Electronic Supplementary Material (ESI) for Lab on a Chip.

Supporting Information:

Injection molded lab on disc platform for screening of genetically modified E. coli using liquid-liquid extraction and surface enhanced Raman scattering

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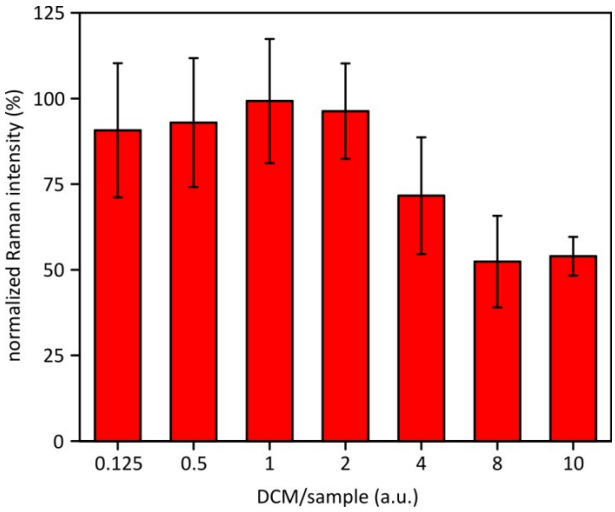

Fig. S1 Normalized Raman intensity at 1169 cm^{-1} for various DCM/sample ratios. Each ratio was tested on 2 SERS substrates, and 3 maps of 48 points were collected from each chip (n = 6), with error bars representing standard deviation. Intensities were normalized by the maximum value obtained.

When applying the PLS model to spiked DCM samples, the analysis of pure components showed that the analyte spectrum (Fig. S2 a)) closely resembled SERS fingerprint of pHCA, detected through SERS in our previous works.[1,2] Therefore, the model was able to isolate the contribution of pHCA from the background (Fig. S2 b)), and enabled good quantification.

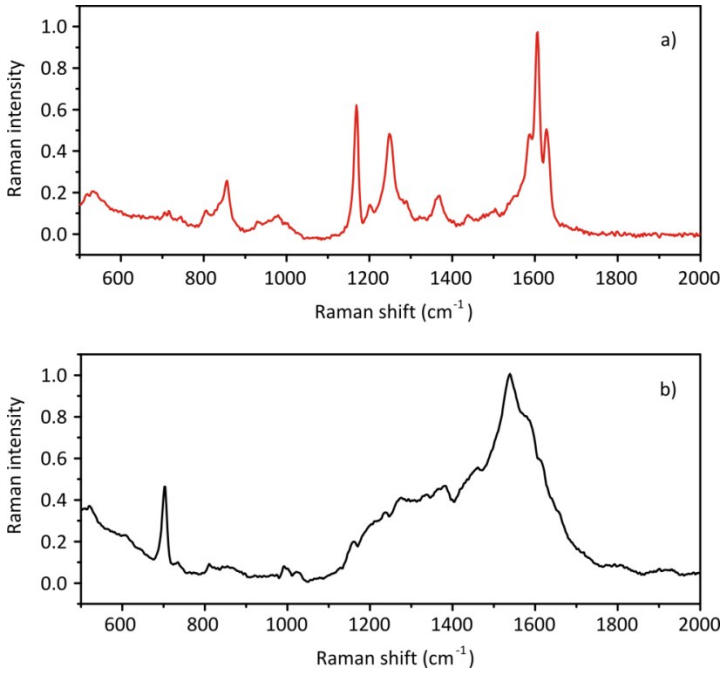

Fig. S2 Graphs of pure components detected in spiked DCM. a) Analyte component and b) background component.

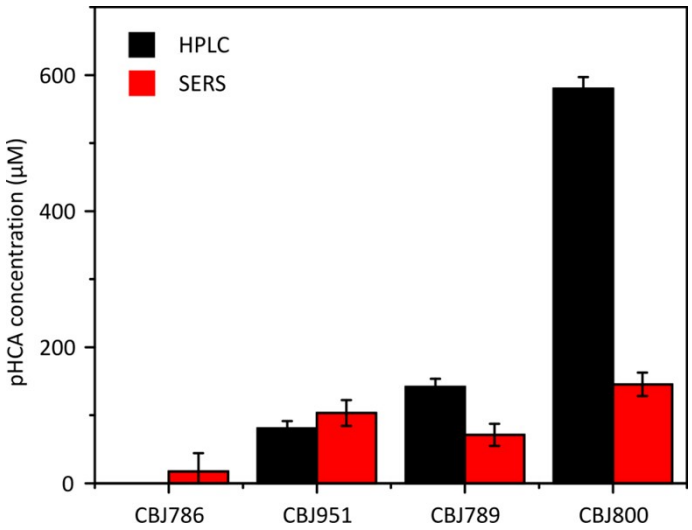

Fig. S3 Quantification of pHCA in supernatant using a calibration model based on spiked DCM standards. Each SERS point is the average of triplicate chips, with 2 maps collected from each chip (n = 6). Each HPLC point is the average of triplicate injections (n = 3).

