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Food metabolomics for improvement of nutrition and well-being

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Abstract. Food metabolomics is an emerging field that employs comprehensive analytical techniques, such as Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography-Mass Spectrometry (LC-MS), and Nuclear Magnetic Resonance (NMR), to identify and quantify essential nutrients and bioactive compounds in foods, and to link their impact on human health. By integrating metabolomic data with nutritional science, researchers can better elucidate how dietary components influence metabolic processes and contribute to overall health and well-being. This review highlights recent studies in food metabolomics, providing a detailed understanding of its application in assessing nutritional value, optimizing dietary recommendations, and improving food quality. The role of food metabolomics in precision nutrition and well-being is significant, and recent advancements in this research area are discussed.

1 Introduction

Metabolomics, the comprehensive study of small molecules or metabolites produced by cells, plays a pivotal role in understanding metabolic processes within biological systems [1] [2]. Over the past decade, metabolomics has emerged as a vital field, distinguishing itself from genomics, transcriptomics, and proteomics by providing direct biomarkers of biochemical activity [3]. This direct approach allows for a more precise linkage between metabolomic data and phenotypic traits, offering invaluable insights into the complex biological changes occurring in organisms [4] [3].

The concept of metabolomics began to emerge from genomics and proteomics, with researchers applying these principles to food science to capture a comprehensive profile of metabolites [5]. Since the early 2000s, advancements in analytical technologies, such as Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography-Mass Spectrometry (LC-MS), and Nuclear Magnetic Resonance (NMR) spectroscopy, have advanced the field significantly [6] [7]. These innovations have led to extensive food metabolite databases and sophisticated analytical methods for handling complex food matrices.

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In food science, metabolomics is employed to analyze the chemical compounds in various food samples, such as fruits [8] [9], spices [10], cocoa [11] [12] [13] [14], coffee [15] [16] [17], and other agricultural products [3], with different study objectives. This field, known as food metabolomics, involves applying metabolomic techniques to study the small molecules (metabolites) present in food. By comprehensively analyzing the chemical composition of foods, including nutrients [6], bioactive compounds [18], and potential contaminants [19], metabolomics provides critical insights into the nutritional value of foods [20]. It identifies and quantifies essential nutrients such as vitamins, minerals, amino acids, and fatty acids, also assessing the impact of agricultural practices, processing methods, and storage conditions on food quality.

The applications of food metabolomics extend to enhancing dietary recommendations [21], improving food labeling [22], and discovering compounds with potential health benefits [23] (Iman et al., 2024), including antioxidants, anti-inflammatory agents, and polyphenols. Additionally, it plays a crucial role in quality control by monitoring changes in food composition during processing and storage to ensure safety and consistency [24]. This paper aims to review recent research in food metabolomics, highlighting its transformative impact on nutrition and well-being and exploring its significance, diverse applications, and future potential.

2 Analytical Techniques in Food Metabolomics

Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography-Mass Spectrometry (LC-MS), and Nuclear Magnetic Resonance (NMR) spectroscopy are analytical techniques commonly used in food metabolomics. Each method offers unique advantages for profiling food metabolites. [25] [6].

GC-MS (Gas Chromatography-Mass Spectrometry) is particularly effective for analyzing both volatile and non-volatile compounds, such as essential oils and aroma compounds [26], making it invaluable for characterizing complex flavor components [8]. This tool offers high resolution and sensitivity, allowing for the detailed characterization of complex mixtures [25]. For example, Ikram et al. [27] employed GC-MS-based metabolomics to reveal 56 metabolites during the ripening stages of pineapple. Padilla-Jimenez et al. [28] used SPME (Solid Phase Microextraction) GC-MS to identify flavor compounds in organic blueberries. Additionally, the flavor and taste of different fruit cultivars were examined using GC-MS-based metabolomics in studies by Sato et al. [29] and Kim et al. [8]. Hanifah et al. [11] and Herrera-Rocha et al. [12] also used GC-MS-based metabolomics to identify chemical components in cocoa subjected to different post-harvest processing methods. These studies highlight the utility of GC-MS in providing comprehensive profiles of chemical components in a wide range of food products, contributing to a deeper understanding of their flavor and nutritional attributes.

