Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supplementary Information

Conformational switch of G-quadruplex as a label-free platform for fluorescence detection of Ag^+ and biothiol

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Procedures for Ag^+ Detection in local tap water and Xiang River

The 300 nM probe P1 (22AG human telomeric DNA) was dissolved with 10 mM Tris-HAc buffer (pH=7.0) containing 50 mM KAc. The DNA solution was heated to 95 °C for 5 min and then cooled down slowly to room temperature. 3 μM ThT was added to this DNA solution, which was incubated at 37 °C for another 15 min. Afterwards, the actual samples (local tap water and water from Xiang River) were previously disposed with 0.22 μm filter membrane (Millipore, Merck), then added to the mixture and incubated at 37 °C for 20 min. The fluorescence spectra of the mixture were recorded at room temperature in a quartz cuvette.

Procedures for Cys Detection.

The 300 nM probe P1 (22AG human telomeric DNA) was dissolved with 10 mM Tris-HAc buffer (pH=7.0) containing 50 mM KAc. The DNA solution was heated to 95 °C for 5 min and then cooled down slowly to room temperature. Fistly, 3 μM ThT was added to this DNA solution and incubated at 37 °C for another 15 min. Then 3.5 μM of freshly prepared Ag^+ was added to the mixture and freshly prepared Cys of different concentrations was then mixed together. The mixture was allowed to react at 37 °C for 20 min. The fluorescence spectra of the mixture were recorded at room temperature in a quartz cuvette.

Table S1. Sequences of DNA oligonucleiotides

Name	Sequences (5′-3′)
P1 (the 22AG human telomeric DNA)	AGGGTTAGGGTTAGGGTTAGGG
P2	TGGGTAGGGCGGGTTGGGAAA
P3	AGGGTTAGGGTTAGGGTTAGGGCTCAACATC

Fig. S1. Optimization of DNA probes. Fluorescence intensity obtained from ThT only (black); P1 incubated with ThT (red); P1 incubated with ThT and Ag^+ (blue). (ThT 3 μM, P1 300 nM, Ag^+ 3.5 μM, in 10 mM Tris-HAc buffer (pH=7.0)).

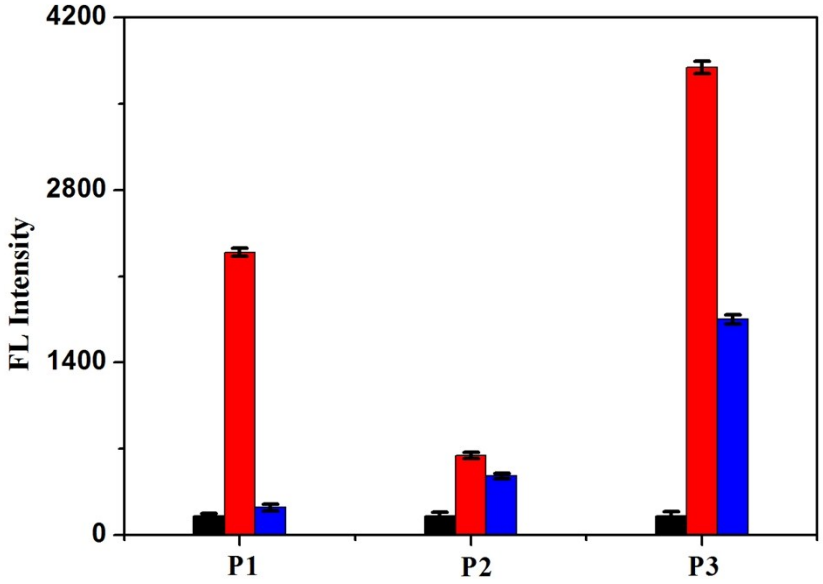


Fig. S2. Fluorescence (A, B) and absorption (C, D) spectra of ThT with P1 under different buffer conditions. (A and B correspond to the presence and absence of K^+ respectively. ThT (Purple line); P1 + ThT (black line); P1 + ThT + Ag^+ (red line); P1 + ThT +Ag^++ GSH (blue line). (ThT 3 μM, P1 300 nM, Ag^+ 3.5 μM, GSH 3.6 μM in 10 mM Tris-HAc buffer (pH=7.0)). C and D correspond to the presence and absence of K^+ respectively. ThT (Black line); P1 + ThT (red line); P1 + ThT + Ag^+ (blue line); P1 + ThT + Ag^++ GSH (purple line). (ThT: 100 μM, P1: 10 μM, Ag^+: 116.7 μM, GSH: 120 μM in 10 mM Tris-HAc buffer (pH=7.0)).

