Supporting Information

A Coordination and Ligand Replacement Based Three-input Colorimetric Logic Gate Sensing Platform for Melamine, Mercury Ions, and Cysteine

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Fig. S1 TEM images of ~13 nm Au NPs upon the combinational additions of melamine (6×10^{-5} M), cysteine (3.6×10^{-4} M) and Hg²⁺ (1.8×10^{-4} M) for the logic operations. The scale bars are 50 nm.

Input (A) (B)		Output		
0	0	0	0	0
0	1	0	1	1
1	0	0	1	0
1	1	1	1	0
Name		AND	OR	INH

Table S1. Truth table of Boolean logic operations of AND, OR, and INH.



Fig. S2 A schematic illustration of the pathways for the discrimination of different analytes based on the colorimetric platform. (A) Discrimination of a single kind of analyte. (B) Discrimination of the combination of two kinds of analytes. The analytes can be discriminated step by step with the help of an additional solution of Hg^{2+} when it is known that how many kinds of targeted species are in the sample solution. There will be only one case when the number of species is three, namely, the coexistence of Hg^{2+} , melamine, and cyeteine. The output of this combination will always be the aggregation of Au NPs (Output 1), so the discrimination of this case is not needed.



Fig. S3 (A) UV-vis absorption spectra of Au NPs solution upon the addition of cysteine at the concentrations ranging from 0 to 404 μ M, (B) Au NPs solution upon the addition of melamine at the concentrations ranging from 0 to 200 μ M in the presence of 6 μ M cysteine, (C) Au NPs solution upon the addition of Hg²⁺ at the concentrations ranging from 0 to 60 μ M in the presence of 6 μ M cysteine, Au NPs solution upon the addition of (D) HCl and (E) NaOH at the concentrations ranging from 0 to 120 μ M in the presence of 6 μ M cysteine. These results imply that cysteine can be served as a stabilizing agent against melamine

induced aggregation of Au NPs. However, this stabilizing effect will be broken when Hg^{2+} is introduced into the system at the same time.



Fig. S4 Control experiments to verify the role of –SH group in the logic gates. (A) Colour readout of the Au NPs solutions upon the combinational addition of melamine $(6 \times 10^{-5} \text{ M})$ and $\text{Hg}^{2+}(1.8 \times 10^{-4} \text{ M})$ in the presence of alanine $(3.6 \times 10^{-4} \text{ M})$ (top) and cysteine $(3.6 \times 10^{-4} \text{ M})$ (bottom). (B) UV-vis absorption spectra responses of melamine $(2 \times 10^{-5} \text{ M})$ – $\text{Hg}^{2+}(6 \times 10^{-5} \text{ M})$ complex solution upon the addition of alanine at the molar ratios (Melamine/Hg²⁺/Alanine) ranging from 1:3:0 to 1:3:8, (C) Hg²⁺ $(6 \times 10^{-5} \text{ M})$ solution upon

the addition of alanine at the molar ratios (Hg²⁺/Alanine) ranging from 3:0 to 3:8, (D) alanine aqueous solution at the concentrations ranging from 4×10^{-5} M to 1.6×10^{-4} M, and (E) melamine (2 × 10⁻⁵ M) aqueous solution upon the addition of (E) alanine and (F) cysteine at the molar ratios ranging from 3:2 to 3:8.

Table S2. Stability constants of complexes of Hg^{2+} with cysteine and alanine. ¹	1
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Amino acid	Stability constant- β (ML ₂)
Alanine	19.6
Cysteine	39.4



Fig. S5 Selectivity to melamine like compounds. (A) UV-vis absorption spectra responses of Au NPs solutions upon the addition of six nitrogen containing compounds with the concentration of 1.5×10^{-6} M, (B) the corresponding signal readouts in the form of A_{650nm}/A_{520nm} , (C) the colour readouts of the Au NPs solutions, and (D) molecular structures of the six compounds.



Fig. S6 Comparison between ~13 nm and ~30 nm Au NPs. (A) SEM image of ~30 nm Au NPs. UV-vis absorption spectra responses of ~30 nm (B) and ~13 nm (C) Au NPs solutions upon the addition of 1.5×10^{-6} M Melamine, (D) the corresponding signal readouts in the form of A_{676nm}/A_{519nm} (13 nm Au NPs) and A_{820nm}/A_{527nm} (30 nm Au NPs), (E) the colour readouts of the Au NPs solutions.



Fig. S7 (A) UV-vis absorption spectra responses of Au NPs solutions upon the addition of 6 $\times 10^{-7}$ M Melamine in the presence of 15 mM NaCl in 30 minutes. (B) Time dependent visual detections of Hg²⁺ by using 6 $\times 10^{-7}$ M melamine as a control sample.



Fig. S8 Visual detection of Hg^{2+} . (A) UV-vis absorption spectra responses of Au NPs solutions upon the addition of 5 × 10⁻⁶ M metal ions in the presence of 1.5 × 10⁻⁶ M melamine, (B) the corresponding signal readouts in the form of A_{650nm}/A_{520nm} , and (C) the colour readouts of the Au NPs solutions. The UV-vis absorption spectra and the photos of Au NPs solutions were collected after 2 minutes. (D) Signal readouts in the form of A_{650nm}/A_{520nm} of the Au NPs solutions upon the addition of Hg^{2+} with different concentrations in the presence of 6 × 10⁻⁷ M melamine and 15 mM NaCl, (E) the corresponding visual colour changes of the Au NPs solutions (The signal readouts in the form of A_{650nm}/A_{520nm} and the photos Au NPs solutions were collected after 15 minutes), and (F) a linear plot of A_{650nm}/A_{520nm} as a function of Hg^{2+} concentration over the range of 0 to 250 nM.

Reference

1. Van Der Linden, W. E.; Beers, C. Determination of the Composition and the Stability Constants of Complexes of Mercury(II) with Amino Acids. *Anal. Chim. Acta.* 1973, 68, 143-154.