

Supporting Information

Cyano-functionalized Small-Molecule Acceptors for High-Efficiency Wide-Bandgap Organic Solar Cells

Jun Zhang,^{‡,a,c} Jie Lv,^{‡,a,b} Xiyue Dong,^{a,b} Tongle Xu,^{a,b} Xuexin Dai,^{a,d} Tainan Duan^{*a}, Zhipeng Kan,^{*a} Ping Liu^c and Shirong Lu^{*a}

^a *Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences, Chongqing, 400714, China*

^b *University of Chinese Academy of Sciences, Beijing 100049, China*

^c *School of Chemistry and Chemical Engineering, The Key Laboratory for Green Processing of Chemical Engineering of Xinjiang Bingtuan, Shihezi University, Shihezi City, 832004, China.*

^d *School of Chemistry and Chemical Engineering, Qiannan Normal University for Nationalities, Duyun, Guizhou Province 558000, China*

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1. General Experimental Details

Instrument: ^1H NMR and ^{13}C NMR spectra were obtained on an AVANCE500 nuclear magnetic resonance (NMR) spectroscope. UV-vis absorption spectra were recorded on a Perkin Elmer Lambda 365 spectrophotometer. Thermogravimetric analysis (TGA) was carried out on a WCT-2 thermal balance under protection of nitrogen at a heating rate of $10\text{ }^\circ\text{C}/\text{min}$.

Cyclic voltammetry (CV) measurements were done on the 600E electrochemical workstation with a three electrode system: a glassy carbon electrode as the working electrode, a platinum wire electrode as the counter electrode and a Ag/AgCl electrode as the reference electrode. The 0.1 M solution of tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) in acetonitrile was used as an electrolyte. The CV curves were recorded and calibrated by the ferrocene-ferrocenium (Fc/Fc^+) redox couple (-4.8 eV versus vacuum level). The materials were measured by coating a film on the surface of working electrode. The HOMO and LUMO levels are calculated by the formula: $E_{\text{HOMO}} = -[E_{\text{OX}} + (4.8 - E_{\text{Fc}/\text{Fc}^+})]$, $E_{\text{LUMO}} = -[E_{\text{RED}} + (4.8 - E_{\text{Fc}/\text{Fc}^+})]$, where $E_{\text{OX}}/E_{\text{RED}}$ means the potential from the first oxidation or reduction peak and $E_{\text{Fc}/\text{Fc}^+}$ means the half-wave potential of the external standard.

Materials: All reagents and solvents, unless otherwise specified, were purchased from Energy Chemical, Tansoole and Derthon Optoelectronic Materials Science Technology Co LTD and were used without further purification. PBDB-T was purchased from Solarmer Energy Inc. IDT-SnMe₃, IDT-C8-SnMe₃ and Br-BC were synthesized according to literature reports,¹⁻³ and the compounds IDT-BC and IDT-C8-BC were synthesized according to reported literature. All reactions were performed under nitrogen atmosphere and solvents were purified and dried from appropriate drying agents using standard techniques prior to use. Flash

chromatography was performed by using Silicycle Silica Flash P60 silica gel. Silica gel on TLC-PET foils from Fluka was used for TLC.

2. Synthetic Protocols and Characterizations

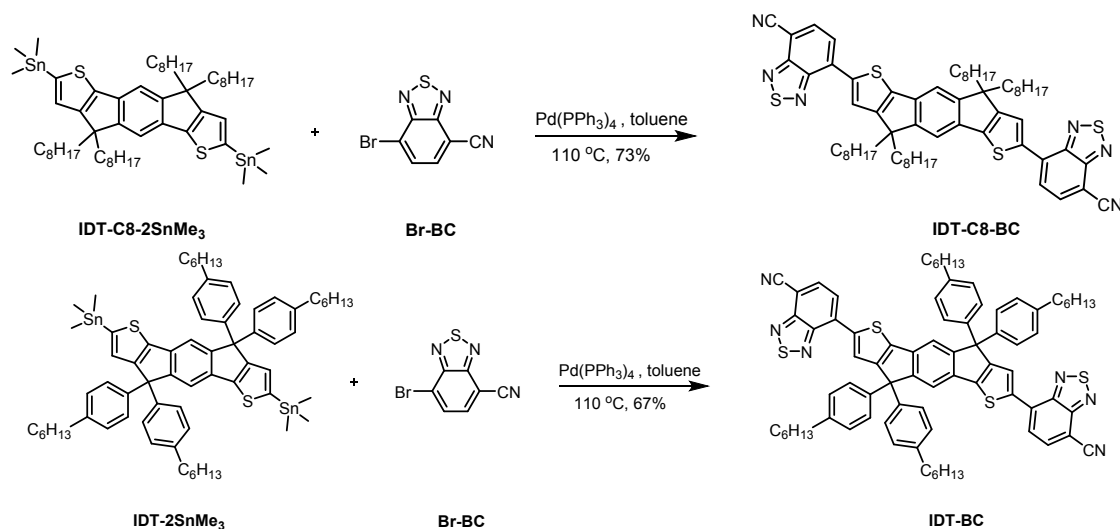


Figure S1. The detailed synthetic routes toward the target structures IDT-BC and IDT-C8-BC.

