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Blue applicability grade index (BAGI) and software: a new tool for the evaluation of method practicality

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In this work, blue applicability grade index (BAGI) is proposed as a new metric tool for evaluating the practicality of an analytical method. BAGI can be considered complementary to the well-established green metrics, and it is mainly focused on the practical aspects of White Analytical Chemistry. This tool evaluates ten main attributes including the type of analysis, the number of analytes that are simultaneously determined, the number of samples that can be analyzed per hour, the type of reagents and materials used in the analytical method, the required instrumentation, the number of samples that can be simultaneously treated, the requirement for preconcentration, the automation degree, the type of sample preparation, and the amount of sample. Through the evaluation of these attributes, an asteroid pictogram is generated, together with the respective score. To facilitate the use of the metric a simple, open-source application was created (mostwiedzy.pl/bagi). It is accompanied by a web application available at bagi-index.anvil.app. The functionality of the tool was demonstrated by evaluating the applicability of five different analytical methods as case studies. All things considered, BAGI can be easily used to identify the weak and strong points of a method in terms of practicality and applicability, as well as to compare the performance of different analytical methods. We believe that BAGI metric tool will gain not only attention but also trust and acceptance from the chemical community.

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1. Introduction

Green chemistry was originally proposed in the 1990s by Paul Anastas and John Warner as a way in which the skills, knowledge, and talents of chemists can be combined to avoid threats to human health and the environment in all types of chemical processes.[1] Green Analytical Chemistry (GAC)[2] is a concept that emerged from green chemistry in 2000 and it concerns the role of analytical chemists in making laboratory practices more environmentally friendly. GAC considers different aspects of an analytical method including the safety of solvents/reagents, the generation of toxic laboratory wastes, the safety of the analysts, and the energy demands, aiming to redefine and reevaluate the analytical methods. Moreover, the ten principles of Green Sample Preparation (GSP) were proposed aiming to chart the path towards the development of greener sample preparation methods, to minimize the environmental impact of this step and to enhance sample throughput.[3] Thus, today compliance with green chemistry, GAC,[2] and GSP[3] principles has become a necessity in the development of analytical methods to reassure sustainability requirements. More recently, the Unified Greenness Theory was presented that merged the principles of green chemistry, GAC, and other sets of principles and introduced a novel set of hierarchal and universal statements.[4]

Several green metric tools have been proposed and already implemented in recent publications to evaluate the green performance of an analytical method and its subsequent impact on the environment. These tools include the National Environmental Method Index (NEMI),[5] analytical eco-scale,[6] green analytical procedure index (GAPI),[7] analytical greenness calculator (AGREE),[8] complementary green analytical procedure index (ComplexGAPI),[9] and analytical greenness metric for sample preparation (AGREEprep).[10] Each of the above-mentioned tools has certain advantages and disadvantages; thus, some of them have prevailed since they provide a more quantitative description of the green character of the method.

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However, none of these tools considers the practicality of the method, which is a very important parameter that is encountered by all routine analysis laboratories. This parameter has been already included in the concept of White Analytical Chemistry (WAC) that was introduced in 2021 by Nowak *et al*.[11] WAC serves as an extension and complement to green analytical chemistry and combines the ecological, analytical, and practical perspectives of an analytical method according to the red-green-blue (RGB) model.[12] The red colour of WAC is related to the analytical efficiency as described by the method's validation criteria (accuracy, precision, sensitivity, and others), while blue represents the productivity and practical/economic efficiency of the method. The four attributes of the 'blue' category correspond to cost-efficiency, time-efficiency, requirements, and operational simplicity.

In this article, we introduce a simple and fast metric tool for the evaluation of the practicality of any analytical method (*e.g.*, conventional, state-of-the-art, newly developed, *etc*.). As such, the blue applicability grade index (BAGI) is developed and proposed herein. The blue colour is inspired by the RGB model, and the proposed index may be considered a complementary concept to the existing green metrics tools. To facilitate its use open-source desktop and web applications were developed, and their functionality was demonstrated based on various analytical methods. The target audience of this new tool includes but is not restricted to analytical method developers and users from academia, industry and routine analysis laboratories. BAGI tool has many advantages with the most important being complementary to the existing green assessment tools such as complexGAPI and AGREEprep. In addition, it is in line with the principles of environmental sustainability. We believe that the BAGI metric tool will gain not only attention but also trust and acceptance from the chemical community.

