Electronic Supplementary Information

Design, synthesis and optical properties of small molecules based on dithieno[3,2-*b*:2',3'-*d*]stannole and stannafluorene

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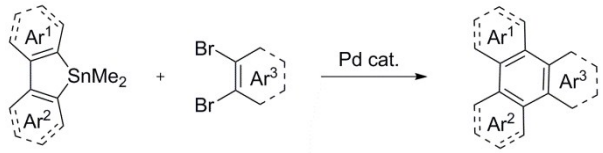

Scheme S1. The reaction of dialkylstannole derivatives with 1,2-dihaloarenes [1].

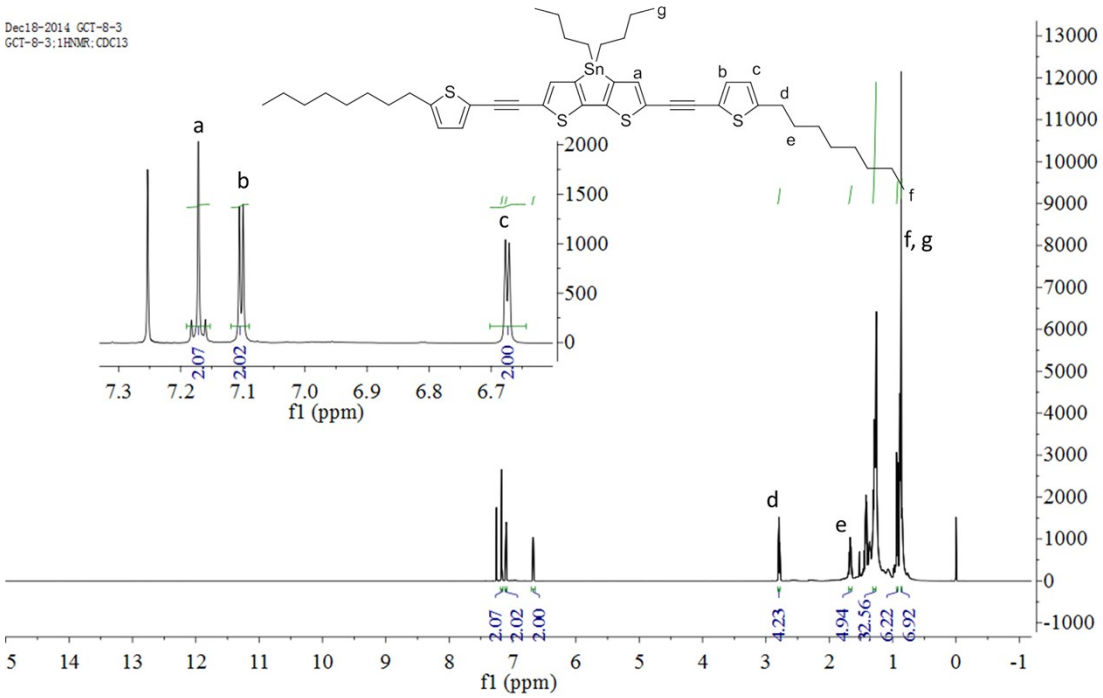

Figure S1. ^{1}H NMR spectrum of **DTSn-1** in $CDCl_3$.

