Supporting Information

Efficient As-Cast Thick Film Small-Molecule Organic Solar Cell with Less Fluorination on Donor

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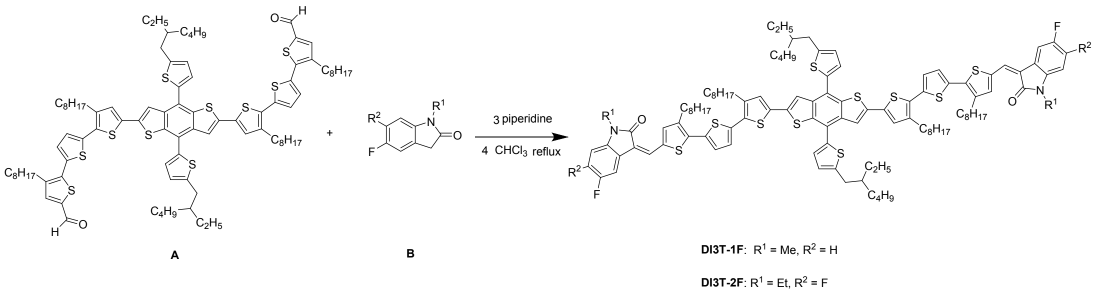
General information

All general 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. Experimental General Information ^{1}H NMR and ^{13}C NMR spectra were measured on a MECUYR-VX300 spectrometer. Elemental analyses of carbon, hydrogen, and nitrogen were performed on a Vario EL III microanalyzer. Mass spectra were measured on a ZAB 3F-HF mass spectrophotometer and Bruker autoflex matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF). UV-Vis absorption spectra were recorded on a Shimadzu UV-2500 recording spectrophotometer. Differential scanning calorimetry (DSC) was performed on a NETZSCH DSC 200 PC unit at a heating rate of 10 ºC min-1 from -40 ºC to 300 ºC under argon. The glass transition temperature (Tg) was determined from the second heating scan. Thermogravimetric analysis (TGA) was undertaken with a NETZSCH STA 449C instrument. The thermal stability of the samples under a nitrogen atmosphere was determined by measuring their weight loss while heating at a rate of 20 ºC min-1 from 25 to 500 ºC. Electrochemical spectra of DI3T and DI3T-2F measured by ionization energy measurement system.



Scheme S1. Synthesis of DI3T-1F and DI3T-2F

Under the protection of N_2, to a solution of 1-methyl-5-fluoro-1H-indole-2-one (533.30 mg,3.24mmol),5'',5'''''-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)benzo[1,2-b:4,5-b']dithiophene-2,6-diyl)bis(3,3''-dioctyl-[2,2':5',2''-terthiophene]-5-carbaldehyde)(**3TBDTT**) (500.00 mg, 0.32 mmol), which was synthesized as it reported [1], in 30 mL chloroform, 0.45mL of piperidine was added and refluxed for 48 hrs. After quenching by water, the solution was extracted with chloroform for three times and the combined organic layer was washed with brine for three times, then dried with Na_2SO_4. After removal of solvent, the crude product was sedimented by methanol and chloroform for 4 times. Then, throught soxhlet extraction for 3 times and recrystallization from chloroform, a black solid was obtained (306 mg, yield: 51.4%). The ^{1}H NMR shows the product are a mixture of rotamers, ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66-7.59 (m, 4H), 7.55 (s, 2H), 7.43 (s, 1H), 7.32 (dd, *J* = 9 Hz,3 Hz, 3H), 7.21 (dd, *J* = 8.5 Hz,2 Hz 2H), 7.15-7.12 (m, 4H), 7.04-6.94 (m, 4H), 6.77-6.73 (m, 2H), 3.32 (s, 6H), 3.29 (s, 2H), 2.95-2.89 (m, 6H), 2.85 (t, 6H), 2.79 (t, 6H), 1.75-1.71 (m, 16H), 1.42-1.28 (m, 84H), 1.00(t, 8H), 0.95(t, 8H), 0.88(t, 16H); ^{13}C NMR (800 MHz, $CDCl_3$) δ 166.41, 159.91, 158.02, 145.97, 145.93, 141.19, 140.87, 140.63, 140.39, 140.26, 139.49, 139.34, 138.62, 138.58, 137.86, 137.85, 137.42, 137.34, 137.30, 137.11, 137.09, 136.87, 135.60, 135.58, 135.54, 135.28, 134.76, 130.80, 128.85, 127.31, 127.11, 126.11, 126.09, 125.50, 125.28, 125.21, 123.24, 120.04, 119.04, 114.33, 114.14, 108.28, 108.22, 106.15, 105.95, 41.49, 34.37, 32.55, 31.93, 30.51, 30.47, 30.36, 30.33, 29.75, 29.72, 29.69, 29.60, 29.49, 29.44, 29.38, 29.34, 29.29, 28.99, 26.39, 25.99, 25.84, 23.11, 22.72, 14.27, 14.15, 11.01, 10.98; HR-MS: calculated: $C_{110}H_{130}F_2N_2O_2S_{10}$, 1670.8588, found: 1670.8633.

