Volume 27
Number 18
14 May 2025
Pages 4801-5390

Green Chemistry

Cutting-edge research for a greener sustainable future

rsc.li/greenchem

ISSN 1463-9262

ROYAL SOCIETY OF CHEMISTRY

PAPER

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25 YEARS ANNIVERSARY

Green Chemistry

PAPER

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Cite this: *Green Chem.*, 2025, **27**, 5015

Advancing green chemistry performance assessment: the Estée Lauder Companies' continuing journey towards meaningful transparency†

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Green chemistry can serve as a key framework to guide cosmetic formulation decision making, as evidenced through the development and portfolio-wide implementation of the Estée Lauder Companies' (ELC) "Green Score" assessment tool. Recent advancements in data quality and availability from regulatory, industry reporting, and wider literature sources have provided the opportunity to improve and refine the underlying scientific robustness of the framework. Consequently, the first significant methodological iteration is described. The environmental impact pillar is greatly strengthened through inclusion of a waste impact metric and refined greenhouse gas and feedstock sourcing metric approaches. The addition of a biodegradability endpoint also builds upon the tool's initial persistence assessment. Exemplified through ingredient selection case studies, the enhanced tool enables provision of more accurate formulation guidance and strengthens the Green Score's utility as a forward-looking product design guide and informed substitution tool. Potential opportunities for leveraging the rapid evolution of the cosmetic and chemical regulatory landscape to facilitate further optimization and refinement of the framework are also discussed. The applicability of the Green Score to catalyze progress in the pursuit of meaningful transparency and empirical data sharing across enterprise supply chain networks is also highlighted.

Received 18th September 2024,
Accepted 3rd March 2025

DOI: 10.1039/d4gc04670f

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Green foundation

1. This work introduces an enhanced methodology for assessing the green chemistry performance of cosmetic ingredients and formulas, thereby providing formulation teams with higher resolution material selection guidance and design analytics.
2. By incorporating new endpoints for biodegradability, waste generation, and manufacturing process hazards, along with more robust environmental impact data sources, the number of green chemistry principles covered by the metric doubled from four to eight. Additionally, the enhanced metric enables improved differentiation between the environmental performance of individual ingredients and can more reliably serve as an 'early warning signal' for materials that may be of potential future concern.
3. Wider availability of empirical human health and environmental impact data across full chemical supply chains will enable further refinement of the metric's assessment methodology and continued improvement in resulting formulation signals.

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† Electronic supplementary information (ESI) available. See DOI: https://doi.org/10.1039/d4gc04670f

Introduction

The overarching ambition of green chemistry since its inception as a scientific field over 30 years ago has been that all chemistry eventually becomes green chemistry.[1,2] Green chemistry has been described as a critical enabler of broader sustainable chemistry and molecular sustainability and continues to play a lead role in humanity's fight against the climate crisis.[3,4]

From a practical standpoint, embedding molecular sustainability across research and development organizations creates synergy with new sustainability frameworks such as the EU Green Deal.[2,3,5] Beyond the Green Deal, global chemical regulations are calling for increased data and transparency with a focus on understanding wider environmental impact. The cosmetics industry exemplifies this evolution, with numerous regulations related to material sustainability and environmental reporting requirements being adopted or proposed in the past four years.[6–9] Hazard based sustainability metrics play a critical role in promoting supply chain transparency and enabling compliance with new and future regulations.[10–12]

While life cycle assessment (LCA) offers the most comprehensive framework for environmental sustainability assessments, it is acknowledged to be data hungry and both resource and computationally intensive, and there remains limited empirical data underlying LCA for fine chemicals.[11,13–17] Proposed regulatory frameworks for product LCA importantly exclude any potential direct consumer hazard impacts, which are increasingly scrutinized by retailers, regulators, and consumers.[18–20] Computationally simple, hazard-oriented green chemistry screening metrics, though not able to match LCA's environmental impact assessment breadth, can complement and aid informed product design by providing a real-time indication of consumer and ecosystem hazard potential along with environmental impact.[13,21,22] These simpler and more streamlined 'green design' tools can further benefit rapidly evolving industries like cosmetics by operationalizing a 'benign by design' approach to product innovation.[11,13,23]

