Supporting Information

Absorption enhancement of oligothiophene dyes through the use of a cyanopyridone acceptor group in solution-processed organic solar cells

Akhil Gupta,[a,b] Abdelselam Ali,[a] Ante Billic,[c] Mei Gao,[a] Katalin Hegedus,[a] Birendra Singh,[a] Scott E. Watkins,*[a] Gerard J. Wilson,[a] Udo Bach,[b] and Richard A. Evans*[a]

[a] *CSIRO Materials Science and Engineering, Flexible Electronics Theme, Bayview Avenue, Clayton South, 3169, Victoria, Australia; Tel:+61 3 9545 2507;*
E-mail: scott.watkins@csiro.au, richard.evans@csiro.au;
[b] *Department of Materials Engineering, Monash University, Wellington Road, Clayton, 3800, Victoria, Australia*
[c] *CSIRO Mathematics Informatics and Statistics, Bayview Avenue, Clayton South, 3169, Victoria, Australia.*

1. Experimental

1.1. Materials

All the reagents and chemicals used, unless otherwise specified, were purchased from Sigma-Aldrich Co. The solvents used for reactions were obtained from Merck Speciality Chemicals (Sydney, Australia) and were used after distillation.

1.2. Instruments and characterisation

Unless otherwise specified, all ^1H and ^{13}C NMR spectra were recorded using a Bruker AV400 spectrometer at 400 MHz and 100.6 MHz, respectively, or a Bruker AV200 spectrometer at 200 MHz and 50 MHz, respectively. Chemical shifts (δ) are measured in ppm. Thin Layer Chromatography (TLC) was performed using 0.25 mm thick plates pre-coated with Merck Kieselgel 60 F_{254} silica gel, and visualised using ultraviolet (UV) light (254 nm and 366 nm). Analytical HPLC analyses were performed using a Waters 2695 alliance system and Waters 2996 photodiode array detector scanning 190-700nm using an Alltima HP C18 column at 30°C with 90% acetonitrile, 0.1% trifluoroacetic acid and water as mobile phase. Waters Empower 2 data management system was used for data processing. Melting points were measured using a Gallenkamp MPD350 digital melting point apparatus and are uncorrected. Positive ion electron impact (EI) mass spectra were measured using a ThermoQuest MAT95XL mass spectrometer using ionisation energy of 70 eV. Ultraviolet-visible (UV-Vis) absorption spectra were recorded using a Hewlett Packard HP 8453 diode array spectrometer. Fluorescence spectra were measured using a Perkin Elmer LS50B fluorimeter. Photoelectron Spectroscopy in Air (PESA) measurements were recorded using a Riken Keiki AC-2 PESA spectrometer with a power setting of 5 nW and a power number of 0.5. Samples for PESA were prepared on glass substrates. Electrochemical measurements were carried out using a PowerLab ML160 potentiostat interfaced via a PowerLab 4/20 controller to a PC running E-Chem For Windows Ver. 1.5.2. The measurements were run in argon-purged dichloromethane with tetrabutylammonium hexafluorophosphate (0.2 M) as the supporting electrolyte. The cyclic voltammograms were recorded using a standard 3 electrode configuration with a glassy carbon (2 mm diameter) working electrode, a platinum wire counter electrode and a silver wire pseudo reference electrode. The silver wire was cleaned in concentrated nitric acid and then in concentrated hydrochloric acid to generate the Ag/AgCl reference. Voltammograms were recorded with a sweep rate of 50–200 mV/s. All the potentials were referenced to $E_{1/2}$ of the ferrocene/ferrocenium redox couple.

1.3 Device fabrication and characterisation of photovoltaic devices

UV/ozone cleaning of glass substrates was performed using a Novascan PDS-UVT, UV/ozone cleaner with the platform set to maximum height. The intensity of the lamp was greater than 36 mW/cm^2 at a distance of 10 cm. At ambient conditions the ozone output of the UV cleaner is greater than 50 ppm. Indium tin oxide (ITO)-coated glass (Kintek, 15 Ω/□) was cleaned by standing in a stirred solution of 5% (v/v) Deconex 12PA detergent at 90 °C for 20 minutes. The ITO-coated glass was then successively sonicated for 10 mins each in distilled water, acetone and isopropanol. The substrates were then exposed to a UV-ozone clean at room temperature for 10 minutes.

Aqueous solutions of PEDOT/PSS (HC Starck, Baytron P AI 4083) were filtered (0.2 µm RC filter) and deposited onto glass substrates in air by spin coating (Laurell WS-400B-6NPP lite single wafer spin processor) at 5000 rpm for 60 seconds to give a layer having a thickness of 38 nm. The PEDOT/PSS layer was then annealed on a hotplate in a glovebox at 145 °C for 10 minutes.

For OPV devices, the newly synthesised organic p-type materials and PCBM (Nano-C) were separately dissolved in individual vials by magnetic stirring. Blend ratios and solution concentrations were varied to optimise device performance, see below. The solutions were then combined, filtered (0.2 µm RC filter) and deposited by spin coating (SCS G3P spin coater) onto the ITO-coated glass substrates inside a glove box. Film thicknesses were determined using a Dektak 6M Profilometer.

The coated substrates were then transferred (without exposure to air) to a vacuum evaporator inside an adjacent nitrogen-filled glovebox (H_2O and O_2 levels both < 1 ppm). Samples were placed on a shadow mask in a tray. The area defined by the shadow mask gave device areas of exactly 0.2 cm^2. Deposition rates and film thicknesses were monitored using a calibrated quartz thickness monitor inside the vacuum chamber. Layers of calcium (Ca) (Aldrich) and aluminium (Al) (3 pellets of 99.999%, KJ Lesker) having thicknesses of 20 nm and 100 nm, respectively, were evaporated from open tungsten boats onto the active layer by thermal evaporation at pressures less than 2×10^{-6} mbar. Where used, C_{60} (Nano-C) and BCP (Aldrich) were evaporated from alumina crucibles.

A connection point for the ITO electrode was made by manually scratching off a small area of the active layers. A small amount of silver paint (Silver Print II, GC Electronics, part no.: 22-023) was then deposited onto all of the connection points, both ITO and Al. The completed devices were then encapsulated with glass and a UV-cured epoxy (Summers Optical, Lens Bond type J-91) by exposing to 365nm UV light inside a glovebox (H_2O and O_2 levels both < 1 ppm) for 10 mins. The encapsulated devices were then removed from the glovebox and tested in air within 1 hour. Electrical connections were made using alligator clips.

