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Path2Green: introducing 12 green extraction principles and a novel metric for assessing sustainability in biomass valorization

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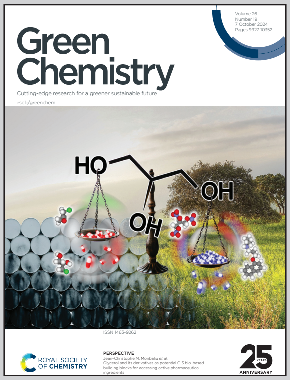

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Path2Green: introducing 12 green extraction principles and a novel metric for assessing sustainability in biomass valorization†

Leonardo M. de Souza Mesquita, *[a] Leticia S. Contieri,[a] Francisca A. e Silva, [b] Rafael Henrique Bagini,[a] Felipe S. Bragagnolo,[a] Monique M. Strieder,[a] Filipe H. B. Sosa,[b] Nicolas Schaeffer, [b] Mara G. Freire, [b] Sónia P. M. Ventura, [b] João A. P. Coutinho [b] and Maurício A. Rostagno[a]

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We propose an innovative approach to address the pressing need for efficient and transparent evaluation techniques to assess extraction processes' sustainability. In response to society's growing demand for natural products and the consequent surge in biomass exploration, a critical imperative arises to ensure that these processes are genuinely environmentally friendly. Extracting natural compounds has traditionally been regarded as a benign activity rooted in ancient practices. However, contemporary extraction methods can also significantly harm the environment if not carefully managed. Recognizing this, we developed a novel metric, *Path2Green*, tailored specifically and rooted in 12 new principles of a green extraction process. *Path2Green* seeks to provide a comprehensive framework beyond conventional metrics, offering a nuanced understanding of the environmental impact of extraction activities from biomass collection/production until the end of the process. By integrating factors such as resource depletion, energy consumption, waste generation, and biodiversity preservation, *Path2Green* aims to offer a holistic assessment of sustainability of an extraction approach. The significance of *Path2Green* lies in its ability to distill complex environmental data into a simple, accessible metric. This facilitates informed decision-making for stakeholders across industries, enabling them to prioritize greener extraction practices. Moreover, by setting clear benchmarks and standards, *Path2Green* incentivizes innovation and drives continuous improvement in sustainability efforts, being a new user-friendly methodology.

1. Introduction

The extraction of bioactive compounds from natural sources has a rich history spanning centuries and has been shaped by civilizations like the Egyptians, Greeks, and Chinese. These civilizations harnessed plants' therapeutic properties, using crude extraction methods such as maceration and infusion to obtain medicinal compounds.[1] The Middle Ages witnessed the emergence of alchemy and a quiet refinement of extraction techniques. Afterward, the scientific and industrial revolution in the 17th and 18th centuries paved the way for significant breakthroughs in extraction methods, pivotal in the isolation and identification of specific compounds.[2] The late 19th and early 20th centuries witnessed the advent of chromatography, a game-changer that continues to advance separation methods. Today, in the metabolomic era, technological progress in extraction methods builds upon this rich history, enhancing our understanding of complex substances and natural extracts.[3] Yet, along with these advancements, the environmental impact of these activities has reached alarming levels.

Today, there is a growing emphasis on an interdisciplinary approach to extract compounds from biomass, especially cost-effectively.[1] By integrating chemistry, biology, engineering, and environmental science expertise, scientists aim to develop innovative and sustainable methods, employing new technologies like ultrasound, microwave, and pressurized liquid extraction. Those approaches are known to improve extraction efficiency and may preserve the bioactivity of the extracted compounds and minimize environmental impact.[4] Despite these advantages, there are still associated burdens. These manifest as economic, social, and environmental impacts, resulting in a range of consequences, including, but not limited to, (i) habitat destruction and depletion of primary resources, (ii) increased energy consumption and greenhouse

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[a] *Multidisciplinary Laboratory of Food and Health (LabMAS), School of Applied Sciences (FCA), University of Campinas, Rua Pedro Zaccaria 1300, 13484-350 Limeira, Sao Paulo, Brazil. E-mail: mesquitalms@gmail.com*
[b] *Department of Chemistry, CICECO – Aveiro Institute of Materials, University of Aveiro Campus Universitário de Santiago, 3810-193 Aveiro, Portugal*

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gas emissions, and (iii) waste generation.[5] The connection of these three dimensions (economic, social, and environmental, representing the 3 Ps in sustainability) highlights the need for a comprehensive understanding of the impacts of extraction activities to develop sustainable practices and mitigate potential harm,[6] ultimately corresponding to the 17 sustainable development goals (SDGs) preconized by the United Nations,[7] which guide the actual global scenario regarding the decision-making of several governments.

The 12 principles of green chemistry, introduced in 1998 by Anastas and Warner in their book "Green Chemistry: Theory and Practice", alerted the scientific community to the need for paradigm shifts. These principles provide a framework for designing and implementing chemical processes and products that are environmentally friendly and sustainable. One notable extension of these principles is the development of the 12 principles of Green Analytical Chemistry.[8] These principles offer a similar framework, but explicitly tailored to analytical chemistry. Other metrics were created to assess sustainability in different fields, like solvents (EcoScale and Chem 21),[9,10] green engineering,[11,12] and products – GreenMotion,[13] and to assess the sustainability of industrial solvent-based processes.[14] However, these existing metrics are highly specific, not allowing the sustainability character or green credentials of extraction activities from biomass to be addressed.

While life cycle analysis (LCA) is regarded as the benchmark for evaluating the environmental implications of processes, it requires costly software, specialized expertise, and databases that present new techniques for conducting the analysis. Thus, considering the need to simplify the analysis without losing effectiveness, devising alternative metrics to address these limitations is necessary.[15] New metrics should provide an understanding of the environmental harm caused by extraction activities and enable a robust evaluation of their sustainability to enhance our ability to assess the environmental consequences of extraction processes.

Due to the lack of a readily accessible method to evaluate the green credentials of extraction processes from biomass, while considering the urgent requirement for a comprehensive, inclusive, user-friendly, and sensitive metric, we herein introduce the 12 green principles of biomass extraction processes. Our goal is to foster the advancement of greener biomass utilization in line with the sustainability pillars. Drawing inspiration from existing metrics and employing an intuitive methodology, we developed a straightforward metric firmly rooted in the three core pillars of sustainability. By defining criteria to assess the environmental impact of an extraction process, this tool aims to promote green chemistry in biomass extraction processes. It has been designed harmoniously with the fundamental sustainable approaches to biomass valorization, ensuring the development of environmentally friendly processes. Hence, we aim to offer valuable guidance to those new to the subject and inspire current researchers to acknowledge the pressing and crucial intellectual challenges we must confront.

2. Principles of a green extraction process

Drawing inspiration from the 12 green chemistry principles and the 12 principles of green analytical chemistry, while considering the previous six principles of green extraction,[16] we formulated the 12 principles of a green extraction process. These principles were established by evaluating attributes throughout the pre- and post-extraction procedures, encompassing parameters that directly influence the extraction approach and its outcome, as illustrated in Fig. 1, and discussed in the following topics.

Principle 1 – Biomass: select biomass that is naturally sourced or requires minimal resource usage for production

The biomass used in the extraction process could be versatile and have multiple roles in many sectors and in the environment. In some cases, the biomass may retain practical applications even after extraction; for example, it can be suitable for bioenergy production, composting, or as feedstock for other processes.[17] A critical point regarding the inherent environmental impact associated with biomass production is centered on land usage. The choice of biomass for extraction predominantly stems from plant-based sources, with extraction processes deeply intertwined with agricultural practices. For example, monoculture, linked to deforestation and heavy pesticide use, contributes to soil degradation, contrasting sharply with polyculture, which aims for crop diversity and sustainability, reducing reliance on agro-pesticides. Additionally, local small-scale cultivation emphasizes eco-conscious practices, fostering environmentally friendly approaches to cultivation.[18–21] In contrast, biomass sourced from the sea often holds a more sustainable edge over land-based biomass. Marine biomass typically involves less competition for resources than land-based agriculture, which often requires greater land, water, and fertilizer inputs.[22] Harvesting sea biomass usually does not demand land conversion or deforestation, reducing the environmental impact. Additionally, marine ecosystems possess a high potential for regeneration.[23] Furthermore, the oceans cover a vast area, potentially accommodating sustainable biomass production without disrupting ecosystems. However, sustainable practices must be implemented to prevent over-harvesting and preserve marine biodiversity.[24]

The assessment considers its abundance and ecological role in cases where biomass is not produced but collected from the environment. While collecting biomass from abundant sources may have minimal consequences for nature, prudent consideration is warranted when dealing with rare, endemic species or those facing extinction risk.[25,26] Conversely, in some cases, the biomass goes to waste despite having significant potential for numerous applications, including in extraction processes.[26] A prominent example is food waste and agriculture residues/byproducts, which are abundant sources of bioactive compounds[27] with high (bio)techno-

