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Supporting Information

Energy Level Modulation of Non-Fullerene Acceptors for Efficient Organic Solar Cells with Small Energy Loss

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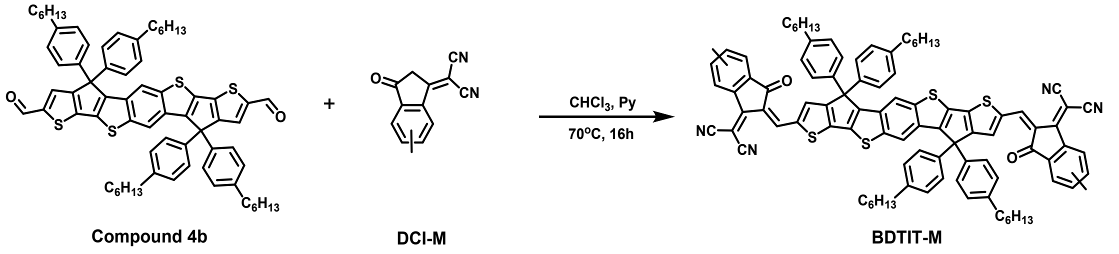
1. Detailed experimental section

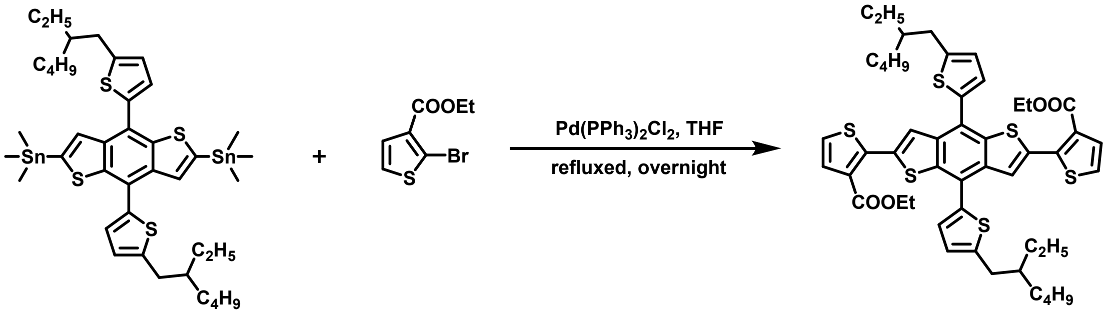
(1) Synthesis

2,6-bis(trimethylstannyl)benzo[1,2-*b*:4,5-*b'*]dithiophene, (4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-*b*:4,5-*b'*]dithiophene-2,6-diyl)bis(trimethylstannane), 1-bromo-4-hexylbenzene and bis(triphenylphosphine) palladium(II) dichloride ($Pd(PPh_3)_2Cl_2$) were purchased from commercial sources. Ethyl 2-bromothiophene-3-carboxylate and 2-(5/6-methyl-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (DCI-M) were synthesized according to literature.[1] THF was dried by using potassium sodium alloy under refluxing condition.



Synthesis of ***BDTIT-M****:* To a 100 ml round bottom flask, compound 4b[2](100 mg, 0.093 mmol) and DCI-M (84 mg, 0.372 mmol) were added under argon protection. Then, deoxidized chloroform (20 ml) was added and stirred for a while when pyridine (1 ml) was added. The mixture was kept stirring at 70 °C for 16h. After removal of chloroform of reaction mixture under reduced pressure, 100 ml methanol was added and the precipitate was collected by filtration. The residue was purified by column chromatography on silica gel using a mixture solvent as eluent (petroleum ether/dichloromethane, vol/vol = 5/4) to give a dark solid (113 mg, 82%). ^1H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.84 (m, 2H), 8.56 (d, J = 8 Hz, 1H), 8.47 (s, 1H), 8.01 (s, 2H), 7.80 (d, J = 8Hz, 1H), 7.69 (m, 3H), 7.54 (m, 2H), 7.17 (d, J = 8Hz, 8H), 7.11 (d, J = 8Hz, 8H), 2.55 (m, 14H), 1. 61 (m, 8H), 1.28 (m, 24H), 0.84 (t, J = 6.4 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm):

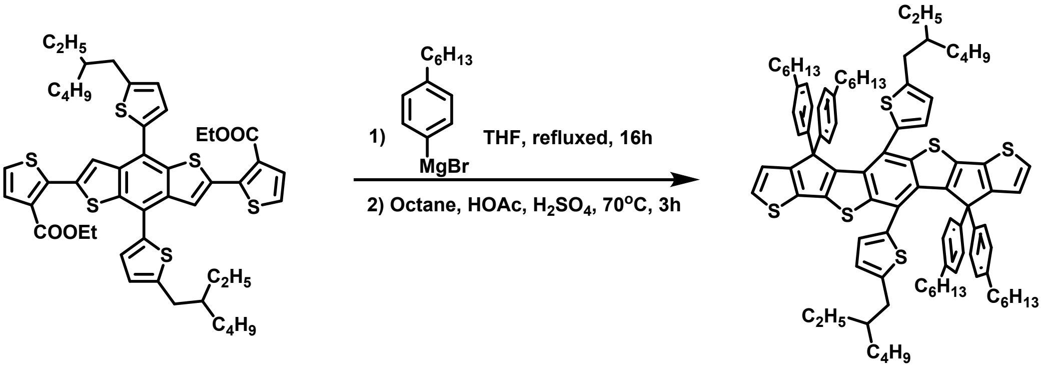
188.71, 188.35, 162.71, 160.48, 155.74, 155.00, 154.88, 146.74, 146.20, 143.88, 142.62, 140.50, 140.37, 138.73, 137.96, 137.63, 137.37, 137.20, 136.03, 135.43, 134.71, 131.66, 128.91, 128.00, 125.67, 125.26, 124.04, 123.62, 122.22, 118.05, 114.94, 114.84, 68.45, 67.91, 62.72, 35.58, 31.71, 31.31, 29.14, 22.62, 14.14. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{96}H_{87}N_4O_2S_4^+$, 1455.57064; found, 1455.57068.



Compound 1a

Compound 2a

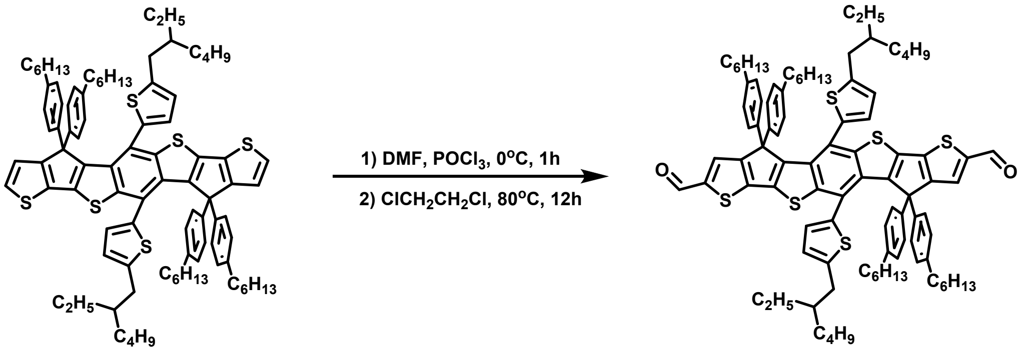
Synthesis of ***Compound 2a*****:** To a 50 ml round bottom flask, compound **1a** (1.0 g, 1.10 mmol), $Pd(PPh_3)_2Cl_2$ (39 mg, 0.055 mmol), ethyl 2-bromothiophene-3-carboxylate (644 mg, 2.75 mmol) and dry THF (15 ml) were added, and then the solution was bubbled with argon for 30 min. The mixture was refluxed overnight under argon protection. After cooling to room temperature, the solvent was evaporated and the residue was purified by silicon chromatography using petroleum ether/ethyl acetate (20:1, vol/vol) as eluent to get the product as an yellow oil (682 mg, 70%). ^1H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.92 (s, 2H), 7.53 (d, J = 5.2 Hz, 2H), 7.33 (d, J = 3.2 Hz, 2H), 7.28 (d, J = 5.2 Hz, 2H), 6.89 (d, J = 3.2 Hz, 2H), 4,27 (q, J = 7.2 Hz, 4H), 2.86 (d, J = 6.8 Hz, 4H), 1.67 (m, 2H), 1.37 (m, 8H), 1.21 (t, J = 7.2 Hz, 6H), 0.93 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 163.12, 146.01, 142.16, 139.83, 136.77, 136.66, 135.30, 130.79, 129.52, 127.98, 125.54, 125.38, 125.26, 123.93, 60.98, 41.45, 34.23, 32.46, 28.91, 25.65, 23.05, 14.21, 14.06, 10.91. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{48}H_{55}O_4S_6^+$, 887.24191; found, 887.24341.