The Estée Lauder Companies (ELC) has created such a framework in the "Green Score" to codify key principles of green chemistry relevant to cosmetics and to provide formulation teams with data-driven molecular sustainability insights in real time.[24] Through more deeply embedding green chemistry within the product development process, more sustainable chemistries can be evaluated and selected early-on and ahead of new regulatory pressures. The Green Score's ability to distil scientific complexity into meaningful, practicable ingredient comparisons and formulation guidance is dependent upon a foundation of robust, ideally empirical data. Furthermore, by rewarding the use of empirical supplier data across its environmental metrics, it can aid in catalyzing a shift towards more meaningful supply chain transparency.

To ensure the Green Score's continued scientific relevance and align with its philosophy of continuous improvement, the tool is periodically updated to include the most recent data and new sources that improve its output resolution. For instance, ingredient suppliers frequently provide updated data on feedstock sourcing and greenhouse gas emissions, and continued scientific advancement also yields improved measurement techniques and impact data across all framework pillars, which benefit the relevance and robustness of the tool once integrated. As part of the periodic Green Score review, ELC convened its inaugural green chemistry Scientific Advisory Group (SAG) in 2021 comprised of global experts in the field of green chemistry. Subsequent work was undertaken to incorporate biodegradability, waste generation, and manufacturing process hazard into the tool, which was validated during the second SAG meeting in late 2023 comprising both global and regional experts from across Asia. This has resulted in "Green Score v.2.0" incorporating four additional green chemistry principles, including waste prevention, material efficiency (atom economy), more benign chemical syntheses, and design for degradation (Fig. 1).

Here, a detailed overview of the Green Score v.2.0 framework is provided, along with representative case studies and discussion exemplifying the enhanced capability of the tool in guiding the proactive selection of chemistries with improved sustainability profiles.

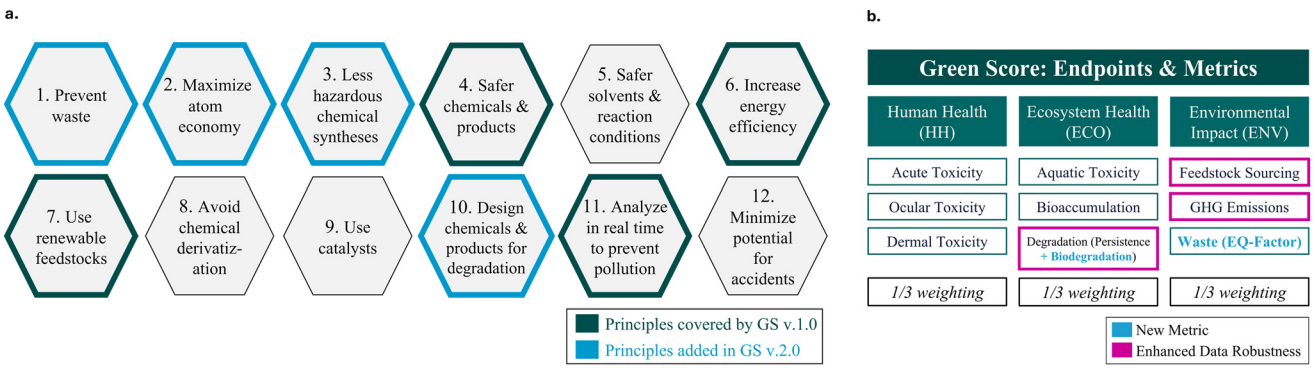


Fig. 1 (a) Green Score v.2.0 doubles the number of green chemistry principles it encompasses from four to eight; (b) overview of Green Score v.2.0, highlighting changes *versus* the original methodology. GS, Green Score; GHG, greenhouse gas; EQ, environmental quotient.

Methods

General methodological framework

The initial Green Score framework quantified the green chemistry alignment of cosmetic ingredients and formulas through equally weighted pillars of human health (HH), ecosystem health (ECO), and environmental impact (ENV).[24] The Green Score v.2.0 iteration follows the previously reported hazard-based scoring framework, with newly incorporated waste and biodegradability endpoints and refined data sources for the feedstock source and greenhouse gas (GHG) emissions metrics. The new and refined ENV endpoints were scaled in a similar manner as v.1.0 to align with the Green Score's 1–5 scoring scale and to account for variation within and between the data ranges (Table S1†). Fig. 2 outlines the Green Score v.2.0 pillars, metrics, endpoints, and respective data sources, while the subsequent sections describe the individual metric constructs.

