

# Book of Abstracts



## 17<sup>th</sup> ANNUAL WORKSHOP ON EMERGING HIGH RESOLUTION MASS SPECTROMETRY (HRMS) AND LC-MS/MS APPLICATIONS IN ENVIRONMENTAL ANALYSIS AND FOOD SAFETY

Organized and hosted virtually by:



Environment and  
Climate Change Canada

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Changement climatique Canada

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**<https://lcmsms2021.ca/>**

Dear Colleagues,

On behalf of the Organizing Committee, it is with pleasure that I welcome you at the 17<sup>th</sup> Annual Workshop on Emerging High-Resolution Mass Spectrometry (HRMS) and LC-MS/MS Applications in Environmental Analysis and Food Safety.

This workshop is a scientific meeting to foster dialogue among scientists in government, academia, and

# Award Certificate

is proudly presented to

**Mireya Granados-Povedano**

in recognition of exceptional performance in the

**Best Student Poster Presentation**

during the 17<sup>th</sup> Annual Workshop on Emerging High-Resolution  
Mass Spectrometry and LC-MS/MS Applications in Environmental  
Analysis and Food Safety

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## UHPLC-HRMS based screening of pesticides degradation and dissipation

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At present, knowledge about the behaviour and persistence of pesticides in the environment such as the soil is very scarce despite the importance that may have on crops and ecosystems. Furthermore, the metabolites that can be produced in the soil can have a higher toxicity than their parent pesticides<sup>1</sup>. In this work, a study was carried out on the dissipation and degradation of two widely used broad-spectrum pesticides, chlorantraniliprole (insecticide) and difenoconazole (fungicide) in two different types of soils (clay and sandy).

After an ultrasound assisted extraction (UAE) of the analytes, the final extracts were analyzed by ultra-high performance liquid chromatography coupled to high resolution mass spectrometry using a Q-Exactive-Orbitrap analyzer (UHPLC-Q-Exactive-Orbitrap MS). The mass spectrometer operated with a heated electrospray interface (HESI) in positive and negative mode. The monitoring of the ions was achieved in two ways: full scan and data independent acquisition scanning (DIA). An exact mass database including mass information regarding the pesticides and 42 metabolites was developed and applied for a fast and accurate analysis of the samples. The data were processed with highly specialized software such as Xcalibur™ version 4.3.73, and TriceFinder 5.1, for the detection and confirmation of the ions.

The proposed methodology allowed for providing evidence of the high persistence of the two parent pesticides in the soil, with difenoconazole the first to decrease in concentration after two months. Thanks to the application of HRMS, retrospective analysis will be carried out in the search for unknown metabolites. In addition, it was studied how these pesticides can affect the soil microbiota.

(1) Wu, M.; Li, G.; Li, P.; Jiang, N.; Wei, S.; Petropoulos, E.; Li, Z. Assessing the Ecological Risk of Pesticides Should Not Ignore the Impact of Their Transformation Byproducts – The Case of Chlorantraniliprole. *J. Hazard. Mater.* 2021, *418*, 126270.

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