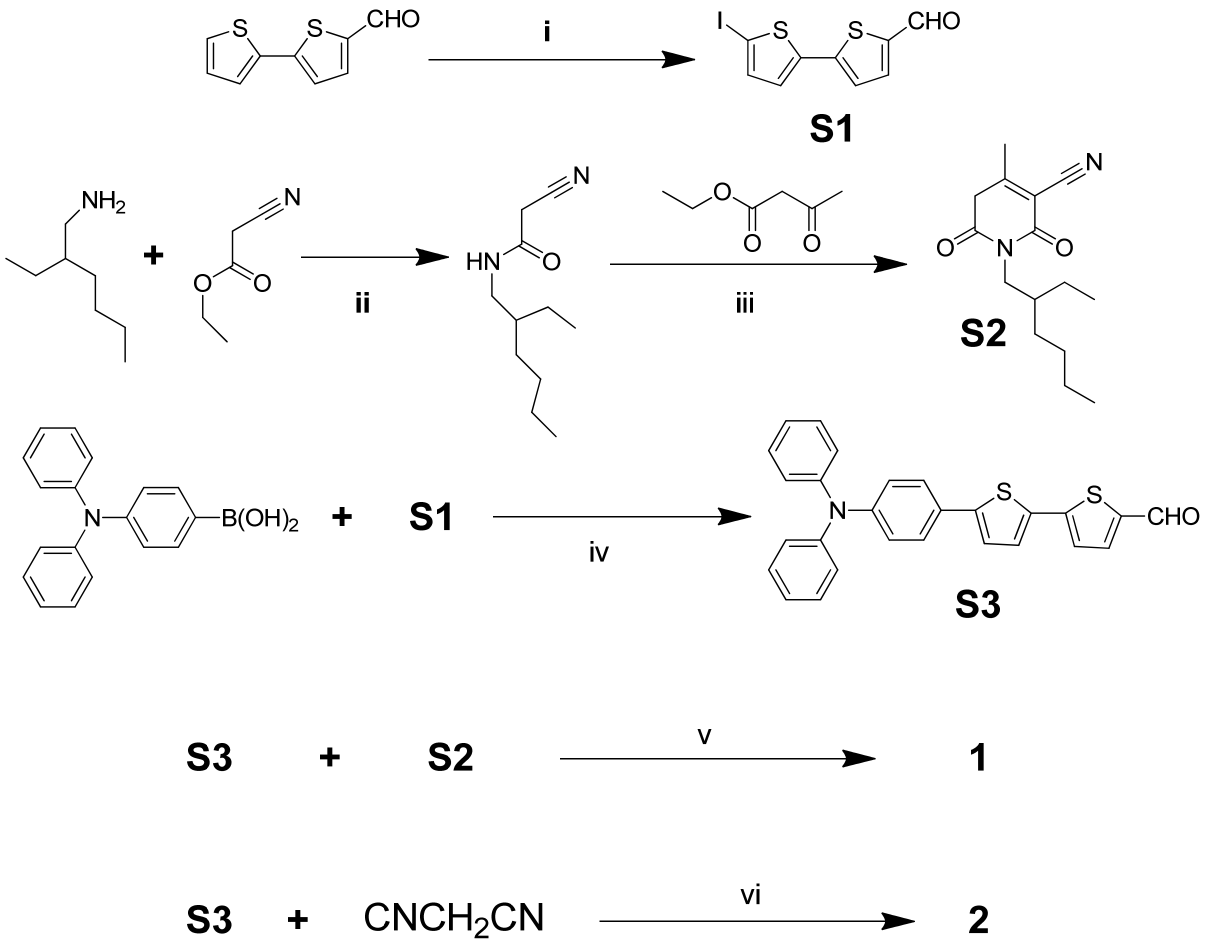
The OPV devices were tested using an Oriel solar simulator fitted with a 1000 W xenon lamp filtered to give an output of 100 mW/cm^2 at simulated AM 1.5. The lamp was calibrated using a standard, filtered silicon (Si) cell from Peccell Limited which was subsequently cross-calibrated with a standard reference cell traceable to the National Renewable Energy Laboratory. The devices were tested using a Keithley 2400 sourcemeter controlled by Lab-view software.

1.4 Device fabrication and characterization of field effect transistors

A doped ($N \sim 3 \times 10^{17}$ cm^{-3}) Si wafer was used as a substrate and as gate electrode. Discrete bottom contact Organic Field Effect Transistors (OFETs) were fabricated on thermally grown smooth silicon dioxide (230 nm). Interdigitated source and drain electrodes were photolithographically patterned from a 50 nm sputtered gold layer. Channel length, L, of the devices was 2.5 μm and the channel width, W, was 2 mm. The SiO_2 layer was first cleaned with acetone, then with 2-propanol and finally treated with UV ozone. Device fabrication was completed by spin coating the organic semiconductor layers at 1500 rpm in the glove box from solutions in chlorobenzene and chloroform. The active layers consisted of either pristine compounds or a blend of compound with $PC_{61}BM$. Without any further treatment, completed devices were transferred (under air-free conditions) to another glove box fitted to probe the devices using a probe station. Electrical measurements were carried out using a Keithley 2612 dual channel SMU. The reproducibility of the OFET preparation procedure was high with a confidence interval for the extracted mobility of ±15% of the values which have been presented. The carrier mobility values presented in this work were generally averaged from measurements done on at least four devices on the same substrate.

2. Synthesis of 1 and 2

The synthetic strategy for compounds 1 and 2 is represented in Scheme 1.



Scheme 1 Synthesis of compounds **1** and **2**: (i) N-iodosuccinimide, acetic acid : chloroform 1 : 1, RT (ii) 0 °C to RT (iii) pyridine, 100 °C; (iv) Pd(C) (10%), $Na_2PO_4.12H_2O$, isopropyl alcohol, 80°C; (v) methanol, 65 °C; (vi) chloroform, pyridine, 70 °C

Synthesis of 5'-iodo-2,2'-bithiophene-5-carbaldehyde (S1)

To the solution of 2,2'-bithiophene-5-carbaldehyde (12g, 61.86 mmol) in 1:1 solvent mixture of chloroform and acetic acid was added n-iodosuccinimide (16.70g, 74.23 mmol) at room temperature (RT). The resulting reaction solution was stirred at RT overnight. The solid that appeared in the reaction was filtered off, washed with diethyl ether and dried under vacuum to afford 18g (90.93%) of the product as a yellow powder.

^{1}H NMR (400MHz, CD_3COCD_3) δ9.93 (s, 1H), 7.91 (m, 1H), 7.44 (m, 1H), 7.38 (m, 1H), 7.24 (m, 1H)

Synthesis of

1-(2-ethylhexyl)-4-methyl-2.6-dioxo-1,2,5,6-tetrahydropyridine-3-carbonitrile (S2)

2-Ethylhexyl amine (38.7g, 0.30 moles) was added to a 500 ml round bottom flask and cooled to 0 °C. Ethyl cyanoacetate (28.3g, 0.25 moles) was added dropwise to this solution while maintaining the same reaction temperature. The reaction was stirred overnight at room temperature. On the following day a mixture of ethyl acetoacetate (39.5g, 0.25 moles) and pyridine (25ml, 0.25 moles) were added dropwise and the reaction was heated to 100 °C overnight. On the following day the reaction was cooled and diluted with water before acidifying with concentrated hydrochloric acid. The thick precipitate was collected by filtration. The precipitate was dried in air before being recrystallised from ethyl acetate and ethanol to give 32 grams (40.8%) of S2 as a pale pink solid. NMR revealed that the compound existed in its enol form in DMSO.

