Trends in Environmental Analytical Chemistry 47 (2025) e00275

Contents lists available at ScienceDirect

Trends in Environmental Analytical Chemistry

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

# Analytical chemistry in the era of sustainability: evaluating tools and challenges for a greener future

Louise Durand, Laure Wiest, Emmanuelle Vulliet *

*Universite Claude Bernard Lyon 1, CNRS, ISA, UMR5280, 5 rue de la Doua, Villeurbanne F-69100, France*

ARTICLE INFO

*Keywords:*
Green analytical chemistry
White analytical chemistry
Sustainability
Metric tools

ABSTRACT

Analytical chemistry plays a crucial role in environmental monitoring, yet its own practices contribute to environmental degradation. To address this paradox, the emergence of the concepts of Green Analytical Chemistry (GAC), White Analytical Chemistry (WAC) and Green Sample Preparation (GSP) has led to the use of tools to evaluate analytical methods. Various tools have been developed to assess the environmental impact of analytical methods, including HPLC-EAT, AES, AMVI, GAPI, AMGS, RGB model and its evolutions, AGREE, AGREEprep, HEXAGON, LCA, SPMS and BAGI. They differ in their scope, assessment criteria, and methodological approach, from qualitative scoring systems to quantitative assessments. This review critically compares these tools, highlighting their strengths and limitations in evaluating sustainability across different stages of the analytical process. Particular attention is given to the assessment of chemical hazards, energy consumption, and impact quantification. The need for standardized, comprehensive, and accessible methodologies is emphasized to guide the transition toward truly sustainable analytical practices.

## 1. Introduction

Analytical chemistry plays a crucial role in environmental monitoring, enabling the monitoring and the assessment of risks associated with anthropogenic activities by detecting, identifying and quantifying substances across different media such as surface water, drinking water, wastewater, sediment, soil, biota, etc. However, like all human activities, analytical chemistry applied to environmental issues is also paradoxically involved in the degradation of the environment and human health. This duality highlights the need for more sustainable practices within the field.

Every stage of an analytical method can contribute to its environmental impact. It begins with the sampling of the studied media which can (i) physically and/or chemically deteriorate the latter, (ii) use of energy-intensive equipment and (iii) require long-distance transport in the case of *ex-situ* analysis. Sample preparation is often considered the most problematic step, even though it is necessary given the complexity of the matrixes and the low concentration of analytes. It necessitates specific extraction, purification and sample concentration steps that frequently rely on chemical reagents and generate significant waste. Instrumental analysis also plays a role in the method’s environmental impacts as it requires energy-intensive instruments such as chromatographic techniques coupled with mass spectrometry which are widely used in environmental analysis. These methods are indispensable for addressing the diversity of micropollutants, the complexity of the matrixes and the low concentrations of the analytes which require high separation, specificity and sensitivity. Finally, data analysis, storage and management also contribute to the overall impact, as they demand substantial energy resources.

This paradox gave birth in 1999 to the Green Analytical Chemistry (GAC) which emerged as an extension of the broader field of Green Chemistry (GC) formalized by Anastas and Warner [1]. While GC initially focused on making chemical synthesis more sustainable, GAC was introduced to apply these principles to the specific context of analytical sciences. As emphasized by Koel et al. [2], although analytical procedures are typically performed at small scales, their cumulative environmental impact can become significant due to their frequent repetition. GAC thus aims to transform analytical methods by promoting the use of safer solvents and reagents, minimizing toxic waste generation in laboratories, enhancing operator safety, and improving energy efficiency. The concept was further developed by Armenta et al. [3], who proposed practical guidelines to improve the greenness of analytical procedures, while also highlighting the critical role of greener sample preparation techniques. These foundational works contributed to the

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* Corresponding author.
*E-mail address:* emmanuelle.vulliet@isa-lyon.fr (E. Vulliet).

https://doi.org/10.1016/j.teac.2025.e00275
Received 12 March 2025; Received in revised form 22 July 2025; Accepted 22 July 2025

formalization of GAC in 2013 with 12 now well-known principles [4] which were tailored to address specific challenges of analytical chemistry, providing the first guideline to help analytical chemists to reduce the environmental and health impacts of their methods. Since then, additional concepts and guidelines have been introduced. White Analytical Chemistry (WAC) [5] exemplifies this evolution, aiming to reconcile the reduction of environmental impact with analytical performances, while addressing the limitations posed by certain GAC principles. Similarly, the 10 principles of Green Sample Preparation (GSP) [6] were introduced to fill the gap left by the first principle of GAC "Direct analytical techniques should be applied to avoid sample treatment", which appears to be overly idealistic when dealing with complex matrixes such as environmental ones.

Thanks to all these guidelines, a great deal of work has turned towards reducing the environmental impact of analytical methods. Nevertheless, many methods are labelled as 'green' or 'sustainable' without sufficient justification for these claims. It is therefore crucial to rigorously assess the sustainability of the developed method [7]. Over the past two decades, numerous tools have been developed for this goal, starting with National Environmental Methods Index (NEMI) in 2002, and then the High Performance Liquid Chromatography Environmental Assessment Tool (HPLC EAT) [8], the Analytical Method Volume Intensity (AMVI) [9], the Analytical Eco-Scale (AES) [10], the Green Analytical Procedure Index (GAPI) [11], the Analytical Method Greenness Score (AMGS) [12], HEXAGON [13], the RGB model and its evolutions [5,14,15], Analytical GREEnness (AGREE) [16], AGREEprep [17], the Life Cycle Assessment (LCA), the Sample Preparation Metric of Sustainability (SMPS) [18] and the Blue Applicability Grade Index (BAGI) [19]. These tools are useful for relativity assessing the sustainability or the greenness of methods. Indeed, they enable the comparison of several methods with the same analytical objectives, facilitate the selection of the most sustainable or the greener one according to predefined criteria and help identifying drawbacks of the studied methods.

