Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Assembly of Gold Nanoparticles Using Turnip Yellow Mosaic Virus as an in-solution SERS Sensor

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Estimation of AuNP numbers

The TEM results showed the spherical structure of synthesized AuNPs, so the concentration of AuNP was calculated applying the Spherical Cluster Approximation as per R. L. Johnston, 'Atomic and Molecular Clusters', Taylor & Francis, 2002

$$V_{NP} = N \times V_{atom} \quad \text{(S1)}$$

$$4/3\ \pi\ (R_{NP})^3 = N \times 4/3\ \pi\ (R_{atom})^3 \quad \text{(S2)}$$

In which, V is the NP or atom volume, R is the NP or atom radius, and N is the number of atoms in each nanoparticle.

Rearranging, we obtain:

$$N = (R_{NP}/R_{atom})^3 \quad \text{(S3)}$$

Knowing that R_{atom} = 0.137 nm, the number of atoms could be estimated using the radius of the synthesized AuNP.

Besides, total number of gold atoms in the synthesis was calculated based on the moles of $HAuCl_4$:

$$N_{atom} = m_{HAuCl4} \times 6.022 \times 10^{23} \quad \text{(S4)}$$

$$\text{Number of AuNPs, } N_{NP} = N_{atom}/N \quad \text{(S5)}$$

Divided by the total volume, the number of AuNPs per milliliter was estimated and used for other experiments.

In addition to this calculation, the result was compared to the calculation using extinction coefficient of gold nanoparticles (Liu X, Atwater M, Wang J, Huo Q. Colloids Surf., B. 2007; 58:3–7)

$$\ln\varepsilon = 3.32 \ln d + 10.8 \quad \text{(S6)}$$

where, ε is the molar absorption coefficient at the wavelength of maximum extinction (L mol^{-1} cm^{-1}) and d is the diameter (nm) of AuNP.

The concentration of AuNP was then calculated via Beer-Lambert law

$$A = \varepsilon c l \quad \text{(S7)}$$

where A is absorbance, ε is the molar absorption coefficient (L mol^{-1} cm^{-1}), c is the concentration of nanoparticles in solution (M), l is the path length of the cuvette (cm).

The number of AuNPs per milliliter calculated applying this method was similar to the one obtained via the Spherical Cluster Approximation.