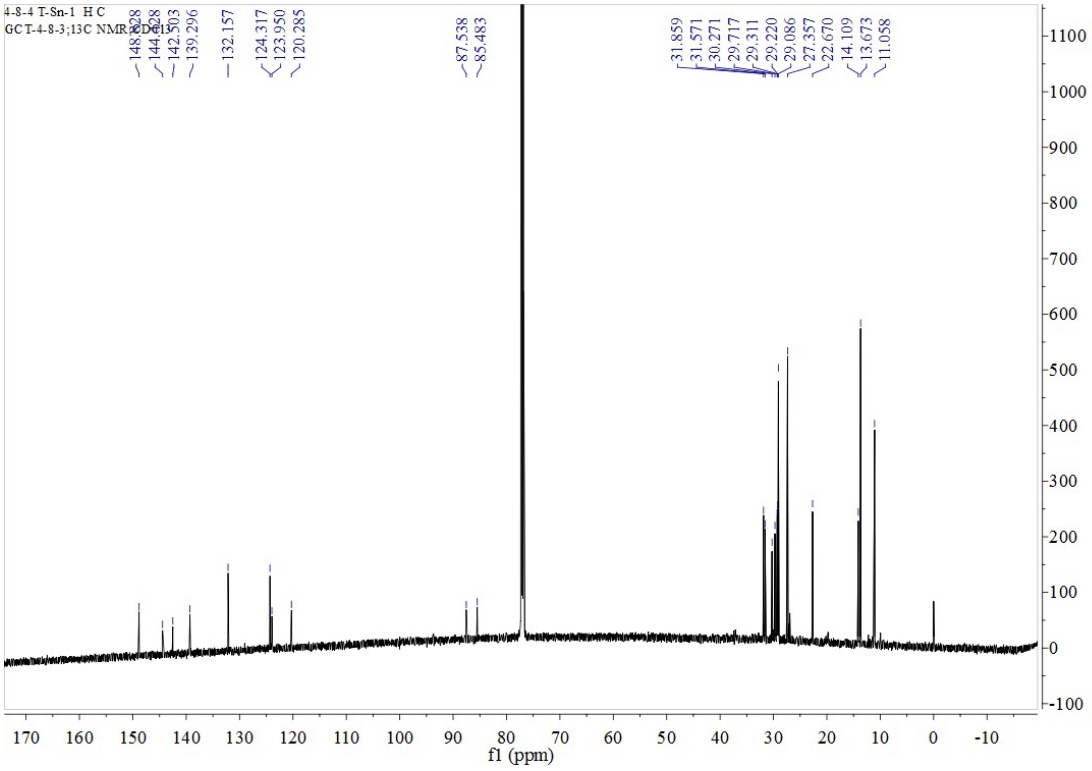

Figure S2. ^{13}C NMR spectrum of **DTSn-1** in $CDCl_3$.

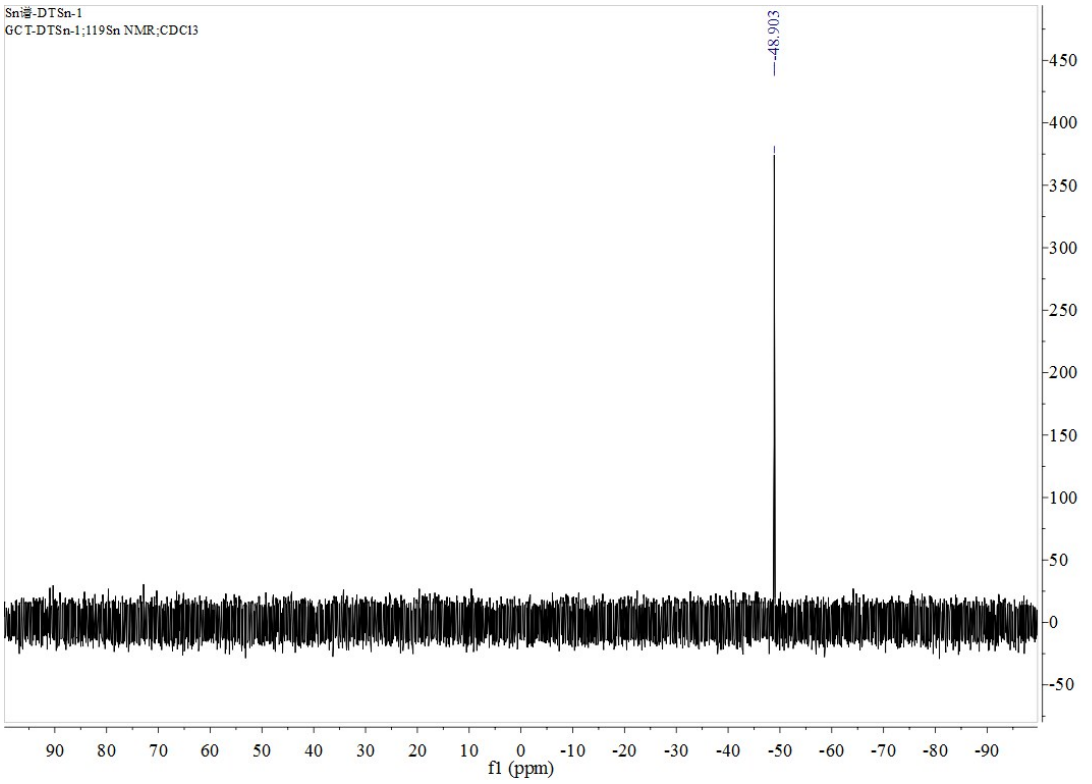

Figure S3. ^{119}Sn NMR spectrum of **DTSn-1** in $CDCl_3$.