While several review articles have already provided detailed presentation of these tools [20–22], the novelty of the present work lies in a comparative and critical analysis of their application scopes and methodologies. The preliminary objective is to briefly introduce each tool (except NEMI, which is now obsolete), in chronological order of publication or of use in the field of analytical chemistry. The main goal, however, remains to systematically compare them in order to (i) identify the specific scope of each tool, (ii) discuss the different methods and references used to assess crucial items, such as chemical hazard, and finally (iii) highlight the need to move towards impact quantification tools. Through this approach, this study aims to emphasize the need to move beyond qualitative rating tools and towards more robust impact quantification approaches, which could provide analytical chemists with clearer guidance when choosing or designing more sustainable methods.

## 2. Tools brief description

### 2.1. HPLC-EAT

HPLC-EAT [8] is a tool that assess the environmental impact of HPLC methods by focusing on solvent consumption during, on the one hand sample preparation, and on the other hand, instrumental analysis. This tool is based on a risk assessment as a function of volumes used and associated hazards. It is calculated according to Eq. (1), with safety, health and environmental (SHE) factors provided by Koller and al. [23].

$$\mathrm{HPLC-EAT} = \sum (S_n m_n + H_n m_n + E_n m_n) \tag{1}$$

With $S_n$ the safety factor, $H_n$ the health factor, $E_n$ the environmental factor and $m_n$ the solvent volume.

HPLC-EAT results enable (i) the direct comparison of different methods, but also illustrate the contribution of (ii) the various SHE factors to the method score, (iii) the sample preparation step and the instrumental step to the overall method score, and (iv) the various solvents to the overall method score.

### 2.2. Analytical eco-scale

The AES [10] is a semi-quantitative tool that allows to compare methods according to their greenness, based on the attribution of penalty points (PP) of an ideal score of 100. The authors defined penalty points to be distributed according to several themes: solvents and reagents used, energy consumed, and management of produced waste. These penalty points are presented in Table S1. If the AES is superior to 75, the method can be considered as "excellent green", whereas if the AES is between 50 and 75 the method is only "acceptable". Under this score, the method is qualified as "inadequate".

### 2.3. Analytical method volume intensity

The goal of the AMVI [9] is to measure the total volume of solvent used as waste produced by a method, during both sample preparation and instrumental analysis steps. The methodology takes into account all the solvents consumed during an analytical batch, i.e. for the preparation of samples, calibration, blanks, injections, etc. The calculated volume is then expressed per analyte: the authors suggest to target a maximum of 90 mL per analyte.

### 2.4. Green Analytical Procedure Index

GAPI [11] is a tool developed to evaluate methods' greenness by taking into account the analytical chain from sampling to instrumental analysis. The assessment is divided into 5 themes: sampling, sample preparation, chemicals used, instrumentation and type of method. Each theme is subdivided into categories that are assessed thanks to a three-level colour scale: green, yellow and red for low, medium and high environmental impact. The different assessed criteria and the allocation of colours are shown in Table S2.

Results are summarized in the shape of five coloured pictograms representing the different assessed themes and reflecting the greenness degree of each category. These results enable to (i) visually identify the steps of the analytical chain that have the greatest impact according to the studied criteria, (ii) easily identify the parts of the method that need to be improved, (iii) globally compare different methods according to the total number of green, yellow and red criteria, and (iv) precisely compare different methods theme by theme according to the same process.

### 2.5. Analytical method greenness score

AMGS [12] aims to assess analytical methods through the consumption of solvents and energy. The score takes into account the SHE assessment of solvents, the waste generation and both instrument and solvent energy consumption. In fact, the AMGS merges the principles of two other tools: AMVI [9], for the solvent consumption, and the SHE factors from the Solvent Selection Guide (SSG) [24], for the solvent assessment. In addition, the AMGS introduces the energetic dimension for both instrument and solvent, with, on the one hand, the Cumulative Energy Demand (CED) which is the total required quantity of energy for the solvent life, from the raw material extraction to the disposal, and on the other hand, the consumed energy during analysis. The AMGS score is calculated by the Eq. (2):

$$AMGS = \frac{1}{N} \times \sum_{n} (mS_n + mI_n) \times (3\sqrt{S_n \times H_n \times E_n} + CED_n + (\sum_{i} E_{i} \times R)) \tag{2}$$

With $m_{Sn}$: mass of solvent n used to prepare a standard or sample, $m_{In}$: mass of solvent n used by the instrument during gradient mobile phase elution, $S_n$: safety factor of solvent n, $H_n$: health factor of solvent n, $E_n$: environmental factor of solvent n, $CED_n$: cumulative energy demand of solvent n based on production and solvent incineration for disposal, $E_i$: instrument energy consumption, R: number of sample injections required for the analysis set (standards, controls, etc.), $N$: number of interest analytes.

As a result, a global greenness score is attributed to the method (the smaller the greener) that allows the direct comparison between methods. In addition, the percentage contributions to the score of (i) the instrument energy, (ii) solvent energy and (iii) of EHS are provided.