Synthesis of IDT-BC

To a three-necked round bottom flask were added (4,4,9,9-tetrakis(4-hexylphenyl)-4,9-dihydro-*s*-indaceno[1,2-*b*:5,6-*b'*]dithiophene-2,7-diyl)bis(trimethylstannane) (150 mg, 0.12 mmol), 7-bromobenzo[*c*][1,2,5]thiadiazole-4-carbonitrile (151 mg, 0.63 mmol) and toluene (20 mL). The mixture was deoxygenated with argon for 15 min, and then Pd(PPh₃)₄ (21 mg, 0.018 mmol) was added. The mixture was refluxed for 24 h and then cooled to room temperature. 40 mL KF solution was added and stirred at room temperature overnight to remove the tin impurity. Water (150 mL) was added and the mixture was extracted with CHCl₃. The organic phase was dried over anhydrous MgSO₄. After removing the solvent, the residue was purified by column chromatography on silica gel using petroleum ether/CHCl₃ (1:2) as eluent yielding a Purple black solid (102 mg, 67%). ¹H NMR (600 MHz, CDCl₃) δ 8.18 (s, 2H), 7.96 (d, *J* = 7.6 Hz, 2H), 7.82 (d, *J* = 7.6 Hz, 2H), 7.58 (s, 2H), 7.24 (d, *J* = 8.1 Hz, 8H), 7.11 (d, *J* = 8.2 Hz, 8H), 2.57 (t, *J* = 7.9 Hz, 8H), 1.59 (m, 8H), 1.35 – 1.27 (m, 24H), 0.88 – 0.84 (m, 12H). ¹³C NMR (151 MHz, CDCl₃) δ 157.59, 154.38, 153.81, 151.08, 146.25, 141.93, 141.23, 140.70, 135.88, 135.72, 132.93, 128.56,

127.86, 126.03, 122.59, 118.30, 115.73, 102.33, 63.25, 35.57, 31.70, 31.32, 29.70, 29.13, 22.58, 14.06. MS (MALDI-TOF): calcd for C₇₈H₇₆N₆S₄ (M⁺): 1225.7480, Found: 1225.5154.

Synthesis of **IDT-C8-BC**

To a three-necked round bottom flask were added (4,4,9,9-tetraoctyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophene-2,7-diyl)bis(trimethylstannane) (200 mg, 0.2 mmol), 7-bromobenzo[c][1,2,5]thiadiazole-4-carbonitrile (124 mg, 0.52 mmol) and toluene (20 mL). The mixture was deoxygenated with argon for 15 min, and then Pd(PPh₃)₄ (35 mg, 0.03 mmol) was added. The mixture was refluxed for 24 h and then cooled to room temperature. 40 mL KF solution was added and stirred at room temperature overnight to remove the tin impurity. Water (150 mL) was added and the mixture was extracted with CHCl₃. The organic phase was dried over anhydrous MgSO₄. After removing the solvent, the residue was purified by column chromatography on silica gel using petroleum ether/CHCl₃ (1:2) as eluent yielding a purple black solid (152 mg, 73%). ¹H NMR (600 MHz, CD₂Cl₂) δ 8.27 (s, 2H), 8.05 (d, *J* = 7.6 Hz, 2H), 7.96 (d, *J* = 7.6 Hz, 2H), 7.51 (s, 2H), 2.13 (m, 4H), 2.00 (m, 4H), 1.11 (s, 40H), 0.96 – 0.86 (m, 8H), 0.77 (t, *J* = 7.1 Hz, 12H). ¹³C NMR (151 MHz, CD₂Cl₂) δ 158.42, 155.59, 155.36, 152.57, 148.21, 141.36, 137.76, 137.47, 134.59, 126.30, 123.80, 117.26, 115.52, 103.12, 55.81, 40.43, 33.11, 31.24, 30.58, 30.47, 25.57, 23.90, 15.10. MS (MALDI-TOF): calcd for C₆₂H₇₆N₆S₄ (M⁺): 1033.5720, Found: 1032.5164.

3. UV-Vis Absorption Spectra and Energy Level Diagram

UV-Vis absorption spectra of IDT-BC and IDT-C8-BC were recorded on PerkinElmer LAMBDA 365 UV-Vis spectrophotometer.

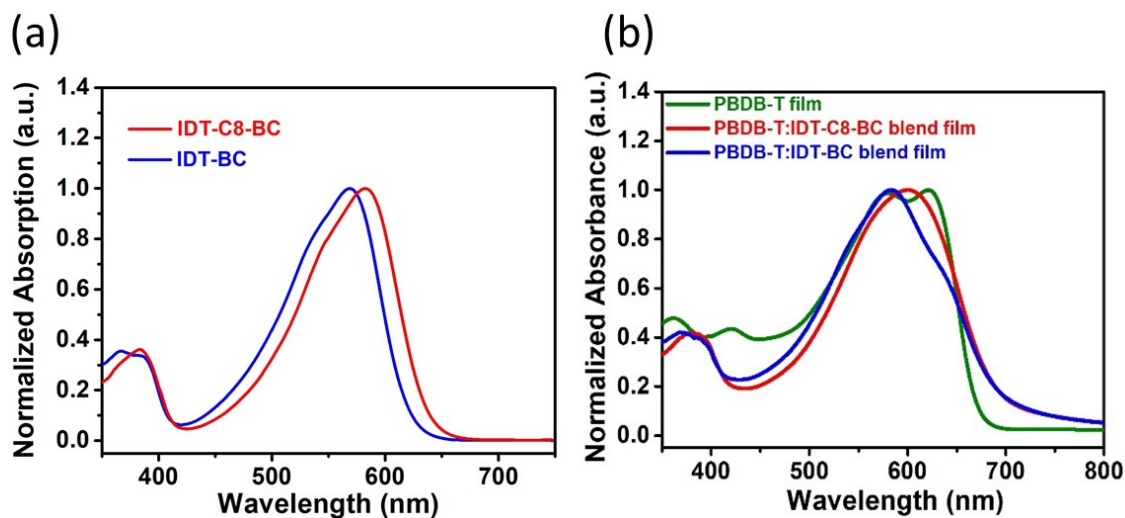


Figure S2. (a) Normalized solution (chloroform) UV-vis absorption spectra of the two SM acceptors. (b) Normalized absorption spectra of the donor PBDB-T and the blend films of PBDB-T:IDT-C8-BC, PBDB-T:IDT-BC.

