

18TH ANNUAL WORKSHOP ON EMERGING HIGH-RESOLUTION MASS SPECTROMETRY (HRMS) AND LC-MS/MS APPLICATIONS IN ENVIRONMENTAL ANALYSIS AND FOOD SAFETY

BARCELONA,
10-11 OCTOBER 2022

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BOOK OF ABSTRACTS

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CERTIFICATE

I HEREBY CERTIFY THE ATTENDANCE OF:

Rosalia Lopez Ruiz



D. BARCELÒ
Damià Barcelò
Chair of the Scientific Committee

BARCELONA, 11 OCTOBER 2020



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Rosalia Lopez-Ruiz, Antonio Jesús Maldonado-Reina, Jesús Marín-Sáez, Roberto Romero-González, José Luis Martínez-Vidal, Antonia Garrido Frenich

Have given the ORAL presentation entitled: *Characterization of agricultural products using chromatographic techniques coupled to high resolution mass spectrometry: more than just the active substance*



Damià Barcelò
Chair of the Scientific Committee

BARCELONA, 11 OCTOBER 2020



Characterization of agricultural products using chromatographic techniques coupled to high resolution mass spectrometry: more than just the active substance

Rosalía Lopez-Ruiz⁽¹⁾, Antonio Jesús Maldonado-Reina⁽¹⁾, Jesús Marín-Sáez^(1,2), Roberto Romero-González⁽¹⁾, José Luis Martínez-Vidal⁽¹⁾, Antonia Garrido Frenich⁽¹⁾

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Plant protection products (PPPs) are essential agricultural tools used for pest control. They are composed of at least an active substance (pesticide) and other components (additives and impurities), which comprise a great part of their composition, and include safeners, synergist, co-formulants and adjuvants. Whereas active substances are completely characterized, information regarding additives and impurities is still notably insufficient, since manufacturers are not enforced to disclose them, even though some of them have been proved to trigger negative effects on health (1). Thus, there is a need of analytical methodologies capable of dealing with the identification of these compounds.

The proposed analytical methodology involves sample treatment, separation and detection, and data analysis including data acquisition (quality control (QC)) and data processing (identification, validation, and quantification). Liquid chromatography (LC) and gas chromatography (GC), coupled to Q-Orbitrap high resolution mass spectrometry (Q-Orbitrap-HRMS) that ensure the cover of a wide range of polarity and volatility are used. This methodology also addresses different acquisition methods, such as full scan MS and data independent acquisition (DIA).

Regarding data analysis, a combination of suspect screening, consisting in a home-made data base, which was built considering previous literature research, and unknown analysis is proposed, focusing on the critical points of these analysis modes. Raw data handling strategies and different software for suspect and unknown analysis are presented to ensure a reliable tentative identification of additives and impurities.

The methodology is supported by examples based on our findings and experience in the study of additives, as co-formulants in PPPs, in which more than 10 PPPs were studied by LC-HRMS and GC-HRMS. The proposed methodology is also highly applicable to other analytical problems focused on sample's characterization.

To conclude, this methodology intends to contribute to the state of the art of the analysis PPPs, as well as to be a resource for further studies concerning PPPs.

1. M.T.K. Tsui and L.M. Chu, *Chemosphere*. 52 (2003) 1189–1197. [https://doi.org/10.1016/S0045-6535\(03\)00306-0](https://doi.org/10.1016/S0045-6535(03)00306-0).

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Topic: 1-Advances in HRMS instrumentation and their applicability in environmental analysis and food authenticity

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