Supporting Information

Rational design of diketopyrrolopyrrole-based oligomers for high performance small molecular photovoltaic materials *via* extended framework and multiple fluorine substitution

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Experimental Section

SCLC device fabrication and characterization:

The structures of hole only and electron only device are ITO/PEDOT/donor materials: $PC_{71}BM/MoO_3$/Al and ITO/ZnO/PFN/ donor materials: $PC_{71}BM$/Ca/Al, respectively. The mobility was determined by fitting the dark current to the model of the filed-independent space charge limited current (SCLC) according to the Mott-Gurney law, given by $J = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_h\frac{V^2}{L^3}$ for hole only device and $J = \frac{9}{8}\varepsilon_0\varepsilon_r\mu_e\frac{V^2}{L^3}$ for electron only device

Where J is the current density, ε_0 is the permittivity of free space, ε_r is the relative

permittivity of the material, μ_h is the hole mobility, μ_e is the electron mobility, L is the film thickness of the active layer, and V is the effective voltage which is determined by subtracting the built-in voltage (V_{bi}) from the applied voltage ($V = V_{appl} - V_{bi}$). The hole and electron mobility can be directly calculated from *J*-V curves.

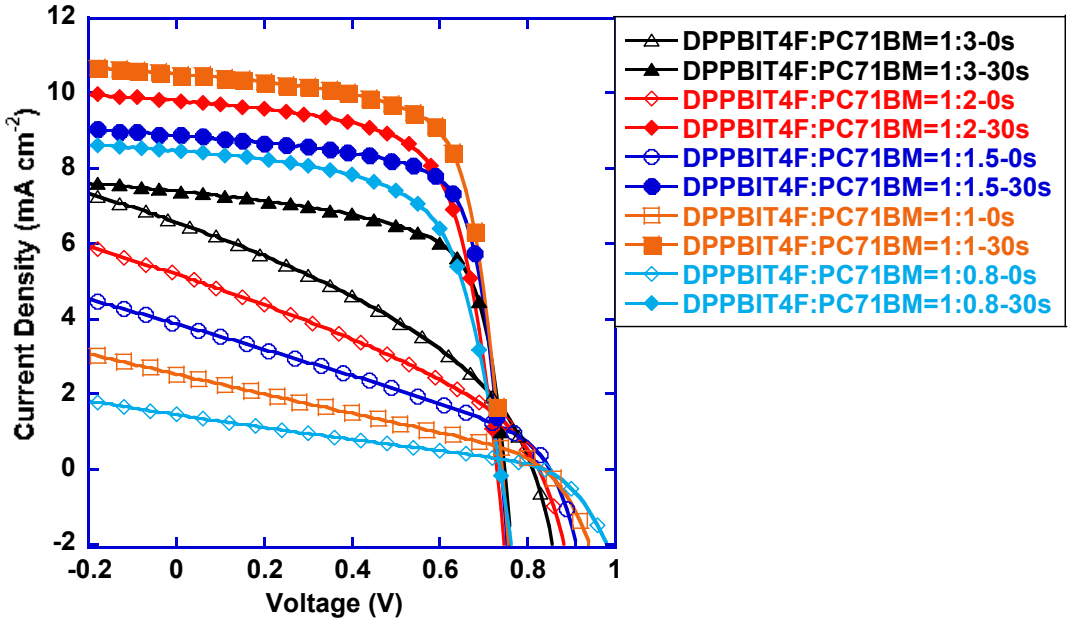


Figure S1. Current density-voltage (*J-V*) characteristics of devices based on **DPPBIT4F** blend with **PC$_{71}$BM** (different blend ratio and before/after solvent treatment).

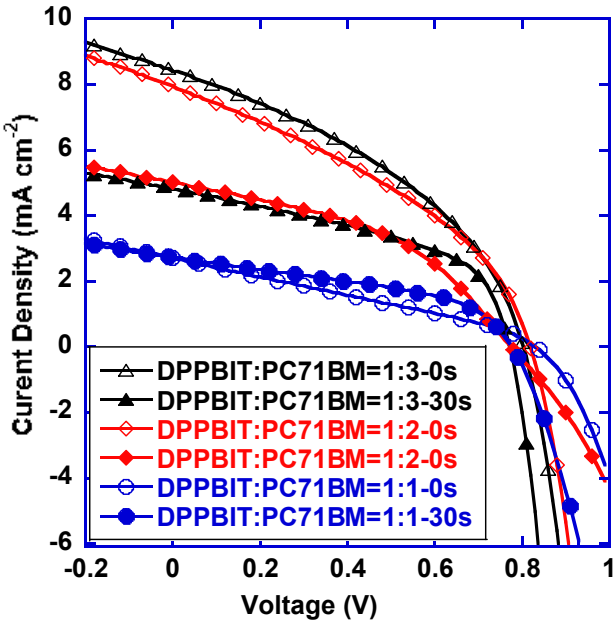


Figure S2. Current density-voltage (*J-V*) characteristics of devices based on **DPPBIT** blend with **$PC_{71}BM$** (different blend ratio and before/after solvent treatment).

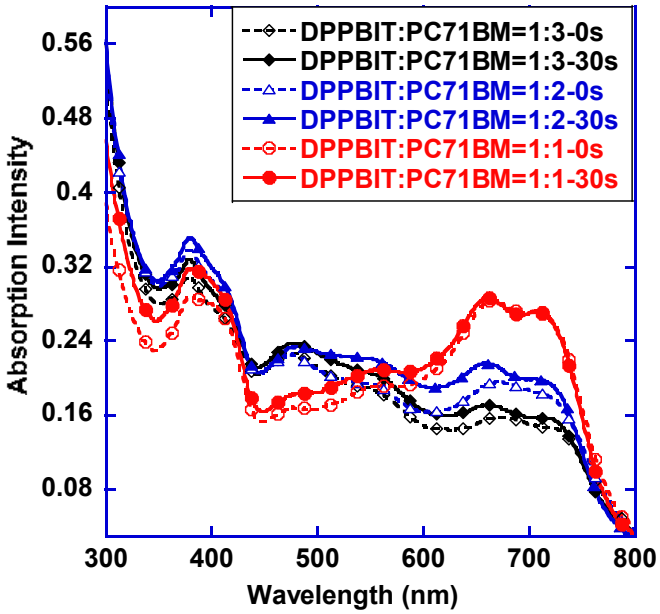


Figure S3. Absorption spectra of **DPPBIT:** $PC_{71}BM$ (1:1, 1:2, and 1:3, w/w) blend films with or without CH_2Cl_2 vapor annealing.

