

**T-Hg²⁺-T metallo-base pair-mediated dual amplification fluorescent
strategy for the selective and sensitive detection of Hg²⁺**

Haiping Wei ^a, Lei Wang ^b, Xiaowen Xu ^a, Jing Zhu ^a, Wei Jiang ^{a,*}

^aKey Laboratory for Colloid and Interface Chemistry of Education Ministry, School
of Chemistry and Chemical Engineering, Shandong University, 250100 Jinan, P.R.
China

^bSchool of Pharmaceutical Sciences, Shandong University, 250012 Jinan, P. R.
China

Corresponding author: Tel: 86-531-88363888; fax: 86-531-88564464.

E-mail: wjiang@sdu.edu.cn

Table S1 Sequences of oligonucleotides used in this work.

Name	Sequence (from 5' to 3')
H-DNA3	<u>CAT CTC TTC TCC GAG CCG GTC GAA ATA GTG GGT AAT GAA</u> <u>GAG ATG GTT TCG</u>
A-DNA3	<u>CGT TTC CAT CTC TTC AAA AAG</u>
H-DNA4	<u>CAT CTC TTC TCC GAG CCG GTC GAA ATA GTG GGT AAT GAA</u> <u>GAG ATG GTT TCG G</u>
A-DNA4	<u>CCG TTT CCA TCT CTT CAA AAA G</u>
H-DNA5	<u>CAT CTC TTC TCC GAG CCG GTC GAA ATA GTG GGT AAT GAA</u> <u>GAG ATG GTT TCG GG</u>
A-DNA5	<u>CCC GTT TCC ATC TCT TCA AAA AG</u>
H-DNA6	<u>CAT CTC TTC TCC GAG CCG GTC GAA ATA GTG GGT AAT GAA</u> <u>GAG ATG GTT TCG GGG</u>
A-DNA6	<u>CCC CGT TTC CAT CTC TTC AAA AAG</u>
H-DNA7	<u>CAT CTC TTC TCC GAG CCG GTC GAA ATA GTG GGT AAT GAA</u> <u>GAG ATG GTT TCG GGG G</u>
A-DNA7	<u>CCC CCG TTT CCA TCT CTT CAA AAA G</u>
H-DNA8	<u>CAT CTC TTC TCC GAG CCG GTC GAA ATA GTG GGT AAT GAA</u> <u>GAG ATG GTT TCG GGG GG</u>
A-DNA8	<u>CCC CCC GTT TCC ATC TCT TCA AAA AG</u>
MB	FAM- <u>CCA CCA CAC TGA AAT TGA CCC ACT ATrA GGA AGA</u> <u>GAT GTT ACG AGG CGG TGG TGG</u> -Dacyl

^a The rose domains in H-DNA are DNAzyme sequences. The gold domains and the blue domains in both H-DNA and A-DNA are T-rich sequences and complementary sequences, respectively. And the coffee domains in A-DNA are protection sequences. The red rA of the MB denotes adenine ribonucleotide at that position. The underlined sequences in H-DNA and MB present

the stem of the structures.

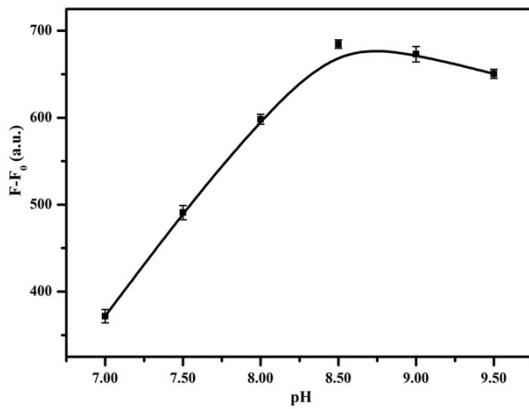


Fig. S1. The effect of the pH values of the TM buffer on Fluorescence Increase. Conditions : $C_{Mg^{2+}} = 5.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$, $C_{A\text{-DNA}} = 1.0 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{H\text{-DNA}} = 1.2 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{MB} = 1.8 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, Exo III = 50 U. T-Hg²⁺-T reaction : 60 min, Target cycle : 120 min, DNAzyme cycle : 30 min.

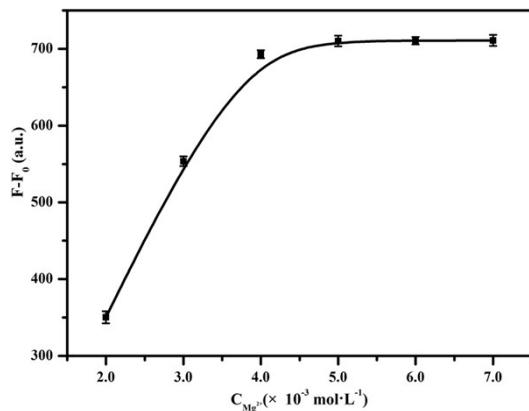


Fig. S2. The effect of the ion strengths of the TM buffer on Fluorescence Increase. Conditions : pH = 8.50, $C_{A\text{-DNA}} = 1.0 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{H\text{-DNA}} = 1.2 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{MB} = 1.8 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, Exo III = 50 U. T-Hg²⁺-T reaction : 60 min, Target cycle : 120 min, DNAzyme cycle : 30 min.