Compound 2a

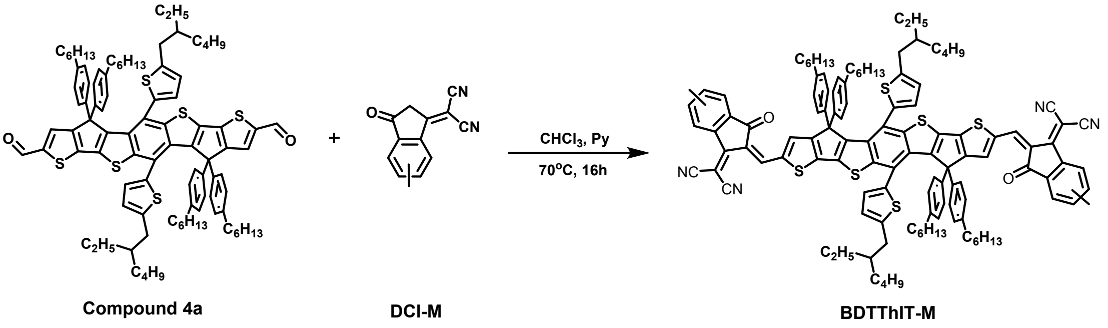
Compound 3a

Synthesis of ***Compound 3a*****:** To a stirring solution of compound **2a** (618 mg, 0.70 mmol) in dry THF (30 ml) was added dropwise a solution of (4-hexylphenyl)magnesiumbromide which was prepared from 1-bromo-4-hexylbenzene (1.7g, 7 mmol) and magnesium (185 mg, 7.7 mmol) at room temperature under argon atmosphere. After adding, the solution was heated to reflux for 16 hours. After the reaction finished, the mixture was poured into water (150 ml) and extracted with ethyl acetate (3 × 100 ml), then washed with saturated salt water three times and dried over anhydrous Na_2SO_4. After removal of the solvent under reduced pressure, the brown crude product was obtained and then used in the next step without further purification. The crude product was dissolved in octane (100 ml) and glacial acetic acid (10 ml), and 1 ml concentrated sulfuric acid in 5 ml glacial acetic acid was dropwise into the solution, then the mixture was stirred at 70 °C for 3 hours. After cooling to room temperature, the mixture was extracted with dichloromethane and washed with water. The collected organic layer was dried over anhydrous Na_2SO_4 and concentrated. The residue was purified by column chromatography on silica gel using a mixture solvent as eluent (petroleum ether/dichloromethane, vol/vol = 20/1) to give a yellow solid (483 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 7.06 (d, J = 4.8 Hz, 2H), 6.95 (m, 16H), 6.78 (dd, J_1 = 1.6 Hz, J_2 = 4.8 Hz, 2H), 6.40 (m, 2H), 6.08 (m, 2H), 2.71 (m, 4H), 2.57 (m, 8H), 1.61 (m, 8H), 1.51 (m, 2H), 1.40 (m, 46H), 0.92 (m, 18H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 164.72, 150.30, 149.37, 145.83, 141.10, 140.81, 140.59, 140.54, 137.14, 137.08, 136.54, 136.49, 136.39, 134.10, 130.90, 130.02, 129.92, 128.36, 127.93, 127.78, 127.42, 124.51, 124.34, 124.23, 122.46, 63.11, 41.49, 41.20, 35.62, 35.48, 34.04, 33.94, 32.41, 32.38, 31.80, 31.78, 31.53, 29.23, 29.19, 28.93, 28.76, 25.63, 25.51, 23.23, 23.13, 22.67, 22.66, 14.32, 14.30, 14.15, 10.86, 10.85, 10.76. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{92}H_{111}S_6^+$, 1407.70046; found, 1407.70023.



Compound 3a **Compound 4a**

Synthesis of ***Compound 4a:*** To a dry 100 mL two-necked round bottom flask, 10 ml anhydrous *N*, *N*-dimethylformamide (DMF) was added, and the solution was cooled to 0 °C and stirred when 2 ml phosphorous oxychloride ($POCl_3$) was added by syringe under argon protection. The mixture was stirred at 0 °C for 1 hour, and then compound **3a** (450 mg, 0.32 mmol) in dry 1, 2-dichloroethane (20 ml) was added. Then, the mixture solution was allowed to reflux overnight. After cooling to room temperature, 100 ml water was added and the mixture was extracted with dichloromethane (DCM), and the organic layer was collected, washed with water and dried with anhydrous Na_2SO_4. After removal of the solvent under reduced pressure, the residue was purified by column chromatography on silica gel using a mixture solvent as eluent (petroleum ether/dichloromethane, vol/vol = 2/1) to give an orange solid (398 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 9.64 (s, 2H), 7.40 (d, J = 1.6 Hz, 2H), 6.94 (m, 16H), 6.39 (m, 2H), 6.06 (m, 2H), 2.70 (m, 4H), 2.57 (m, 8H), 1.59 (m, 8H), 1.49 (m, 2H), 1.32 (m, 46H), 0.95 (m, 18H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 182.66, 164.85, 154.49, 150.97, 146.66, 146.63, 145.75, 144.14, 141.62, 141.38, 140.95, 135.75, 135.68, 135.52, 135.38, 135.17, 135.11, 131.33, 130.98, 130.38, 130.27, 128.33, 128.27, 128.13, 126.03, 124.55, 124.45, 63.49, 41.58, 41.29, 35.64, 35.51, 34.08, 33.98, 32.42, 31.82, 31.80, 31.55, 29.24, 29.19, 28.96, 28.80, 25.72, 25.59, 23.26, 23.15, 22.71, 22.69, 14.36, 14.34, 14.19, 10.91, 10.83. HRMS (ESI) m/z: $[M+H]^+$ calcd. for $C_{94}H_{111}O_2S_6^+$, 1463.69028; found, 1463.68994.



Synthesis of ***BDTThIT-M*****:** To a 100 ml round bottom flask, compound **4a** (150 mg, 0.10 mmol) and DCI-M (90 mg, 0.40 mmol) were added under argon protection. Then, deoxidized chloroform (25 ml) was added and stirred for a while when pyridine (1 ml) was added. The mixture was kept stirring at 70 °C for 16 h. After removal of chloroform of reaction mixture under reduced pressure, 100 ml methanol was added and the precipitate was collected by filtration. The residue was purified by column chromatography on silica gel using a mixture solvent as eluent (petroleum ether/dichloromethane, vol/vol = 5/4) to give a dark solid (150 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$), δ (ppm): 8.67 (s, 2H), 8.51 (s, J = 8.4 Hz, 1H), 8.42 (s, 2H), 7.75 (d, J = 7.8 Hz, 1H), 7.63 (s, 1H), 7.49 (m, 2H), 7.36 (S, 2H), 6.93 (m, 16H), 6.41 (m, 2H), 6.11 (m, 2H), 2.51 (m, 12H), 1.61 (m, 10H), 1.33 (m, 46H), 0.95 (m, 18H). ^{13}C NMR (100 MHz, $CDCl_3$), δ (ppm): 188.50, 188.15, 165.62, 160.42, 156.69, 152.93, 152.80, 152.08, 146.86, 146.68, 146.56, 146.07, 142.13, 141.83, 141.46, 141.04, 140.28, 137.82, 137.71, 137.52, 137.14, 135.87, 135.51, 135.43, 135.31, 135.08, 134.93, 134.87, 134.66, 131.61, 130.35, 128.38, 128.21, 128.06, 126.69, 125.59, 125.17, 124.61, 123.98, 123.56, 122.03, 114.96, 114.86, 114.81, 68.14, 67.61, 63.34, 41.39, 41.17, 35.66, 35.53, 33.83, 32.52, 32.40, 31.82, 31.81, 31.59, 31.53, 29.27, 29.09, 28.99, 25.64, 25.31, 23.26, 23.21, 22.72, 22.70, 22.56, 22.06, 14.41, 14.37, 14.20, 10.94, 10.72. HRMS (ESI) m/z: $[M]^+$ calcd. for $C_{120}H_{122}N_4O_2S_6^+$, 1842.78865; found, 1842.78835.

