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Supplementary Information

Donor polymer based on alkylthiophene side chains for efficient non-fullerene organic solar cells: Insights into fluorination and side chain effects on polymer aggregation and blend morphology

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Solar cell fabrication and testing. Pre-patterned ITO-coated glass with a sheet resistance of ~15 Ω per square was used as the substrate. It was cleaned by sequential sonications in soap deionized water, deionized water, acetone, and isopropanol for 30 min at each step. After UV/ozone treatment for 60 min, a ZnO electron transport layer was prepared by spin-coating at 5000 rpm from a ZnO precursor solution (diethyl zinc). Active layer solutions (D/A ratio 1:1.5, polymer concentration 8 mg/ml) were prepared in chlorobenzene (CB). To completely dissolve the polymer, the active layer solution should be stirred on hotplate at 90 °C for at least 1 hour. Before spin coating, both the polymer solution and ITO substrate are preheated on a hotplate at about 100 °C. Active layers were spin-coated from the warm polymer solution on the preheated substrate in a N_2 glovebox at 2000 rpm to obtain thicknesses of ~115 nm. The polymer:SMA blend films were then thermally annealed before being transferred to the vacuum chamber of a thermal evaporator inside the same glovebox. At a vacuum level of 3×10^{-6} Torr, a thin layer (20 nm) of V_2O_5 was deposited as the anode interlayer, followed by deposition of 100 nm of Al as the top electrode. All cells were encapsulated using epoxy inside the glovebox. Device J-V characteristics was measured in forward direction under AM1.5G (100 mW cm^{-2}) at room temperature using a Newport solar simulator. The dwell times is 2 s and the speed is 0.8 V/s. The light intensity was calibrated using a standard Si diode (with KG5 filter, purchased from PV Measurement) to bring spectral mismatch to unity. J-V characteristics were recorded using a Keithley 236 source meter unit. Typical cells have devices area of 5.9 mm^2, which is defined by a metal mask with an aperture aligned with the device area. EQE was characterized using a Newport EQE system equipped with a standard Si diode. Monochromatic light was generated from a Newport 300W lamp source.

AFM analysis. AFM measurements were acquired by using a Scanning Probe Microscope-Dimension 3100 in tapping mode. All film samples were spincast on ITO/ZnO substrates.

Optical characterizations. Film ultraviolet–visible absorption spectra were acquired on a Perkin Elmer Lambda 20 ultraviolet/visible Spectrophotometer. All film samples were spincast on ITO/ZnO substrates. Solution ultraviolet-visible absorption spectra at elevated temperatures were collected on a Perkin Elmer Lambda 950 ultraviolet/visible/NIR Spectrophotometer. The temperature of the cuvette was controlled with a Perkin Elmer PTP 6+6 Peltier System, which is supplied by a Perkin Elmer PCB 1,500 Water Peltier System. Before each measurement, the system was held for at least 5 min at the target temperature to reach thermal equilibrium. A cuvette with a stopper (Sigma Z600628) was used to avoid volatilization during the measurement.

Cyclic voltammetry. Cyclic voltammetry was performed in an electrolyte solution of 0.1M tetrabutylammonium hexafluorophosphate, both working and counter electrodes were platinum electrode. Ag/AgCl electrode was used as the reference electrode; the Fc/Fc^+ redox couple was used as an external standard.

GIWAXS characterizations. GIWAXS measurements[1] were performed at beamline 7.3.3 at the Advanced Light Source (ALS). Samples were prepared on Si substrates using identical blend solutions as those used in devices. The 10k eV X-ray beam was incident at a grazing angle of 0.13^o -0.17^o, which maximized the scattering intensity from the samples. The scattered X-rays were detected using a Dectris Pilatus 2 M photon counting detector.

R-SoXS characterization. R-SoXS transmission measurements were performed at beamline 11.0.1.2 at the

ALS.[2] Samples for R-SoXS measurements were prepared on a PSS modified Si substrate under the same conditions as those used for device fabrication, and then transferred by floating in water to a 1.5×1.5 mm, 100 nm thick Si_3N_4 membrane supported by a 5×5 mm, 200 mm thick Si frame (Norcada Inc.). Two dimensional scattering patterns were collected on an in-vacuum CCD camera (Princeton Instrument PI-MTE). The beam size at the sample is ~100 mm by 200 mm. The composition variation (or relative domain purity) over the length scales probed can be extracted by integrating scattering profiles to yield the total scattering intensity. The median domain spacing is calculated from 2π/q, where q here corresponds to half the total scattering intensity.[3] The purer the average domains are, the higher the total scattering intensity. Owing to a lack of absolute flux normalization, the absolute composition cannot be obtained by only R-SoXS.

