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### **Supporting information**

Solution processed bulk heterojunction based on A-D-A small molecules with dihydroindoloindole (DINI) central donor with different acceptor end groups

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# Experimental Section Synthesis of core unit [1]



**1,2-Bis(2-nitrophenyl)ethylene (1).** 2-Iodonitrobenzene (24.9 g, 0.10 mol) was dissolved in dry toluene (220mL) and triethylamine (25 mL), the solution was purged with nitrogen, and  $PdCl_2(Ph_3P)_2$  (230 mg, 0.4 mmol) and CuI (115 mg, 0.6 mmol) were added, followed by (trimethylsilyl)acetylene (15.5 mL, 0.11 mol). The mixture was stirred for 12 h, hexane (80 mL) was added, and the suspension was filtered through a Celite plug. The resulting eluate was concentrated, the oily residue was dissolved in methanol (100 mL), and a solution of KOH (7.0 g) in methanol (60 mL) was slowly added while maintaining the temperature below 25 °C. The mixture was stirred for 0.5 h, concentrated to ca. 100 mL, poured into water (500 mL), and the product was extracted with ethyl acetate. The extract was dried with sodium sulfate and filtered through a short plug of silica prior to evaporation. The resulting crude (2) was dissolved in toluene (200 mL) containing triethylamine (25 mL) and 2-iodonitrobenzene (23.0 g), the solution was purged with nitrogen, and  $PdCl_2(Ph_3P)_2$  (230 mg, 0.4 mmol) were added. The mixture was stirred for 12 h at rt,

and the resulting yellow precipitate was isolated by filtration and crystallized from toluene to give 13.67 g (51% yield) of light-yellow solid; mp 187–189 °C dec. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  7.51–7.56 (m, 2H), 7.63–7.69 (m, 2H), 7.83 (d, J = 7.8 Hz, 2H), 8.14 (d, J = 8.3 Hz, 2H).



**1,2-Bis(2-nitrophenyl)ethane-1,2-dione(2)**. Compound 1 (19.94g, 74 mmol) was added to a mixture of potassium permanganate (35.2 g, 222 mmol), water (600 mL), TBAB (0.48 g, 1 mmol), methylene chloride (800 mL), and acetic acid (40 mL). The mixture was vigorously stirred at reflux for 7 h, cooled, and carefully decolorized with NaHSO<sub>3</sub>. The organic and aqueous were separated, and the yellow organic was dried with Na<sub>2</sub>SO<sub>4</sub> and filtered through Celite plug. After removal of solvent the resulting yellow crystalline solid was washed with methanol to give 18.90 g (85% yield) of the title compound; mp 206–207 °C. <sup>1</sup>H NMR (300

MHz, CDCl<sub>3</sub>): δ 7.68 (dd, J1 = 7.6 Hz, J2 = 1.2 Hz, 2H), 7.73–7.79 (m, 2H), 7.86–7.91 (m, 2H), 8.28 (dd, J1 = 8.3 Hz, J2 = 0.5 Hz, 2H).



Figure S2<sup>1</sup>H NMR spectra of compound 2



**5,10-Dihydroindolo[3,2-b]indole (3).** To a stirred mixture containing acetic acid (360 mL) and Zn powder (45.8 g, 700 mmol) was added 12 N HCl (3 mL) followed by 4 (21.00 g, 70 mmol), which was added in portions over 0.5 h while maintaining temperature below 40 °C. The mixture was stirred at 80 °C for 1 h, an additional amount of Zn (9.81 g, 200 mmol) was

added, and stirring was continued for another 2 h, before the reaction mixture was cooled to rt. The solids containing unreacted Zn and the product were isolated by filtration and washed twice with methanol, and the product was eluted with hot DMF (70–80 °C,  $3 \times 50$  mL). The cold eluent was poured slowly to stirred cold water (1200 mL), precipitated white solid was isolated by filtration, washed with water, several times with methanol, and dried initially in air and then under vacuum to yield 13.06 g (91%) of the title compound. <sup>1</sup>H NMR (300 MHz, THF):  $\delta$  8.03(s, 2H), 7.79 (d, J = 8.1 Hz, 2 H), 7.55 (d, J = 7.8 Hz, 2H), 7.19–7.22 (m, 2 H), 7.06–7.11 (m, 2 H).



