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Metabolomics In Modern Food Science: Techniques, Applications, And Emerging Trends

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ABSTRACT

The high-throughput study of small molecule metabolites in biological matrices is the focus of metabolomics, a rapidly expanding field of omics research. As a result, metabolomics is well situated to be employed in food nutrition and food science research. Technology and databases are the two factors that now limit the potential impact of metabolomics. For metabolite detection and quantification systems to become more accurate, automated, and comprehensive, significant equipment changes are obviously needed. Food quality, monitoring of food intake, food component analysis, physiological supervision in food intercession, food authenticity assessment, and diet challenge research are imperative fields of food science and technology. The study's main emphasis is on metabolomics' present potential future usage and trends.

Keywords: Food, Technology, Metabolomics, Analysis, Nutrition, Quality

1. INTRODUCTION

The high-throughput quantification/identification of metabolites (small molecules) in the metabolome is the focus of the relatively new branch of omics research known as "metabolomics." The collection of all small molecule compounds or metabolites that may be discovered in a cell, organ, or organism is known as the "metabolome," according to formal definitions. These molecules have diverse exogenous and endogenous components, including carbohydrates, amino acids, peptides, alkaloids, vitamins, organic acids, polyphenols, minerals, and nucleic acids pretty much any other substance that can be utilized, ingested, or produced by a specific cell or organism. [1]

Metabolomics, also known as metabonomics or metabolic profiling, was only made practical recently by advances in the technology of small molecule isolation and identification. These include reliable, high-resolution mass spectrometry devices for accurate mass determination, high-resolution, high-throughput

NMR spectrometers, capillary electrophoresis, and ultra-high pressure liquid chromatography systems for quick compound separation, as well as new software tools for quickly processing spectral or chromatographic patterns. The creation of electronic databases with spectral and descriptive data on the chemicals present in various metabolomes has been crucial to the advancement of metabolomics. These advances in technology and software have made it feasible to quickly identify and analyze dozens of small molecule metabolites rather than just one or two at a time. [2]

Similar to other emerging "omics" domains, there is sometimes a propensity for quick technological advancement, which is then followed by a protracted phase of consolidation and methodological development. No exclusion pertains to metabolics. There are several metabolomics technologies available, and numerous analytical methods can be applied, each with unique benefits and drawbacks (**Table 1**). In reality, for metabolomic data analyzing and processing, two different schools of thought have evolved in recent years. In one form, just the spectral patterns and intensities of chemical compounds are recorded, statistically compared, and utilized to determine the pertinent spectral properties that separate sample classes. Unsupervised clustering or supervised categorization are frequently used in these statistical analyses and feature identification methods. [3]

Table 1. Comparison of different metabolomics technologies.

TECHNOLOGY	**ADVANTAGES**	**DISADVANTAGES**
Liquid Chromatography-Mass Spectroscopy (LC-MS)	Quantitative Non-destructive Fast (2-3 minutes/sample); Necessitates neither derivitization nor separation; identifies every organic class; ID of new compounds is permitted; dependable, advanced technology; Large amount of databases/software and for metabolite ID; and Metabolite imaging (fMRI)	Lacking in sensitivity; high-cost instrumentation substantial instrument footprint; unable to identify salts and inorganic ions; non-protonated substances cannot be detected; and bigger (0.5 mL) samples are necessary
Gas Chromatography-Mass Spectroscopy (GC-MS)	Robust, established technology, reasonably priced, quantitative (with calibration), small sample size need, and high sensitivity; extensive databases and software for metabolite identification; Most organic and some inorganic compounds are detected, and the separation repeatability is excellent	Sample not recoverable; sample derivitization is necessary; needs to be separated; (20–30 minutes per sample); not suitable for imaging; and Novel compound ID is difficult
Nuclear Magnetic Resonance Spectroscopy	Excellent sensitivity; Highly adaptable technology; most organic and some inorganic compounds are detected;	Unrecoverable sample not very numerical; high-cost instrumentation Slow (20–30 min/sample); Poor

(NMR)	Minimum sample size necessary metabolite imaging (MALDI) is a possible use; direct injection, which can be performed without separation; and has the capacity to identify the majority of the metabolome	resolution and repeatability of the separation (compared to GC); less durable equipment than NMR or GC-MS; databases and software for metabolite identification are few; Novel compound ID is challenging

Identification of several compounds simultaneously in sample specimens is made possible by metabolomics, which gives nutrition and food explorers a fantastic opportunity to build up a much more detailed and comprehensive molecular picture of food composition, food consumption, and the metabolomic effects of various diets. To put it another way, metabolomics essentially opens the door to studying many facets of "molecular nutrition," such as: (1) food component analysis; (2) food quality/authenticity sensing; (3) food intake monitoring; and (4) work in science in food interference or diet conundrum research.

