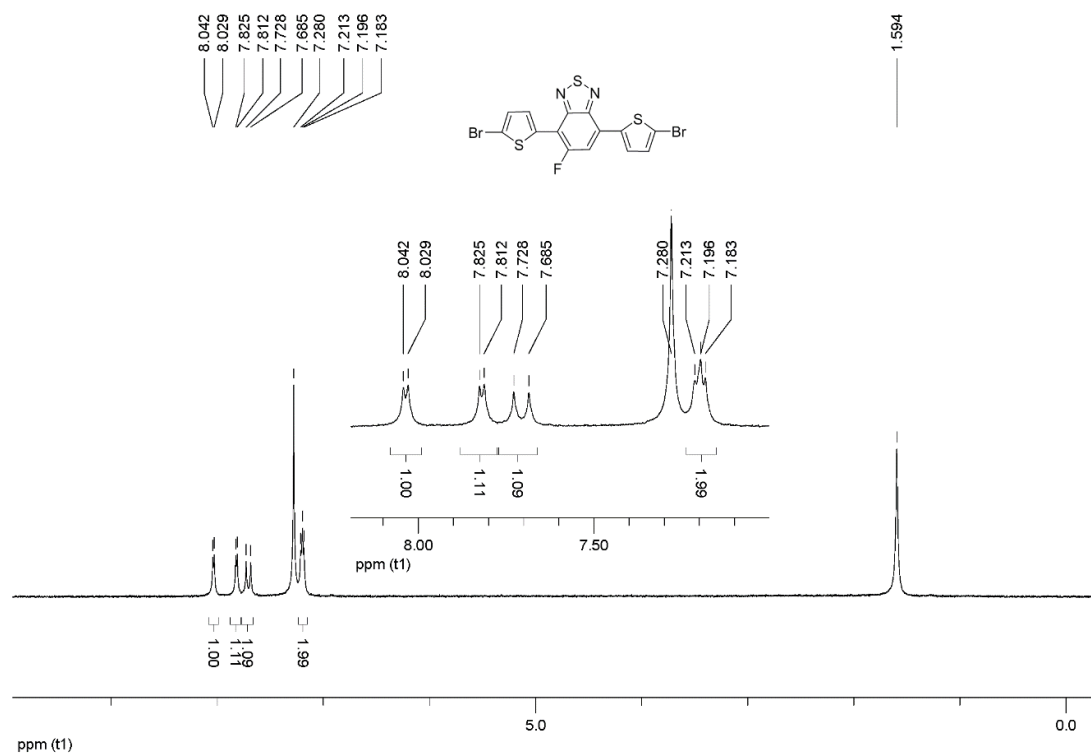
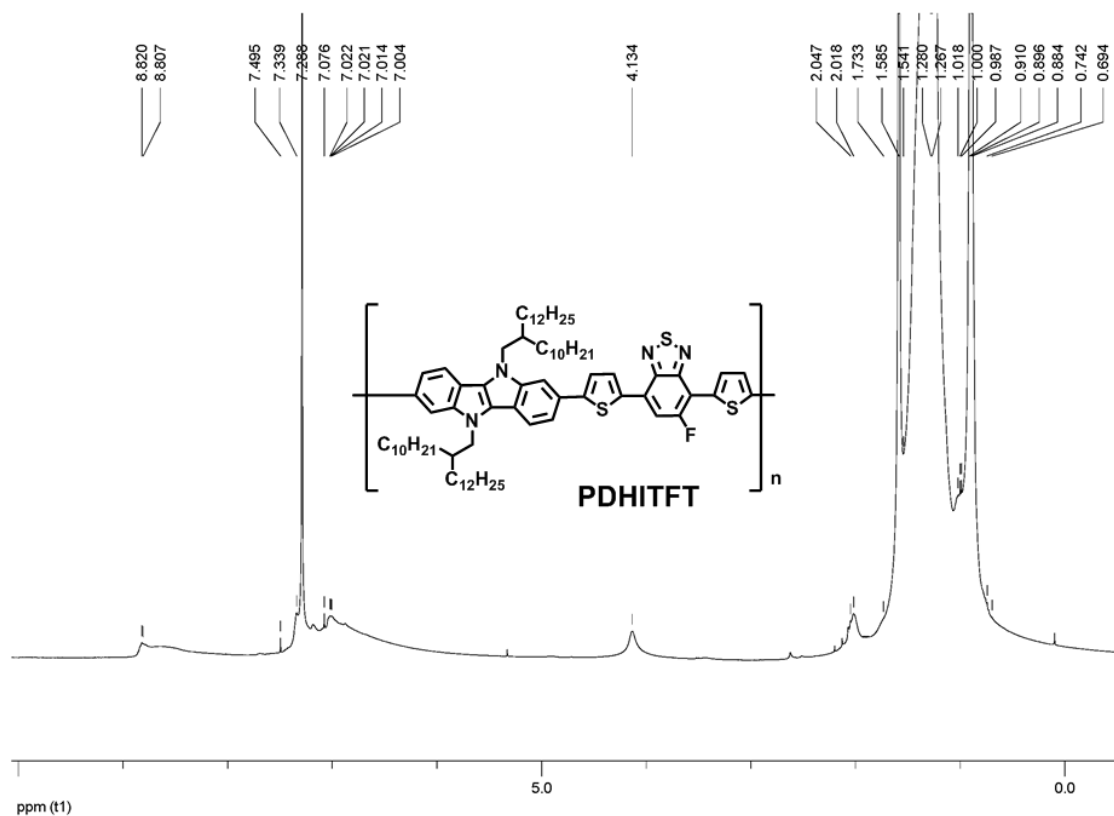
