Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Applying direct heteroarylation synthesis to evaluate organic dyes as the core component in PDI-based molecular materials for fullerene-free organic solar cells

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SUPPORTING INFORMATION

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Materials and methods

General synthetic details: Reactions were carried out on a bench top or under an atmosphere of dry, O_2-free N_2 where indicated. For reactions requiring heat, the conventional method involved submerging reaction vial in a LabArmor® bead bath and heating on a hot plate at the desired temperature. For reactions that made use of microwave-assisted synthesis a Biotage® Initiator+ microwave reactor was used. The operational power range of this instrument is 0-400 W using a 2.45 GHz magnetron.

Materials: All materials and solvents were purchased from Sigma-Aldrich unless indicated otherwise. Heterogeneous catalyst Silia*Cat*® DPP-Pd was purchased from SiliCycle. *NH*-diketopyrrolopyrrole was purchased from Brilliant Matters. 2EH-TII and PTB7-Th were purchased from 1-Material. Isoindigo starting materials were purchased from Ontario Chemicals Inc.

Nuclear Magnetic Resonance (NMR): Final material ^{1}H and ^{13}C NMR spectra were acquired on a Bruker Ascend 500 mHz. For precursor organic dye synthesis, NMR spectra were acquired on a Nanalysis Corp NMReady™ 60 mHz spectrometer. Chemical shifts are reported in parts per million (ppm) and are referenced to the external standard $SiMe_4$. All experiments were performed in deuterated chloroform ($CDCl_3$). Multiplicities are reported as: singlet (s), doublet (d), triplet (t), multiplet (m), and overlapping (ov).

High-resolution Mass Spectrometry (HRMS): High-resolution MALDI mass spectrometry measurements were performed courtesy of Jian Jun (Johnson) Li in the Chemical Instrumentation Facility at the University of Calgary. A Bruker Autoflex III Smartbeam MALDI-TOF (Na:YAG laser, 355nm), setting in positive reflective mode, was used to acquire spectra. Operation settings were all typical, e.g. laser offset 62-69; laser frequency 200Hz; and number of shots 300. The target used was Bruker MTP 384 ground steel plate target. Sample solution (~ 1 µg/ml in dichloromethane) was mixed with matrix trans-2-[3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) solution (~ 5mg/ml in methanol). Pipetted 1µl solution above to target spot and dried in the fume hood.

Cyclic Voltammetry (CV): All electrochemical measurements were performed using a CH Instruments potentiostat in a standard three-electrode configuration equipped with a silver wire pseudo-reference, platinum wire counter electrode and glassy carbon working electrode. The cyclic voltammetry experiments were performed in an anhydrous solution of dichloromethane (CH_2Cl_2) with ~ 0.1 M tetrabutylammoniumhexafluorophosphate ($TBAPF_6$) supporting electrolyte. Samples were scanned at a rate of 100 mV/s following a dry N_2 purge to deoxygenate the solution. Solution CV measurements were carried out with a sample concentration of ~ 0.5 mg/mL in CH_2Cl_2. Estimations of the energy levels were obtained by correlating the onset (E_{ox} Fc/Fc+, E_{red} Fc/Fc+) to the normal hydrogen electrode (NHE), assuming a HOMO energy level of 4.80 eV for Fc/Fc+.

$E(HOMO) = -(E_{ox}+4.80)$, $E(LUMO) = -(E_{red}+4.80)$

UV-Visible Spectroscopy (UV-vis): All absorption measurements were recorded using an Agilent Technologies Cary 60 UV-vis spectrometer at room temperature. All solution UV-vis experiments were run in chloroform ($CHCl_3$) using 2 mm quartz cuvettes and diluted 1 % wt/v solutions. Thin-films were prepared by spin-coating 1 % wt/v solutions from $CHCl_3$ onto Corning glass micro slides. Prior to use, glass slides were cleaned with soap and water, acetone and isopropanol, and followed by UV/ozone treatment using a Novascan UV/ozone cleaning system.

Photoluminescence (PL): All emission measurements were recorded using an Agilent Technologies Cary Eclipse fluorescence spectrophotometer at room temperature. Thin-films were prepared by spin-coating 1 % wt/v solutions from $CHCl_3$ on Corning glass micro slides. Prior to use, glass slides were cleaned with soap and water, acetone and isopropanol and followed by UV/ozone treatment using a Novascan UV/ozone cleaning system.

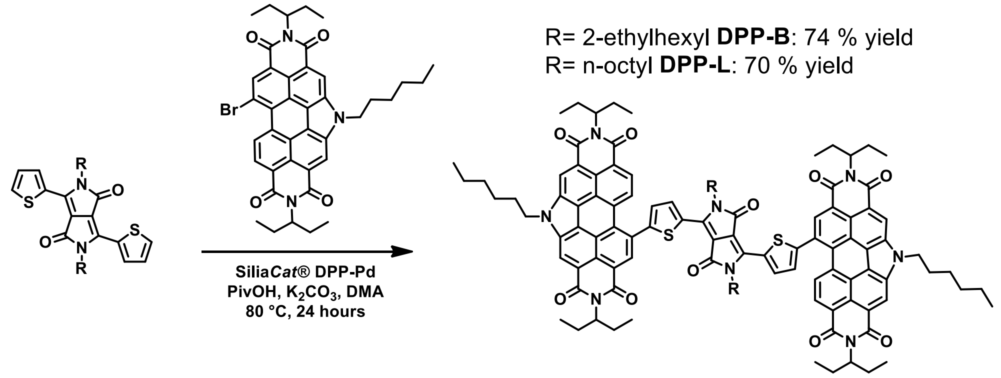
Melting Point Determination (mp): The melting or decomposition points were determined using a Stuart SMP40 apparatus operating from 50 to 400 °C with a ramp rate of 20 °C per minute.

Power Conversion Efficiency (PCE) and External Quantum Efficiency (EQE): The current density-voltage (J-V) curves were measured by a Keithley 2420 source measure unit. The photocurrent was measured under AM 1.5 illumination at 100mW/cm^2 under a Solar Simulator (Newport 92251A-1000). The standard silicon solar cell (Newport 91150V) was used to calibrate light intensity. EQE was measured in a QEX7 Solar Cell Spectral Response/QE/IPCE Measurement System (PV Measurement, Model QEX7, USA) with an optical lens to focus the light into an area about 0.04cm^2, smaller than the dot cell. The silicon photodiode was used to calibration of the EQE measurement system in the wavelength range from 300 to 900 nm.

Atomic Force Microscopy (AFM): AFM measurements were performed by using a Scanning Probe Microscope-Agilent Technologies 5500 in contact mode. We used probe with contact aluminum coated (PEN-0054-00, NanoInk, Inc). Thin film samples for AFM measurement were deposited on ITO/ZnO substrates following the same procedures as used for OPV devices fabrication.

Synthesis

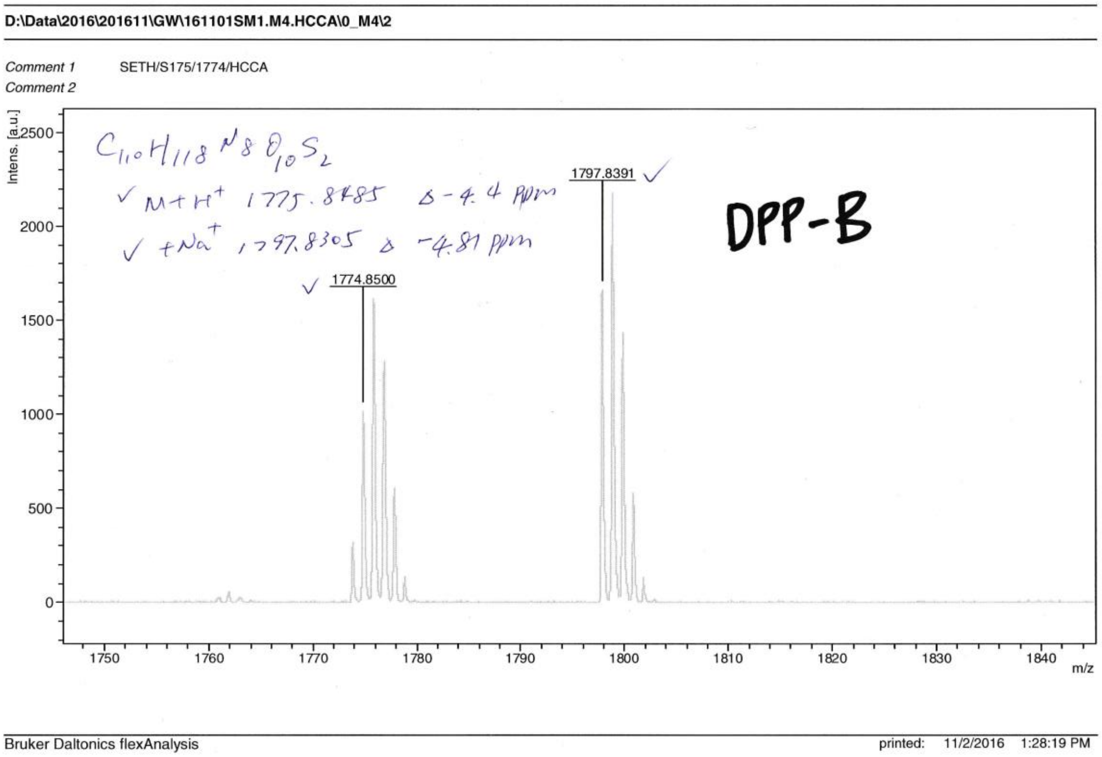
Precursor Synthesis: Isoindigo, diketopyrrolopyrrole and thienoisoindigo precursor materials were synthesized according to literature procedures. N-annulated perylene diimide precursor materials were synthesized according to literature procedure.[1] Complete characterization data for **DPP-L** can be found in its original reported synthesis.[2]



Scheme S1. Direct heteroarylation coupling of **PDI** and **DPP**

Synthesis of DPP-B: In a 12-15 mL pressure vial 2,5-bis(2-ethylhexyl)-3,6-di(thiophen-2-yl)diketopyrrolopyrrole (1 eq.), 11-bromo-5-hexyl-2,8-bis(1-ethylpropyl)perylene diimide (2.2 eq.), Silia*Cat*® DPP-Pd (5 mol %), pivalic acid (30 mol %) and potassium carbonate (2.5 eq.) were added with a stir bar and sealed with a crimp sealed septa cap. The contents were purged with N_2 gas followed by the addition of degassed anhydrous *N,N'*-dimethylacetamide (7 mL) via syringe. The reaction mixture was heated at 80 °C in a LabArmor® beads bath for 24 hours. After 24 hours the reaction mixture was poured into MeOH and allowed to stir overnight. The precipitated product was collected by filtration and the filtrate was discarded. The solid product was subsequently washed with dichloromethane to solubilize the product and isolate it from the insoluble silica-supported catalyst. The filtrate was concentrated by rotary evaporation and prepared for purification by flash column chromatography. With a petroleum ether to dichloromethane gradient residual impurities and a small fraction of mono-substituted product can be removed from 50-90 % dichloromethane. The product begins to elute slowly at 100 % dichloromethane and was more rapidly eluted following the addition of 5 % triethylamine. The product fractions were slurried with a small amount of aluminum oxide and filtered. The filtrate was concentrated by rotary evaporation to a solid which was stirred in acetone overnight to remove residual polar impurities that eluted upon the use of triethylamine. The final product was collected by filtration from acetone as a dark green solid.

DPP-B: 0.24 g, 0.14 mmol, 74 % yield
HRMS (MALDI): DPP-B: m/z: 1774.9 calc'd: 1775.8



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Comment 2

$C_{110}H_{118}N_8O_{10}S_2$

✓ $M+H^+$ 1775.8485 Δ -4.4 ppm

✓ $+Na^+$ 1797.8305 Δ -4.81 ppm

DPP-B

Bruker Daltonics flexAnalysis

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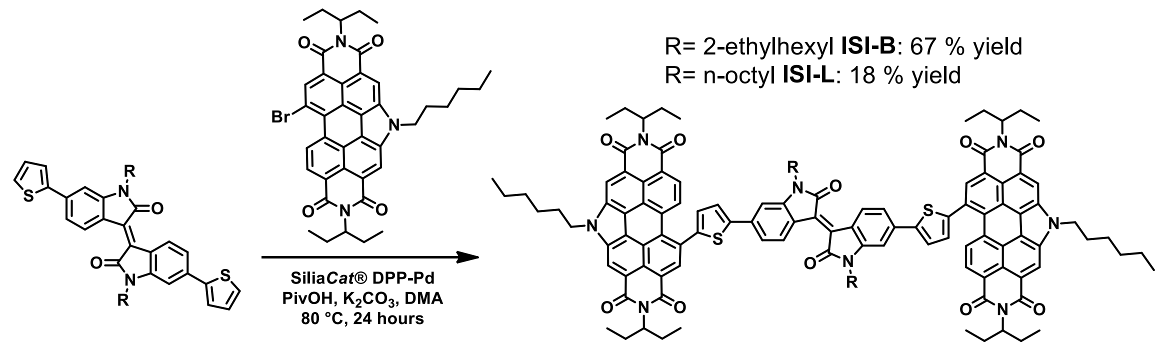
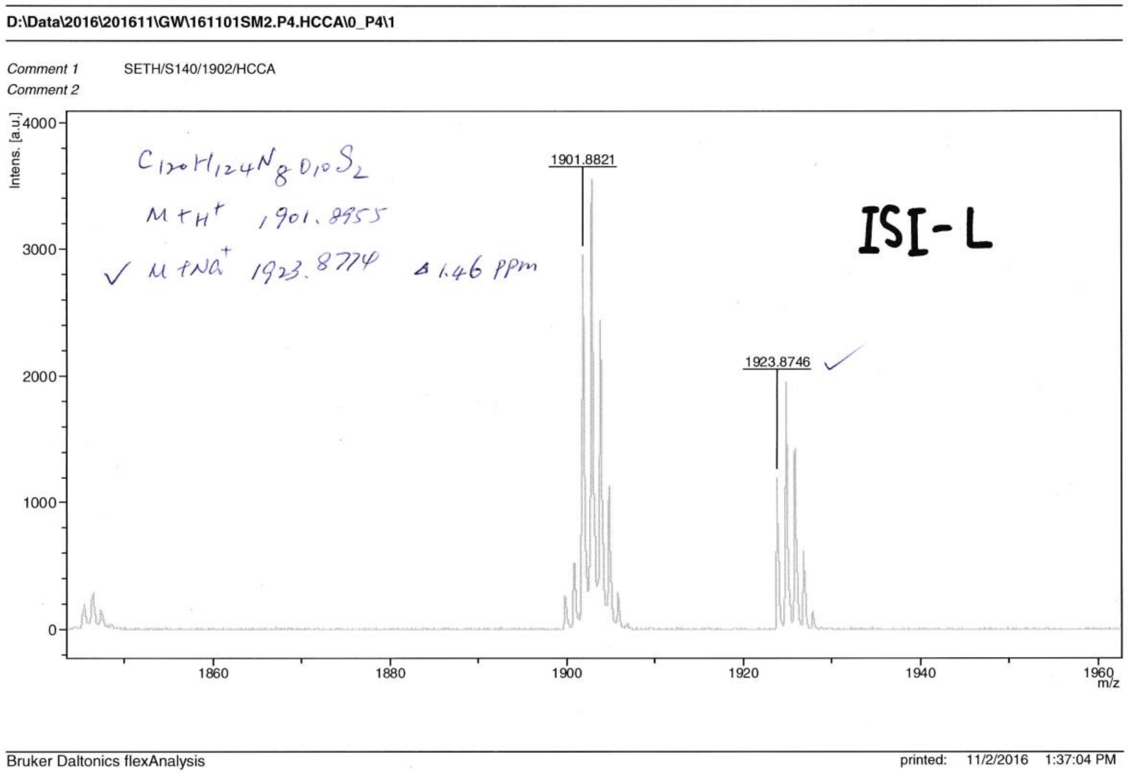


Scheme S2. Direct heteroarylation coupling of **PDI** and **ISI**

Synthesis of ISI-B and ISI-L: In a 12-15 mL pressure vial 2,5-bis(*N*-alkyl)-3,6-di(thiophen-2-yl)isoindigo (1 eq.), 11-bromo-5-hexyl-2,8-bis(1-ethylpropyl)perylene diimide (2.2 eq.), Silia*Cat*® DPP-Pd (5 mol %), pivalic acid (30 mol %) and potassium carbonate (2.5 eq.) were added with a stir bar and sealed with a crimp sealed septa cap. The contents were purged with N_2 gas followed by the addition of degassed anhydrous *N,N'*-dimethylacetamide (7 mL) via syringe. The reaction mixture was heated at 80 °C in a LabArmor® beads bath for 24 hours. After 24 hours the reaction mixture was poured into MeOH and allowed to stir overnight. The precipitated product was collected by filtration and the filtrate was discarded. The solid product was subsequently washed with dichloromethane to solubilize the product and isolate it from the insoluble silica-supported catalyst. The filtrate was concentrated by rotary evaporation and prepared for purification by flash column chromatography. With a petroleum ether to dichloromethane gradient residual impurities and a small fraction of mono-substituted product can be removed from 50-90 % dichloromethane. The product begins to elute slowly at 100 % dichloromethane and was more rapidly eluted following the addition of 5 % triethylamine. The product fractions were slurried with a small amount of aluminum oxide and filtered. The filtrate was concentrated by rotary evaporation to a solid which was stirred in acetone overnight to remove residual polar impurities that eluted upon the use of triethylamine. The final product was collected by filtration from acetone as a dark green solid.

