SUPPORTING INFORMATION

Silver Nanoparticle-Based Surface-Enhanced Raman Spectroscopy for the Rapid and Selective Detection of Trace Tropane Alkaloids in Food

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Figure S1(A) and (B) show the extinction spectra of Ag seeds and Ag NPs in the range of 300 nm to 800 nm respectively. One clearly observed that the extinctive peak was red shifted from 412.5 nm (A) to 477.5 nm (B), and the FHHM (full-width of half maximum) of Ag seeds was broadened of 15 nm due to the enlarged diameter of Ag NPs, accordingly. Inset SEM images displayed the size distributes and morphology of these two NPs: both displayed quasi-spherical shape, with the size increased from 50±5.3 nm (seeds) to 100±8.8 nm (Ag NPs) averaged from 100 nanoparticles.

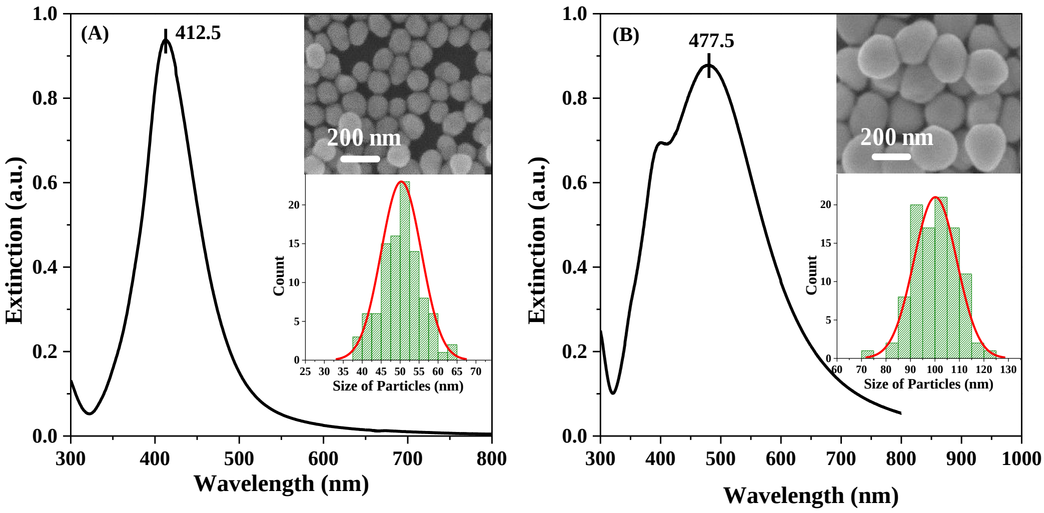

Figure S1. Extinction spectra of the Ag NPs. (A) Ag seeds, and (B) grown Ag NPs.

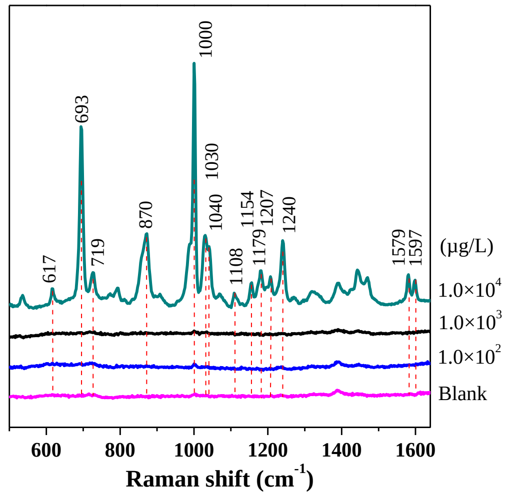

Figure S2. Concentration dependent SERS spectra of SB by using 1 M NaCl as aggregating agent.

Figure S3 (A)-(C) show the effects from concentrations of KI and Ag NPs and aggregation time for SERS signal by using 1.0×10^2 μg/L SB as target. The concentration of KI was varied from 0.1 M to 3 M, the results (A) show the SERS intensity increased with concentration increasing between 0.1-1.0 M. Then the signal decreased because of large aggregates produced by too fast aggregation. For Ag NPs (B), with the increasing of Ag NPs, the SERS intensity increased slowly and then decreased. At the low concentration of Ag NPs, increasing the number of nanoparticles can improve amount of absorbed molecules, which induced enhancement of SERS signal. After particles reached a high concentration, total molecules absorbed on each Ag NPs began to decrease, which weakened the signal. In addition, a large number of nanoparticles aggravated the absorption and scattering of incident light. Therefore, Ag NPs with concentration of 1.5×10^{-8} mol/L were used. The result of aggregating time (C) indicated the SERS signal decreased slowly after mixing. Therefore, the sample should be detected immediately after mixture.

