Electronic Supplementary Information

Fluorine-induced high-performance narrow bandgap polymer based on thiadiazolo[3,4-*c*]pyridine for photovoltaic application

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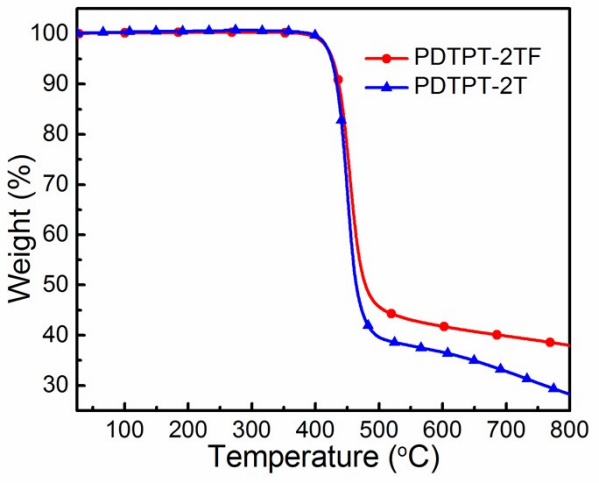

Fig. S1 TGA plots of PDTPT-2T and PDTPT-2TF.

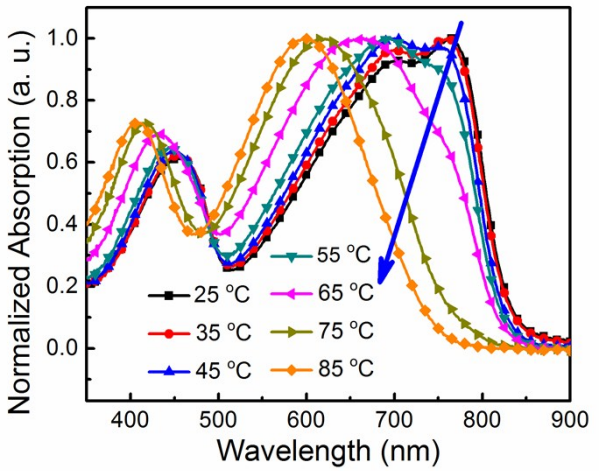

Fig. S2 Temperature-dependent absorption spectra of PDTPT-2TF in DCB solution.

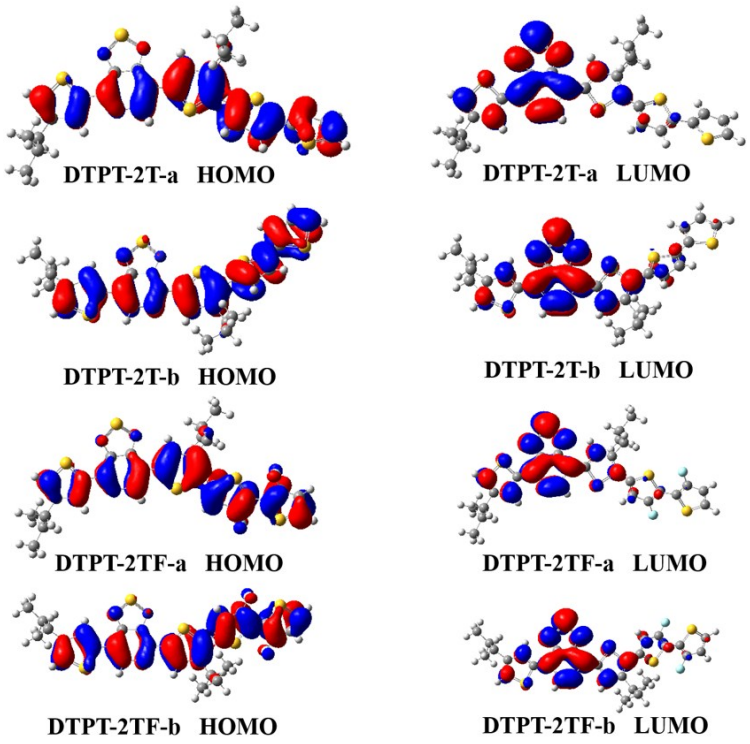

Fig. S3 The distributions of HOMO and LUMO of the molecular models.[1]

Hole Mobility Measurements.

