

Definition of food quality by NMR-based foodomics

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Quality definition of food includes several complex factors like physical, compositional and microbial features, modifications induced by technological processes or storage, nutritional value and safety. Foodomics is a holistic approach applying omics technologies to observe food along the entire production/consumption chain. In the present review, we present key applications of nuclear magnetic resonance in foodomics described in the 2012–2015 period, in the quest for robust and thorough information required by the scientific community. In doing so, we summarize the issues connected to food traceability and authenticity, composition and physical characteristics, processing and storage and health, that mostly impact food quality.

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Current Opinion in Food Science 2015, 4:99–104

This review comes from a themed issue on **Foodomics technologies**

Edited by **Alejandro Cifuentes**

For a complete overview see the [Issue](#) and the [Editorial](#)

Available online 18th June 2015

<http://dx.doi.org/10.1016/j.cofs.2015.06.008>

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Introduction

Soon after the advent of genomics, transcriptomics, proteomics and metabolomics, aimed to a holistic understanding of the complex human biology and physiology, it has been natural to apply the same approaches to food. The information collected in this way at each step of the production/consumption chain has been enclosed into the single definition of foodomics, which now is defined as ‘the 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’ [1]. Among the techniques used for this discipline, Nuclear Magnetic Resonance (NMR) has given a great boost to the new approach, thanks, in particular, to the high reproducibility of its observations [2*].

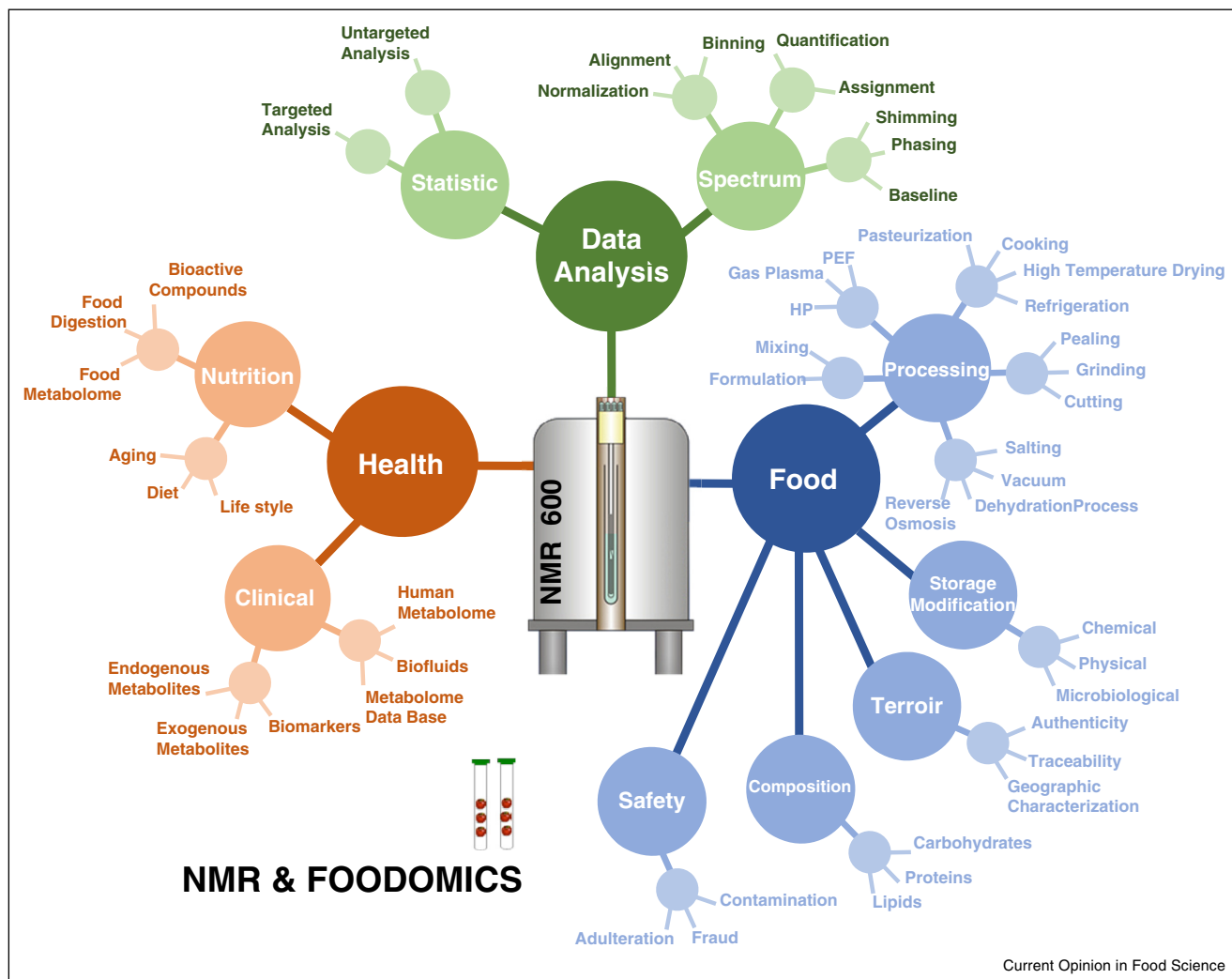
Goodacre [3], in a recent divertissement, has noted that the growth of the metabolomics literature reminded that of microorganisms. The lag phase is represented by a handful of papers, listed by Goodacre [3], which created the conceptual framework. A key element of the initial phase can be identified also in the development of software and algorithms (i.e. Projection on Latent Structures [4]) specifically tailored to highlight the useful features in the overwhelming information represented by large experimental datasets. The phase of rapid growth can be felt in the works focusing on the most diverse biofluids, foods and raw materials, aiming at verifying the applicability of the metabolomics approach. A common trait of these papers is some degree of failure in making each step of the investigation (i.e. experimental design, data generated and analytical tools) totally transparent. The stationary, desirable, phase is represented by works where experimental design, data generated and the means of analysis are made publicly available, and the level of metabolite identification is properly assigned [5], as well as the level of confidence of each key statement. Papers actively contribute to a generalized increase of quality, when they fulfill such requirements better than any other of their own field, by forcing the scientific community to adapt.

