- Supporting Information -

A Flexible Plasmonic SERS Hydrogel Patch for Metabolite Sensing on Bio-interfaces

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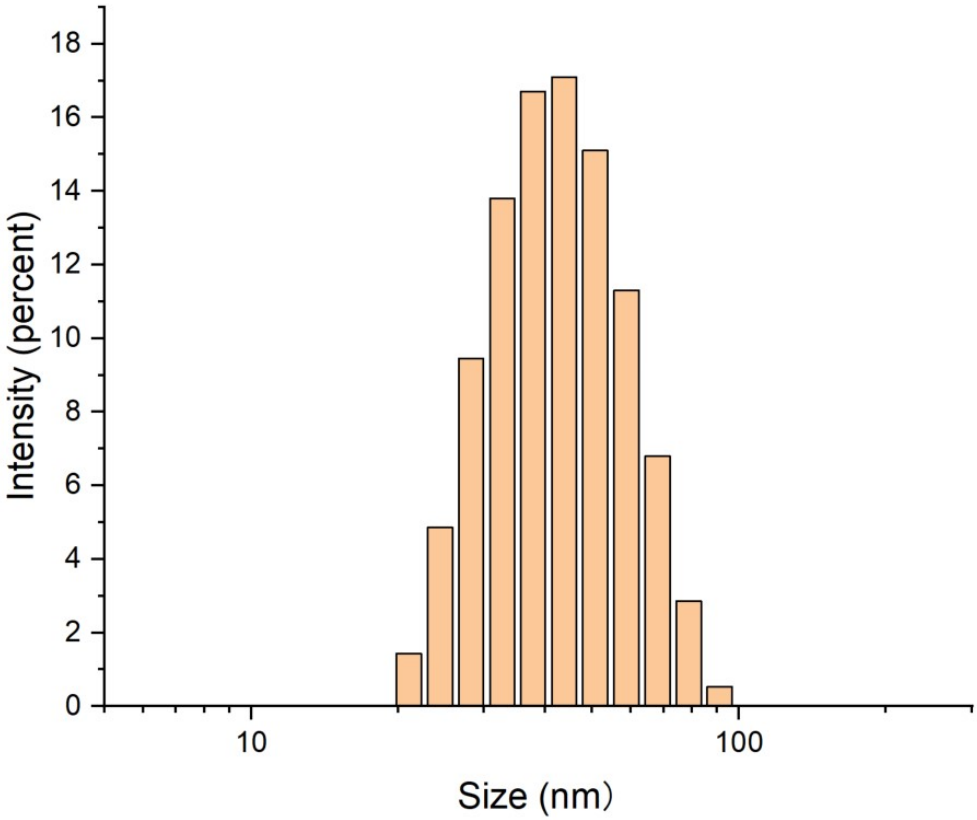

Figure S1. Hydrodynamic size distribution of Ag NPs, with the peak value at 44 nm.

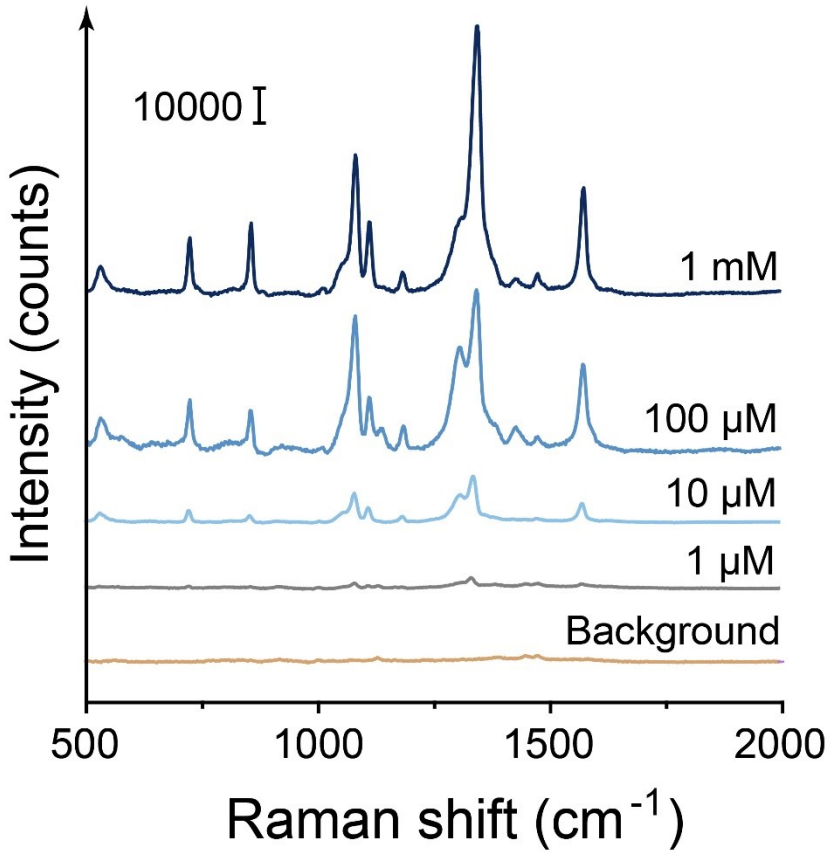

Figure S2. Raman signals of 4-NBT molecules at different concentrations on the SERS hydrogel. The measurements were using 785 nm excitation, 50 mW power, and 500 ms integration time.