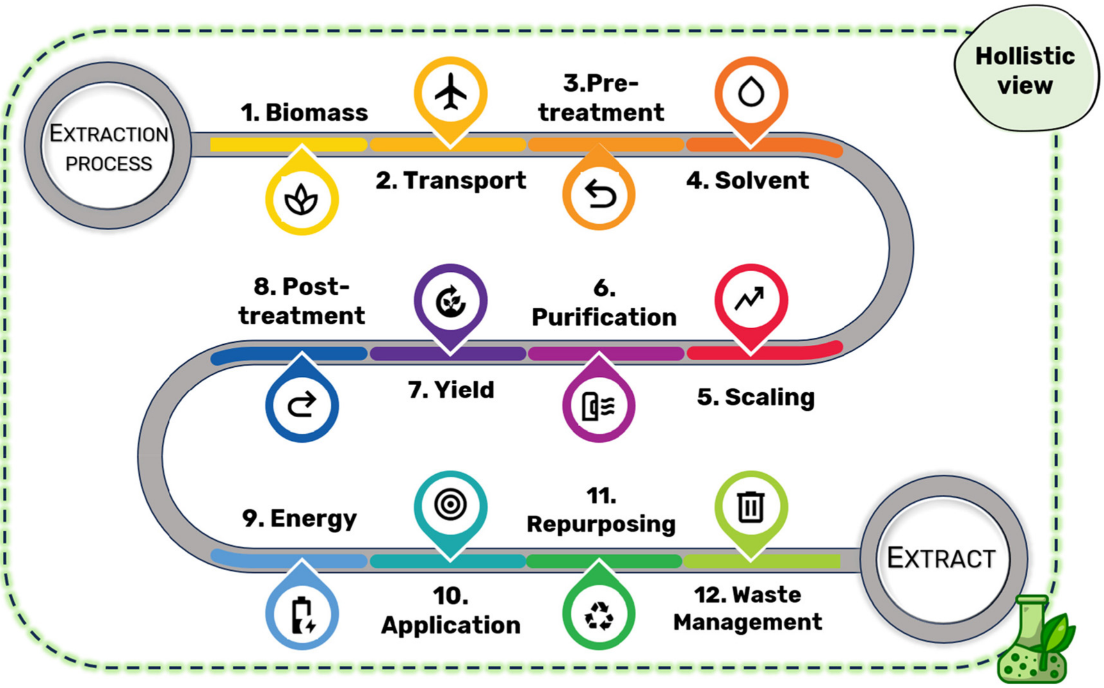

Fig. 1 The 12 principles of a green extraction process evaluated by the *Path2Green* metric.

logical value. By extracting these valuable compounds from waste and residues, we add value to what was once considered refuse, and mitigate the environmental impact associated with its disposal, often conducted in environmentally detrimental ways.[28] This approach creates a win–win situation, benefiting all sustainability pillars.

Microorganisms are another source of biomass typically explored in extraction processes, usually preferred for their advantages, such as easy cultivation in controlled environments, facilitating automation, and ensuring reproducibility between batches, thereby providing a consistent and reliable supply.[29,30] Nonetheless, the successful production of microorganisms demands adherence to specific protocols for each strain, necessitating resources and efforts dedicated to their cultivation for extraction purposes. Thus, it is essential to recognize the impact associated with microorganism production. Despite not requiring vast soil areas like monoculture plant production, the cultivation of microorganisms still carries an environmental footprint that cannot be overlooked, having an inherent impact on the environment that must be considered.

Considering the arguments presented, we recognize the challenges in converting qualitative data into quantitative scores, particularly when evaluating the role of biomass in extraction processes. However, by assessing the significance of biomass in specific sustainability niches, a more holistic approach to scoring its importance in the extraction process becomes viable. In this regard, we propose a set of values depicted in Fig. 2, which aims to assist users in attributing the relevant scores. This approach allows for a more comprehensive and user-friendly metric utilization, enabling a nuanced evaluation of biomass's contribution to sustainable extraction practices.

Principle 2 – Transport: preserving biomass integrity while minimizing transport's environmental impact

Before extraction, biomass transportation must be appropriately designated for the handling site (laboratory, industry, research center, *etc.*). However, the route between the biomass's point of origin and the extraction site is not always straightforward or short. The ease of accessing the biomass source varies based on its origin, and this accessibility can pose challenges.[31] This situation arises due to the distinctive regional nature of the biomass's origin, which can lead to a significant geographical gap between the source and the extraction site. This scenario can also occur when the biomass is widely distributed but distant from the intended extraction location. Additionally, it is crucial to consider the transportation process's inherent environmental impact when evaluating each journey step. The biomass must reach its destination with high quality and minimal environmental impact, ensuring that the desired compounds remain intact for extraction. This emphasizes the need to incorporate effective transport management once the biomass faces stressors during transit that can lead to losses and increased production costs.[32] Several vehicles come into play in transportation, encompassing containers, trucks, automobiles, motorcycles, planes, boats, and (non-)electric freight trains.[33] In this sense, prioritizing a transportation option with minimal environmental

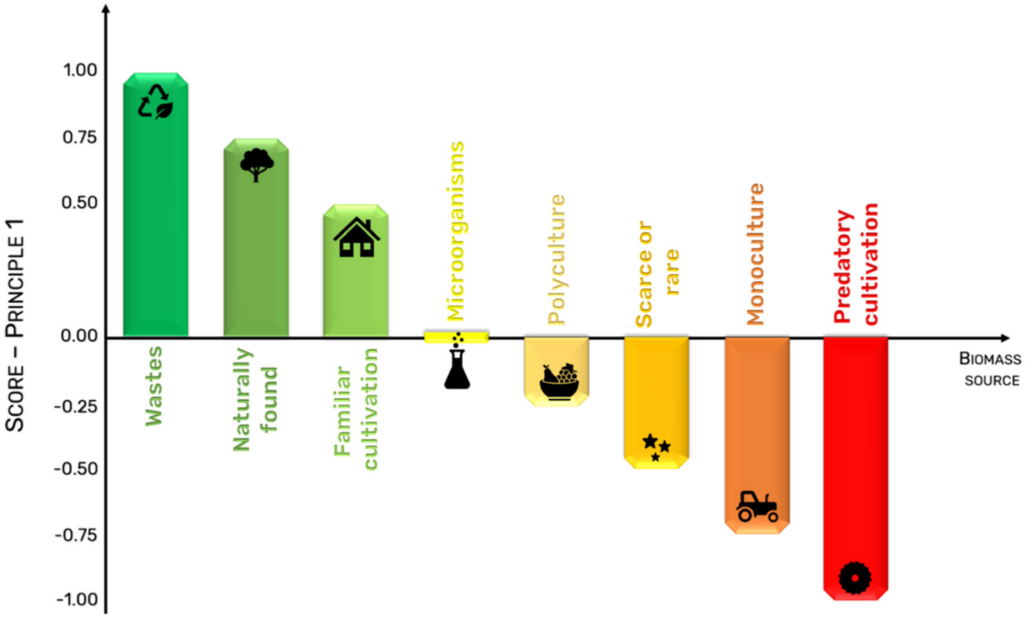

Fig. 2 Representative scheme of biomass sources and their respective score.

impact is essential while ensuring the biomass's unblemished quality remains the paramount objective.[34]

Considering those arguments, some reports categorize the carbon footprint of several means of transport.[35] Besides, the comprehensive classification of parameters influencing transportation environmental impact presents a significant challenge, especially when implementing a scoring system like the one proposed in this metric. Therefore, our present strategy revolves around pinpointing key factors, with travel distance taking precedence as it significantly shapes our selection of transportation methods. This principle highlights the substantial complexities involved in transporting raw materials for extraction. Our objective is to consolidate essential assessment criteria, enabling an initial evaluation of biomass transportation's impact. Considering this perspective, we have undertaken a regression analysis concerning simulated travel distances. Using a CO_2 emission calculator for varying means of transport (**https://www.carbonfootprint.com/calculator.aspx**), we simulated long and short journeys *via* different modes (cars, planes, trains, and even walking). With those results, a regression was conducted using the highest and the lowest CO_2 emission, which can be converted into scores between −1 and +1 (Fig. 3).

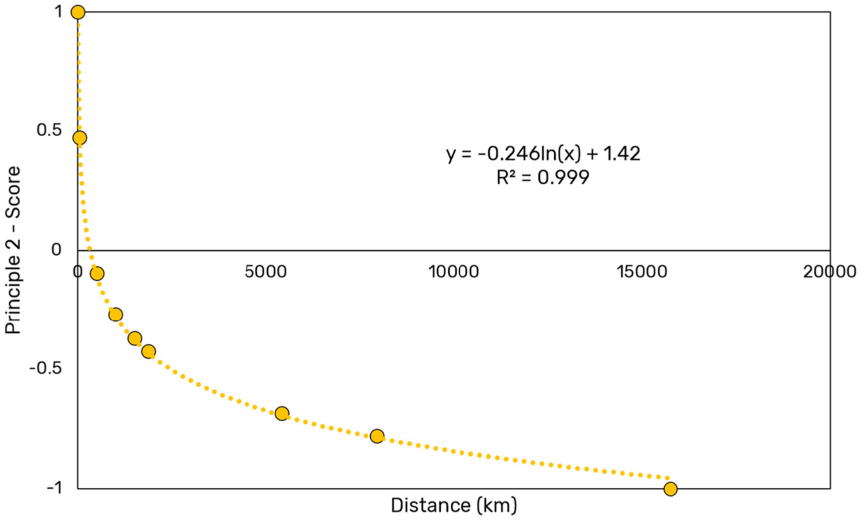

Fig. 3 Graphical representation of the function applied to convert distance (km) to scores in the scale ranging from −1.00 to 1.00.

Principle 3 – Pre-treatment: optimization for pre-treatment avoidance and cost-effective techniques

Before the extraction process begins, pre-treatment is often necessary to prepare the raw material (biomass) for an efficient extraction. Pre-treatment involves several physical, chemical, or/and biological processes to enhance the accessibility to the target bioactive compounds while ideally removing unwanted components (contaminants or impurities, which to facilitate will be called interferents). The choice of the pre-treatment method in extraction hinges on factors like biomass (morphological) characteristics, target compounds, and extraction goals. When purity is paramount, pre-treatment steps should help separate interfering substances without compromising the desired compound's quality/bioactivity and stability. These steps should enhance extraction selectivity, allowing for a more precise approach. The pre-treatment complexity varies based on the nature of biomass and desired compounds, sometimes necessitating multiple steps for an effective extraction, and even combining more than one pre-treatment strategy. While pre-treatment adds to costs and energy requirements, optimizing yield and quality underscores its importance.