### 2.6. *RGB model, RGB 12 et RGB fast*

The goal of the RGB model [14] is to evaluate analytical methods by considering not only green analytical chemistry principles, but also analytical performance and productivity/practicality criteria. A primary colour is related to these three components (respectively green, red and blue) that are individually assessed. If a method is well-balanced according to these 3 components, by additive colour synthesis, it can be described as white. This model also gave birth to the concept of WAC, which aims to reconcile GAC concepts with analytical needs (precision, sensitivity, etc.) and practical and economic aspects of analytical methods. For each component (red, green and blue), the user has to define evaluation criteria and then assign a score ranging from 0 to 100 for each criterion (100 being the score assigned to the ideal method).

The RGB model has faced criticism for being overly flexible, as it allows users to choose their own criteria, potentially compromising the objectivity of evaluations. In response, the authors introduced the RGB 12 algorithm [5], an updated version that retains the original model's framework but uses fixed criteria determined by the authors. These criteria are based on the 12 principles of WAC and are listed in Table S3.

A latest update was developed in 2024: RGBfast [15]. Still based on the principles of WAC, this tool offers improvements on the criticisms of complexity, lack of guideline, and too much subjectivity. The assessment is now only based on 6 criteria: (1) trueness, (2) precision and (3) sensitivity for analytical performances (red), (4) ChlorTox Scale for greenness (green), (5) electricity consumption for the greenness linked to economical aspect (green-blue) and (6) sample throughput for practical considerations. To reduce the subjectivity of the user's assignment of a score from 0 to 100 for each criterion, the formula presented in Eq. (3) helps to assign this score (provided that at least two methods with the same analytical purpose are compared):

$$Score = 100 \quad \times \quad \frac{1}{1 + \frac{result}{average\ result}} \tag{3}$$

The output display makes it possible to (i) identify the satisfaction level of each RGB component and criterion, while (ii) allowing global discrimination between the different tested methods thanks to an overall score called the 'whiteness'.

The ChlorTox scale [25] is an indicator of chemical risk developed by Nowak and al. The concept is to estimate the chemical risk associated with the use of a substance by comparing it with the chemical risk posed by chloroform, which is a well-known substance whose toxicity and safety aspects have been widely tested, and which represents numerous hazards for the environment and human health. ChlorTox is therefore calculated according to Eq. (4).

$$ChlorTox = \frac{CH_{sub}}{CH_{CHCl3}} \times m_{sub} \tag{4}$$

With $CH_{sub}$ a chemical hazard estimation of the studied substance, $CH_{CHCl3}$ a chemical hazard estimation of chloroform, $m_{sub}$ the mass (in g) of the studied substance

The choice of the model to estimate the chemical hazard (CH) of the substances, such as CHEMS-1 [26], is left to the user, as long as the same is used for the studied substances and the chloroform. Nevertheless, the authors suggest to use a model they have developed: the Weighted Hazards Number (WHN) which consists to sum the different hazards identified in the Safety Data Sheets (SDS) weighting to take into account the degree of potential danger according to the hazard categories.

Consequently, the result of Chlortox Scale gives a quantified estimation of the chemical risk degree posed by the used chemicals in comparison to the chemical risk degree that would be posed by using the same quantity of chloroform, as a standardised unit.

### 2.7. *HEXAGON*

HEXAGON [13] is a tool that has been developed to assess the sustainability of methods, taking into account not only operator health and the environment, but also economic, practicality and performance aspects. The assessment is based on 6 different themes: figures of merits 1 (sample preparation, methods and calibration), figures of merits 2 (analytical performances), risk, waste generation, carbon footprint and annual cost. As for the AES assessment [10], penalty points are distributed to methods according to the guidelines described in Table S4, with the exception of the carbon footprint that needs to be calculated. For each theme, the total of penalty points is therefore transformed into an overall qualification (OQ) ranging from 0 to 4 (0 being the best score) thanks to Table S5.

Finally, the results are illustrated in the form of a hexagon composed of six triangles with the OQ that correspond to the assessed themes. This representation allows to (i) visually identify themes that have the greatest impact according to the criteria studied, (ii) easily identify the parts of the method that need to be improved, (iii) globally compare different methods according to the sum of OQs and (iv) precisely compare different methods theme by theme.

### 2.8. *AGREE and AGREEprep*

AGREE [16] is a tool based on the 12 principles of GAC [4]. A criterion, that can be weighted, is established for all principles, and a score between 0 and 1 is assigned to each one (1 being attributed to the ideal method) thanks to the guidelines presented in Table S6. The final score is then obtained by calculating the weighted mean of the scores obtained for each principle. The result is described in the form of a clock whose centre contains the final score obtained against a coloured background. The more the method meets the criteria, the closer the score is to 1 and the greener the background. In addition, the periphery of the clock is made up of coloured segments which indicate in the same way the agreement of the method with each principle.

This result makes it possible to (i) visually identify the compliance of the method with the different GAC principles, (ii) easily identify what need to be improved, (iii) compare different methods according to the global score, and (iv) compare methods in a discriminating way using continuous mathematical models.

AGREEprep [17] aims to assess the environmental impact of sample preparation. It is based on the 10 principles of GSP [6], each of which is assigned a criterion. The assessment process and results are based on the same concepts as AGREE. The criteria and evaluation procedure are presented in Table S7. The final score is also obtained by calculating the weighted mean of the scores obtained for each principle. The result is described mostly in the same form as AGREE results. However, the periphery of the clock is made up of coloured segments whose size varies according to the weight given to the principles.