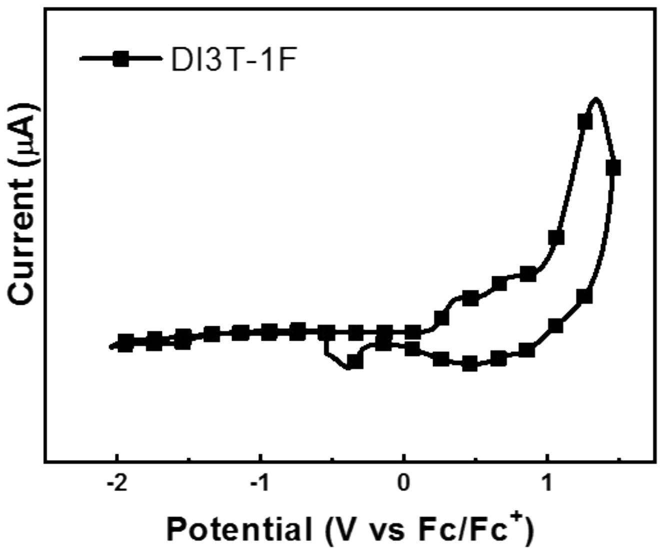


Figure S1. Cyclic voltammogram of DI3T-1F in dichloromethane solution with 0.1mol/L *n*-Bu_4NPF_6 at a scan rate of 100 mV s^{-1}.