^{1}H NMR (400MHz, CD_3SOCD_3) δ5.65 (s, 1H), 3.86-3.76 (m, 2H), 2.21 (s, 3H), 1.80-1.71 (m, 1H), 1.30-1.11 (m, 8H), 0.84-0.79 (m, 6H)

Synthesis of 5'-[(4-diphenylamino)phenyl]-2, 2'-bithiophene-5-carbaldyde (S3)

Compound S2 (5.2g, 16.24 mmol), 4-(diphenylamino)phenylboronic acid (8.0g, 26.83 mmol), sodium phosphate dodecahydrate (7.6g, 19.48 mmol) and 10% Pd(C) (0.70g) were mixed in isopropanol (300 ml) in a 500 ml round bottom flask at RT. The mixture was heated at 80°C in an oil bath for 24 hours and the reaction progress was followed by thin-layer chromatography (TLC) that indicated the consumption of the starting aldehyde. The reaction mixture was cooled to room temperature, filtered through celite (0.05g) and eluted with dichloromethane (180ml). The solution was allowed to stand at room temperature for half an hour upon which an orange solid crystallised. The precipitate was collected by filtration and washed with petroleum ether to afford 4.5g of S3 as an orange solid.

The filtrate was evaporated under reduced pressure and purified by flash chromatograph, eluted with a gradient eluent of 50% $CHCl_3$/ petroleum ether (60°-80 °C) to 100% $CHCl_3$, to give the title product (S3) as an orange solid, 1.8g;

Total solid = 4.5 g + 1.8 g = 6.3g (89%) yield.

^{1}H NMR (400MHz, CD_2Cl_2) δ 9.85 (s, 1H), 7.70 (d, 1 H *J*= 3.92 Hz), 7.52-7.48 (m, 2H,), 7.36 (d, 1 H *J*= 11.48 Hz) 7.32-7.28 (m, 6H,), 7.23 (d, 1 H *J*= 3.92 Hz,), 7.14-7.04 (m, 8H).

Synthesis of 5-((5'-(4-(diphenylamino)phenyl)-2,2'-bithiophen-5-yl)methylene)-1-(2-ethylhexyl)-4-methyl-2,6-dioxo-1,2,5,6-tetrahydropyridine-3-carbonitrile (1)

Compound S2 (113mg, 0.432mmol) was added to the mixture of S3 (104mg, 0.24mmol) in methanol (20 ml) at room temperature and the resulting mixture was heated at reflux overnight. The precipitated solid was collected by filtration, washed with methanol and dried under vacuum to give 125mg (77.3%) of compound 1 as a black powder.

Melting Point: 212-218 °C; IR (neat, cm^{-1}) 3061, 2952, 2925, 2854, 2220, 1634, 1541, 1527, 1409, 1371, 1327, 1297, 1274, 1150, 1080, 810, 787, 696; ^{1}H NMR: (400MHz, CD_3SOCD_3) δ 8.33 (s, IH), 8.21 (d, J=4.4Hz, 1H), δ 7.71-7.74 (m, 2H), δ 7.65 (m, 2H), δ 7.52 (m, 1H), δ 7.36-7.323 (m, 4H), 7.12-7.06 (m, 6H), 6.95 (m, 2H), 3.79 (m, 2H), 2.6(s, 3H), 1.80-1.70 m, 1H), 1.35-1.15 (m, 8H), 0.90-0.81 (m, 6H); ^{13}C NMR (200 MHz, $CDCl_3$) δ163.53, 161.21, 158.26, 154.84, 148.61, 148.24, 147.36, 147.10, 144.18, 136.30, 134.50, 129.67, 128.79, 126.96, 126.91, 125.20, 124.60, 123.88, 123.07, 116.05, 115.33, 103.61, 44.21, 37.68, 30.73, 28.67, 24.12, 23.32, 19.10, 14.37, 10.84; HRMS/EI: Calcd for $C_{42}H_{39}N_3O_2S_2$ (m/z) 681.2478; found = 681.2477. HPLC analysis (normal phase, eluent 9:1 acetonitrile:water, 0.1% trifluroacetic acid), 96.61%. A large scale preparation (8g) gave a HPLC purity of 99.26%.

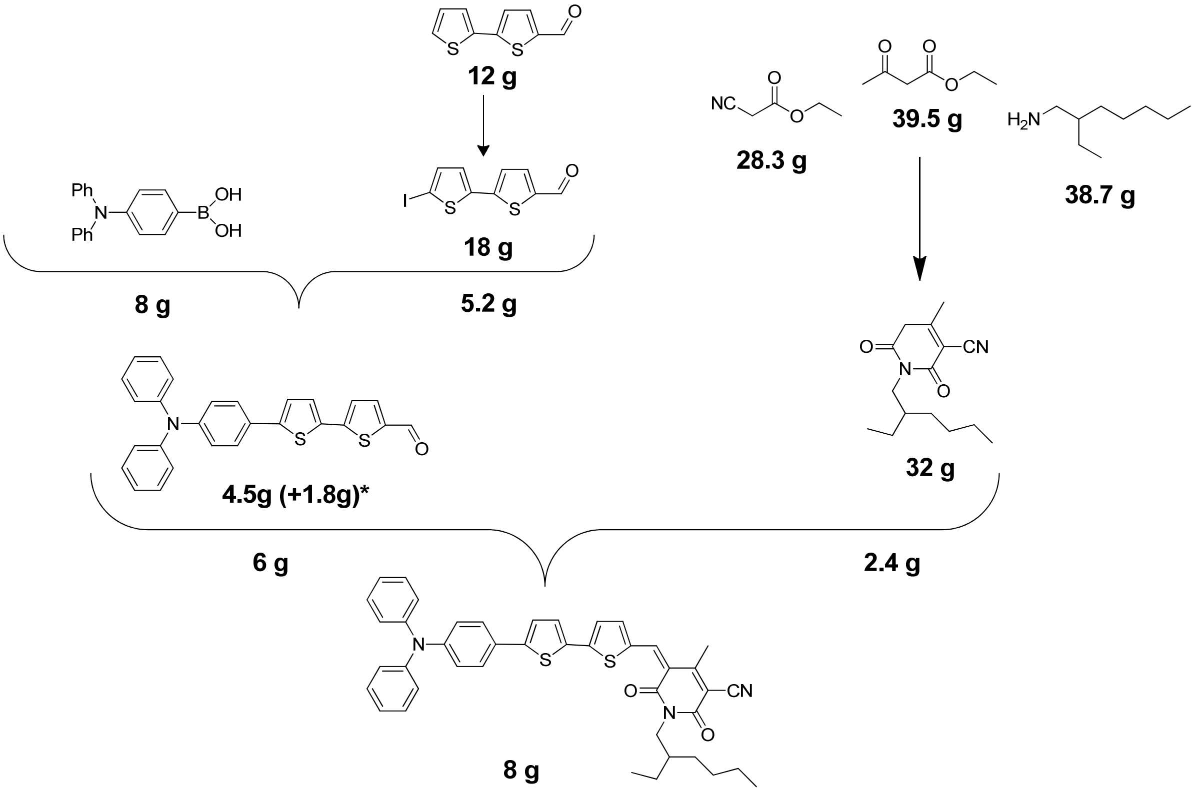
Synthesis of

2-((5’-(4-diphenylamino)phenyl)-[2,2’-bithiophene]-5-yl)methylene)malononitrile (2)

