Supporting Information

Fluorescent Silver Nanoclusters in Hybridized DNA Duplexes for the Turn on Detection of ${ m Hg}^{2+}$ ion

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1. Experimental

1.1 Materials and preparation: All DNA strands were synthesized by Shanghai Sangon Biotechnology Co. Ltd. (Shanghai, China). Other chemicals were commercially available and of analytical grade. All DNA samples were prepared with phosphate buffer (20 mM phosphate, 1 mM magnesium acetate, pH 7.0). All the solutions were prepared with water purified by a Milli-Q system (Millipore, Bedford, MA, USA) and stored at 4 °C. In a typical hybridization experiment, 2 μ M probe DNA was first mixed with 2 μ M Str-A or Str-B, respectively. Then DNA mixture solutions were denatured at 95 °C for 15 minutes, followed with a slow annealing treatment for 1 hour to form DNA duplex. Then, different concentrations of Hg²⁺ were added to this solution respectively, and the mixture was allowed to incubate at 25 °C for 1 h. Next, AgNO₃ [6:1 Ag⁺/DNA molar ratio] was added to the DNA duplex solutions. After mixing, the solutions were stirred for 15 min and then reduced with NaBH₄ [1:1 Ag⁺/NaBH₄ molar ratio] for another 7 hours. 1.2 Characterization: The FL spectra were recorded by a Perkin-Elmer LS55 Luminescence Spectrometer (Perkin-Elmer Instruments U.K.) using a 1-cm path length quartz cell at room temperature. The slot widths of the excitation and emission both were set at 10.0 nm. UV/vis absorption spectra were recorded by a CARY 500 UV/vis-near-IR Varian spectrophotometer. The melting point was determined from the first derivative plot of absorption versus temperature curve.

2. FL spectra of Str-A/Str-B/Hg²⁺ system

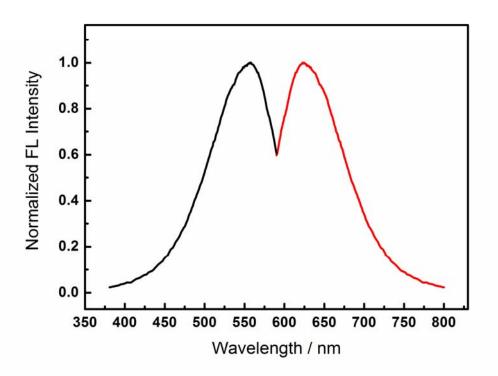


Figure S1. Excitation and emission spectra of fluorescent Ag NCs obtained using the Str-A /Str-B/Hg²⁺ duplex as the synthetic scaffold.

3. UV spectra of Str-A/Str-B/Hg²⁺ system

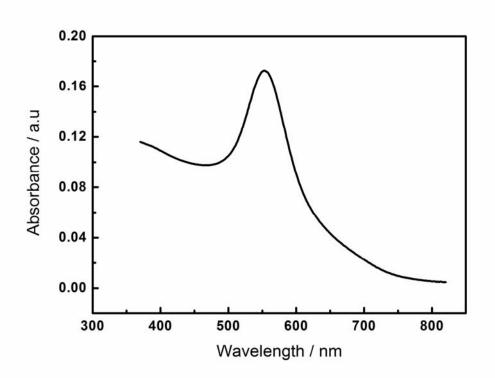


Figure S2. UV-vis spectra of fluorescent Ag NCs obtained using the Str-A/Str-B/Hg²⁺ duplex as the synthetic scaffold.

