Supporting information

Optimal Bulk Morphology *via* Side-chain Engineering on Non-fullerene Acceptor for Efficient Organic Solar Cells

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1. General characterization

All ¹H, ¹³C nuclear magnetic resonance spectra (NMR) were measured in CDCl₃ on a Bruker Advance III HD system operating at 400 MHz. Solution and film UV-Vis absorption spectra were performed on Lambda 25 spectrophotometer. All film samples were spin-cast on ITO substrates. UV-Vis absorption spectra were collected from the solution of three small molecules with a concentration of less than 10⁻⁶ M in chloroform. Cyclic voltammetry (CV) measurements were taken on a CHI660D electrochemical workstation. The CV experiments were carried out at room temperature with a conventional three-electrode system using a glassy carbon electrode as the working electrode, Pt wire as the counter electrode, and a saturated calomel electrode as the reference electrode. Tetrabutylammonium phosphorus hexafluoride (Bu4NPF6, 0.1 M) in acetonitrile solution was used as the supporting electrolyte, and the scan rate was 100 mV/s. Ferrocene/Ferrocenium (Fc/Fc⁺) was used as the internal standard, and their energy levels are assumed at -4.8 eV relative to vacuum. Small molecules were dropped and cast onto the glassy carbon electrode from chloroform solutions (1 mg/mL) to form thin films. Thermal gravimetric analysis (TGA) measurements were performed on STA-409 at a heating rate of 10 °C min⁻¹. Differential scanning calorimetry (DSC Q200 V24.4) measurements were performed with a heating/cooling rate of 10 $^{\circ}$ C min⁻¹ under N_2 . The number-average molecular weight (M_n) and polydispersity index (PDI) of PM6 donor was characterized using gel permeation chromatography (GPC) at 80 °C using odichlorobenzene as the eluent relative to polystyrene standards. 2D GIWAXS measurements were performed at the 9A (U-SAXS) beamline at the Pohang Accelerator Laboratory, Korea. The surface morphology of the films was characterized using AFM (Advanced Scanning Probe Microscope, XE-100, PSIA) in tapping mode.

2. Synthesis

Brominated 1,1-dicyanomethylene-3-indanone (IC-Br) was purchased from SunaTech Inc. (Suzhou, China). 4,7-dibromo-5,6-dinitrobenzo[c][1,2,5]-thiadiazole and tributyl(6-undecylthieno[3,2-b]thiophene-2-yl)stannane were purchased from Derthon Optoelectronic Materials Science Technology Co. LTD. The other chemicals and solvents were reagent grades purchased from Aladdin or Energy Chemical and used without further purification. 5,6-dinitro-4,7-bis(6-undecylthieno[3,2-b]thiophen-2yl)benzo[c]-[1,2,5]thiadiazole (Compound 1), 12-(2-hexyldecyl)-13-(pentadecan-7yl)-3,9-diundecyl-12,13-dihydro-[1,2,5]thiadiazolo[3,4

e]thieno[2",3":4',5']thieno[2',3':4,5]pyrrolo[3,2-g]thieno[2',3':4,5]thieno[3,2-b]indole-2,10-dicarbaldehyde (Compound 3a), 12-(nonadecan-9-yl)-13-(2-octyldodecyl)-3,9diundecyl-12,13-dihydro-[1,2,5]thiadiazolo[3,4-

e]thieno[2",3":4',5']thieno[2',3':4,5]pyrrolo[3,2-g]thieno[2',3':4,5]thieno[3,2-b]indole-

2,10-dicarbaldehyde (Compound 3b), and 12-(2-decyltetradecyl)-13-(tricosan-11-yl)-

3,9-diundecyl-12,13-dihydro-[1,2,5]thiadiazolo[3,4-

e]thieno[2",3":4',5']thieno[2',3':4,5]pyrrolo[3,2-g]thieno[2',3':4,5]thieno[3,2-b]indole-

2,10-dicarbaldehyde (Compound 3c) were synthesized according to literature.¹



Scheme 1. Synthetic routes to the Y-2Br-HD, Y-2Br-OD, and Y-2Br-DT.

