



# Green food analysis: Current trends and perspectives

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Green Chemistry and Green Analytical Chemistry principles have been promoting the development of environmentally friendly processes to achieve a more sustainable society. This boost to sustainability has been given thanks to the strong relationship between Sustainable Development Goals, Green Chemistry, and Food Bioeconomy. In particular, the analytical approaches based on Green Analytical Chemistry have contributed to food safety and quality assessment as well as to food bioactivity studies improving the nutritional status quality of communities while they interact in a more sustainable way with their environment. This opinion article describes, exemplifies, and discusses some recent advances and new applications of Green Analytical Chemistry for food analysis.

## Addresses

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## Abbreviations

EPA, U.S. Environmental Protection Agency; FAAS, flame atomic absorption spectrometry; GAC, green analytical chemistry.

## Introduction—Green Analytical Chemistry and green food analysis

The Sustainable Development Goals (SDGs), particularly SDG 2: Zero hunger by 2030 [1], require efficient and sustainable food production systems that are also able to meet the four dimensions of food security: (i) food availability; (ii) food access; (iii) food utilization; and (iv) stability over time [2]. Food bioeconomy (FB) is a powerful food production approach founded in the circular biobased economy that “use renewable

biological resources from land and sea in a responsible way but with the aim at benefitting businesses, society and nature alike” [3]. In the FB processes, the biotic resources are optimized closing production loops, since input (biomass and energy) and output (products, by-products, and wastes) are reduced [4]. The potential of FB for large-scale production of high-quality foods is increased by biorefinery processes, since these involve improved utilization of biological resources by generating value from all parts of particular biomass feedstock sources [5].

Considering this background, the question is how Green Analytical Chemistry (GAC) can contribute to ensure food security and SDG 2 [6,7]. As can be seen in [Figure 1](#), analytical methodologies based on GAC could promote at least two dimensions of food security: food availability and food utilization. GAC facilitates the bioprospecting of compounds with nutritional or functional value in biorefinery processes using, among others, predictive models to ascertain the solubility of these compounds in green solvents employed in environmentally friendly extraction techniques. On the other hand, GAC strategies promote safer, cheaper, and sustainable analytical methods for reliable detection of food components and harmful compounds ensuring the food quality and safety. For instance, Green Foodomics approaches integrate the GAC principles in each of the -omics platforms during method development to determine food constituents and nutrients at the molecular level [8,9]. GAC principles and Green Chemistry principles are closely correlated, and their implementation not only promotes food security and SDG 2 achievement but also contributes to the consolidation of other SDGs, as can be seen in [Figure 2](#). Those principles could improve health and welfare, clean water, clean-energy production and consumption, promoting the sustainable cities and communities’ development, industrial innovation and infrastructure, as well as responsible consumption and production [10].

These ideas somehow run parallel to those already reported by Marcinkowska et al. [11] and De la Guardia and Garrigues [6] in which they realize on the importance of the social dimension of GAC and its linkage with sustainability that lead to interesting and new definitions such as “Equitable Analytical Chemistry” or “Democratic Analytical Chemistry” emphasizing the role of GAC in making analytical procedures

more affordable, accessible to every person, institution and country that needs to, and therefore, beneficial for the whole society.

### Goals of this work and coverage

In the present opinion paper, we want to emphasize the importance of GAC principles in food analysis to really contribute to a more sustainable world. To do so, it is important to detect the main challenges the society is facing nowadays, in terms of sustainable food production and food security, to provide with some solutions in the light of Green Food Analysis. It is interesting to mention here that many of the concepts, ideas and strategies to generate a greener food analysis can be directly extrapolated to get a greener food production, so, in this paper both concepts will be used indistinctly, although, clearly we focus on the food analytical part.