ISI-B: 0.38 g, 0.20 mmol, 67 % yield
ISI-L: 0.08 g, 0.04 mmol, 18 % yield
HRMS (MALDI): ISI-B: m/z: 1901.9 calc'd: 1901.9 **ISI-L**: m/z: 1901.9 calc'd: 1901.9



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Comment 2

$C_{120}H_{124}N_8O_{10}S_2$

$M+H^+$ 1901.8955

✓ $M+Na^+$ 1923.8774 Δ 1.46 ppm

ISI-L

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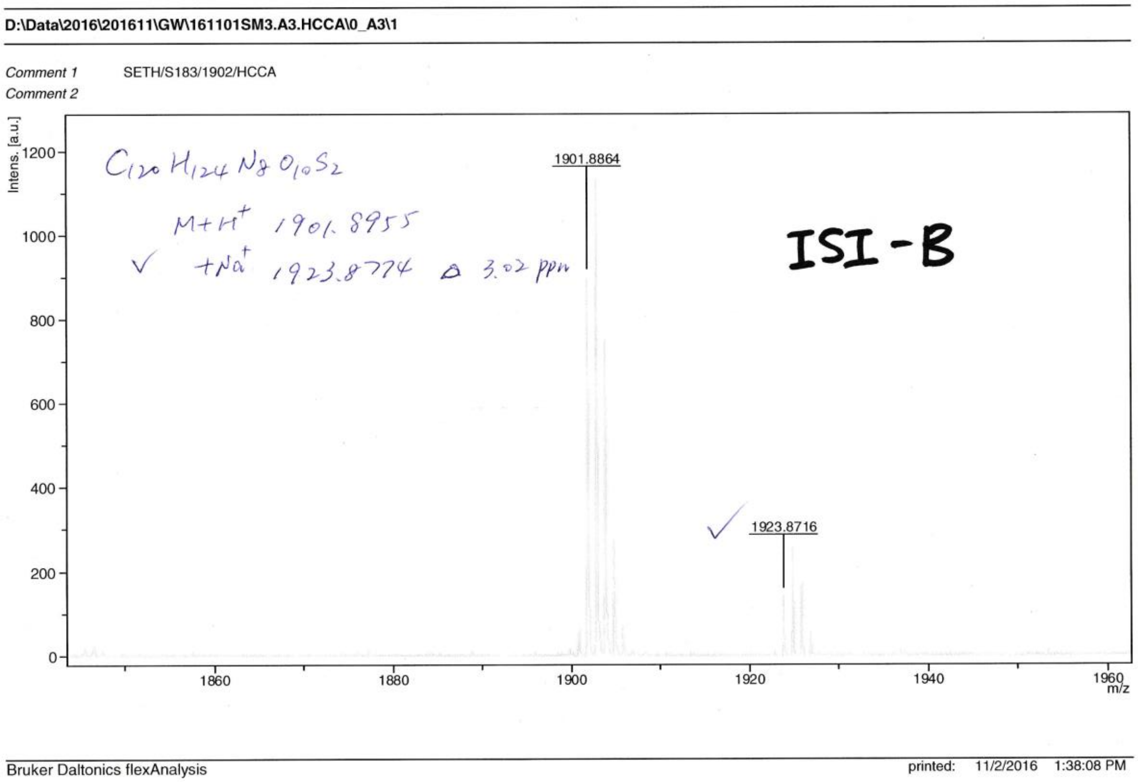

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Comment 2

$C_{120}H_{124}N_8O_{10}S_2$

$M+H^+$ 1901.8955

✓ $+Na^+$ 1923.8774 Δ 3.02 ppm

ISI-B

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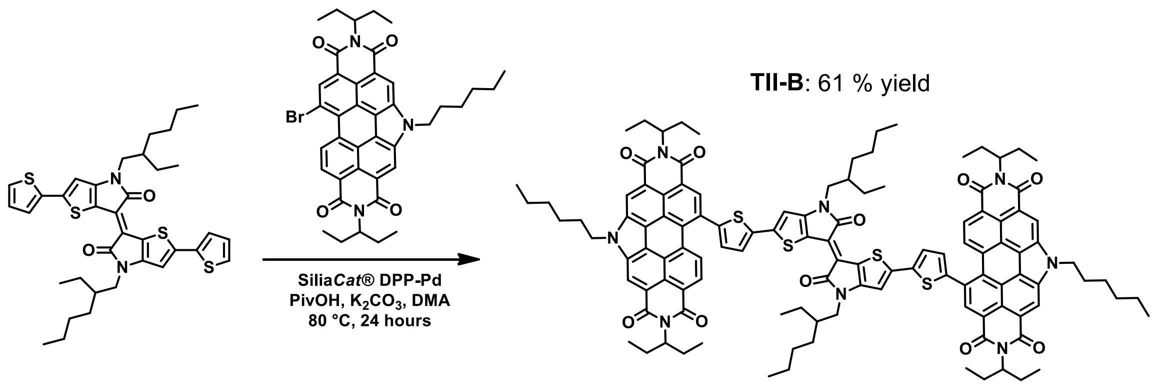

Scheme S3. Direct heteroarylation coupling of **PDI** and **TII**

Synthesis of TII-B: In a 12-15 mL pressure vial 2,5-bis(2-ethylhexyl)-3,6-di(thiophen-2-yl)thienoisoindigo (1 eq.), 11-bromo-5-hexyl-2,8-bis(1-ethylpropyl)perylene diimide (2.2 eq.), Silia*Cat*® DPP-Pd (5 mol %), pivalic acid (30 mol %) and potassium carbonate (2.5 eq.) were added with a stir bar and sealed with a crimp sealed septa cap. The contents were purged with N_2 gas followed by the addition of degassed anhydrous *N,N'*-dimethylacetamide (7 mL) via syringe. The reaction mixture was heated at 80 °C in a LabArmor® beads bath for 24 hours. After 24 hours the reaction mixture was poured into MeOH and allowed to stir overnight. The precipitated product was collected by filtration and the filtrate was discarded. The solid product was subsequently washed with dichloromethane to solubilize the product and isolate it from the insoluble silica-supported catalyst. The filtrate was concentrated by rotary evaporation and prepared for purification by flash column chromatography. With a petroleum ether to dichloromethane gradient residual impurities and a small fraction of mono-substituted product can be removed from 50-90 % dichloromethane. The product begins to elute slowly at 100 % dichloromethane and was more rapidly eluted following the addition of 5 % triethylamine. The product fractions were slurried with a small amount of aluminum oxide and filtered. The filtrate was concentrated by rotary evaporation to a solid which was stirred in acetone overnight to remove residual polar impurities that eluted upon the use of triethylamine. The final product was collected by filtration from acetone as a dark green solid.

TII-B: 0.44 g, 0.23 mmol, 61 % yield
HRMS (MALDI): TII-B: m/z: 1912.8 calc'd: 1913.8

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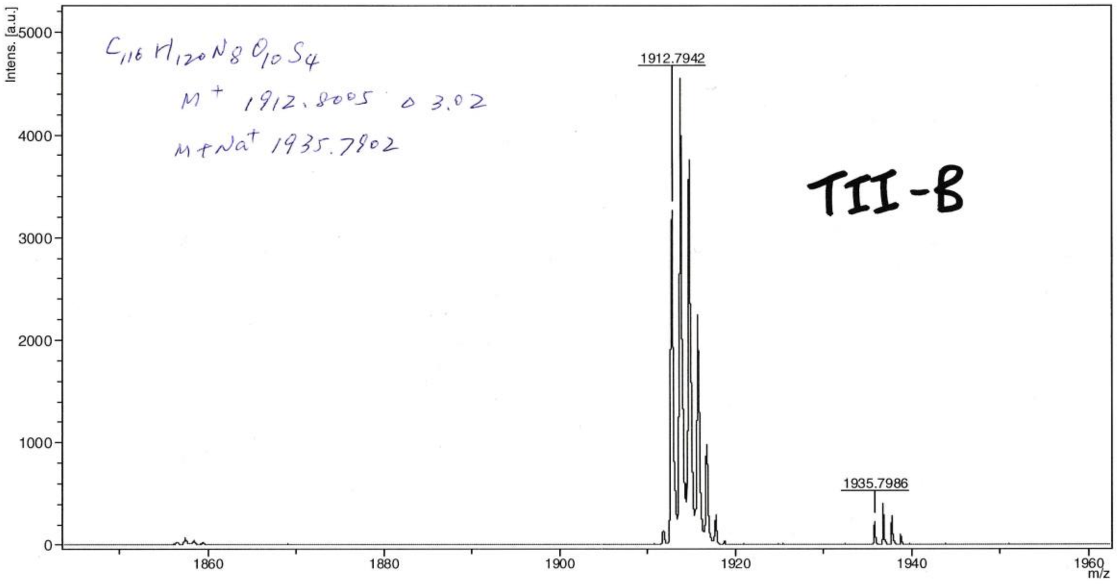
Comment 2



$C_{116}H_{120}N_8O_{10}S_4$

M^+ 1912.8005 Δ 3.02

$M+Na^+$ 1935.7902

TII-B

Bruker Daltonics flexAnalysis

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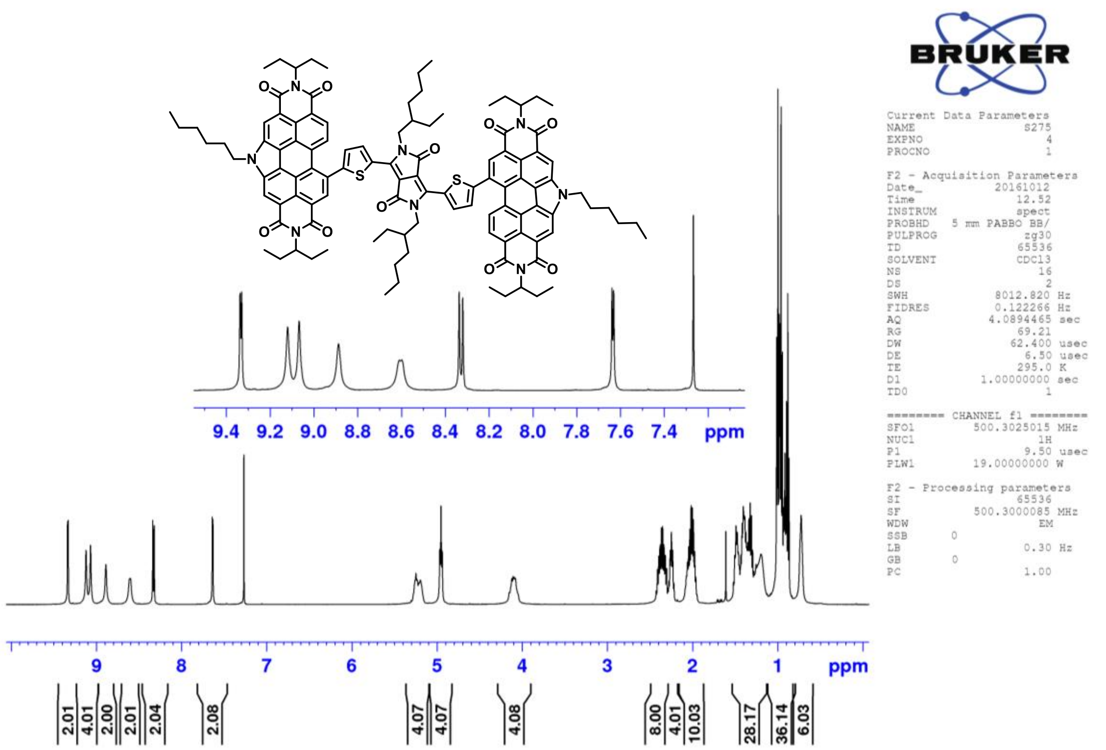
Solution ^{1}H and ^{13}C NMR spectra



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PLW1          19.00000000 W

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Figure S1. ^{1}H NMR spectra of **DPP-B**

^{1}H NMR: 9.33 (d, $J_{H\text{-}H}$= 4 Hz, 2H); 9.12 (s, 2H); 9.07 (s, 2H); 8.89 (s, 2H); 8.60 (s, 2H); 8.33 (d, $J_{H\text{-}H}$= 8 Hz, 2H); 7.63 (d, $J_{H\text{-}H}$= 4 Hz, 2H); 5.25-5.19 (m, 4H); 4.9 (t, 4H); 4.11 (t, 4H); 2.36 (m, 8H); 2.25 (m, 4H); 2.01 (m, 10H); 1.49-1.19 (m, 28H); 1.00-0.88 (m, 36H); 0.72 (t, 6H).

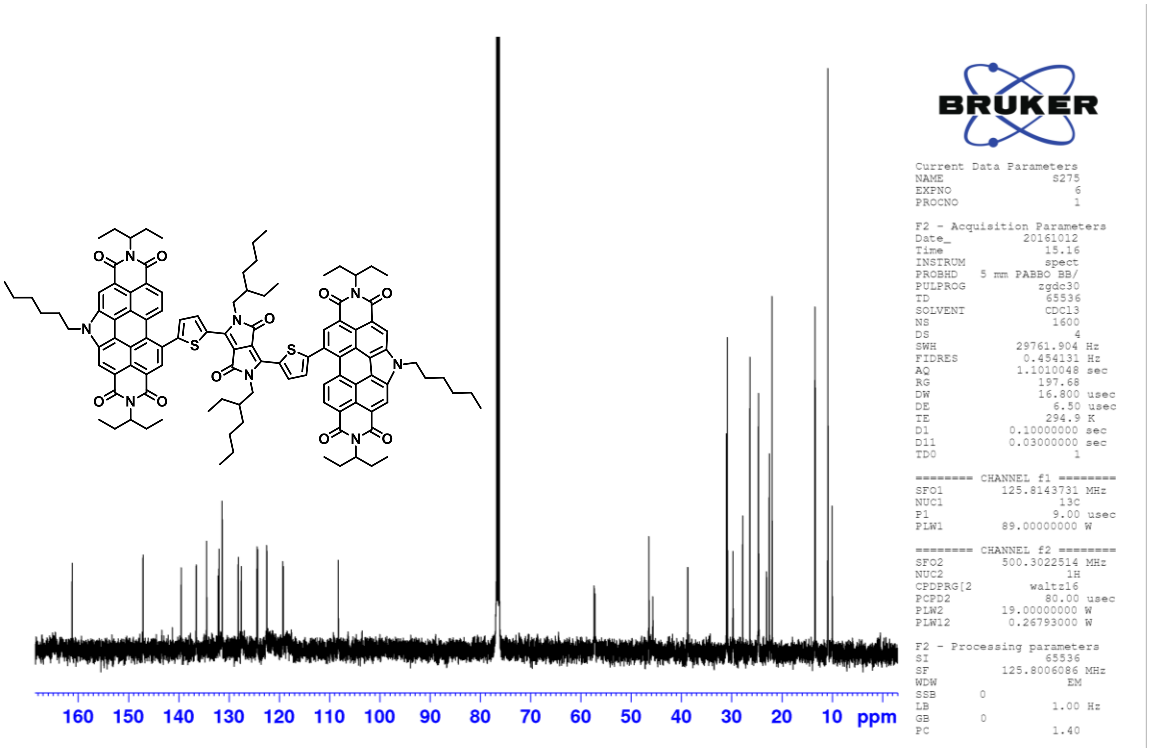

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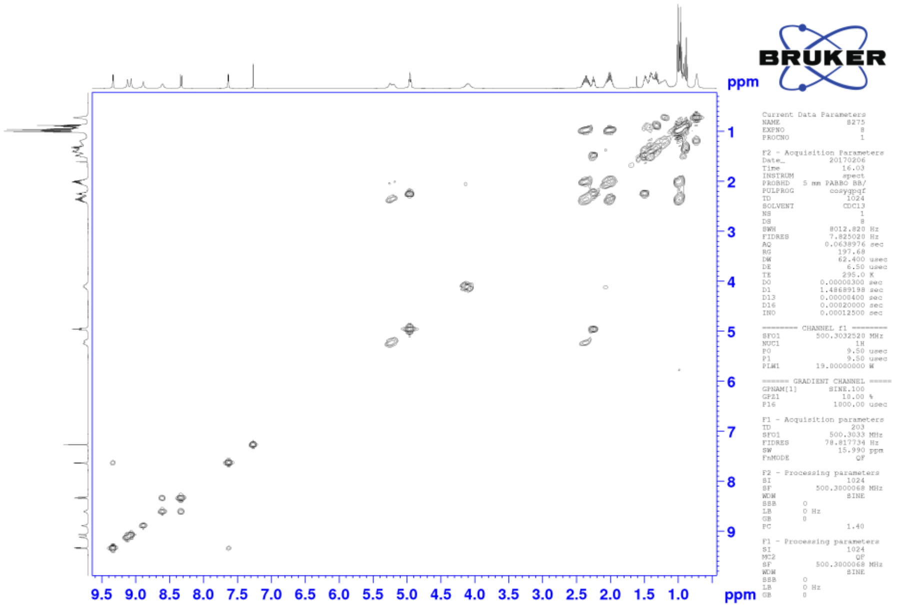
Figure S2. ^{13}C NMR spectra of **DPP-B**

^{13}C NMR: 161.2; 147.1; 139.5; 136.5; 134.5; 132.1; 132.0; 131.3; 128.1; 127.5; 124.4; 124.3; 122.5; 122.4; 119.3; 119.2; 108.2; 57.3; 57.2; 46.4; 45.7; 38.7; 31.0; 30.8; 29.8; 27.7; 26.3; 24.6; 23.0; 22.5; 21.9; 13.4; 13.3; 10.9; 10.8; 10.0; 9.9. Expected: 56 Found: 37.



