Supplementary Material

# Application of Aluminum Hydroxide for Improvement of Label-Free SERS Detection of Some Cephalosporin Antibiotics in Urine

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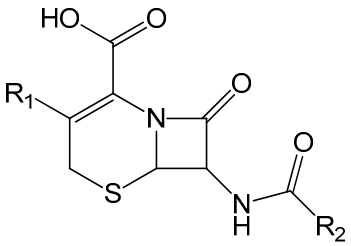
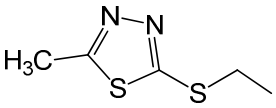
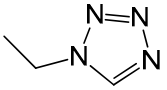
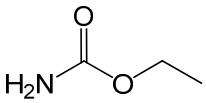
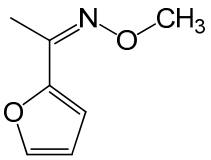
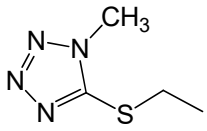
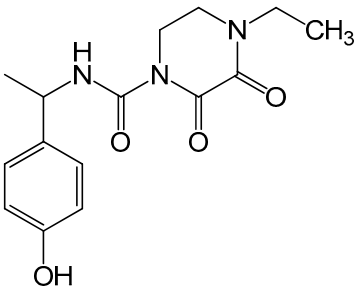
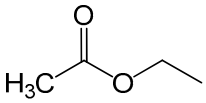
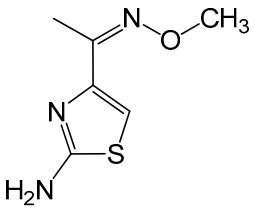
**Table 1.** Chemical structures of the analytes (cephalosporins):.



| Analyte | $R_1$ – | – $R_2$ | Generation | Molecular weight, g/mol |
|---|---|---|---|---|
| CZL |  |  | 1 | 454.5 |
| CRX |  |  | 2 | 424 |
| CPR |  |  | 3 | 646 |
| CTX |  |  | 3 | 455.5 |



*Biosensors* **2019**, *9*, 91; doi:10.3390/bios9030091 www.mdpi.com/journal/biosensors

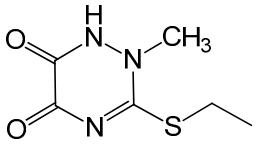
| | | | |
|---|---|---|---|
| CTR |  | 3 | 554.5 |

**Table S2.** Description of the Raman spectrometer used in the study.

| Detail | Description |
|---|---|
| Spectrometer | QEPro |
| Diffraction gratings | 1200 g/mm (Grating H35) |
| Raman shift range | 150–3100 $cm^{-1}$ |
| Slit | 100 μm |
| Laser | 638 nm<br>18 mW (power at the sample)<br>(Laser-638-LAB-FCA) |
| Raman probe | FC excitation and SMA 905 collection<br>(RIP-RPB-638-SMA-SMA) |
| Holder | Universal for Raman, fluorescence,<br>and absorbance measurements (OOA-HOLDER-RFA) |
| Software | OceanView |

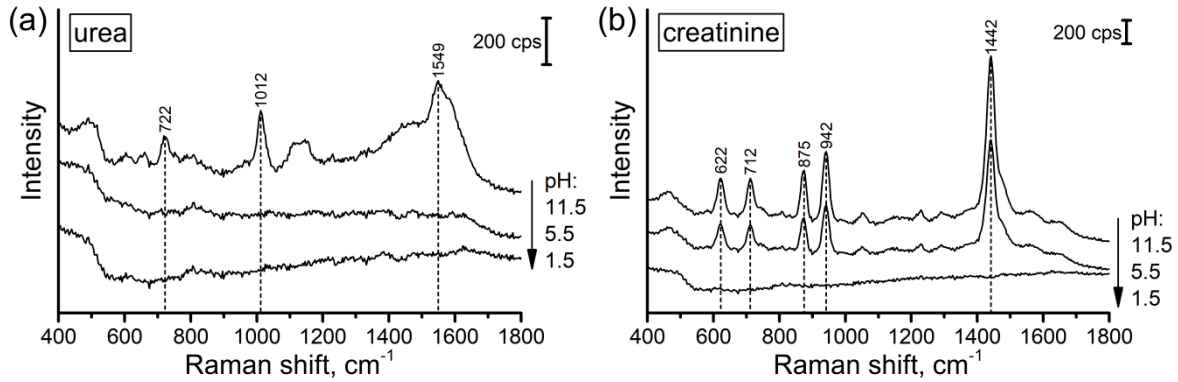



**Figure S1.** SERS spectra of (**a**) urea (1000 μg/mL) and (**b**) creatinine (2 μg/mL) aqueous solutions at different pH values.