Physical pre-treatments are preferred for preparing biomass for extraction due to their simplicity, cost efficiency, and minimal requirements of reagents, high-energy techniques, or extended durations, resulting in a low environmental impact associated with those activities. These methods involve mechanical actions to break down the biomass structure, increase surface area, and aid in releasing target compounds. Techniques like grinding, drying, freezing, microwave, and ultrasound treatment are commonly employed.[36] Alternatively, chemical pre-treatments offer another approach to prepare biomass for extraction processes, commonly utilized in industries such as papermaking. The primary goal of chemical pre-treatment involves dissolving unwanted compounds using specialized solutions to improve access to desired ones. Depending on the dissolving solution used, these treatments are categorized as either acid or alkaline. Acid pre-treatment, for instance, employs substances like sulfuric or hydrochloric acid to break down the biomass's cell walls.[37] However, chemical pre-treatments often raise concerns regarding their environmental impact due to the use of chemicals, which lead to the generation of hazardous waste and the release of pollutants into the environment.[36] The disposal of these chemicals must be carefully managed to minimize ecological harm, highlighting the need for environmentally conscious approaches in utilizing chemical pre-treatments.

The third pre-treatment method involves using living organisms to prepare the biomass for extraction. These techniques are commonly employed when there is a need to break down complex structures, such as proteins and polysaccharides, making the extraction process more efficient and effective in releasing the desired compounds.[36] Among the set of biological pre-treatments, two methods stand out: the use of microorganisms to induce chemical structure modifications in the biomass[38] and the application of enzymes, which can catalyze the breakdown of complex components, such as cellulose and hemicellulose, and favor the extraction. Typically, in the former, non-pathogenic bacteria and fungi are employed for these approaches. Depending on their nature, these microorganisms can facilitate biotransformation through oxidation or fermentation, converting certain compounds in the biomass into more desirable forms before the extraction process.

When the complete elimination of pre-treatment procedures is not possible, to minimize their environmental impacts it is essential to adopt sustainable methods, such as using renewable energy sources for physical pre-treatments, employing environmentally friendly chemicals in chemical pre-treatments, and optimizing biological pre-treatment conditions to minimize resource usage. Table 1 summarizes the main advantages and disadvantages of known pre-treatment methods. This information can serve as a guide for researchers to explore potential improvements in each technique. By identifying the strengths and weaknesses of existing pre-treatment methods, researchers can focus on enhancing the efficiency and sustainability of the extraction processes. Fig. 4 illustrates the conversion of pre-treatment methods into scores, facilitating the evaluation of this principle based on the frequency and variety of pre-treatments employed.

Principle 4 – Solvents: minimize solvent usage, prioritizing those of biological origin, biodegradable and non-toxic

After completing the biomass pre-treatment, the extraction process begins, wherein the careful selection of an optimal solvent becomes paramount for sustainable approaches under development. Various challenges arise concerning the efficiency of extracting compounds, particularly in achieving selective extraction once specific compounds are extracted in a precise and targeted manner, which poses significant difficulties that need to be overcome for optimal results.[39] The solvent choice must align with the principles of a circular economy, as their biodegradability ensures that they do not persist after use.[40] In addition to being environmentally safe, ensuring safety during handling is crucial, considering factors such as flammability, odor, and volatility.[41]

Considering the green approach of a solvent, the most recommended is water, known as the universal solvent,[42] being the most recommended choice. On the other hand, for many years, various types of Volatile Organic Solvents (VOS) like alcohols, ketones, ethers, esters, hydrocarbons, halogenated, and aromatic solvents were extensively utilized.[43] Despite their effectiveness across diverse industries, these solvents are associated with a high inherent environmental impact, affecting all three sustainability pillars. As their name suggests, the high volatility of VOS poses significant risks to the environmental, social, and economic pillars of sustainability.[44] Embracing non-volatile alternative solvents offers a promising pathway toward a more sustainable future, minimizing environmental and human health impacts while supporting resource efficiency and long-term economic viability.[45,46] In this context, considerable progress has already been made in exploring alternative solvents such as ionic liquids (ILs), deep

Table 1 Advantages and disadvantages of biomass pre-treatment methods, and recommendations for a more sustainable approach

Pre-treatments	Advantages	Disadvantages	Recommendations
Physical	Generally, they require less or no chemicals, making them relatively eco-friendly.	Demands significant energy inputs, leading to higher greenhouse gas emissions if derived from fossil fuel-based sources.	Use renewable energy sources.
Chemical	Breaking down complex structures enhances the accessibility of target compounds.	Generation of hazardous waste; depending on the type and amount of chemicals used, concerns about their toxicity and long-term effects on ecosystems might arise.	Use safer solvents and raw materials.
Biological	Biological pre-treatments often apply environmentally friendly microorganisms and enzymes, reducing the need for chemicals.	May require specific growth conditions or the use of substrates, which could increase resource consumption and environmental footprints; disposal of residual microorganisms or enzymes after pre-treatment needs to be properly managed.	Perform an eco-friendlier microorganism cultivation.
Combined	Synergize their benefits, leading to improved extraction efficiency.	Complex pre-treatment strategies may introduce additional complexities and costs, potentially increasing the overall environmental burden.	Avoid when the up-cited recommendations are not applicable.

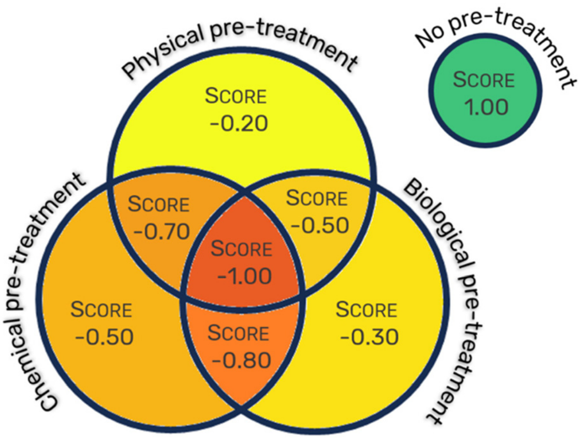

Fig. 4 Scoring based on the pre-treatment options and their combined use.

eutectic solvents (DES), supercritical fluids (CO_2), aqueous solutions of surfactants, and even edible oils.[6] These alternatives show significant potential for application across diverse industries, providing greener and more environmentally friendly options for various processes and products and modulating the water's chemical parameters, increasing its hydrophobicity.[47,48]

In selecting these solvents as extractant media, careful consideration of criteria for efficiency and benignity is crucial. It is essential to prioritize solvents derived from sustainable starting materials to ensure the safety and eco-friendliness of the extraction process. Furthermore, it is essential to eliminate overgeneralizations about the greenness of ILs and DES solely based on their non-volatile nature.[6] While non-volatility reduces organic contaminant emissions, it does not guarantee these solvents' overall environmental impact or sustainability. To accurately assess their eco-friendliness, it is crucial to consider other factors, such as the origin of their raw materials, toxicity, biodegradability, and energy efficiency.[49,50]

Considering the alternatives to avoid using VOS and enhance water extraction performance, a promising green path emerges. However, it is worth noting that these solvents are relatively recent compared to VOS, and the literature still lacks extensive studies on extracting bioactive compounds from biomass using non-volatile alternatives and even biobased solvents. While various research groups have been actively exploring eco-friendlier pathways with non-volatile solvents, significant challenges remain. As previously discussed, there is a complexity in choosing the most suitable solvent for the process that meets all the requirements. Table 2 highlights the main advantages and disadvantages of the different solvents to assist the reader in this choice. Furthermore, recommendations for the use of each solvent are proposed. This valuable information can serve as a guide for researchers to explore the potential of each solvent.

Our proposal involves assessing solvents' environmental, social, and economic aspects to determine their sustainable character. This evaluation is inspired by the guide provided by CHEM21, which focuses on classical and less-classical solvents.[10] In this article, a precise evaluation enables us to make informed decisions about the sustainability and eco-friendliness of the solvents used in extraction. Their overall impact on the environment, society, and economy is considered, enabling the reader to classify solvent usage as recommended, problematic, or hazardous. By employing such a comprehensive metric, we can identify and prioritize solvents that align with the principles of green chemistry and contribute to a more sustainable and responsible approach in extractions. Table 3 enables the scoring of principle 4, which evaluates the environmental sustainability of solvents used in biomass extraction processes.