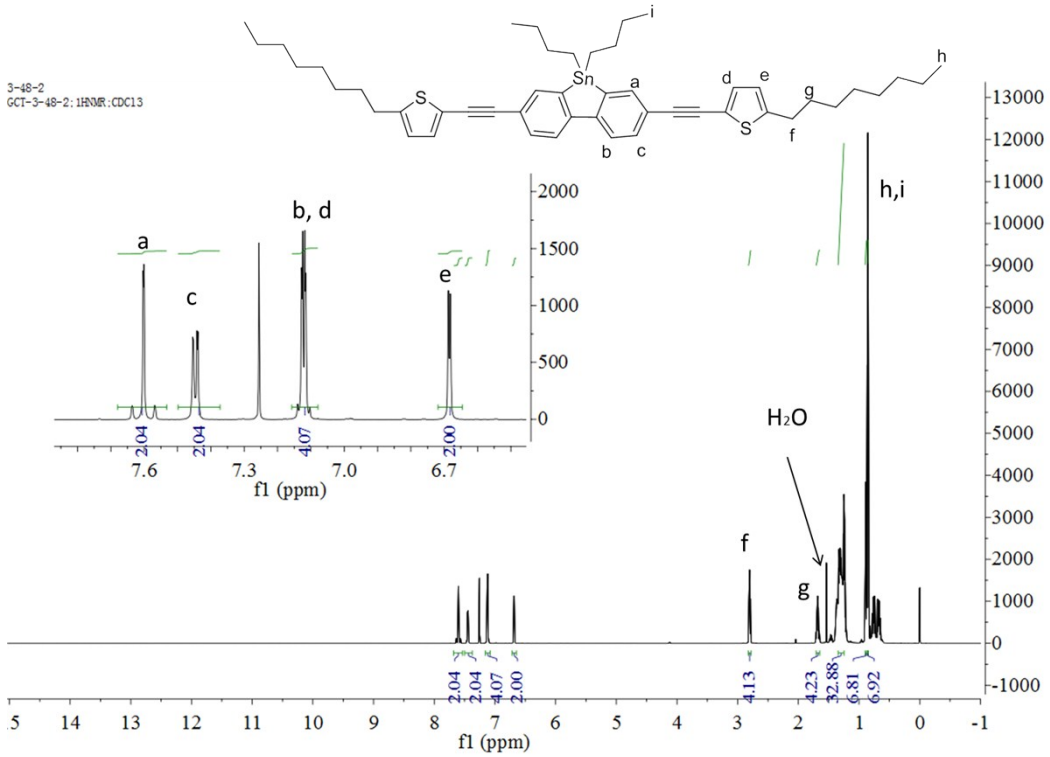

Figure S4. ^{1}H NMR spectrum of **SnF-1** in $CDCl_3$.

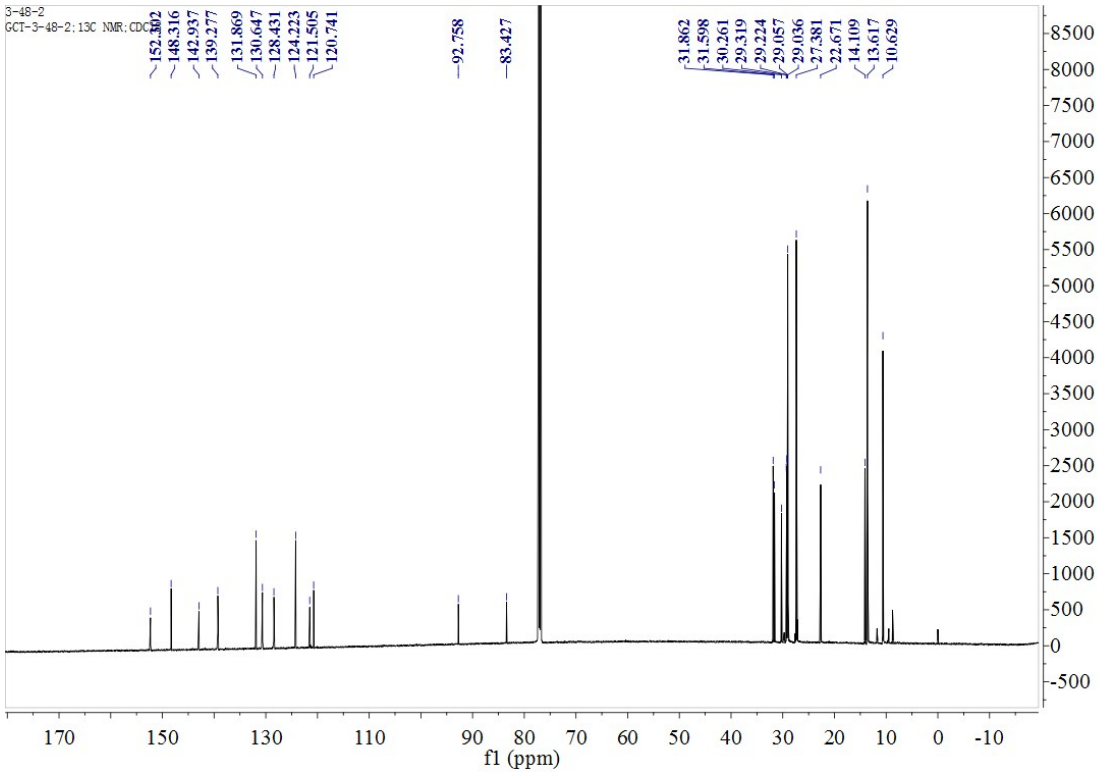

Figure S5. ^{13}C NMR spectrum of **SnF-1** in $CDCl_3$.