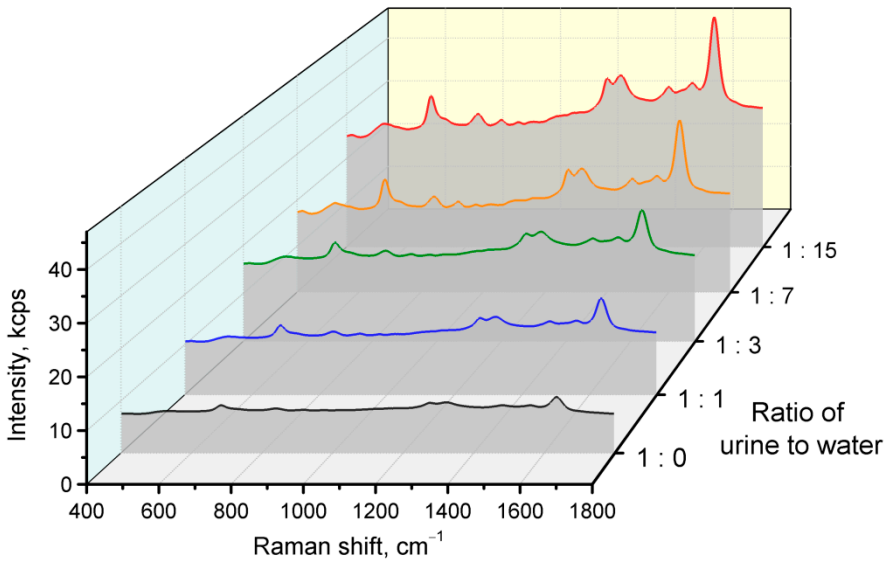



**Figure S2.** An influence of urine dilution on SERS signals of the pure urine with acidic pH (1.5).

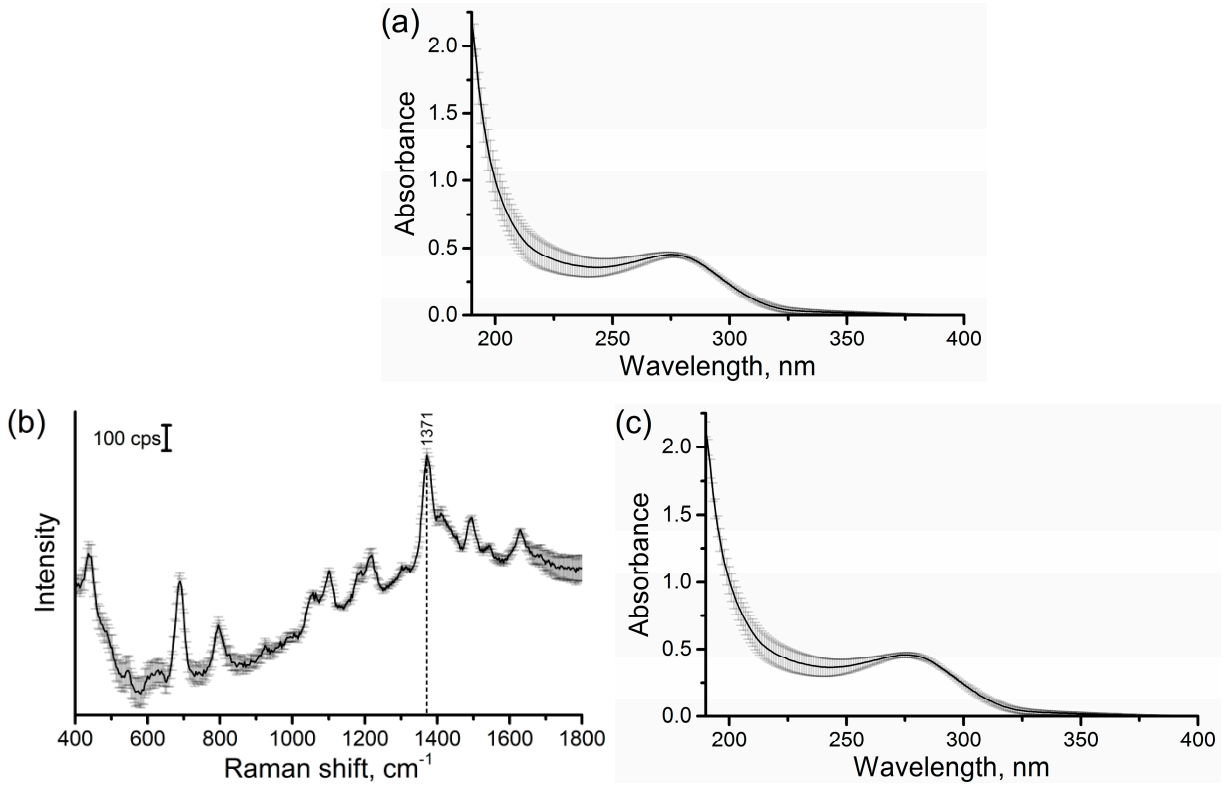



**Figure S3.** (**a**) Absorbance spectrum of CZL obtained during the study of temporal stability of AHG. (**b,c**) SERS and absorbance spectra of CZL obtained during the study of batch-to-batch reproducibility of AHG synthesis.