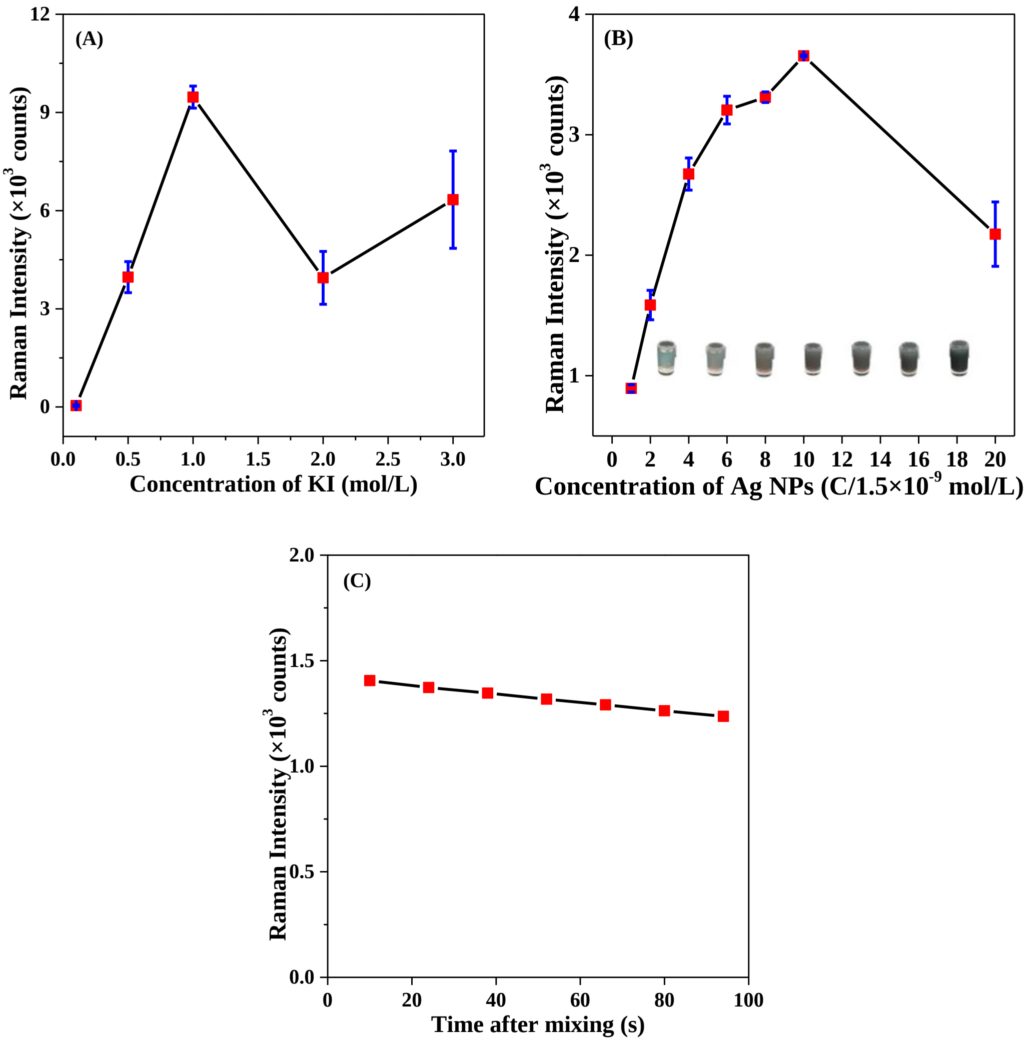

Figure S3. Optimization of detection conditions by using 1.0×10^2 μg/L SB. (A) SERS intensity of the 693 cm^{-1} peak with different concentrations of KI, (B) SERS intensity of the 693 cm^{-1} peak with different concentrations of Ag NPs, and (C) SERS intensity of the 693 cm^{-1} peak with different aggregating time.