(2) Photovoltaic Device Fabrication

The patterned indium tin oxide (ITO) glass coated substrates (sheet resistance 15 Ω/□) were consecutively cleaned in ultrasonic baths containing detergent, de-ionized water and ethanol, respectively. The cleaned ITO substrates were blow-dried by high pure nitrogen gas and then treated by oxygen plasma for 1 min to improve its work function and clearance. Then, poly-(3,4-ethylenedioxythiophene):poly-(styrenesulphonicacid) (PEDOT:PSS) (clevios P VP Al 4083, purchased from H.C. Starck co. Ltd.) thin films were fabricated on the cleaned ITO substrates by spin-coating method at 5000 round per minute (RPM) for 40 s, and then annealed at 150 °C for 10 minutes in ambient conditions. After annealing treatment, the ITO substrates coated PEDOT:PSS films were transferred to a high-purity nitrogen-filled glove box to fabricate active layers. The donor materials PBDB-T was purchased from Solarmer Materials Inc and used as received. The materials PBDB-T:BDTIT-M and PBDB-T:BDTThIT-M were all dissolved in chlorobenzene (with or without 1,8-diiodooctane) to prepare 20 mg/ml blend solutions. The blend solutions were spin-coated on PEDOT:PSS films at 2500 rpm in a high purity nitrogen-filled glove box to fabricate the active layers. Subsequently, the active layers were then annealed for 5 min under different temperatures. The optimized thickness of the active layer is ~100 nm, which was measured by Ambios Technology XP-2 stylus Profiler. After that, PDIN solution (2 mg ml^{-1} in methanol with 0.25 vol% acetic acid) was spin-coated on the top of active layers at 5000 RPM for 30 s. The cathode of Al was deposited by thermal evaporation with a shadow mask under 10^{-4} Pa and the thickness of 100 nm was monitored by a quartz crystal microbalance. Therefore, organic solar cells (OSCs) were fabricated with the architecture of ITO/PEDOT:PSS/active layer/PDIN/Al. The active area of OSCs is about 3.8 mm^2, which is defined by the vertical overlap of ITO anode and Al cathode.

(3) Space charge-limited current (SCLC) device fabrication

The structure of electron-only devices is ITO/ZnO/active layer/Al and the structure of hole-only devices is ITO/PEDOT:PSS/active layer/MoO_3/Ag. The fabrication conditions of the active layer films are same with those for the solar cells. The charge mobilities are generally described by the Mott-Gurney equation:[3]

$$J = \frac{9}{8}\varepsilon_r \varepsilon_0 \mu \frac{V^2}{L^3} \qquad (1)$$

where J is the current density, ε_0 is the permittivity of free space (8.85×10^{-14} F/cm), ε_r is the dielectric constant of used materials, μ is the charge mobility, V is the applied voltage and L is the active layer thickness. The ε_r parameter is assumed to be 3, which is a typical value for organic materials. In organic materials, charge mobility is usually field dependent and can be described by the disorder formalism, typically varying with electric field, E=V/L, according to the equation:

$$\mu = \mu_0 \exp[0.89\gamma\sqrt{\frac{V}{L}}] \qquad (2)$$

where μ_0 is the charge mobility at zero electric field and γ is a constant. Then, the Mott-Gurney equation can be described by:

$$J = \frac{9}{8}\varepsilon_r \varepsilon_0 \mu_0 \frac{V^2}{L^3} \exp[0.89\gamma\sqrt{\frac{V}{L}}] \qquad (3)$$

In this case, The charge mobilities were estimated using the following equation:[4]

$$\ln(\frac{JL^3}{V^2}) = 0.89\gamma\sqrt{\frac{V}{L}} + \ln(\frac{9}{8}\varepsilon_r \varepsilon_0 \mu_0) \qquad (4)$$

(4) Solution, Film and Device Characterization

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Advanced II (400 MHz) spectrometer using tetramethylsilane (TMS) as internal standard. The high resolution mass spectra (HRMS) were performed on Thermo Scientific LTQ Orbitrap Xl using ESI. The ultraviolet-visible (UV-Vis) absorption spectra of neat and blend films were obtained using a Shimadzu UV-3101 PC spectrometer. cyclic voltammetry (CV) curves of targeted donor and acceptor thin films were conducted on a CHI voltammetric analyzer in acetonitrile solution with 0.1 M tetrabutylammonium hexafluorophosphate (*n*-Bu$_4$NPF$_6$) as supporting electrolyte at room temperature by using a scan rate of 100 mV s^{-1} and conventional three-electrode configuration consisting of a platinum working electrode with 2 mm diameter, a platinum wire counter electrode and a Ag/AgCl wire reference electrode. The current density-voltage (*J*-*V*) curves of all OSCs were measured in a high-purity nitrogen-filled glove box using a Keithley 2400 source meter. AM 1.5G irradiation at 100 mW/cm^2 provided by An XES-40S2 (SAN-EI Electric Co., Ltd.) solar simulator (AAA grade, 70×70 mm^2 photobeam size), which was calibrated by standard silicon solar cells (purchased from Zolix INSTRUMENTS CO. LTD). The external quantum efficiency (EQE) spectra of solar cells were measured in air conditions by a Zolix Solar Cell Scan 100. The morphology of the active layers was investigated by atomic force microscopy (AFM) using a Dimension Icon AFM (Bruker) in a tapping mode. Transmission electron microscopy (TEM) images of the active layers were obtained by using a JEOL JEM-1400 transmission electron microscope operated at 80 kV.

2. Additional Experimental Results

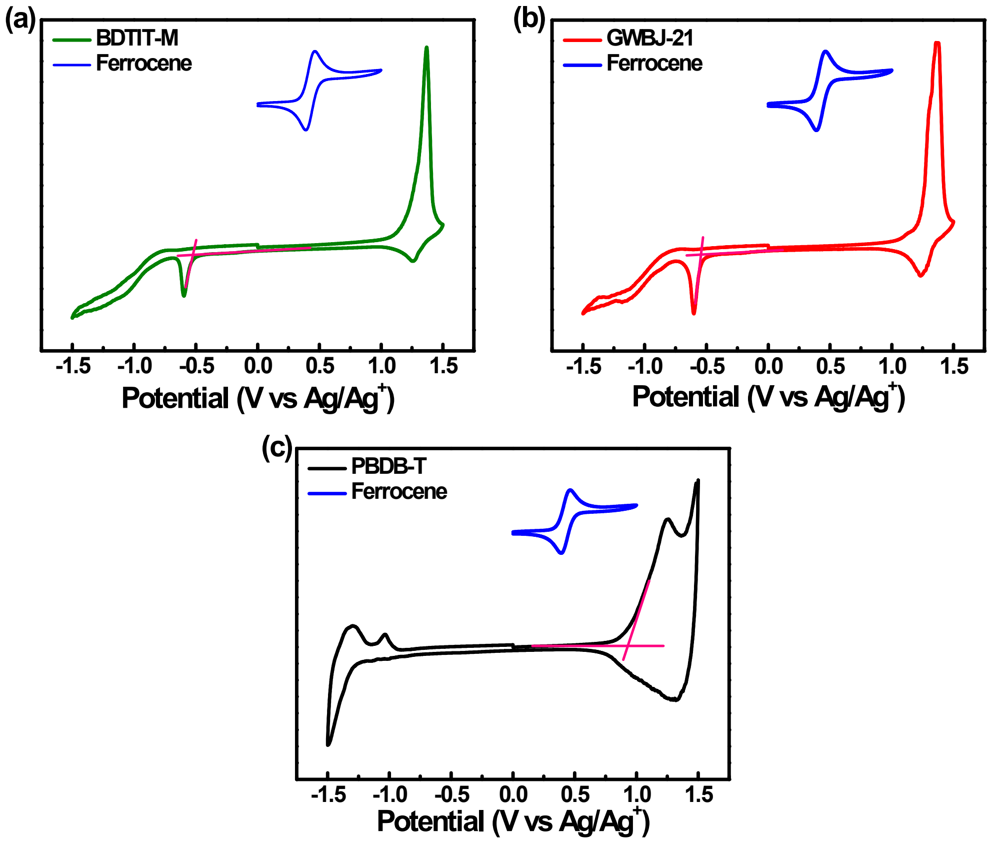


Figure S1. CV curves of (a) BDTIT-M (b) BDTThIT-M and (c) PBDB-T in CH3CN/0.1 M [n-Bu4N]$^+$[PF6]$^-$ solution at a scan rate of 100 mV s^{-1}.