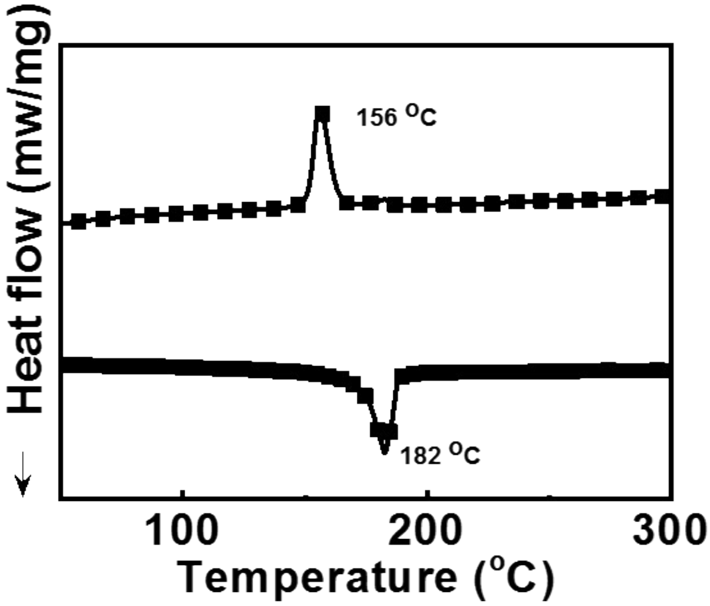


Figure S2. DSC traces of DI3T-1F

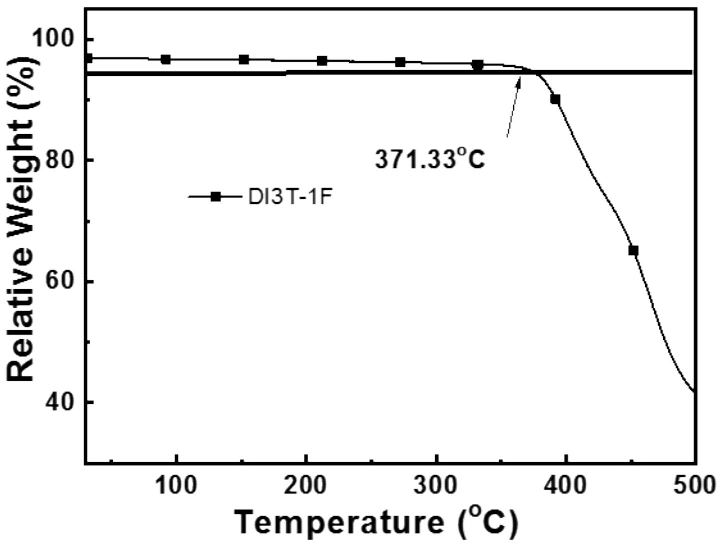


Figure S3. TGA curves of DI3T-F. Td with 5% weight loss: 371.33°C.

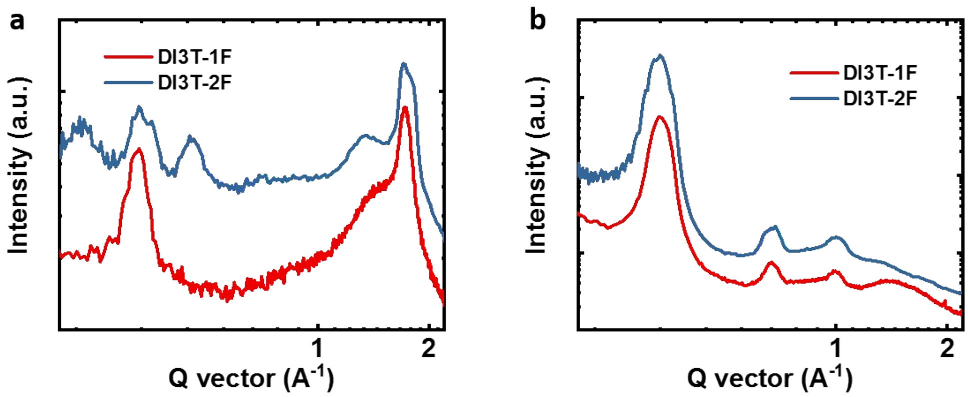


Figure S4. a) the in-plane (IP) profiles of DI3T-1F and DI3T-2F; b) the out-of-plane (OOP) profiles of DI3T-1F and DI3T-2F.

