Bacteria discrimination at strain level by PCA analysis based on the SERS spectra

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Raman spectroscopy is a powerful characterization and identification technique for biological molecules and structures such as bacteria and living cells. The compatibility with water and easy sample preparations are some of its advantages, while its inherent weak nature is maybe one of the well-known disadvantages. A viable alternative is **surface-enhanced Raman scattering (SERS) spectroscopy**, when the Raman effect is enhanced in the close proximity of noble metal surfaces. In this work, vibrational spectroscopic methods and chemometrics were employed to classify bacterial species. Raman spectra on biomass by using 785 nm **(3)** laser line and SERS spectra on biomass **(1)** and at single bacterium level **(2)**, respectively, by using the 633 nm laser line, were acquired. Principle Component Analysis (PCA) was applied on the processed spectra for bacteria accurate identification and discrimination at strain level. The PCA scores obtained indicate a clear discrimination between different bacterial genera and between different strains.

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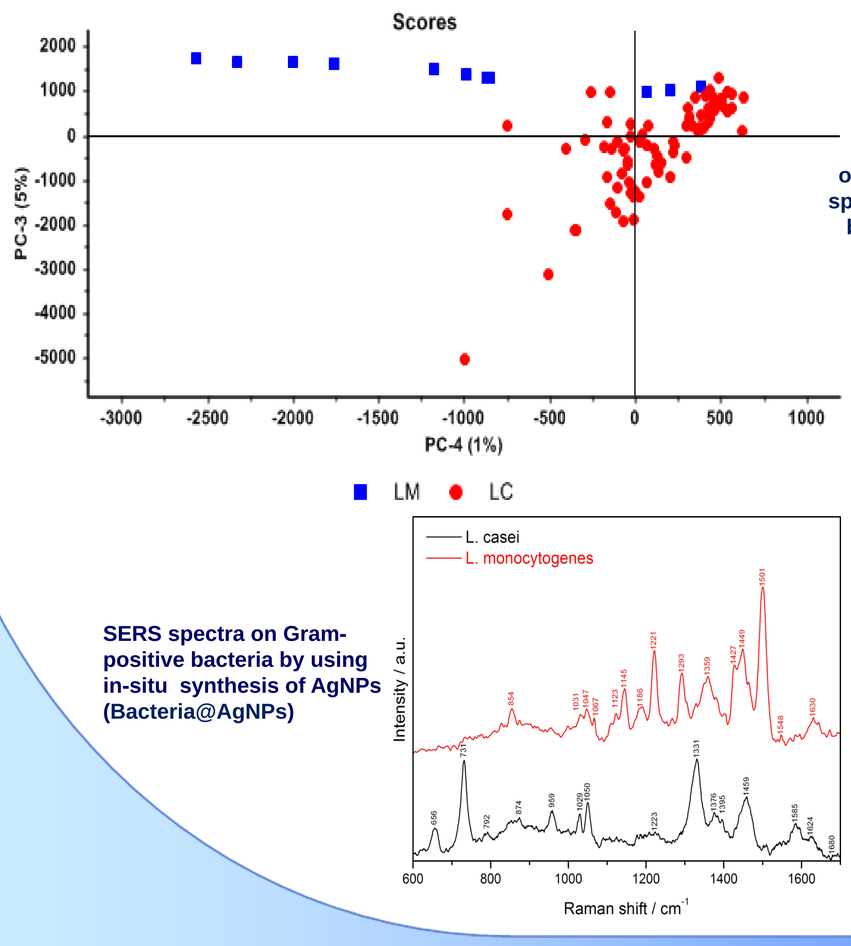
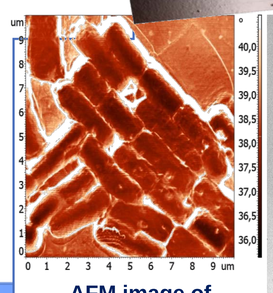
Discrimination of Gram-positive bacteria by using PCA on SERS spectra



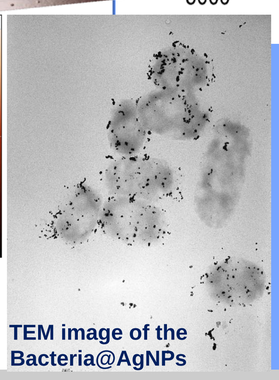
PC3 and PC4 scores obtained for the SERS spectra of Gram-positive bacteria (*L. casei* , *L. monocytogenes*)

SERS spectra on Gram-positive bacteria by using in-situ synthesis of AgNPs (Bacteria@AgNPs)