### 2.9. *Life cycle assessment*

LCA is a method of environmental impact assessment and quantification normalized by the International Organization for Standardization with the norms ISO 14040/44 [27]. While this method is widely used in chemical industries in the field of organic chemistry in order to identify eco-design solutions and to evaluate quantitatively the impact of new materials, its use remains marginal in the evaluation of analytical methods. However, Tobiszewski et al. [28] emphasized the relevance and potential of LCA in the field of analytical chemistry, highlighting its ability to provide comprehensive and quantitative environmental assessments. Recentely, Raccary and al. provided new perspectives by conducting LCA in order to compare two sample preparation methods [29] and by proposing a tutorial to help analytical chemists to conduct LCA in this field [30]. Unlike the other tools, LCA relies on a more comprehensive inventory of every use (energy, solvents, etc.) that are included in the defined scope of the assessment. Indeed, this inventory includes a larger scope than the other tools given that for each item considered, production, use and end-of-life data are taken into account. In addition, data linked to the background processes of the primary data can be collected using LCA database such as Ecoinvent [31]. These secondary data are necessary to extend the assessment and to involve the processes and places of production of the different items used, their end of life, etc. By using dedicating softwares, such as SimaPro or OpenLCA, the different data are linked and converted into environmental impacts that are defined by the chosen calculation methodology. By using the ReCiPe 2016 [32] method, 17 categories of impact are quantified with equivalent units. They are presented in Table 1.

LCA results can then (i) indicate which parts/items of the method contribute most to the different types of impact, which is very useful to find impacting changes to set up, (ii) allow to compare the quantified impacts of different methods, and (iii) identify impact transfers between different impact categories or between key stages of the process during a method improvement study.

### 2.10. *Sample preparation metric of sustainability*

The goal of SPMS [18] is to assess the sustainability of the sample preparation step exclusively. It considers 9 parameters grouped into four categories: (i) sample information, (ii) extractant information, (iii) procedure information, and (iv) energy consumption and waste. Each parameter is assigned a score based on the guidelines presented in Table S8. These scores are then summed, weighted according to the relative impact of each category on sustainability as defined by the authors, and finally adjusted to a 10-point scale to obtain a global score. The tool provides a visual output in the form of a clock-like diagram, where parameters are represented by small colored squares grouped by category (green for successful, yellow for acceptable, orange for tolerable, and red for inadequate), with the overall score displayed in the center.

These results allow users to (i) visually identify the categories of the sample preparation process that contribute most to its sustainability profile, (ii) easily detect areas of the method that require improvement, (iii) accurately compare different sample preparation techniques based on the distribution of green, yellow, orange, and red parameters, and (iv) globally compare procedures using the final score.

**Table 1**
ReCiPe 2016 impact categories and units.

| Impact category | Unit |
|---|---|
| Global warming | kg $CO_2$ eq |
| Stratospheric ozone depletion | kg CFC11 eq |
| Ionizing radiation | kg Co−60 eq |
| Ozone formation, human health | kg $NO_x$ eq |
| Fine particulate matter formation | kg PM 2.5 eq |
| Terrestrial acidification | kg $SO^2$ eq |
| Freshwater eutrophication | kg P eq |
| Terrestrial ecotoxicity | kg 1,4-DCB eq |
| Freshwater ecotoxicity | kg 1,4-DCB eq |
| Marine ecotoxicity | kg 1,4-DCB eq |
| Human carcinogenic toxicity | kg 1,4-DCB eq |
| Human non-carcinogenic toxicity | kg 1,4-DCB eq |
| Marine eutrophication | kg N eq |
| Land use | $m^2$a crop eq |
| Mineral resource scarcity | kg Cu eq |
| Fossil resource scarcity | kg oil eq |
| Water consumption | $m^3$ |

### 2.11. *Blue Applicability Grade Index*

BAGI [19] is a tool that aims to evaluate the practicality of a method in complementarity with tools which evaluate their greenness. It is therefore part of the WAC framework where the “blue” component is related to cost-efficiency, time-efficiency and operational simplicity. BAGI assesses 10 main criteria, each rated from 2.5 to 10 points, according to their compliance with the practicality of an analytical method. The criteria and evaluation procedure are presented in Table S9. Each criterion is represented visually in an asteroid-shaped pictogram with segments coloured according to a blue gradient, from dark blue (10 points, best compliance) to white (2.5 points, non-compliant). In addition, an overall score is attributed to methods at the centre of the pictogram ranging between 25 (not compliant) and 100 (best compliance).

The authors suggest that a method is considered as practical of the overall score is at least 60 points. This pictogram provides the possibility to (i) identify levers for action to make a method more practical, (ii) globally compare the practicality of different methods according to the global score, and (iv) visually compare methods criterion by criterion.

## 3. Comparisons of the tools

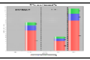
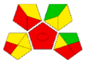
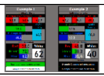
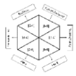
To better understand the relevance and limitations of the various presented tools, it is essential to compare their scopes, criteria, and underlying principles. This section provides a detailed comparison of the tools, focusing on the steps of the analytical process and the pillars of sustainability they cover, the way they assess chemical risk and energy consumption, and their ability to quantify environmental impacts. These comparative insights are summarized in Table 2, in addition to the ease of use of the tools. Currently, the most widely used tools tend to be those that are the simplest and most user-friendly, even if they lack methodological comprehensiveness.

### 3.1. *Scope of the tool*

The analytical process is defined as the succession of the following steps: (1) sampling, (2) sample preparation, (3) instrumental analysis, (4) data processing and finally (5) data storage and management. This entire chain is not assessed by all the tools, with the exception of LCA, depending on the objectives set and the scope defined at the beginning of the assessment. For this reason, it is not relevant to discuss the scope of LCA in this section. Depending on their goals, the other tools cover different stages of the analytical process (Fig. 1).