Compound S3 (0.40g, 0.92 mmol) and malononitrile (0.18g, 2.76 mmol were dissolved in chloroform (50 ml) in a 250 ml round bottom flask at room temperature followed by the addition of pyridine (0.2 ml). The resulting reaction mixture was heated at reflux overnight and the solvent was evaporated under reduced pressure. The crude solid was purified through column chromatography on silica gel (hexane:ethyl acetate, 8:2) to give 0.35g (78.3%) of compound **2** as a deep red solid.

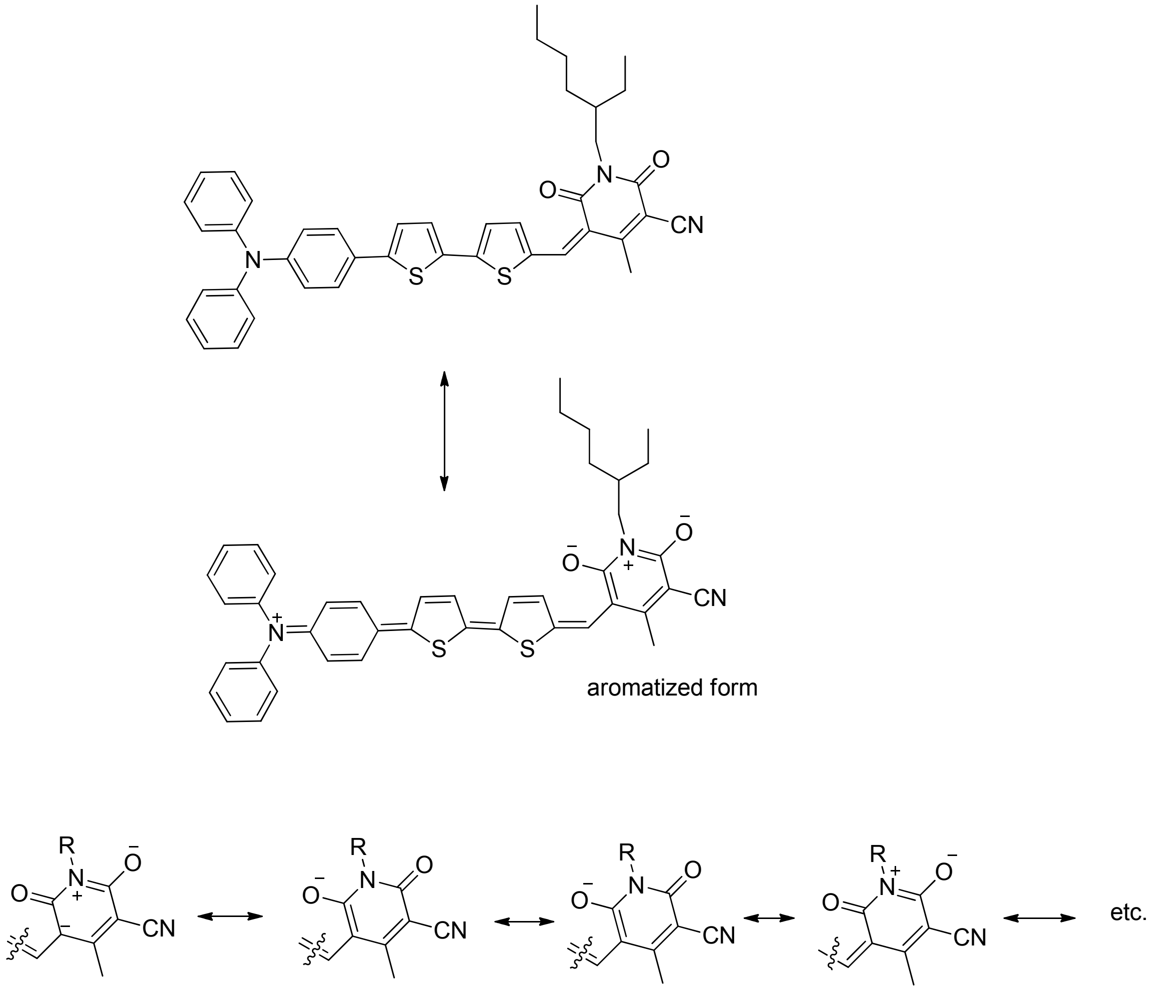
Melting Point: 186-189 °C; IR (neat, cm^{-1}) 3024, 2212, 1590, 1569, 1537, 1485, 1436, 1419, 1319, 1270, 1228, 1193, 1078, 1059, 790, 753, 695; ^1H NMR (400MHz, CD_3COCD_3) δ 8.40 (s, 1H), 7.95 (m, 1 H), 7.68-7.64 (m, 3H), 7.59 (m, 1H), 7.49 (m, 1H), 7.39-7.34 (m, 4H), 7.16-7.11 (m, 6 H), 7.08-7.04 (m, 2H); ^{13}C NMR (200MHz, $CDCl_3$): δ 149.93, 149.74, 148.39, 147.86, 147.10, 140.19, 133.13, 133.04, 129.41, 128.46, 126.66, 126.53, 124.94, 124.03, 123.62, 123.47, 122.81, 113.54, 75.49; HRMS/EI: calcd for $C_{30}H_{19}N_3S_2$ (m/z) 485.1015; found = 485.1011

3. The convergent synthesis of 1



1

Figure S1 Chromatography-free scaled-up synthetic strategy for **1**. * indicates additional material that can easily be recovered from the filtrate by straightforward chromatography if desired and economically appropriate.



A selection of other canonical forms of the cyanopyridone

Figure S2 Canonical structures of **1** illustrating how cyanopridone provides strong electron accepting properties in donor(amine)-acceptor molecule via contribution of aromatized and other resonance forms.[1,2]

---

[1] F. Würthner, R. Wortmann, R. Matschiner, K. Lukaszuk, K. Meerholz, Y. DeNardin, R. Bittner, C. Bräuchle and R. Sens, *Angew. Chem. Int. Ed. Engl.*, 1997, **36**, 2765-2768.

