

Supporting information

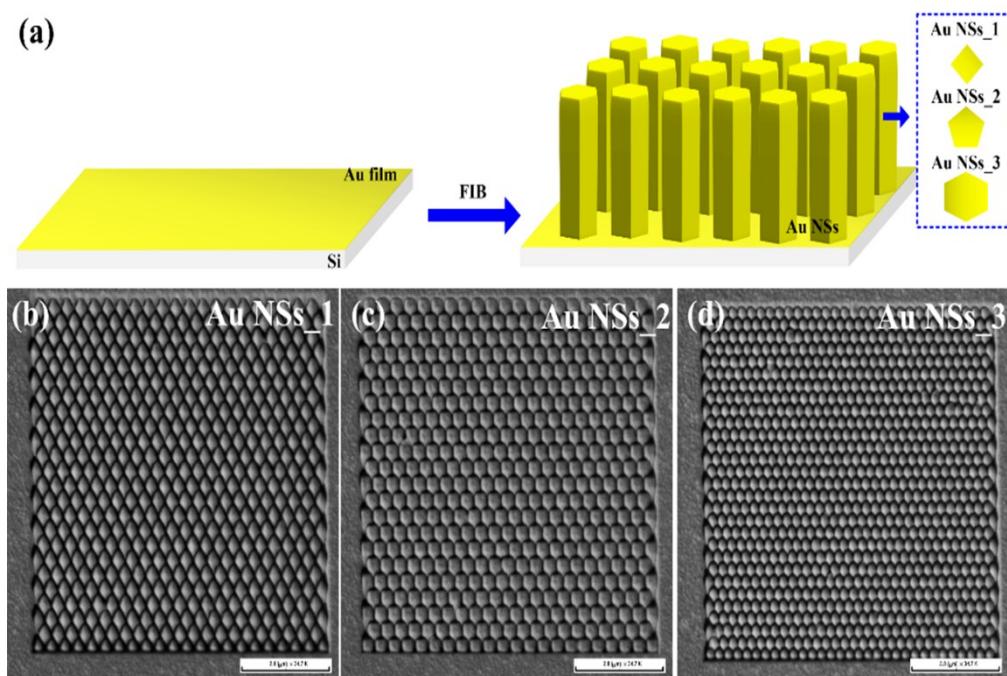


Figure S1 (a) Schematic drawing of focus ion beam (FIB) fabrication process of gold nanorods (AuNRs) array. Scanning Electron Microscope (SEM) images of (b) square, (c) pentagonal, and (d) hexagonal AuNRs array within $14 \mu\text{m} \times 14 \mu\text{m}$ pattern size.