2. METABOLOMICS IN FOOD QUALITY/AUTHENTICITY ASSESSMENT

Metabolic profiling's ability to detect food elements exploited to evaluate food quality and food adulteration. In particular, the detection of tainted or adulterated food items takes use of the fact that specific chemicals or chemical concentrations are particularly typical of particular types of juices, extracts, and oils. Food items with desired qualities that cannot be recognized by flavor, fragrance, or color can be distinguished from those with less desirable attributes using similar chemical composition criteria. Food quality control is impacted by food quality evaluation as well. In reality, batch-to-batch product reproducibility monitoring or quality control monitoring may be where metabolomic approaches in the food business are most useful. [4]

The majority of metabolomic research on food quality and food adulteration that have been published so far have centered on describing oils or drinks such vegetable oils, fish oils, fruit juices, wines, and beers. Because it is so challenging to tell if fruit juice is adulterated by flavor or color, it happens rather frequently. For instance, orange juice and less expensive grapefruit juice can be mixed without any discernible flavor or color changes. However, those who are on specific drugs may experience substantial side effects if grapefruit juice is present in an ostensibly pure orange juice product. Numerous coumarin-like flavanoids and other potent CYP450 inhibitors can be found in grapefruit juice. Therefore, it is particularly crucial to identify and stop this sort of adulteration. Traditional methods for detecting this form of juice mixing involve time-consuming HPLC procedures. Recently, an NMR-based chemometric method utilizing Independent Component Analysis (ICA), a PCA version, has been created. The main idea behind this strategy is to examine certain areas of the ^{1}H-NMR spectrum that are known to have distinctive flavanoid glycoside signals. 92 juices comprising of 59 orange, 23 grape, and 10 combinations, were used to evaluate the approach. It was discovered to be highly accurate, properly classifying 98% of the samples. Additionally, the time required by this NMR technique was less than half that of conventional chromatographic methods. [5]

The difference between juices made from pulp washes and juices that have just been squeezed is another frequent problem with juice production. Similar to how pulp wash is used to cut expenses while producing grapefruit juice, pulp might adjoined to freshly squeeze orange juice without leaving a noticeable taste, texture, or visual difference. Scientists employed 1H-NMR and principal component analysis to separate more than 300 samples of freshly squeezed and pulp-washed orange juice in order to solve this problem. The accuracy of the approach was found to be close to 95%. Furthermore, compared to freshly squeezed juice, pulp-wash juice was found to contain considerably greater amounts of the particular biomarker component dimethylproline. The creation of a test to identify this changed amino acid might make the detection of pulp-wash relatively straightforward and low-cost. [6]

Additionally, NMR has been used successfully to track variations in beer production sites and batch-to-batch quality. Large multinational or pannational brewers are required to produce their brews across a wide geographic range. It is crucial to create methods for quality control that can be performed at a more precise molecular level rather than merely at the level of color, alcohol content, or specific gravity given the need to make beers that taste and are of comparable quality at these various locations. The study found that various manufacturing locations, likely producing the same beer, could be easily recognized based on their concentration of lactic acid, pyruvic acid, dextrans, adenosine, inosine, uridine, tyrosine, and 2-phenylethanol. By quantifying these chemicals, the researchers are familiar with one production site that had far poorer quality control than the other production sites and shown considerably more variability in these compounds. Other international firms might use these techniques to enhance quality control in the manufacture of juice, soft drinks, and vegetable oils. The quality control of functional foods and nutraceuticals—food extracts with favorable therapeutic effects—harvested from various geographical regions may also be monitored using comparable techniques. [7]

In order to detect and categorize samples, the majority of published food/beverage adulteration studies to date have used NMR in conjunction with PCA, artificial neural networks, or other multivariate statistical approaches. Mass spectrometry may also be used to look for food adulteration, though. In example, beet sugar detection and exogenous citric acid to fruit juices has long been done using isotope ratio mass spectrometry, as well as the adulteration of wines and olive oils. The comparative loads of isotopes or isotope fractionation in a particular sample is measured using the mass spectrometry instrument in IRMS, a specialized variant of the technique. Isotope abundances can alter based on material's age, physical source, geographic location, and metabolic response. As a result, isotope abundances can be utilized to determine the biological or geographical origins of numerous substances when compared to a known internal isotope reference. [8]

