Supporting Information:

Regioregular Electroactive Polyolefins with Precisely Sequenced π-Conjugated Chromophores

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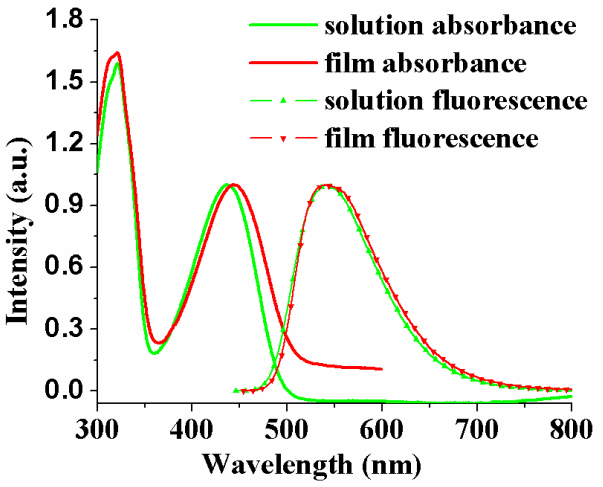

Figure S1. Normalized UV-Vis absorption and photoluminescence spectra of **PFBTF-9** in chlorobenzene.

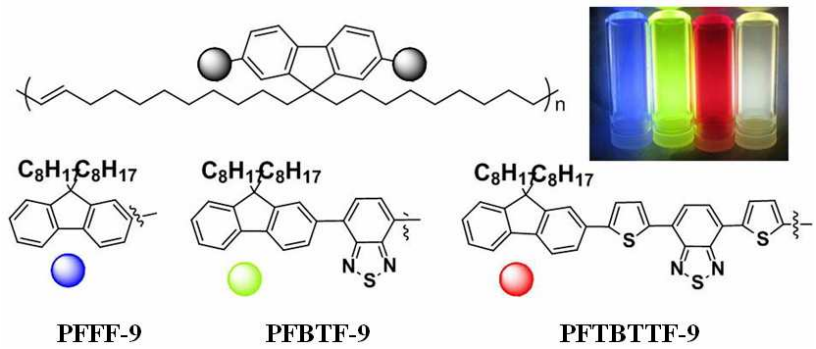

Figure S2. Chemical structures of blue, green, red and white-light emitting polymers and their chloroform solutions under UV illumination (λ_{exc} = 365 nm)

Synthesis and Characterization.

All reagents and starting materials were purchased from commercial sources and used without further purification, unless otherwise noted. Anhydrous solvents were obtained from an anhydrous solvent system. All ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on a Varian Mercury 300 spectrometer. Chemical shifts for ^{1}H and ^{13}C NMR were referenced to residual signals from $CDCl_3$ (^{1}H 7.25 ppm and ^{13}C 77.00 ppm). Mass spectrograms were recorded on either a Finnigan MAT95Q Hybrid Sector (EI, HRMS) or a Bruker Reflex II (MALDI-TOF) mass spectrometer operated in linear mode with delayed extraction. Elemental analyses were carried out by Atlantic Microlab, Inc. UV-vis spectra were recorded on a Varian Cary 500 Scan UV-vis-near-IR spectrophotometer. Thermogravimetric analysis (TGA) was performed on TA Instruments TGA Q1000 Series using dynamic scans under nitrogen. Differential scanning calorimetry (DSC) analysis was performed using a TA Instruments Q1000 series equipped with a controlled cooling accessory (liquid nitrogen cooling system) at 10 °C/min. Gel permeation chromatography (GPC) was performed at 40 °C using a Waters

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Associates GPCV2000 liquid chromatography system with an internal differential refractive index detector and two Waters Styragel HR-5E columns (10 μm PD, 7.8 mm i.d., 300 mm length) using HPLC grade THF as the mobile phase at a flow rate of 1.0 mL/min.

