Supporting Information for

Interfacial Chemistry Governs SERS Detectability of Trimethoprim and Ketoprofen: Adsorption Geometry and Chloride-Mediated Activation

Dao Thi Nguyet Nga[a,1], Ha Anh Nguyen[a,*,1], Mai Quan Doan[a], Anh-Tuan Le[a,**]

[a]*Phenikaa University Nano Institute (PHENA), Phenikaa School of Engineering (PSE), Phenikaa University, Hanoi 12116, Vietnam*

Corresponding authors:

*anh.nguyenha@phenikaa-uni.edu.vn (H.A.Nguyen)

**tuan.leanh@phenikaa-uni.edu.vn (A.T.Le)

[1] D.T.N. Nga and H.A. Nguyen contributed equally to this work

Calculation of limit of detection (LOD)

The standard curve of linear detecting range was given as:

$$Y = A + B \times Log(X) \quad (1)$$

where A and B are intercept and slope of regression equation obtained through the plot of the logarithmic SERS intensity (Y) – logarithmic concentration (X).

The LOD is calculated using the following equation [1]

$$LOD = 10^{\left[(Y_{blank} + 3SD)/Y_{blank} - A\right]/B} \quad (2)$$

where Y_{blank} and SD are the SERS signal and the standard deviation of blank sample, respectively.

SD is calculated via the well-known formula:

$$SD = \sqrt{\frac{1}{n-1} \times \sum_{i}^{n} (x_i - x_{average})^2} \quad (3)$$

where x_i if the "i" sample of the series of measurements, $x_{average}$ is the average value of SERS signal obtained from the blank sample repeated n times.

Calculation of relative standard deviation (RSD)

The RSD value of repeatability and reproducibility is calculated via the well-known formula:

$$\text{RSD} = \frac{SD \times 100}{x_{average}} \quad (4)$$

where SD is the standard deviation that calculates using equation 4 and $x_{average}$ is the average value of SERS signal obtained from each measurement.

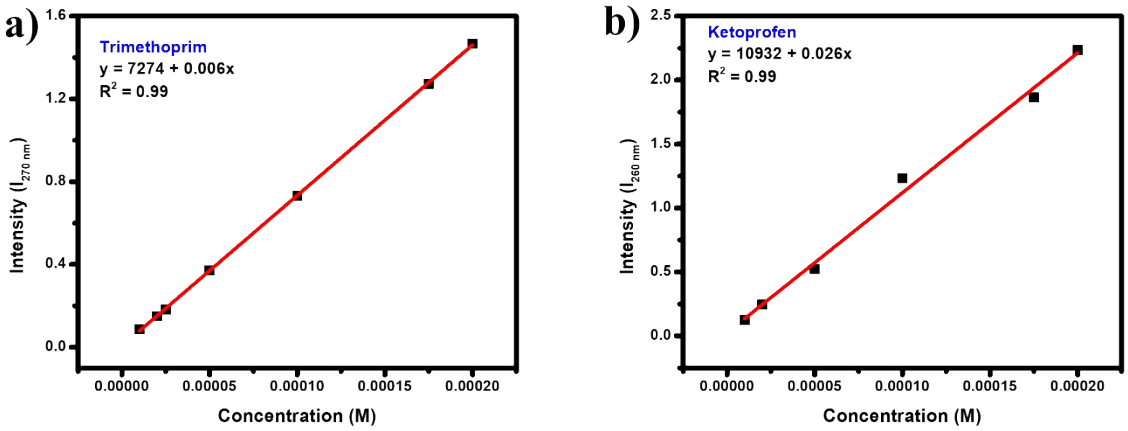

Figure S1: Plot of the SERS intensity at 270nm and 260 nm against (a) Trimethoprim and (b) Ketoprofen concentration in the standard solution.