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F1 - Processing parameters
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Figure S3. ^{1}H-^{1}H COSY NMR spectra of **DPP-B**

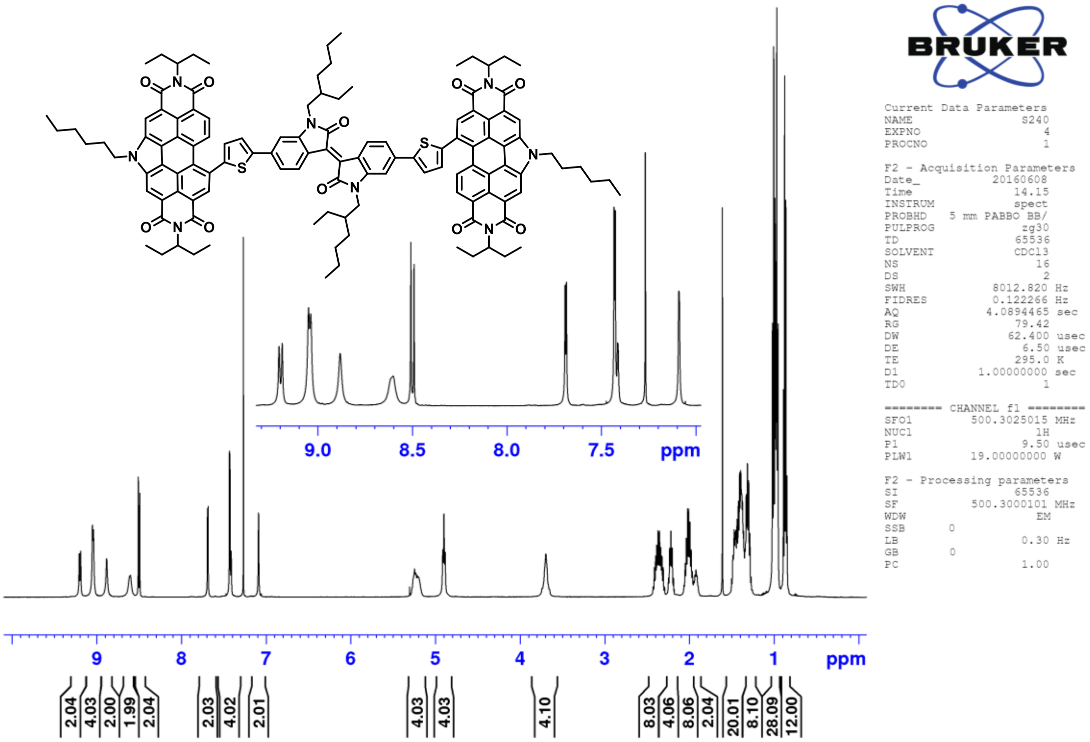

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Figure S4. ^{1}H NMR spectra of **ISI-B**

^{1}H NMR: 9.20 (d, $J_{H\text{-}H}$= 8 Hz, 2H); 9.05 (s, ov, 2H); 9.04 (s, ov, 2H); 8.60 (s, br, 2H); 8.50 (d, $J_{H\text{-}H}$= 8 Hz, 2H); 7.69 (d, $J_{H\text{-}H}$= 4 Hz, 2H); 7.43 (d, ov, $J_{H\text{-}H}$= 4 Hz, 2H); 7.42 (d, ov, $J_{H\text{-}H}$= 8 Hz, 2H); 7.09 (s, 2H); 5.24-5.22 (m, 4H); 4.90 (t, 4H); 3.70 (m, 4H); 2.36 (m, 8H); 2.22 (m, 4H); 2.01 (m, 8H); 1.92 (m, 2H); 1.40 (m, 20H); 1.32 (m, 8H); 1.01 (t, ov, 12H); 0.97 (m, ov, 4H); 0.96 (t, ov, 12H) 0.88 (t, ov, 6H) 0.86 (t, ov, 6H).

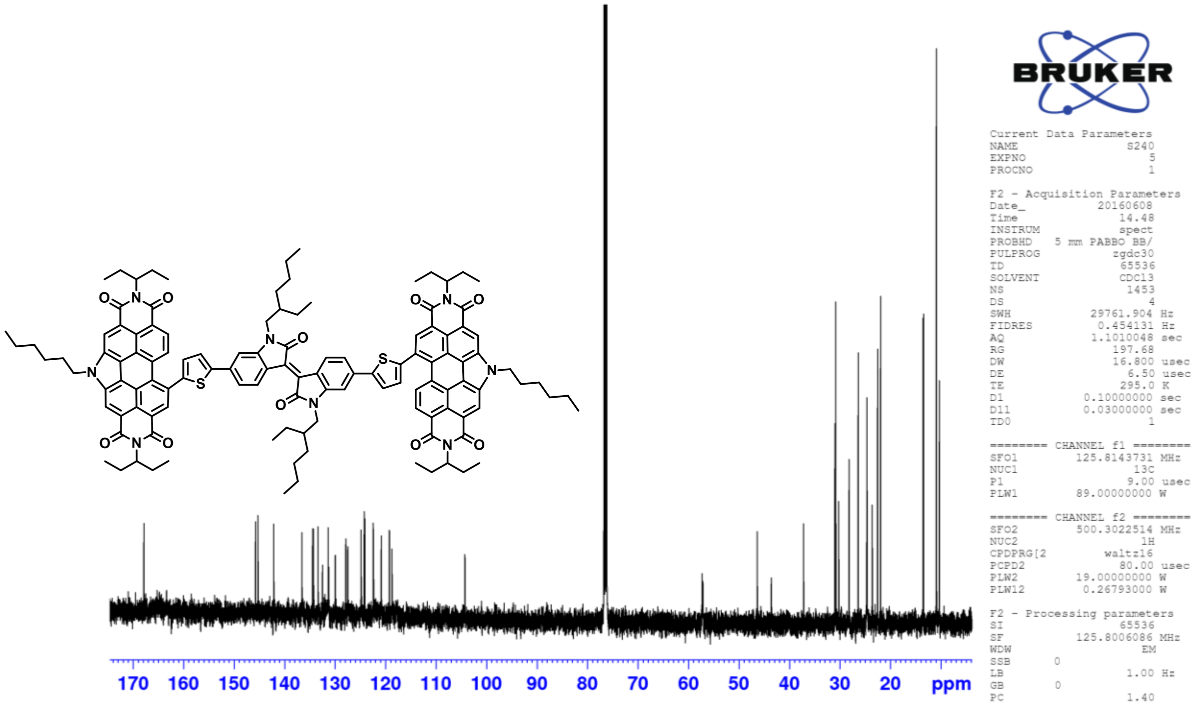

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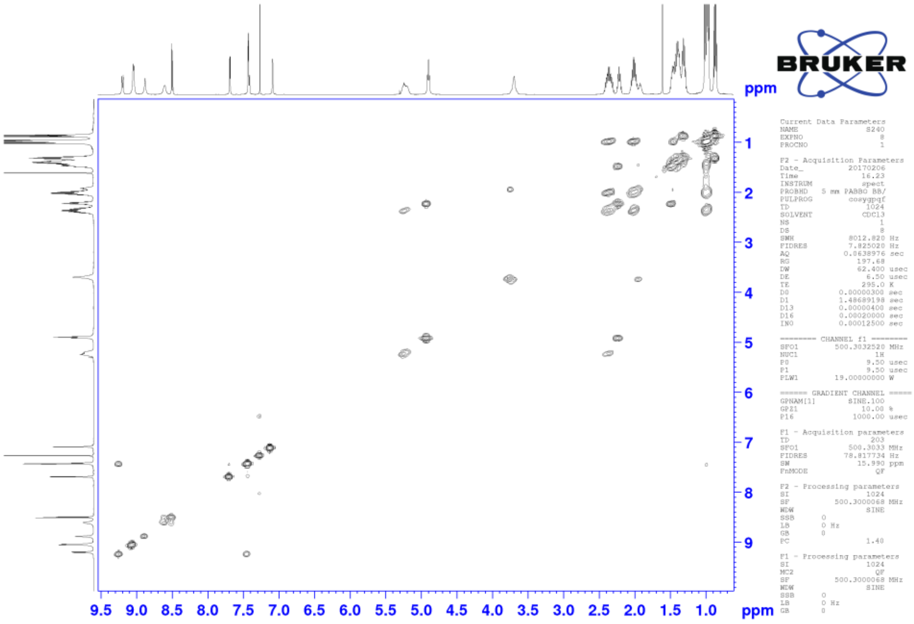
Figure S5. ^{13}C NMR spectra of **ISI-B**

^{13}C NMR: 167.8; 145.7; 145.2; 142.2; 136.6; 134.4; 134.3; 133.4; 132.5; 131.3; 131.2; 130.0; 127.9; 127.5; 124.8; 124.2; 124.1; 122.5; 122.4; 120.8; 119.3; 119.2; 118.7; 104.3; 57.3; 57.1; 46.4; 43.6; 37.2; 31.0; 30.8; 30.2; 28.2; 26.3; 24.6; 23.6; 22.5; 22.0; 13.5; 13.4; 11.0; 10.9; 10.3. Expected: 60 Found: 43.



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FnMODE                QF

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LB       0 Hz
GB       0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           500.3000068 MHz
WDW                 SINE
SSB      0
LB       0 Hz
GB       0
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Figure S6. ^{1}H-^{1}H COSY NMR spectra of **ISI-B**

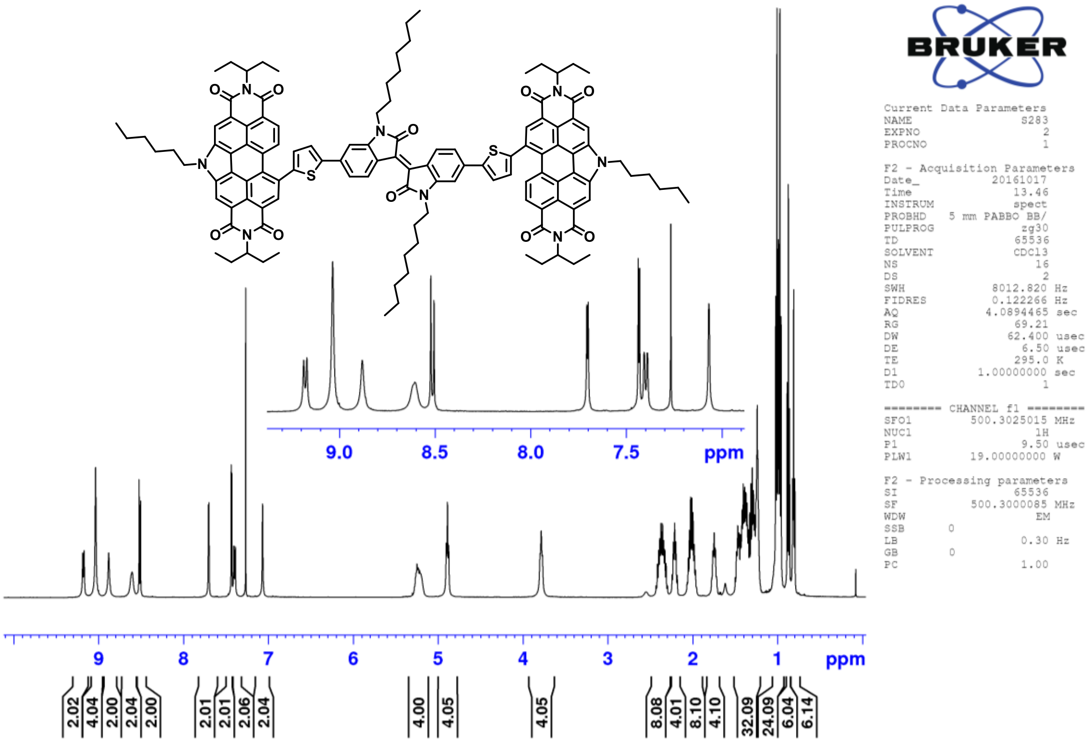


Figure S7. ^{1}H NMR spectra of **ISI-L**

^{1}H NMR: 9.18 (d, $J_{H\text{-}H}$= 8 Hz, 2H); 9.03 (s, ov, 4H); 8.88 (s, br, 2H); 8.61 (s, br, 2H) 8.51 (d, $J_{H\text{-}H}$= 8 Hz, 2H); 7.70 (d, $J_{H\text{-}H}$= 4 Hz, 2H); 7.43 (d, $J_{H\text{-}H}$= 4 Hz, 2H); 7.40 (d, $J_{H\text{-}H}$= 8 Hz, 2H); 7.07 (s, 2H); 5.25-5.22 (m, 4H); 4.90 (t, 4H); 3.78 (t, 4H); 2.36 (m, 8H); 2.21 (m, 4H); 2.01 (m, 8H); 1.74 (m, 4H); 1.47-1.24 (m, 32H); 1.01-0.97 (t, ov, 24H); 0.87 (t, 6H); 0.81 (t, 6H).

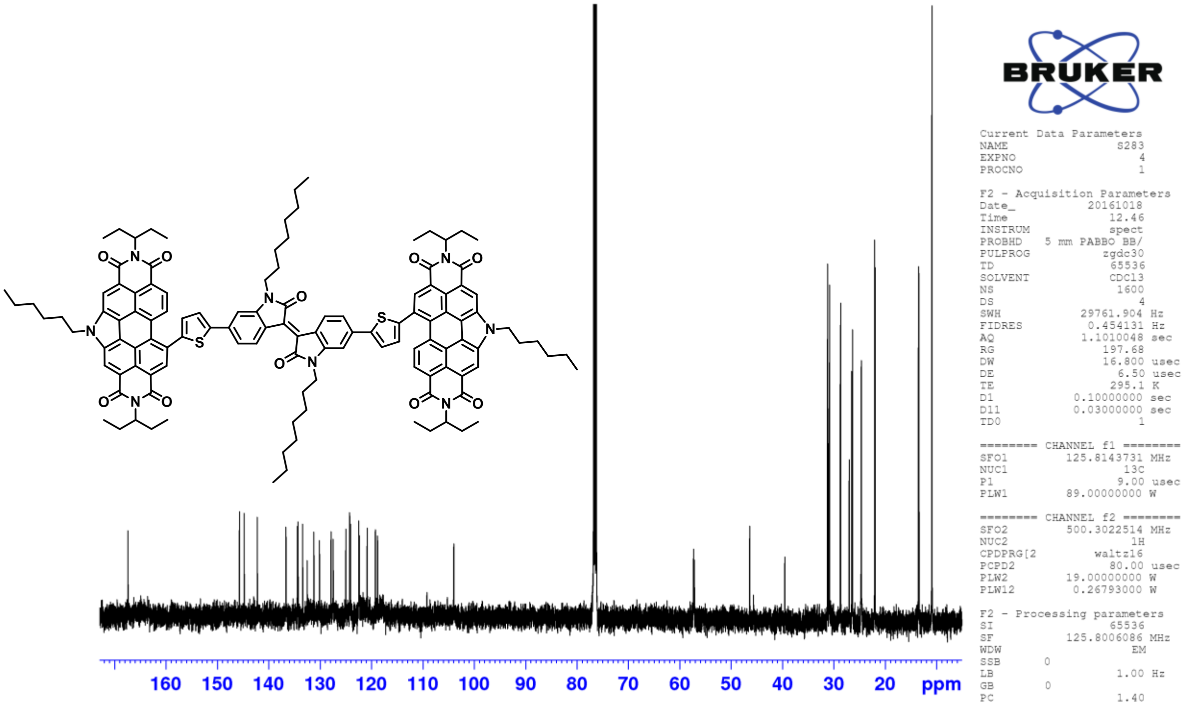


Figure S8. ^{13}C NMR spectra of **ISI-L**

^{13}C NMR: 167.4; 145.7; 144.7; 142.2; 136.6; 134.4; 134.3; 133.4; 132.5; 131.2; 131.1; 130.1; 127.8; 127.5; 124.9; 124.2; 124.1; 122.4; 122.3; 120.8; 119.3; 119.2; 118.8; 103.9; 57.3; 57.1; 46.4; 39.5; 31.2; 31.0; 30.8; 28.7; 28.6; 27.0; 26.5; 26.3; 24.6; 22.0; 21.9; 13.5; 13.4; 10.9; 10.8. Expected: 60 Found: 42.

