

Toward SERS-based Point-of-Care approaches for Therapeutic Drug Monitoring: the case of Methotrexate.

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Supplementary information

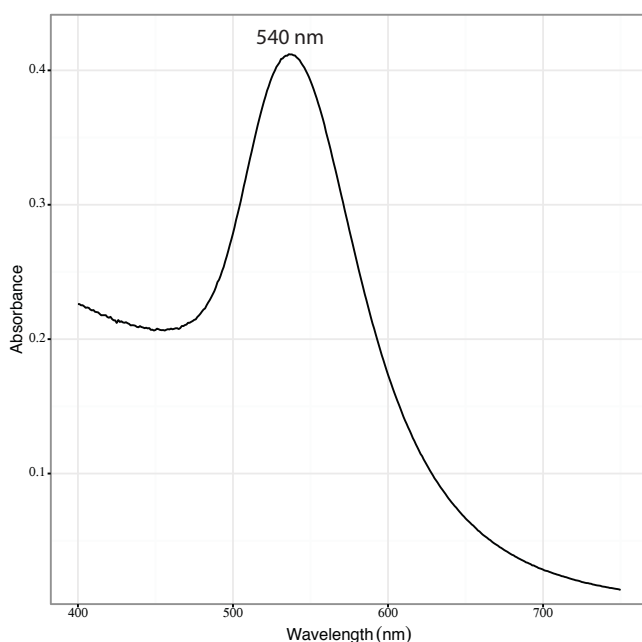


Figure S1 UV/VIS Spectra of the citrate-reduced gold colloid.

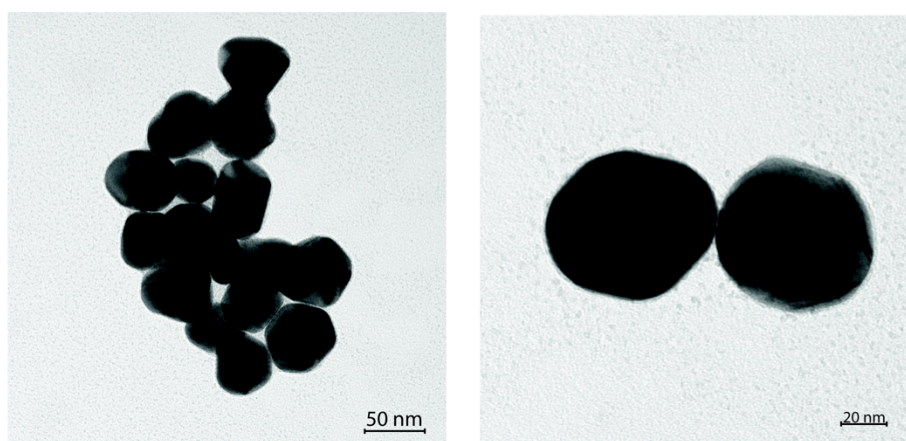


Figure S2 Representative TEM images of gold colloid.

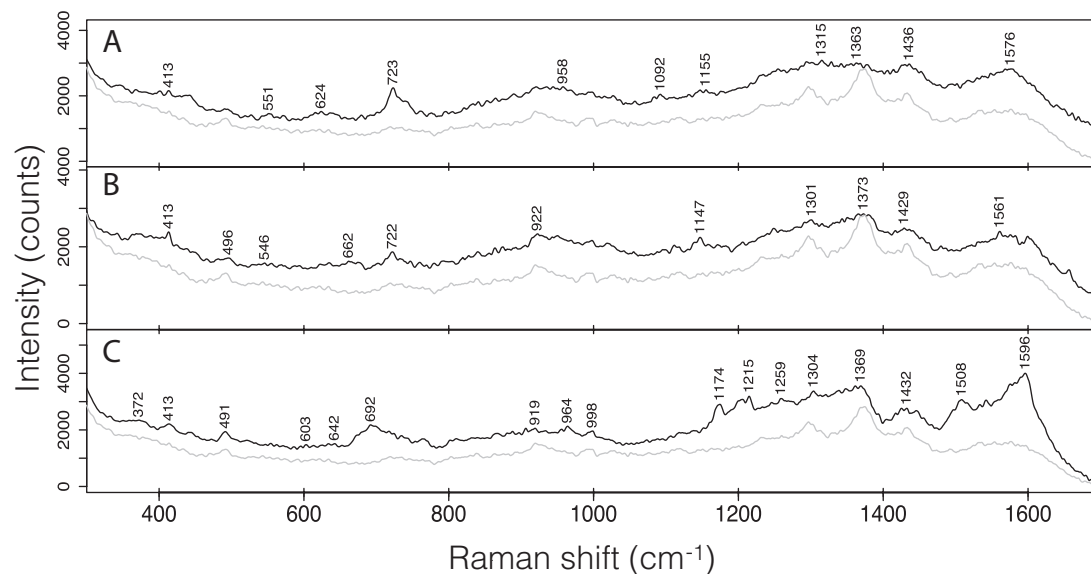


Figure S3 (A) SERS spectrum of human serum, (B) SERS spectrum of diluted human serum (1:4, v/v, PBS), and (C) SERS spectrum of MTX diluted in human serum (1:4, v/v, PBS). The background signal of the substrate (grey line) is reported for comparison together with SERS spectra. All spectra were collected using an excitation at 785 nm.