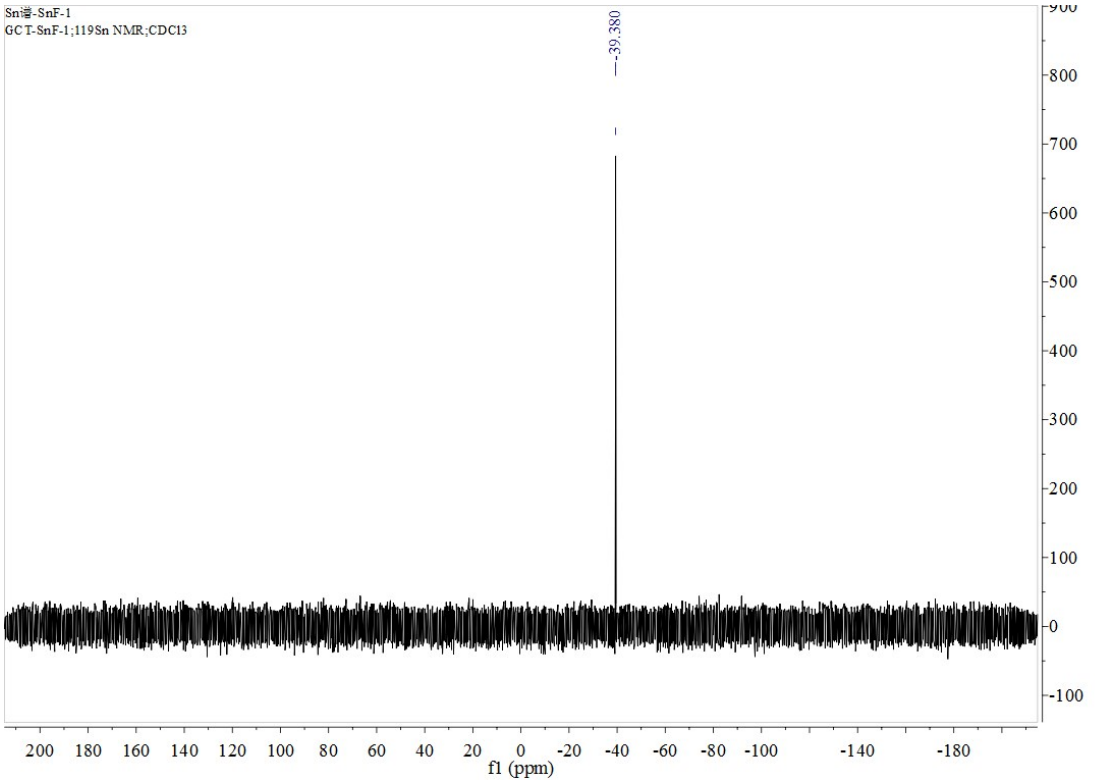

Figure S6. ^{119}Sn NMR spectrum of **SnF-1** in $CDCl_3$.