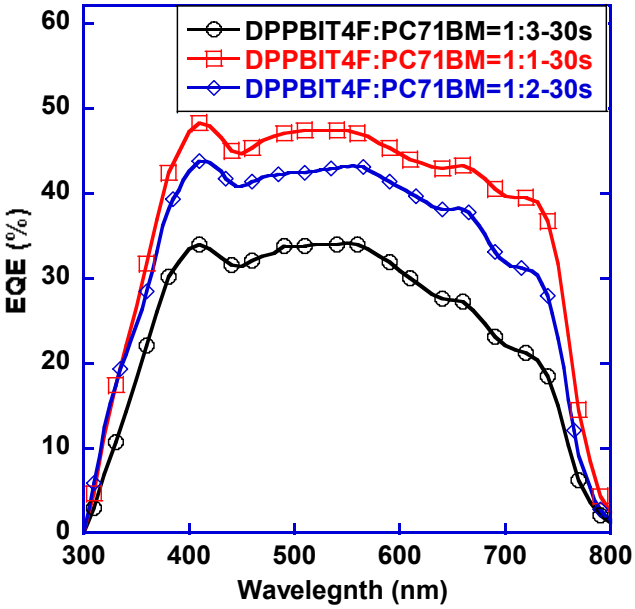


Figure S4. EQE plots of devices based on **DPPBIT4F** blend with **$PC_{71}BM$** (1:1, 1:2, and 1:3, w/w) after CH_2Cl_2 vapor annealing.

