Supplementary Information

A biomimetic colorimetric logic gate system based on multi-functional peptide-mediated gold nanoparticles assembly

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Content

Table S1 Peptides used in this work

Name	Sequence of peptide	Isoelectric point	Application
P-1	CAAR-NH_2	9.51	Control peptide with positive charge
P-2	CCPGCAR-NH_2	8.71	YES-Zn^{2+} gate
P-3	CAYRA-NH_2	9.31	YES-Chy and INHIBIT gate
P-4	ARYCCPGC-NH_2	8.69	OR and INHIBIT-OR gate
P-5	ACYRCCPGC-NH_2	8.54	AND gate
P-6	DAYRCCPGC-CH_3	6.72	IMPLICATION gate
P-7	DDDCCPGCYRACC-NH_2	4.41	NAND gate
P-8	DDDYCCPGC-NH_2	3.93	Control peptide with negative charge
P-9	Ac-CCPGC-CH_3	6.71	Control peptide without charge

Noted: Isoelectric point was calculated according to the website of http://web.expasy.org/compute_pi/, referring to "*Electrophoresis 1993, 14, 1023-1031*".

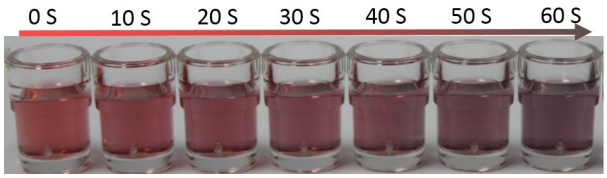


Fig. S1. The colour change of AuNPs varying with time after addition of P-4 (ARYCCPGC, 1.2 μM). The experiment was carried in borate buffer (50 mM H_3BO_3-$Na_2B_4O_7.10H_2O$, 25 mM $NaClO_4$, 50 μM TCEP, pH 7.4).

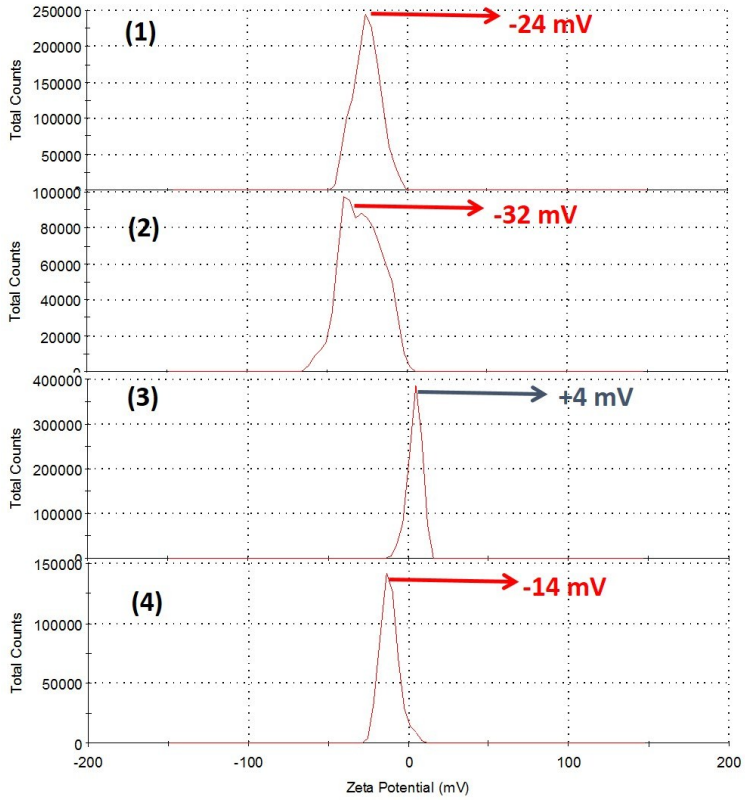


Fig. S2. Zeta potential of AuNPs before or after the addition of peptide from up to down corresponding to no peptide (1), DDDYCCPGC (2 μM, 2), CAAR (2 μM, 3), and CCPGC (2 μM, 4) as noted in figure, respectively.