Quantifying waste generation: waste metric development

The incorporation of a view on waste generation represents a significant methodological evolution. Reducing, or ideally eliminating, chemical waste generation during manufacturing processes, and across supply chains, is a key pillar of green chemistry, often yielding decreased costs and reduced process hazards.[23] While upstream waste generation is a fundamental component of chemical GHG emissions as utilized within the ENV pillar, its specific proportional influence is significantly diluted, subsumed into a single carbon emissions factor that encompasses a plethora of other variables including energy demand, electricity generation, transportation, *etc*.[15,30,31] And, as waste generation is so integral to green chemistry performance and a direct methodological improvement advocated by ELC's SAG, it was incorporated as a new standalone metric within ENV.[32,33]

Green Score v.2.0 not only assesses for waste generation volume, but also includes an evaluation of the hazard potential of both generated waste and the manufacturing process, by introducing the "*EQ*-factor" as the third ENV metric. As established in the literature, the *EQ*-factor is comprised of an "*E*-factor", or waste volume assessment, and "*Q*" as a hazard measure.[23] Only the *E*-factor is commonly used across the wider chemical industry as routes to quantifying "*Q*" have not yet been standardized.[11,34,35]

The *E*-factor is intended to comprehensively quantify all waste generated during a given process or process sequence; therefore, waste was defined within the Green Score framework as any manufacturing process byproduct or auxiliary (*e.g.*,