Hole mobility was obtained using the SCLC method:[2]

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

where ε_0 is the vacuum permittivity, ε_r is the relative dielectric constant, μ is the hole mobility, V is the electric field, L is the thickness of the organic layer, and J is the current density.

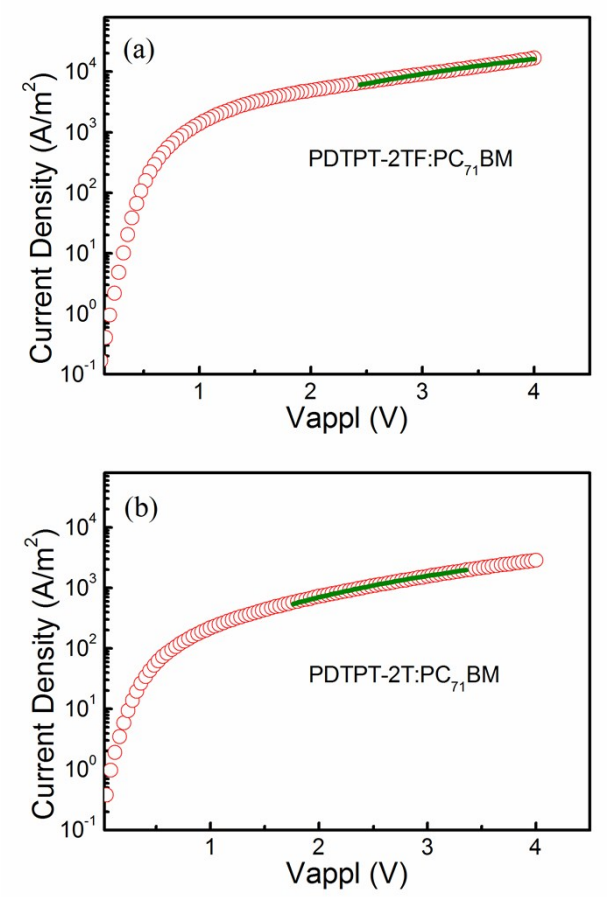

Fig. S4 The dark *J*-*V* plots of the hole-only devices based on (a) PDTPT-2TF:$PC_{71}BM$ (1:2) and (b) PDTPT-2T:$PC_{71}BM$ (1:2). The experimental data (red circles) are fitted (olive lines) using SCLC modified Mott-Gurney model.

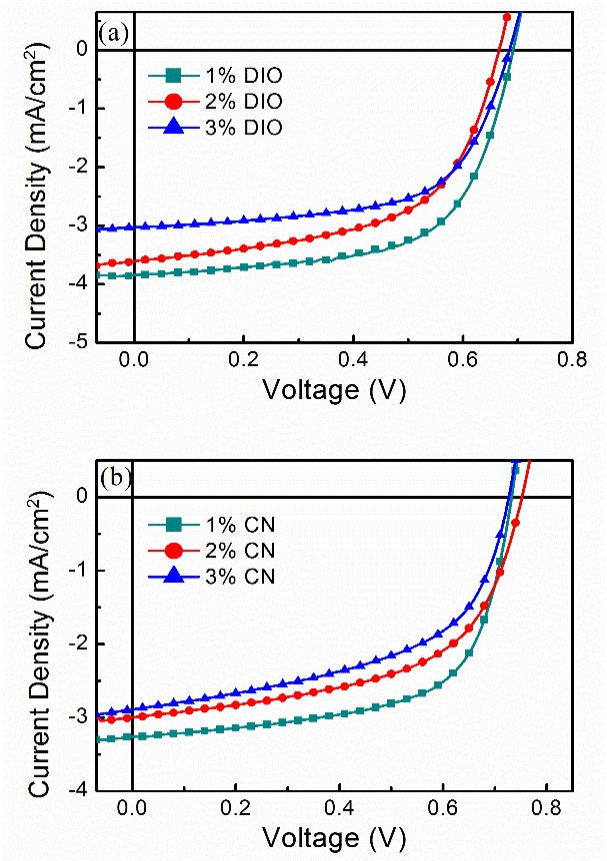

Fig. S5 *J-V* characteristics of the PDTPT-2T-based devices processed with (a) 1,8-diiodooctane (DIO) and (b) 1-chloronaphthalene (CN) additives.