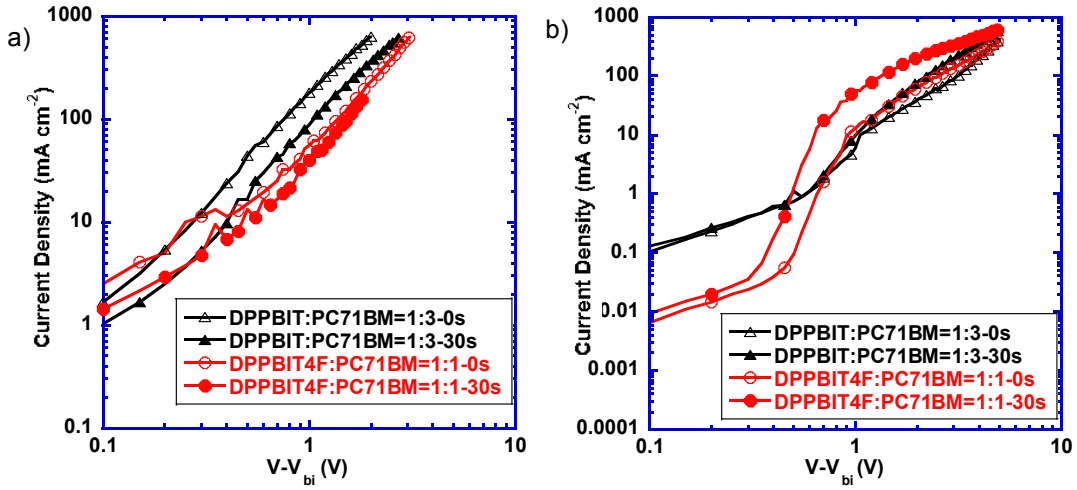
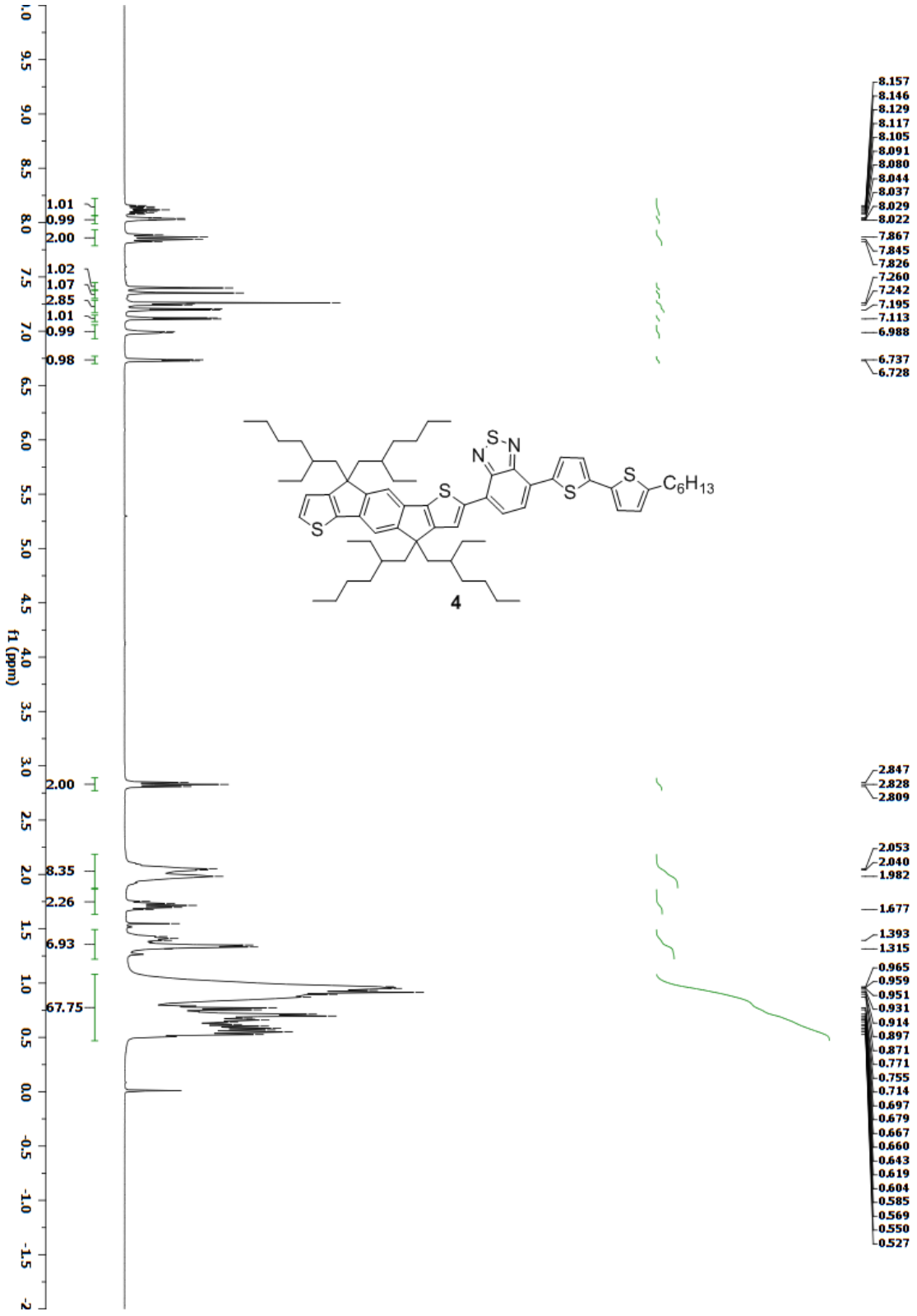
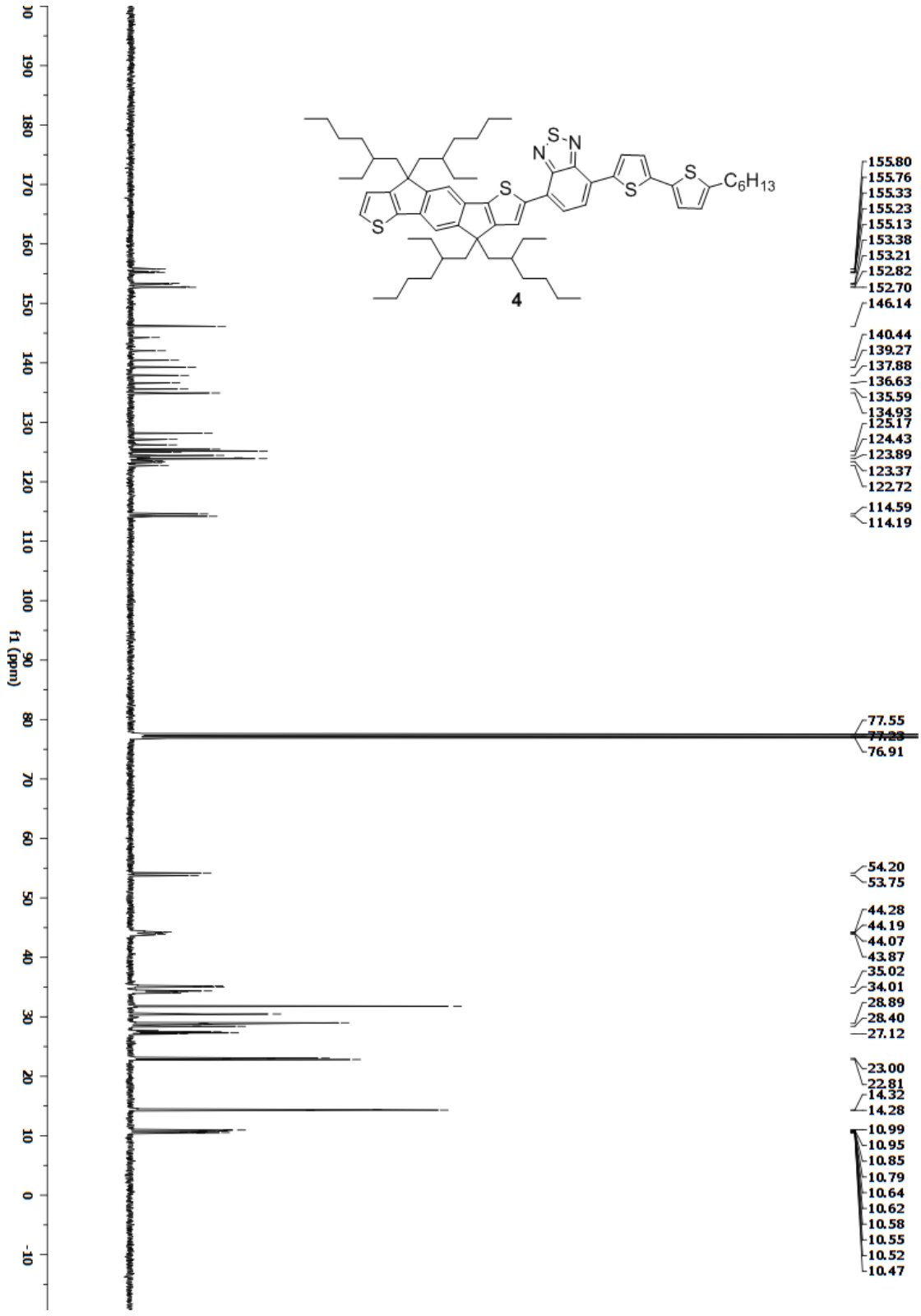


Figure S5. The *J-V* plots of the devices with a configuration of ITO/PEDOT/donor materials: $PC_{71}BM/MoO_3/Al$ for hole only device (a) and ITO/ZnO/PFN/ donor materials: $PC_{71}BM$/Ca/Al for electron only device (b) before and after CH_2Cl_2 vapor annealing, respectively.