First, only GAPI, AGREE and HEXAGON include sampling in their assessment thanks to qualitative data. While AGREE evaluates the type of sampling and sample transport, and HEXAGON focuses on sample preservation and storage, GAPI takes all four aspects into account. Then, sample preparation is assessed by all the presented tools, which is consistent with the fact that it is judged to be the step in the analytical chain with the greatest environmental impact. However, this stage is not assessed in the same way. For instance, HPLC-EAT, AMVI and AMGS, which are designed exclusively for solvent-based instrumental analyses, only consider solvents. In contrast, the other tools account for all chemicals (at least as waste). Criteria concerning other materials such as consumables are included in AES, RGB, GAPI, AGREE, AGREEprep, SPMS and HEXAGON (at least as waste). Electricity consumption is taken into account by AES, RGB, GAPI, AGREE, AGREEprep, SPMS and HEXAGON. Concerning the instrumental analysis stage, the only tool that does not assess it is SPMS. It is important to note that although

**Table 2**
Comparative summary of the presented assessment tools.

| Tool | Sustainability scope | | | Chemical hazard | Energy consumption | Impact(s) quantification | Ease of use | Graphical output |
|---|---|---|---|---|---|---|---|---|
| | Environmental and human health | Analytical performances | Practicality and economic efficiency | | | | | |
| HPLC-EAT | ✓ | | | ✓ | | | A user-friendly software is available at: https://pubs.rsc.org/en/content/articlelanding/2011/gc/c0gc00667j |  |
| AES | ✓ | | | ✓ | ✓ | | Easy to understand, but there is no template or software. | |
| AMVI | ✓ | | | | | | Relies on simple calculations, but there is no template or software. | |
| GAPI | ✓ | | | | ✓ | | Intuitive, as it is supported by a detailed guideline. |  |
| AMGS | ✓ | | | ✓ | ✓ | | Complex due to the level of understanding required for data collection and the calculation formula. | |
| RGBfast | ✓ | ✓ | ✓ | ✓ | ✓ | ✓<br>Toxicity ($CHCl_3$-eq in g) | Easy to understand, but as it requires experimental data, the assessment is longer. It also requires more calculations. An Excel file is available. |  |
| HEXAGON | ✓ | ✓ | ✓ | ✓ | ✓ | ✓<br>Environmental ($CO_2$-eq in kg)<br>Economic (€) | Data collection can be lengthy due to the complexity of the criteria and the need for experimental data. No template is available. |  |
| AGREE | ✓ | | ✓ | | ✓ | | Intuitive, as it is supported by a detailed guideline and a dedicated application: https://agree-index.anvil.app/ |  |
| AGREEprep | ✓ | | ✓ | | ✓ | | Intuitive, as it is supported by a detailed guideline and a dedicated application: https://agreeprep.anvil.app/ |  |
| LCA | ✓ | | | ✓ | ✓ | ✓<br>See Table 2 | Complex and time-consuming tool as it requires detailed quantitative data, specialized software (often at a cost) and more reflexion on the scope of the assessment. | |
| SPMS | ✓ | | ✓ | | ✓ | | Intuitive, as it is supported by a detailed guideline and a dedicated Excel file. |  |
| BAGI | | | ✓ | | | | Intuitive, as it is supported by a detailed guideline and a dedicated application: https://bagi-index.anvil.app/ |  |

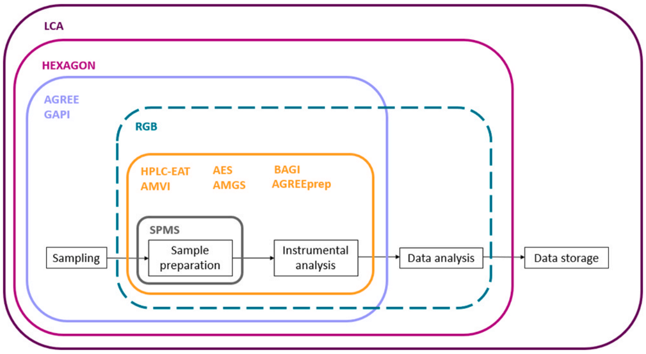


**Fig. 1.** Steps of the analytical process covered by the presented tools.

AGREEprep aims to assess the environmental impact of sample preparation, it does include an evaluation criterion on the choice of post-sample preparation configuration for analysis, in accordance with the 9th principle of the GSP. The data analysis stage is considered by RGB and HEXAGON, which incorporate criteria such as sensitivity, precision, etc. Finally, none of these tools include data storage in their assessment.

Furthermore, the three pillars of sustainability should ideally be considered: environment, economy and society. The concept of WAC is similar in this sense. Indeed, it tends to integrate (i) the red component which is assigned to analytical efficiency, and aligns with the economic pillar of sustainability by focusing on performance, (ii) the green component which follows the principles of GAC and corresponds to the environmental and social pillars of sustainability, aiming to minimize environmental impact and safeguard human health, and (iii) the blue component assigned to the productivity, practicality and economic efficiency of the methods, corresponding to both the economic and societal pillars of sustainability. With the exception of BAGI, all the tools assess methods from environmental and social perspectives, since their primary aim is to evaluate the impacts or hazards of methods on operator health and on the environment, or to determine their green/white characteristics. Nevertheless, the other aspects of sustainability are missing with a few exceptions. HEXAGON includes criteria related to GAC principles, analytical performance and economic factors. For example, the electricity consumption is assessed from both environmental and economic point of view. RGB also includes GAC, practicality and analytical performances aspects, while AGREE, AGREEprep and SPMS do not include the latter one. BAGI only considers practicality.