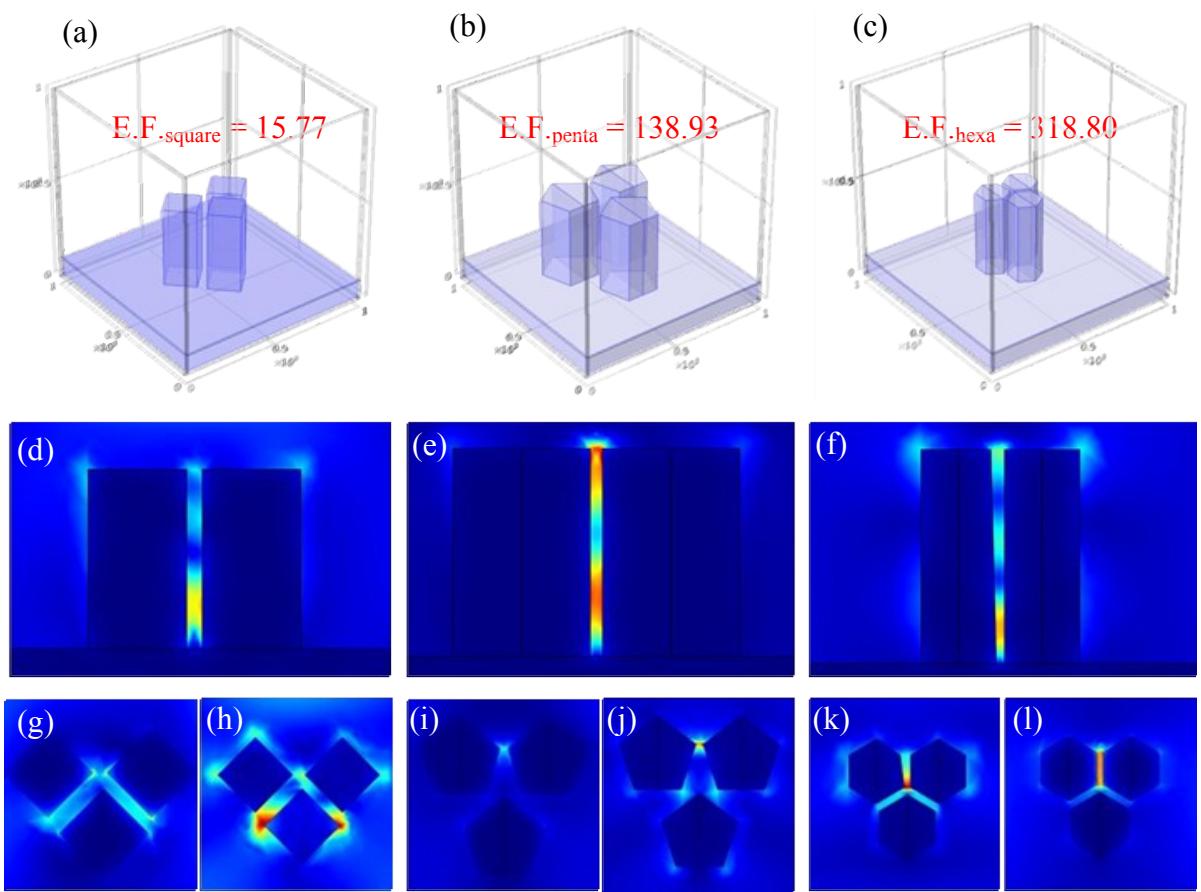


Figure S2. (a-c) COMSOL Multiphysics® simulation model geometry structures of square, pentagonal, and hexagonal AuNRs array (400 nm height). Electromagnetic field distribution side views (d-f), top view from bottom-up 10 nm (g,i,k), and top view from bottom-up 390 nm of square, pentagonal, and hexagonal AuNRs array.