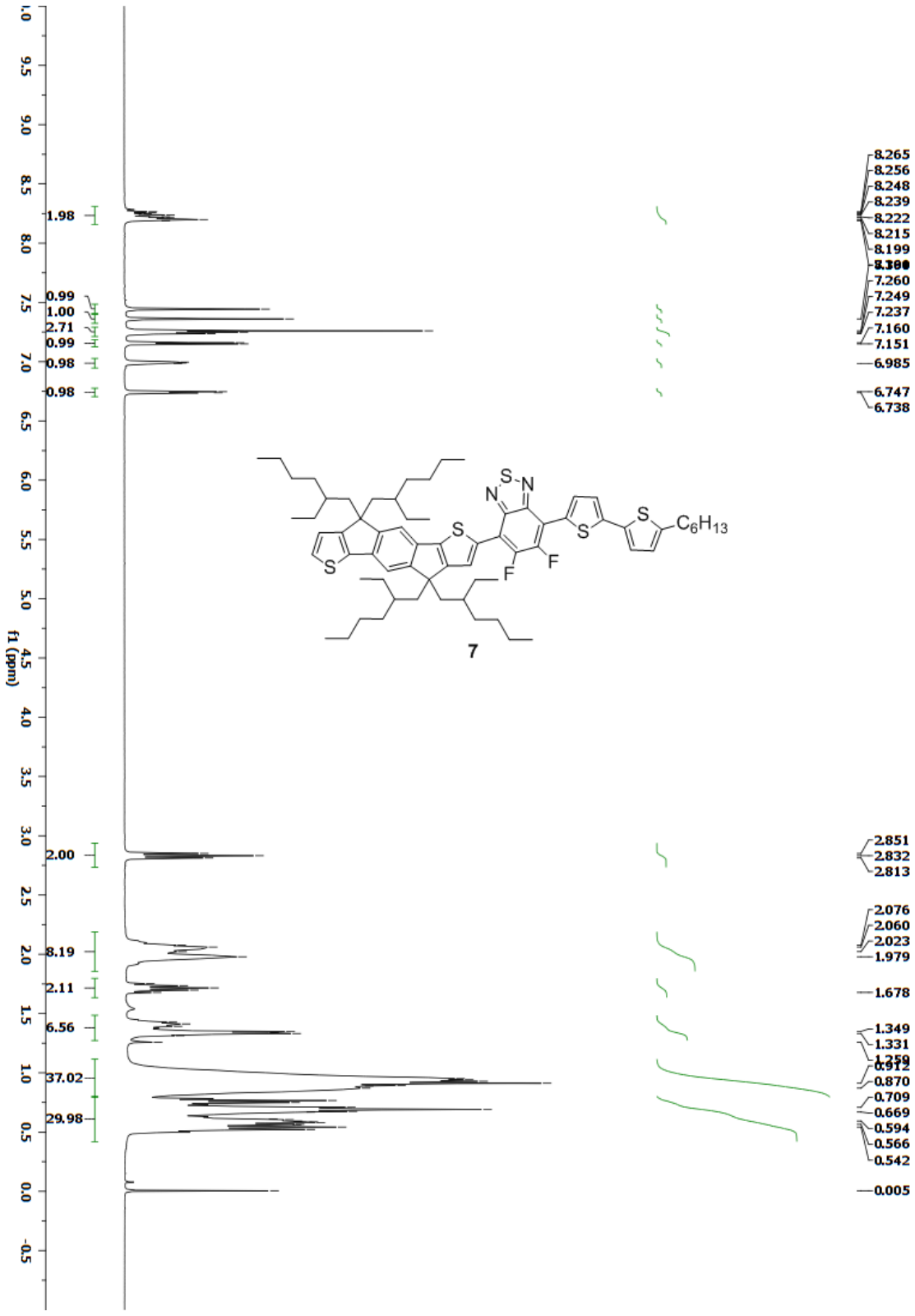
Copies of ^{1}H and ^{13}C NMR, and MALDI-TOF MS Spectra