	PDI
TYMV	0.198
AuNP20-TYMV	0.354
AuNP20	0.234
AuNP10-TYMV	0.377
AuNP10	0.260
AuNP5	0.375
AuNP5-TYMV	0.457
AuNP NH2	0.137

Table S1: Polydispersity index (PDI) value of DLS experiments

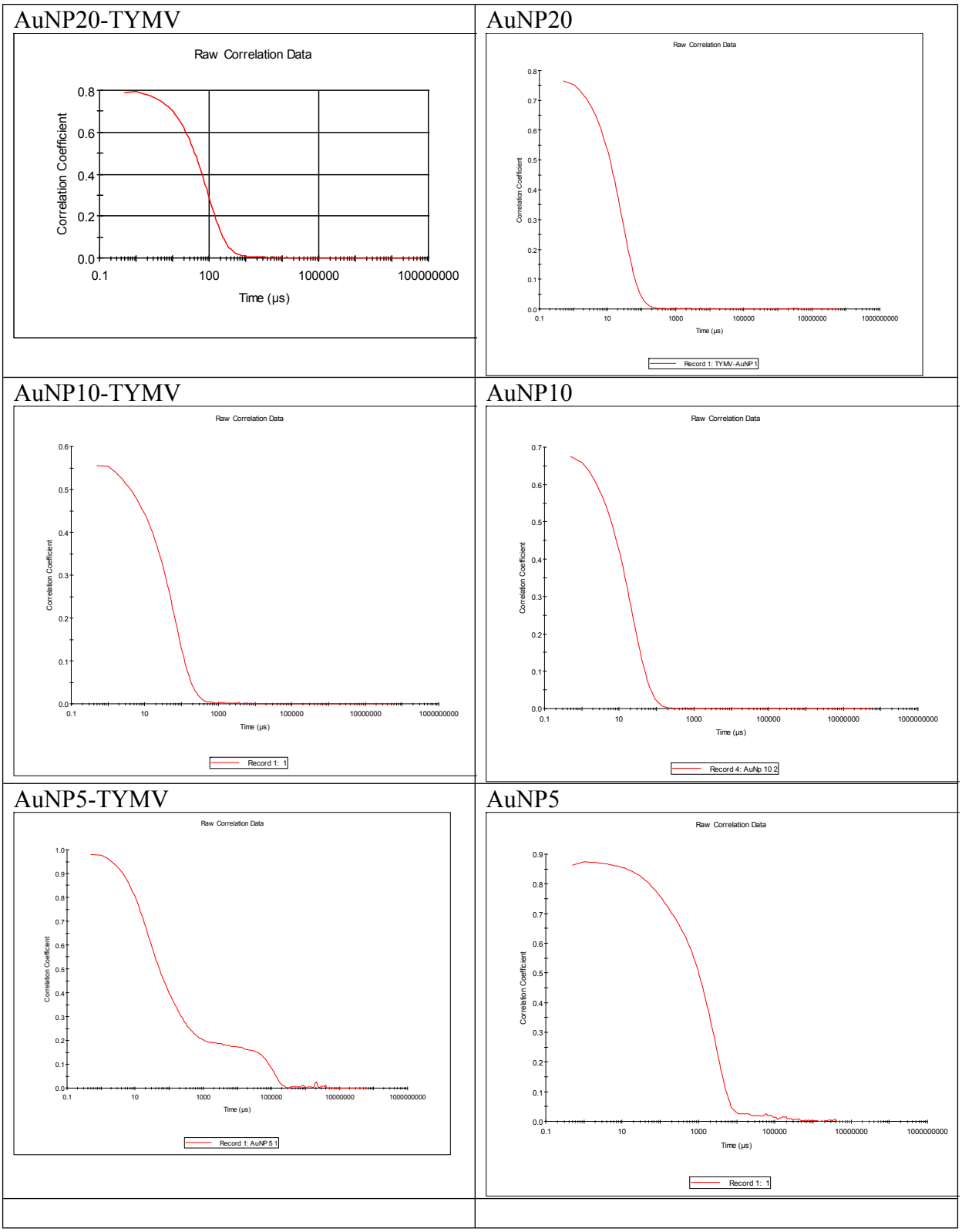


Fig. S1: DLS autocorrelation curves of (A) AuNP20-TYMV (B) AuNP 20 nm (C) AuNP20-TYMV (D) AuNP 10 nm (E) AuNP5-TYMV (B) AuNP 5nm