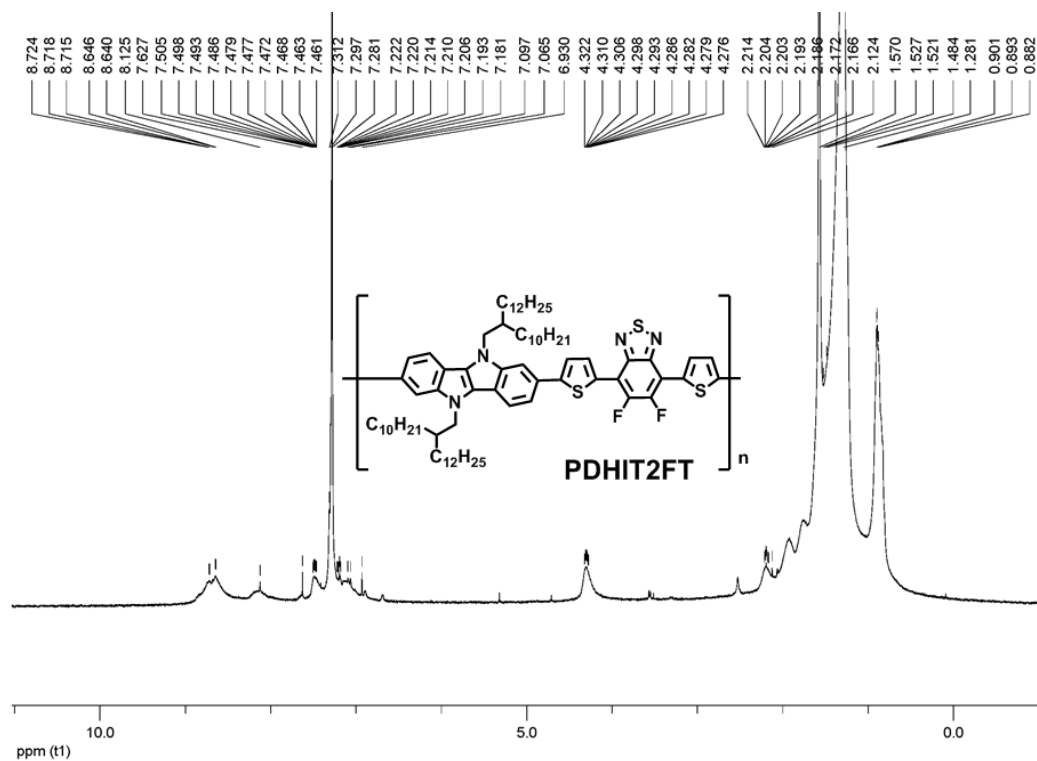


