

Supplementary Information For:

**Aminopyrine Raman spectral features characterised by
experimental and theoretical methods: Toward rapid SERS
detection of synthetic antipyretic-analgesic drug in traditional
Chinese medicine**

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LC-MS conditions

Chromatographic separation was performed on a 3.5 μm Agilent Zorbax SB-C18 column (100 mm \times 2.1 mm) at 30 $^{\circ}\text{C}$, with 55: 45 (v/v) methanol-water as mobile phase at a flow rate of 0.3 mL min^{-1} . Drying gas flow and nebuliser pressure was adjusted to 7 L min^{-1} and 25 psi, respectively. Dry gas temperature and capillary voltage of the system was set to 350 $^{\circ}\text{C}$ and 3500 V, respectively. LC-MS/MS was performed in the multiple reactions monitoring mode using target ions at m/z 231.8 \rightarrow 110.8 for AP and m/z 236.7 \rightarrow 193.7 for carbamazepine (IS) with a positive ion electrospray ionization interface.

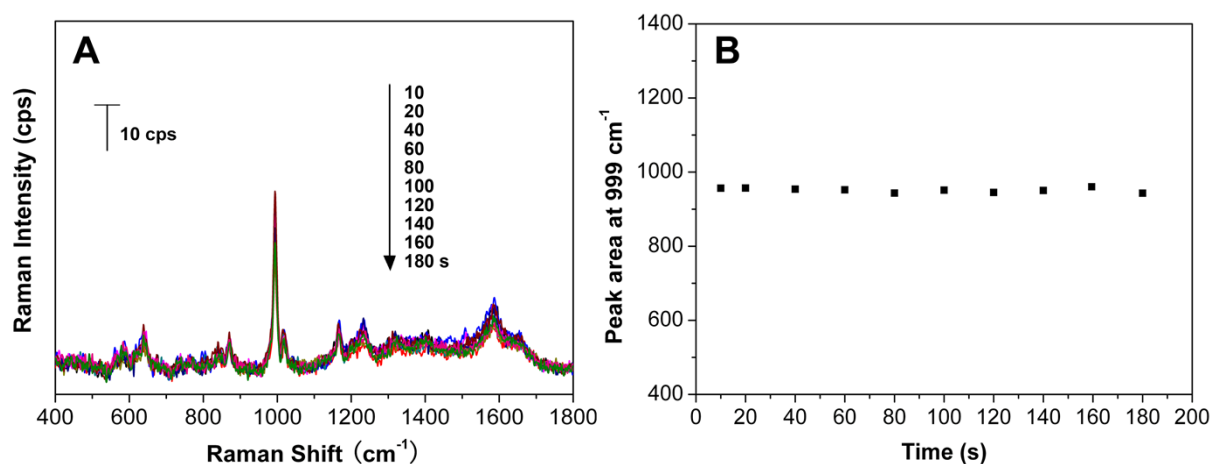


Fig. S1 (A) Variation of the SERS spectral profile of AP (1.00×10^{-2} M) absorbed on Au@Ag NPs colloids with the irradiation time. (B) Evolution of the SERS peak (999 cm^{-1}) area of AP (1.00×10^{-2} M) absorbed on Au@Ag NPs colloids with the irradiation time.

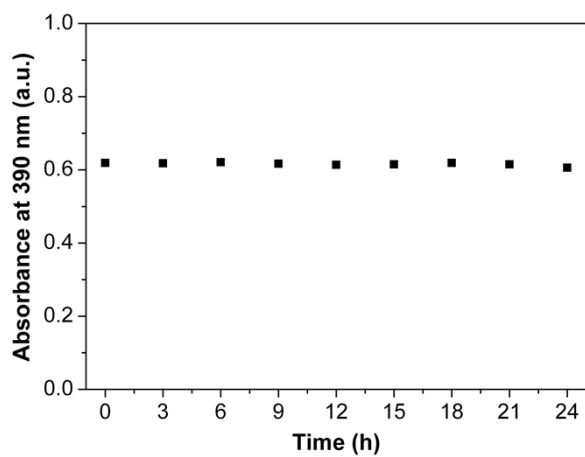


Fig. S2 UV-vis absorbance stability of Au@Ag NPs colloids against time.

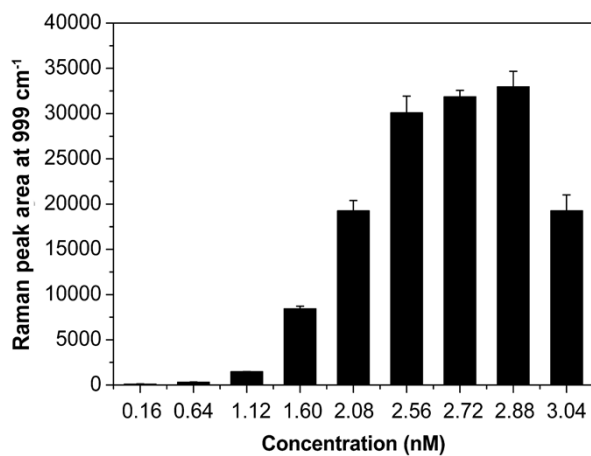


Fig. S3 Evolution of AP (1×10^{-3} M) Raman peak area (at 999 cm⁻¹) with concentration of Au@Ag NPs.

