Optimization of gold nanorod arrays for surface enhanced Raman spectroscopy (SERS) detection of atrazine

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Supporting Information

Abstract

Recently, increasing concern over the widespread use of atrazine, which has been reported to have problematic side effects on local ecosystems has highlighted the need for rapid and accurate point-of-need assessment tools for analytical determination of herbicides in ground and surface waters. Surface enhanced Raman spectroscopy (SERS) is a sensitive vibrational spectroscopy technique which has recently been employed for the analysis of a variety of analytes in water, ranging from pharmaceuticals to pesticides. In this work, SERS sensors constructed using gold nanorod (AuNR) arrays are optimized and then utilized for the rapid and sensitive detection of atrazine. In this study, the effect of relative humidity on the self-assembly of the gold nanorods into arrays was explored, and the SERS performance was assessed using *para*-aminothiophenol as a SERS probe. Once the performance of the substrates was deemed optimal, the detection of atrazine was highlighted. This work represents the first time that relative humidity is explored as an optimization strategy for controlled alignment of gold nanorods for SERS analysis of atrazine.

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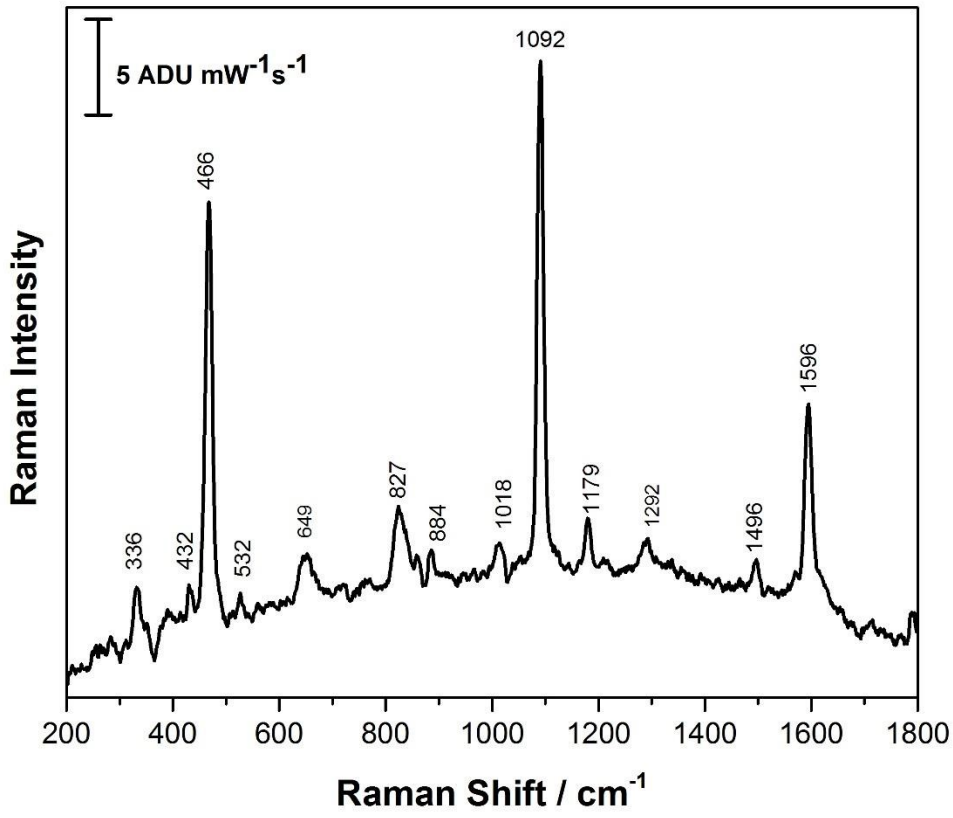

Figure S-1: Normal Raman spectrum of *p*-ATP powder at 785 nm. Laser power was 54.77 mW for an acquisition time of 60s.