Table S1 Photovoltaic parameters of the PDTPT-2T-based PSCs processed with DIO and CN additives under AM 1.5G illumination (100 mW/cm^2)

Processing additive	V_{oc} (V)	J_{sc} (mA/cm^2)	*FF* (%)	PCE_{max} (PCE_{ave})[a] (%)
1% DIO	0.69	3.84	62.71	1.66 (1.59)
2% DIO	0.67	3.62	56.83	1.38 (1.32)
3% DIO	0.68	3.04	61.63	1.27 (1.21)
1% CN	0.73	3.27	63.25	1.51 (1.49)
2% CN	0.75	3.00	55.98	1.26 (1.20)
3% CN	0.73	2.89	52.98	1.12 (0.85)

[a]The average PCE value was obtained from 5 devices.

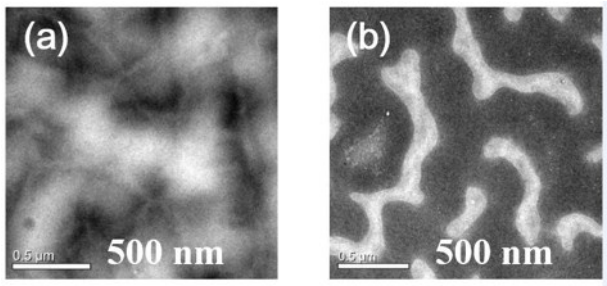

Fig. S6 TEM images of PDTPT-2T:$PC_{71}BM$ processed with 1% (a) DIO and (b) CN additives.

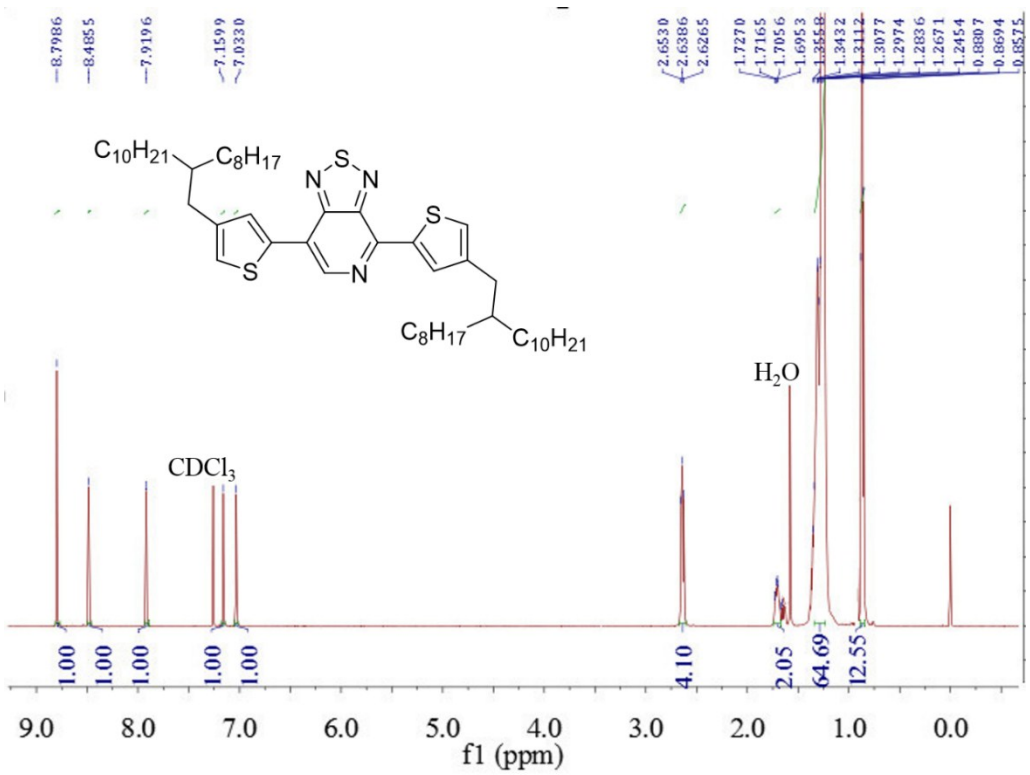

Fig. S7 ^1H NMR spectrum of compound **3**.