Figure S3 <sup>1</sup>H NMR spectra of compound 3



**5,10-Di(n-hexyl)-5,10-dihydroindolo[3,2-b]indole (4).** NaH (2.64 g, 55 mmol, 50% in mineral oil) was stirred with hexane (25 mL) under nitrogen for a few minutes before stirring was turned o to allow NaH to settle at the bottom of the flask. After 30 min, the hexane solution was removed under a slight nitrogen pressure, using cannula tipped with a soft filter paper. The activated NaH was mixed with dry DMF (45 mL). Subsequently, 3 (4.08 g, 20 mmol) was added to the mixture in portions, followed by n-hexyl bromide (7.8 mL, 45 mmol), while maintaining temperature of the reaction mixture below 35 °C. The mixture was then stirred for 10 h at rt before it was poured slowly into cold water (600 mL). The precipitated solid material was isolated by filtration, washed with water and methanol, and dried under vacuum to yield 8.10 g (94%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  7.86 (d, 2H, J = 7.8 Hz), 7.48 (d, 2H, J = 8.1 Hz), 7.29–7.35 (t, 2H), 7.17–7.22 (t, 2H), 4.48–4.53 (t, 4H, J = 7.2 Hz), 1.94–2.04 (m, 4H), 1.18–1.44 (m, 12H), 0.86 (t, 6H, J = 7.2 Hz).



Figure S4<sup>1</sup>H NMR spectra of compound 4



**2,7-Dibromo-5,10-bis(n-hexyl)-5,10-dihydroindolo[3,2-b]indole (5).** To a solution of the crude 6 (4.30 g, 10 mmol) in a mixture of pyridine (8 mL) and chloroform (10 mL) was added Br<sub>2</sub> (1.1 mL, 21.5 mmol) in chloroform (10 mL) over a period of 30 min. After 2 h, the mixture was poured into 1 N HCl (200 mL) and ice, the product was extracted twice with ethyl acetate, and the combined organic layers were washed twice with water and dried over Na<sub>2</sub>SO<sub>4</sub> prior to evaporation. The crude product was crystallized from methanol–ethyl acetate to yield 3.59 g (61%) of the title compound as a yellow solid. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  7.63 (d, 2H, J = 8.4 Hz), 7.58 (d, 2H, J = 1.6 Hz), 7.27 (dd, 2H, J1 = 8.4 Hz, J2 = 1.6 Hz), 4.36–4.41 (t, 4H, J = 7.2 Hz), 1.93 (m, 4H), 1.17–1.41 (m, 12H), 0.85 (t, 6H, J = 7.0 Hz).



Figure S4<sup>1</sup>H NMR spectra of compound 5



#### 5,10-Bis(n-hexyl)-2,7-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan2-

yl)-5,10-dihydroindolo[3,2-b]indole (6). To a solution of compound 10 (2.35 g, 4.0 mmol) in THF (40 mL) was added dropwise 3.60 mL (9.0 mmol) of n-butyllithium (2.5 M in hexane) at -70 °C. The mixture was stirred at -78 °C for 2 h, and 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (2.65 mL, 13,0 mmol) was added rapidly to the suspension of the bis-lithium salt in THF. After an additional 1 h at -78 °C, the resulting mixture was warmed up to rt and stirred for 6 h, before it was poured into cold water (300 mL), extracted with ethyl acetate, and dried over sodium sulfate. The solvent was removed under reduced pressure, and the residue was purified by crystallization form methanol/ethyl acetate to yield the title product as light yellow crystals (1.73 g, 63%). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>):  $\delta$  7.93 (s, 2H), 7.89 (d, 2H, J = 7.8 Hz), 7.53 (d, 2H, J = 7.9 Hz), 4.60–4.65 (t, 4H, J = 7.2 Hz), 1.98 (m, 2H), 1.40 (s, 20H), 1.14–1.50 (m, 16H).