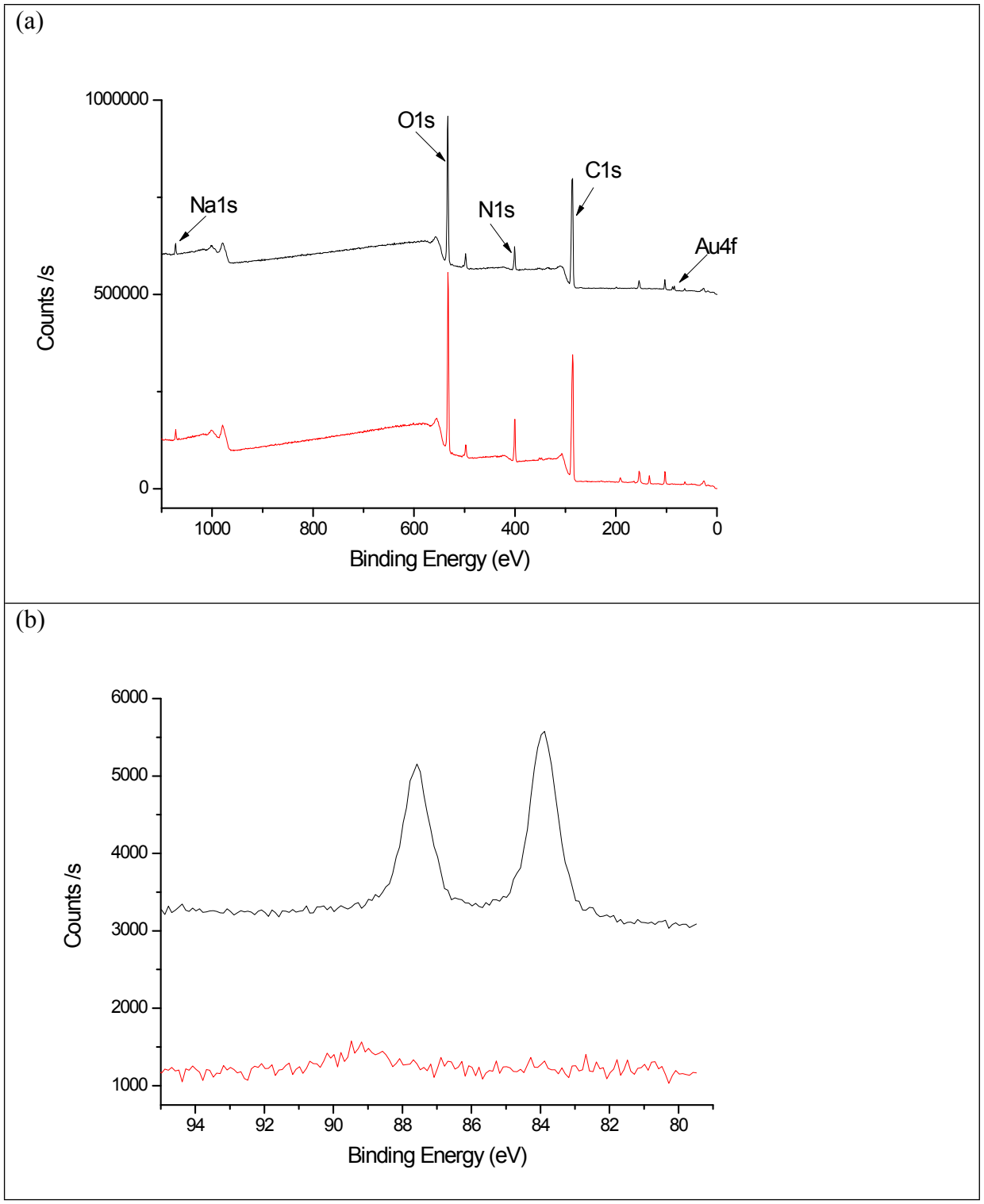
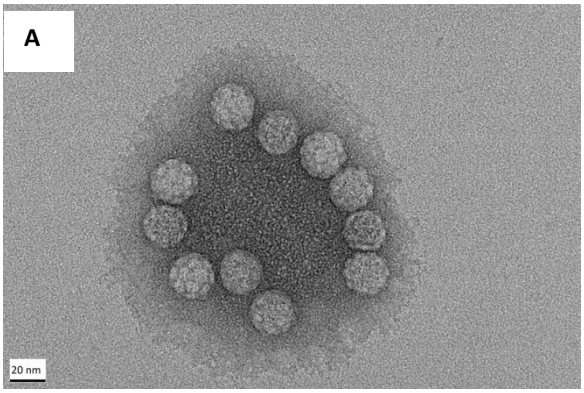
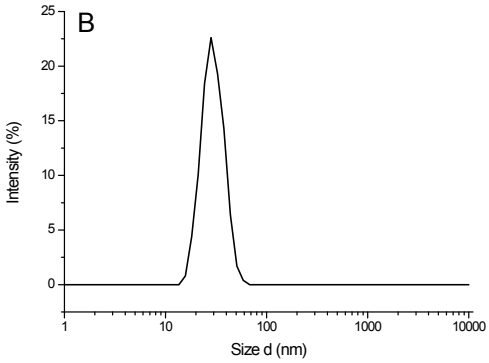


Fig. S2. XPS spectra of AuNP-TYMV (black) and TYMV (red): (a) Survey Spectra, (b) HR-Au4f region.





