Supporting Information

for

Fluorine Substituents Reduce Charge Recombination and Drive Structure and Morphology Development in Polymer Solar Cells

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EXPERIMENTAL

Reagents and instrumentation. All reagents and chemicals were purchased from commercial sources (Aldrich, Acros, Strem, Matrix Scientific) and used without further purification. Reagent grade solvents were dried when necessary and purified by distillation. Microwave assisted polymerizations were conducted in a CEM Discover Benchmate microwave reactor. Gel permeation chromatography (GPC) measurements were performed on a Polymer Laboratories PL-GPC 220 instrument (at Cornell University) The obtained molecular weight is relative to the polystyrene standard. ^{1}H nuclear magnetic resonance (NMR) measurements were recorded either with a Bruker Avance 300MHz AMX or Bruker 400 MHz DRX spectrometer. ^{13}C nuclear magnetic resonance (NMR) measurements were carried out with a Bruker 400 MHz DRX spectrometer. Chemical shifts were expressed in parts per million (ppm), and splitting patterns are designated as s (singlet), d (doublet), m (multiplet) and br (broad). Coupling constants *J* are reported in Hertz (Hz).

UV-Vis & Fluorescence Spectroscopy. For both measurements, thin films of each polymer were spin-coated at 600 RPM onto pre-cleaned glass slides from 10 mg mL^{-1} polymer solution in o-dichlorobenzene, and dried slowly in a petri dish for 3 hours. UV-visible absorption spectra were obtained by a Shimadzu UV-2401PC spectrophotometer. Steady state emission spectra were acquired with a PTI 4SE-NIR QuantaMaster emission spectrometer equipped with a Xenon light source and Hamamatsu R928P photomultiplier tube (PMT). Excitation was at 600nm, with a 650nm long-pass optical filter inserted before the detector. Emission intensities at each wavelength were corrected for system spectral response.

Cyclic voltammetry. Cyclic voltammetry measurements were carried out using a Bioanalytical Systems (BAS) Epsilon potentiostat equipped with a standard three-electrode configuration. Typically, a three-electrode cell equipped with a glassy carbon working electrode, a $Ag/AgNO_3$ (0.01 M in anhydrous acetonitrile) reference electrode, and a Pt wire counter electrode was employed. The measurements were done in anhydrous acetonitrile with tetrabutylammonium hexafluorophosphate (0.1 M) as the supporting electrolyte under an argon atmosphere at a scan rate of 100 mV/s. Polymer films were drop-cast onto the glassy carbon working electrode from a 3 mg/mL chlorobenzene solution and dried under house nitrogen stream prior to measurements. The potential of $Ag/AgNO_3$ reference electrode was internally calibrated by using the ferrocene/ferrocenium redox couple (Fc/Fc+). The electrochemical onsets were determined at the position where the current starts to differ from the baseline. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy levels of polymers were calculated from the onset oxidation potential (E^{ox}) and onset reductive potential (E^{red}), respectively, according to **eqs. 1** and **eqs. 2**.

$$HOMO = -(E^{ox} + 4.8)\ \text{(eV)} \tag{1}$$

$$LUMO = -(E^{red} + 4.8)\ \text{(eV)} \tag{2}$$

Polymer solar cell fabrication and testing. Glass substrates coated with patterned indium-doped tin oxide (ITO) were purchased from Thin Film Devices, Inc. The 150 nm thick sputtered ITO pattern had a sheet resistance of 15Ω/□. Prior to use, the substrates were ultrasonicated for 20 minutes in 2-propanol. The substrates were then dried under a stream of nitrogen and placed in a UV-Ozone cleaner for 20 minutes. A 0.45 μm PVDF filtered dispersion of PEDOT:PSS in water (Baytron PH500) was then spun cast onto clean ITO substrates at 4000 rpm for 60 seconds and baked at 140 °C for 20 minutes yielding a thin film with a thickness of 40 nm. A 1:1 w/w blend of polymer and PCBM at 10 mg/mL was dissolved in dichlorobenzene 120 °C for overnight, filtered through a 1.0 μm poly(tetrafluoroethylene) (PTFE) filter, and spun cast between 400 – 1000 rpm for 60 seconds onto a PEDOT:PSS layer. The substrates were then left to dry at room temperature under N_2 for 12 hours. The devices were finished for measurement after thermal deposition of a 30 nm film of calcium and a 70 nm aluminum film as the cathode at a pressure of ~ 1 × 10^{-6} mbar. There are 8 devices per substrate, with an active area of 12 mm^2 per device. The thicknesses of films were recorded by a profilometer (Alpha-Step 200, Tencor Instruments). Device characterization was carried out under AM 1.5G irradiation with the intensity of 100 mW cm^{-2} (Oriel 91160, 300 W) calibrated by a NREL certified standard silicon cell. I-V curves were recorded with a Keithley 2400 digital source meter. All fabrication steps after adding the PEDOT:PSS layer onto ITO substrate, and characterizations were performed in gloveboxes under nitrogen atmosphere. For mobility measurements, the hole-only devices in a configuration of ITO/PEDOT:PSS (45 nm)/polymer-PCBM/Pd (40 nm) were fabricated. The experimental dark current densities J of polymer: PCBM blends were measured when applied with voltage from 0 to 6 V. The applied voltage V was corrected from the built-in voltage V_{bi} which was taken as a compensation voltage $V_{bi}=V_{oc}$ + 0.05 V and the voltage drop V_{rs} across the indium tin oxide/poly(3,4-ethylene-dioxythiophene):poly(styrene sulfonic acid) (ITO/PEDOT:PSS) series resistance and contact resistance, which is found to be around 35 Ω from a reference device without the polymer layer. From the plots of $J^{0.5}$ vs. V (supporting information Figure S6), hole mobilities of copolymers can be deduced from

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

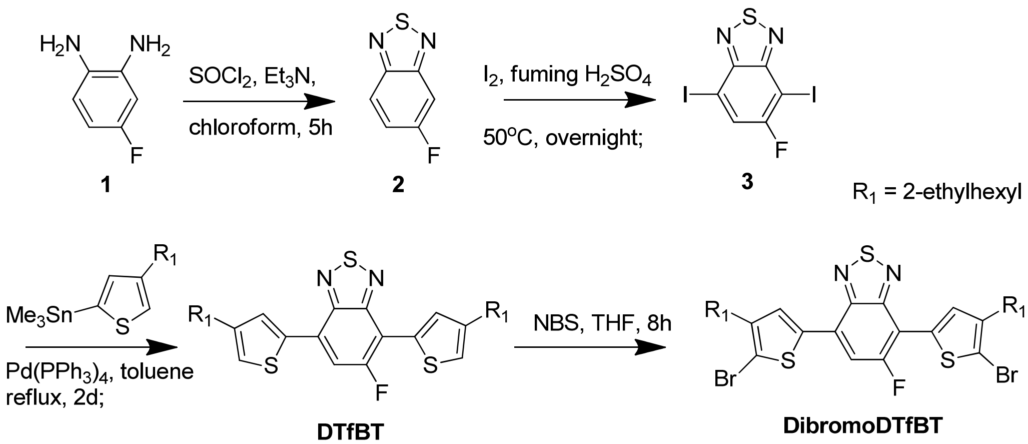
where ε_0 is the permittivity of free space, ε_r is the dielectric constant of the polymer which is assumed to be around 3 for the conjugated polymers, μ_h is the hole mobility, V is the voltage drop across the device, and L is the film thickness of active layer. AFM Images were taken using an Asylum Research MFP3D Atomic Force Microscope. Varied light intensity studies were performed by using neutral density filters ranging from 0.1 up to 1.0 optical density. Light intensity for each filter was calculated by the ratio of measured current of an NREL certified stardard silicon solar cell under each filter to the current collected under 1-sun condition. A total of 7 different light intensities were used as I-V curves were collected in series from each individual device.

Single crystal preparation and analysis. The crude product after column chromatography was dissolved in hot ethanol (DTBT and DTfBT) or 2-propanol (DTffBT) upon stirring, and the solution was cooled to room temperature slowly and then to -10 °C in the fridge overnight. A suitable needle-like crystal was mouted on Bruker-AXS SMART Apex-II diffractometer. The crystal was kept at 100 K during data collection. Using Olex2,[1] the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the XL [3] refinement package using Least Squares minimisation.

Computational Details. All quantum chemical calculations were performed using density functional theory (DFT) B3LYP functional with the 6-311+G(d) basis set. A full structure optimization for each of these model structures in gas phase at 0 K was first carried out, and a frequency calculation for each of the systems was performed to check that the optimized structure was indeed a minimum (i.e., with no imaginary frequency). Time-dependent DFT calculations at the same level of theory were performed to obtain the optimized structure and dipole moments of the first excited state for BnDT-DTBT, BnDT-DTfBT and BnDT-DTffBT monomers. All calculations are performed with the Gaussian 09 package Version C01[4] with tight self-consistent field convergence and ultrafine integration grids.

X-ray Characterization. Resonant soft X-ray scattering (R-SoXS) characterization was conducted at Beamline 11.0.1.2 of the Advanced Light Source (ALS). Films were cast on PEDOT:PSS-coated Si substrates and processed with the same conditions as those used to make devices. A section of the film was then floated onto 1.5 mm X 1.5 mm silicon nitride windows. Grazing incidence wide angle X-ray scattering (GIWAXS) was carried out at Beamline 7.3.3. of the ALS. Blend films were measured on PEDOT:PSS-coated Si substrates at an incident angle of 0.15º, above the critical angle to ensure X-ray penetration to the substrate. The beamline energy was 10 keV. Air scatter was reduced using helium gas. Scanning transmission X-ray microscopy was conducted at Beamline 5.3.2.2 of the ALS. Films cast on PEDOT:PSS-coated Si substrates were floated onto TEM grids. During measurement, the chamber was filled with 1/3 ATM He.

Scheme S1. Synthetic Route for **DibromoDTfBT**.



Monomer and Polymer Synthesis.

5-fluorobenzo[c][1,2,5]thiadiazole (2). To a round bottom flask were added **1** (0.33 g, 2.6 mmol), $CHCl_3$ (30 mL) and triethylamine (0.7 mL, 7 mmol). The solution was stirred until compound **1** was completely dissolved. Thionyl chloride (0.7 g, 5.2 mmol) was added dropwise and the mixture was heated to reflux for 5 h. The mixture was then cooled to room temperature before it was extracted with $CHCl_3$ (10 mL×3). The organic layer was combined and dried over $MgSO_4$. A short silica plug was used to remove most of the impurities, then solvent was evaporated and the product as white needle-like crystal (0.29 g) was obtained by column chromatography using hexane/dichloromethane (1:3 v/v) as the eluent. Yield:72%. ^{1}H NMR (400MHz, $CDCl_3$): δ 7.96 (dd, 1H, $J_{H\text{-}H}$= 5.2 Hz, $J_{H\text{-}F}$= 9.6 Hz), 7.58 (dd, 1H, $J_{H\text{-}H}$= 2 Hz, $J_{H\text{-}F}$= 8.8 Hz), 7.40 (m, 1H). *Note*: this compound is now commercially available from Matrix (catalog number 003286)

5-fluoro-4,7-diiodobenzo[c][1,2,5]thiadiazole (3). A mixture of **2** (0.29 g, 1.9 mmol), I_2 (2.5 g, 10 mmol) and fuming sulfuric acid (10 mL) in a RB flask was stirred at 50°C for 8

h. After cooling to room temperature, the reaction mixture was poured into a 500 mL beaker with crushed ice. Chloroform was added and the mixture was transferred into a separatory funnel and washed with distilled water, followed by 1M NaOH solution several times to remove excess iodine and finally washed with saturated $NaHCO_3$. The organic layer was then dried over $MgSO_4$. After the solvent removal, the yellow needle-like crystalline product was used without further purification. Reaction temperature and reaction time were screened and the reported condition gave highest yield of the product.