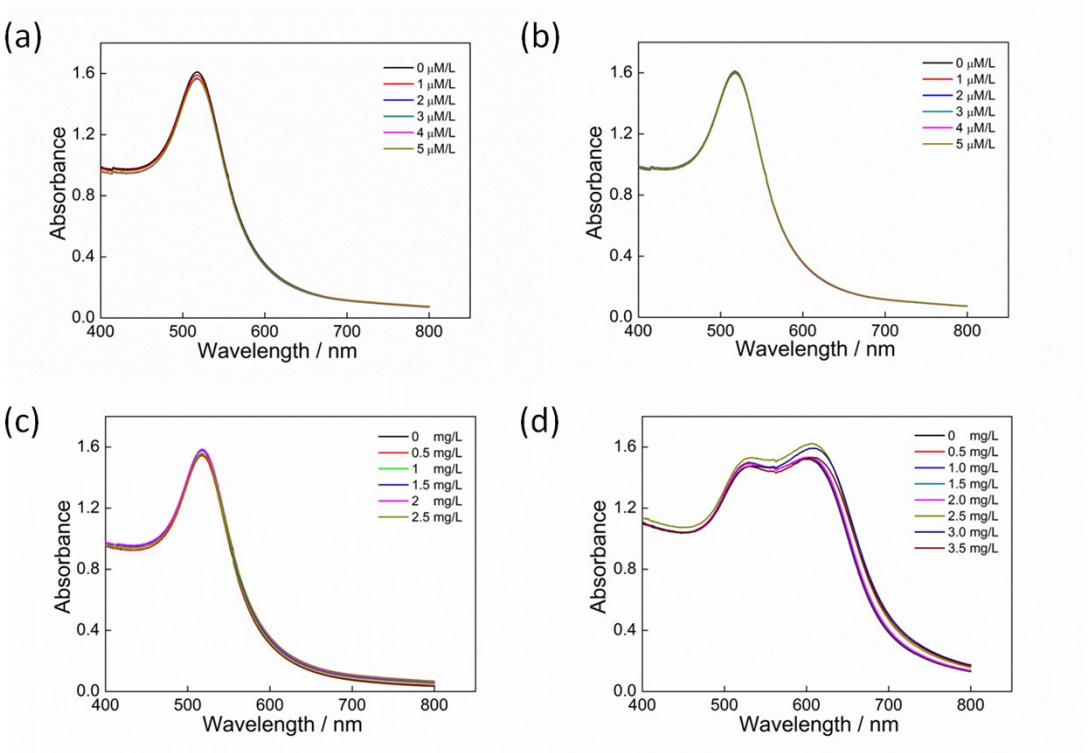


Fig. S3. The effect of Zn^{2+} (a), EDTA (b), and Chy (c) on the dispersions of AuNPs and the effect of Chy on aggregation of AuNPs (d), and the absorption spectra from 400 nm to 800 nm were measured.

