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Green foodomics. Towards a cleaner scientific discipline

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ABSTRACT

In the present review, we have tried to highlight foodomics' goals with regards to green chemistry principles providing an update (from mid-2013 up to 2017) on the novelties and new approaches that can be employed to make foodomics greener. Although Foodomics covers different fields of research included in food science approached using advanced -omics technologies and associated to sustainability, in the present work only those directly related to green analytical chemistry (GAC) and novel foods development are discussed. Aspects treated in the present work deal with new trends in production of functional food ingredients (through the use of alternative solvents and design of biorefinery processes) and with green alternatives mainly for metabolomics and proteomics. Moreover, different methodologies to quantify the greenness of the processes are presented.

1. Foodomics and green chemistry

Since its first definition in 2009 [1], interest in Foodomics has greatly increased; for instance, from the 27 manuscripts dealing with Foodomics in the period 2009-mid 2013, numbers have moved to more than 110 manuscripts published in the last years (mid 2013-beginning 2017), thus showing a great adoption of the discipline as a framework to assess several important aspects in food science and nutrition, such as those related to food safety, quality, production and processing [2–4], novel foods development and the binomial food-health [5,6], including the study of human gut microbiota and its relationship with host physiology and environmental modulating factors [7], among others.

The present contribution highlights foodomics goals with regards to green chemistry principles and provides an update on the previous work [8], emphasizing the novelties and new approaches that can be employed to make foodomics greener. Even if there are many aspects covered by foodomics that are associated to sustainability, only those directly related to green analytical chemistry (GAC) and novel foods development will be discussed in the present work. Therefore, the basic concepts of Green Chemistry and GAC should be borne in mind in order to improve the greenness of a process and/or the analytical methodologies involved in any foodomics study [9–11].

As in our previous work, special emphasis has been put in the new possibilities to quantify the greenness of a process and/or analytical methodology.

Abbreviations: AIMS, ambient ionization mass spectrometry; AMVI, analytical method volume intensity; ASE, accelerated solvent extraction; CE, capillary electrophoresis; CV, coefficient of variance; DART, direct analysis in real time; DES, deep eutectic solvents; FWHM, full width at half maximum; GAC, green analytical chemistry; GC, gas chromatography; GHS, globally harmonized system of classification and labeling of chemicals; GXL, gas-expanded liquid; HILIC, hydrophilic interaction liquid chromatography; HPLC-EAT, HPLC environmental assessment tool; HRMS, high-resolution mass spectrometry; HS, headspace; HSE, health, safety and environmental impact; ILs, ionic liquids; IMS, ion mobility spectrometry; IR, infrared; LC, liquid chromatography; LCA, life cycle assessment; LIT, linear ion trap; LLE, liquid–liquid extraction; SLE, solid–liquid extraction; LPME, liquid-phase microextraction; LTP, low-temperature plasma; MAE, microwave-assisted extraction; MCDA, multicriteria decision analysis; MALDI, matrix-assisted laser desorption/ionization; MALDI-MSI, MALDI-MS imaging; MS, mass spectrometry; MSPD, matrix solid-phase dispersion; NADES, natural deep eutectic solvents; NEMI, national environmental methods index; NMR, nuclear magnetic resonance; NPLC, normal phase liquid chromatography; PHWE, pressurized hot water extraction; PLE, pressurized liquid extraction; PROMETHEE, preference ranking organization method for enrichment evaluations; PS-MS, paper spray mass spectrometry; PTR, proton transfer reactions; QuEChERS, Quick, easy, cheap, effective, rugged and safe; Q-TOF, quadrupole–time of flight; RPLC, reversed-phase liquid chromatography; RTILs, room temperature ionic liquids; SC-CO_2, supercritical carbon dioxide; SFC, supercritical fluid chromatography; SFE, supercritical fluid extraction; SLE, solid–liquid extraction; SPE, solid phase extraction; SPME, solid phase microextraction; SWE, subcritical water extraction; TOF, time of flight; UAE, ultrasound assisted extraction; UHPLC, ultra-high performance liquid chromatography.

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2. Green processes to produce functional food ingredients

As defined, Foodomics is a "new discipline that studies the food and nutrition domains through the application and integration of advanced -omics technologies to improve consumer well-being, health and knowledge" [1,12] (see Fig. 1), and therefore, the rational design of new foods and/or food ingredients able to improve our health is one of the main goals, together with unraveling the mechanisms involved in the observed bioactivity. Thus, the extraction of bioactives from natural sources (such as plants, algae, food by-products, among others) is a key step in a foodomics work.

In this context, it is important to consider how foodomics can integrate the ideas behind the sustainability concept, understood as a rational way of improving processes to maximize production while minimizing the environmental impact and "maintaining the appropriate conditions between humans and nature that permit fulfilling the social, economic and other requirements of present and future generations" [13]. Among the different possibilities that can help foodomics moving towards a cleaner scientific discipline, the replacement of toxic solvents for green solvents with lower environmental impact, the design of new biorefinery processes and the intensification and integration of processes will be discussed in this section.

