Sustainable Chemistry and Pharmacy 45 (2025) 102031

Contents lists available at ScienceDirect

Sustainable Chemistry and Pharmacy

journal homepage: www.elsevier.com/locate/scp

Ten principles for developing and implementing tools in the context of white analytical chemistry

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ARTICLE INFO

Keywords:
Tools
Metrics
White analytical chemistry
Green analytical chemistry
Analytical methods
Principles
PRISM

ABSTRACT

This work presents a structured framework of ten principles designed to guide the development and implementation of analytical tools within the context of white analytical chemistry. Despite the growing availability of various metric tools such as AGREE, AGREEprep, GAPI, ComplexGAPI, MoGAPI, and BAGI, the absence of standardized guidelines for their development has resulted in inconsistencies in applicability and effectiveness. The ten principles proposed in this study, framed within the PRISM approach—Practical, Reproducible, Inclusive, Sustainable, & Manageable—aim to bridge this gap by promoting standardization, usability, and sustainability in the design of analytical tools. Each principle is explored emphasizing the importance of simplicity, clear guidance, visual clarity, comparability, dual quantitative and qualitative evaluation, open accessibility, and adaptability. Additionally, an evaluation of recently developed tools using the PRISM framework, identifying their strengths, limitations, and areas for improvement is included. This assessment highlights the necessity for tools that are dynamic and capable of integrating emerging methodologies. By establishing these principles, it is expected to contribute to advancing a more standardized and sustainable future for analytical chemistry, ensuring that tools effectively support the field's progress while adhering to white analytical chemistry's holistic goals.

1. Introduction

Analytical tools designed for green chemistry have become indispensable tools in evaluating the environmental footprint of analytical methods across industrial and academic settings (Locatelli et al., 2023; Tobiszewski, 2016). Over time, specialized metrics for green analytical chemistry (GAC) have emerged, such as analytical method volume intensity (AMVI) (Hartman et al., 2011), high performance liquid chromatography-environmental assessment tools (HPLC-EAT) (Gaber et al., 2011), national environmental methods index (NEMI) (Tobiszewski et al., 2015) or analytical eco-scale (Gałuszka et al., 2012). Some of these metrics are tailored for specific types of analytical procedures, while others are more general and applicable to a wide range of methods (Sajid and Płotka-Wasylka, 2022). Among these, a few have gained significant popularity with the most notable being analytical greenness calculator metric (AGREE) (Pena-Pereira et al., 2020), analytical greenness metric for sample preparation (AGREEprep) (Wojnowski et al., 2022), green analytical procedure index (GAPI) (Płotka-Wasylka, 2018), and its derivatives complementary GAPI (ComplexGAPI) (Płotka-Wasylka and Wojnowski, 2021), and modified GAPI (MoGAPI) (Mansour et al., 2024a, 2024b). These GAC metrics provide

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https://doi.org/10.1016/j.scp.2025.102031
Received 7 January 2025; Received in revised form 3 April 2025; Accepted 18 April 2025
Available online 25 April 2025
2352-5541/

visual assessments, often through intuitive pictograms, to determine how environmentally friendly a given analytical method is (Silva et al., 2023). They evaluate key aspects such as the amount and toxicity of reagents, waste generation, energy consumption, procedural complexity, as well as the degree of miniaturization and automation (Locatelli et al., 2024). By applying these metrics, analysts can identify environmental weaknesses in their processes and implement strategies to mitigate negative impacts, ultimately fostering sustainable practices and environmental conservation. A variety of GAC tools are now available, each adapted to specific analytical objectives or laboratory requirements (Imam and Abdelrahman, 2023; Shi et al., 2023). Many of these tools use straightforward visual representations, often employing color gradients to communicate environmental performance at a glance. However, the most commonly used green metrics often fail to address other critical dimensions of analytical methods, such as practicality and analytical performance (Manousi et al., 2023). In this regard, the concept of white analytical chemistry (WAC) offers a holistic framework that integrates analytical (red), ecological (green), and practical (blue) attributes into a unified Red-Green-Blue (RGB) model (see Fig. 1; Nowak et al., 2021). According to that, 12 WAC principles were proposed condensing the existing GAC principles into four broad and mutually independent "green" guidelines (G1–G4), each addressing a key aspect of sustainability in analytical methods. These are complemented by four "red" principles (R1–R4), which focus on analytical efficiency, and four "blue" principles (B1–B4), which address practical and economic aspects (see Table 1).