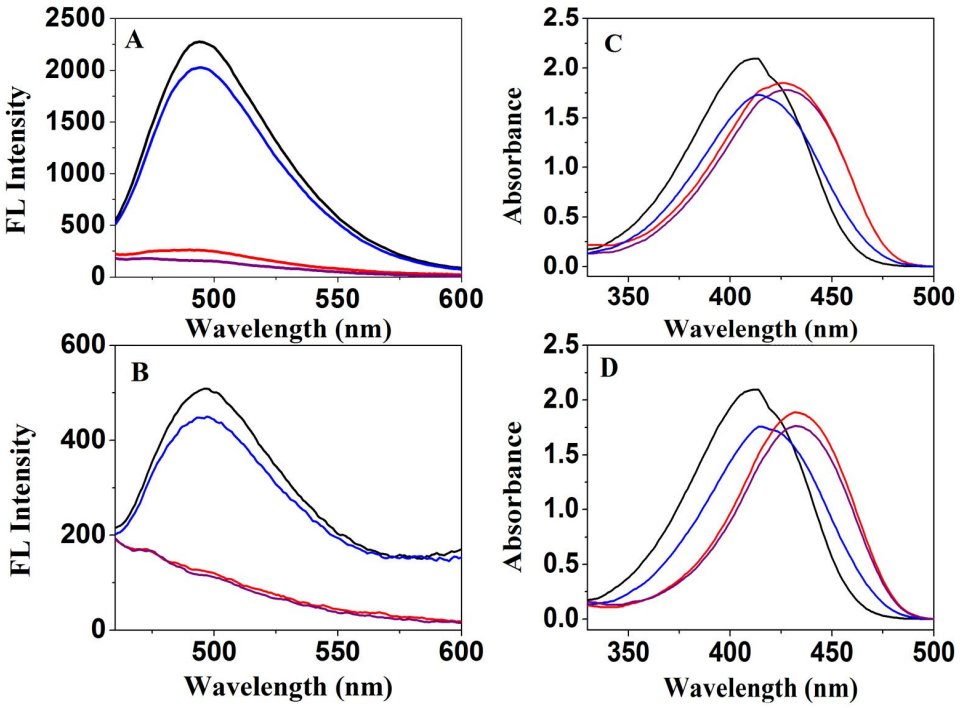


Fig. S3. CD measurements. (A): (red and black line are in the presence and absence K^+ respectively) P1 + ThT (ThT: 100 μM, P1: 10 μM in 10 mM Tris-HAc buffer); (B) CD spectra of P1 under different conditions in 10 mM Tris-HAc buffer: P1 (red line); P1 + ThT (purple line); P1 + ThT + Ag^+ (black line); P1 + ThT + Ag^++ GSH (blue line). (ThT: 100 μM, P1: 10 μM, Ag^+: 116.7 μM, GSH: 120 μM)

