Electronic Supplementary Information

Assessment of ATR-FTIR spectroscopy with multivariate analysis to investigate the binding mechanisms of Ag and TiO_2 nanoparticles to Chelex®-100 or Metsorb™ for DGT technique

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Summary

- **Number of pages: 8**
- **Number of Figures: 7**

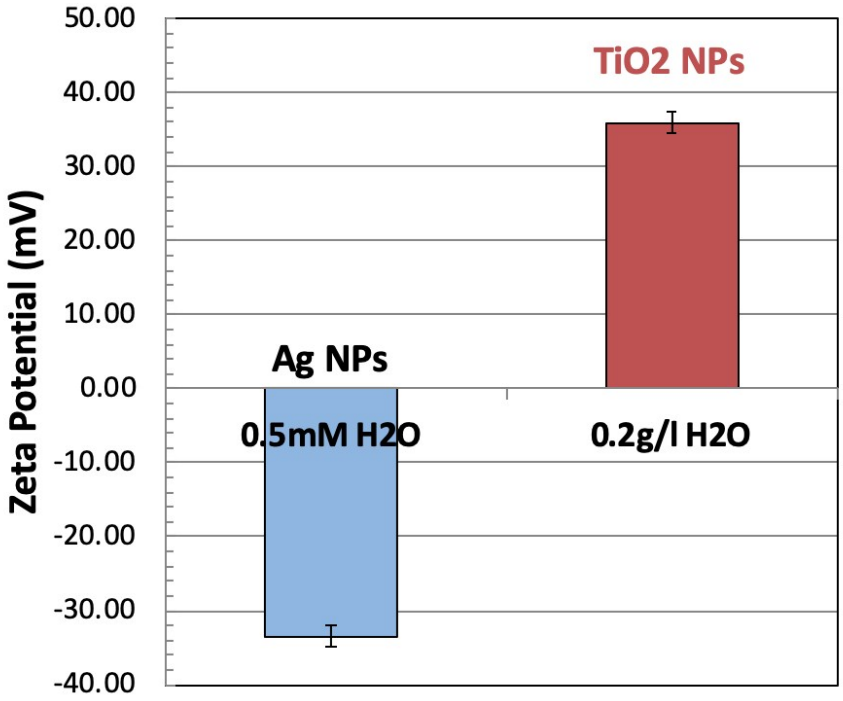

Figure S1. This Figure shows surface potential of Ag and TiO_2 NPs, under the experimental conditions.

Figures S2. shows IR spectra for Metsorb exposed to titanium oxide nanoparticles. Metsorb is a titanium oxide-based commercial resin with TiO_2 and $Ti(OH)_4$ as its main constituents and small quantities of other chemicals including polymers. Limited information is available about the chemical components of this resin. It's worth noting that the aim of investigating the binding mechanism of titanium dioxide nanoparticles to Metsorb was to explore the detection limits of this resin rather than to develop a Metsorb based DGT for measuring these nanoparticles in soil and water. This finding is important if a fully developed DGT for measuring NPs is deployed in a contaminated environment with unknown types of contaminants.