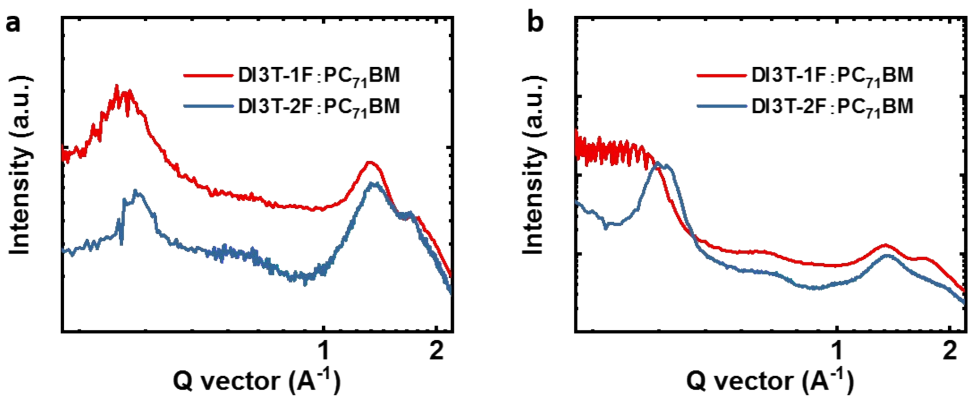


Figure S5. a) the in-plane (IP) profiles of DI3T :$PC_{71}BM$ and DI3T-2F :$PC_{71}BM$; b) the out-of-plane (OOP) profiles of DI3T:$PC_{71}BM$ and DI3T-2F:$PC_{71}BM$.

Table S1. The performance dependent on the thickness of active layer based DI3T-2F

Thickness (nm)	***Jsc*** (mA·cm^{-2})	***Voc (mV)***	***FF (%)***	**PCE (%)**
162	12.8	835	68.5	7.32
216	10.2	832	58.2	4.94
232	9.6	830	56.2	4.48
272	9.0	833	52.1	3.90
303	8.4	835	51.6	3.62

Table S2. The performance dependent on the thickness of active layer based DI3T-1F

Thickness (nm)	***Jsc*** **(mA·cm^{-2})**	***Voc*** **(mV)**	**FF (%)**	**PCE (%)**
153 nm	13.6	815	75.1	8.33
205 nm	13.0	814	71.2	7.53
234 nm	12.0	814	69.7	6.81
278 nm	11.5	809	65.4	6.08
307 nm	10.6	815	62.9	5.43

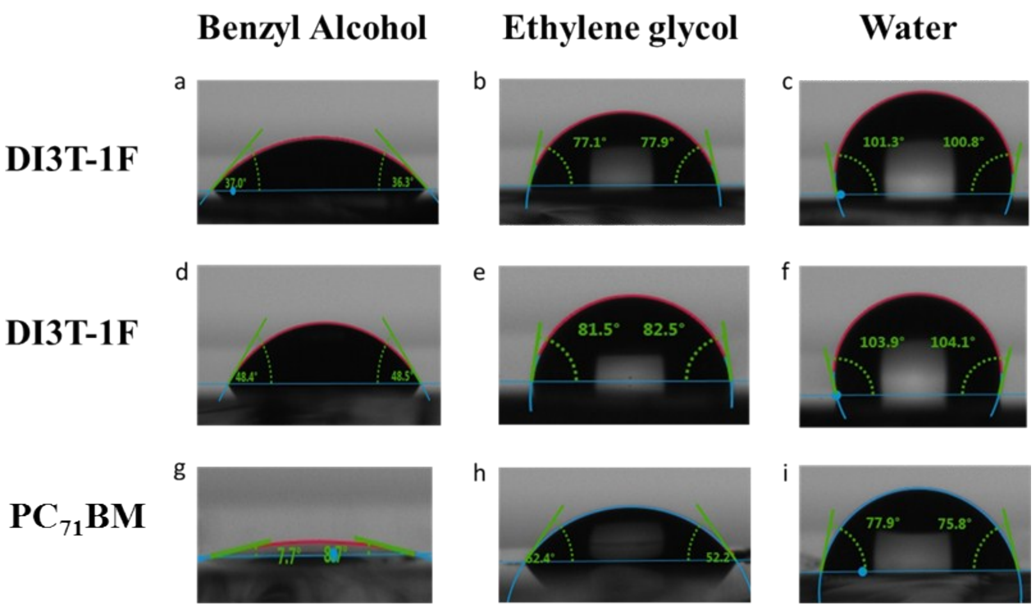


Figure S6. Contact angles of small molecules with benzyl alcohol, ethylene glycol and water