Compound 2a: Compound 1 (0.50 g, 0.62 mmol) and triethyl phosphate (1.10 g, 6.62 mmol) were dissolved in the *o*-dichlorobenzene (*o*-DCB, 10 mL) under nitrogen. After being heated at 180 °C overnight, the aqueous phase was extracted with dichloromethane, and the organic layer was dried over MgSO₄ and filtered. After removing the solvent, the red residue was added to a three-necked round bottom flask. 1-Bromo-2-hexyldecyl (1.50 g, 4.96 mmol), potassium hydroxide (0.3 g, 4.96 mmol), and DMF (15 mL) were added, and the mixture was deoxygenated with argon for 15 min. The mixture was refluxed at 95 °C for 15 h. After removing the solvent from the filtrate, the residue was extracted with DCM and H₂O. The organic layers were combined and dried over MgSO₄, filtered, and purified with column chromatography on silica gel using dichloromethane /petroleum ether (1/15, v/v) as the eluent to give a red solid (0.36 g, 48.8%). ¹H NMR (400 MHz, CDCl₃), δ (ppm): 7.01 (s, 2H), 4.58-4.60 (d, 4H), 2.80-2.84 (t, 4H), 2.06 (m, 2H), 1.84-1.88 (m, 4H), 1.25-1.30 (m, 38H), 0.97-1.02 (m, 24H), 0.66-0.77 (m, 18H).

Compound 2b: Synthesis of 2b was carried out in a similar manner to that of 2a. ¹H NMR (400 MHZ, CDCl₃), δ (ppm): 7.01 (s, 2H), 4.58-4.60 (d, 4H), 2.80-2.84 (t, 4H),

2.06 (m, 2H), 1.84-1.88 (m, 4H), 1.25-1.30 (m, 60H), 0.97-1.02 (m, 34H), 0.66-0.77 (m, 18H).

Compound 2c: Synthesis of 2c was carried out in a similar manner to that of 2a. ¹H NMR (400MHZ, CDCl₃), δ(ppm): 7.00 (s, 2H), 4.57-4.59 (d, 4H), 2.80-2.83 (t, 4H), 2.06 (m, 2H), 1.84-1.88 (m, 4H), 1.16-1.27 (m, 62H), 0.85-0.90 (m, 32H).

Compound 3a: To a solution of compound 2a (0.30 g, 0.25 mmol) in DCE (5 mL) and DMF (3.30 mL) at 0 °C, phosphorous oxychloride (0.40 mL, 3.75 mmol) was added slowly under the protection of argon. After stirring at 0 °C for 1 h and then refluxed at 85 °C overnight. The reaction mixture was poured into deionized water (10 mL) and then extracted with dichloromethane three times. The combined organic layer was washed with water, dried over MgSO₄, and the solvents were distilled under reduced pressure. The residue was purified by silica gel column chromatography, using petroleum ether/dichloromethane (4/1, v/v) as the eluent to give 3a as a red solid (0.30 g, 96.20%). ¹H NMR (400 MHZ, CDCl₃), δ (ppm): 10.14 (s, 2H), 4.61-4.63 (d, 4H), 3.18-3.20 (d, 2H), 1.93 (m, 2H), 1.21-1.29 (m, 64H), 0.87 (t, 18H).

Compound 3b: Synthesis of 3b was carried out in a similar manner to that of 3a. ¹H NMR (400 MHZ, CDCl₃), δ(ppm): 10.14 (s, 2H), 4.61-4.63 (d, 4H), 3.18-3.20 (d, 2H), 1.93 (m, 2H), 1.21-1.29 (m, 64H), 0.87 (t, 18H).

Compound 3c: Synthesis of 3c was carried out in a similar manner to that of 3a. ¹H NMR (400 MHZ, CDCl₃), δ(ppm): 10.14 (s, 2H), 4.61-4.63 (d, 4H), 3.18-3.20 (d, 2H), 1.93 (m, 2H), 1.21-1.29 (m, 64H), 0.87 (t, 18H).