Principle 5 – Scaling: ensure reproducibility and a continuous extraction flow

The extraction strategy and its operational parameters have a pivotal influence on the success of the extraction process: the

Table 2 Advantages and disadvantages of solvents, and recommendations for a more sustainable extraction approach

Solvent type	Advantages	Disadvantages	Recommendations
Renewable solvents of biological origin	Biodegradable and environmentally safe	Limited availability and higher cost compared to traditional solvents	Prioritize research and development in renewable solvents
Water	Abundant, low-cost and non-toxic	Ineffective for extracting high-medium hydrophobicity compounds	Prioritize water-based extraction processes and explore methods to enhance their effectiveness
Aqueous solutions of surfactants	Creation of micelles in water, allowing the solubilization of hydrophobic compounds	Choice of surfactant determines eco-friendliness	Prioritize for biobased surfactants and thoroughly assess their environmental impact and renewability
Volatile organic solvents (VOS)	Efficient in extracting various compounds with different polarities and from different classes	Depending on the VOS used (mainly those with high volatility) inherent high environmental impacts and health risks can be observed	Actively seek greener alternatives to VOS, and invest in research for sustainable replacements
Ionic liquids (ILs) and (deep) eutectic solvents (DES)	Tailorable properties for specific applications	Potential toxicity and non-renewable options	Focus on green synthesis of ILs and DES from renewable sources, and prioritize non-toxic options
Supercritical CO_2	Highly effective for extracting hydrophobic compounds	Substantial initial investment and longer extraction times	Consider supercritical CO_2 extraction for specific applications where its benefits outweigh the drawbacks
Edible oils	Non-volatile, providing an alternative to VOS	High viscosity may hinder mass transfer efficiency	Use non-volatile edible oils for specific applications and employ advanced techniques for efficient extraction

Table 3 Scores of solvents according to criteria outlined in the CHEM21 guideline,[10] categorizing them as recommended, problematic, or hazard

Solvents	Scores
Recommended: water, ethanol, propanol, *n*-butanol, *t*-butanol, i-butanol, i-amyl alcohol, i-butyl acetate, i-amyl acetate, glycol diacetate, tertiary amyl methyl ether, dimethyl carbonate, biobased solvents, vegetable oils from non-predatory cultivation systems, DES formulated using biobased starting materials, ILs synthetized using biobased raw materials, biobased surfactants.	1.00
Problematic: methanol, benzyl alcohol, ethylene glycol, glycerol, 1,3-propane diol, acetone, cyclohexane, methyl acetate, tetrahydrofuran, methyl tetrahydrofuran, anisole, heptane, cyclohexane, toluene, xylene, acetonitrile, dimethyl propylene urea, dimethyl sulfoxide, formic acid, acetic acid, γ-valerolactone, diethyl succinate, cyclopentyl methyl ether, ethyl *tert*-butyl ether, limonene, turpentine, cymene, ethylene carbonate, propylene carbonate, cyrene, ethyl lactate, lactic acid, supercritical CO_2, vegetable oils from monoculture systems, DES formulated using non-biobased or problematic starting materials, ILs synthetized using non-biobased raw materials, non-biobased surfactants.	0.00
Hazard: diethyl ether, diisopropyl ether, methyl *tert*-butyl ether, 1,4-dioxane, dimethyl ether, pentane, hexane, benzene, dichloromethane, chloroform, chloroform, dichloroethane; dimethylformamide, dimethylacetamide, methyl-2-pyrrolidone, sulfolane, hexamethylphosphoramide, nitromethane, methoxy-ethanol, carbon disulfide, pyridine, triethylamine, furfuryl alcohol, chlorobenzene	−1.00

choice of the extraction technique involves enhancing the efficiency of compound extraction but safeguarding the integrity of the final extract. Various challenges are faced with the intent to develop a valuable and eco-friendly extraction approach, underscoring the importance of establishing strategies applicable to large-scale systems.[47] In this context, prioritizing more straightforward techniques enabling continuous and efficient operations becomes the benchmark for success. The decision to opt for a particular technique able to operate at a high-scale mode should be informed by a holistic assessment encompassing factors beyond extraction yield, including cost-effectiveness, reproducibility, and the overall economic feasibility of the process.

The goal of scalability is to ensure that as demand grows, the process or system can be easily adapted to meet new requirements while maintaining optimal efficiency, performance, and resource usage.[51] Indeed, scalability can be performed in all extraction methods, but their effectiveness ultimately depends on two critical factors: time and reproducibility.[52] Efficient extraction methods must consider factors like time and technology to achieve high yields consistently. The time directly impacts production volume—the faster the process, the more extract can be produced in a given timeframe, resulting in higher gains per unit of time and increased profitability.[53] However, this variable does not operate alone; it is futile to prioritize speed without ensuring reproducibility.[52]

In this context, the most readily scalable extraction techniques involve minimal steps and operate within a continuous flow framework *in situ* and with automated systems.[54] Such techniques offer enhanced efficiency, reduced idle periods, and consistent operational continuity.[55] Furthermore, this approach minimizes process interruptions, enhancing predictability and productivity.[47] Once optimized, adjustments can be seamlessly implemented to augment production without significantly altering the fundamental configuration. On the other hand, the non-continuous production mode is performed in batches, *i.e.*, the biomass and the solvent are added for the first extraction approach. After that, the system is emptied and prepared for another batch.[56] In semi-continuous production mode, extraction occurs in batches. However, continuous processes can work in combination with other batch processes or even in parallel reactors.[56] Nevertheless, asserting that one system lends itself more readily to scalability than the other is reasonable. Consequently, when considering this principle alone, scoring a continuous system with a non-handling dependence with the highest score (score +1) is intuitive. In contrast, the batch system, being more challenging to scale, receives a lower score (score −1). Therefore, the operating mode selection should be founded upon a comprehensive evaluation of these advantages and disadvantages in addition to the application's specific context, available resources, production objectives, and materials' attributes. In this sense, Fig. 5 highlights the scores to evaluate principle 5.

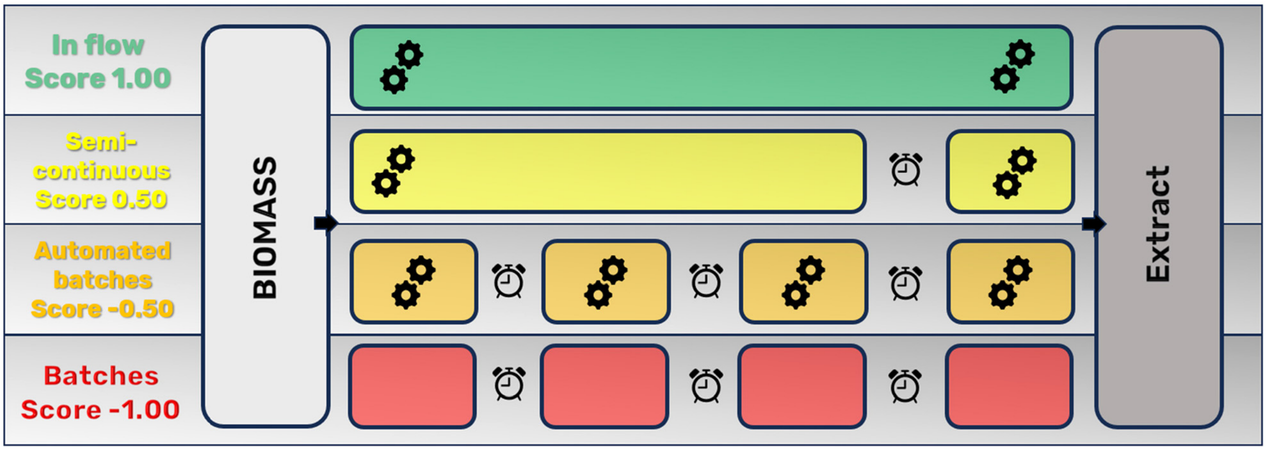

Fig. 5 Scoring based on the scaling options. The gears represent automated systems, and the clocks the time requested between the approaches.

Principle 6 – Purification: final application dictates the extent of purification

The product acquired by extraction is usually a complex mixture of several components from the biomass material solubilized in the chosen solvent, typically called crude extract. Some applications, such as food, feed, and nutraceutical applications, allow the employment of these crude extracts since their compounds can act symbiotically towards a specific aim. However, in cases where the interaction between compounds in the crude extract is unfavorable or in fine applications, such as in the pharmaceutical industry, it becomes essential to isolate target bioactive compounds. In this sense, purification strategies within extraction processes play a dual role, impacting product quality, quantity, and environmental aspects. While enhancing the concentration and purity of target compounds can broaden the potential applications of extracts, these techniques frequently require substantial energy and solvent volumes and lead to waste generation. Thus, reducing the number of steps in a process chain leads to reduced costs and better use of energy and raw materials, which means that a single-stage process yielding a ready-to-use extract would appear ideal.[16] Obtaining ready-to-use extracts is complex, and purification strategies are often requested. For example, methods like chromatography, molecular distillation, crystallization, and ultrafiltration, while effective in isolating specific compounds, even on an industrial scale, require substantial energy inputs and/or high solvent volumes.[57] Disposing of solvents and waste materials from purification steps can pose environmental risks if not managed properly, contributing to a high environmental impact of the extraction process. However, advancements in purification technologies strive to minimize these impacts, focusing on solvent recovery and reuse, and the development of greener, more sustainable purification methods.[58] Innovations such as green solvents, membrane-based separations, and continuous processing aim to reduce energy usage, cost, waste generation, and the overall environmental footprint of purification strategies, ensuring a balance between product purity and eco-friendliness.[59,60]

Principle 6 straightforwardly addresses the necessity of purification strategies. The highest score (+1.00) is assigned if no purification is required. Conversely, when purification is essential, the evaluation considers whether it is conducted using environmentally benign alternatives, like chromatography with renewable materials and solvents, and in a few steps (up to two), or if any measures are taken to minimize the associated environmental impact (like the reuse of raw materials and solvents). Table 4 shows the detailed scores assigned to this principle.

Table 4 Scoring based on the purification strategies

Biomass source	Score
Ready-to-use extracts	1.00
Purification without using solvents[a]	0.50
Purification performed based on recommended solvents[a]	0.00
Purification performed based on problematic solvents[a]	−0.50
Purification performed based on hazard solvents[a]	−1.00

[a] Refer to Table 3 to determine the hazard classification of a chemical.