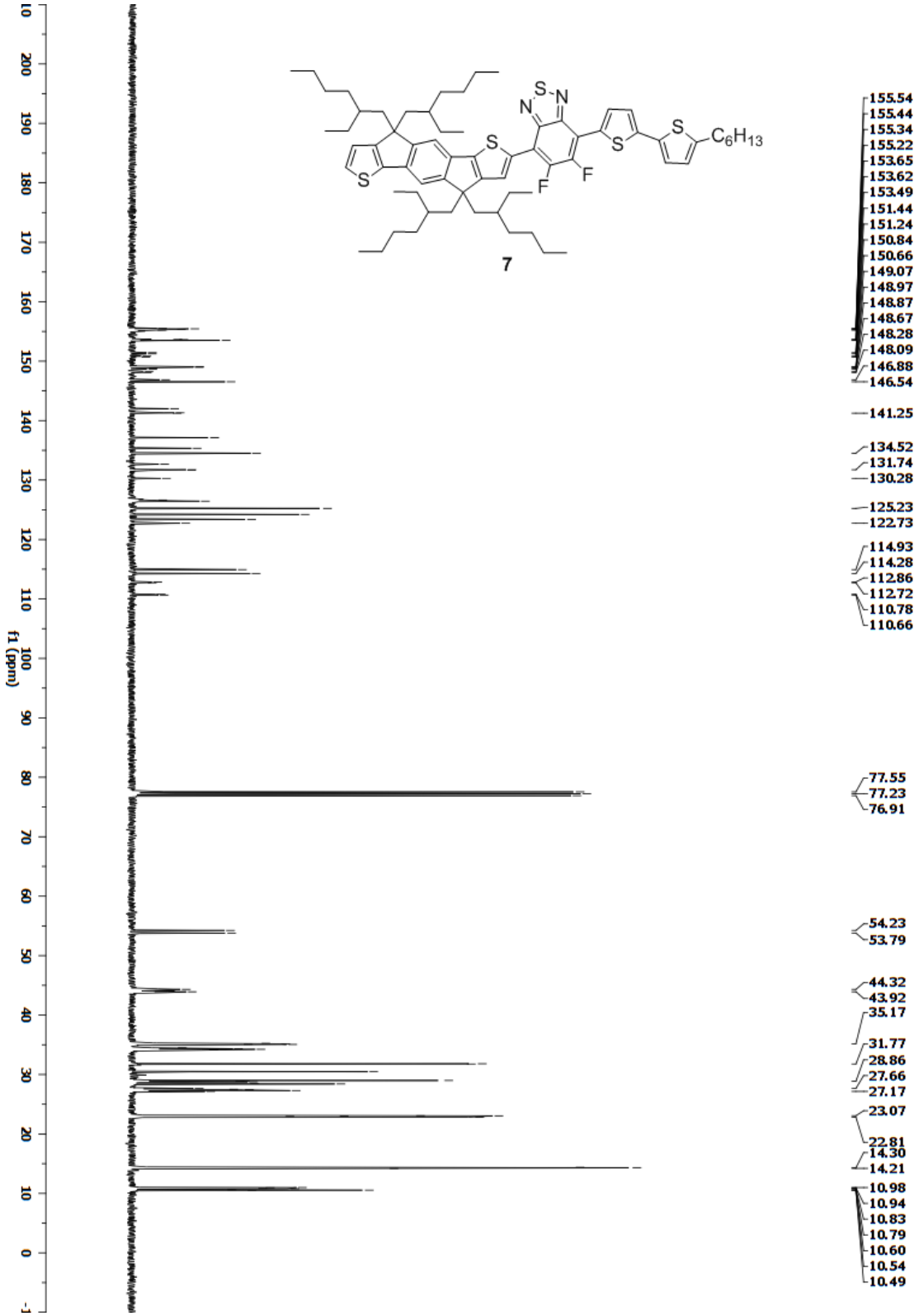
^{1}H NMR spectrum for compound **4**



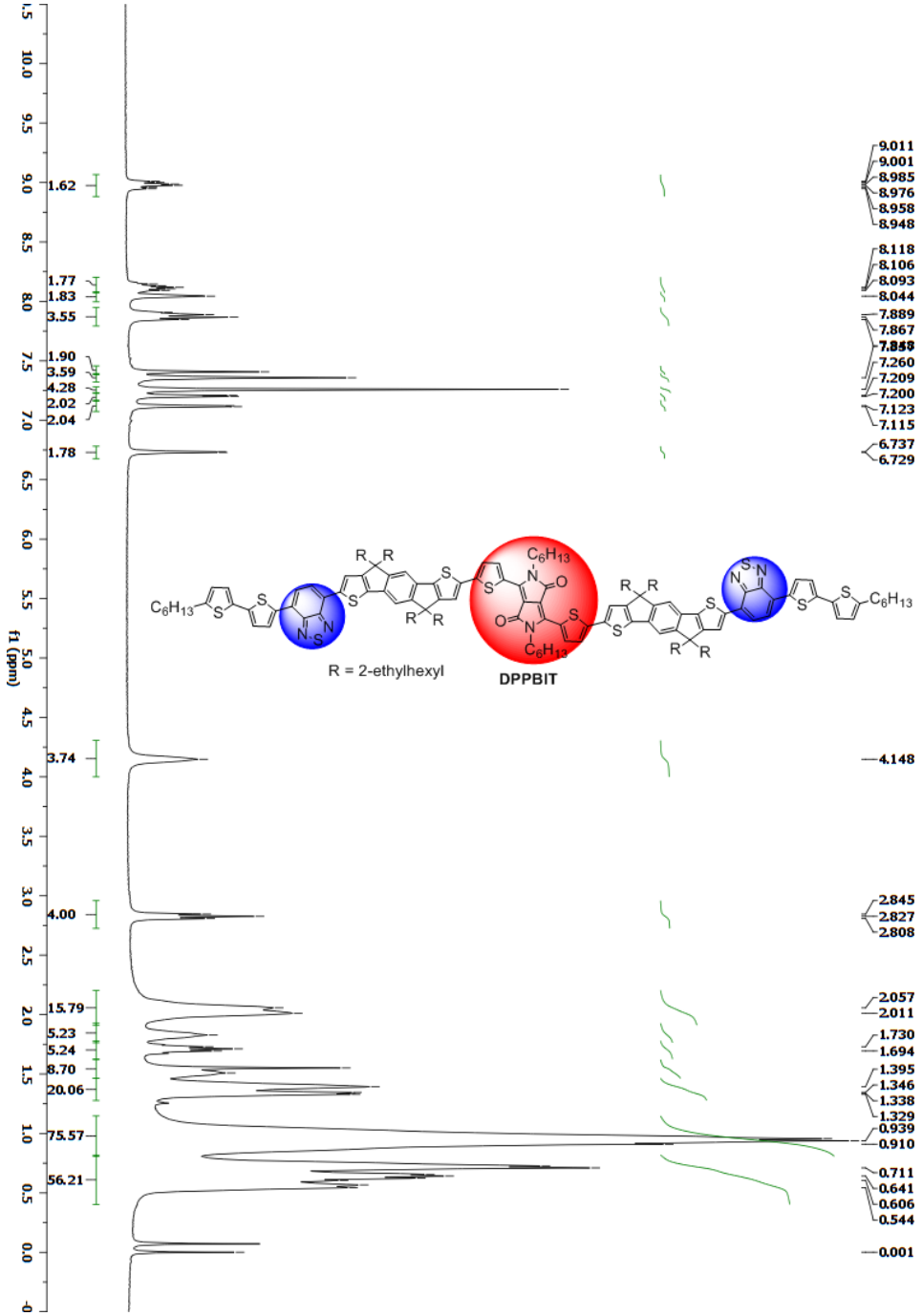
^{13}C NMR spectrum for compound **4**.