LC-MS excels in the analysis of non-volatile and thermally labile metabolites, including amino acids, peptides, and polyphenols [24]. The technique's ability to separate compounds based on their chemical properties before mass spectrometric detection enhances its capability to analyze diverse metabolite classes. For instance, Drira et al. [26] identified adulteration in olive oil samples using HPLC-based metabolomics. Jiang et al. [30] employed LC-MS to detect compound changes in jujube leaf trees during post-harvest processing.

NMR spectroscopy provides a non-destructive method for identifying and quantifying metabolites by measuring the magnetic properties of atomic nuclei [31]. It is particularly useful for studying food matrices as it offers a comprehensive view of the molecular composition and allows for the analysis of metabolites in their native state [32]. Together, these techniques enable a thorough investigation of food metabolomes, facilitating the identification of key nutritional components, bioactive compounds, and potential contaminants, and providing insights into the effects of food processing and storage on nutritional quality [33].

Analyzing complex food matrices using GC, LC, and NMR spectroscopy-based metabolomics presents unique challenges due to the diverse and intricate nature of food constituents [24]. GC and LC require efficient separation of metabolites, complicated by the wide range of chemical properties and concentrations in food samples [25][31]. Sample preparation and derivatization steps must be meticulously optimized to ensure accurate and reproducible results. NMR, while highly informative, often faces sensitivity limitations, difficulties in signal identification, and requires large sample volumes [34]. Solutions to these challenges include the development of advanced chromatographic techniques, such as multidimensional gas chromatography (MDGC), which offers excellent separation efficiency for advanced characterization of volatiles and semi-volatiles in food samples [35]. Improved sample preparation protocols and the use of internal standards can reduce variability and matrix effects [24], [25]. For NMR, the use of cryoprobes and advanced pulse sequences can significantly enhance sensitivity. Additionally, combining GC, LC, and NMR data with sophisticated bioinformatics tools for multivariate analysis can provide a more comprehensive and accurate metabolic profile, thereby overcoming individual technique limitations and improving the reliability of metabolomic studies in complex food matrices [36].

3 Food Metabolomics Applications

3.1 Nutritional profiling of food

Nutritional profiling of foods involves a detailed analysis of their chemical composition to assess nutritional value [20]. This process utilizes advanced metabolomic techniques to identify and quantify essential nutrients, such as vitamins, minerals, amino acids, and fatty acids, as well as bioactive compounds with potential health benefits. It also offers personalized nutrition based on individual factors such as genetics, metabolism, and environmental exposure. Metabolomic profiling has been employed to analyze the nutrient composition of various foods, including fruits [8] [34], vegetables [37], and grains [4], to better understand their contribution to dietary requirements and health outcomes, as well as their chemical profiles for quality control [38].

Several studies have focused on revealing the nutrient content, particularly flavonoid components and antioxidant properties, in various foods and agricultural products using a metabolomic approach [39] [37] [40]. For instance, Iman et al. [18] identified the metabolites of germinated green soybean, green soybean, and green soybean tempeh as functional foods, highlighting the bioactive metabolites related to nutrition. Similarly, Rahmawati et al. [41] profiled the metabolites of tempeh made from various legumes, providing insights into improving the nutritional value of tempeh and legumes.

Metabolomic profiling has also been conducted on fruits and other agricultural products [27] [29] [42] . For example, profiling different types of coconuts, such as normal and kopyor varieties, highlighted the functional components of the kopyor variety, which was found to have more nutritional components compared to the normal one. Additionally, metabolomic studies on cocoa and coffee have identified biochemical markers related to the unique properties of luwak coffee [43]. Another study on chocolate from different origins and fermentation temperatures [11] revealed important metabolites that contribute to its nutritional value.

According to various studies on food profiling, integrating this data with dietary guidelines allows researchers and nutritionists to develop more accurate dietary recommendations and food labels that reflect the true nutritional value of foods. Additionally, understanding the impact of agricultural practices and food processing on nutrient levels helps optimize food quality and ensure consumer health [44].