2. Characteristics of the BAGI attributes

To evaluate the applicability of an analytical method, the BAGI metric tool takes into consideration the following main attributes:

1. The type of analysis.
2. The number of analytes that are simultaneously determined.
3. The analytical technique and required analytical instrumentation.
4. The number of samples that can be simultaneously treated.
5. The sample preparation.
6. The number of samples that can be analyzed per hour.
7. The type of reagents and materials used in the analytical method.
8. The requirement for preconcentration
9. The automation degree.
10. The amount of sample.

Attributes 1–3 correspond to the step of the analytical determination, attributes 4 and 5 correspond to the sample preparation step, while attributes 6–10 correspond to both steps. The selection of the main attributes and their respective levels was based on a consideration of a wide range of different analytical methods that were reported in the literature. To ensure the simplicity of the performance, four discrete scores of equal weights are used in the assessment. Each score corresponds to a different hue (for the qualitative evaluation of the method's applicability) and contributes to the final, overall score (for the quantitative evaluation of the method's applicability). In this sense, 10, 7.5, 5.0, and 2.5 points correspond to dark blue (#0c305b), blue (#3a89c1), light blue (#adcffd), and white (#FFFFFF), respectively. The BAGI tool also takes into consideration the field of application to adjust the bias and treat all methods at realistic ranges. For example, it distinguishes the differences between bioanalytical methods that can be applied to low sample amounts requiring low reagents amounts and food or environmental samples, where the sample amount can be easily increased to achieve the criteria required by legislation and the necessary sensitivity.

2.1 Description of attributes

2.1.1 Type of analysis. The type of analysis is classified into the following categories: qualitative (white), screening (light blue), quantitative (blue), and quantitative and confirmatory (dark blue). According to the European Commission Decision 657/2002/EC,[13] a confirmatory method can provide full or complementary information enabling the substance to be unequivocally identified and if necessary quantified at the level of interest by providing information regarding the chemical structure of the analyte. Thus, quantitative and confirmatory methods get the highest score (*i.e.*, 10 points), while only quantitative methods that can determine the amount or mass fraction of a substance so that it may be expressed as a numerical value of appropriate units with simple detection techniques, get 7.5 points. Screening methods that are used for the detection of the presence of a substance or class of substances at the level of interest and are specifically designed to avoid false compliant results get 5 points, while simple qualitative methods that are used to identify a substance based on its chemical, biological, or physical properties get 2.5 points.

2.1.2 Number of analytes that are simultaneously determined. According to the 12 principles of GAC,[2] multi-analyte methods are preferred over methods that are used for the determination of one analyte at a time. In the BAGI metric tool, a multi-element analysis targeting more than 15 analytes at a time gets the highest score of 10 points, while a single-element analysis gets the lowest score of 2.5 points. For multi-element methods that are used for the determination of 6–15 analytes of the same chemical class or 2–15 analytes of different chemical class 7.5 points are attained, while 5 points are attained for a method that leads to the multi-element analysis for 2–5 compounds of the same chemical class.

2.1.3 Analytical technique-instrumentation. The analytical technique and the relevant instrumentation that is required

also play a crucial role in the selection of an analytical method. When simple in operation, portable instrumentation (*e.g.*, smartphone-based detectors, portable gas chromatographs, *etc.*) is used, the method gets 10 points. The score of 7.5 is reached by a method that uses simple instrumentation available in most labs (*e.g.*, ultraviolet spectrometry, high-performance liquid chromatography-ultraviolet detection, high-performance liquid chromatography-diode array detection, ultra-high performance liquid chromatography, flame atomic absorption spectrometry, electrothermal atomic absorption spectrometry, inductively coupled plasma-optical emission spectrometry, gas chromatography-flame ionization detection *etc.*). If sophisticated instrumentation (*e.g.*, liquid chromatography-mass spectrometry, gas chromatography-mass spectrometry, inductively coupled plasma-mass spectrometry, homemade interfaces, homemade automatic systems *etc.*) is required, then 5 points are attained. Finally, in the case of instrumentation that is not commonly available in most laboratories (*e.g.*, supercritical fluid chromatography, two-dimensional gas and liquid chromatography, liquid chromatography-tandem mass spectrometry, gas chromatography-tandem mass spectrometry *etc.*) the method attains 2.5 points.