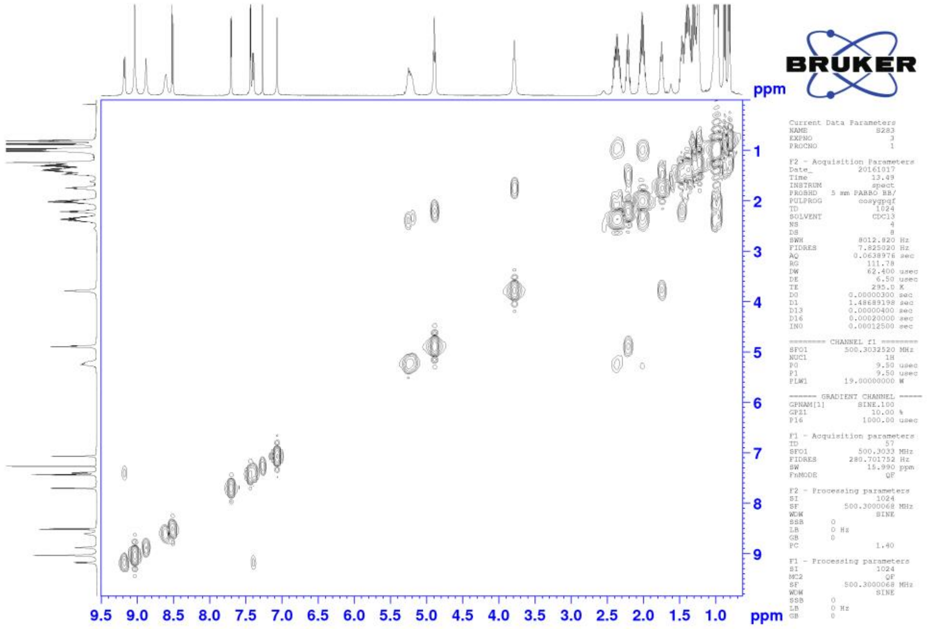
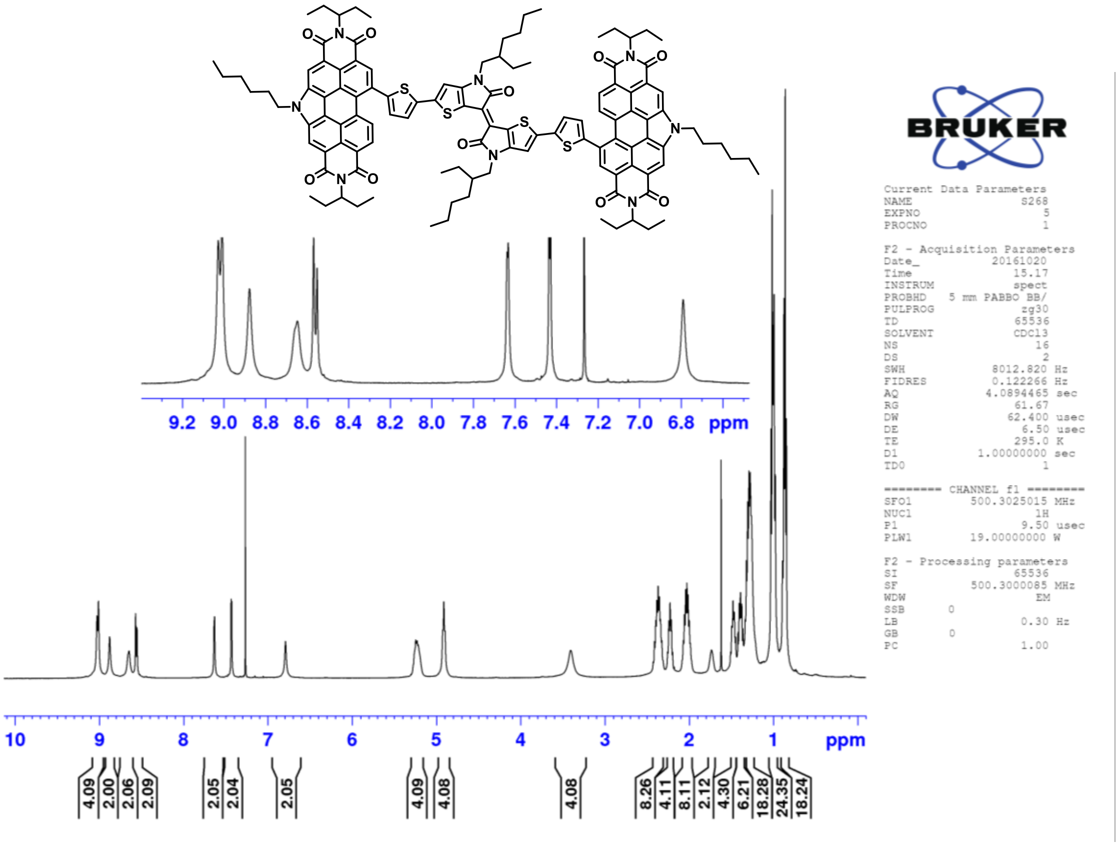


Figure S9. ^{1}H-^{1}H COSY NMR spectra of **ISI-L**



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TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
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FIDRES           0.122266 Hz
AQ              4.0894465 sec
RG                  61.67
DW                 62.400 usec
DE                   6.50 usec
TE                  295.0 K
D1             1.00000000 sec
TD0                     1

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NUC1                   1H
P1                   9.50 usec
PLW1          19.00000000 W

F2 - Processing parameters
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SF            500.3000085 MHz
WDW                    EM
SSB      0
LB                   0.30 Hz
GB       0
PC                   1.00
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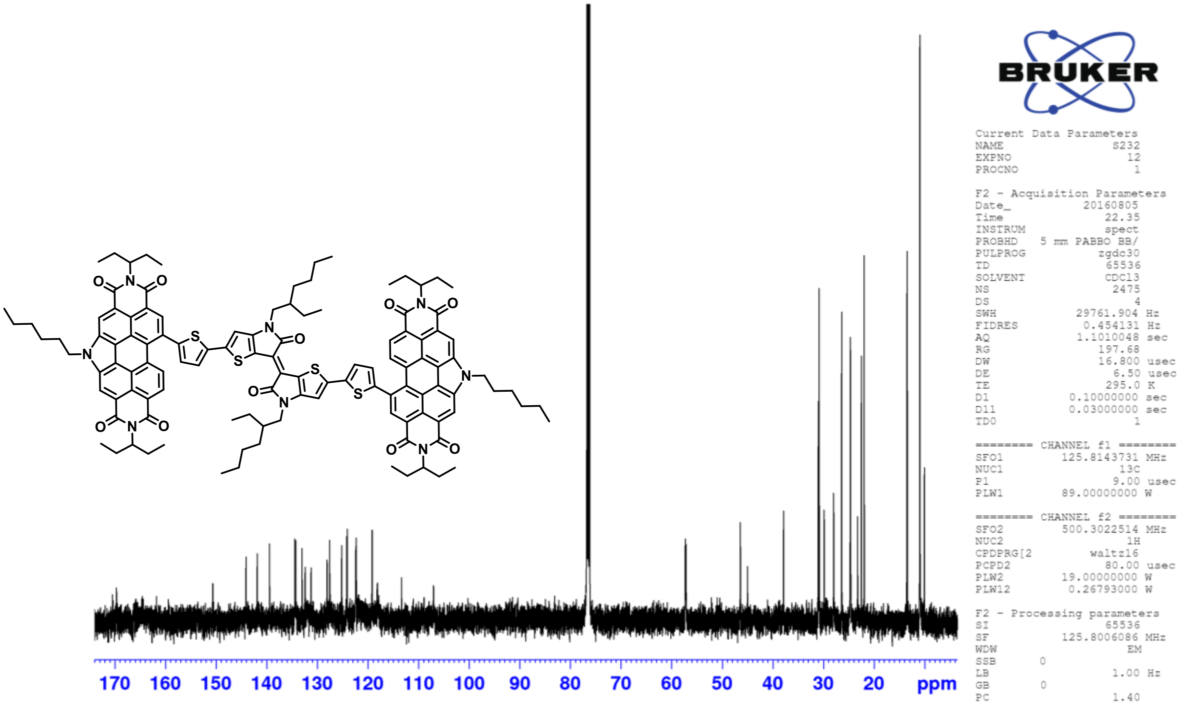
Figure S10. ^{1}H NMR spectra of **TII-B**

^{1}H NMR: 9.02 (s, 2H); 9.01 (s, 2H); 8.88 (s, ov, 2H); 8.65 (s, br, 2H); 8.55 (d, $J_{\text{H-H}}$= 8 Hz, 2H); 7.63 (d, $J_{\text{H-H}}$= 3 Hz, 2H); 7.43 (d, ov, $J_{\text{H-H}}$= 3 Hz, 2H); 6.79 (s, 2H); 5.25-5.23 (m, 4H); 4.91 (t, 4H); 3.41 (s, br, 4H); 2.37 (m, 8H); 2.23 (m, 4H); 2.03 (m, 8H); 1.73 (m, 2H); 1.46 (m, 4H); 1.39 (m, 6H); 1.28 (m, 18H); 1.01 (t, ov, 24H); 0.86 (t, ov, 18H).



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DS                     4
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FIDRES          0.454131 Hz
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D1            0.10000000 sec
D11           0.03000000 sec
TD0                    1

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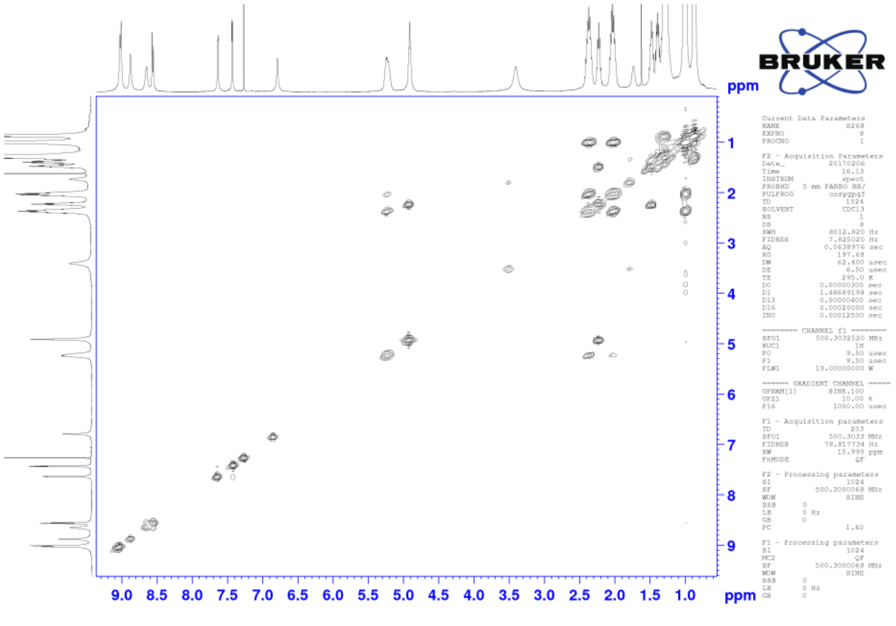
NUC1                 13C
P1                  9.00 usec
PLW1         89.00000000 W

======== CHANNEL f2 ========
SFO2         500.3022514 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         19.00000000 W
PLW12         0.26793000 W

F2 - Processing parameters
SI                 65536
SF           125.8006086 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```

Figure S11. ^{13}C NMR spectra of **TII-B**

^{13}C NMR: 150.6; 144.0; 141.8; 139.4; 134.4; 134.3; 133.0; 132.4; 131.2; 128.1; 127.6; 125.1; 124.2; 124.1; 122.4; 122.3; 119.1; 118.0; 113.3; 106.7; 57.3; 57.1; 46.4; 44.9; 37.8; 31.0; 30.8; 29.8; 27.9; 26.4; 24.5; 23.2; 22.5; 21.9; 13.5; 13.4; 10.9; 10.0. Expected:58 Found: 38.



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PROCNO                 1

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PULPROG         cosygpqf
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NS                     1
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FIDRES          7.825020 Hz
AQ             0.0638976 sec
RG                197.68
DW                62.400 usec
DE                  6.50 usec
TE                 295.0 K
D0            0.00000300 sec
D1            1.48689198 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012500 sec

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NUC1                  1H
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P1                  9.50 usec
PLW1         19.00000000 W

====== GRADIENT CHANNEL =====
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GPZ1               10.00 %
P16              1000.00 usec

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FIDRES         78.817734 Hz
SW                15.990 ppm
FnMODE                QF

F2 - Processing parameters
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SF           500.3000068 MHz
WDW                 SINE
SSB      0
LB       0 Hz
GB       0
PC                  1.40

F1 - Processing parameters
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MC2                   QF
SF           500.3000068 MHz
WDW                 SINE
SSB      0
LB       0 Hz
GB       0
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Figure S12. ^{1}H-^{1}H COSY NMR spectra of **TII-B**

Cyclic voltammograms

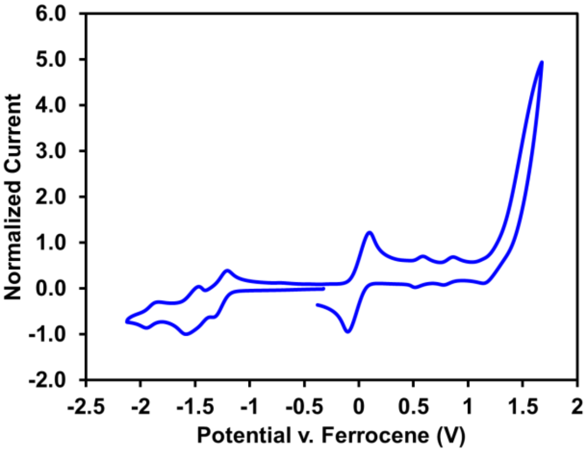

Figure S13. Cyclic voltammogram of **DPP-B** with ferrocene reference.

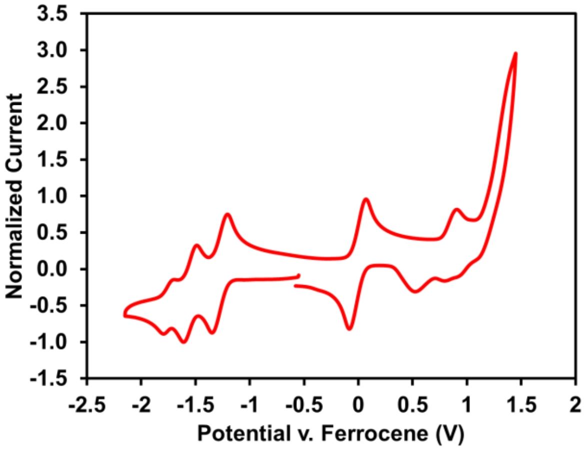

Figure S14. Cyclic voltammogram of **ISI-B** with ferrocene reference.

