

# Identification of Proteins and Bacteria Based on Metal Ions- Gold Nanoclusters Sensor Array

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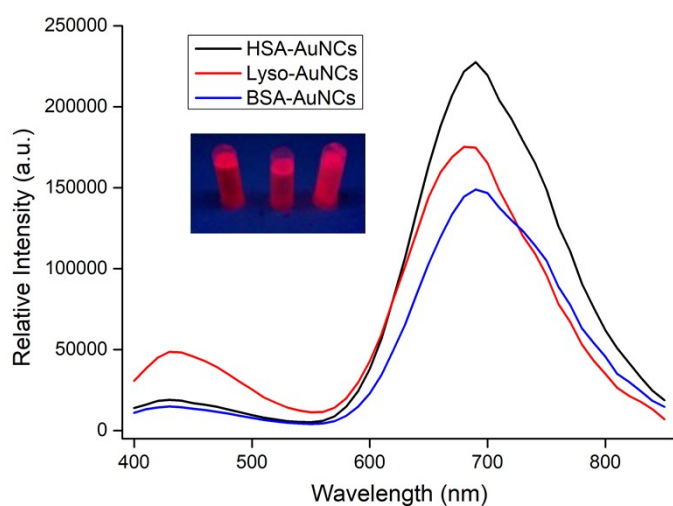


Figure S1. Fluorescence emission spectra of protein-stabilized AuNCs (BSA-AuNCs, HAS-AuNCs and Lys-AuNCs) at the excitation wavelength at 365nm.

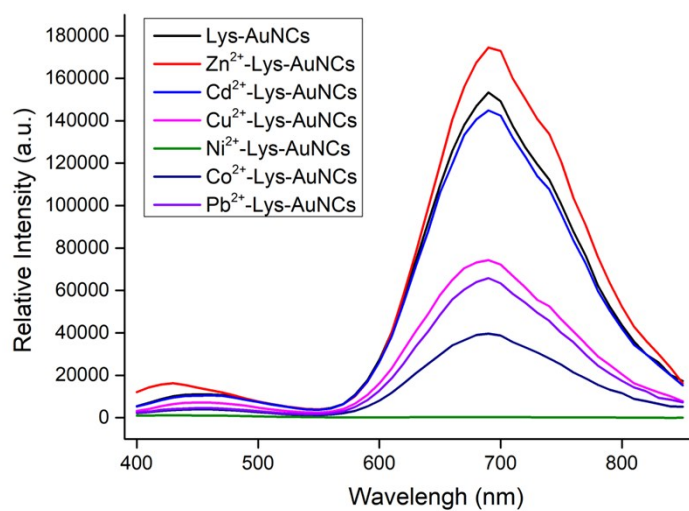


Figure S2. Fluorescence emission spectra of Lys-AuNCs after co-precipitation with different cations. The concentration of  $Zn^{2+}$ ,  $Cd^{2+}$ ,  $Cu^{2+}$ ,  $Ni^{2+}$ ,  $Co^{2+}$ , and  $Pb^{2+}$  is  $0.02 \text{ mol L}^{-1}$ .

Table S1 The results of precipitation formation after co-precipitation of BSA-AuNCs with various cations at different concentrations.

Cations added	0.005 (mol L <sup>-1</sup> )	0.01 (mol L <sup>-1</sup> )	0.02 (mol L <sup>-1</sup> )	0.04 (mol L <sup>-1</sup> )	0.06 (mol L <sup>-1</sup> )	0.08 (mol L <sup>-1</sup> )	0.1 (mol L <sup>-1</sup> )
Zn <sup>2+</sup>	-	*	+	+	+	+	+
Cd <sup>2+</sup>	-	*	+	+	+	+	+
Mg <sup>2+</sup>	-	-	-	-	-	-	-
Co <sup>2+</sup>	-	-	*	+	+	+	+
Cu <sup>2+</sup>	-	-	*	*	*	*	*
Ca <sup>2+</sup>	-	-	-	-	-	-	-
Ni <sup>2+</sup>	-	*	+	+	+	+	+
Pb <sup>2+</sup>	-	*	*	*	*	*	*

“-” No precipitation, “\*” Partial precipitation, “+” Complete precipitation.

Table S2 The results of precipitation formation after co-precipitation of Lys-AuNCs with various cations at different concentrations.

Cations added	0.005 (mol L <sup>-1</sup> )	0.01 (mol L <sup>-1</sup> )	0.02 (mol L <sup>-1</sup> )	0.04 (mol L <sup>-1</sup> )	0.06 (mol L <sup>-1</sup> )	0.08 (mol L <sup>-1</sup> )	0.1 (mol L <sup>-1</sup> )
Zn <sup>2+</sup>	-	*	+	+	+	+	+
Cd <sup>2+</sup>	-	*	+	+	+	+	+
Mg <sup>2+</sup>	-	*	+	+	+	+	+
Co <sup>2+</sup>	-	*	+	+	+	+	+
Cu <sup>2+</sup>	-	*	+	+	+	+	+
Ca <sup>2+</sup>	-	-	-	-	-	-	-
Ni <sup>2+</sup>	*	+	+	+	+	+	+
Pb <sup>2+</sup>	-	-	*	+	*	*	*