In a very recent document, the Spanish National Research Council (CSIC) analyzed the Scientific Challenges towards a Sustainable Primary Production in 2030 [12] including the following key points that need to be addressed (some of them are discussed in Sections [Food safety and quality assessment](#) and [Food bioactivity](#)):

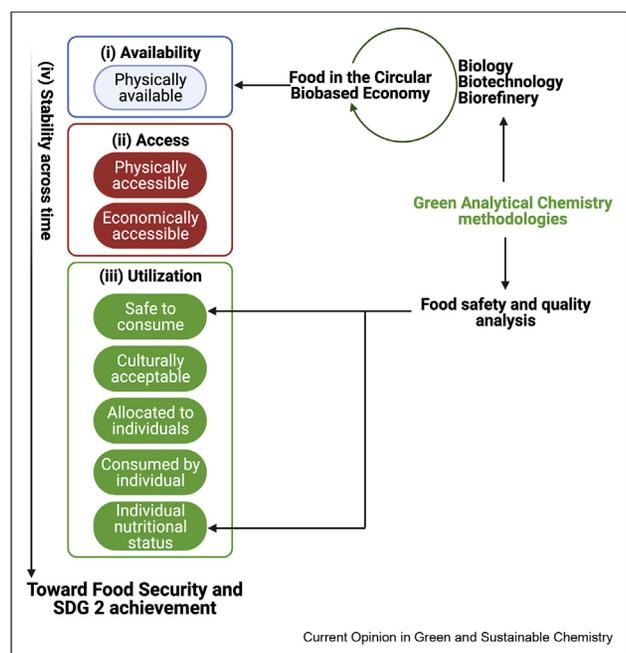
1. In terms of food safety and quality:
  - a. Identify and prevent frauds and emerging risks related to changes to more sustainable production systems (reuse of wastes and by-products, effect of minimal processed foods, reduction in the use of additives, etc).

- b. Verification of the absence of toxicity and risk of bioaccumulation of new compounds and ingredients and mixtures.
  - c. Real-time safety control along the different production steps for a comprehensive characterization of food products.
  - d. Discovery of new markers of authenticity and origin.
2. In terms of food bioactivity:
    - a. Recovery of bioactive compounds from underused biomasses and food wastes
    - b. Evaluation of the bioactivity of the compounds/foods.
    - c. Knowledge of the relationships between food, nutrition and health.
    - d. Development of new food products able to meet the responses for different societal needs (from undernourished populations to health promoting foods).

### Green food analysis or how GAC can contribute to meet SDGs

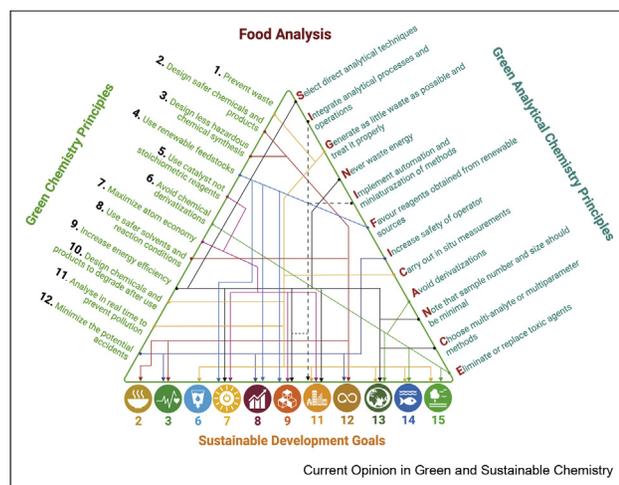
As mentioned above, many challenges arise for a sustainable food analysis, so, this area should evolve to get ready to answer the complex demands coming from the application of GAC principles. In this sense, it is worth mentioning that analytical methods applied to food analysis should be validated and optimized by determining parameters such as accuracy, sensitivity, reproducibility, simplicity, cost-effectiveness, flexibility, and speed (inherent to all of them) and fulfilling the

Figure 1



Contribution of GAC to food security dimensions.

Figure 2



Correlation of Green Chemistry principles and GAC principles and their contribution to SDGs consolidation. SDG 2: Zero Hunger; SDG 3 Good Health and Well-being; SDG 6: Clean Water and Sanitation; SDG 7: Affordable and Clean Energy; SDG 8: Decent Work and Economic Growth; SDG 9: Industry, Innovation and Infrastructure; SDG 11: Sustainable Cities and Communities; SDG 12: Responsible Consumption and Production; SDG 13: Climate Action; SDG 14: Life Below Water; SDG 15: Life on Land.