Table S3. Surface free energies of DI3T-1F, DI3T-2F and PC71BM

	Surface free energy (mN/m)
DI3T-1F	31.8

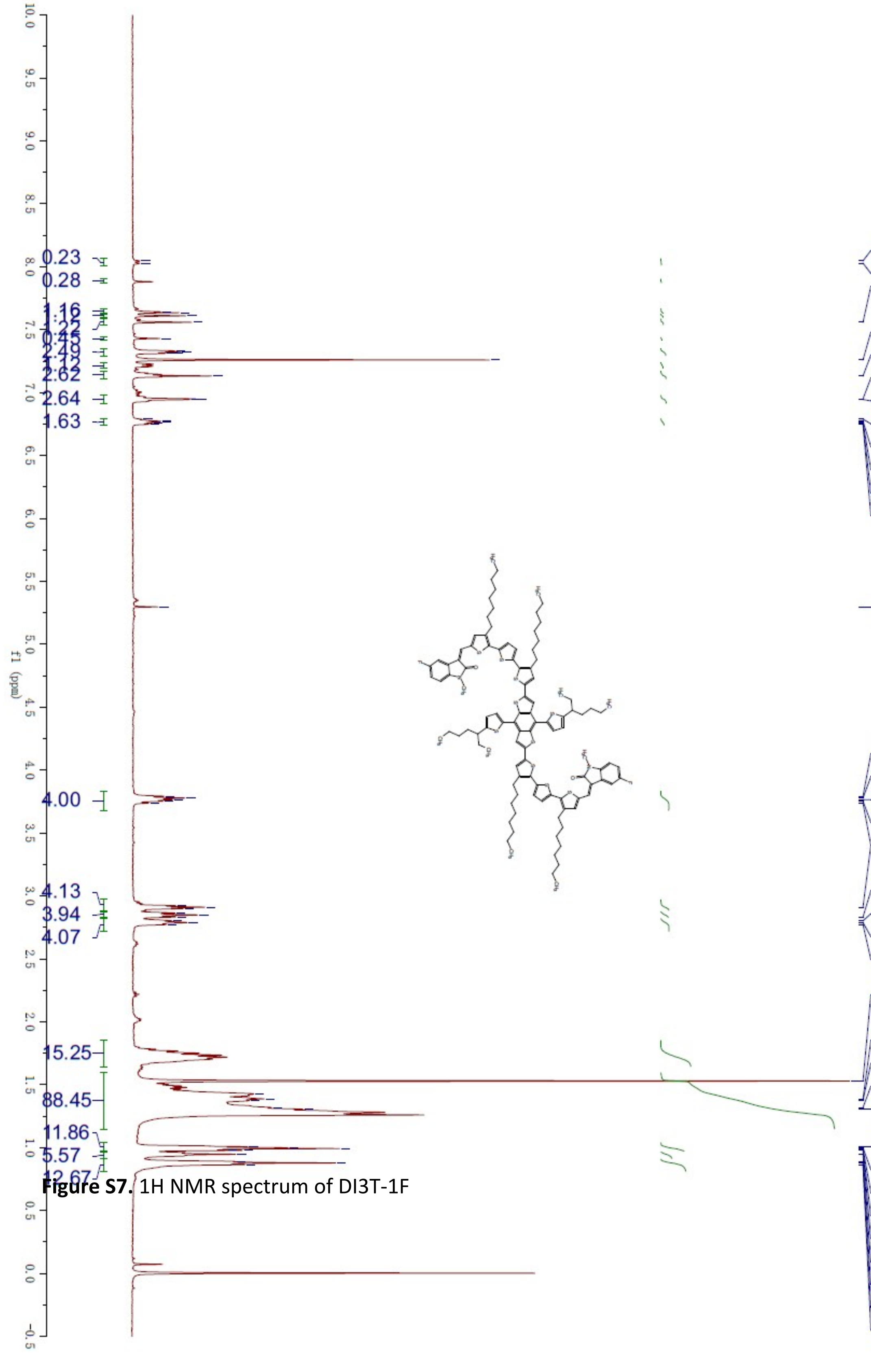


