Supporting Information

Sensitive and specific detection of clinical bacteria via vancomycin-modified Fe_3O_4@Au nanoparticles and aptamer-functionalized SERS tags

Chuyue Zhang[a,c], Chongwen Wang[b], Rui Xiao[b], Li Tang[a], Jing Huang[a], Di Wu[a], Shuwen Liu[a], Yong Wang[a], Dong Zhang[a], Shengqi Wang[b,*] and Xiangmei Chen[a,*]

a Department of Nephrology, Chinese PLA General Hospital, Chinese PLA Institute of Nephrology, State Key Laboratory of Kidney Diseases, National Clinical Research Center for Kidney Diseases, Beijing Key Laboratory of Kidney Diseases, Beijing 100853, China.

b Beijing Institute of Radiation Medicine, Beijing 100850, China.

c Medical College, Nankai University, Tianjin, China.

The authors Chuyue Zhang, Chongwen Wang and Rui Xiao contributed equally to this work.

*Corresponding Author. *E-mail address:*

sqwang@bmi.ac.cn (S. Wang),

xmchen301@126.com (X. Chen).

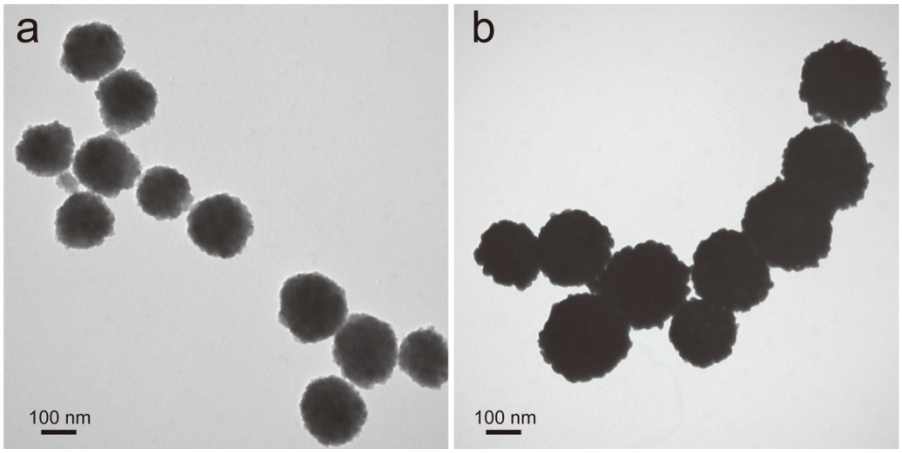

Fig. S1 TEM images of (a) Fe_3O_4 and (b) Fe_3O_4@Au MNPs.

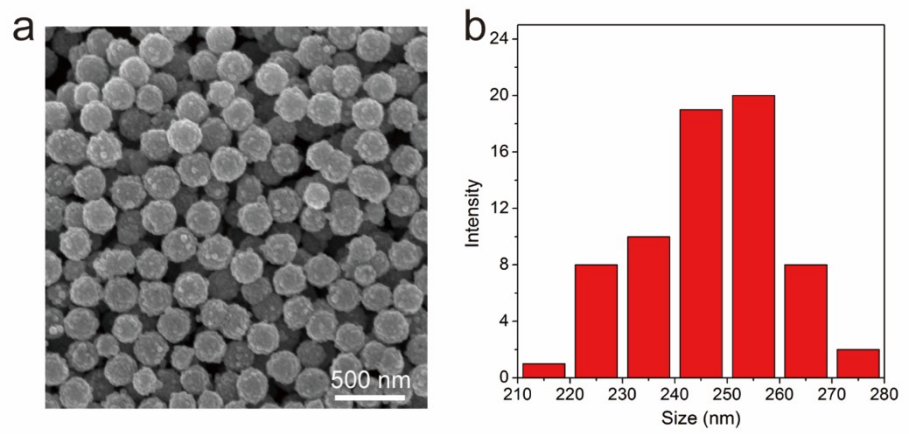

Fig. S2 SEM image (a) and particle size distribution diagram (b) of Fe_3O_4@Au MNPs.