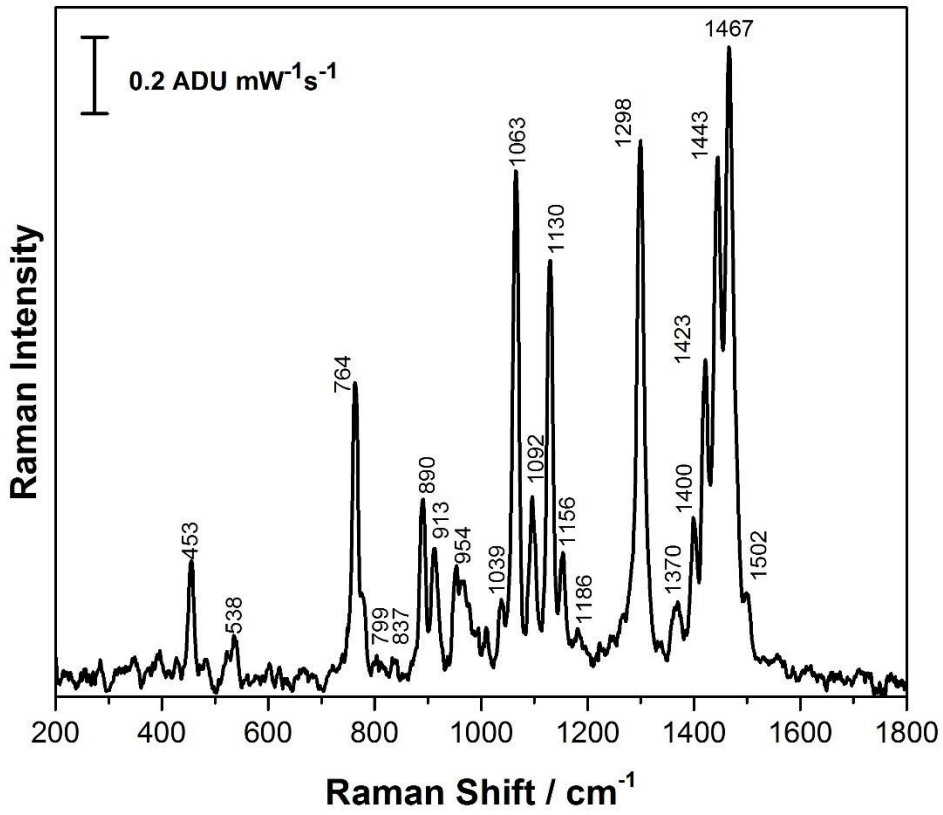

Figure S-2: Normal Raman spectrum of CTAB powder recorded at 785 nm. Laser power was 12.17 mW for an acquisition time of 30s.

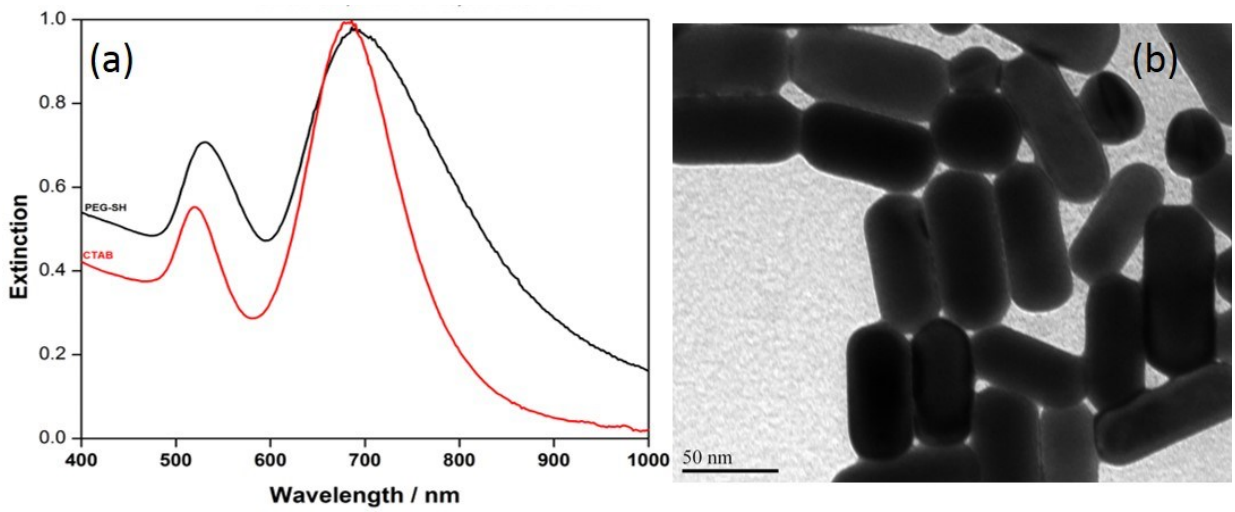

Figure S-3: (a) Extinction spectrum of CTAB coated AuNRs and PEGylated AuNRs in water **(**b) TEM image of AuNRs at 300kX.