[2] F. Würthner, R. Wortmann, and K. Meerholz, CHEMPHYSCHEM, 2002, **3**, 17-31.

4. Thin Film Absorption spectra of 1 and 2

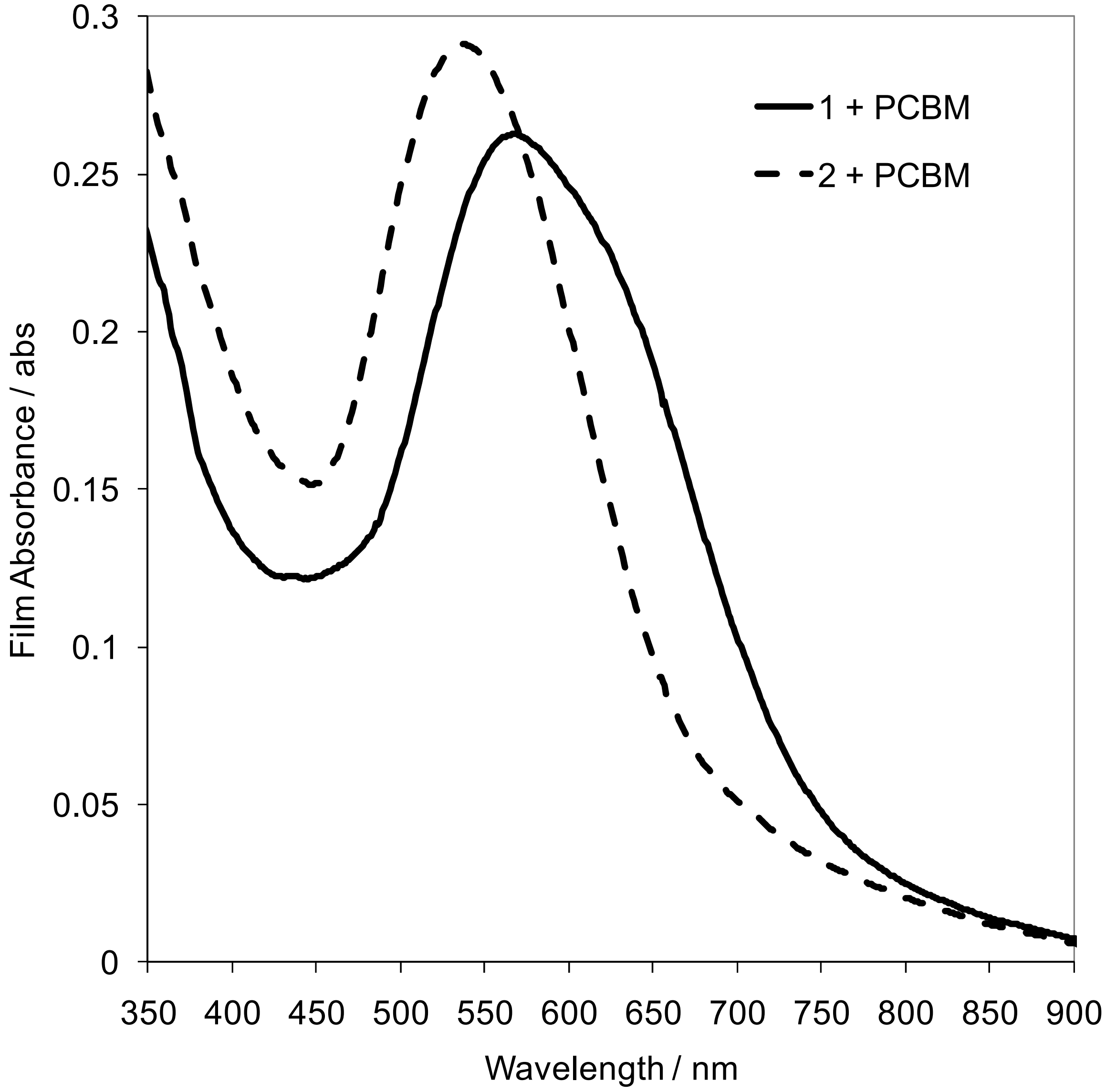
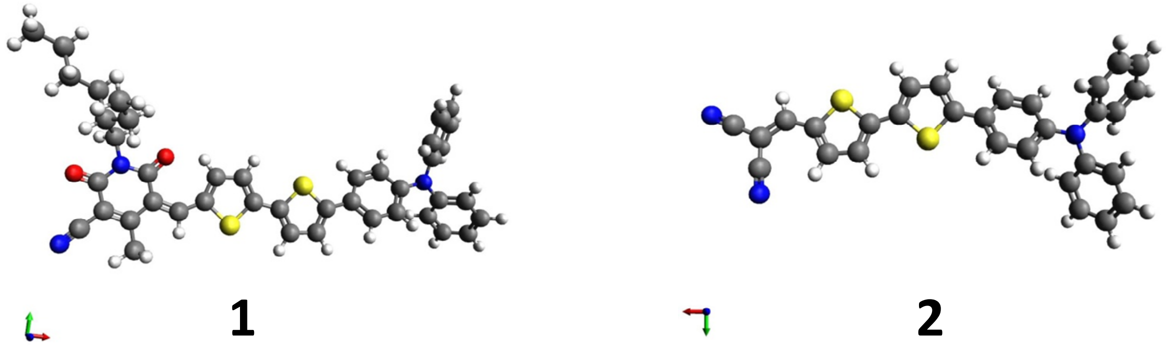


Figure S3 UV-Vis absorption spectra of films of **1** and **2** spun using conditions for the best performing devices. Blends of the materials and PCBM were spun on top of films of PEDOT:PSS. For compound **1** a 1:1 solution of **1** and PCBM (20 mg:20 mg) in chlorobenzene (1 mL) was spin-cast at 4000 rpm to give a film thickness of 46 nm. For compound **2** a 1:1 solution of **2** and PCBM (10 mg:10 mg) in chloroform (1 mL) was spin-cast at 4000 rpm to give a film thickness of 56 nm. Devices based films prepared under these conditions gave power conversion efficiencies of 2.25% (**1**) and 1.64% (**2**), see Section 7.2 and Section 7.3**.**

