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Evaluating the whiteness of spectroscopy-based non-destructive analytical methods – Application to food analytical control

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ABSTRACT

Recent advancements in analytical chemistry in the food quality field have emphasized ecofriendly analytical techniques eschewing chemicals and solvents. Various methodologies exist for assessing the sustainability of analytical methods, however none has provided guidance for appraising non-destructive methods, especially pre-development. Among these, the RGB approach stands out, evaluating method colour via three main criteria: analytical performance, environmental impact, and practical efficiency. This framework offers a comprehensive evaluation, aiming for a "white" colour denoting excellence across all three categories.

This article introduces an adapted RGB method for *ex-ante* evaluation of new non-destructive analytical methods pre-development. It outlines key steps for evaluating method "whiteness". As a guiding example, the approach was applied to three analytical methods focussed on quality and authenticity control of edible vegetable oils utilizing solvent-free spectroscopic techniques. Results underscored a priori feasibility assessment value, aligning evaluative objectives with intended method goals.

1. Introduction

Ensuring food quality and safety is crucial along the entire food chain: from raw materials through all production stages to the final product reaching consumers. Food fraud is a scourge as old as food production itself. And just as food technology is advancing by leaps and bounds, the ways of committing food fraud are becoming increasingly sophisticated. The most common acts of food fraud encompass counterfeiting, mislabelling, misrepresentation, dilution, unauthorized enhancement, or adulteration; this information can be expanded by referring to literature, as the recent review by Bannor et al. [1]. However, the analytical methods used to ensure proper food quality control and authentication are not keeping pace with this growth. Instrumental techniques such as liquid or gas chromatography coupled to mass spectrometry are nowadays commonly used for these types of analysis. Those analytical techniques undoubtedly provide accurate results. Nevertheless, there are some disadvantages associated with these techniques. These include time-consuming analysis, several sample preparation steps (separation and/or dissolution processes), allowing off-line analysis only (some instances also on-line analysis), the need to use chemical solvents, which can be environmentally hazardous and pose risks to analysts, and the requirement for expertise due to their complexity [2].

Against this background, there is undoubtedly an urgent demand for analytical methods involving the use of alternative techniques to the widely employed ones mentioned above. The most important requirement is to enable rapid, non-destructive analysis and *in-situ* if possible. In such a way that it should be non-destructive, including the total or partial absence of chemical solvents and minimising waste as much as possible, thus fostering a more sustainable analytical chemistry, also known as green chemistry. Current research in the field of food analysis does follow this trend from several years ago [3]. Many studies can be found in the scientific literature exploring the potential of different alternatives to conventional analytical techniques, providing the possibility of rapid and non-destructive analysis [4]. Moreover, some advanced techniques even enable non-invasive analysis [5]. The difference between a non-destructive technique and a non-invasive one is worth noting. In the former, the sample remains in the same physical and chemical state after measurement. It requires only a minimal amount of sample, resulting in hardly any wasted product and allowing for potential future re-measurement. Whereas with a non-invasive technique, the measurement is performed directly on the food

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product, i.e., no sampling is necessary. The tested foodstuff remains unaltered, as the non-destructive, but also remains fully intact, e.g., the packaging is not opened to measure the food in the case of final product analysis, and it could even be consumed. So, any non-invasive technique is in turn a non-destructive technique, but not vice versa. A general example of what a destructive (conventional), non-destructive and non-invasive analytical technique would consist of is illustrated in Fig. 1, taking as an example the analytical measurement of a vegetable oil at the final stage of production, i.e., already packaged.

Generally, the most commonly used techniques that meet the aforementioned requirements include spectroscopic techniques, sensing techniques (such as e-nose or e-tongue) and techniques based on image analysis (e.g., computer vision, multi- or hyper-spectral imaging) or nanotechnology [2,6]. Among them, the spectroscopic techniques such as infrared [7], Raman [8,9] or nuclear magnetic resonance (NMR) [10,11] spectroscopies are the most investigated. All these techniques yield substantial chemical information by generating corresponding spectra, enabling rapid acquisition of results. The utilization of solvents is dispensable, except in the case of NMR, although low-field benchtop equipment is now accessible to facilitate solvent-free measurements [12].

