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EDITORIAL

High-resolution mass spectrometry in food and environmental analysis

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In 1968 Finnigan introduced the first commercial quadrupole mass spectrometer equipped with a computerized data-processing unit. Since then, the coupling of gas chromatography to mass spectrometry (GC–MS) for the analysis of contaminants in environmental and biological samples has achieved impressive success, and at the end of the last millennium it was in routine use in many laboratories. Furthermore, GC–MS was used to determine food composition, and thus it was a tool to guarantee food authenticity and safety while also providing information about the nutritional value.

The discovery of atmospheric-pressure ion sources during the mid-80s was another important development, because it made the effective coupling of high-performance liquid chromatography (HPLC) to MS possible. With this technique available, the analysis of low-volatility and thermolabile compounds became possible without the need for a long derivatization procedure, which was sometimes difficult to perform and not always successful. However, after the initial excitement, the limitations of the technique soon became evident; these result from the relatively low efficiency of HPLC compared with GC and the large number of compounds present in samples that can interfere with the determination of the analytes of interest. Therefore, the need for higher MS selectivity was soon realized by the research community. The technology to overcome this problem was fortunately already available. Collision-induced dissociation (CID) was

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introduced by Jennings and McLafferty at end of the 60s; tandem MS (MS–MS) was made possible with the triple-stage quadrupole (QqQ) introduced by Yost, Henke, and Morrison at end of the 70s; and finally multi-stage MS was provided by the Paul ion trap, patented in 1953. The addition of one more dimension in separation greatly increased selectivity; furthermore, rapid advances were made toward the design of mass spectrometers with improved sensitivity, in parallel with advances in separation technology and the development of columns with improved efficiency. Currently, HPLC and ultra HPLC (UHPLC) coupled to QqQ working in selected-reaction-monitoring (SRM) mode are the most widespread techniques in both environmental and food analysis because they provide the analyst with a high degree of selectivity and sensitivity. Hence, complex and labor-intensive sample-processing techniques could be substantially simplified. However, the use of SRM mode on QqQ instruments proved to have some limitations, including a limit to the number of compounds monitored per analysis, the inability to screen for unknowns, and the reliance on reference standards. To overcome these limitations, there is a need for an alternative approach using instruments capable of providing full spectral information and high mass resolution and mass accuracy.

Classic high-resolution (HR) mass spectrometers, for example double-focus sector or Fourier-transform ion cyclotron resonance (FT-ICR), were too slow, complex to handle, and expensive to buy and to maintain. However, the introduction of modern time-of-flight (TOF) and electrostatic FT trap (Orbitrap) instrumentation totally changed the situation. TOF and Orbitrap have undergone tremendous technological advances giving—in addition to improved mass resolution, accuracy, and sensitivity—fast scan velocity, sufficient dynamic range, and the possibility of MS–MS when part of hybrid instruments. Because of their unrivaled resolution, modern FT-ICR mass spectrometers also have their advocates in the

field of HRMS. The major advantage of HRMS instruments is their ability to record a theoretically unlimited number of compounds in full-scan mode. The hybrid instruments can record fewer compounds, but can provide structural information. These characteristics enable the development of screening strategies, based on accurate-mass and MS–MS database searches, for the identification of unexpected, non-target compounds with the additional advantage of retrospective data mining.

Environmental and food analysis will greatly benefit from these capabilities. For example, in environmental analysis, monitoring a few known compounds does not provide a comprehensive description of a sample, whereas untargeted analysis enables the determination of unexpected compounds, or metabolites of licit or illicit drugs, even in samples previously analyzed. In the field of food sciences, quality, safety, and authenticity are topics of increasing importance, where accurate analytical results are critical. The use of HRMS has greatly improved the detection and identification of compounds in food. Because of the increasing globalization of the market, food quality and safety have become increasingly important for consumers, food suppliers, food manufacturers, and regulatory authorities. There is a greater pressure than in the past to test more food products, and also to search for more contaminants and authenticity markers. Higher levels of sensitivity, together with the ability to simultaneously monitor a range of contaminants and/or natural components with improved throughput, can certainly help to cope with this urgent request.

Given the above considerations, in the topical collection hosted in this issue of *Analytical and Bioanalytical Chemistry* we are glad to present crucial recent developments in HRMS applied in the fields of environmental and food analysis. We did our best to provide high-level publications, and hope that the readers will enjoy the selected papers.

We thank all the authors for their contributions to this special topical collection and the referees for their excellent and accurate work. Finally, special thanks must be given to the editorial team of *ABC* for their invaluable cooperation.

Aldo Laganà is Full Professor of Analytical Chemistry at the University of Rome "La Sapienza" and Head of the Department of Chemistry. His research fields are the development and validation of novel analytical methods based on LC coupled to advanced mass-spectrometric instrumentation (for example UHPLC–MS–MS and nanoLC–HRMS with Orbitrap technology) for the characterization and quantification of natural and anthropogenic substances (e.g. flame retardants, pesticides, mycotoxins, polyphenols, phytoestrogens, estrogens, etc.) in environmental, food, plant, and biological samples. His scientific interests also include proteomic studies (in particular differential proteome analysis), and the study of the interactions between biomolecules and nanoparticles for nanomedicine applications.

Chiara Cavaliere has been a Researcher at Department of Chemistry of University of Rome "La Sapienza" since 2009. Her research field is the development of innovative analytical methods based on liquid chromatography coupled to tandem mass spectrometry to determine substances present in various matrices such as food, water, animal and plant tissues. In particular, she has dealt with the determination of contaminants in water and food, and mycotoxin analysis in food by LC-MS/MS; characterization of different polyphenol classes in plants by LC-high-resolution MS/MS; and protein profiling in plant and animal samples by nanoLC- high-resolution MS/MS.