3.2 Developing personalized nutrition related to health benefits

Food metabolomics also advances personalized nutrition and health by enabling a deeper understanding of individual metabolic responses to diet [21]. Through comprehensive profiling of metabolites in biological samples, metabolomics can reveal unique metabolic signatures that reflect a person's nutritional status, dietary habits, and overall health [45]. This information allows for the customization of dietary recommendations to meet specific nutritional needs, enhance metabolic health, and prevent diet-related diseases [46]. For example, metabolomic data can identify biomarkers associated with metabolic disorders such as diabetes and obesity [23] [45], leading to more targeted and effective interventions. Additionally, personalized nutrition based on metabolomic insights can optimize dietary intake to improve athletic performance [47], manage chronic conditions, and support healthy aging [48]. By using metabolomics in nutrition plans, healthcare providers can offer personalized advice based on each person's unique metabolism, genetics, and lifestyle, leading to better health and well-being [49]. Research about nutrition particularly unraveling the connection between diet and human health has been conducted [48]. These research was employed omic technology to provide individual nutrition based on antropometrics parameters such as gender, age, physiological status, environmental and biological condition. A study about identification metabolites related to human health has been employed [23]. This research was successfully discovered six metabolites which can prevent LDL colesterol. This result offers aplication in personal dietary recommendation for illness prevention.

3.3 Food Quality Control and Safety

Metabolomics is also crucial for food quality control and safety. By profiling the metabolite composition of food, metabolomics can detect adulteration, contamination, and spoilage with high sensitivity and specificity in various food samples [19]. This approach enables the identification of chemical markers associated with food freshness [50], authenticity, and quality, which are critical for maintaining consumer trust and meeting regulatory standards. For instance, by using GC-MS profiling can revealed the chemical compounds of different manggo cultivars [29]. This study provide understanding for the consumer preferences by comparing with high quality cultivar which already established in the market. Another study using metabolomic techniques can differentiate between organically and conventionally grown produce by identifying specific metabolic fingerprints [51]. Study of Syukri et al. [50] using HPLC-MS/MS technique could reveal biomarker in the feshness degree of soybean sproud. Additionally, they can detect harmful substances such as pesticides, mycotoxins, and pathogens [52], providing a comprehensive assessment of food safety [44]. Metabolomics also facilitates the monitoring of production processes and storage conditions [53], ensuring that food products retain their nutritional value and safety throughout the supply chain. By integrating metabolomics into food quality control systems, producers and regulators can achieve more precise and efficient monitoring, ultimately safeguarding public health and enhancing the overall quality of the food supply [44].

4 Challenges and Future Directions

Food metabolomics faces several challenges in improving nutrition and wellbeing [54], but the future holds promising directions. One of the primary challenges is the complexity of food matrices and the vast diversity of metabolites [55], which require sophisticated analytical technique and extensive databases for accurate identification and quantification. Additionally, inter-individual variability in metabolism poses a significant challenge, necessitating large-scale studies to establish reliable biomarkers and dietary recommendations [56]. Data integration and interpretation also remain complex due to the multidimensional nature of metabolomic data. Additionally, it is challenging to achieve reliable validation from the results [57]. However, future directions are poised to address these issues through advancements in analytical technologies such as high-resolution mass spectrometry and nuclear magnetic resonance spectroscopy, which can provide more detailed and accurate metabolic profiles [35]. The development of more comprehensive and standardized metabolomic databases will enhance data comparability and reliability [36]. Furthermore, integrating metabolomics with other omics technologies and leveraging artificial intelligence for data analysis can provide deeper insights into the interactions between diet, metabolism, and health [58]. As these innovations progress, food metabolomics will become increasingly effective in tailoring nutritional strategies to individual needs, ultimately enhancing health and well-being.

5 Conclusion

Recent advancements in food metabolomics have provided crucial insights into the chemical composition of various foods, identifying essential nutrients, bioactive compounds, and potential contaminants. To fully realize the benefits of food metabolomics, further research and application are necessary. Continued exploration in this field will deepen our understanding of food-health interactions and drive innovations in food science, leading to better global nutrition and well-being. Researchers and industry professionals should engage in collaborative studies to maximize the potential of metabolomics for a healthier future.

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