AFM image of *L. casei* bacteria



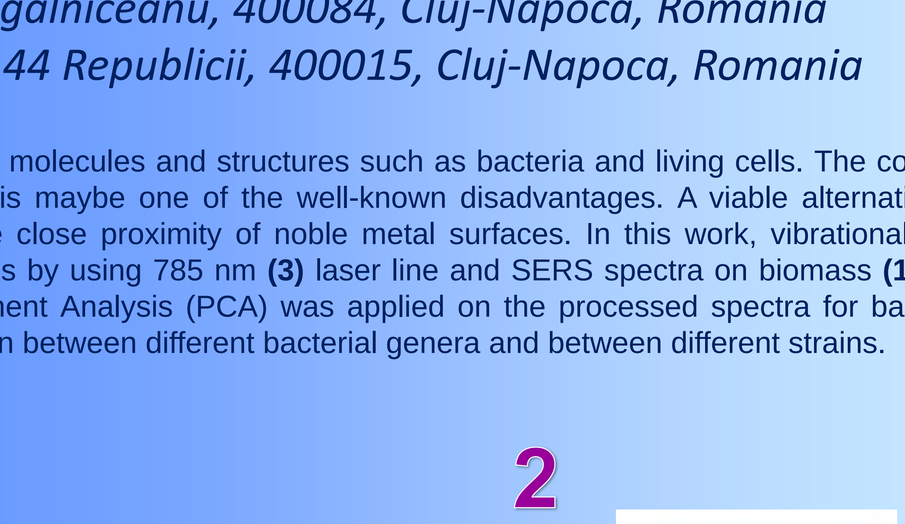
AFM image of *L. monocytogenes* bacteria



TEM image of the Bacteria@AgNPs

2

Microscope image of *E. coli* bacteria (spot obtained on silanized-antibody treated glass slide)



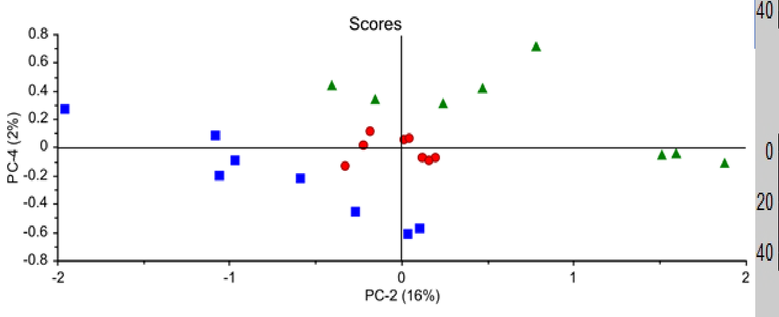
PC1 and PC3 scores and the loadings used to discriminate the single-bacterium SERS spectra of uropathogens (*E. coli* – *DH5α, UTI89, P. mirabilis*)

Discrimination of uropathogens by using PCA on single-bacterium SERS spectra

N. E. Mircescu, H. Zhou, N. Leopold, V. Chiş, N. P. Ivleva, R. Niessner, A. Wieser, C. Haisch, Anal Bioanal Chem, 406 (13), 2014

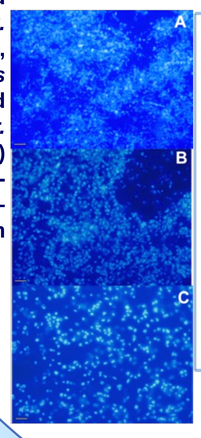
3

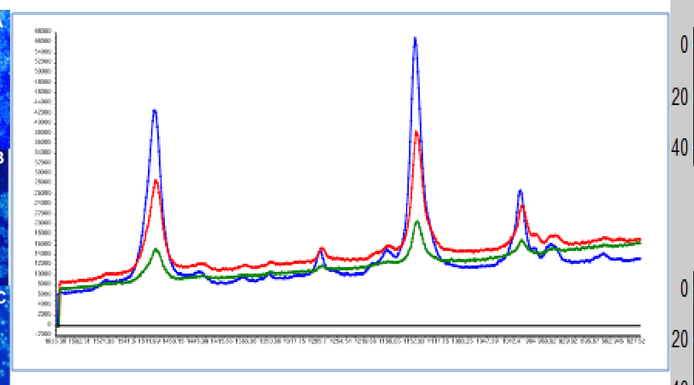
Discrimination of haloarchaeal genera by using PCA on Raman spectra