Hole-mobility measurements. The hole-mobilities were measured using the SCLC method, employing a device architecture of ITO/V2O5/blend film/V2O5/Al. The mobilities were obtained by taking current-voltage curves and fitting the results to a space charge limited form, where the SCLC is described by:

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

Where ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material (assumed to be 3), μ is the hole mobility, V_{appl} is the applied voltage, V_{bi} is the built-in voltage (0V), V_S is the voltage drop from the substrate's series resistance ($V_S = IR$, R is measured to be 10.8 Ω) and L is the thickness of the film. By linearly fitting $J^{1/2}$ with $V_{appl} - V_{bi} - V_S$, the mobilities were extracted from the slope and L:

$$\mu = \frac{slope^2 \times 8L^3}{9\varepsilon_0\varepsilon_r}$$

Electron mobility measurements. The electron mobilities were measured using the SCLC method, employing a device architecture of ITO/ZnO/blend film/Ca/Al. The mobilities were obtained by taking current-voltage curves and fitting the results to a space charge limited form, where the SCLC is described by:

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

Where ε_0 is the permittivity of free space, ε_r is the relative permittivity of the material (assumed to be 3), μ is the hole mobility and L is the thickness of the film. From the plots of $J^{1/2}$ versus V, electron mobilities can be deduced. The mobilities were extracted from the slope and L:

$$\mu = \frac{slope^2 \times 8L^3}{9\varepsilon_0\varepsilon_r}$$

Molecular interaction parameter (χ) calculation. We can obtain an estimate of the Flory-Huggins interaction parameter, χ, following the Flory-Huggins equation:[4, 5]

$$\frac{1}{T_m} - \frac{1}{{T_m}^0} = \frac{R}{\Delta H_f}\frac{v_m}{v_s}(\Phi_s - \chi{\Phi_s}^2)$$

where T_m is the melting point of the mixture, T_m^0 is the melting point of pure polymer, R is the ideal gas constant, ΔH_f is the heat of fusion of pure polymer, Φs is the volume fraction of the small molecule, v_m is the monomer molar volume of polymer and v_s is the solvent molar volume (polymer and small molecule density was found to be ~1.15 and ~1.3 g/cm^3, respectively, and the small molecule is regarded as the solvent for the polymer). The molecular mass of the polymer divided by its density (1.15 g/cm^3) is the monomer molar volume v_m.

The PT4FB:IDIC and PTT4FB:IDIC were dissolved in CB and stirred on hotplate at 90 °C for at least 1 hour to guarantee sufficient mixing. The solvent of two solutions was then removed from the system at 90 °C, which is similar to the film processing temperature, to yield the solid of two blends for DSC characterizations. Based on the DSC data as shown in Fig. 5, interaction parameters χ of 1.45 and 0.81 are calculated for the PT4FB:IDIC and PTT4FB:IDIC blends, respectively.

Supplementary figures and tables

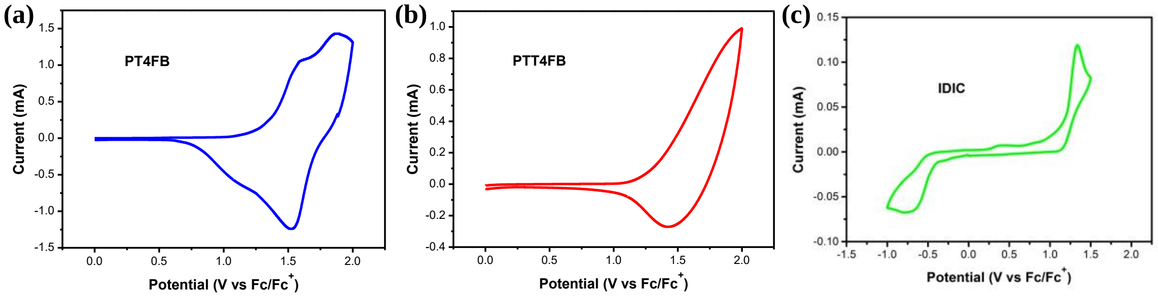


Fig. S1 Cyclic voltammetry of (a) PT4FB, (b) PTT4FB and (c) IDIC.

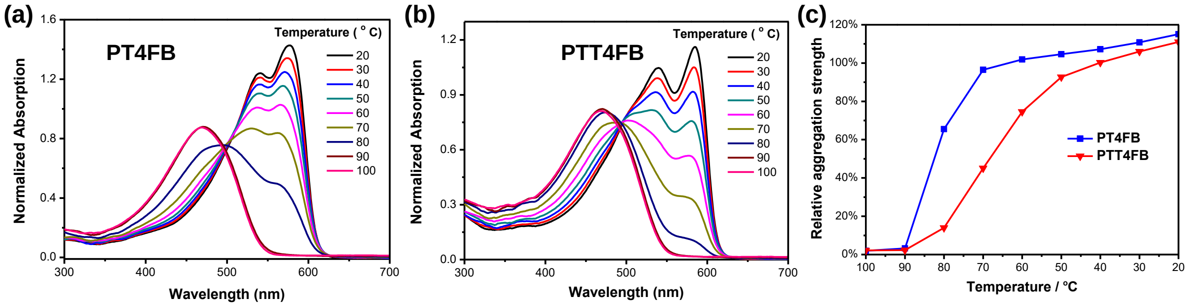


Fig. S2 Temperature-dependent UV-vis absorption spectra of 0.02 mg/mL (a) PT4FB and (b) PTT4FB in chlorobenzene solutions. (c) “Relative aggregation strength” plots of PT4FB and PTT4FB in chlorobenzene solutions at different temperature. The “relative aggregation strength” is defined as the ratio of the second absorption peak to the first absorption peak in two polymer absorption curves.