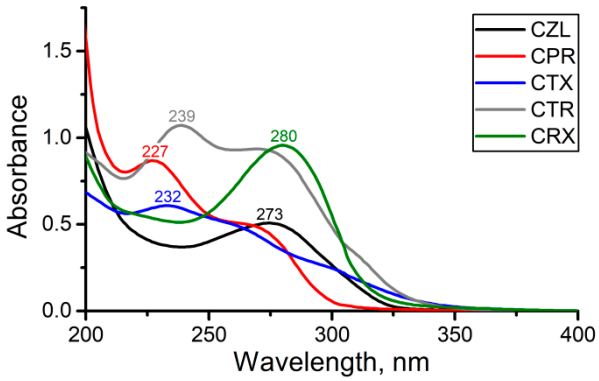



**Figure S4.** Profiles of absorbance spectra of the analytes (50 μg/mL)

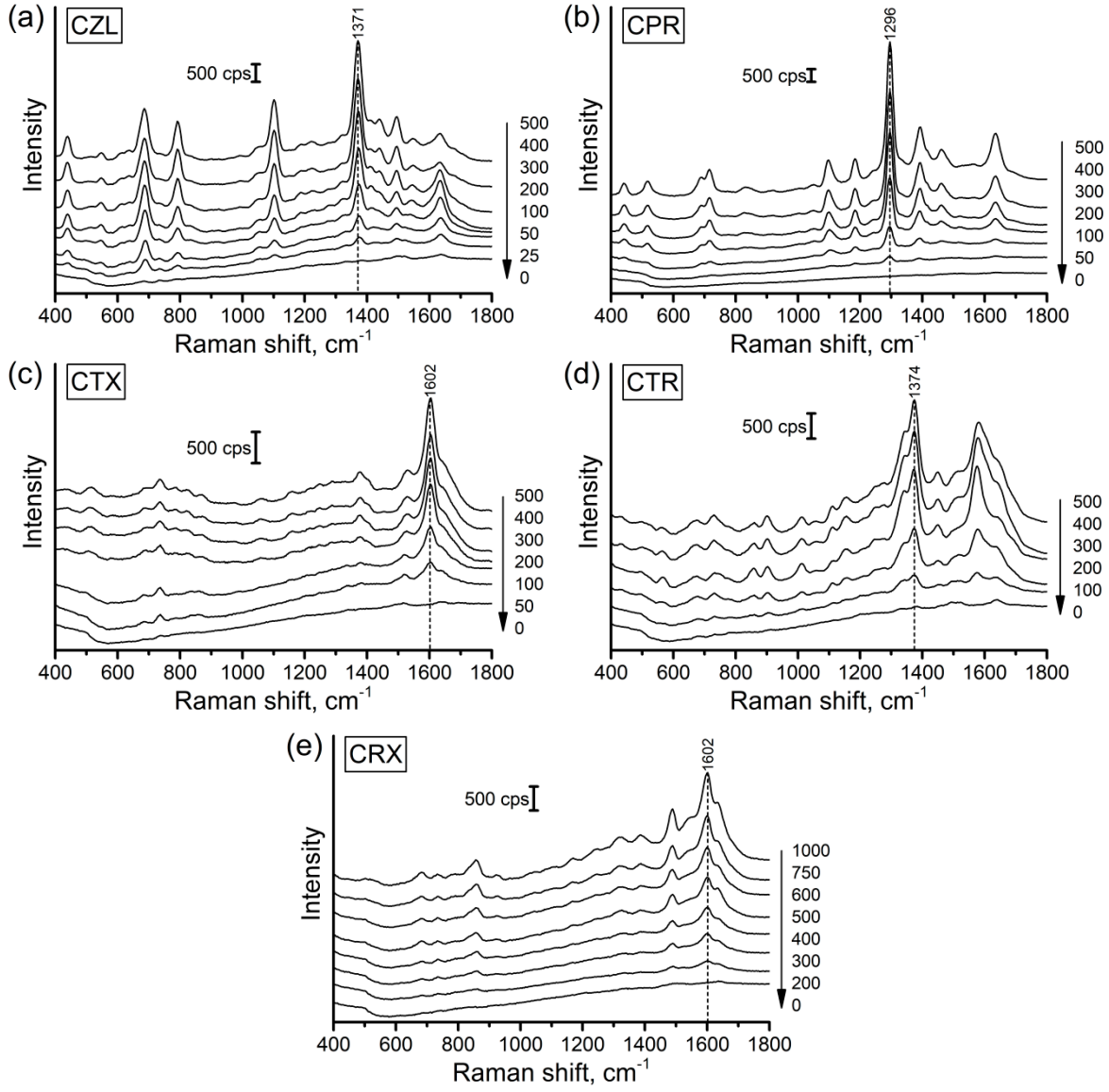



**Figure S5.** SERS spectra of the spiked urine samples after pretreatment with AHG and pH adjusting to 1.5. Marked bands were used to plot calibration curves (Figure 4 in the main text).

