Direct use of TXRF spectral signal for multivariate data analysis: a new strategy for food fingerprint

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Total-reflection X-ray fluorescence (TXRF) spectroscopy is a well-established technique used for the elemental analysis of samples in several scientific fields. Respect to other atomic spectroscopies (ICP-OES, ICP-MS, AAS and XRF), TXRF allows to perform a fast analyze on different kinds of matrixes (water, organic tissues and fluids, minerals, composites and ores) using very small amount of sample prepared using a simple procedures. These advantages make the technique very suitable for the analysis of food where a reliable and fast analysis is crucial to detect pollutants and toxic elements, to trace the food and to identify frauds. For these purposes, and in particular in the case of food traceability, detected elements are quantified (using different approaches which can influences the accuracy of the quantification) and the results are then processed with multivariate analysis. By using this approach, TXRF has more or less the same applicability of the other atomic spectroscopies which, on the other hand, have the capability to achieve better limits of detection and offer a wider number of quantifiable elements, in particular trace elements. However, respect to other atomic spectroscopies, TXRF has the possibility to give a continuum spectrum (generally in the range from 0 to 20kV) as an output, which can be used, in combination with chemometric approaches, as a fingerprint of the sample. If this approach was already applied on EDXRF spectra [1,2], it has never been applied on TXRF ones. Moreover, on the basis of authors' knowledge, XRF spectra, and in particular TXRF ones, have never been used as food fingerprint.

For this reason, the present work aims at developing, testing and validating a new method of food fingerprint and traceability using TXRF spectra. In order to fulfill this goal, a group of 24 different genotypes of beans (*Phaseolus vulgaris*) coming from two growing sites were analyzed. The elemental quantitative data as well as the TXRF signals were processes by unsupervised and supervised multivariate techniques with the aim at developing a classification method for geographical origin of beans according to the growing site.

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[2] I. Allegretta, B. Marangoni, P. Manzari, C. Porfido, R. Terzano, O. De Pascale, G.S. Senesi, Talanta 212, 2020, 120785

PREFERENCE*: ORAL