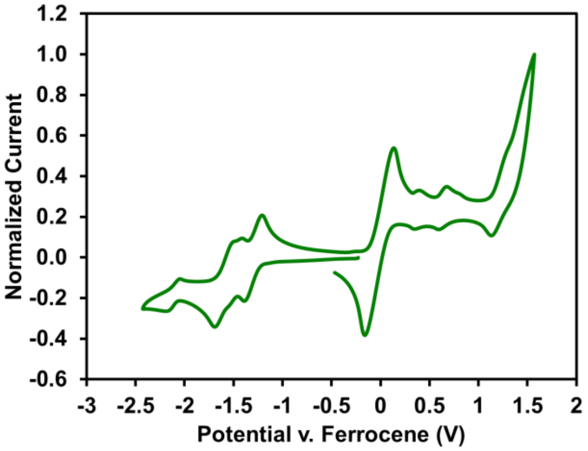

Figure S15. Cyclic voltammogram of **TII-B** with ferrocene reference.

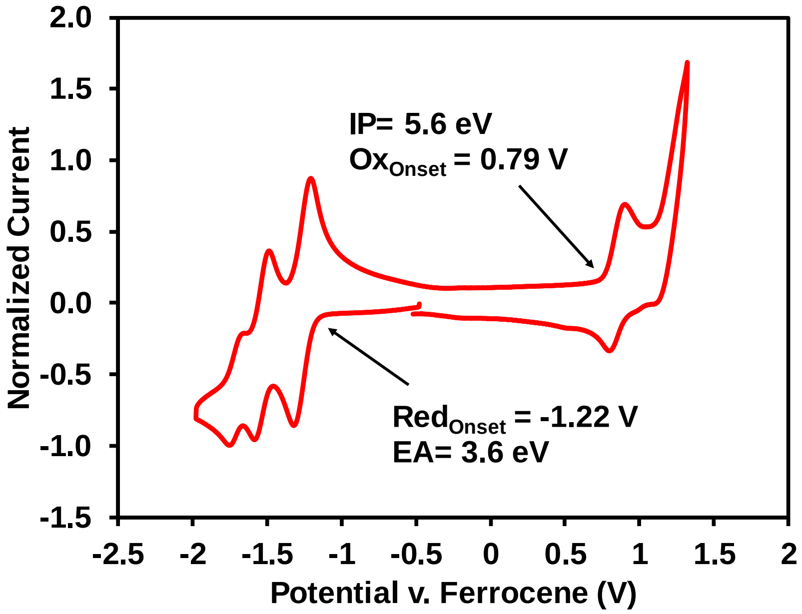

Figure S16. Cyclic voltammogram of **ISI-L**.

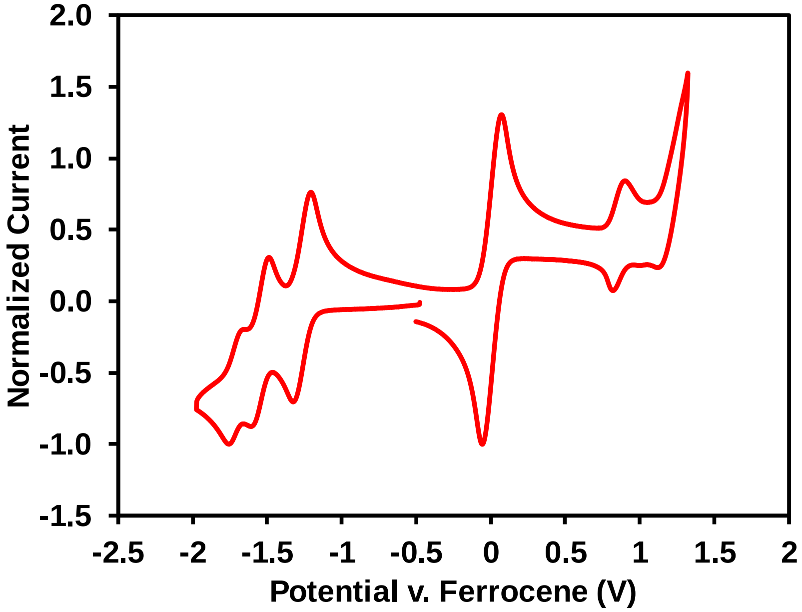

Figure S17. Cyclic voltammogram of **ISI-L** with ferrocene reference.

TD-DFT Calculations

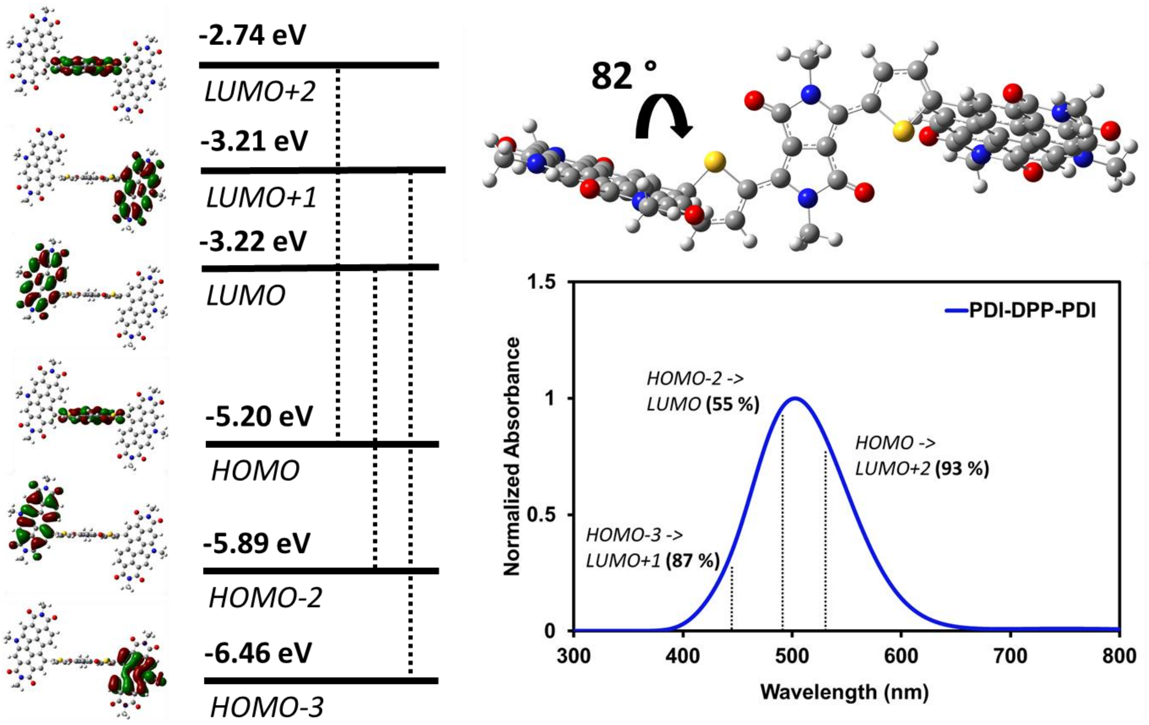

Figure S18. TD-DFT calculations of **DPP-B**, including optimized geometry, predicted orbital transitions and predicted energy levels with π-orbital distributions.

Table S1. Predicted electronic transitions of **DPP-B**.

State	E_{opt} (eV)	λ (nm)	f	Composition
S_3	2.33	533	0.7684	H →L+2 (93 %)
S_7	2.54	489	0.9987	H-2 →L (55 %)
S_{10}	2.82	440	0.1014	H-3 →L+1 (87 %)

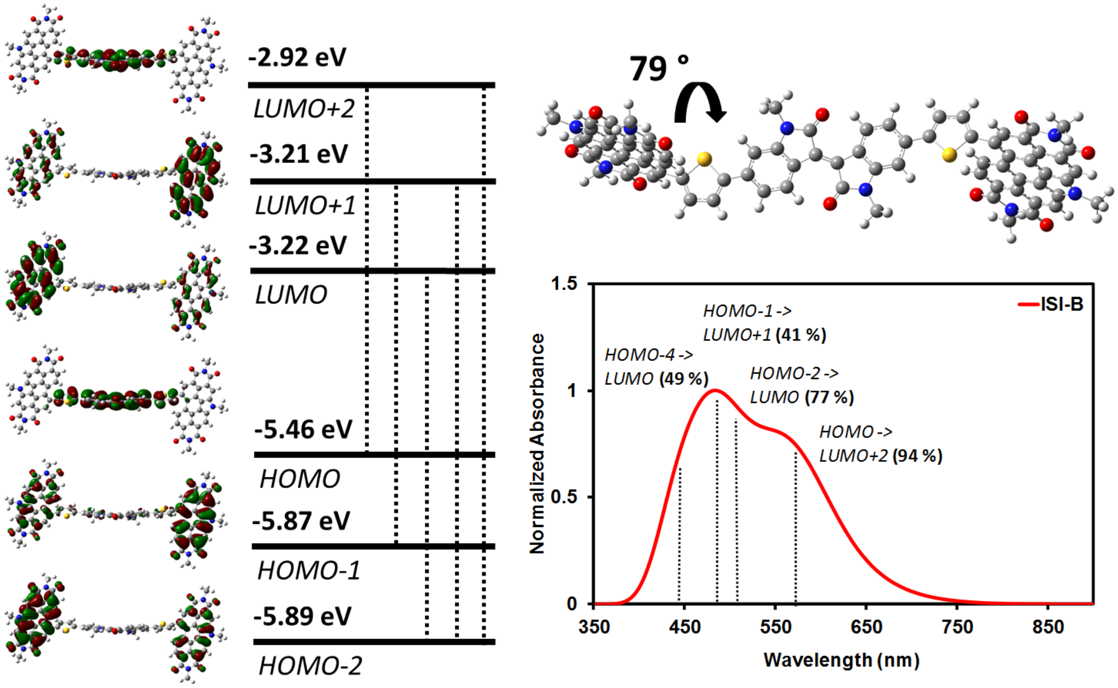

Figure S19. TD-DFT calculations of **ISI-B**, including optimized geometry, predicted orbital transitions and predicted energy levels with π-orbital distributions.

Table S2. Predicted electronic transitions of **ISI-B**.

State	E_{opt} (eV)	λ (nm)	f	Composition
S_3	2.19	567	0.8798	H → L+2 (95 %)
S_5	2.48	499	0.1846	H-1 → L+1 (41 %)
S_7	2.52	492	0.5930	H-2 → L (77 %)
S_8	2.53	491	0.1319	H-2 → L+1 (48 %)
S_{11}	2.71	457	0.1014	H-2 → L+2 (58 %)
S_{13}	2.73	454	0.2249	H-4 → L (49 %)
S_{15}	2.82	440	0.3680	H-6 → L (33 %)

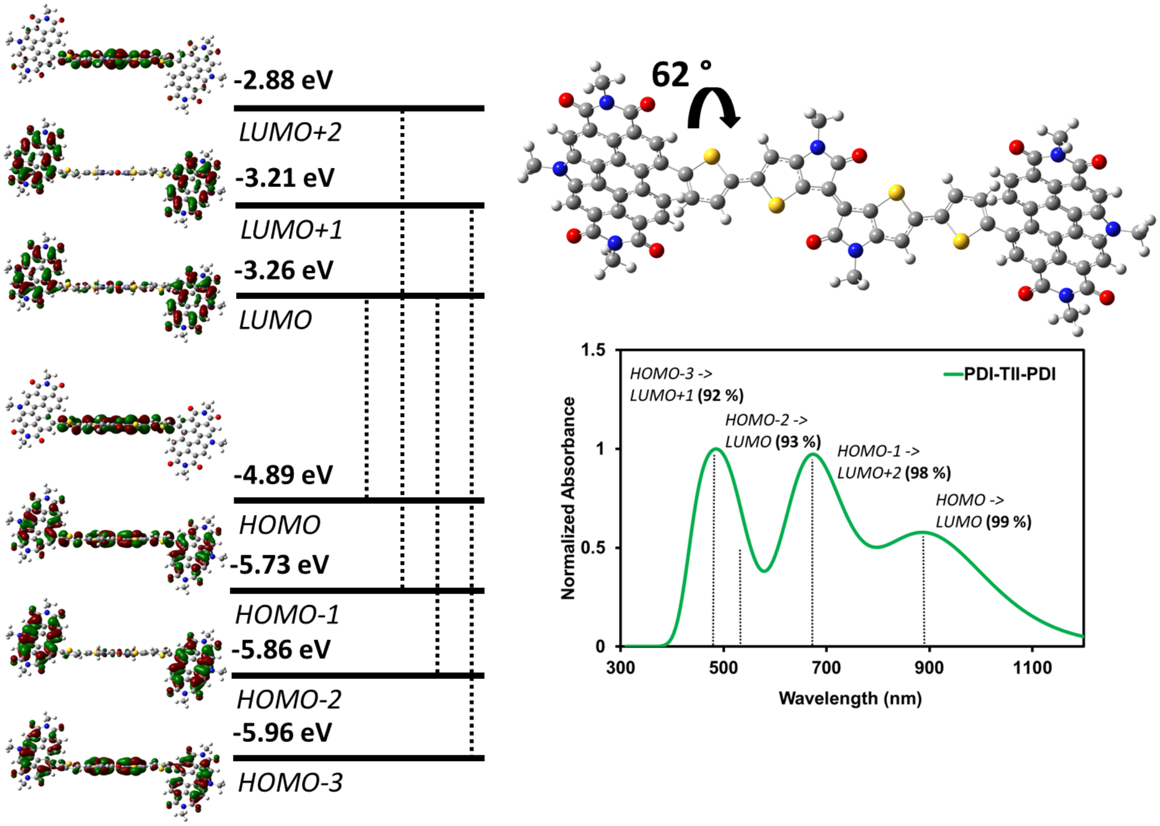

Figure S20. TD-DFT calculations of **TII-B**, including optimized geometry, predicted orbital transitions and predicted energy levels with π-orbital distributions.

Table S3. Predicted electronic transitions of **TII-B**.

State	E_{opt} (eV)	λ (nm)	f	Composition
S_1	1.38	896	0.5373	H →L (99 %)
S_3	1.84	673	0.9212	H-1 →L+2 (98 %)
S_5	2.30	538	0.1839	H-1 →L+1 (91 %)
S_7	2.43	510	0.4705	H-2 →L (93 %)
S_{10}	2.57	482	0.2750	H-3 →L+1 (92 %)
S_{11}	2.72	457	0.1088	H-2 →L+2 (92 %)
S_{13}	2.76	452	0.4384	H-4 →L (61 %)

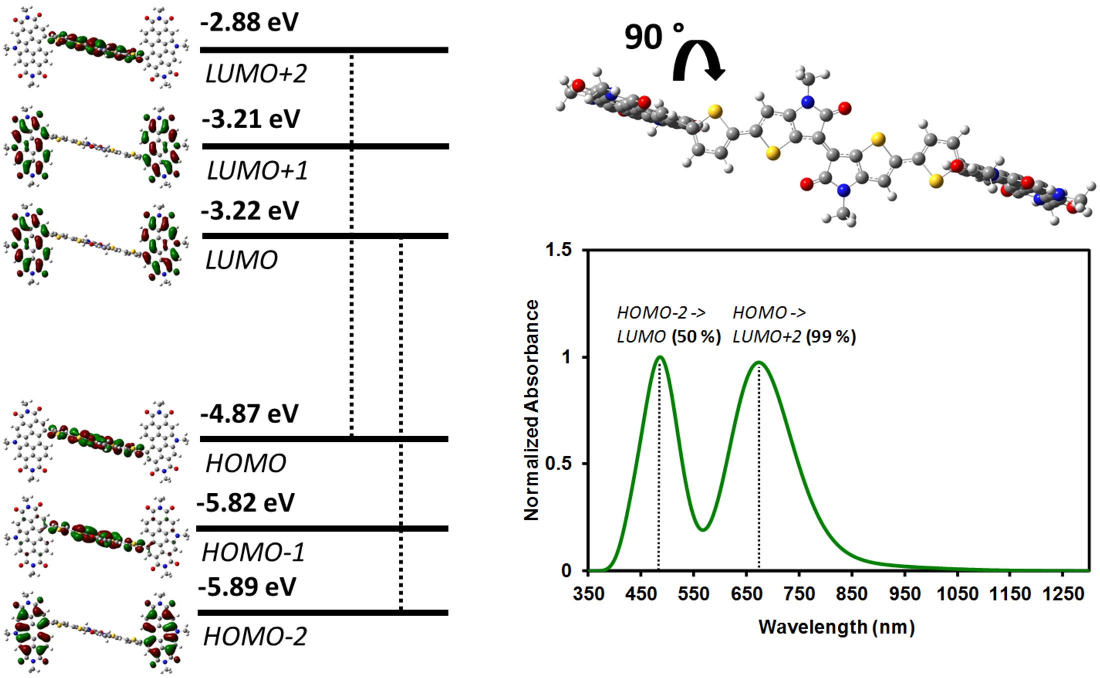

Figure S21. TD-DFT calculations of **TII-B** at 90°, including optimized geometry, predicted orbital transitions and predicted energy levels with π-orbital distributions.

Table S4. Predicted electronic transitions of **TII-B** at 90 ° dihedral angles.