In this regard, these analytical techniques would adhere to the principles of sustainability and green chemistry mentioned earlier. However, guaranteeing this alignment requires the availability of appropriate tools for their assessment. For this purpose, some developed indexes can be found in scientific literature. These include the Life Cycle Assessment (LCA) or the National Environmental Methods Index (NEMI), both have been applied to assess analytical chemistry methods, even though they are not exclusive to the field [13,14]. Other tools have been developed specifically for analytical chemistry, such as the analytical Eco-scale, which is intended to rank any analytical procedure as: excellent, acceptable, or inadequate from the green analysis standpoint [15]. Also, the Green Analytical Procedure Index (GAPI) and the ComplexGAPI evaluate the green profile of an analytical method based on several criteria, involving the sample preparation and analysis procedures [16]. Another recent index is the Analytical GREEnness Metric Approach (AGREE), which responds to the 12 principles of the Green Analytical Chemistry (GAC) [17,18]. Nevertheless, all the mentioned metrics only assess the ecofriendly aspect of the methods, based on the 12 GAC principles, overlooking other important aspects such as cost, time, or analytical performance.

Consequently, new methodologies for the comprehensive assessment of analytical methods have recently been proposed. For instance, HEXAGON algorithm, an extension of the Eco-scale which not only assess the green profile, but also the characteristics of the analytical method such as the technical reliability, and the economic cost [19]. Despite, some limitations are presented such as not considering key sampling aspects, thus it has not been widely employed by the scientific community [16]. A group of algorithms named Multi-Criteria Decision Analysis (MCDA) [20] has also been applied for this purpose [21], although it primarily emphasizes decision-making rather than the evaluation of the analytical method itself. Lastly, Nowak et al. [22] developed the novel RGB algorithm based on the three primary colours, each embodying a set of criteria to be evaluated: analytical performance, safety and environmental friendliness, and practical efficiency and productivity. This methodology provides the capacity to assess an analytical method both qualitatively and quantitatively. The authors subsequently re-versioned this algorithm to the new RGB 12, including the 12 GAC principles by grouping them into 4, alongside other aspects, leading to the 12 principles of White Analytical Chemistry (WAC) [23].

Within this framework and to the best of our knowledge, RGB algorithm has not been applied to assess an analytical method based on a non-destructive technique for food quality control purposes. Besides, all the above-mentioned approaches have been founded on an *ex-post* evaluation, i.e., assessment conducted after the method development. However, it would be advantageous to have the possibility to perform an *ex-ante* evaluation of the method, enabling the decision-making process regarding its development before initiation. Therefore, the aim of this paper is to establish the key points on which to base the *ex-ante* evaluation of a new analytical method based on non-destructive/non-invasive techniques for food control, although could also be useful for non-food analytical chemistry fields. For this purpose, a proposal based on the RGB methodology is presented together with a practical example, as it was considered the most suitable of the indexes listed above for evaluating this type of analytical method, due to its flexibility and the ability to evaluate not only the ecology of the method, but also other critical and important points.

2. Analytical method whiteness

The RGB algorithm is based on the three primary colours: red, green, and blue. Each of one represents a set of evaluable items categorised into