5-fluoro-4,7-bis(4-(2-ethylhexyl)-2-thienyl)-2,1,3-benzothiadiazole (DTfBT). In a 250 mL flame-dried 2-neck round-bottom flask with a condenser, the light yellow crystal from last step (1.9 mmol), excess of (4-(2-ethylhexyl)thiophen-2-yl)trimethylstannane (1.90 g, 4 mmol) and dry toluene 20 mL were added. The mixture was purged with argon for 15min. Then $Pd(PPh_3)_4$ (30 mg) was added and the reaction mixture was heated to reflux for 1d. The reaction mixture was then cooled to room temperature and the solvent was evaporated. The crude orange product was purified by column chromatography with hexane/dichloromethane (50:1 v/v) as eluent. The solvent was evaporated and the product was recrystallized from ethanol as orange solid. Yield: 0.237g (23% from compound **2**). ^1H NMR (300MHz, $CDCl_3$): δ 8.08 (s, 1H), 7.96 (s, 1H), 7.77&7.73 (d, 1H, J=12.9 Hz), 7.14 (s, 1H), 7.08 (s, 1H), 2.65 (dd, 4H, J=6.9 Hz), 1.66 (m, 2H), 1.21-1.44 (m, 16H), 0.80-0.94 (m, 12H). ^{13}C NMR (400MHz, CDCl3): δ 160.0, 157.8, 153.2, 149.6, 143.1, 142.1, 137.3, 132.0, 130.2, 125.7, 125.6, 123.9, 123.8, 116.8, 116.5, 111.1, 40.2, 34.5, 32.5, 29.0, 28.9, 26.6, 25.7, 23.1, 16.3, 14.2, 13.5, 10.9.

160.1, 153.0, 149.4, 142.4, 141.5, 136.9, 132.0, 131.9, 131.6, 131.5, 129.3, 125.1,125.0, 116.2, 115.9, 113.7, 40.0, 33.9, 33.8, 32.5, 28.8, 25.7, 23.1, 14.2, 10.9

Synthesis of 5-fluoro-4,7-bis(5-bromo-4-(2-ethylhexyl)-2-thienyl)-2,1,3-benzothiadiazole (dibromoDTfBT).

DTfBT (0.237 g, 0.44 mmol) and N-bromosuccinimide (NBS) (178 mg, 1 mmol) were added into THF under stirring. The reaction mixture was stirred at a room temperature for 8 h, and then the reaction mixture was washed with brine and dried over anhydrous sodium sulfate. The solvent was removed under a reduced pressure to give the product as an orange solid. Needle-like crystal was obtained by recrystallization from iso-propanol. Yield: 255 mg (83%). ^{1}H NMR (400MHz, $CDCl_3$): δ 7.93 (s, 1H), 7.73 (s, 1H), 7.69&7.65 (d, 1H, J=13.2 Hz), 2.59 (d, 4H), 1.70 (m, 2H), 1.18-1.45 (m, 16H), 0.79-0.91 (m, 12H). ^{13}C NMR (400MHz, CDCl3): δ 160.1, 153.0, 149.4, 142.4, 141.5, 136.9, 132.0, 131.9, 131.6, 131.5, 129.3, 125.1,125.0, 116.2, 115.9, 113.7, 40.0, 33.9, 33.8, 32.5, 28.8, 25.7, 23.1, 14.2, 10.9

Synthesis of PBnDT-DTfBT via Microwave-assisted Stille Coupling Polymerization.

To a 10 mL Microwave pressurized vial equipped with a stir bar, distannylated BnDT (154 mg, 0.175 mmol), dibromoDTfBT (123 mg, 0.175 mmol), $Pd_2(dba)_3$ (2.5%) and $P(o\text{-}tol)_3$ (20%) were added. Then the tube was sealed and evacuated and refilled with argon for three cycles and then o-xylene was added inside a glovebox. Reaction tube was put into microwave reactor and heated to 150 °C under 300 watt microwave for 20 min. After cooling to room temperature, the organic solution was added dropwise to 200 mL of methanol to obtain precipitate, which was collected by filtration and washed with methanol and dried. The crude polymer was then extracted subsequently with methanol, acetone, hexane and $CHCl_3$ in a Soxhlet's extractor. The residue after extracting with $CHCl_3$ was collected and dried under reduced pressure and to give the polymer **PBnDT-DTfBT** (148 mg, 77%) as a dark green solid. ^{1}H NMR (500 MHz, $CDCl_2CDCl_2$, 373K):8.16 (s, 1H), 8.03(s,1H), 7.78(d, 1H), 7.76(s, 2H), 3.18(br, 4H), 2.96(br,4H), 1.85(br, 6H), 1.65-1.21(br, 48H), 0.93(br, 12H), 0.85(br, 12H)

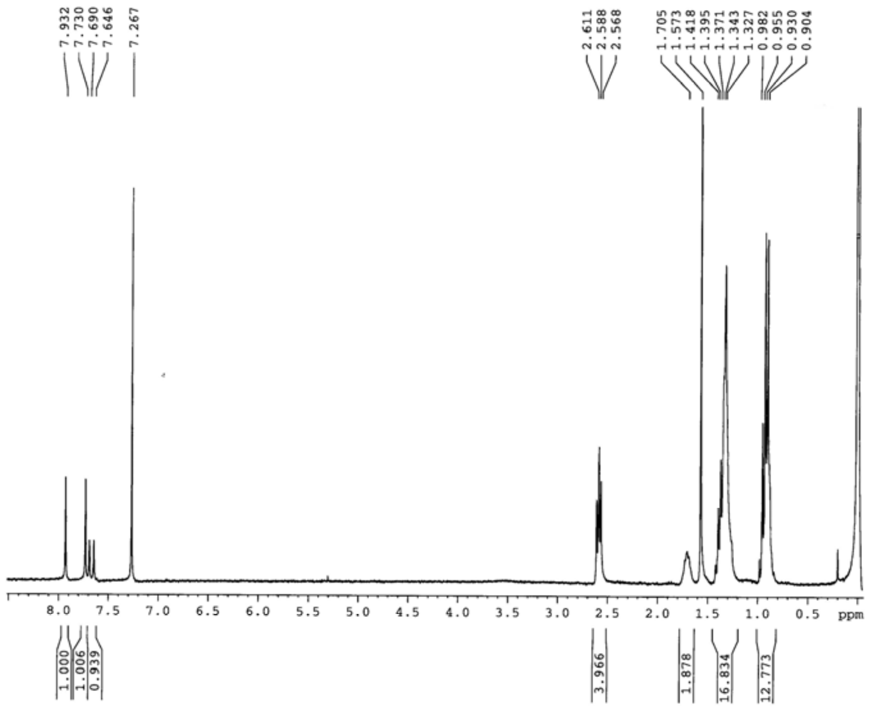


Figure S1. 1H NMR of **dibromoDTfBT**

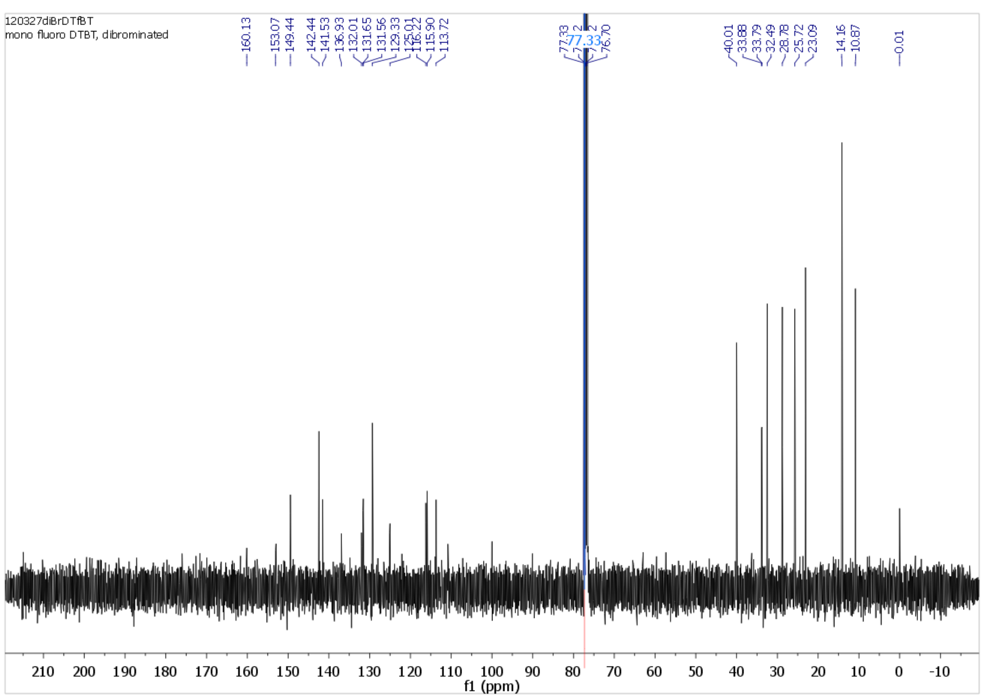


Figure S2. 13C NMR of **dibromoDTfBT**

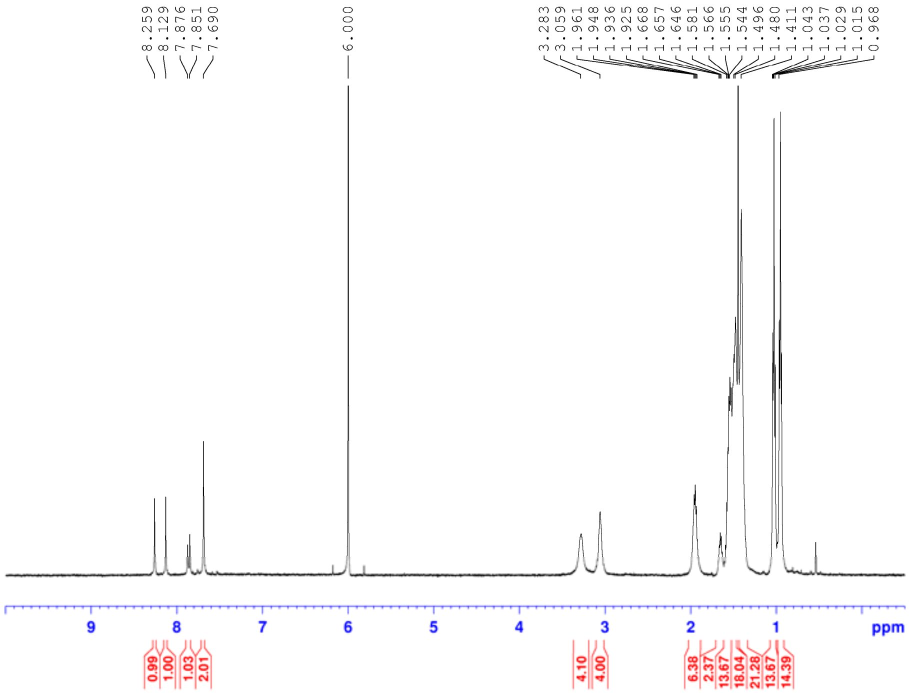


Figure S3. 1H NMR of **PBnDT-DTfBT.**

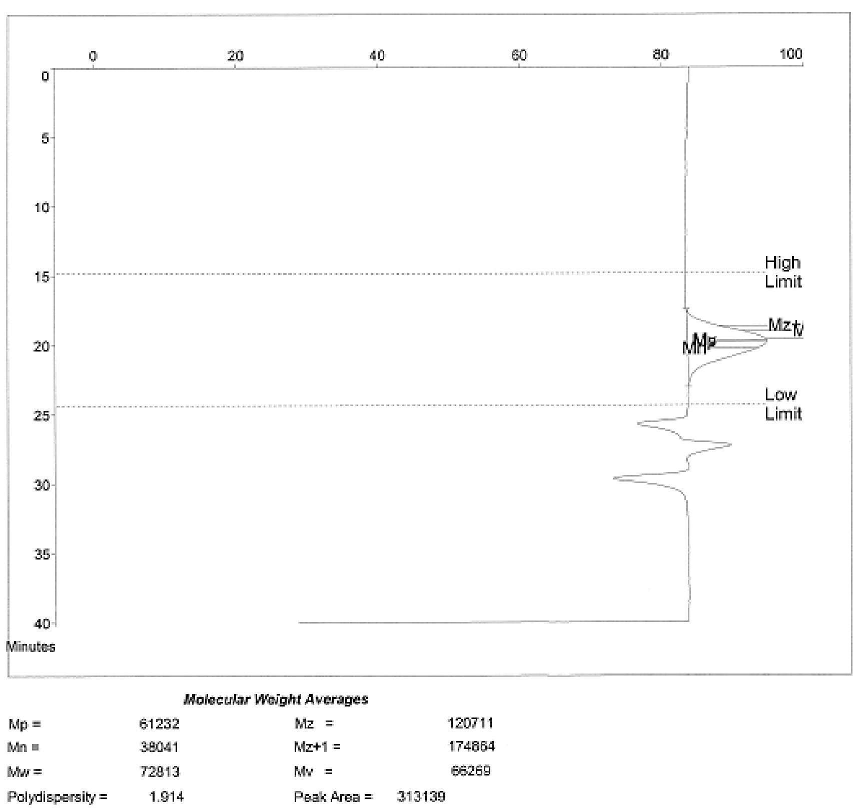


Figure S4. GPC trace of **PBnDT-DTfBT** polymer.