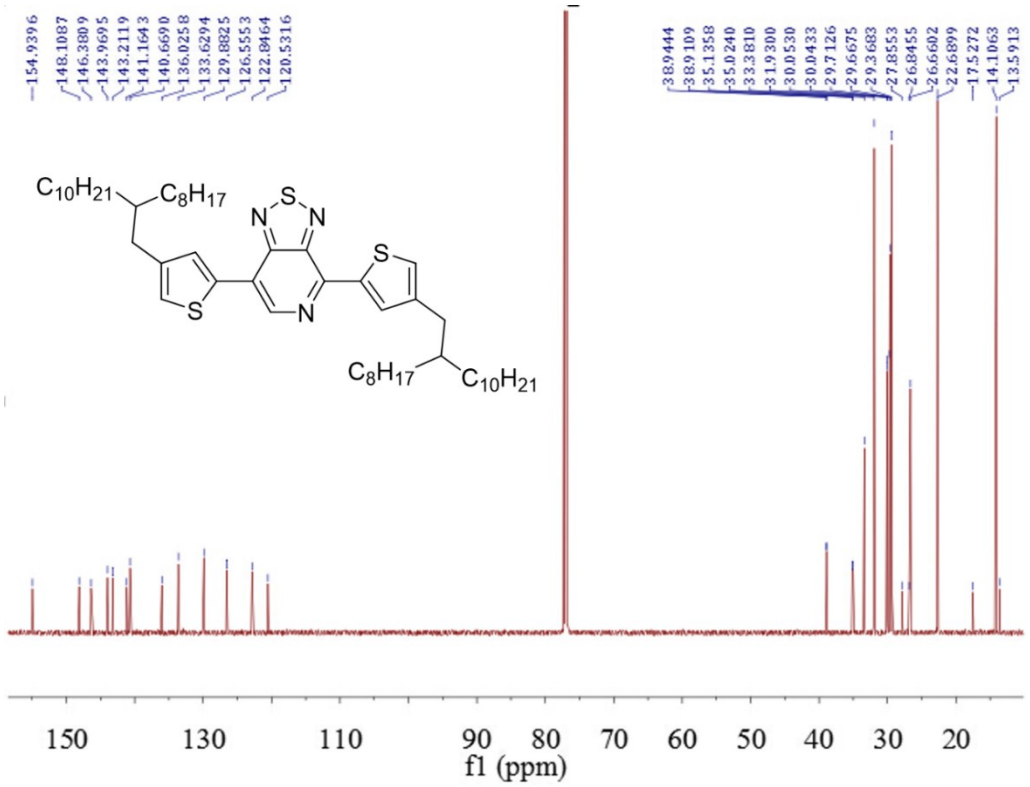

Fig. S8 ^{13}C NMR spectrum of compound **3**.