Energy Level Diagram

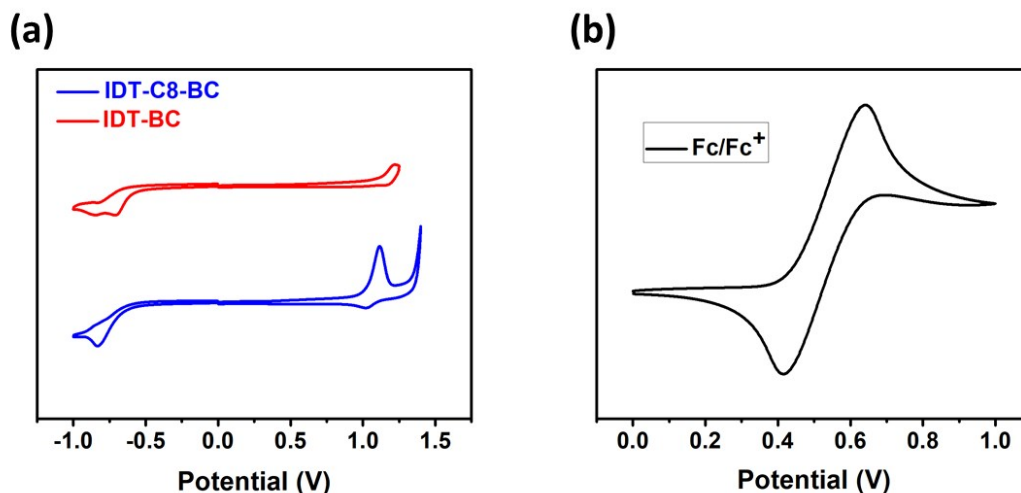


Figure S3. (a) Cyclic voltammograms of IDT-BC, IDT-C8-BC and (b) Fc/Fc⁺ in CH₃CN solutions.

4. TGA curves of IDT-BC and IDT-C8-BC

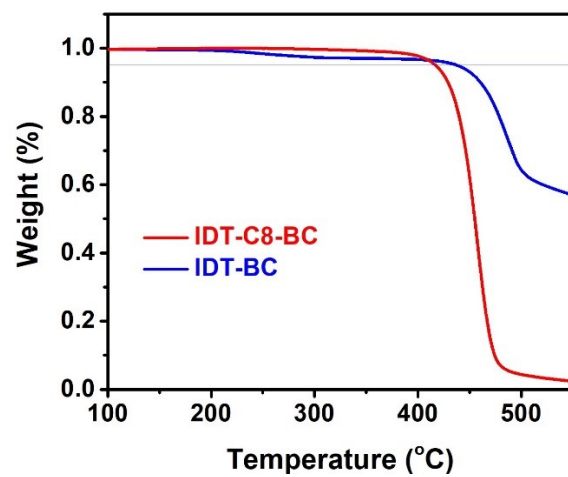


Figure S4. TGA curves of IDT-BC and IDT-C8-BC.

5. Device Fabrication and Characterization

The organic solar cells were prepared on glass substrates with tin-doped indium oxide (ITO, 15 Ω /sq) patterned on the surface (device area: 0.11 cm²). Substrates were prewashed with isopropanol to remove organic residues before immersing in an ultrasonic bath of soap for 15 min. Samples were rinsed in flowing deionized water for 5 min before being sonicated for 15 min each in successive baths of deionized water, acetone and isopropanol. Next, the samples were dried with pressurized nitrogen before being exposed to a UV-ozone plasma for 20 min. ZnO precursor solution (ZnO precursor solution (ZnAc \cdot 2H₂O of 0.4g was dissolved in 5mL ethylene glycol monomethyl ether, and the ethanolamine of 107.8uL was added to prepare a 0.36 mol/L ZnO precursor solution, and then filtered through a 0.45 μ m PVDF filter) was spin-coated on to ITO substrates at a spinning rate of 4000 rpm for 30s in dried air, followed by baked on a hot plate at 150°C for 30 min to form a thin ZnO layer (\approx 40 nm), and the substrates were then transferred into the glovebox for active layer deposition. ($<$ 0.1 ppm O₂).

All solutions were prepared in the glovebox using the polymer donor PBDB-T and the SM acceptors IDT-BC and IDT-C8-BC; the polymer donor PBDB-T was purchased from Brilliant Matters. Optimized devices were obtained by dissolving PCE10, IDT-BC and IDT-C8-BC in chlorobenzene (CB) using a D/A ratio of 1:1.5 and 1:1.5 (wt/wt), respectively, total concentration of 15mg/ml. Note: The as-prepared CB solutions were stirred for 8 hours at 80°C before being cast on the (room temperature) substrates. The active layers with CB solutions were spin-coated at an optimized speed of 2500 rpm for time period of 40s, resulting in films of 100 to 110 nm in thickness. After annealing of 150°C, 10 min and 90°C, 10 min, respectively, the substrates were immediately moved into an evaporator. A molybdenum trioxide interlayer (MoO₃, 8 nm) and Ag layer (100 nm) were deposited onto the surface of

the active layer through a shadow mask under high vacuum (less than 2×10^{-6} Torr). The area for each device is 0.11 cm^2 .

Following electrode deposition, samples underwent $J-V$ testing. J-V measurements of solar cells were performed in the glovebox with a Keithley 2400 source meter. A 300 W xenon arc solar simulator (Oriel) with an AM 1.5 global filter operated at 100 mW/cm^2 was used to simulate the AM 1.5G solar irradiation. The illumination intensity was corrected by using a silicon photodiode with a protective KG5 filter calibrated by the National Institute of Metrology (NIM). The EQE spectra were measured using a Solar Cell Spectral Response Measurement System QE-R3011 (Enlitech Co., Ltd.). The light intensity at each wavelength was calibrated using a standard monocrystalline Si photovoltaic cell.