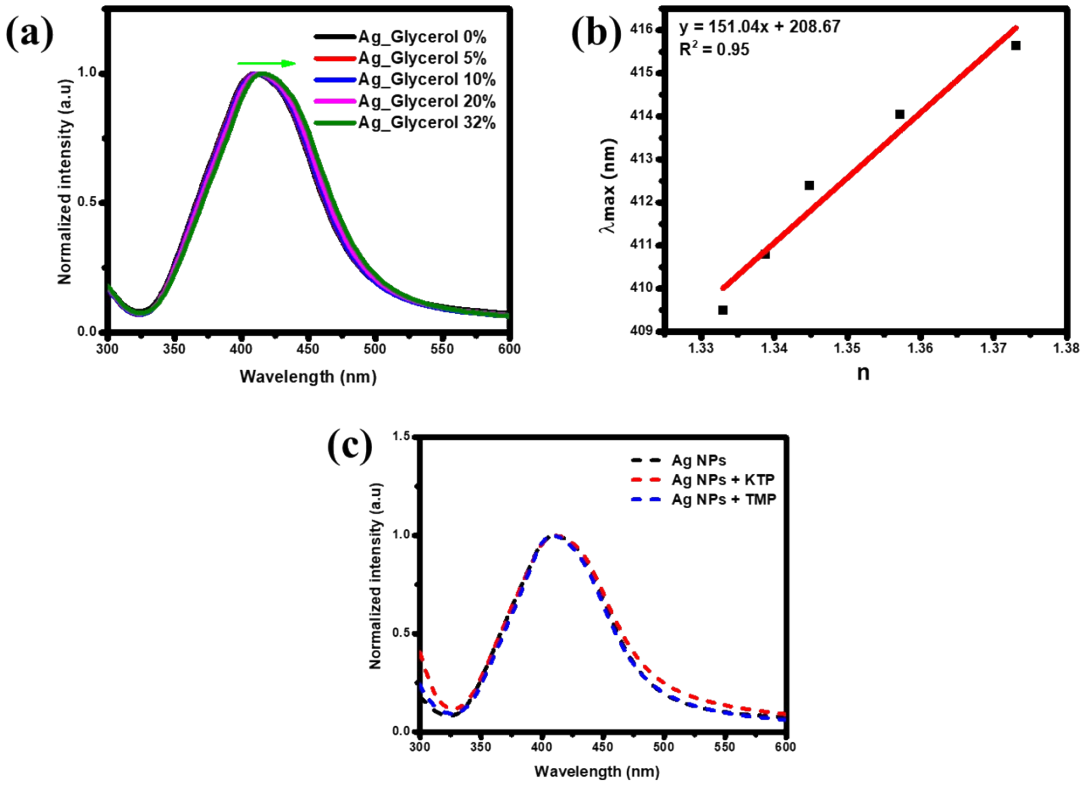

Figure S2: (a) Normalized adsorption spectra of e-AgNPs in glycerol (0 – 32%); (b) Plot of λ_{max} of the absorption spectra of e-AgNPs in glycerol (0 – 32%) versus n measured by refractometer; (c) Normalized adsorption spectra of e-AgNPs in the presence of TMP and KTP (1.75×10^{-4} M) in comparison with that of pure e-AgNPs.

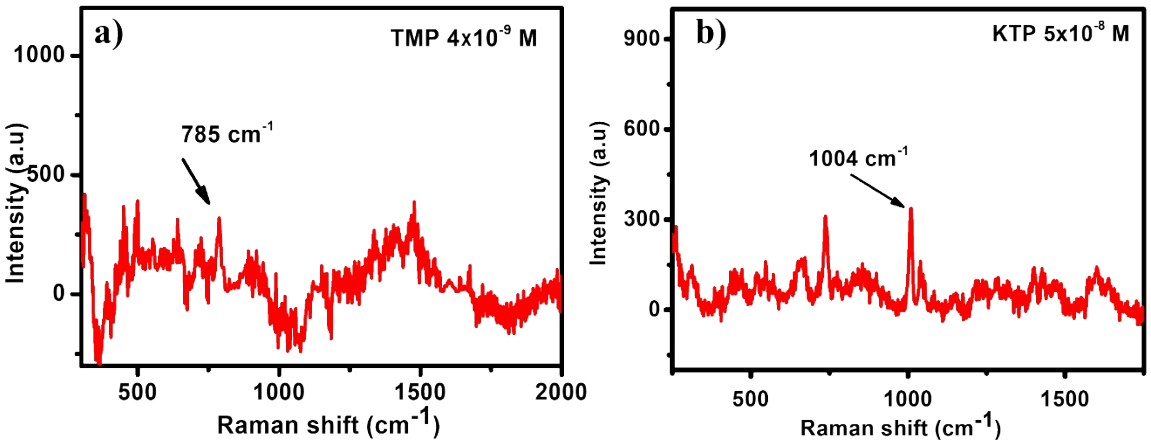

Figure S3: SERS spectra of (a) TMP (4×10^{-9} M) and (b) KTP (5×10^{-8} M) on e-AgNPs