WAC emphasizes balance and synergy, ensuring that environmental sustainability is not pursued at the expense of functionality, reliability, or quality. The holistic nature of WAC aligns closely with the principles of sustainable development, aiming to harmonize ecological objectives with the practical and analytical demands of modern methods (Jain et al., 2024). As the analytical chemistry community increasingly recognizes the importance of sustainability, the WAC paradigm provides a forward-thinking solution. It facilitates a nuanced understanding of what constitutes a "white" method—one that balances analytical, ecological, and practical considerations (Hussain et al., 2023). The incorporation of blue and red aspects within WAC has led to the development and application of tools like the blue applicability grade index (BAGI) (Manousi et al., 2023) and the red analytical performance index (RAPI) (Płotka-Wasylka, 2024), which specifically assess the practicality and analytical performance of the methods (Kalogiouri et al., 2024; Kubica et al., 2025; Manousi et al., 2024; Samanidou, 2024). Moreover, the violet innovation grade index (VIGI) (Fuente-Ballesteros et al., 2025b) and GLANCE (Fuente-Ballesteros et al., 2025a), a novel graphical tool of analytical chemistry evaluation, have been recently introduced. This growing interest in metrics has led several researchers to incorporate a WAC perspective into their work (Prajapati et al., 2024a, 2024b).

Multiple metrics have been developed to evaluate various facets of analytical methods over the past few years, with the trend expected to grow (Martínez et al., 2022). However, no standardized guidelines, norms, or principles have yet been implemented to govern the comprehensive development of these tools—be they metrics, indices, or other complementary resources. This lack of universal frameworks represents a significant gap, as these tools, despite their growing popularity and utility, lack the consistency, quality, and applicability ensured by standardization. The novelty of this work lies in its proposal to address this need by presenting a structured set of ten principles to guide the design, development, and implementation of new tools. These principles were inspired by and built upon the ones established in earlier studies (Gałuszka et al., 2013; López-Lorente et al., 2022; Prajapati et al., 2023). This approach not only promotes standardization, but also fosters the adoption of more sustainable, efficient, and holistic practices, addressing the pressing challenges of modern analytical chemistry. The need for standardization has been previously highlighted by other authors as a critical step towards ensuring consistency and reliability in the development of analytical tools (Gamal et al., 2021; Locatelli et al., 2024; Sajid and Płotka-Wasylka, 2022). By filling this critical gap in the literature, this work establishes a foundation for a new direction in the development of analytical tools, contributing to a more standardized and sustainable future for the field.

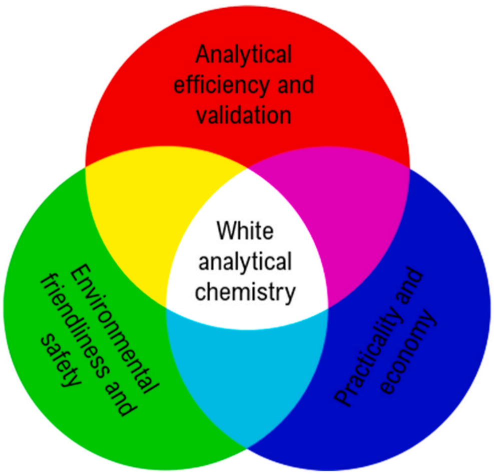

Fig. 1. The three components of white analytical chemistry.

Table 1
Description of the 12 principles of white analytical chemistry (Nowak et al., 2021).

Red		
R1	Scope of application	- Analytical methods should have the widest possible range of applicability expressed in the number of simultaneously determined analytes, range of linearity of the determinations, compatibility with various types of samples and resistance to the presence of potential interferences
R2	LOD and LOQ	- Analytical methods should have the lowest possible limits of detection and quantification
R3	Precision	- Analytical methods should be characterized by the best possible precision expressed in repeatability and reproducibility of the results
R4	Accuracy	- Analytical methods should be as accurate as possible
Green		
G1	Toxicity of reagents	- Analytical methods should be characterized by the lowest possible toxicity of reagents used and the maximum share of biodegradable/renewable reagents and materials
G2	Number and amount of reagents and waste	- Analytical methods should be characterized by the lowest possible consumption of reagents and production of waste
G3	Energy and other media	- Analytical methods should be characterized by the lowest possible consumption of electricity and other utilities. On-site, automated and high-throughput methods are preferred for saving energy
G4	Direct impacts	- The use of analytical methods should not directly affect humans, animals, and genetic naturalness. Exposure of humans to harmful factors and the use of animals and/or genetic modifications should be avoided
Blue		
B1	Cost-efficiency	- Analytical methods should be as cost-efficient as possible
B2	Time-efficiency	- Analytical methods should be characterized by the highest possible time-efficiency
B3	Requirements	- Analytical methods should be characterized by the minimal practical requirements including the amount of sample used, access to advanced equipment, personnel qualifications, and laboratory infrastructure
B4	Operational simplicity	- Analytical methods should be characterized by the highest possible level of miniaturization, integration, automation, and portability

