Supporting Information *for*

Finite-difference time-domain to screen Au NPs as SERS active substrate for sensitive determination of prohibited drugs in fish via solvent cleaning

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Experimental section

Materials and Reagents.

$HAuCl_4 \cdot 4H_2O$ (99.9%) and trisodium citrate ($Na_3C_6H_5O_7 \cdot 2H_2O$, 99%) were purchased from Sinopharm Chemical Reagent Co., Ltd., China. Ascorbic acid (AA, 99%) was received from Shanghai Aladdin Biochemical Technology Co., Ltd. Teflon membrane (polytetrafluoroethylene, PTFE) with 0.22 μm pore size was purchased from Tianjin Keyilong Experiment Equipment Co., Ltd. The illegal additive of CV was purchased from Tianjin Damao Chemical Reagent Co., Ltd. The fish were obtained from Shijiazhuang Yunda Biological Technology Co., Ltd. Methanol was purchased from Thermo Fisher Scientific Co., Ltd., China. All chemicals were used without any further purification. Millipore Ultrapure water (18.25 MΩ•cm) was used in all experiments.

Instrument Characterization.

In order to obtain the morphology and structure of Au NPs (16, 50, 120 nm), scanning electron microscope (SEM) (Hitachi, S-4800) and transmission electron microscope (TEM) (Hitachi, H-7650) were used for characterization. Optical properties of Au NPs (16, 50, 120 nm) were measured by UV−Vis spectrophotometer (Aglient, Carry 60). The particle size distribution of Au NPs was measured by the dynamic light scattering (DLS) instrument (Malvern, ZS90). The fish puree was grinded by a vertical mill (TenCan Powder XQM-0.4) at the speed of 700 r/min for 20 min. In order to obtain the SERS signal of CV in fish, a laser confocal Raman spectrometer (Horiba Scientific, XploRA PLUS) was used for testing. The test parameters included laser wavelength of 638 nm, focusing objective of 50X, The scanning parameters included a grating of 1200 mm^{-1}, integration

time of 1 s, scanning number 1 time. Each sample collected Raman spectra in the range of 400-1800 cm^{-1} for analysis.

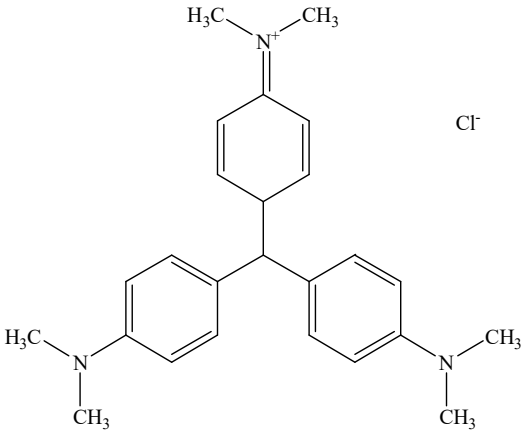

Figure S1: Molecular structure of crystal violet (CV).

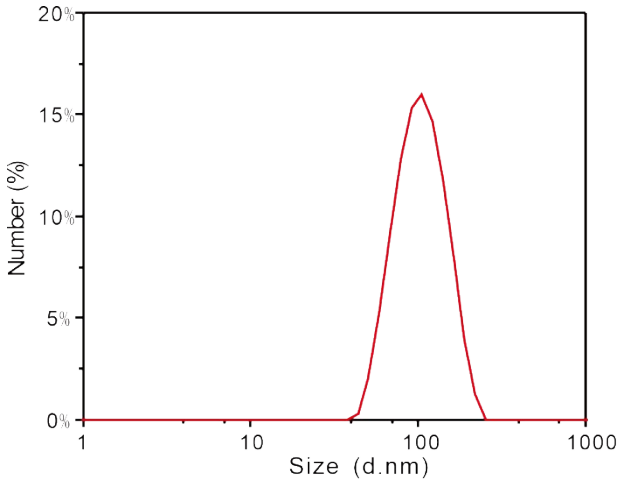

Figure S2: Hyrodynamic particle size of Au NPs through dynamic light scattering (DLS) analysis.

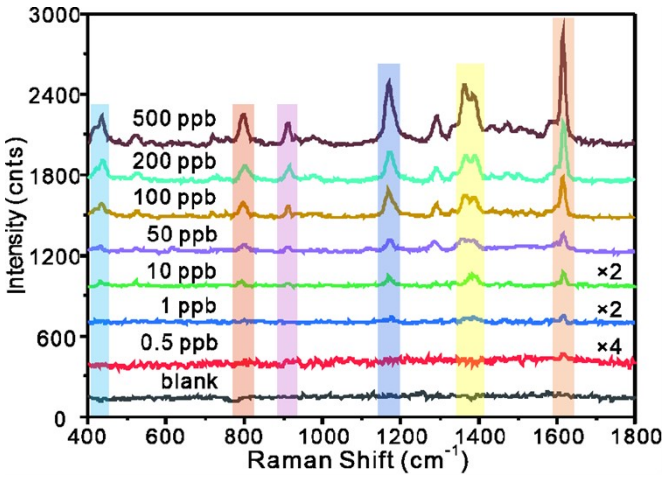

Figure S3: SERS spectra of ~100 nm Au NPs absorbing CV standard solutions with different concentrations from 500 ppb to 0.5 ppb.

Table 1： Wavenumbers of SERS spectra of CV and band assignments [1, 2].

Wavenumber/cm^{-1}	Band Assignment
436	γ (phenyl-C-phenyl)
803	γ (C-H)
915	Ring-breathing
1170	υ (C-H)
1376	υ (N-phenyl), υ (C-C)
1536	υ (C-C)
1616	υ (C-C)

◆ ν, stretching vibration; γ, out-of-plane bending.

References

1. J. Song, Y. Huang, Y. Fan, Z. Zhao, W. Yu, B. A. Rasco and K. Lai, *Nanomaterials*, 2016, **6**, 175.
2. H. K. Turley, Z. Hu, D. W. Silverstein, D. A. Cooper, L. Jensen and J. P. Camden, *The Journal of Physical Chemistry C*, 2016, **120**, 20936-20942.