Y-2Br-HD: To a solution of 3a (100 mg, 0.08 mmol) in CHCl3 (10 mL) was added IC-

Br-*m* (a mixture of IC-Br- γ and IC-Br- δ , 74 mg, 0.32 mmol), and pyridine (1 mL) at room temperature. The mixture was heated to 70 °C reflux for 15 h. After removal of the solvent, the crude product was purified via column chromatography (silica gel) by using petroleum ether/dichloromethane (3/1, v/v) as eluent to give Y-2Br-HD as a blue-black solid with metallic luster (125.23 mg, 88.6%). The corresponding ¹H NMR spectra were shown in Fig. S1, and ¹³C NMR was shown in Fig. S2. ¹H NMR (400 MHz, CDCl₃), δ (ppm): 9.18 (s, 2H), 8.84 (s, 1H), 8.52 (d, J = 8.4 Hz, 1H), 8.03 (d, J =1.6 Hz, 1H), 7.78-7.89 (m, 3H), 4.77 (m, 4H), 3.20 (t, *J* = 7.5 Hz, 4H), 2.14 (m, 2H), 1.91-1.83 (m, 4H), 1.55-1.49 (m, 4H), 1.38-1.36 (m, 4H), 1.33-1.23 (m, 30H), 1.24-1.12 (m,14H), 1.04-0.99 (m, 30H), 0.88-0.81(m, 18H). ¹³C NMR (400 MHz, CDCl₃), δ (ppm): 187.34, 160.01, 159.40, 153.63, 147.51, 145.13, 141.40, 138.36, 137.74, 137.65, 137.20, 135.95, 135.49, 134.18, 133.51, 130.14, 129.44, 128.20, 126.70, 126.43, 124.51, 120.26, 115.27, 115.12, 114.57, 113.57, 68.88, 68.35, 55.60, 39.19, 31.92, 31.83, 31.63, 31.58, 31.21, 30.60, 29.86, 29.83, 29.79, 29.75, 29.70, 29.66, 29.62, 29.52, 29.45, 29.39, 29.34, 29.20, 29.18, 25.57, 22.69, 22.60, 22.51, 22.48, 14.11, 14.04, 14.02.

Y-2Br-OD: The synthesis of Y-2Br-OD was carried out similarly to that of Y-2Br-HD. The corresponding ¹H NMR spectra were shown in Fig. S3 and 13C NMR in Fig. S4. ¹H NMR (400 MHz, CDCl₃), δ (ppm): 9.20 (s, 2H), 8.86 (s, 1H), 8.58-8.60 (d, J = 8.4Hz, 1H), 8.04 (d, J = 1.6 Hz, 1H), 7.87-7.89 (m, 2H),7.78-7.80 (d, 1H), 4.75 (m, 4H), 3.22-3.26 (t, J = 7.5 Hz, 4H), 2.10 (m, 2H), 2.00-2.02 (m, 4H), 1.87-1.89(m, 4H), 1.11-1.27 (m, 76H), 0.81-0.87 (m, 26H). ¹³C NMR (400 MHz, CDCl₃), δ (ppm): 187.35, 159.99, 153.64, 147.50, 145.13, 141.39, 137.76, 137.20, 135.47, 134.15, 133.50, 130.15, 128.20, 126.70, 124.52, 120.22, 120.14, 115.11, 113.57, 77.21, 68.85, 55.67, 39.12, 31.92, 31.83, 31.24, 30.53, 29.89, 29.77, 29.67, 29.63, 29.55, 29.46, 29.42, 29.36, 29.33, 29.22, 29.19, 25.56, 22.70, 22.61, 14.13.

Y-2Br-DT: The synthesis of Y-2Br-DT was carried out similarly to that of Y-2Br-HD. The corresponding ¹H NMR spectra were shown in Fig. S5, and ¹³C NMR was shown in Fig. S6. ¹H NMR (400 MHz, CDCl₃), δ(ppm): 9.20 (s, 2H), 8.86 (s, 1H), 8.58-8.60 (d, *J* = 8.4 Hz, 1H), 8.04 (d, *J* = 1.6 Hz, 1H), 7.87-7.89 (m, 2H), 7.78-7.80 (d, 1H), 4.76 (m, 4H), 3.22-3.24 (t, *J* = 7.5 Hz, 4H), 2.10 (m, 2H), 2.00-2.02 (m, 4H), 1.89-1.90 (m, 4H), 1.11-1.27 (m, 80H), 0.81-0.87 (m, 26H). ¹³C NMR (400 MHz, CDCl₃), δ(ppm): 186.89, 159.92, 158.58, 153.61, 147.50, 145.13, 137.77, 138.84, 137.69, 137.62, 137.16, 135.92, 135.47, 133.49, 130.84, 129.43, 126.70, 126.39, 120.14, 115.24, 113.56, 77.21, 68.33, 55.74, 39.17, 31.95, 31.92, 31.23, 30.59, 29.89, 29.78, 29.69, 29.67, 29.63, 29.55, 29.43, 29.42, 29.40, 29.35, 29.33, 25.59, 25.53, 22.70, 22.68, 14.10.