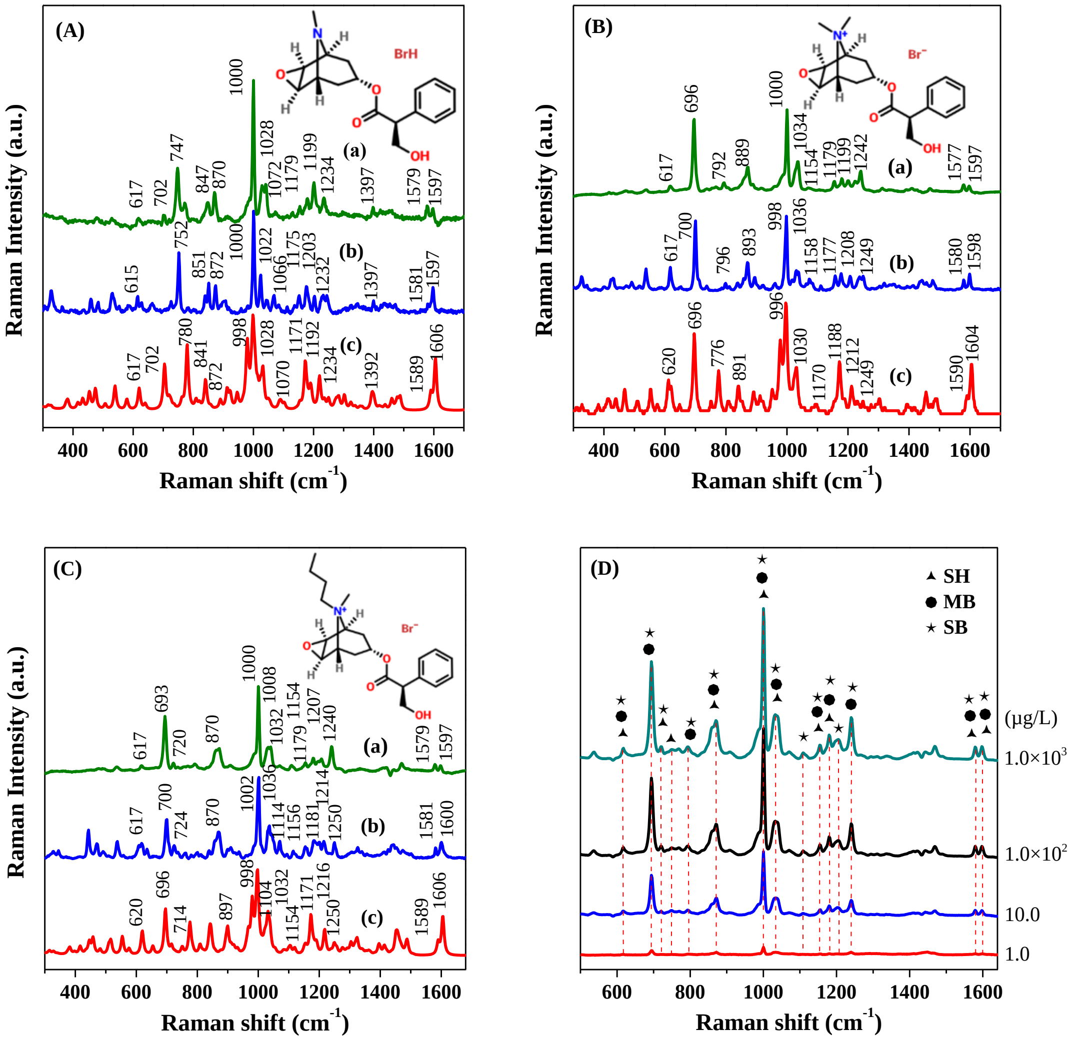

Figure S4. Raman spectra of TAs. (A) SH, (B) MB, (C) SB, and (D) Mixture. (a) SERS of spectra of aqueous solution, (b) solid normal Raman spectra, and (c) calculated Raman spectra.