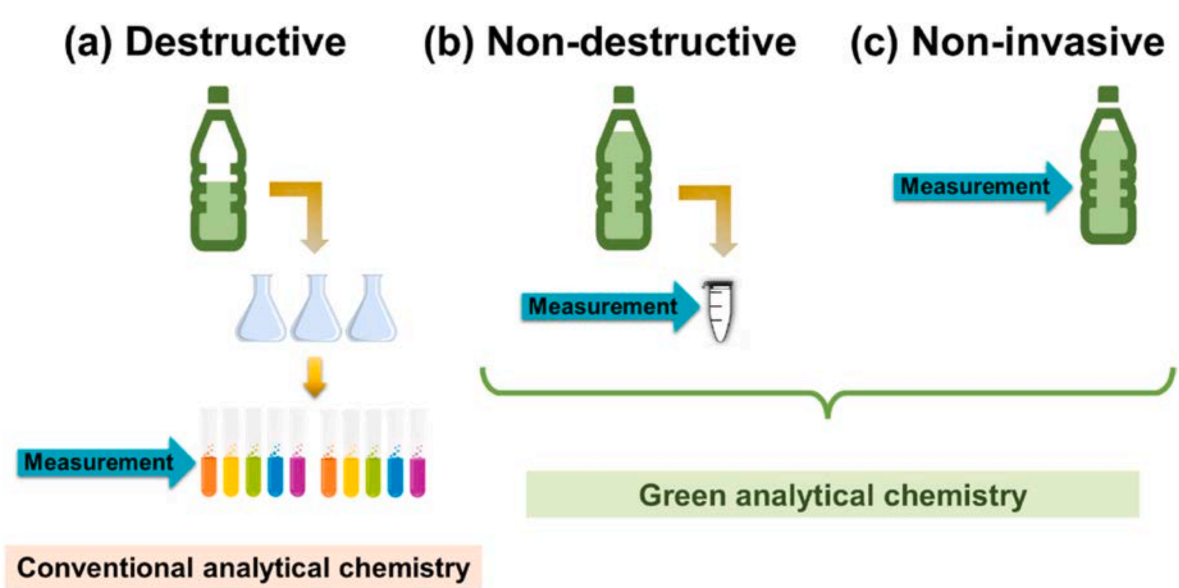

Fig. 1. Illustrative example of an analytical measurement of a packaged vegetable oil by using (a) destructive, (b) non-destructive and (c) non-invasive analytical technique.

three groups: RED to assess the analytical performance; GREEN to evaluate the sustainability (greenness) of the method; and BLUE for the productivity and practical efficiency assessment. The mixture of these three primary colours at 100 % scoring results in the colour WHITE. This is where the concept of the "white analytical method" arises, representing the optimal solution. Consequently, the RGB algorithm appraises the method whiteness, a concept initially introduced by the authors responsible for devising the RGB 12 algorithm [23].

Note that the assessment of the analytical method may result in different colours depending on the scores obtained in each of the three RGB colour parameters, spanning from black (0 % scoring) to white (100 % scoring). To quantitatively assess the colour score, the authors devised an index termed Method Brilliance (MB) in the RGB algorithm and whiteness in the RGB 12 algorithm, both of which are estimated differently. More details about RGB and RGB 12 algorithms can be found in the source proposal, in Refs. [22,23] respectively.

Given the aforementioned considerations, the RGB algorithm was deemed the most appropriate methodology for assessing new analytical method based on non-destructive/non-invasive analytical techniques for food analysis. On one hand, this methodology offers the advantage of assessing not only the method greenness but also encompasses other crucial issues, including its practicality concerning time, cost, and performance, as well as result reliability. On the other hand, it provides flexibility in assigning weights to each evaluable item according to the pursued objective, in contrast to the rigidity of the RGB 12 algorithm.

In this context, it is crucial to emphasize a significant aspect: thus far, the RGB algorithm has been employed *ex-post*, meaning it has been applied only after the analytical method development. However, a more reasonable approach would involve assessing the method prior its development. In other words, defining acceptable and satisfactory limits for each evaluable item, and assigning the expected scores based on the intended procedure. Once the outcome is determined, the analyst should decide whether the candidate analytical method is valid to achieve the proposed goal and develop it or whether it is preferable to seek a better alternative.

Considering this matter, this paper proposes to use the RGB algorithm in a novel way, aimed at defining the minimum whiteness scoring that the candidate analytical method should have before developing it. In addition, intermediate values for acceptable and satisfactory results of the main items evaluated for each colour have been set at 50 % and 80 % respectively, instead of the 33.3 % and 66.6 % used so far. The proposal is also based on establishing several secondary items (or sub-items) within main item comprising each of the three colour parameters. It should be borne in mind that *ex-ante* evaluation of a non-destructive/non-invasive analytical method requires careful selection of the evaluable items. In the following section the main evaluable items and sub-items proposed here will be presented and discussed.