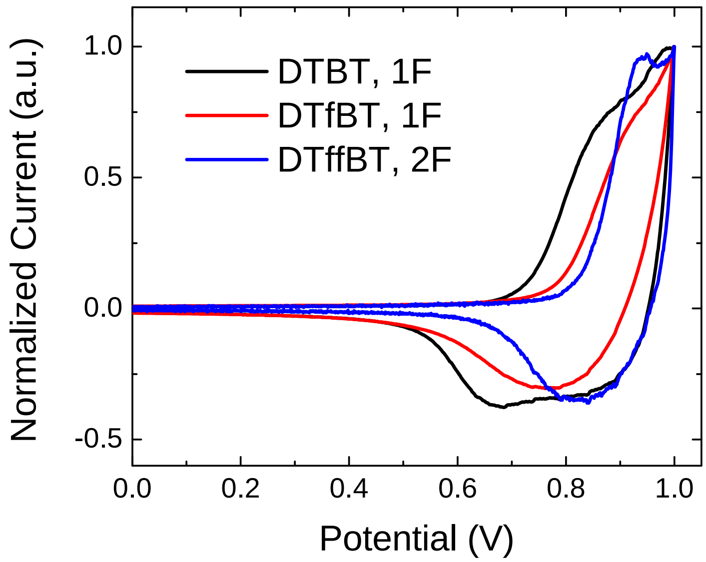


Figure S5. The oxidative portion of the cyclic voltammogram for 0F, 1F and 2F polymers. Ferrocene/ferrocenium redox couple is used as a standard (–4.8 eV) to evaluate polymer HOMO levels measured by CV.

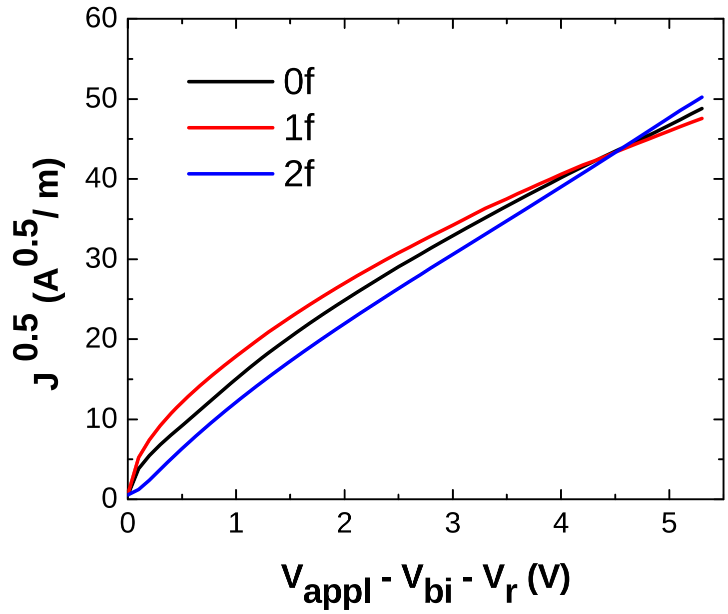


Figure S6. Example SCLC hole mobility measurements for each polymer. Curves correspond to 3.2, 2.6, and 3.7 × 10^{-4} $cm^2/V\cdot s$ for 0f, 1f and 2f polymers, respectively.

Table S1. Photovoltaic characteristics of **DTBT**, **DTfBT**, and **DTffBT** 100nm thick films at incremental light intensities where Jsat represents the photocurrent at high reverse bias voltage.

DTBT 100nm							
Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.15	2.10	0.73	55.8	5.51	8.83	2.50	83.9
0.39	4.96	0.74	53.5	5.10	7.90	6.25	79.3
0.50	6.11	0.75	52.5	4.84	7.66	7.78	78.4
0.62	7.65	0.75	51.3	4.76	7.33	9.75	78.4
0.77	9.71	0.75	50.1	4.75	6.94	12.44	78.1
1.00	11.93	0.76	48.7	4.43	6.65	15.19	78.5
1.26	14.21	0.76	47.6	4.07	6.30	18.30	77.7
1.55	17.22	0.76	46.3	3.92	5.98	22.24	77.4
DTfBT 100nm							
Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.15	2.02	0.80	57.6	6.03	5.98	2.34	86.3
0.39	4.96	0.82	55.1	5.80	5.68	5.82	85.2
0.50	6.21	0.83	54.2	5.61	5.53	7.32	84.8
0.62	7.69	0.83	53.9	5.58	5.38	9.25	83.1
0.77	9.94	0.84	52.9	5.71	5.21	12.08	82.3
1.00	12.11	0.84	51.8	5.30	5.03	14.83	81.6
1.26	14.37	0.85	51.1	4.95	5.04	17.91	80.2
1.55	17.66	0.85	50.4	4.89	4.78	22.32	79.1
DTffBT 100nm							
Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.15	2.12	0.85	63.0	7.33	7.81	2.56	82.7
0.39	5.11	0.87	63.5	7.29	6.94	6.13	83.3
0.50	6.44	0.88	63.1	7.18	6.61	7.63	84.4
0.62	8.13	0.88	63.1	7.31	6.25	9.59	84.7
0.77	10.65	0.89	61.8	7.55	5.86	12.39	86.0
1.00	13.17	0.89	61.1	7.18	5.49	15.36	85.8
1.26	15.71	0.90	61.4	6.87	5.13	18.40	85.4
1.55	19.41	0.90	59.8	6.75	4.83	24.02	80.8

Table S2. Photovoltaic characteristics of **DTBT**, **DTfBT**, and **DTffBT** 150nm thick films at incremental light intensities

DTBT 150nm							
Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.17	2.09	0.76	52.48	4.92	5.41	2.53	82.66
0.41	4.77	0.78	50.78	4.57	5.22	6.17	77.37
0.52	5.93	0.78	49.73	4.42	5.18	7.78	76.14
0.64	7.27	0.78	48.87	4.34	5.13	9.61	75.70
0.81	9.25	0.79	47.22	4.24	5.08	12.15	76.17
1.00	11.17	0.79	46.32	4.09	5.01	14.96	74.65
1.16	13.08	0.79	45.22	4.02	4.90	17.41	75.15
1.45	16.06	0.79	44.02	3.88	4.83	21.65	74.21
DTfBT 150nm							
Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.15	2.03	0.80	58.59	6.16	5.10	2.30	88.15
0.39	4.90	0.82	56.45	5.86	4.87	5.80	84.55
0.50	6.08	0.82	55.90	5.66	4.78	7.28	83.56
0.62	7.62	0.83	54.79	5.60	4.70	9.15	83.27
0.77	9.72	0.84	53.39	5.60	4.59	11.84	82.09
1.00	11.74	0.84	52.58	5.18	4.48	14.42	81.44
1.26	14.23	0.84	51.18	4.88	4.36	17.50	81.30
1.55	17.34	0.85	50.03	4.74	4.20	21.40	81.03
DTffBT 150nm							
Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.17	2.07	0.85	56.43	5.82	5.94	2.60	79.31
0.41	4.96	0.88	55.91	5.96	5.78	6.21	79.93
0.50	6.15	0.88	55.60	5.98	5.72	7.68	80.16
0.63	7.75	0.89	54.96	5.99	5.69	9.60	80.74
0.81	10.01	0.89	54.07	5.95	5.65	12.35	81.04
1.00	12.25	0.90	53.61	5.89	5.63	15.23	80.46
1.20	14.66	0.90	52.65	5.78	5.58	18.26	80.27
1.47	17.99	0.90	51.93	5.73	5.51	22.36	80.44

Table S3. Photovoltaic characteristics of **DTBT**, **DTfBT**, and **DTffBT** 200nm thick films at incremental light intensities

DTBT 200nm

Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.18	2.20	0.78	46.28	4.49	7.41	2.89	76.06
0.43	4.94	0.80	43.36	4.03	7.15	6.96	71.09
0.53	6.08	0.81	42.31	3.94	7.03	8.60	70.77
0.65	7.39	0.81	41.52	3.82	6.90	10.62	69.61
0.82	9.21	0.81	40.49	3.68	6.74	13.45	68.43
1.00	11.03	0.82	39.49	3.56	6.52	16.31	67.62
1.19	12.95	0.82	38.75	3.45	6.41	19.42	66.67
1.44	15.22	0.82	38.10	3.29	6.33	23.49	64.79

DTfBT 200nm

Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.17	2.15	0.78	55.82	5.42	3.58	2.66	80.98
0.42	5.09	0.80	52.56	5.14	3.52	6.43	79.13
0.52	6.32	0.81	51.56	5.09	3.50	7.96	79.42
0.64	7.81	0.81	50.34	5.01	3.45	9.81	79.58
0.83	10.12	0.82	48.27	4.83	3.44	12.71	79.61
1.00	12.14	0.82	47.07	4.69	3.39	15.39	78.89
1.21	14.64	0.82	45.76	4.55	3.35	18.66	78.45
1.48	17.74	0.83	43.94	4.36	3.27	22.75	78.01

DTffBT 200nm

Light Intensity (Fraction of 1 Sun)	Jsc (mA/cm^2)	Voc (V)	FF (%)	Efficiency (%)	Series R (Ohm*cm2)	Jsat (mA/cm^2)	Jsc/Jsat (%)
0.16	2.24	0.84	50.34	5.86	3.94	2.87	78.02
0.40	5.28	0.87	49.64	5.64	3.85	7.13	74.05
0.50	6.61	0.87	49.05	5.61	3.75	8.91	74.11
0.63	8.25	0.88	48.48	5.60	3.70	11.10	74.31
0.81	10.54	0.89	47.87	5.54	3.62	14.26	73.95
1.00	13.01	0.89	47.13	5.46	3.50	17.69	73.53
1.18	15.19	0.90	46.55	5.38	3.66	20.82	73.00
1.43	18.56	0.90	45.63	5.32	3.59	25.30	73.37

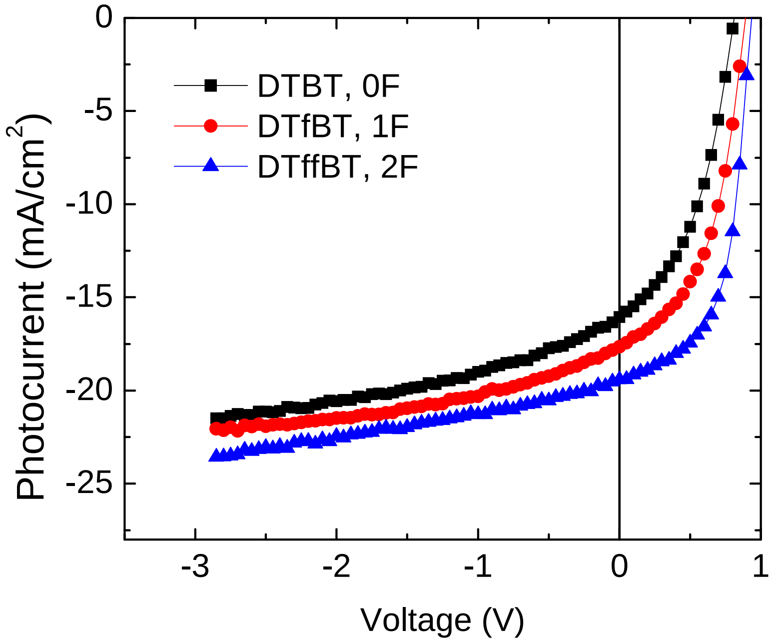


Figure S7. J-V curves of 0F, 1F and 2F polymers, 100nm thick film devices. Displayed photocurrent data are from the highest light intensity (1.55 Suns, see Table S1).