State	E_{opt} (eV)	λ (nm)	f	Composition
S_3	1.84	673	1.1448	H→L+2 (99 %)
S_8	2.53	491	1.0649	H-2 →L (58 %)

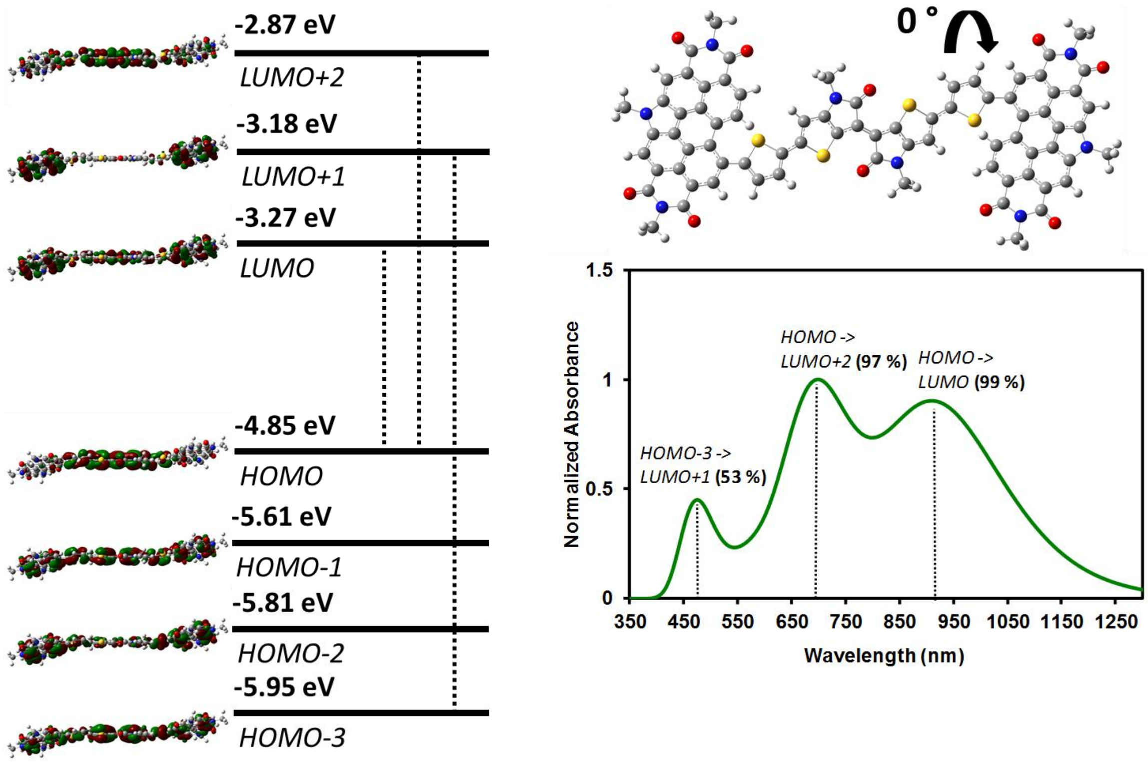

Figure S22. TD-DFT calculations of **TII-B** at 0°, including optimized geometry, predicted orbital transitions and predicted energy levels with π-orbital distributions.

Table S5. Predicted electronic transitions of **TII-B** at 0 ° dihedral angles.

State	E_{opt} (eV)	λ (nm)	f	Composition
S_1	1.35	920	0.8838	H→L (99 %)
S_3	1.78	697	0.9690	H →L+2 (97 %)
S_5	2.12	585	0.1795	H-2 →L (36 %)
S_{12}	2.58	480	0.1771	H-3 →L+1 (53 %)
S_{15}	2.68	463	0.2258	H→L+4 (31 %)

Thin-film UV-vis

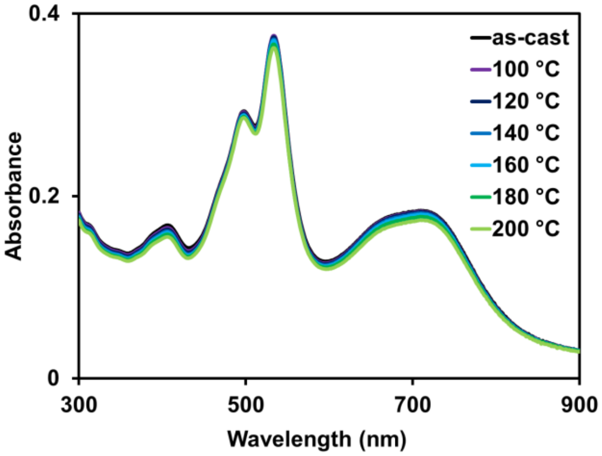

Figure S23. Thin-film UV-vis after thermal annealing of **TII-B**.

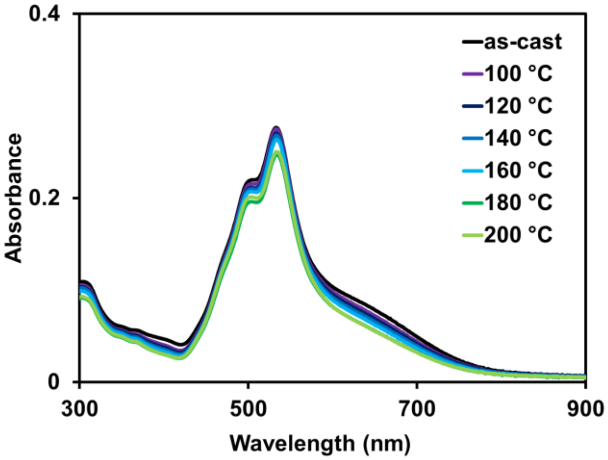

Figure S24. Thin-film UV-vis after thermal annealing of **DPP-B**.

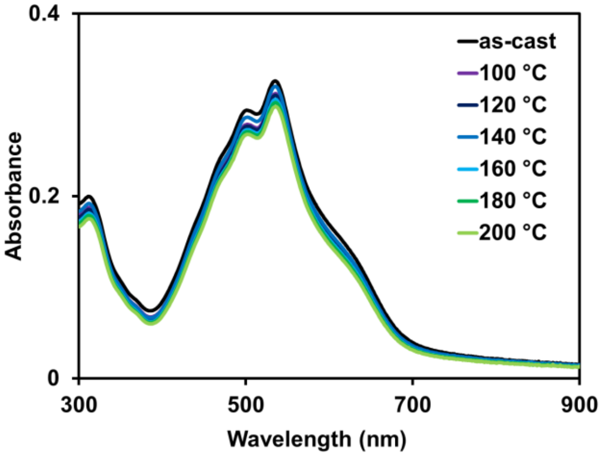

Figure S25. Thin-film UV-vis after thermal annealing of **ISI-B**.

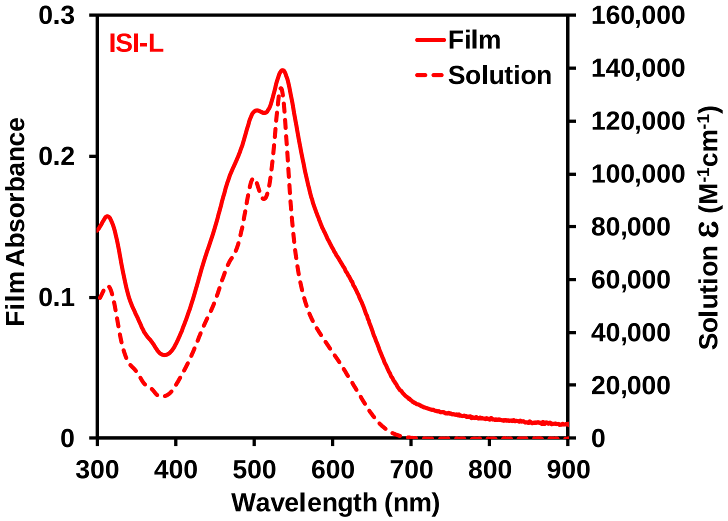

Figure S26. Solution and film UV-vis of **ISI-L**.

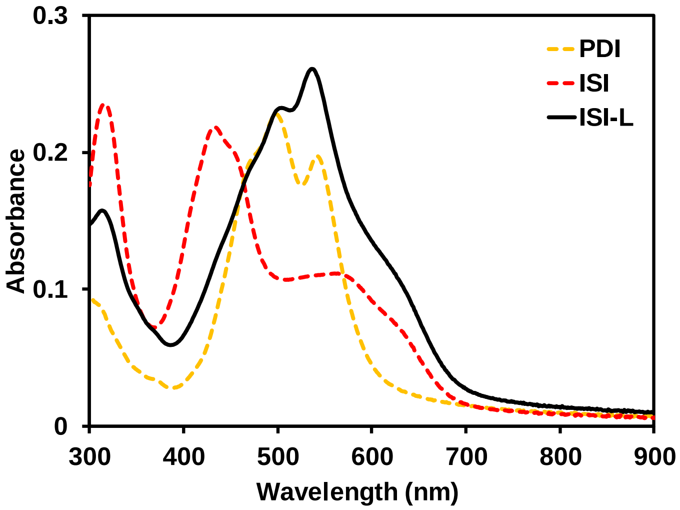

Figure S27. Thin-film UV-vis of **ISI-L** and the individual components (PDI and ISI).

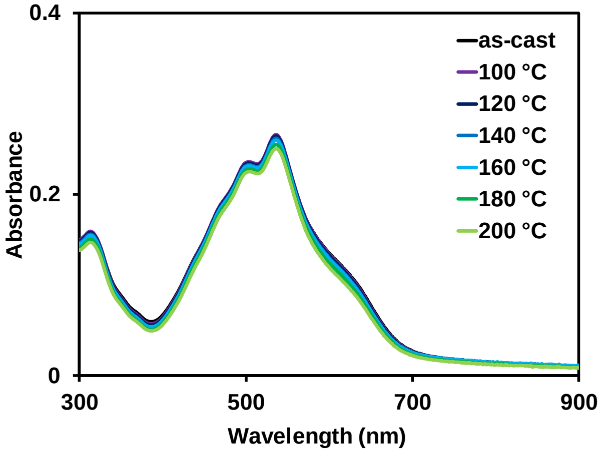

Figure S28. Thin-film UV-vis after thermal annealing of **ISI-L**.

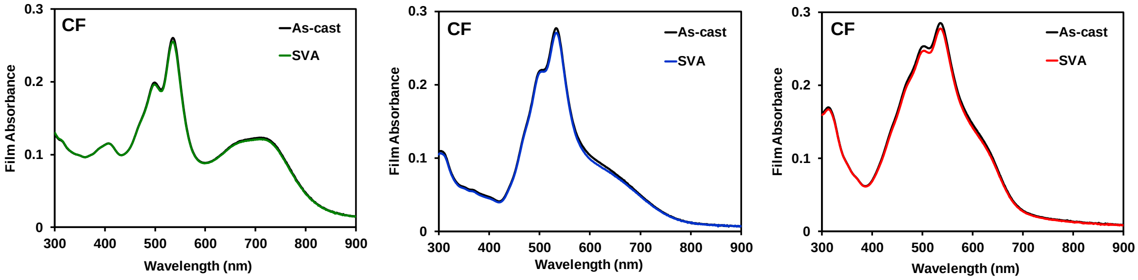

Figure S29. Thin-film UV-vis of $CHCl_3$ vapour annealing of **TII-B**, **DPP-B** and **ISI-B** cast from $CHCl_3$.

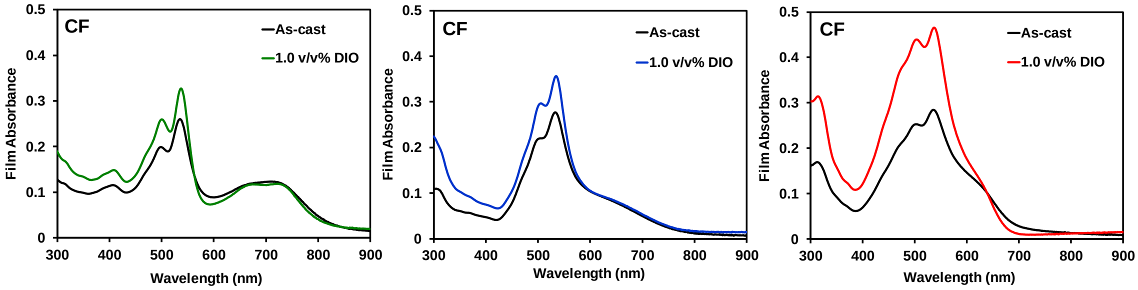

Figure S30. Thin-film UV-vis of **TII-B**, **DPP-B** and **ISI-B** cast from $CHCl_3$ with 1.0 v/v% DIO additive.

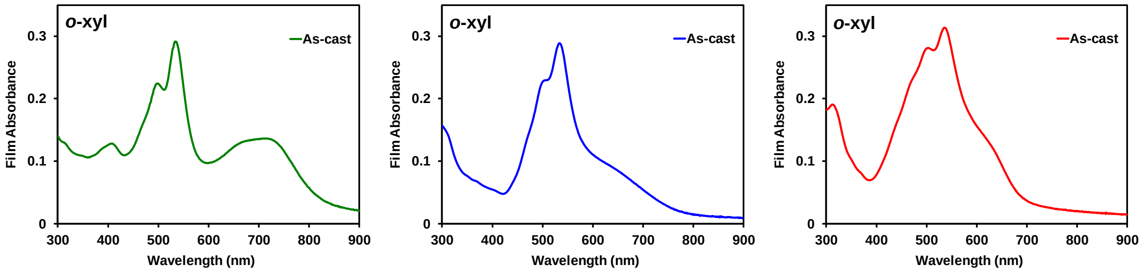

Figure S31. Thin-film UV-vis of **TII-B**, **DPP-B** and **ISI-B** cast o-xylenes.

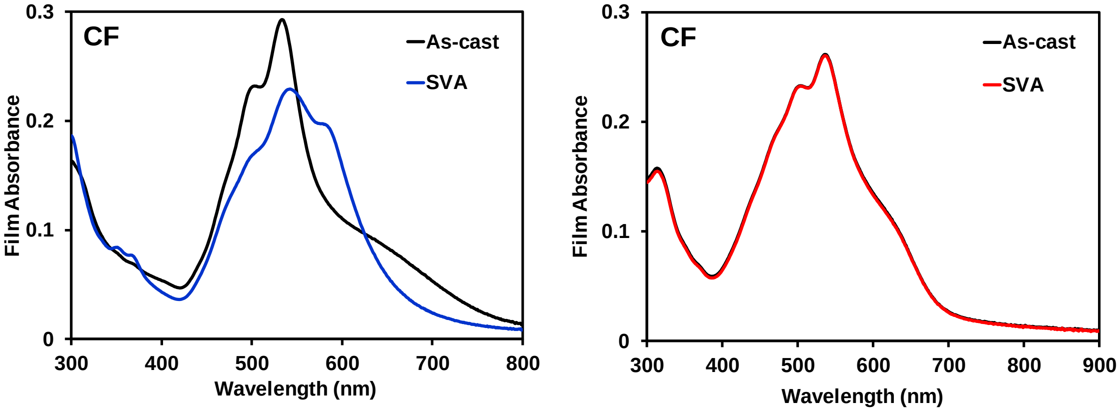

Figure S32. Thin-film UV-vis of $CHCl_3$ vapour annealing of **DPP-L** and **ISI-L** cast from $CHCl_3$.

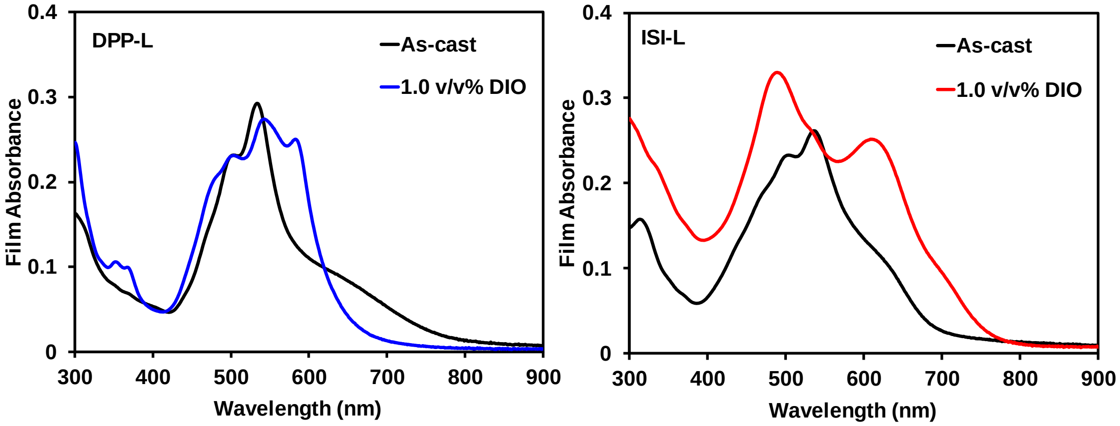

Figure S33. Thin-film UV-vis of **DPP-L** and **ISI-L** cast from $CHCl_3$ with 1.0 v/v% DIO.

