Electronic Supplementary Material (ESI) for Analyst.

ZnO oxide films for ultrasensitive, rapid, and label-free detection of Neopterin by surface–enhanced Raman spectroscopy

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Supporting Information

1. Characterization of Si/ZnO/Au surface

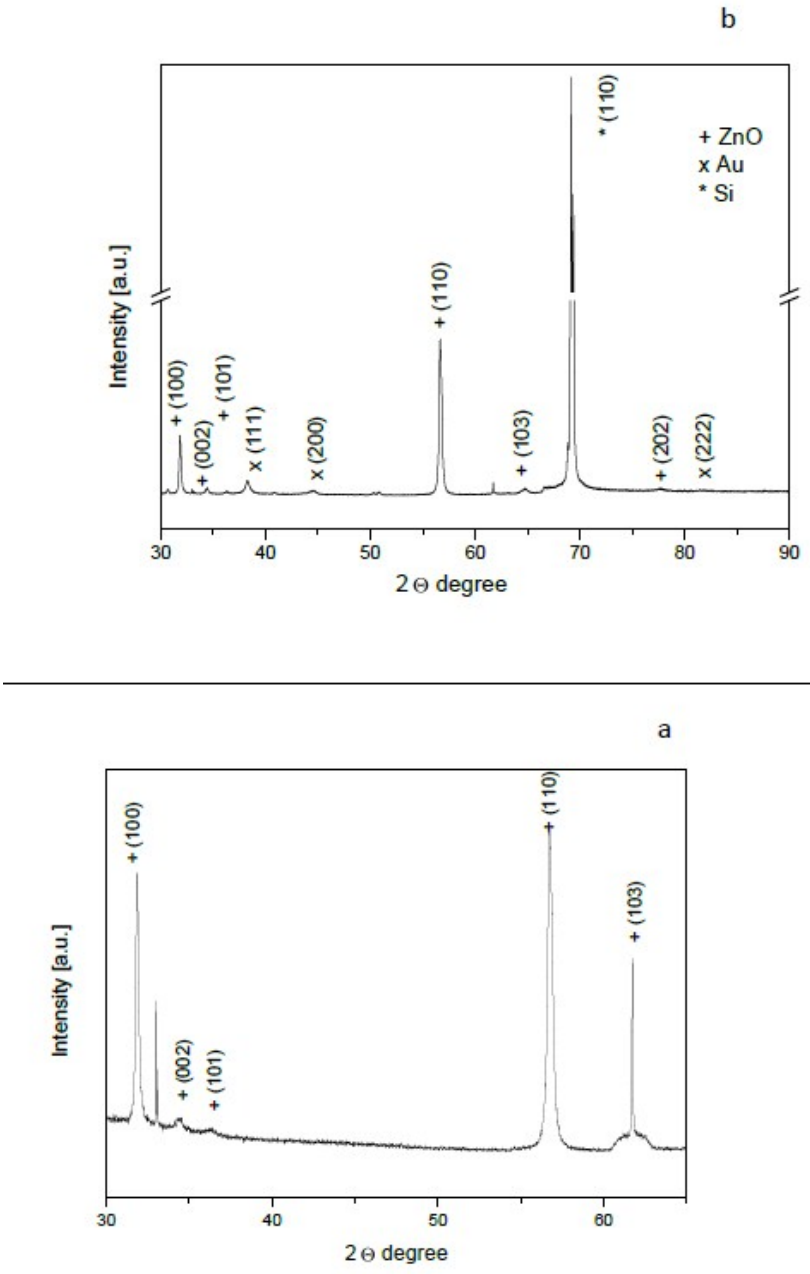

Figure S1. EDX results for ZnO/Si (a) and ZnO/Si covered with 80 nm of gold (b).

2. SERS properties of Si/ZnO/Au substrate: *p*-MBA band assignment.

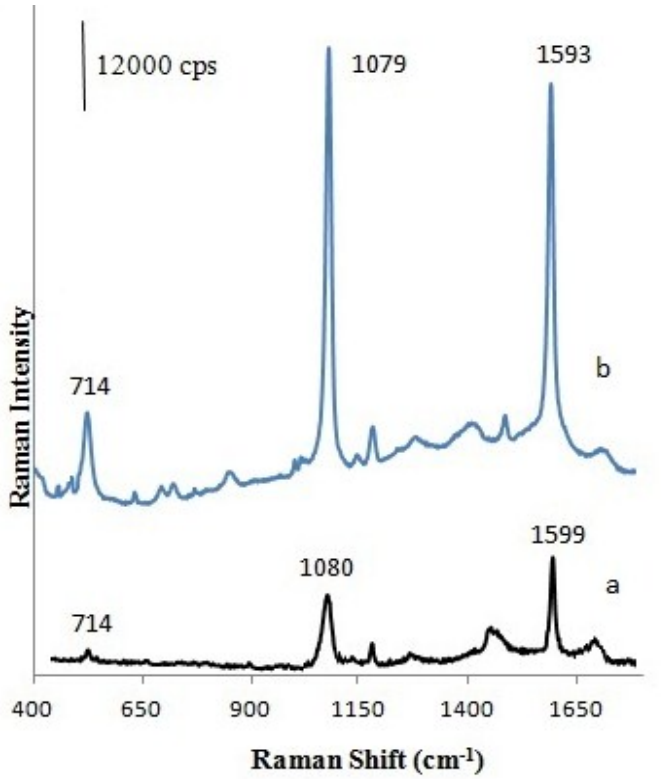

Figure S2. (a) normal Raman spectrum of 10^{-3}M *p*-MBA solution, (b) SERS spectrum of 1.0 × 10^{-6} M *p*-MBA solution on the Si/ZnO/Au substrates. Experimental conditions: 5mW of 785 nm excitation, 4 x 10 seconds acquisition time. The SERS spectra have been baseline-corrected and shifted vertically for better visualization. Each SERS spectrum was averaged from seven measurements at different places of the SERS platform. Normal Raman spectrum was obtained with 15 accumulations of 50s each, using 50mW of 785 nm excitation.