It is expected that stricter and more accurate food monitoring systems will need to be put in place over the next years due to the international nature of food production and processing as well as the rising concerns about food safety and food quality. Metabolomics may soon play a significant role in many aspects of food quality assessment and quality control, as evidenced by the proven ability of metabolomic techniques to quickly and affordably recognize adulterated oils and beverages as well as their capacity to precisely scrutinize previously undetectable quality control issues. [9]

3. METABOLOMICS IN PHYSIOLOGICAL MONITORING OF DIET AND NUTRITION STUDIES

The identification of the crucial nutrients required for human growth and survival has advanced significantly over the past century thanks to the work of food scientists and biochemists. Most nutritional "deficiencies" have been successfully treated with improved dietary recommendations and required food supplements of critical minerals and vitamins. Today's nutritional experts are faced with the task of developing novel methods for treating or preventing illnesses including obesity, diabetes, chronic inflammation, and cardiovascular disease that are brought on by dietary "oversufficiencies." Additionally, they are expected to name any bioactive dietary ingredients that may lengthen life, lower weight, improve physical or mental performance, and shield against ailments including atherosclerosis, heart disease, cancer, and arthritis. [10]

In order to investigate how diet or bioactive food ingredients affect human health, nutrition experts might choose one of two approaches. One way is through retrospective epidemiological studies that aim to link a person's long-term food intake to their health or susceptibility to disease. The other way is by conducting research with shorter-term prospective dietary interventions or diet challenges. Epidemiological studies designated several positive connections between diet and better health status, however these correlations do not always imply causality. Therefore, diet-challenge studies that concentrate on quantitatively detecting molecular biomarkers and physiological impacts have emerged as the ideal method for examining the mechanisms behind the unfavorable or favorable effects of important nutrients. [11]

In many diet-challenge or food intervention investigations, genomic, proteomic, and most recently metabolomic approaches are increasingly often employed. Small molecule indicators of inflammation, redox potential, anti-oxidant activity, oxidative stress, and cardiovascular disease risk may all be quantified using metabolomic tests, based upon the physiological reaction under examination. The benefit of using small molecule biomarkers is that the same small molecule monitoring techniques can be used to look at the short-term concentration changes of diet-related chemicals or metabolites. Although proteomic and transcriptomic markers are also available for tracking these responses, small molecule biomarkers have this advantage over them. To measure dietary intakes and physiological outputs, just one technological platform is required. [12]

The molecules that are utilized as biomarkers of physiological response to meals are usually non-polar and most are detected in blood, in contrast to the urine polar compounds that can be employed as biomarkers of food ingestion. This is due to the fact that blood is often a more consistent and trustworthy indication of physiological processes. Additionally, compared to urine, blood contains a lot more non-polar molecules. NMR or MS approaches haven't historically been used to find all of the chemicals. In reality, some are often evaluated using centrifugation techniques or identified using immunoassays. However, improvements in MS-based lipidomic technologies and lipoprotein characterisation now make it possible to identify and/or quantify these compounds using relatively conventional, high-throughput MS or NMR methods. [13]

One of the initial investigations on the effects of soy-derived proteins and soy isoflavones in a diet-intervention experiment used metabolomic methods. Pre-menopausal women on a multi-week soy diet had their blood plasma alterations examined using ^{1}H-NMR and chemometric methods. The findings demonstrated that distinct variations in lipoprotein, amino acid, and carbohydrate profiles associated to the metabolic pathways governing osmolyte fluctuation and energy consumption could be observed. The effects of whole-grain and wheat flour diets on rats were investigated in a related study utilizing both NMR-based chemometric techniques. These experiments demonstrated that the rats given whole grains had increased urine levels of hippuric acid, aromatic acids, and Kreb's cycle intermediates. Both a change in the animal's basal metabolic rate and a change in the metabolism of the gut microbiota may be indicated by these metabolites. Increases in glutathione and betaine, two markers of a healthy redox state and lessened oxidative stress, were seen in NMR tests on plasma and liver. [14]

Many of the more recent studies have concentrated on employing more sensitive MS techniques or immunoassays since many of the effects of food modification are likely to be more subtly expressed and the biomarkers of interest will be at lower concentrations. The impact of concentrated red grape juice on oxidative stress, lipidemic, and inflammatory markers in blood, the impact of extra virgin olive oil on plasma inflammatory and oxidative stress markers, the effects of macadamia nut consumption on markers for cardiovascular disease, and the impact of gazpacho soup consumption on plasma oxidative biomarkers are a few of the studies included in this list. The findings of prior retrospective epidemiological research were essentially confirmed by all of these investigations, all of which demonstrated some statistically significant, favorable effect. Many of these researches measured the physiological effects of interest using both small molecule and large molecule protein biomarkers. [15]

Future investigations on the physiological effects of foods or diet-intervention trials are expected to utilize less varied food sources or specific bioactive components as diet supplements as a result of advances in perceptive of bioactives present in many foods. The physiological elucidations are frequently simplified, and the outcomes are frequently more repeatable, when pure or partly purified bioactive components are used. Studies of this nature are already being conducted. For instance, researchers looked at how plasma homocysteine levels were affected by two distinct compounds from food, betaine and choline. A known risk factor for heart disease and several other chronic illnesses is homocysteine.