5. Energy Level Calculations



1

2

LUMO = -3.06 eV
HOMO = -5.20 eV

LUMO= -2.94 eV
HOMO= -5.21 eV

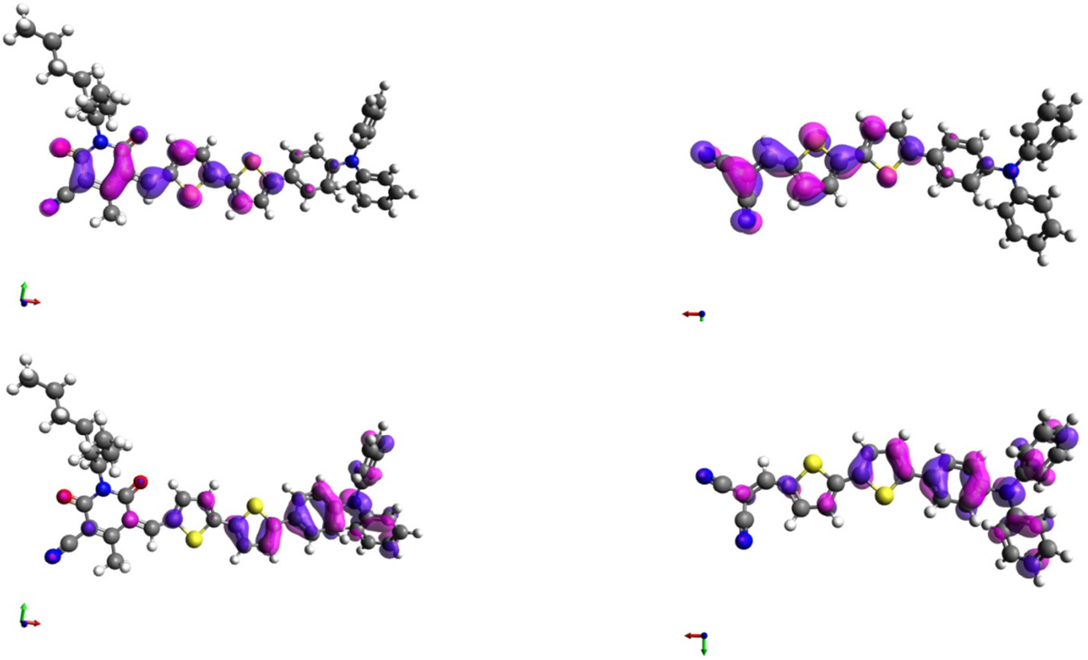


Figure S4 HOMO and LUMO orbital densities for **1** and **2** based on theoretical energy level calculations using the Gaussian 03 suite of programs and the B3LYP/6-311+G(d,p) // B3LYP/6-31G(d) level of theory

6. Cyclic-voltammograms

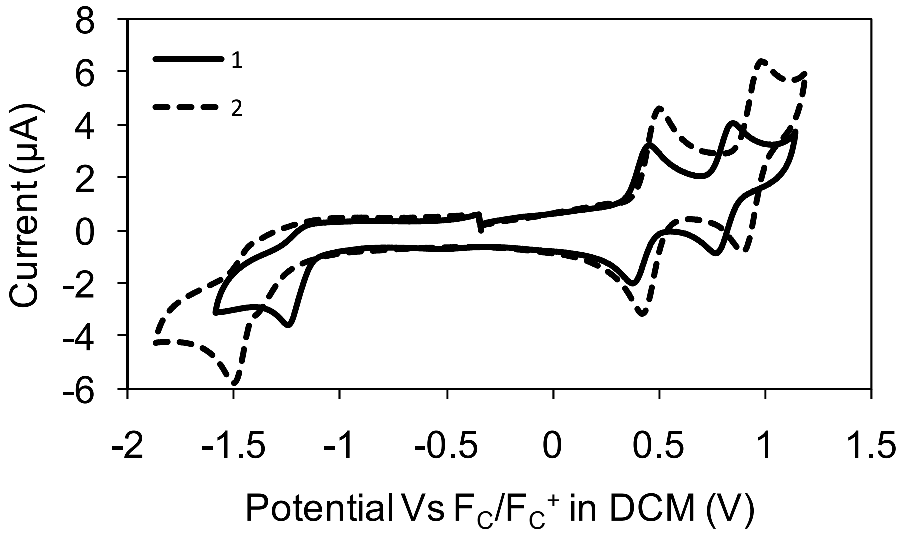


Figure S5 Cyclic-voltammograms in dichloromethane for **1** and **2**, at a sweep rate of 50 mV sec^{-1}, showing two reversible oxidation processes and one irreversible reduction process.

7. Detailed device fabrication results

7.1 Bi-layer device study for compound 1

Spin speed (rpm)	**C_{60} (nm)**	**V_{oc} (mV)**	**J_{sc} (mA/cm^2)**	**FF**	**η (%)**
4000[a]	20	655	2.44	0.56	0.89
4000[b]	20	525	2.47	0.56	0.72
4000[a]	25	590	2.83	0.59	1.00
4000[b]	25	585	3.02	0.58	1.02
4000[a]	30	595	3.51	0.51	1.06
4000[b]	30	595	3.37	0.55	1.13
4000[a]	**35**	**595**	**3.90**	**0.55**	**1.29**
4000[b]	35	570	3.69	0.54	1.14
5000[b]	35	610	3.02	0.62	1.14
4000[b]	35	600	3.04	0.63	1.14
3000[b]	35	550	2.88	0.60	0.96
2000[b]	35	540	2.63	0.58	0.82

Table S1: OPV device parameters for bilayer devices of compound **1**

Device Structure: ITO / PEDOT:PSS (38 nm) / **1** / C_{60} / BCP (10nm) / Al (100 nm)

Compound 1 was deposited by spin coating from a solution in chlorobenzene (20 mg / mL)

a: Layer of **1** was annealed at 120 ˚C for 10 mins prior to evaporation of the remaining layers

b: Layer of **1** was not annealed

7.2 Detailed BHJ device study based on compound 1

Blend ratio	Spin speed rpm	V_{oc} (mV)	J_{sc} (mA/cm^2)	FF	η (%)
1:4	2000^a	822	5.64	0.32	1.50
1:4	2000^b	643	4.43	0.32	0.90
1:2	3000^c	832	5.29	0.33	1.45
1:2	4000^c	871	5.7	0.33	1.62
1:1	3000^d	852	6.77	0.38	2.18
1:1	**4000^d**	**872**	**6.77**	**0.38**	**2.25**
1:1	5000^d	852	6.48	0.39	2.14
1:1	6000^d	862	5.9	0.38	1.95
1:1	1000^e	463	3.78	0.37	0.65
1:1	800^f	901	5.3	0.39	1.87
1:1	1000^f	901	5.73	0.43	2.20
1:1	1200^f	891	5.19	0.41	1.89
1:1	3000^g	901	7.09	0.35	2.23
1:1	4000^g	891	7.32	0.36	2.34
1:1	5000^g	911	7.16	0.35	2.29
1:1	6000^g	901	6.89	0.36	2.24

Table S2: OPV device parameters for BHJ devices of compound **1**

Device Structure: ITO / PEDOT:PSS (38 nm) / Active layer / Ca (20 nm) / Al (100 nm)

a: 10mg:40mg **1**: PCBM in 1 mL chlorobenzene, no annealing

b: 10mg:40mg **1**: PCBM in 1 mL chlorobenzene, annealed at 150 ˚C for 10 mins prior to evaporation of the remaining layers

c: 20mg:40mg **1**: PCBM in 1 mL chlorobenzene, no annealing

d: 20mg:20mg **1**: PCBM in 1 mL chlorobenzene, no annealing

e: 10mg:10mg **1**: PCBM in 1 mL chlorobenzene, annealed at 150 ˚C for 10 mins prior to evaporation of the remaining layers

f: 10mg:10mg **1**: PCBM in 1 mL chlorobenzene

g: 20mg:20mg **1**: PC$_{70}$BM in 1 mL chlorobenzene

IPCE spectrum for the **bold** device is shown in the figure in Section 7.4

The large-scale route to compound **1**, shown in Figure S1, resulted in a material with higher purity (HPLC purity ≥99% vs 98% for the smaller batch prepared by the route shown in Scheme 1). Devices fabricated using this batch showed slightly improved performances compared with devices prepared using the lower purity batches.

