Simultaneous quantification of multi-class contaminants in tea leaves and brews by UHPLC-HRMS as a springboard to a new « omics » approach of food chemical safety

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The routes of food chemical contamination are complex (agricultural practices, transformation processes, environment, toxins, food contact materials,) and assessing the chemical safety of a food product is an everyday challenge considering the large number of molecules to monitor and the diversity of their physico-chemical properties. Nowadays, strategies to ensure chemical food safety always imply an addition of single-class analytical methods. Some of the main drawbacks of this approach are cost, duration and the disability to perform *a posteriori* data analysis, meaning that the detection of unexpected compounds is very unlikely since those methods are highly selective. Thus, there is a strong need in developing global, untargeted methods to address food chemical safety issues. The development of such an approach starts with the quantification of multi-class trace contaminants in a complex matrix.

The method presented here shows, for the very first time, the simultaneous quantification in a complex matrix (tea leaves and brews) of trace (ng/g) contaminants from four distinct classes: pesticides (n=23); mycotoxins (n=4); packaging contaminants (n=5); process-induced contaminants (n=2).

These molecules have been chosen for their structural diversity (both in terms of size, polarity and functionality) and their relevance in tea samples. For regulated compounds such as pesticides, concentrations as low as the maximum residue limits (few ng/g) were targeted when feasible.

Ultra-High Performance Liquid Chromatography (UHPLC) coupled with High Resolution Mass Spectrometry (HRMS) was used. Compounds were first separated on a C18-PFP (PentaFluoroPhenyl) column, since it allows an enhanced retention for more polar compounds. Electrospray ionization and Time-of-Flight mass analyzer were then used. Generic sample preparation techniques commonly used in metabolomics (Liquid/Liquid Extraction and Dilute & Shoot) were compared in order to have the widest analytical scope as possible.

Beyond the quantification of multi-class contaminants, this study aims at being the springboard to a more global fingerprinting approach of chemical safety for food products.