Application of advanced molecular spectroscopies and chemometric analysis to emerging food metrology challenges

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The background in which this doctoral study is located is the emerging field of food metrology. This project started in conjunction with the birth of the Food Metrology Program within the Metrology for the Quality of Life Division at the Italian National Institute of Metrological Research (INRiM). The main goal of this thesis is the assessment of advanced vibrational spectroscopies and chemometrics in food metrology framework. Vibrational spectroscopies, in general, represent valuable candidate methods for food analysis because they are known to be sensitive and selective molecular fingerprint technologies which enable rapid, simple and non-destructive analytical determinations (1). The challenge is to reach the best compromise between smart screening methods, suitable for routine application, and the rigorous metrology requirements. If, from one side, the development of rapid and simple methods for *in-situ* analysis is the priority, on the other side, there is the outstanding need of reproducible and non-method-dependent measurement results. The lack of robustness and wide range validation typical of just born analytical methods can be overcome following the metrology principles of traceability to the SI units, calibration, validation and measurement uncertainty (2). Hyperspectral imaging is the mainly explored technique in this thesis, ranging from near infrared spectroscopy to Raman and Surface Enhanced Raman Scattering Spectroscopy (SERS). Chemometric methods were widely used as powerful tools to extract useful information from a big amount of analytical data and to produce valid models for the classification of food samples and the quantification of food contaminants (3). Different topics were studied to attest the versatility and wide range application of the mentioned techniques. First, spectral imaging was coupled with discriminant analysis to set-up a detection method for animal origin components in feed samples (4); second, SERS strategies for the detection of pesticides traces directly on fruits' peel were developed and tested (5), for example a flexible semi-transparent SERS tape was developed (Fig.1); last, chemometric explorative and classification methods were exploited to investigate the influence of geographical origin on the chemical composition of cocoa shells powder. In conclusion this thesis is devoted to investigate some emerging analytical strategies to face the food safety, food security and food provenience issues.

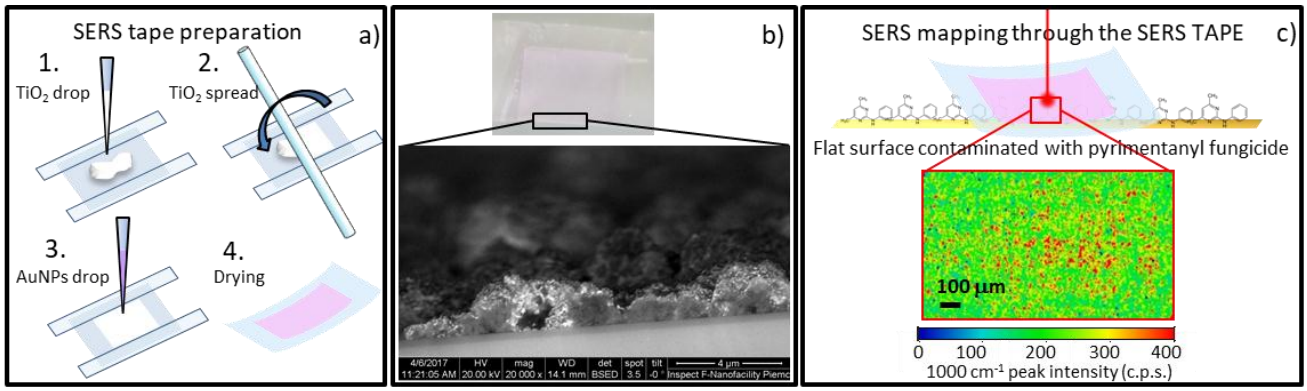

Figure 1:a) preparation steps of a flexible SERS tape: porous layer of TiO_2 and gold nanoparticles are deposited on a sticky scotch tape; b) SEM images of the cross section of the tape; c) SERS mapping through the tape laid on a surface contaminated with pyrimethanil fungicide.

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