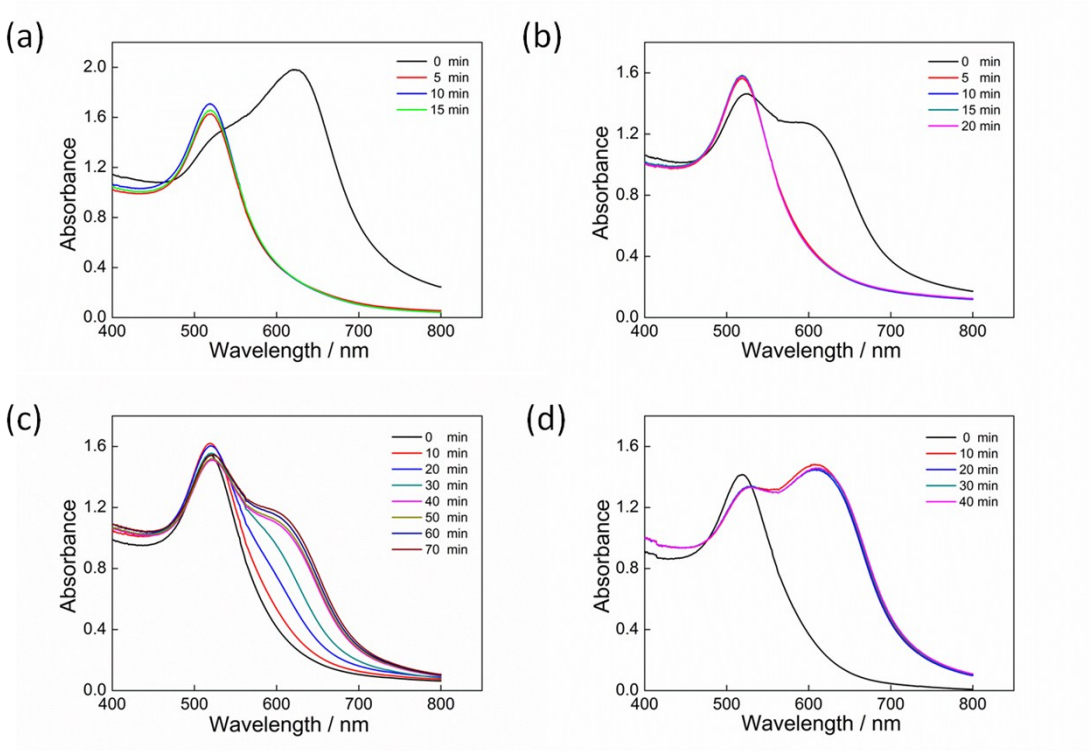


Fig. S4. Optimization of the Chy cleaving time for different peptides: 5 μM P-2 (CAYRA-NH_2) (a); 1.2 μM P-4 (ARYCCPGC-NH_2) (b); 2.2 μM P-6 (DAYRCCPGC-NH_2) (c); 2.4 μM P-7 (DDCCPGCYRACC) (d).

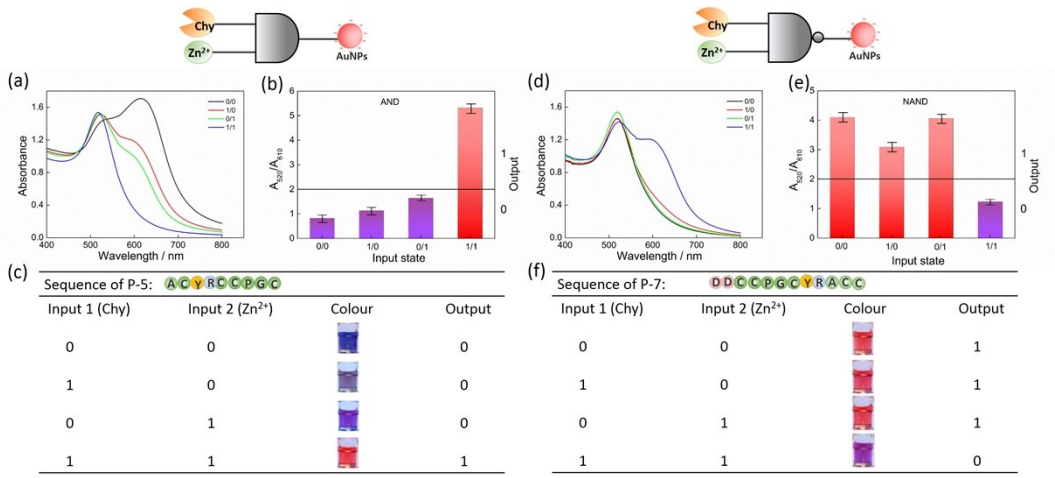
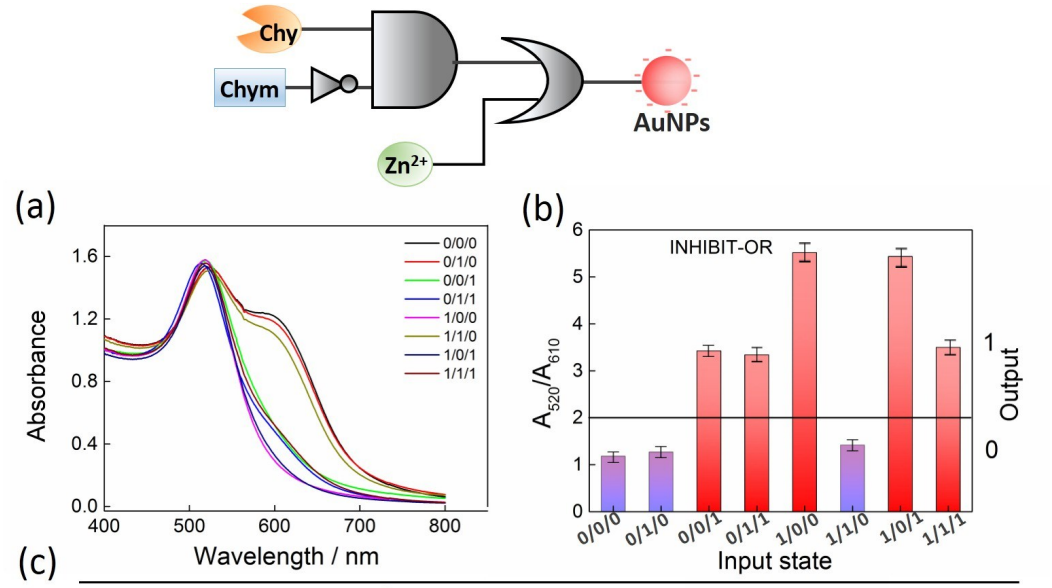