Optical characterization

Absorption spectra were measured with a PerkinElmer Lambda 25 UV-Vis spectrometer. The photoluminescence spectra were obtained using a Horiba Jobin Yvon Fluorolog-3 fluorimeter and exciting at the λ_{max} between 400 and 450 nm. For film measurements thin films were spin-coated from chlorobenzene onto cleaned, PEDOT:PSS (Baytron P VP Al4083) coated glass slides.

Device Fabrication and characterization

PLEDs were fabricated on pre-patterned indium tin oxide (ITO) coated glass substrates with a sheet resistance of ~ 20 Ω/□. The ITO substrates were cleaned sequentially with a sodium dodecyl sulfate solution, acetone, and isopropanol followed by exposure to an oxygen plasma. A layer of PEDOT:PSS (Baytron P VP Al4083) was spin-coated on the ITO immediately following oxygen plasma exposure, and then annealed at 120°C under vacuum for 2 hours. The active layer solutions were prepared and spin-coated from chlorobenzene in an MBraun glovebox with < 0.1 ppm oxygen and water. The cathode consisting of LiF (1 nm), Ca (10 nm), and Al (80 nm) was deposited in a thermal evaporator under a vacuum of 10^{-6} Torr. Radiant emittance (R) - voltage (V) measurements were carried out using a calibrated UDT Instruments silicon photodiode. Current density (J) - voltage (V) measurements were made using a Keithley 2400 sourcemeter. The electroluminescence (EL) spectra were collected using an ISA SPEX

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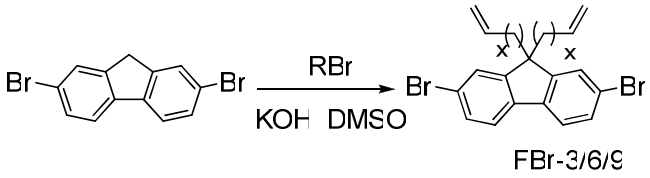
Triax 180 spectrograph with the device driven using the Keithley sourcemeter. Luminance measurements were collected with a calibrated Minolta CS100 chromameter. Each 25 x 25 mm substrate features 8 independently addressable pixels with an area of 0.071 cm^2 each.

General method for alkylation



FBr-3/6/9. To a round bottom flask (250 ml) charged with 2,7-dibromo-9H-fluorene (6.48 g, 20 mmol), RBr (44 mmol) and potassium hydroxide (6.73 g, 120 mmol), dimethylsulfoxide (DMSO) (60 mL) was added. The resulting mixture was stirred under 60 ^oC for 25 h, and then poured into 500 ml ice-water. The organic phase was extracted with ethyl acetate (50 mL x 3). The combined red solution was dried over magnesium sulfate. The solvent was removed under reduced pressure to yield viscous oil. The crude product was purified by silica gel chromatography, eluting with pure hexane to give white solids.

FBr-9 (2,7-dibromo-9,9-di(undec-10-enyl)-9H-fluorene) (11.3 g, 90%) ^{1}H-NMR ($CDCl_3$) δ: 7.53-7.44 (m, 6H), 5.89-5.75 (m, 2H), 5.05-4.93 (m, 4H), 2.08-1.93 (m, 8H), 1.40-1.08 (m, 24H),0.65 (brs, 4H); ^{13}C-NMR ($CDCl_3$) δ: 152.7, 139.2, 130.3, 126.3, 121.7, 121.2, 114.3, 55.8, 40.3, 34.0, 30.0, 29.63, 29.55, 29.3, 29.2, 29.1, 23.8; HRMS (ESI-TOF) Calculated for $C_{35}H_{48}Br_2$ $(M+H)^+$: 626.2115, found: *m/z* 626.2123; Anal. Calcd for $C_{35}H_{48}Br_2$: C, 66.88; H, 7.70, found: C, 66.89; H, 7.68.