2.1.4 Number of samples that can be simultaneously treated. Undoubtedly, sample preparation is considered the bottleneck of the analytical procedure, however, it is also the cornerstone of an efficient analytical method. Moreover, it is the most tedious and laborious step that accounts for a significant part of the total time that is required for the determination of the target analyte(s). In this frame, various formats have been developed to enable the simultaneous sample preparation of an increased number of samples leading to high-throughput methods. Since well plate formats are currently commercially available, making the sample pretreatment simpler, faster, and safer for the analytical scientist,[14] 10 points are assigned to a method that enables the simultaneous sample preparation of more than 95 samples (*e.g.*, 96-well plates). Such a method is considered the most practical and thus it gets the highest score. In the case of single sample preparation, only 2.5 points are reached. For the simultaneous sample preparation of 2–12 samples (*e.g.*, using the 12 ports of conventional solid-phase extraction manifolds), 5 points are assigned to the method, while 7.5 points are assigned in the case of the simultaneous sample preparation of 13–95 samples.

2.1.5 The sample preparation scale. The sample preparation scale is another significant aspect of the analytical method since it clearly affects the reagents consumption and waste generation. Apart from the impact of these two aspects on the environment, they can also affect the selection of a method by a routine analysis laboratory since they are closely related to the cost of the method. If on-site sample preparation can be performed or if no sample preparation is required, 10 points are added to the total score. When simple, low-cost sample preparation is required (*e.g.*, protein precipitation) the method gets 7.5 points, while a miniaturized extraction sample preparation technique (*e.g.*, solid-phase microextraction, dispersive liquid–liquid microextraction, microextraction by packed sorbents, stir bar sorptive extraction, fabric phase sorptive extraction) gets 5 points. A score of 2.5 points is assigned to the method when conventional sample preparation is required in one or more steps (*e.g.* liquid–liquid extraction, solid-phase extraction, matrix solid-phase dispersion and/or derivatization).

2.1.6 Number of samples that can be analysed per hour. An analytical method that is characterized by high sample throughput is highly desired in routine analysis laboratories. A method with which more than 10 samples can be analysed per hour (including all the steps from sample pre-treatment to the final step of the determination) gets 10 points. For analytical methods that can be implemented for the analysis of 5–10 samples 7.5 points are added, while when the throughput of 2–4 samples per hour results in 5 points. In case at least one hour or more is needed for a single sample to be prepared and analyzed a score of 2.5 points is attained.

2.1.7 Type of reagents and materials. The availability and cost of the reagents and materials that are required is an important aspect that affects the selection of an analytical method by a laboratory. In BAGI, the indirect approach of the implementation of cost analysis which is reflected on different attributes of this tool (*e.g.*, instrumentation, sample preparation, reagents *etc.*) was adopted to ensure the practicality of the blue assessment since the accurate of the cost is a complicated and disputable. It is well known that the cost of common commercially available reagents can vary significantly among different classes of chemicals, however, the practicality of being able to use a commercial reagent without having to synthesize it in the lab is undeniable. This is very important for accredited laboratories that are only able to use commercially available reagents and standard methods.

Taking all into consideration, the analytical method gets 10 points in cases where common commercially available reagents (*e.g.* methanol, acetonitrile, HNO_3, nitrogen or other common gases), are used. When commercially available reagents are required that are non-common in quality control laboratories (*e.g.*, derivatization reagents, solid-phase extraction cartridges, solid-phase microextraction fibres), a score of 7.5 is attained. However, in cases where reagents are needed to be synthesized in the laboratory, a score of 5 or 2.5 points is added to the total, considering whether this can be performed in a simple way using common laboratory equipment or involves the use of advanced equipment/know-how (*e.g.*, specially designed metal–organic frameworks), respectively.