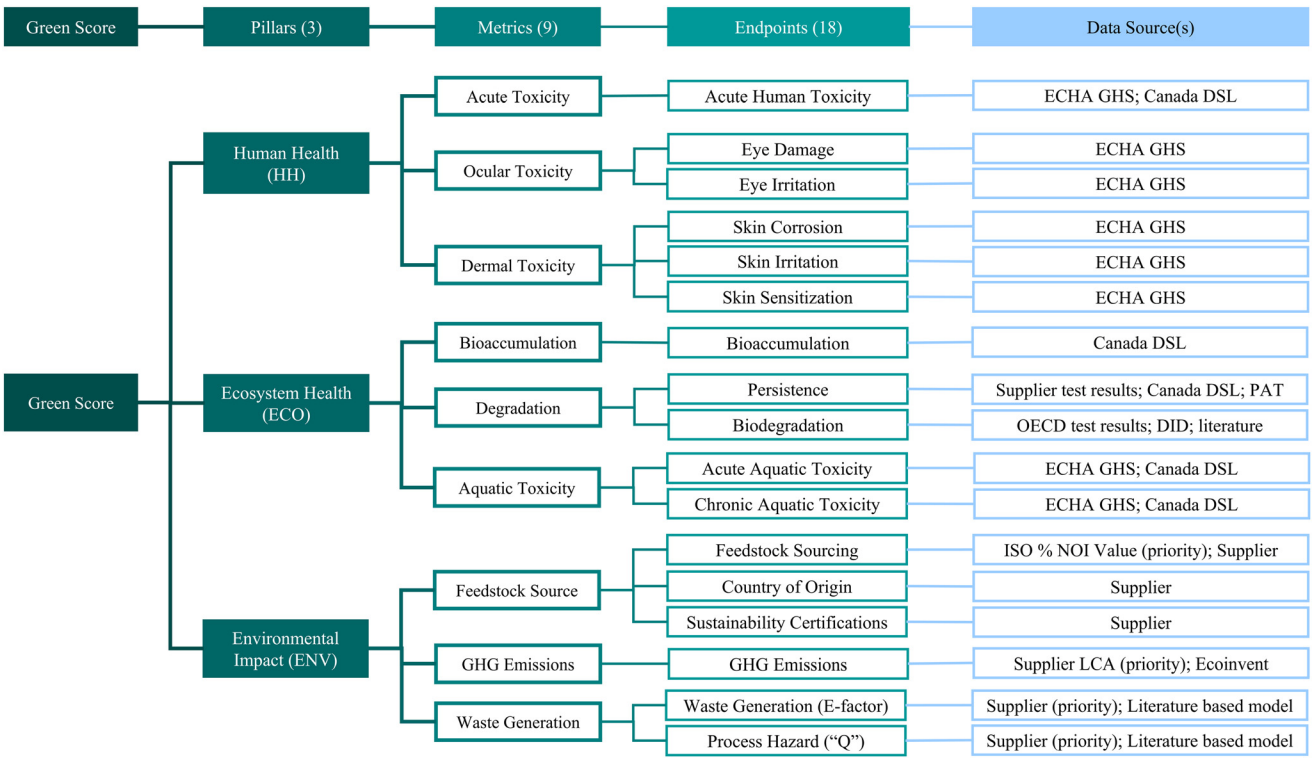


Fig. 2 Overview of Green Score v.2.0 pillar, metric, and endpoint hierarchy with respective endpoint data sources. As per the initial framework, final Green Scores were calculated as an equally weighted average of the three pillar scores, with each pillar similarly calculated as an equally weighted average of its respective metric scores.[24] ECHA, European Chemical Agency;[25] GHS, Globally Harmonized System of Classification and Labelling of Chemicals; DSL, Domestic Substance List;[26] PAT, Ricardo Persistence Assessment Tool;[27] OECD, Organization of Economic Cooperation and Development; DID, Detergent Ingredients Database;[28] ISO, International Standards Organization; NOI, natural origin index; GHG, greenhouse gas; LCA, life cycle assessment; Ecoinvent, ecoinvent life cycle inventory database version 3.10.[29]

solvent, catalyst, *etc.*) not directly incorporated into the final ingredient.[23] Materials that were otherwise repurposed or upcycled, such as biomass or recycled solvents, were not considered waste as this valorization positively contributes to a circular economy. Specific *E*-factor calculation parameters are detailed in the ESI, Table S2.† *E*-factor contributions spanning each chemical's full manufacturing supply chain were assessed, as opposed to solely considering the waste impact of processing steps performed by ingredient suppliers. Such a holistic view on waste generation is important because the relevance of individual process *E*-factors is limited without the context of overall waste generation throughout the supply chain.[11,23]

A simplified derivation of "*Q*" was employed, reflecting the current paucity of transparent data across full ingredient supply chains and exemplifying the need to obtain more meaningful transparency across the chemical industry.[36] Manufacturing process hazard was used as a proxy for the hazardous nature of generated waste, since they are generally correlated and process hazard data is more widely available.[23,37,38] A standard bonus was assigned if the ingredient processing conditions entailed low hazard (*e.g.*, benign reagents, solvents, byproducts, *etc.*), with a penalty assigned if processing was highly hazardous. Neither bonus nor penalty was assigned if process conditions entailed intermediate hazard or if there was insufficient data to perform a full assessment.

The waste metric scoring rubric is visualized in Table S1,† with Table S3† depicting the assigned certainty scores. Empirical supplier *E*-factors and process hazard data were prioritized for scoring, as obtained through separate supplier surveys. Due to their proprietary nature and the ambition to attain a view on waste across the full supply chain of each ingredient, availability of high quality empirical data was very limited.[15,36] In lieu of waiting for more meaningful supply chain transparency into ingredient waste impact, and while working with suppliers to promote the gathering and sharing of this data, a modelling approach analogous to life cycle inventory (LCI) was employed to conservatively estimate *EQ*-factors.[15,39,40] This initial screening level impact evaluation entailed derivation of a literature-based *E*-factor and "*Q*" model.

The waste model approach was predicated on the assumption that many chemistries used in cosmetic formulation are sufficiently similar in feedstock origin and manufacturing process as to be assigned equivalent *EQ*-factor estimates.[41–44] This assumption is a pragmatic way forward in the absence of empirical supplier data or an LCI-style waste database, and was reviewed and ratified by ELC's SAG. Relevant literature examples of *E*-factor and process hazard were leveraged to derive conservative *EQ*-factor proxies for those components and ingredients lacking empirical data. A detailed overview of the waste model development is provided in section 4 of the ESI.† While the output accuracy and specificity are limited, the waste model represents a valuable interim solution while working towards greater supply chain transparency and maturity.