6. Additional OPV Device Performance Data

From **Table S1** to **Table S4**, a summary of the photovoltaic performance parameters of IDT-C8-BC under various preparation process conditions and the photovoltaic performance parameters of IDT-BC with different process conditions from **Table S5** to **Table S8**.

Table S1. The photovoltaic parameters of the IDT-C8-BC for the devices with the different condition treatment. All the Data were obtained under illumination of AM 1.5G, 100 mW/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1	As Cast	1.05 (1.05±0.00)	7.75 (7.65±0.09)	40.2 (39.5±0.7)	3.3 (3.2±0.1)
1:1	100°C, 10 min	1.06 (1.05±0.01)	10.59 (10.51±0.08)	58.5 (56.7±1.8)	6.6 (6.3±0.3)
1:1	0.5% CN	1.06 (1.05±0.01)	10.07 (9.65±0.42)	57.1 (55.8±1.3)	6.1 (5.6±0.5)
1:1	0.5% DIO	1.06 (1.05±0.01)	9.64 (9.60±0.04)	64.2 (59.0±5.2)	6.5 (6.0±0.5)
1:1	0.5% DPE	1.08 (1.06±0.02)	9.98 (9.85±0.13)	54.7 (53.3±1.4)	5.9 (5.6±0.4)
1:1	0.5% NMP	1.06 (1.05±0.01)	9.90 (9.95±0.05)	55.6 (52.3±3.3)	5.8 (5.5±0.3)

a) The average parameters were calculated over 10 independent cells.

Table S2. The photovoltaic parameters of the IDT-C8-BC for the devices with the different D:A ratio at thermal treatment 100°C, 10 min. All the Data were obtained under illumination of AM 1.5G, 100 mW/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1	100°C, 10 min	1.06 (1.05±0.01)	10.59 (10.51±0.08)	58.5 (56.7±1.8)	6.6 (6.3±0.3)
1:1.5	100°C, 10 min	1.05 (1.05±0.01)	10.02 (9.30±0.71)	65.6 (64.9±0.7)	6.9 (6.4±0.5)
1:2	100°C, 10 min	1.05 (1.04±0.01)	8.77 (8.68±0.09)	68.5 (66.7±1.8)	6.3 (6.0±0.3)

a) The average parameters were calculated over 10 independent cells.

Table S3. The photovoltaic parameters of the IDT-C8-BC for the devices with the different thermal treatment. All the data were obtained under illumination of AM 1.5G, 100 mW/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1.5	60°C, 10 min	1.10 (1.08±0.02)	9.69 (9.56±0.13)	58.7 (58.5±0.2)	6.3 (6.1±0.2)
1:1.5	70°C, 10 min	1.08 (1.06±0.02)	10.50 (10.17±0.33)	62.3 (61.5±0.8)	7.1 (6.7±0.4)
1:1.5	80°C, 10 min	1.05 (1.05±0.00)	10.70 (10.45±0.25)	64.3 (60.9±3.4)	7.2 (6.7±0.5)
1:1.5	90°C, 10 min	1.05 (1.05±0.01)	10.27 (10.06±0.21)	67.6 (65.4±2.2)	7.3 (7.0±0.3)
1:1.5	100°C, 10 min	1.05 (1.05±0.01)	10.02 (9.30±0.71)	65.6 (64.9±0.7)	6.9 (6.4±0.5)

a) The average parameters were calculated over 10 independent cells.

Table S4. The photovoltaic parameters of the IDT-C8-BC for the devices with the different amount of DIO treatment. All the data were obtained under illumination of AM 1.5G, 100 Mw/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1.5	0.5% DIO	1.06 (1.05±0.01)	9.58 (9.53±0.05)	60.7 (57.8±2.9)	6.2 (5.8±0.4)
1:1.5	1% DIO	1.08 (1.06±0.02)	9.97 (9.86±0.11)	58.4 (55.2±3.3)	6.3 (5.8±0.5)
1:1.5	1.5% DIO	1.08 (1.07±0.01)	9.78 (9.69±0.09)	55.3 (52.5±2.8)	5.9 (5.5±0.4)
1:1.5	2% DIO	1.03 (1.02±0.01)	9.34 (9.30±0.04)	54.3 (50.2±3.9)	5.2 (4.8±0.4)

a) The average parameters were calculated over 10 independent cells.

Table S5. The photovoltaic parameters of the IDT-BC for the devices with the the different thermal treatment. All the data were obtained under illumination of AM 1.5G, 100 mW/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1	As Cast	1.11 (1.08±0.03)	8.52 (8.49±0.03)	41.9 (40.0±1.9)	4.0 (3.7±0.3)
1:1	100°C, 10 min	1.09 (1.05±0.04)	9.05 (8.97±0.08)	42.7 (42.1±0.6)	4.2 (3.9±0.3)
1:1	120°C, 10 min	1.09 (1.07±0.02)	9.16 (9.02±0.14)	46.2 (41.9±4.3)	4.6 (4.1±0.5)
1:1	140°C, 10 min	1.05 (1.05±0.01)	10.27 (10.03±0.24)	44.9 (43.0±1.9)	4.8 (4.5±0.3)

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1	150°C, 10 min	1.06 (1.05±0.01)	10.87 (10.37±0.50)	54.0 (49.1±4.9)	6.2 (5.4±0.8)
1:1	160°C, 10 min	1.05 (1.05±0.00)	10.11 (10.09±0.02)	55.5 (53.5±2.0)	5.9 (5.7±0.2)

a) The average parameters were calculated over 10 independent cells.