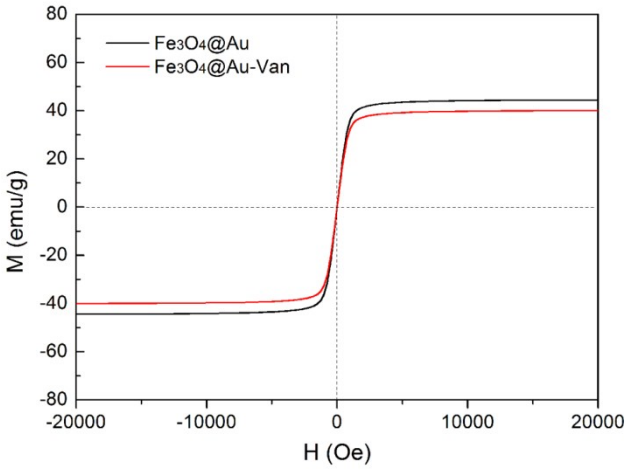

Fig. S3 Magnetic hysteresis curves of the prepared Fe_3O_4@Au and Fe_3O_4@Au-Van MNPs.

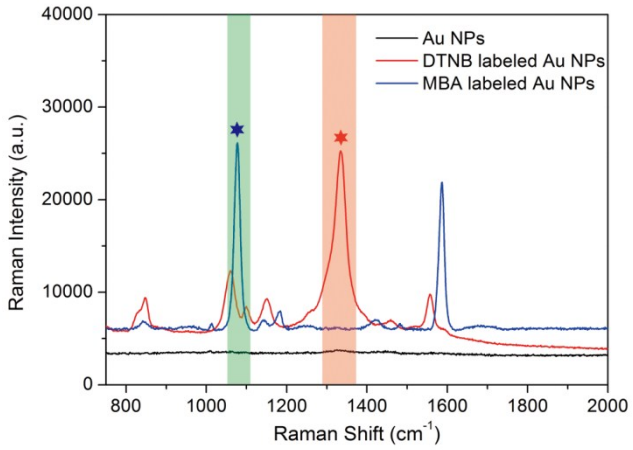

Fig. S4 Raman spectra of Au NPs (black line), DTNB-labeled Au NPs (red line), and MBA-labeled Au NPs (blue line). Characteristic and the strongest Raman peaks of DTNB (1331 cm^{-1}) and MBA (1074 cm^{-1}) were used for quantitative detection of *E. coli* and *S. aureus*, respectively.

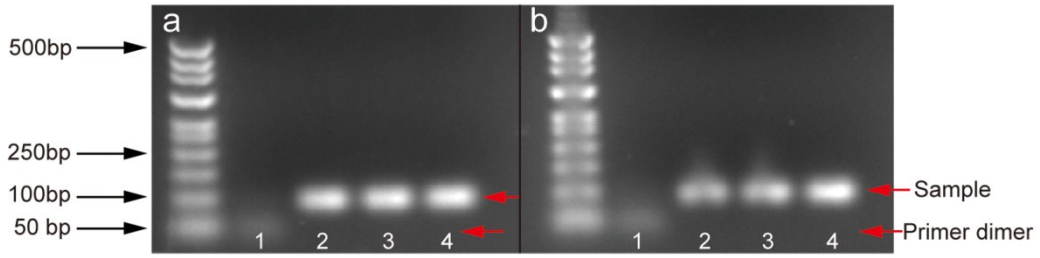

Fig. S5 Agarose gel electrophoresis bands of in situ PCR amplification (35 cycles) using *E. coli* SERS tags (a) and *S. aureus* SERS tags (b) as the DNA template. In each group, sample1 is blank and sample 2-4 is under the same condition. Upstream primer: GCA ATG GTA CGG TAC TTC CTC. Downstream primer: TTA GCA AAG TAG CGT GCA CTT.

