Supporting information

Highly sensitive determination of ethyl carbamate in alcoholic beverages by surface-enhanced Raman spectroscopy combined with molecular imprinting polymer

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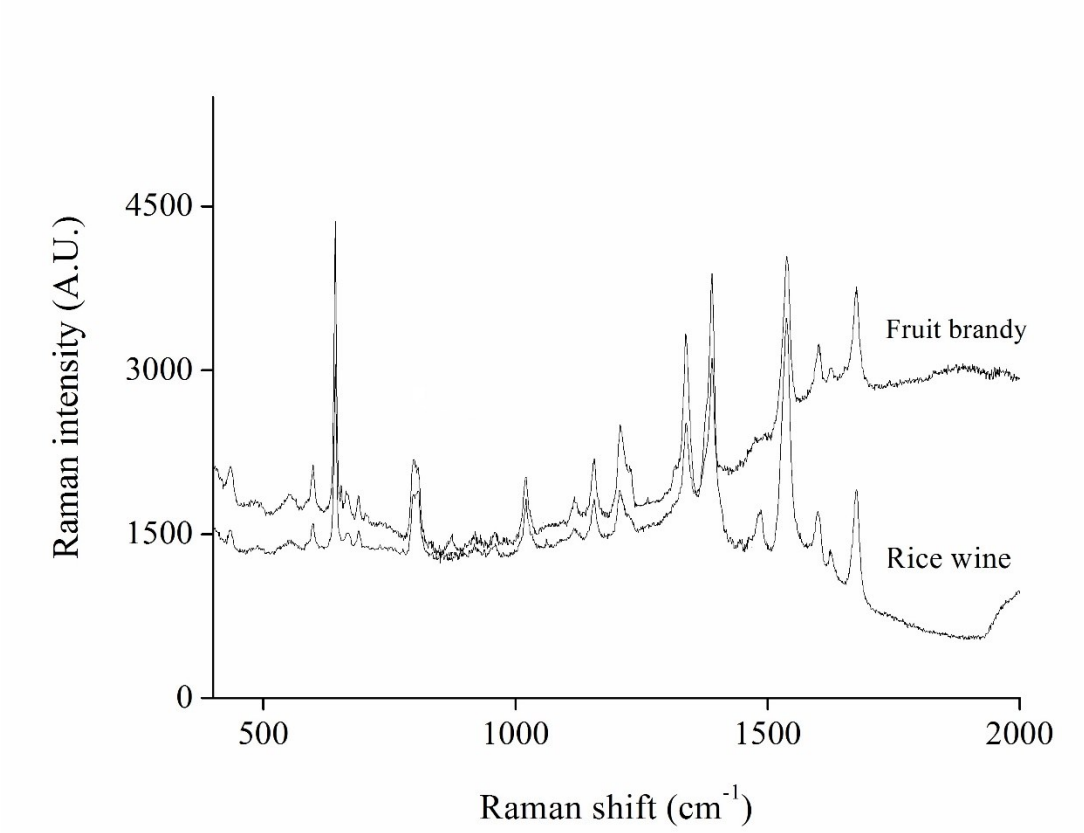


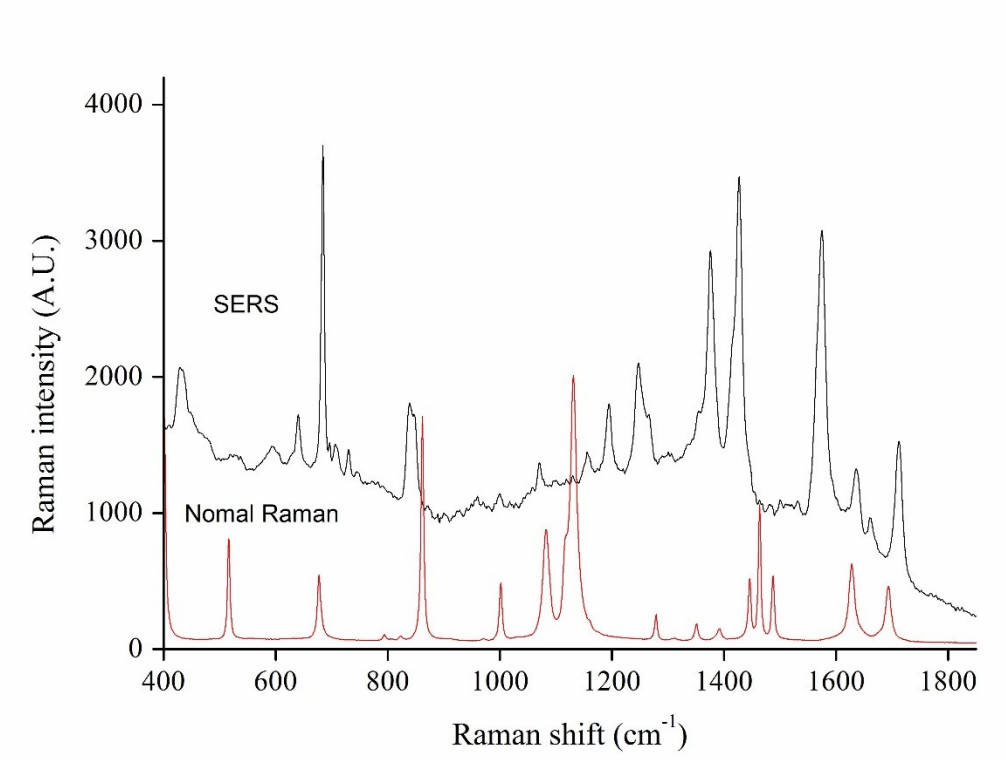
Fig. S1 Raw SERS spectra of EC extracted form rice wine and fruit bandy using the MIPs synthesized in our study.