3. Practical applications

As a practical instance, three analytical methods based on non-destructive/non-invasive techniques for analysing food quality and authenticity have been selected for *ex-ante* evaluation using a proposed RGB-modified algorithm. The main aim of these methods is to serve as a screening method based on a multivariate classification for identification purposes. The difference among the three lay in the analytical technique involved on each method: near infrared spectroscopy (NIR), spatially offset Raman spectroscopy (SORS) and low-field nuclear magnetic resonance (LF-NMR). NIR was selected for its widespread use and versatility in the field of food analysis [24]. SORS is an advanced mode of conventional Raman spectroscopy that allows through-container measurements, making it a non-invasive technique [25]. And LF-NMR was selected for its increasing interest in recent times, which in the low frequency field mode allows for non-destructive solvent-free measurements [26].

All three analytical methods pursued the same aim: the quality and/or authentication control of virgin olive oils. Therefore, the target material to be analysed was vegetable oils at the final stage of the production process, i.e., already marketed. The reader should take this as a practical example of how the algorithm should be applied using the approach described here, to serve as an implementation guideline but it could be applied to any other foodstuff. Moreover, it should be emphasized that the three spectroscopic techniques provide a large amount of chemical information, especially in food products which are chemically very complex materials. Thus, there was no doubt that data treatment should be addressed from a non-targeted approach by using data mining chemometric tools [27–29], also in line with green chemistry [30].

In order to perform an *ex-ante* comprehensive evaluation of an analytical method being developed, an estimate of the scores for each of the three colour parameters, ranging from 0 to 100, is estimated. However, redness cannot be properly assessed, as depends on the final results. To overcome this drawback, two alternatives can be considered. The first, and easier to apply, considers the value of 80 % as the starting point for all evaluable sub-items. Moreover, according to the published scientific literature, the three spectroscopic techniques coupled with chemometrics obtain high performance metrics in the analysis of vegetable oils [31–33]. On the other hand, from a more analytical standpoint, the critical values of the performance metrics defining the fitness for purpose of the analytical method under study, which had to be previously established in order to be applied for validation, could now be considered.

Considering a method applying machine learning/chemometrics can be oriented toward developing either a classification or quantitation model, each evaluated by different analytical metrics, two options are proposed to evaluate the redness, shown in Fig. 2. Option one is designed for classification/discrimination models and four main evaluable items are proposed, where each score represents the 0–1 scaled metric value expressed as a percentage. The metrics are sensitivity, specificity, precision (positive predictive value) and accuracy or efficiency, although more metrics could be added [34]. While option two intends to evaluate quantitation models, by using four alternative metrics as main evaluable items: determination coefficient of the model (R^2), standard error validation (SEV), standard deviation of validation residuals (SDV) and relative bias. These quantitation metrics agree with the recommendations outlined in the ASTM Standard Practice [35].

Depending on the scenario, the critical values of the performance metrics to be considered may be different. For instance, in a screening method based on a multivariate classification regarding an official conformity evaluation scenario, values of 0.95, 0.50, 0.95 and 0.90 could be set for sensitivity, specificity, precision and accuracy, respectively [36]. Likewise, regarding a method of quantifying an adulterant (e.g., a cheaper vegetable oil) in extra virgin olive oil, values of 0.95, 0.90, 0.90 and 0.95 could be set for R^2, SEV, SDV and bias, respectively [37,38]. Practitioners are encouraged to review recent literature to ascertain the performance of the candidate analytical technique on the particular sample being analysed in order to define consistent critical values for *ex-ante* evaluation.

Further on, specific evaluable items for assessing greenness and blueness are proposed. Within each of them, several sub-items that should be considered have been included. Upon meeting these sub-items, a score up to 100 is assigned for each item, contributing to the overall evaluation of each colour parameter. Note that the proposal is based on a simple “yes” or “no” (Y/N column) response for each evaluable sub-item, as shown in Fig. 3, thus rendering the tool user-friendly. The template for colour evaluation to be filled in, along with brief instructions can be found in the supplementary material (note that the sub-items of cost-effectiveness and sample destruction are adapted to the objective stated here, and may be modified at the analyst’s request).