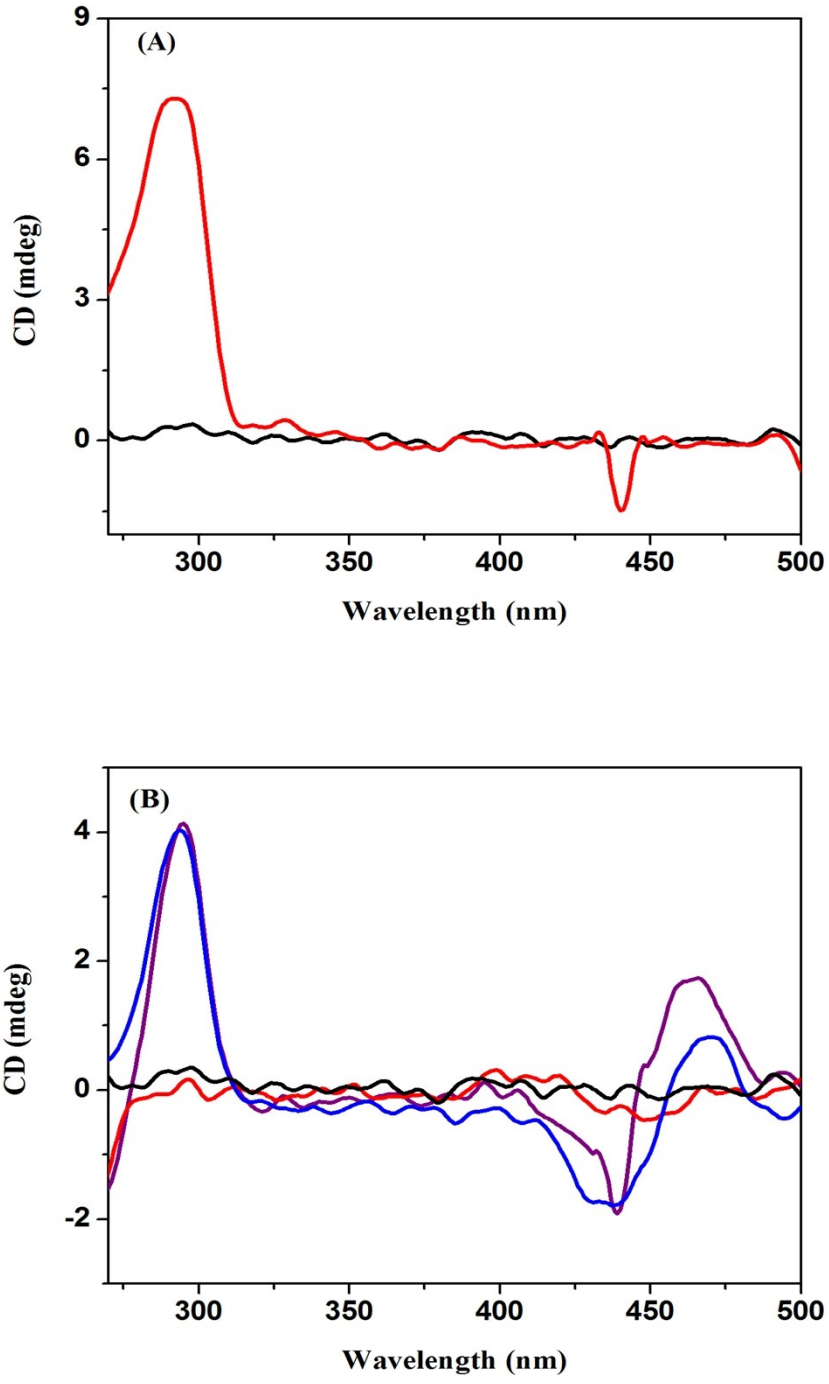
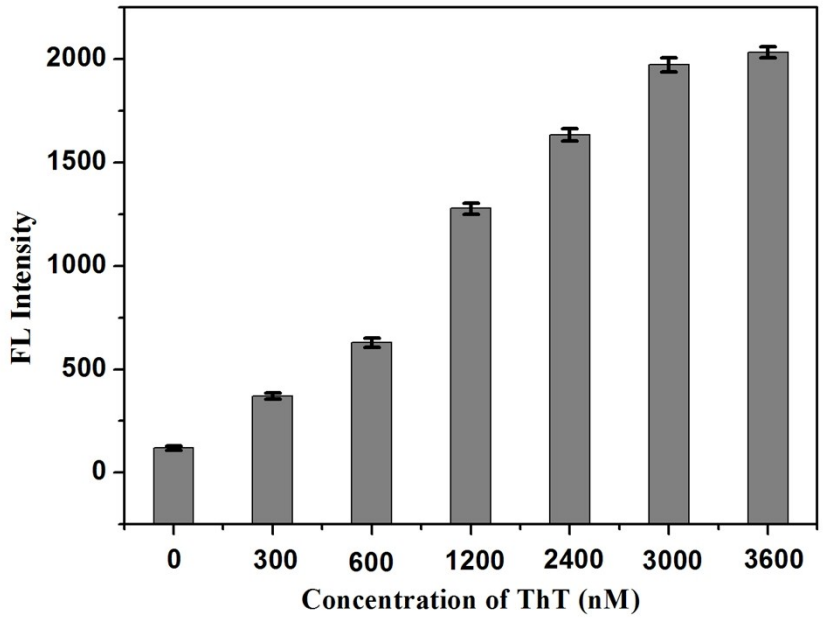


Fig. S4. (A) The optimized concentration of ThT. (P1: 300 nM); (B) Influence of the concentration of K^+. (ThT: 3 μM, P1: 300 nM).