2. Ten principles for developing and implementing tools in the context of white analytical chemistry

Every analytical procedure, method, and instrumentation may encounter challenges in fully adhering to the principles of GAC. To address these issues, numerous tools have been developed to evaluate a plethora of parameters in analytical chemistry field. Assessing the "redness", "greenness", or "blueness" of an analytical procedure enables comparisons between different methods, helping to identify the most suitable option for specific applications (Locatelli et al., 2024; Zughaibi, 2024). For a tool to be effective and widely adopted, it should meet certain principles and considerations following the PRISM (**P**ractical, **R**eproducible, **I**nclusive, **S**ustainable, & **M**anageable) framework (see Table 2). The selection of these principles was based on two criteria: (1) information gathered from the various metrics published and reviewed in the literature, and (2) the authors' experience in the use and application of different metrics within this field.

2.1. Principle 1: simplicity

The first principle underscores the critical importance of simplicity and usability in the design and implementation of analytical tools in WAC. Tools must be easy to understand, apply, and execute, enabling their seamless integration into the workflows of the scientific community. A user-friendly and intuitive design minimizes the time required for training and reduces the cognitive load on users, allowing them to focus on the analytical process rather than the complexities of the tool itself. This simplicity is especially important given the diverse expertise levels of potential users, from seasoned researchers to students and industry professionals. Tools that are quick to implement and operate not only enhance efficiency, but also ensure their accessibility to laboratories with varying levels of resources and expertise. An intuitive design fosters broader adoption and minimizes the risk of errors or misinterpretation, which can compromise the reliability of results. By facilitating straightforward adoption, such tools can bridge the gap between advanced theoretical principles and practical applications, aligning with WAC's goal of promoting sustainable, efficient, and inclusive practices. Ultimately, this principle ensures that analytical tools become valuable assets in advancing the field, promoting their widespread use and contributing to a culture of innovation and sustainability.

2.2. Principle 2: guidance

A detailed guide explaining the use and scope of an analytical tool is fundamental to ensure its proper implementation and maximize its impact. Such a guide provides users with clear instructions on how to operate the tool, interpret its outputs, and apply its insights effectively, thereby reducing the potential for errors and inconsistencies. Additionally, a well-structured guide clarifies the specific scenarios, methodologies, and analytical contexts for which the tool is best suited, helping users determine its applicability to their needs. This is particularly important given the diversity of analytical methods and laboratory setups across the scientific community. Moreover, the inclusion of practical examples, case studies, or tutorials in the guide can further enhance user comprehension and confidence in the tool's capabilities. Defining the tool's limitations and boundaries within the guide is equally critical, as it helps users understand what the tool cannot achieve and prevents its misuse in inappropriate contexts.

Table 2
Core principles of PRISM for analytical chemistry tool design.

Acronym	Principle No.	Description
P (Practical)	1	-Be easy to understand, apply, and execute quickly and intuitively, facilitating its adoption by the scientific community
	2	-Include a detailed guide explaining its use and scope
	3	-Offer a clear and visually appealing design to facilitate interpretation
R (Reproducible)	4	-Deliver results that are easily comparable across different methods, enabling standardized and reproducible evaluations
	5	-Provide a quantitative and/or qualitative measure to comprehensively assess the method's suitability and potential
I (Inclusive)	6	-Be accessible through open platforms or user-friendly software, ensuring availability to a broad audience
S (Sustainable)	7	-Incorporate attributes that account for not only environmental sustainability but also economic and social aspects, providing a holistic view of the evaluated method
M (Manageable)	8	-Evaluate and consider the key elements of an analytical method
	9	-Be flexible and adaptable to different instrumental configurations and specific needs
	10	-Allow for updates and expansions as the field evolves