Table 1

## Recent applications of sustainable analytical procedures for the evaluation of food safety and quality.

Technique(s)	Objective of the study	GAC principles achieved <sup>a</sup>	Remarks	Reference
Sweep metallic probe + (ESI)-MS/MS	Multiresidue analysis of pesticides (15) in fruit and vegetables	S, I, G, I, N, C, E,	- Sample preparation and chromatography were avoided. - Reasonable detection limits (<50 ppb). Comparison with GC-MS, LC-MS.	[17]
Bain-Marie extraction (70 °C, 5 min) + CIC-CD	Analysis of preservatives in solid, semi-solid and liquid foods	G, N, F, I, E	- Reagent-free - Different extraction methods were compared (vortex and ultrasound-assisted extractions, magnetic stirring, and bain-marie extraction). - No organic solvents were used in chromatography or extraction.	[18]
Online- biosorbent-SPE-FAAS	Analysis of Pb in tea	I, G, I, F, A, N, E	- Hazardous plants from the environment were removed. - Low cost and easy to operate FAAS. - The use of complexing agents was avoided. - Miniaturization (3 cm column). - HCl solution as elution solvent.	[19]
LADI-MS	Analysis of furan 5-hydroxymethylfurfural in unroasted and roasted coffee beans	S, I, G, N, E	- Confirmation by GC-MS and argon-DART-MS. - No organic solvents were used.	[20]
Near-infrared hyperspectral imaging	Characterization of narrow-leaved oleaster dry fruit (geographical origin prediction)	S, I, G, C, E	- Use of machine learning. - Without sample pretreatment.	[21]
SLE + LC-MS	Analysis of sulfadiazine and trimethoprim in bovine meat and chicken muscles	G, I, F, N, E	- Green Metrics: NEMI, GAPI, Analytical Eco-Scale. - Comparison of LC (a) ethanol/water; b) micellar, c) UHPLC (acetonitrile, ammonium acetate). - b and c were the best. - The SLE for b method did not use organic solvents.	[22]

CD: conductivity detection; CIC: capillary ion chromatography; ESI: electrospray ionization; FAAS: flame atomic absorption spectrometry; GAPI: Green Analytical Procedure Index; GC: gas chromatography; LADI: Laser ablation direct analysis in real time imaging spectrometry; LC: liquid chromatography; MS: mass spectrometry; MS/MS: tandem mass spectrometry; NEMI: National Environmental Methods Index; SLE: solid-liquid extraction; SPE: solid-phase extraction.

<sup>a</sup> See Figure 2 for further description.

requirements of GAC should never go against this rule; on the opposite, GAC should be able to provide with methods having similar figures of merit but with improved characteristics in terms of environmental and societal impacts.

In this section, we have selected some relevant applications in light of the current trends and main challenges of “food safety and quality assessment” and “food bioactivity” but discussed considering how they adhere to the GAC principles and how they improved previous “not so green” approaches. In our attempt to understand the correlation among Green Chemistry-GAC-SDGs, a detailed analysis of the GAC principles achieved in the selected examples has been included with the final

objective to realize what is being achieved and what is still lacking in this race towards 2030 SDGs.

### Food safety and quality assessment

Requirements for a sustainable food production are challengingly increasing in this area with the growth of world population and globalization of the food market. In this context, food security, traceability, and authenticity assurance become of utmost importance to guarantee consumers safety [13,14]. One of the main problems for implementing GAC principles to analyze complex samples as foods is, for instance, to determine the existence and toxicity of contaminants, new chemicals, additives, etc., due to the low levels at which these toxic substances are found, which makes difficult to

avoid sample preparation steps and the development of direct or just simpler procedures, according to GAC [15]. Despite these drawbacks, diverse approaches have been developed to reach successful procedures fulfilling the action lines of green chemistry, even involving the participation of the general population as it is shown in initiatives such as “Citizen science” [16]. As can be seen in Table 1, in which some recent green food analysis applications for food safety and quality determination are compiled, different strategies have been proposed for the analysis of organic and inorganic contaminants [17–19], hazardous substances generated during food processing [20] or for products characterization [21].

One of the proposed strategies is the combination of direct analytical imaging techniques with computer tools that allow reducing the complexity of the analytical procedure for fruit geographical origin prediction [21]. Similar strategy was applied by Fowble et al. [20] who studied the spatial distribution of furan and 5-hydroxymethylfurfural in unroasted and roasted *Coffea arabica*, while Cheng et al. [17] carried out the simultaneous identification of more than 300 pesticides and the quantification of 15 of them in vegetables and fruits.