Table S6. The photovoltaic parameters of the IDT-BC for the devices with the different additive treatment. All the data were obtained under illumination of AM 1.5G, 100 mW/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1	As Cast	1.11 (1.08±0.03)	8.52 (8.49±0.03)	41.9 (40.0±1.9)	4.0 (3.7±0.3)
1:1	150°C, 10 min	1.06 (1.05±0.01)	10.87 (10.37±0.50)	54.0 (49.1±4.9)	6.2 (5.4±0.8)
1:1	0.5% CN	1.14 (1.09±0.05)	8.39 (8.25±0.14)	44.7 (42.2±2.5)	4.3 (3.8±0.5)
1:1	0.5% DIO	1.11 (1.10±0.01)	9.66 (9.16±0.50)	49.2 (45.3±3.9)	5.3 (4.6±0.7)
1:1	0.5% DPE	1.11 (1.10±0.01)	8.66 (8.53±0.13)	46.8 (43.7±3.1)	4.5 (4.1±0.4)
1:1	0.5% NMP	1.11 (1.11±0.01)	7.87 (7.39±0.48)	38.4 (36.9±1.5)	3.8 (3.1±0.3)

a) The average parameters were calculated over 10 independent cells.

Table S7. The photovoltaic parameters of the IDT-BC for the devices with the different amount of DIO treatment. All the data were obtained under illumination of AM 1.5G, 100 mW/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1.5	0.5% DIO	1.14 (1.11±0.03)	9.13 (8.91±0.22)	54.3 (51.7±2.6)	5.7 (5.2±0.5)
1:1.5	1% DIO	1.11 (1.10±0.01)	8.97 (8.59±0.38)	52.4 (49.1±3.3)	5.2 (4.6±0.6)
1:1.5	1.5% DIO	1.11 (1.10±0.01)	9.48 (9.17±0.31)	48.6 (47.7±0.9)	5.1 (4.9±0.2)
1:1.5	2% DIO	1.11 (1.10±0.01)	9.07 (8.90±0.17)	49.7 (47.5±2.2)	5.0 (4.7±0.4)

a) The average parameters were calculated over 10 independent cells.

Table S8. The photovoltaic parameters of the IDT-BC for the devices with the different D:A ratio at thermal treatment 150°C, 10 min. All the data were obtained under illumination of AM 1.5G, 100 mW/ cm² light source.

D:A ratio	Condition	^{a)} V _{OC} [V]	^{a)} J _{SC} [mA/cm ²]	^{a)} FF [%]	^{a)} PCE [%]
1:1	150°C, 10 min	1.06 (1.05±0.01)	10.87 (10.37±0.50)	54.0 (49.1±4.9)	6.2 (5.4±0.8)
1:1.5	150°C, 10 min	1.08 (1.06±0.01)	10.53 (10.46±0.06)	55.5 (54.9±0.6)	6.3 (6.1±0.2)
1:2	150°C, 10 min	1.05 (1.05±0.01)	7.43 (7.36±0.07)	50.1 (49.1±1.0)	3.9 (3.81±0.1)

a) The average parameters were calculated over 10 independent cells.

7. Light-Intensity Dependence Statistics

Table S9. Summary of n and a values for the light intensity dependent J_{SC} and V_{OC} .

Active layer	n	a
PBDB-T:IDT-C8-BC=1:1.5	1.00	1.00
PBDB-T:IDT-BC=1:1.5	1.26	1.00

8. SCLC Measurements

Hole-only devices were fabricated for the dark J-V measurements with device structure of ITO/PEDOT: PSS/ Active layer /MoOx/Ag. Electron-only devices were fabricated for the dark J-V measurements with device structure of ITO/ZnO/PhenoNaDPO/ Active layer /PhenoNaDPO/Ag. The single-carrier device was connected to a Source Measure Unit (Keithley, Model 2400 source meter), which provided DC voltage to the hole-only devices. The 2400 was also used to record the currents under different DC voltage conditions. The J-V signals was detected and recorded. The J-V characteristics were further analyzed by the space-charge-limited-current (SCLC) method to extract zero-field carrier mobilities, where SCLC is described by:

$$j = \frac{9\varepsilon_0\varepsilon_r\mu_0V^2}{8L^3} \exp\left[0.89\beta\sqrt{\frac{V}{L}}\right] \quad (\text{E1})$$

where J is the current density, L is the film thickness of the active layer, μ_0 is the hole or electron mobility, ε_r is the relative dielectric constant of the transport medium, ε_0 is the permittivity of free space (8.85×10^{-12} F m⁻¹), V (= V_{appl} - V_{bi}) is the internal voltage in the device, where V_{appl} is the applied voltage to the device and V_{bi} is the built-in voltage due to the relative work function difference of the two electrodes.

Table S10. Hole and electron mobilities of the binary/ternary OSCs

Active layer	μ_h [$\times 10^{-4}$ cm ² V ⁻¹ s ⁻¹]	μ_e [$\times 10^{-4}$ cm ² V ⁻¹ s ⁻¹]	μ_h/μ_e
PBDB-T:IDT-C8-BC=1:1.5	2.85±0.1	3.00±0.1	0.95
PBDB-T:IDT-BC=1:1.5	2.75±0.1	1.36±0.1	2.02

9. Transmission Electron Microscopy (TEM) Characterization.

Films were spun-cast on PEDOT:PSS-coated glass substrates. The IDT-C8-BC-based and IDT-BC-based BHJ films were floated off the substrates in deionized water and collected on lacey carbon coated TEM grids (Electron Microscopy Sciences). Middle range TEM images were recorded in bright field mode with a microscope operating at 120 keV (JEM-2100F), using eagle CCD camera (FEI).