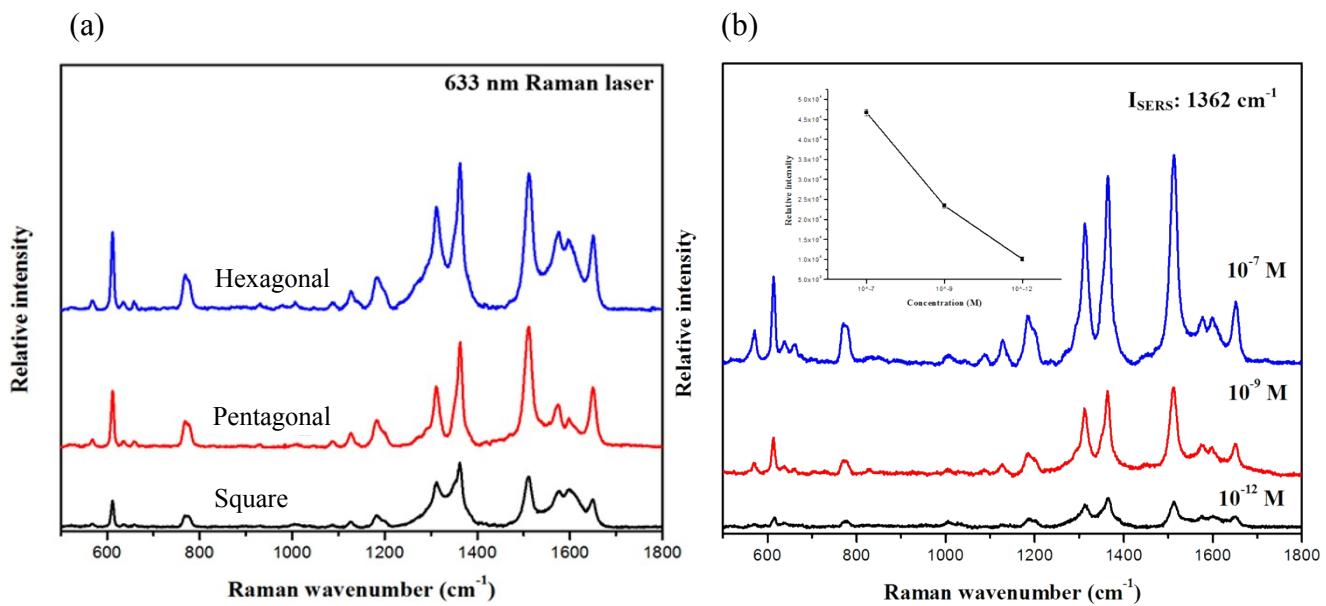


Figure S3. (a) Raman spectra of three different shapes AuNRs applied for R6G molecules SERS analysis with 633 nm laser light irritation. (b) $10^{-7}, 10^{-9}, 10^{-12}$ M R6G aqueous solution Raman spectra for hexagonal AuNRs active SERS substrates detection limit verification.

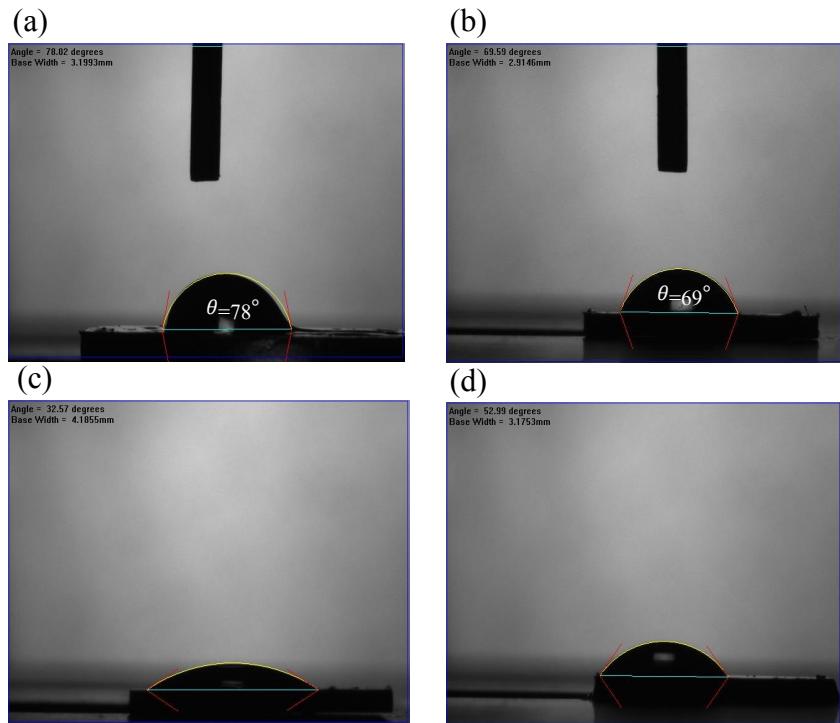


Figure S4. Contact angle measurement of (a) gold nanorods array (AuNRs), (b) AuNRs modified with EDT (c) m-PEG-thiol grafted AuNRs, and (d) PGMA-r-PSBMA grafted AuNRs for the confirmation of polymer grafting onto substrate.