Table S3. Jackknifed Classification Matrix of LDA analysis in 9 proteins differentiation (5 $\mu$ M)

	BS A	Casei n	Lysozy me	Papai n	Hemoglob in	Lipas e	Myoglobi n	Pepsi n	Trypsi n	%corre ct
BSA	6	0	0	0	0	0	0	0	0	100
Casein	0	6	0	0	0	0	0	0	0	100
Lysozyme	0	0	6	0	0	0	0	0	0	100
Papain	0	0	0	6	0	0	0	0	0	100
Hemoglobi n	0	0	0	0	6	0	0	0	0	100
Lipase	0	0	0	0	0	6	0	0	0	100
Myoglobin	0	0	0	0	0	0	6	0	0	100
Pepsin	0	0	0	0	0	0	0	6	0	100
Trypsin	0	0	0	0	0	0	0	0	6	100
Total	6	6	6	6	6	6	6	6	6	100

The jackknifed classification illustrates no overlap between the groups at all, and all the cases are classified with 100% classification accuracy.

Cumulative proportion of total dispersion

0.506	0.970	0.993	0.998	1.000	1.000
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From the above table, the values of different factors can be calculated. The first and second factors contribute largely to the classification, 50.6% and 46.4% (0.970-0.506) respectively. The third factor and fourth factor account for 2.3% (0.993-0.970) and 0.5% (0.998-0.993). So, it could be easily found that the first two factors can make a good identification to 8 proteins.

Table S4. Jackknifed Classification Matrix of LDA analysis in 9 proteins differentiation (0.5 $\mu$ M)

	BS A	Casei n	Lysozy me	Papai n	Hemoglob in	Lipas e	Myoglobi n	Pepsi n	Trypsi n	%corre ct
BSA	6	0	0	0	0	0	0	0	0	100
Casein	0	6	0	0	0	0	0	0	0	100
Lysozyme	0	0	6	0	0	0	0	0	0	100
Papain	0	0	0	6	0	0	0	0	0	100
Hemoglobi n	0	0	0	0	6	0	0	0	0	100
Lipase	0	0	0	0	0	6	0	0	0	100
Myoglobin	0	0	0	0	0	0	6	0	0	100
Pepsin	0	0	0	0	0	0	0	6	0	100
Trypsin	0	0	0	0	0	0	0	0	6	100
Total	6	6	6	6	6	6	6	6	6	100

The jackknifed classification illustrates no overlap between the groups at all, and all the cases are classified with 100% classification accuracy.

Cumulative proportion of total dispersion

0.630	0.895	0.990	0.995	0.999	1.000
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The first and second factors account for 63% and 26.5% (0.895-0.630). These figures are clearly larger than the third and fourth factors, 9.5% (0.990-0.895) and 0.5% (0.995-0.990).

Table S5. Jackknifed Classification Matrix of LDA analysis in 8 proteins differentiation (50  $\mu$ M)

	BS A	Casei n	Lysozy me	Papai n	Hemoglob in	Lipas e	Myoglobi n	Pepsi n	Trypsi n	%corre ct
BSA	6	0	0	0	0	0	0	0	0	100
Casein	0	6	0	0	0	0	0	0	0	100
Lysozyme	0	0	6	0	0	0	0	0	0	100
Papain	0	0	0	6	0	0	0	0	0	100
Hemoglobi n	0	0	0	0	6	0	0	0	0	100
Lipase	0	0	0	0	0	6	0	0	0	100
Myoglobin	0	0	0	0	0	0	6	0	0	100
Pepsin	0	0	0	0	0	0	0	6	0	100
Trypsin	0	0	0	0	0	0	0	0	6	100
Total	6	6	6	6	6	6	6	6	6	100

The jackknifed classification illustrates no overlap between the groups at all, and all the cases are classified with 100% classification accuracy.

Cumulative proportion of total dispersion

0.735	0.887	0.997	0.999	1.000	1.000
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The first three factors account for 73.5%, 15.2% (0.887-0.735) and 11% (0.997-0.887) respectively. And the fourth factor just contribute little to the classification (0.2%, 0.999-0.997).

Table S6. Jackknifed Classification Matrix of LDA analysis in 5 bacteria differentiation

	Bacillus aceticus	Bacillus natto	Bacillus	Escherichia coli	Pseudomonas aeruginosa	%correct
Bacillus aceticus	2	0	4	0	0	33
Bacillus natto	0	6	0	0	0	100
Bacillus	2	0	4	0	0	67
Escherichia coli	0	0	0	6	0	100
Pseudomonas aeruginosa	0	0	0	0	0	100
Total	4	6	8	6	6	80

The jackknifed classification illustrates overlap between Bacillus aceticus and Bacillus. Four cases of Bacillus aceticus were misclassified to Bacillus, and the accuracy is just 33%. Similarly, two cases of Bacillus were misclassified to Bacillus aceticus, and the accuracy is around 67%. Besides, the rest of cases can be totally classified.

Cumulative proportion of total dispersion

0.813	0.931	0.997	1.000
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It is worth noting that the first factor (81.3%) is significantly larger than other factors. The second factor accounts for 11.8% (0.931-0.813), and this figure is larger than the third factor (6.6%, 0.997-0.931).