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COMPONENT IDENTIFICATION OF LIQUID MIXTURES BY USING COMPUTATIONAL MODELS

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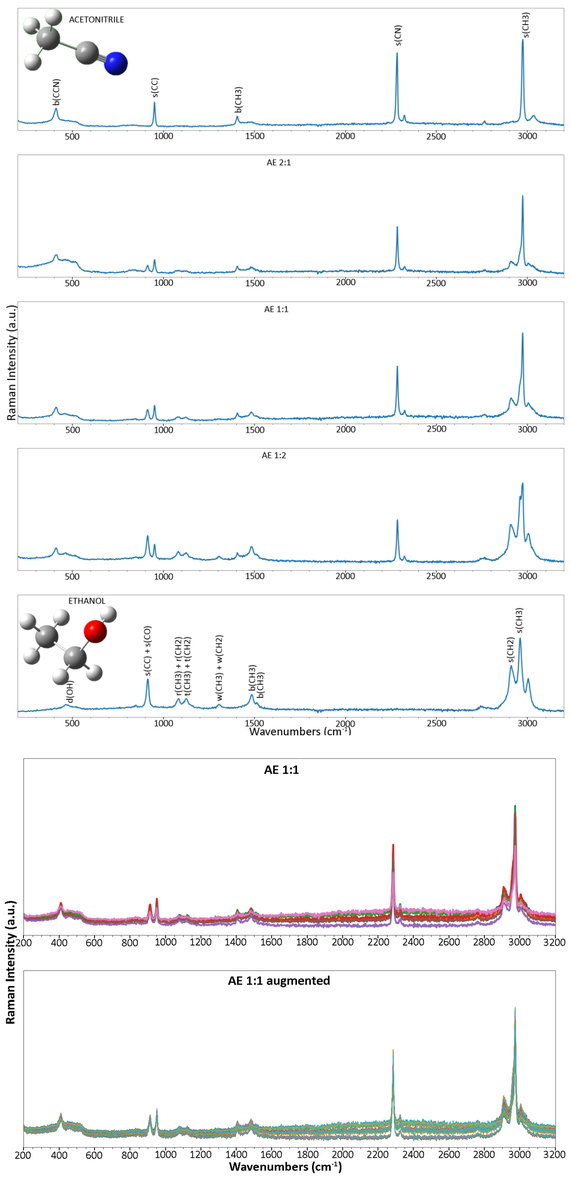
ABSTRACT

Our experience in detecting complex biological samples such as microorganisms in biofluids by means of vibrational (Raman and Surface-enhanced Raman scattering - SERS) spectroscopies generated the need of component identification for such samples. The complexity involved in deciphering the information from the vibrational spectra lays in how many biological components and/or their derivatives are combined in the investigated biomass or specific byproducts. The complementarity of the Raman and IR fingerprints assigned to common biochemical species found mixed in different ratios as composing complex samples was explored. Herein, we are looking to identify individual components present in liquid samples by creating an *in silico* model. A robust algorithm was developed and tested on the vibrational response of two different classes: mixtures of (i) solvents and (ii) antibiotics.

acetonitrile – ethanol (AE)