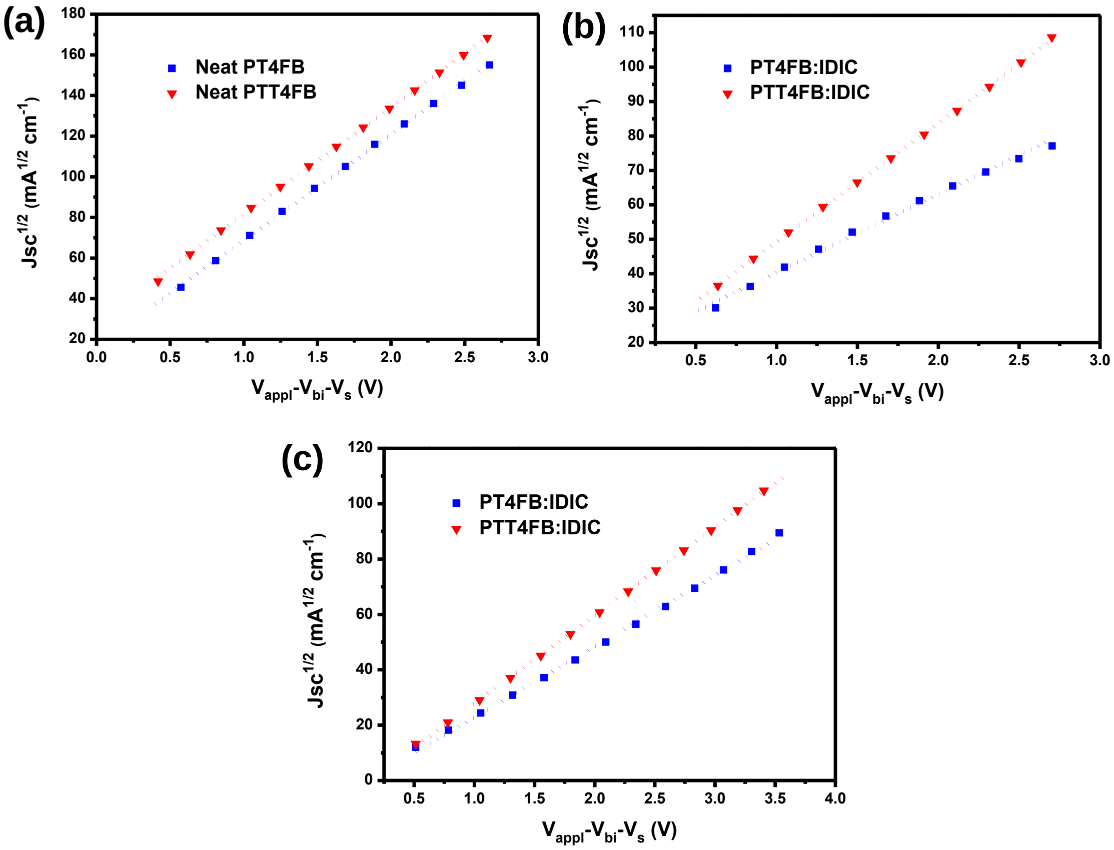


Fig. S3 $J^{1/2} \sim V_{appl} - V_{bi} - V_S$ characteristics of (a) hole-only for neat PT4FB and PTT4FB polymer films. (b) hole-only and (c) electron-only for PT4FB:IDIC and PTT4FB:IDIC devices. Dash lines are fits. The hole mobilities for two polymers PT4FB and PTT4FB are $(1.57\pm 0.12)\times10^{-4}$ cm^2 V^{-1} S^{-1} and $(1.27\pm 0.22)\times10^{-4}$ cm^2 V^{-1} S^{-1}. The hole and electron mobilities for PT4FB:IDIC blend are $(7.00 \pm 0.33)\times10^{-4}$ cm^2 V^{-1} S^{-1} and $(6.16 \pm 0.20)\times10^{-4}$ cm^2 V^{-1} S^{-1}, and are $(5.67 \pm 0.22)\times10^{-4}$ cm^2 V^{-1} S^{-1} and $(5.59 \pm 0.18)\times10^{-4}$ cm^2 V^{-1} S^{-1} for PTT4FB:IDIC blend, respectively.

Table S1. Thermal and optical properties of Donors.

Materials	T_m^0 (°C)	ΔH_m (J/g)	λ_{onset} (nm)	HOMO (eV)$^{a)}$	LUMO (eV)$^{b)}$
PT4FB	293.38	21.44	625	-5.59	-3.61
PTT4FB	319.24	23.79	620	-5.58	-3.58

a) is extracted from cyclic voltammetry results and b) is calculated from a) values and polymer optical band gaps.

Table S2. The ratio of 2nd peak and 1st peak extracted from the UV absorption curves of PT4FB and PTT4FB solutions.