Principle 7 – Yield: maximize the utilization and valorization of the biomass

Achieving high extraction yields has become critical in extraction processes, as the search for bioactive compounds from natural sources increased substantially.[61] However, achieving these optimal yields is not a simple task. Detailed planning is required, including proper choice of solvents (when necessary), management techniques, and optimization of the operational variables. Due to the diversity of factors, it is challenging to determine an acceptable extraction yield that applies to different proposals. The complex nature of the biomass and the diverse factors involved make it difficult to establish a single and standardized measure for yield. In this context, the optimal yield being synonymous with full utilization of the initial raw material seems to be the correct path. In addition, optimizing extraction to maximize the use of all the compounds in the raw material reduces waste and promotes more efficient use of natural resources.[62,63]

When we state the full benefit of biomass, we refer to an exhaustive extraction process and how much of the biomass is valorized. An exhaustive extraction process is a method or procedure that takes the maximum advantage of the biomass, *i.e.* by extracting the maximum number of compounds with the maximum yield. The proportion of target compounds successfully extracted and recovered from the original sample is an excellent factor in evaluating whether the extraction was exhaustive. This measure quantifies the efficiency of the process, indicating the degree of use of available resources.

A high biomass valorization suggests that many of the desired compounds were extracted from the biomass. On the other hand, the low utilization indicates that a significant portion of the compounds was not recovered. In addition, making the most of the raw material is also related to the sustainability of the generation process. The more efficient the process, the less natural resources will be wasted, which is expected to reduce the environmental impact and more responsible use of natural resources. Nevertheless, the efficient use of biomass does not necessarily imply the capture of all compounds present in the sample, as some compounds may be more difficult to extract or may not be of interest for the specific application. Therefore, defining the compounds of interest clearly before the application is crucial. As depicted in Fig. 6, we propose a scaling to assess the yield of an extraction process, which aims to assist users in attributing the relevant scores.

Principle 8 – Post-treatment: functionalization of natural products post-extraction to maximize their benefits

High-value compounds extracted from natural matrices can enhance their properties by applying different post-treatment methods. Considering the purpose of the application, higher stability and activity and lower toxicity might be desirable. Crude extracts could already contain the properties required for their utilization related to greener options, and a post-treatment and/or purification step is thus not required. In this sense, ready-to-use extracts, which can be directly used as, for example, additives in nutraceuticals, cosmetics, and food, represent one promising approach and must be encouraged.

In scenarios requiring post-treatment, methods involving microorganisms or isolated/immobilized enzymes are frequently used, representing greener alternatives compared to chemical modifications that may involve potentially harmful solvents.[64] In this post-treatment category, enzyme-mediated biotransformation reactions are performed, which modify

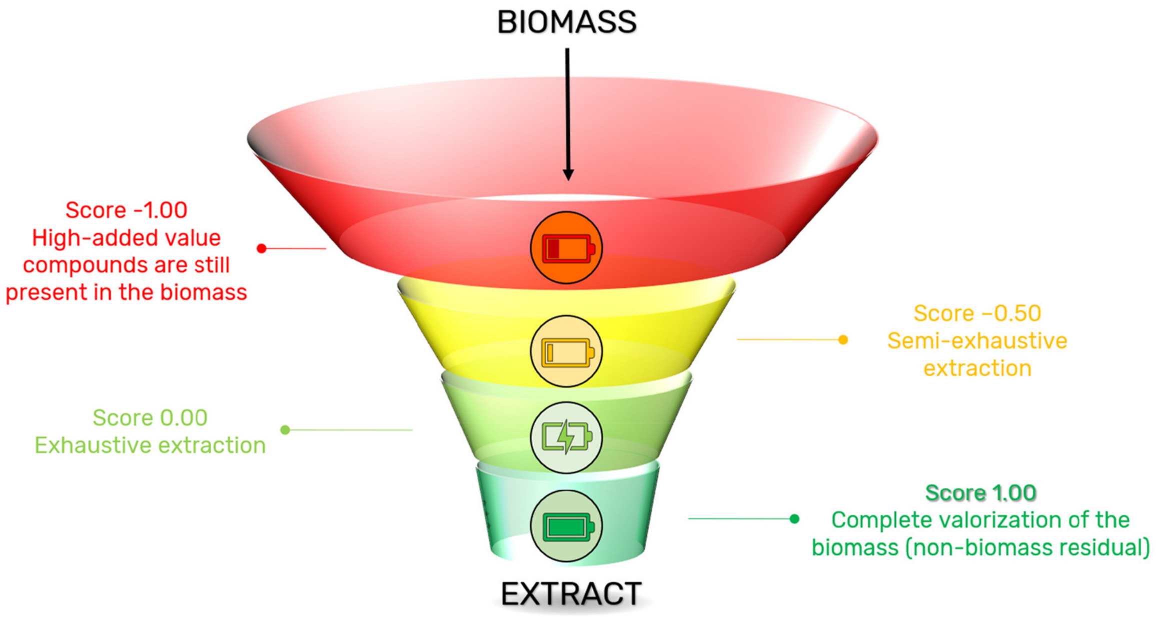

Fig. 6 Scoring based on the obtained yields from biomass.

metabolites to generate potential products with increased biological effects (higher antioxidant activity, higher bioavailability, just to mention a few). On the other hand, post-treatment modifications in metabolites from natural products can result from a semisynthetic route, which is widely used, for example, for drug discovery.[65] Such a strategy can enhance therapeutic properties, improve pharmacokinetics, or reduce potential side effects.[66] However, most organic solvents and reagents are usually classified as harmful, volatile, and derived from non-renewable sources while being often required for performing semi-synthesis, ultimately imposing a limitation to their application and an inherent increased environmental impact. In this sense, Table 5 shows the proposed scores for post-treatment strategies.

Principle 9 – Energy: prioritize using clean energy sources and high-efficiency extraction techniques

Currently, energy consumption represents a significant challenge for industries across various sectors. This concern arises from its implications for environmental sustainability and the scaling of production costs, which can impact process profitability. In this scenario, there is a new challenge in developing processes with low energy requirements. However, this is not straightforward, as the biomass to be extracted can present diverse characteristics that hinder the release of the target compounds into the solution. When this occurs, extraction techniques with high energy demands are often employed, such as ultrasound-assisted extraction (UAE), pressurized-liquid extraction (PLE), and microwave-assisted extraction (MAE).[67,68] Therefore, in this context, despite the energy applied to generate benefits in facilitating extraction and maximizing extraction yield, it can also play a negative role in the process once high-energy-demand techniques increase the inherent cost of the process. In this sense, researchers have focused on developing extraction strategies with low (or zero) energy demand without sacrificing extraction process efficiency. Typically, strategies to achieve this goal focus on optimizing existing processes by applying statistic tools of process optimization, recovering the energy used during the process, and developing innovative approaches that maximize the extraction process yield without high energy demands.[69]

Curbing energy consumption and integrating inventive technologies into extraction processes is a promising avenue. Nonetheless, surpassing the mere reduction of energy use in extraction, the pivotal consideration lies in the energy employed to develop the process. When concentrating solely on the type of energy for extraction, opting for a renewable energy source (clean energy), even if demanding a high-energy intensity, invariably bears a lower environmental impact than extracts generated using non-renewable sources.[69] Consequently, aside from concentrating on advancing energy-efficient extractions, the ecological repercussions of extract production are intricately tied to the energy category employed throughout the operation. Naturally, the energy expense for both methods and the intrinsic cost of generating that energy cannot be factored in this scenario due to variations in investment contingent on location. However, the investment in clean energy, not only to perform extraction approaches, could be a considerable win–win relationship towards a green economy. In this context, our metric emphasizes the judicious utilization of energy in crafting energy-efficient extraction processes and underscores the significance of employing clean energy sources. Table 6 displays the proposed scores for energy utilization.

Principle 10 – Application: ensure safety for applications in several domains

The natural extracts application spans various industries. From cosmetics to nutraceuticals/pharmaceuticals, food and beverages to agriculture, and biomaterials, these extracts are versatile ingredients enriched in bioactive compounds,[70] as illustrated in Fig. 7. As scientific understanding advances, the potential of natural extracts continues to expand, influencing innovation across industries and supporting the quest for healthier, more natural lifestyles, meeting the actual market demand.[65,71,72] Nevertheless, owing to their inherent complexity, natural products demand meticulous consideration across

Table 6 Scoring based on the energy options

Energy usage options	Score
Non-energy extraction approach	1.00
Low-energy extraction technique using renewable energy	0.50
Low-energy extraction technique using non-renewable energy	0.00
High-energy extraction technique using renewable energy	−0.50
High-energy extraction technique using non-renewable energy	−1.00

Table 5 Scoring based on the post-treatment strategies

Post-treatment strategies	Score
Ready-to-use extracts	1.00
Combining up two post-treatments based on recommended solvents[a]	0.50
Combining more than two post-treatments based on recommended solvents[a]	0.25
Combining up two post-treatments based on microorganisms and enzymes biotransformation	0.10
Combining more than two post-treatments based on microorganisms and enzymes biotransformation	0.00
Combining up two post-treatments and based on problematic solvents[a]	−0.50
Combining more than two post-treatment and based on problematic solvents[a]	−0.80
Post-treatment was performed based on hazard solvents[a]	−1.00

[a] Refer to Table 3 to determine the hazard classification of a chemical.