Figure S5<sup>1</sup>H NMR spectra of compound 6

#### Synthesise of Ligand [2]



**2-(4-Hexylthiophen-2-yl)-4,4,5,5-tetramethyl1,3,2-dioxaborolane (1a).** To a solution of 3-Hexylthiophene (4.0 mmol) in THF was added dropwise (4.4 mmol) of t-butyllithium at–78 °C. The mixture was stirred at -78 °C for 1 h, and 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.8 mmol) was added. The resulting mixture was warmed up to rt and stirred for 8 h, before it was poured into cold water , extracted with ethyl Et<sub>2</sub>O, and dried over sodium sulfate. The solvent was removed under reduced pressure, and the residue was purified by column chromatography on a silica gel. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, d, ppm) 7.53 (s, 1H), 7.02 (s, 1H), 2.75 (t, 2H), 1.62 (m, 2H), 1.31 (s, 12H), 0.85 (t, 3H)



**3,4' -Dihexyl-2,2'-bithiophene (2a).**  $Pd(PPh_3)_4$  (0.097 g, 0.084 mmol) was inserted into a two-necked 100-mL round-bottomed flask in a dry box. A mixture of 2-(4-hexylthiophen-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1.0 g, 3.39 mmol), 2-bromo-3-hexylthiophene (1.26 g, 5.08 mmol), toluene (10 mL), and THF (20 mL) was added to the reactor. Aliquat 336 (0.113 g, 0.28 mmol) as the phase-transfer catalyst and 2 M aqueous sodium carbonate solution (8 mL) were also added to the reaction mixture, and the reaction solution was stirred at 80°C for 24 h. Then, the reaction was quenched with methanol, the solvent was removed by rotary evaporation, and the residue was purified by reprecipitation several times in

methanol, affording the product as a pale liquid (65%, yield). <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>, d, ppm) 7.62 (d, 1H), 7.60 (d, 1H), 7.09 (s, 1H), 6.98 (d, 1H), 2.78 (m, 2H), 2.42 (m, 2H), 1.53 (m, 4H), 1.21 (m, 12H), 0.88 (t, 6H).



**3,4'-dihexyl-[2,2'-bithiophene]-5-carbaldehyde (3a)** [3]. 3,4'-dihexyl-2,2'-bithiophene (3 g, 9 mmol) was dissolved in dry THF solution under N2. n-BuLi (4.5 ml, 11.25 mmol) was dropwised at  $-78^{\circ}$ C, then the mixture was stirred for 1 h. DMF (1.31 g, 18 mmol) was added and the result mixture was kept for 2 h at room temperature. When the reaction was finished, water was added, and the mixture was extracted by EtOAc. After removing the solvent by rotary evaporation, the crude product was purified by CH<sub>2</sub>Cl<sub>2</sub> / petroleum ether (2 : 1) to give compound 1 (2.7 g, 82%) as yellow oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  9.81 (s, 1H), 7.58 (s, 1H), 7.10 (s, 1H), 7.01 (s, 1H), 2.59 – 2.81 (m, 4H), 1.61 – 1.68 (m, 4H), 1.32 – 1.38 (m, 12H), 0.87 – 0.91 (m, 9H)



Figure S6<sup>1</sup>H NMR spectra of compound 3a



**5'-Iodo-3,4'-dihexyl-[2,2'-bithiophene]-5-carbaldehyde (4a).** Compound 3a (5.68 mmol) was dissolved in THF and AcOH at 0°C , NIS (5.68 mmol) was added slowly and the result mixture was stirred for 3 h. When the reaction was finished, water was added and the mixture was extracted by  $CH_2Cl_2$ , organic layer was collected and concentrated by rotary evaporation. Crude product was purified by  $CH_2Cl_2$  / petroleum ether (2 : 1) to give compound 4 as yellow oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  9.82 (s, 1H), 7.57 (s, 1H), 6.91 (s, 1H), 2.72 – 2.77 (t, 2H), 2.52 – 2.57 (t, 2H), 1.53 – 1.65 (m, 4H), 1.34 – 1.28 (m, 12H), 0.91 –0.87 (m, 6H).