Figure S1-10. <sup>1</sup>H NMR spectrum of compound (9)





**Figure S1-13.** <sup>1</sup>H NMR spectrum of PDHITFT



**Figure S1-14.** <sup>1</sup>H NMR spectrum of PDHIT2FT

**Table S1.** Molecular weight of the polymers

Polymer	M <sub>n</sub> (g/mol)	M <sub>w</sub> (g/mol)	PDI
PDHITHT	31,732	97,002	3.06
PDHITFT	25,777	78,610	3.05
PDHIT2FT	22,503	66,008	2.93



**Figure S1-15** Gel permeation chromatogram of the PDHITHT polymer run in chloroform solution

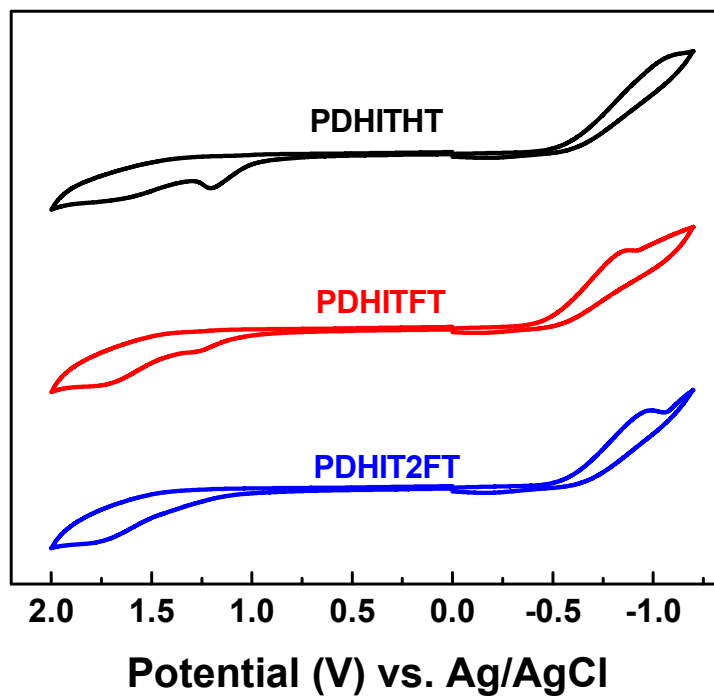


**Figure S1-16** Gel permeation chromatogram of the PDHITFT polymer run in chloroform solution





**Figure S1-17.** Gel permeation chromatogram of the PDHIT2FT polymer run in chloroform solution



**Figure S2.** Cyclic voltammograms of PDHITHT, PDHITFT and PDHIT2FT.

**Table S2.** Summary of electrochemical properties of PDHITHT, PDHITFT and PDHIT2FT.

Compound	HOMO (eV)	Ox onset	LUMO (eV)	E <sub>g</sub> optical (V)
PDHITT	5.38	0.95	3.62	1.76
PDHITFT	5.46	1.03	3.75	1.71
PDHIT2FT	5.53	1.10	3.79	1.74

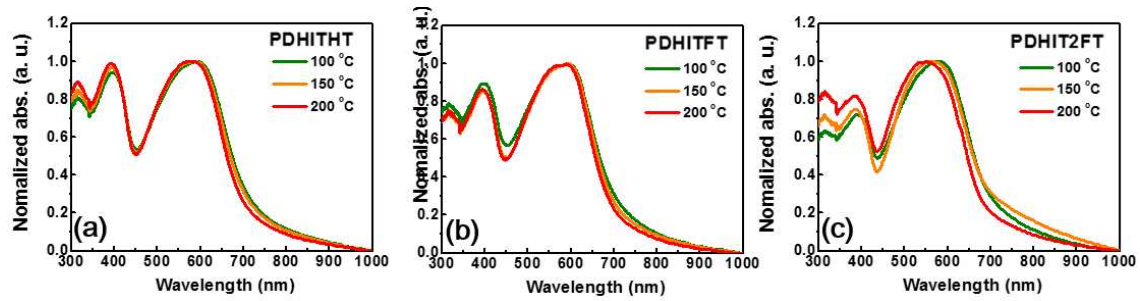


Figure S3. Normalized UV-Vis absorption spectra of (a) PDHITHT, (b) PDHITFT, and (c) PDHIT2FT as a thin film prepared under various thermal treatment.