2.3. Principle 3: clarity

A clear and visually appealing design is crucial for analytical tools, as it significantly enhances their usability and impact. Tools that incorporate intuitive visual elements, such as charts, graphs, or pictograms, help users quickly grasp complex data and concepts without requiring extensive explanation. A well-thought-out visual design can bridge the gap between technical information and practical understanding, making the tool accessible to a broader range of users with varying expertise levels. Furthermore, effective visuals reduce the likelihood of misinterpretation by presenting results in a structured and logical format, allowing users to focus on decision-making rather than deciphering data. The aesthetic aspect of the design is also key to capturing and maintaining user engagement; tools that are visually appealing are more likely to attract attention, encourage consistent use, and foster positive perceptions within the scientific community. Simplicity in visuals does not mean sacrificing detail, but rather ensuring that key information is highlighted in a way that is both functional and elegant. A visually coherent tool aligns with the principles of standardization and reproducibility, as it facilitates consistent interpretation across different users and contexts.

2.4. Principle 4: comparability

Comparability ensures that results obtained from distinct methods or laboratories can be evaluated on a common platform, facilitating meaningful assessments and benchmarking. This is especially important in WAC, where achieving a balance between ecological, analytical, and practical attributes requires clear and consistent metrics. Tools that generate standardized outputs enable researchers to identify strengths and limitations of various methods, aiding in the selection of the most appropriate approach for specific applications. Moreover, comparability enhances collaboration within the scientific community, as shared data and insights can be interpreted uniformly across different teams and contexts. For this to be achieved, tools must incorporate universal criteria and metrics that transcend individual methodological nuances, thus maintaining their relevance across a wide spectrum of analytical techniques. Clear visual outputs and structured reporting formats further enhance the interpretability of results, making them accessible to users with varying levels of expertise. By enabling standardized and reproducible evaluations, tools adhering to this principle not only improve the reliability of analytical processes, but also promote transparency and progress in the development of sustainable methodologies.

2.5. Principle 5: assessment

Quantitative measures, such as numerical indices or scores, offer a standardized and objective way to evaluate key attributes of a method, including its efficiency, sustainability, and reproducibility. These measures allow for precise comparison across different methods and highlight specific areas of strength or improvement. On the other hand, qualitative assessments complement this numerical approach by capturing nuanced factors that may not be fully reflected in quantitative metrics, such as practical challenges during implementation or the contextual relevance of the method. Together, these dual forms of evaluation provide a comprehensive understanding of a method's overall performance, ensuring that both measurable outcomes and subjective insights are considered. A robust evaluation framework that integrates quantitative and qualitative measures also supports decision-making by helping users determine whether a given method aligns with their specific goals and constraints. Importantly, these measures must be presented in a clear and user-friendly manner, ensuring that they can be interpreted effectively by a wide range of users.

2.6. Principle 6: accessibility

Making tools available through open platforms or user-friendly software significantly broadens their reach and impact within the scientific community. Open access eliminates barriers related to cost and exclusivity, allowing researchers, educators, and industry professionals from diverse backgrounds to benefit from these resources. This democratization of knowledge enhances inclusivity and collaboration, enabling a wider adoption of sustainable and innovative practices. Equally important is the usability of the tool's platform or software. Intuitive interfaces, straightforward navigation, and minimal technical requirements ensure that users with varying levels of expertise and resources can efficiently integrate the tool into their workflows. For example, tools compatible with commonly used operating systems or accessible via cloud-based platforms can enhance usability and eliminate the need for specialized hardware or extensive training. Additionally, accessible tools facilitate educational initiatives by providing students and early-career researchers with the opportunity to engage with advanced methodologies.

2.7. Principle 7: sustainability

In the framework of WAC, sustainability extends beyond green chemistry principles to include broader considerations that impact the overall feasibility and societal relevance of a method. From an environmental perspective, tools must assess factors such as waste generation, energy consumption, and the use of hazardous reagents, with the aim of minimizing the ecological footprint of the methods. However, focusing solely on environmental criteria risks overlooking the practical and societal dimensions that influence a method's adoption and long-term success. Economic attributes, such as cost-effectiveness, are equally critical, as methods must be viable within the financial constraints of laboratories, particularly in resource-limited settings. Affordability ensures that sustainable practices can be implemented widely, rather than being restricted to well-funded institutions. Social aspects, including accessibility, equity, and safety, further expand the scope of sustainability. Methods that prioritize user safety, inclusivity, and accessibility foster greater collaboration and engagement across diverse communities. The integration these three dimensions—environmental, economic, and social—tools can offer a comprehensive perspective that aligns with the multifaceted goals of WAC.