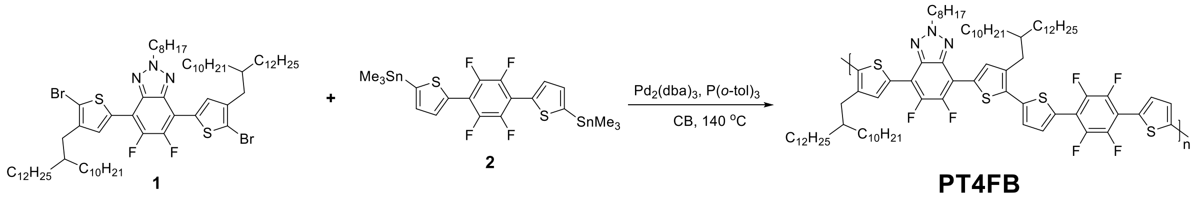
	PT4FB			PTT4FB		
Temperature (°C)	Max. value$^{a)}$ at 1st peak	Max. value$^{a)}$ at 2nd peak	**Ratio of 2nd Peak to 1st Peak**	Max. value$^{a)}$ at 1st peak	Max. value$^{a)}$ at 2nd peak	**Ratio of 2nd Peak to 1st Peak**
100	0.875	0.018	**0.020**	0.812	0.018	**0.022**
90	0.879	0.028	**0.032**	0.823	0.019	**0.023**
80	0.756	0.495	**0.655**	0.804	0.113	**0.140**
70	0.868	0.837	**0.965**	0.749	0.338	**0.451**
60	1.009	1.028	**1.019**	0.760	0.567	**0.746**
50	1.103	1.155	**1.046**	0.817	0.757	**0.927**
40	1.164	1.248	**1.072**	0.915	0.917	**1.003**
30	1.211	1.341	**1.108**	0.991	1.051	**1.060**
20	1.240	1.427	**1.151**	1.047	1.162	**1.110**

a) The max. values of 1st peak and 2rd peak are extracted from Fig. S2(a) and (b).

Synthesis Section

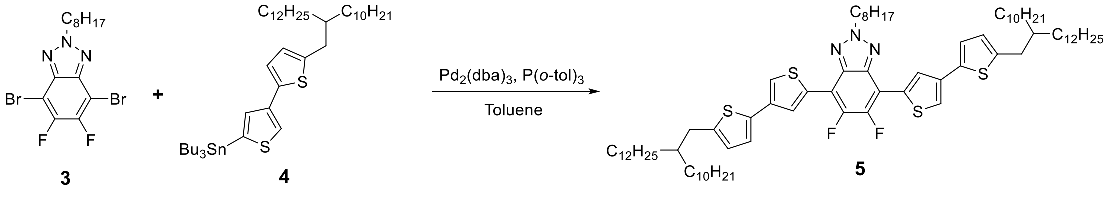
General information. All reagents and solvents were purchased from commercial sources (Aldrich, Acros, solarmer and J&K) and used without further purification unless stated otherwise. Solvents were purified by distillation when necessary. IDIC, 4,7-bis(5-bromo-4-(2-decyltetradecyl)thiophen-2-yl)-5,6-difluoro-2-octyl-2H-benzo[d][1,2,3]triazole (**1**) and ((perfluoro-1,4-phenylene)bis(thiophene-5,2-diyl))bis(trimethylstannane) (**2**) were synthesized according to literature procedure.[6-8] Microwave assisted polymerizations were conducted in a CEM Discover microwave reactor. ^{1}H, ^{19}F and ^{13}C NMR spectra were recorded on a Bruker AV-400 MHz NMR spectrometer. Chemical shifts were reported in parts per million (ppm, δ). ^{1}H NMR and ^{13}C NMR spectra were referenced to tetramethylsilane (0 ppm) for $CDCl_3$. Mass spectra were collected on a MALDI Micro MX mass spectrometer.

Synthesis of PT4FB and PTT4FB



Polymerization of PT4FB. A mixture of 4,7-bis(5-bromo-4-(2-decyltetradecyl)thiophen-2-yl)-5,6-difluoro-2-octyl-2*H*-benzo[*d*][1,2,3]triazole (1) (31.6 mg, 0.025 mmol), ((perfluoro-1,4-phenylene)bis(thiophene-5,2-diyl))bis(trimethylstannane) (2) (16.0 mg, 0.025 mmol), $Pd_2(dba)_3$ (1.1 mg, 0.00125 mmol) and P(*o*-tol)$_3$ (1.5 mg, 0.005 mmol) were added to a microwave vial equipped with a stirring bar and then 0.25 mL of chlorobenzene was added in a glove box protected with N_2.The reaction mixture was then sealed and heated to 140 °C for one day by thermal heating. Then the mixture was cooled to room tempearture and 20 mL of chlorobenzene was used to dissolve the mixture before the mixture was precipitated with methanol. The solid was collected by filtration, subsequently subjected to soxhlet extraction with acetone, hexane, chloroform and toluene. This toluene solution was then concentrated by rotary evaporator, precipitated into methanol. Finally it was collected by filtration and dried in vacuum to get the polymer as dark purple solid (20.1 mg, 57 %).

GPC: Mn: 56.2 kDa; Mw: 114.2 kDa; PDI=2.03.