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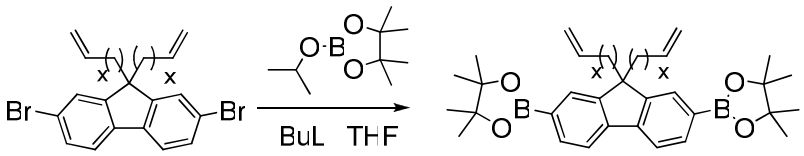
FBr-6 (2,7-dibromo-9,9-di(oct-7-enyl)-9H-fluorene) (9.7 g, 90%) ^{1}H-NMR ($CDCl_3$) δ: 7.53-7.43 (6H), 5.80-5.66 (m, 2H), 4.96-4.85 (m, 4H), 1.96-1.88 (m, 8H), 1.24-1.02 (m, 12H), 0.59 (brs, 4H); ^{13}C-NMR ($CDCl_3$) *δ*: 152.7, 139.3, 130.4, 126.4, 121.7, 121.3, 114.4, 55.9, 40.3, 33.9, 29.9, 29.0, 28.9, 23.8; HRMS (ESI-TOF) Calculated for $C_{29}H_{36}Br_2$ $(M+H)^+$: 545.1238, found: *m/z* 545.1254; Anal. Calcd for $C_{29}H_{36}Br_2$: C, 63.98; H, 6.67, found: C, 64.11; H, 6.75.

FBr-3 (2,7-dibromo-9,9-di(pent-4-enyl)-9H-fluorene) (8.1 g, 88 %) ^{1}H-NMR ($CDCl_3$) δ: 7.54-7.45 (m, 6H), 5.64-5.48 (m, 2H), 4.89-4.84 (m, 4H), 2.01-1.80 (m, 8H), 0.78-0.67 (m, 4H); ^{13}C-NMR ($CDCl_3$) *δ*: 152.3, 139.2, 138.3, 130.5, 126.3, 121.8, 121.3, 114.9, 55.6, 39.7, 33.9, 23.0; HRMS (ESI-TOF) Calculated for $C_{23}H_{24}Br_2$ $(M+H)^+$: 461.0303, found: *m/z* 461.0311; Anal. Calcd for $C_{23}H_{24}Br_2$: C, 60.02; H, 5.26, found: C, 60.02; H, 5.27.

General method for borylation



FBr-3/6/9 (10 mmol) was dissolved into anhydrous THF (100 mL), BuLi (22 mmol) was added dropwise over 30 min under argon atmosphere at -78 ^{o}C. After stirring for 90 min, 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.46 g, 24 mmol) was injected in one portion. The reaction mixture was allowed to warm up to room temperature and stirred overnight. THF was removed under reduced pressure and water (100 mL) was added. The organic phase was extracted with ethyl acetate (60 mL x 4). The combined

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organic phase was dried over magnesium sulfate. The solvent was removed under reduced pressure to yield yellowish viscous oil. The crude product was purified by silica gel chromatography, eluting with EtOAc: hexane (8:92) to give white solids.

FB-9 (2,2'-(9,9-di(undec-10-enyl)-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)) (4.7 g, 65 %). ^{1}H-NMR ($CDCl_3$) δ: 7.81-7.70 (m, 6H), 5.82-5.65 (m, 2H), 4.98-4.85 (m, 4H), 2.02-1.95 (m, 8H), 1.38 (s, 24H), 1.35-1-0.98 (m, 24H), 0.54 (brs, 4H); ^{13}C-NMR ($CDCl_3$) δ: 150.7, 144.1, 139.5, 133.9, 129.1, 119.6, 114.2, 83.9, 55.4, 40.3, 34.0, 30.2, 29.7, 29.6, 29.4, 29.3, 29.1, 25.2, 23.9; HRMS (ESI-TOF) Calculated for $C_{47}H_{72}B_2O_4$ $(M+H)^+$: 723.5705, found: *m/z* 723.5653; Anal. Calcd for $C_{47}H_{72}B_2O_4$: C, 78.11; H, 10.04, found: C, 78.01; H, 10.23.

