Supporting information for

Fluorinated Dithienyl-Diketopyrrolopyrrole: A New Building Block for Organic Optoelectronic Materials

Xiaohua Wang,‡ Bin Jiang,‡ Chenchen Du, Xiaolei Ren, Zhiming Duan, Hongyu Wang*

Department of Chemistry, College of Science, and Center for Supramolecular Chemistry & Catalysis, Shanghai University, 99 Shangda Road, Shanghai, 200444, P. R. China.

‡ Both authors contributed equally to this work.

E-mail: wanghy@shu.edu.cn

NMR and mass spectra of the fluorinated compound

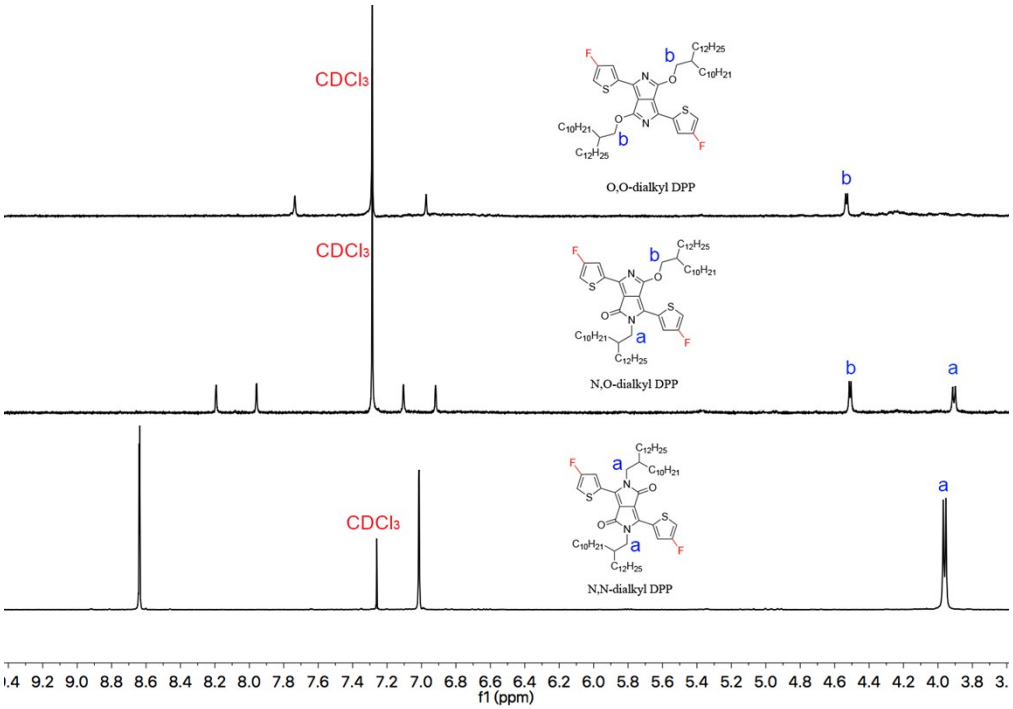
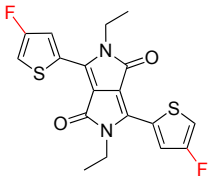


Figure S1. The partial ^{1}H NMR spectra of the DPP isomers.



12a

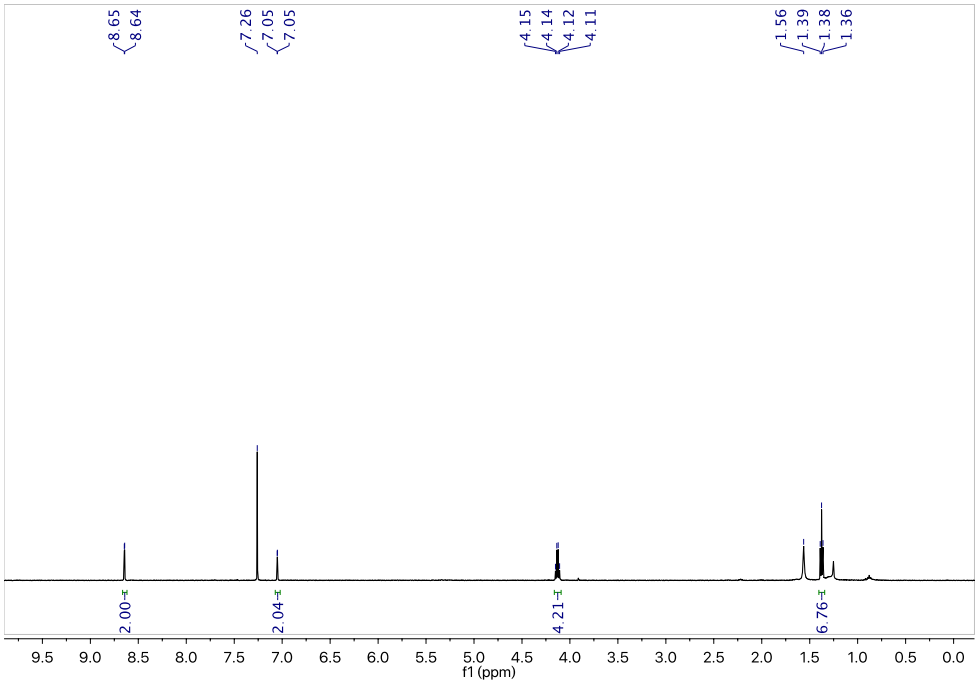


Figure S2. ^{1}H NMR spectrum of **12a** in $CDCl_3$.