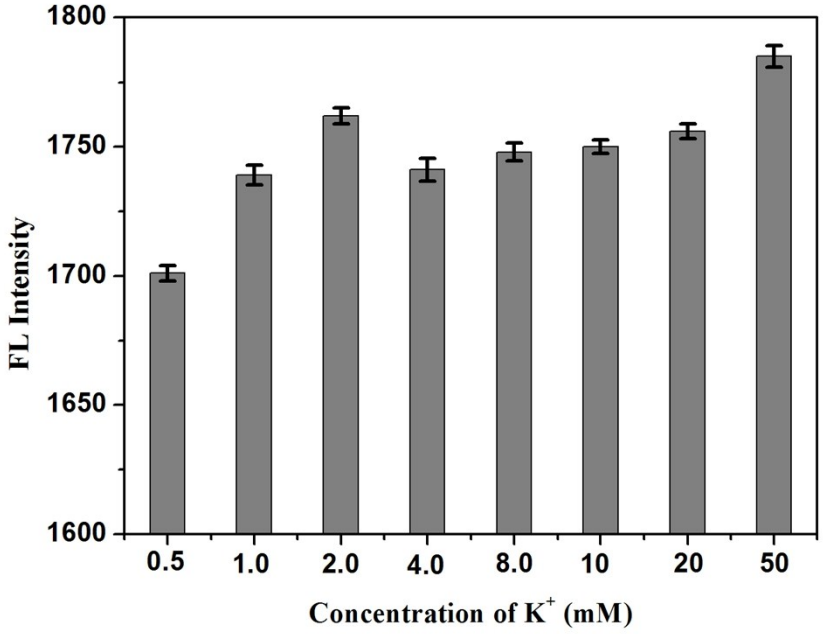
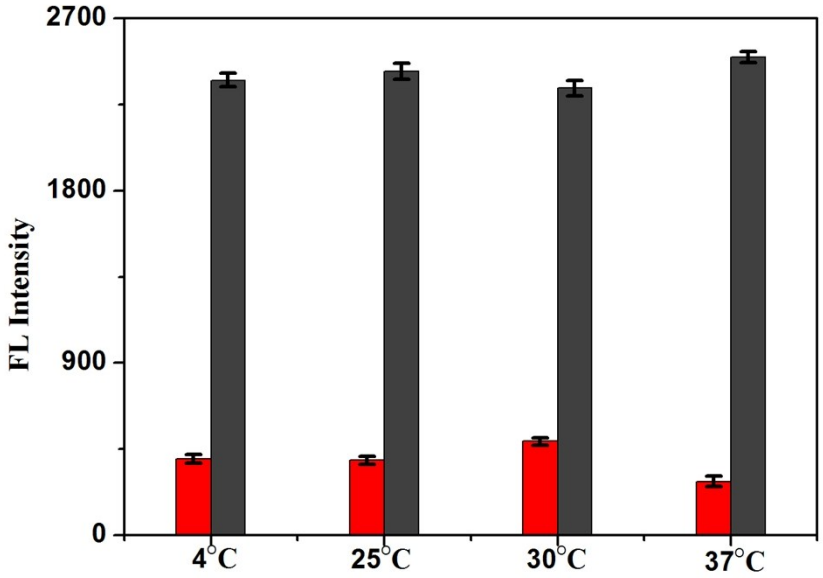


Fig. S5. The effects of temperature and pH of the reaction buffer. Probe incubated with ThT (gray); probe incubated with ThT and Ag^+ (red). (ThT: 3 μM; P1: 300 nM; Ag^+: 3.5 μM)