Figure S7 <sup>1</sup>H NMR spectra of compound 4a



**5,10-Di(n-hexyl)-5,10-dihydroindolo[3,2-b]indolebis(7-3,4'-dihexyl-[2,2'-bithiophene]-5carbaldehyde (5a).** 5'-Iodo-3,4'-dihexyl-[2,2'-bithiophene]-5-carbaldehyde (1.8mmol) was dissolved in dry THF. A solution of 4M K<sub>2</sub>CO<sub>3</sub> and 4 mol% Pd(PPh<sub>3</sub>)<sub>4</sub> were added into the reaction mixture and then 5,10-Bis(n-hexyl)-2,7-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan2-yl)-5,10-dihydroindolo[3,2-b]indole, (0.85mmol) was added under a nitrogen atmosphere. The solution was stirred at 80 ° C for 36 h. The mixture was poured into water and extracted with dichloromethane. The organic layer was then dried over anhydrous MgSO<sub>4</sub>. After evaporation of the solvent, the residue was purified by column chromatography on a silica gel (ethylacetate : hexane = 1:10 ) to afford a red oil. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>)  $\delta$  9.83 (s, 1H), 7.86 (d, J = 8.4Hz, 1H), 7.61 (s, 1H), 7.54 (s, 1H), 7.29(d, J = 8.4Hz, 1H), 7.23(s, 1H), 4.49 - 4.54 (t, 2H), 2.84 - 2.89 (t, 2H), 2.76 - 2.81 (t, 2H), 1.72 - 2.01(t, 2H), 1.70-1.74(t, 4H), 1.25 - 1.43 (m, 18H), 0.85 - 0.92 (m, 9H).



Figure S8 <sup>1</sup>H NMR spectra of compound 5a



# 2,2'-(5',5''-(5,10-dihexyl-5,10-dihydroindolo[3,2-b]indole-2,7-diyl)bis(3,4'-dihexyl-2,2'-bithiophene-5',5-diyl))bis(methan-1-yl-1-ylidene)dimalononitrile(DINI-DCV):

Malononitrile (120 mmol) dissolved in CHCl<sub>3</sub> (40 mL) was added to **5a** (20 mmol) followed by 2 drops of piperidine. The reaction was stirred for 2 h at room temperature. The mixture was poured into water and extracted with dichloromethane. The organic layer was then dried over anhydrous MgSO<sub>4</sub>. After evaporation of the solvent, the residue was purified by column chromatography on a silica gel (ethylacetate : hexane = 1:5 ). The crude product was washed with MeOH to afford a purple solid in 65% yield. <sup>1</sup>H NMR (300 MHz, CD<sub>2</sub>Cl<sub>2</sub>) :  $\delta$  7.87 (d, J = 8.4Hz, 1H), 7.73 (s, 1H), 7.57 (s, 1H), 7.53 (s, 1H), 7.33(s, 1H), 7.29 (dd, J = 8.4Hz, 1H), 4.53 - 4.57 (t, 2H), 2.88 - 2.94 (t, 2H), 2.79 - 2.84 (t, 2H), 2.03 - 2.05 (t, 2H), 1.72-1.77(t, 4H), 1.28 - 1.48 (m, 18H), 0.86 - 0.93 (m, 9H). <sup>13</sup>C NMR ( 75 MHz, CDCl<sub>3</sub>) :  $\delta$  150.20, 145.08, 143.73, 142.14, 142.01, 140.97, 140.47, 139.75, 131.92, 131.36, 127.25, 127.07, 119.97, 114.71, 114.08, 113.78, 110.75, 75.49, 45.69, 31.73, 31.25, 30.49, 30.23, 29.45, 29.30, 29.09, 27.06, 26.33, 22.68, 14.20. MS: m/z 1190.61 [M<sup>+</sup>]. Anal. calcd for C<sub>74</sub>H<sub>90</sub>N<sub>6</sub>S<sub>4</sub> : C, 74.58; H, 7.61. Found: C, 74.18; H, 7.58.