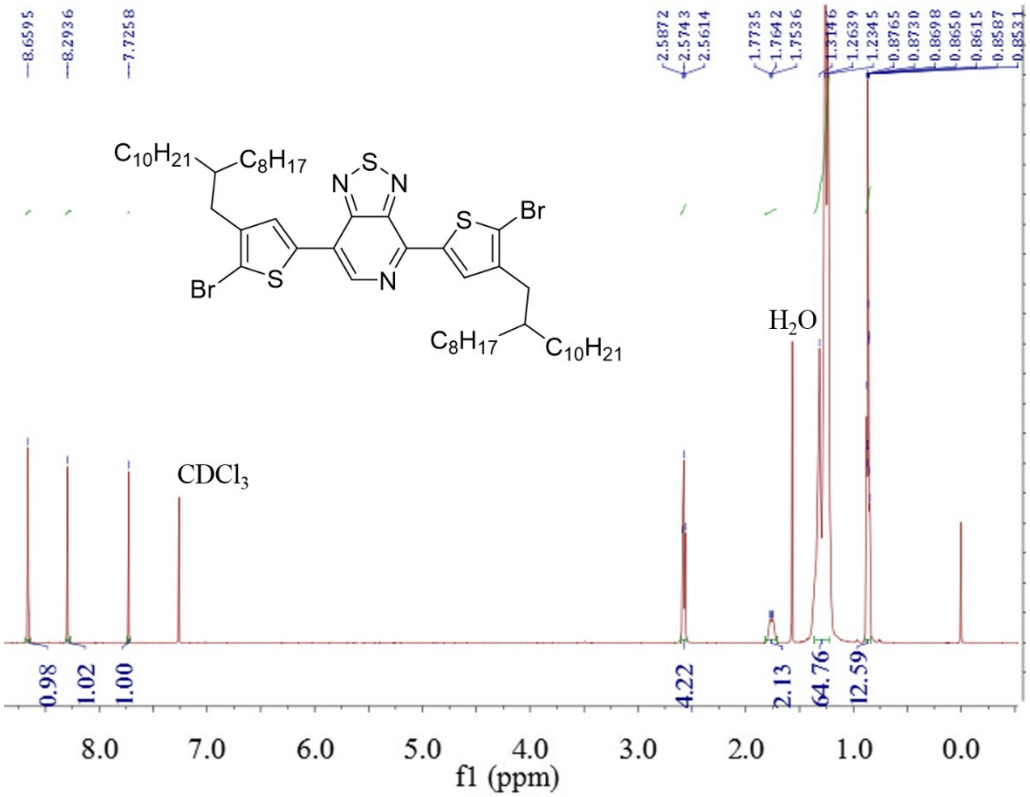

Fig. S9 ^{1}H NMR spectrum of compound **4**.

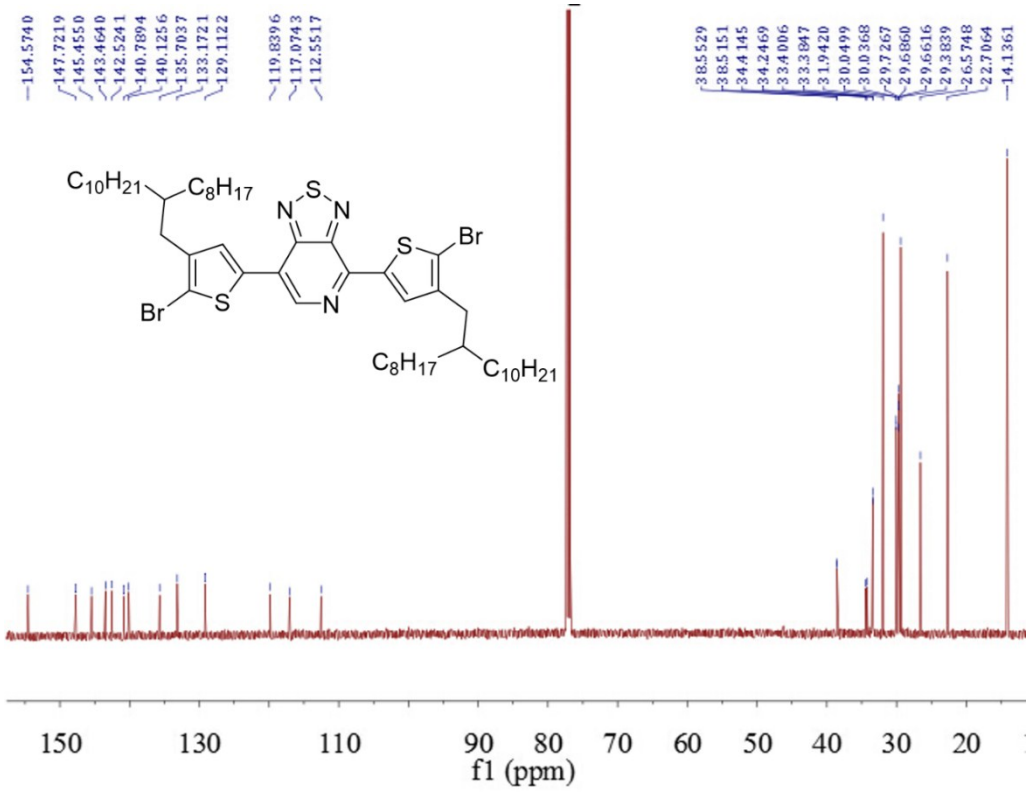

Fig. S10 ^{13}C NMR spectrum of compound **4**.