7.3 Compound 2 device optimisation including variation of solvents

Annealing of the devices at 120°C led to a drastic drop in V_{oc} resulting in conversion efficiencies close to zero. Data for optimised devices are shown below:

Active layer	**Spin speed rpm**	**V_{oc} (mV)**	**J_{sc} (mA/cm^2)**	**FF**	**η (%)**
a	4000	840	2.6	0.40	0.88
b	4000	980	4.7	0.36	1.64

Table S3: OPV device parameters for BHJ devices of compound **2**

a: 10mg:10mg **2**: PCBM in 1 mL chlorobenzene

b: 10mg:10mg **2**: PCBM in 1 mL chloroform

Device Structure: ITO / PEDOT:PSS (38 nm) / active layer / Ca (20 nm) / Al (100 nm)

IPCE spectrum for the **bold** device is shown in the figure in Section 7.4

7.4 BHJ Device IPCE spectra

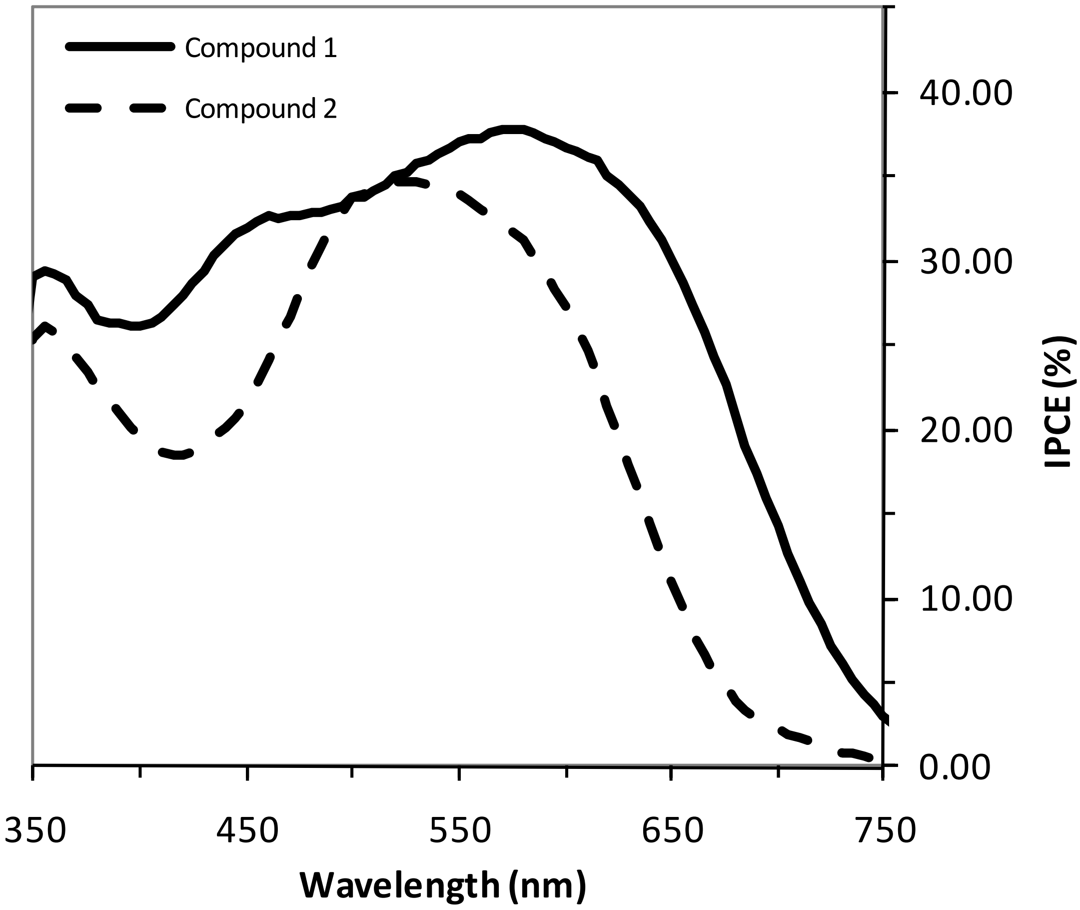


Figure S6 The Incident Photon Collection Efficiency (IPCE) data were collected using an Oriel 150W Xe lamp coupled to a monochromator and an optical fibre. The output of the optical fibre was focussed to give a beam that was contained within the area of the device. The IPCE was calibrated with a standard, unfiltered Si cell and the data was corrected to the output of the calibrated AM1.5 solar simulator response. IPCE data are for the **bold** devices described in Section 7.2 and 7.3.

7.5 Device fabrication details of compound 1 in air

Aqueous solutions of PEDOT/PSS (HC Starck, Baytron P AI 4083) were filtered (0.2 µm RC filter) and deposited onto glass substrates in air by spin coating (Laurell WS-400B-6NPP Lite Single Wafer Spin Processor) at 5000 rpm for 60 sec to give a layer having a thickness of 38 nm. The PEDOT/PSS layer was then optionally annealed on a hotplate in air at 145 °C for 10 minutes.

Blend solutions (20mg of **1** : 20mg PCBM in 1 ml chlorobenzene) were prepared in air (or N_2) for comparison. The solutions were heated at 70 °C for 1 h in air (or N_2) and cooled down to room temperature prior to spin coating. The blend solutions were deposited by spin coating at 4000 rpm (acceleration 10000 rpm/sec) for 1 min in air and films were annealed in air at 120 °C for 10 min. Deposition of Ca/Al was carried out in an evaporator inside a nitrogen-filled glove-box.