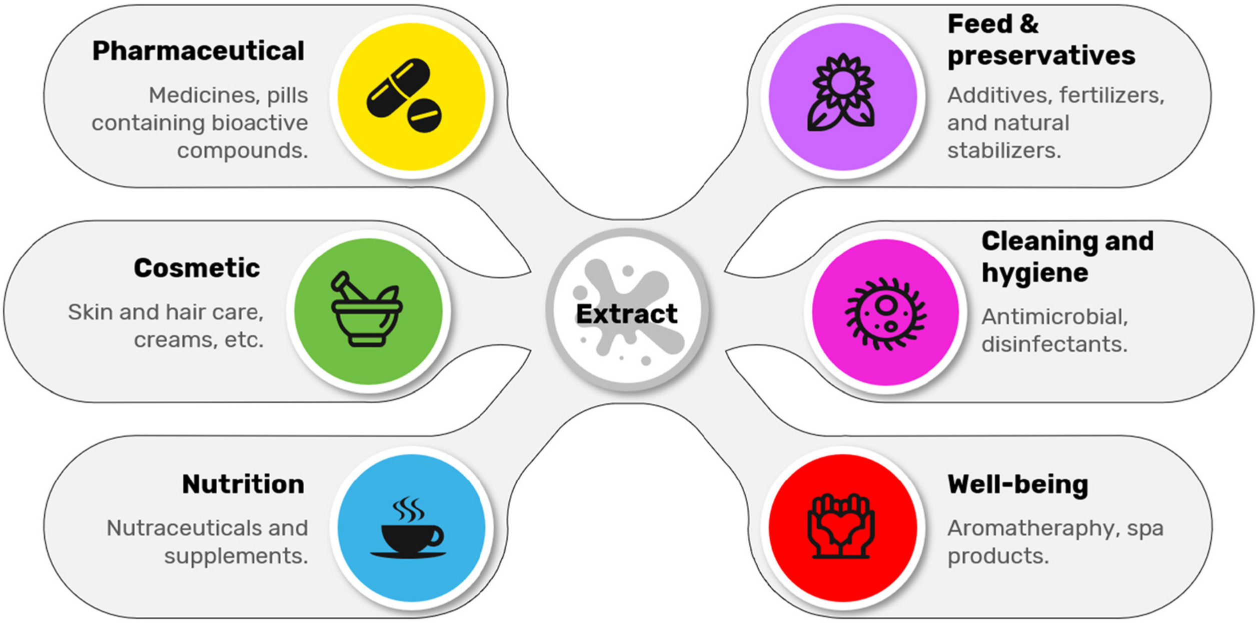

Fig. 7 Set of possible applications of natural extracts obtained from biomass.

various facets for every application. These facets encompass significance within a given context, the distinctive chemical attributes of prominent compounds, and potential underlying mechanisms of action.[65] The safety of natural extracts is a crucial concern in their various applications across industries. While they are derived from botanical, marine, microorganisms, or other natural sources, it is essential to recognize that natural does not always equate to safe. The developed extraction process plays a pivotal role in determining the safety of natural extracts; the method used to obtain bioactive compounds/extracts from their source materials can significantly impact the composition, purity, and potential contaminants within the extract, which can impair the desired application.[67] An accurately planned extraction process considers the target compounds and the undesirable elements that could put safety at risk. For example, using solvents that are not eliminated during the process could lead to solvent residues in the final extract, adversely affecting its intended application.[73]

Specific extraction techniques can alter the chemical structure of compounds, potentially creating unintended by-products that might have safety implications.[69] Careful selection of extraction methods, coupled with rigorous quality control and the process's steps, is essential to ensure that the final natural extract maintains its efficacy while meeting stringent safety standards. A well-executed extraction process produces extracts that deliver the desired benefits and prioritize consumer health and well-being. In this sense, a specific extract application must be directed after safeguarding the extract's safety. Moreover, it is crucial to emphasize that utilizing a natural extract extends beyond a singular domain. For instance, natural colorants hold the potential as additives to enhance food coloration while also serving as significant nutraceutical or active cosmetic ingredients. This accomplishment spans three out of the six general applications of natural extracts. Another tangible illustration pertains to essential oils, frequently encountered in well-being commodities yet equally pivotal in cleaning and cosmetics. Hence, after procuring the natural extract and ensuring its safe use, many potential applications can be directed, thereby increasing the extract's capacity to contribute across diverse economic sectors.

In the proposed metric, concerning the six overarching application domains of natural extracts as depicted in Fig. 7, and in alignment with principle 7, which preconizes a maximal utilization of biomass and the broad spectrum of potential applications for an extract, the highest score (score +1) of this principle is attained when the obtained extract exhibits viability across the most comprehensive array of domains. This criterion can be regarded as the benchmark for optimal application. Conversely, an extract lacking proposed applications or deemed unsafe for use remains unprepared for the market, consequently receiving the lowest score within this metric (score −1), as depicted in Table 7.

Table 7 Scoring based on the possible application domains

Application possibilities	Score
The extract has the potential to be applied in all domains	1.00
The extract has the potential to be applied in at least five domains	0.83
The extract has the potential to be applied in four domains	0.66
The extract has the potential to be applied in three domains	0.50
The extract has the potential to be applied in two domains	0.33
The extract has the potential to be applied in one domain	0.00
The extract cannot be applied to any domain or/and has safety concerns	−1.00

Principle 11 – Repurposing: trace strategies to perform closed-loop extraction systems, preferably using non-virgin materials

Biomass extraction often entails a considerable expenditure of resources, encompassing water, solvents, energy, and technological apparatus. The significance of recovering and reusing raw materials cannot be ignored and must be encouraged, especially regarding the extraction or purification solvents. However, reusing solvents substantially promotes environmental stewardship and resource efficiency. Repurposing solvents for subsequent applications (in new extraction steps or even for other applications) significantly reduces waste generation, mitigates environmental pollution, and restricts the need for new solvent production.[74] However, successfully implementing solvent reuse requires addressing challenges such as contamination degree (which could impair its repurposing), purity restoration, and process optimization. This became even more challenging when non-volatile alternative solvents, such as ILs and DES, are used in the extraction approaches.[6,75] In this sense, through innovative technologies, rigorous quality control, and careful solvent management, the reuse of solvents stands as a pragmatic approach to minimize the ecological footprint of extraction processes and advance sustainable practices.[58,76] These practices interlink with sustainability, prudent resource management, heightened energy efficiency, and substantial economic advantages.

Following biomass extraction, the leftovers display substantial ecological damage when not subject to appropriate disposal.[77] In this context, the actions of recovery and reuse work against the build-up of waste, prevent the release of harmful pollutants and reduce the depletion of natural resources. This approach promotes the overall health of ecosystems and lessens the environmental strain associated with disposal. That's why retrieving and reusing these resources from the waste spectrum counterbalances the demand for virgin materials, conserving them for further applications.[78,79] A noteworthy instance emerges when reuse involves energy-intensive processing methods.[80–82] Hence, the establishment of closed-loop systems, wherein non-virgin materials fuel novel production processes and magnify the sustainability of extraction practices, meets the sustainable practices towards green extraction approaches. This paradigm mitigates the incessant call for raw materials and curtails the ecological pressures linked to production cycles. Simultaneously, the advancement of recovering/reuse technologies brings innovation to various fields, making them more cost-effective, mitigating the impact of disposal, and driving positive progress in the area.[83] The strategy of recovery and reuse stemming from biomass activities serves as effective conduits for diverting a substantial volume of material from disposal. These endeavors orchestrate a harmonious synergy among ecological preservation, resource optimization, energy efficiency, and economic prosperity.[84]

Considering the vital role in repurposing raw materials within extraction processes, this metric assigns positive scores when non-virgin raw materials (such as reused solvents) are employed for the extraction process. Moreover, even if strategies for reusing raw materials are proposed, the approach envisioned is guided toward a sustainable extraction pathway. Conversely, using virgin raw materials without a repurposing strategy results in a negative score, contradicting the effort to mitigate the repurposing of raw materials utilized in the extraction process. The detailed scores of this principle are provided in Fig. 8.

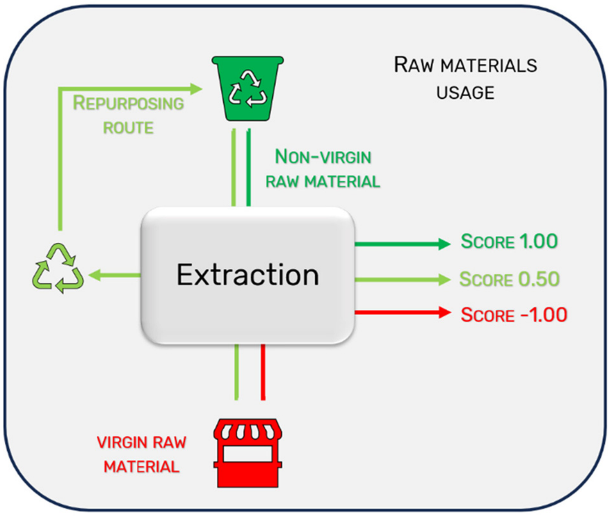

Fig. 8 Scoring based on the repurposing of raw materials.

Principle 12 – Waste management: refine waste reduction and ensure effective waste management

Upon the completion of the extraction process, there is a residual fraction of the raw materials, including leftover biomass debris and solvents employed in the pre-treatment/extraction/purification process. Should these elements not be repurposed for secondary applications, they will fall into the waste category. This underscores the significance of identifying alternative functionalities for these residual components. By optimizing the extraction process to obtain the most significant quantity of desired components from raw materials, the overall efficiency is heightened, reducing the volume of unused or leftover material that might transform into waste. Another essential strategy involves recovery and reusing. Rather than discarding residual biomass debris, reagents, and solvents, these materials are repurposed for secondary applications or integrated into subsequent extraction cycles, diminishing their potential classification as waste.

The concept of process integration plays a key role. By designing extraction processes that synergistically use the outputs of one stage as the inputs of another, the overall material flow is streamlined, curbing waste creation at various points in the process. By harmoniously integrating these strategies, extraction processes can be transformed into resource efficiency and waste reduction models. However, when these strategies are not achieved, waste generation is unavoidable, directly affecting the three pillars of sustainability.

