Electronic Supplementary Information for:

Revealing Effects of Molecular Packing on the Performances of Polymer Solar Cells Based on A-D-C-D-A Type Non-Fullerene Acceptors

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Materials and Methods

Instrument. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were obtained on a Bruker Advance III 400 (400 MHz) or an Agilent 600 MHz DD2 nuclear magnetic resonance (NMR) spectroscope. MALDI-TOF MS spectra were measured on a Walters Maldi Q-TOF Premier mass spectrometry. UV-vis absorption spectra were recorded on a Shimadzu UV-2450 spectrophotometer. Thermogravimetric analysis (TGA) was carried out on a WCT-2 thermal balance under protection of nitrogen at a heating rate of 10 ^{o}C/min. Differential scanning calorimetry (DSC) was recorded on a Pekin-Elmer Pyris 1 differential scanning calorimeter. Cyclic voltammetry (CV) was done on a CHI600A electrochemical workstation with Pt disk, Pt plate, and standard calomel electrode (SCE) as working electrode, counter electrode, and reference electrode, respectively, in a 0.1 mol/L tetrabutylammoniumhexafluorophosphate (Bu_4NPF_6) CH_2Cl_2 solution. The CV curves were recorded versus the potential of SCE, which was calibrated by the ferrocene-ferrocenium (Fc/Fc^+) redox couple (4.8 eV below the vacuum level). Topographic images of the films were obtained on a VeecoMultiMode atomic force microscopy (AFM) in the tapping mode using an etched silicon cantilever at a nominal load of ~2 nN, and the scanning rate for a 10 μm×10 μm image size was 1.5 Hz. Single crystal diffraction meansurement was performed on Gemini A Ultra with Atlas CCD as the detector.

Materials. All reagents and solvents, unless otherwise specified, were purchased from J&K Scientific, Derthon Tech, Suna Tech, Aldrich and Energy Chemical Ltd. and were used without further purification. **PBDB-TF**,[1] compound **1** and **4**[2] were synthesized according to the reported literatures.

DFT Calculation. Geometry optimizations were carried out by the density functional theory (DFT) method at the B3LYP/6-31G level. All the calculations were performed using Gaussian 03 program. All ethylhexyl substituents were replaced with methyl groups in calculations.

GIWAXS Measurements. Grazing-incidence wide-angle X-ray scattering (GIWAXS) measurements were carried out with a Xeuss 2.0 SAXS/WAXS laboratory beamline using a Cu X-ray source (8.05 keV, 1.54 Å) and a Pilatus3R 300K detector. The incidence angle is 0.2^{o}.

GISAXS Measurements. Grazing-incidence small-angle X-ray scattering (GISAXS) measurements were carried out at BL19U2 in the Shanghai Synchrotron Radiation Facility. The wavelength is 1.03 Å. The incidence angle is 0.1^{o}.

Device Fabrication and Characterization. Polymer solar cells were fabricated on glass substrates commercially pre-coated with a layer of indium tin oxide (ITO) with the inverted structure of ITO/ZnO/PBDB-TF:Acceptor/MoO_3/Ag. Prior to fabrication, the substrates were cleaned using detergent, deionized water, acetone and isopropanol consecutively for every 15 min, and then treated in an ultraviolet ozone generator for 15 min. A thin layer of ZnO was spin coated onto precleaned ITO-coated glass substrates at 3500 rpm for 60 s and then annealed at 170 ^{o}C for 20 min. Then the substrates were transferred to a glovebox, the PBDB-TF:Acceptor active layer was spin coated from 20 mg/mL chlorobenzene solution (PBDB-TF:Acceptor = 1:1.2, 1.0% CN) at 2000 rpm for 60 s. Then an extra pre-annealing at 110 ^{o}C for 10 min was performed. Finally, a layer of MoO_3 (10 nm) and the Ag (100 nm) electrode were deposited by thermal evaporation to complete the device with an active area of 6 mm^2. For the chloroform processed devices, the PBDB-TF:HF-PCIC active layer was spin coated from 17.6 mg/mL chloroform solution (PBDB-TF:HF-PCIC = 1:1.2, 0.5% DIO) at 3500 rpm for 40 s. And the pre-annealing was performed at 100 ^{o}C for 10 min.

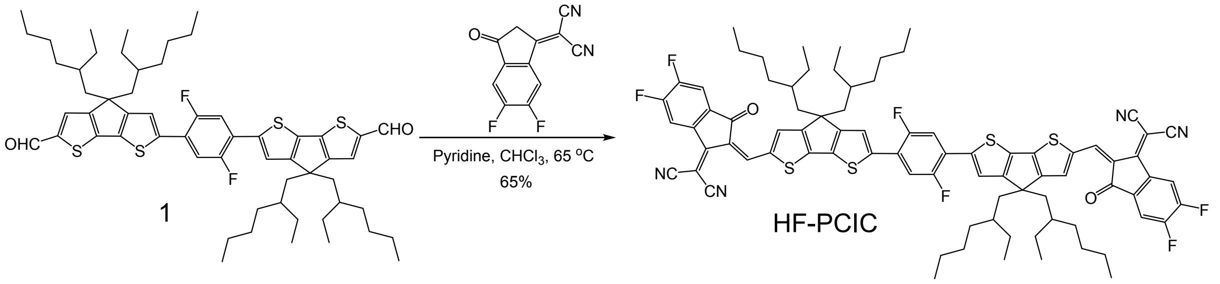
The current density-voltage (*J-V*) curves of PSCs were measured with Keithley 236 measurement source units under 1 sun, AM 1.5 G spectra from a solar simulator (Taiwan, Enlitech), and the light intensity was calibrated with a standard photovoltaic (PV) reference cell. The external quantum efficiency (EQE) spectra were measured with a Stanford lock-in amplifier 8300 unit.

The charge carrier mobilities of the PBDB-TF:Acceptor films were measured using the space-charge-limited current (SCLC) method. Hole-only devices were fabricated in a structure of ITO/PEDOT:PSS/PBDB-TF:Acceptor (1:1.2)/MoO_3/Ag, electron-only devices were fabricated in a structure of ITO/ZnO/PBDB-TF:Acceptor (1:1.2)/PFN-Br/Al. The device characteristics were extracted by modeling the dark current under forward bias using the SCLC expression described by the Mott-Gurney law:

$$J = \frac{9}{8}\varepsilon_r \varepsilon_0 \mu \frac{V^2}{L^3} \qquad (1)$$

Here, $\varepsilon_r \approx 3$ is the average dielectric constant of the blend film, ε_0 is the permittivity of the free space, μ is the carrier mobility, $L \approx 100$ nm is the thickness of the film, and V is the applied voltage.

Synthesis of HF-PCIC

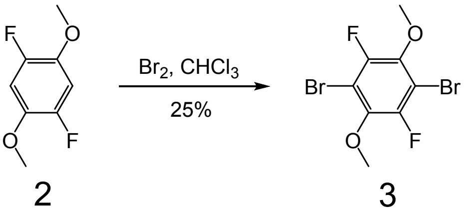


2,2'-((2Z,2'Z)-(((2,5-difluoro-1,4-phenylene)bis(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-6,2-diyl))bis(methanylylidene))bis(5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile (HF-PCIC).

To a two-necked round bottom flask were added compund **1** (0.3g, 0.3 mmol), 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (0.35 g, 1.5 mmol) and dried $CHCl_3$ (50 mL). The mixture was frozen with liquid nitrogen, followed by three times of successive vacuum and nitrogen fill cycles, then under the protection of nitrogen, 0.6 mL pyridine was added. The resulting mixture was refluxed at 65 °C for 12 h. After removing the solvent, the residue was purified using silica gel column chromatography with hexane/dichloromethane (1:3) as the eluent, yielding a deep brown solid (0.27 g, 65%). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.91 (s, 2H), 8.53 (dd, J = 9.8, 6.5 Hz, 2H), 7.68 (t, J = 7.3 Hz, 4H), 7.54-7.50 (m, 2H), 7.48 (t, J = 6.6 Hz, 2H), 2.07-1.94 (m, 8H), 1.09-0.89 (m, 32H), 0.79-0.68 (m, 16H), 0.64 (t, J = 7.3 Hz, 12H). ^{13}C NMR (600 MHz, $CDCl_3$): δ = 186.08, 165.70, 159.75, 158.41, 157.66, 155.93, 155.15, 154.28, 153.50, 153.41, 143.06, 139.29, 138.25, 137.97, 136.52, 134.46, 122.65, 119.91, 114.98, 114.84, 114.54, 112.55, 112.42, 107.35, 68.53, 54.27, 43.24, 43.13, 35.55, 35.50, 34.31, 34.05, 28.50, 27.53, 27.29, 22.79, 22.78, 14.06, 13.98, 10.61, 10.59. ^{19}F NMR (600 MHz, $CDCl_3$): δ = -116.86, -123.37, -124.48. MS (MALDI-TOF): Calcd for

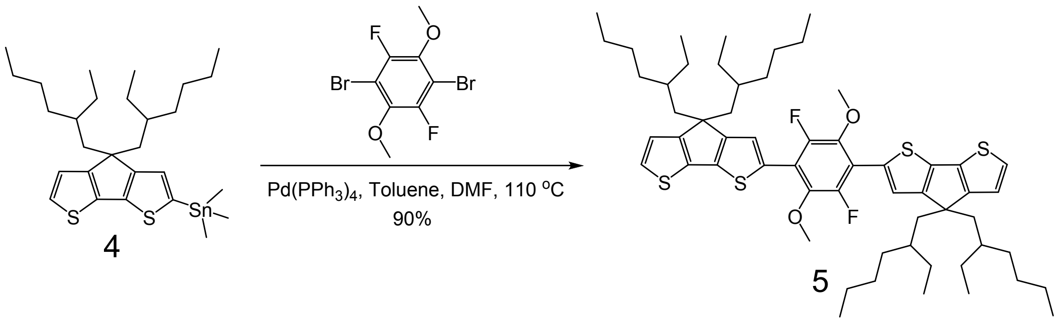
$C_{82}H_{80}F_6N_4O_2S_4$ (M^+): 1395.80, Found: 1396.57.

Synthesis of HFO-PCIC



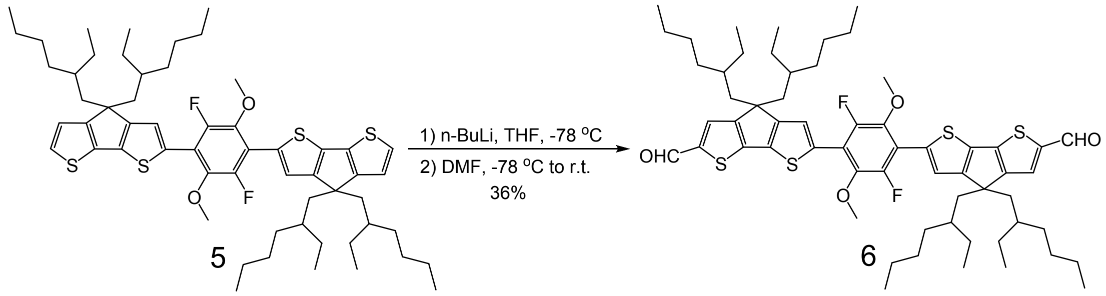
1,4-dibromo-2,5-difluoro-3,6-dimethoxybenzene (3)

To a solution of compound **2** (1.74 g, 10 mmol) in 30 mL $CHCl_3$ was added 5 mL Br_2 (100 mmol) and the resulting mixture was stirred at room temperature overnight. After pouring into ethanol, the mixture was extracted with chloroform and washed with NaOH saturated solution. The combined organic phase was evaporated under vacuum and the residue was purified using silica gel column chromatography with hexane/dichloromethane (10:1) as the eluent, yielding a white solid (0.82 g, 25%). ^1H NMR (400 MHz, $CDCl_3$): $\delta = 3.95$ (s, 6H).