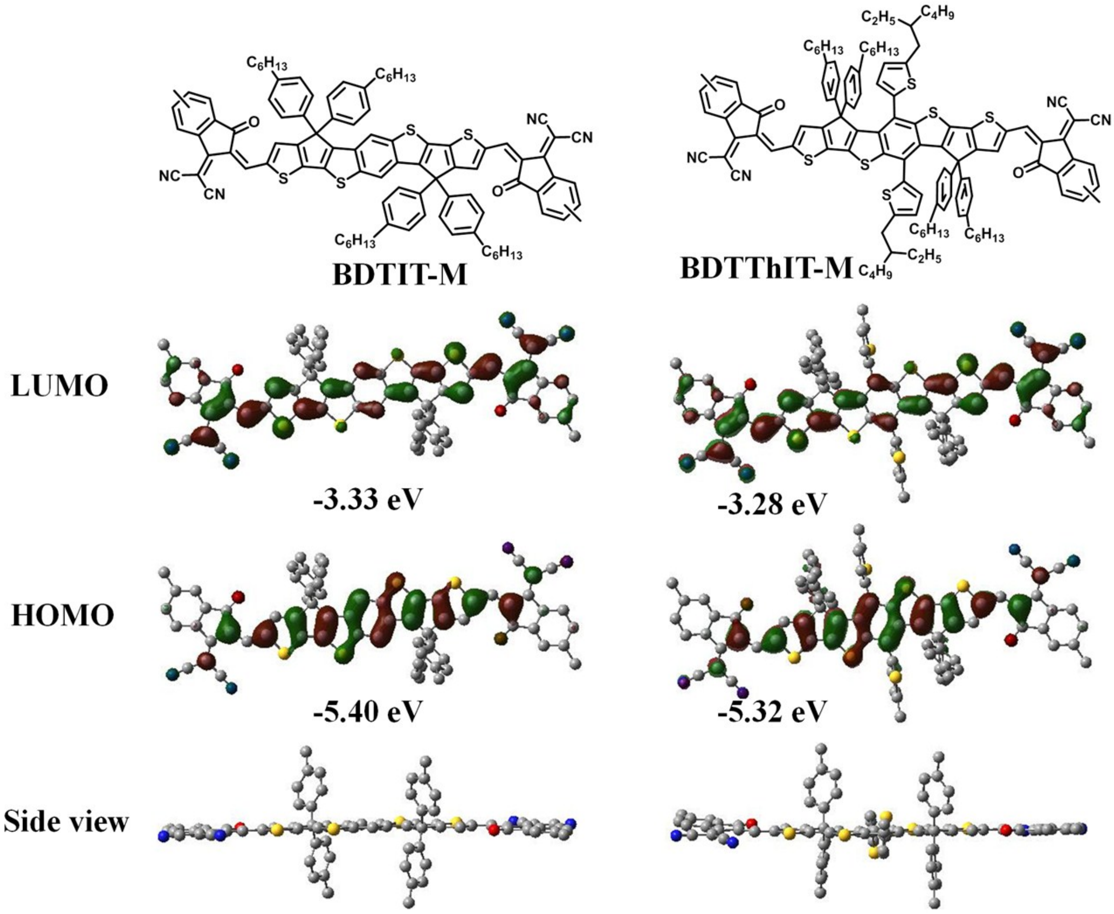


Figure S2. The structures, LUMO and HOMO distributions, corresponding calculated energy levels and side views of BDTIT-M and BDTThIT-M.

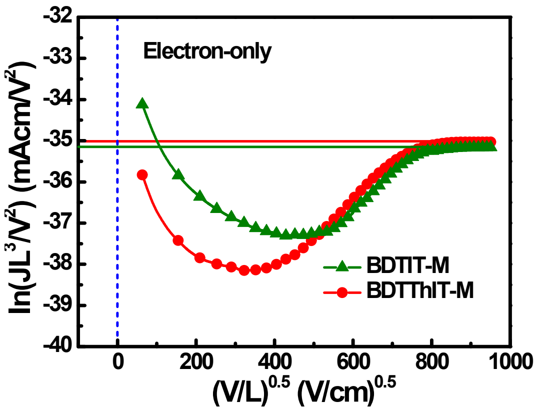


Figure S3. The $\ln(JL^3/V^2)$ vs $(V/L)^{0.5}$ curves of electron-only ITO/ZnO/BDTIT-M or BDTThIT-M/Al device.

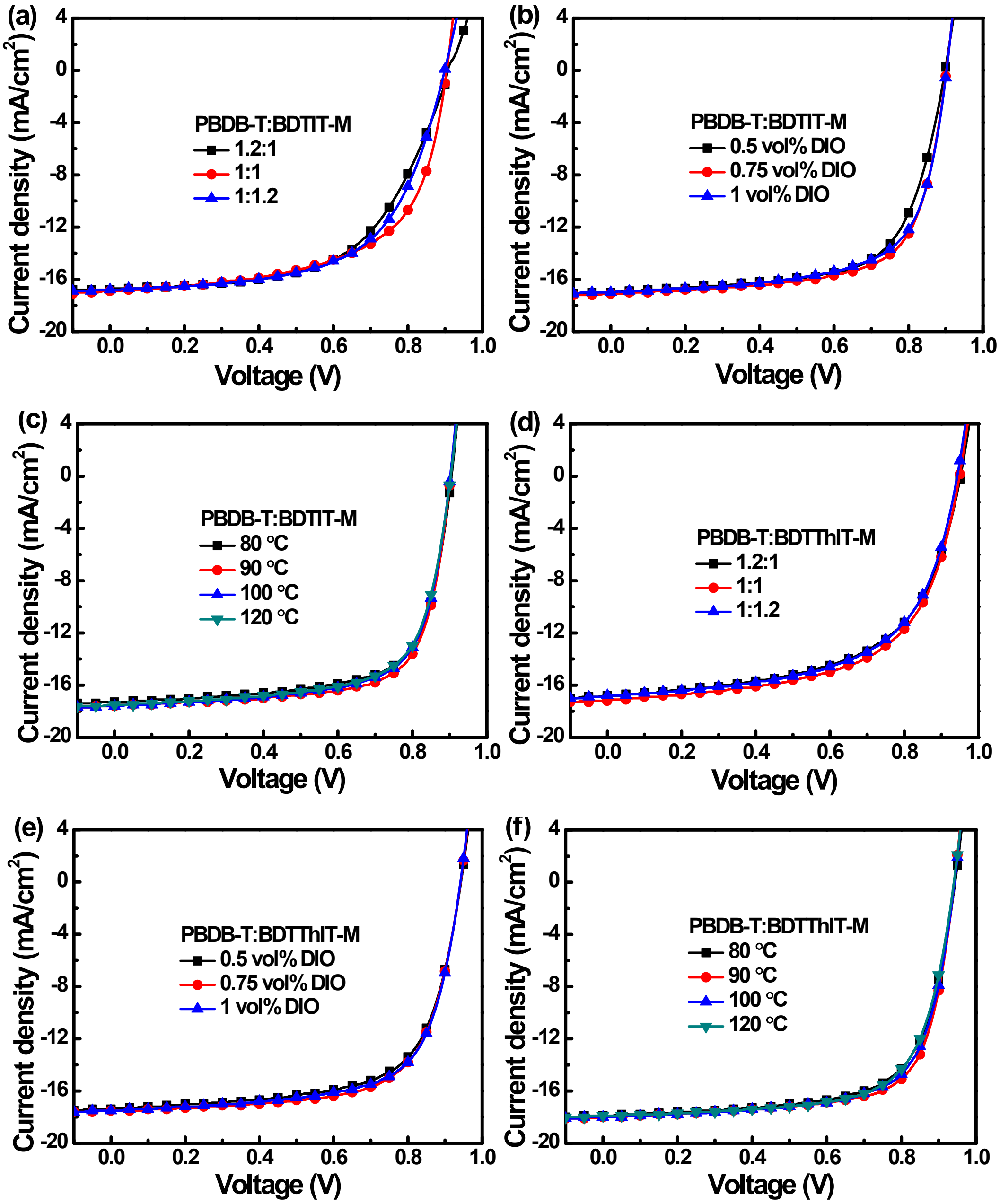


Figure S4. The *J-V* curves of BDTIT-M or BDTThIT-M based OSCs with (a or d) different ratios of donor to acceptor, (b or e) different contents of DIO as additive and (c or f) different annealing temperature under AM 1.5 G illumination at intensity of 100 mW cm^{-2}.

Table S1 The photovoltaic parameters of the BDTIT-M or BDTThIT-M based OSCs under AM 1.5 G illumination at intensity of 100 mW cm^{-2}.