The selected evaluable items for greenness do not differ widely from their predecessor RGB methods [22,23], while the considered sub-items

EX-ANTE EVALUATION

OPTION 1*	Sensitivity	Specificity	Precision	Accuracy
OPTION 2*	R^2 (fitting)	SEV	SDV	Bias
value (%)				
	w=3	w=3	w=2	w=2

Abbreviations:
SEV: *Standard Error of Validation (also known as Standard Error or Prediction, SEP)*
SDV: *Standard Deviation of Validation residuals*

EX-POST EVALUATION

OPTION 1*	Sensitivity	Specificity	Precision	Accuracy
OPTION 2*	R^2 (fitting)	SEV	SDV	Bias
value (%)				
	w=3	w=3	w=2	w=2

Fig. 2. Proposed items for redness rating of an analytical method according to its main purpose: classification or quantitation.
**Note that OPTION 1 addresses the metrics to be considered in classification/discrimination methods for identification or detection purposes and OPTION 2 in quantitation methods for prediction purposes.*

(A)

Use of chemicals			Use of resources			Safety of operator			Analytical waste		
Sub-items	Y/N	Max score	Sub-items	Y/N	Max score	Sub-items	Y/N	Max score	Sub-items	Y/N	Max score
No sample clean-up needed		50	Not require electricity when not in use		50	No biologic hazards		50	No hazardous waste		50
No chemical reactions caused		30	Not require electricity when performing		30	No chemical hazards		30	No sample waste		20
No sample dilution needed		20	No water consumption while applying		20	No physical hazards		20	Reusable consumables		30
Final score per sub-item		0			0			0			0

(B)

Sample throughput & time of analysis			Cost effectiveness *			Sample destruction			Easy operation			Specialized staff requirements		
Sub-items	Y/N	Max score	Sub-items	Y/N	Max score	Sub-items	Y/N	Max score	Sub-items	Y/N	Max score	Sub-items	Y/N	Max score
< 1 h/sample		40	< $200 / sample		50	Non destructive technique		40	Allow *in situ* measure [benchtop]		30	No high level		50
< 30 min/sample		30	< $100 / sample		30	Non invasive technique		30	Allow on line measure [portable]		30	No medium level		30
< 10 min/sample		20	< $20 / sample		20	< 10 ml used		10	Multiparameter		40	No required (basic)		20
< 1 min/sample		10				< 1 ml used		20						
Final score per sub-item		0			0			0			0			0

** Excluding depreciation expenses*

Fig. 3. Proposed items and sub-items for the greenness and blueness rating of a non-destructive/non-invasive analytical method.

have been carefully chosen according to what the authors find most critical in requiring an analytical method to achieve 100 % greenness scoring. As for blueness, it was deemed appropriate to include a main item considering the analyst's specialization requirements. Besides, it is worth noting that the sub-items within the cost-effectiveness shown in Fig. 3B have been adapted to the specific case of the full analysis of a virgin olive oil. It is understood that a method pursuing this goal will be cost-effective when is at least cheaper than the total cost ($200/sample). Observe that, this information was provided from an official laboratory dedicated to the analysis of olive oil. Our recommendation to the reader is either seek a reliable source knowing this information (cost of the official or recognized method/s normally used for the food or sample under study) or estimate the cost as close to reality as possible. The datum will be well-known in the case of an industry aiming to evaluate a new method to perform an analysis already carried out by another conventional analytical method that is destined to be substituted.

The following sections provide a breakdown of the scores obtained for each of the three methods selected to evaluate their whiteness with our proposal as a practical example. Some aspects to be considered for the application of this proposal are discussed. In accordance with the pursued aim of the three proposed methods under consideration (screening method), the aforementioned critical values for multivariate classification metrics have been established in the redness assessment [36]. Note that, based on the objective of the analytical methods evaluated, the authors have established a minimum whiteness requirement of 80 % scoring. If this criterion is met, i.e., the whiteness result exceeds 80 % once completing the *ex-ante* evaluation, the next step is to proceed with the method's development in order to conduct a comprehensive *ex-post* evaluation, and compare the results with the *ex-ante* evaluation.