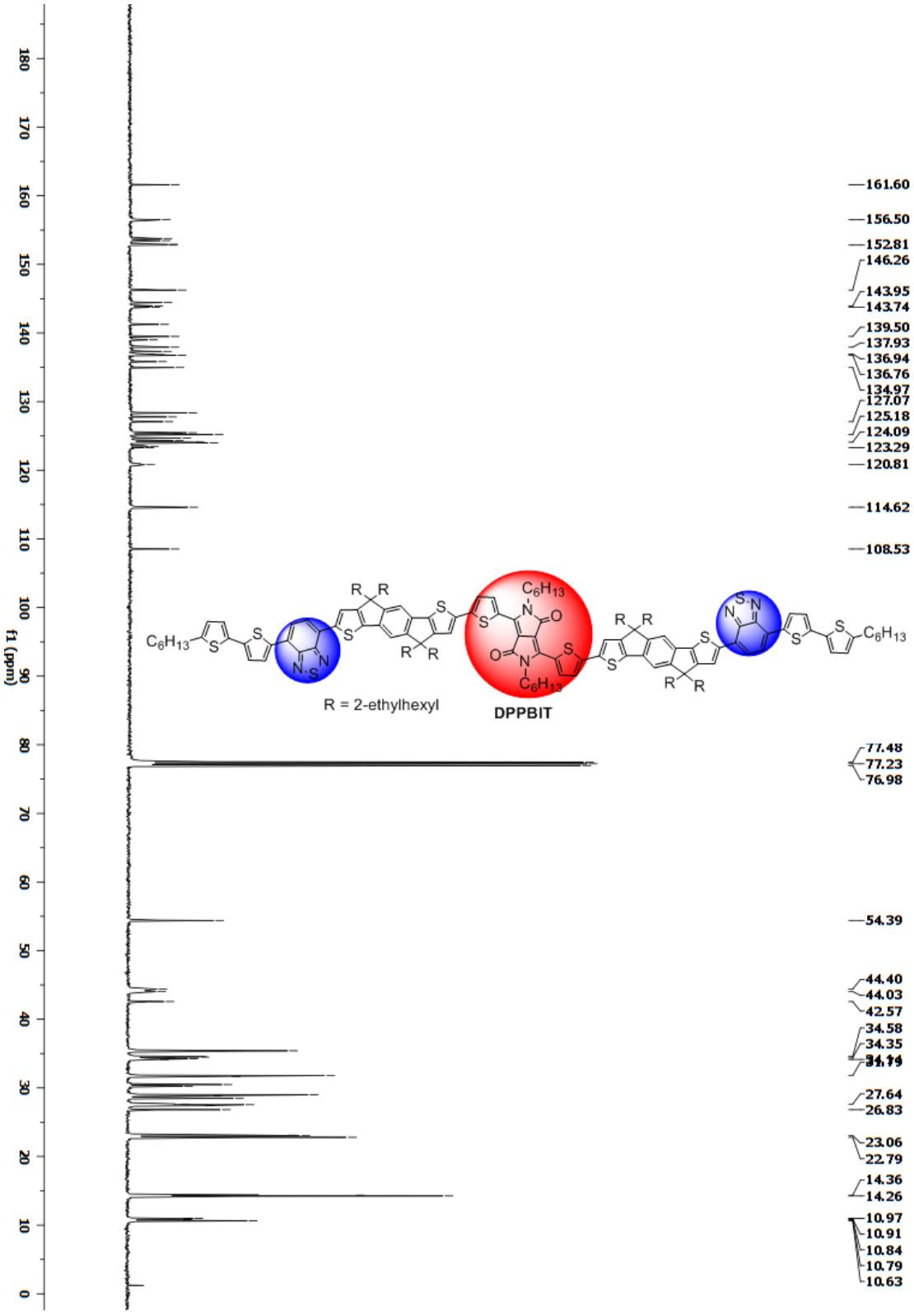
^{1}H NMR spectrum for compound **7**



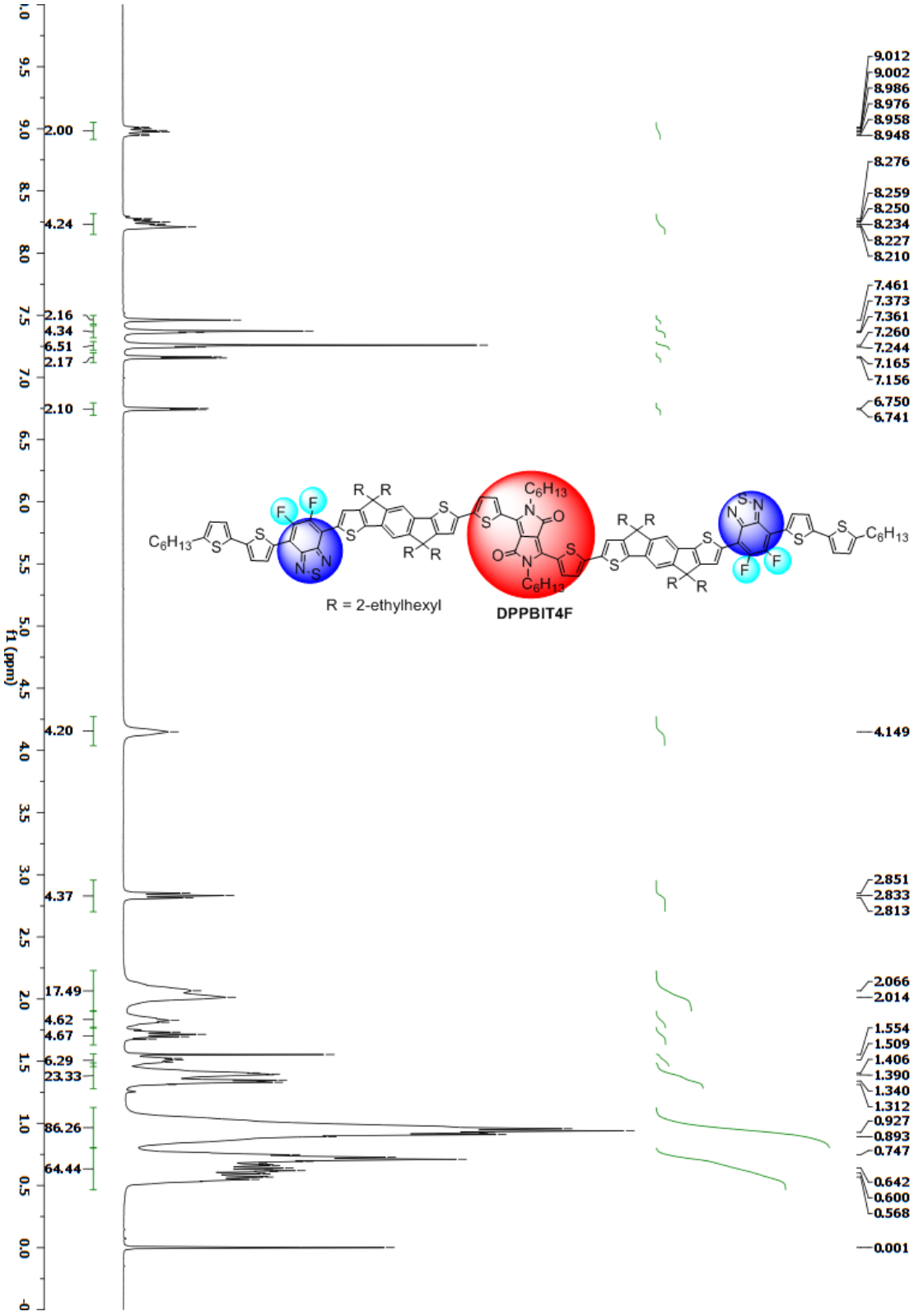
^{13}C NMR spectrum for compound **7**.