Figure S7. 1H NMR spectrum of DI3T-1F

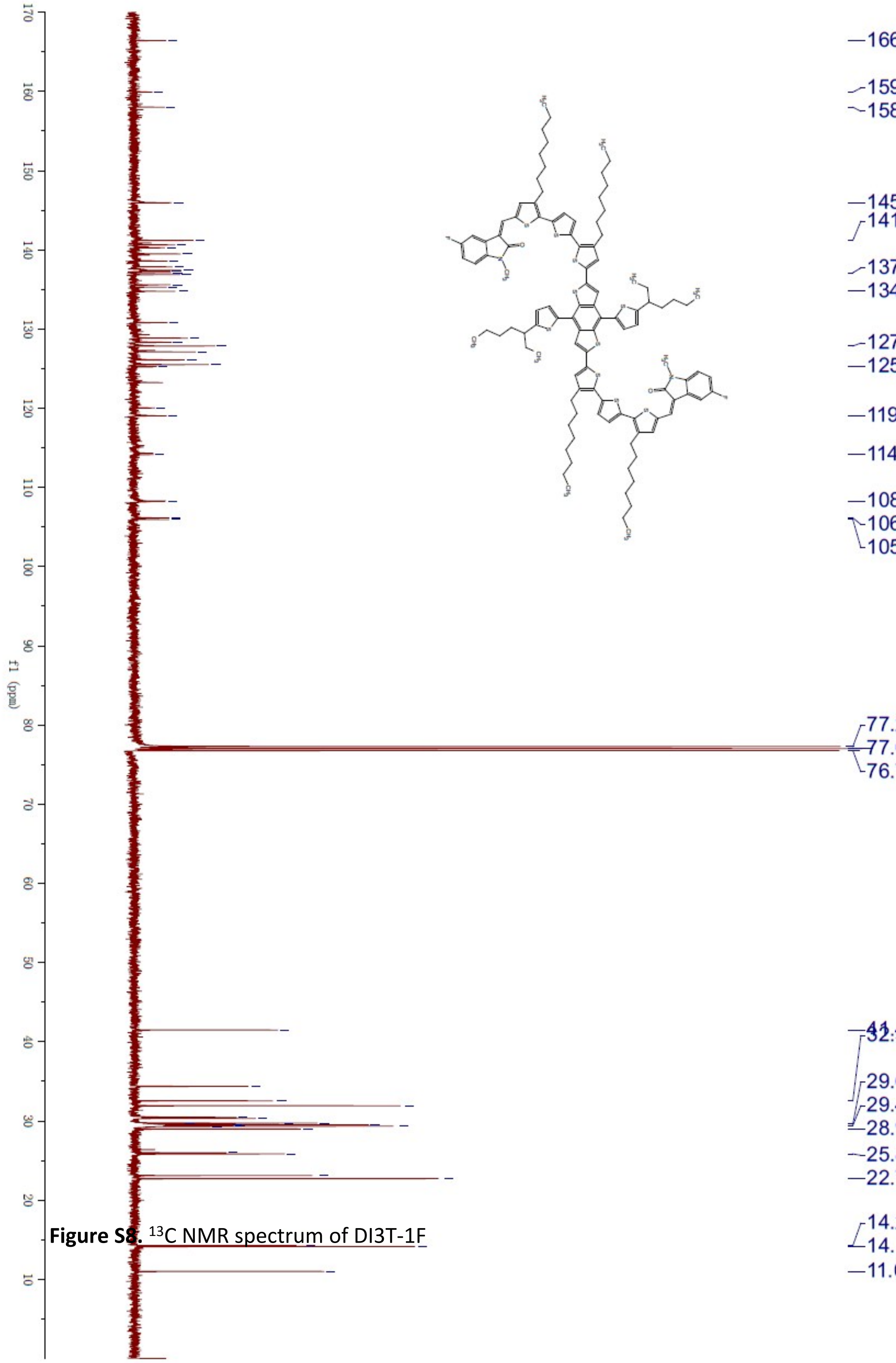


Figure S8. ^{13}C NMR spectrum of DI3T-1F