

XVI SCIENTIFIC MEETING

OF THE SPANISH SOCIETY
OF CHROMATOGRAPHY
AND RELATED TECHNIQUES

ALMERÍA 25TH-27TH OCTOBER 2022

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PLENARY LECTURE 4

FROM TARGETED TO NON-TARGETED ANALYSIS IN FOOD SAFETY: WHAT'S UP, DOC?

Roberto Romero-González*

Department of Chemistry and Physics, Research Centre for Mediterranean Intensive Agrosystems and Agrifood Biotechnology (CIAIMBITAL), Agrifood Campus of International Excellence (ceiA3), University of Almería. Ctra. de Sacramento s/n, E-04120, Almería, Spain.

*rromero@ual.es, Tel: +34 950 214 278

Food and feed analysis is needed to support their authenticity, quality, and/or safety. Different analytical strategies have been developed to monitor food and feed composition, nutritional value as well as to detect the presence of undesirable or harmful compounds or foodborne pathogens. The analysis of toxic chemical substances in food and feed is a challenging task, taking into account the great number of matrices and the diverse properties of potential contaminants. Additionally, most of these substances must be detected and/or quantified at trace levels with sufficient accuracy and robustness according to current legislation. Therefore, analytical methods have been evolving over the last few decades, and instead of developing a method that allows the determination of one type of compound or a family of compounds in one single matrix, nowadays, multiresidue methods that allow the simultaneous determination of different families of compounds in several matrices have been developed, increasing the scope of the analysis, and minimizing the number of analyses to characterize food samples, developing the so-called “generic” or “all-in-one” methods. In addition to conventional targeted analysis, more analytical methods focused on non-targeted analysis (NTA) have been developing, using high resolution mass spectrometry coupled to chromatographic techniques [1], where theoretically, an unlimited number of compounds could be determined in only one chromatographic run, applying generic conditions for sample, chromatographic and mass spectrometric step. Thus, suspect and unknown methods can be performed, where in the first approach, the compounds are identified based on a suspected compound list, whereas in the case of unknown analysis, the compounds are identified without any previous list of targeted or suspect compounds. The main issues related to sample preparation, instrumental analysis (chromatographic separation and MS acquisition) and post-acquisition data processing, when NTA is developed, will be described, bearing in mind that these three stages require optimization to minimize false positives while keeping an acceptable rate of false negatives. Special attention will be paid to different aspects of data processing [2] as feature extraction, semi-quantitation and quality control. Several applications will be described, showing the capabilities that NTA have in order to obtain as much information as possible of potential toxic compounds (known and unknown substances) in food matrices.

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References:

- [1] R. López-Ruiz, R. Romero-González, A. Garrido Frenich, *TrAC Trends in Analytical Chemistry*, 118 (2019) 170-181.
- [2] C. M. Fisher, T. R. Croley, A. M. Knolhoff, *TrAC Trends in Analytical Chemistry*, 136 (2022) 116188.