4,7-bis(5-(2-decyltetradecyl)-[2,3'-bithiophen]-5'-yl)-5,6-difluoro-2-octyl-2*H*-enzo[*d*][1,2,3]triazole (5). A mixture of 4,7-dibromo-5,6-difluoro-2-octyl-2*H*-benzo[*d*][1,2,3]triazole (3) (850 mg, 2 mmol), tributyl(5-(2-decyltetradecyl)-[2,3'-bithiophen]-5'-yl)stannane (4) (3484 mg, 4.4 mmol), $Pd_2(dba)_3$ (92 mg, 0.1 mmol) and P(*o*-tol)$_3$ (122 mg, 0.4 mmol) were added to a flask. After adding 50 mL toluene, the mixture was refluxed at 100 °C overnight under N_2. Then a solution of KF in water was added and the system was stirred for another half an hour. The reaction mixture was filtered, diluted with hexane and washed with KF solution, water and brine. The organic layer was dried over Na_2SO_4, filtered and concentrated. Then the residue was purified with silica gel column chromatography by hexane to give the crude product of yellow oil (1904 mg, 75%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 1.4 Hz, 2H), 7.46 (d, *J* = 1.3 Hz, 2H), 7.12 (d, *J* = 3.4 Hz, 2H), 6.72 (d, *J* = 3.5 Hz, 2H), 4.81 (t, *J* = 7.1 Hz, 2H), 2.77 (d, *J* = 6.6 Hz, 4H), 2.31 – 2.11 (m, 2H), 1.78 – 1.51 (m, 2H), 1.17 – 0.48 (m, 109 H), 1.10 – 0.48 (m, 15H).

^{13}C NMR (101 MHz, CDCl3) δ 148.37 (d, J = 80.6 Hz), 146.03 (dd, J = 56.1, 43.4 Hz), 143.48 (d, J = 56.2 Hz), 138.22 – 137.52 (m), 136.73 (d, J = 7.2 Hz), 136.33 (d, J = 31.2 Hz), 132.71 (d, J = 45.5 Hz), 128.46 (d, J = 41.0 Hz), 125.70 (d, J = 41.5 Hz), 122.92 (d, J = 52.0 Hz), 121.22 (d, J = 33.4 Hz), 110.77 – 109.21 (m), 56.87 (d, J = 49.5 Hz), 40.09 (d, J = 26.9 Hz), 34.63 (d, J = 36.9 Hz), 33.20 (d, J = 46.9 Hz), 32.57 – 31.73 (m), 30.70 – 28.41 (m), 27.60 – 26.53 (m), 23.30 – 21.97 (m), 14.71 – 13.67 (m).

^{19}F NMR (376 MHz, $CDCl_3$) δ -133.62 (s).

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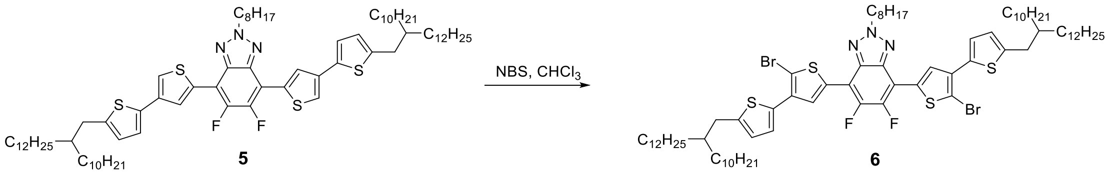


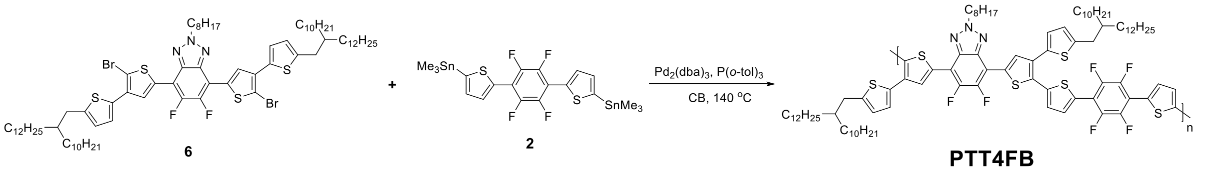
4,7-bis(2'-bromo-5-(2-decyltetradecyl)-[2,3'-bithiophen]-5'-yl)-5,6-difluoro-2-octyl-2*H*-benzo[*d*][1,2,3]triazole (6). Chemical 5 (1904 mg, 1.5 mmol) was added to a 100 mL flask. 30 mL chloroform was added to dissolve 5. The N-Bromosuccinimide (534 mg, 3 mmol) was then added to the system at 0 °C. After reacting for two hours, the reaction mixture was warmed to r.t. and stirred overnight. 10 mL water was added to quench the reaction. After washing with water, the organic phase was dried with Na_2SO_4 and the solvent was removed by rotary evaporator. Then the residue was purified with silica gel chromatography to get the pure product as yellow liquid (1.969 g, 92 % yield).

^{1}H NMR (400 MHz, CDCl3) δ 8.25 (s, 2H), 7.37 (d, J = 3.6 Hz, 2H), 6.77 (d, J = 3.6 Hz, 2H), 4.80 (t, J = 7.1 Hz, 2H), 2.78 (d, J = 6.6 Hz, 4H), 2.32 – 2.04 (m, 2H), 1.86 – 0.84 (m, 96H), 0.87 (dd, J = 7.9, 5.6 Hz, 15H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 148.66 (d, *J* = 13.3 Hz), 146.12 (d, *J* = 10.1 Hz), 145.12 (d, *J* = 26.0 Hz), 137.27 (s), 135.02 (d, *J* = 27.0 Hz), 134.11 (d, *J* = 15.9 Hz), 132.36 (d, *J* = 21.4 Hz), 130.50 (s), 126.17 (d, *J* = 15.9 Hz), 125.44 (d, *J* = 20.2 Hz), 110.70 (s), 109.42 (s), 57.09 (s), 40.09 (d, *J* = 24.5 Hz), 34.54 (d, *J* = 48.9 Hz), 33.39 (d, *J* = 13.7 Hz), 32.12 (d, *J* = 8.5 Hz), 31.90 (d, *J* = 19.1 Hz), 30.88 – 28.56 (m), 27.10 – 26.62 (m), 23.41 – 22.50 (m), 14.71 – 13.96 (m).