In those cases, in which sample preparation and separation cannot be omitted, the use of environmentally friendly solvents and the application of miniaturized methods are interesting strategies to develop greener procedures (see Ref. [18] in Table 1).

Regarding the application of alternative solvents or sorbents, diverse biocompatible materials have been recently developed and applied. In general terms, the most suitable approaches are those in which different strategies are combined enhancing the sustainable character of the procedure. A remarkable application based on that concept is the methodology developed by de Almeida et al. [19] in which an invasive plant was converted into a new sorbent for the online extraction and subsequent analysis of lead in water by flame atomic absorption spectrometry (FAAS).

From the aforementioned examples, it can be seen that one of the main problems in the evaluation of food safety and quality from a quantitative point of view is the inability to remove sample preparation and pre-concentration steps. The technological development of more sensitive and specific instruments could be a suitable alternative, as well as the implementation of strategic proposals that allow the development of effective methodologies for every step of the analytical procedure. In this sense, the application of initiatives such as the Triad approach, developed by the U.S. Environmental Protection Agency (EPA) to manage chemically contaminated site remediation, could be also

a good tool to reach the aims of GAC in this area, especially for its application in routine analysis. This approach is based on the application of systematic planning, dynamic work strategies, and real-time measurement systems, which would allow simplifying analytical strategies, reducing analysis times and costs, as well as improving procedure efficiency and flexibility [23].

A good example for real-time control and monitoring along the food production chain is the development of portable instrumentation [24] that can integrate multi-sensors (and bio-sensors) and analytical tools combined with databases and predictive mathematical models that allow a real-time quality and safety control along the different production steps. Portable systems greatly reduce sampling, sample stockage and transport, while avoiding environmental side effects and risks and helps improving decision-making by carrying out *in situ* measurements. Moreover, considering that portable systems are commonly less expensive, their use can be more accessible and widespread worldwide (including low-income countries), thus contributing to reach SDGs in a more fair and responsible way. A clear example of this trend is the wide application of smartphones as colorimetric platforms for the evaluation of food quality [25].

#### Food bioactivity

As we stated above, important challenges can be encountered in terms of food bioactivity such as those related to the search and recovery of bioactive compounds for food products innovation (functional foods, new foods, nutraceuticals, etc.) and those helping us to understand how food can contribute to good health and well-being. In this sense, researchers are carrying out important efforts to obtain and characterize the main bioactive compounds that can be found in natural products, wastes and agri-food industrial by-products, together with the implementation of analytical platforms for (foodomics) evaluation of bioactivity. But the most appealing is the increasing number of interesting applications in which classical methodologies have been substituted by novel procedures to improve the environmental performance of the approach, and the attention paid to its quantification through the use of Green metrics. A selection of recent publications regarding the application of GAC in food bioactivity assessment is listed in Table 2.

As already emphasized in Section [Food safety and quality assessment](#), Green Food Analysis can greatly contribute to the attainment of the SDGs from different perspectives which also include the democratization and reduction in costs (of any kind) of classical methods. A pioneer work, based on such principles, was developed by Vaher and Kaljurand who used a mobile phone camera

Table 2

## Recent applications of sustainable analytical procedures for the evaluation of food bioactivity.

Technique(s)	Objective of the study	GAC principles achieved <sup>a</sup>	Remarks	Reference
Paper microzone plates	Antioxidant capacity and total phenolic content	G, I, F, N, C, E	<ul style="list-style-type: none"> <li>- NADES as extraction medium.</li> <li>- Simplicity, miniaturization, easy disposal, fastness.</li> <li>- Green metrics calculation.</li> <li>- Previous extraction.</li> </ul>	[27]
HAE, UAE and MAE, UHPLC-PDA	Flavonoids from <i>Passiflora</i> waste	N, I, F, C, E	<ul style="list-style-type: none"> <li>- Circular economy (BIOREFINERY) + GAC.</li> <li>- Energy consumption as Green Chemistry metric.</li> <li>- Renewable solvents (EtOH/water).</li> </ul>	[29]
Two-liquid-phase ultrasound-assisted and extraction with probe and two-liquid-phase dynamic maceration. UHPLC-MS, GC-MS	Bioactive metabolites in sugarcane solid by-products	N,C,E	<ul style="list-style-type: none"> <li>- Comparison of 9 extraction techniques.</li> <li>- Green metric calculation: Analytical-Eco Scale; the Analytical Greenness Calculator.</li> <li>- Simplicity, greener solvents.</li> <li>- Circular economy.</li> </ul>	[30]
SFE (CO <sub>2</sub> )	Carotenoids and neuroprotective compounds	N, F, E	<ul style="list-style-type: none"> <li>- Comparison with conventional extraction.</li> <li>- No cosolvent used.</li> <li>- Life cycle assessment for environmental performance.</li> </ul>	[31]
PLE + UHPLC-(QTOF)-MS/MS	Polyphenols (flavonoids, flavanols and proanthocyanidins)	G, I, C, E	<ul style="list-style-type: none"> <li>- Comparison with conventional extraction.</li> <li>- Circular economy (BIOREFINERY) + GAC.</li> <li>- Time saving.</li> </ul>	[33,34]