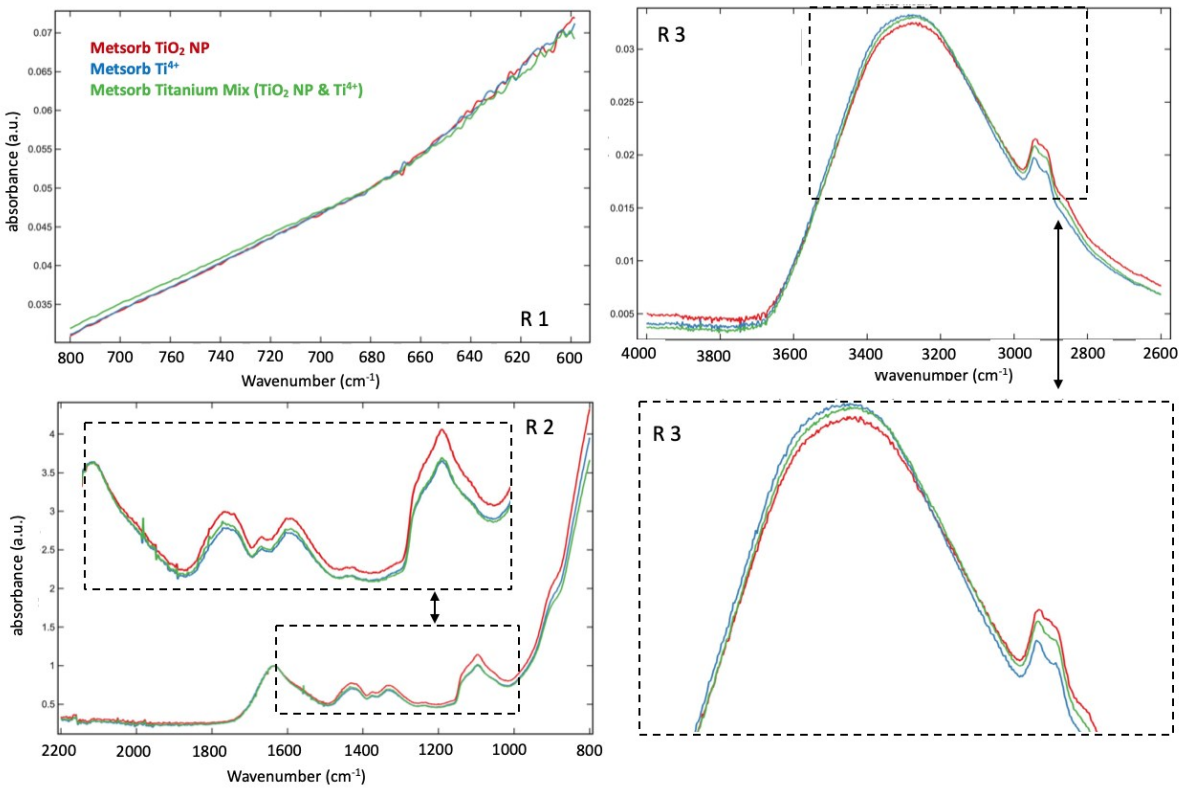

Figure S2. Comparison between derived infrared (IR) spectra for Metsorb exposed to the titanium dioxide nanoparticle treatments. The IR spectra (600−4000cm−1) is divided into three spectral regions: Region 1 (600−800 cm−1), Region 2 (800−2200 cm−1), and region 3 (2600−4000 cm−1) for comparison purpose.