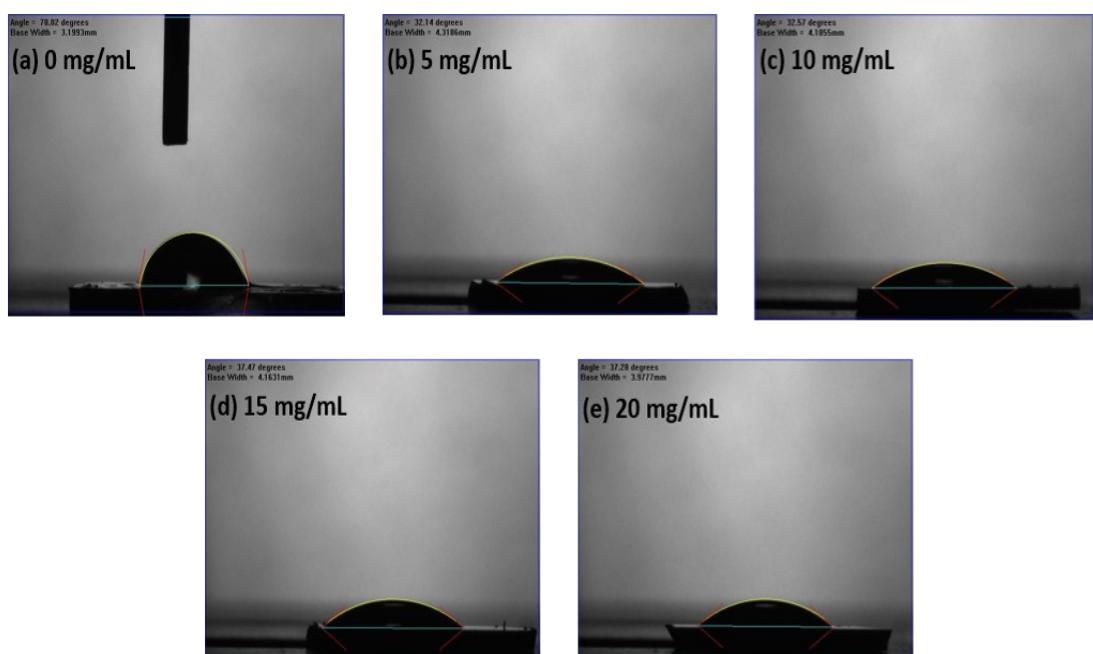


Figure S5. Contact angle measurement of (a) pristine gold nanorods array (AuNRs), and AuNRs with (b) 5 mg/mL, (c) 10 mg/mL, (d) 15 mg/mL, and (e) 20 mg/mL mPEG-thiol surface modification.