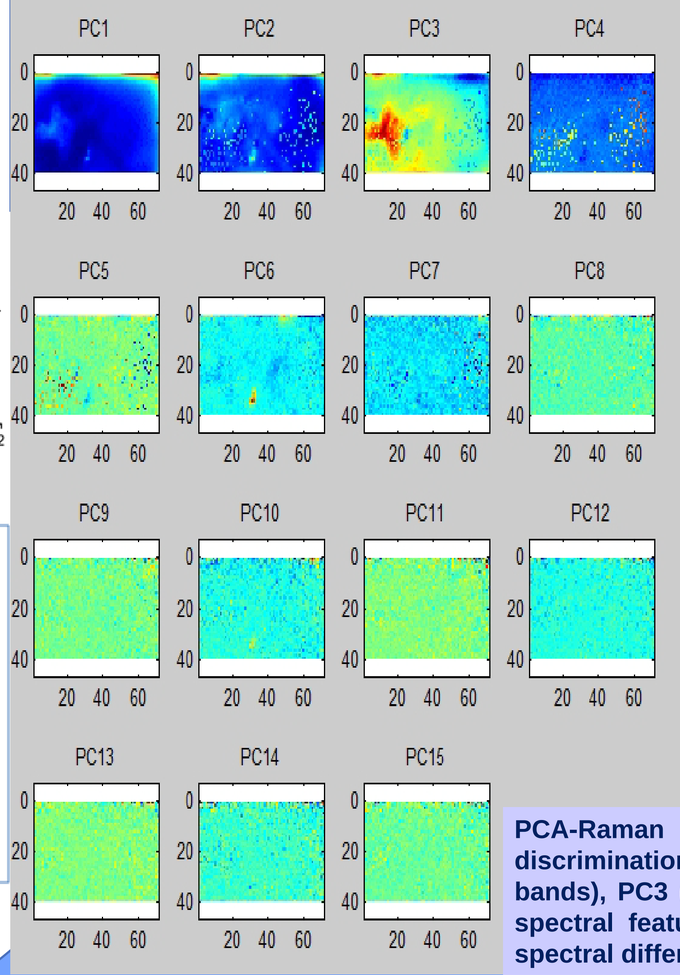
Scores plot showing discrimination between three haloarchaeal genera

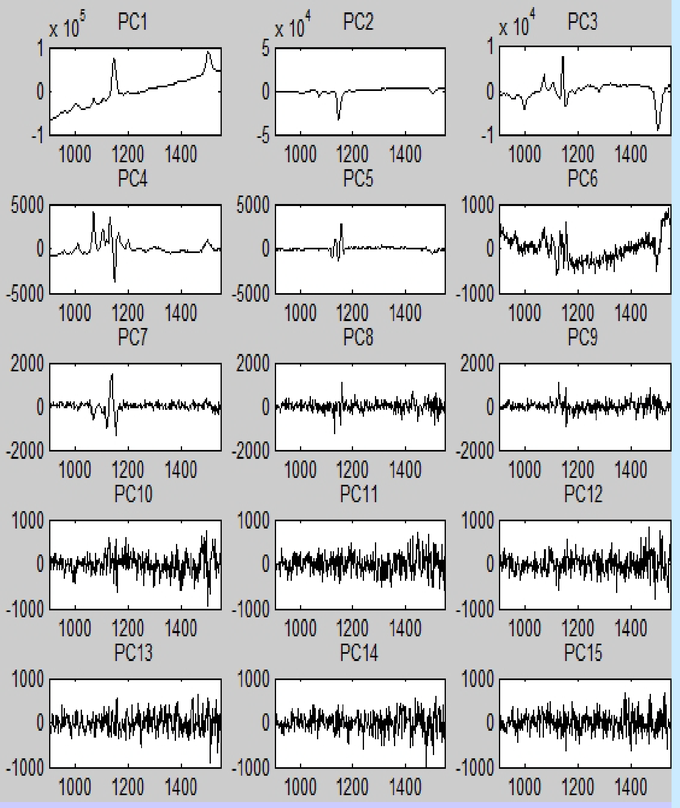
Epifluorescence micrographs of DAPI stained cultures of *Hbt. salinarum* (A), *Hfx. sulfurifontis* (B) and *Hrr. sodomense* (C) - scale bars – 10 µm





Raman spectra of three representative of the haloarchaeal genera *Halobacterium* (blue), *Haloferax* (green) and *Halorubrum* (red)





PCA-Raman based mapping of 15 PCs and their contribution in the discrimination algorithm: PC1 (mainly background spectrum), PC2 (marker bands), PC3 (separating the marker bands contribution from the particular spectral features of each sample), PC4-PC7 (taking into account smaller spectral differences), PC8-PC15 (mainly noise signal)

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