Space charge limited current (SCLC):

A solution of neat molecular acceptors **PDI-dye-PDI** (15 mg/mL) in chloroform, filtered through a 0.45 µm PTFE membrane (Millex®), was spun cast at 1000 rpm on the cleaned ITO substrates, providing organic layers of *ca* 120 nm (measured with a Dektak 3M profilometer). In addition, to assess the impact of solvent vapor annealing (SVA), several substrates were exposed to chloroform vapors for 5 minutes (controlled by UV-vis spectroscopy). Then, lithium fluoride (1 nm) and aluminum (100 nm) were thermally and successively evaporated under a vacuum of 5.5 x 10^{-6} Torr, through a shadow mask defining actives area of 12.60 mm², 3.10 mm² and 0.78 mm² per substrates. Electrons mobilities μ_e were evaluated using the Mott-Gurney law, *ie*, $J_{SCLC} = (9/8)\varepsilon_0\varepsilon_r\mu_e(V^2/d^3)$ where ε_r is the static dielectric constant of the medium ($\varepsilon_r = 3$) and d, the thickness of the active layer.[3] From the J-V characteristics (Figure 1), μ_e values of 1.0×10^{-4} (**TII-B**), 1.2×10^{-4} (**DPP-B**) and 1.1×10^{-4} cm^2 V^{-1} s^{-1} (**ISI-B**) were estimated for as-cast based films.

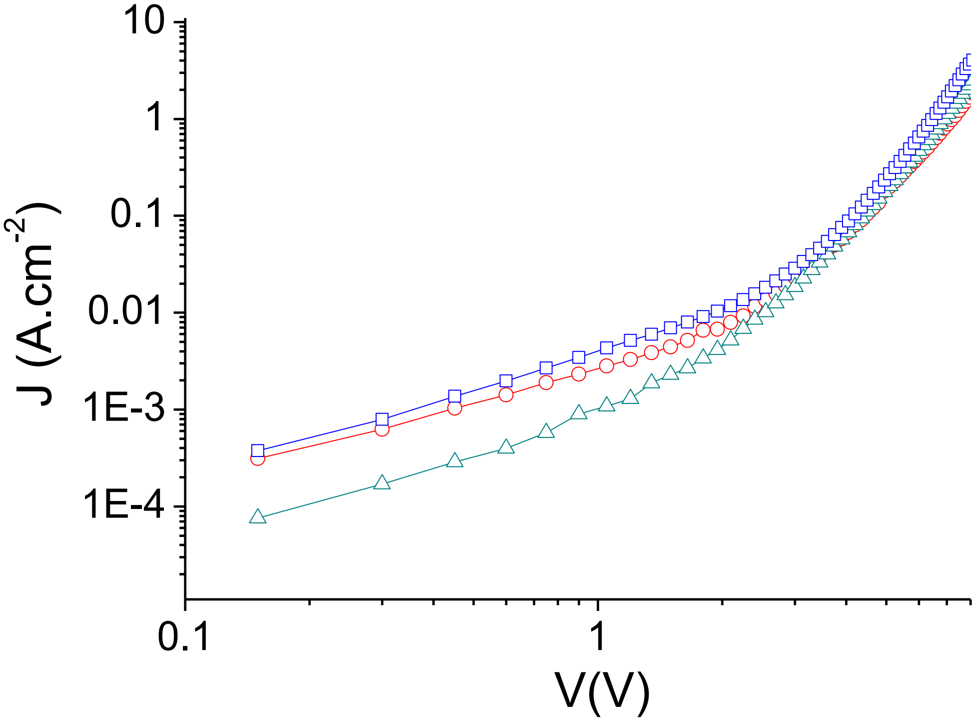

Figure S34. Current-voltage characteristics of as-cast **TII-B** (green), **DPP-B** (blue) and **ISI-B** (red).

Device fabrication

Devices were fabricated using ITO-coated glass substrates cleaned by sequentially ultra-sonicating detergent and de-ionized water, acetone and isopropanol followed by exposure to UV/zone for 30 minutes.

ZnO was deposited as a sol-gel precursor solution in air following the method of Sun *et al.*[4] The room temperature solution was filtered and spin-cast at a speed of 4000 rpm and then annealed at 200 °C in air for 1 hour.

Active layer solutions of **PTB7-Th** and **PDI-dye-PDI** were prepared in air with a total concentration of 10 mg/mL in $CHCl_3$ or *o*-Xylene. Solutions were stirred overnight at room temperature prior to filtration through a PTFE filter. Active layer materials were combined in 40:60 ratios and cast at room temperature in air at a speed of 1500 rpm for 60 seconds from $CHCl_3$ or 600 rpm for 60 seconds followed by a neat drying spin at 1500 rpm for 20 seconds when casting from *o*-Xylene.

Post-deposition solvent vapour annealing where indicated was carried out by containing a raised as-cast substrate within a screw cap glass jar with 0.5 mL of $CHCl_3$ as a solvent in the bottom of the jar. Substrates were left exposed to the solvent vapour for pre-determined durations.

The substrates were then kept in an N_2 atmosphere glovebox overnight before evaporating MoO_3 and Ag. The evaporation of 10 nm of MoO_3 followed by 100 nm of Ag were thermally deposited under vacuum ($1x10^{-6}$ Torr). Devices that used DIO as an additive were kept under vacuum ($1x10^{-6}$ Torr) for 2 hours prior to evaporation. The active areas of resulting devices were 0.09 cm^2. Completed devices were then tested in air using a Newport 92251A-1000 AM 1.5 solar simulator which had been calibrated using a standard silicon solar cell (Newport 91150V) to obtain an irradiance level of 1000 W/m^2.

Device optimization

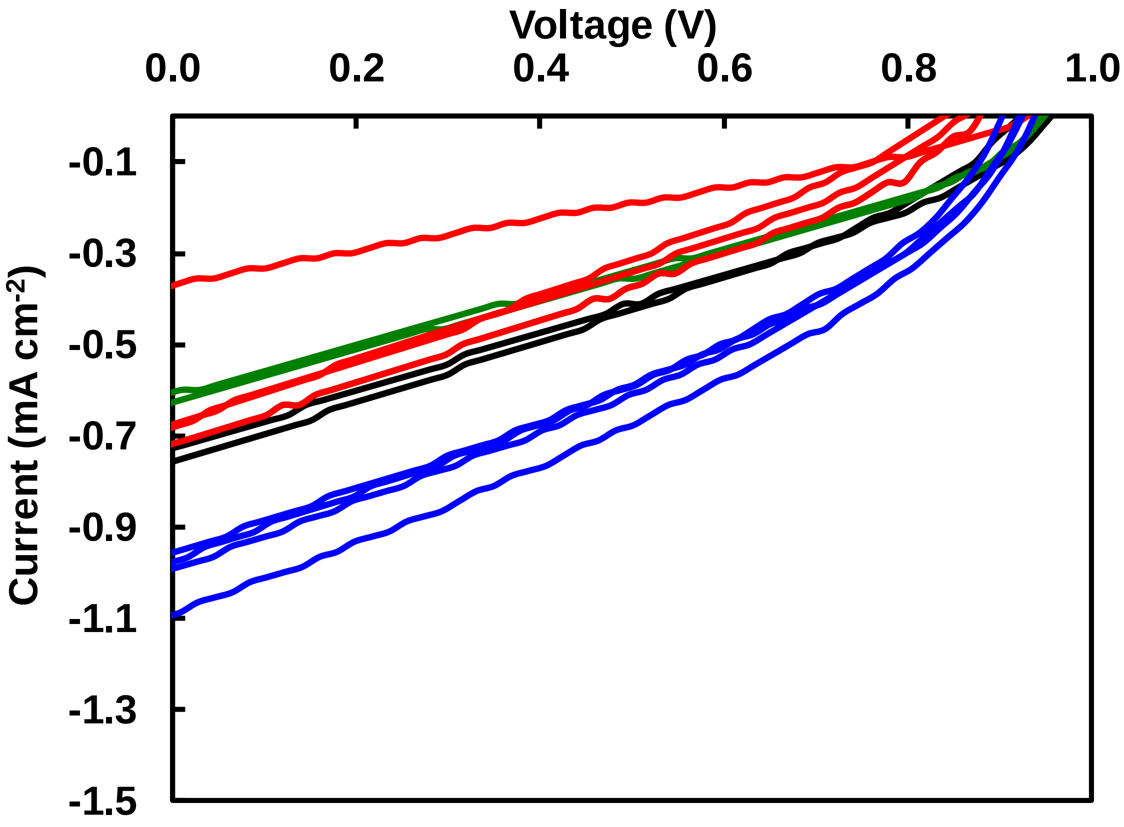

Figure S35. Current voltage curves for **PTB7-Th:TII-B**.

Black – As-cast $CHCl_3$
Green – $CHCl_3$ Solvent Vapour Annealing
Red – 0.5 v/v% DIO additive
Blue – As-cast *o*-Xylene

Table S1. Device statistics for **PTB7-Th:TII-B**.

Acceptor	**Solvent**	**Processing**	**V_{OC} (V)**	**J_{SC} (mAcm^{-2})**	**FF (%)**	**PCE (%)**
TII-B[a]	CHCl$_3$	As-cast	0.92	0.76	30.4	0.21
TII-B[a]	CHCl$_3$	As-cast	0.96	0.73	30.0	0.21
TII-B[a]	CHCl$_3$	As-cast	0.88	0.72	29.4	0.19
			0.92	***0.74***	***29.9***	***0.20***
TII-B[a]	CHCl$_3$	CHCl$_3$ SVA	0.94	0.63	30.5	0.18
TII-B[a]	CHCl$_3$	CHCl$_3$ SVA	0.95	0.61	29,9	0.17
			0.94	***0.62***	***30.2***	***0.18***
TII-B[a]	CHCl$_3$	0.5 v/v% DIO	0.92	0.37	28.0	0.10
TII-B[a]	CHCl$_3$	0.5 v/v% DIO	0.86	0.67	29.3	0.17
TII-B[a]	CHCl$_3$	0.5 v/v% DIO	0.88	0.72	29.4	0.19
TII-B[a]	CHCl$_3$	0.5 v/v% DIO	0.84	0.68	28.1	0.16
			0.87	***0.61***	***28.7***	***0.15***
TII-B[a]	*o*-Xylene	As-cast	0.91	0.97	34.0	0.30
TII-B[a]	*o*-Xylene	As-cast	0.92	0.96	34.4	0.30
TII-B[a]	*o*-Xylene	As-cast	0.93	1.09	34.2	0.35
TII-B[a]	*o*-Xylene	As-cast	0.92	1.00	34.2	0.31
			0.92	***1.00***	***34.2***	***0.32***

[a] Individual, ***Average***. Device size = 9 mm^2. Substrate size = 15 x 15 x 0.7 mm.

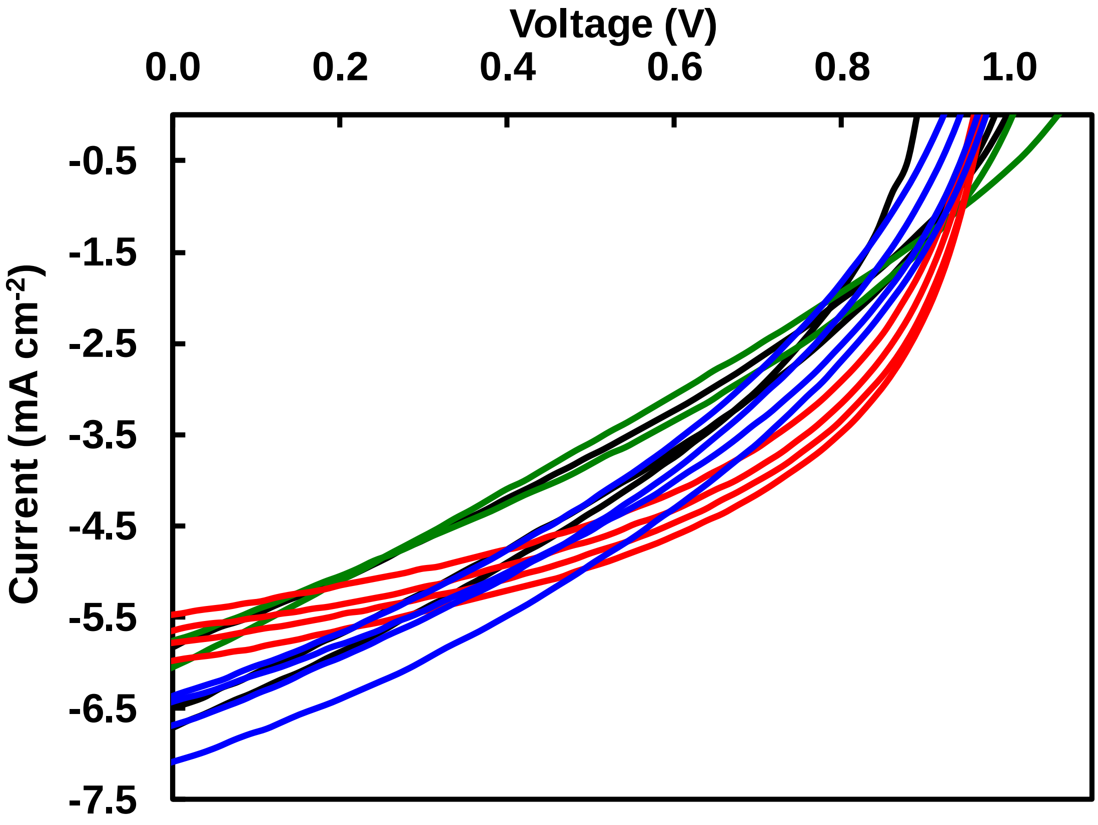

Figure S36. Current voltage curves for **PTB7-Th:DPP-B**.

Black – As-cast $CHCl_3$
Green – $CHCl_3$ Solvent Vapour Annealing
Red – 0.5 v/v% DIO additive
Blue – As-cast *o*-Xylene

Table S2. Device statistics for **PTB7-Th:DPP-B**.

Acceptor	**Solvent**	**Processing**	**V_{OC} (V)**	**J_{SC} (mAcm^{-2})**	**FF (%)**	**PCE (%)**
DPP-B[a]	$CHCl_3$	As-cast	0.89	6.71	37.6	2.25
DPP-B[a]	$CHCl_3$	As-cast	0.98	6.51	34.5	2.21
DPP-B[a]	$CHCl_3$	As-cast	1.00	5.81	33.4	1.94
			0.96	***6.35***	***35.2***	***2.13***
DPP-B[a]	$CHCl_3$	$CHCl_3$ SVA	1.00	5.76	34.8	2.01
DPP-B[a]	$CHCl_3$	$CHCl_3$ SVA				
			1.00	***5.76***	***34.8***	***2.01***
DPP-B[a]	$CHCl_3$	0.5 v/v% DIO	0.97	5.98	50.3	2.91
DPP-B[a]	$CHCl_3$	0.5 v/v% DIO	0.97	5.78	50.2	2.80
DPP-B[a]	$CHCl_3$	0.5 v/v% DIO	0.96	5.63	49.8	2.70
DPP-B[a]	$CHCl_3$	0.5 v/v% DIO	0.96	5.44	48.9	2.55
			0.96	***5.70***	***49.8***	***2.74***
DPP-B[a]	*o*-Xylene	As-cast	0.94	6.69	37.1	2.34
DPP-B[a]	*o*-Xylene	As-cast	0.92	6.36	36.9	2.16
DPP-B[a]	*o*-Xylene	As-cast	0.97	7.09	37.6	2.59
DPP-B[a]	*o*-Xylene	As-cast	0.96	6.41	39.2	2.41
			0.95	***6.64***	***37.7***	***2.38***

[a] Individual, ***Average***. Device size = 9 mm^2. Substrate size = 15 x 15 x 0.7 mm.