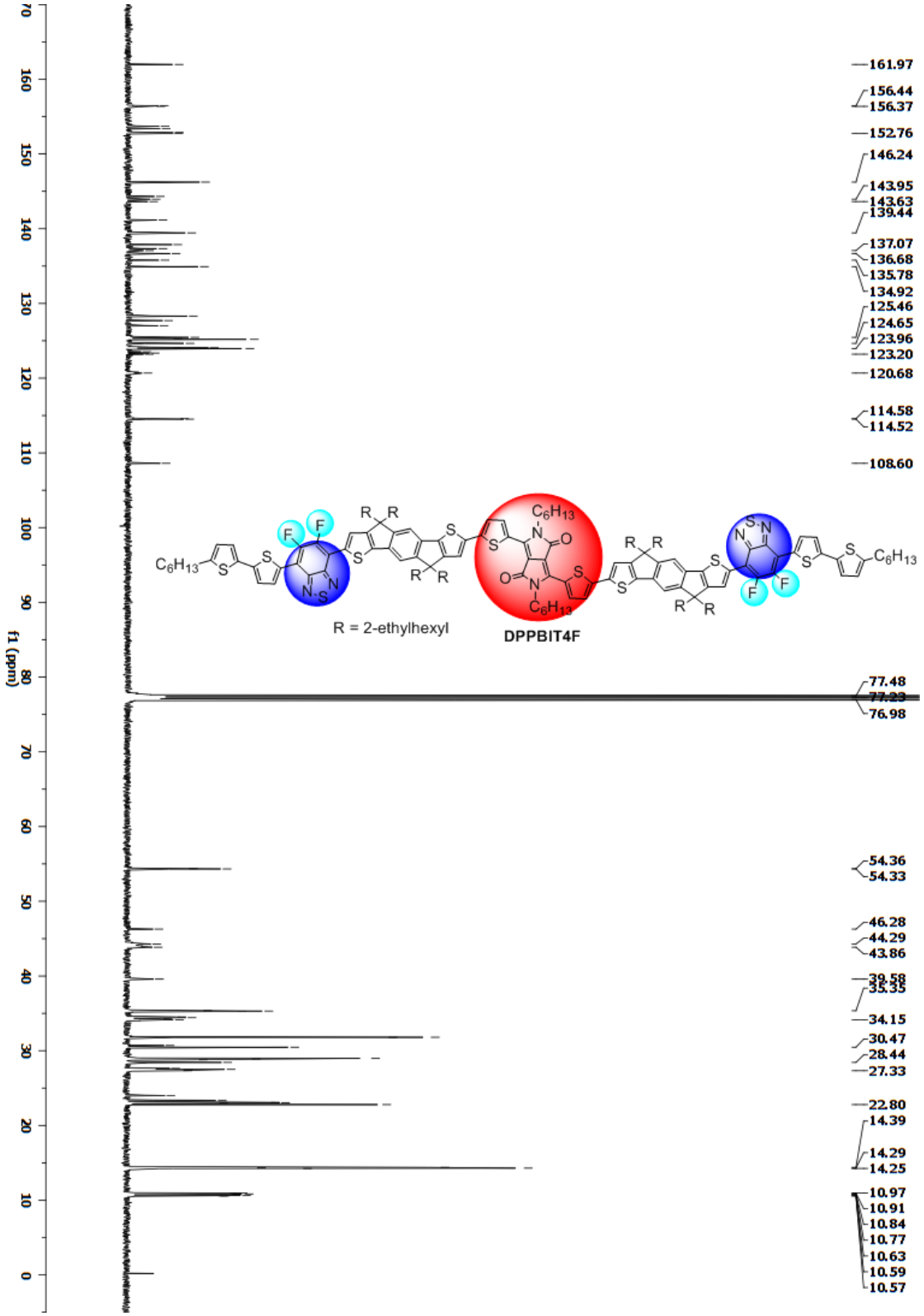
^{1}H NMR spectrum for **DPPBIT**



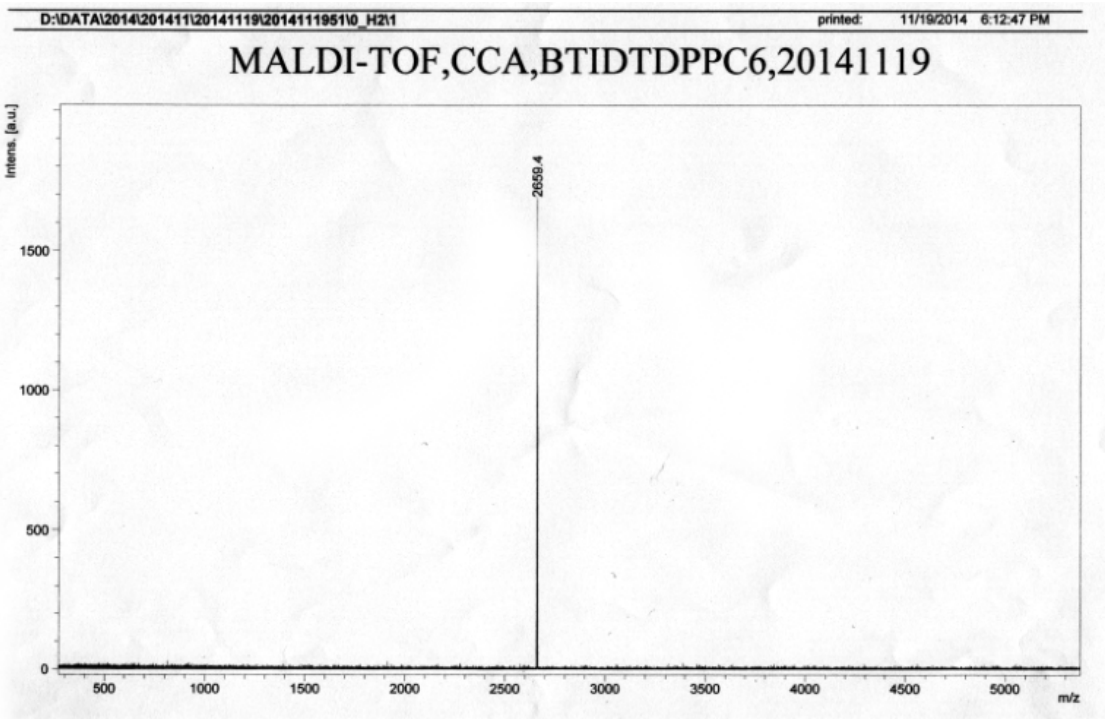
^{13}C NMR spectrum for **DPPBIT**.