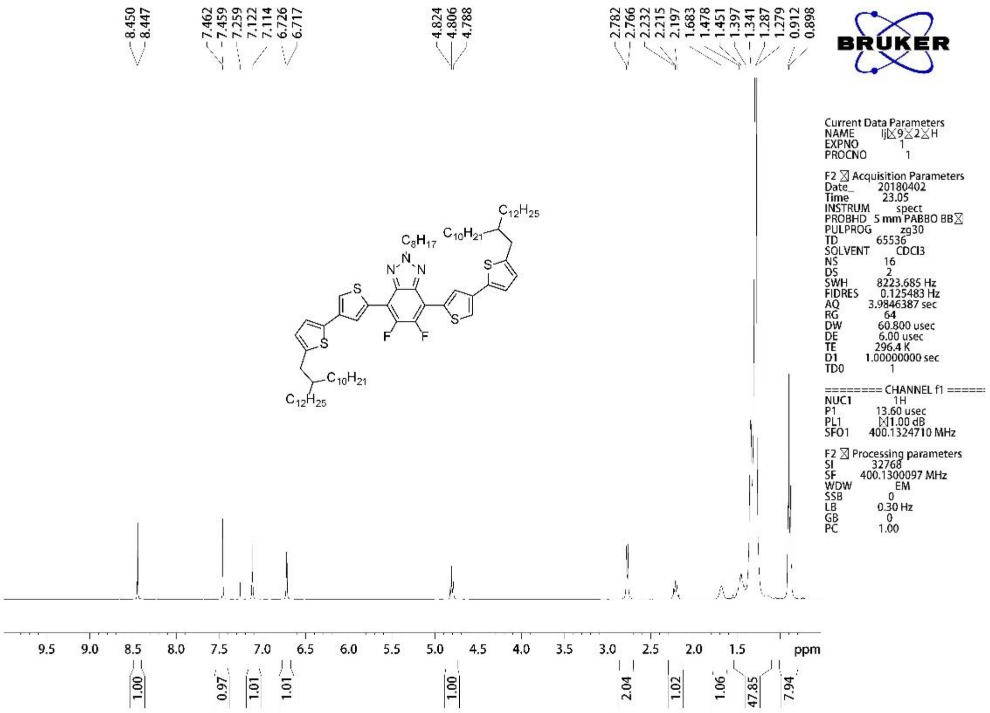
^{19}F NMR (376 MHz, $CDCl_3$) δ -133.66 (s).

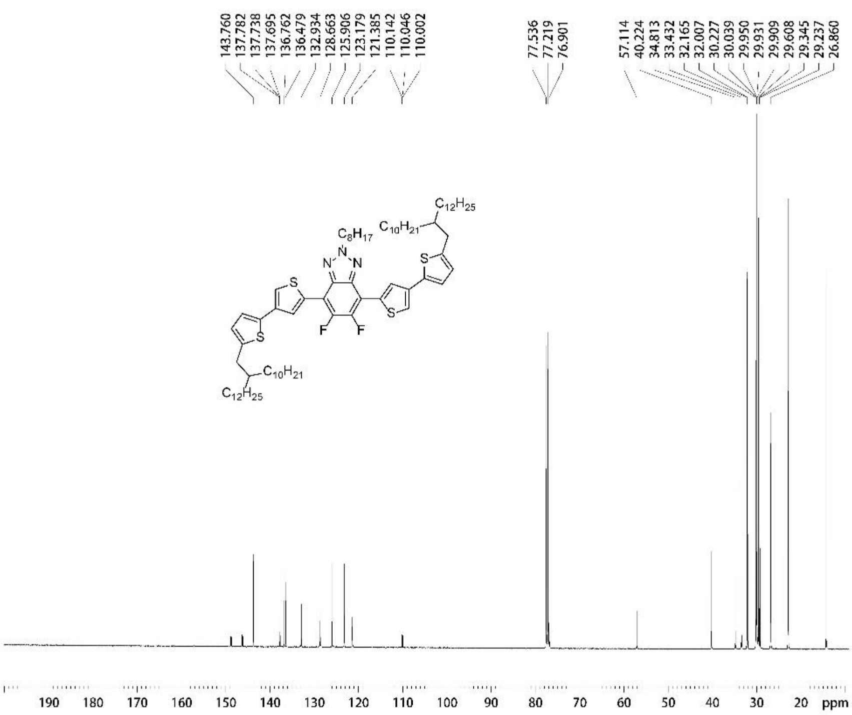
HRMS (MALDI+) Calcd for $C_{78}H_{121}Br_2F_2N_3S_4$ (M +): 1423.6778, Found: 1424.7444.