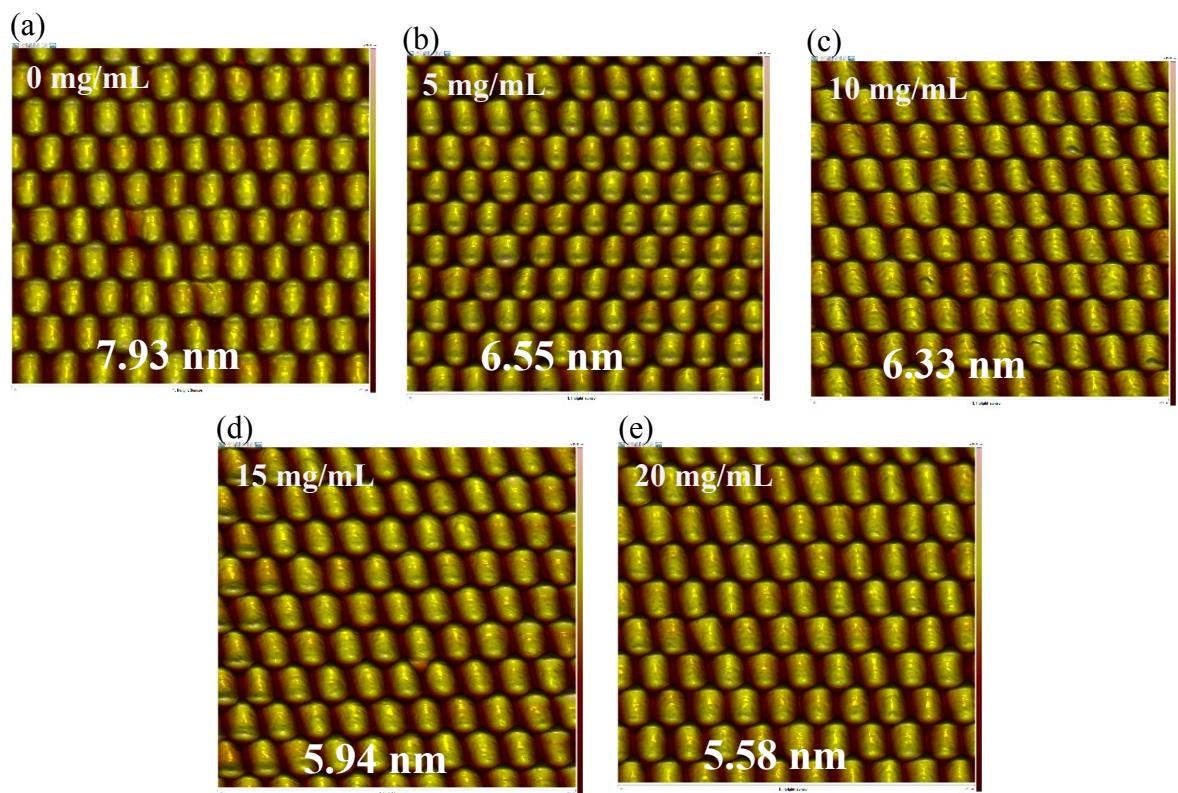


Figure S6. AFM analysis of AuNRs array surface root-mean-square roughness with a series of PGMA-r-PSBMA precursor solution concentrations (a)0, (b)5, (c)10, (d)15, (e)20 mg/ml grafting modification.