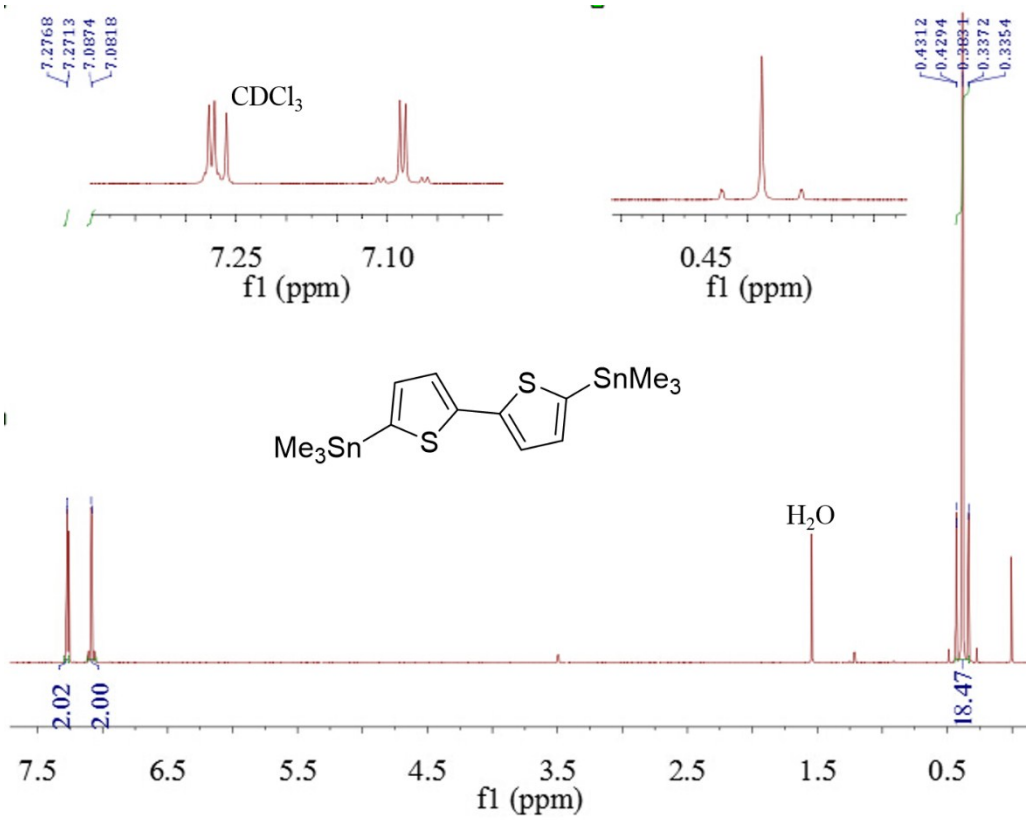

Fig. S11 ^{1}H NMR spectrum of 2T-Sn.