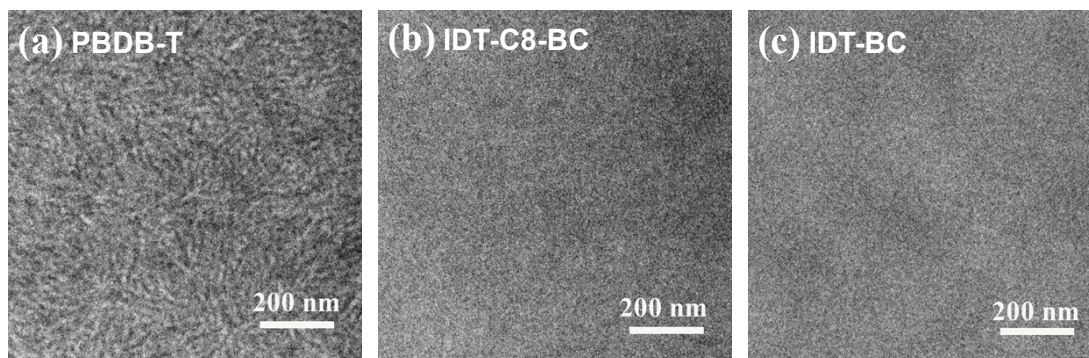
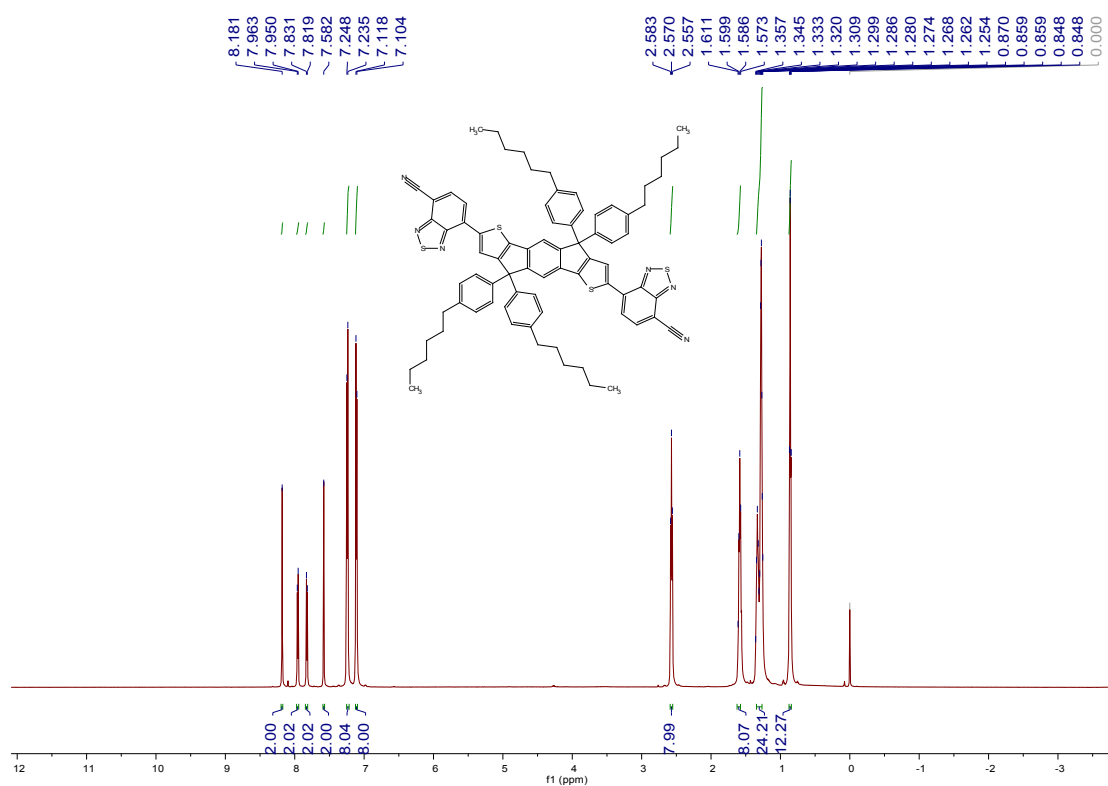
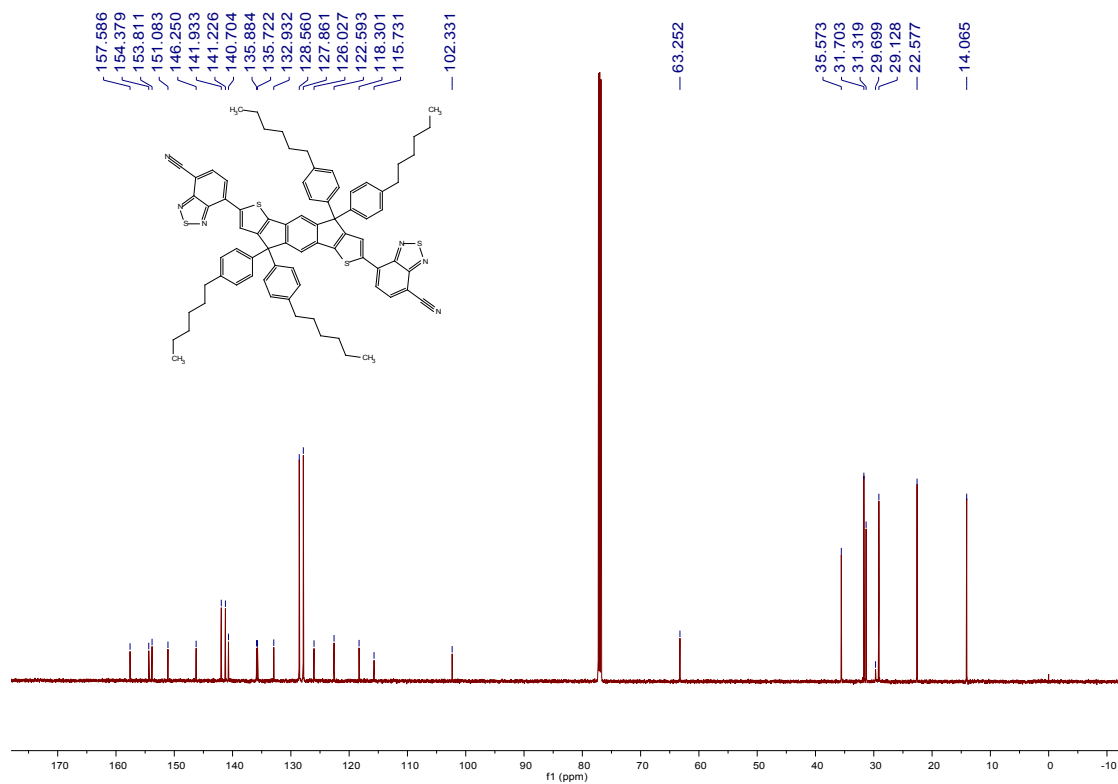


