

**BOOK OF ABSTRACTS**



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# **APPLICATION OF DOE AND MULTIVARIATE ANALYSIS FOR A TXRF METHOD DEVELOPMENT AND DATA ANALYSIS. A CASE-STUDY FROM THE AGRI-FOOD SECTOR**

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Total-reflection X-ray fluorescence (TXRF) spectroscopy is a suitable analytical method for the determination of the elemental composition of different kind of samples. In recent years, the technique has been widely used for agri-food products (Borgese et al., 2015). However, despite the growing application of TXRF, few studies have considered and applied multivariate strategies for improving method performance and usability. In particular, at least two critical steps could profit from the application of chemometric tools: i) sample preparation and ii) signal analysis. As for the first step, our goal was to find the best sample preparation for an organic material. In literature there is no accordance among the amounts of sample/suspender to be used. Thus, the design of experiments has been used as a rational approach to find suitable conditions of sample preparation (mass of the sample and dispersant volume). A 2<sup>2</sup> full factorial design was set up having as responses the recovery of twelve elements. The obtained response surfaces allowed to identify the region(s) of the experimental domain in which a suitable recovery (80-120%) was reached for most of the elements.

For what concern the second aspect, the output of TXRF is a continuous spectrum which is multivariate in its nature. Nonetheless, in literature these signals are seldom



treated directly by multivariate methods, while, most commonly, a quantitation of the single elements is carried out. Thus, we aimed at evaluating the feasibility of TXRF coupled with multivariate data analysis for the discrimination of beans (twenty-four genotypes) from two growing sites comparing this analytical approach with the most common one, i.e., by using the quantified elemental composition for the multivariate analysis. The elemental dataset ( $144 \times 12$ ) and the spectral dataset ( $144 \times 2312$ ) were subjected to different preprocessing methods (according to the different nature of the data), explored by PCA and then different classification models were built and tested (Allegretta et al., 2023). The results showed that good discrimination between the growing sites could be achieved with both the datasets and approaches. In the case of the spectral dataset, the great variability associated to the bean genotypes masked that related to the growing sites which could be highlighted by using the GLSW filter. The practical advantage of the direct use of TXRF signals for classification purposes lied in the possibility to avoid the elemental quantification procedure (and related errors) thus speeding up the analysis and the classification assessment.

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## References

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