Fig. S1 ¹H NMR spectrum of Y-2Br-HD (400 MHz, CDCl₃).





Fig. S2 ¹³C NMR spectrum of Y-2Br-HD (400 MHz, CDCl₃).

Fig. S3 ¹H NMR spectrum of Y-2Br-OD (400 MHz, CDCl₃).



f1 (ppm)

Fig. S4 ¹³C NMR spectrum of Y-2Br-OD (400 MHz, CDCl₃).



Fig. S5 ¹H NMR spectrum of Y-2Br-DT (400 MHz, CDCl₃).



Fig. S6¹³C NMR spectrum of Y-2Br-DT (400 MHz, CDCl₃).

4. TGA measurements



Fig. S7 TGA curves of the Y-2Br-HD, Y-2Br-OD and Y-2Br-DT.

5. DSC measurements



Fig. S8 Differential scanning calorimetry (DSC) characteristics for Y-2Br-HD (a), Y-

2Br-OD (b), and Y-2Br-DT (c).

6. CV measurements



Fig. S9 Cyclic voltammograms of the ferrocene (Fc/Fc⁺).



Fig. S10 Cyclic voltammogram of the donor polymer PM6.

7. Device fabrication and measurements

Conventional solar cells

The device structures were ITO/PEDOT: PSS/Active layer/PDINO/Al. ITO-coated glass substrates were cleaned with detergent water, deionized water, acetone, and isopropyl alcohol in an ultrasonic bath sequentially for 30 min and further treated with UV exposure for 20 min in a UV-ozone chamber. A thin layer (ca. 40 nm) of PEDOT: PSS (Baytron P VP AI 4083, H. C. Starck) was first spin-coated on the substrates at 4000 rpm and baked at 150 °C for 15 min under ambient conditions. The substrates were then transferred into a nitrogen-filled glove box. The optimized concentration was 17 mg/ml chloroform solution with the solvent additive of 1-chloronaphthalene (CN) (0.5%, v/v), the weight ratio of PM6: acceptor is 1:1.2. After spin coating, the blend films were thermalannealed at 85 °C for 5 min. The active layer thickness was around 100 nm. Then PDINO (\sim 15 nm) as the electron transporting layer was spin-coated on the active layer by 3000 rpm from methanal solution. Finally, the substrates were transferred to a thermal evaporator, and top electrode was evaporated at a pressure of 2×10^{-4} Pa. The current density-voltage characteristics of the photovoltaic cells were measured using a Keithley 2400 (I-V) digital source meter under a simulated AM 1.5

G solar irradiation at 100 mW/cm² (SAN-EI Electric Co., LTD, AAA Class Solar Simulator, XES- 40S3). The film thickness data were obtained via a surface profilometer (Dektak XT, Bruker). The light intensity is calibrated by a certified Oriel Reference Cell (91150 V) and verified with an NREL calibrated Hamamatsu S1787-04 diode. The external quantum efficiency (EQE) was determined by solar cell spectral response measurement system QE-R3011 (Enli Technology Co., Ltd.)

Hole- and electron-only devices

The hole or electron mobilities were measured using the space charge limited current (SCLC) method. The hole-only or electron-only devices were fabricated using the following architectures: ITO/PEDOT: PSS(40 nm)/active layer (100 nm) /MoO₃(10 nm)/A1 (100 nm) for holes and ITO/ZnO(40 nm)/active layer(100 nm) /Ca(4 nm) /Al(100 nm) for electrons. The films were prepared under the same fabrication conditions as the optimized devices, and the measured *J-V* characteristics were fitted to the Mott-Gurney equation:

$$J = \frac{9\varepsilon_0 \varepsilon_r \mu (V_{appl} - V_{bi})^2}{8L^3}$$

Where J is the current density of the hole-only or electron-only devices, ε_0 is the permittivity of free-space, ε_r is the relative permittivity of the material, μ is the mobility, V_{appl} is the applied voltage, V_{bi} is s the built-involtage and L is the thickness of the active layer.

