

## **APPLICATION OF WIDE SCOPE TARGET, SUSPECT AND NON-TARGET HIGH RESOLUTION MASS SPECTROMETRIC METHODS COUPLED WITH ADVANCED CHEMOMETRICS IN FOOD AUTHENTICITY STUDIES**

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Foodomics was defined for the first time in 2009 as “a new discipline that studies the food and nutrition domains through the application of advanced omics technologies to improve consumer’s well-being, health and confidence [1]. Foodomics, more than a simple term covering the panel of the “omic” sciences, also includes the nutritional aspects. Foodomics allows the simultaneous characterization of large numbers of compounds in food matrices, offering to food and nutrition scientists the opportunity to acquire a far more detailed and comprehensive molecular picture of food composition [2]. The concept of authentic, applied to food, certifies that the product is in accordance with standards and regulations [2]. Thus, the development of analytical methods which ensure the authenticity of foods plays a fundamental role in modern society. This can be achieved by the development of analytical methods that apply advanced “omics” technologies to investigate the metabolite profile of different food matrices. High Resolution Mass Spectrometry (HRMS) has been proved to have excellent analytical performance allowing the analysis of a wide range of constituents and assisting identification for both non-target and target compounds. In non-target screening, when there are no reference standards commercially available, the semi-quantification of new compounds remains a challenge. To such an end, chemical similarity analysis can be applied to rank the most appropriate reference standards for semi-quantification purposes [3]. Non-targeted methods combined with chemometrics improve the quality and reliability of the conclusions by suggesting markers. Non-target screening workflows combined with supervised chemometric techniques, such as Partial Least Square – Discriminant Analysis (PLS-DA) and Counter Propagation Artificial Neural Network (CP-ANNs) have been successfully applied for the establishment of classification models that discriminate between defective and EVOOs [4]. Moreover, Ant Colony Optimization Random Forest (ACO-RF/RF) was developed to investigate alterations between organic and conventional EVOOs and introduced one marker with a concentration threshold [3]. HRMS screening workflows coupled to chemometrics reveal the chemical profile (fingerprint) of food products and hence, can be widely applied in food authenticity studies, as complimentary methods.

### References

- [1] N.P. Kalogiouri and N.S. Thomaidis, in *Food Authentication: Management, Analysis and Regulation*, C. A. Georgiou and G.P. Danezis, John Wiley & Sons, West Sussex, UK (2017) 453-470.
- [2] J. Dennis, *Analyst*, 123, 9 (1998) 151-156.
- [3] N.P. Kalogiouri, N.A. Alygizakis, R. Aalizadeh and N.S. Thomaidis, *Analytical and Bioanalytical Chemistry*, 408, 28 (2016), 7955-7970.
- [4] N.P. Kalogiouri, R. Aalizadeh and N.S. Thomaidis, *Analytical and Bioanalytical Chemistry* (2017) Accepted.

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