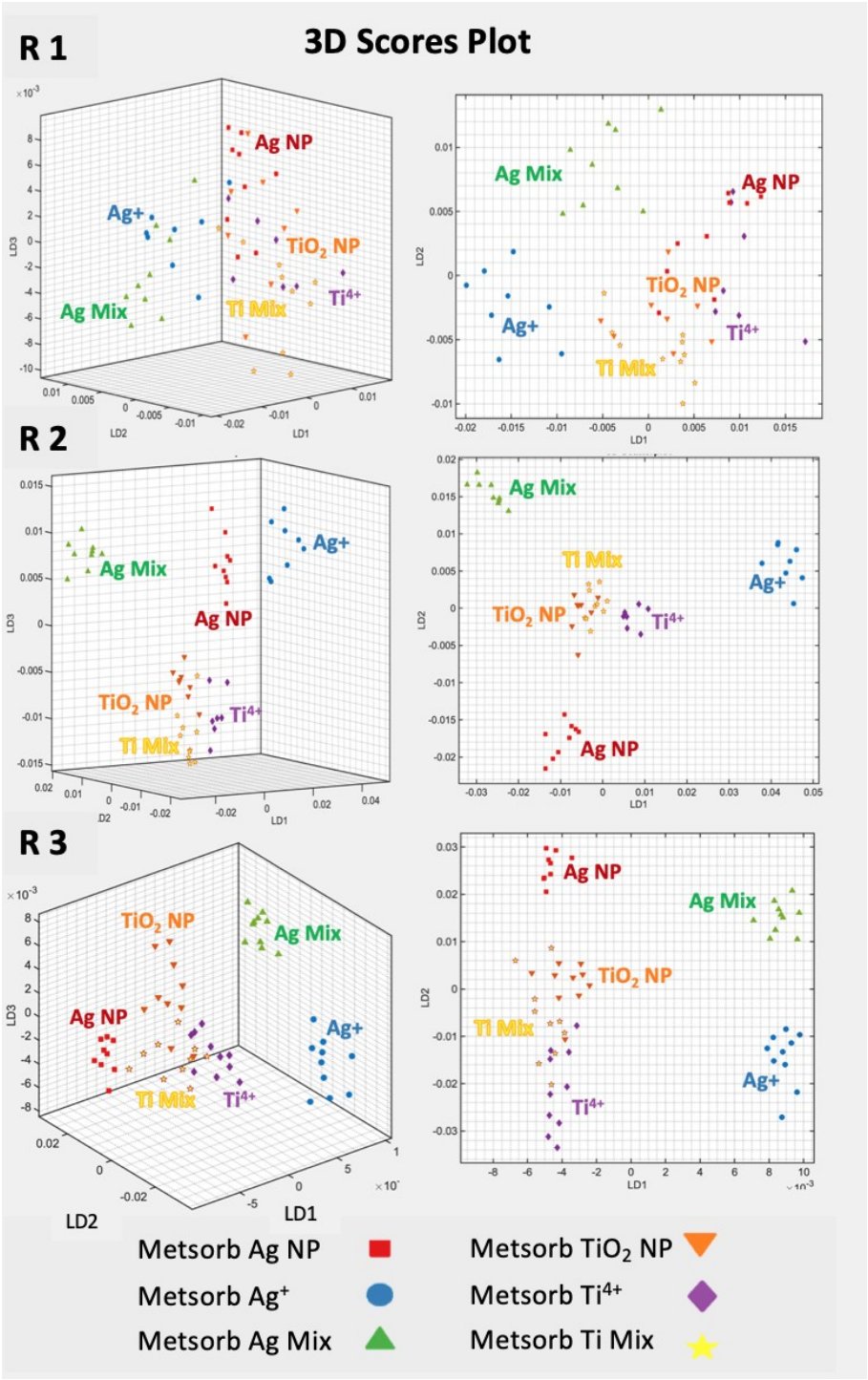

Figure S3. Three-dimensional scores plot visualization of principal component analysis and linear discriminant analysis (PCA-LDA) of Metsorb when exposed to Ag and TiO_2 treatments R1 (600−800 cm−1), R2 (800−2200 cm− 1), and R3 (2600−4000 cm− 1), respectively, represent three spectral regions of the spectra. Scales for X, Y, and Z-axis are arbitrary units. The graphs on the right show the top views of these scores' plots.