Polymerization of PTT4FB. A mixture of 4,7-bis(5-bromo-4-(2-decyltetradecyl)thiophen-2-yl)-5,6-difluoro-2-octyl-2*H*-benzo[*d*][1,2,3]triazole (6) (35.7 mg, 0.025 mmol), ((perfluoro-1,4-phenylene)bis(thiophene-5,2-diyl))bis(trimethylstannane) (2) (16.0 mg, 0.025 mmol), $Pd_2(dba)_3$ (1.1 mg, 0.00125 mmol) and P(*o*-tol)$_3$ (1.5 mg, 0.005 mmol) were added to a microwave vial equipped with a stirring bar and then 0.25 mL of chlorobenzene was added in a glove box protected with N_2.The reaction mixture was then sealed and heated to 140 °C for one day by thermal heating. Then the mixture was cooled to room tempearture and 20 mL of chlorobenzene was used to dissolve the mixture before the mixture was precipitated with methanol. The solid was collected by filtration, subsequently subjected to soxhlet extraction with acetone, hexane and chloroform. This chloroform solution was then concentrated by rotary evaporator, precipitated into methanol. Finally it was collected by filtration and dried in vacuum to get the polymer as dark purple solid (24.9 mg, 63 %).

GPC: Mn: 54.1 kDa; Mw: 98.0 kDa; PDI=1.81.





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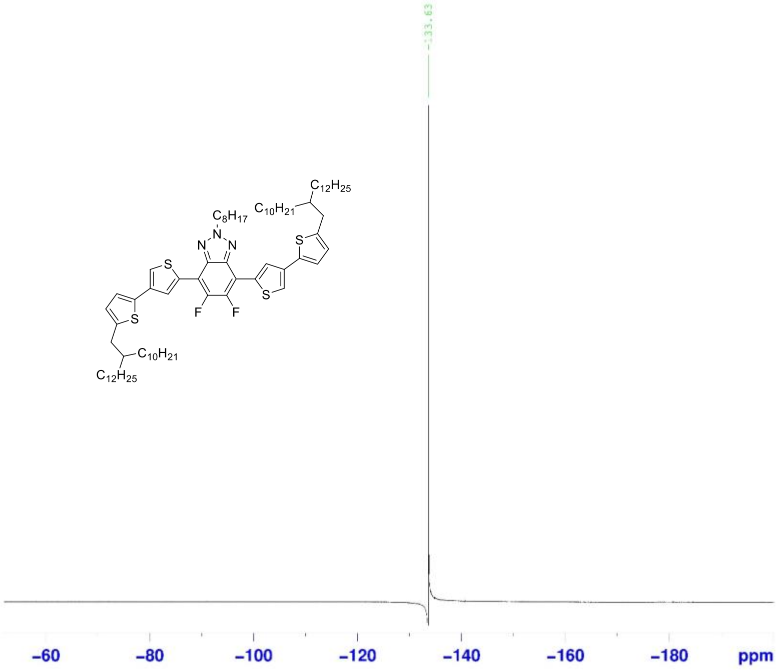

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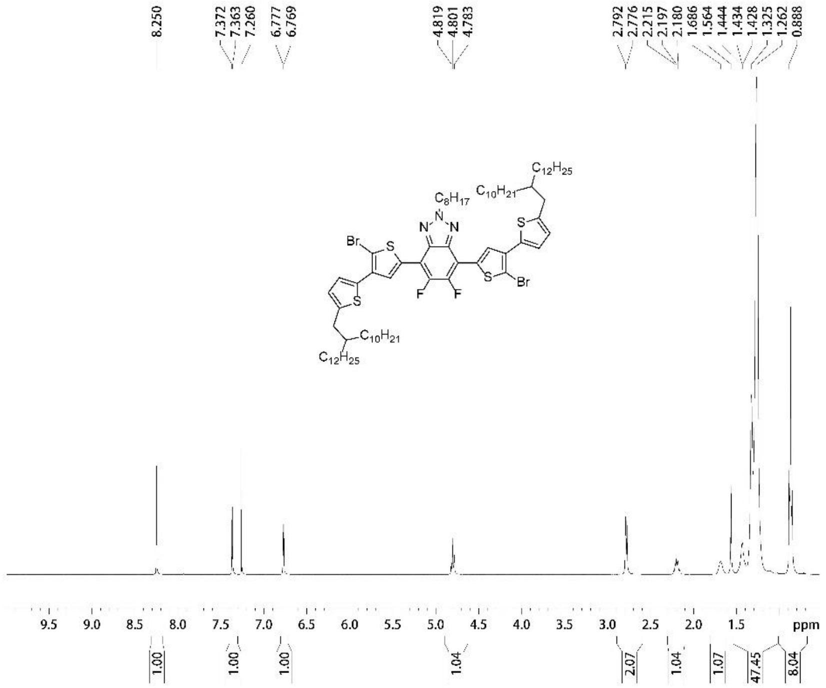