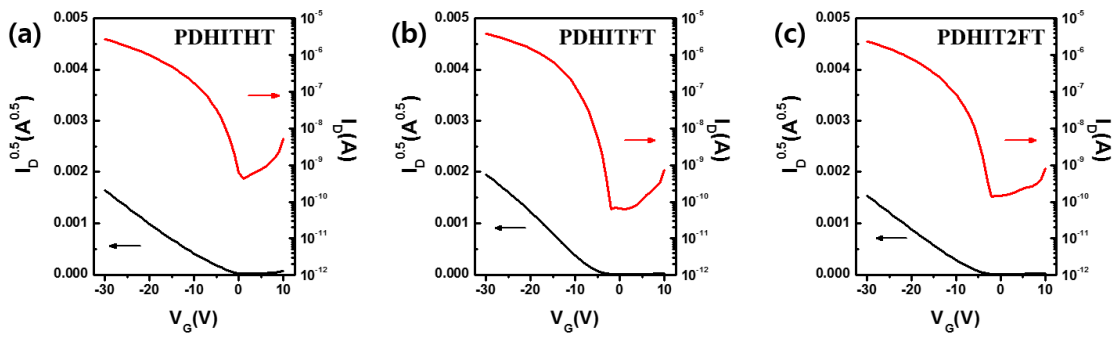
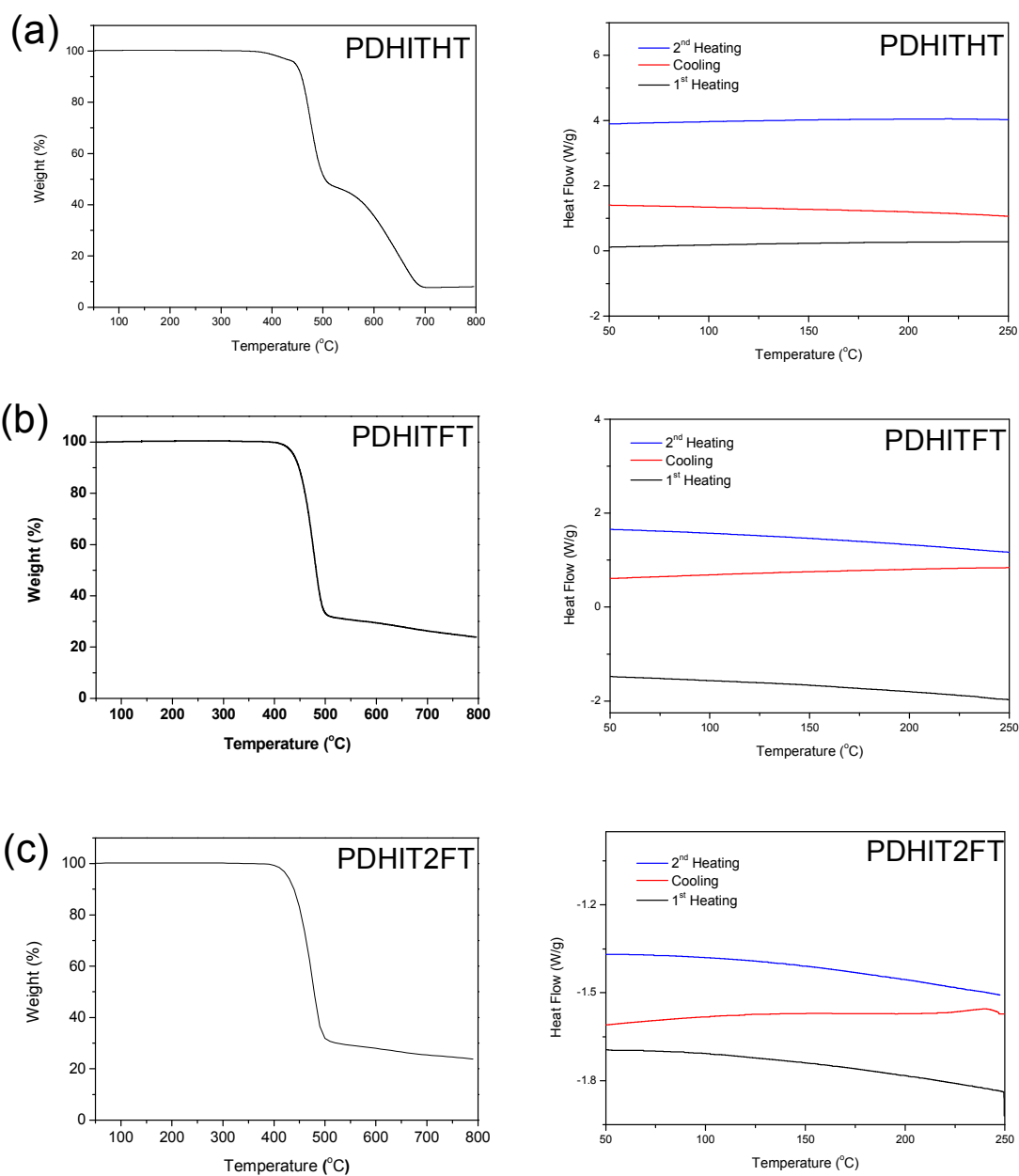