PBDB-T:BDTIT-M [wt%]:[wt%]	DIO [vol%]	Annealing [°C]	PCE [%]	J_{sc} [mA cm^{-2}]	V_{oc} [V]	FF
1.2:1	w/o	w/o	8.88	16.74	0.906	0.586
1:1	w/o	w/o	9.29	16.91	0.904	0.608
1:1	0.5	w/o	10.14	16.95	0.901	0.664
1:1	0.75	w/o	10.58	17.11	0.902	0.686
1:1	0.75	80	10.89	17.32	0.905	0.695
1:1	0.75	100	11.31	17.56	0.903	0.713
1:1	0.75	120	11.01	17.59	0.902	0.694
1:1	0.75	140	10.90	17.51	0.900	0.689
1:1	1	w/o	10.29	17.59	0.902	0.673
1:1.2	w/o	w/o	9.12	16.78	0.900	0.604
PBDB-T:BDTThIT-M [wt%]:[wt%]	**DIO [vol%]**	**Annealing [°C]**	**PCE [%]**	**J_{sc} [mA cm^{-2}]**	**V_{oc} [V]**	**FF**
1.2:1	w/o	w/o	9.38	16.81	0.952	0.586
1:1	w/o	w/o	9.77	17.16	0.949	0.600
1:1	0.5	w/o	10.91	17.36	0.943	0.667
1:1	0.75	w/o	11.29	17.54	0.942	0.683
1:1	0.75	80	11.58	17.89	0.944	0.687
1:1	0.75	100	12.12	18.03	0.942	0.714
1:1	0.75	120	11.84	18.00	0.942	0.698
1:1	0.75	140	11.68	17.91	0.941	0.692
1:1	1	w/o	11.17	17.51	0.942	0.677
1:1.2	w/o	w/o	9.46	16.85	0.943	0.595

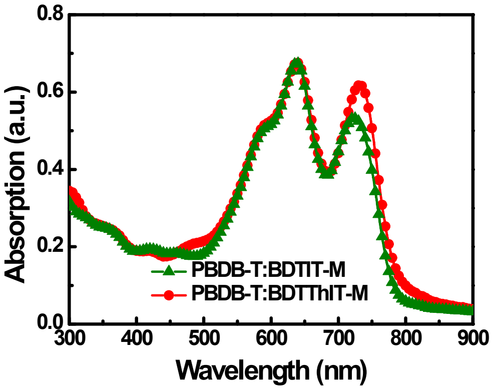


Figure S5. UV-vis absorption spectra of PBDB-T:BDTIT-M and PBDB-T:BDTThIT-M blend films.

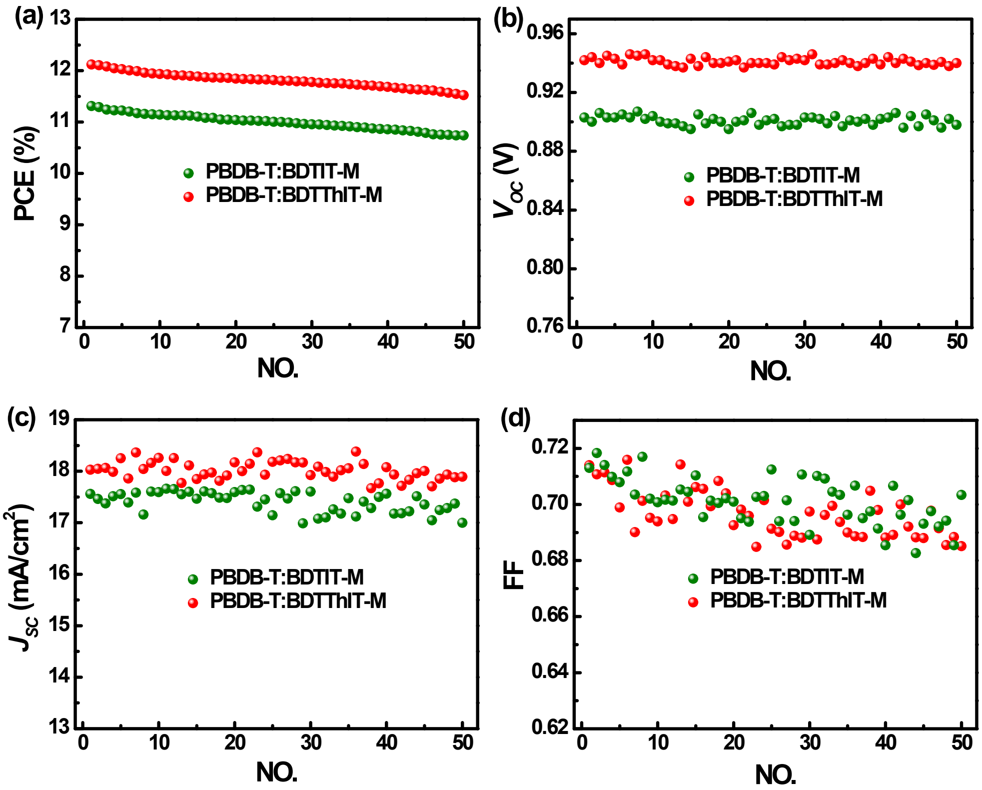


Figure S6. The distribution of photovoltaic parameters (PCE, J_{SC}, V_{OC} and FF) for the 50 optimzied BDTIT-M and BDTThIT-M based OSCs.

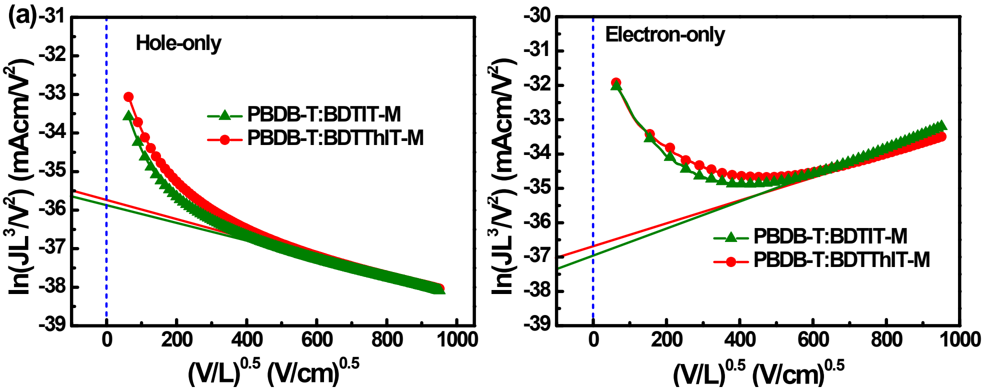


Figure S7. The ln(JL^3/V^2) vs $(V/L)^{0.5}$ curves of a) electron-only ITO/ZnO/active layer/Al device and b) hole-only ITO/PEDOT:PSS/active layer/MoO_3/Ag devices.

Table S2 The μe, μh and μe/μh in the BDTIT-M and BDTThIT-M based OSCs.

	μ_e [cm^2 Vs^{-1}]	μ_h [cm^2 Vs^{-1}]	μ_e/μ_h
PBDB-T:BDTIT-M	3.00×10^{-4}	8.84×10^{-4}	0.34
PBDB-T:BDTThIT-M	3.93×10^{-4}	9.97×10^{-4}	0.39

Table S3 Photovoltaic results of polymer donors and NF-acceptors.

Donor:NF	E_g [eV]	V_{oc} [V]	E_g - eV_{oc} [eV]	FF	EQE_{max} [%]	PCE_{max} [%]	Ref.
PBDB-T:BDTIT-M	1.53	0.942	0.588	0.714	78	12.12	This work
PBDB-T:BDTThIT-M	1.55	0.903	0.647	0.713	77.5	11.31	This work
PBDB-T-SF:IT-4F	1.52	0.88	0.64	0.719	83	13.10	[5]
PBDB-T:NITI	1.49	0.86	0.63	0.71	82	12.74	[6]
PBDB-TF:IDTN	1.59	0.946	0.644	0.78	73	12.2	[7]
FTAZ:ITIC-Th1	1.55	0.849	0.701	0.737	80	12.10	[8]
PBDBT:IT-M	1.60	0.94	0.66	0.735	78	12.05	[9]
PBDB-T:IT-OM-2	1.59	0.93	0.66	0.73	78.1	11.9	[10]
PB3T:IT-M	1.61	1.00	0.61	0.630	82	11.9	[11]
PBT1-EH:ITCPTC	1.58	0.95	0.63	0.751	72	11.8	[12]
J61:m-ITIC	1.58	0.912	0.668	0.705	81	11.77	[13]