Figure S5. TEM images of (a) PBDB-T film, (b) IDT-C8-BC film and (c) IDT-BC film.

10. Solution NMR and HR-MS spectra



¹H NMR Spectrum of IDT-BC



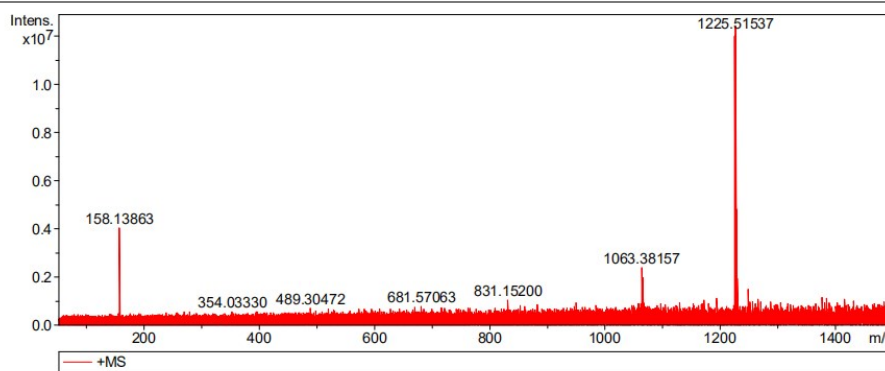
¹³C NMR Spectrum of IDT-BC

Mass Spectrum List Report

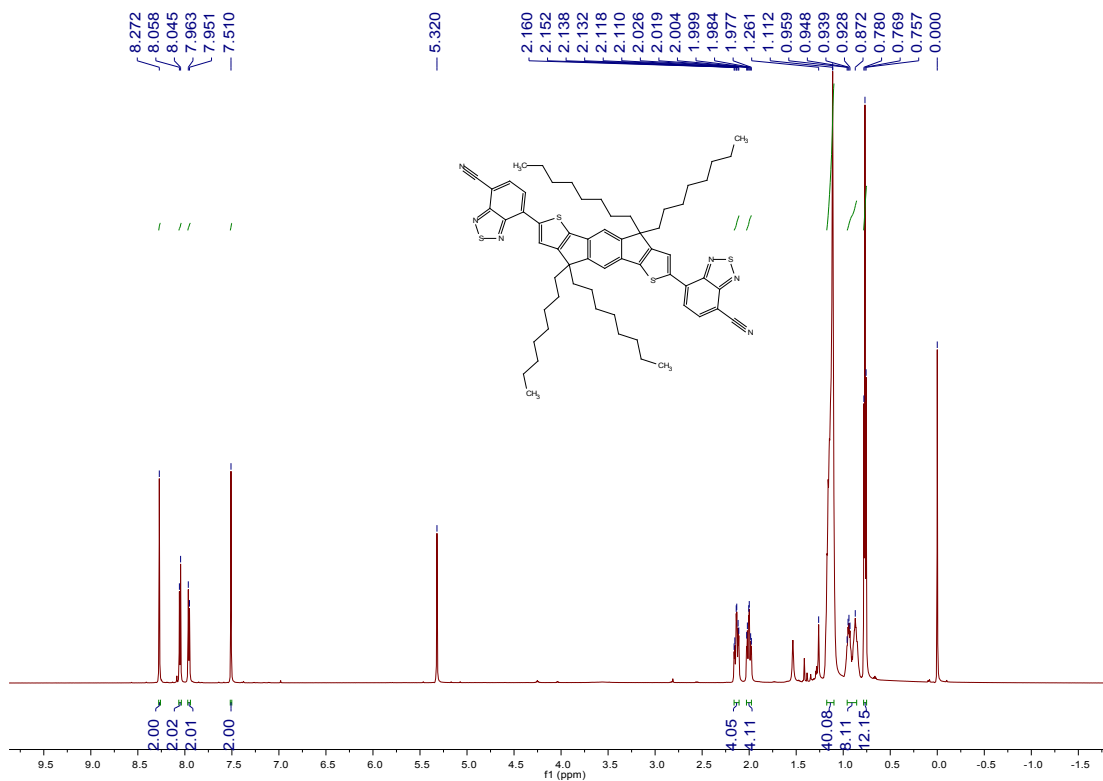
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Sample Name: 2018-6-7-MD
Comment: PeptideMix NS=8 TF=1.2
Acquisition Date: 8/25/2019 3:57:03 PM
Operator: solarix
Instrument: solarix