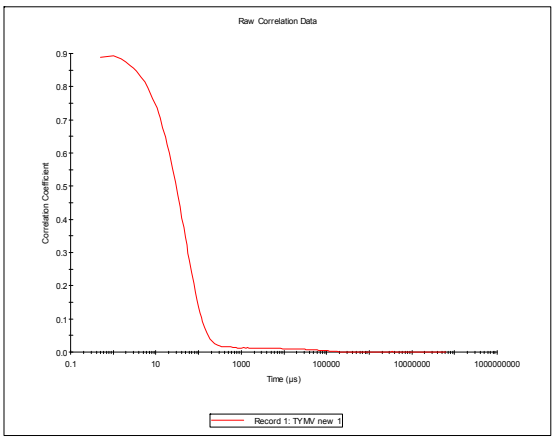
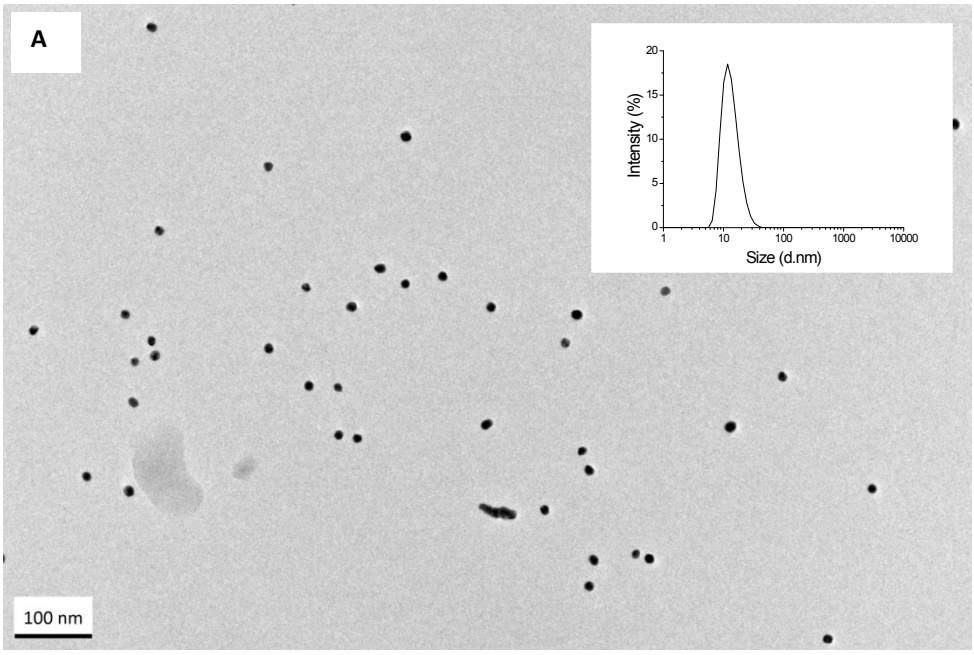
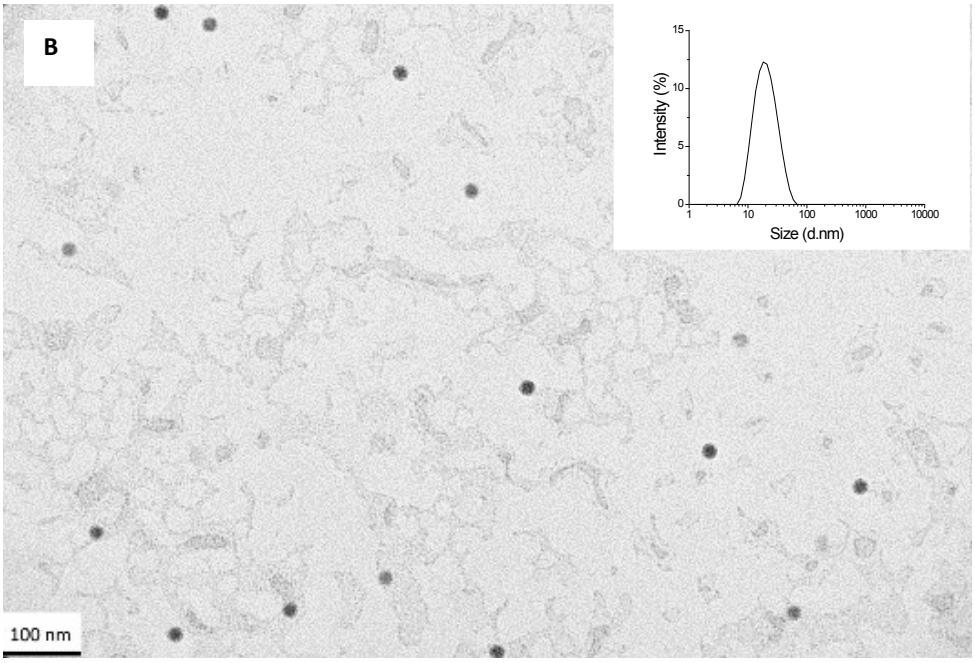