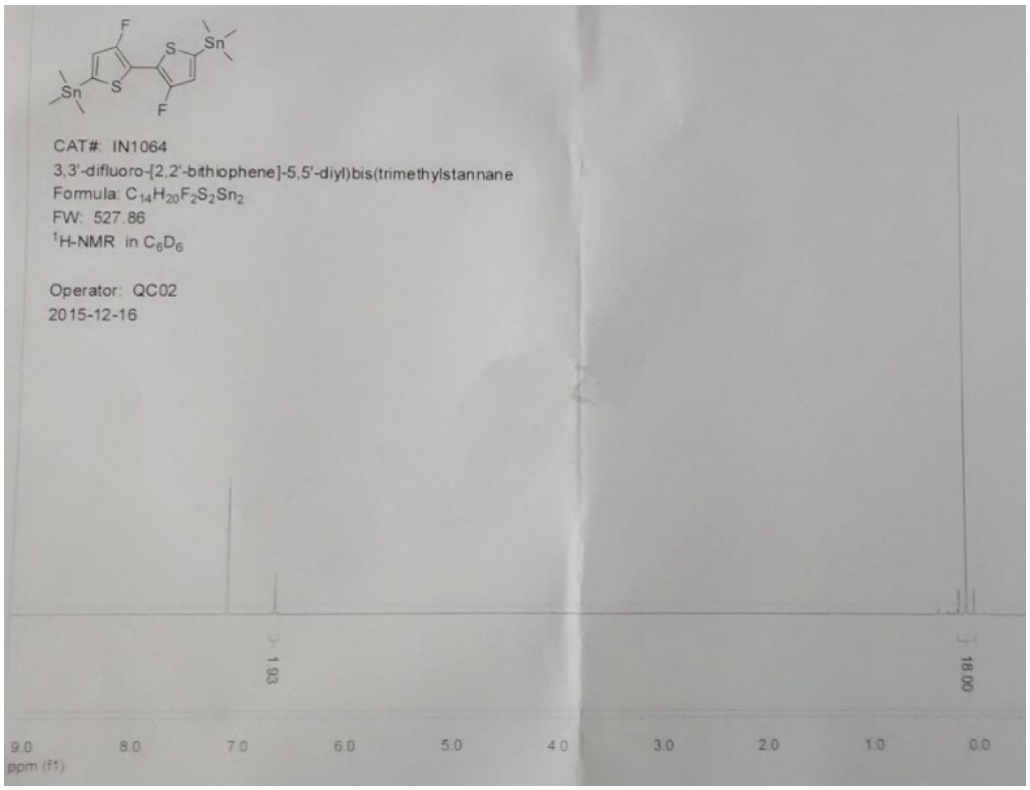

Fig. S12 ^{1}H NMR spectrum of 2TF-Sn.

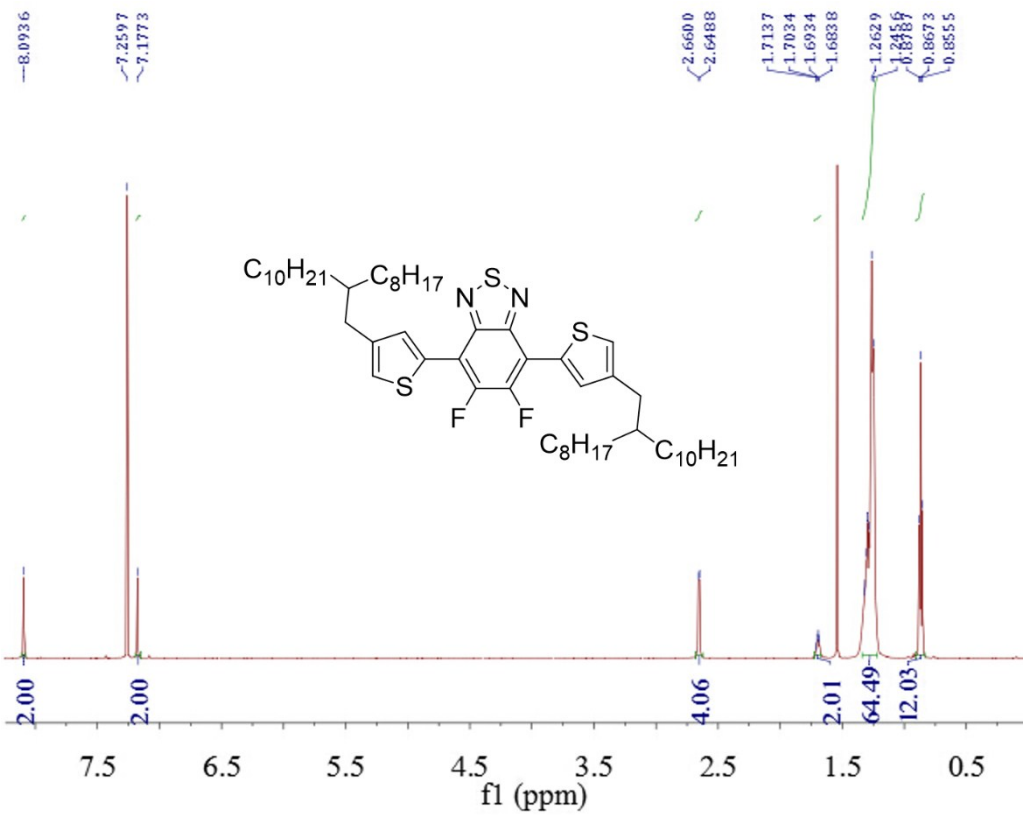

Fig. S13 ^{1}H NMR spectrum of compound **5**.

References

(1) Gaussian 09, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.

(2) Murgatroyd P N. Theory of Space-Charge-Limited Current Enhanced by Frenkel Effect. *J Phys. D Appl. Phys.* 1970, **3**, 151-156.