EXPERIMENTAL DETAILS

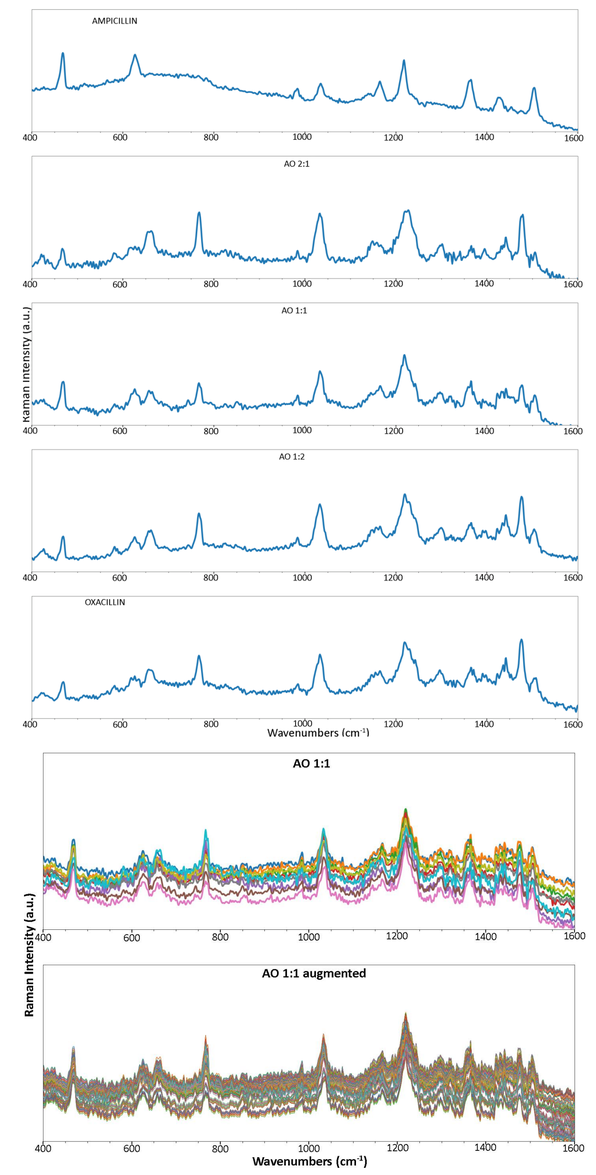
Instrument for Raman/SERS spectra acquisition: portable BW-TEK *i*-Raman spectrometer coupled with a BW-TEK optical microscope having a 20x objective (N.A. 0.4, D = 12 mm). The spectrometer is equipped with a 532 nm laser line having a total power of 50 mW.

AE acquisition details: 10 seconds; 1 acquisition; 50 % laser line power; ratios: A, AE 1:2, AE 1:1, AE 2:1, E.

AO acquisition details: 60 seconds; 1 acquisition; 100 % laser line power; 10^{-4} M in Ag NPs prepared by Leopold- Lendl recipe [J. Phys Chem B, 2003, 107 (24), 5723-5727]; ratios A, AO 1:2, AO 1:1, AO 2:1, O.

AE: acetonitrile – ethanol series
AO: ampicillin – oxacillin series

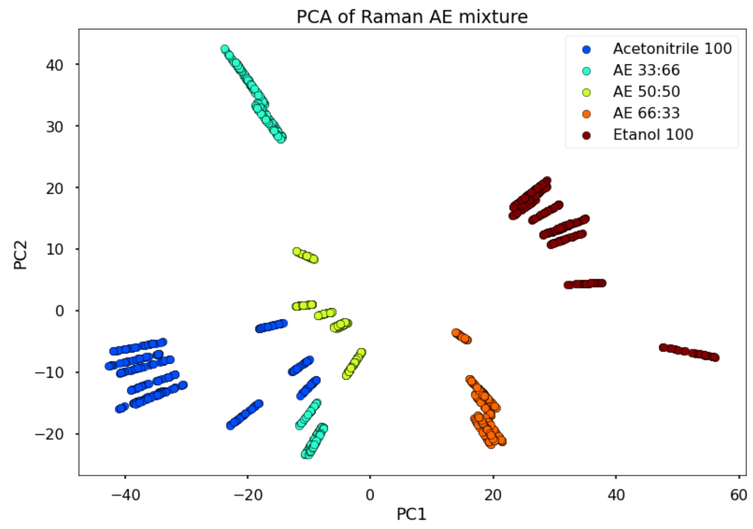
ampicillin – oxacillin (AO)