Similar research on people, animals, and other cell systems have been done with other pure bioactives, such as folate, omega-3 polyunsaturated fatty acids, and a range of purified fruit polyphenols. [16]

While long-term food exposure eventually affects human health and illness, the most efficient way to employ metabolomics to investigate diet-health interactions is probably to use short-term diet challenges to assess their expected consequences on long-term health outcomes. Sensitive metabolomic techniques combined with experiments using glucose, fructose, fat, and high-calorie diet challenges are likely to yield some important insights into the temporal progression of chronic diseases like obesity, diabetes, cardiovascular disease, and metabolic syndrome. Additionally, studies using fish/olive oil, flaxseed, cruciferous vegetables, polyphenol-rich fruit, and low-calorie diet challenges may provide similarly significant insights into their effectiveness for treating metabolic syndrome, preventing cardiovascular disease, and prolonging life. [17]

Diet-challenge studies will aid in revealing the range of individual responses to these various dietary perturbations if they are adequately and thoroughly tracked by the more sensitive metabolomic approaches. Certain disease-risk biomarkers or metabolites will undoubtedly exhibit far bigger or longer-lasting disturbances in certain "high-risk" individuals, whilst other "low-risk" persons would show essentially none. The assimilated utilization of transcriptomic, SNP-profiling, copy-number variation, gut metagenomic, and proteomic/enzymatic studies in these diet-challenge experiments will also allow for a much more thorough understanding of the inter-individual differences or proclivities due to epigenetic and genetic effects, albeit metabolomics undertake to endow with a much more chemically and quantitative comprehensive perceptive of phenotypic alterations. [18]

As was previously said, there many different kinds of actively responding coordination to nutrition in addition to a wide range of dietary preferences among people. Certainly, this variation creates profiling of metabolites and metabolite "standardization" challenging. Gender, diurnal influences, and specifically age also affect the concentrations and even the existence of several metabolites, complicating consistencies, and inter-subject comparability. This might be substantially aided by the development of specialized metabolite or metabolomic databases that incorporate these gender-specific ranges, age-specific variances, or temporal impacts. This kind of database building would undoubtedly be made much simpler by the establishment and exchange of extensive, longitudinal metabolomic data sets gathered from well-designed and well-documented diet-challenge trials. Additionally, it could strengthen group comparisons and metabolite calibrations, making their results considerably more reliable. [19]

4. FUNCTIONAL PERSPECTIVES OF METABOLOMICS IN FOOD SCIENCE

The creation of equipment with extremely low limits of detection and high sample throughput, as well as sample production and manipulation, has frequently been the bottleneck despite enormous advancements in analytical methodologies. It is obvious that metabolomics participate in a critical function in plant improvement, whether conventional hybridization or transgenic plants are utilized, from the standpoint of producing plant meals with improved quality. However, it is very challenging to demonstrate cause-and-effect since there are several metabolic pathways and outside influences. Metabolomics plays an even more important function in nutrition, however it is outside the purview of this book chapter. In fact, it doesn't matter how many more vitamins, antioxidants, or probiotics may be added to a meal or food composition; what matters is whether human absorption improves consumer health. Similar to this, describing not only the metabolome of a specific plant, animal, or microbe but also the interaction that takes place when the metabolomes interact, such as in plant and animal infection, may prove to be the greatest difficulty in the future. Large interdisciplinary teams are required to tackle these problems and put the "omics" puzzle together logically. [20]

5. CONCLUSION

In several fields of food nutrition and food science research, such as food intake monitoring, food quality, food component analysis, food authenticity evaluation, and physiological monitoring in food intervention studies, metabolomics is well-positioned to be applied. Metabolomics' potential influence is currently constrained by two elements, namely technology and databases. It is obvious that considerable apparatus upgrades are required to make metabolite detection and quantification technologies more reliable, automated, and thorough. It is true that having access to resources like databases pertaining to nutritional phenotype or food metabolome that might be just as beneficial to the explorers (molecular biologists).

CONFLICT OF INTEREST

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