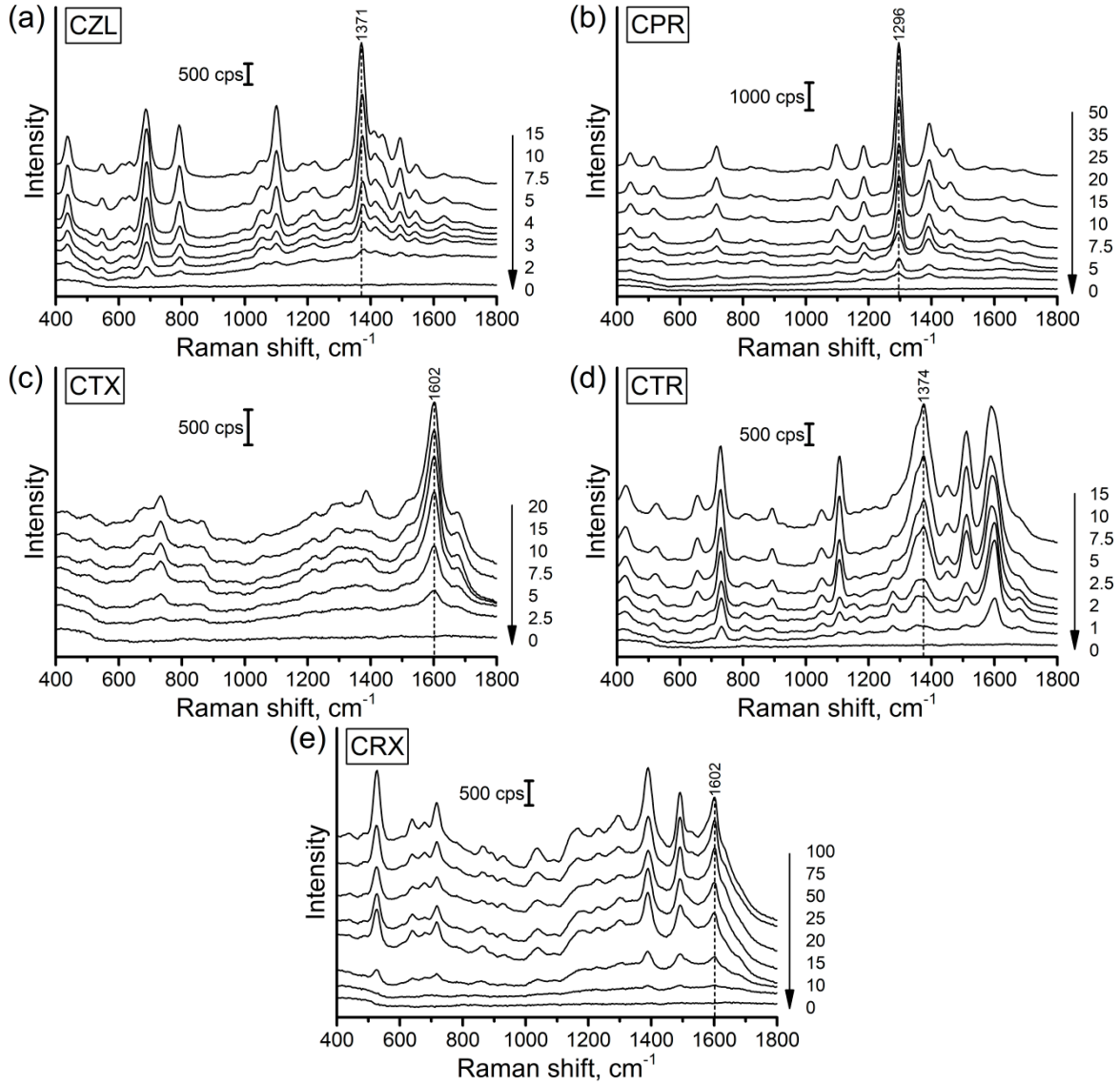



**Figure S6.** SERS spectra of the pure analytes solutions. Marked bands were used for plotting calibration curves (Figure S7).

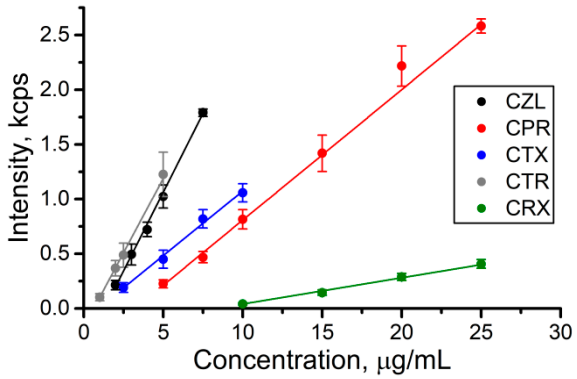



**Figure S7.** Linear parts of the calibration curves obtained using registered SERS spectra of the pure analyte solutions (Figure S6).

**Table S3.** The equations of calibration curves/plots obtained by registration of SERS signals of analyte solutions in pure water and the urine sample spiked by the analytes. $I_{SERS}$, C, and σ are the intensity of SERS signal, the analyte concentration, and the level of background signal, respectively. The intensity of SERS and background signals is measured in counts per second (cps).

| Analyte | Pure water | σ | Spiked urine | | |
|---|---|---|---|---|---|