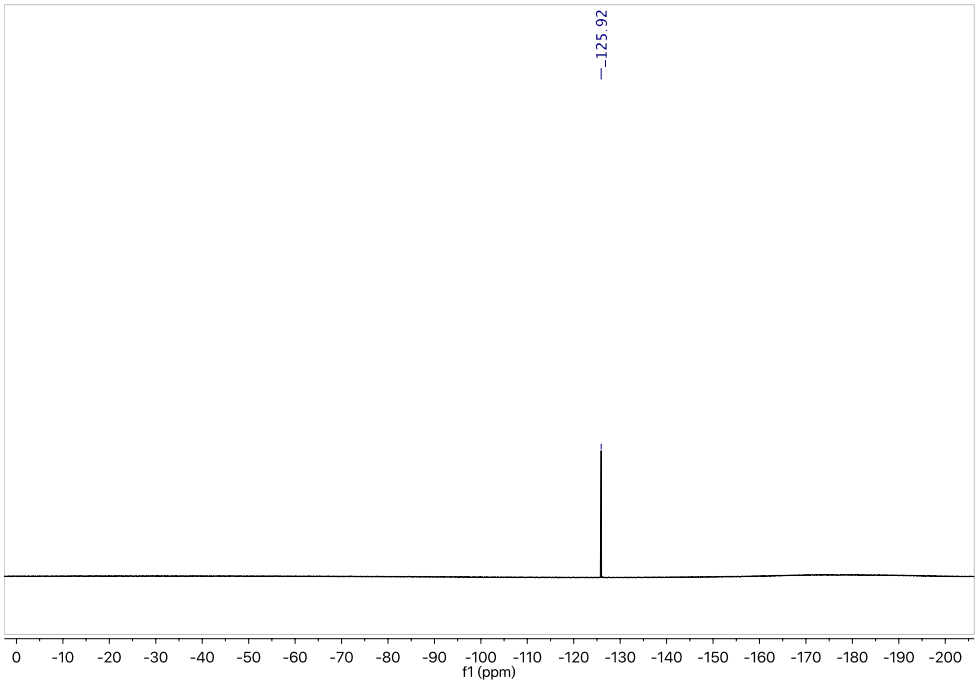


Figure S3. ^{13}C NMR spectrum of **12a** in $CDCl_3$.

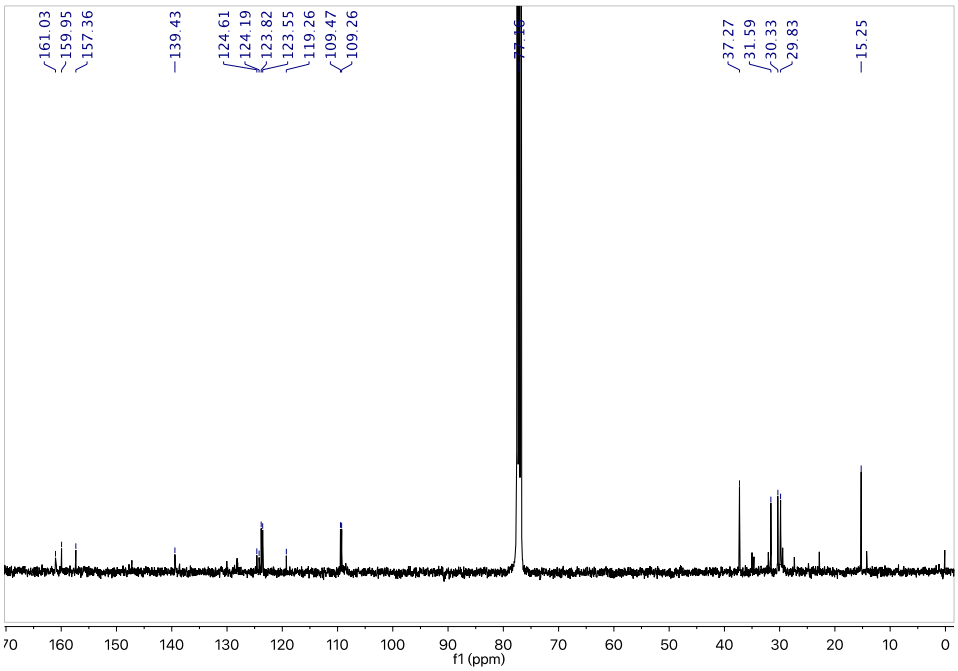
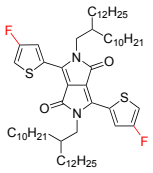


Figure S4. ^{19}F NMR spectrum of **12a** in $CDCl_3$.



12b

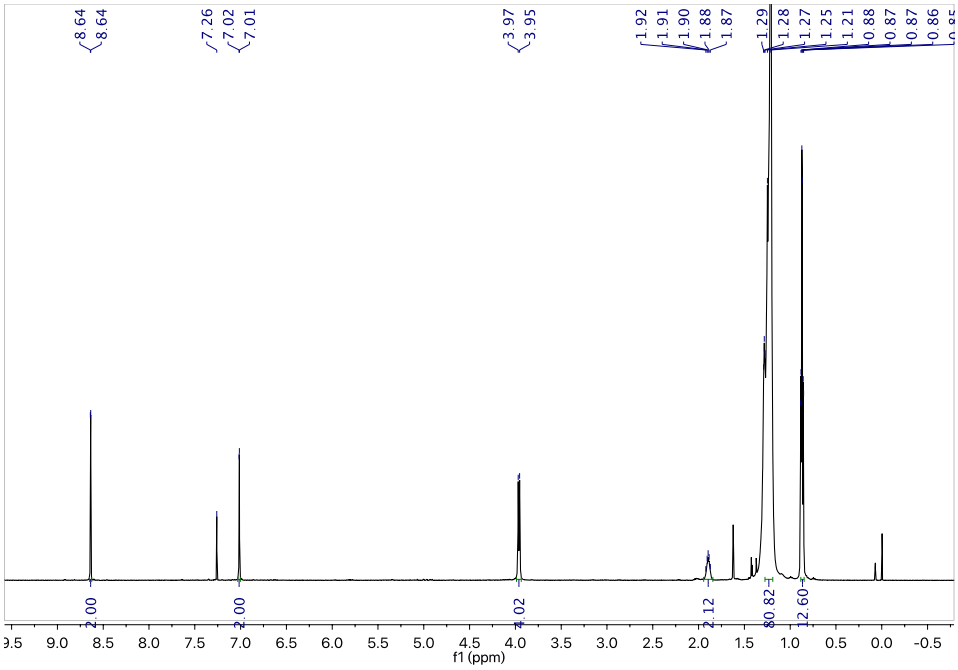


Figure S5. ^{1}H NMR spectrum of **12b** in $CDCl_3$.