FB-6 (2,2'-(9,9-di(oct-7-enyl)-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)) (3.1 g, 49 %). ^{1}H-NMR ($CDCl_3$) δ: 7.84-7.71(m, 6H), 5.80-5.64 (m, 2H), 4.95-4.84 (m, 4H), 2.05-2.01 (m, 4H), 1.94-1.76 (m, 4H), 1.39 (s, 24H), 1.70-1.01 (m, 12H), 0.58 (brs, 4H); ^{13}C-NMR ($CDCl_3$) δ: 150.5, 144.1, 139.3, 133.9, 129.1, 119.6, 114.2, 83.9, 55.3, 40.2, 33.9, 29.9, 29.0, 28.8, 25.1, 23.7; HRMS (ESI-TOF) Calculated for $C_{41}H_{60}B_2O_4$ $(M+H)^+$: 639.4770, found: *m/z* 639.4792; Anal. Calcd for $C_{41}H_{60}B_2O_4$: C, 77.12; H, 9.47, found: C, 77.25; H, 9.32.

FB-3 (2,2'-(9,9-di(pent-4-enyl)-9H-fluorene-2,7-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)) (3.0 g, 54 %). ^{1}H-NMR ($CDCl_3$) δ: 7.86-7.74 (m, 6H), 5.62-5.48 (m, 2H), 4.84-4.79 (m, 4H), 2.08-2.03 (m, 4H), 1.87-1.75 (m, 4H), 1.45-1.40 (m, 24H). 0.70 (brs, 4H); ^{13}C-NMR ($CDCl_3$) δ: 150.132, 144.1, 138.7, 134.0, 129.0, 119.6, 114.3, 83.8, 55.1, 39.8, 34.1, 25.1, 23.0; HRMS (ESI-TOF) Calculated for $C_{35}H_{48}B_2O_4$

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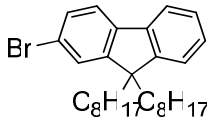
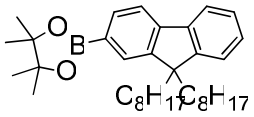
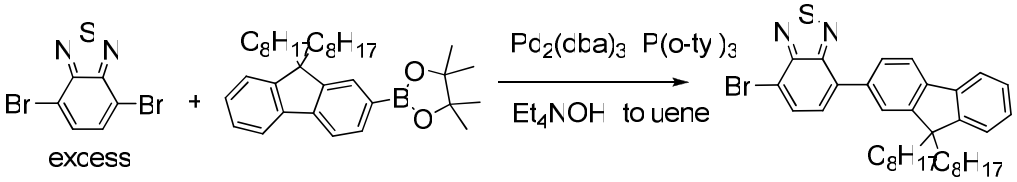
$(M+Na)^+$:577.3643, found: *m/z* 577.3669; Anal. Calcd for $C_{35}H_{48}B_2O_4$: C, 75.83; H, 8.73, found: C, 75.78; H, 8.80.



2-bromo-9,9-dioctyl-9H-fluorene (**F8Br**) was prepared by following the literature procedure. Liu, S.; Zhao, Q.; Chen, R.; Deng, Y.; Fan, Q.; Li, F.; Wang, L.; Huang, C.; Huang, W. Chemistry - A European Journal 2006, 12, 4351-4361.



2-(9,9-dioctyl-9H-fluoren-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**F8B**) was prepared by following the literature procedure. Li, T.; Yamamoto, T.; Lan, H.; Kido, J. Polymers for Advanced Technologies 2004, 15, 266-269.



4-bromo-7-(9,9-dioctyl-9H-fluoren-2-yl)benzo[c][1,2,5]thiadiazole (**F8BTBr**). To a Schlenk flask charged with 4,7-dibromobenzo[c][1,2,5]thiadiazole (1.47 g, 5.0 mmol), $Pd_2(dba)_3$ (2.5 mol %, 45 mg), P(o-tyl)$_3$ (5 mol %, 30 mg) under argon atmosphere, degassed toluene solution of 2-(9,9-dioctyl-9H-fluoren-2-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (**F8B**) (1.03 g, 2 mmol, 20 mL) was injected. Subsequently, degassed tetraethylammonium hydroxide aqueous solution (20 wt %, 4.8 mL, 6 mmol) was added. The reaction mixture was heated up to 80 ^oC and stirred for 16 h. After cooling back to