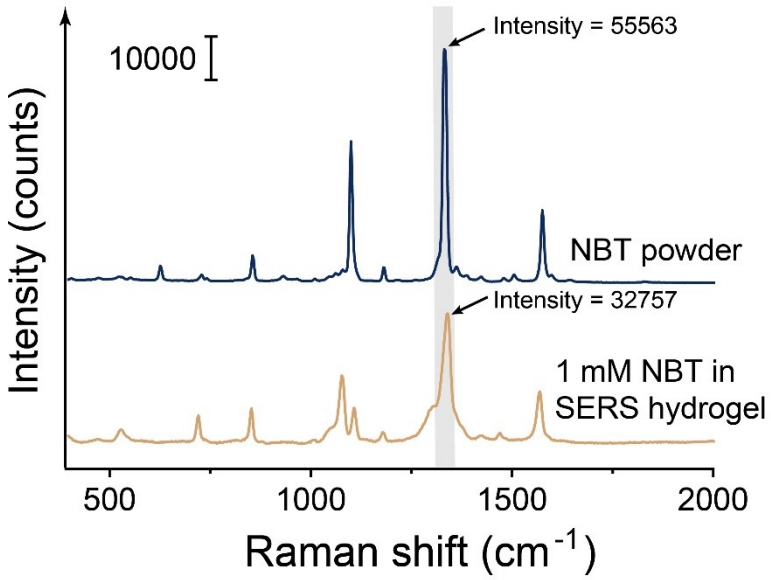

Figure S3. Comparison the normal Raman intensity of NBT powder (integration time = 50 ms) and SERS signal of 1 mM 4-NBT solution dropping on the SERS hydrogel (integration time = 300 ms). The enhancement factor (EF) was calculated to be 10^5, by peak intensity at 1340 cm^{-1}.

EF was calculated using the following formula.

$$EF = \frac{I_{SERS}/N_{SERS}}{I_{Raman}/N_{Raman}} = \frac{I_{SERS}}{I_{Raman}} \cdot \frac{N_{Raman}}{N_{SERS}}$$

In the formula, the ratio of I_{SERS} to I_{Raman} can be calculated using peak intensity at 1340 cm^{-1}.

$$\frac{I_{SERS}}{I_{Raman}} = \frac{32757\ counts/300\ ms}{55563\ counts/50\ ms} = 0.098$$

Meanwhile, N_{SERS} and N_{Raman} represent the effective number of molecules in SERS and Raman tests. N_{SERS} can be estimated based on the area occupied by each molecule on the substrate. Assume the diameter of the light spot d_{spot} = 2 μm, packing area of each molecule $S_{molecule}$ = 0.2 nm^2, then

$$N_{SERS} = \frac{\pi \cdot (\frac{d_{spot}}{2})^2}{S_{molecule}} = \frac{\pi \cdot (\frac{2\ \mu m}{2})^2}{0.2\ nm^2} = 1.57 \times 10^7$$

For N_{Raman}, the experiment is conducted on NBT powder. The density of the powder ρ_{NBT} = 1.2 g/cm^3, molar mass of NBT M_{NBT} = 125.19 g/mol and the volume of the excited molecules can be estimated using d_{spot} and focal depth of the lens l = 1.2 mm [1].

$$N_{Raman} = \frac{\pi \cdot \left(\frac{d_{spot}}{2}\right)^2 \cdot l \cdot \rho_{NBT}}{M_{NBT}} \cdot N_A = \frac{\pi \cdot \left(\frac{2\ \mu m}{2}\right)^2 \times 1.2\ mm \times 1.2\ g/cm^3}{125.19\ g/mol} \times 6.02 \times 10^{23} \times 10^{13}$$

Therefore, the EF of the substrate,

$$EF = \frac{I_{SERS}}{I_{Raman}} \cdot \frac{N_{Raman}}{N_{SERS}} = 0.098 \times \frac{2.17 \times 10^{13}}{1.57 \times 10^{7}} = 1.36 \times 10^{5}$$

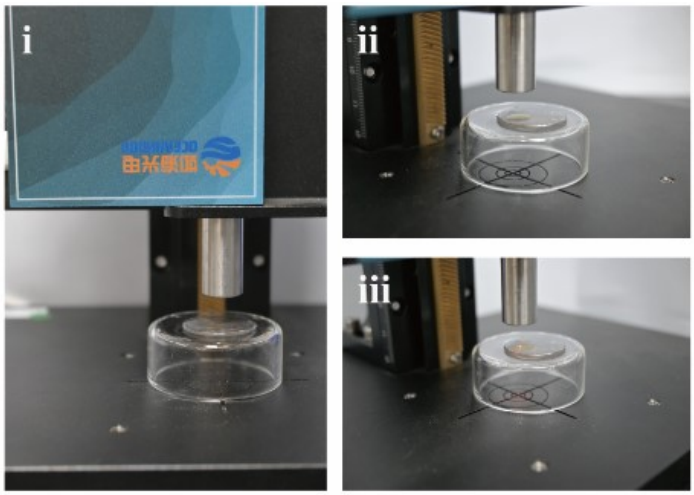

Figure S4. Photographs showing the SERS measurement. The SERS hydrogel is attached to a quartz plate for testing. The entire assembly is placed on a glass container for easy handling.

Reference:

[1] Li Lin, Haoqi He, Ruiyang Xue, et al. Direct and quantitative assessments of near-infrared light attenuation and spectroscopic detection depth in biological tissues using surface-enhanced Raman scattering[J]. *Med-X*, 2023, 1(1): 9-9 https://doi.org/10.1007/s44258-023-00010-2