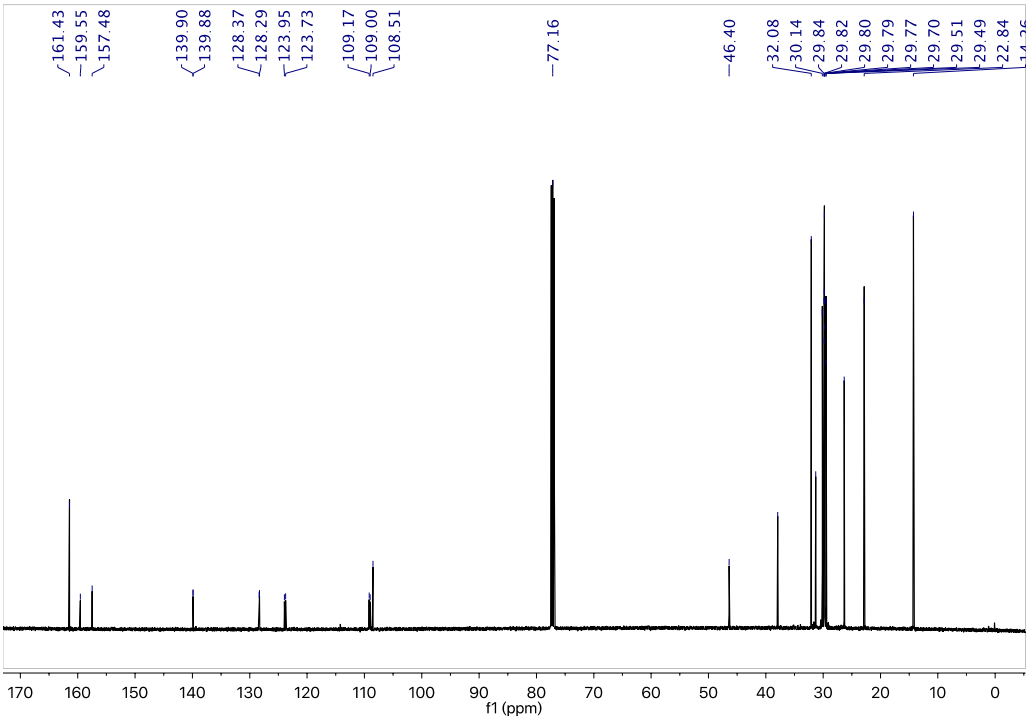


Figure S6. ^{13}C NMR spectrum of **12b** in $CDCl_3$.

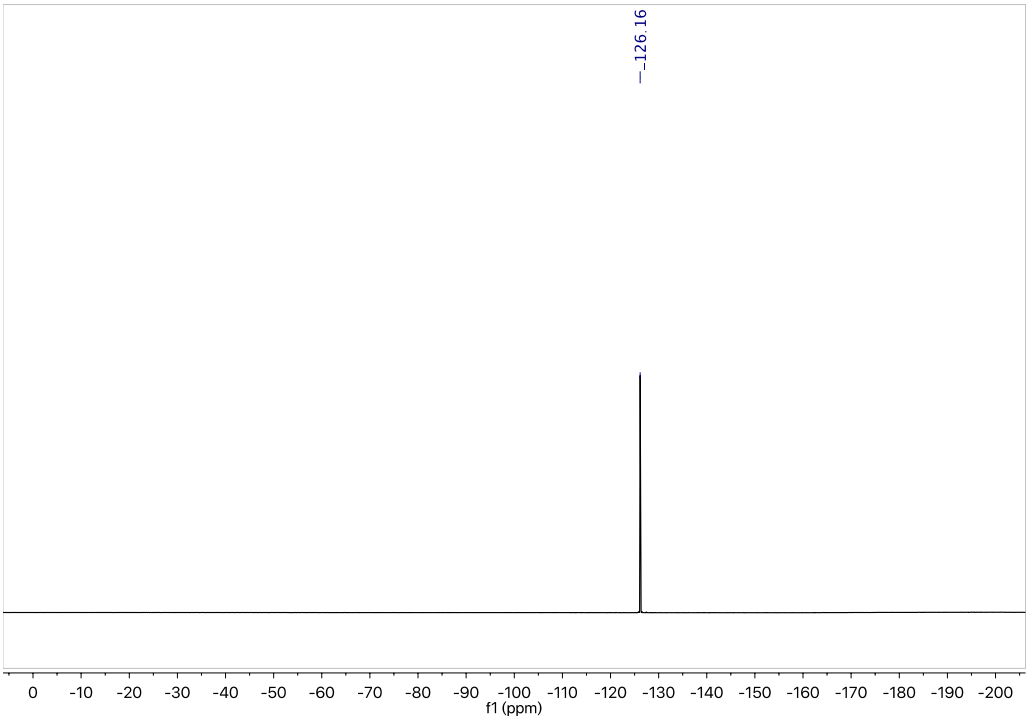


Figure S7. ^{19}F NMR spectrum of **12b** in $CDCl_3$.