Table S1. Raman and SERS bands assignments for *p*-MBA (data based on [42]).

SERS of PMBA on Au/ZnO/Si (Wavenumber [cm^{-1}])	Band assignment
~714	γ(CCC) aromatic ring vibrations
~845	$\delta(COO^-)$
~1000	substitued benzene ring vibrations
~1079	ν_{12} aromatic ring vibrations
~1374	$\nu_s(COO^-)$
~1593	ν_{8a} aromatic ring vibrations

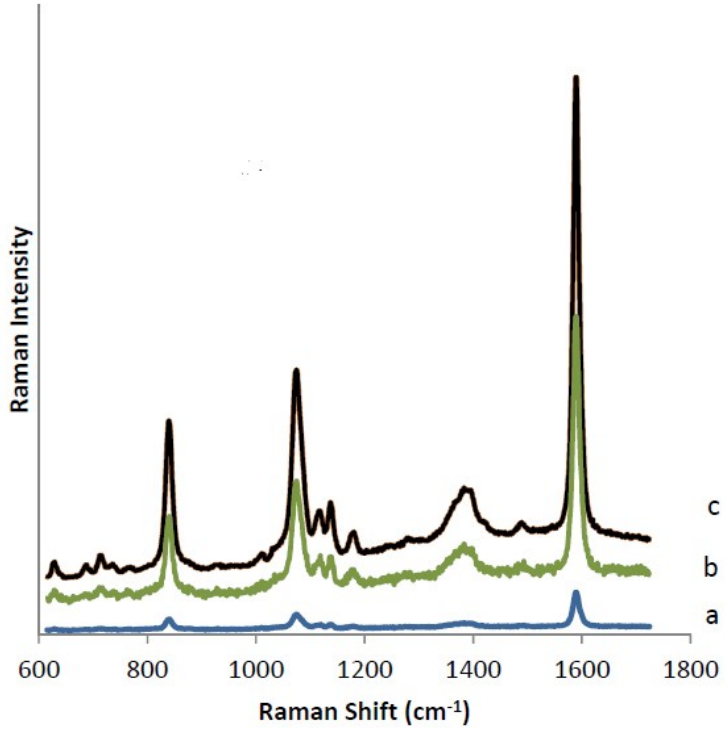

Figure S3. SERS spectra of *p*-MBA from three different thickness of ZnO layers: (a) 630nm, (b) 1 μm, and (c) 1.4 μm. Experimental conditions: 5mW of 785 nm excitation, 4 x 10 seconds acquisition time. Each SERS spectrum was averaged from seven measurements in different places of SERS surface.The *p*-MBA spectra have been baseline corrected and shifted vertically for better visualization.

Table S2. The RMS and EF factors for three different thickness of ZnO layers.

Thickness of ZnO layer	RMS/nm	EF
630 nm	24	3.3×10^2
1 μm	38.5	1.4×10^6
1.4 μm	68	4.2×10^7

Reproducibility of SERS-based immunoassay.

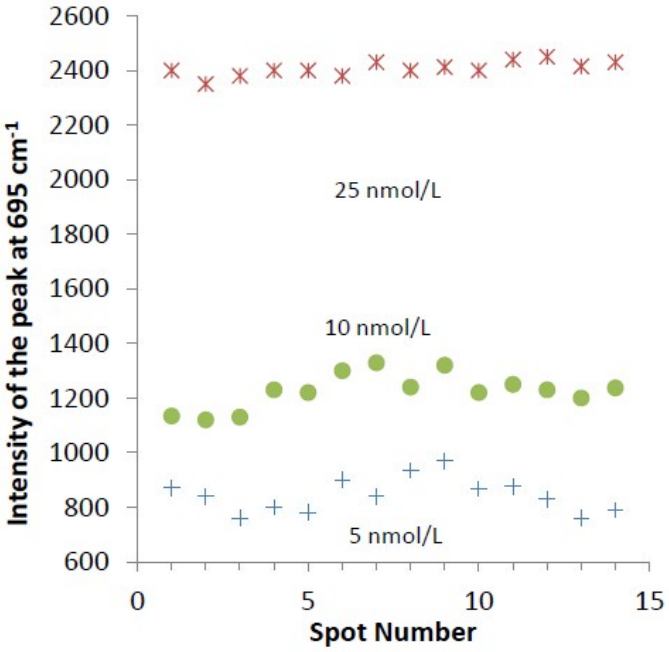

Figure S4. Reproducibility of three separately prepared SERS immunoassays exposed to different concentrations of neopterin in the buffer solution s (5.0, 10.0, and 25.0 nmol/L). The marker band of at 695 cm^{-1} was chosen to present the uniformity of the SERS signal for label-free detection of neopterin and, subsequently, to calculate the relative standard deviation (RSD). The SERS spectra were recorded from 15 randomly selected spots across each SERS surface.