Fig. S3: (A) TEM picture of TYMV stained with uranyl acetate. (B) DLS of TYMV; PDI value = 0.198 (C) DLS autocorrelation curve.


A
Intensity (%)
Size (d.nm)
100 nm


B
Intensity (%)
Size (d.nm)
100 nm

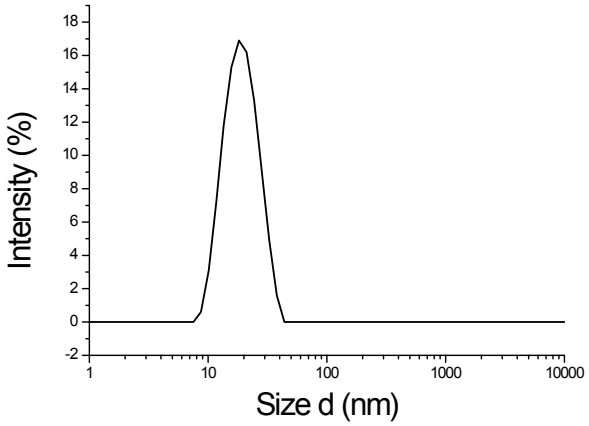


Fig. S4: TEM picture and DLS of (A) 10 nm-AuNP (B) 20 nm-AuNP. (C) DLS of 20 nm-AUNP coated with 6-amino-1-hexanethiol.