| | | | Whole range | Linear range | σ |
| CZL | $I_{SERS} = 288\ C - 378$<br>$R^2 = 0.999$ | 10 | $I_{SERS} = -0.007\ C^2 + 8.6\ C + 30$<br>$R^2 = 0.999$ | $I_{SERS} = 7.4\ C + 66$<br>$R^2 = 0.994$ | 20 |
| CPR | $I_{SERS} = 119\ C - 385$<br>$R^2 = 0.992$ | 10 | $I_{SERS} = -0.009\ C^2 + 15\ C - 479$<br>$R^2 = 0.999$ | $I_{SERS} = 13\ C - 362$<br>$R^2 = 0.999$ | 22 |
| CTX | $I_{SERS} = 118\ C - 107$<br>$R^2 = 0.996$ | 13 | $I_{SERS} = -0.005\ C^2 + 4.4\ C + 68$<br>$R^2 = 0.994$ | $I_{SERS} = 3.6\ C + 97$<br>$R^2 = 0.991$ | 22 |
| CTR | $I_{SERS} = 272\ C - 171$<br>$R^2 = 0.998$ | 11 | $I_{SERS} = -0.006\ C^2 + 7.0\ C - 409$<br>$R^2 = 0.995$ | $I_{SERS} = 5.0\ C - 266$<br>$R^2 = 0.999$ | 20 |
| CRX | $I_{SERS} = 24.0\ C - 199$<br>$R^2 = 0.996$ | 11 | $I_{SERS} = 0.99\ C - 74$<br>$R^2 = 0.999$ | $I_{SERS} = 1.0\ C - 74$<br>$R^2 = 0.999$ | 20 |