J91:m-ITIC	1.59	0.984	0.61	0.655	79	11.63	[14]
PvBDTTAZ:O-IDTBR	1.63	1.08	0.55	0.636	71	11.6	[15]
FTAZ:INIC3	1.48	0.852	0.628	0.674	77	11.5	[16]
J71:ITIC	1.59	0.94	0.65	0.698	76.5	11.41	[17]
PBDB-T:ITCC	1.67	1.01	0.66	0.71	78	11.4	[18]
PBQ-4F:ITIC	1.57	0.95	0.62	0.668	82	11.34	[19]
PBDBT:ITIC	1.57	0.90	0.67	0.742	75	11.2	[20]
PBDB-T:FTIC-C6C8	1.63	0.93	0.70	0.647	80	11.12	[21]
PTFBDT-BZS:IDIC	1.62	0.905	0.715	0.708	80	11.03	[22]
FTAZ:ITIC2	1.53	0.925	0.605	0.626	78	11.00	[23]
PBPD-Th:ITIC	1.55	1.01	0.54	0.590	78	10.8	[24]
J71:BT-IC	1.43	0.90	0.53	0.657	68	10.46	[25]
PBDB-T:NFBDT	1.56	0.868	0.692	0.672	75	10.42	[2]
HFQx:ITTC	1.61	0.88	0.73	0.710	73	10.4	[26]
PFBZ:ITIC	1.57	0.89	0.68	0.620	84	10.4	[27]
PTZ6:ITIC	1.59	1.01	0.58	0.723	62	10.3	[28]
PTzBI:ITIC	1.57	0.87	0.70	0.643	75	10.24	[29]
PDCBT:ITIC	1.57	0.94	0.63	0.657	73	10.16	[30]
PTB7-Th:ATT-1	1.54	0.87	0.67	0.700	74	10.07	[31]
PBDB-T:FDICTF	1.63	0.94	0.69	0.660	75	10.06	[32]
PBDTTT-EFT:IEICO-4F	1.24	0.739	0.501	0.594	74	10.0	[33]
PffBT4T-2DT:IDTBR	1.63	1.07	0.56	0.620	76	9.95	[34]
3MT-Th:ITIC	1.57	0.95	0.62	0.601	78	9.73	[35]
PDBT-T1:ITIC-Th	1.60	0.88	0.72	0.671	80	9.6	[36]
PBDB-T:IDT-BOC6	1.63	1.01	0.62	0.540	72	9.60	[37]
PTB7-Th:ATT-2	1.32	0.73	0.59	0.630	71	9.58	[38]
J61:ITIC	1.57	0.89	0.68	0.615	78	9.53	[39]
P3TEA:SF-PDI2	1.72	1.11	0.61	0.643	66	9.5	[40]
PffBT4T-B:ITIC-Th	1.60	0.972	0.628	0.618	72	9.4	[41]
PDBT-T1:TPH-Se	1.78	1.0	0.78	0.717	75	9.28	[42]
J51:ITIC	1.57	0.82	0.75	0.690	74	9.26	[43]
PTzBI:N2200	1.44	0.844	0.596	0.703	74	9.16	[44]
PBDB-T1:ITTIC	1.46	0.92	0.54	0.620	65	9.12	[45]
PffQx-PS:ITIC	1.57	0.97	0.60	0.629	66	9.12	[46]
PBDTS-DTBTO:ITIC	1.57	0.843	0.727	0.649	78	9.09	[47]

PDBT-T1:IDIC	1.62	0.89	0.73	0.650	76	8.71	[48]
PTB7-Th:NDP-V	1.61	0.74	0.87	0.670	80	8.59	[49]
J51:IDSe-T-IC	1.52	0.91	0.61	0.620	66	8.58	[50]
PTB7-Th:TPB	1.61	0.79	0.82	0.581	75	8.47	[51]
PDBT-T1:SdiPBI-Se	1.77	0.96	0.81	0.697	73.3	8.42	[52]
PBDTTT-E-T:IEICO	1.34	0.82	0.52	0.580	66	8.4	[53]
J51:N2200	1.48	0.83	0.65	0.702	75	8.27	[54]
PBDTS-Se:SdiPBI-S	1.77	0.91	0.86	0.688	72	8.22	[55]
PSEHTT:DBFI-EDOT	1.77	0.93	0.84	0.630	81.6	8.10	[56]
J51:IDTIDSe-T-IC	1.52	0.91	0.61	0.580	65	8.02	[57]

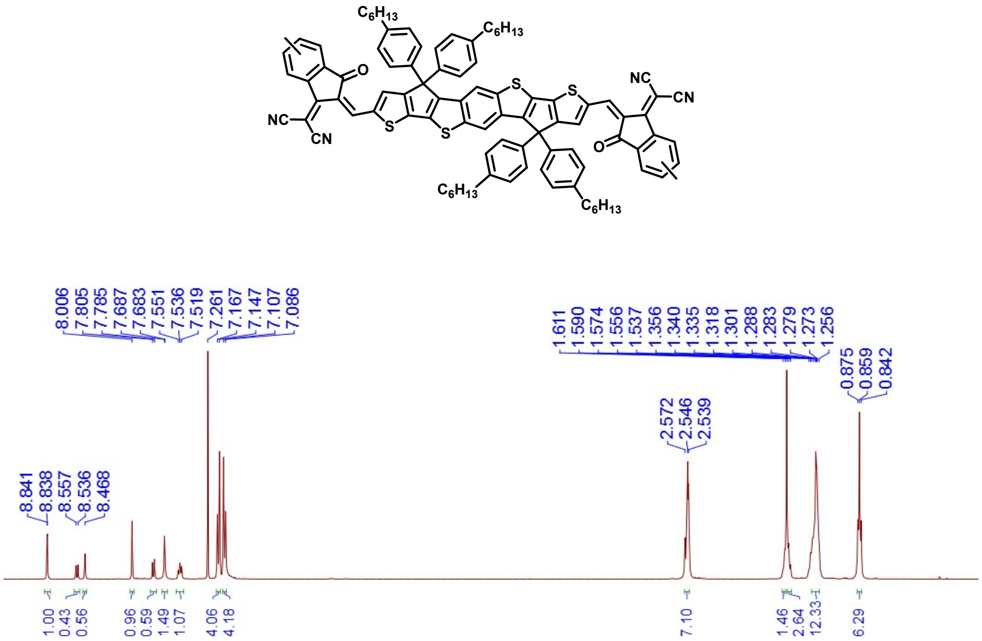


Figure S8. The ^{1}H NMR spectrum of BDTIT-M in $CDCl_3$.

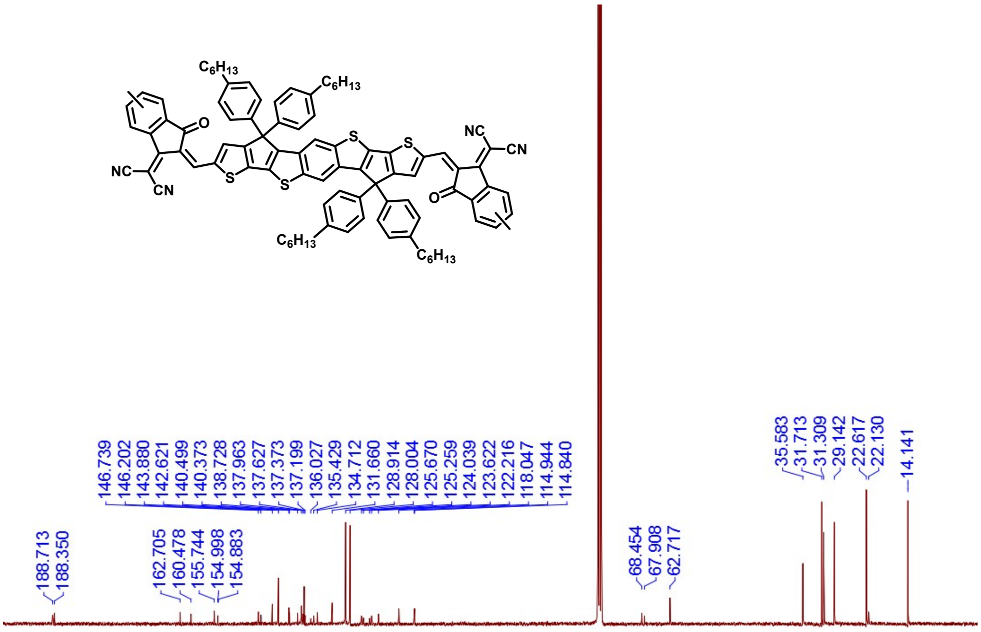


Figure S9. The ^{13}C NMR spectrum of BDTIT-M in $CDCl_3$.