In the present review, we mainly focus on the literature of the 2012–2015 period and present key applications of NMR in foodomics, in the quest for robust and thorough information required by the scientific community. In doing that, we will run through the steps of the food production chain, from the origin of the raw material to the transformation that food undergoes during storage, that mostly affect food quality, as summarized in [Figure 1](#).

Traceability, authenticity and safety of food

A relevant percentage of the commercial value of several foods and beverages relies on the ensemble of climate, land, cultural practices and history of the raw material, collectively enclosed in the term ‘terroir’. NMR has been used from the eighties with the purpose of geographic characterization, by studying the distribution of stable isotopes of the bio-molecules [6]. A natural consequence of the advent of the ‘omic’ analytical techniques has been to consider the entire metabolome in the perspective of terroir characterization. This is generally observed in a non-targeted fashion [7], that is without focusing on specific molecules but letting features of the NMR spectra emerge from the entire spectrum profile, through the appropriate mathematical treatments. Examples of this

Figure 1



Infographic of the information that can be obtained along the food production/consumption chain by NMR, through a foodomic approach. For the spectra, processing steps see Ref. [2].

approach are the work by Gallo *et al.* [8] on table grape, and the work by Hohman *et al.* [9] about tomato.

Unfortunately, each aspect of a food terroir potentially affects the metabolome, so that general applicability represents the weak point of any mathematical model trying to relate features of an NMR spectrum with a single aspect of the origin of a food. This is probably why no method based on non-targeted fingerprinting has been accepted for food official controls [7]. The recently published work that can be considered a to-date benchmark in this respect is the one by Godelmann *et al.* [10^{••}] testing wine screening method WineScreener™. The analysis of 600 German wine samples, produced during 2 years in 5 areas from 10 grape varieties, led to the maximum correct prediction of geographical origin,

year of vintage and grape variety (89%, 97% and 95% respectively).

It has been suggested that the studies on food safety, similarly to those on terroir, would bring information to a higher level if including an omic-untargeted approach, because many features that raise concerns about the healthiness of food, as genetic modification [11] or microorganisms development [12,13], are likely to influence large portions of food or raw material molecular profile [14].

The main challenge for scientists facing non-targeted analysis is to correctly define appropriate biomarkers from raw NMR spectra containing hundreds of metabolites. The rationale of this practice is that the inclusion of a

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