2.1.8 Requirement for preconcentration. Conforming with the concept of fit-for-purpose is essential for a method to be practical. When no pre-concentration is needed in order to meet the required sensitivity and/or the legislation criteria, a score of 10 points is assigned to the method. In cases where preconcentration is required, 7.5 points are assigned if the desired sensitivity is met with one step (*e.g.*, simultaneous sample preparation and preconcentration by choosing appropriate initial and final sample volumes during extraction). Finally, if the legislation criteria are met after the combination of different stages of preconcentration (*e.g.*, extraction, evaporation, reconstitution), 2.5 points are assigned.

2.1.9 The automation degree. The automation of an analytical procedure is also an important feature based on the requirements of GAC[2] and GSP.[3] In the context of applicability, automated methods are highly desired to minimize human intervention resulting in potential errors, while also reducing the exposure of the analyst to hazardous chemicals. Fully automated methods (with novel technologies, advanced devices, *etc.*) get 10 points, semi-automated methods with common devices (*e.g.*, HPLC autosampler) get 7.5 points, and semi-automated methods that require the special design of novel systems (*e.g.*, homemade) get 5 points. Manual treatment and analysis get only 2.5 points as the worst-case scenario.

2.1.10 The amount of sample. The amount of sample can directly affect the sensitivity of the analytical method, as well as the waste generation. The sample availability clearly depends on the type of the sample. In general, low sample quantities are available for bioanalytical samples, while for food and environmental samples, higher volumes can be easily utilized. As such, 10 points are attained for sample volumes below 100 μL or 100 mg for bioanalytical samples, or below 10 mL or 10 g for food or environmental samples. When the required amount is 101–500 μL for bioanalytical samples or 10.1–50 g for food/environmental samples, the score is 7.5 points, while 5 points are added to the total score in cases where a method requires 501–1000 μL for bioanalytical samples or 51–100 g for food/environmental samples. Just 2.5 points are added to the score for a method that uses more than 1000 μL of bioanalytical samples or more than 100 g of food/environmental samples. It must be noted that in case of samples that do not directly fall into the above-mentioned categories (*e.g.*, cosmetic products, plastic leachates) their size availability must be considered, and they can be categorized either as low quantity (similar to the bioanalytical matrices) or as normal quantity (similar to food/environmental matrices) samples.

The attributes along with their respective hues and score points are summarized in Table 1. It should be noted that when clear score cannot be given or the researcher are on the verge of two options, they have to choose the one that is closer to the available scores, based on their expertise.

2.2 Explanation of the obtained results

Two different types of results can be obtained using the BAGI metric tool which are correlated to the obtained pictogram and the obtained score. The overall assessment result is an asteroid pictogram with the number in its centre. The hue scale of the pictogram shows the compliance of the method with the set criteria (*i.e.*, dark blue for high compliance, blue for medium compliance, light blue for low compliance, and white for no compliance). The number in the inner part of the BAGI pictogram reveals the assigned overall score of the analytical method and it ranges between 25–100. The worst method performance in terms of applicability is assigned to a score value of 25, while a score value of 100 reveals the excellent performance of the method. In order to be considered practical", it is recommended that the method attains at least 60 points. This score is recommendable, but not determinant. The ten parts of the asteroid pictogram are related to the different performance criteria, and they are considered of equal importance. The attributes 1–5 that correspond either to the step of the analytical determination or to the step of the sample preparation are in the inner part of the pictogram, while the attributes 6–10 that correspond to both steps are in the outer part. The central field containing the score is assigned a hue based on the value of the total score by sampling from the whole range of the matplotlib 'blues' sequential colourmap[15] mapped to the 25–100 scale. The discrete hues for the individual fields of the pictogram were sampled from the same colour map. This allowed to obtain a perceptually uniform mapping of hues to values that is colour-blind-safe and legible when reproduced in grayscale.[16] This is akin to the approach used in the AGREE and AGREEprep tools.[8,10]

Using the overall BAGI pictogram it is easy to find the weak and strong points of an analytical method by evaluating its applicability in terms of practicality to further improve them and to compare the performance of different methods.