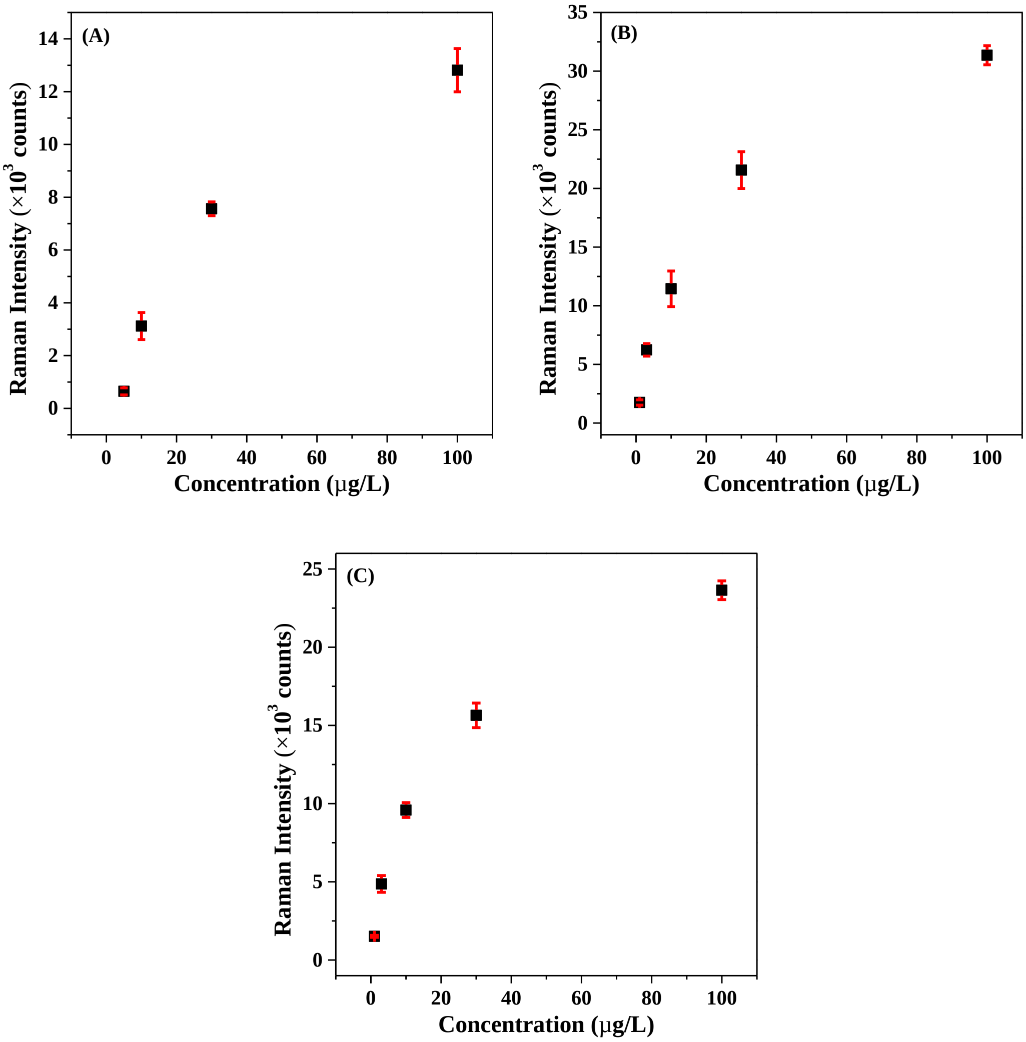

Figure S5. SERS intensity of the 693 cm^{-1} peak with different concentrations. (A) SH, (B) MB, and (C) SB.