Ultimately, even if alternative approaches to prevent waste are ineffective, inherent waste generation in the extraction process becomes inevitable. This challenge is compounded by the complex nature of assessing residual waste, necessitating a multifaceted evaluation encompassing various factors. Acknowledging the inherent difficulty in eliminating waste from extraction processes, this principle can be evaluated using the E-factor equation (eqn (1)). The E-factor, or environmental factor, is a tool used in industries to measure the environmental impact of processes or products. It quantifies waste generation, where lower values indicate environmentally friendly processes with reduced waste, while higher values signify inefficiency and a larger environmental impact. Embracing this approach, and as illustrated in the AGREE metric, when evaluating a proposed parameter poses challenges, regressions considering both positive and negative extremes are computed to simplify the scoring process. In this context, envisioning the most optimistic scenario where waste generation is absent is scored as +1 (low E-factor). In contrast, the most adverse situation with a higher 100% waste generation rate is assigned −1 (high E-Factor). The regression derived from the E-factor aids in assessing and setting a score to this principle (Fig. 9).

$$\text{E-factor}\,(\%) = 100 \times \left(\frac{\text{total waste (mass)}}{\text{total product (mass)}}\right) \qquad (1)$$

3. *Path2Green* metric

Every time society depends on goods produced by a biomass-dependent process, evaluating their adherence to sustainability pillars becomes crucial. Although each pillar is significant, their relative importance may vary when creating a genuine green extraction process, which consequently influences the score of the green metric developed here. In crafting a metric to assess biomass valorization, it is imperative to acknowledge and delineate the distinct importance of the three sustainability pillars: environment, society, and economy. While all three are interconnected, the environmental pillar stands out as paramount due to its overarching impact on global sustainability. Prioritizing environmental considerations in biomass valorization metrics underscores the critical need to mitigate climate change, preserve biodiversity, and safeguard natural resources.[85] Such metrics incentivize practices that minimize ecological harm and promote long-term ecological resilience by emphasizing the environmental aspect. However, this does not diminish the significance of the social and economic pillars. The social dimension is crucial as it ensures equitable access to benefits and opportunities generated by biomass valorization, fostering community well-being and inclusivity.[86] Simultaneously, the economic pillar remains essential for driving innovation, creating jobs, and ensuring the viability and scalability of biomass valorization initiatives. While each pillar has its unique importance, an integrated approach that prioritizes the environmental aspect acknowledges the interconnectedness of these dimensions and fosters holistic sustainability in biomass valorization efforts. In this sense, despite the significant role played by each pillar in sustainability, the environmental component can be seen as the major force that sets the other pillars in motion, meeting social needs and ensuring economic stability.

In the proposed *Path2Green* metric, each principle was evaluated individually. To create a more robust distinction between the developed principles, different weights were attributed, namely the environmental aspect carrying a more pronounced weight (weight 3), followed by society (weight 2), and, ultimately, the economic (weight 1). Hence, the cumulative weight of each principle in determining the score results from the sum of its weights across the pillars it directly associates with. However, when the principle does not directly influence the pillar, we considered only half of the weight of the principle. Table 8 provides a detailed elucidation of the direct connections between each principle and its corresponding pillar, outlining the rationale behind these associations.

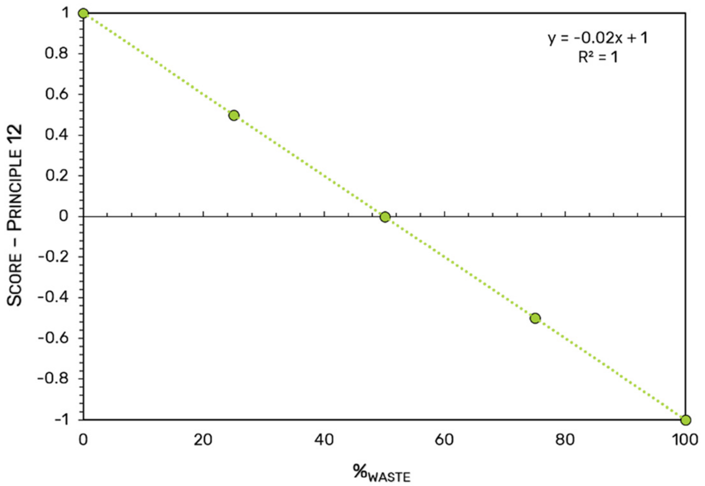

Fig. 9 Graphical representation of the function applied to convert the % of waste in score between −1.00 to +1.00.

Table 8 Recommended weights assigned to each principle for the Path2Green metric, reflecting their direct and indirect impacts across environmental, social, and economic sustainability pillars in addition to the rationale behind these associations

Principles	Environmental (weight 3)	Social (weight 2)	Economic (weight 1)	Total weight of the principle
Principle 1 – Biomass: Select biomass that is naturally sourced or requires minimal resource usage for production	Ensuring sustainable harvesting, harvesting practices, or production is essential not to compromise ecosystems. (*Direct impact → weight 3.0*)	Depending on how it is collected/produced and used, biomass can have significant social impacts. It can benefit local communities by providing extracts for various applications if managed responsibly. (*Direct impact → weight 2.0*)	Using biomass can boost local economies, especially in areas with abundant biomass. This can create employment and economic development opportunities as long as it is managed responsibly and equitably. (*Direct impact → weight 1.0*)	6.0
Principle 2 – Transport: Preserving biomass integrity while minimizing transport's environmental impact	Biomass transportation can have significant environmental impacts, especially related to carbon emissions and carbon footprint. Efficient and sustainable transport strategies, such as using cleaner modes of transport or optimized logistics routes, can reduce this impact. (*Direct impact → weight 3.0*)	Biomass transport can affect communities along transport routes, especially if there are impacts on health, safety, or access to local resources. Strategies that minimize negative impacts on communities, ensuring safety and respect for local rights, are essential for sustainable social development. (*Indirect impact → weight 1.0*)	Biomass transportation can influence the local and global economy. It can generate jobs in logistics and transportation and create economic opportunities in areas where biomass is produced, as long as it is done efficiently and economically viable. (*Direct impact → weight 1.0*)	5.0
Principle 3 – Pre-treatment: Optimization for pre-treatment avoidance and cost-effective techniques	Pre-treatment can significantly influence the environmental impact of biomass extraction. Pre-treatment methods that minimize waste, reduce the consumption of natural resources, and limit the release of polluting substances contribute to more sustainable practices. (*Indirect impact → weight 1.5*)	Non-direct or indirect impact (weight 0.0)	Pre-treatment can affect the economic viability of biomass extraction. Efficient and economically viable pre-treatment processes can reduce operational costs, and increase biomass use efficiency. (*Direct impact → weight 1.0*)	2.5
Principle 4 – Solvent: minimize solvent usage, prioritizing those of biological origin, biodegradable and non-toxic	The type of solvent chosen can have a significant impact on the environment. Organic solvents, for example, can have adverse effects if released into the environment. Opting for less toxic, biodegradable solvents or aqueous solutions can reduce the environmental impact. (*Direct impact → weight 3.0*)	The use of solvents can impact the health of workers involved in the extraction process. Toxic solvents can pose occupational health risks. Choosing safer solvents can protect the health and safety of workers, contributing to a healthier work environment. (*Direct impact → weight 1.0*)	The choice of solvent can influence the costs of the extraction process. More sustainable solvents can increase process efficiency and reduce long-term operating costs, even though they may initially be more expensive. (*Direct impact → weight 1.0*)	6.0
Principle 5 – Scaling: Ensure reproducibility and a continuous extraction flow	Increasing production scale may imply greater consumption of natural resources and the generation of waste and emissions. Therefore, it is essential to implement practices that minimize environmental impacts, such as the efficient use of resources, waste reduction, and emissions control. (*Direct impact → weight 3.0*)	Scaling a biomass extraction process can significantly impact society, affecting areas such as employment, local economy, energy security, environment, health, and social equity. (*Indirect impact → weight 1.0*)	The scaling of the extraction process seeks to optimize large-scale production, which can result in economies of scale, reduced production costs, and economic viability. This can open opportunities for investment, jobs and economic growth if done efficiently and sustainably. (*Direct impact → weight 1.0*)	5.0