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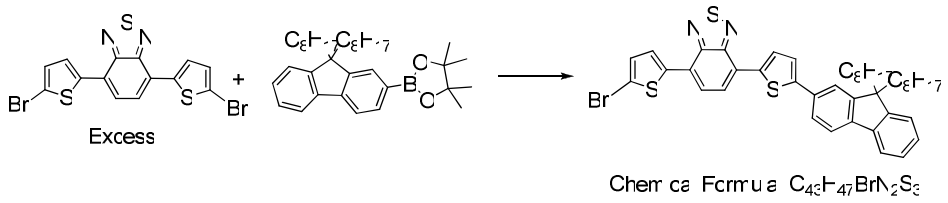
room temperature, the organic phase was washed with water, extracted with ethyl acetate, dried over magnesium sulfate. The solvent was removed under reduced pressure to yield yellow-greenish viscous oil. The crude product was purified by silica gel chromatography, eluting with toluene: hexane (2:8) to give viscous oil (955 mg, 79.5 %). ^{1}H-NMR ($CDCl_3$) δ: 7.98-7.95 (m, 3H), 7.94 (d, J = 7.5 Hz, 1H), 7.83-7.80 (m, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.45-7.38 (m, 3H), 2.20-2.03 (m 4H), 1.27-1.13 (m, 20H), 0.88-0.78 (m, 10H); ^{13}C-NMR ($CDCl_3$) δ: 154.1, 153.5, 151.45, 151.36, 141.9, 140.6, 135.4, 134.7, 132.4, 128.4, 128.3, 127.6, 124.0, 123.1, 120.2, 120.0, 112.8, 55.4, 40.5, 32.0, 30.2, 29.4, 24.0, 22.8, 14.2; HRMS (ESI-TOF) Calculated for $C_{35}H_{43}BrN_2S$ $(M+H)^+$: 605.2388, found: *m/z* 605.2335.



4-(5-bromothiophen-2-yl)-7-(5-(9,9-dioctyl-9H-fluoren-2-yl)thiophen-2-yl)benzo[c][1,2,5]thiadiazole (**F8TBTTBr**) was prepared using the same procedure as F8BTBr. ^{1}H-NMR ($CDCl_3$) δ: 8.05 (d, J = 4.2 Hz, 1H), 7.73-7.61 (m, 7H), 7.41-7.33 (m, 4H), 7.09 (d, J = 4.2 Hz, 1H), 2.08-2.02 (m, 4H), 1.24-1.09 (m, 20H), 0.84-0.63 (m, 10H); ^{13}C-NMR ($CDCl_3$) δ: 152.4, 152.3, 151.8,151.1, 146.8, 141.4, 140.9, 140.7, 138.1, 133.0, 130.8, 129.0, 127.4, 127.1, 127.07, 126.3, 125.1, 125.0, 124.7, 124.0, 123.1, 120.3, 120.1, 120.0, 114.6, 55.4, 40.6, 32.0, 30.2, 29.4, 24.0, 22.8, 14.3; HRMS (ESI-TOF) Calculated for $C_{43}H_{47}BrN_2S_3$ $(M+H)^+$: 769.2143, found: *m/z* 769.2163.

General procedure for ADMET.

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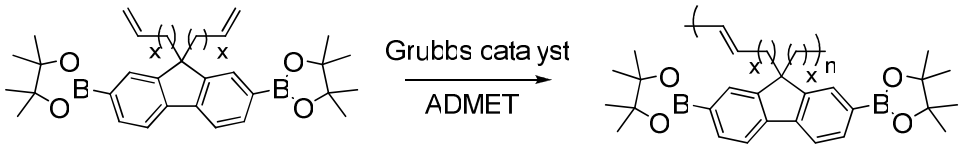