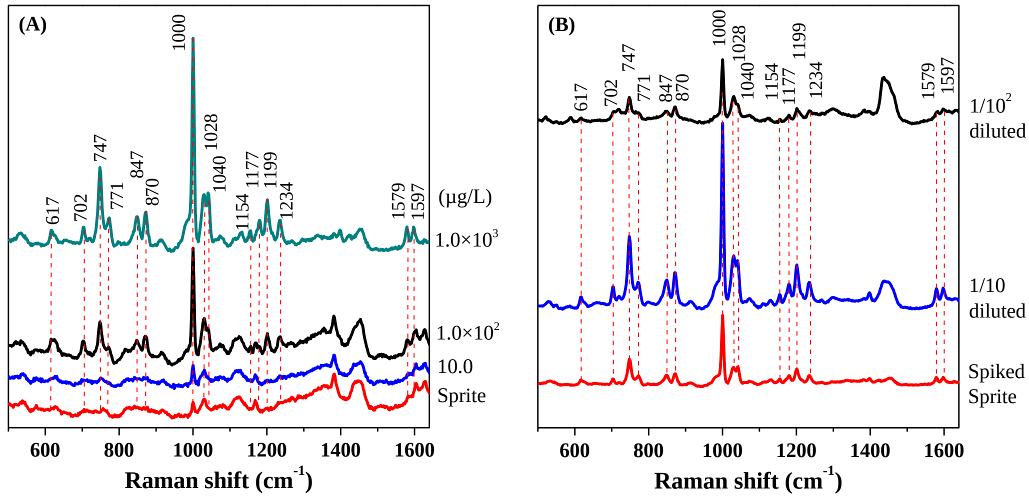

Figure S6. SERS spectra of SH. (A) Sprite spiked with different concentrations of SH, and (B) Sprite Spiked at 1.0×10^3 μg/L was diluted to different times by ultrapure water.

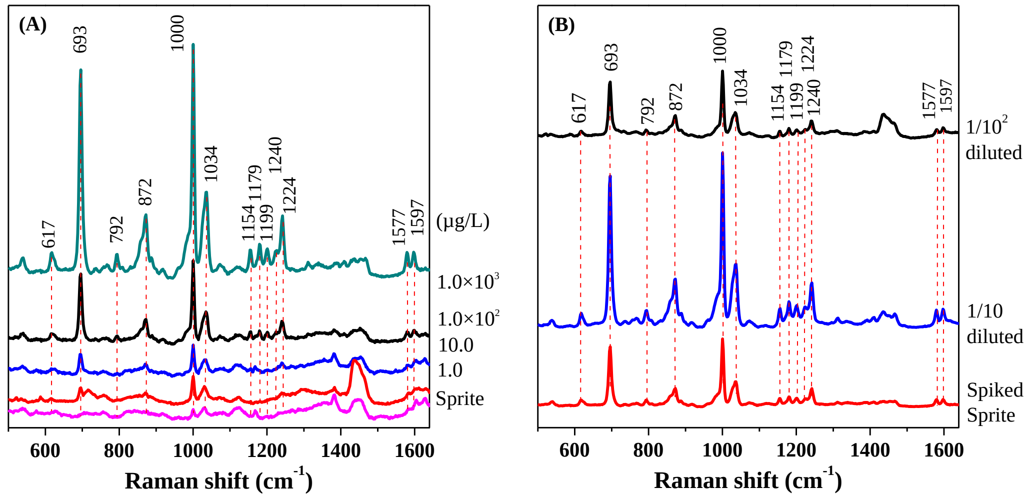

Figure S7. SERS spectra of MB. (A) Sprite spiked with different concentrations of MB, and (B) Sprite Spiked at 1.0×10^3 μg/L was diluted to different times by ultrapure water.

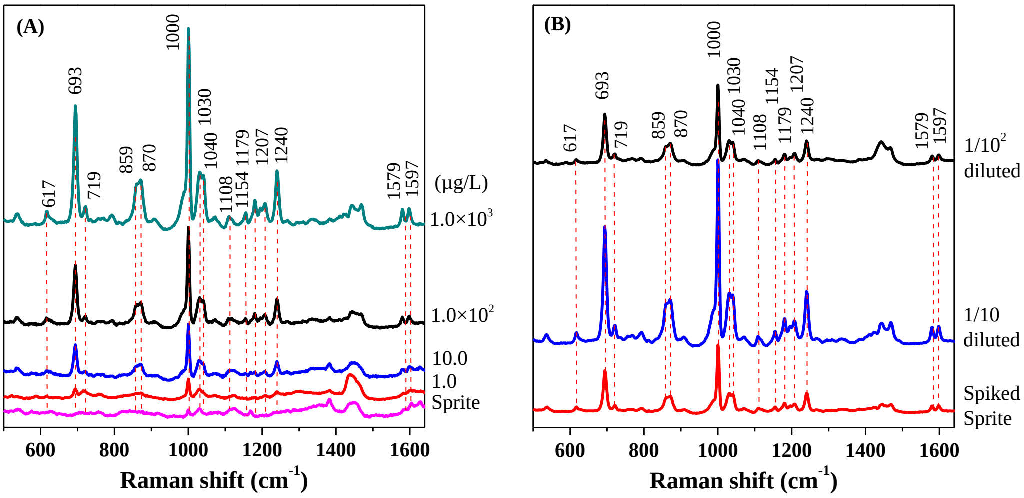

Figure S8. SERS spectra of SB. (A) Sprite spiked with different concentrations of SB, and (B) Sprite Spiked at 1.0×10^3 μg/L was diluted to different times by ultrapure water.