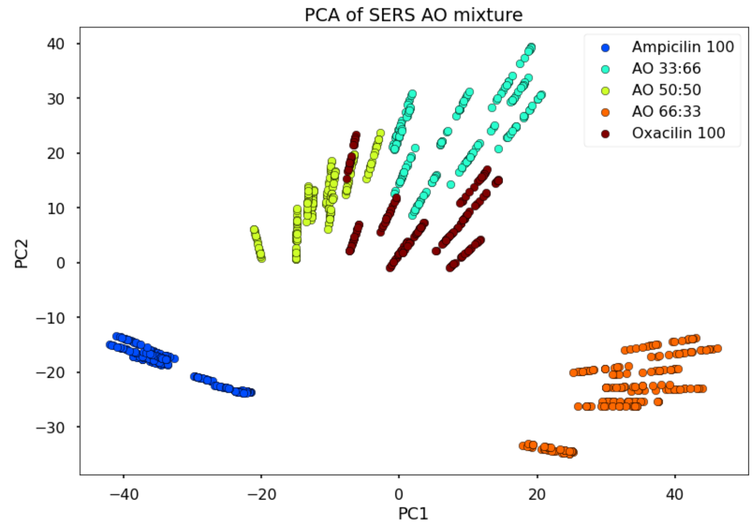


COMPUTATIONAL DETAILS

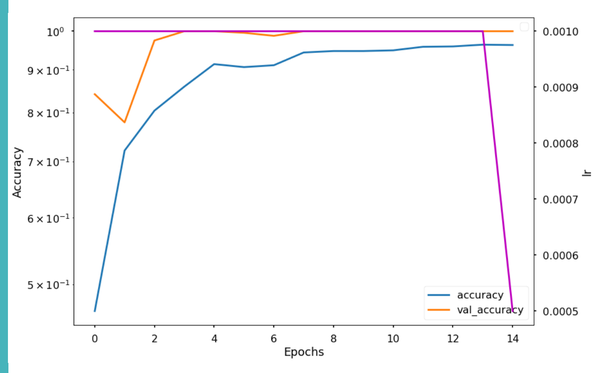
Data augmentation was applied to the registered Raman/SERS spectra in order to construct a big enought database for further statistical analyses.

A spectrum obtained by running the developped code for data augmentation was obtained after finding the min and max for each peak and obtaining its mean intensity from all original spectra considered as starting point. After this, each peak in a simulated spectrum will have a random intensity between the mean of the originals and the min and max values. [ref: https://arxiv.org/abs/1710.01927]

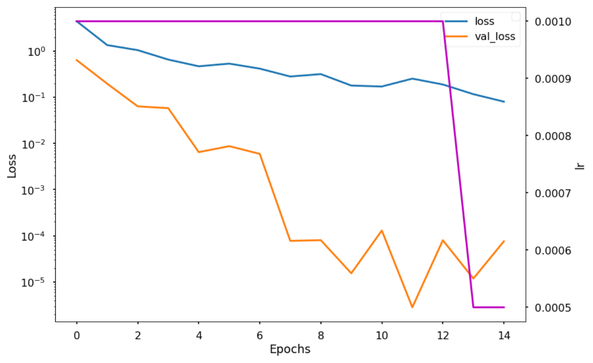




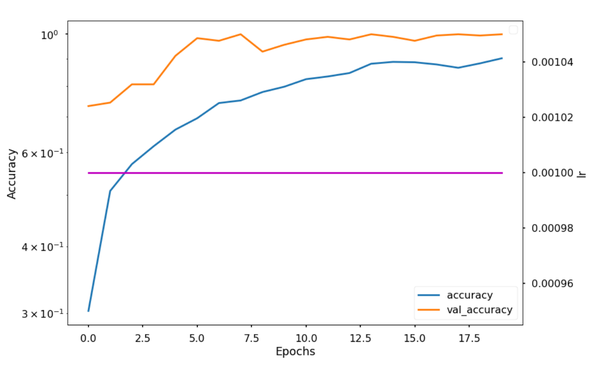
CNN accuracy AE



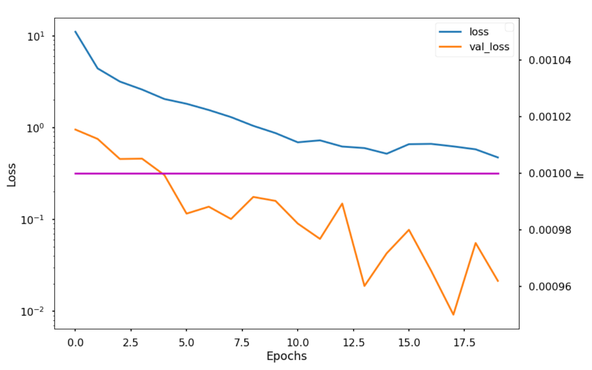
CNN loss AE



CNN accuracy AO



CNN loss AO



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