3. Application of BAGI to selected methods

In this section, the utilization of the BAGI index web app is demonstrated. For this purpose, the new tool was used to evaluate the applicability of five different analytical methods dealing with the determination of antidepressants in post-mortem whole blood and cerebrospinal liquor,[17] bisphenol A (BPA) in food contact materials' leachates,[18] androgens and progestogens in environmental water samples,[19] ibuprofen in milk-containing simulated gastrointestinal media,[20] and quinine in soft drinks.[21] The BAGI index pictograms for these methods are depicted in Fig. 1.

In the first case study, a fabric phase sorptive (FPSE) extraction method combined with high-performance liquid chromatography-diode array detection (HPLC-DAD) was used for the quantification of seven different antidepressant drugs in human whole blood, plasma, and urine.[17] The information of the analysis was both quantitative and confirmatory due to the employment of the DAD detector that was set in the range of 200–400 nm. The determination enabled the quantification of seven compounds belonging to three different classes (*i.e.*, serotonin and norepinephrine reuptake inhibitor; selective serotonin reuptake inhibitors and tricyclic antidepressants). Since the FPSE membranes are not commercially available, they need to be synthesized in the lab in a relatively simple and straightforward way using simple equipment. Regarding the instrumentation, simple equipment available in most labs was employed. The simultaneous sample preparation of almost 20 samples was assumed, which can be easily performed using two magnetic stirrers. Following the simultaneous sample preparation of the 20 samples that requires a time span of around 40 min, the total analysis time by HPLC-DAD is

Table 1 Main attributes, corresponding hues, and score points of the BAGI index

Criterion	Attribute	Dark blue (10 points)	Blue (7.5 points)	Light blue (5 points)	White (2.5 points)
1	Type of analysis	Quantitative and confirmatory	Quantitative	Screening	Qualitative
2	Multi- or single-element analysis	Multi-element analysis for >15 compounds	Multi-element analysis for 6–15 compounds of the same chemical class or 2–15 compounds of different chemical classes	Multi-element analysis for 2–5 compounds of the same chemical class	Single element
3	Analytical technique[a]	Simple in operation portable instrumentation (*e.g.*, smart-phone based detectors, portable GC)	Simple instrumentation available in most labs (*e.g.*, UV, HPLC-UV, HPLC-DAD, UHPLC, FAAS, ETAAS, ICP-OES, GC-FID)	Sophisticated instrumentation (*e.g.*, LC-MS, GC-MS, ICP-MS, homemade interfaces, homemade automatic systems)	Instrumentation that is not commonly available in most labs (*e.g.*, SFC, 2D-GC, 2D-LC, LC-MS/MS, GC-MS/MS)
4	Simultaneous sample preparation	>95	13–95	2–12	1
5	Sample preparation[b]	Not required or on-site sample preparation if required	Simple low-cost sample preparation is required (protein precipitation *etc.*)	Miniaturized extraction sample preparation (*e.g.*, SPME, DLLME, MEPS, SBSE, d-SPE, FPSE)	Multi-step sample preparation is required (*e.g.*, LLE, SPE and/or derivatization)
6	Samples per h (sample preparation + analysis time)	>10	5–10	2–4	≤1
7	Reagents and materials	Common commercially available reagents (methanol, acetonitrile, HNO_3, nitrogen or other common gases *etc.*).	Commercially available reagents that are non-common in QC labs (*e.g.*, derivatization reagents, SPE cartridges, SPME fibres)	Need to be synthesized in the lab with common instrumentation and in a simple way.	Need to be synthesized in the lab with advanced equipment or know-how (*e.g.*, specially designed metal–organic frameworks, modified nanomaterials).
8	Preconcentration	No preconcentration is required. Required sensitivity and/or legislation criteria are directly met.	Preconcentration is required. Required sensitivity is met with one-step preconcentration.	—	Preconcentration is required. Legislation criteria are met after complicated stages (*e.g.*, extraction, evaporation, and reconstitution).
9	Automation degree	Fully automated with novel technology advanced devices (*e.g.*, robotics, lab-in-syringe)	Semi-automated with common devices (HPLC autosampler, *etc.*)	Semi-automated with non-common devices (homemade systems, *etc.*)	Manual treatment and analysis.
10	Amount of sample	≤100 μL (or mg) bioanalytical samples ≤10 mL (or g) food/environmental/other.	101–500 μL (or mg) bioanalytical samples 10.1–50 mL (or g) food/environmental.	501–1000 μL (or mg) bioanalytical samples 51–100 mL (or g) food/environmental.	>1000 μL (or mg) bioanalytical samples >100 mL (or g) food/environmental.