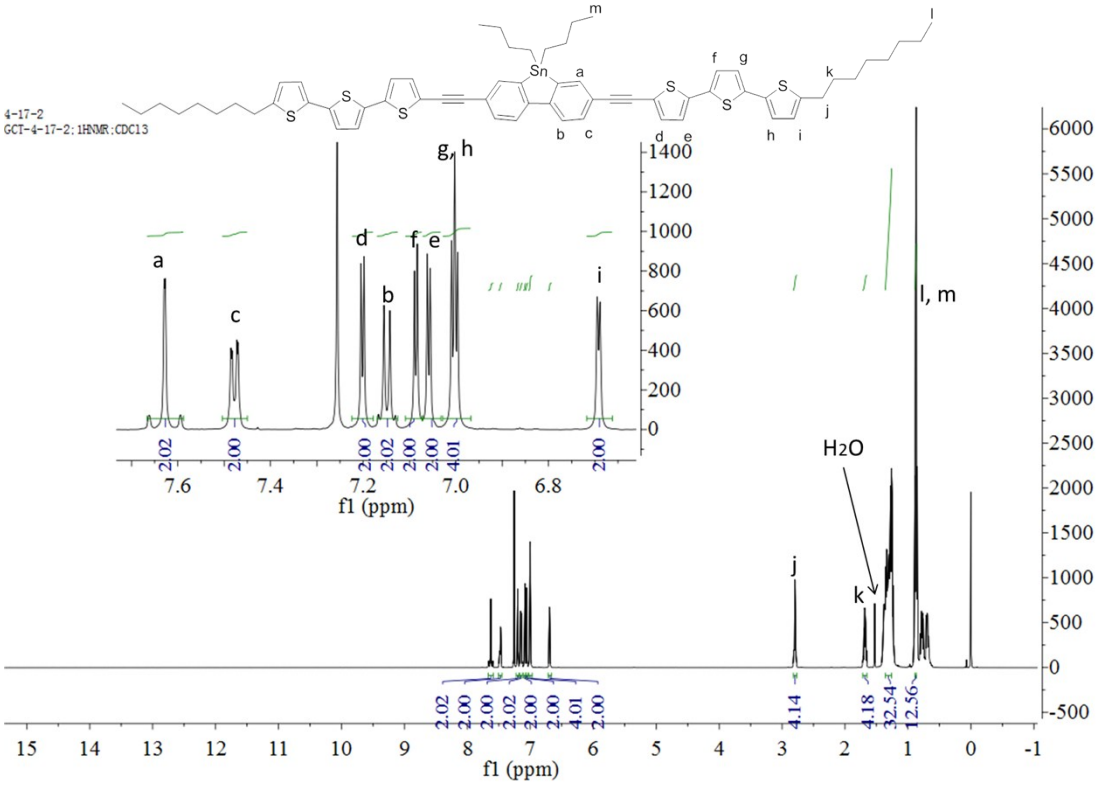

Figure S7. ^{1}H NMR spectrum of **SnF-3** in $CDCl_3$.

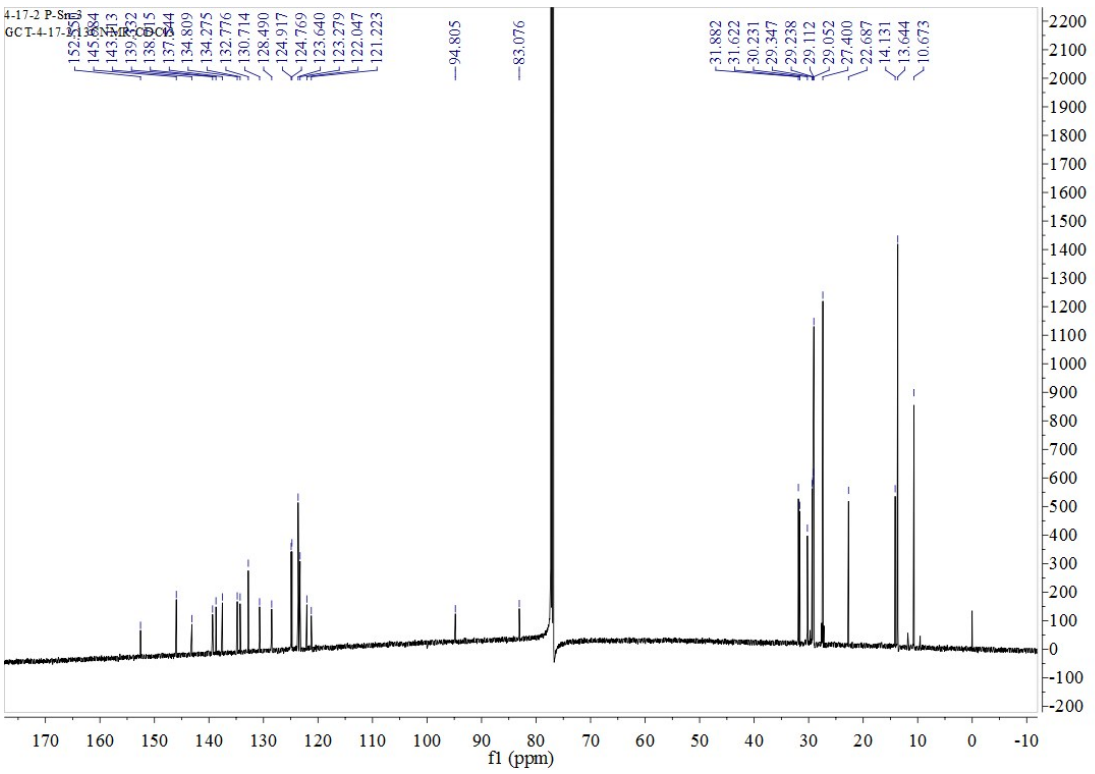

Figure S8. ^{13}C NMR spectrum of **SnF-3** in $CDCl_3$.