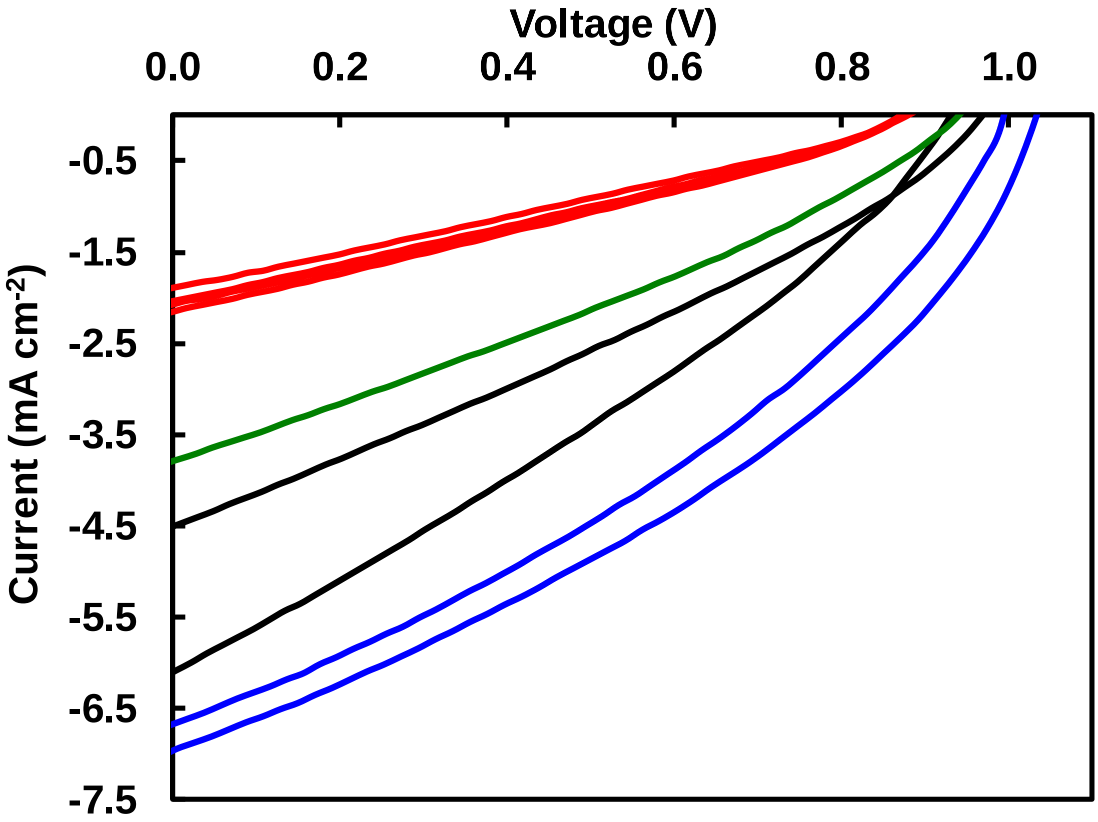

Figure S37. Current voltage curves for **PTB7-Th:ISI-B**.

Black – As-cast $CHCl_3$
Green – $CHCl_3$ Solvent Vapour Annealing
Red – 0.5 v/v% DIO additive
Blue – As-cast *o*-Xylene

Table S3. Device statistics for **PTB7-Th:ISI-B**

Acceptor	**Solvent**	**Processing**	**V_{OC} (V)**	**J_{SC} (mAcm^{-2})**	**FF (%)**	**PCE (%)**
ISI-B[a]	$CHCl_3$	As-cast	0.93	6.11	30.0	1.71
ISI-B[a]	$CHCl_3$	As-cast	0.97	4.51	29.7	1.30
ISI-B[a]	$CHCl_3$	As-cast				
			0.95	***5.31***	***29.9***	***1.51***
ISI-B[a]	$CHCl_3$	$CHCl_3$ SVA	1.06	6.05	28.6	1.84
ISI-B[a]	$CHCl_3$	$CHCl_3$ SVA				
			1.06	***6.05***	***28.6***	***1.84***
ISI-B[a]	$CHCl_3$	0.5 v/v% DIO	0.87	2.07	28.1	0.51
ISI-B[a]	$CHCl_3$	0.5 v/v% DIO	0.88	1.89	27.5	0.45
ISI-B[a]	$CHCl_3$	0.5 v/v% DIO	0.87	2.15	28.6	0.53
ISI-B[a]	$CHCl_3$	0.5 v/v% DIO	0.87	2.05	28.3	0.50
			0.87	***2.04***	***28.1***	***0.50***
ISI-B[a]	*o*-Xylene	As-cast	0.99	6.68	35.4	2.33
ISI-B[a]	*o*-Xylene	As-cast	1.03	6.97	36.7	2.63
ISI-B[a]	*o*-Xylene	As-cast				
ISI-B[a]	*o*-Xylene	As-cast				
			1.01	***6.82***	***36.1***	***2.48***

[a] Individual, ***Average***. Device size = 9 mm^2. Substrate size = 15 x 15 x 0.7 mm.

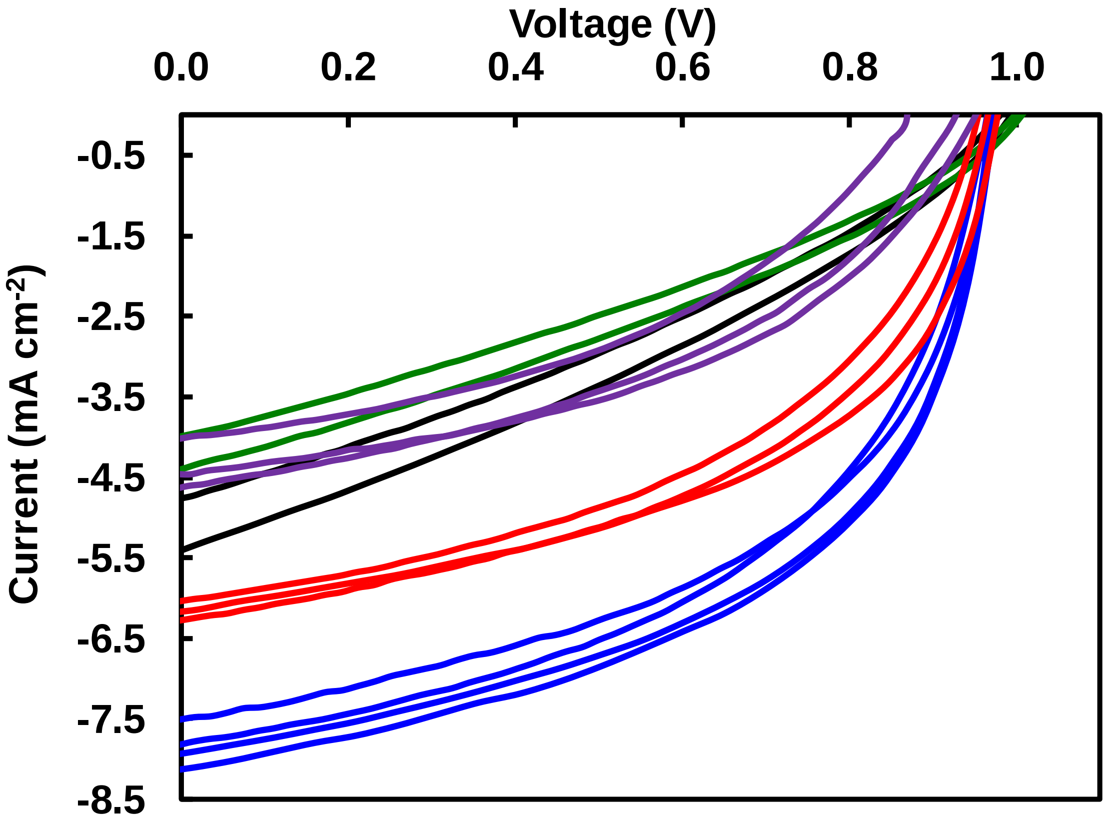

Figure S38. Current voltage curves for **PTB7-Th:DPP-L**.

Black – As-cast $CHCl_3$
Green – 0.1 v/v% DIO additive
Blue – 0.5 v/v% DIO additive
Red – 1.0 v/v% DIO additive
Purple – 3.0 v/v% DIO additive

Table S4. Device statistics for **PTB7-Th:DPP-L**

Acceptor	**Solvent**	**Processing**	**V_{OC} (V)**	**J_{SC} (mAcm^{-2})**	**FF (%)**	**PCE (%)**
DPP-L[a]	$CHCl_3$	As-cast	0.99	5.41	32.1	1.72
DPP-L[a]	$CHCl_3$	As-cast	0.98	4.78	32.2	1.51
			0.99	***5.09***	***32.2***	***1.62***
DPP-L[a]	$CHCl_3$	0.1 v/v% DIO	1.00	4.40	32.4	1.43
DPP-L[a]	$CHCl_3$	0.1 v/v% DIO	1.00	4.00	32.2	1.29
			1.00	***4.20***	***32.3***	***1.36***
DPP-L[a]	$CHCl_3$	0.5 v/v% DIO	0.96	7.77	50.4	3.78
DPP-L[a]	$CHCl_3$	0.5 v/v% DIO	0.97	7.93	52.9	4.07
DPP-L[a]	$CHCl_3$	0.5 v/v% DIO	0.98	7.48	51.1	3.73
DPP-L[a]	$CHCl_3$	0.5 v/v% DIO	0.97	8.11	52.4	4.14
			0.97	***7.82***	***51.7***	***3.93***
DPP-L[a]	$CHCl_3$	1.0 v/v% DIO	0.97	6.24	48.8	2.94
DPP-L[a]	$CHCl_3$	1.0 v/v% DIO	0.95	6.02	47.6	2.74
DPP-L[a]	$CHCl_3$	1.0 v/v% DIO	0.98	6.16	50.9	3.06
			0.97	***6.14***	***49.1***	***2.91***
DPP-L[a]	$CHCl_3$	3.0 v/v% DIO	0.95	4.46	45.8	1.94
DPP-L[a]	$CHCl_3$	3.0 v/v% DIO	0.87	4.00	42.6	1.49
DPP-L[a]	$CHCl_3$	3.0 v/v% DIO	0.92	4.62	42.8	1.83
			0.91	***4.36***	***43.7***	***1.75***

[a] Individual, ***Average***. *De*vice size = 9 mm^2. Substrate size = 15 x 15 x 0.7 mm.

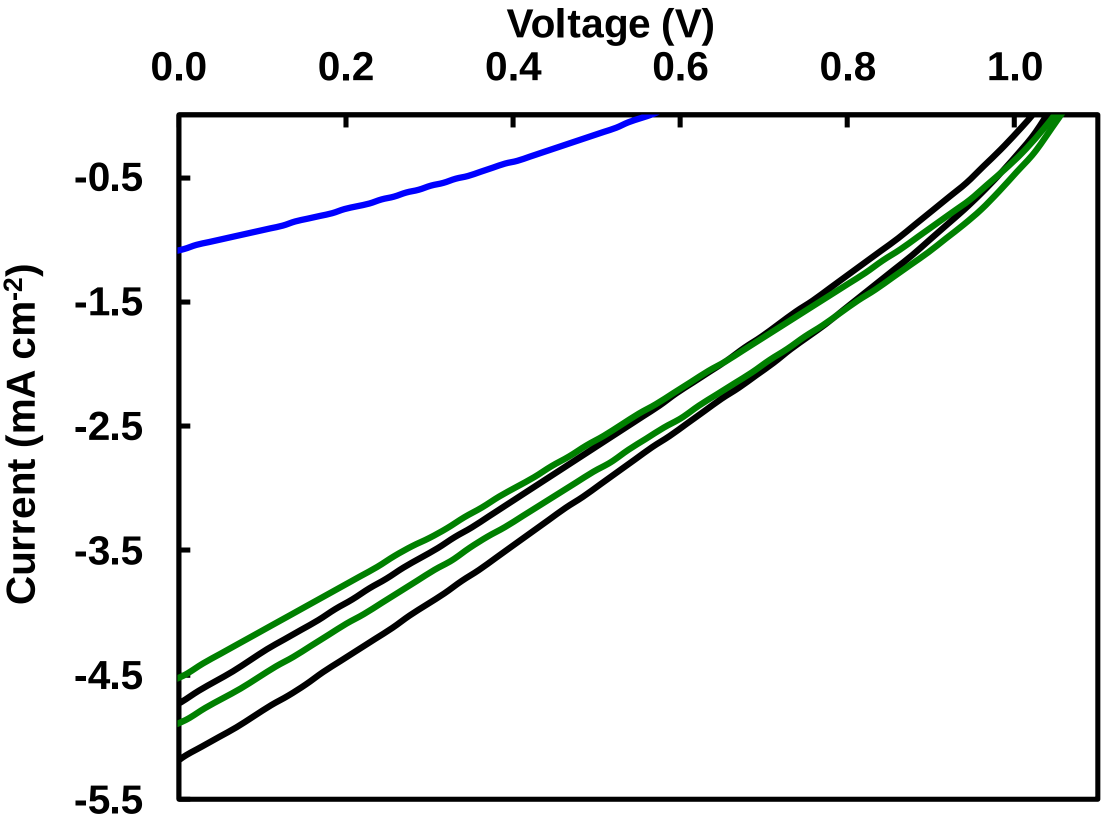

Figure S39. Current voltage curves for **PTB7-Th:ISI-L**.

Black – As-cast $CHCl_3$
Green – 0.1 v/v% DIO additive
Blue – 0.5 v/v% DIO additive

Table S5. Device statistics for **PTB7-Th:ISI-L**

Acceptor	**Solvent**	**Processing**	**V_{OC} (V)**	**J_{SC} (mAcm^{-2})**	**FF (%)**	**PCE (%)**
ISI-L[a]	$CHCl_3$	As-cast	1.04	5.20	28.1	1.52
ISI-L[a]	$CHCl_3$	As-cast	1.02	4.72	27.9	1.34
			1.03	***4.96***	***28.0***	***1.43***
ISI-L[a]	$CHCl_3$	0.1 v/v% DIO	1.05	4.89	28.4	1.46
ISI-L[a]	$CHCl_3$	0.1 v/v% DIO	1.05	4.52	28.0	1.33
			1.05	***4.71***	***28.2***	***1.39***
ISI-L[a]	$CHCl_3$	0.5 v/v% DIO	0.56	1.08	28.3	0.17
			0.56	***1.08***	***28.3***	***0.17***

[a] Individual, ***Average***. *De*vice size = 9 mm^2. Substrate size = 15 x 15 x 0.7 mm.

Atomic force microscopy images

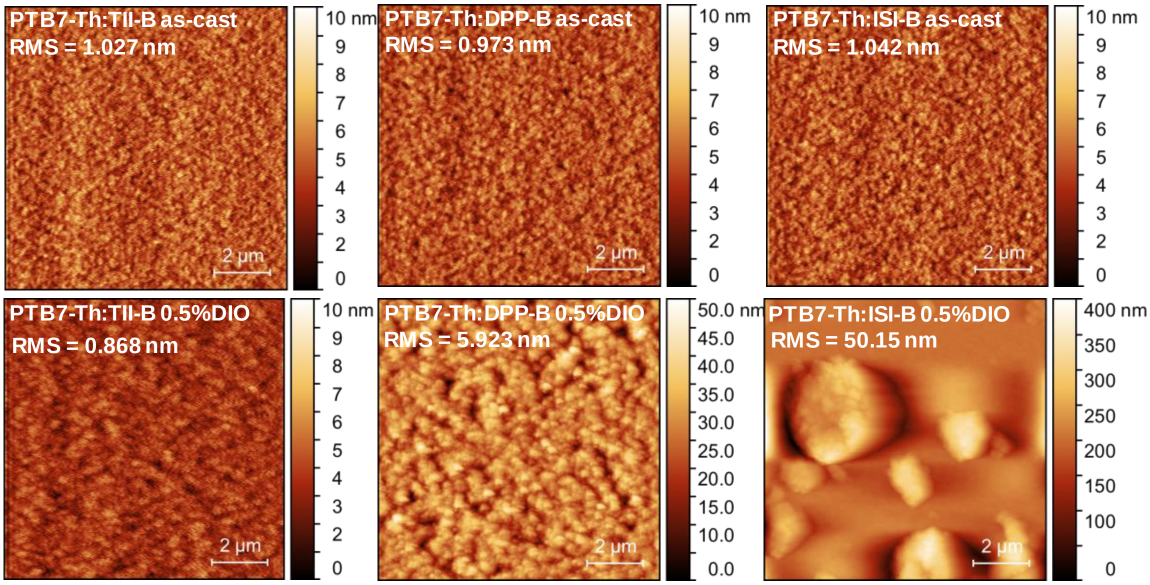

Figure S40. AFM images for as-cast active layer blends **PTB7-Th:TII-B** (top, left) **PTB7-Th:DPP-B** (top, centre) and **PTB7-Th:ISI-B** (top, right) and with 0.5 % DIO additive **PTB7-Th:TII-B** (bottom, left) **PTB7-Th:DPP-B** (bottom, centre) and **PTB7-Th:ISI-B** (bottom, right)

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