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$_3$. 

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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 spectra of DTSn-1 with different concentrations of Al$^{3+}$ (excitation at 360 nm).
Figure S12. The fluorescence spectra of SnF-1 in absence and presence of $5 \times 10^{-5}$ mol/L metal ions (excitation at 320 nm).

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

Figure S14. The structure of pre-DTSn-1 and the fluorescence spectra 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 spectra 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 spectra 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$^3$:

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

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: