

Supporting information for

Molecular imaging of biothiols and in vitro diagnostics based on an
organic chromophore bearing terbium hybrid probe

Zhan Zhou,^b Qianming Wang,^{a,b,c*} Cheng Cheng Zhang^d, Jinwei Gao^e

- a. Key Laboratory of Theoretical Chemistry of Environment, Ministry of Education, School of Chemistry & Environment, South China Normal University, Guangzhou 510006, China*
- b. School of Chemistry & Environment, South China Normal University, Guangzhou 510006, China*
- c. Guangzhou Key Laboratory of Materials for Energy Conversion and Storage Guangzhou 510006, P.R. China*
- d. Departments of Physiology and Developmental Biology, University of Texas, Southwestern Medical Center, Dallas, TX 75390-9133, USA*
- e. Institute for Advanced Materials, Academy of Advanced Optoelectronics, South China Normal University, Guangzhou 510006, P.R. China*

* To whom the correspondence should be addressed. E-mail: qmwang@scnu.edu.cn

Tel: 86-20-39310258; Fax: 86-20-39310187

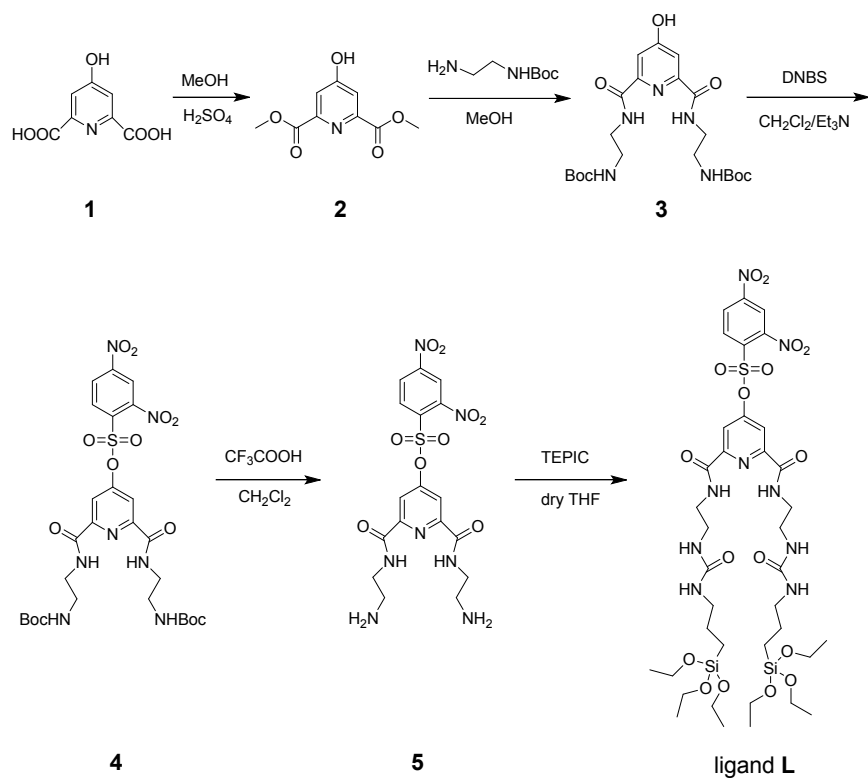


Figure S1 Reaction pathway for the synthesis of ligand L.

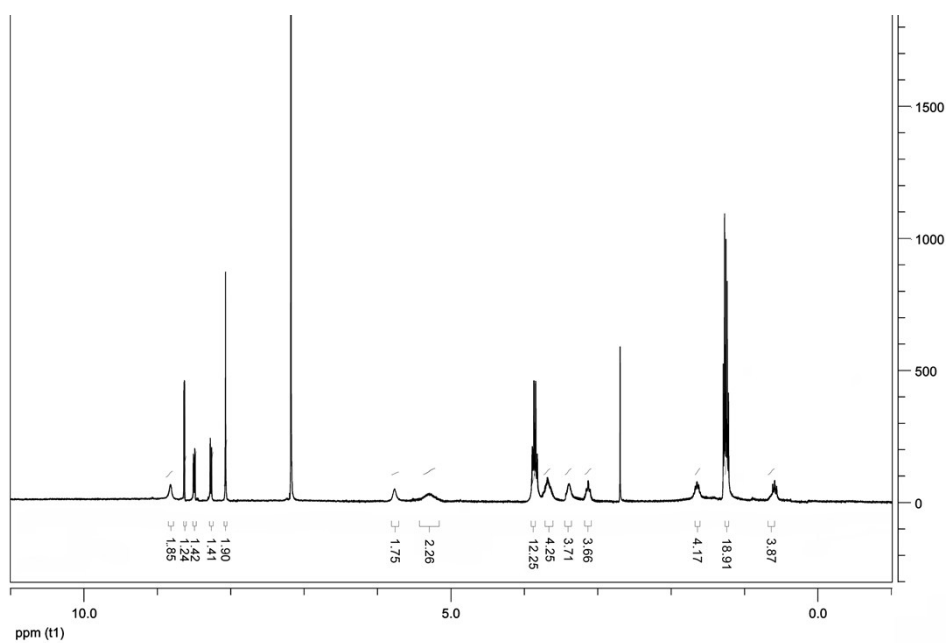


Figure S2 ^1H NMR spectra of ligand L.

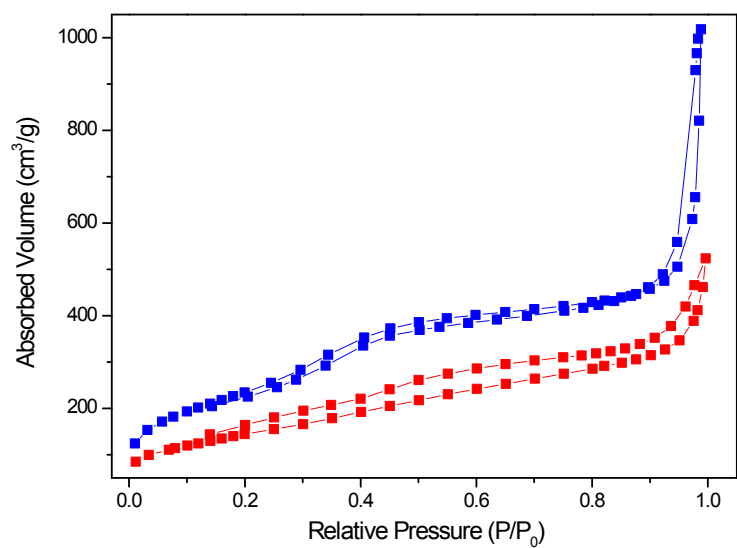


Figure S3 Nitrogen adsorption-desorption curves of MSN in the absence of terbium complex structure (blue) and H-MSN-Tb (red).

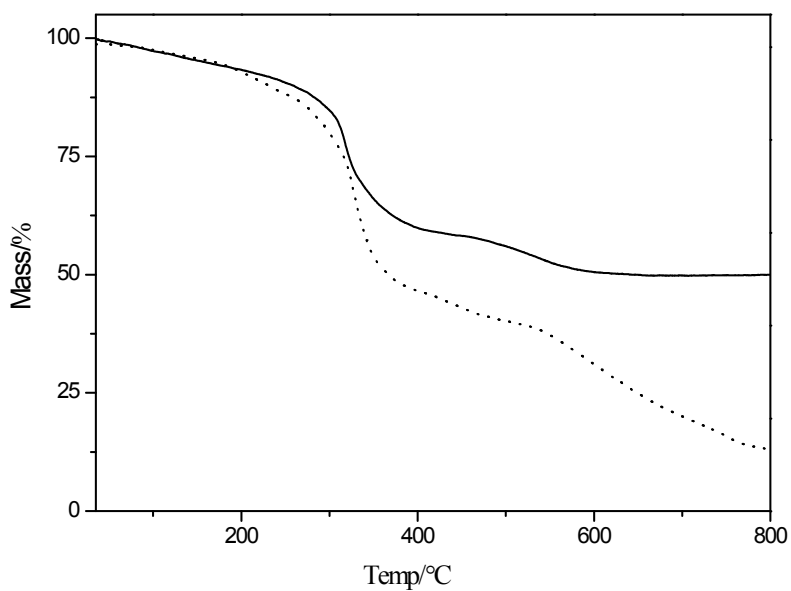


Figure S4 Thermogravimetric analysis traces of Tb-L (dotted line) and H-MSN-Tb (solid line).

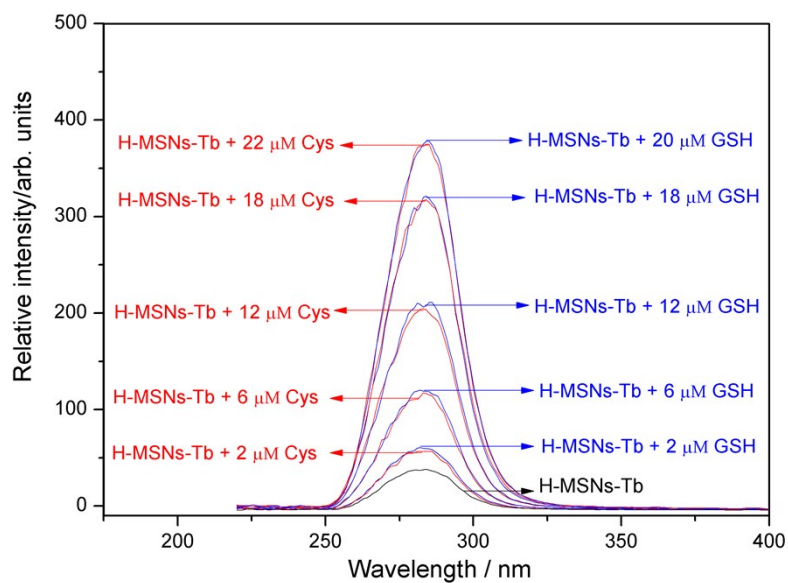


Figure S5 Excitation spectra of 50 $\mu\text{g/mL}$ H-MSNs-Tb without (black line) or with 2, 6, 12, 18, 22 μM Cys (red lines) or 20 μM GSH (blue lines) in water ($\lambda_{\text{em}} = 545 \text{ nm}$).

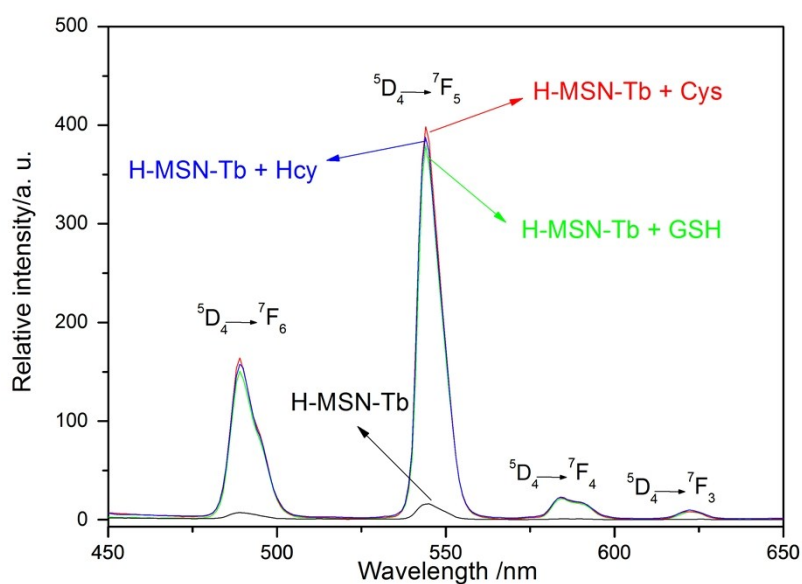


Figure S6 Emission spectra of H-MSN-Tb (50 $\mu\text{g/mL}$) in the absence and in the presence of biothiol (20 μM) in 30 mM HEPES buffer, pH 7.0 ($\lambda_{\text{ex}} = 284 \text{ nm}$).

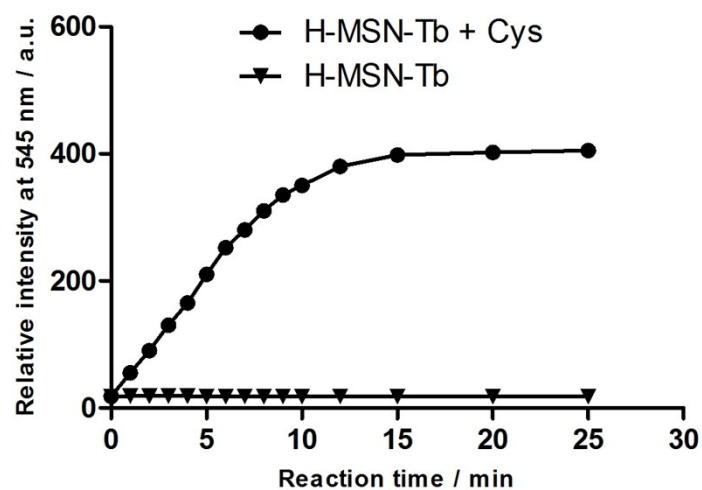


Figure S7 Fluorescence response of H-MSN-Tb (50 µg/mL) as a function of time with or without Cys (20 µM) treatment in 30 mM HEPES buffer, pH 7.0 ($\lambda_{\text{ex}} = 284 \text{ nm}$).

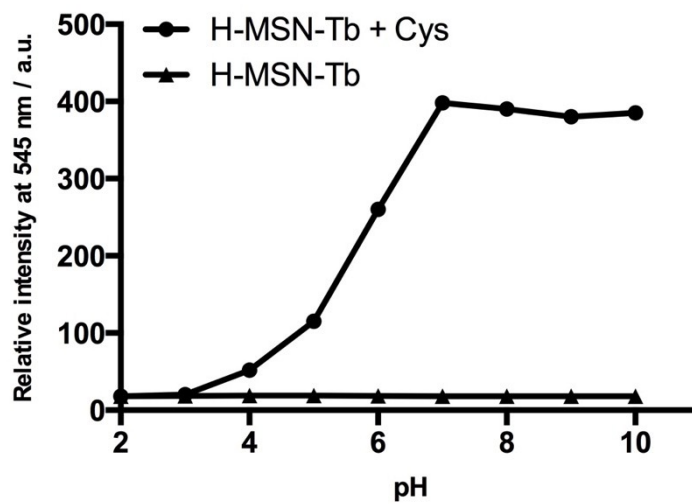


Figure S8 The fluorescence intensity of H-MSN-Tb at 545 nm in the presence and absence of Cys (20 µM) at different pH.