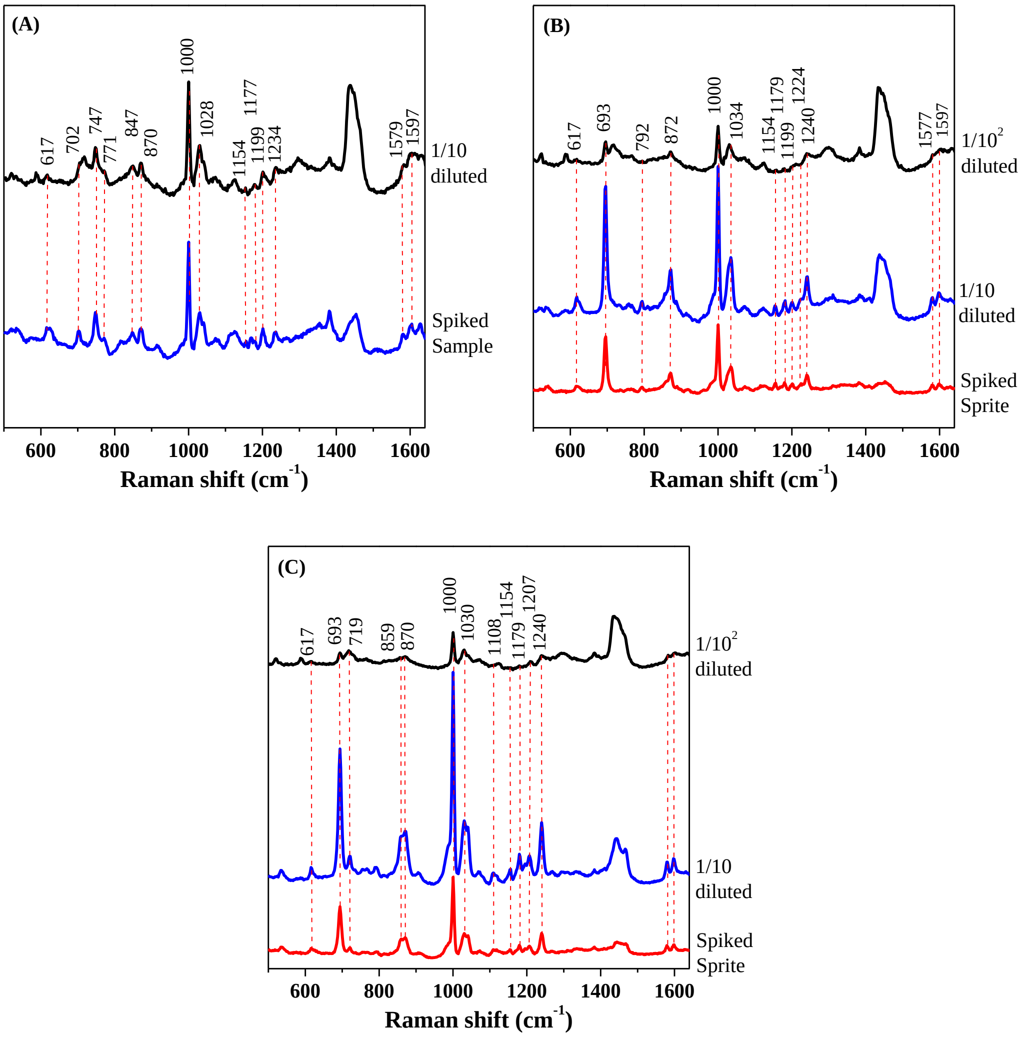

Figure S9. Sprite Spiked at 1.0×10^2 μg/L was diluted to different times by ultrapure water. (A) SH, (B) MB, and (C) SB.

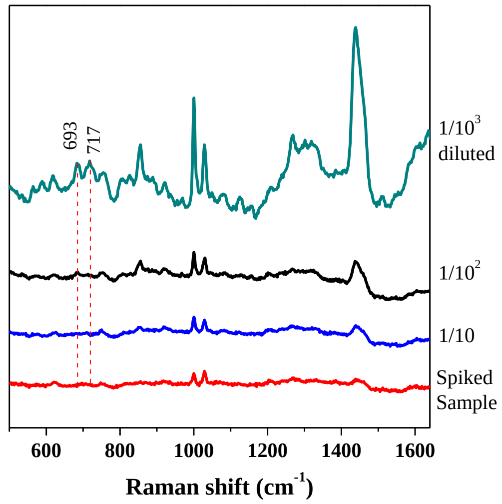

Figure S10. SERS spectra of SB in Minute Maid Spiked at 1.0×10^3 μg/L.