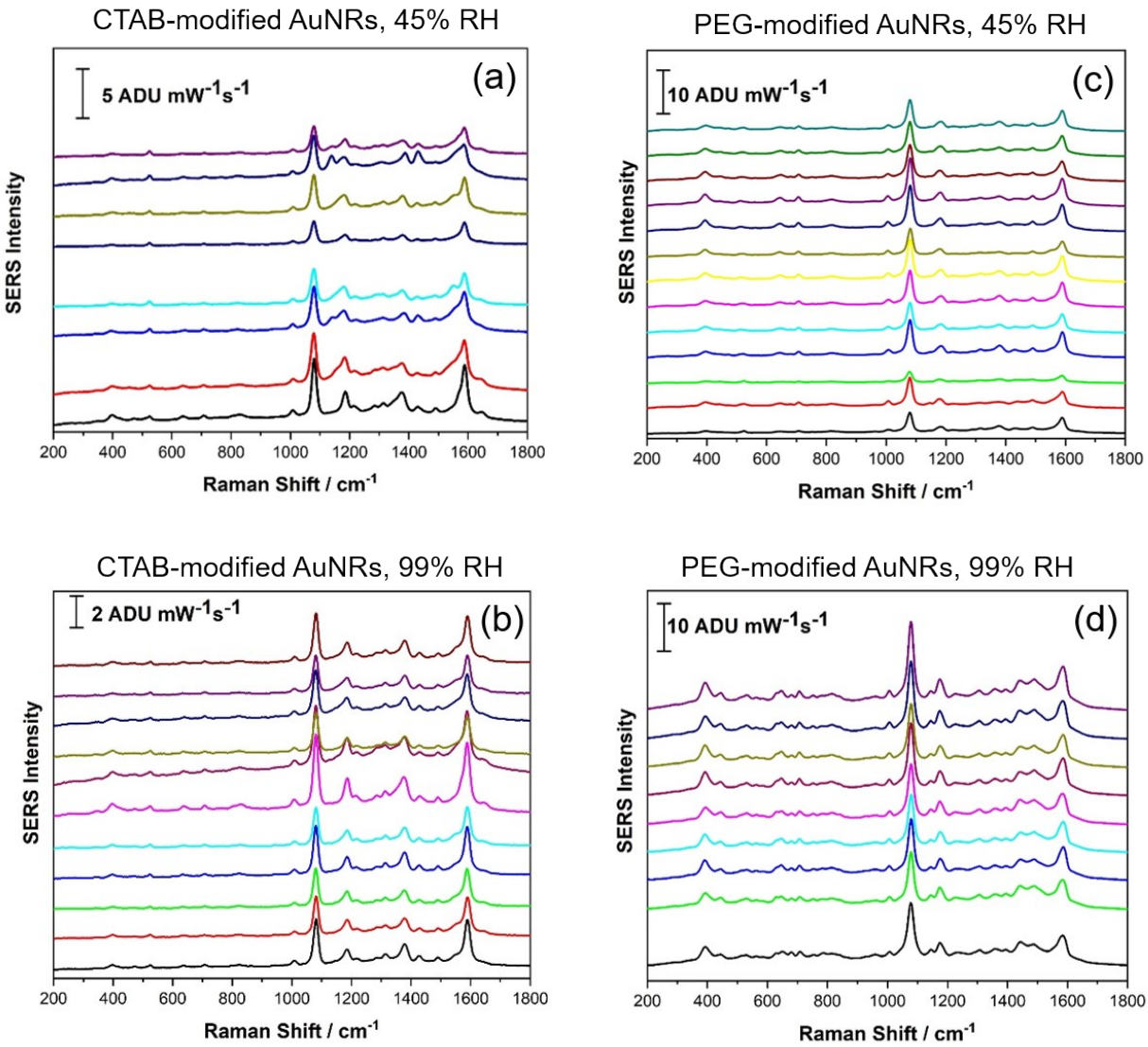

Figure S-4: Raw SERS data for 1.0 mM p-ATP recorded for CTAB-modified AuNRs at 45% RH (a) and 99% RH (b) and PEG-modified AuNRs at 45% RH (c) and 99% RH.