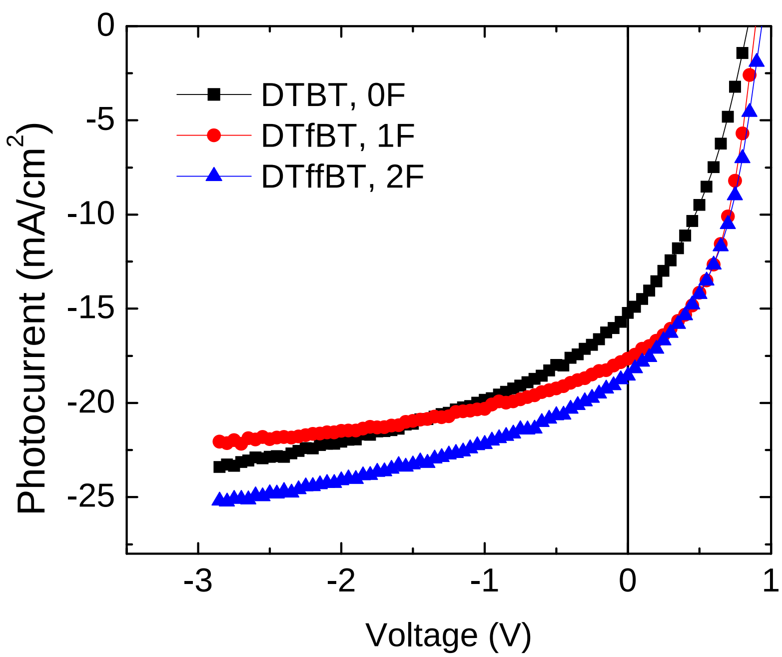


Figure S8. J-V curves of 0F, 1F and 2F polymers, 150nm thick film devices. Displayed photocurrent data are from the highest light intensity (1.45-1.55 Suns, see Table S2).

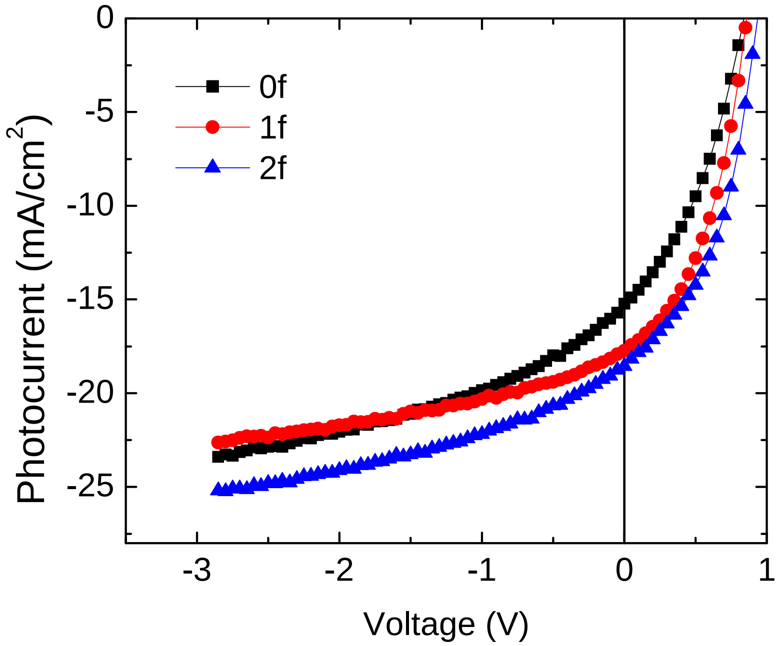


Figure S9. J-V curves of 0F, 1F and 2F polymers, 200nm thick film devices. Displayed photocurrent data are from the highest light intensity (1.43-1.48 Suns, see Table S3).

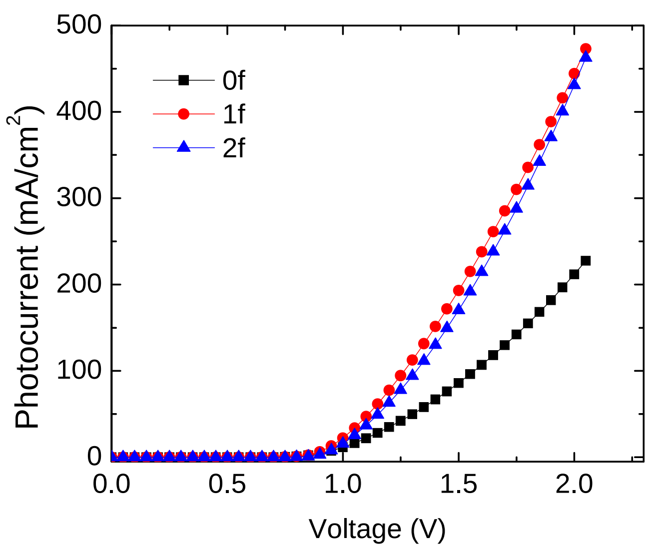


Figure S10. Dark J-V curves of 0F, 1F and 2F polymer, 100nm thick film devices.

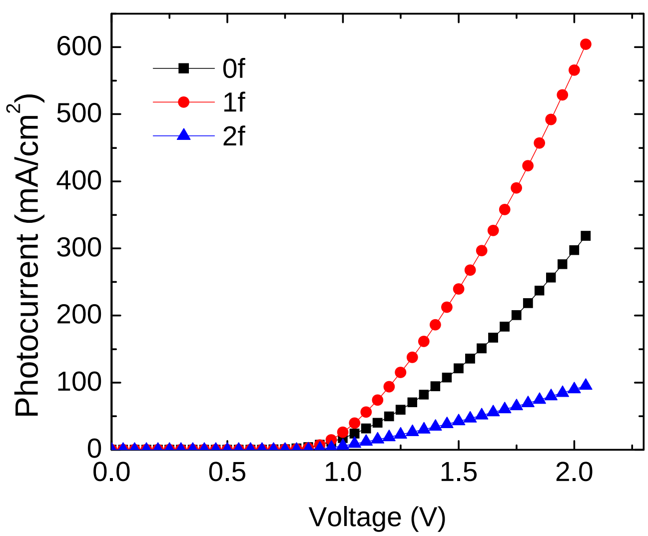


Figure S11. Dark J-V curves of 0F, 1F and 2F polymer, 150nm thick film devices.

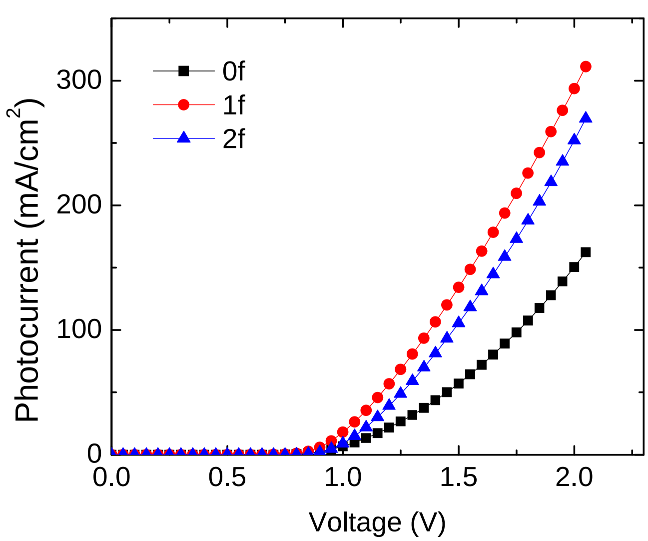


Figure S12. Dark J-V curves of 0F, 1F and 2F polymer, 200nm thick film devices.

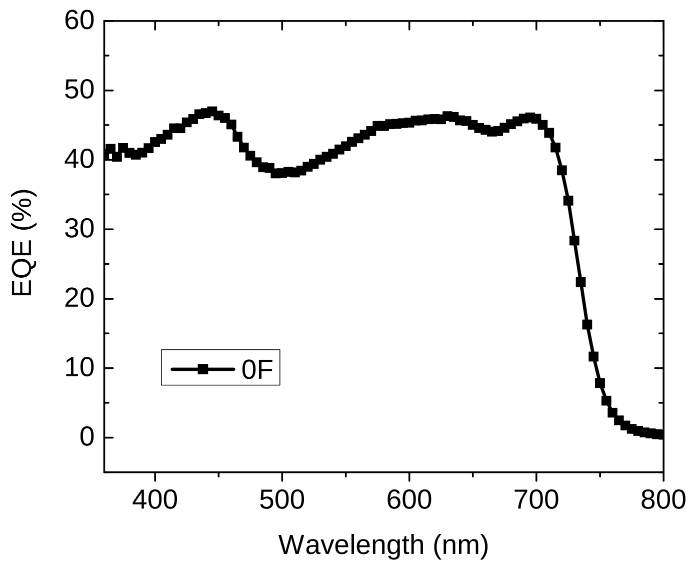


Figure S13. EQE of 0F polymer, 100nm thick film device.

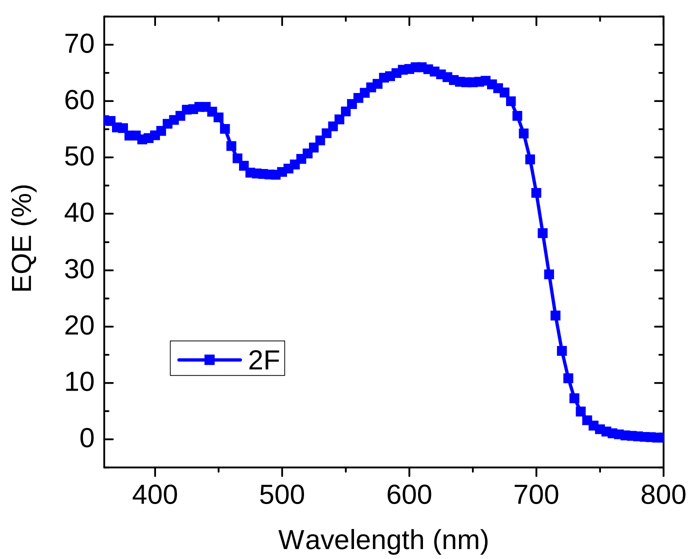


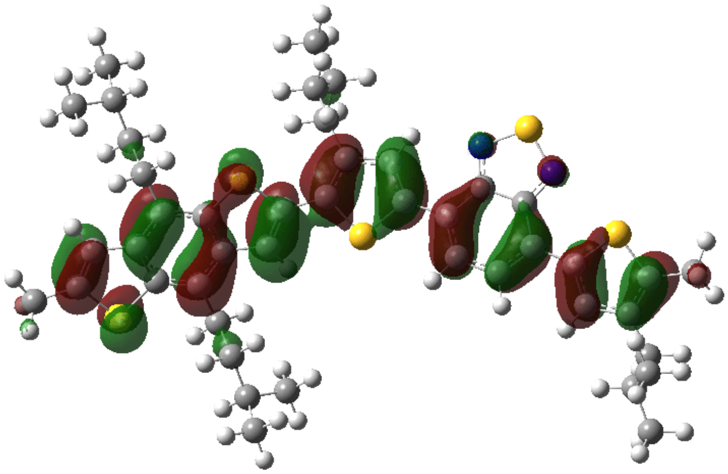
Figure S14. EQE of 2F polymer, 100nm thick film device.