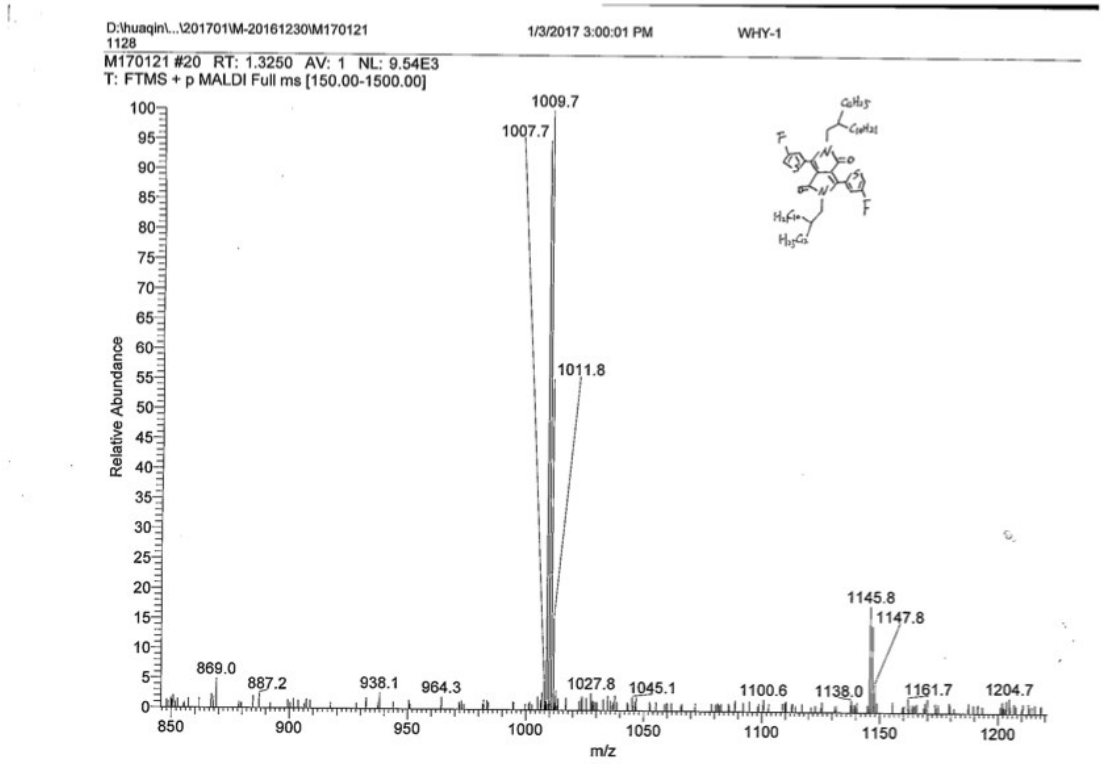
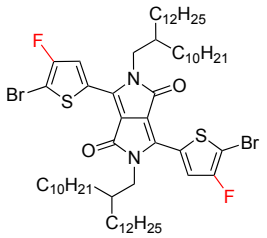


Figure S8. Mass spectrum of **12b**.



13

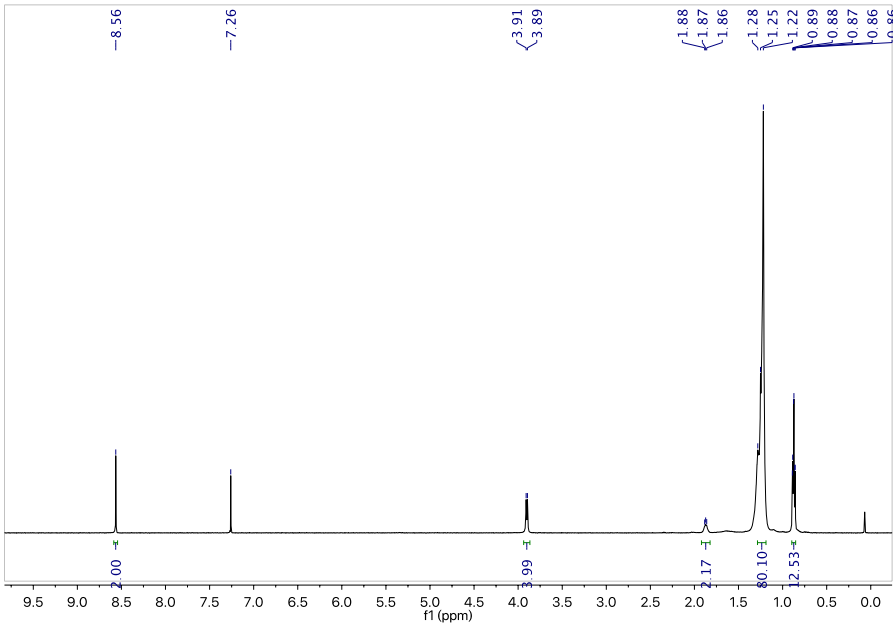


Figure S9. ^{1}H NMR spectrum of **13** in $CDCl_3$.