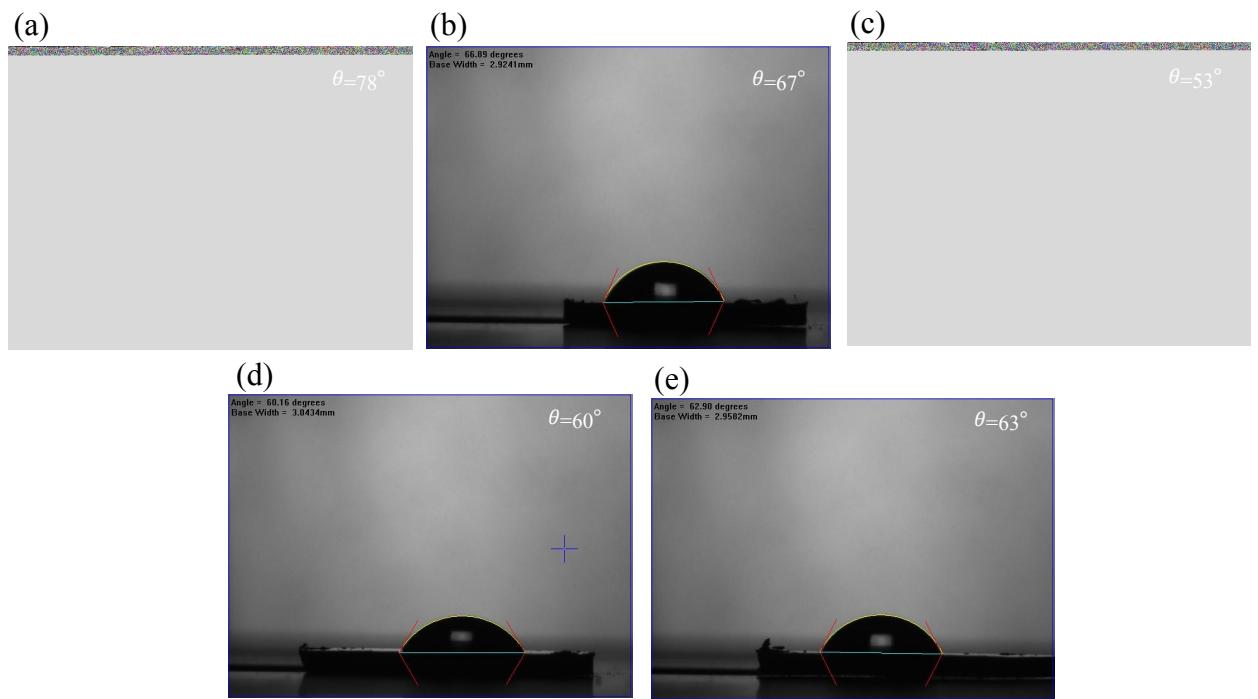


Figure S7. Contact angle measurement of AuNRs SERS substrate surface hydrophilicity with a series of PGMA-r-PSBMA precursor solution concentrations (a)0, (b)5, (c)10, (d)15, (e)20 mg/ml grafting modification.

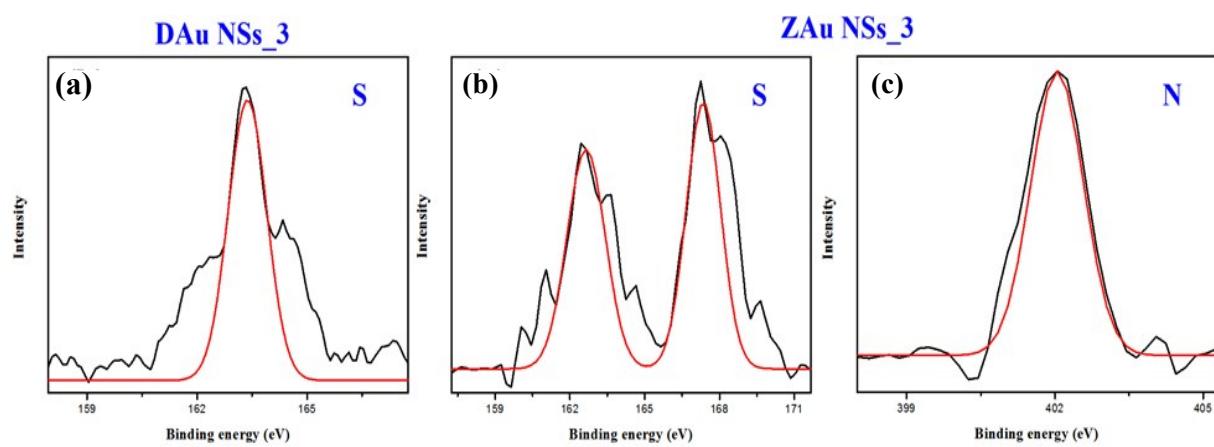


Figure S8. XPS spectra of Au NRs S 2p, N 1s with (a) EDT modification, (b-c) 10 mg/mL PGMA-*r*-PSBMA zwitterionic-modified modification