Figure S9b <sup>13</sup>C NMR spectra of compound **DINI-DCV** 



(2E,2'E)-dihexyl3,3'-(5',5''-(5,10-dihexyl-5,10-dihydroindolo[3,2-b]indole-2,7diyl)bis(3,4'-dihexyl-2,2'-bithiophene-5',5-diyl))bis(2-cyanoacrylate) (DINI-CA): Hexyl 2-cyanoacetate (120 mmol) dissolved in CHCl<sub>3</sub> (40 mL) was added to **5a** (20 mmol) followed by 2 drops of piperidine. The reaction was stirred overnight at room temperature. The mixture was poured into water and extracted with dichloromethane. The organic layer was then dried over anhydrous MgSO<sub>4</sub>. After evaporation of the solvent, the residue was purified by column chromatography on a silica gel (dichloromethane : hexane = 1:1 ). The crude product was washed with hexane and MeOH to afford a deep red solid in 53% yield. <sup>1</sup>H NMR (300 MHz, acetone)  $\delta$  8.35(s, 1H), 7.99 (d, J = 7.5Hz, 1H), 7.86 (s, 1H), 7.68 (s, 1H), 7.40 (s, 1H), 7.31( dd, J = 7.5Hz, 1H), 4.66 - 4.71 (t, 2H), 4.26 - 4.31 (t, 2H), 2.93 - 2.98 (t, 2H), 2.85 - 2.90 (t, 2H), 1.76 - 1.78 (m, 8H), 1.33-1.49(m, 24 H), 0.85 - 0.96 (m, 12H). <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) :  $\delta$  177.99, 177.42, 163.45, 159.13, 156.47, 147.06, 146.28, 143.02, 142.64, 140.90, 140.16, 139.45, 132.60, 132.47, 127.43, 126.97, 120.88, 116.33, 114.01, 97.26, 78.71, 66.66, 31.78, 31.55, 30.51, 29.49, 29.35, 29.12, 28.71, 27.08, 25.64, 22.78, 14.28. MS: m/z 1396.79 [M<sup>+</sup>]. Anal. calcd for C<sub>86</sub>H<sub>116</sub>N<sub>4</sub>O<sub>4</sub>S<sub>4</sub> : C, 73.88; H, 8.36. Found: C, 73.56; H, 8.30.



Figure S10b <sup>13</sup>C NMR spectra of compound DINI-CA



# 2,2'-(5',5''-(5,10-dihexyl-5,10-dihydroindolo[3,2-b]indole-2,7-diyl)bis(3,4'-dihexyl-2,2'bithiophene-5',5-diyl))bis(methan-1-yl-1-ylidene)bis(1H-indene-1,3(2H)-dione)