Activity	**Conditions 1**	**Conditions 2**	**Conditions 3**	**Conditions 4**
PEDOT:PSS	no anneal	no anneal	no anneal	anneal
Active layer prepared in	air	N_2	air	N_2
Active layer spin coated in	air	air	air	air
Active layer annealed at 120°C in air	no anneal	no anneal	anneal	no anneal
V_{oc} (V)	0.92	0.92	0.91	0.89
J_{sc} (mA/cm^2)	6.38	6.87	6.15	6.34
FF	0.42	0.415	0.39	0.4
Best device η (%)	**2.44**	**2.62**	**2.18**	**2.24**
Average η (%)	2.31	1.68	1.94	1.20

Table S4: OPV device parameters for BHJ devices of compound **1**

8 AFM images of blend films

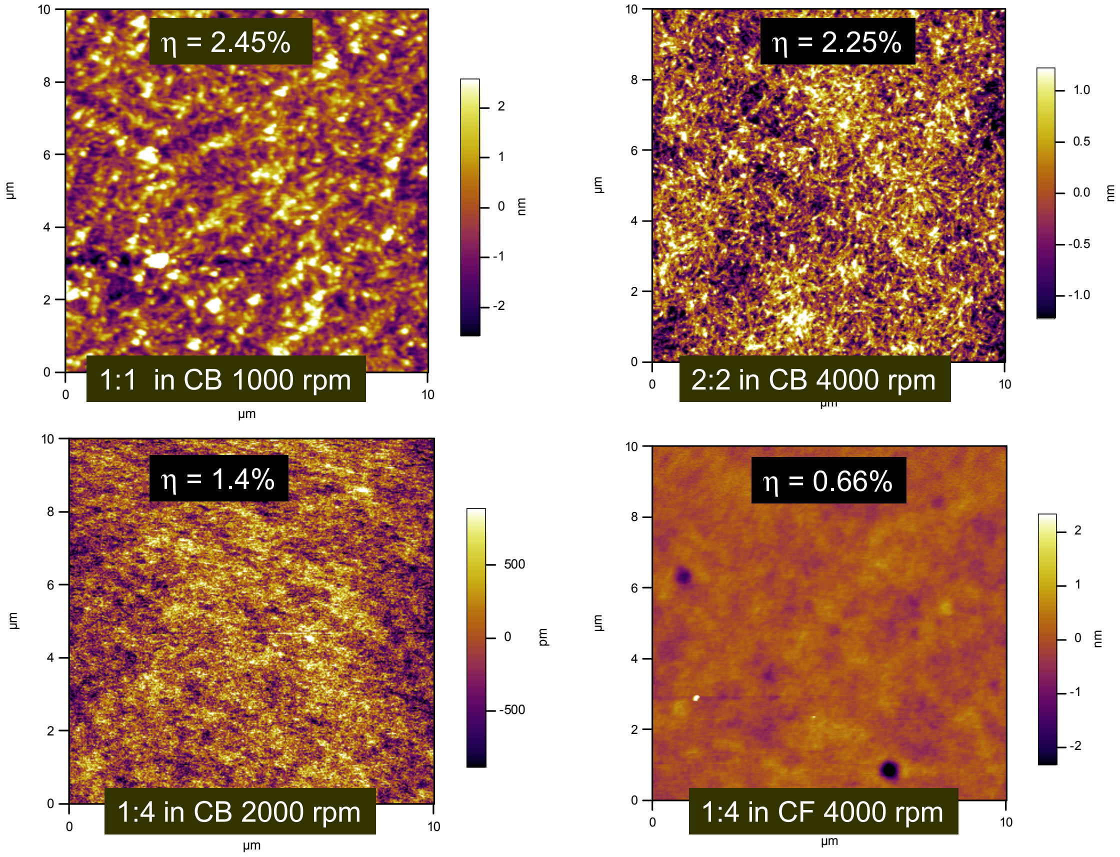
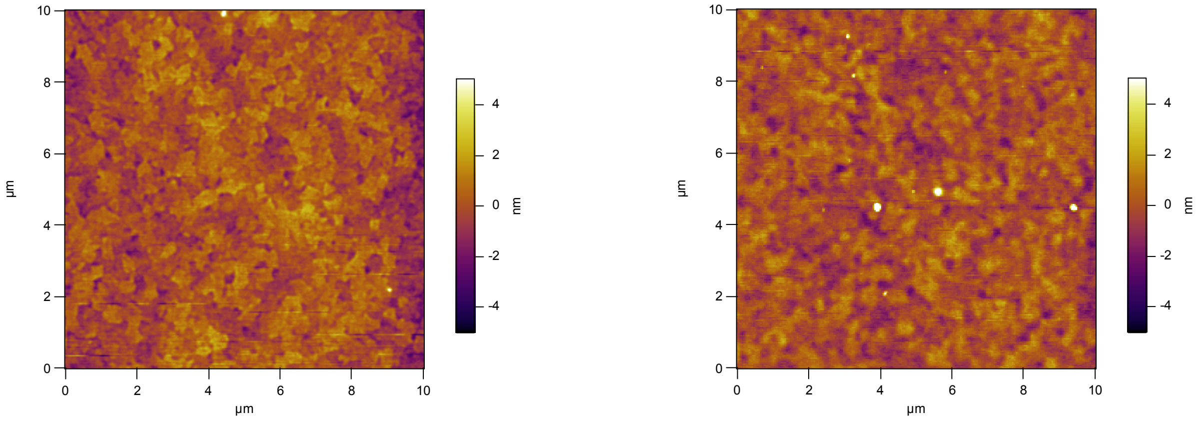


Figure S7 AFM images of $PC_{61}BM$-blended films of compound **1** spun at various spin speeds in different solvents. Unit for the AFM images is µm. CB=chlorobenzene, CF=chloroform, blend ratios and device power conversion efficiencies are as indicated.



(a) (b)

Figure S8 AFM images of $PC_{61}BM$-blended films of compound **2** spun from different solvents. Unit for the AFM images is µm. Solvents were chlorobenzene (a) and chloroform (b). Solution concentrations, blend ratios and device power conversion efficiencies were as indicated below.

Active layer	**Spin speed rpm**	V_{oc} **(mV)**	J_{sc} **(mA/cm^2)**	**FF**	**η (%)**
a	4000	840	2.6	0.40	0.88
b	4000	980	4.7	0.36	1.64

Table S5: OPV device parameters for BHJ devices of compound **2**

a: 10mg:10mg **2**: PCBM in 1 mL chlorobenzene

b: 10mg:10mg **2**: PCBM in 1 mL chloroform

Device Structure: ITO / PEDOT:PSS (38 nm) / active layer / Ca (20 nm) / Al (100 nm)

8 Mobility Measurements

Compound	**Hole Mobility (cm^2/Vs)**	**Electron Mobility (cm^2/Vs)**
1 pristine	1.8×10^{-6}	Not active
2 pristine	4.7×10^{-7}	Not active
1 blend (1:1 chlorobenzene)	4.2×10^{-6}	2.4×10^{-6}
2 blend (1:1 chlorobenzene)	8.2×10^{-7}	2×10^{-6}
2 blend (1:1 chloroform)	2.07×10^{-7}	1.19×10^{-5}

Table S6: OFET mobilities from devices based on compound **1** and **2**