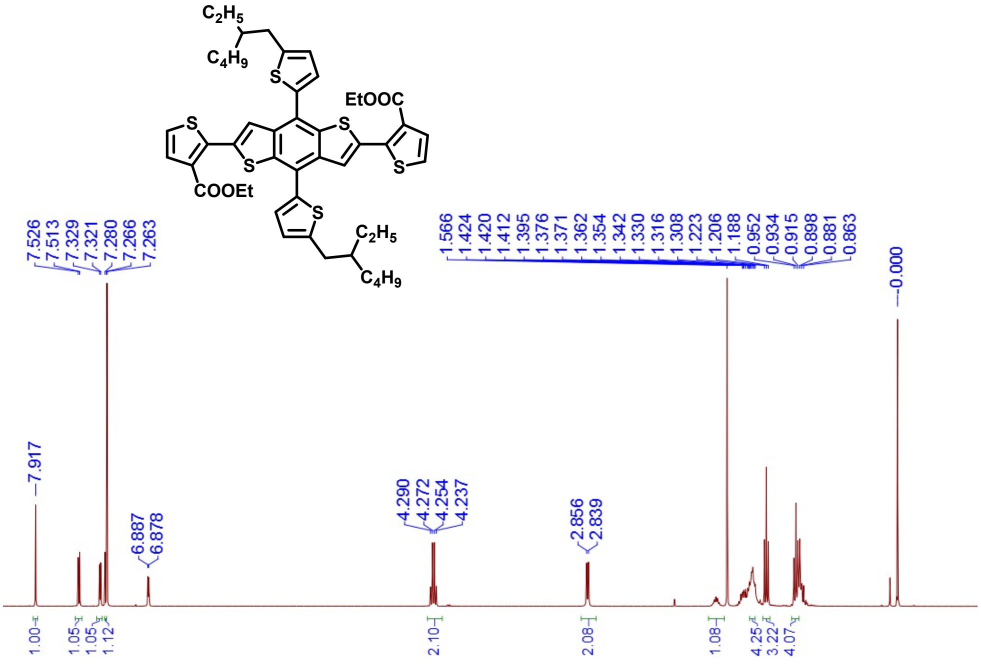


Figure S10. The ^{1}H NMR spectrum of compound **2a** in $CDCl_3$.

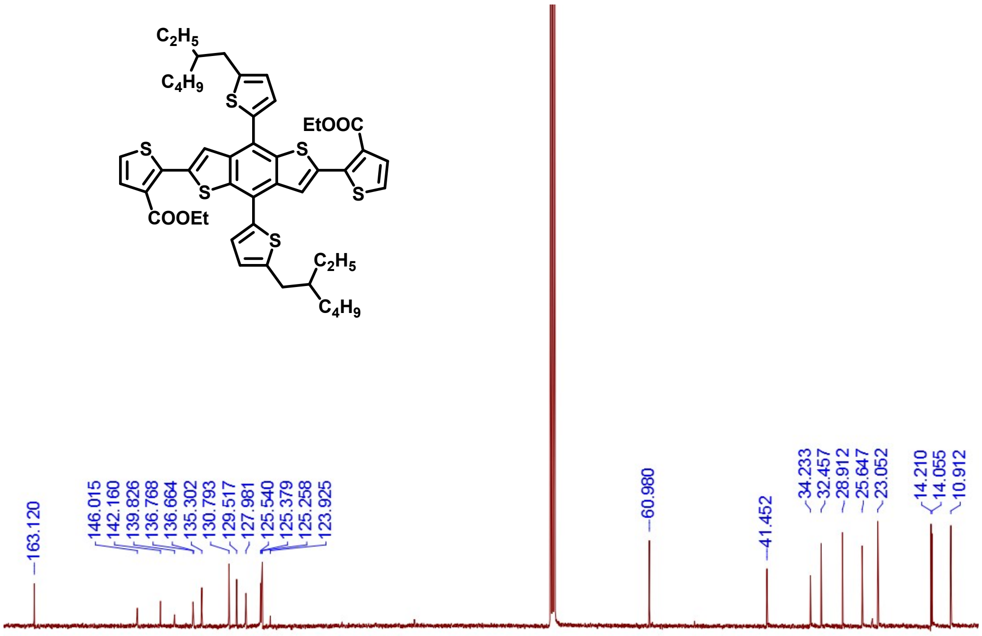


Figure S11. The ^{13}C NMR spectrum of compound **2a** in $CDCl_3$.

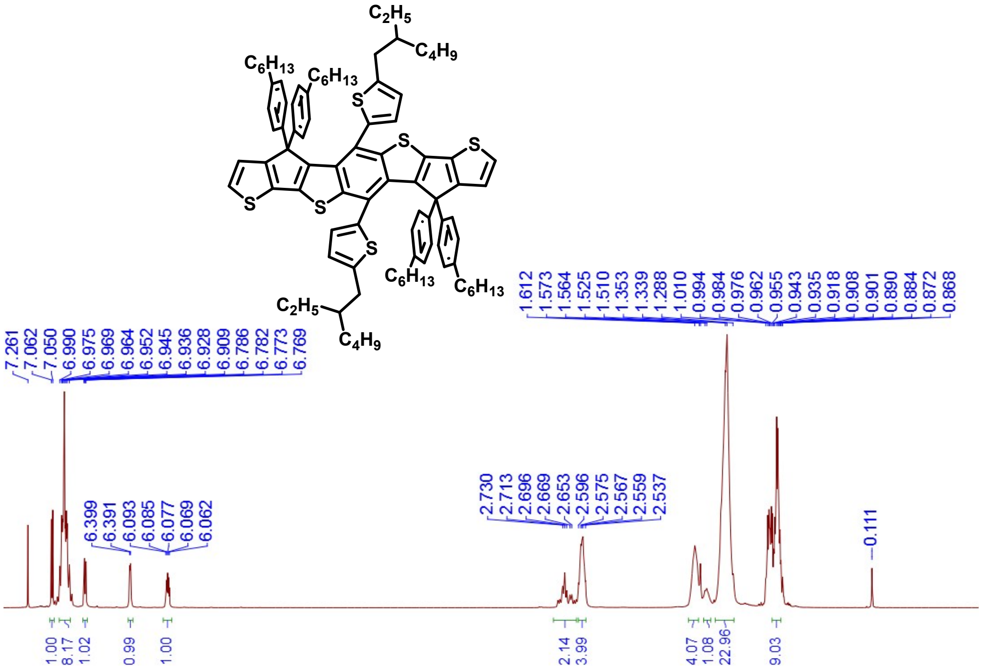


Figure S12. The ^{1}H NMR spectrum of compound **3a** in $CDCl_3$.

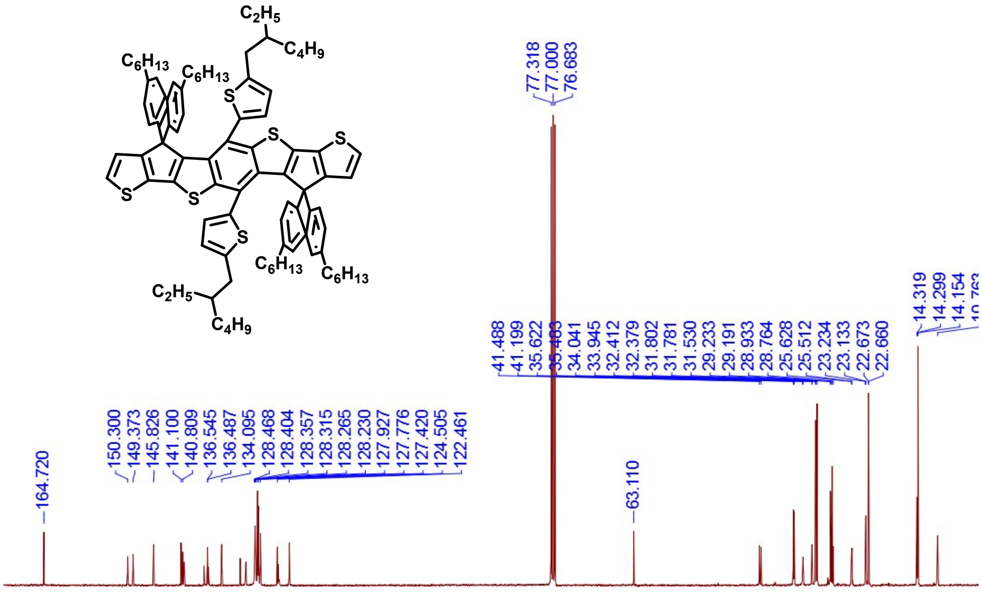


Figure S13. The ^{13}C NMR spectrum of compound **3a** in CDCl$_3$.