2.8. Principle 8: evaluation

This principle emphasizes the importance of identifying the foundational aspects that define the method's performance, reliability, and overall applicability. Central components such as accuracy, precision, sensitivity, selectivity, and robustness must be carefully assessed, as these parameters directly influence the method's ability to deliver meaningful and reproducible results. By prioritizing these elements in the evaluation process, tools can provide a structured approach to highlight the strengths and limitations of a method. Moreover, this principle encourages a systematic review of how these key elements interact within the broader analytical workflow. For instance, a method's accuracy cannot be isolated from its practicality or environmental impact. Instead, tools should integrate these elements into a cohesive framework, allowing users to see the trade-offs and interdependencies that may affect decision-making. This approach is particularly valuable in the development of tools aimed at balancing analytical rigor with the sustainable and practical priorities of WAC. Principle eight promotes a deeper understanding of what makes an analytical method effective and reliable.

2.9. Principle 9: flexibility

Flexibility and adaptability are indispensable attributes for any analytical tool intended for widespread use. A tool's value significantly increases when it can accommodate diverse instrumental configurations and meet the specific needs of various users or laboratories. Analytical methods often rely on different instruments, ranging from high-end, automated setups to more basic or manual setups, depending on the resources available. Tools that account for such variability ensure that they are not limited to a single context or overly specialized setting. Instead, they remain applicable across a wide spectrum of scenarios, making them practical and inclusive. This adaptability extends beyond instrumentation to address variations in procedural requirements or environmental constraints. Laboratories may have different priorities, such as speed, cost, or sensitivity, and a flexible tool can align with these diverse objectives without compromising its core function. Importantly, adaptability also fosters resilience, allowing tools to remain relevant as analytical technology advances. A tool designed with modular or scalable features can easily integrate new advancements or accommodate adjustments, making it future-proof.

2.10. Principle 10: adaptability

The dynamic nature of analytical chemistry demands tools that can adapt to ongoing advancements in the field. A tool that allows for updates and expansions supports its continued relevance and utility in a constantly changing scientific landscape. As new technologies emerge, analytical methods improve, and sustainability standards grow more rigorous, tools must be designed to adapt. This adaptability can take many forms, such as the incorporation of new metrics, refinement of evaluation criteria, or integration of updated methodologies. Moreover, the ability to expand a tool's scope is equally critical. What might initially address a specific analytical need should, over time, be capable of evaluating broader applications or accommodating additional functionalities. For instance, a tool might start by focusing on environmental sustainability but later expand to include social or economic aspects, aligning more closely with the holistic goals of WAC. Ensuring that updates and expansions are seamless requires tools to be built on flexible, modular frameworks. Such frameworks not only simplify the process of incorporating changes, but also reduce the risk of obsolescence.

3. Assessment by PRISM of last accepted tools in the WAC field

In this section, an evaluation of recently developed analytical tools in the context of WAC is presented using the PRISM framework. The aim is to analyze whether these tools align with the core principles of PRISM—**P**ractical, **R**eproducible, **I**nclusive, **S**ustainable, & **M**anageable. By systematically comparing these tools against the defined principles, this assessment provides valuable insights into their strengths, limitations, and potential areas for improvement. The results of this evaluation are summarized in Table 3, offering a

Table 3
Evaluation of recently accepted tools in the WAC field using the PRISM principles.

Principle No.	AGREE	AGREEprep	GAPI	ComplexGAPI	MoGAPI	BAGI
1	✔	✔	✘	✘	✔	✔
2	✔	✔	✔	✔	✘	✔
3	✔	✔	✔	✘	✔	✔
4	✔	✔	✔	✔	✔	✔
5	✔	✔	✔	✔	✔	✔
6	✔	✔	✔	✔	✔	✔
7	✘	✘	✔	✔	✔	✘
8	✘	✔	✘	✔	✔	✔
9	✘	✔	✘	✔	✔	✔
10	✔	✘	✔	✘	✔	✔