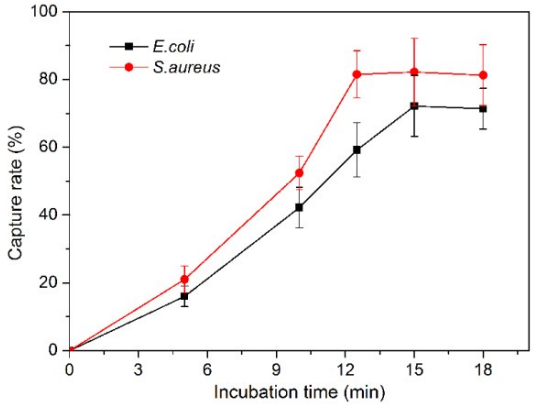

Fig. S6 Capture rates of the Fe_3O_4@Au-Van MNPs for *E.coli* (black line) and *S. aureus* (red line) at different incubation times. The error bars represent the standard deviations from 3 measurement.

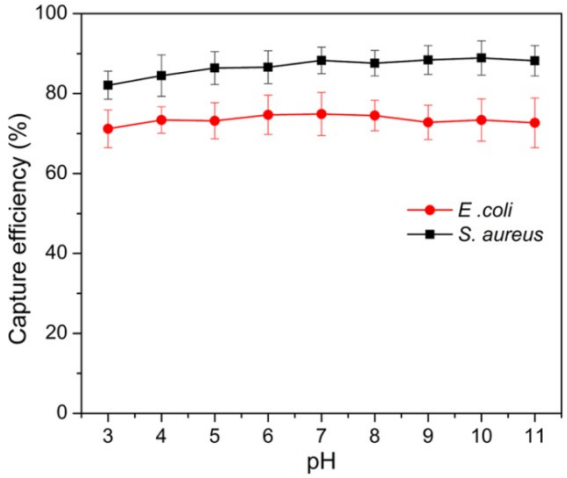

Fig. S7 The capture effciency of Fe_3O_4@Au-Van MNPs for *E. coli* and *S. aureus* in PBS buffer at varying pH. The error bars represent the standard deviations from 3 measurements.

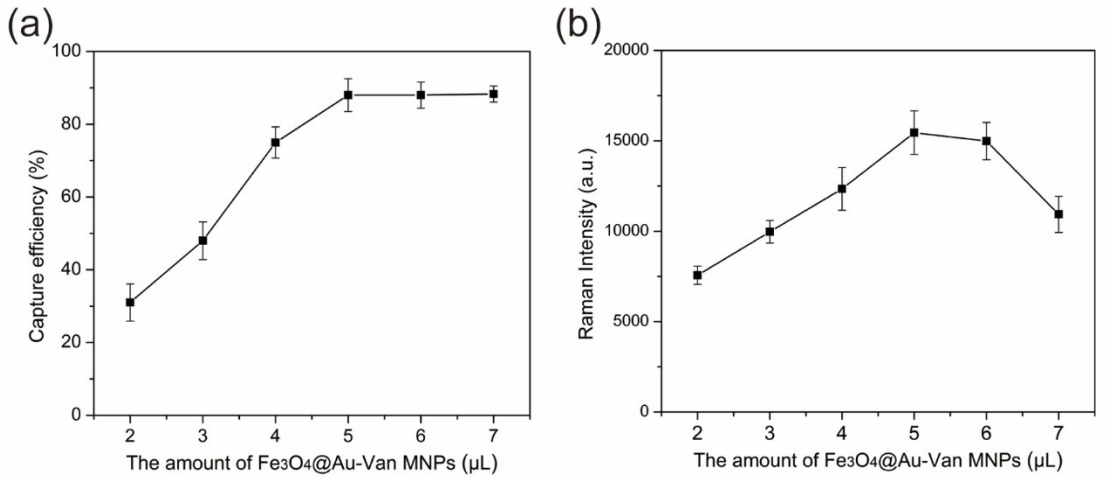

Fig. S8 The capture efficiency (a) and SERS intensity at 1074 cm^{-1} (b) versus the amount of Fe_3O_4@Au-Van MNPs (20 mg/mL) with 15 min interaction time for *S. aureus*. The error bars represent the standard deviations from 3 measurements.