2,2'-(2,5-difluoro-3,6-dimethoxy-1,4-phenylene)bis(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene) (5)

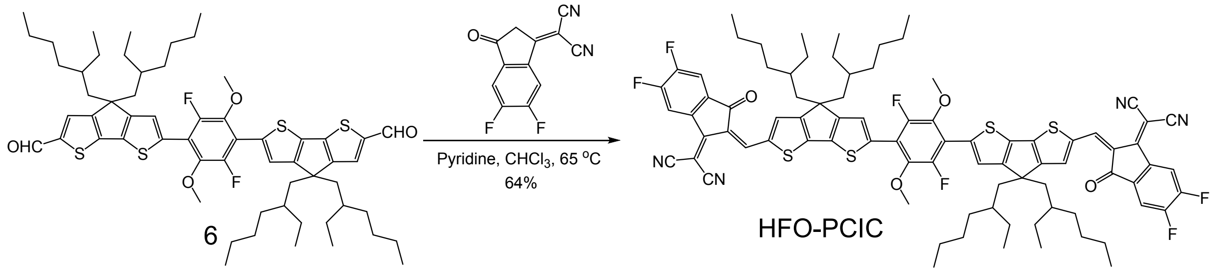
To a two-necked round bottom flask were added compound **4** (1.2 g, 2.1 mmol), compound **3** (0.32 g, 1 mmol), toluene (50 mL) and N, N-dimethylformamide (DMF, 5 mL). The mixture was frozen with liquid nitrogen, followed by three times of successive vacuum and nitrogen fill cycles, then under the protection of nitrogen, $Pd(PPh_3)_4$ (50 mg, 0.042 mmol) was added, and another three times of successive vacuum and nitrogen fill cycles were performed. Then, the mixture was refluxed at 110 ^oC for 24 h. The crude product was extracted with dichloromethane and washed with water. After removing the solvent, silica gel column chromatography was used to purify the product with hexane as the eluent, yielding an orange oil (0.87 g, 90%). ^1H NMR (400 MHz, $CDCl_3$): δ = 7.60-7.53 (m, 2H), 7.18 (d, J = 4.9 Hz, 2H), 6.98-6.94 (m, 2H), 3.92 (s, 6H), 2.00-1.85 (m, 8H), 1.06-0.85 (m, 32H), 0.79-0.69 (m, 12H), 0.67-0.57 (m, 16H).



6,6'-(2,5-difluoro-3,6-dimethoxy-1,4-phenylene)bis(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2-carbaldehyde) (6)

To a solution of compound **5** (0.87 g, 0.9 mmol) in 30 mL THF, n-BuLi (1 mL, 2.4M, 2.4 mmol) was added dropwise under the protection of nitrogen at -78 ^oC. After the mixture was stirred at -78 ^oC for 1 h, 0.5 mL DMF was added quickly. Then the mixture was warmed to room temperature and stirred overnight. After pouring into water, the mixture was extracted with dichloromethane. After removing the solvent of the organic phase on a rotary evaporator, the residue was purified using silica gel column chromatography with hexane/dichloromethane (1:1~1:3) as the eluent, yielding a red solid (0.33g, 36%). ^1H NMR (400 MHz, $CDCl_3$): δ =

9.86 (s, 2H), 7.68-7.57 (m, 4H), 3.97 (s, 6H), 2.05-1.91 (m, 8H), 1.07-0.85 (m, 32H), 0.80-0.69 (m, 12H), 0.67-0.57 (m, 16H).

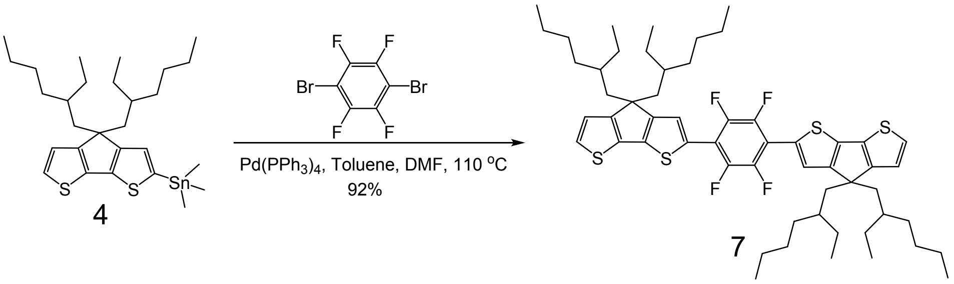


2,2'-((2Z,2'Z)-(((2,5-difluoro-3,6-dimethoxy-1,4-phenylene)bis(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-6,2-diyl))bis(methanylylidene))bis(5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile (HFO-PCIC)

To a two-necked round bottom flask were added compund **6** (0.3 g, 0.3 mmol), 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (0.35 g, 1.5 mmol) and dried $CHCl_3$ (50 mL). The mixture was frozen with liquid nitrogen, followed by three times of successive vacuum and nitrogen fill cycles, then under the protection of nitrogen, 0.6 mL pyridine was added. The resulting mixture was refluxed at 65 °C for 12 h. After removing the solvent, the residue was purified using silica gel column chromatography with hexane/dichloromethane (1:3) as the eluent, yielding a deep brown solid (0.28 g, 64%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.93 (s, 2H), 8.54 (dd, J = 10.0, 6.5 Hz, 2H), 7.76-7.63 (m, 6H), 4.02 (s, 6H), 2.09-1.94 (m, 8H), 1.10-0.85 (m, 32H), 0.81-0.69 (m, 16H), 0.68-0.59 (m, 12H). ^{13}C NMR (600 MHz, $CDCl_3$): δ = 186.08, 164.58, 160.03, 158.55, 158.38, 155.19, 155.10, 153.45, 153.36, 150.38, 148.73, 141.06, 139.35, 139.22, 138.56, 138.28, 136.48, 134.51, 125.09, 119.69, 117.10, 114.96, 114.65, 112.49, 68.26, 61.64, 54.14, 43.29, 43.20, 35.53, 35.47, 34.07, 28.54, 28.49, 27.48, 22.78, 14.08, 14.00, 10.66, 10.58. ^{19}F NMR (400 MHz, $CDCl_3$): δ = -123.54, -124.58, -

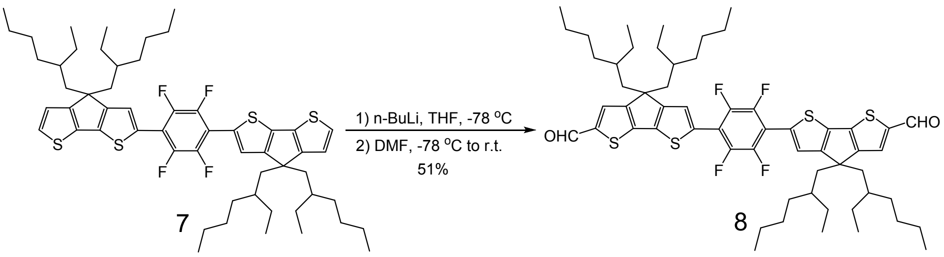
132.02. MS (MALDI-TOF): Calcd for $C_{84}H_{84}F_6N_4O_4S_4$ (M^+): 1455.85, Found: 1456.74.

Synthesis of OF-PCIC



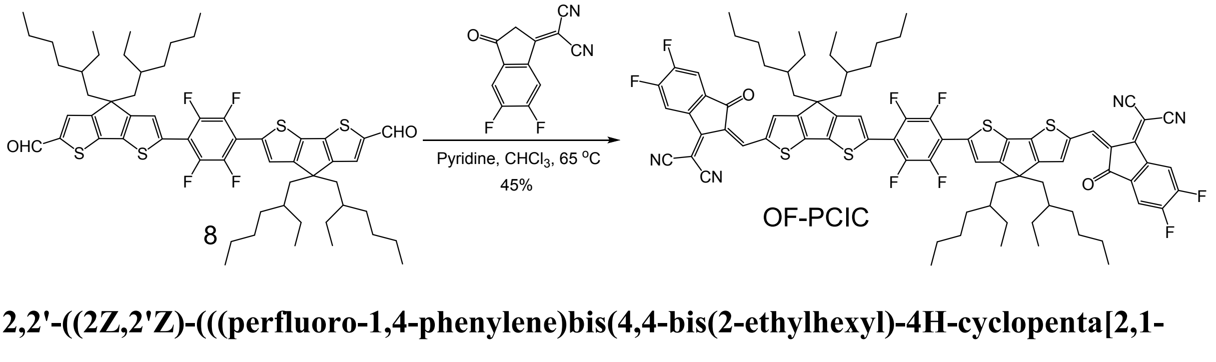
2,2'-(perfluoro-1,4-phenylene)bis(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene) (7)

To a two-necked round bottom flask were added compound **4** (1.4 g, 2.5 mmol), 1,4-dibromo-2,3,5,6-tetrafluorobenzene (0.35g, 1.12 mmol), toluene (50 mL) and N, N-dimethylformamide (DMF, 5 mL). The mixture was frozen with liquid nitrogen, followed by three times of successive vacuum and nitrogen fill cycles, then under the protection of nitrogen, $Pd(PPh_3)_4$ (50 mg, 0.042 mmol) was added, and another three times of successive vacuum and nitrogen fill cycles were performed. Then, the mixture was refluxed at 110 °C for 24 h. The crude product was extracted with dichloromethane and washed with water. After removing the solvent, silica gel column chromatography was used to purify the product with hexane as the eluent, yielding an orange oil (0.98 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.57-7.51 (m, 2H), 7.22 (d, J = 4.9 Hz, 2H), 6.99-6.95 (m, 2H), 1.98-1.86 (m, 8H), 1.06-0.83 (m, 32H), 0.79-0.69 (m, 12H), 0.67-0.54 (m, 16H).



6,6'-(perfluoro-1,4-phenylene)bis(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-2-carbaldehyde) (8)

To a solution of compound **7** (1.1 g, 1.2 mmol) in 30 mL THF, n-BuLi (1.2 mL, 2.4M, 2.88 mmol) was added dropwise under the protection of nitrogen at -78 °C. After the mixture was stirred at -78 °C for 1 h, 0.5 mL DMF was added quickly. Then the mixture was warmed to room temperature and stirred overnight. After pouring into water, the mixture was extracted with dichloromethane. After removing the solvent of the organic phase on a rotary evaporator, the residue was purified using silica gel column chromatography with hexane/dichloromethane (1:1~1:3) as the eluent, yielding a red solid (0.62 g, 51%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.88 (s, 2H), 7.64-7.58 (m, 4H), 2.06-1.91 (m, 8H), 1.07-0.84 (m, 32H), 0.79-0.69 (m, 12H), 0.67-0.56 (m, 16H).