Expanded ingredient degradation assessment: biodegradability integration

Incorporation of a biodegradability endpoint is the second significant v.2.0 methodological addition. Ingredient degradation into environmentally benign byproducts is intrinsically important to the cosmetics industry and is captured by the green chemistry principle "design for degradation".[45,46] Green Score v.2.0 provides an expanded view on ingredient degradation by integrating a biodegradation assessment that better rewards materials which most rapidly and completely degrade. Certain 'levels' of material degradation were defined (Table 1) and utilized for scoring to ensure alignment with the Organization for Economic Cooperation and Development (OECD) harmonized

Table 1 Definition of relevant (bio)degradation terms, as used in this work[47]

Term	Definition *(as used in this work)*	Indicative test thresholds
Readily biodegradable	Classification for chemicals that pass certain stringent screening tests which is indicative of the rapid and complete breakdown of the chemical in aerobic environmental aquatic conditions	OECD 301 & 310 series: >60–70% degradation within 28 days & meets 10-day window (where relevant)
Inherently biodegradable	Classification for chemicals that pass certain screening tests entailing favorable conditions for microbial metabolism which is indicative of the potential for ultimate (complete) chemical breakdown under favorable, aerobic environmental aquatic conditions	OECD 302 series: >70% degradation within 60 days
Ultimate biodegradation	The complete breakdown of chemicals into water, CO_2, biomass, and inorganic salts *via* aerobic microbial metabolism. Ready and inherent biodegradability (above) are sub-categories of ultimate biodegradation	See ready & inherent test thresholds (above)
Non persistent	Classification for chemicals that fail ultimate biodegradation tests but with sufficient evidence available to demonstrate an environmental degradation rate that does not meet criteria for persistence	All environmental half-lives sufficiently short (*e.g.*, <60 days in marine water)
Potentially persistent	Classification for chemicals lacking sufficient data to determine whether they are not environmentally persistent	No data available
Environmentally persistent	Classification for chemicals that resist environmental degradation processes, resulting in the potential for prolonged environmental exposure. Persistence is typically evaluated by comparing degradation rates against threshold values established in regulation	Certain environmental half-lives exceed criteria (*e.g.*, >60 days in marine water)

approach to material biodegradation assessment.[47] The OECD series of test protocols (Table S7†) represent the current 'state of the science' in biodegradation testing and are ubiquitously recognized by global regulatory authorities.[48] The degradation metric scoring rubric is provided in Table S1.† To ensure that inorganic materials were not overly penalized due to not being applicable for microbial biodegradation, an average score of 3 was assigned to all wholly inorganic components.

Overall, data requirements for the degradation metric were significantly more complex than the v.1.0 persistence assessment. V.2.0 utilized a hierarchical data preference framework that prioritized empirical OECD biodegradation test results, such as provided by ingredient suppliers or obtained from publicly accessible databases (*e.g.*, European Chemicals Agency).[25] When evaluating component OECD test outcomes, preference was given to positive readily biodegradable results, superseding any inherently biodegradable data, as is standard practice within the cosmetics industry.[49] Similarly, some consideration of variability in results around the inherent biodegradation threshold value was performed on an individual component basis. The Detergent Ingredients Database (DID) was also leveraged as a source of biodegradability data due to its established role in informing components of the EU Detergent Regulations.[28]

If ultimate biodegradation of a component could not be proven (*e.g.*, due to insufficient data), further investigation of environmental persistence and/or non-persistence was performed, using a weight of evidence approach. Relevant screening level sources (*e.g.*, Canada DSL), scientific literature, and supplier provided data were leveraged to assess the persistence potential of individual chemical components.[26] The metric certainty score assignment rubric is presented in Table S3.†