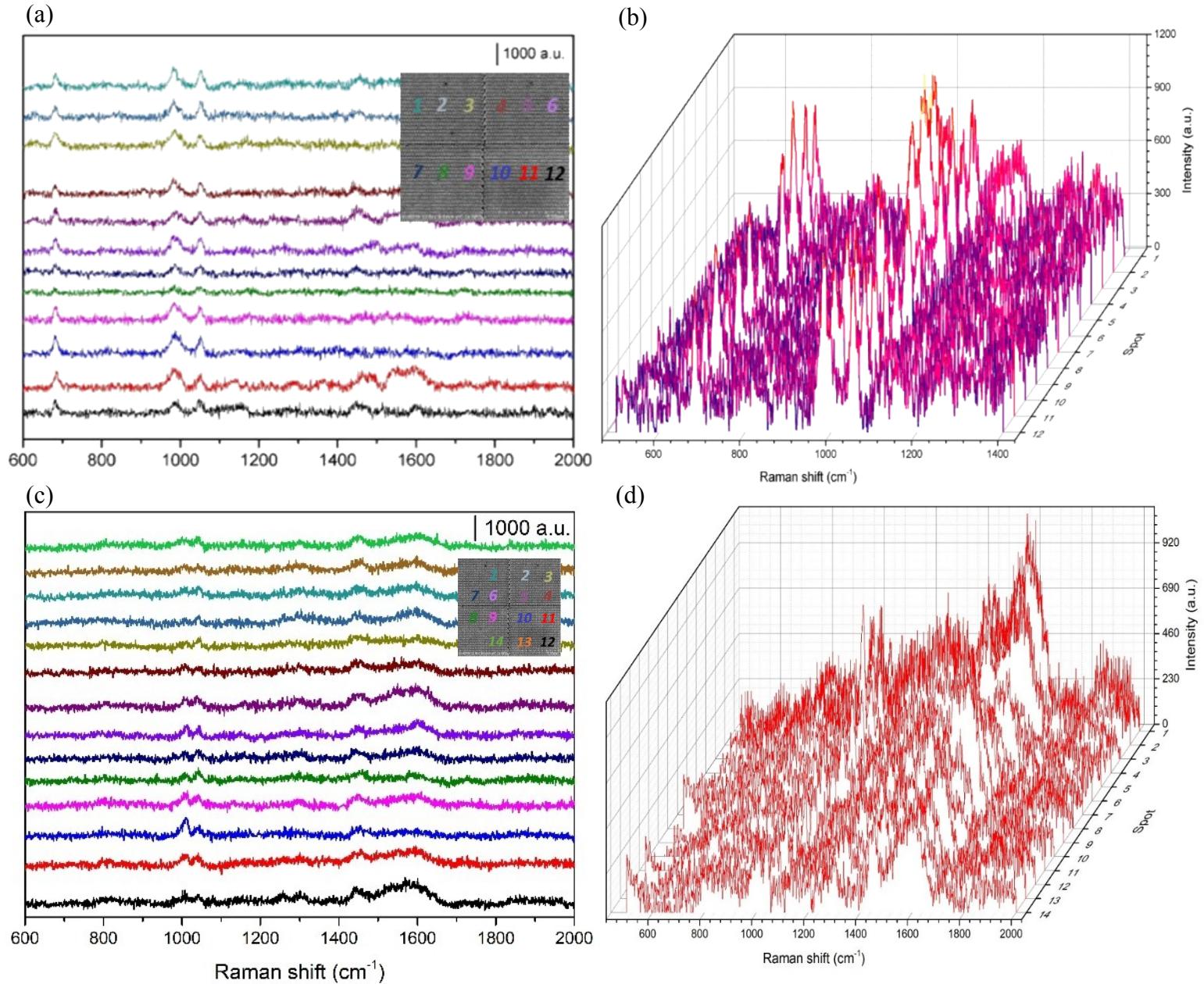


Figure S9. (a-b) Twelve points selection on PGMA-r-PSBMA-AuNR SERS substrate for 10^{-3} M NDMA detection. (c-d) fourteen points selection on PGMA-r-PSBMA-AuNR SERS substrate for 10^{-3} M NDEA detection to confirm SERS substrates uniformity and reproducibility.

Table S1. The enhancement factors (EF) of three Au NRs SERS substrates calculated via COMSOL Multiphysics® electromagnetic field simulation

| Sample | Shape | EF |
|----------|------------|-------|
| Au NRs_1 | Square | 15.8 |
| Au NRs_2 | Pentagonal | 138.9 |
| Au NRs_3 | Hexagonal | 318.8 |