FTIR: Fourier-transform infrared spectroscopy; GC: gas chromatography; HAE: homogenizer-assisted, HPLC: high-performance liquid chromatography; MALDI: matrix-assisted laser desorption/ionization; MAE: microwave-assisted; MS: mass spectrometry; MS/MS: tandem mass spectrometry; PDA: photodiode array; PLE: Pressurized liquid extraction; Q: single quadrupole; SFE: supercritical fluids extraction; TGA: thermogravimetric analysis; TOF: time of flight; UAE: ultrasound-assisted; UHPLC: ultra-high performance liquid chromatography.

<sup>a</sup> See Figure 2 for further description.

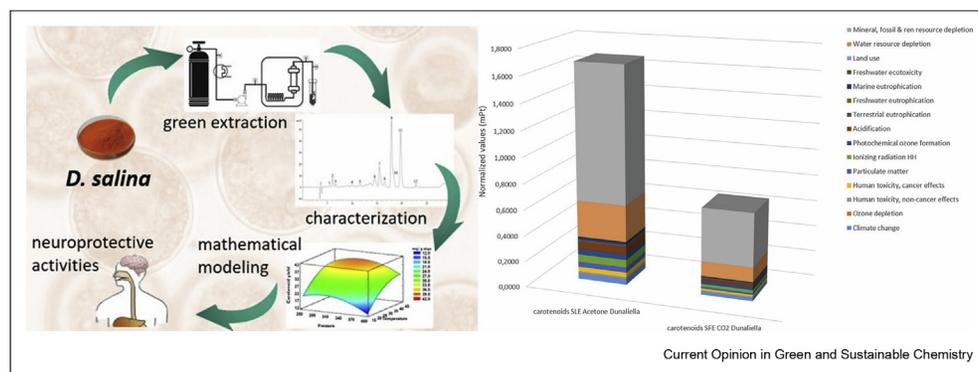
for sample spot capture on a paper microzone for the evaluation of wine samples [26]. A recent and updated example of this statement can be seen in the work developed by Espino *et al.* [27] integrating Natural Deep Eutectic Solvents (NADES) with the inexpensive analysis of paper zone microplates using a smartphone camera as detector and free open source software for data processing [28]. NADES can be defined as mixtures of natural compounds that are solid at room temperature separately but liquid when mixed; the use of these type of natural solvents contribute to SDGs 13, 14 and 15 related to Climate Action, Life Below Water and Life on Land respectively (see Figure 2). In this particular example, lactic acid and dextrose (5:1) were selected as extraction medium. The authors used the paper zone microplates to compare with a well-known spectrophotometric method for total phenolic compounds determination (Folin-Ciocalteu method) in terms of Green metrics based on penalty points. Results showed an important reduction of 22 times the penalty points of the proposed approach compared to the classical method. Benefits of the proposed approach deal with little or no waste generation, miniaturized method,

use of reagents obtained from renewable sources and replacement of toxic organic solvents, among others.

As the recovery of valuable compounds from underused biomasses and agricultural by-products, some examples have been selected not only for the interest of the application by itself, but also because they employed different tools for quantifying the eco-friendliness of the approach. This aspect is relevant when thinking about the scaling up of the processes in order to produce the desired fractions/metabolites or to set the basis for e.g., a biorefinery, aiming at biomass processing into value-added products (foods and ingredients, feed, materials, chemicals) and/or energy.

