

Concours de l'Ecole Doctorale de Chimie de Lyon - 2023

(Semi) quantification de traces de micropolluants dans des matrices environnementales complexes par couplages CPG ou CL avec la spectrométrie de masse : des challenges à relever !

(Semi) quantification of traces of micropollutants in complex environmental matrices by coupling GC or LC with mass spectrometry (LRMS, HRMS): still challenges to face!

Keywords : mass spectrometry, semi-quantification, targeted and suspected analyses, high and low mass resolution, LC-QTRAP, LC-QqQ, LC-QToF, GC-Orbitrap

Contact : Emmanuelle VULLIET (emmanuelle.vulliet@isa-lyon.fr)

Trace and ultra-trace analysis is an important driver of progress in analytical chemistry, particularly in the field of the environmental exposome. This requires constant innovation of analytical strategies in terms of sensitivity, identification, resolution, speed and reliability. The scientific progress made over the last fifteen years regarding sensitivity and identification is mainly linked to technical advances in the coupling of chromatography and mass spectrometry, and to the improvement of the resolution of analysers.

However, quantification of trace levels remains a real analytical challenge due to the complexity of non-aqueous environmental matrices and the lack of hindsight on the impact of spiking and incorporation of an internal standard. Another major difficulty for scientists is the lack of analytical standards for many metabolites or transformation products (TPs), which escape environmental monitoring and for which no quantitative data are available.

In this context, the objectives of this thesis are:

- With the aim of semi-quantifying metabolites or TPs, the response factors of an analyte and its by-products from the main degradations (conjugation, oxidation, dealkylation, hydrolysis,...) will be studied in order to evaluate the impact of adding or removing a functional group on the electrospray ionisation efficiency, electron impact response factor, and fragmentation patterns. Different methodologies will be developed and compared, such as the closest eluting compound approach, the structurally similar compound approach, the use of an internal standard, the ionisation efficiency of suspect compounds present (Kiefer et al., 2019; Liigand et al., 2021; Wiest et al., 2021).
- The impregnation of the matrix with the analytes and/or isotopically labelled internal standards will be explored in terms of representativeness and matrix effects generated in mass spectrometry. The response of analytes and internal standards will be studied during LC-MS/MS (triple quadrupole analyzer) and GC-HRMS (Orbitrap analyzer) couplings. In

particular, the ionization competition between matrix interferents, analytes and their isotopically labelled internal standards will be investigated.

The thesis will be carried out within the TRACES team of the Institute of Analytical Sciences, whose research activities focus on the development of analytical methods, based on mass spectrometric detection, to improve the characterisation of chemical pollution markers in environmental matrices, including sentinel species. The combination of targeted or global analytical strategies allows a better understanding of the Exposome and its consequences on the environment.

References:

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