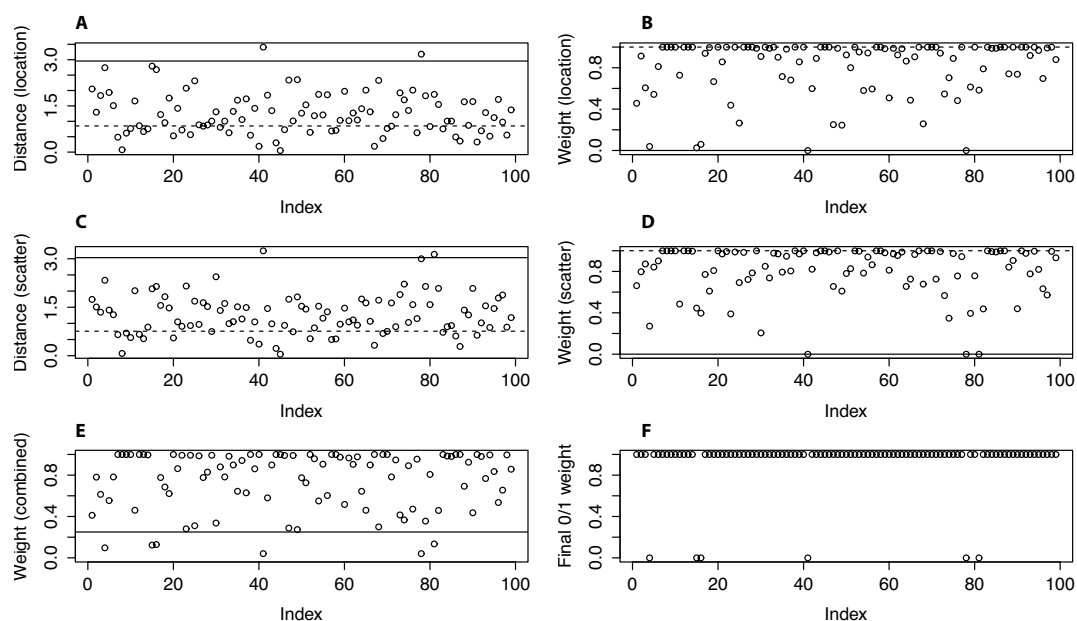


Figure S4 Visualization of the intermediate steps in the *pcout* algorithm (distances and weights) for outlier detection in the HS dataset. For the first step, aimed to detect location outliers, kurtosis distances, together with the weight boundaries are shown in panels A and B, respectively. Similarly, the distances and weights from the second step (detection of scatter outliers) are shown in the C and D panel, respectively. The E panel shows the combined weights (step 1 and 2 combined) together with the default outlier boundary 0.25 (solid line), which results in 0/1 weights (F panel). At the end of the procedure, six spectra are identified as multivariate outliers.