Table S4. Computed HOMO/LUMO levels, HOMO-LUMP gaps, ground and excited state dipole moments of BnDT-DTBT, BnDT-DTfBT and BnDT-DTffBT monomers at the DFT B3LYP/6-311+G(d) level of theory:

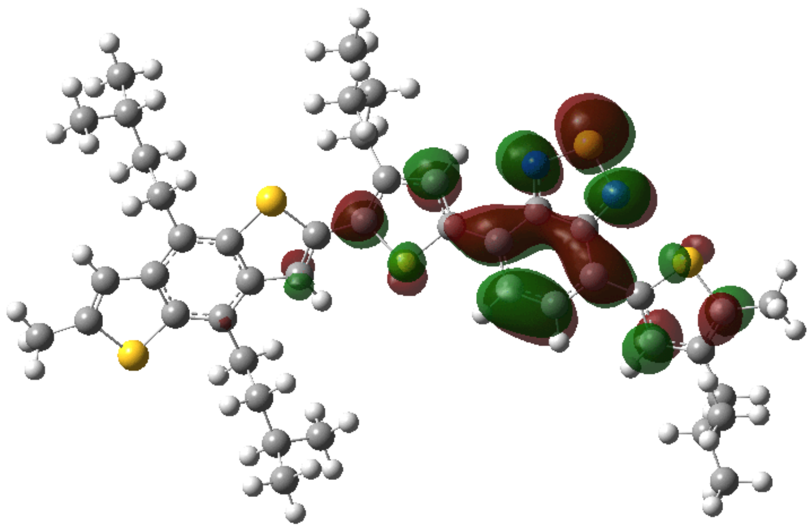
	HOMO(eV)	LUMO (eV)	GAP (eV)	Dipole (Debye)				
				x	y	z	Total	Difference
Ground State								
1FF	-5.28355	-2.97144	2.31211	-0.5963	0.3434	0.2979	0.7498	
1F	-5.21362	-2.93361	2.28001	-0.8502	-1.2250	-0.1052	1.4948	
1	-5.21389	-2.84055	2.37334	0.9873	-1.1025	-0.4266	1.5402	
Excited State								
1FF	-5.00410	-3.17770	1.82640	14.2310	4.9870	-3.5874	15.5003	16.02
1F	-4.91403	-3.12545	1.78858	13.4272	2.8945	-3.2028	14.1042	15.18
1	-4.91022	-3.04300	1.86722	11.8304	0.8941	-2.3820	12.1009	11.20

Difference=$[(\mu_{gx} - \mu_{ex})^2 + [(\mu_{gy} - \mu_{ey})^2\ [(\mu_{gz} - \mu_{ez})^2]^{½}$

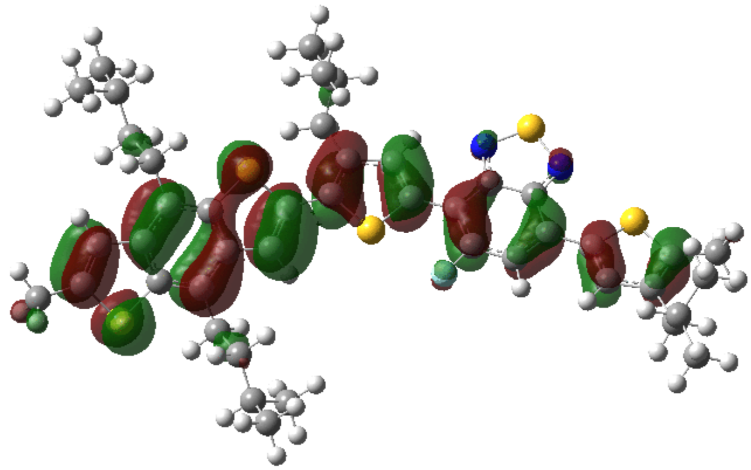
Figure S15. Calculated Frontier Orbitals in the Ground State



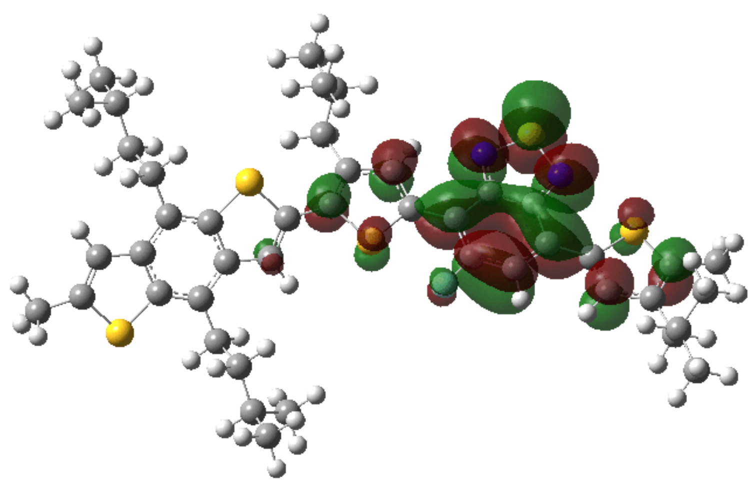
0F, BnDT-DTBT, Ground State, HOMO



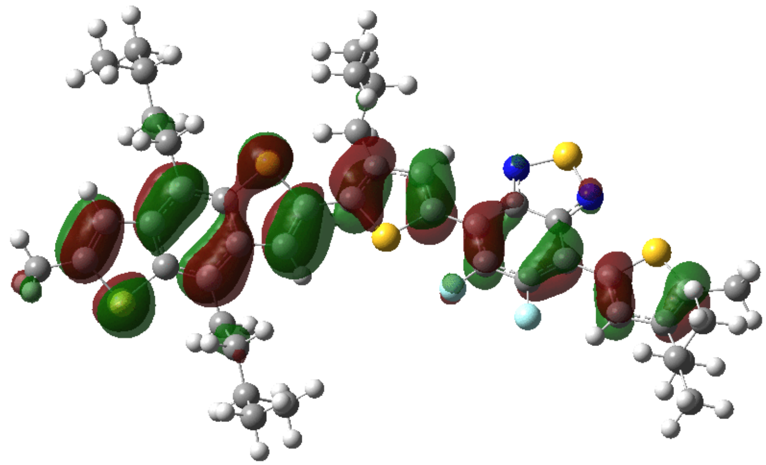
0F, BnDT-DTBT, Ground State, LUMO



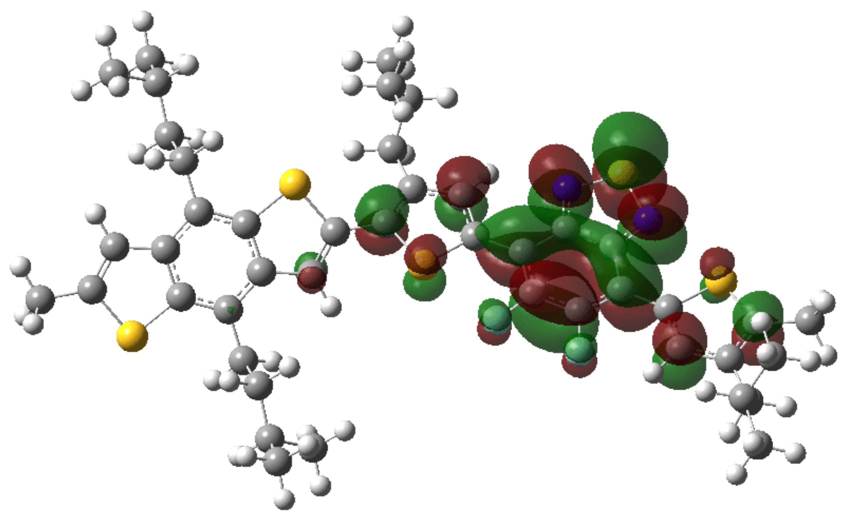
1F, BnDT-DTfBT, Ground State, HOMO



1F, BnDT-DTfBT, Ground State, LUMO



2F, BnDT-DTffBT, Ground State, HOMO



2F, BnDT-DTffBT, Ground State, LUMO

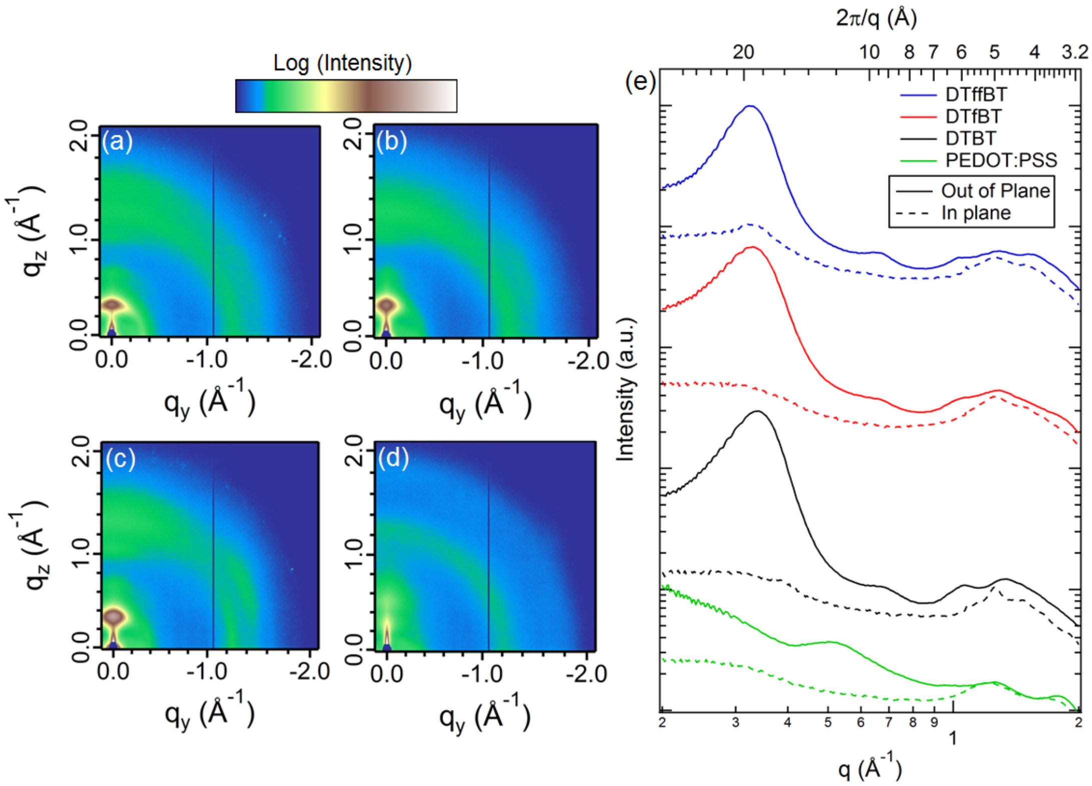


Figure S16: Two dimensional pure film GIWAXS data of (a) DTffBT, (b) DTfBT, and (c) DTBT on PEDOT:PSS-coated silicon substrates. (d) GIWAXS of reference PEDOT:PSS on silicon. (e) 20 degree in-plane and out-of-plane sector averages corresponding to (a)-(d). As with the device data in the main text, DTffBT shows the highest intensity in-plane (100) peak. Please note that the 2D data have not been corrected for the ‘‘missing wedge’’ of data along the out-of-plane direction.