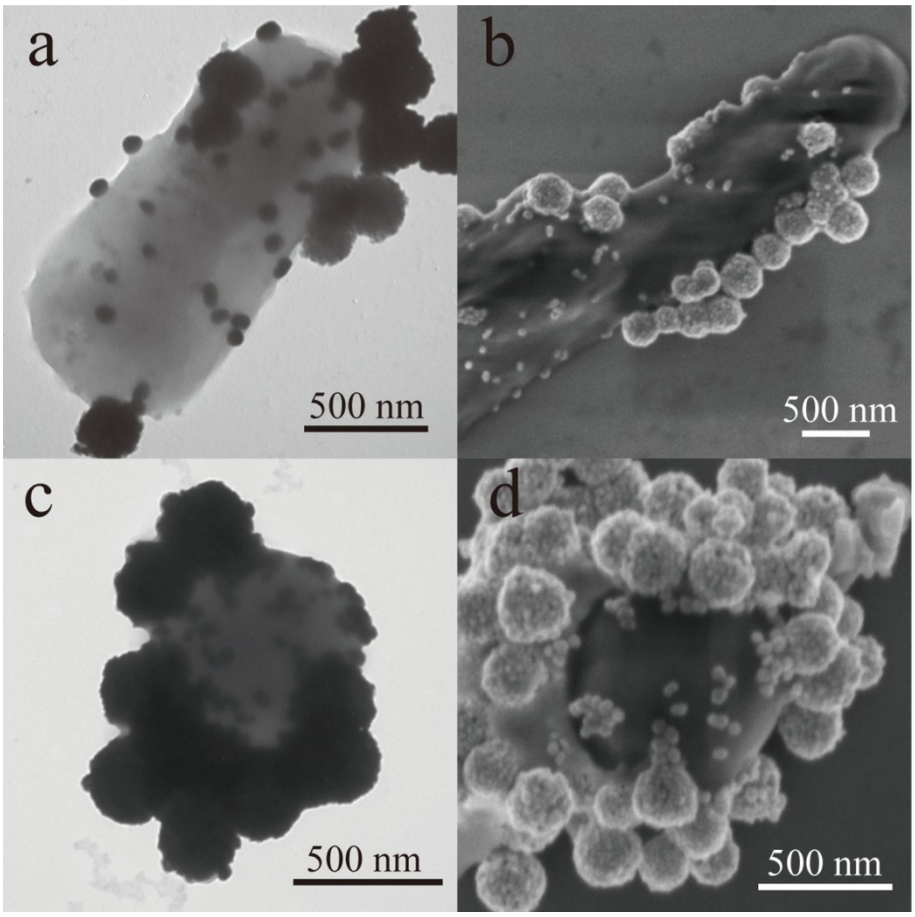

Fig. S9 The enlarged TEM and SEM images of Fe_3O_4@Au-Van/*E. coli*/SERS tags complexes (a-b) and Fe_3O_4@Au-Van/*S. aureus*/SERS tags complexes (c-d).

Table S1 Aptamer sequences used in this study.