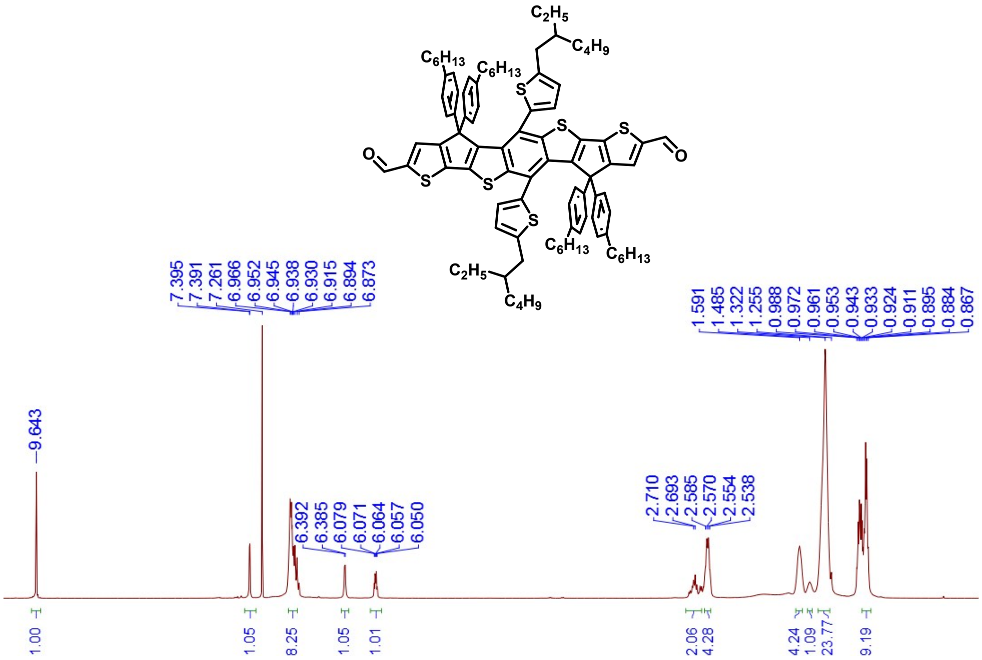


Figure S14. The ^{1}H NMR spectrum of compound **4a** in CDCl$_3$.

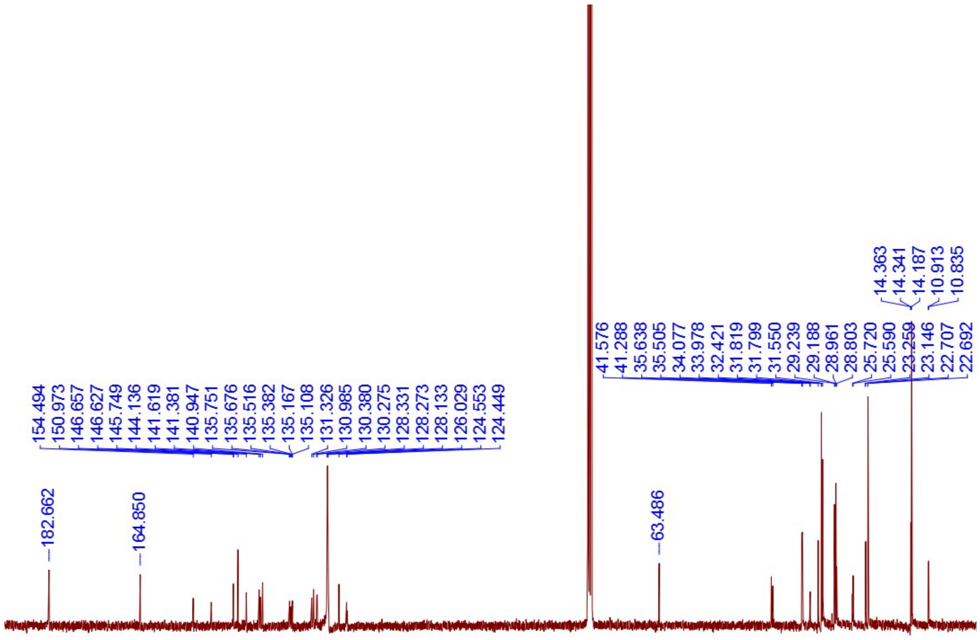


Figure S15. The ^{13}C NMR spectrum of compound **4a** in $CDCl_3$.

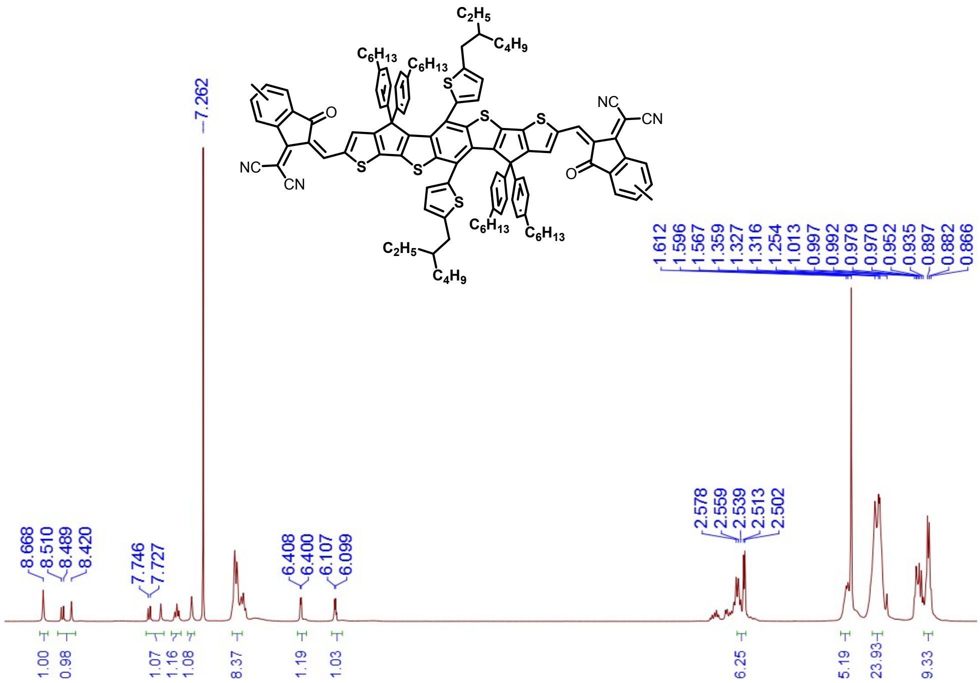


Figure S16. The ^{1}H NMR spectrum of BDTThIT-M in $CDCl_3$.

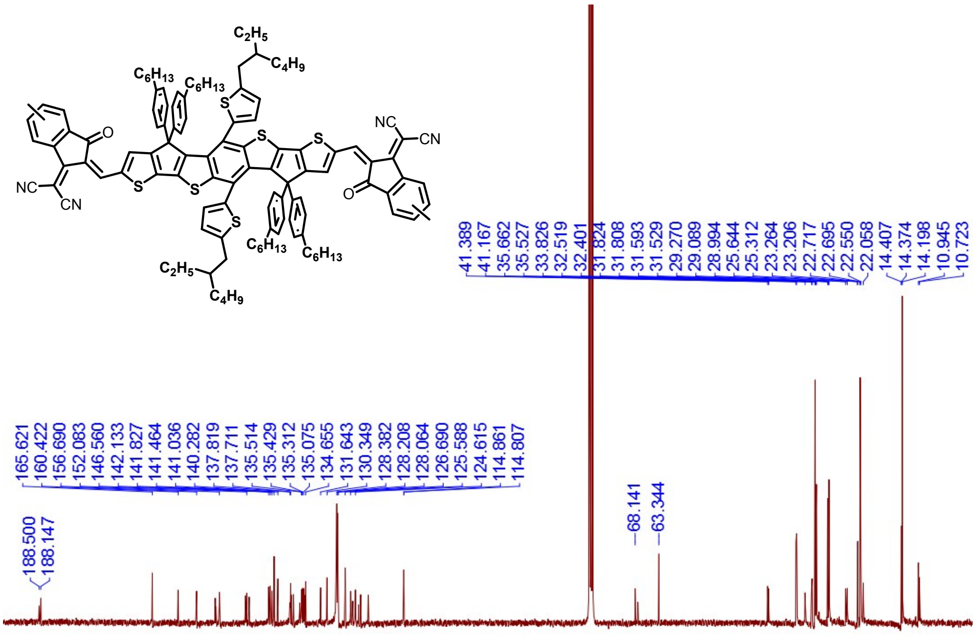


Figure S17. The ^{13}C NMR spectrum of BDTThIT-M in CDCl$_3$.

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