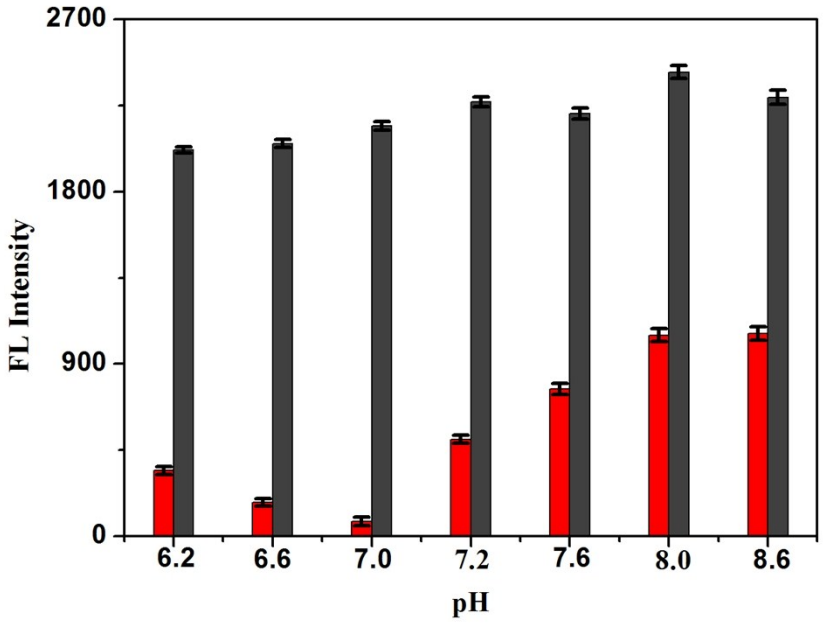


Fig. S6. Selectivity of the method for the detection of Ag^+. The concentration of Ag^+ and other metal ions is 3.5 μM (P1: 300 nM, ThT: 3 μM).

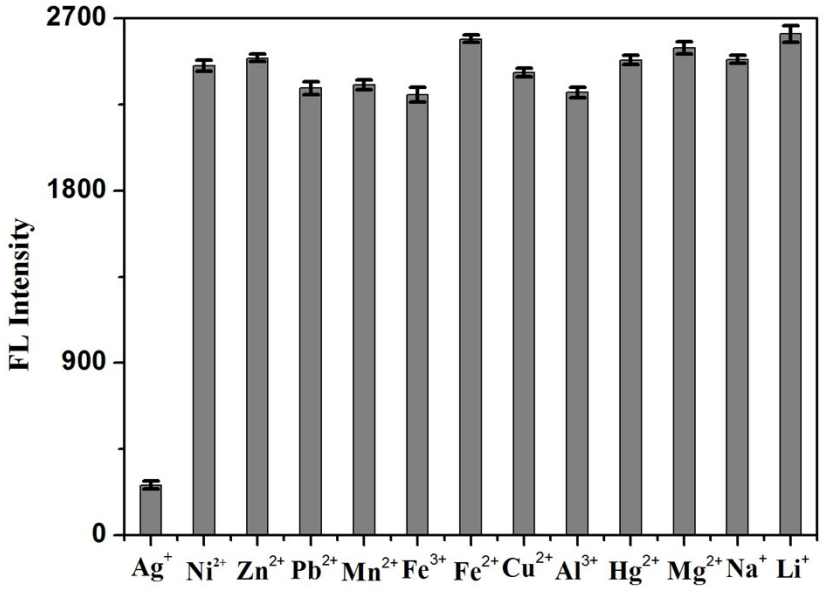


Fig. S7. Detection of Ag^+ from local tap water and Xiang River. Fluorescence emission spectra of ThT under different conditions: ThT: (purple line); P1 + ThT: (black line); P1 + ThT + treated Xiang River: (blue line); P1 + ThT + treated tap water: (olive line). (ThT: 3 μM, P1: 300 nM, in 10 mM Tris-HAc buffer (pH=7.0) containing 50 mM KAc). From the figure and the calibration equation of Ag^+, we could know that the content of Ag^+ in the Xiang River water and local tap water samples were 22.4 nM and 42.9 nM respectively.

