



## Review article

## The evolution of analytical chemistry methods in foodomics

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## ABSTRACT

The methodologies of food analysis have greatly evolved over the past 100 years, from basic assays based on solution chemistry to those relying on the modern instrumental platforms. Today, the development and optimization of integrated analytical approaches based on different techniques to study at molecular level the chemical composition of a food may allow to define a 'food fingerprint', valuable to assess nutritional value, safety and quality, authenticity and security of foods. This comprehensive strategy, defined foodomics, includes emerging work areas such as food chemistry, phytochemistry, advanced analytical techniques, biosensors and bioinformatics.

Integrated approaches can help to elucidate some critical issues in food analysis, but also to face the new challenges of a globalized world: security, sustainability and food productions in response to environmental world-wide changes. They include the development of powerful analytical methods to ensure the origin and quality of food, as well as the discovery of biomarkers to identify potential food safety problems. In the area of nutrition, the future challenge is to identify, through specific biomarkers, individual peculiarities that allow early diagnosis and then a personalized prognosis and diet for patients with food-related disorders.

Far from the aim of an exhaustive review of the abundant literature dedicated to the applications of omic sciences in food analysis, we will explore how classical approaches, such as those used in chemistry and biochemistry, have evolved to intersect with the new omics technologies to produce a progress in our understanding of the complexity of foods. Perhaps most importantly, a key objective of the review will be to explore the development of simple and robust methods for a fully applied use of omics data in food science.

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## 1. Introduction: analytical chemistry in food science

In 1894, Wilhelm Ostwald, future Nobel prize in chemistry, defined analytical chemistry as the art of separating, recognizing different substances and determine the constituents of a sample. Since then, analytical chemistry evolved from art to a branch of chemical science of greatest theoretical and practical utility for industry, medicine and in general for all applied sciences (Fig. 1). Over the years, applications in food technology led to the development of analytical approaches aimed to the global characterization of a food to define its chemical, physical and sensory characteristics and to ensure its quality and safety for consumers, supporting and implementing the laws and regulations of the field.

Recently, this comprehensive strategy has been termed 'foodomics' [1–3]. Foodomics is defined as 'a discipline that studies the food and nutrition domains through the application and integration of advanced omics technologies to improve consumer's well-being, health and confidence' [3]. In the development of the advanced foodomic platforms, because of their potential to profile complex mixtures of biomolecules, mass spectrometry techniques have assumed an unquestionable role. The analytical capability of MS have made highly resolving, hyphenated separation devices (HPLC, GC, CE, SFC, PAGE) able to characterize at the molecular level the entire panel of the components of a complex system. For these reasons MS, together with NMR and other spectroscopic techniques, is the core of the omic technologies.

This paper illustrates the development and evolution of analytical methods which led to modern foodomic platforms (MS, NMR, biosensors and ancillary techniques), based on high-throughput instrumentation and computational methods, and the revolution they introduced in food analysis. We also review the significant technological advances which are opening new and important areas in food technology, food biotechnology and nutrigenomics.

## 2. Sources of information

Researchers in the foodomic field must identify and select the best methodology among those available to address their specific questions. The main sources of information and general approach to a literature search are detailed below.

### 2.1. Books, reviews and journals

Recent discoveries in molecular biology, analytical chemistry, and biochemistry have led to the development of new tools that are likely to revolutionize the study of foods. The fast development of food chemistry and technology over the last two decades is described in the book *Food Chemistry* [4]. The book *Foodomics: Advanced Mass Spectrometry in Modern Food Science and Nutrition* presents this rapidly emerging field [5]. The book *OMICs Technologies: Tools for Food Science* explores how these tools reveal the fundamental pathways and biochemical processes that drive food and nutrition sciences [6].

Omic methods are gaining in importance for process development and validation in food technology and biotechnology as well as corresponding quality control of starting materials and final products (Fig. 2). Therefore, the number of reviews and journals dealing with use of omics methods in food processing and

nutrition has also rapidly increased, for instance: *Food Technology and Biotechnology*, *Journal of Agricultural and Food Chemistry* (ACS Publications), *Food Chemistry*, *Food Analytical Methods* (Springer), *Food Research International* (Elsevier). Special Issues of the most eminent analytical chemistry journals – *Journal of Chromatography*; *Trends in Analytical Chemistry* (Elsevier); *Electrophoresis* (Wiley) are regularly dedicated to update methods and applications in food analysis.

### 2.2. Web sites and databases

Current informatic systems allow the generation, processing, circulation and storage of various scientific information. Generally, several websites are available for information on a particular subject. A non-exhaustive list of relevant sites on foodomics and its applications includes: (<http://www.foodomics.eu>; <http://www.chancefood.eu>; <http://www.foodomics.org>; <http://www.allergome.com>; <http://www.foodchem.it>; <http://www.safefoods.nl>).

Databases together with statistical systems with thematic character provide a comprehensive and accurate vision of the phenomenon under investigation. Each database is accompanied by various information (methodologies, classifications, definitions) on the subject. Foodomics is based on molecular characterization by metabolomic and proteomic approach; therefore, some databases are [www.expasy.ch](http://www.expasy.ch); GeneBank, EBI, GEO and also BioPEP, PepBank, EROP or APD.

## 3. From classical to instrumental approaches to food analysis

Food chemistry deals with the themes related to the qualitative and quantitative characterization of foods and their (bio)chemical transformations during production, maturation and storage (Fig. 1). The roots of modern food chemistry trace back to the XIX century, when chemists began studying foods and isolate their macro-components.

Most modern food analysis has been advanced by food safety issues. The U.S. Food and Drug Administration (FDA) was created in the early XX century to protect consumers from food adulteration. In that period, nearly all food analysis was carried out using classical chemistry in solution [for an extensive review see 7], based on specific chemical reactions and using only chemicals and the basic equipment easily available in all laboratories. From these bases, Henneberg developed the classification scheme to determine food composition in terms of macro-components (moisture, proteins, carbohydrates, lipids) still in use today (Fig. 3). Later, the basic Kjeldhal procedure for determining the food protein content, the golden standard for over 100 years, is based on acid–base titration after conversion of protein nitrogen to ammonia. The limitation of the method, demanding and laborious, as also recently exploited by its inability to identify the poisonous adulteration of feed and milk powder with melamine, are those common to all the chemistry in solution

It is not an overstatement to say that the demand from food and agriculture sector was one of the driving forces for the instrumental developments. The first electronic, portable pH meter was built by Beckman to meet the request of a consortium of fruit

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