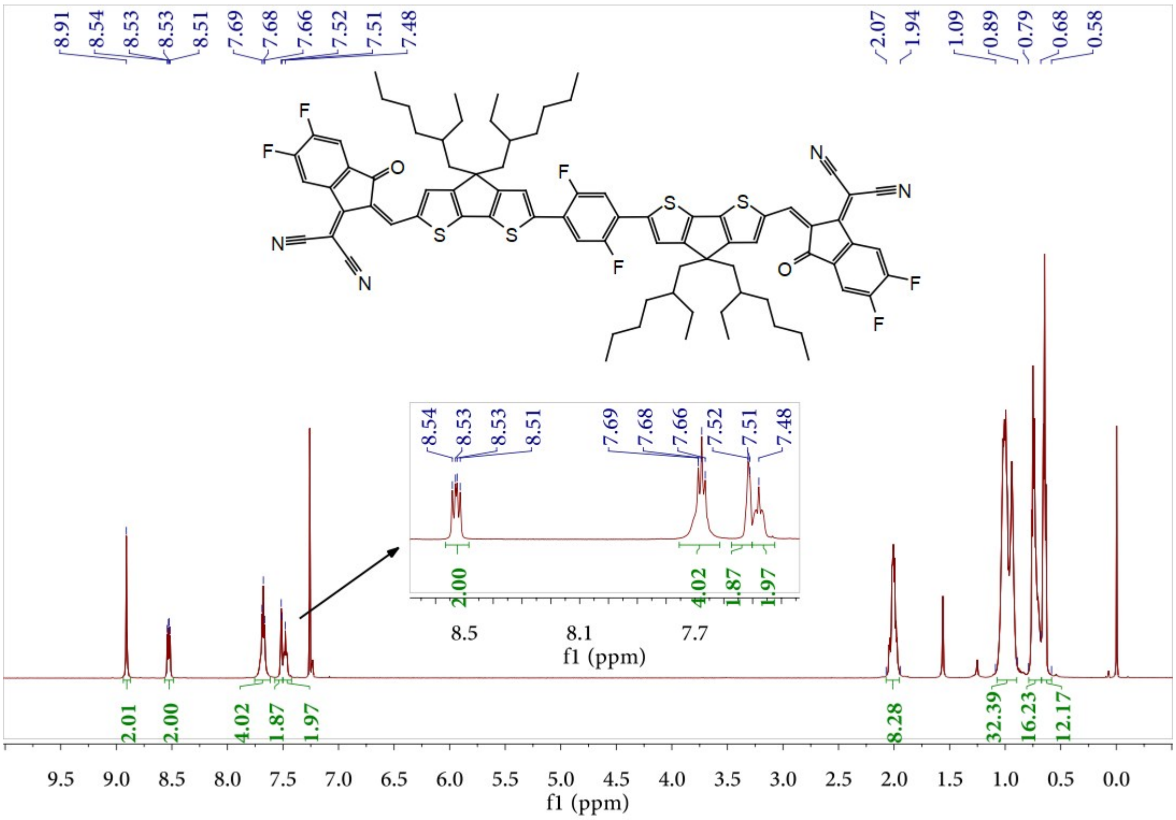


2,2'-((2Z,2'Z)-(((perfluoro-1,4-phenylene)bis(4,4-bis(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b']dithiophene-6,2-diyl))bis(methanylylidene))bis(5,6-difluoro-3-oxo-2,3-dihydro-1H-indene-2,1-diylidene))dimalononitrile (OF-PCIC)

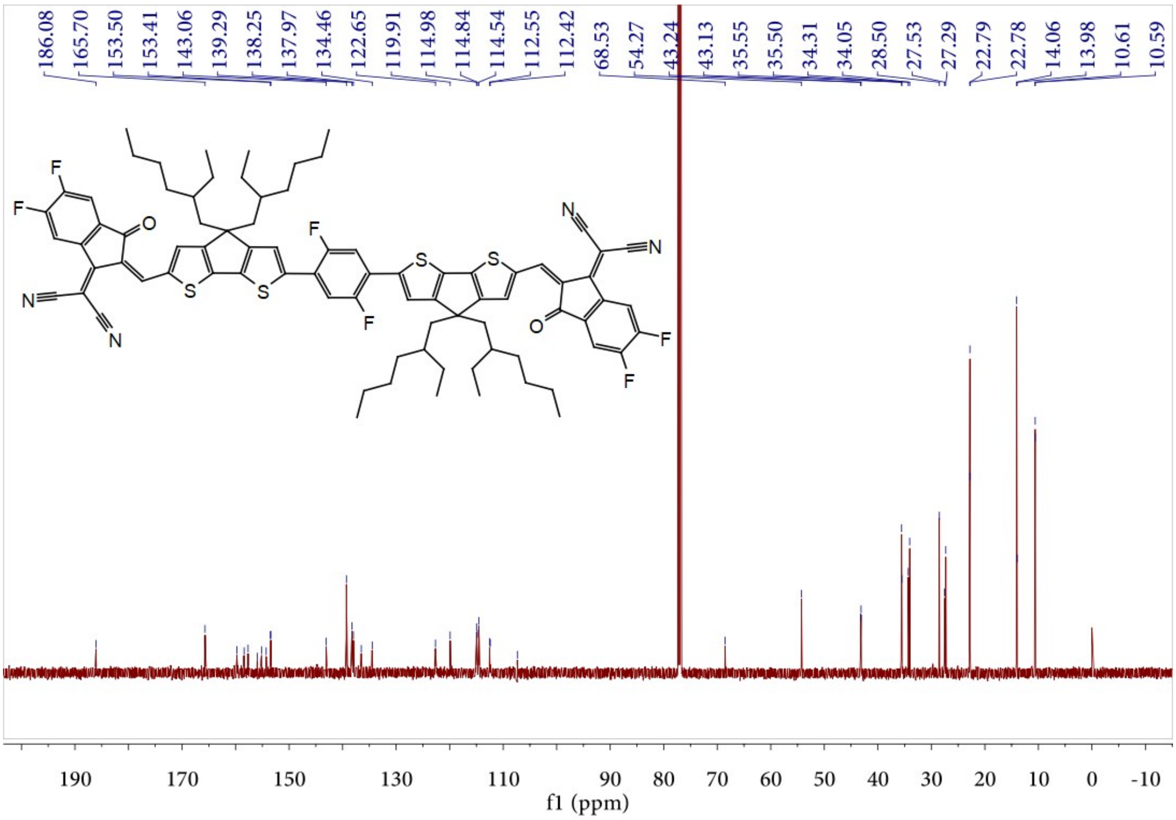
To a two-necked round bottom flask were added compund **8** (0.28 g, 0.28 mmol), 2-(5,6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile (0.35 g, 1.5 mmol) and dried $CHCl_3$ (50 mL). The mixture was frozen with liquid nitrogen, followed by three times of successive vacuum and nitrogen fill cycles, then under the protection of nitrogen, 0.6 mL pyridine was added. The resulting mixture was refluxed at 65 ^{o}C for 12 h. After removing the solvent, the residue was purified using silica gel column chromatography with hexane/dichloromethane (1:3) as the eluent, yielding a deep green solid. (0.18 g, 45%). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 8.91 (s, 2H), 8.53 (dd, J = 9.6, 6.5 Hz, 2H), 7.77-7.62 (m, 6H), 2.09-1.95 (m, 8H), 1.09-0.86 (m, 32H), 0.79-0.71 (m, 12H), 0.7-0.59 (m, 16H). ^{13}C NMR (600 MHz, $CDCl_3$): δ = 186.02, 164.26, 160.18, 158.38, 156.71, 155.32, 155.23, 153.57, 153.47, 144.83, 143.13, 139.89, 139.60, 138.24, 136.49, 134.62, 125.57, 120.41, 115.02, 114.88, 114.43, 113.02, 112.64, 112.51, 69.00, 54.33, 43.29, 43.11, 35.54, 34.09, 28.53, 28.50, 22.78, 22.76, 14.06, 13.93, 10.59. ^{19}F NMR (400 MHz, $CDCl_3$): δ = -123.04, -124.13, -139.04. MS (MALDI-TOF): Calcd for $C_{82}H_{78}F_8N_4O_2S_4$ (M^+): 1431.78, Found: 1432.22.