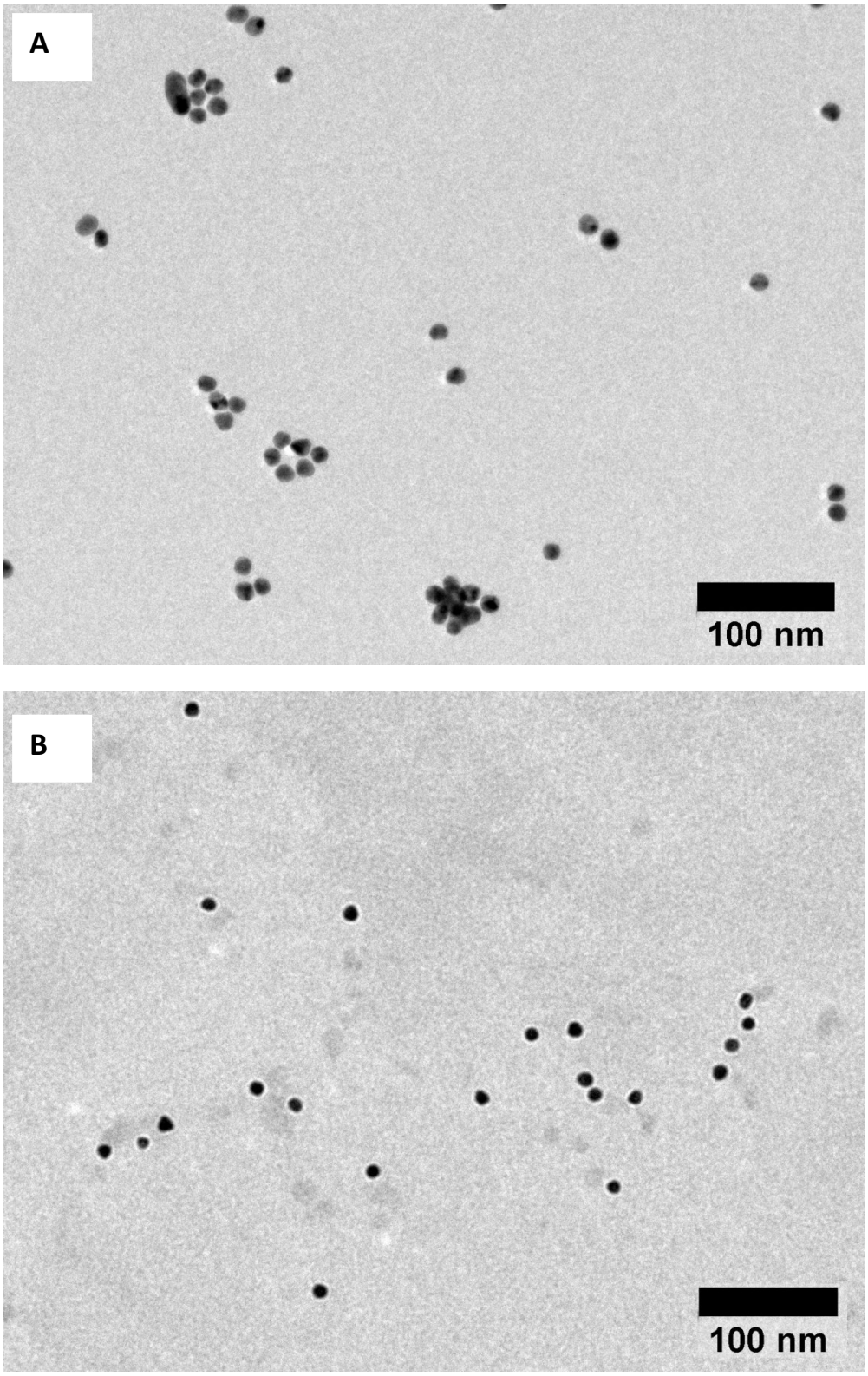


Fig. S5. TEM pictures of AuNP grafted onto TYMV (A) or ungrafted (B)