### 3.2. *Assessment of the chemical risk*

Reducing and replacing hazardous chemicals to ensure the safety and health of operators and protect the environment are one of the main goals of sustainable analytical chemistry. This objective is embodied in various principles in the concepts of:

- GAC, with principles 7. “Generation of large volume of analytical waste should be avoided", 11. “Toxic reagents should be eliminated” and 12. “The safety of the operator should be increased”.
- GSP with principles 2. “Use safer solvents and reagents”, 4. “Minimize sample, chemical and material amounts” and 10. “Ensure safe procedures for the operator”.
- WAC with principles 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 (regardless of how toxic they are) "and G4. "Direct impacts: The use of analytical methods should not directly affect humans, animals, and genetic naturalness. Exposure of humans (operator) to harmful factors and the use of animals and/or genetic modifications should be avoided."

In this context, chemical substances must be considered as part of the global assessment of analytical methods in order to evaluate the risks they pose to operators or on the environment. These risks are a function of their intrinsic properties to cause harmful effects, i.e., hazards, and of the exposure to them. Therefore, all the presented tools dedicate part of their assessment to chemicals, based on their quantities and at least one type of hazard contributing to chemical hazard (environmental, health or safety), except AMVI and BAGI. Indeed, on the one hand, AMVI takes into account the volume of consumed solvents (other chemicals are not covered) and does not include their hazards in its evaluation. On the other hand, BAGI evaluates the use of chemicals according to their practicality, i.e., their availability on the market. Moreover, it is worth noting that misunderstandings can arise in sustainable analytical chemistry, where conventional petrochemical solvents are often considered more practical than biobased solvents, even though biobased solvents are generally regarded as having a lower environmental impact than their petrochemical counterparts.

Different methods and datasets are used in order to assess hazards associated to chemicals. One first approach relies on data from the Global Harmonized System (GHS). AGREE, AES, HEXAGON and certain versions of RGB use the number of GHS pictograms as an input. They have the advantage of being easy to collect and widely used. AGREE, AGREEprep and RGB12 focus on the total number of unavoidable hazards (pictograms) in a method. This approach may be criticised for being overly simplistic, as it fails to reflect levels and characteristics of hazards. For SPMS, toxicity is assessed in conjunction with the origin of the species (petrochemical, biobased, etc.) using the 'degradable' and 'persistent' indications on the SDS, based on the principle that degradable species have a lesser impact than persistent species. It is important to note that care must be taken to avoid confusion between origin and toxicity: a natural/biobased origin is not synonymous with non-toxicity or degradability (e.g. limonene). AES and the WHN, which is used by ChlorTox Scale in the RGB model, for their part, take into account the differences in levels of potential danger attributed to the chemicals by weighting the number of hazards according to the hazard category mentioned on the SDS (1, 2, 3 or 4). Only HEXAGON includes a differentiation of the hazard characteristics based on the prioritisation work of Phan et al. [33]. For example, carcinogenic substances are assigned higher penalty points (3) compared to eye irritants (2). But this tool does not include categories of hazard considerations. Similar to GHS-based methods, GAPI uses the NFPA classification to assess health and safety hazards, but does not include environmental assessment.

In contrast to methods relying primarily on SDS data or hazard pictograms, LCA evaluates toxicity using standardized impact assessment models, such as USEtox®[34]. These models calculate characterization factors for human toxicity (carcinogenic and non-carcinogenic) and freshwater ecotoxicity, based on fate–exposure–effect modelling. Input data include physicochemical properties (e.g., half-lives, partition coefficients), emission quantities, and toxicological endpoints such as EC50, NOAEL or LD50. Another approach is the use of SHE factors, which assign a specific factor to each hazard category: S for safety, H for health, and E for the environment. This method is used by HPLC-EAT with SHE factors calculated by Koller and al. [23], and by AMGS where SHE factors are presented in the SSG. Incorporating SHE factors into chemical assessments enhances the understanding and differentiation of chemical hazards while providing semi-quantitative data. The last approach is CHEMS-1 which can be used in the ChlorTox Scale within the RGB model, and is supplemented by Tobwieski and al. [35]. It calculates a "Hazard Value" for each chemical based on data from SDS. This algorithm considers factors related to oral toxicity, inhalation toxicity, carcinogenicity, aquatic acute and chronic toxicities and exposure-related factors such as biodegradability, hydrolysis and bioconcentration. These methods are based on concrete toxicity data, and differentiate between the various hazards and their levels.

In the modern sense of the word, "risk" relates to the likelihood of a danger occurring and the potential consequences it may cause. Since risk involves both hazard and exposure, these two factors should not be assessed separately. However, most tools studied in this work fail to fully assess the risk associated with chemical use because they evaluate hazards and quantities independently. Tools such as GAPI, HEXAGON, AGREE, AGREEprep, SPMS and RGB (apart from the version that uses ChlorTox) assess hazards and quantities separately. In addition, their evaluations take a holistic approach, focusing on the overall hazards and quantities rather than assessing each chemical individually. Thus, two methods using a total volume of 50 mL of solvents (for example, chloroform and methanol) but using different individual volumes (for example (i) 10 mL of chloroform and 40 mL of methanol for the first method and (ii) 10 mL of methanol and 40 mL of chloroform for the second) will have the same assessment, even though the second is more toxic than the first. One the other hand, HPLC-EAT, AMGS, AES, LCA and the RGB model integrate these two aspects by multiplying a score or a factor for hazards and another for quantities, thus enabling a more accurate risk assessment of analytical methods.

### 3.3. Assessment of the electrical consumption

Minimizing energy consumption is also a key objective of sustainable analytical chemistry, as reflected in several principles within the frameworks of:

- GAC with principles 4. "Integration of analytical processes and operations saves energy and reduces the use of reagents" and 9. "The use of energy should be minimized".
- GSP with principles 8. "Minimize energy consumption" and 9. "Choose the greenest possible post-sample preparation configuration for analysis".
- WAC with principle G3. "Energy and other media: analytical methods should be characterized by the lowest possible consumption of electricity and other utilities".