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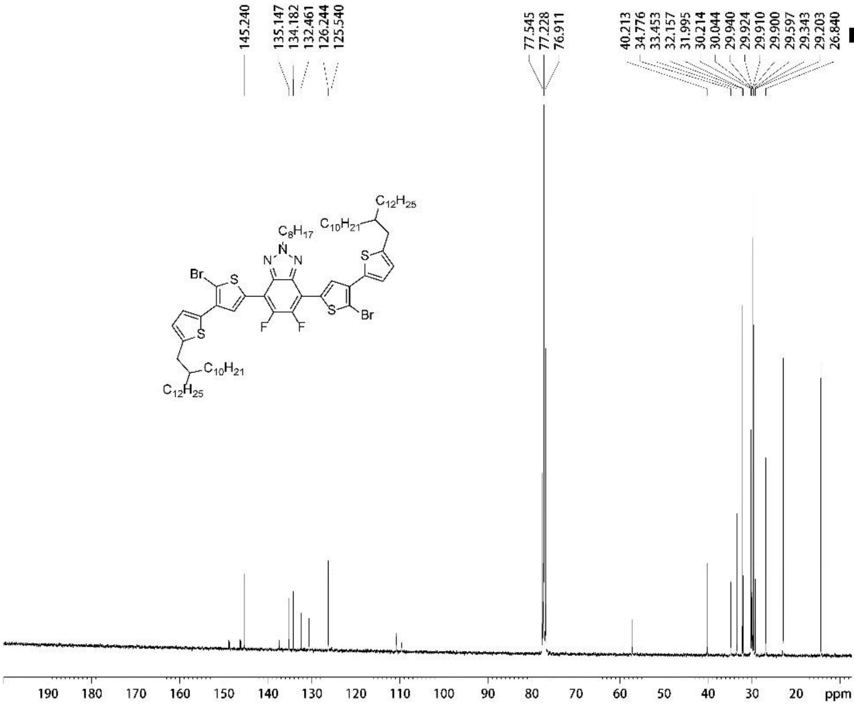

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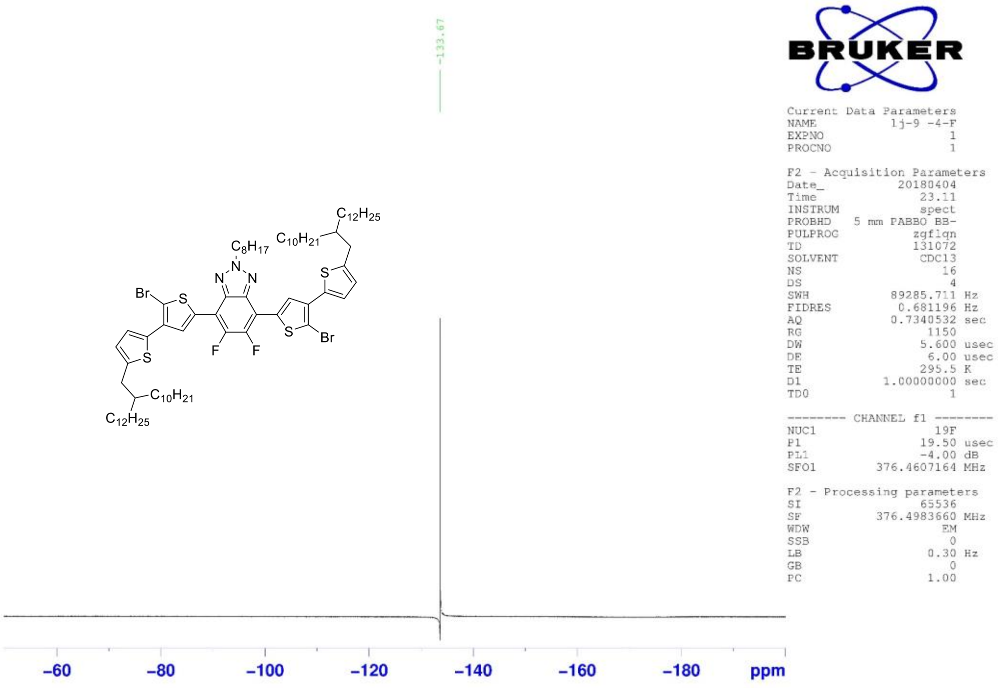
Time          8.39
INSTRUM        spect
PROBHD  5 mm PABBO E
PULPROG       zgpg30
TD          65536
SOLVENT        CDCl3
NS          10000
DS             2
SWH       24038.461 Hz
FIDRES      0.366798 Hz
AQ        1.3631988 sec
RG             64
DW         20.800 usec
DE          6.00 usec
TE          297.6 K
D1       2.00000000 sec
d11      0.03000000 sec
DELTA     1.89999998 se
TD0            1

======== CHANNEL f1
NUC1           13C
P1           9.25 usec
PL1          ☒3.00 dB
SFO1    100.6228298 M

======== CHANNEL f2
CPDPRG2      waltz16
NUC2            1H
PCPD2       80.00 usec
PL12        12.45 dB
PL13        18.00 dB
PL2          ☒1.00 dB
SFO2    400.1316005 M

F2 ☒ Processing parame
SI          32768
SF     100.6127473 MH:
WDW             EM
SSB            0
LB          1.00 Hz
GB             0
PC          1.40
```



```
Current Data Parameters
NAME           1j-9 -4-F
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180404
Time               23.11
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgflqn
TD                131072
SOLVENT            CDC13
NS                    16
DS                     4
SWH           89285.711 Hz
FIDRES         0.681196 Hz
AQ            0.7340532 sec
RG                  1150
DW                 5.600 usec
DE                  6.00 usec
TE                 295.5 K
D1            1.00000000 sec
TD0                    1

-------- CHANNEL f1 --------
NUC1                 19F
P1                 19.50 usec
PL1                -4.00 dB
SFO1         376.4607164 MHz

F2 - Processing parameters
SI                 65536
SF           376.4983660 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

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