clear and structured overview of how well these tools adhere to the proposed principles. It is worth noting that no tool fully adheres to all PRISM principles, as each has its own strengths and weaknesses. Most of the developed tools demonstrate strong alignment with PRISM principles, particularly in prioritizing user-friendly designs, accessibility through open platforms, and consideration of environmental impacts. Regarding Principle 10, the GAPI tool (Płotka-Wasylka, 2018) has been updated over time, resulting in derivatives such as ComplexGAPI (Płotka-Wasylka and Wojnowski, 2021) and MoGAPI (Mansour et al., 2024b). Similarly, AGREEprep (Wojnowski et al., 2022) expands upon the original AGREE tool (Pena-Pereira et al., 2020), highlighting how these tools can be refined to meet new analytical needs and challenges. However, certain tools fall short in addressing specific principles. In terms of Principle 3, which emphasizes clarity and user-friendliness, some tools present notable weaknesses. GAPI (Płotka-Wasylka, 2018) and ComplexGAPI (Płotka-Wasylka and Wojnowski, 2021) are often criticized for being difficult to interpret and potentially overwhelming due to their complexity. Additionally, their functionality has been described as challenging, as noted by S. Imam (Imam and Abdelrahman, 2023). For MoGAPI, a lack of transparency regarding the scoring credits undermines its usability, leaving users without a clear understanding of how the scoring is derived. For Principle 8, which focuses on evaluating key elements of an analytical method, significant shortcomings are observed in GAPI and AGREE. Both tools fail to account for the synthesis stage prior to sample preparation, leaving the overall greenness of the analytical methodology unclear. Furthermore, the results generated by these tools often lack detailed information on the structure of hazardous substances, limiting their ability to provide a comprehensive assessment of analytical methods (Sajid and Płotka-Wasylka, 2022). While most tools exhibit commendable adherence to PRISM principles, there remains variability in their flexibility and adaptability, which highlights an area for future development. Efforts should focus on ensuring that tools remain dynamic, capable of integrating emerging methodologies and addressing changing requirements. Enhancing these aspects will reinforce their value in promoting sustainable and effective analytical practices.

While the PRISM framework aims to provide a standardized and practical guideline for the development and evaluation of analytical tools in the context of WAC, it is not without limitations. One key challenge lies in the subjective interpretation of certain principles, especially those related to qualitative assessments such as clarity, usability, or sustainability across different contexts. Moreover, the implementation of PRISM relies heavily on the availability of transparent information regarding each tool's design and performance, which is not always accessible in the literature.

4. Conclusions

A comprehensive framework of ten principles to guide the development and implementation of analytical tools within the context of WAC is established. By addressing the critical gap in standardized guidelines, these principles promote tools that balance analytical, ecological, and practical dimensions. The evaluation of recently developed tools using the PRISM framework demonstrates that while many adhere strongly to core principles, others reveal notable weaknesses—particularly in adaptability, transparency, and interpretability. It is important to emphasize that PRISM is not intended to replace existing greenness or sustainability metrics, but rather to complement them by providing a conceptual guideline that promotes clarity, usability, and consistency in their development. Looking ahead, research should focus on developing PRISM-based tools tailored to specific analytical contexts. Moreover, there is a need to redefine existing tools to overcome their limitations, design modular frameworks to enhance adaptability, and expand their scope to meet the growing demands of sustainable and effective analytical practices. Establishing training programs and user guidelines will also be crucial to ensure effective implementation and widespread adoption, especially in resource-limited settings. Progress in this area may also benefit from the creation of a consensus or task force to refine and standardize these principles collaboratively, ensuring their broad acceptance and practical relevance.

CRediT authorship contribution statement

Adrián Fuente-Ballesteros: Writing – review & editing, Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Conceptualization. **Victoria Samanidou:** Writing – review & editing. **Ana M. Ares:** Writing – review & editing, Supervision. **José Bernal:** Writing – review & editing, Supervision.

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.

Acknowledgements

Adrián Fuente-Ballesteros thanks the University of Valladolid (Spain) for his PhD contract.

Abbreviations

AGREE, analytical greenness calculator metric; **AGREEprep**, analytical greenness metric for sample preparation; **AMVI**, analytical method volume intensity; **BAGI**, blue applicability grade index; **GAC**, green analytical chemistry; **GAPI**, green analytical procedure index; **GLANCE**, graphical layout tool for analytical chemistry evaluation; **ComplexGAPI**, complementary GAPI; **HPLC-EAT**, high performance liquid chromatography-environmental assessment tools; **MoGAPI**, modified GAPI; **NEMI**, national environmental methods index; **RAPI**, red analytical performance index; **RGB**, Red-Green-Blue; **VIGI**, violet innovation grade index; **WAC**, white analytical chemistry.

Data availability

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

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