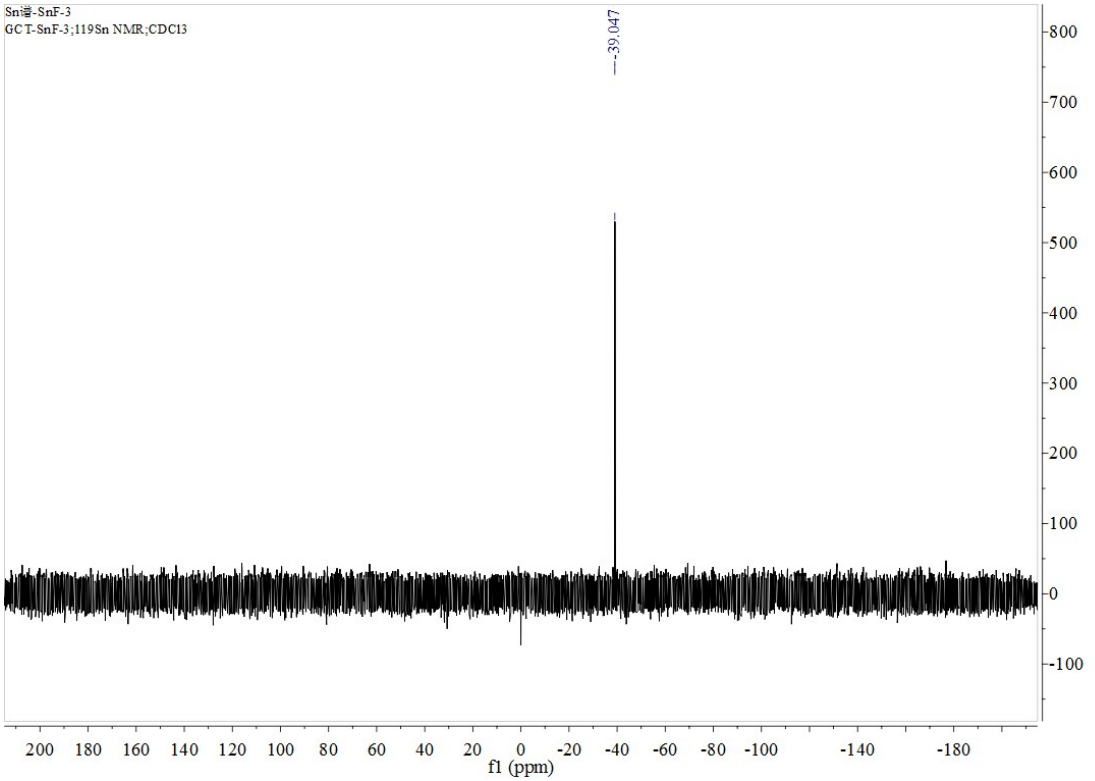

Figure S9. ^{119}Sn NMR spectrum of **SnF-3** in $CDCl_3$.

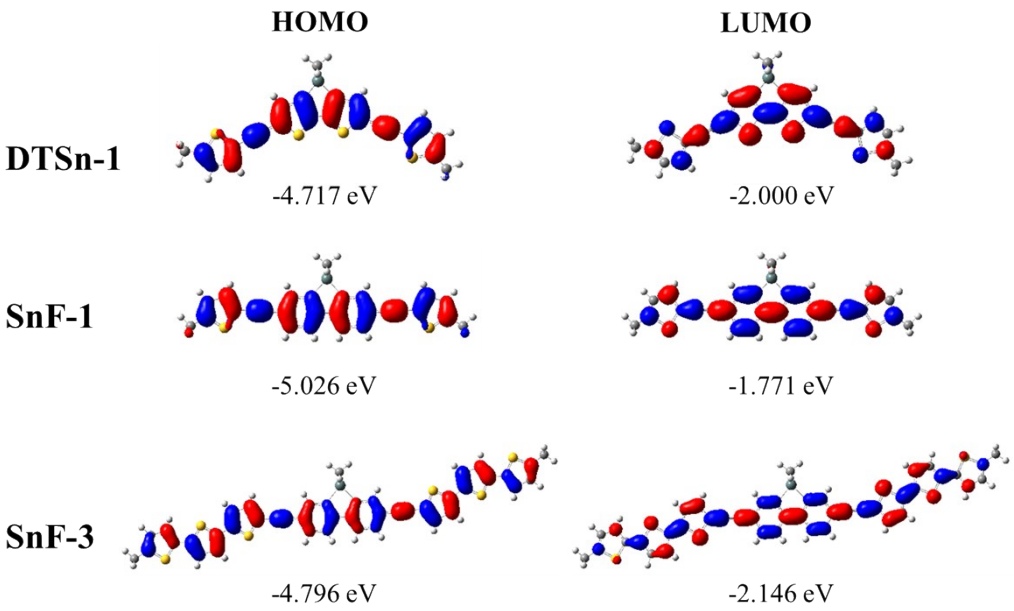

Figure S10. The energies and distributions of the frontier molecular orbitals of the Sn-containing small molecules [2]. The optimized molecular geometries were confirmed to be minimum-energy conformations since there were no imaginary frequencies by vibrational frequencies calculation at the same level.

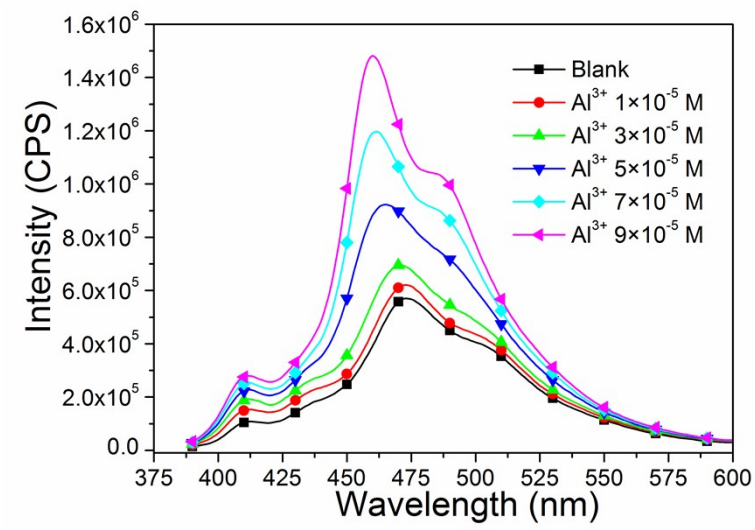

Figure S11. The fluorescence specra of **DTSn-1** with different concentrations of Al^{3+} (excitation at 360 nm).