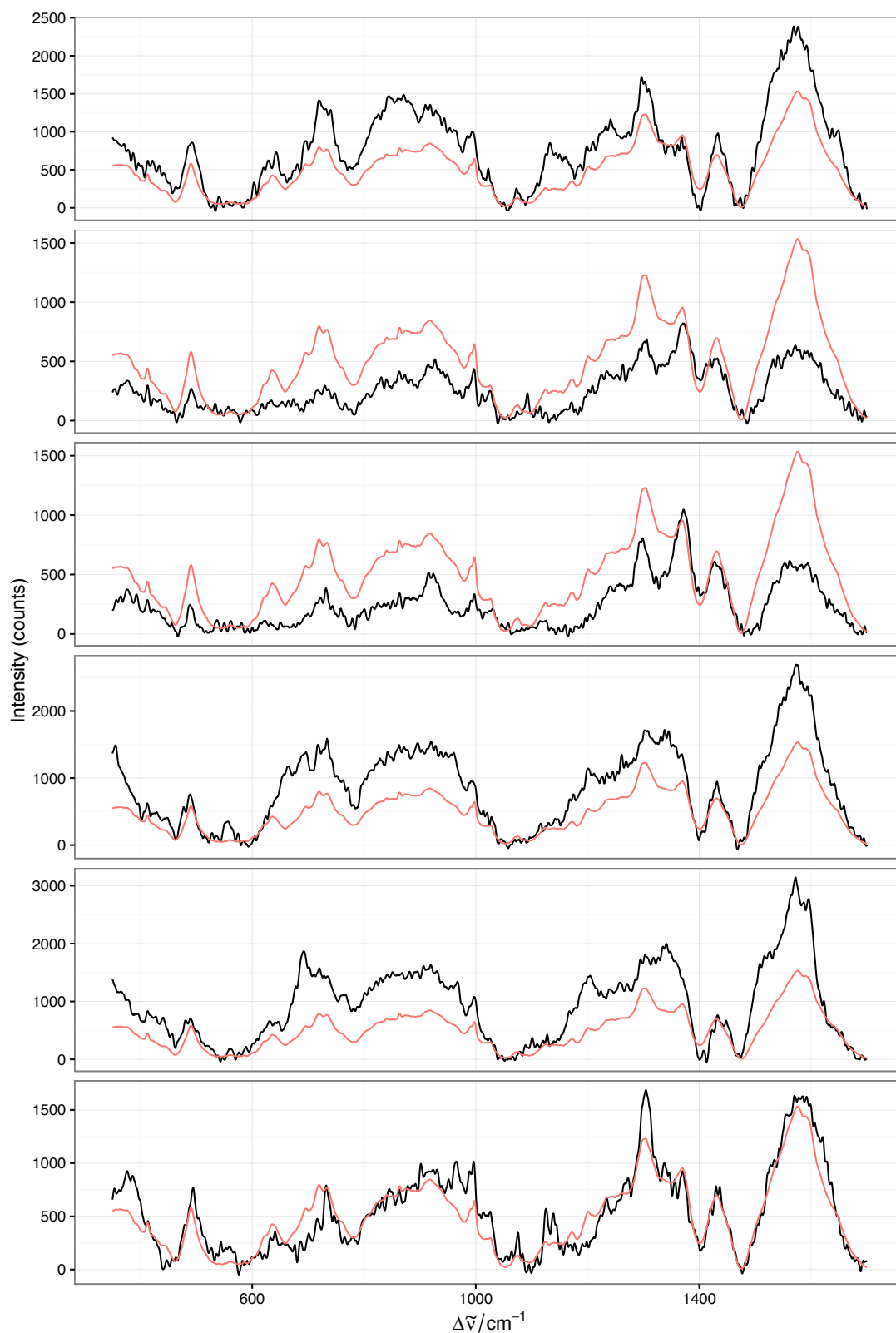


Figure S5. Multivariate outliers detected by the *pcout* function. Mean spectra (red line) of the HS dataset is reported for comparison

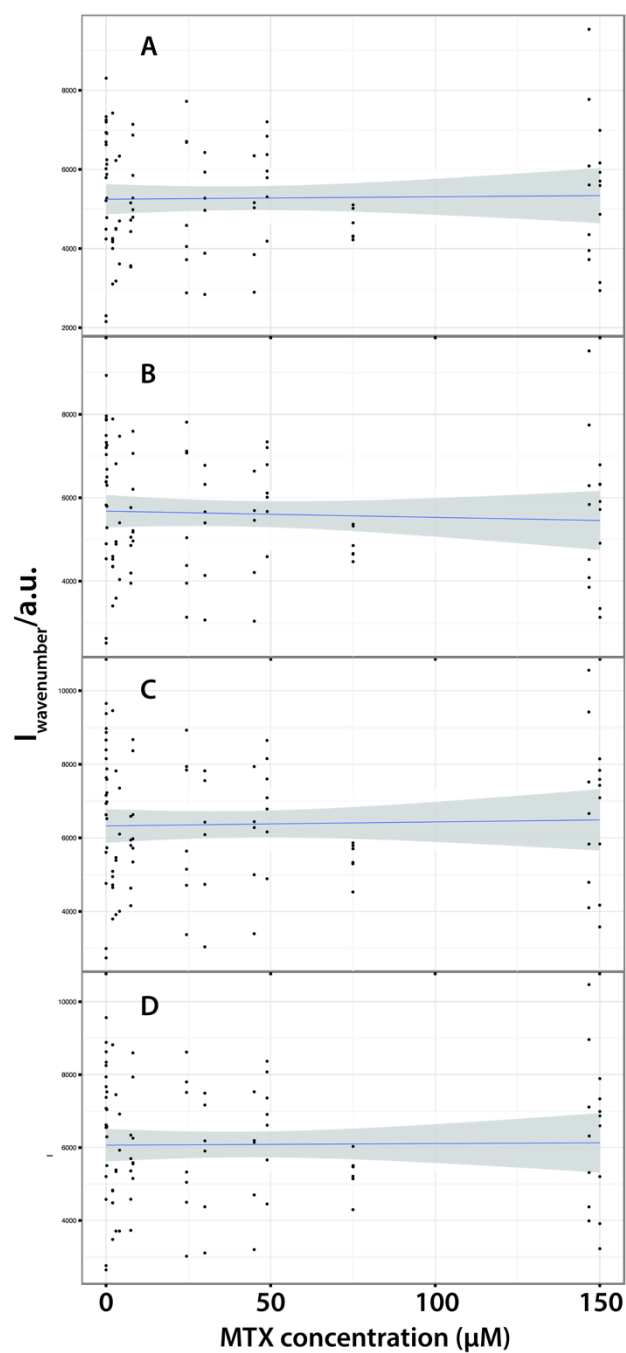


Figure S6 Conventional linear univariate evaluation of the spectral response was performed using specific Raman bands [(A) 692 cm^{-1} ; (B) 965 cm^{-1} , (C) 1508 cm^{-1} (D) 1596 cm^{-1}] in the SERS spectrum of MTX in human serum. The signal intensities were plotted against the reference concentrations, and a first-order least-squares regression line was calculated.