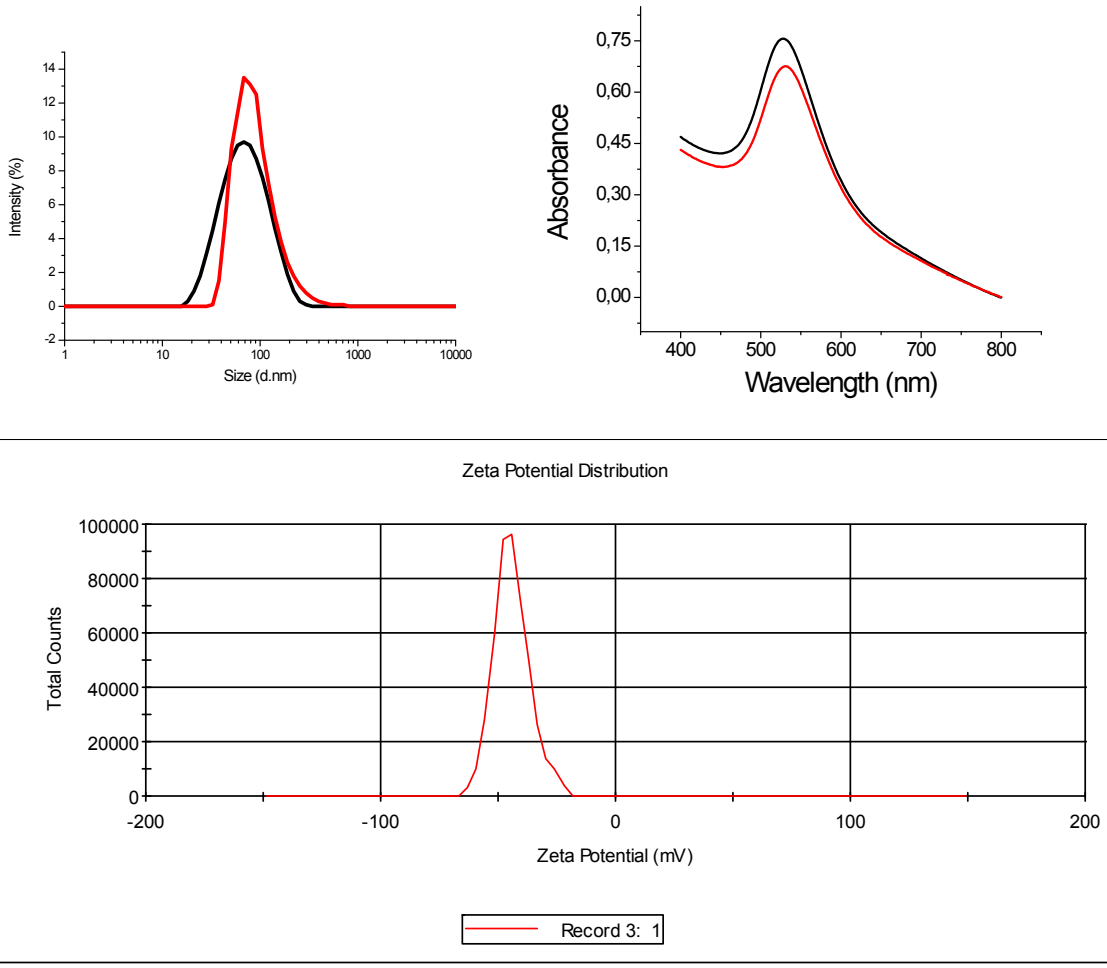


Fig. S6: DLS, absorption spectra and zeta potential of 20 nm-AuNP-TYMV after three months (red) compared to those of new synthetized ones (black)