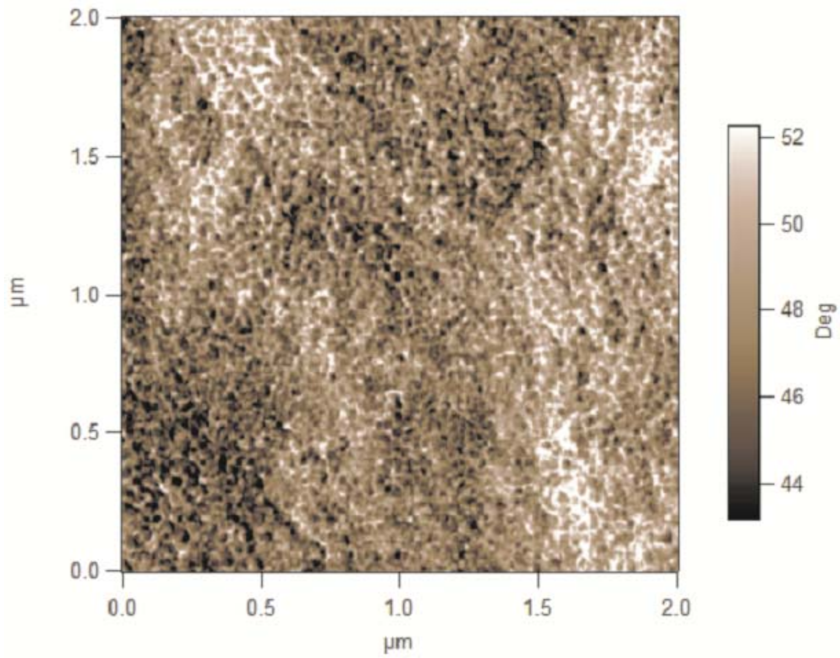


Figure S17. AFM phase image of 100nm thick **DTBT**:PCBM film

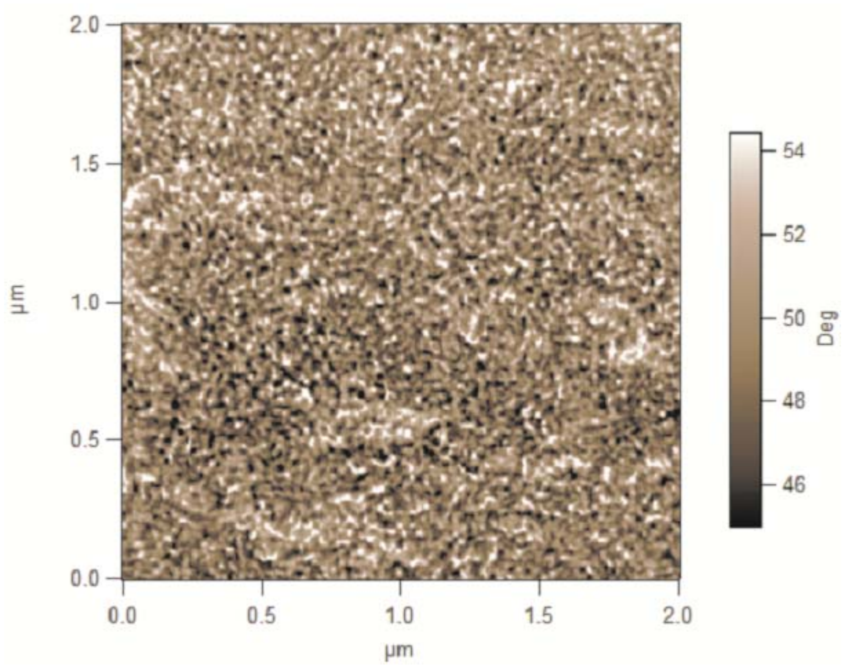


Figure S18. AFM phase image of 100nm thick **DTfBT**:PCBM film

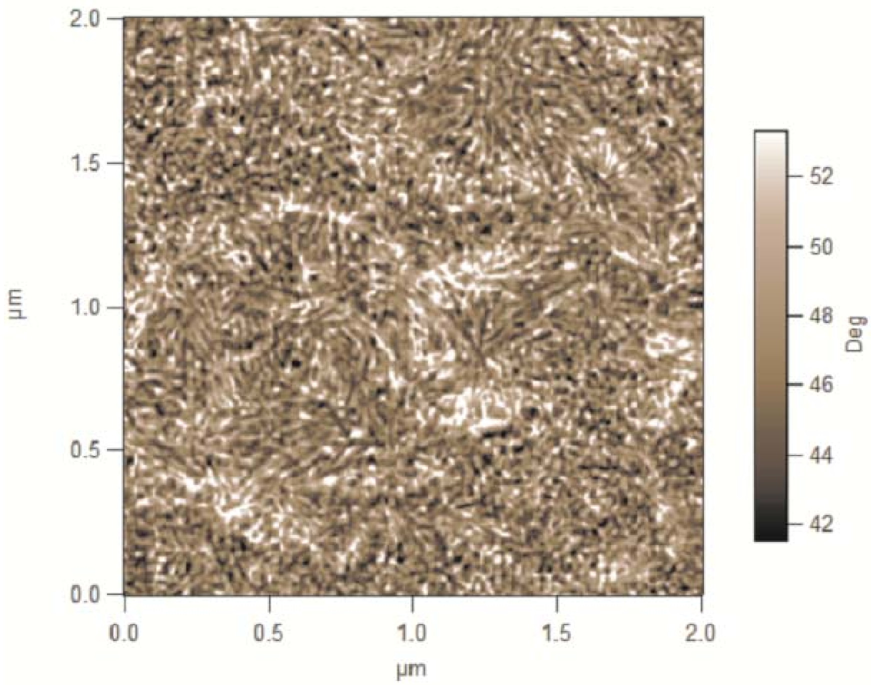


Figure S19. AFM phase image of 100nm thick **DTffBT**:PCBM film

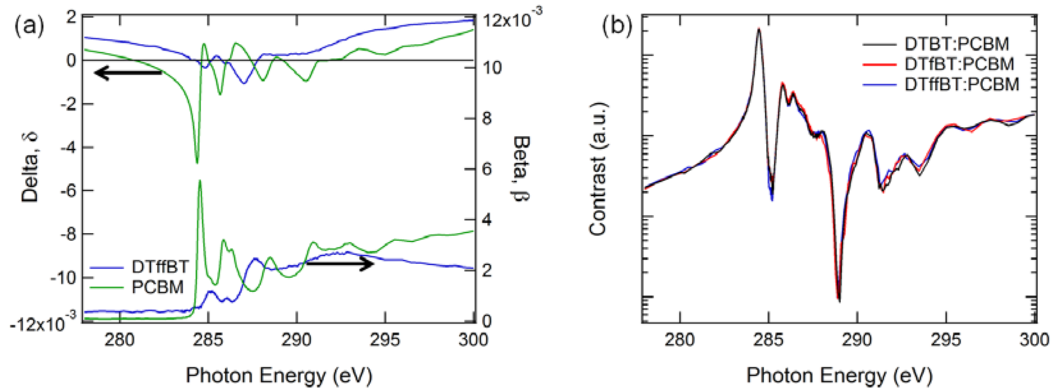


Figure S20: (a) Real (δ) and imaginary (β) parts of the complex index of refraction of PCBM and DTffBT. The imaginary part is determined from NEXAFS transmission scans of pure films using scanning transmission x-ray microscopy of at Beamline 5.3.2.2 of the Advanced Light Source.[5] The real part is then calculated from a Kramers-Kronig transformation of the imaginary part. The assumed densities of polymer and PCBM are 1.1 and 1.3 g/cm^3, respectively, consistent with measurements of P3HT and PCBM.[6] (b) Contrast functions, $E^4 \cdot ((\Delta\delta)^2+(\Delta\beta)^2)$, for the three polymers used in this study with PCBM. No significant differences are noted indicating that the complex index of refraction for each polymer is similar regardless of fluorine substitution over this energy range.

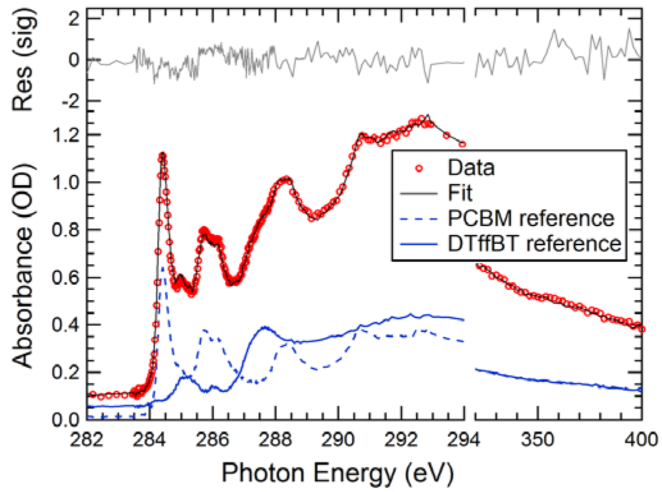


Figure S21: PCBM percentage by weight in polymer:PCBM thin films prior to long-term solvent annealing for miscibility measurements (equivalent to those used for device and X-ray characterization measurements). Blend film based on DTffBT is shown above with similar results for DTBT and DTfBT-based blends. In all cases PCBM is ~50% ($50.8 \pm 0.5\%$ for fit above) by weight, the same as measured during solution preparation since the target blend weight ratio was 1:1.

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Appendix

The Cartesian coordinates of optimized structures of the ground and excited states BnDT-DTBT, BnDT-DTfBT and BnDT-DTffBT monomers:

A. BnDT-DTBT ground state

C	6.54646	0.93791	-1.17922
C	6.76771	-0.36906	-0.65839
C	5.27394	1.53160	-1.09020
C	4.28539	0.76439	-0.47624
C	4.50612	-0.54228	0.04322
C	5.78235	-1.13514	-0.04236
C	2.22306	-0.27042	0.57234
C	7.74864	1.49015	-1.75347
H	7.80161	2.47571	-2.20054
C	-3.56654	-2.65919	2.19288
C	-4.55467	-3.72606	2.30308
C	8.82992	0.67394	-1.68857
C	10.21792	0.93290	-2.18355
H	10.95183	0.89455	-1.37232
H	10.52512	0.19714	-2.93352
H	10.27615	1.92250	-2.64173
S	2.60914	1.25735	-0.23754
S	8.44762	-0.85888	-0.90464
C	3.31344	-1.09169	0.62298
H	3.26805	-2.06813	1.08824
C	5.30819	4.01888	-0.54717
H	6.37251	3.98078	-0.28202
H	4.76234	3.77576	0.37133
C	4.94193	5.45090	-0.97799
H	3.88195	5.45022	-1.26992
C	5.76142	5.93378	-2.18244
H	5.60497	5.31377	-3.06896
H	5.49275	6.95893	-2.45443
H	6.83375	5.92647	-1.95500
C	5.10013	6.41853	0.20227
H	4.80393	7.43536	-0.07289
H	4.48785	6.11407	1.05633
H	6.14129	6.45994	0.54122
C	5.74568	-3.62358	-0.57815
H	4.67924	-3.59082	-0.83516

H	6.28395	-3.37975	-1.50085
C	6.12193	-5.05297	-0.14733
H	7.18494	-5.04704	0.13344
C	5.31663	-5.53619	1.06647
H	5.48057	-4.91434	1.95031
H	4.24195	-5.53195	0.85101
H	5.59142	-6.56011	1.33722
C	5.95605	-6.02376	-1.32396
H	6.55894	-5.71870	-2.18448
H	6.25895	-7.03879	-1.04932
H	4.91182	-6.06993	-1.65267
C	-2.25030	-2.91780	1.66777
C	-4.26550	-5.07187	1.89066
C	0.87600	-0.58186	1.02835
C	-0.05743	0.16023	1.72829
S	0.27245	-2.19715	0.69702
C	-1.23540	-0.58900	2.01006
C	-1.23358	-1.88378	1.54201
H	-2.06903	-0.18798	2.56754
C	-5.21617	-6.17074	2.00641
C	-4.93269	-7.51822	1.96369
S	-6.94766	-5.94920	2.17888
C	-6.06571	-8.37692	2.04556
H	-3.91985	-7.90031	1.90437
C	-7.24006	-7.66618	2.15859
C	-8.65000	-8.16975	2.25779
H	-9.27743	-7.49736	2.84784
H	-9.11674	-8.26760	1.27149
H	-8.68576	-9.15187	2.73409
N	-5.71701	-3.31306	2.80875
N	-4.02882	-1.48137	2.61819
C	5.00550	2.92978	-1.59676
H	3.95657	3.01211	-1.90445
H	5.59225	3.10679	-2.50195
C	6.05172	-2.53148	0.46759
H	7.10199	-2.61213	0.77075
H	5.46820	-2.70631	1.37530
S	-5.57473	-1.71088	3.11293
C	-2.02980	-4.23019	1.28068
H	-1.06207	-4.50234	0.87233