Consequently, electricity consumption has been included as a criterion to be assessed in most of the presented tools , with the exception of HPLC-EAT, AMVI and BAGI. Depending on the tool, this energy consumption is either estimated or calculated. Some of them rely on reference data that indicate average consumption according to the type of instrument used. In 2009, Raynie and al. reported data [36] on the energy consumption of different types of devices that can be used during analytical development. Among the presented tools, AES, GAPI, AGREE, AGREEprep integrate these data. It is worth noting, however, that these latter were determined almost 20 years ago. Technological advancements over the intervening years may have significantly altered the energy consumption of the instruments. The SPMS is based on similar approach, but proposes to detail consumption by extraction protocol step: (i) dispersion/stir, (ii) separation and (iii) temperature. HEXAGON (power data) and AMGS (energydata) also provide similar data based on their own, more recent measurements. However, the specific instruments used for these measurements are not disclosed. Importantly, it is possible to calculate the actual energy consumed and provide this data rather than relying on estimates from tables, using Eq. (5).

$$Energy(kWh) = Power(kW) \times Time(h) \tag{5}$$

The authors of AGREE recommend, for example, considering the power specified in the technical documentation, which is often the maximum power. However, the authors of AMGS demonstrated that actual power usage is often significantly lower than this maximum. According to their measurements, the average power consumption of instruments is approximately 40 % of their maximum power. Moreover, actual power consumption can considerably vary depending on the various parameters applied to the instruments (temperature, etc.). Therefore, the only way to get accurate estimations is to take direct measurements. For LCA, the methodology does not formally specify a way of estimating energy consumption, but it does state that the data used may be external or derived from direct measurements.

### 3.4. Towards the quantification of impacts

The quantification of the environmental impact of analytical methods is built on two main points: (i) defining the effects that the method may have on the environment and health (e.g., global warming) and (ii) measuring the magnitude of these effects, which requires the use of specific units (e.g., kg $CO_2$-eq). Most of the presented tools do not quantify the impact of methods, as their assessment results are expressed as overall scores that, in most cases, neither specify the nature of the impacts nor their magnitude. In practice, this is not the intended purpose of these tools, which are designed primarily to facilitate comparisons and to assess green and/or sustainable nature of different methods.

Only a few of the discussed tools provide a partial or complete quantification of the impacts of analytical methods. The first is HEXAGON, which (i) encourages estimating the real costs of methods and therefore to quantify their economic impact and (ii) introduces the concept of the carbon footprint (CF) to quantify the environmental impact of methods. The CF is initially an indicator designed to quantify the greenhouse gases (GHGs) emitted throughout the life cycle of an activity-in this case, an analytical method. This includes direct emissions (e.g., those associated with energy consumption to operate instruments, the use of chemical reagents, waste production) as well as indirect emissions (e.g., those related to the manufacture of equipment, production of consumables, the transport of samples and reagents). The authors suggest to calculate the CF according to Eq. (6) with an emission factor of 0.247 kg $CO_2$-eq/kWh for electricity [37].

$$CF = \quad EF_{elec} \sum_{n} P_n t_n \tag{6}$$

With $EF_{electricity}$ the emission factor for electricity in Kg-CO2 per kWh, $P_n$ the power of instrument n, $t_n$ the operating time of instrument n

Nevertheless, this factor is not universal and varies significantly from one country to another. This variation is due to differences in electricity mix, which is the proportion of different energy sources used in electricity production (fossil fuels, nuclear and renewables), as well as the varying emission factors of each source/fuel. For example, as shown in Fig. 2 and Table 3, in 2021 France had a relatively low emission factor for electricity of 0.087 kg $CO_2$-eq/kWh because its mix relied mainly on nuclear power (69 %), a low carbon source. In contrast, Germany's emission factor was much higher, at 0.438 kg $CO_2$-eq/kWh, due to its reliance on fossil fuels for 48 % of its electricity mix [38,39].

Additionally, to calculate the CF, the authors suggest focusing solely on emissions related to the use of instrumental devices, that is, the energy consumption within the laboratory. However, other components of the analytical process also contribute to GHG emissions. This is the case for reagents and consumables such as solvents, whose GHG emissions are linked to their production, use and end-of-life, as well as to the transportation of samples, waste treatment, etc. To provide a more comprehensive and accurate evaluation of environmental impacts of analytical method, the scope of these assessments must be expanded.

While calculating the carbon footprint (CF) of a method is valuable for assessing its contribution to global warming through the quantification of GHG emissions, it does not provide a comprehensive picture of the method's overall environmental impact. In this sense, LCA is a tool that enables a broader assessment of environmental impact by considering a wider range of environmental impacts, depending on the method used, such as those outlined in Table 1 if ReCiPe 2016 is used. LCA quantifies all impacts using a standardised unit, enabling direct comparisons between methods and highlighting opportunities for improvements to reduce these impacts. Furthermore, LCA takes into account the entire life cycle (production, use and end-of-life) and all the processes related to items (consumables, energy, etc.) used. This is in contrast to other tools, which primarily focus on laboratory use, with a few exceptions. This broader perspective enables a more complete evaluation of environmental impacts and reduces the risk of overlooking potential

**Table 3**
Emission factors for electricity of France, Germany, Spain, Sweden and Hungary in 2021, calculated according to LCA GHG method [38].