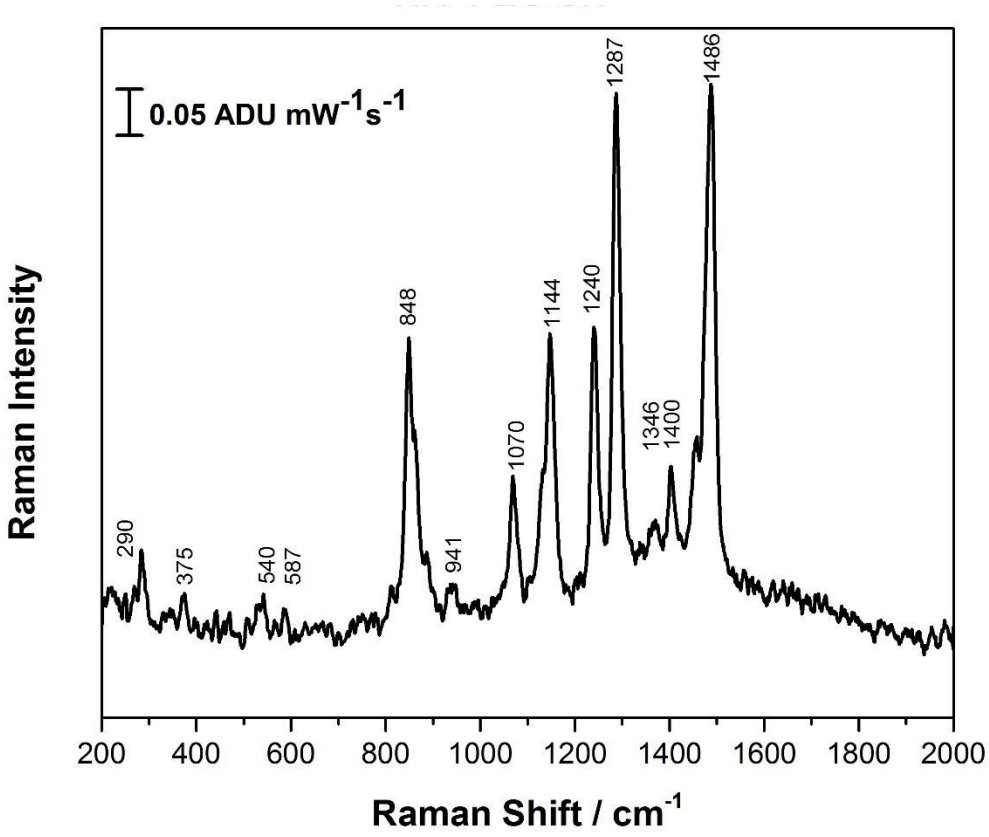

Figure S-5: Normal Raman spectrum of PEG-SH powder recorded at 785 nm. Laser power was 54.77 mW for an acquisition time of 60s.