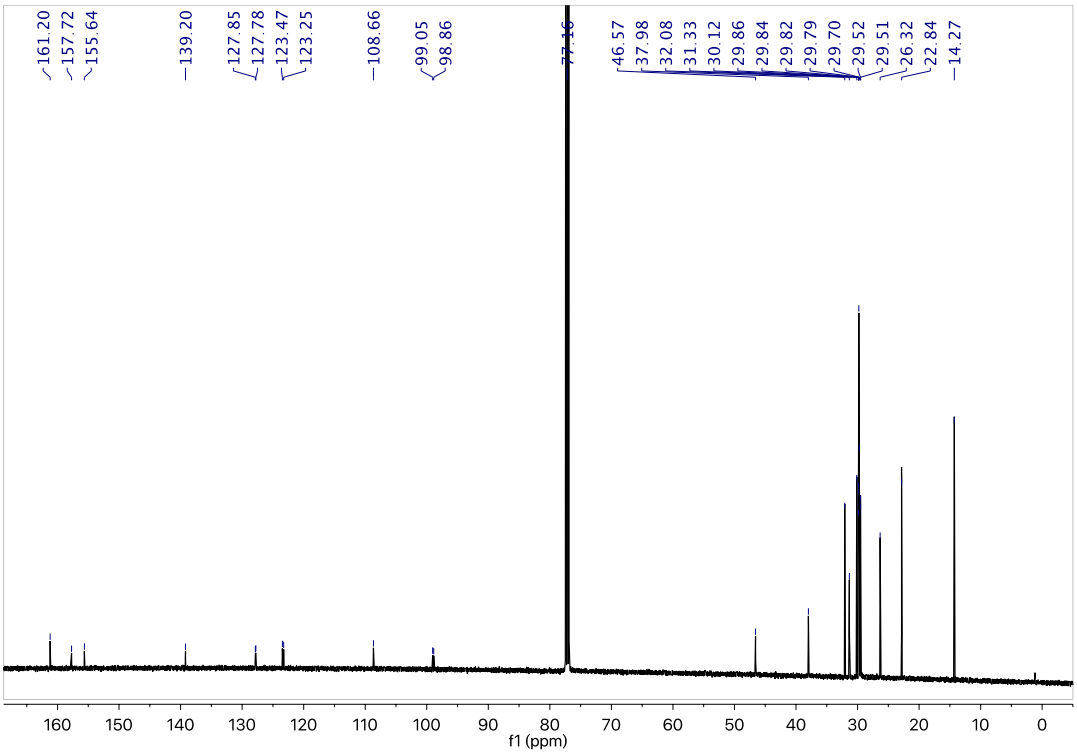


Figure S10. ^{13}C NMR spectrum of **13** in $CDCl_3$.

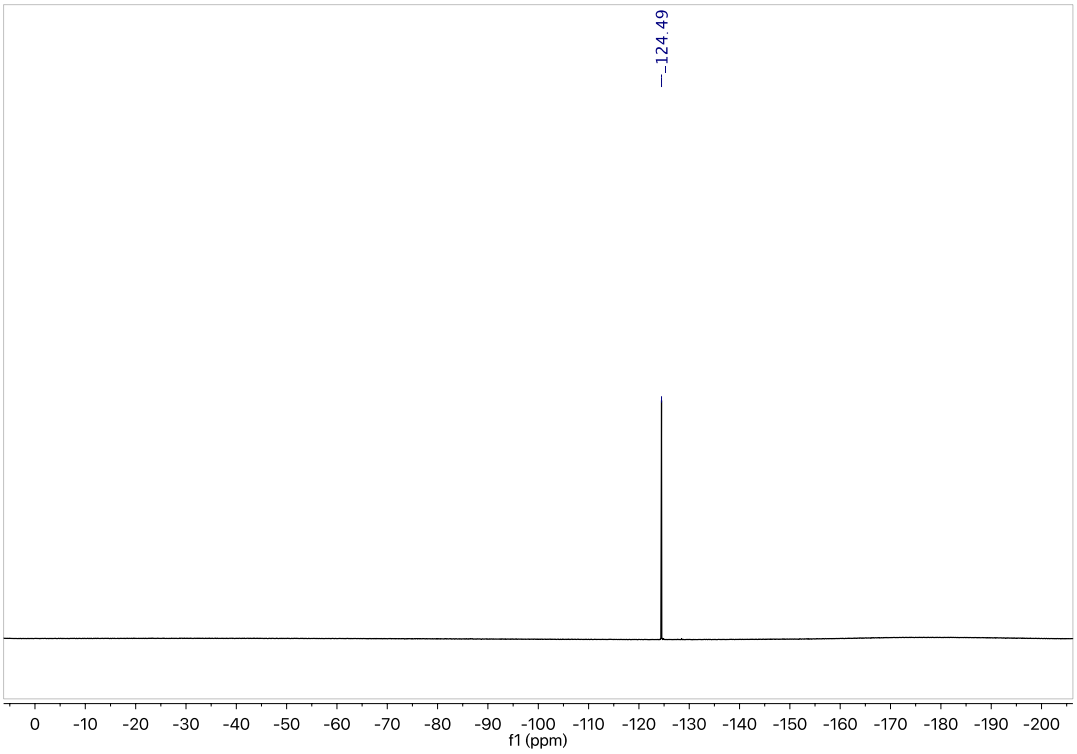


Figure S11. ^{19}F NMR spectrum of **13** in $CDCl_3$.

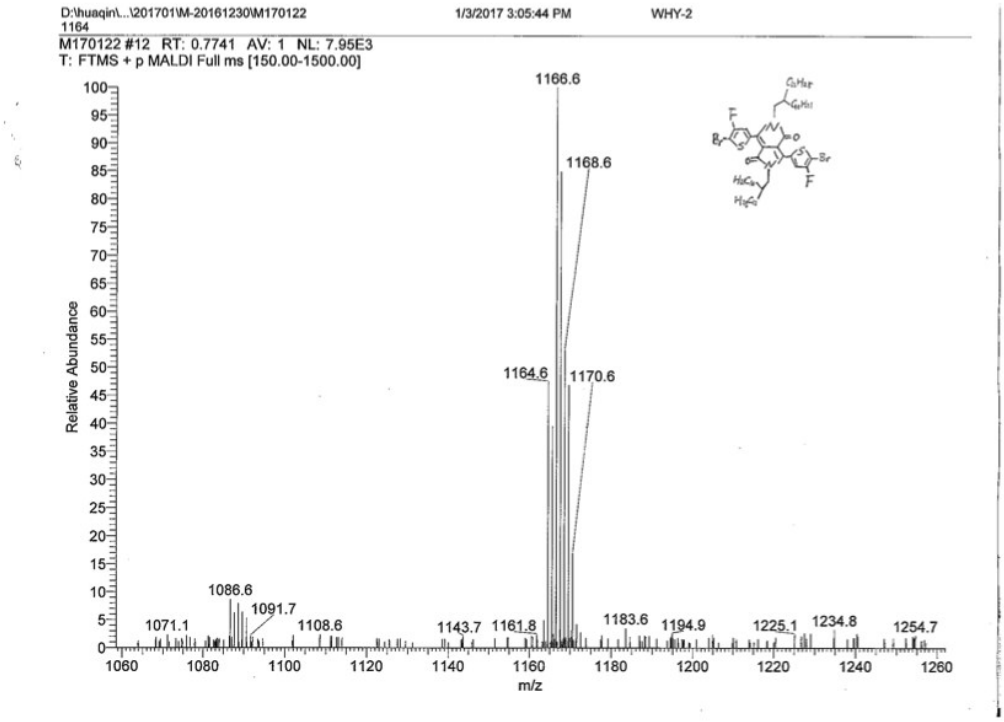


Figure S12. Mass spectrum of **13**.