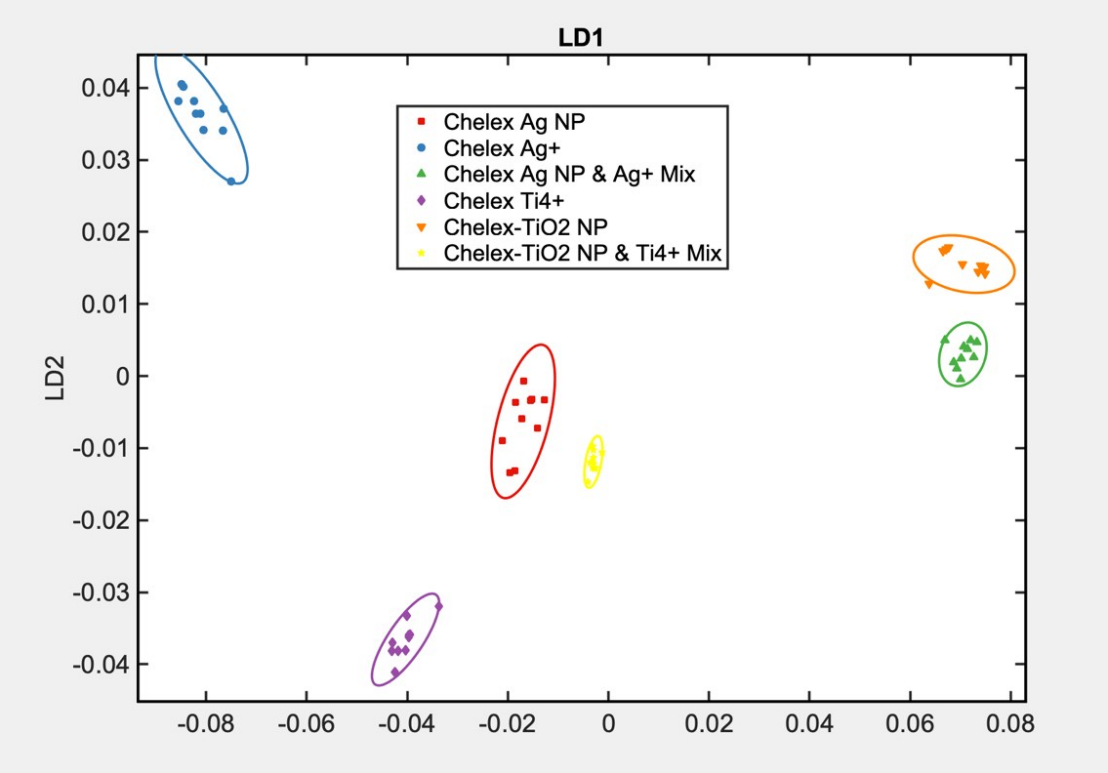

Figure S4. Two-D visualization of principal component analysis and linear discriminant analysis (PCA-LDA) of Chelex®-100 when exposed to the Ag and TiO_2 treatments. The figure represents region 2 of the spectra (R2). Scales for X, Y and Z-axis are arbitrary units. Ellipsoids around each class of spectral points = 95% confidence interval.

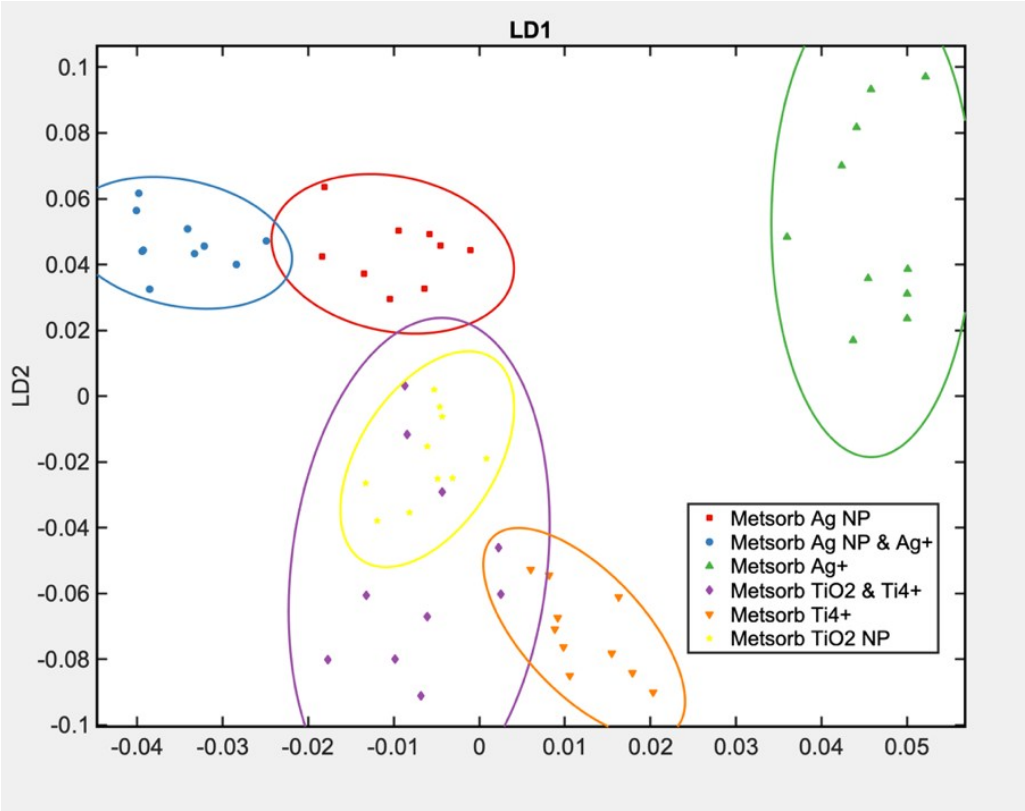

Figure S5. Two-D visualization of principal component analysis and linear discriminant analysis (PCA-LDA) of Metsorb when exposed to the Ag and TiO_2 treatments. The figure represents region 2 of the spectra (R2). Scales for X, Y and Z-axis are arbitrary units. Ellipsoids around each class of spectral points = 95% confidence interval.