NMR Spectra

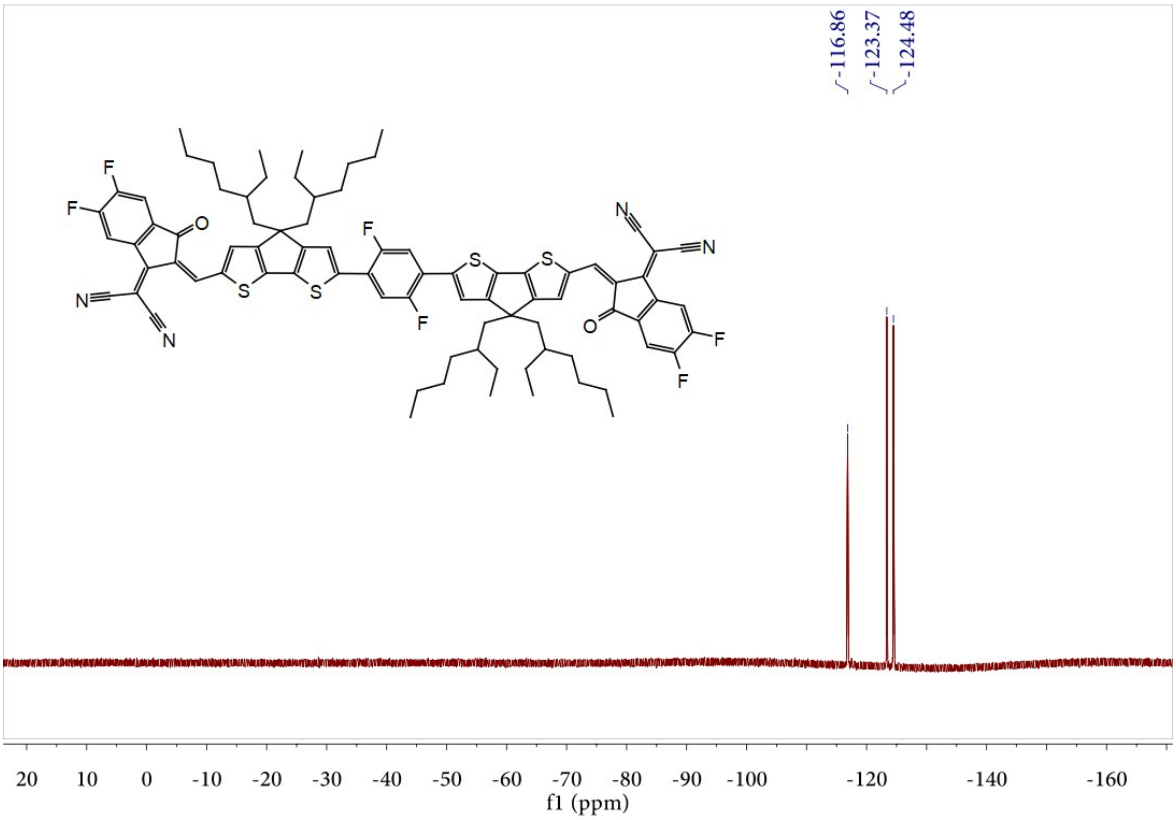
^{1}H NMR Spectrum of HF-PCIC



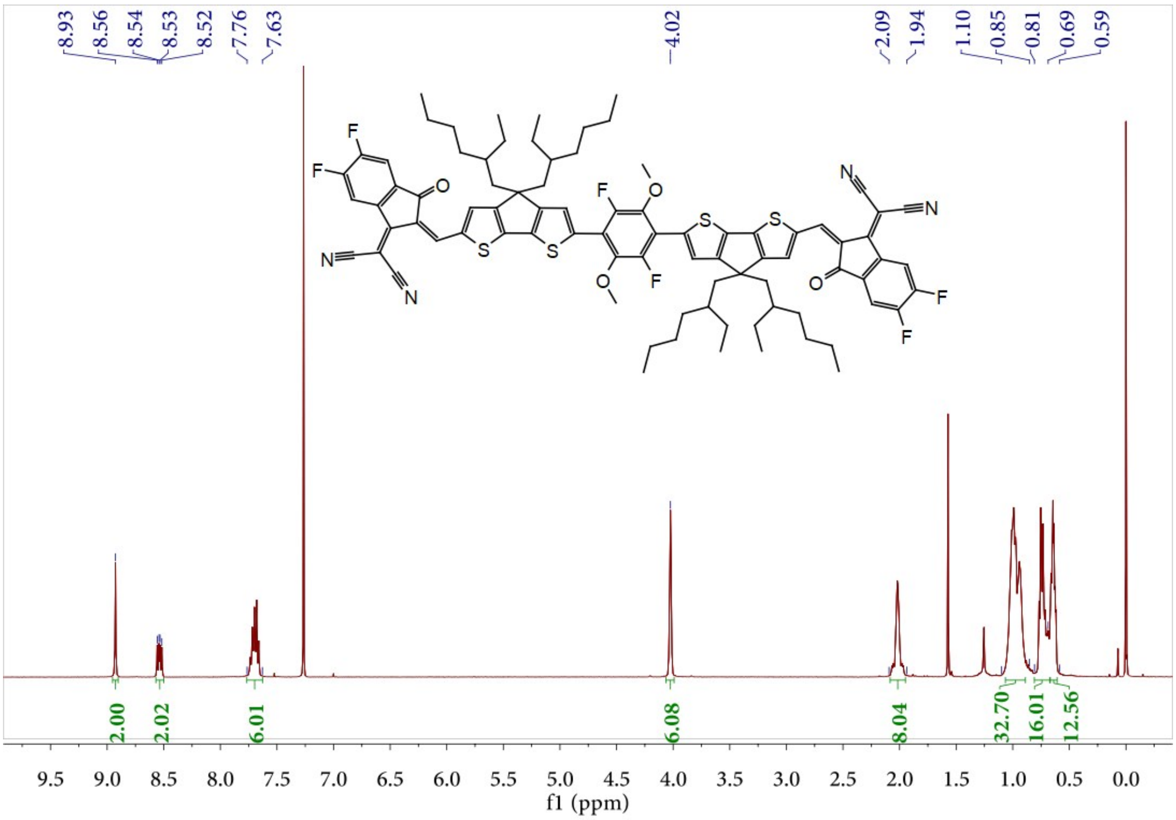
^{13}C NMR Spectrum of HF-PCIC



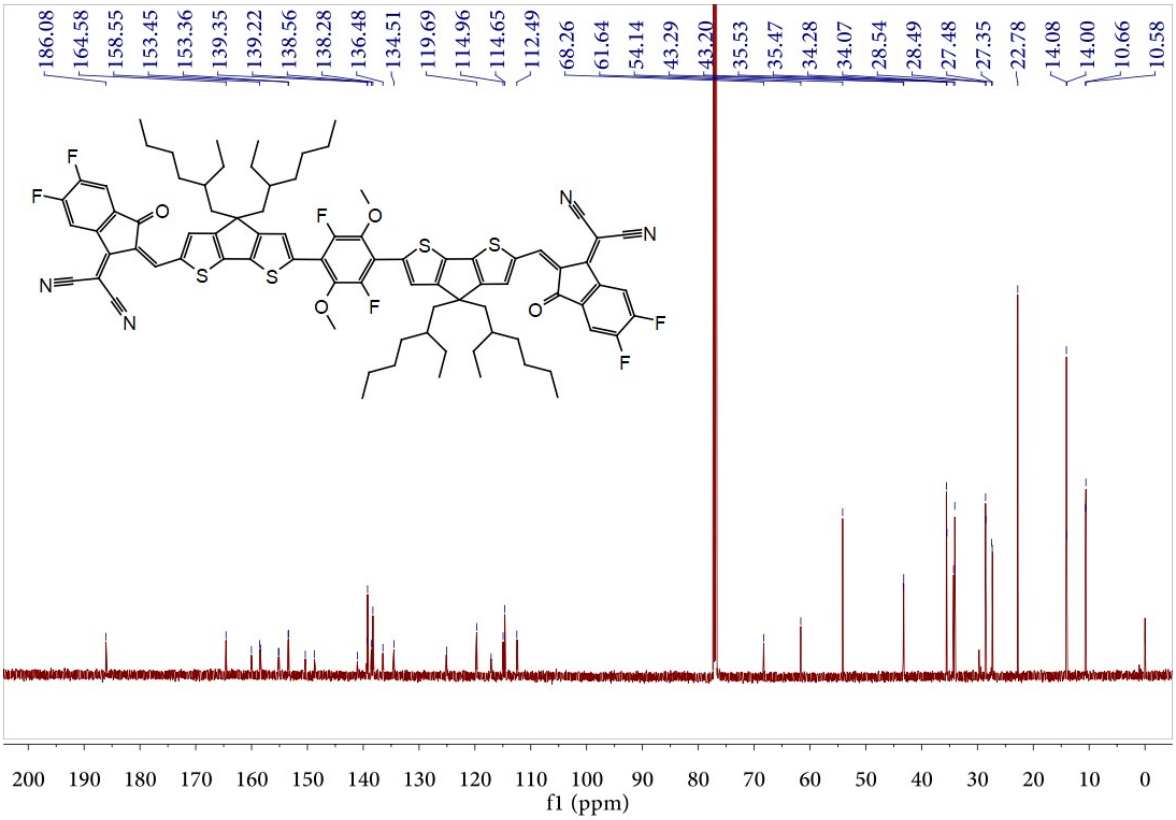
^{19}F NMR Spectrum of HF-PCIC



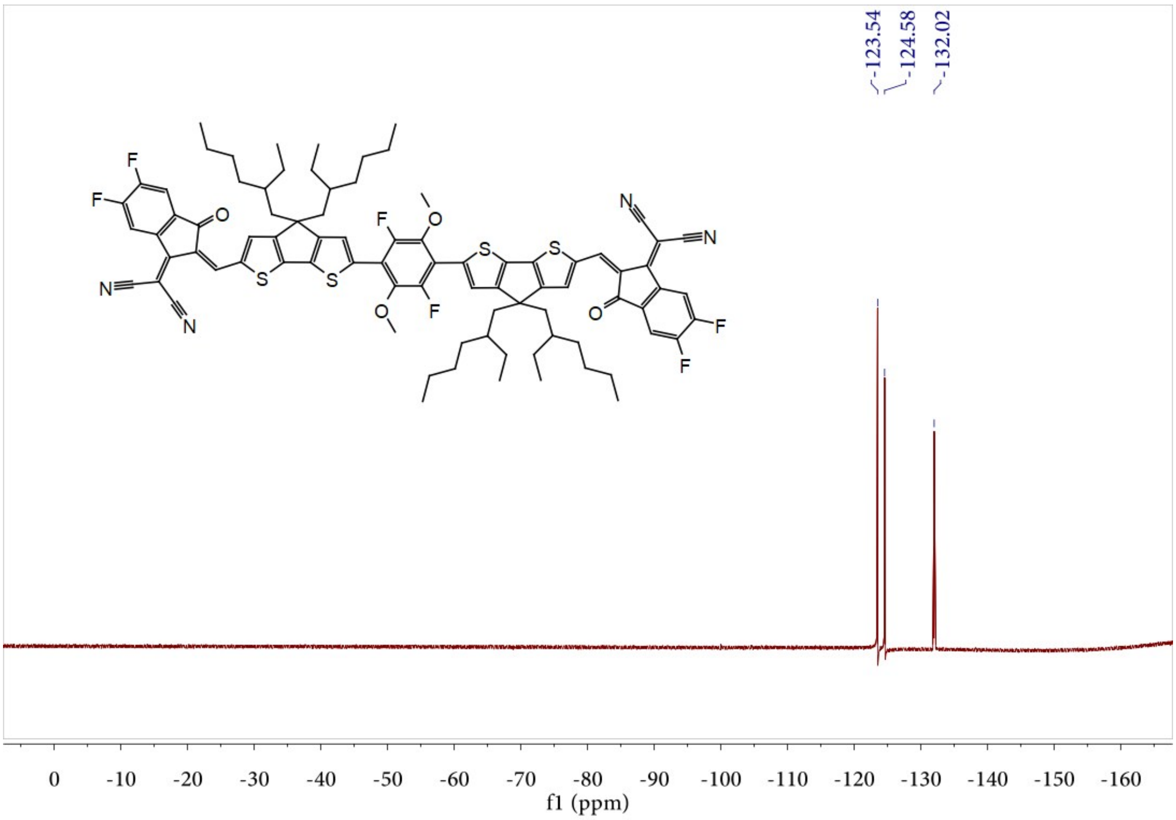
^{1}H NMR Spectrum of HFO-PCIC



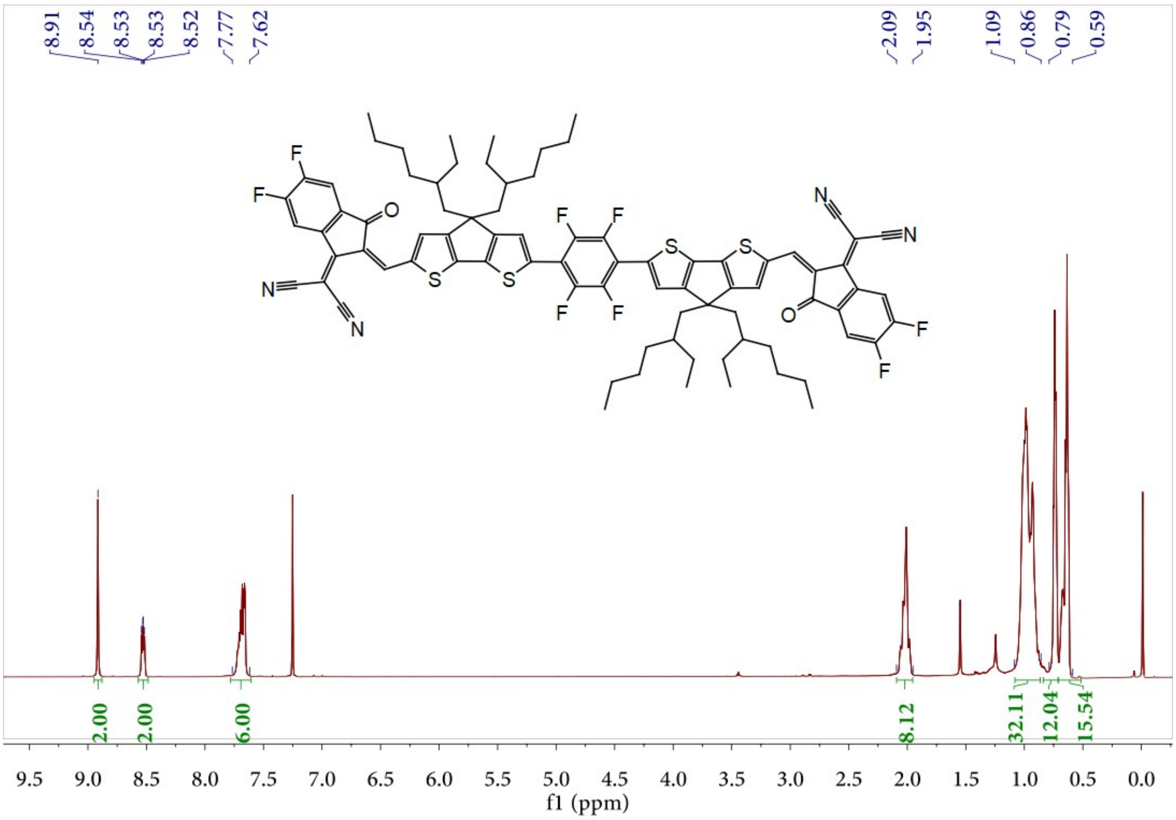
^{13}C NMR Spectrum of HFO-PCIC



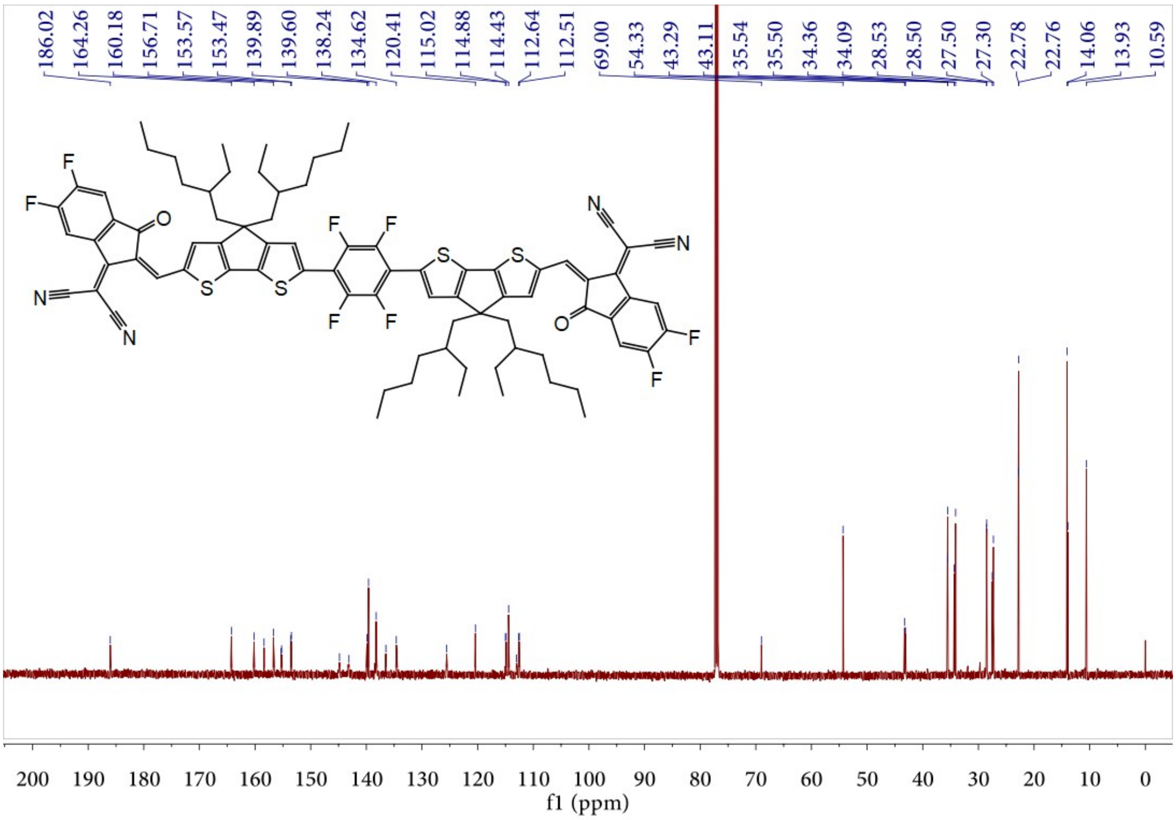
^{19}F NMR Spectrum of HFO-PCIC