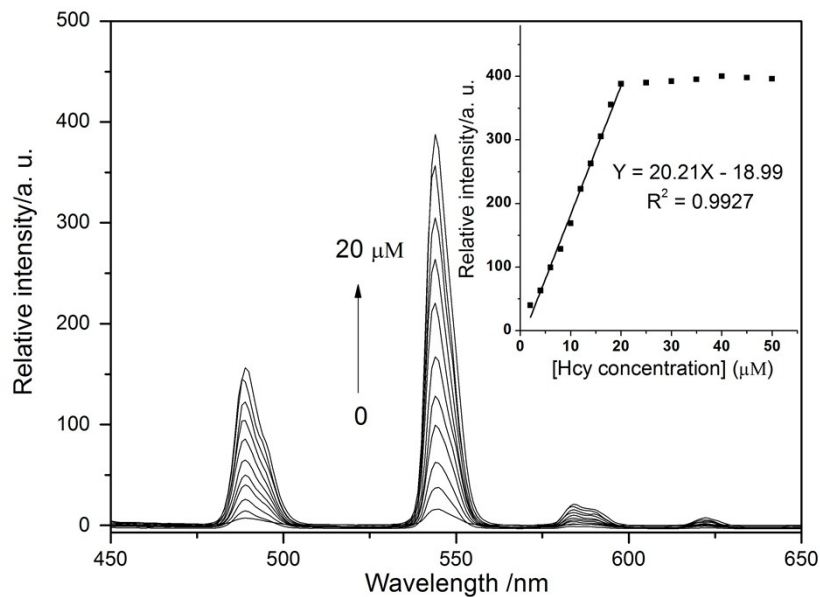


Figure S9 Emission spectra of H-MSN-Tb (50 $\mu\text{g/mL}$) upon addition of Hcy (from 0 to 20 μM) in 30 mM HEPES buffer, pH 7.0 ($\lambda_{\text{ex}} = 284 \text{ nm}$). Inset: Relative intensity of H-MSN-Tb at 545 nm as a function of Hcy concentration from 2 to 20 μM .

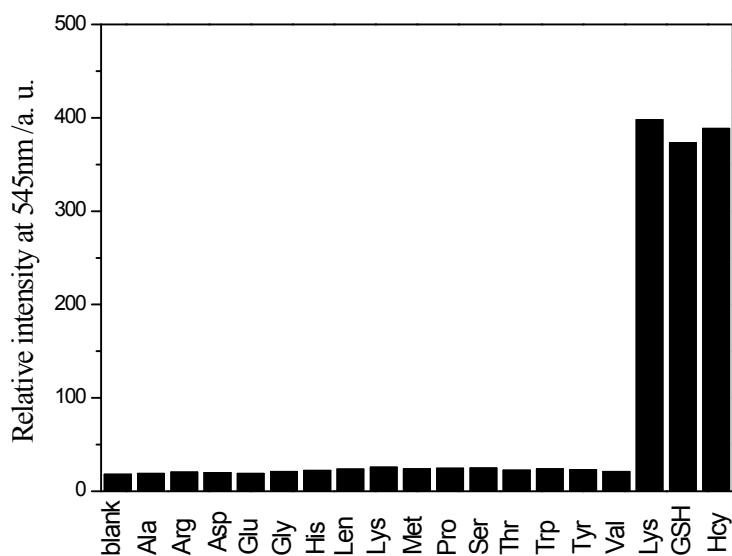


Figure S10 Emission intensities of H-MSNs-Tb at 545 nm in the presence of various amino acids (20 μM for Cys, GSH and Hcy, 100 μM for other amino acids) in 30 mM HEPES buffer, pH 7.