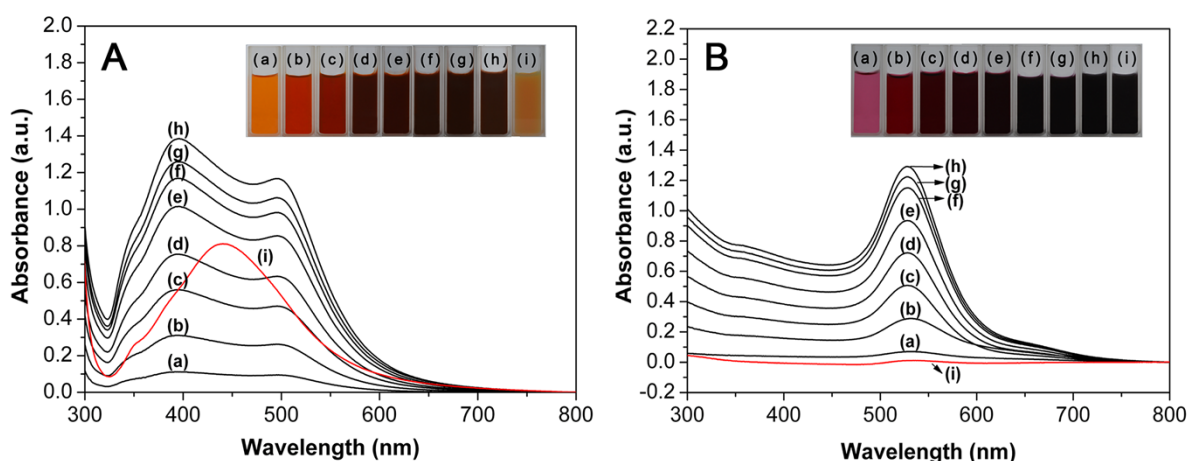


Fig. S4 (A) UV-vis absorption spectra of Au@Ag NPs: 0.016 nM (a), 0.064 nM (b), 0.112 nM (c), 0.160 nM (d), 0.208 nM (e), 0.256 nM (f), 0.272 nM (g), 0.288 nM (h), and 0.304 nM (i). The inset images show that the color of Au@Ag NPs changes from orange to reddish brown obviously, and then light yellow. (B) UV-vis absorption spectra of Au NPs: 0.024 nM (a), 0.096 nM (b), 0.168 nM (c), 0.240 nM (d), 0.312 nM (e), 0.384 nM (f), 0.408 nM (g), 0.432 nM (h), and aggregation (i). The insets show the colors change from pink to black. The above NPs were diluted ten times with water prior to investigation.

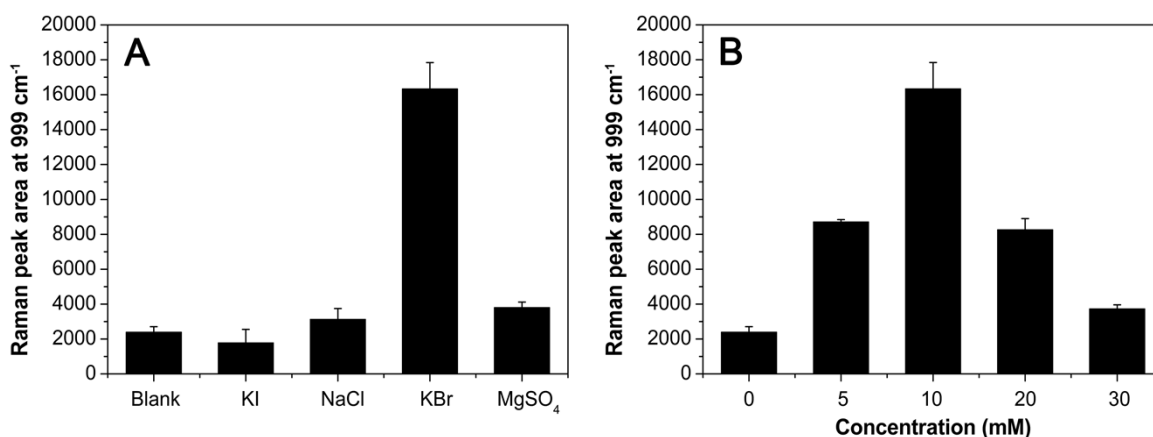


Fig. S5 (A) Variation of AP Raman peak area (at 999 cm^{-1}) with aggregating agent (Concentration of each aggregating agent is 10 mM). (B) Evolution of AP Raman peak area

(at 999 cm^{-1}) with concentration of KBr. (AP concentration is $1 \times 10^{-4}\text{ M}$ in Au@Ag NPs colloids).