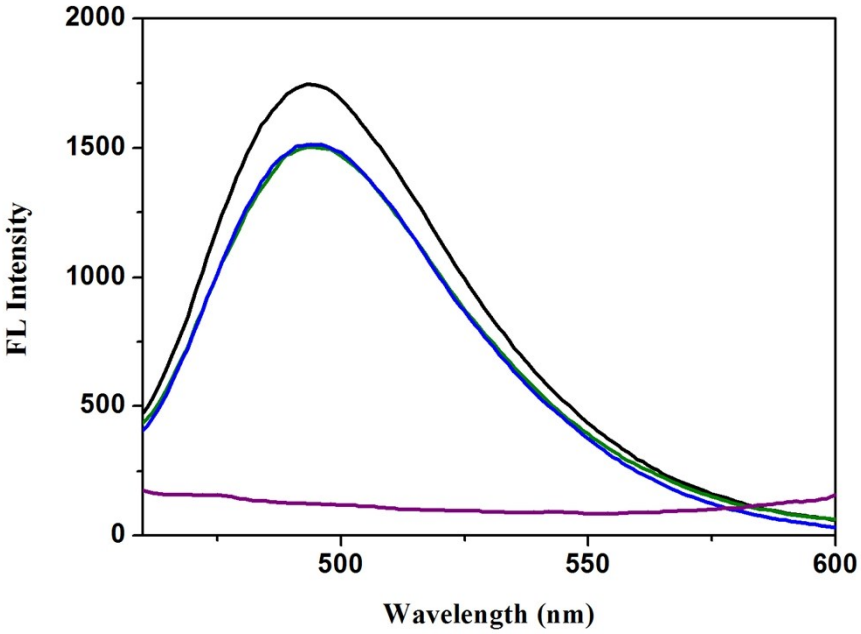


Fig. S8. Selectivity of the method for the detection of GSH. (P1: 300 nM, Ag^{+}: 3.5 μM, GSH: 3.6 μM).

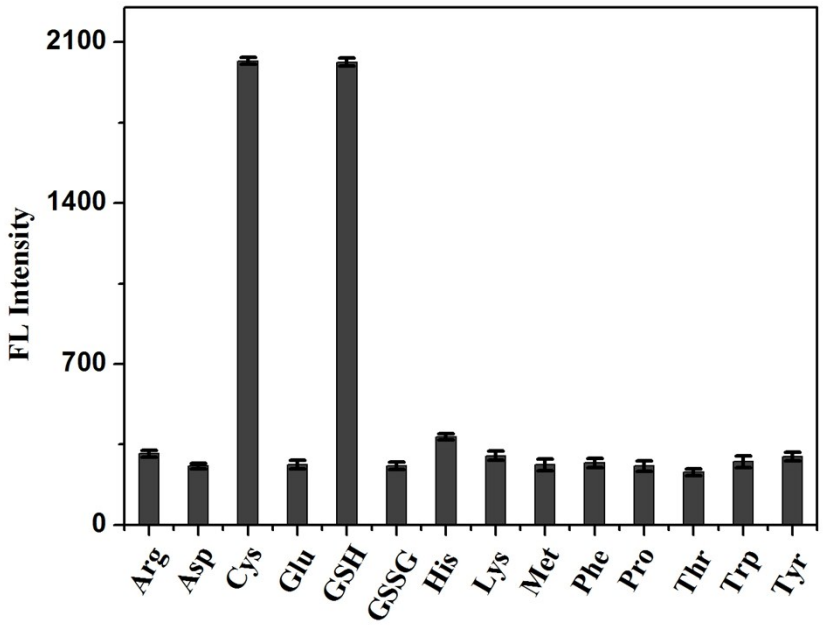


Fig. S9. Feasibility of the sensing system for the quantitative determination of Cys. (ThT: 3 μM, P1: 300 nM, Ag^{+}: 3.5 μM)

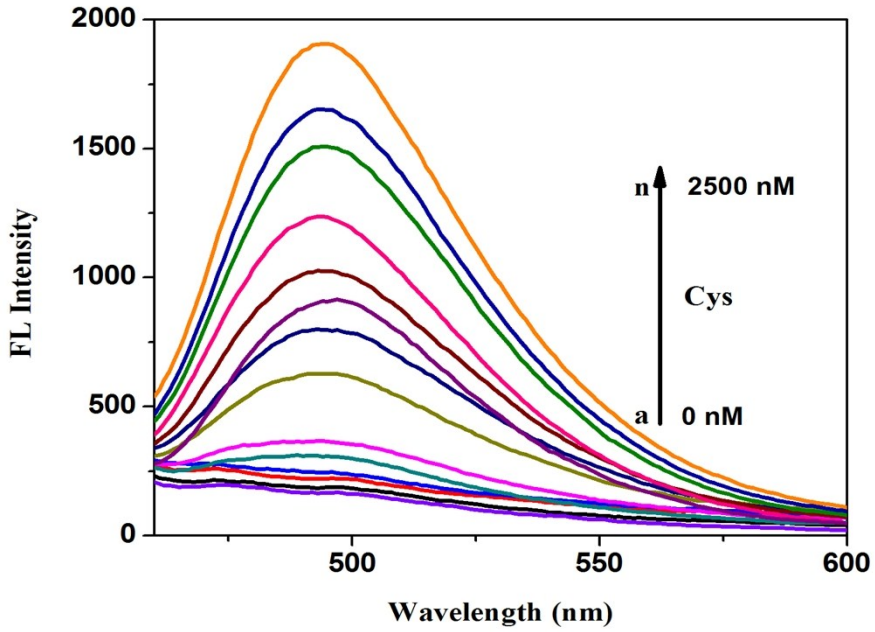


Fig. S10. Sensitivity of the method for the detection of Cys. (ThT: 3 μM, P1: 300 nM, Ag^{+}: 3.5 μM). A linear relationship (correlation coefficient R^2 =0.9992) was obtained at Cys concentration in the range of 50-2000 nM with the detection limit of 11 nM.