Refinement of GHG emissions data

Data quality and robustness within the ENV pillar was further enhanced through GHG metric refinement. Increasing the energy efficiency of products and processes is fundamental to improving sustainability performance, encompassed by the green chemistry principle "design for energy efficiency".[11,50] Ingredient GHG (*i.e.*, carbon) emissions impact is used as a proxy for energy efficiency within the Green Score as it offers a broader view on production efficiency than electricity use alone.[35,51,52] Green Score v.1.0 provided an initial view on GHG impact by averaging each ingredient supplier's overall (corporate) scope 1 & 2 carbon emissions with a component specific cradle-to-gate emissions factor estimate.[24] Supplier emissions were tracked through a separate survey, and component emissions factors were obtained from the Ecoinvent life cycle inventory database.[29] While this approach enabled high-level supplier differentiation (*e.g.*, rewarding those suppliers using renewable energy across their corporate operations), supplier emissions data were not ingredient specific, highlighting a shortfall in meaningful transparency.

Under Green Score v.2.0, the GHG metric was refined to enable direct empirical comparison of ingredient emissions by integrating newly available, ingredient specific cradle-to-gate carbon footprints as obtained from supplier LCA results. This data represents the state of the science in emissions assessment across the cosmetic and wider chemicals industries.[15] If an empirical supplier emissions factor was not available or was not in alignment with enterprise standards for supplier emissions reporting, the cradle-to-gate carbon footprint was estimated through optimized assignment of component emissions factors, as based upon feedstock source and manufacturing process. Emissions factor estimates were derived from life cycle inventory databases relevant to cosmetic chemistries, such as Ecoinvent.[29] The previously utilized supplier emissions endpoint was superseded by the greater accuracy and relevance offered by empirical supplier data, complementing ELC's standardized approach to enterprise GHG accounting. The v.2.0 GHG metric scoring rubric is provided in Table S1,† with Table S3† depicting the updated certainty score assignment.

Refinement of feedstock sourcing data

Feedstock sourcing metric refinement provides the final v.2.0 data robustness enhancement. Selection of ingredient feedstock is a critical formulation decision within the development of cosmetic products, with the use of renewables wherever feasible explicitly included as a green chemistry principle.[11] Green Score v.1.0 accounted for feedstock source through binary, non-standardized supplier reported source designations. To better differentiate between ingredients with varying levels of renewable (*i.e.*, natural) derived content, Green Score v.2.0 prioritized newly available, harmonized ISO 16128 natural origin index (NOI) data, which has become the cosmetic industry standard for naturality assessment.[53] Ingredient NOI values were calculated and validated internally according to the ISO protocol and supplier provided feedstock and manufacturing process data. The metric scoring rubric (Table S1†) was evolved to reflect the continuous scale of ingredient NOI values and the ISO stipulation that any ingredient less than 50% NOI must be considered non-natural.[53] ISO NOI values excluding the influence of water were utilized for scoring, as water is considered natural under the ISO protocol but is otherwise excluded from the Green Score calculation. The metric's additional country of origin and sustainability certifications points were assessed as per the original methodology, employing supplier provided data at the component and ingredient levels.[24] Table S3† depicts the refined certainty score assignment rubric.

Descriptive analyses

All descriptive analyses used to assess the impact of the v.2.0 methodological enhancement on resulting in-house formulation signals were performed in Microsoft Excel.

Results and discussion

The minimization of both toxicological hazard and potential environmental impact, while simultaneously maintaining chemical function and efficacy, may be one of the most chal-

lenging aspects of designing more sustainable products. However, by providing formulation chemists with both a real-time indication of green chemistry performance and continued education on its use and refinement over time, 'benign by design' approaches can successfully be employed. Such upfront design can then lessen the need for costly and time-consuming reformulation after the fact.

This context highlights the opportunity afforded by the Green Score in providing quantitative real-time molecular sustainability guidance to product formulators throughout the product development cycle, complementing existing product safety and regulatory compliance requirements. In measuring progress towards internal green chemistry goals and against product benchmark standards, development teams can better understand the broader impact of their ingredient selections and efficiently evaluate options for optimizing performance.

