Disease Diagnosis using multimodal FTIR spectroscopy

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ABSTRACT

The use of infrared (IR) spectroscopy for studying biological specimens is nowadays a wide and active area of research. The IR microspectroscopy has proved to be an ideal tool for investigating the biochemical composition of biological samples at the microscopic scale, as well as its fast, sensitive, and label-free nature [1]. IR image spectral histopathology has shown great promise as an important diagnostic tool, with the potential to complement current pathological methods, reducing subjectivity in biopsy samples analysis [2]. In this talk, I shall introduce the basis why FTIR spectroscopy is becoming a non-invasive optical tissue diagnosis tool and particularly show that clinical investigations related to malignancy and cancer detection by spectroscopic means have attracted attention both by the clinical and non-clinical researchers. The FTIR datasets are imported from the spectrometer into software written in-house in the Python or MATLAB environments. Data pre-processing is a very sensitive matter, with imposition of selection criteria to avoid pixels not covered by tissue and/or those that displayed excessively strong scattering effects. Spectra are usually vector normalized and phase corrected. In some cases, they are converted to second derivatives using a Savitzky–Golay smoothing filter, using a second order polynomial filter. Spectral datasets are subsequently converted to pseudocolor images using for instance hierarchical cluster analysis (HCA), which clusters patterns in a dataset based on their spectral similarity, and the most suitable method of clustering is chosen. Principal Component Analysis (PCA) is used for data exploration and dimensionality reduction for prediction models, thus decreasing training time and overfitting. Linear Discriminant Analysis (LDA), Partial Least Squares (PLS), Support Vector Machine (SVM) and Random Forest (RF) algorithms are commonly trained as classification methods, where their accuracy, sensitivity and specificity are assessed through cross validation tests. I will describe our research in Dentistry area in which we have a fundamental interest in identifying the chemical origin of all the bands present in the infrared region to study the chemical and thermal action on the hard dental tissues, that together to other techniques such as infrared thermography, determine the safety several clinical uses of lasers (caries/erosion prevention and treatment, prosthodontics, etc)[2]. I will describe our ongoing research using FTIR of thin tissue slice samples exposed to infrared radiation, thus allowing to monitor the collagen during the healing process when evaluating burned skin as well as the diagnose and molecular differentiation between thyroid [3]and different breast cancer subtypes: positive and negative for estrogen (ER) and progesterone (PR) receptors. The spectra region and conditions which are important to differentiate cutaneous tumor tissue from healthy skin, treated by ALA-MEALA Photodynamic Therapy [4] will be discussed. In the last example, I will present our proposal for biodoimetry in bone submitted to gamma radiation using ATR-FTIR.

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