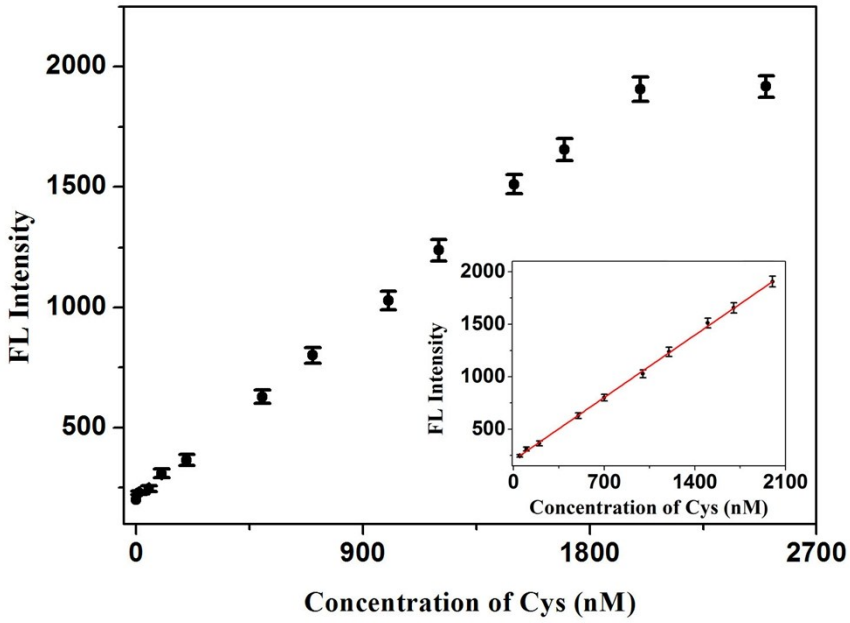


Fig. S11. Selectivity of the method for the detection of Cys. (ThT: 3 μM, P1: 300 nM, Ag^{+}: 3.5 μM, Cys: 2 μM)

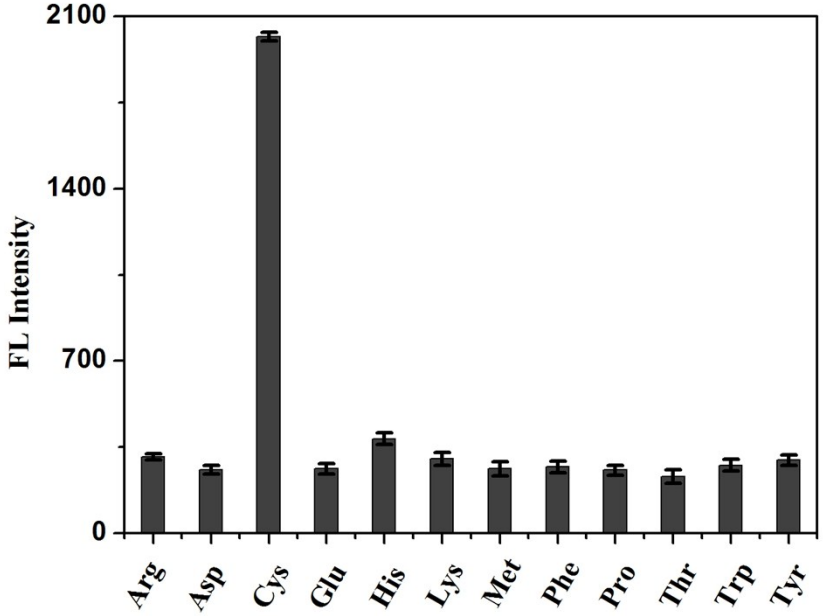


Fig. S12. A kinetic experiment of the method for the detection of Ag^+. (ThT: 3 μM, P1: 300 nM, Ag^+: 3 μM)