Acquisition Parameter

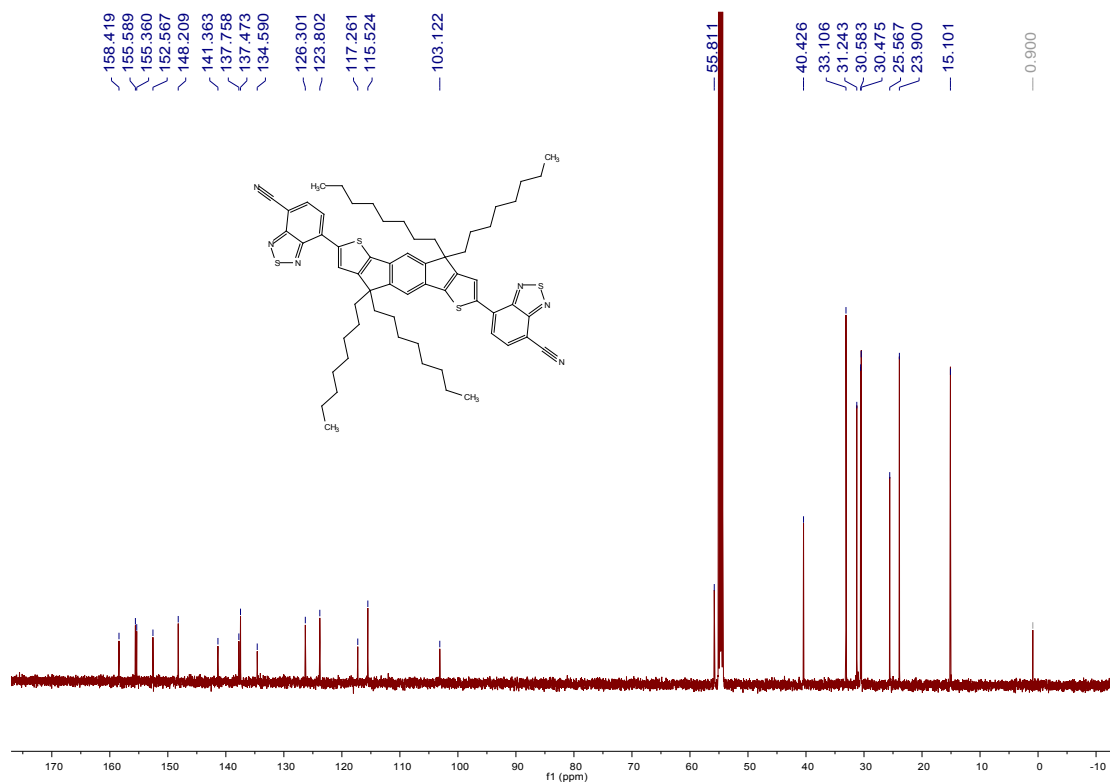
Polarity	Positive	n/a	n/a	No. of Laser Shots	100
n/a	n/a	No. of Cell Fills	1	Laser Power	75.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Fri Feb 21 02:36:54 2014
Pulse Program	basic	n/a	n/a	Data Acquisition Size	1048576
Source Accumulation	0.100 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.500 sec	n/a	n/a	Apodization	Apodization
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		



HR-MS spectrum of IDT-BC



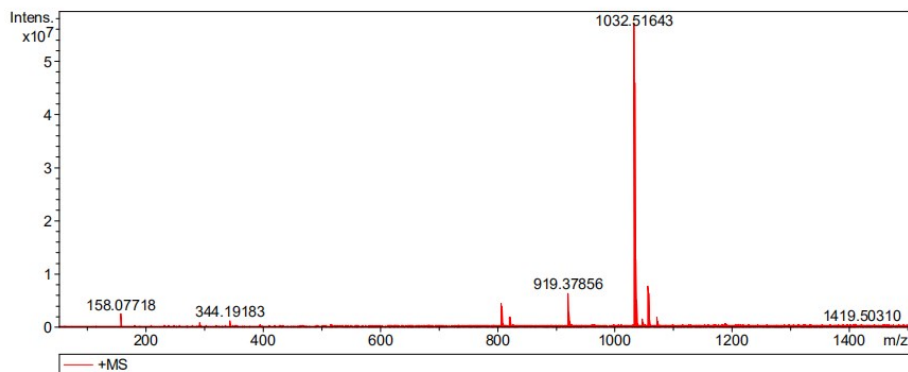
¹H NMR Spectrum of IDT-C8-BC



¹³C NMR Spectrum of IDT-C8-BC

Mass Spectrum List Report

Analysis Info				Acquisition Date	
Analysis Name	D:\Data\HYYSKD_0_I3_000008.d			8/25/2019 4:05:53 PM	
Method	5-12-DADOU			Operator	
Sample Name	2018-6-7-MD			Instrument	solariX
Comment	PeptideMix NS=8 TF=1.2				
Acquisition Parameter					
Polarity	Positive	n/a	n/a	No. of Laser Shots	100
n/a	n/a	No. of Cell Fills	1	Laser Power	75.0 lp
Broadband Low Mass	53.8 m/z	n/a	n/a	n/a	n/a
Broadband High Mass	1500.0 m/z	n/a	n/a	n/a	n/a
Acquisition Mode	Single MS	n/a	n/a	Calibration Date	Fri Feb 21 02:36:54 2014
Pulse Program	basic	n/a	n/a	Data Acquisition Size	1048576
Source Accumulation	0.100 sec	n/a	n/a	Apodization	Sine-Bell Multiplication
Ion Accumulation Time	0.500 sec	n/a	n/a	Apodization	Apodization
Flight Time to Acq. Cell	0.001 sec	n/a	n/a		



HR-MS spectrum of IDT-C8-BC

11. Supporting Information References

1. S. Shi, P. Chen, Y. Chen, K. Feng, B. Liu, J. Chen, Q. Liao, B. Tu, J. Luo, M. Su, H. Guo, M. G. Kim, A. Facchetti and X. Guo, *Adv. Mater.*, 2019, **31**, 1905161.
2. A. M. Thooft, K. Cassaidy and B. VanVeller, *J. Org. Chem.*, 2017, **82**, 8842-8847.
3. W. Wen, L. Ying, B. B. Hsu, Y. Zhang, T. Q. Nguyen and G. C. Bazan, *Chem. Commun.*, 2013, **49**, 7192-7194.