FB-x **PFB-x** x = 3 6 and 9

A saturated solution of monomer in 1,2-dichlorobenzene (50 wt. % for 9,9 and 30 wt. % for 6,6) was degassed by bubbling argon through the solution for 20 minutes. Under strong argon flow, 1.1 ml of this solution and 15 mg of Grubbs 1st generation catalyst (1-2 mol %) was then placed in a flat bottomed mechanical stirring high vacuum reactor capable of continuously spreading the viscous polymerization matrix as a thin film. The reactor was then placed under dynamic vacuum at 70 torr absolute pressure via an aspirator attached to one arm and ~1 ml/min argon flow through the opposing arm. The reactor was then heated to 45 ^{o}C and left to stir at 350 rpm for 12 hours. After this time, ADMET was terminated by dissolving the polymer and all remaining 1,2-dichlorobenzene in 15 ml of chloroform, 1 ml of ethyl vinyl ether was then added, and the solution was allowed to stir for 4 hours. After 4 hours, the solutions were precipitated into methanol to produce polymers. The precipitates were then subjected to Soxhlet with methanol, hexane and chloroform. From chloroform fraction, 630 mg for PFB-9 (>95%) and 570 mg for PFB-6 (> 90%) were obtained.

PFB-9: SEC (THF, light scattering detector, PS standards calibration): M_n = 39 kDa, PDI = 1.8.; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.77-7.9 (d, 2H, br), 7.6-7.77 (m, 4H, br), 5.3 (s, 2H, br), 2.0 (s, 4H, br), 1.9 (s, 4H, br), 1.4 (s, 26H, br), 1.1-1.6 (m, 14H, br), 1.0 (s, 12H, br),0.5 (s, 4H, br); ^{13}C NMR (75 MHz, $CDCl_3$): δ 150.7, 144.1, 133.9, 130.5, 130.0, 129.1, 128.0, 119.6, 83.9, 55.4, 40.4, 32.8, 30.2, 23.9, 29.9, 29.8, 29.6, 29.5, 25.2, 27.4, 29.4. Anal. Calcd for **PFB-9**: C, 77.48; H, 9.68, found: C, 77.84; H, 9.92.

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PFB-6: SEC (THF, light scattering detector, PS standards calibration): M_n = 30 kDa, PDI = 2.0; 1H NMR (300 MHz, CDCl3) δ: 7.75-7.82 (d, 2H, br), 7.65-7.75 (m, 4H, br), 5.2 (t, 2H, br), 2.0 (s, 4H, br), 1.8 (s, 4H, br), 1.6 (s, 4H, br), 1.4 (m, 26H, br), 0.9-1.1 (s, 12H, br), 0.5 (s, 4H, br); ^{13}C NMR (75 MHz, CDCl3): δ 150.7, 144.1, 133.9, 130.5, 130.0, 129.1, 128.0, 119.6, 83.9, 55.4, 40.4, 32.9, 30.3, 29.9, 29.8, 29.7, 29.5, 29.4, 25.2, 23.9.

PFB-3: A solution of 30 wt. % monomer, 30 wt. % 1,1,2,2-tetrachloroethane, and 40 wt. % 1,2-dichlorobenzene was degassed by bubbling argon through the solution for 20 minutes. Under strong argon flow, 1.5 ml of this solution and 40 mg of Grubbs 1st generation catalyst (2.5 mol %) were then placed in a flat bottomed mechanical stirring high vacuum reactor capable of continuously spreading the viscous polymerization matrix as a thin film. The reactor was then placed under dynamic vacuum at 85 torr absolute pressure via an aspirator attached to one arm and ~1 ml/min argon flow through the opposing arm. The reactor was then heated to 40 ^{o}C and left to stir at 350 rpm for 12 hours. After this time, ADMET was terminated by dissolving the polymer and all remaining solvents in 15 ml of chloroform, 1 ml of ethyl vinyl ether was then added, and the solution was allowed to stir for 4 hours. After 4 hours, the solution was reprecipitated into room temperature methanol to produce 341 mg (~60%. SEC: M_n = 11 kDa, PDI = 1.4 (THF, light scattering detector, PS standards calibration). ^{1}H NMR (300 MHz, CDCl3): δ 7.80-7.83 (d, 2H, br), 7.71-7.75(m, 4H, br), 5.3 (s, 2H, br), 2.0 (s, 4H, br), 1.9 (s, 4H, br), 1.4 (s, 26H, br), 1.0-1.3 (m, 24H, br), 0.6 (s, 4H, br); ^{13}C NMR (75 MHz, CDCl3): δ 150.8, 144.4, 133.9, 133.6, 131.9, 129.5, 119.6, 83.9, 55.5, 38.9, 32.1, 25.2, 22.3.