4. T_m spectra of Str-A/Str-B/Hg²⁺ system

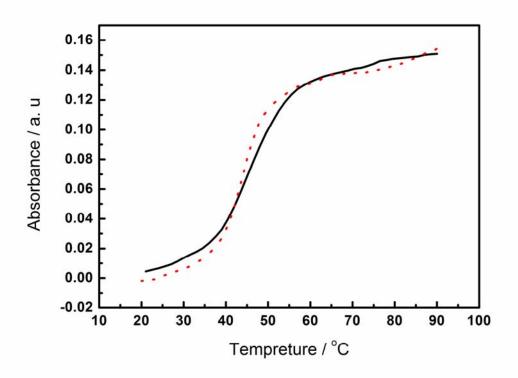
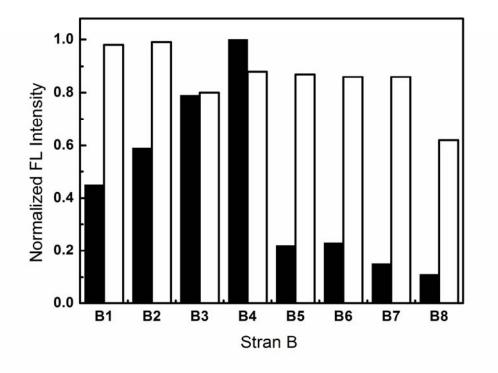


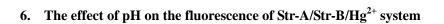
Figure S3. Relative absorbance $A = [(A_t - A_{31}^{\circ}_{C})/(A_{70}^{\circ}_{C} - A_{31}^{\circ}_{C})]$ at 260 nm vs temperature (t) for Str-A/Str-B (black line) and Str-A /Str-B/Hg²⁺ (red dot line) duplexes (2µM in 20 mM phosphate buffer (pH 7.0) containing 1 mM magnesium acetate).



5. The effect of different Str-B on the fluorescence of Str-A/Str-B/Hg²⁺ system

Figure S4 The normalized FL intensity in the absence (black bars) or presence (white bars) of Str-A/Str-B/Hg²⁺ duplex in presence of 100 nM Hg²⁺ when a different strand B was used.

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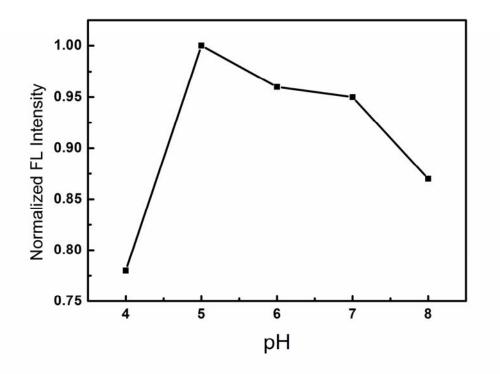


Figure S5 Influence of pH value on the generation of the fluorescence silver species in $Str-A/Str-B/Hg^{2+}$ duplex with 100 nM Hg²⁺ addition.

7. The oligonucleotide sequences applied in this work

Table S1	The olig	onucleotides	used in	this work

- Str-A 5'-CCCACTTTCCCCCCTCCTACCC
- Str-A' 5'-CCC ACT TT TCC TA CCC
- Str-B 5'-GGG TAG A<u>T TT</u>A GTG GG
- Str-B1 5'-GGG TAG AA TAA GTG GG
- Str-B2 5'-GGG TAG AA A<u>T</u>A GTG GG
- Str-B3 5'-GGG TAG AA AAT GTG GG
- Str-B4 5'-GGG TTG AA AAA GTG GG
- Str-B5 5'-GGG TAG AA <u>TT</u>A GTG GG
- Str-B6 5'-GGG TAG A<u>T T</u>AA GTG GG
- Str-B7 5'-GGG TAG A<u>T TT</u>A GTG GG
- Str-B8 5'-GGG TAG TT TTA GTG GG

The underlined bold letters identify mismatched bases.

8. The results of the proposed method in the practical samples

Table S2 Recoveries of Hg²⁺ by utilization the proposed method in the practical samples

Samulas	$\mathrm{Hg}^{2+}(\mathrm{nM})$		
Samples	Added	Recovery (%)	
Lake water ^a	30 105.2±3.3		
Lake water	50 106.8±3.2		
Ten weter ^b	30 101.1±2.1		
Tap water ^b	50	102.9±1.8	
Purified water ^c	30	98.7±1.2	
Fuillied water	50 101.3±3.2		
Spring water ^d	30	101.1±4.1	
Spring water ^d	50	102.8 ± 1.9	

^a Obtained from the south lake in ChangChun; ^b Obtained from the Laboratory Building; ^c Obtained from the Milli-Q water; ^d Obtained from the commercial "Wahaha" spring water.