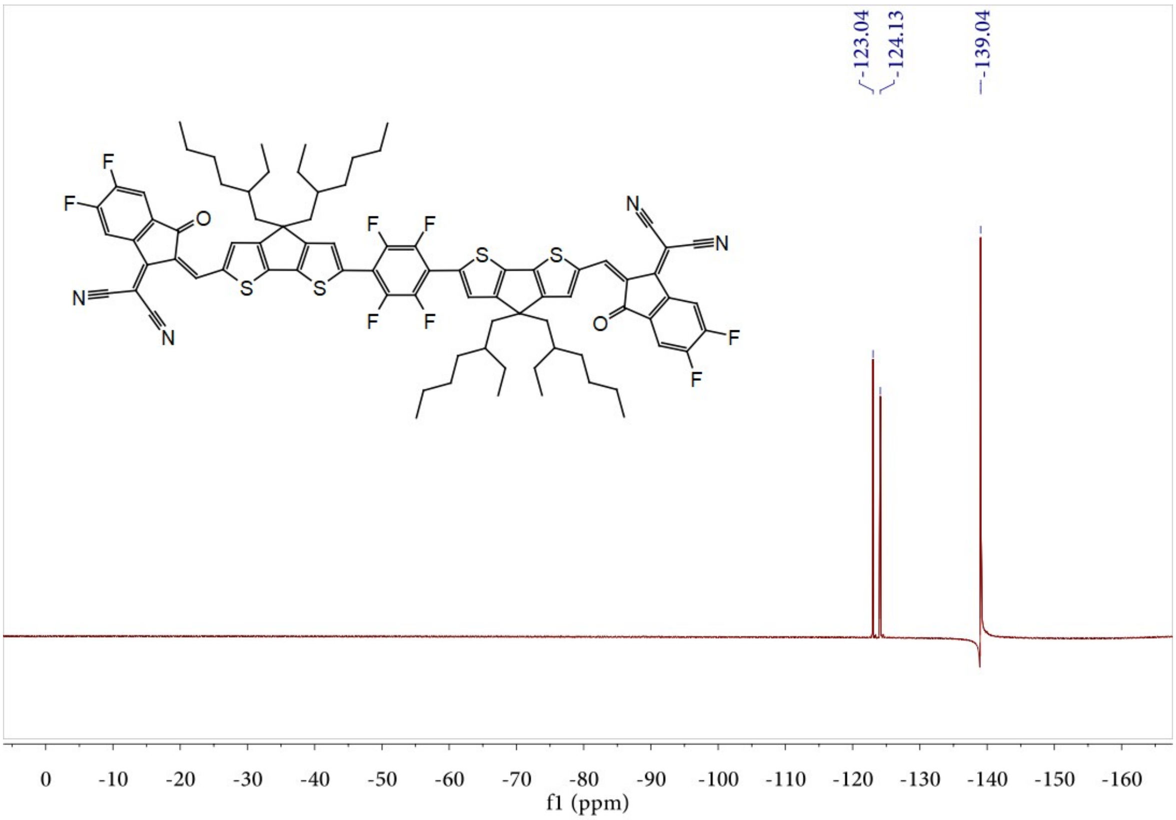
^{1}H NMR Spectrum of OF-PCIC



^{13}C NMR Spectrum of OF-PCIC



^{19}F NMR Spectrum of OF-PCIC



Supporting Figures and Tables

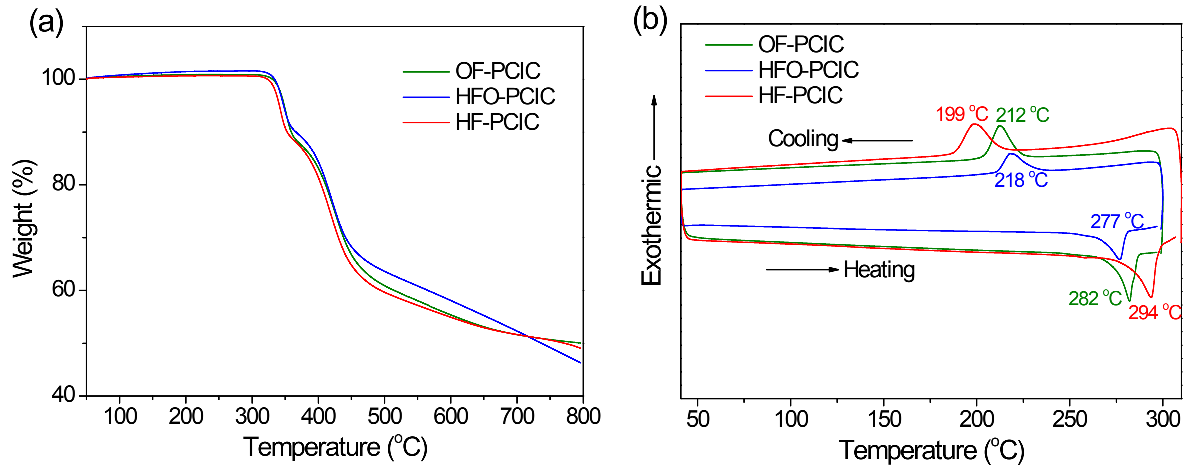


Figure S1. (a) TGA curves of HF-PCIC, HFO-PCIC and OF-PCIC. (b) DSC curves of HF-PCIC, HFO-PCIC and OF-PCIC.

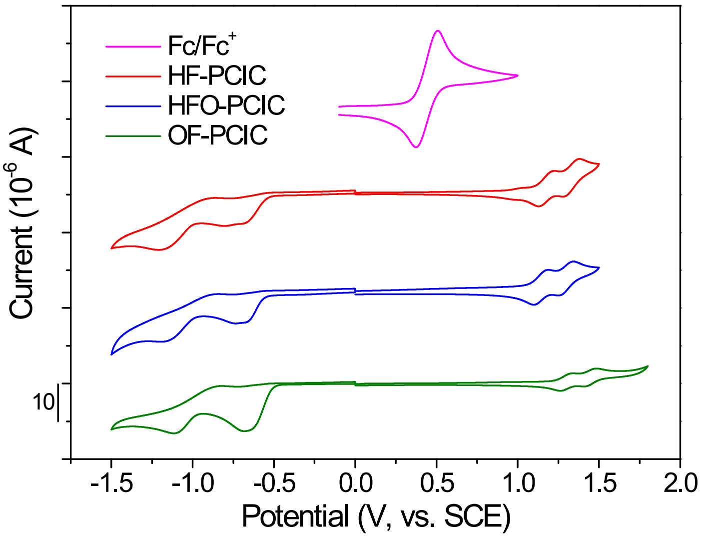


Figure S2. Cyclic voltammograms of HF-PCIC, HFO-PCIC, OF-PCIC and Fc/Fc$^+$ in dichloromethane solutions.