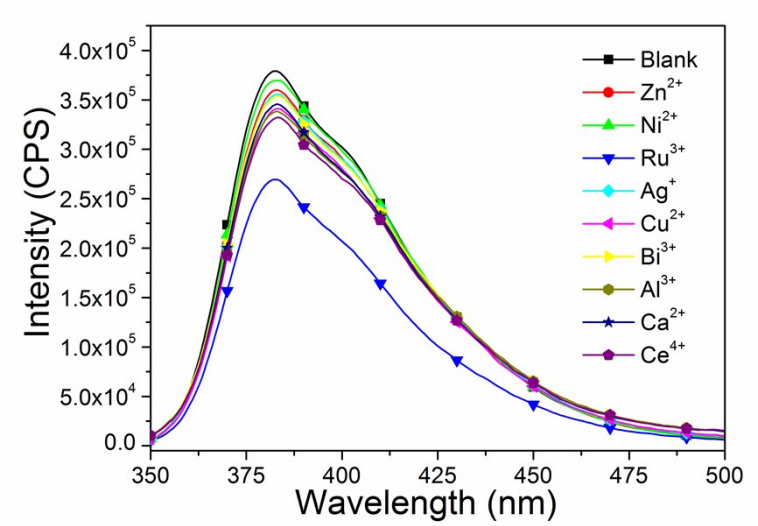

Figure S12. The fluorescence specra of **SnF-1** in absence and presence of 5×10^{-5} mol/L metal ions (excitation at 320 nm).

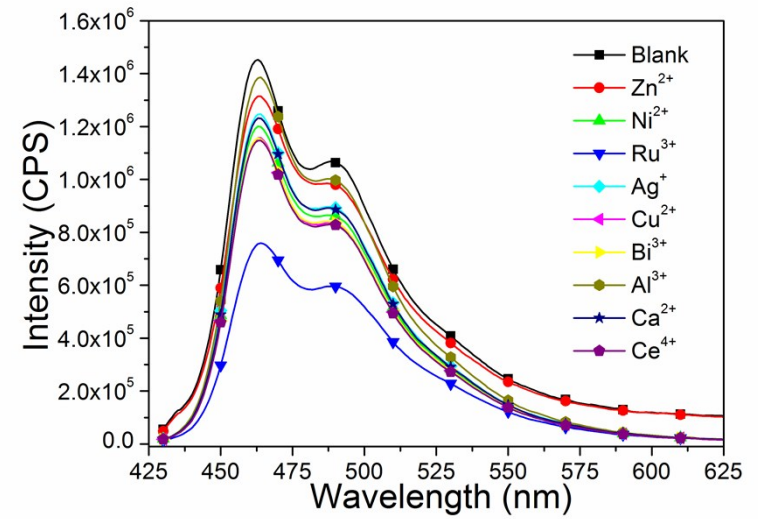

Figure S13. The fluorescence specra of **SnF-3** in absence and presence of 5×10^{-5} mol/L metal ions (excitation at 400 nm).

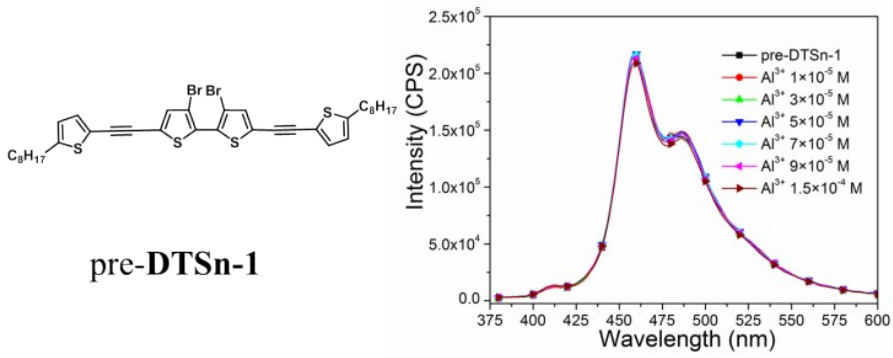

Figure S14. The strusture of pre-**DTSn-1** and the fluorescence specra of pre-**DTSn-1** with different concentrations of Al^{3+} (excitation at 350 nm).

