

Abstract

Analytical metabolomics approaches for the assessment of food safety and quality

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The Max Rubner-Institute (MRI) is the Federal Research Institute of Nutrition and Food and advises the Federal Ministry of Food and Agriculture in questions about food and nutrition. Research regarding consumer health protection focuses also on bioprocessing and technology, microbiology and biotechnology and safety and quality of food. Since questions regarding authenticity and traceability are of special concern there are four departments within the MRI that work on respective research within this field. These departments investigate influences regarding quality and safety along the entire food production chain. Different analytical approaches are used to characterize and confirm the authenticity of products. While the conventional approach lies in the targeted analyses of one or few marker substances, the metabolomics approach strives to analyze a product as comprehensive as possible. Subsequently large amount of data are generated, which can be stored in Databases for subsequent use of metabolomic fingerprinting. Another option is metabolite profiling, which provides a comprehensive characterization of food and facilitates the search for characteristic patterns and markers which give proof of the foods' identity or quality. The metabolomics platform established at the MRI in Karlsruhe uses different methods and instruments, while the comprehensive two-dimensional gas chromatography (GCxGC-MS) has been found to be most versatile(1).

An example for the application of the GCxGC-MS method for the characterization and differentiation of apple cultivars is presented. Samples from 14 different cultivars were taken; peel and pulp were sampled separately. After freeze-drying, grinding and extraction with methanol, samples were centrifuged, evaporated and derivatized for subsequent GCxGC-MS analyses. Results revealed a different profile for apple flesh and peel. Up to 240 analytes were detected. Using multivariate analysis it was possible to differentiate the apple cultivars based on their metabolite profile of peel and flesh. Analytes with quantitative differences between the cultivars were found, but most mentionable some analytes were cultivar-specific. These compounds are potential markers to identify apple cultivars. Data and findings in this experiment have been confirmed by parallel NMR analyses(2). Thus GCxGC-MS has proven to be a valuable tool for the assessment of authenticity.

1. Weinert CH, Egert B, Kulling SE. On the applicability of comprehensive two-dimensional gas chromatography combined with a fast-scanning quadrupole mass spectrometer for untargeted large-scale metabolomics. *J Chromatogr A*. 2015;1405:156-67.
2. Eisenmann P, Ehlers M, Weinert CH, Tzvetkova P, Silber M, Rist MJ, Luy B, Muhle-Goll C. Untargeted NMR spectroscopic analysis of the metabolic variety of new apple cultivars. *Metabolites*. 2016;6(3).