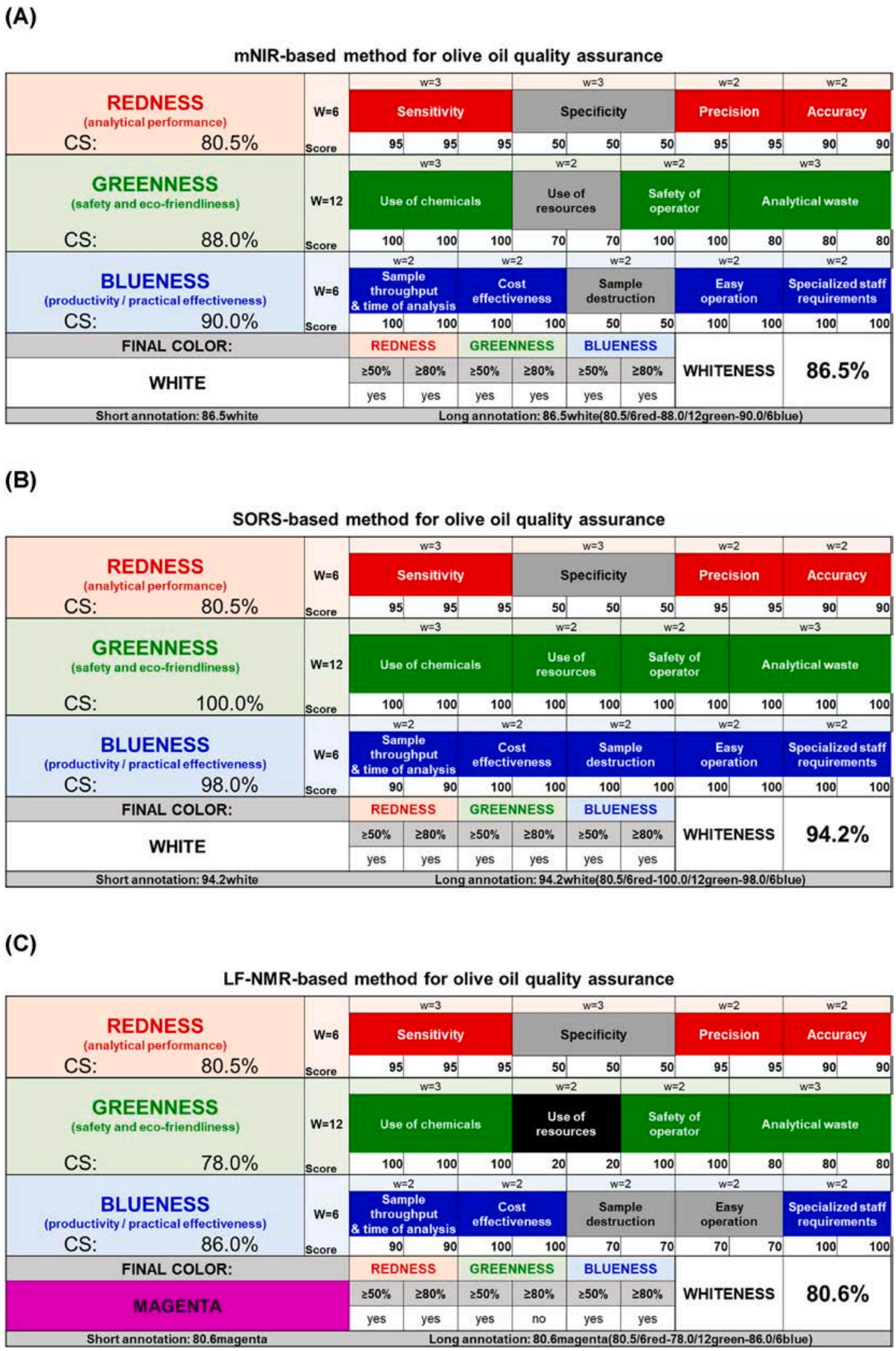

Fig. 4. Overall whiteness scoring obtained by *ex-ante* evaluation of a: (**A**) mNIR-based method, (**B**) SORS-based method, and (**C**) LF-NMR-based method for virgin olive oils quality and/or authenticity analytical assessment.