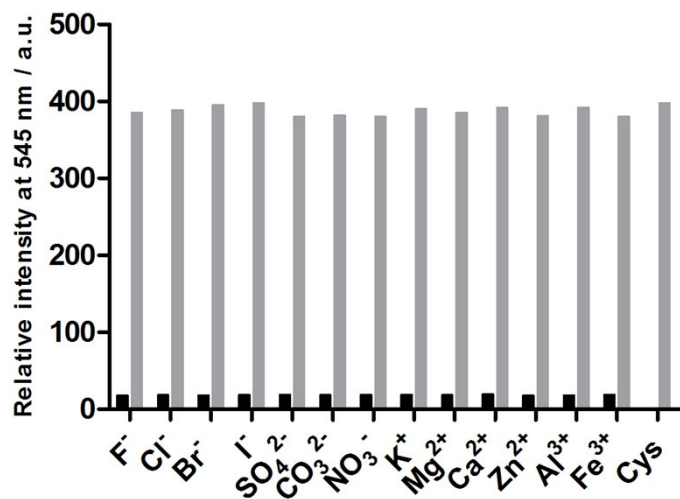


Figure S11 Emission intensities of H-MSNs-Tb at 545 nm to various ions in 30 mM HEPES buffer, pH 7. The black bars represent the fluorescence intensity of H-MSNs-Tb in the presence of miscellaneous ions (20 μ M). The grey bars represent the fluorescence enhancement upon the subsequent addition of Cys (20 μ M) to the above solution.

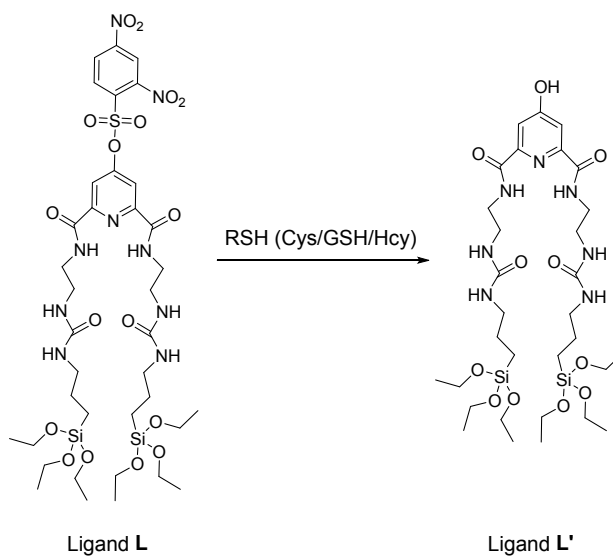


Figure S12 Molecular structures of **L** and **L'**.

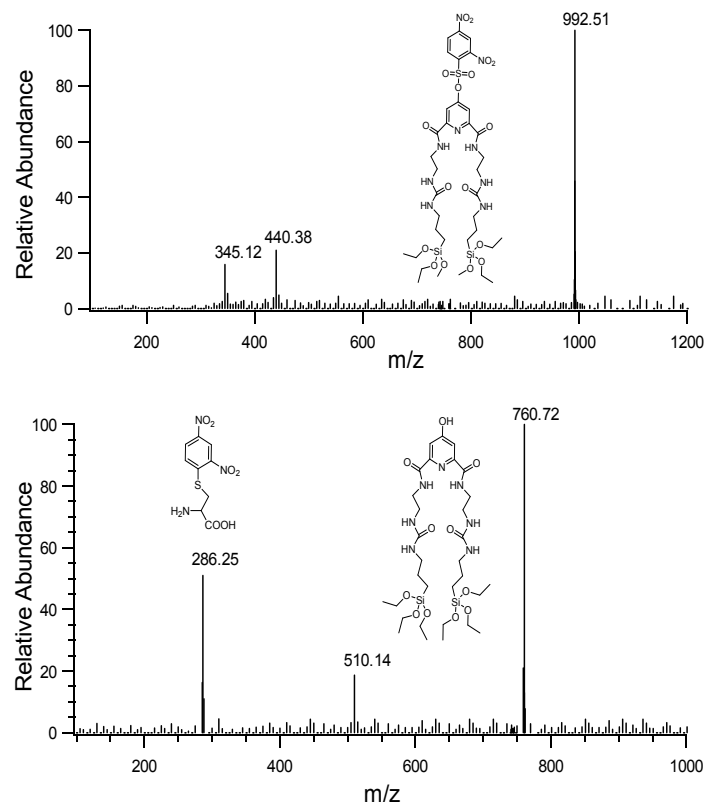


Figure S13 Mass spectra of ligand **L** in the absence (top) and presence of Cys (bottom).