Figure S4. Transfer characteristics of polymer field effect transistors with (a) PDHITHT, (b) PDHITFT, and (c) PDHIT2FT as an active layer.



**Figure S5.** TGA and DSC curves of PDHITHT (a), PDHITFT (b) and PDHIT2FT (c).

**Table S3.** Summary of OPV performances for each single cell

Polymer:PC <sub>71</sub> BM		<i>V</i> <sub>oc</sub> (V)	<i>J</i> <sub>sc</sub> (mA / cm <sup>2</sup> )	FF (%)	PCE (%)
PDHITHT:PC <sub>71</sub> BM	cell_1	0.88	15.4	51.8	7.01
	cell_2	0.88	15.6	52.2	7.16
	cell_3	0.89	14.9	51.5	6.82
	cell_4	0.88	15.5	50.8	6.92
	cell_5	0.87	13.9	48.9	5.91
	cell_6	0.89	16.1	52.3	7.49
	cell_7	0.88	16.2	51.2	7.29
	cell_8	0.87	14.7	50.1	6.40
	cell_9	0.88	15.0	51.1	6.74
	cell_10	0.86	14.6	49.2	6.17
	cell_11	0.86	14.5	51.1	6.37
	cell_12	0.85	14.2	49.7	5.99
Polymer:PC <sub>71</sub> BM		<i>V</i> <sub>oc</sub> (V)	<i>J</i> <sub>sc</sub> (mA / cm <sup>2</sup> )	FF (%)	PCE (%)
PDHITFT:PC <sub>71</sub> BM	cell_1	0.88	17.9	52.8	8.31
	cell_2	0.89	16.8	51.5	7.70
	cell_3	0.89	17.1	51.8	7.88
	cell_4	0.89	18.4	53.4	8.84
	cell_5	0.89	18.2	53.4	8.59
	cell_6	0.89	17.4	52.3	8.09

	cell_7	0.88	16.9	51.7	7.68
	cell_8	0.87	17.0	50.1	7.40
	cell_9	0.87	17.6	51.9	7.94
	cell_10	0.88	18.0	53.0	8.39
	cell_11	0.88	18.1	53.2	8.47
	cell_12	0.88	17.9	52.8	8.31
Polymer:PC <sub>71</sub> BM		<i>V</i> <sub>oc</sub>	<i>J</i> <sub>sc</sub>	FF	PCE
		(V)	(mA / cm <sup>2</sup> )	(%)	(%)
	cell_1	0.87	17.9	51.8	8.06
	cell_2	0.88	17.4	52.2	7.99
	cell_3	0.88	16.8	50.4	7.45
	cell_4	0.89	17.1	51.2	7.79
	cell_5	0.89	16.5	50.1	7.35
PDHIT2FT:PC <sub>71</sub> BM	cell_6	0.89	17.3	51.9	8.00
	cell_7	0.88	16.9	52.7	7.84
	cell_8	0.89	17.5	52.5	8.17
	cell_9	0.89	17.6	52.9	8.28
	cell_10	0.88	17.0	50.8	7.60
	cell_11	0.88	16.4	49.8	7.10
	cell_12	0.87	16.2	49.2	6.93

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