One of the key factors for a successful biorefinery is to start with a low-cost biomass or by-product, easily available, produced in important amounts and chemically characterized in order to obtain its full potential; and to develop sustainable processes with minimum environmental and economic costs (thus fulfilling the Green Chemistry Principles). These processes can be studied and optimized at analytical scale and scaled up

Figure 3



Scheme of the optimized green extraction platform for neuroprotective carotenoids' recovery from the edible microalga *D. salina*. Comparison of its environmental impacts with a classical extraction by means of Life Cycle Assessment (LCA). Reprinted from Bueno et al. [28,31] with permission of ACS.

later for producing the co-products. In this sense, Da Silva Francischini et al. [29] compared green extractions of bioactive compounds from passion fruit by-products considering their extraction yield, energy and solvent efficiencies as a method for green quantification. On the other hand, Assirati et al. [30] implemented a green and efficient experimental set up to extract and tentatively identify a wide range of metabolites (from highly polar sucrose to nonpolar wax ester C53 in a single extraction) from sugarcane solid by-products. Their final selection was based on two environmental performance tools, Eco Scale and Analytical Greenness Calculator.

The last example dealing with the recovery of bioactive compounds to develop new food products with potential neuroprotective activity was carried out in our research group [31]. In this work, we optimized the extraction of carotenoids with neuroprotective potential from edible microalga *Dunaliella salina* by means of supercritical fluids extraction (SFE) and compared with a classical method of extraction using acetone at room conditions. We also evaluated the environmental impact of both processes by using Life Cycle Assessment (LCA), probably the most complete approximation of environmental impacts quantification and the only standardized methodology (ISO14040 and ISO14044). Results showed that, despite acetone solid-liquid extraction (SLE) is a simpler method, SFE process ( $\text{CO}_2$  at 302 bar and  $45.0^\circ\text{C}$ ) produces only 39% of the impacts found for SLE in the recovery of neuroprotective compounds from microalga (Figure 3).

One of the most difficult challenges to reach in food bioactivity assessment is the understanding of the relationships between food, nutrition, and health. Foodomics is a discipline whose main goals are to improve

consumer well-being, knowledge, and confidence through the use of omics tools to investigate food safety, quality and the complex binomial food & health; many of the principles, applications and challenges of this discipline have been collected in a huge major reference work recently published [32]. Very recent applications carried out in our research group on Foodomics allowed the development of a complete strategy for i) green extraction of bioactive compounds from plants, food matrices and/or food by-products, ii) profiling and chemical characterization of bioactive metabolites, and iii) foodomics evaluation of their bioactivity. This strategy has successfully been applied recently to investigate the antiproliferative potential of *Passiflora mollissima* seeds against colon cancer cell lines [33,34]. The described platform can be very useful for the scientific development of new food products with health-promoting effects, also contributing to some of the SDGs via the development of Green Foodomics strategies [9]. In this sense, the basic concepts of Green Chemistry and GAC should be considered in order to improve the greenness of a process and/or the analytical methodologies (metabolomics, proteomics, etc.) involved in any foodomics study.

## Conclusions

In the present work, we have described the challenges Food Analysis is facing nowadays not only in terms of food safety, quality, and bioactivity assessment by itself but also in how implementation of Green Chemistry and GAC principles can contribute in achieving SDGs. For the first time, the relationship among them (Green Chemistry, GAC and SDGs principles) is proposed as a way of realizing how Green Food Analysis can contribute to sustainability. Although new approaches, ideas, and methodologies have been recently developed for Green

Food Analysis, as it has been exemplified in this work, more research is needed in order to produce a real change in our society. In this sense, we believe that a different way of thinking is needed to effectively contribute to sustainability while addressing increasing challenges related to greener food production. For instance, 1) the requirement of new methods giving the same importance to a) objective of the measurement (risk detection, biomarkers discovery, safety and quality control, etc.), b) method requirements in terms of sensitivity, figures of merit, etc., and c) greenness; 2) the development of methodologies with a wide applicability even in low-income countries (cheaper devices, affordable technologies); 3) the promotion of methods able to fulfill the GAC principles; 4) the support and encouragement from the authorities of these type of new developments. In this era towards SDGs by 2030, there is still a long way to go and we, as food analytical scientists, have a great responsibility and enormous opportunities for making this goal possible.

### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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