# Electronic Supplementary Information

## New metal-coordination-inhibited charge transfer emission for terfluorenes: highly sensitive and selective detection for $Hg^{2+}$ with ratiometric "turn-on" fluorescence response

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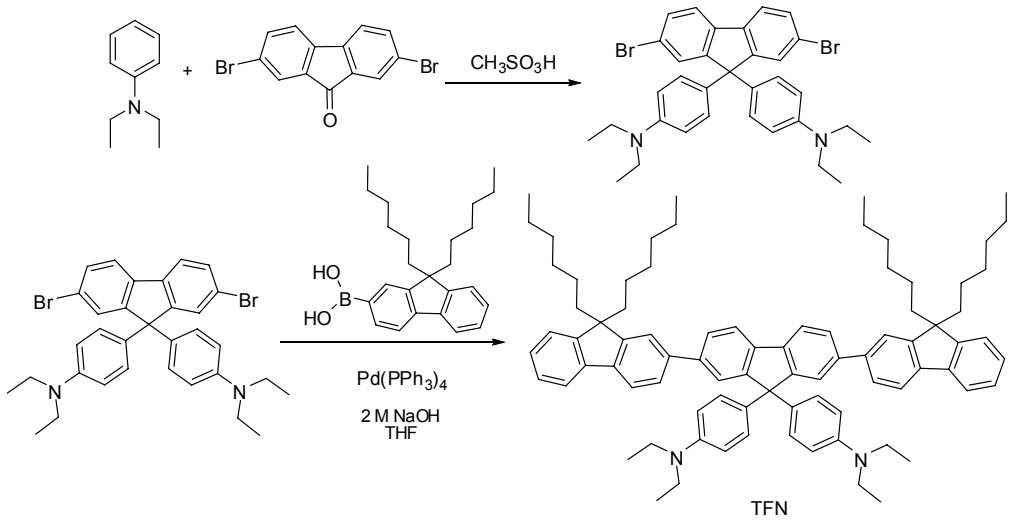
# *1. General Information*

The $^{1}H$ NMR and $^{13}C$ NMR spectra were recorded on a MECUYRVX300 spectrometer in $CDCl_3$, using tetramethylsilane as an internal reference. Elemental analyses of carbon, hydrogen, and nitrogen were performed on a Carlorerba-1106 microanalyzer. MALDI TOF was measured on a Voyager-DE STR MALDI TOF instrument, using α-cyano-4-hydroxyclinnamic acid (CHCA) as a matrix. EI Mass was recorded on a Finnigan TRACE Mass Spectrometer. UV-Vis absorption spectra were recorded on Shimadzu 160A recording spectrophotometer. PL spectra were recorded on Hitachi F-4500 fluorescence spectrophotometer. The PL quantum yields were measured from dilute THF solution of the terfluorenes (ca. $10^{-6}$ mol/L) by an absolute method using the Edinburgh Instruments (FLS 920) integrating sphere excited with Xe lamp. The concentration of TFOH and TFN in fluorescence titration tests are $5\times10^{-6}$ M with THF as solvent, and metal ions are all at a concentration of $5\times10^{-3}$ M in MeOH.

9,9'-bis(4-aminophenyl)-2,7-dibromofluorene and 9,9-dihexyl-9H-fluoren-2-ylboronic acid were prepared according to the literature procedures. Other materials were used as received without further purification unless otherwise stated.

Fluorescence titration experiments were carried out, with the terfluorenes in THF solution (5 μM) and the metal ions in MeOH solution (5 mM). During titration, metal ions were added using the micro injector into a solution of terfluorene (2 mL), and the whole volume of the terfluorene and metal ions could be considered as 2 mL because the volume of metal ions could be ignored compared to that of terfluorenes. After stirring, the fluorescence spectra were collected. In the non-linear fitting experiment, the samples were prepared as in the titration experiment, with the terfluorenes in a concentration of 5 μM in THF.

## *2. Synthesis and Characterization of TFN*




Scheme S1. Synthesis of terfluorene TFN.