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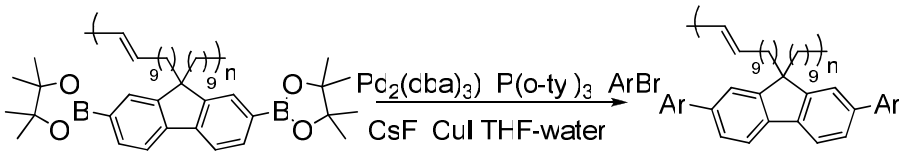
General method for Suzuki Reaction:



PFB - 9

A Schlenk flask charged with **PFB-9** (0.2 mmol), $Pd_2(dba)_3$ (2.5 mol %), $[(C_4H_9)_3PH]^+BF4^-$ (5 mol %,), CuI (10 mol %), and were purged with argon atmosphere and vacuum for three cycles, and then filled with argon. Ar-Br (2.1 eq, in the case of $P_{white,}$ 2 eq was used) in degassed tetrahydrofuran (8 mL) was added through a septum, followed by an aqueous solution of CsF (6 eq, 1.2 mmol, 0.6 mL). The reaction mixture was heated up to 85 ^oC and stirred for 48 h. After cooling back to room temperature, the mixture was poured into methanol (200 mL) and stirred for 1h. The precipitates were collected, washed with methanol and dried (294 mg, 99%). The crude polymer was put inside a thimble for Soxhlet extraction with methanol, hexane and chloroform. The chloroform fraction was concentrated and precipitated into methanol. The solids were then collected by vacuum filtration and dried under vacuum at 60 ^0C for 12h to yield the corresponding polymers (225 mg, 75%).

PFBTF-9 M_n = 56 kDa, PDI = 1.6 ^1H NMR (300 MHz, $CDCl_3$) δ: 8.05-7.83 (m, 16H), 7.60 (d, J = 5.7 Hz), 7.36-7.32 (m, 6H), 5.23 (bs, 2H), 2.19-1.78 (m, 16H), 1.25-0.64 (m, 88H); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 154.6, 151.9, 151.5, 151.3, 141.6, 141.1, 140.9, 136.7, 136.4, 133.9, 133.7, 130.4, 128.6, 128.2, 127.5, 127.1, 124.2, 124.1, 123.2, 120.2, 119.9, 55.7, 55.4, 40.5, 32.8, 32.0, 30.4, 30.3, 29.8, 29.7, 29.6, 29.4, 24.1, 22.8, 14.3.

PFFF-9 M_n = 51 kDa, PDI = 1.6. ^1H NMR (300 MHz, $CDCl_3$) δ : 7.4-8 (m, 14H), 7.3-7.45 (d, 6H), 5.38 (s, 2H, br), 1.9-2.2 (m, 16H, br), 1.0-1.4 (s, 64H, br), 0.5-0.9 (s, 22H,

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br); ^{13}C NMR (75 MHz, $CDCl_3$) δ: 152.0, 151.7, 151.3, 141.1, 140.7, 140.6, 140.3, 130.5, 130.1, 127.3, 127.1, 126.4, 126.3, 123.2, 121.7, 120.2, 120.0, 55.6, 55.4, 40.7, 32.9, 32.1, 30.3, 30.0, 29.9, 29.8, 29.6, 29.5, 27.5, 24.2, 24.1, 22.9, 14.4.

PFTBTTF-9 M_n = 30 kDa, PDI = 2.1.

P_{white} = 51 kDa, PDI = 1.7. The selected optimized mole ratio of F8Br, F8BTBr and F8TBTTBr was 99.5 : 0.4 : 0.1, where an equal equivalent PFB-9 was used as the precursor polymer.

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