| | France | Germany | Spain | Sweden | Hungary |
|---|---|---|---|---|---|
| Emission factor (in kg $CO_2$-eq/kWh) | 0.087 | 0.438 | 0.236 | 0.027 | 0.226 |

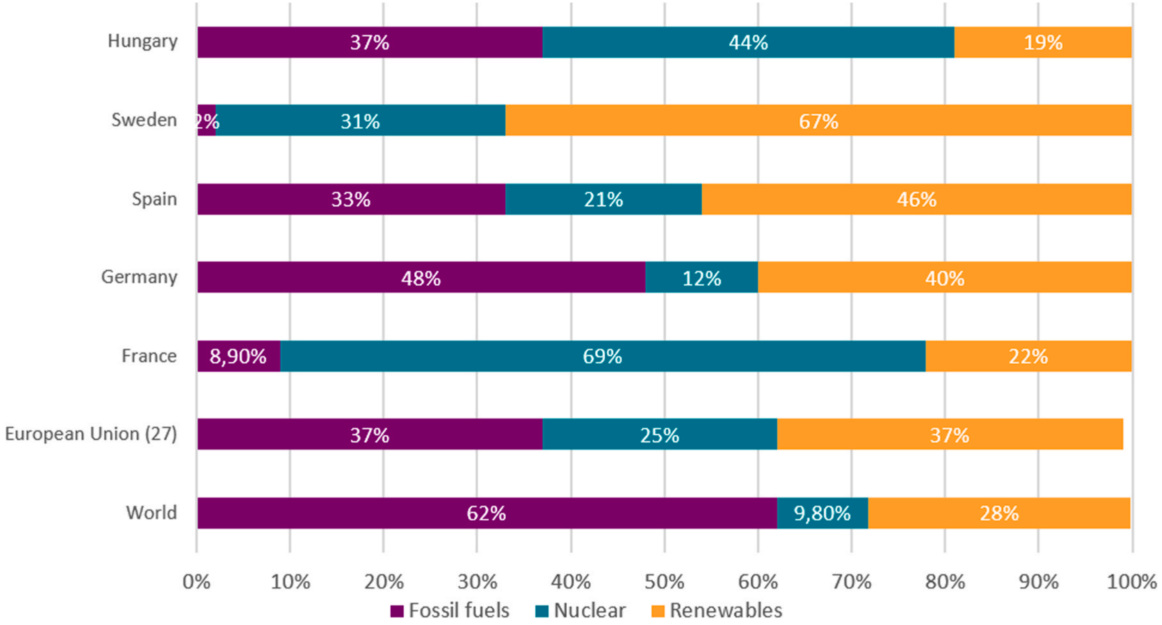


**Fig. 2.** Electric mixes of the world, the European Union, France, Germany, Spain, Sweden and Hungary in 2021 [38].

environmental hotspots, which could otherwise lead to suboptimal or even counterproductive eco-design decisions. However, LCA remains inherently global in scope, making it challenging to translate quantified impacts to the laboratory scale, particularly in terms of operator safety.

The last tool able to quantify impact is ChlorTox Scale used by RGBfast. The aim of this tool is to quantify the chemical risk associated with an analytical method using a standardised unit: the chloroform equivalent ($CHCl_3$-eq in g). The result given by Chlortox Scale indicates the degree of chemical risk posed by using an equivalent amount of chloroform. This tool therefore provides quantified data on the direct chemical impact, specifically in the laboratory. It could therefore be used as a complement to other tools, such as LCA.

## 4. Conclusions

Assessing the sustainability of analytical methods has become a priority in a context of heightened awareness of environmental and health impacts, especially as it relates to environmental monitoring. Numerous tools have been developed to assess and improve the greenness, whiteness or the sustainability of analytical methods. However, despite the large diversity of available tools, no single approach comprehensively addresses the entire analytical process while simultaneously integrating all dimensions of sustainability, i.e. environmental, performance, practical and economic aspects in the case of analytical chemistry. However, it is questionable whether it is really necessary to include analytical performance criteria in this field, given that these are already well-established in method development. This leads to the question of whether practical, economic and environmental aspects should take priority over analytical performance, or vice versa.

Focusing solely on GAC considerations, efforts need to be done to assess the impact of data analysis as well as the data storage. There is also a need to focus on quantifying environmental and health impacts. For instance, tools like LCA offer a holistic and promising approach as a standardised tool, offering flexibility that allows adaptation to different types of method evaluation (comparison, calculation of overall impact, etc.). Although LCA may appear complex, this complexity should not be viewed as a limitation, but rather as an opportunity to encourage the rigorous quantification of impacts and the integration of eco-design of our methods. However, its holistic nature means that, at present, it cannot be applied at a laboratory scale to determine the impact of the methods on operators. That is why it still needs to be used in combination with other tools.

## CRediT authorship contribution statement

**Durand Louise:** Writing – original draft, Methodology, Investigation, Formal analysis, Conceptualization. **Wiest Laure:** Writing – review & editing, Validation, Supervision, Methodology, Investigation, Conceptualization. **Vulliet Emmanuelle:** Writing – review & editing, Supervision, Project administration, Methodology, Investigation, Funding acquisition.

## Declaration of Competing Interest

The authors declare that the wok described has not been published previously, that it is not under consideration for publication elsewhere, that its publication is approved by all authors and tacitly or explicitly by the responsible authorities where the work was carried out, and that, if accepted, it will not be published elsewhere in the same form.

## Acknowledgments

This work has been supported by BIOSYSMO project from the European Union's Horizon Europe research and innovation program under grant agreement No 101060211. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or REA. Neither the European Union nor the granting authority can be held responsible for them.

## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.teac.2025.e00275.

## Data availability

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

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