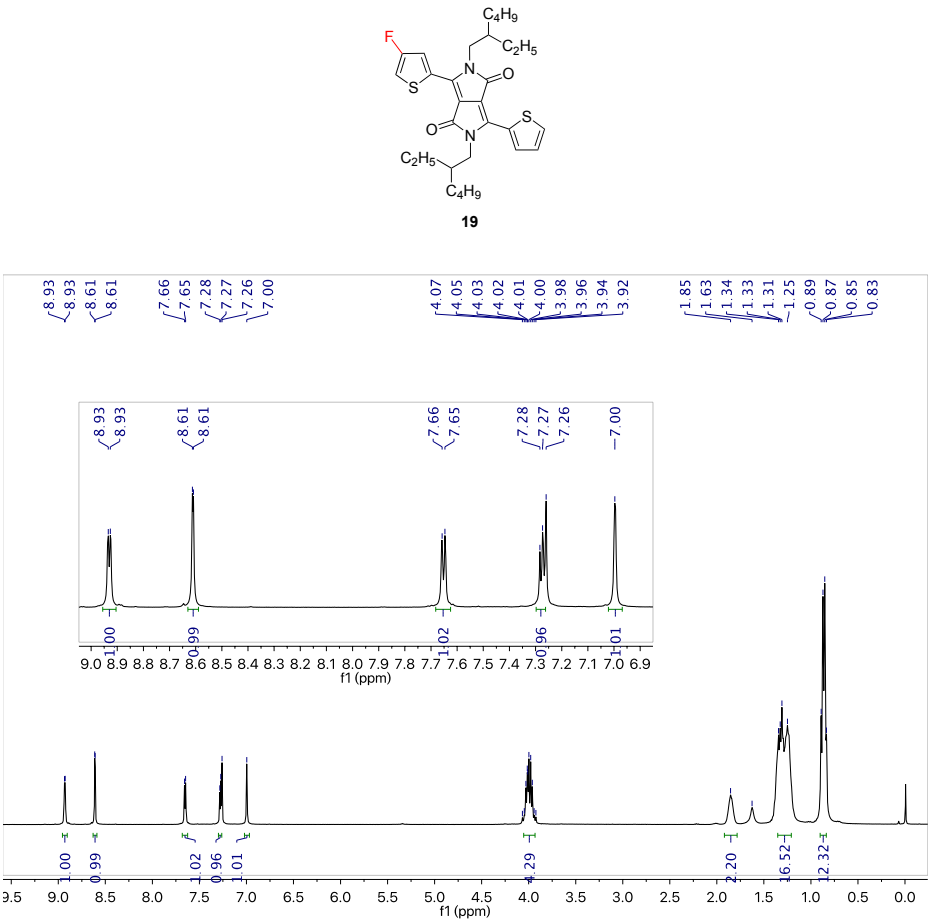


Figure S13. ^{1}H NMR spectrum of **19** in $CDCl_3$.

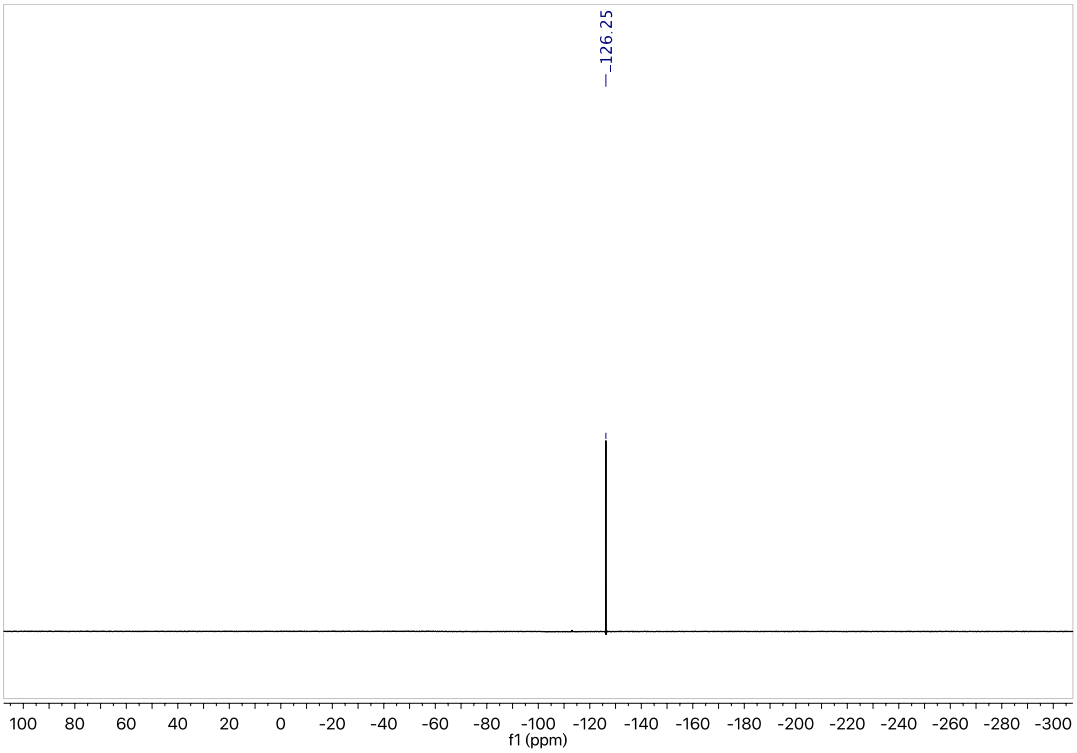


Figure S14. ^{19}F NMR spectrum of **19** in $CDCl_3$.