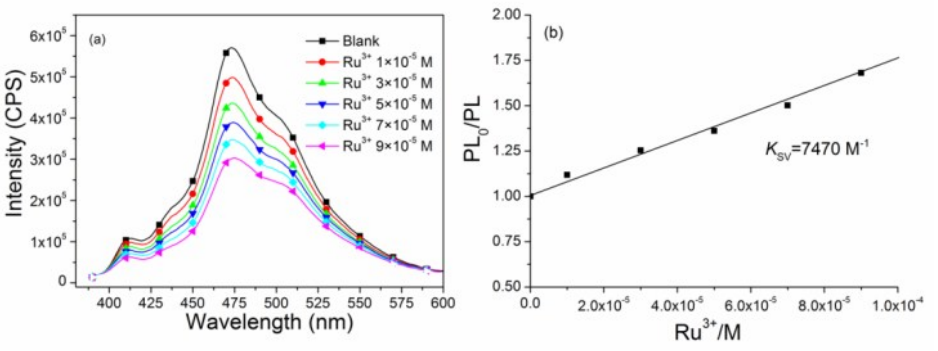

Figure S15. (a) The fluorescence spectra of **DTSn-1** with different concentrations of Ru^{3+} (excitation at 360 nm) and (b) Stern-Volmer plot of the quenching efficiency.

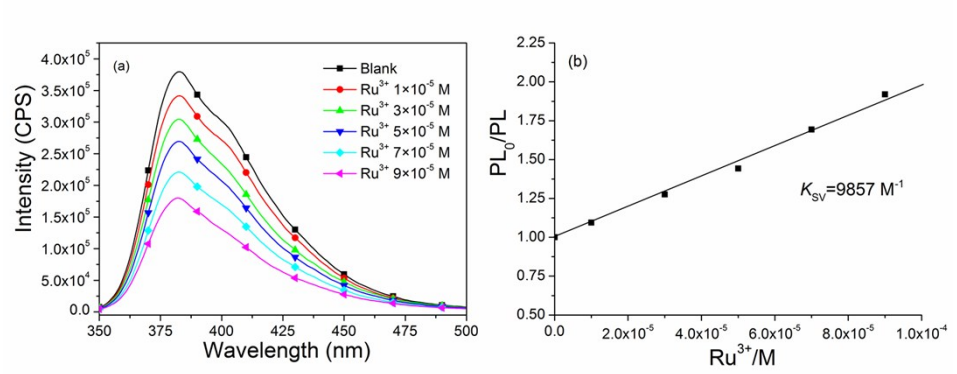

Figure S16. (a) The fluorescence specra of **SnF-1** with different concentrations of Ru^{3+} (excitation at 320 nm) and (b) Stern-Volmer plot of the quenching efficiency.

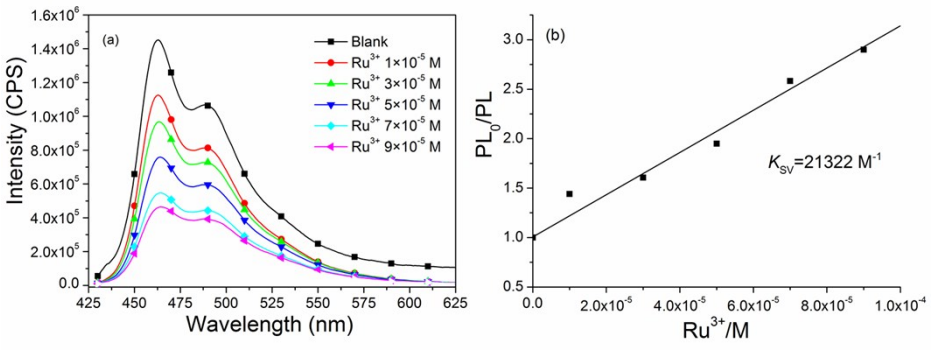

Figure S17. (a) The fluorescence specra of **SnF-3** with different concentrations of Ru^{3+} (excitation at 400 nm) and (b) Stern-Volmer plot of the quenching efficiency.

The quenching process can be quantitatively described by the Stern-Volmer equation[3]:

$$\frac{PL_0}{PL} = 1 + K_{SV}[Q] \qquad (1)$$

where the PL_0 refers to the overall integrated emission intensity of fluorescence in the

absence of the quencher, PL corresponds to the integrated emission intensity of fluorescence in the presence of the quencher, K_{SV} is the Stern-Volmer constant. Here, the quencher was Ru^{3+}.

References:

1. I. Nagao, M. Shimizu, T. Hiyama, *Angew. Chem. Int. Ed.,* 2009, **48**, 7573-7576.
2. 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.
3. (a) J. Wang, D. Wang, E. K. Miller, D. Moses, G. C. Bazan and A. J. Heeger, *Macromolecules*, 2000, **33**, 5153; (b) S. Wang, B. S. Gaylord and G. C. Bazan, *Adv. Mater.*, 2004, **16**, 2127.