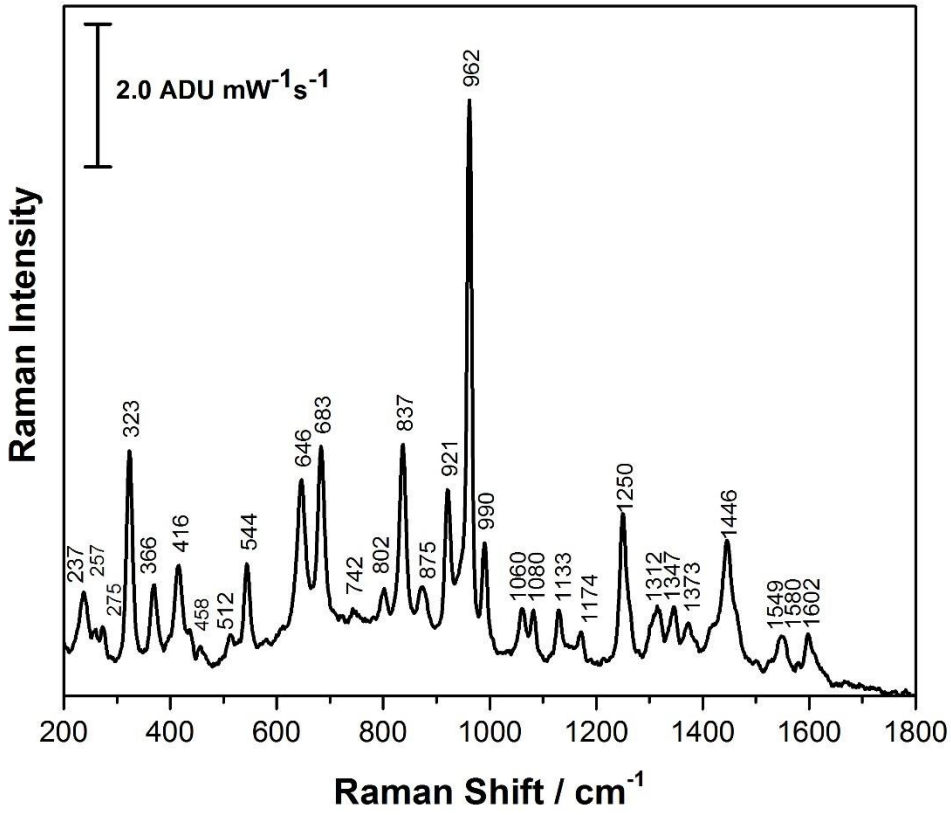

Figure S-6: Normal Raman spectrum of atrazine powder measured at 785 nm. Laser power was 12.17 mW for an acquisition time of 30s.

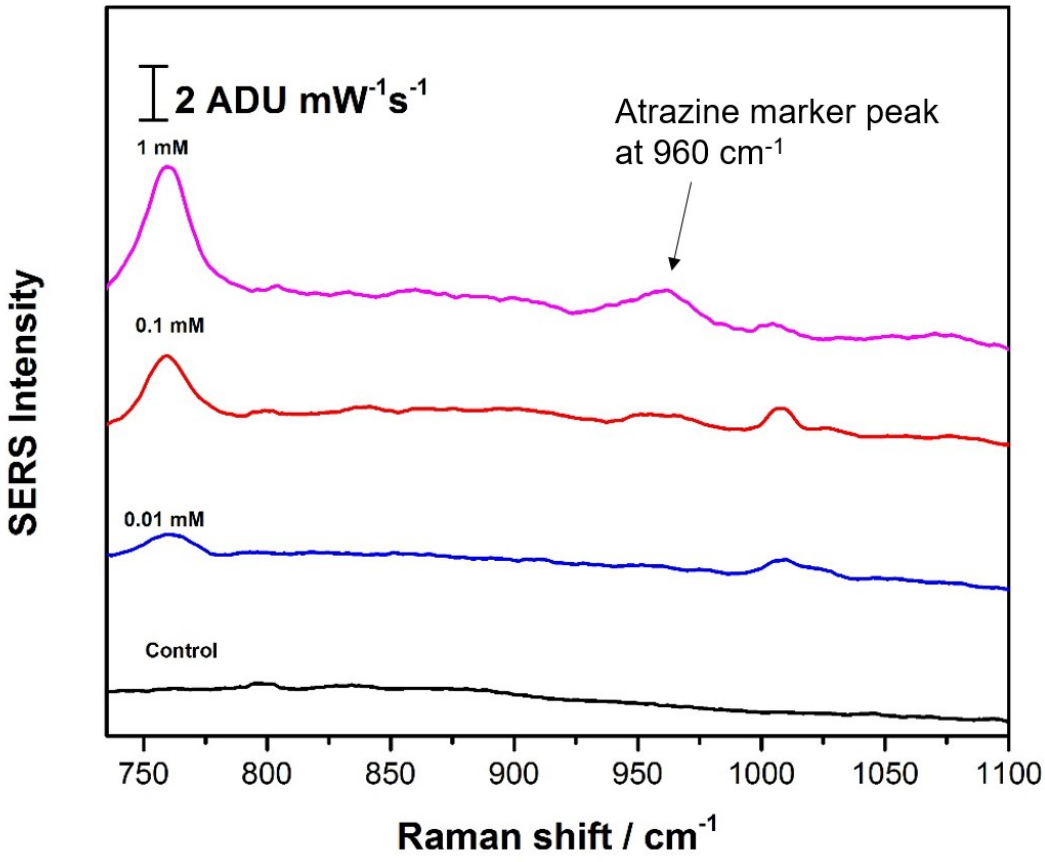

Figure S-7: SERS signal for atrazine recorded at 1 mM, 0.1 mM and 0.01 mM. Control signal is for the PEGylated AuNR array in the absence of atrazine, highlighting signals from the surface of the rods.