Label-Free Surface-Enhanced Raman Spectroscopy of Biofluids: Diagnostic Applications in Oncology

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Label-free Surface-enhanced Raman scattering (LF-SERS) spectroscopy of biofluids (e.g. blood, urine) has recently raised interest for its potential in the field of diagnostics [1]. Being portable and having a fast response, SERS is particularly appealing for *point-of-care* applications.

LF-SERS spectra of biofluids can be viewed as "partial metabolic fingerprints" due to a subset of metabolites which spontaneously adsorb on a SERS substrate, and thus they could be exploited for diagnosis [1,2]. Identification of most (if not all) of the metabolites contributing to the SERS signal is crucial, but because of the difficulties concerning a correct interpretation of SERS spectra, it has been only partially achieved [2]. Despite a complete interpretation and assignment of LF-SERS spectra of most common biofluids is still missing, recent works by our group showed how such spectra do indeed have the potential to be used for diagnosis of different types of cancer. Preliminary results showed how LF-SERS can detect prostate cancer from urine samples with promising sensitivity and specificity [3]. We also reported that both early and locally advanced breast cancer could be detected by LF-SERS of serum [4], with a sensitivity, specificity and overall accuracy higher than 80% (i.e. better than mammography, the currently used method for screening).

Data analysis is a key aspect of such LF-SERS diagnostic approach, as adequate chemometrics methods must be applied to spectra to build and validate consistent predictive models. In our preliminary reports, we used Principal Component Analysis (PCA) to reduce the dimensionality of spectroscopic data, and Linear Discriminant Analysis (LDA) to build the predictive model, which was validated using a "leave-one-out" (i.e. leave-one-patient-out) cross validation method.

Overall, the LF-SERS diagnostic approach still has several issues to be settled in further studies, but results so far are very promising, and in our opinion it has a great potential to be used in “point-of-care” diagnostic tests.

References

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