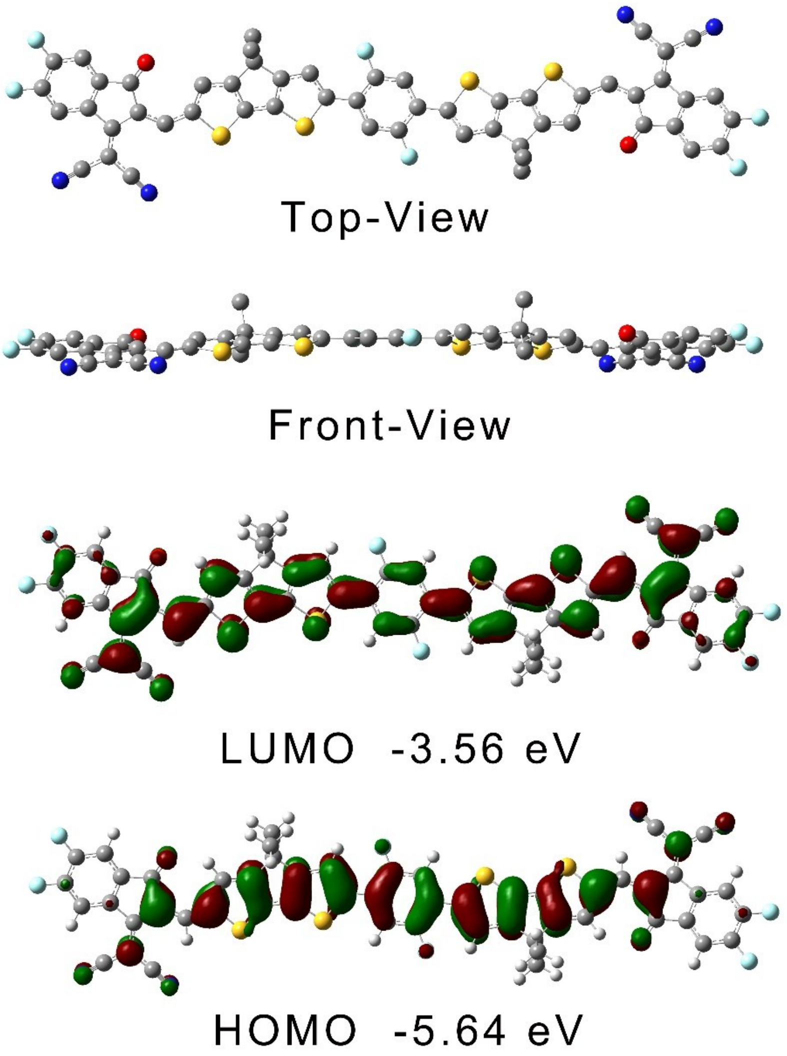
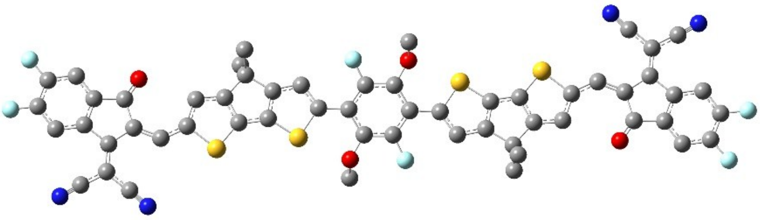
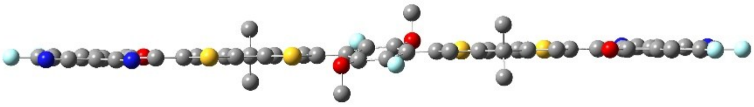


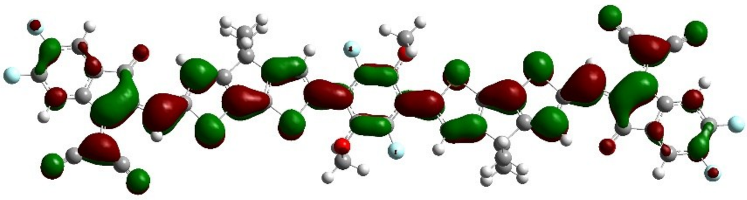
Figure S3. Simulated molecular geometries (Top-View and Front-View) and frontier molecular orbitals by DFT calculation for HF-PCIC.



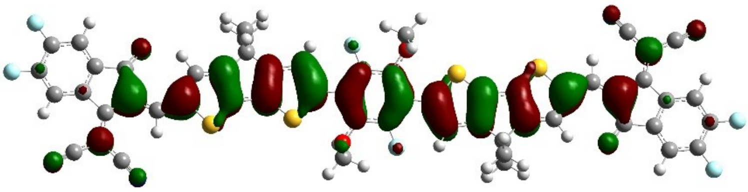
Top-View



Front-View



LUMO -3.48 eV



HOMO -5.56 eV

Figure S4. Simulated molecular geometries (Top-View and Front-View) and frontier molecular orbitals by DFT calculation for HFO-PCIC.

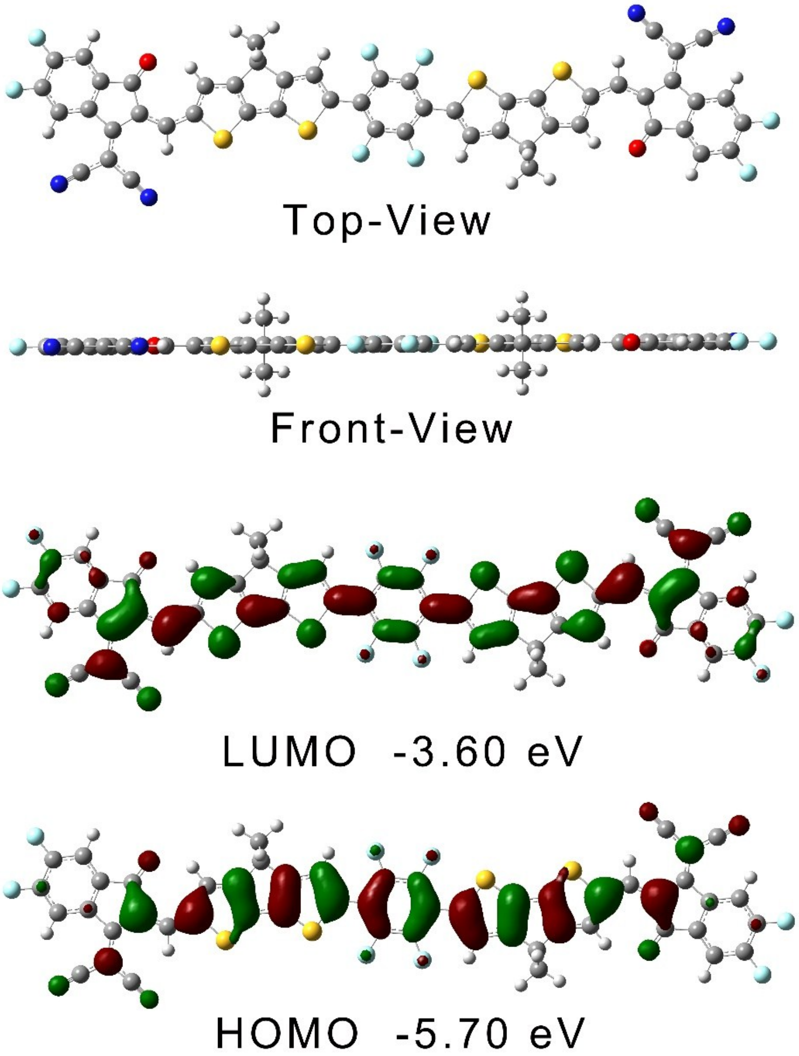


Figure S5. Simulated molecular geometries (Top-View and Front-View) and frontier molecular orbitals by DFT calculation for OF-PCIC.

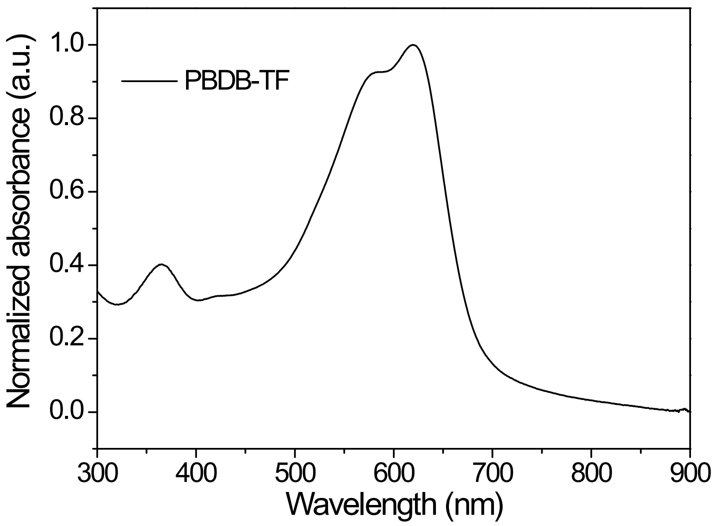


Figure S6. UV-vis absorption spectrum of PBDB-TF thin film.

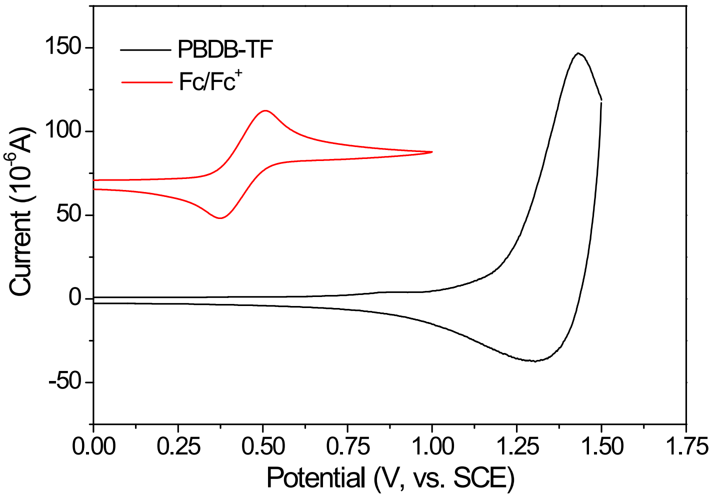


Figure S7. Cyclic voltammograms of PBDB-TF and Fc/Fc$^+$.