Name	Length (Mer)	Sequence(5'-3')	Modification
E1	88	GCAATGGTACGGTACTTCCTCGGCACG TTCTCAGTAGCGCTCGCTGGTCATCCC ACAGCTACGTCAAAAGTGCACGCTACT TTGCTAA	5'-NH_2-C6
E1-cy3	88		5'-Cy3
Sa1	88	GCAATGGTACGGTACTTCCACTTAGGT CGAGGTTAGTTTGTCTTGCTGGCGCAT CCACTGAGCGCAAAAGTGCACGCTAC TTTGCTAA	5'-NH_2-C6
Sa1-FITC	88		5'-FITC

Table S2 Classification and quantification in clinical samples of *E. coli* determined by the SERS platform and standard quantitative urine culture.

Clinical samples	**SERS biosensor**		**Standard quantitative urine culture**	
	Classification	**Quantification**	**Classification**	**Quantification**
1	*E. coli*	1.3×10^3 cfu mL^{-1}	*E. coli*	2×10^3 cfu mL^{-1}
2	*E. coli*	5.1×10^4 cfu mL^{-1}	*E. coli*	8×10^4 cfu mL^{-1}
3	*E. coli*	3.7×10^4 cfu mL^{-1}	*E. coli*	5×10^4 cfu mL-1
4	*E. coli*	9.4×10^4 cfu mL^{-1}	*E. coli*	8×10^4 cfu mL^{-1}
5	*E. coli*	3.8×10^4 cfu mL^{-1}	*E. coli*	5×10^4 cfu mL^{-1}
6	*E. coli*	over 10^5 cfu mL^{-1}	*E. coli*	over 10^5 cfu mL^{-1}
7	*E. coli*	8.7×10^3 cfu mL^{-1}	*E. coli*	3×10^3 cfu mL^{-1}
8	*E. coli*	over 10^5 cfu mL^{-1}	*E. coli*	over 10^5 cfu mL^{-1}
9	*E. coli*	10^4 cfu mL^{-1}	*E. coli*	10^4 cfu mL^{-1}
10	*E. coli*	6.2×10^4 cfu mL^{-1}	*E. coli, A. baumannii*	10^5 cfu mL^{-1}
11	*E. coli*	4.4×10^3 cfu mL^{-1}	*E. coli*	2×10^3 cfu mL^{-1}
12	*E. coli*	7.9×10^4 cfu mL^{-1}	*E. coli*	5×10^4 cfu mL^{-1}
13	*E. coli*	6.6×10^3 cfu mL^{-1}	*E. coli*	8×10^3 cfu mL^{-1}
14	*E. coli*	over 10^5 cfu mL^{-1}	*E. coli*	over 10^5 cfu mL^{-1}
15	*E. coli*	8.7×10^3 cfu mL^{-1}	*E. coli*	10^4 cfu mL^{-1}
16	*E. coli*	9.3×10^4 cfu mL^{-1}	*E. coli*	8×10^4 cfu mL^{-1}
17	*E. coli*	over 10^5 cfu mL^{-1}	*E. coli*	over 10^5 cfu mL^{-1}
18	*E. coli*	10^4 cfu mL^{-1}	*E. coli*	10^4 cfu mL^{-1}
19	*E. coli*	over 10^5 cfu mL^{-1}	*E. coli*	over 10^5 cfu mL^{-1}
20	*E. coli*	2.3×10^4 cfu mL^{-1}	*E. coli*	10^4 cfu mL^{-1}

Table S3 Classification and quantification in clinical samples of *S. aureus* determined by the SERS platform and standard quantitative urine culture.

Clinical samples	SERS biosensor		Standard quantitative urine culture	
	Classification	**Quantification**	**Classification**	**Quantification**
1	*S. aureus*	over 10^5 cfu mL^{-1}	*S. aureus*	over 10^5 cfu mL^{-1}
2	*S. aureus*	10^4 cfu mL^{-1}	*S. aureus*	10^4 cfu mL^{-1}
3	*S. aureus*	3.3×10^3 cfu mL^{-1}	*S. aureus*	10^3 cfu mL^{-1}
4	*S. aureus*	10^4 cfu mL^{-1}	*S. aureus*	10^4 cfu mL^{-1}