Figures S6 shows scanning electron microscopy (SEM) image of Chelex®-100 exposed to the nanoparticles. As seen retention of TiO_2 NPs on the resin surface is clear, the image also indicates Ag NPs sorption on Chelex®-100. Figure S7 belongs to Metsorb™, unlike Chelex®-100, its physical appearance combined with our SEM instrument detection limits prevented us from distinguishing between the structural, nanoscale titanium dioxide forming this resin and Ag or TiO_2 NPs treatments.

For the SEM imaging purpose, the surface and morphologies of the powder samples were examined using a Zeiss EVO 50, under a high vacuum setting and using a 20 KV acceleration voltage, a 100 mA of beam current and a secondary electron detector. Finally, the samples for SEM observation were golds sputtered to reduce electrostatic charging of the surface.

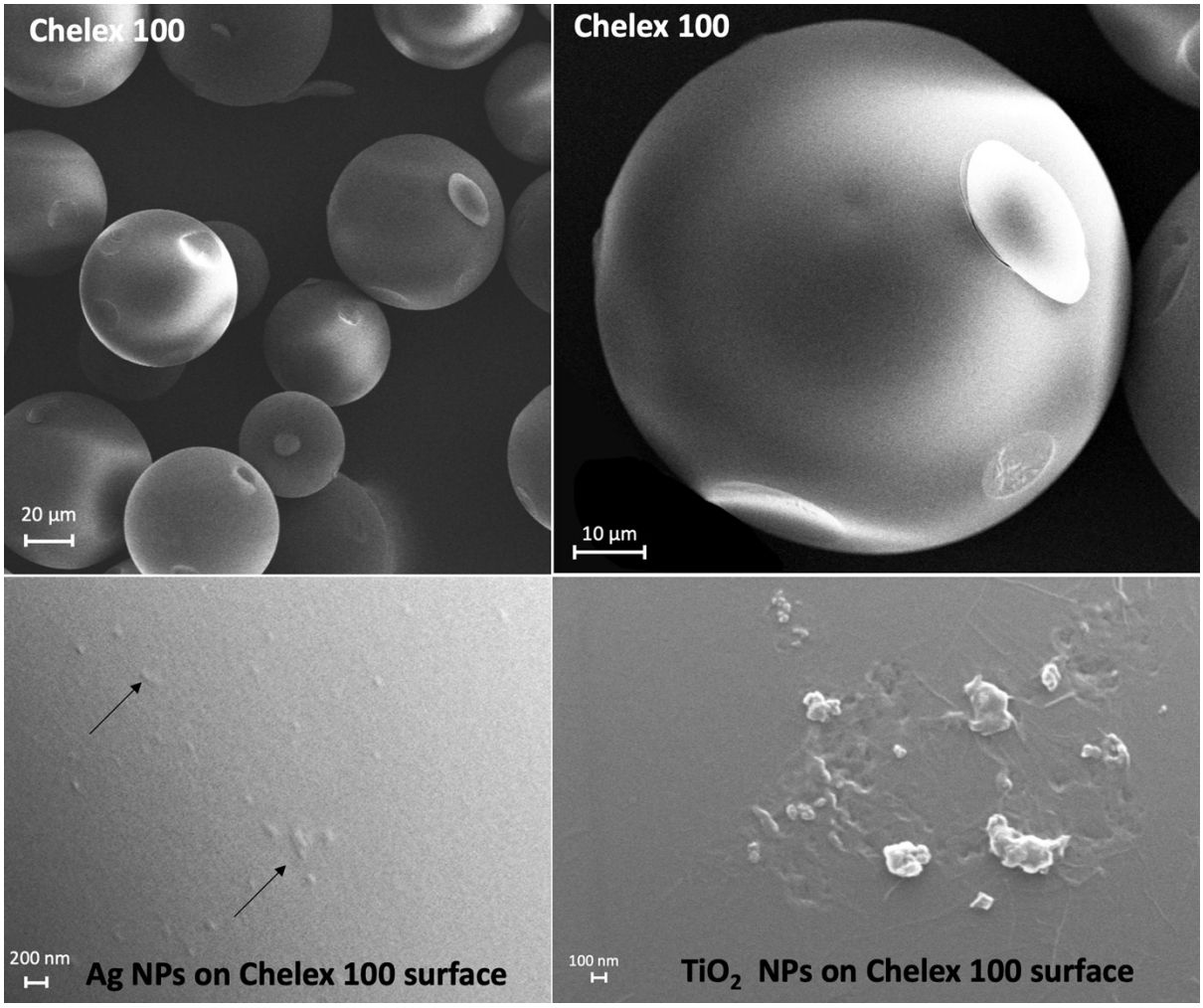

Figure S6. SEM images of Chelex®-100, which the blank Chelex®-100 beads and the samples exposed to Ag and TiO_2 NPs.