C	-2.99398	-5.25743	1.37431
H	-2.71179	-6.23773	1.00802
C	0.11856	1.56925	2.24244
H	0.07579	1.53623	3.33877
H	1.11458	1.94414	1.99422
C	-0.94426	2.58088	1.75081
H	-1.93145	2.18705	2.02500
C	-0.91857	2.76100	0.22900
H	-1.05846	1.81203	-0.29497
H	-1.71290	3.43928	-0.09686
H	0.03412	3.18665	-0.10287
C	-0.76248	3.92419	2.46773
H	-0.82615	3.81380	3.55472
H	0.21301	4.36644	2.23707
H	-1.52878	4.64288	2.16238
C	-5.94175	-9.88028	2.00964
H	-5.16507	-10.18597	2.72129
H	-6.86876	-10.34605	2.36122
C	-5.58975	-10.46938	0.62209
H	-4.66824	-9.97979	0.27920
C	-5.31024	-11.97251	0.73741
H	-6.19745	-12.51373	1.08491
H	-5.02463	-12.39900	-0.22875
H	-4.50035	-12.17987	1.44367
C	-6.68309	-10.19020	-0.41490
H	-6.87440	-9.11962	-0.52201
H	-6.40063	-10.57747	-1.39835
H	-7.62566	-10.67243	-0.13146

B. BnDT-DTBT excited state

C	6.68380	1.05884	-0.51711
C	6.69777	-0.36013	-0.65659
C	5.47708	1.73770	-0.22274
C	4.35392	0.93802	-0.07855
C	4.36611	-0.48284	-0.21371
C	5.57447	-1.16302	-0.51561
C	2.07110	-0.12976	0.24798
C	7.98773	1.62102	-0.71014
H	8.20157	2.68053	-0.64206
C	-3.72332	-2.54694	1.60386

C	-4.62213	-3.60850	1.96500
C	8.96029	0.70851	-0.98708
C	10.41242	0.95889	-1.24118
H	11.04501	0.44450	-0.51113
H	10.71452	0.61057	-2.23372
H	10.62855	2.02701	-1.17991
S	2.72772	1.51438	0.29205
S	8.32861	-0.93000	-1.02805
C	3.07860	-1.04378	-0.02738
H	2.87423	-2.10225	-0.11582
C	5.75142	3.67401	1.40582
H	6.76872	3.35531	1.66566
H	5.08499	3.13331	2.08673
C	5.60883	5.18486	1.66679
H	4.59384	5.48052	1.36571
C	6.60476	6.02203	0.85292
H	6.47047	5.90038	-0.22505
H	6.49190	7.08748	1.07230
H	7.63767	5.74659	1.09482
C	5.75508	5.47978	3.16533
H	5.61505	6.54379	3.37654
H	5.02159	4.92494	3.75727
H	6.75089	5.20101	3.52683
C	5.28025	-3.08785	-2.15197
H	4.26079	-2.76631	-2.39826
H	5.94051	-2.54494	-2.83724
C	5.41697	-4.59787	-2.42107
H	6.43564	-4.89641	-2.13522
C	4.43026	-5.43688	-1.59795
H	4.58104	-5.32305	-0.52133
H	3.39482	-5.15692	-1.82188
H	4.53680	-6.50117	-1.82599
C	5.24961	-4.88481	-3.91907
H	5.97529	-4.32748	-4.51857
H	5.38578	-5.94791	-4.13727
H	4.24910	-4.60388	-4.26503
C	-2.32526	-2.81503	1.44992
C	-4.15307	-4.94601	2.17830
C	0.70245	-0.44916	0.51907
C	-0.46862	0.32266	0.53248

S	0.33177	-2.13053	0.92086
C	-1.61028	-0.43450	0.85411
C	-1.38248	-1.78676	1.09322
H	-2.60870	-0.02823	0.92069
C	-5.03189	-6.02747	2.54223
C	-4.68327	-7.35135	2.78872
S	-6.77130	-5.84305	2.75143
C	-5.75676	-8.20263	3.12844
H	-3.66096	-7.70556	2.73657
C	-6.96298	-7.52046	3.15111
C	-8.32842	-8.05754	3.46033
H	-9.05266	-7.25328	3.60372
H	-8.70391	-8.69504	2.65247
H	-8.32290	-8.66050	4.37328
N	-5.90942	-3.23900	2.07952
N	-4.32221	-1.34885	1.43845
C	5.43149	3.23602	-0.03887
H	4.43725	3.60683	-0.31232
H	6.12513	3.70855	-0.73901
C	5.61792	-2.65872	-0.70768
H	6.61524	-3.03119	-0.44885
H	4.93198	-3.13571	-0.00308
S	-5.95773	-1.59955	1.73765
C	-1.90137	-4.14533	1.66392
H	-0.84964	-4.38919	1.55334
C	-2.76699	-5.16555	2.01155
H	-2.35954	-6.15818	2.15454
C	-0.60754	1.78738	0.19891
H	-1.13975	2.27045	1.02640
H	0.36132	2.28382	0.13430
C	-1.38705	2.06270	-1.11274
H	-2.36096	1.56608	-1.02995
C	-0.66566	1.49072	-2.33815
H	-0.51681	0.41142	-2.25384
H	-1.24223	1.67343	-3.24933
H	0.31792	1.95444	-2.47056
C	-1.63413	3.56784	-1.26741
H	-2.18507	3.97589	-0.41494
H	-0.69044	4.11866	-1.34829
H	-2.21588	3.77976	-2.16886

C	-5.57957	-9.67264	3.41791
H	-4.76845	-9.79378	4.14621
H	-6.47804	-10.07263	3.90071
C	-5.25502	-10.54191	2.17852
H	-4.36375	-10.11408	1.70059
C	-4.91997	-11.97583	2.60563
H	-5.77517	-12.45076	3.09910
H	-4.65397	-12.59501	1.74394
H	-4.07902	-12.00255	3.30530
C	-6.39162	-10.52402	1.15069
H	-6.62459	-9.50739	0.82496
H	-6.12772	-11.10486	0.26211
H	-7.30539	-10.96154	1.56855

C. BnDT-DTfBT ground state

C	6.66968	0.97613	-0.99780
C	6.92412	-0.26476	-0.34701
C	5.36547	1.50274	-1.03723
C	4.38095	0.73878	-0.41297
C	4.63536	-0.50146	0.23718
C	5.94275	-1.02708	0.27977
C	2.31214	-0.31588	0.60331
C	7.87564	1.54167	-1.55065
H	7.90635	2.48520	-2.08240
C	-3.42629	-2.83820	2.21894
C	-4.40758	-3.90807	2.36874
C	8.99078	0.79632	-1.34929
C	10.39151	1.08867	-1.78679
H	11.07567	1.16222	-0.93554
H	10.78077	0.30882	-2.44893
H	10.42664	2.03634	-2.32826
S	2.66971	1.15446	-0.31875
S	8.63863	-0.68002	-0.45148
C	3.43847	-1.06434	0.79485
H	3.41382	-1.99708	1.34359
C	5.23797	4.02645	-0.72508
H	6.28318	4.07018	-0.39345
H	4.64539	3.83704	0.17686
C	4.83155	5.39195	-1.30869
H	3.79494	5.30701	-1.66503

C	5.70574	5.80995	-2.49903
H	5.64167	5.10442	-3.33136
H	5.40443	6.78941	-2.88223
H	6.75890	5.88397	-2.20426
C	4.86244	6.46841	-0.21541
H	4.53732	7.43905	-0.60196
H	4.20877	6.20852	0.62244
H	5.87499	6.59566	0.18339
C	6.05746	-3.55159	-0.02669
H	5.00845	-3.59586	-0.34549
H	6.63994	-3.36440	-0.93566
C	6.47041	-4.91567	0.55559
H	7.51251	-4.83094	0.89588
C	5.61292	-5.32873	1.75971
H	5.69174	-4.62193	2.58971
H	4.55524	-5.40003	1.48198
H	5.91780	-6.30820	2.14021
C	6.42198	-5.99496	-0.53433
H	7.06388	-5.73822	-1.38228
H	6.75140	-6.96491	-0.14959
H	5.40348	-6.12180	-0.91760
C	-2.11326	-3.07846	1.66550
C	-4.12417	-5.26278	1.97621
C	0.95605	-0.66612	1.00309
C	-0.05614	0.08204	1.57869
S	0.46926	-2.33269	0.78599
C	-1.20529	-0.70518	1.85551
C	-1.10941	-2.03696	1.50329
H	-2.09017	-0.30447	2.32552
C	-5.07696	-6.35670	2.09699
C	-4.93209	-7.63780	1.60850
S	-6.59932	-6.23685	2.96141
C	-6.00192	-8.52462	1.91074
H	-4.06830	-7.95275	1.03427
C	-6.98550	-7.90542	2.65114
C	-8.28436	-8.46253	3.15537
H	-8.61437	-7.95496	4.06473
H	-9.08516	-8.35816	2.41528
H	-8.19257	-9.52530	3.38909
N	-5.55853	-3.49678	2.89488

N	-3.88746	-1.66074	2.64226
C	5.05835	2.83271	-1.68565
H	4.02814	2.82769	-2.06009
H	5.69147	2.96152	-2.56731
C	6.24942	-2.35602	0.92951
H	7.28299	-2.35331	1.29428
H	5.62309	-2.48038	1.81667
S	-5.41977	-1.89049	3.18237
C	-1.92867	-4.40484	1.31655
C	-2.85721	-5.45140	1.45912
H	-2.52011	-6.43129	1.14515
C	0.01431	1.53852	1.97244
H	-0.09230	1.59997	3.06310
H	1.00266	1.94616	1.74636
C	-1.06721	2.44163	1.33270
H	-2.04774	2.01846	1.58664
C	-0.95870	2.48807	-0.19561
H	-1.01945	1.49021	-0.63726
H	-1.76412	3.09090	-0.62573
H	-0.00960	2.93373	-0.51090
C	-0.99792	3.85115	1.93298
H	-1.11961	3.83317	3.02042
H	-0.03456	4.32561	1.71604
H	-1.78089	4.49545	1.52226
C	-6.01969	-9.95843	1.44092
H	-5.05717	-10.42186	1.68916
H	-6.77599	-10.52785	1.99173
C	-6.27141	-10.14125	-0.07575
H	-5.51496	-9.55123	-0.61040
C	-6.08885	-11.61136	-0.47131
H	-6.81632	-12.25125	0.04052
H	-6.22808	-11.75279	-1.54702
H	-5.08995	-11.97725	-0.21508
C	-7.65200	-9.62491	-0.49587
H	-7.78444	-8.57081	-0.23960
H	-7.79686	-9.72500	-1.57550
H	-8.44988	-10.19317	-0.00431
F	-0.73890	-4.78128	0.78700

D. BnDT-DTfBT excited state

C	6.70645	1.08676	-0.59718
C	6.75756	-0.33759	-0.61376
C	5.48038	1.75832	-0.35249
C	4.38144	0.94567	-0.13469
C	4.43008	-0.48087	-0.14835
C	5.65725	-1.15470	-0.39700
C	2.12852	-0.14743	0.30438
C	7.99074	1.66382	-0.84673
H	8.17686	2.73030	-0.87293
C	-3.63816	-2.60959	1.70767
C	-4.56705	-3.66117	2.03110
C	8.98823	0.75494	-1.05059
C	10.43121	1.02326	-1.33553
H	11.08133	0.59071	-0.56886
H	10.73803	0.59973	-2.29680
H	10.61729	2.09819	-1.36714
S	2.73991	1.50715	0.19450
S	8.40156	-0.89393	-0.94494
C	3.16331	-1.05701	0.09564
H	2.99138	-2.12440	0.11114
C	5.72633	3.83088	1.10259
H	6.75323	3.55722	1.37552
H	5.07953	3.33658	1.83564
C	5.55352	5.35526	1.23475
H	4.52914	5.60271	0.92245
C	6.52212	6.14004	0.33976
H	6.37799	5.92540	-0.72233
H	6.38921	7.21765	0.46990
H	7.56337	5.90716	0.59042
C	5.70968	5.78026	2.70074
H	5.54856	6.85520	2.82195
H	4.99510	5.26305	3.34732
H	6.71528	5.55454	3.07194
C	5.38966	-3.22150	-1.85406
H	4.35807	-2.95005	-2.10929
H	6.02443	-2.72412	-2.59577
C	5.56395	-4.74540	-1.99070
H	6.59577	-4.98995	-1.70061
C	4.61597	-5.53366	-1.07706
H	4.78396	-5.32388	-0.01761