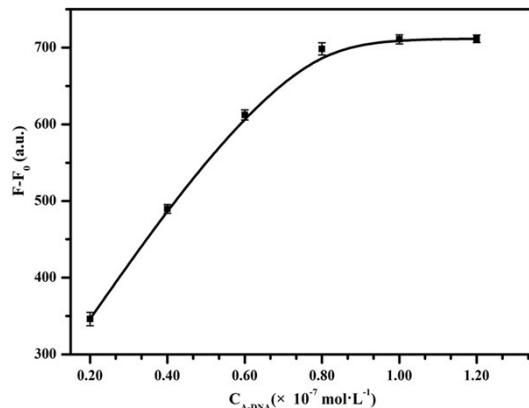


Fig. S3. The effect of the A-DNA concentrations on Fluorescence Increase. Conditions : pH = 8.50, $C_{Mg^{2+}} = 5.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$, $C_{H\text{-DNA}} = 1.2 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{MB} = 1.8 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, Exo III = 50 U. T-Hg²⁺-T reaction : 60 min, Target cycle : 120 min, DNAzyme cycle : 30 min.

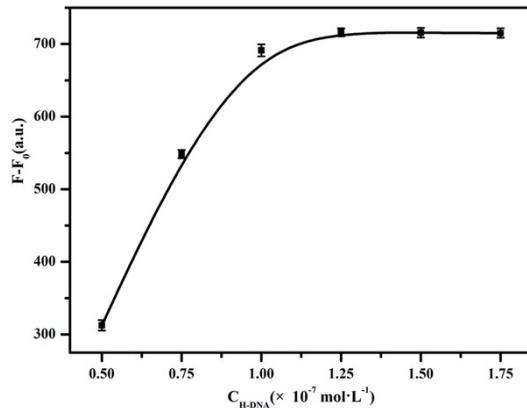


Fig. S4. The effect of the H-DNA concentrations on Fluorescence Increase. Conditions : pH = 8.50, $C_{Mg^{2+}} = 5.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$, $C_{A\text{-DNA}} = 1.0 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{MB} = 1.8 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, Exo III = 50 U. T-Hg²⁺-T reaction : 60 min, Target cycle : 120 min, DNAzyme cycle : 30 min.

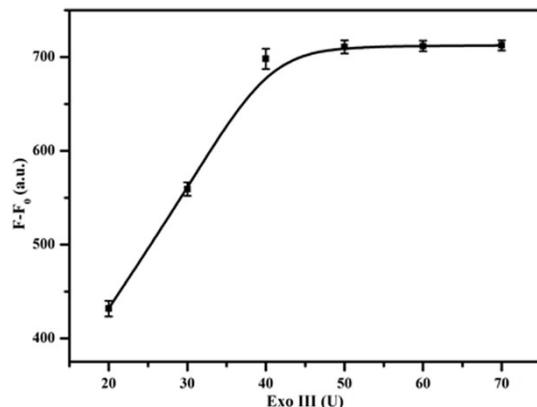


Fig. S5. The effect of the amounts of Exo III on Fluorescence Increase. Conditions : pH = 8.50, $C_{Mg^{2+}} = 5.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$, $C_{A\text{-DNA}} = 1.0 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{H\text{-DNA}} = 1.2 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{MB} = 1.8 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$. T-Hg²⁺-T reaction : 60 min, Target cycle : 120 min, DNAzyme cycle : 30 min.

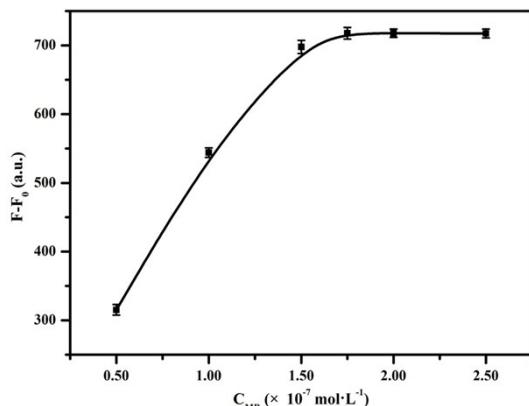


Fig. S6. The effect of the MB concentrations on Fluorescence Increase. Conditions : pH = 8.50, $C_{\text{Mg}^{2+}} = 5.0 \times 10^{-3} \text{ mol}\cdot\text{L}^{-1}$, $C_{\text{A-DNA}} = 1.0 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, $C_{\text{H-DNA}} = 1.2 \times 10^{-7} \text{ mol}\cdot\text{L}^{-1}$, Exo III = 50 U. T-Hg²⁺-T reaction : 60 min, Target cycle : 120 min, DNAzyme cycle : 30 min.

Table S2. Detection of Hg²⁺ in environmental water samples using the proposed strategy and ICP-MS method^a.

Sample Name	Added ($\times 10^{-9}$ mol·L ⁻¹)	Found Mean ^b ($\times 10^{-9}$ mol·L ⁻¹)	Found RSD (%) (n = 3)	Found Recovery (%)	ICP-MS Mean ^b ($\times 10^{-9}$ mol·L ⁻¹)	ICP-MS RSD (%) (n = 3)	ICP-MS Recovery (%)
Tap Water1	2.5	2.4	3.1	92	2.4	3.8	92
Tap Water2	8.0	8.1	2.3	101	8.3	2.1	104
Lake Water1	2.5	2.3	2.4	92	2.4	4.5	92
Lake Water2	8.0	7.9	1.8	99	8.2	2.5	103
River Water1	2.5	2.4	4.2	96	2.6	3.3	104
River Water2	8.0	7.8	3.7	98	7.9	2.9	99
Waste Water	0	7.0	3.5	NO ^c	7.1	4.0	NO ^c

^a The Hg²⁺ in tap, lake and river water was not detected with the proposed strategy and ICP-MS method.

^b All found values were obtained as an average of three repetitive determinations.

^c The results were not obtainable.