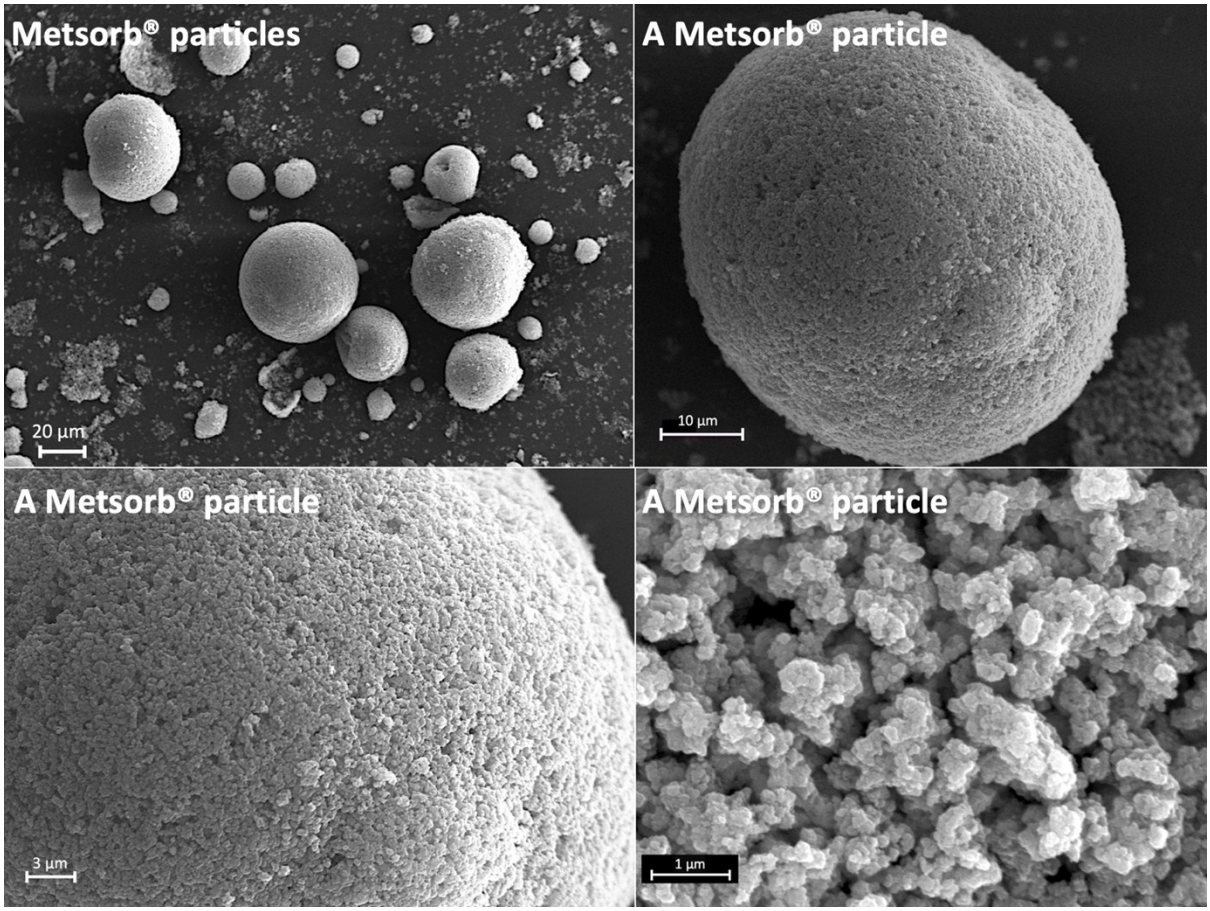

Figure S7. SEM images of the blank Metsorb particles presented in different magnification levels. We could not distinguish between the blank Metsorb samples and those exposed to Ag and TiO_2 NPs using the current SEM instrument.