8. SCLC measurements for PM6:Y-2Br-HD, PM6:Y-2Br-OD, and PM6:Y-2Br-DT blend films



Fig. S11 The experimental current density-applied voltage characteristics for (a) holeonly and (b) electron-only devices.

Table S1 The electron and hole mobility results measured by SCLC method.

Device	$\mu_{e} (\times 10^{-4} \text{ cm}^{2} \text{V}^{-1} \text{s}^{-1})$	$\mu_{\rm h} (\times 10^{-4}{\rm cm}^2{\rm V}^{-1}{\rm s}^{-1})$	$\mu_{\rm e}^{\prime}/\mu_{\rm h}$
PM6:Y-2Br-HD	11.7±0.28	2.19±0.20	5.3
PM6:Y-2Br-OD	10.8±0.50	1.56±0.53	6.9
PM6:Y-2Br-DT	8.35±0.48	1.38±0.24	6.1

9. Optimization of device performance

Table S2 Photovoltaic performances of the OSCs based on PM6 donors: acceptros(1:1.2, w/w) with different annealing temperatures under the illumination of AM 1.5G,

100 mW cm⁻²

Active layer	T (°C)	$V_{ m oc}\left({ m V} ight)$	$J_{\rm sc} ({\rm mA/cm}^2)$	FF (%)	PCE (%)
PM6:Y-2Br-HD	25	0.904±0.008	21.36±0.13	69.4±0.5	13.39±0.16
	85	0.909±0.004	23.45±0.23	66.3±0.5	14.13±0.03
	100	0.856±0.011	22.19±0.15	69.8±0.7	13.25±0.21

	125	0.832 ± 0.008	21.51±0.16	69.2±0.5	12.39±0.11
	150	0.774±0.009	21.38±0.32	65.2±0.9	10.78±0.11
	25	0.900±0.012	21.30±0.61	67.5±0.4	12.95±0.46
	85	0.903±0.018	21.91±1.30	68.2±2.2	13.48±0.10
PM6:Y-2Br-OD	100	0.841±0.012	22.46±0.23	66.4±0.5	12.55±0.25
	125	0.802±0.019	21.24±0.48	66.5±1.5	11.33±0.26
	150	0.746±0.012	17.36±0.25	62.8±0.5	8.13±0.22
	25	0.887±0.005	21.68±0.07	67.0±0.3	12.89±0.16
	85	0.904±0.012	22.52±0.17	66.1±2.7	13.46±0.27
PM6:Y-2Br-DT	100	0.813±0.010	22.33±0.45	67.7±0.1	12.28±0.12
	125	0.824±0.011	21.65±0.44	68.4±0.8	12.19±0.14
	150	0.791±0.009	20.65±0.13	65.5±0.2	10.70±0.10

Table S3 Photovoltaic parameters of the OSCs based on PM6 donors: acceptros (1:1.2, w/w) with with different volume ratios of CN under the illumination of AM 1.5G, 100 mW cm⁻².

Active layer	CN(%)	$V_{\rm oc}$ (V)	$J_{\rm sc} ({\rm mA/cm}^2)$	FF (%)	PCE (%)
PM6:Y-2Br-HD	0	0.909±0.004	23.45±0.23	66.3±0.5	14.13±0.03
	0.5	$0.897 {\pm} 0.007$	23.30±0.03	70.9±0.5	14.80±0.23
	1	0.903±0.011	22.26±0.16	68.2±0.6	13.71±0.28

PM6:Y-2Br-OD	0	0.903±0.018	21.91±1.30	68.2±2.2	13.48±0.10
	0.5	0.898±0.005	22.21±0.14	68.1±0.8	13.59±0.15
	1	0.896±0.011	22.28±0.59	67.3±0.7	13.43±0.33
PM6:Y-2Br-DT	0	0.904±0.012	22.52±0.17	66.1±2.7	13.46±0.27
	0.5	0.889±0.006	22.40±0.09	69.0±0.4	13.74±0.07
	1	0.910±0.008	22.73±0.12	64.9±0.9	13.42±0.13

Table S4 Photovoltaic parameters of the OSCs based on PM6 donors: acceptros (1:1.2, w/w) with different active layer thickness under the illumination of AM 1.5G, 100 mW cm⁻².