3.1. The colour of a mNIR-based method

NIR spectroscopy instruments have come a long way in recent years, to the point where miniaturised, portable, cost-effective instruments are now available that can be used to measure anywhere, including in-line production analysis [39,40]. In this method, a miniaturised portable NIR equipment (mNIR) is used to measure vegetable oil samples placed in glass vials. The samples are measured directly and at room temperature, so there is no sample treatment, and they remain unaffected after measure, in a non-destructive way. Following these premises, the template developed to establish the greenness and blueness of this method has been filled in, and some details are given below.

Regarding the greenness scoring of this method, 100 % was not achieved. The items not scoring full goals were the use of resources and analytical waste. The 70 % scoring on the first item was related to the need to be plugged into the electricity supply to be able to measure, even though it is a portable device. Besides, it is a non-destructive technique, but invasive since the vegetable oil bottle must be opened to collect a small sample. Consequently, it lacks 100 % blueness and is not compliant with the "no sample waste" sub-item (see Fig. 3A). Nevertheless, considering all the evaluable items as a whole by calculating the weighted average, white was the colour achieved (see Fig. 4A), and the whiteness scoring of this method would be at least 86.5 %, assuming that the established critical values will be satisfied or exceeded after developing the method in the *ex-post* evaluation of the redness.

3.2. The colour of a SORS-based method

The emergence of portable and handheld Raman measurement equipment has opened up the possibility of using this technique for at-line production control and exploring its potential in food analysis [41]. In addition, portable equipment based on the non-invasive SORS technique is already commercially available and currently used for the control of raw materials in the pharmaceutical industry [42], so its use in the food industry is becoming more real and nearer [25]. Following the same methodology, an *ex-ante* evaluation was performed on this method, achieving the 100 % greenness scoring. This is coherent given that SORS allows to measure through the original container, therefore the sample is not altered in any way as long as the inside food product is insensitive to laser irradiation. The only evaluable item not reaching full scoring was the analysis time (blueness group) as it requires around 2 min for spectrum acquisition, although it is still a fast technique compared to conventional ones and is reflected with almost 100 % blueness scoring. As outcome, the SORS-based analytical method resulted in a 94.2 % whiteness scoring. The overall result can be seen in Fig. 4B.

3.3. The colour of an LF-NMR-based method

The advent of current LF-NMR equipment opens up the possibility of NMR implementation in control laboratories for non-destructive, fast, and much more affordable measurements than conventional high-field NMR, which also requires higher maintenance costs and takes up more space than benchtop LF-NMR equipment [43]. Consequently, the *ex-ante* evaluation of the method based on LF-NMR yielded an 80.6 % whiteness scoring (see Fig. 4C). Even so, on this occasion the resulting colour was not white, and this is due to the requirement of these devices to be connected to electricity continuously, even if not measuring. Thus, the method scored low on one of the greenness evaluable items, however it should be noted that weight assigned to greenness was higher than for blueness and redness, which may explain the non-white final colour of this proposed method. Nevertheless, it is always possible to modify this based on the user's aim. Given that the NMR specifications yield good performance, it is likely that better analytical performance metrics will be obtained and therefore redness scoring would be larger than with other analytical techniques. If this is the goal of the method, it is recommended to increase the redness weighting.

4. Final remarks

An *ex-ante* evaluation of a new method should be mandatory before addressing an analytical method development and implementation milestone. On the one hand it allows to identify risks, and on the other hand it helps to improve efficiency especially in the use of resources, since if the method fails to give the expected results after development, a loss of time and certainly economic loss may have been avoided by performing the *ex-ante* evaluation and making decisions according to what has been achieved. It is crucial not to be swayed by the analyst preferences, and to be as objective as possible. The authors consider that by following this simple evaluation method, in which a yes or no answer is easily given, it is possible to evaluate the whiteness of a new non-destructive method.

Through practical application to three analytical methods pursuing the same aim, it has been demonstrated that this approach is sufficiently objective, and amply flexible to be applied in *ex-ante* evaluation under specific user requirements. The proposal described in this paper represents a step forward, applicable in any field of analytical chemistry as it does not only consider GAC principles, but goes beyond them.

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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.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.trac.2023.117463.

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