Metabolomics as a Tool for Exploring Natural Compounds in Food Safety

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ABSTRACT:
Metabolomics provides a comprehensive framework for the systematic characterisation of small molecules that define biological systems. Because metabolites are the downstream products of gene and protein activity, their analysis offers direct insight into biochemical regulation and the influence of environmental and physiological factors. Liquid chromatography coupled to high-resolution mass spectrometry (LC–HRMS) has become a key analytical platform for metabolomics, combining high selectivity, sensitivity, and mass accuracy. The integration of ion mobility spectrometry (IMS) further improves molecular resolution by enabling the separation of isomeric species and the generation of multidimensional datasets.

A metabolomic workflow typically merges targeted, suspect, and non-targeted acquisition strategies to quantify known metabolites, annotate theoretically expected compounds, and detect unknown molecular entities. Computational developments such as feature-based molecular networking (FBMN) and in silico fragmentation prediction have expanded annotation capabilities, transforming spectral data into structured chemical information and enhancing reproducibility across laboratories.

This integrated LC–HRMS/IMS–FBMN approach is particularly effective for the study of secondary metabolites in plants and fungi, where chemical diversity underpins ecological interactions and toxicological outcomes.
This communication will present a workflow applied to the annotation of fungal toxins produced by Fusarium spp. High-resolution MS data were processed through FBMN to visualise chemical relationships between detected metabolites. Known mycotoxins served as reference nodes linking to uncharacterised features with comparable fragmentation profiles, facilitating the identification of structural analogues and potential metabolic transformations. The combined use of retention behaviour, isotopic patterns, and collision cross-section data increased annotation confidence and revealed novel molecular analogues.

Overall, the integration of LC–HRMS, IMS, and molecular networking constitutes a robust and scalable analytical strategy for exploring the chemodiversity of natural matrices. The approach enhances structural elucidation, supports the discovery of new toxin analogues, and provides a reproducible foundation for the comparative study of fungal secondary metabolism within food-relevant systems under changing environmental conditions.

KEYWORDS:
Mass spectrometry, metabolomics, mycotoxins, fungal metabolites