Active layer	Thickness(nm)	$V_{\rm oc}$ (V)	$J_{\rm sc} ({\rm mA/cm}^2)$	FF (%)	PCE (%) ^a
	103	0.900±0.007	23.65±0.34	70.90±0.5	15.11±0.17
PM6:Y-2Br-HD	92	0.906±0.011	23.41±0.51	67.2±1.0	14.25±0.17
	84	0.912±0.008	22.52±0.39	67.5±0.5	13.86±0.15
PM6:Y-2Br-OD	106	0.910±0.009	22.54±0.16	68.2±0.4	14.03±0.11
	95	0.919±0.009	21.81±0.30	66.3±0.4	13.28±0.25
	87	0.911±0.011	22.22±0.14	64.7±0.8	13.08±0.14
PM6:Y-2Br-DT	104	0.900±0.007	22.70±0.22	68.8±0.5	14.01±0.13
	94	0.913±0.010	22.53±0.10	64.3±0.6	13.21±0.21

^a The devices were fabricated by spin-coating a mixed solvent of CF/CN (100:5 by volume) solution, the blend films were thermal annealed at 85 °C for 5 min. Average value in brackets was obtained from 10 devices.



Fig. S12 Composition distribution as a function of film depth for (a) PM6:Y-2Br-HD,

(b) PM6:Y-2Br-OD, and (c) PM6:Y-2Br-DT blend films.

11. GIWAXS data for PM6, Y-2Br-HD, Y-2Br-OD, and Y-2Br-DT pure films and

PM6:Y-2Br-HD, PM6:Y-2Br-OD, and PM6:Y-2Br-DT blend films

Table S5 Summary of the parameters for the neat and blend films obtained from the

		Out of pla	ne		In plane			
			FWHM	CCL			FWHM	CCL
Materials	d-spacing	d-spacing	(010)	(010)	<i>d</i> -spacing	d-spacing	(100)	(100)
((010) (Å)	(010)' (Å)	(Å)	(Å)	(100) (Å)	(200) (Å)	(Å)	(Å)
PM6	3.8	N/A	0.334	17.1	21.7	N/A	0.102	55.5

2D-GIWAXS measurements.

	(1.662 Å^{-1})				(0.289 Å^{-1})			
V 2Br HD	3.6	3.9	0.110	51.0	21.2	10.4	0.066	86.5
1-201-110	(1.748 Å^{-1})	(1.593 Å^{-1})	0.110	51.9	(0.297 Å^{-1})	(0.603 Å^{-1})	0.000	80.5
V AD OD	3.8		0.410	12.0	22.9		0.140	40.4
Y-2Br-OD	(1.687 Å^{-1})	N/A	0.412	13.9	(0.274 Å^{-1})	N/A	0.140	40.4
	3.6	4.0	0.092	(1.(21.2	10.5	0.029	195.3
Y-2BF-D1	(1.766 Å^{-1})	(1.560 Å^{-1})		01.0	(0.296 Å^{-1})	(0.597 Å^{-1})		
DMG V 2D- HD	3.7		0.204	10.0	21.3	NT/A	0.074	76 4
PM6:Y-2Br-HD	(1.697 Å^{-1})	N/A	0.304	304 18.8	(0.295 Å^{-1})	IN/A	0.074	/0.4
DMGY 2Dr OD	3.7		0.220	16.0	21.3	NT/A	0.070	00.0
PM6:Y-2Br-OD	(1.690 Å^{-1})	IN/A	0.339	16.9	(0.295 Å^{-1})	IN/A	0.070	80.8
DM6.V 2Dr DT	3.6	4.1	0.152	27.0	21.6		0.071	70.7
PM6:Y-2Br-DT	(1.741 Å^{-1})	(1.533 Å^{-1})	0.153	57.0	(0.291 Å ⁻¹)	IN/A	0.071	/7./

Reference

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