[a] GC: gas chromatography, UV: ultraviolet spectrometry, HPLC-UV: high-performance liquid chromatography-ultraviolet detection, HPLC-DAD: high-performance liquid chromatography-diode array detection, UHPLC: ultra-high performance liquid chromatography, FAAS: flame atomic absorption spectrometry, ETAAS: electrothermal atomic absorption spectrometry, ICP-OES: inductively coupled plasma-optical emission spectrometry, GC-FID: gas chromatography-flame ionization detection, LC-MS: liquid chromatography-mass spectrometry, GC-MS: gas chromatography-mass spectrometry, ICP-MS: inductively coupled plasma-mass spectrometry, SFC: supercritical fluid chromatography, 2D-LC: two-dimensional liquid chromatography, 2D-GC: two-dimensional gas chromatography, LC-MS/MS: liquid chromatography-tandem mass spectrometry, GC-MS/MS: gas chromatography-tandem mass spectrometry. [b] SPME: solid phase microextraction, DLLME: dispersive liquid–liquid extraction, MEPS: microextraction by packed sorbents, SBSE: stir bar sorptive extraction, d-SPE: dispersive solid-phase extraction, FPSE: fabric phase sorptive, LLE: liquid–liquid extraction, SPE: solid-phase extraction.

20 min, resulting in a sample throughput of 2.7 h^{-1}. As demonstrated by the results, no preconcentration was needed and the required sensitivity was directly achieved. Manual treatment and analysis were performed, which can be considered a drawback of the method, and it can be further improved by automating some steps of the analytical procedure. As for the sample preparation, miniaturized extraction was employed and the sample volume for the bioanalytical matrix was 500 μL. Thus, a BAGI score of 67.5 is attained for the method and the whole protocol shows good applicability potential.

In the second case study, an automatic lab-in-syringe sol–gel coated foam microextraction platform was used for monitoring BPA in food contact materials' leachates during migration studies.[18] The separation and determination of the target analyte were conducted using high-performance liquid chromatography-ultraviolet detection (HPLC-UV), resulting in quantitative analysis. Using this approach, a single element

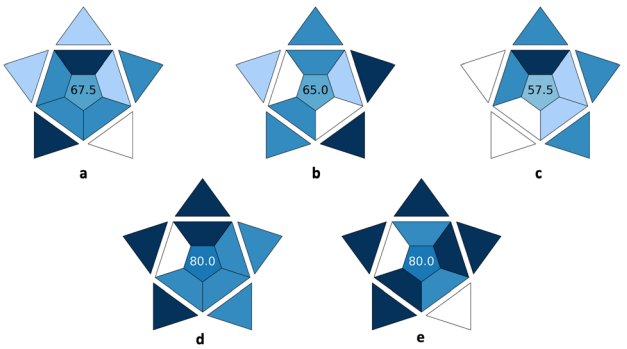

Fig. 1 BAGI index pictograms for five different analytical methods for the (a) determination of antidepressants in post-mortem whole blood and cerebrospinal liquor,[17] (b) bisphenol A (BPA) in food contact materials' leachates,[18] (c) androgens and progestogens in environmental water samples,[19] (d) ibuprofen in milk-containing simulated gastrointestinal media,[20] and (e) quinine in soft drinks.[21]

could be determined, which can be considered as a drawback of the method that can be potentially expanded to include other bisphenols. The sample throughput (sample preparation and analysis) was 5 h^{-1}. The foam microextraction media were not commercially available, and their synthesis in the lab was required. Like the FPSE membranes, this can be performed in a relatively simple way using common reagents. The HPLC-UV system that is required belongs to the category of simple equipment which is available in most labs. Using the lab-in-syringe system, one sample can be treated at a time. The legislation criteria for the migration studies were achieved after the one-step extraction and preconcentration. The whole procedure was fully automatic, and it required the miniaturized extraction of BPA from 10 mL of sample solution. The assigned BAGI score for the developed method was 65, demonstrating its applicability.