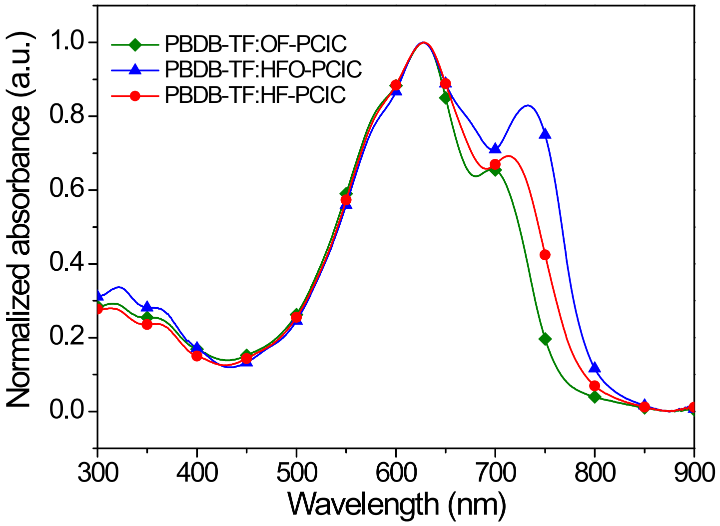


Figure S8. UV-vis absorption spectra of PBDB-TF:Acceptor blended films with different non-fullerene acceptors.

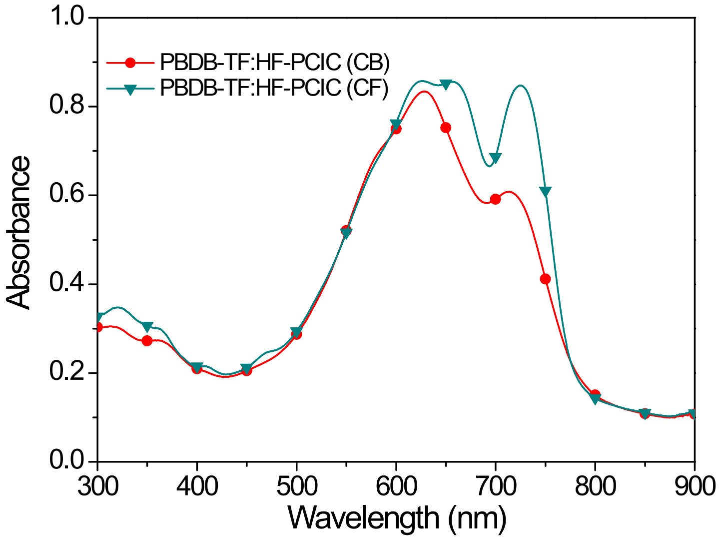


Figure S9. UV-vis absorption spectra of PBDB-TF:HF-PCIC blended films spin-coated from chlorobenzene or chloroform solutions.

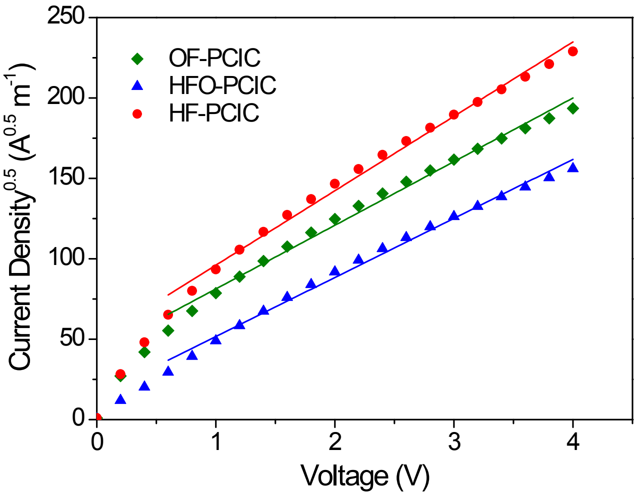


Figure S10. $J^{0.5}$-V curves of the electron-only devices based on pure acceptor films.

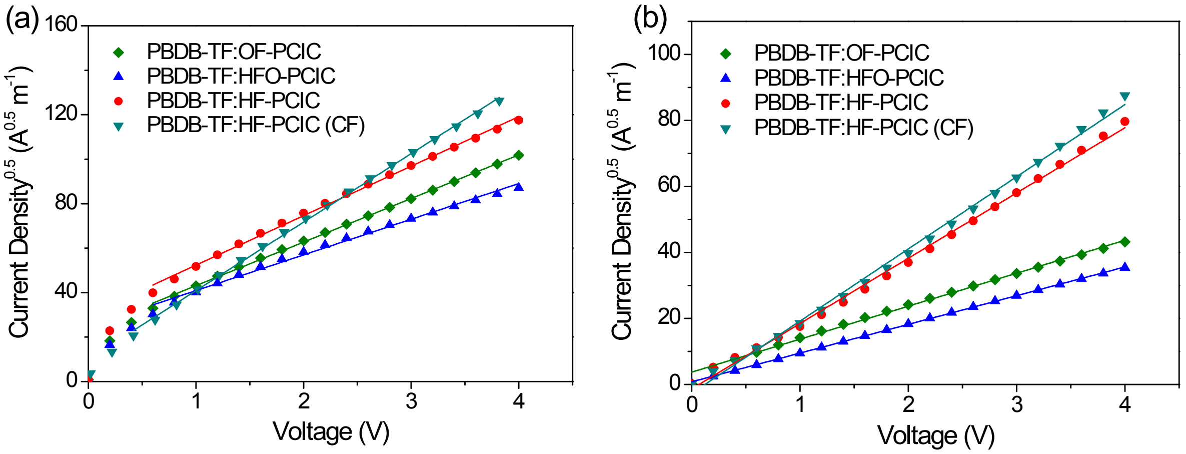


Figure S11. (a) $J^{0.5}$-V curves of the hole-only devices based on PBDB-TF:Acceptor blended films. (b) $J^{0.5}$-V curves of the electron-only devices based on PBDB-TF:Acceptor blended films.

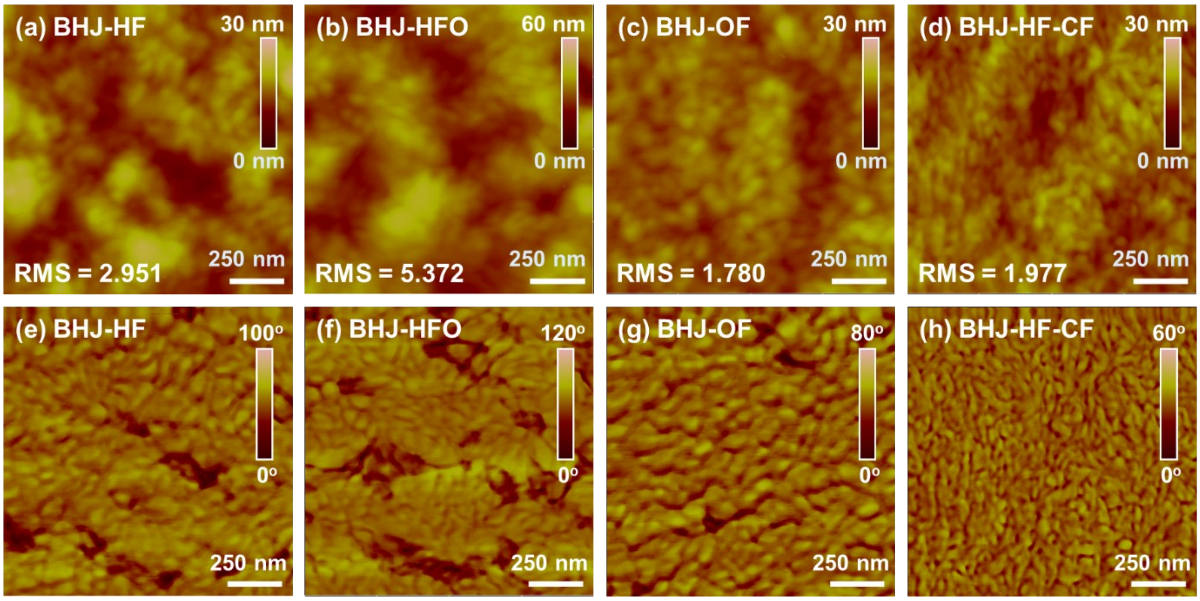


Figure S12. AFM height (a-d) and phase (e-h) images of PBDB-TF:HF-PCIC (BHJ-HF), PBDB-TF:HFO-PCIC (BHJ-HFO), PBDB-TF:OF-PCIC (BHJ-OF) and PBDB-TF:HF-PCIC CF (BHJ-HF-CF) blended films.

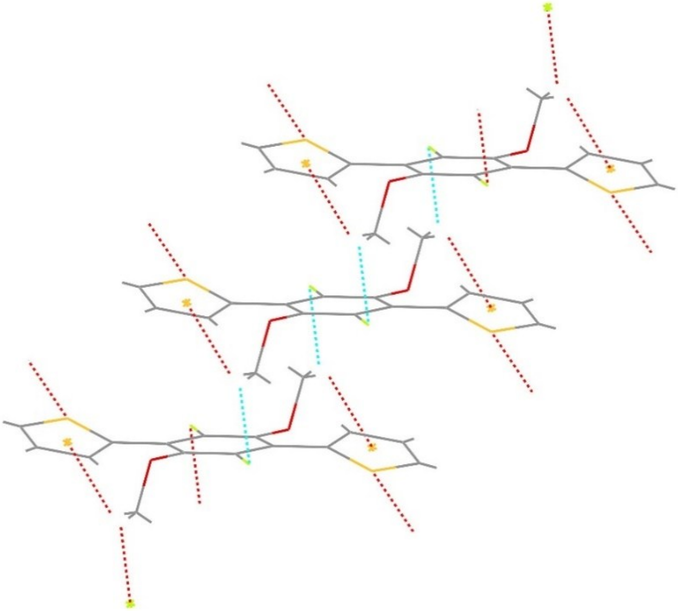


Figure S13. Diagram of intermolecular noncovalent interactions (dot lines) among model compound FPT-O extracted from single crystal data.