The number of factors used for the spiked supernatant calibration model was chosen based on the predicted residual error sum of squares (PRESS), calculated through the TQ Analyst software and represented in Fig. S4. The suggested number of factors to avoid overfitting was three, corresponding to the minimum PRESS value in the graph.

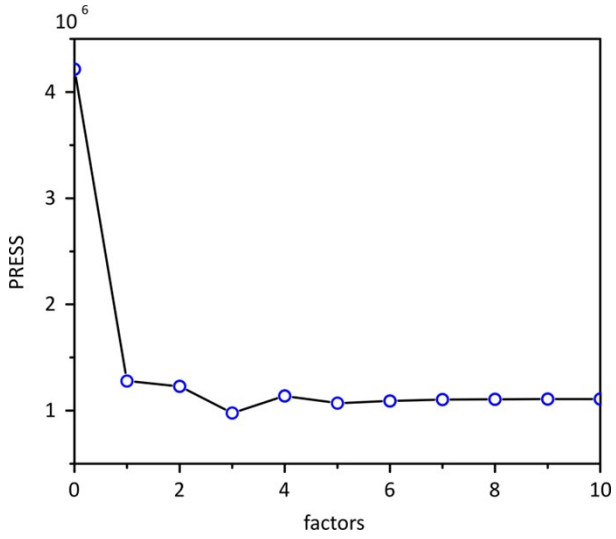

Fig. S4 The predicted residual error sum of squares (PRESS) for the spiked supernatant calibration model.

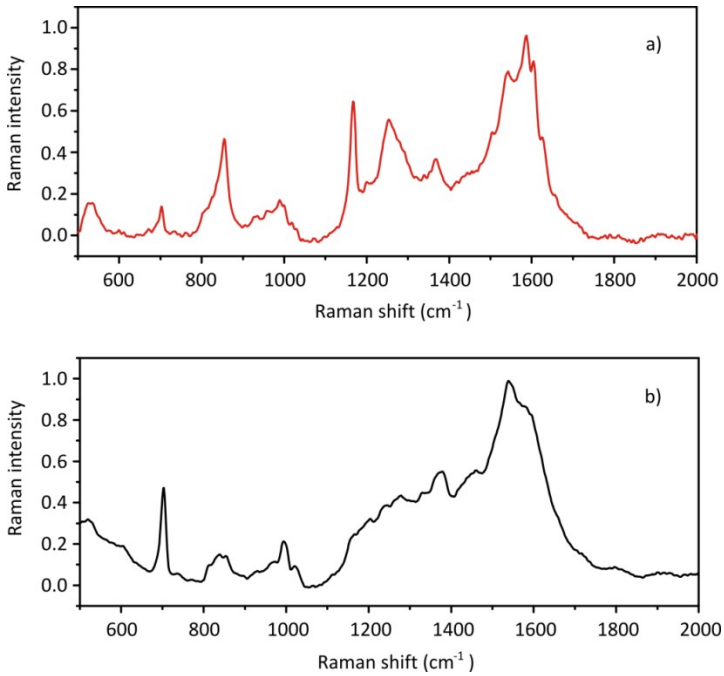

Fig. S5 Graphs of pure components detected in spiked supernatant (CBJ786). a) Analyte component and b) background component.

Fig. S6 shows the mean spectra and standard variations of each bacterial strain in the spectral region used for the PLS model. Since all the spectra share the same peak positions and band intensity variations, the SERS measurements were considered suitable for pHCA quantification.

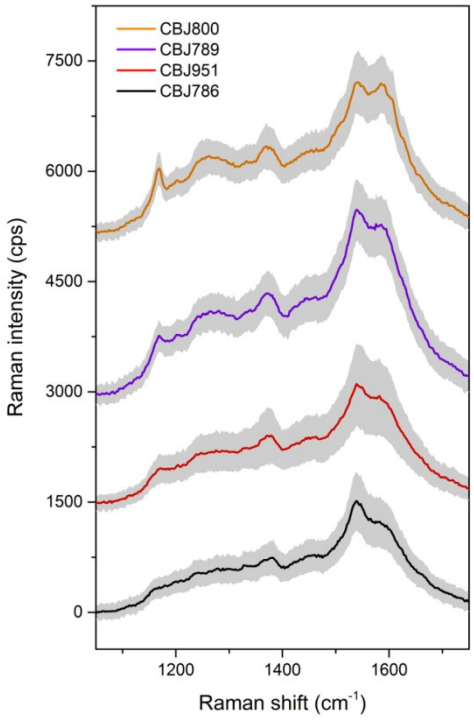

Fig. S6 Mean SERS spectra of *E. coli* samples collected on disc after data pre-processing, with the distribution of all individual spectra (n = 240) represented by the standard deviation in a grey shade.

References

1 L. Morelli, K. Zór, C. B. Jendresen, T. Rindzevicius, M. S. Schmidt, A. T. Nielsen and A. Boisen, *Anal. Chem.*, 2017, **89**, 3981–3987.

2 L. Morelli, S. Z. Andreasen, C. B. Jendresen, A. T. Nielsen, J. Emneus, K. Zor and A. Boisen, *Analyst*, 2017.