### *Synthesis of TFN*

A mixture of 9,9'-bis(4-aminophenyl)-2,7-dibromofluorene (160 mg, 0.26 mmol), 9,9'-dihexyl-9*H*-fluoren-2-ylboronic acid (215 mg, 0.57 mmol), $Pd(PPh_3)_4$ (23 mg) in THF (9 ml) and 2 M KOH aqueous solution (3 ml) were stirred at 75 ℃ for 48 h. After reaction, the organic layer was extracted with $CHCl_3$, and washed with saturated brine, then dried over anhydrous $Na_2SO_4$. The crude product was purified by column chromatography on silica gel using EtOAc/PE (1:10, v/v) as eluent to give a white powder. Yield: 58 %. $^1$H NMR (300 MHz, $CDCl_3$): δ ppm: 7.83 (d, *J* = 6 Hz, 2H, fluorene *H*), 7.72-7.63 (m, 8H, fluorene *H*), 7.58-7.53 (m, 4H, fluorene *H*), 7.35-7.28 (m, 6H, fluorene *H*), 7.22 (d, *J* = 6 Hz, 4H, phenyl *H*), 6.57 (d, *J* = 6 Hz, 4H, phenyl *H*), 3.29 (q, *J* = 6 Hz, 8H, NC*H*$_2$), 2.01-1.96 (m, 8H), 1.14-1.06 (m, 32H), 0.77-0.64 (m, 24H). $^{13}$C NMR (75 MHz, $CDCl_3$): δ ppm: 154.00, 151.48, 151.24, 146.67, 141.07, 140.68, 140.36, 139.01, 132.83, 129.50, 127.07, 126.92, 126.44, 126.33, 125.01, 123.07, 121.58, 120.36, 119.95, 119.85, 111.50, 64.40, 58.41, 55.34, 44.39, 40.60, 31.69, 29.93, 23.97, 22.80, 14.20, 12.90. Anal. Calcd. for $C_{83}H_{100}N_2$ (%): C, 88.56; H, 8.95; N, 2.49; Found: C 88.84, H 8.91, N 2.40. MALDI-TOF-MS: *m/z* 1125.71 ($M^+$+1).

## *3. Photophysical Properties*

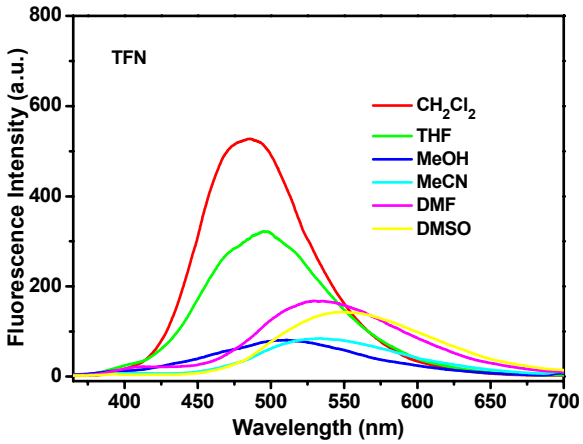



Figure S1. Fluorescence emission spectra of TFN in different solvents.