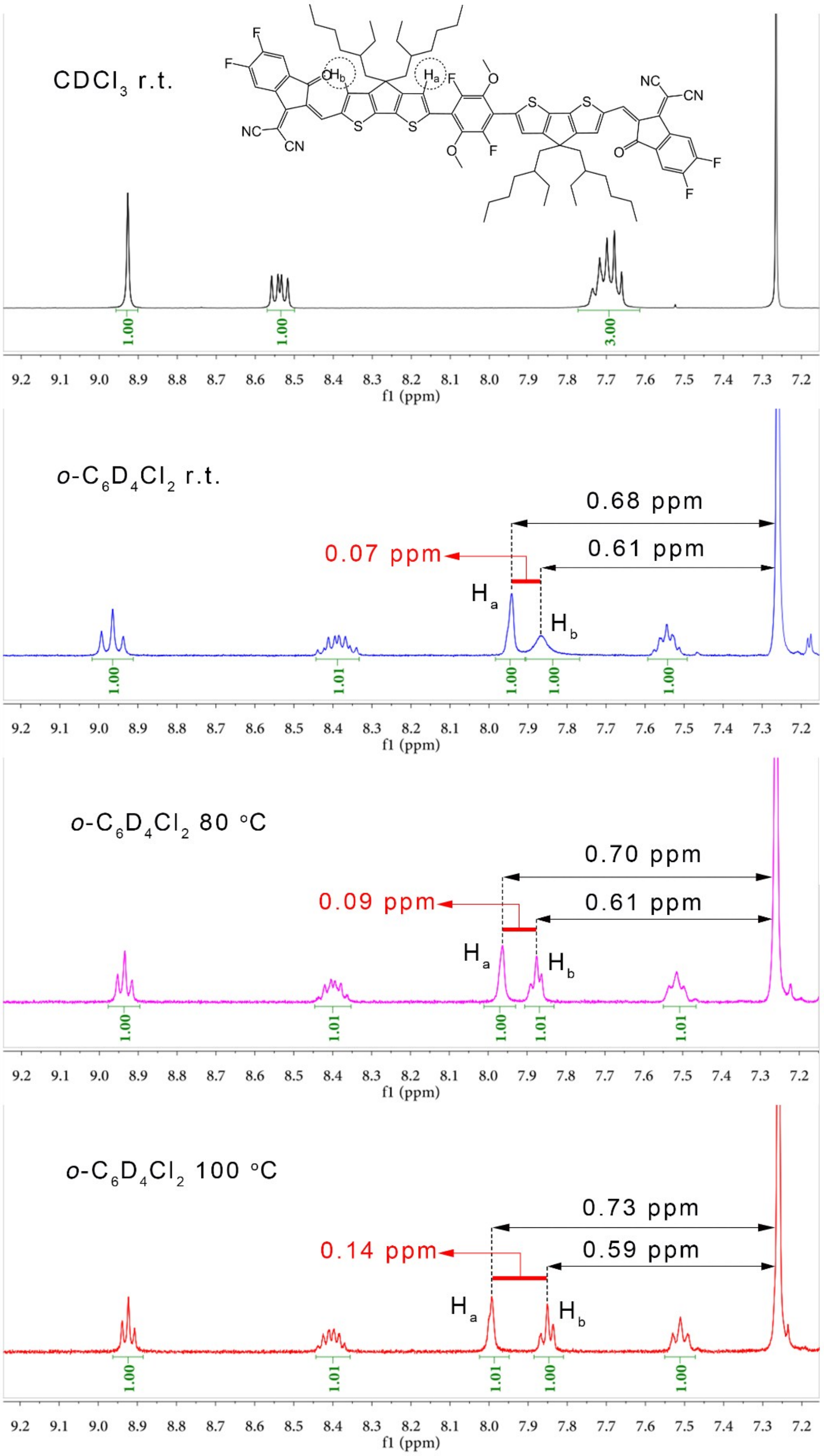


Figure S14. Comparison of ^{1}H NMR spectra of HFO-PCIC in different solvents and at differenet temperatures.

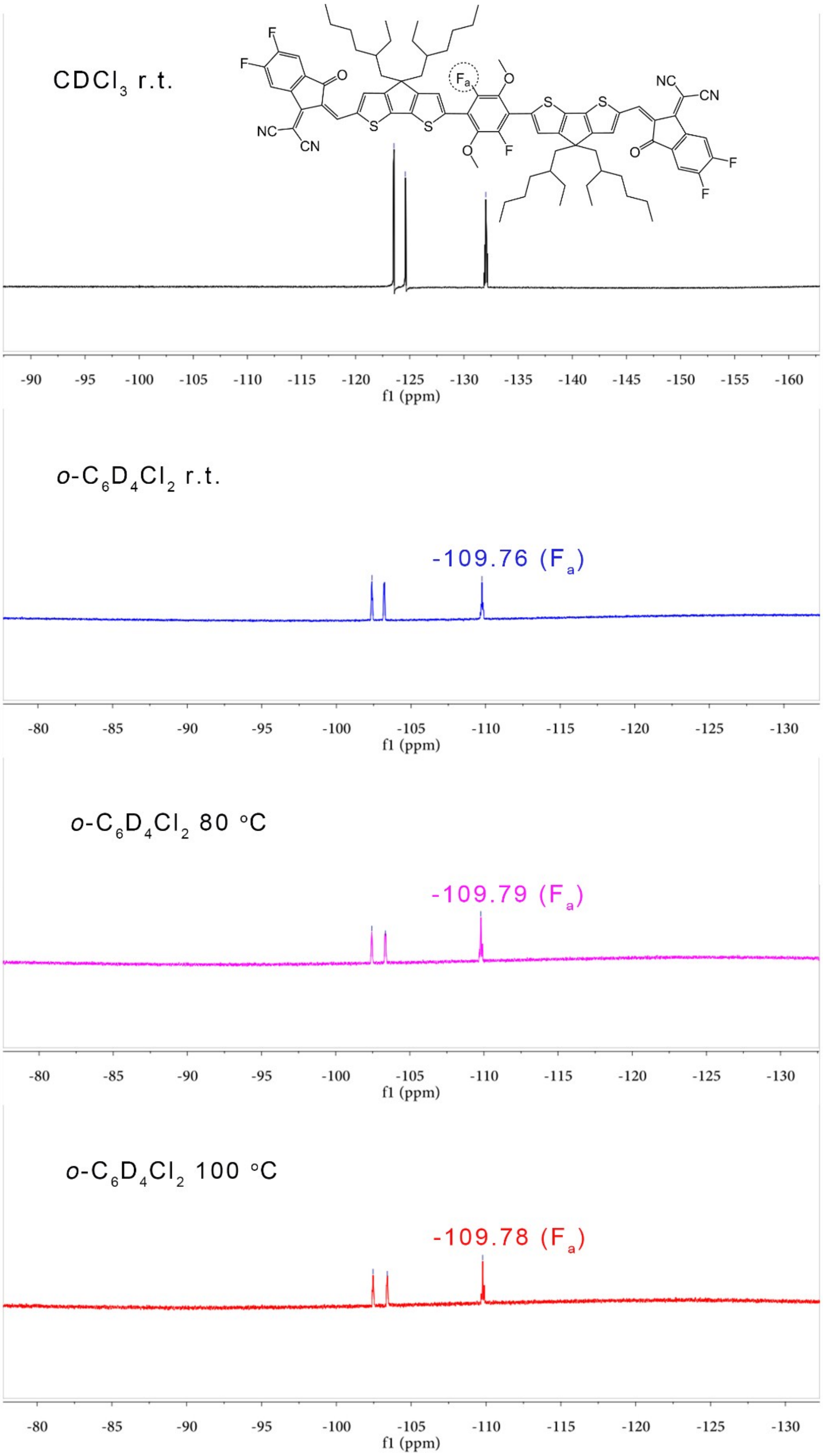


Figure S15. Comparison of ^{19}F NMR spectra of HFO-PCIC in different solvents and at different temperatures.

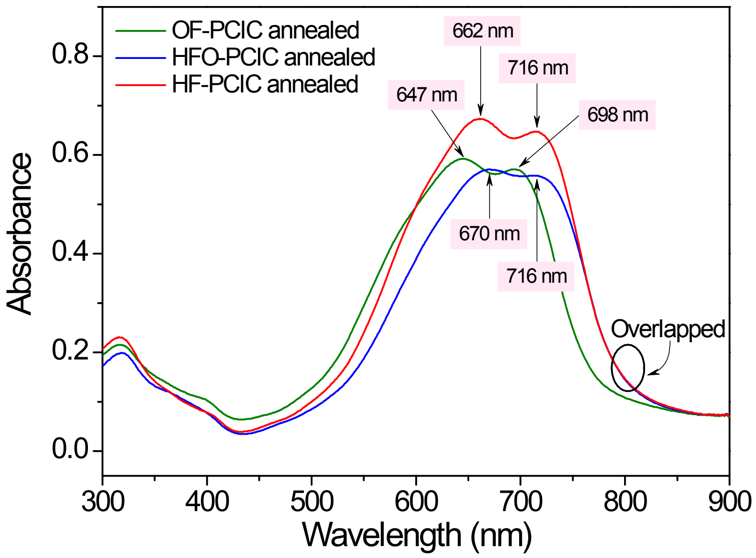


Fig. S16 UV-vis absorption spectra of OF-PCIC, HFO-PCIC and HF-PCIC thin films after thermal annealing at 110 ^oC for 10 min.

Table S1 Photovoltac parameters of PSCs based on PBDB-TF:HF-PCIC with chlorobenzene as the processing solvent

D/A	CN (%)	Annealing Temp. (°C)	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
1:1	w/o	w/o	0.92	13.94	61.08	8.20
1:1.2	w/o	w/o	0.91	14.71	65.68	9.23
1:1.5	w/o	w/o	0.91	14.03	68.29	9.08
1:1.2	1.0	w/o	0.92	14.49	70.46	9.59
1:1.2	1.2	w/o	0.92	15.15	71.65	10.11
1:1.2	1.4	w/o	0.91	14.07	72.78	9.57
1:1.2	1.0	100	0.91	15.25	71.46	10.23
1:1.2	1.0	110	0.92	16.01	72.42	10.97
1:1.2	1.0	130	0.91	16.03	68.77	10.28
1:1.2	1.2	100	0.91	15.39	73.92	10.45
1:1.2	1.2	110	0.90	16.25	72.46	10.91
1:1.2	1.2	130	0.91	15.67	70.65	10.45

Table S2 Hole and electron mobilities of PBDB-TF:Acceptor blended films

Blend	μ_h (× 10^{-4} cm^2 V^{-1} s^{-1})	μ_e (× 10^{-4} cm^2 V^{-1} s^{-1})	μ_h / μ_e
PBDB-TF:HF-PCIC	1.68 ± 0.04	1.35 ± 0.02	1.24
PBDB-TF:HFO-PCIC	0.86 ± 0.02	0.25 ± 0.00	3.44
PBDB-TF:OF-PCIC	1.29 ± 0.02	0.32 ± 0.01	4.03
PBDB-TF:HF-PCIC (CF)	3.28 ± 0.31	1.67 ± 0.06	1.96

Table S3. Crystal data, data collection and structure refinement for FPT-O

Identification code	171207_fpt_o
Crystal data	
Chemical formula	$C_{16}H_{12}F_2O_2S_2$
M_r	338.38
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, b, c (Å)	5.5646 (6), 6.9441 (8), 18.902 (2)
β (°)	98.039 (12)
V (Å^3)	723.22 (15)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.39
Crystal size (mm)	0.36 × 0.18 × 0.1
Data collection	
Diffractometer	Xcalibur, Atlas, Gemini ultra
Absorption correction	Multi-scan *CrysAlis PRO*, Agilent Technologies, Version 1.171.35.11 (release 16-05-2011 CrysAlis171 .NET) (compiled May 16 2011,17:55:39) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.904, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4341, 1326, 1052
R_{int}	0.045
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.602
Structure refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.115, 1.06
No. of reflections	1326
No. of parameters	101
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.32

References

(1) Zhang, M., Guo, X., Ma, W., Ade, H. and Hou, J., *Adv. Mater.*, **2015**, *27*, 4655.

(2) Li, S., Zhan, L., Liu, F., Ren, J., Shi, M., Li, C.-Z., Russell, T. P. and Chen, H., *Adv. Mater.*, **2018**, *30*, 1705208.