H	3.56910	-5.30109	-1.30105
H	4.74703	-6.61057	-1.21459
C	5.37803	-5.16760	-3.45418
H	6.07645	-4.64623	-4.11536
H	5.54073	-6.24170	-3.58053
H	4.36368	-4.94589	-3.80260
C	-2.24782	-2.90079	1.49769
C	-4.14547	-5.02493	2.15436
C	0.76988	-0.48456	0.59681
C	-0.39746	0.27877	0.70947
S	0.41892	-2.19475	0.89939
C	-1.52161	-0.50671	1.02911
C	-1.28024	-1.87081	1.16960
H	-2.51522	-0.10875	1.16735
C	-5.05445	-6.09765	2.47773
C	-4.74359	-7.44076	2.63585
S	-6.77849	-5.86976	2.74589
C	-5.83724	-8.27854	2.95582
H	-3.73506	-7.82380	2.53529
C	-7.01724	-7.56257	3.05248
C	-8.39621	-8.06832	3.35601
H	-9.04632	-7.26837	3.71692
H	-8.87354	-8.50003	2.46916
H	-8.37523	-8.84566	4.12433
N	-5.83680	-3.25396	2.20078
N	-4.20040	-1.38776	1.62960
C	5.39907	3.26485	-0.29551
H	4.39263	3.58706	-0.58440
H	6.07180	3.69268	-1.04317
C	5.73760	-2.65905	-0.45819
H	6.74805	-2.98240	-0.18519
H	5.07454	-3.08923	0.29648
S	-5.83691	-1.59963	1.95732
C	-1.91104	-4.25622	1.63290
C	-2.77896	-5.28369	1.94114
H	-2.36926	-6.28182	2.00801
C	-0.56241	1.76390	0.50284
H	-1.09330	2.16269	1.37475
H	0.39666	2.28336	0.47747
C	-1.36682	2.13923	-0.76857

H	-2.33302	1.62462	-0.70855
C	-0.66659	1.68118	-2.05267
H	-0.49654	0.60174	-2.05873
H	-1.27029	1.92411	-2.93165
H	0.30440	2.17355	-2.17258
C	-1.63450	3.64861	-0.79130
H	-2.17271	3.97637	0.10290
H	-0.69913	4.21697	-0.84371
H	-2.23683	3.92775	-1.66034
C	-5.69417	-9.76800	3.14975
H	-4.85295	-9.95605	3.82792
H	-6.58017	-10.17068	3.65292
C	-5.45812	-10.57107	1.84738
H	-4.57686	-10.14269	1.35169
C	-5.15088	-12.03746	2.17322
H	-5.99737	-12.51515	2.67900
H	-4.94568	-12.61177	1.26503
H	-4.27963	-12.13120	2.82867
C	-6.64109	-10.45742	0.87987
H	-6.85229	-9.41675	0.62272
H	-6.44087	-10.99560	-0.05125
H	-7.54921	-10.88662	1.31820
F	-0.60879	-4.61440	1.44518

E. BnDT-DTffBT ground state

C	6.60277	1.06373	-1.14387
C	6.88108	-0.21229	-0.57552
C	5.30057	1.59442	-1.09478
C	4.34194	0.79850	-0.47009
C	4.62000	-0.47689	0.09727
C	5.92565	-1.00678	0.05141
C	2.31721	-0.30645	0.57910
C	7.78490	1.65705	-1.71862
H	7.79563	2.62851	-2.19836
C	-3.34681	-2.90746	2.32480
C	-4.31730	-3.98830	2.47146
C	8.90461	0.89930	-1.60994
C	10.28567	1.21177	-2.09335
H	11.00770	1.23575	-1.27100
H	10.64062	0.46894	-2.81472

H	10.30201	2.18809	-2.58239
S	2.63869	1.21213	-0.27474
S	8.58729	-0.62388	-0.78008
C	3.44709	-1.06785	0.67612
H	3.44366	-2.02958	1.17305
C	5.20330	4.09697	-0.63742
H	6.26388	4.12019	-0.35615
H	4.65562	3.85835	0.28120
C	4.77475	5.49399	-1.12226
H	3.72050	5.43181	-1.42810
C	5.58792	5.97523	-2.33163
H	5.47453	5.31890	-3.19833
H	5.27452	6.97646	-2.64215
H	6.65587	6.02745	-2.08995
C	4.86843	6.50750	0.02595
H	4.52750	7.49879	-0.28791
H	4.25906	6.20247	0.88190
H	5.90124	6.61113	0.37693
C	6.01463	-3.51044	-0.39971
H	4.95111	-3.53787	-0.66880
H	6.55192	-3.27198	-1.32444
C	6.45323	-4.90485	0.08362
H	7.51199	-4.83904	0.37297
C	5.65890	-5.38401	1.30624
H	5.78532	-4.72592	2.16987
H	4.58751	-5.43772	1.08203
H	5.97843	-6.38422	1.61392
C	6.34479	-5.92163	-1.06044
H	6.94075	-5.61737	-1.92614
H	6.69300	-6.91104	-0.74862
H	5.30712	-6.02900	-1.39521
C	-2.05775	-3.11839	1.70683
C	-4.07001	-5.33465	2.01521
C	0.97976	-0.67554	1.02218
C	-0.00343	0.04246	1.68134
S	0.48063	-2.32854	0.74239
C	-1.13919	-0.75846	1.97197
C	-1.06132	-2.07049	1.54795
H	-2.00015	-0.38260	2.50301
C	-5.02552	-6.42319	2.15456

C	-4.88893	-7.74088	1.75707
S	-6.59909	-6.21465	2.91804
C	-6.00426	-8.57453	2.04267
H	-4.00050	-8.11746	1.27293
C	-7.01382	-7.88547	2.67641
C	-8.35606	-8.37864	3.13123
H	-8.75503	-7.76909	3.94517
H	-9.09061	-8.35844	2.31889
H	-8.29672	-9.40812	3.49187
N	-5.44219	-3.59937	3.06265
N	-3.78978	-1.75118	2.81392
C	4.97071	2.95943	-1.65291
H	3.92377	2.97868	-1.97736
H	5.56159	3.13489	-2.55572
C	6.25546	-2.37050	0.61156
H	7.30454	-2.39003	0.92853
H	5.66983	-2.54293	1.51838
S	-5.29664	-2.00513	3.40793
C	-1.88209	-4.42159	1.28822
C	-2.82648	-5.46851	1.43101
C	0.08673	1.47693	2.14569
H	0.02882	1.48208	3.24173
H	1.06486	1.89621	1.89743
C	-1.02084	2.41063	1.60168
H	-1.98979	1.97394	1.87658
C	-0.98038	2.53640	0.07472
H	-1.06040	1.56291	-0.41579
H	-1.80456	3.15833	-0.28743
H	-0.04673	3.00075	-0.25923
C	-0.92336	3.78710	2.27050
H	-0.99821	3.71311	3.35986
H	0.03044	4.27301	2.03713
H	-1.72225	4.45145	1.92791
C	-6.03432	-10.03525	1.66526
H	-5.10418	-10.50569	2.00618
H	-6.84236	-10.54718	2.19931
C	-6.19184	-10.30953	0.14998
H	-5.38387	-9.77598	-0.36802
C	-6.02954	-11.80648	-0.13886
H	-6.80795	-12.39259	0.36262

H	-6.10274	-12.01426	-1.21043
H	-5.06093	-12.18139	0.20572
C	-7.52527	-9.78487	-0.39372
H	-7.64205	-8.71325	-0.21342
H	-7.60189	-9.94975	-1.47249
H	-8.37133	-10.29890	0.07682
F	-0.73289	-4.78453	0.68768
F	-2.41722	-6.65386	0.94202

F. BnDT-DTffBT excited state

C	6.72308	1.11475	-0.58249
C	6.77998	-0.30892	-0.60924
C	5.49250	1.78011	-0.33694
C	4.39653	0.96123	-0.12913
C	4.45101	-0.46452	-0.15332
C	5.68231	-1.13221	-0.40261
C	2.14723	-0.14332	0.29315
C	8.00478	1.69868	-0.82316
H	8.18695	2.76597	-0.84127
C	-3.60643	-2.65030	1.67875
C	-4.52520	-3.71006	2.00434
C	9.00744	0.79453	-1.03010
C	10.45006	1.07163	-1.30796
H	11.09933	0.63626	-0.54222
H	10.76202	0.65653	-2.27120
H	10.63134	2.14755	-1.33096
S	2.75132	1.51273	0.19929
S	8.42733	-0.85600	-0.93822
C	3.18596	-1.04775	0.08117
H	3.01775	-2.11579	0.08696
C	5.72973	3.84210	1.13401
H	6.75676	3.56875	1.40665
H	5.08277	3.34132	1.86247
C	5.55347	5.36521	1.27617
H	4.52918	5.61268	0.96364
C	6.52222	6.15805	0.38852
H	6.38078	5.95058	-0.67538
H	6.38664	7.23440	0.52577
H	7.56347	5.92586	0.63983
C	5.70596	5.78016	2.74543

H	5.54244	6.85388	2.87368
H	4.99115	5.25714	3.38704
H	6.71129	5.55396	3.11700
C	5.42286	-3.18948	-1.87425
H	4.39109	-2.91844	-2.12905
H	6.05772	-2.68635	-2.61203
C	5.60006	-4.71229	-2.01950
H	6.63193	-4.95667	-1.72944
C	4.65205	-5.50761	-1.11209
H	4.81779	-5.30429	-0.05102
H	3.60505	-5.27613	-1.33638
H	4.78528	-6.58336	-1.25575
C	5.41706	-5.12567	-3.48587
H	6.11552	-4.59913	-4.14293
H	5.58182	-6.19865	-3.61832
H	4.40276	-4.90389	-3.83435
C	-2.21481	-2.92402	1.47910
C	-4.10818	-5.08112	2.14486
C	0.78756	-0.48838	0.58045
C	-0.38509	0.26584	0.67857
S	0.44987	-2.19803	0.89352
C	-1.50655	-0.52741	0.99672
C	-1.25332	-1.88603	1.14899
H	-2.50445	-0.13691	1.12503
C	-5.02646	-6.14569	2.47056
C	-4.75880	-7.49882	2.65107
S	-6.75306	-5.86561	2.71571
C	-5.88293	-8.29538	2.96814
H	-3.76483	-7.91042	2.56567
C	-7.04193	-7.54476	3.04052
C	-8.43751	-8.00729	3.33784
H	-9.08686	-7.17350	3.61280
H	-8.89174	-8.50258	2.47255
H	-8.45241	-8.72172	4.16559
N	-5.79673	-3.31377	2.16288
N	-4.18220	-1.43328	1.58834
C	5.40566	3.28555	-0.26886
H	4.39839	3.60636	-0.55612
H	6.07768	3.72128	-1.01254
C	5.76816	-2.63545	-0.47408

H	6.77947	-2.95729	-0.20279
H	5.10599	-3.07308	0.27699
S	-5.81543	-1.66039	1.90766
C	-1.85336	-4.26961	1.62301
C	-2.73683	-5.29230	1.93588
C	-0.56079	1.74761	0.45815
H	-1.09613	2.15063	1.32543
H	0.39444	2.27396	0.42911
C	-1.36492	2.10517	-0.81856
H	-2.32663	1.58238	-0.75765
C	-0.65582	1.64299	-2.09629
H	-0.47616	0.56509	-2.09307
H	-1.25811	1.87348	-2.97953
H	0.31118	2.14323	-2.21647
C	-1.64611	3.61183	-0.85451
H	-2.19050	3.94197	0.03504
H	-0.71575	4.18822	-0.90830
H	-2.24779	3.87836	-1.72791
C	-5.78729	-9.78556	3.18503
H	-4.96756	-9.98762	3.88496
H	-6.69640	-10.15581	3.67201
C	-5.54324	-10.61208	1.89905
H	-4.63975	-10.21390	1.41910
C	-5.28331	-12.08165	2.25065
H	-6.15326	-12.52966	2.74382
H	-5.07391	-12.67348	1.35470
H	-4.42920	-12.18948	2.92610
C	-6.70054	-10.48011	0.90315
H	-6.87924	-9.43746	0.62959
H	-6.49275	-11.03379	-0.01720
H	-7.62914	-10.88149	1.32487
F	-0.56050	-4.63306	1.45106
F	-2.19551	-6.53205	2.02890