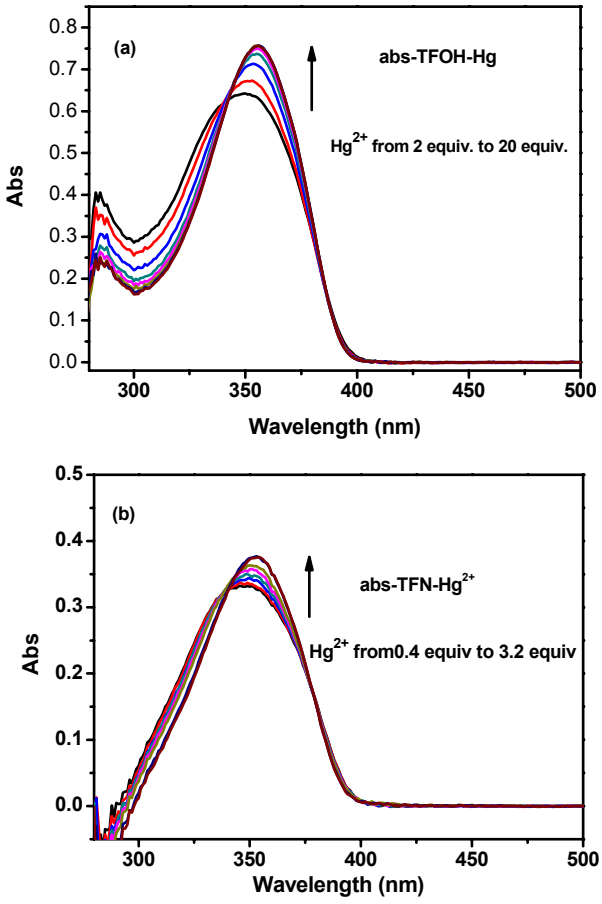



**Figure S2**. UV-vis spectra of **TFOH** (a) and **TFN** (b) upon addition of $Hg^{2+}$.

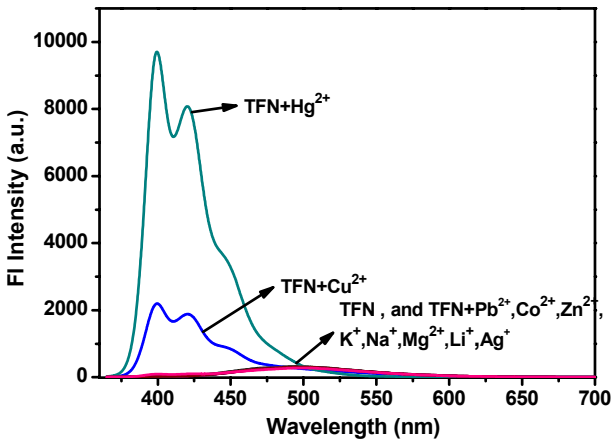



**Figure S3.** Fluorescence spectra of TFN (5 μM in THF) toward different metal ions (5 mM in MeOH, each metal ion was of 50 equiv of TFN). $\lambda_{ex}$= 350 nm.