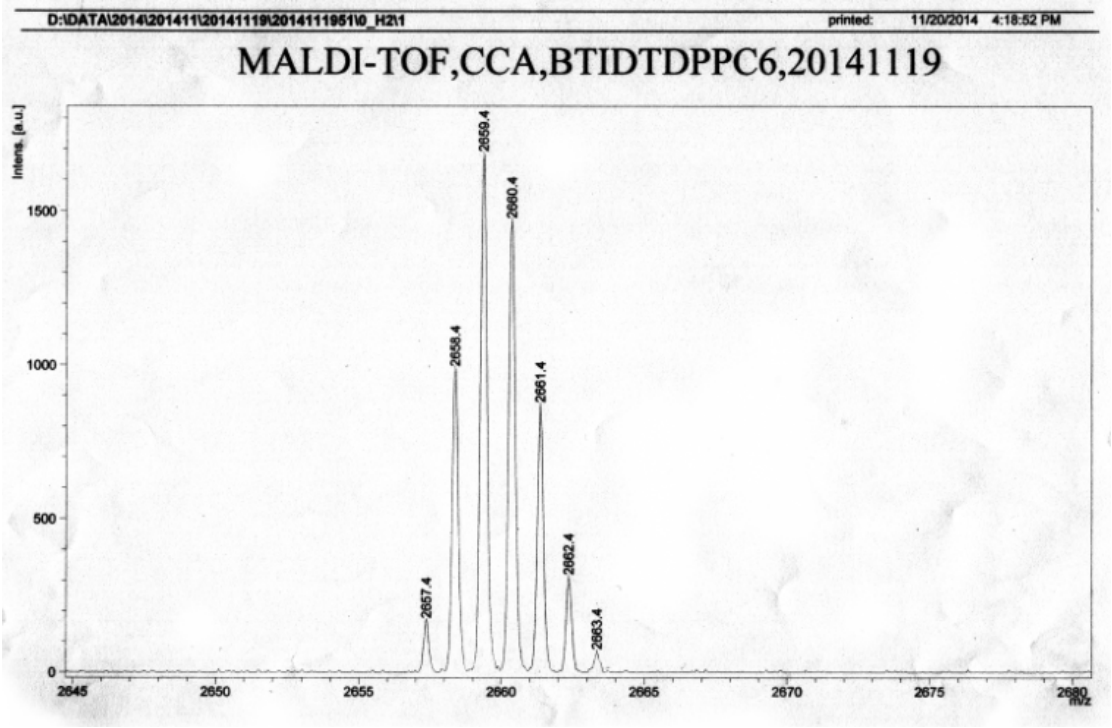


^{1}H NMR spectrum for **DPPBIT4F**

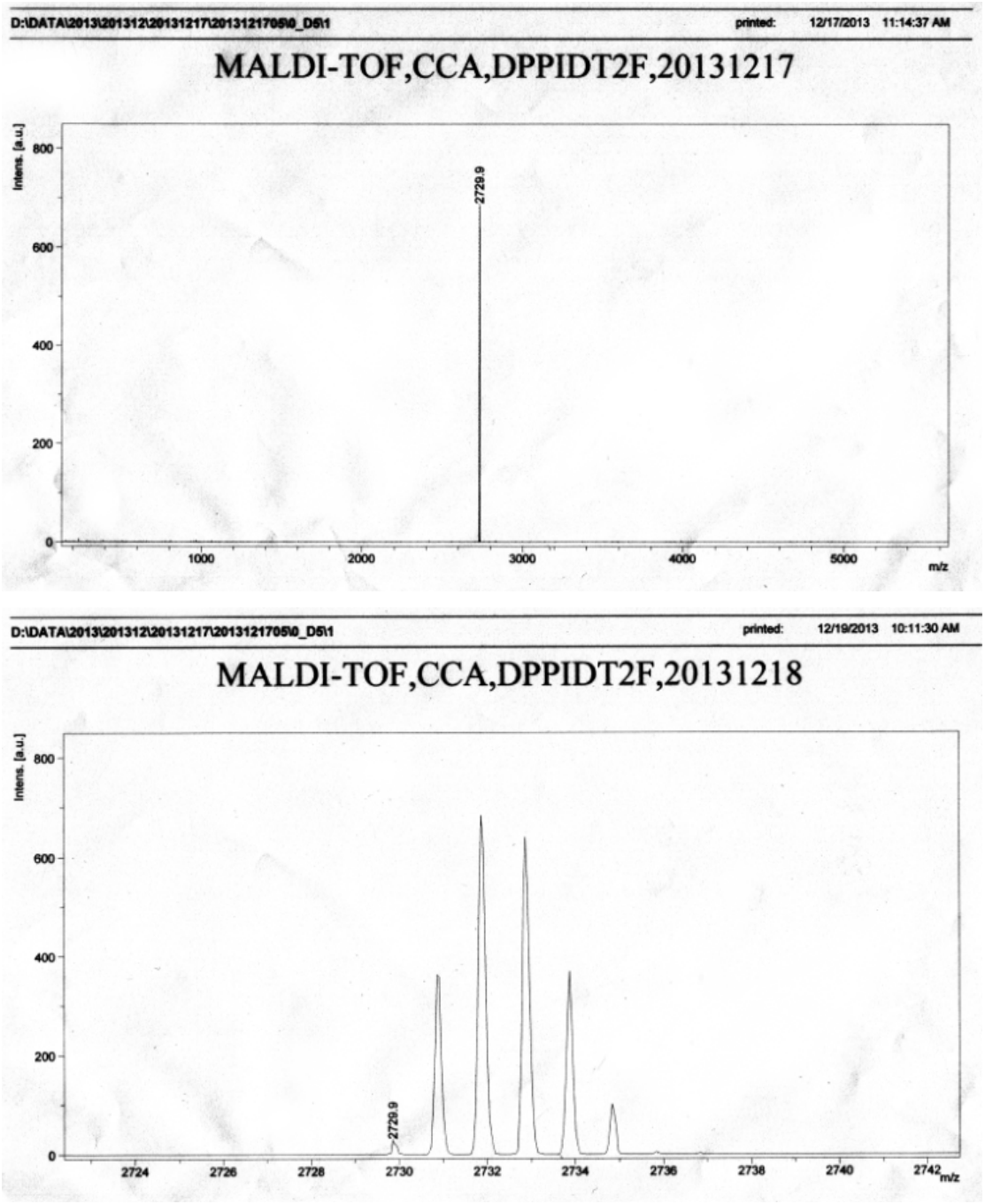


^{13}C NMR spectrum for **DPPBIT4F**.





MALDI-TOF mass spectrum of **DPPBIT**.



MALDI-TOF mass spectrum of **DPPBIT4F**.