

Metabolomics Analysis in Food Authentication

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Editorial

Verification of food authenticity establishes consumer trust in food ingredients and components of processed food. Next to genetic or protein markers, chemicals are unique identifiers of food components. Non-targeted metabolomics is ideally suited to screen food markers when coupled to efficient data analysis. This study explored feasibility of random forest (RF) machine learning, specifically its inherent feature extraction for non-targeted metabolic marker discovery. The distinction of chia, linseed, and sesame that have gained attention as "superfoods" served as test case. Chemical fractions of non-processed seeds and of wheat cookies with seed ingredients were profiled. RF technology classified original seeds unambiguously but appeared overdesigned for material with unique secondary metabolites, like sesamol or rosmarinic acid in the Lamiaceae, chia. Most unique metabolites were diluted or lost during cookie production but RF technology classified the presence of the seed ingredients in cookies with 6.7% overall error and revealed food processing markers, like 4-hydroxybenzaldehyde for chia and succinic acid monomethylester for linseed additions.

RF based feature extraction was adequate for difficult classifications but marker selection should not be without human supervision. Combination with alternative data analysis technologies is advised and further testing of a wide range of seeds and food processing methods. Food authenticity and nutritional quality are of great interest to the food industry, producers, distributors, and consumer trust in nutritional value, origin, and production processes. A food product can be sold at a premium price if label claims and declarations of origin and ingredient identity are certified by producers and can independently be verified by regulatory authorities or consumer's organizations using validated analytical technologies [1].

Authenticity of foods that are based on animal tissues can be traditionally verified by immunological methods. The high diversity of plant derived foods or food additives can be monitored in addition by molecular markers that may be either metabolic or genetic. Genetic markers can be designed to authenticate species, genus, or even plant variety. Indeed, the detection of DNA is considered one of the most potent tools in food integrity research not least due to the considerable chemical stability of DNA. The use of DNA markers as diagnostic tools of validating ingredient authenticity in foods has been investigated by an increasing number of studies. Complementary to genetic and protein markers, metabolomics enables marker searches and validation by spectroscopic and hyphenated analytical techniques⁵, such as Liquid Chromatography (LC) or Gas Chromatography (GC) coupled to Mass Spectrometry (MS). Specialized software is used for compound targeted and non-targeted analyses of the large analytical data sets that are typically created by non-targeted metabolomic

technologies⁹. Tools are in place to predict class membership of plant samples by statistical models that are based on metabolome profiles [2,3].

Metabolomics profiling identifies even plant varieties and crop cultivars according to their chemical composition. Moreover, metabolomics may directly assess the nutritional composition of foods. If combined with hydrolysis procedures, the amino acid composition, fatty acid content and carbohydrate composition of proteins, fats and polysaccharides can be determined. This information is indispensable to both consumers and food producers that take interest in potential health benefits and basic nutritional value of foods seen as "nutraceuticals". The large diversity of primary and specialized secondary metabolites makes plant-based food and food additives highly amenable to the search for metabolic markers of food authenticity or nutritional quality. Consequently, metabolomics approaches and especially non-targeted fingerprinting are expected to become potent tools of food authentication and discovery of food adulteration. As a test case of our current study, we analysed three types of non-processed seed materials, namely chia, linseed and sesame which are typically added as ingredients to baked cookies or other marketed bakery products, such as crackers, breadsticks or bread. Linseed and especially chia gained consumer attention and are frequently labelled "superfoods" because these seeds may have health benefits, however, with so far limited evidence [4,5].

Conflict of interest

None.

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