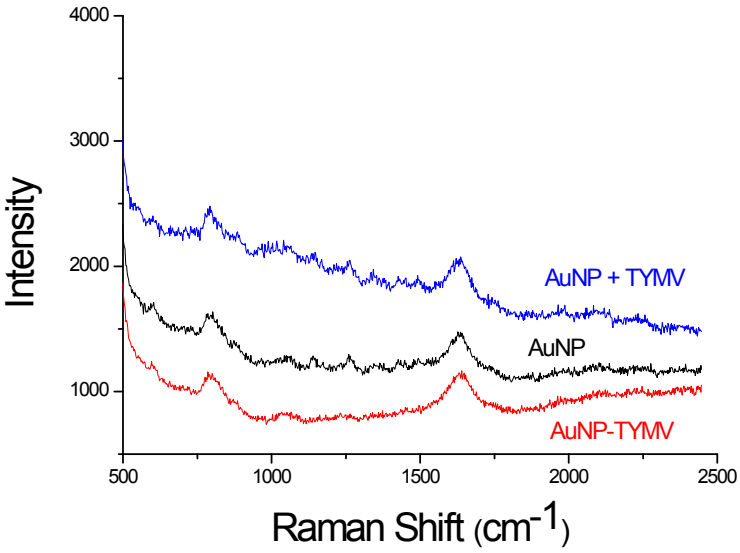


Fig. S7: Raman spectra of AuNP (black), of AuNP in the presence of 0.24 mg/mL of TYMV (blue) and of AuNP grafted onto TYMV (red).

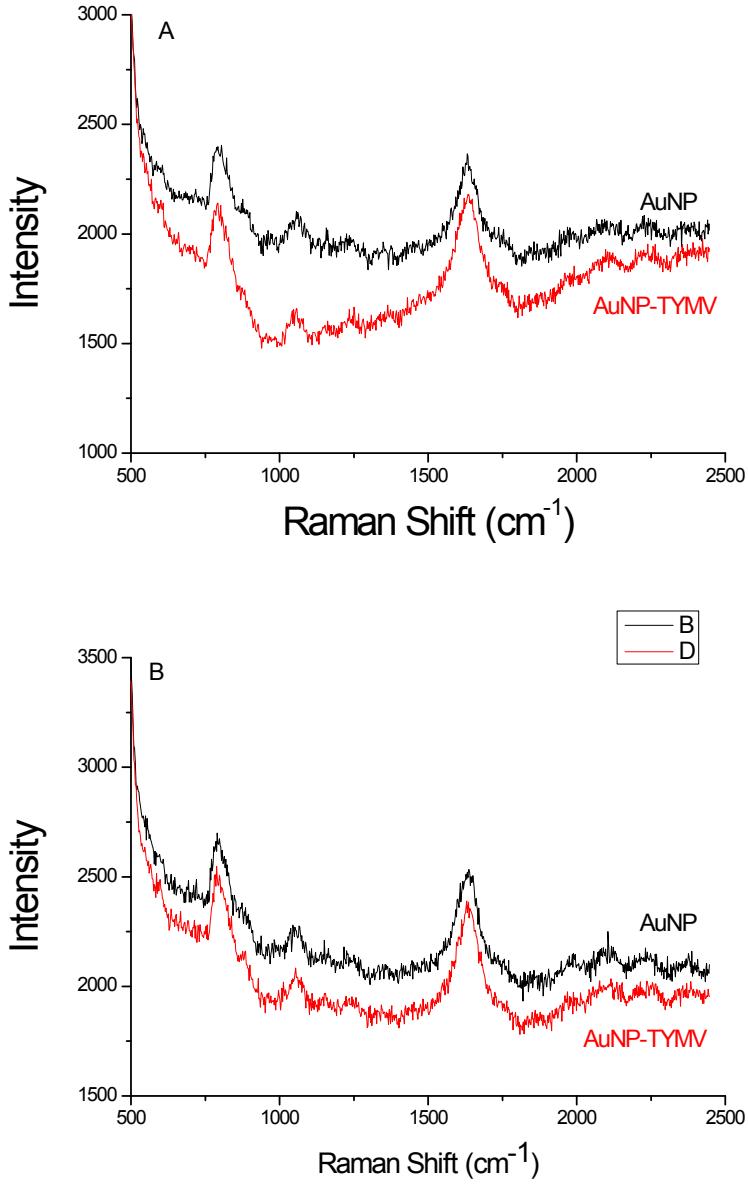


Fig. S8: Raman spectra of BPE at 10^{-5} M in solution in the presence of AuNP (black) and TYMV grafted to AuNP (red), (a) 10 nm-AuNP (b) 5 nm-AuNP