Fig. S5. The AND logic gate reflected by the absorption spectra (a) and the bar graph of the absorbance ratio (A_{520}/A_{610}) corresponding to the four input states (b); the truth table corresponding to the AND gate containing the sequence of computing peptide, four input/output states of the gate and the corresponding solution colour of each output signal. The absorption spectra (d) and the bar graph of the absorbance ratio (A_{520}/A_{610}) (e) of NAND logic gate; the truth table corresponding to the NAND gate containing the sequence of computing peptide, four input states and output states of the gate, and the corresponding colour of each output (f).



(c)

Sequence of P-4: A R Y C C P G C

Input 1 (Chy)	Input 2 (Chym)	Input 3 (Zn^{2+})	Colour	Output
0	0	0		0
0	1	0		0
0	0	1		1
0	1	1		1
1	0	0		1
1	1	0		0
1	0	1		1
1	1	1		1

Fig. S6. The INHIBIT-OR combinational logic gate based on the peptide-mediated AICC of AuNPs. The absorption spectra (a), the absorption ratios (A_{520}/A_{610}) (b), and the truth table of the INHIBIT-OR logic gate (c).

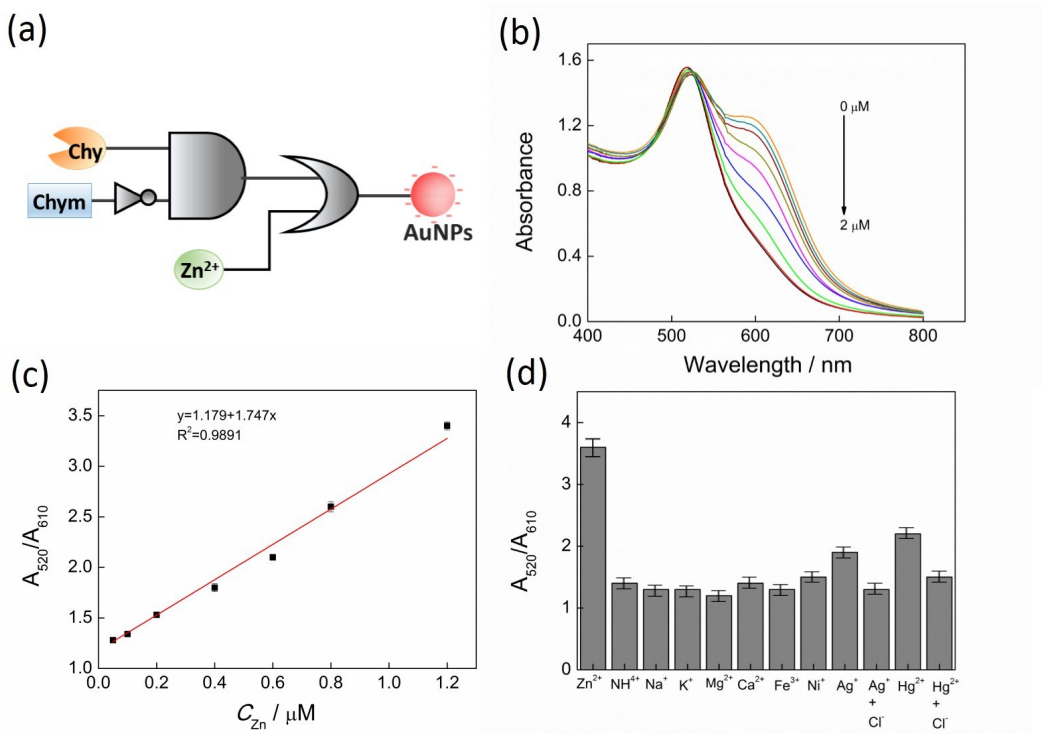


Fig. S7. The INHIBIT-OR logic gate for the Zn^{2+} detection. The symbol of INHIBIT-OR logic gate (a).The absorption spectra of AuNPs with P-4 (1.2 μM) and Zn^{2+} (0 μM – 2 μM) (b). The linear relationship between the absorption ratio (A_{520}/A_{610}) and the concentrations of Zn^{2+} (0.05 μM– 1.2 μM) (c). The absorption ratio (A_{520}/A_{610}) of AuNPs with P-4 and different metal ions (2 μM), while Ag^{+} and Hg were added extra Cl^{-} to prohibit the interference (d).

Table S2. The comparison of AuNPs-based Chy detecting method with other previous methods.

Methods	Detection principle	Detection range	Limit of detection	Disadvantage	Advantage
This method	AuNPs-based colorimetry sensing	0.2 μg–8 μg/L (8.5 pM-340 pM)	0.13 μg/L (5.5 pM)	Discontinous detection	Facile, Economic, Time-saving, High-selective, Homogenous
Chymotrypsin fluormetric assay kit[4]	Utilizing dye-labelled substrate	0.7-3 nM	0.2 nM	Low selective, Low sensitive Expensive	Convenient, Real-time, Commercially available
Electrochemistry[5]	Based on substrate-modified electrodes	5.5–250 μg/L (0.23 nM-10.6 pM)	1.6 μg/L (67.6 pM)	Low sensitive, Unstable	Continuous, Sensitive, Selective
Mass spectrometry[6]	Identification by molecular mass	6-60 pM	1.5 pM	Heterogeneous, Time-costing, High-cost, Discontinous detection	Sensitive, Selective

Table S3. The comparison of AuNPs-based Zn^{2+} detecting method with other previous methods.

Methods	Detection principle	Detection range	Limit of detection	Disadvantage	Advantage
This method	AuNPs-based colorimetry sensing	0.05-1.2 μM	17 nM	Discontinous detection	Facile, Economic, Time-saving, High selectivity, Homogenous
Atomic absorption/emission spectroscopy[1]	Utilizing the characteristic of element	0.7-3 μM	200 nM	Heterogeneous, Time-consuming, High-cost, Discontinous detection	Selective, Repeatable
Fluorescence[2]	Using fluorescent molecule as probe	0.01-0.28 μM	1 nM	Low selective, Toxicant	Sensitive, Convenient, Real-time
Electrochemistry[3]	Based on ion selective electrode	50-750 μM	10 μM	Unstable, Low sensitive	Selective, Cost-effective

Reference

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4. The assay kit was purchased from company of Abcam (ab112154 Proteasome 20S Activity Assay Kit (Fluorometric)).
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6. X. Yan, L. Yang, and Q. Wang, *Angew. Chem. Int. Ed.*, 2011, 50, 5130.