Table 8 *(Contd.)*

Principles	Environmental (weight 3)	Social (weight 2)	Economic (weight 1)	Total weight of the principle
Principle 6 – Purification: Final application dictates the extent of purification	Purification processes may involve using solvents, separation, or filtration techniques that can potentially impact the environment. Choosing cleaner purification methods, with less waste generation and less environmental impact, is crucial for sustainability. (*Indirect impact → weight 1.5*)	Non-direct or indirect impact (weight 0.0)	The efficiency of purification processes directly influences production costs. More efficient and economical methods can reduce waste, minimize resource consumption, and reduce production costs, making the process more economically viable. (*Direct impact → weight 1.0*)	2.5
Principle 7 – Yield: Maximize the utilization and valorization of the biomass	Extraction yield can be associated with the efficient use of natural resources. More efficient extraction processes may require less biomass or solvents, thus reducing resource consumption and minimizing the environmental impact of extracting large quantities of raw materials. (*Direct impact → weight 3.0*)	Non-direct or indirect impact (weight 0.0)	Extract yield directly influences production costs. A higher yield means greater extraction efficiency, which can reduce costs per product unit. This can make the process more economically viable and positively impact its profitability. (*Direct impact → weight 1.0*)	4.0
Principle 8 – Post-treatment: Extract functionalization maximizing natural compound benefits	Post-treatment may include purification, concentration, separation or other techniques to improve the extract's quality, bioavailability or stability. Choosing cleaner post-treatment methods, which minimize the use of harmful substances or reduce waste generated, is essential to reduce environmental impact. (*Indirect impact → weight 1.5*)	Non-direct or indirect impact (weight 0.0.)	Post-treatment processes can influence production costs. More efficient and economical post-treatment strategies can reduce operational costs and improve the economic viability of the process, as long as they do not compromise the quality of the final product. (*Direct impact → weight 1.0*)	2.5
Principle 9 – Energy: Prioritize using clean energy sources and high-efficiency extraction techniques	The source and type of energy used can significantly impact the environment. Choosing renewable energy sources, such as solar or wind, to power biomass extraction processes can reduce carbon emissions and minimize environmental impact. (*Direct impact → weight 3.0*)	Non-direct or indirect impact (weight 0.0.)	The energy efficiency of extraction processes influences operational costs. Strategies to minimize energy use or adopt cheaper and more sustainable sources can reduce long-term costs and increase the economic viability of the process. (*Direct impact → weight 1.0*)	4.0
Principle 10 – Application: Ensure safety for applications in several domains.	The application of the extract may impact the environment, depending on the context and use. If the application results in more sustainable agricultural practices, such as promoting natural pesticides rather than synthetic chemicals, this could positively impact the environment. (*Indirect impact → weight 1.5*)	The application of the extract can have social implications, especially in terms of health and well-being. If the extract is used in the production of food or medicine, for example, its safety and effectiveness can directly influence people's health. (*Direct impact → weight 2.0*)	The application of the extract can create economic opportunities in the food, pharmaceutical, cosmetics industry or other areas. Developing products derived from biomass extracts can represent new markets and business opportunities, generating jobs and stimulating economic growth. (*Direct impact → weight 1.0*)	4.5
Principle 11 – Repurposing: Trace strategies to perform closed-loop extraction systems, preferably using non-virgin materials	Recycling and reusing materials reduce the need for new natural resources, decreasing the environmental pressure. This contributes to the conservation of natural resources, reducing the extraction of raw materials and minimizing the volume of discarded waste, which can help mitigate environmental impacts. (*Direct impact → weight 3.0*)	Recycling and reuse can positively impact local communities, creating jobs in waste management and promoting a culture of environmental responsibility. Furthermore, it can reduce pollution and improve the quality of life in the surrounding areas. (*Direct impact → weight 2.0*)	Recycling and reuse can reduce costs associated with purchasing new materials and waste disposal costs. This can result in economic efficiency, making the process more profitable in the long term and potentially opening up opportunities for new business models based on the circular economy. (*Direct impact → weight 1.0*)	6.0

Table 8 (*Contd.*)

Principles	Environmental (weight 3)	Social (weight 2)	Economic (weight 1)	Total weight of the principle
Principle 12 – Waste management: Refine waste reduction efforts and ensure effective waste management	Proper waste management can reduce environmental impact by minimizing soil, water, and air pollution. Strategies such as recycling, composting, or appropriate waste treatment can reduce the volume of waste sent to landfills, contributing to preserving natural resources and ecosystems. (*Direct impact → weight 3.0*)	Responsible waste management can improve the health and well-being of local communities while preventing environmental contamination. Furthermore, recycling practices and adequate waste treatment can promote jobs in waste management, contributing to local socioeconomic development. (*Direct impact → weight 2.0*)	Effective waste management can reduce costs associated with treatment and final disposal. Furthermore, reusing or recycling waste can create economic opportunities, such as producing marketable by-products or generating energy from organic waste. (*Direct impact → weight 1.0*)	6.0

Fig. 10 Pictogram depicting the final score of the *Path2Green* metric.

To enhance clarity and ease of understanding when showcasing the metric's outcomes, a pictogram was proposed (Fig. 10). The 12 principles are depicted within this visual representation, each colored according to its respective score. At the heart of the pictogram lies the overall score, ranging from −1.0, denoting a poor rating, to +1.0, signifying an excellent rating. This final score is determined by the weighted average of each principle, reflecting their assigned importance, thus indicating whether they garnered a positive, neutral, or negative assessment. The use of green, yellow, and red aligns with their universally understood meanings. Each principle is associated with a specific color, offering a clear visual cue to identify areas requiring enhancements or spotlighting positive attributes. While this metric does not replace the need for a comprehensive LCA, we believe it is an exciting strategy to encourage the scientific community to consider the principles associated with extraction processes, contributing to further advancements in this field and generating improvements in the development of green extraction approaches. A mobile app has been created to streamline the calculation of the *Path2Green* score. It's possible to download it from the ESI (a brief of instruction highlights is also depicted in Fig. S1 – ESI†). Within the app, users can input scores for each principle and, subsequently, the app generates a pictogram displaying the final score, enabling the evaluation of the environmental friendliness of the developed process in alignment with the 12 principles outlined in this article.

4. Validation of the *Path2Green* metric

To validate the proposed metric in line with the proposed 12 principles of green extraction processes, we evaluated various articles on extracting bioactive compounds from biomass to assess their *Path2Green* scores (Table S1 – ESI†). Subsequently, we performed a linear regression analysis comparing out-

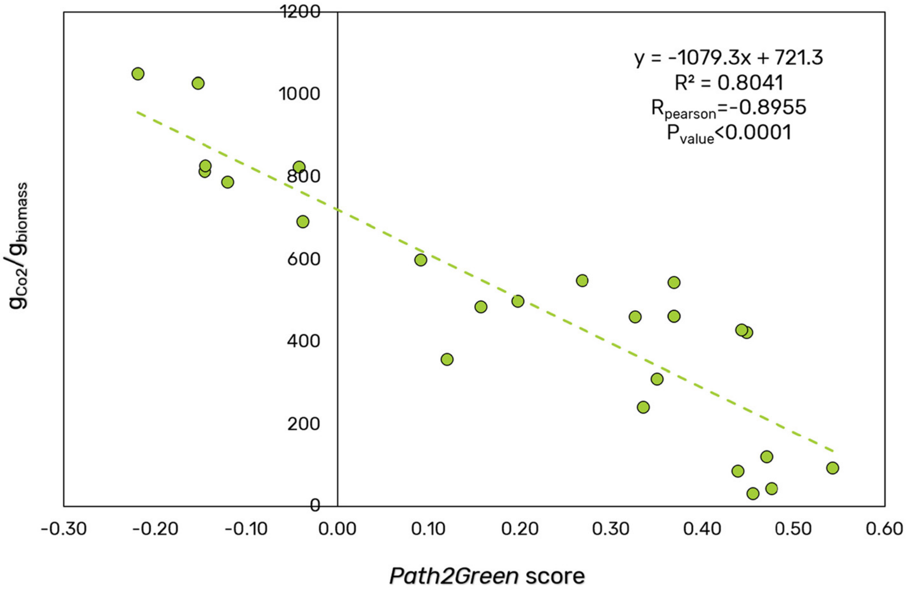

Fig. 11 Linear regression concerning the $g_{CO_2}/g_{biomass}$ *vs. Path2Green* score ($r_{pearson}$ = −0.8955). The individual results of each analysis are reported in ESI.†

comes obtained from our new metric with the carbon footprint emitted per gram of biomass used in the extraction procedure (measured in $g_{CO_2}/g_{biomass}$). Fig. 11 presents the results of this analysis, demonstrating a correlation between the grams of carbon emitted during the process and the *Path2Green* scores. Thus, considering the emitted g_{CO_2} during extraction as a valid metric for assessing the greenness of the extraction procedure and the confidence derived from this analysis, we can assert that the *Path2Gree*n metric could serve as a strategic approach to evaluating the greenness of a new extraction approach. It is essential to emphasize that this metric does not replace the comprehensive results depicted by LCA analysis, which is indeed more robust and trustworthy. A complete LCA accurately demonstrates the real impact of the process, providing precise results regarding various environmental impacts such as ozone depletion, terrestrial warming, and scarcity of fossil resources, among others. However, access to this type of analysis is not always feasible, primarily due to the requirement for specific software, which can be costly, and the need for highly qualified personnel to conduct the analysis. In this context, the *Path2Green* metric can serve as a simpler alternative to identify the main drawbacks associated with a given extraction process. It enables the identification of weaknesses in the process, like a SWOT analysis, thereby assisting researchers in pinpointing areas for improvement in extraction techniques. This contribution facilitates the development of greener extraction approaches, even when access to comprehensive LCA is limited.

5. Conclusion

The *Path2Green* as a metric for assessing extraction approaches presents several advantages. Firstly, it offers a clear and measurable evaluation of the environmental impact associated with extraction processes, considering the three sustainability pillars: environmental, social, and economic. This comprehensive approach aids in defining the relative importance of each principle, considering key characteristics from biomass collection to post-extraction waste management. By delineating principles for each step of the extraction procedure, *Path2Green* facilitates nuanced comparisons between different methods, enabling researchers to pinpoint greener alternatives at every stage. Furthermore, it functions as a practical tool, providing insights into both the strengths and weaknesses of extraction procedures, analogous to a SWOT analysis. Its simplicity and accessibility render it particularly valuable in scenarios where conducting comprehensive life cycle assessments is impractical due to financial or expertise limitations. A cellphone app was developed to assist users in conducting the analysis and provide colorful pictograms. In conclusion, *Path2Green* represents a significant advancement in pursuing sustainable extraction practices. It not only fosters environmentally friendly approaches within the scientific community but also catalyzes stimulating further research in this important field.

Data availability

The data supporting this article have been included as part of the ESI† – *Path2Green* app.

Conflicts of interest

There are no conflicts to declare.

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