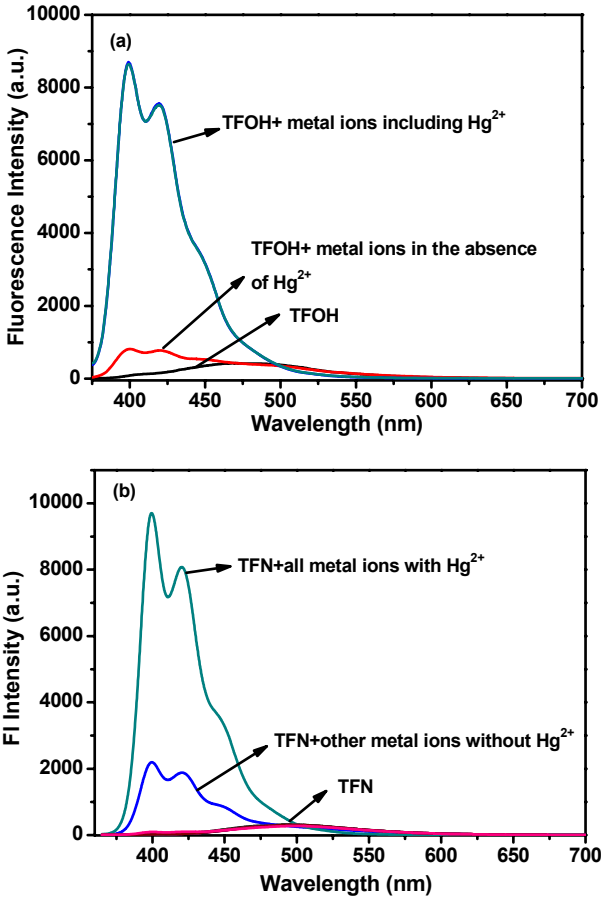



**Figure S4**. The interference of other metal ions toward $Hg^{2+}$ detection for **TFOH** (a) and **TFN** (b).

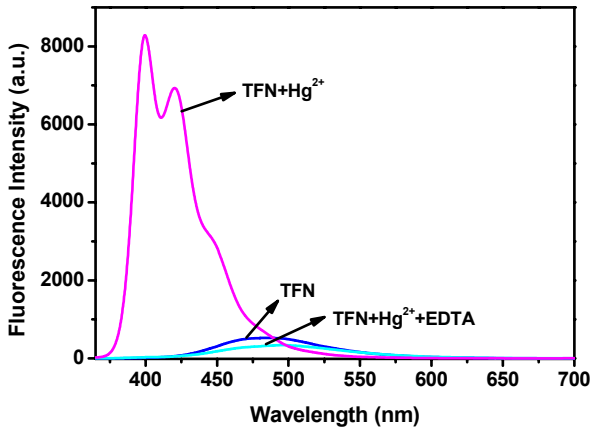



**Figure S5**. Fluorescence reversibility of TFN (5 μM in THF) on detection of $Hg^{2+}$ (5 mM in MeOH).

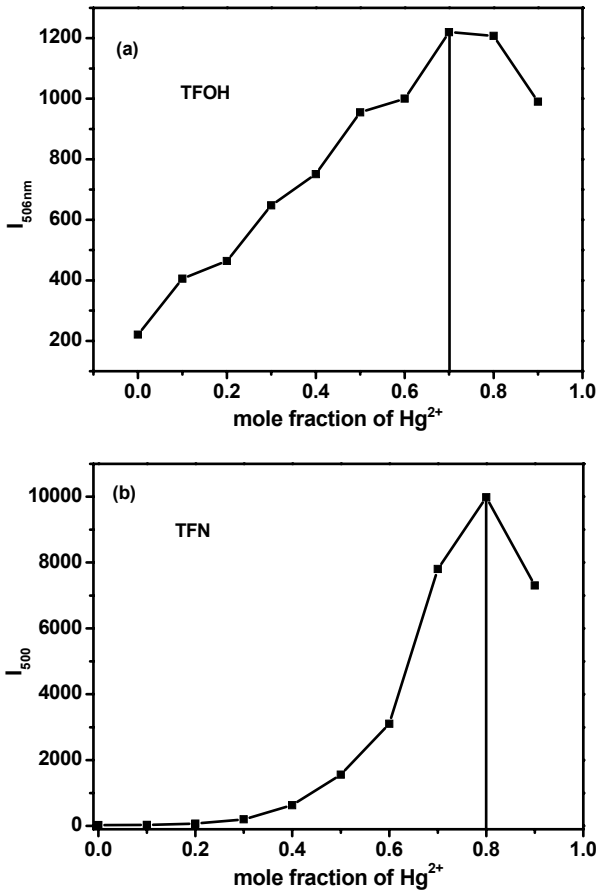



**Figure S6**. Job's plots of **TFOH** (a) and **TFN** (b) in THF solution. The total concentration of sensor and metal ions is 50 μM for the two terfluorenes.

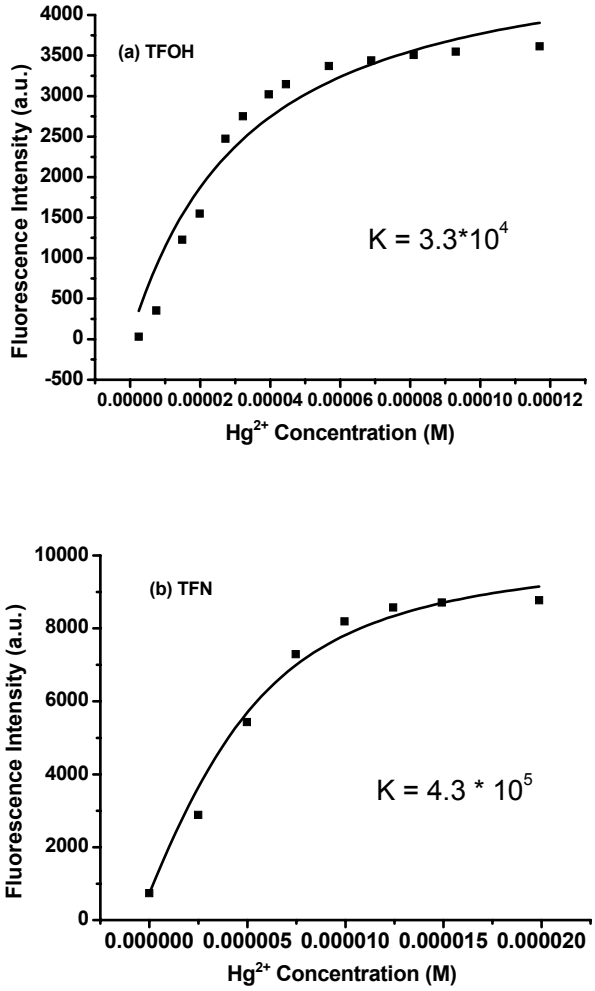



**Figure S7**. Non-Linear Fitting of **TFOH** (a) and **TFN** (b) toward $Hg^{2+}$, respectively.