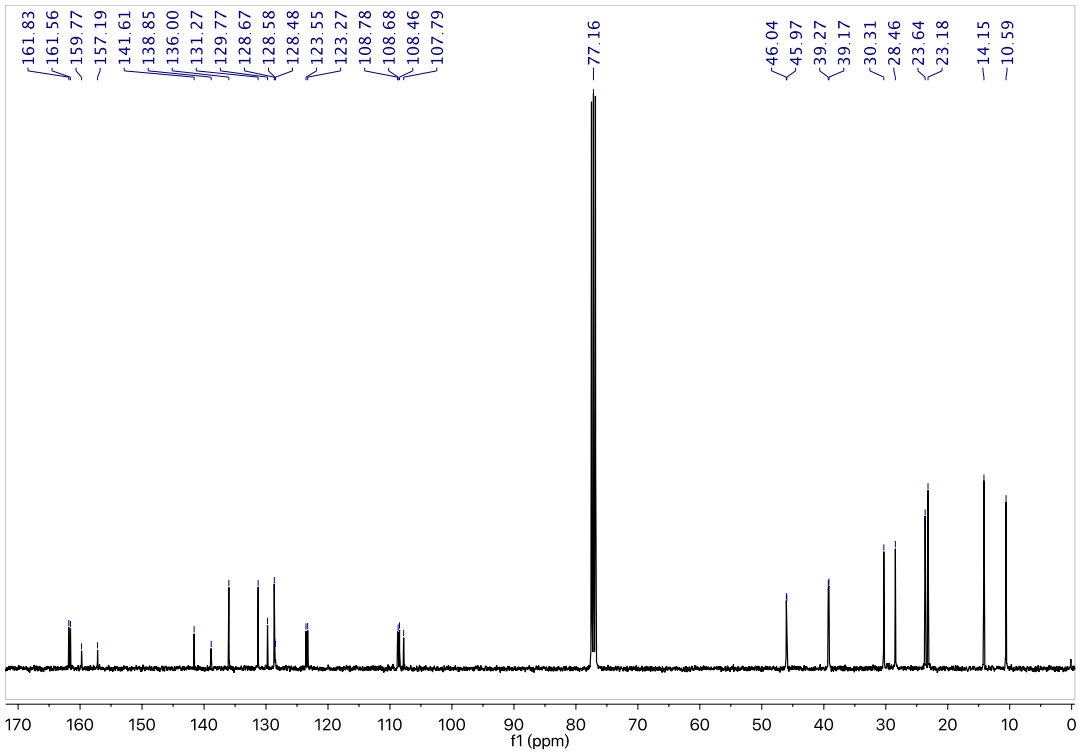


Figure S15. ^{13}C NMR spectrum of **19** in $CDCl_3$.

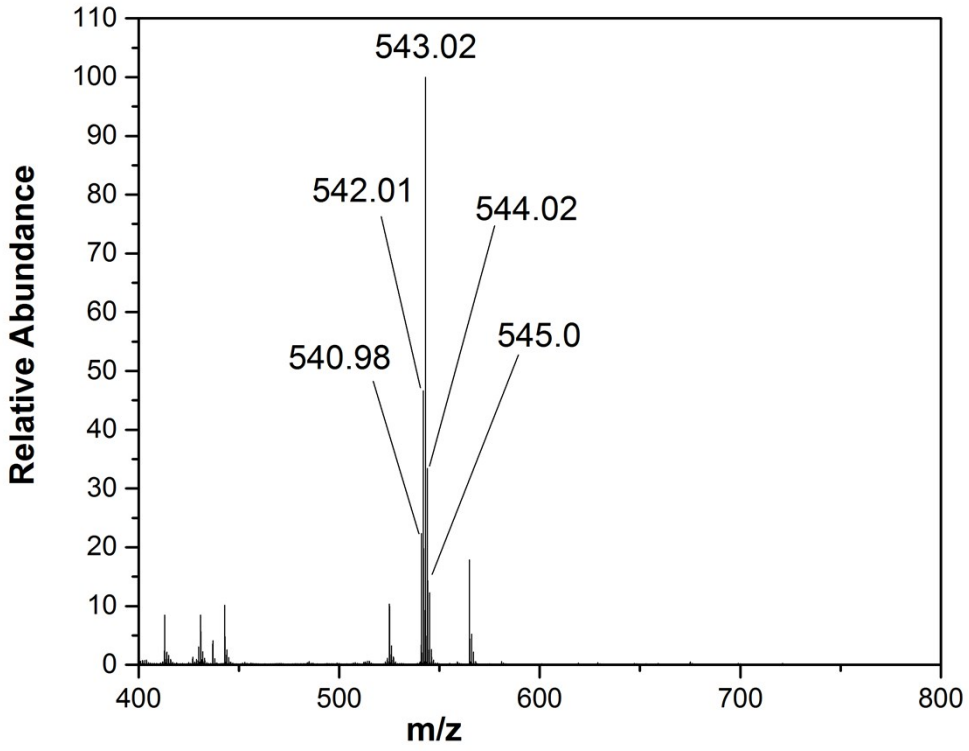


Figure S16. Mass spectrum of **19**.

Table S1 Crystal data and structure refinement for **12a**.