In the third case study, the metal–organic framework UiO-66(Zr) was used as a sorbent for the porous membrane-protected micro-solid-phase extraction of androgens and progestogens from environmental water samples prior to their determination by liquid-chromatography tandem mass spectrometry (LC-MS/MS).[19] Using this technique, both quantitative and confirmatory data can be obtained. As target analytes, four compounds belonging to more than one different class were included. Regarding MOF synthesis, advanced know-how and/or instrumentation are typically required for their preparation in the lab. Simultaneous sample preparation of around 10 samples was assumed for the micro-solid-phase extraction procedure that required around 90 min. Since a time span of 2.5 min was required for the LC-MS/MS analysis, the sample throughput (sample preparation and analysis) was between 5–10 h^{-1}. Preconcentration was required after complicated stages including extraction, evaporation, and reconstitution. The LC-MS/MS systems are not commonly available in most labs. Finally, manual systems were used for the sample preparation and analysis, miniaturized extraction was proposed for sample preparation and 20 mL of water sample was required. The method had a BAGI score of 57.5, demonstrating that improvements are required to make it practical in laboratories.

In the fourth case study, the BAGI index was employed for the evaluation of an ultra-performance liquid chromatography-diode array detection (UPLC-DAD) analytical method for the determination of ibuprofen in milk-containing simulated gastrointestinal media.[20] The rapid protein precipitation scheme and the analysis (2.5 min) resulted in a sample throughput of more than 10 h^{-1}. Common, commercially available reagents were used, while instrumentation currently available in most labs was required. Simultaneous sample preparation of approx. 40 samples was assumed. No pre-concentration was required, manual treatment took place, an autosampler was used resulting in semi-automation, simple and low-cost sample preparation was chosen, and a sample volume of 200 μL was used. The BAGI score of 80 that was assigned to the method demonstrates its good applicability.

In the fifth case study, the applicability of an equipment-free paper-based fluorometric method for the determination of quinine in soft drinks was examined.[21] The method was used for the quantification of a single analyte with only common, commercially available reagents and simple in operation instrumentation. The sample throughput of the method was higher than 10 h^{-1}, while a simultaneous sample preparation of around 50 samples was assumed. No preconcentration was required to achieve the required sensitivity, as well as minimal sample preparation (*i.e.*, dilution of the sample). An aliquot of only 1 μL of the sample was required for the analysis, and the whole operation was performed in manual mode. Thus, a BAGI score of 80 was assigned to the method demonstrating its superiority in terms of practicality and applicability .

4. Conclusions

In this work, a novel index that can efficiently assess the practicality and applicability of an analytical method is proposed. BAGI is complementary to the green assessment tools (*e.g.*, GAPI, ComplexGAPI, AGREE, AGREEprep) and it revolves around the "blue" principles of white analytical chemistry, which are mainly related to practical aspects. BAGI considers ten criteria to produce a pictogram and a score that depicts the applicability and functionality of an analytical method. A sequential blue colour scale was used to represent the final score, with discrete hues of dark blue, blue, light blue, and white used to demonstrate high, medium, low, and no compliance of the method with the set criteria, respectively. Regarding the obtained total score, it is recommended to be higher than 60, so that the analytical method can be considered "practical". The proposed index was used to evaluate the applicability in five different analytical methods. The assessment of the applicability of the analytical method is facilitated by using a desktop application (mostwiedzy.pl/bagi) or a corresponding web application (bagi-index.anvil.app) and enables the comparison of different analytical methods at a first glance. The biggest advantage of BAGI is the simplicity and ease of application, which was achieved by preparing an interesting web application that allows to quickly evaluate the

method and copy a colourful pictogram presenting the results of the evaluation. We believe that the BAGI tool will gain attention and acceptance from the chemical community.

Author contributions

N. Manousi: data curation, formal analysis, methodology, writing – original draft, W. Wojnowski: software, visualization, writing – review & editing, J. Płotka-Wasylka: methodology, supervision, visualization, writing – review & editing, V. Samanidou: conceptualization, data curation, formal analysis, methodology, supervision, visualization, writing – review & editing.

Conflicts of interest

There are no conflicts to declare.

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