The substitution of conventional toxic solvents (which are not only dangerous for health but also flammable, corrosive and negatively contribute to environmental pollution) by green and sustainable solvents is a hot topic nowadays concerning not only the extraction of valuable components from natural sources but also all the research in chemical processes. Other than some very interesting reviews published recently [14,15], a specially devoted themed issued on Green Solvents appeared recently in Current Opinion in Green and Sustainable Chemistry journal [16]. In this special issue, the properties and some application of new solvents such as gas expanded liquids (GXLs) and switchable solvents [17] and dimethyl carbonate [18], among others, are presented. Moreover, an interesting article about molecular modeling of environmentally benign solvents is also discussed [19] in which an overview of the recent applications of different green solvents such as room temperature ionic liquids (RTILs), supercritical carbon dioxide (SC-CO_2), organic carbonates and deep eutectic solvents (DES) is shown.

The design of biorefinery processes has been a quite active field of research in the last few years, with the main idea of revalorizing the whole biomass through the development of different value chains in order to generate new products, co-products and services; by including the production of high-added value products from natural sources/biomass, we are able to move towards a circular bio-economy. The use of compressed fluids for this purpose was anticipated by King and Srinivas [20] and recently promoted through process intensification [21] and integration [22]. Different articles have been published involving the use of compressed fluids for biorefinery of, for instance, microalgae [23] or plants' leaves [24]. For an in depth discussion on the most recent applications of compressed fluids for the extraction of bioactives from different natural sources, through single, intensified, integrated or biorefinery approaches, readers are referred to Refs. [25,26].

3. Development of green analytical methods for foodomics

As stated before, a foodomics study is based on the use of -omics platforms such as transcriptomics, proteomics and metabolomics to provide integral information, among others, about the effects of food in health at three levels of expression: genes, proteins and metabolites. An interesting overview of the evolution of analytical methods in foodomics is provided in a recent review [27]. As mentioned, the green foodomics approach integrates the principles of green analytical chemistry [11] in each of the -omics platforms during method development. In brief, within the framework of GAC, while maintaining high standards in analytical figures of merit, efforts are taken (i) to replace toxic reagents, (ii) to avoid or at least, to reduce, the amount of reagents and solvents employed to do the analytical determinations, (iii) to evaluate and reduce the energy consumed, and (iv) to avoid or minimize the volume of

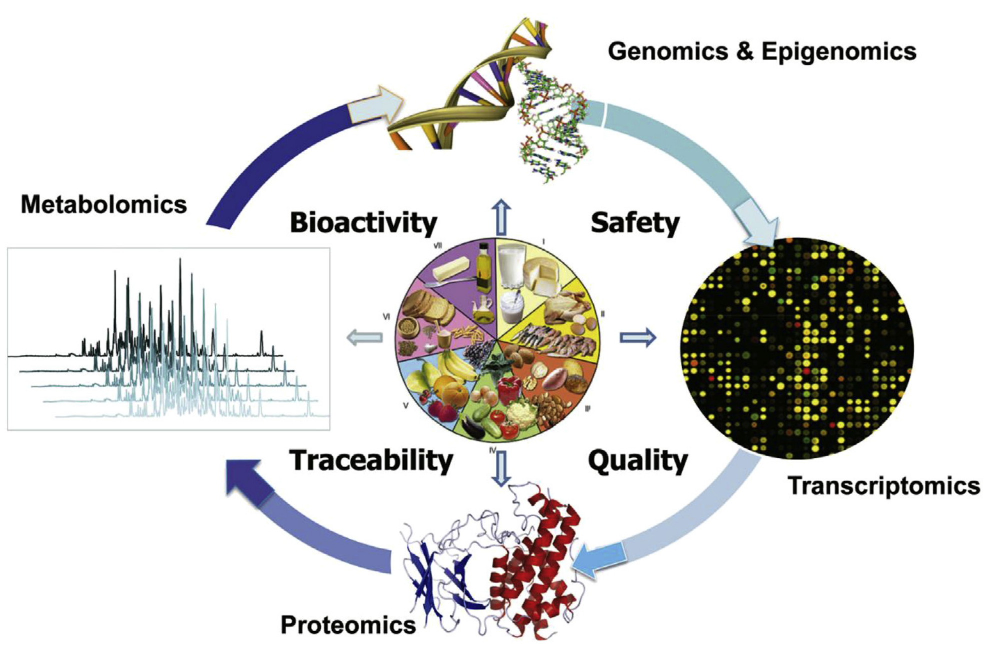

Fig. 1. Foodomics analytical process.
Reproduced with permission from Ref. [12].

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