(**DINI-Ind**): 1,3-Indandione (120 mmol) dissolved in CHCl<sub>3</sub> (40 mL) was added to **5a** (20 mmol) followed by 2 drops of piperidine. The reaction was stirred at room temperature. The mixture was poured into water and extracted with dichloromethane. The organic layer was then dried over anhydrous MgSO<sub>4</sub>. After evaporation of the solvent, the residue was purified by column chromatography on a silica gel (ethylacetate : hexane = 1:5 ). The crude product was washed with MeOH to afford a purple solid in 62% yield. <sup>1</sup>H NMR (300 MHz, THF)  $\delta$  7.99(s, 1H), 7.87 - 7.95 (m, 4H), 7.77 - 7.85 (m, 2H), 7.61 (s, 1H), 7.39 (s, 1H), 7.28 (d, J = 7.8Hz, 1H), 4.60 - 4.62 (t, 2H), 2.91 - 2.96 (t, 2H), 2.82 - 2.88 (t, 2H), 1.80 - 2.04 (m, 4H), 1.67 - 1.80 (m, 2H), 1.40-1.46(m, 18H), 0.90 - 0.96 (m, 9H). <sup>13</sup>C NMR (400 MHz, CDCl<sub>3</sub>) :  $\delta$  190.00, 189.79, 146.49, 143.33, 142.12, 141.79, 141.23, 140.36, 140.04, 135.81, 135.74, 134.10, 131.30, 125.13, 123.51, 120.76, 118.92, 115.12, 111.56, 46.11, 32.89, 32.19, 32.13, 31.51, 31.28, 30.81, 30.47, 30.23, 29.93, 27.91, 26.01, 25.88, 25.61, 25.29, 25.09, 23.74, 23.66, 14.62, 1.53. MS: m/z 1350.64 [M<sup>+</sup>]. Anal. calcd for C<sub>86</sub>H<sub>98</sub>N<sub>2</sub>O<sub>4</sub>S<sub>4</sub> : C, 76.40; H, 7.31. Found: C, 76.33; H, 7.27.



Figure S11a <sup>1</sup>H NMR spectra of compound **DINI-IND** 



Figure S11b<sup>13</sup>C NMR spectra of compound **DINI-IND** 



(5E,5'E)-5,5'-(5',5''-(5,10-dihexyl-5,10-dihydroindolo[3,2-b]indole-2,7-diyl)bis(3,4'dihexyl-2,2'-bithiophene-5',5-diyl))bis(methan-1-yl-1-ylidene)bis(3-ethyl-2thioxothiazolidin-4-one)(DINI-Rho): 3-Ethylrhodanine(100 mmol) and AcONH<sub>4</sub>)dissolved in AcOH (40 mL) was added to 5a (5 mmol). The reaction was refluxed overnight. Then the product were isolated by filtration and washed with H<sub>2</sub>O and MeOH. The deep red product was dissolved in CHCl<sub>3</sub> and dried over anhydrous Na<sub>2</sub>SO<sub>4</sub>. After evaporation of the solvent, the residue was purified by column chromatography on a silica gel (dichloromethane : hexane = 2 : 3 ). The crude product was washed with hexane and MeOH to afford a red-purple solid in 74% yield. <sup>1</sup>H NMR (300 MHz, CD<sub>2</sub>Cl<sub>2</sub>) δ 7.88(d, J = 7.5 Hz, 1H), 7.81 (s, 1H), 7.56 (s, 1H), 7.30 - 7.32 (m, 2H), 7.24(s, 1H), 4.54 - 4.56 (t, 2H), 4.14 - 4.21 (q, 2H), 2.86 - 2.91 (t, 2H), 2.78 - 2.84 (t, 2H), 2.00 - 2.03 (t, 2H), 1.70 - 1.74 (m, 4H), 1.27-1.41(m, 18H), 0.85 -0.94 (m, 12H). <sup>13</sup>C NMR ( 400 MHz, CDCl<sub>3</sub>) :192.41, 185.87, 184.43, 168.22, 150.46, 138.90, 130.61, 125.97, 40.12, 31.95, 31.85, 30.52, 29.92, 29.58, 29.44, 27.14, 22.87, 22.84, 22.78, 14.31, 14.24, 12.52. MS: m/z 1380.56 [M<sup>+</sup>]. Anal. calcd for C<sub>78</sub>H<sub>100</sub>N<sub>4</sub>O<sub>2</sub>S<sub>8</sub>: C, 67.78; H, 7.29. Found: C, 67.53; H, 7.22.



Figure S12a <sup>1</sup>H NMR spectra of compound **DINI-Rho** 



Figure S12b <sup>13</sup>C NMR spectra of compound DINI-Rho



Figure S13 cyclic voltammograms for the DINI-CN, DINI-CA, DINI-Ind and DINI-Rho.



Figure S14 Normalized absorption and emission spectra of **DINI-CN**, **DINI-CA**, **DINI-Ind** and **DINI-Rho** in solution.

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