Evaluate the performance of silver dendrite nanostructure

Enhancement Factor (EF) was calculated by using the standard formula:

$$EF=(I_{SERS}/ C_{SERS})\times(C_{NR/INR})$$

where I_{SERS} and I_{NR} are the intensity at the chosen wavenumber in obtained SERS and normal Raman spectrum, respectively. C_{SERS} and C_{NR} are the concentration of analytes used for SERS and normal Raman scattering measurements, respectively. The characteristic peak (677 cm^{-1}) was considered for EF calculation.



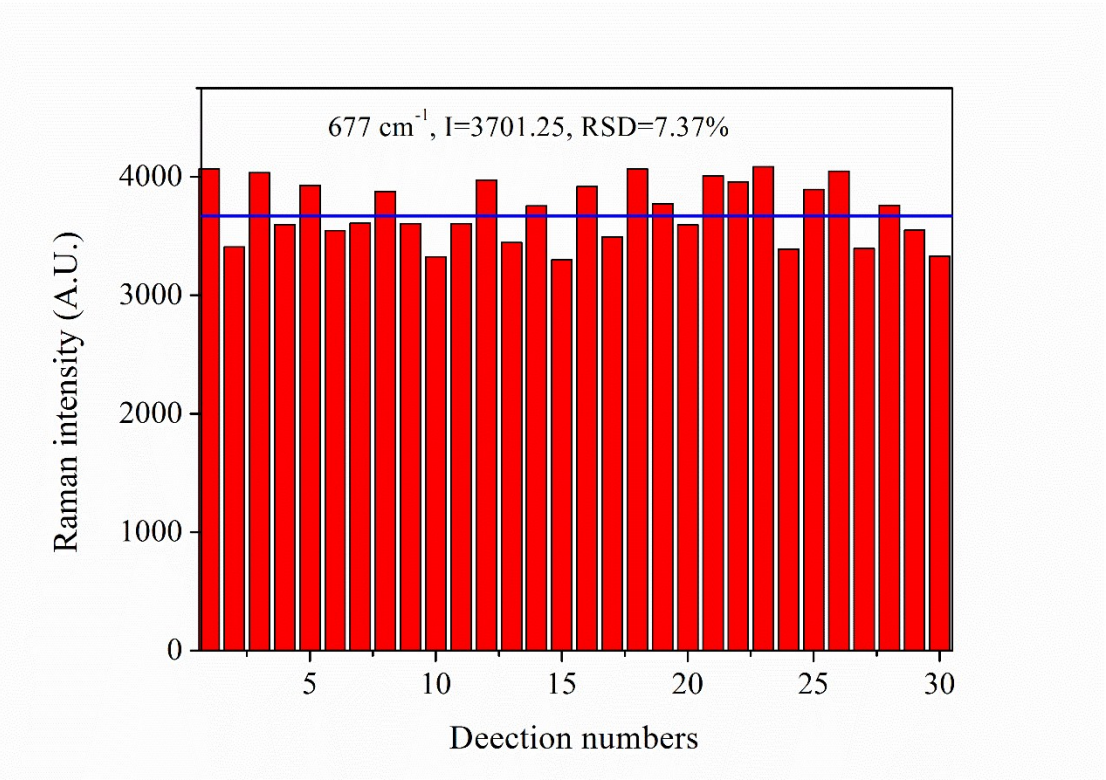
The figure is the typical SERS and normal Raman spectra of ethyl carbamate. The concentration of ethyl carbamate for SERS and normal Raman spectrum is 5.0×10^{-5} g/L and 2 g/L, respectively.

EF=$(3768.09/5\times10^{-5})\times(2/515.53)$

The EF was calculated to about 2.92×10^{5}.

For the reproducibility of the proposed method, SERS detection of substrate at different detect position and substrates from several synthesis batches were performed. For the same substrate, seven different detection spots were random chosen and their spectrum were obtained. For the substrate from different batches, we synthesized five substrates from five batches. Detection was assessed at seven different positions for each substrate. The obtained spectrums were used for the evaluation the reproducibility of our proposed substrate.

The reproducibility experiments results for the used method is shown below.



The RSD was about 7.37% (data at 677 cm^{-1} for 35 replications), shows good homogeneity and reproducibility of the method.

Isotherm models

Scatchard model:

$$\frac{Q}{C_e} = \frac{Q_{\max}}{k_d} - \frac{Q}{k_d}$$

Freundlich model:

$$\lg Q = m \lg C_e + \lg a$$

Langmuir isotherm model:

$$\frac{C_e}{Q} = \frac{C_e}{Q_{\max}} + \frac{1}{Q_{\max} b}$$

C_e (mg/L) is the free EC concentration (mg/L) at equilibrium, Q_{max} is the saturated adsorption capacity (mg/g), k_d is the dissociation constant (mg/L), m is the adsorption intensity of surface

heterogeneity, a is the adsorption capacity of EC (mg/g) and b is the Langmuir adsorption equilibrium constant (L/mg).

Parameters used to evaluate models

$$RMSEC = \sqrt{\frac{\sum_{i=1}^{n}\left(c_i - \hat{c}_i\right)^2}{n}}$$

$$RMSEP = \sqrt{\frac{\sum_{i=1}^{n}\left(c_i - \hat{c}_i\right)^2}{n}}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(c_i - \hat{c}_i)^2}{\sum_{i=1}^{n}(c_i - \overline{c})^2}$$

where n is the number of samples, c_i refers to the actual EC value (ppm) for the sample *i*, $\hat{c}_i$ represents the predicted value (ppm) by SERS spectra for sample *i* by the model developed when the *i*th sample is left out and $\overline{c}$ means the mean of the reference measurement results for all samples.