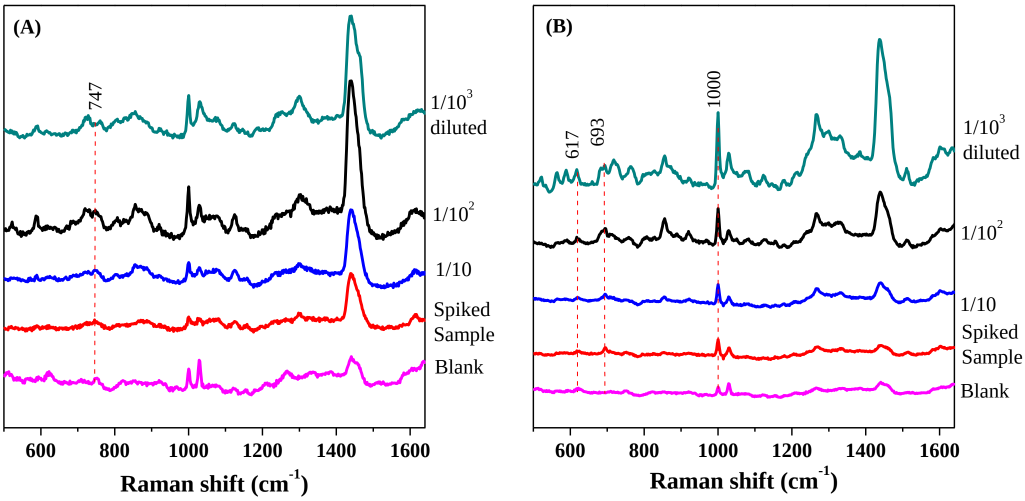

Figure S11. SERS spectra of TAs in Spiked Minute Maid. (A) 1.0×10^4 μg/L SH, and (B) 1.0×10^3 μg/L MB.

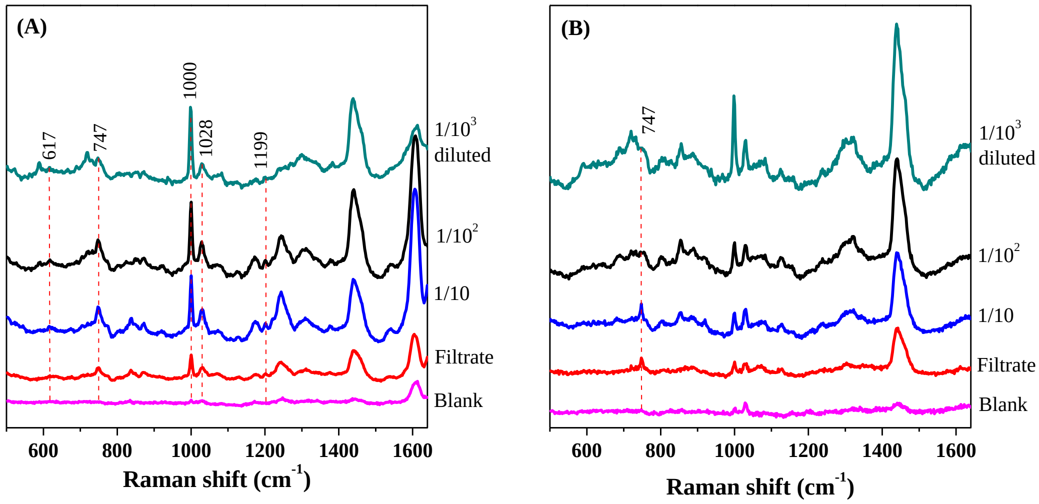

Figure S12. SERS spectra of 2.0×10^4 μg/L SH in spiked foods. (A) Cauliflower roast pork, and (B) Pumpkin Spiked.