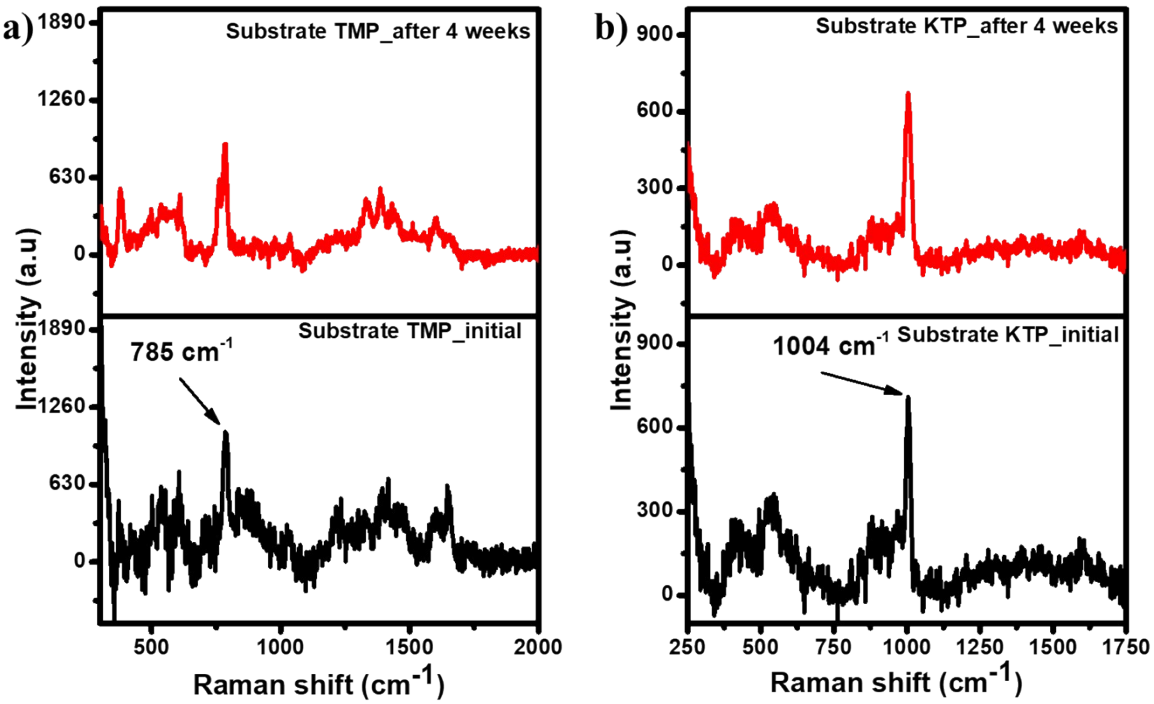

Figure S4: SERS spectra of (a) TMP and (b) KTP on freshly prepared and 4-week stored e-AgNPs.

Table S1: The recovery values for four concentrations of trimethoprim in the tap-water sample.

Real sample	Analyte	Concentration of TCZ (M)	Recovery (%)
Tap-water	Trimethoprim	10^{-4}	96
		10^{-5}	89
		10^{-6}	91
		10^{-7}	93

Table S2: The recovery values for four concentrations of ketoprofen in the tap-water sample.

Real sample	Analyte	Concentration of TCZ (M)	Recovery (%)
Tap-water	Ketoprofen	10^{-4}	93
		10^{-5}	95
		10^{-6}	92
		10^{-7}	88

References

(1) Chen, R.; Shi, H.; Meng, X.; Su, Y.; Wang, H.; He, Y. Dual-Amplification Strategy-Based SERS Chip for Sensitive and Reproducible Detection of DNA Methyltransferase Activity in Human Serum. *Anal. Chem.* **2019**, *91* (5), 3597–3603. https://doi.org/10.1021/acs.analchem.8b05595.