Identification code	**12a**
Empirical formula	$C_{18}H_{14}F_2N_2O_2S_2$
Formula weight	392.43
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	4.5260(9)
b/Å	18.489(4)
c/Å	19.838(4)
α/°	90
β/°	97.22(3)
γ/°	90
Volume/Å^3	1646.9(6)
Z	4
ρ_{calc}g/cm^3	1.583
μ/mm^{-1}	0.286
F(000)	808.0
Crystal size/mm^3	0.155 × 0.045 × 0.010
Radiation	synchrotron (λ = 0.65251)
2Θ range for data collection/°	2.774 to 53.038
Index ranges	$0 \le h \le 6$, $-25 \le k \le 0$, $-27 \le l \le 26$
Reflections collected	4388
Independent reflections	4388 [R_{int} = 0.0000, R_{sigma} = 0.0202]
Data/restraints/parameters	4388/0/237
Goodness-of-fit on F^2	1.022
Final R indexes [I>=2σ (I)]	R_1 = 0.0385, wR_2 = 0.1069
Final R indexes [all data]	R_1 = 0.0401, wR_2 = 0.1091
Largest diff. peak/hole / e Å^{-3}	0.49/-0.41

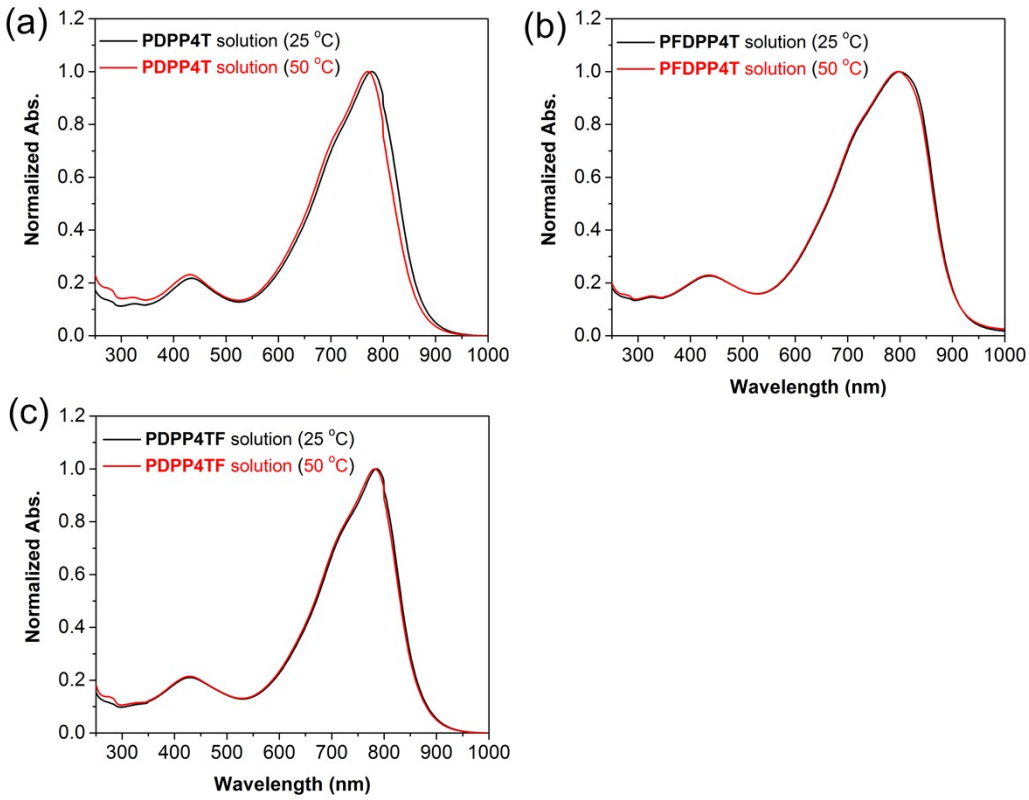


Figure S17. Normalized UV-Vis absorption spectra of the polymers in chloroform solutions at 25 °C and 50 °C, respectively.

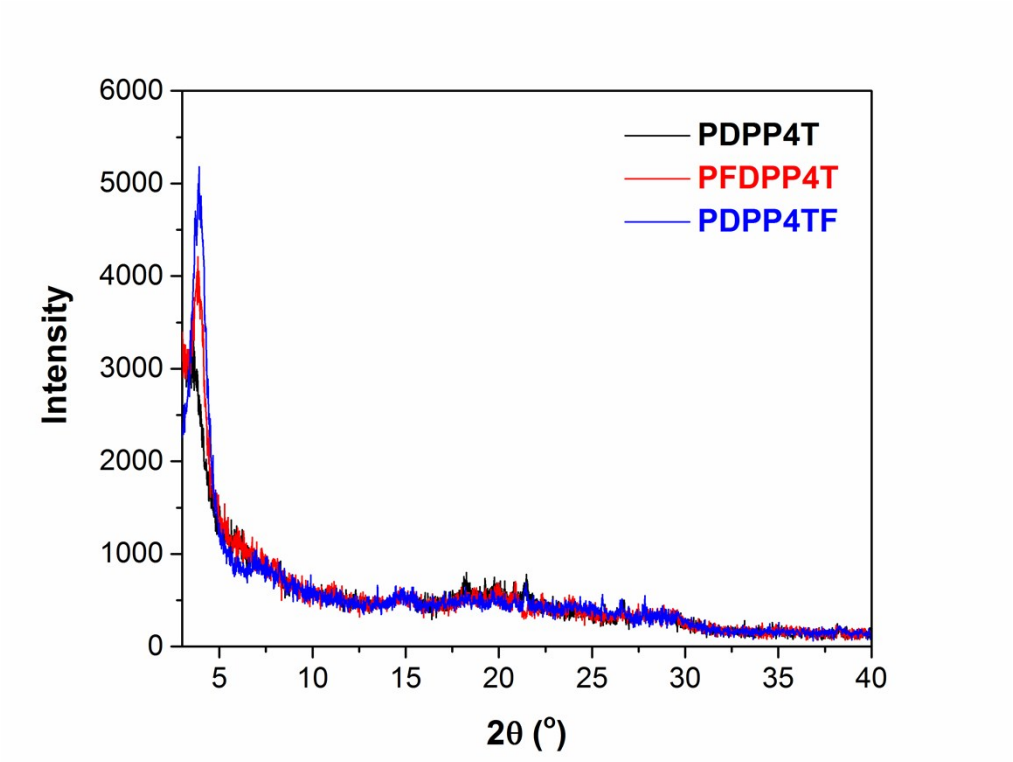


Figure S18. XRD patterns of polymer thin films.