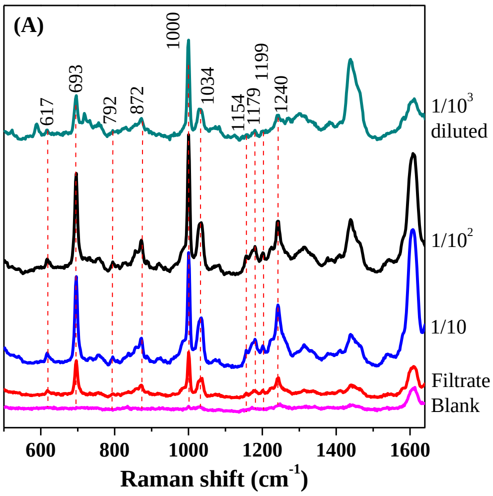

Figure S13. SERS spectra of 2.0×10^4 μg/L MB in spiked foods. (A) Cauliflower roast pork, and (B) Pumpkin Spiked.

Table S1 Experimental and calculated vibrational frequencies (cm^{-1}) and assignment for TAs

mode / *Species*		ω_1 (cm^{-1})	ω_2 (cm^{-1})	ω_3 (cm^{-1})
R-H (SH)	Expt	1000	752	1203
	Theory	998	780	1192
	Assignment	The trigonal deformation of the phenyl ring	The wagging vibration of $-CH_3$ around N atom	The deformation vibration of $-CH_3$ around N atom
R-CH_3(MB)	Expt	998	700	1249
	Theory	996	696	1230
	Assignment	The trigonal deformation of the phenyl ring	The wagging vibration of $-CH_3$ around N atom, the out-of-plane bending of CH in the phenyl ring	The deformation vibration of $-CH_3$ around N atom
R-C_4H_9 (SB)	Expt	1000	698	1249
	Theory	998	696	1217、1249
	Assignment	The trigonal deformation of the phenyl ring	The out-of-plane bending of CH in the phenyl ring	The wagging vibration of CH in the epoxy group

Table S2. Recovery of TAs in Spiked Samples.

Spiked Samples	Dilution	SH			MB			SB		
		Calculated Concentration (μg/L) /Recovery (%)/RSD (%) (n=3)								
Sprite	1	5.6	0.56	1.4	2.4	0.24	4.3	2.4	0.24	3.1
(spiked 1.0×10^3	1/10	114.1	11.41	2.6	156.4	15.63	0.7	221.3	22.13	2.1
μg/L)	$1/10^2$	466.6	46.66	5.3	222.6	22.26	2.3	300.1	30.01	1.0
Minute Maid	1	3.4	0.03	8.6	0.4	0.04	2.6	0.4	0.04	3.7
(spiked 1.0×10^3	1/10	34.8	0.35	7.3	4.2	0.42	10.3	4.2	0.42	5.5
μg/L, but 1.0×10^4 μg/L for SH)	$1/10^2$	356.3	3.56	4.3	44.6	4.46	4.8	52.7	5.27	6.8
Cauliflower roast pork (spiked 20.0 mg/kg)	1	3.7	0.07	2.6	1.0	0.02	2.1	1.0	0.02	2.6
	1/10	42.1	0.84	8.5	14.9	0.30	5.7	9.8	0.20	6.5
	$1/10^2$	406.1	8.12	4.6	160.3	3.21	10.3	101.2	2.02	5.8
	$1/10^3$	ND	ND	ND	1072.5	21.45	6.8	1016.4	20.33	8.7
Pumpkin (spiked 20.0 mg/kg)	1	3.7	0.07	6.3	0.9	0.02	3.6	1.0	0.02	3.6
	1/10	40.6	0.81	8.7	9.3	0.19	8.9	9.9	0.20	5.8
	$1/10^2$	ND	ND	ND	91.9	1.84	4.6	100.6	2.01	9.7
	$1/10^3$	ND	ND	ND	911.7	18.23	7.3	1011.3	20.23	10.6

ND=Not detected.

Table S3. Recovery of TAs in Sprite spiked at 1.0×10^2 μg/L.

	Dilution	SH			MB			SB		
		Calculated Concentration (μg/L) /Recovery (%)/RSD (%) (n=3)								
Sprite	1	4.1	4.12	2.3	1.1	1.11	2.3	1.4	1.36	2.2
	1/10	38.2	38.24	5.4	17.3	17.33	3.3	36.7	36.72	6.8
	$1/10^2$	ND	ND	ND	87.9	87.95	1.8	83.6	83.62	4.6

ND=Not detected.