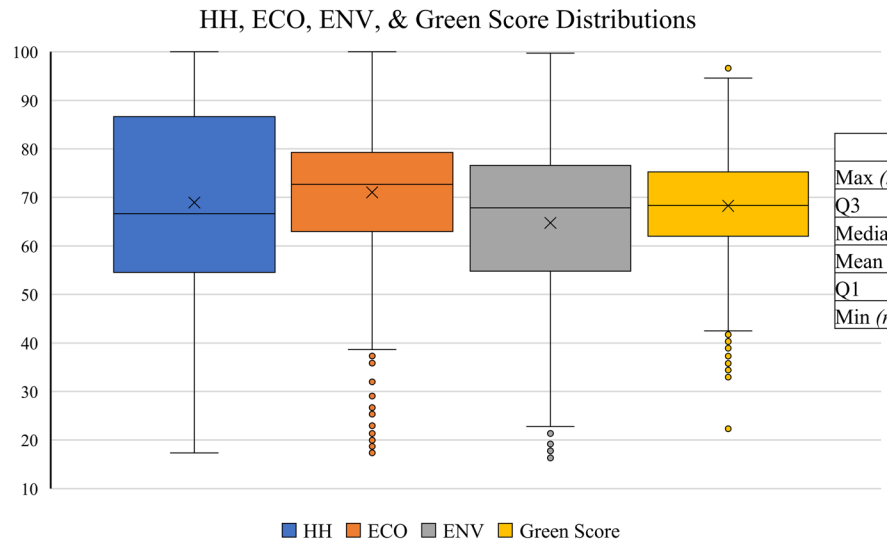
Refinement of the Green Score framework to account for evolution in underlying scientific endpoints and general green chemistry advancement is essential to ensure the tool's continued relevance and scientific robustness.[24] While implementation requires appropriate change management processes for both system and formulator user, this is greatly facilitated by the tool's computational simplicity and flexible architecture, thereby delivering consistent formulation guidance reflective of the current state of the science. A general characterization of the Green Score v.2.0 output data is subsequently provided.

General descriptive analysis of Green Score v.2.0

Box-and-whisker distribution plots of ingredient Green Scores and the HH, ECO, and ENV pillars are depicted in Fig. 3. The conservative directionality of scores (negative skew) reflects the evolved view on material performance resulting from both the degradation and ENV refinements. ENV is generally characterized as the most conservative pillar, reflecting the GHG metric evolution and the addition of a conservative view on waste generation.

While scores are not directly comparable between Green Score v.1.0 and v.2.0 due to the extensive degree of methodological evolution, the reliability and directional accuracy of resulting formulation guidance has significantly improved. For instance, the integration of a biodegradability assessment enables a higher resolution view on chemical end-of-life fate and better rewards those ingredients with lower potential environmental impact. Furthermore, the waste metric addition enables tracking of chemical waste generation and manufacturing process hazard, which was not previously possible due to data availability limitations. In combination with the improved accuracy of GHG emissions and feedstock source accounting, ENV now affords a significantly more robust and accurate material characterization and may now be considered equal in discriminatory power to the well characterized ECO and HH pillars.[24]

The enhanced indication of molecular sustainability performance provided by Green Score v.2.0 proves especially beneficial to practical ingredient comparisons when interrogated in parallel with existing functional material characterization parameters. Fig. 4a and b highlight the variation in Green Scores observed between individual ingredient functional categories and chemical categories, respectively. It is evident that certain functional classes, including sun protection factor (SPF) agents, film formers, and solvents have lower green chemistry performance compared to much of the functional cosmetic portfolio. Similarly, certain chemical classes such as polycyclics and siloxanes have lower green chemistry performance in comparison to other cosmetic chemistries, such as biological products (*i.e.*, non-botanical natural materials such as honey and yeast extract) and fats/oils (*i.e.*, majority triglyceride materials derived from commodity crops). Beyond inherent variation in material green chemistry alignment, the observed ranges and directionality in category performance result from the intersection of cosmetic ingredient structure and function.



	HH	ECO	ENV	GS v.2.0
Max *(non-outlier)*	100	100	99.71	94.63
Q3	86.67	79.27	76.57	75.23
Median	66.67	72.67	67.8	68.31
Mean	69.01	71.01	64.77	68.27
Q1	54.67	63	54.78	62.03
Min *(non-outlier)*	17.3	38.67	22.77	42.45

Fig. 3 Box-and-whisker plots of v.2.0 ingredient HH, ECO, ENV, and Green Scores (GS), with associated data labels.

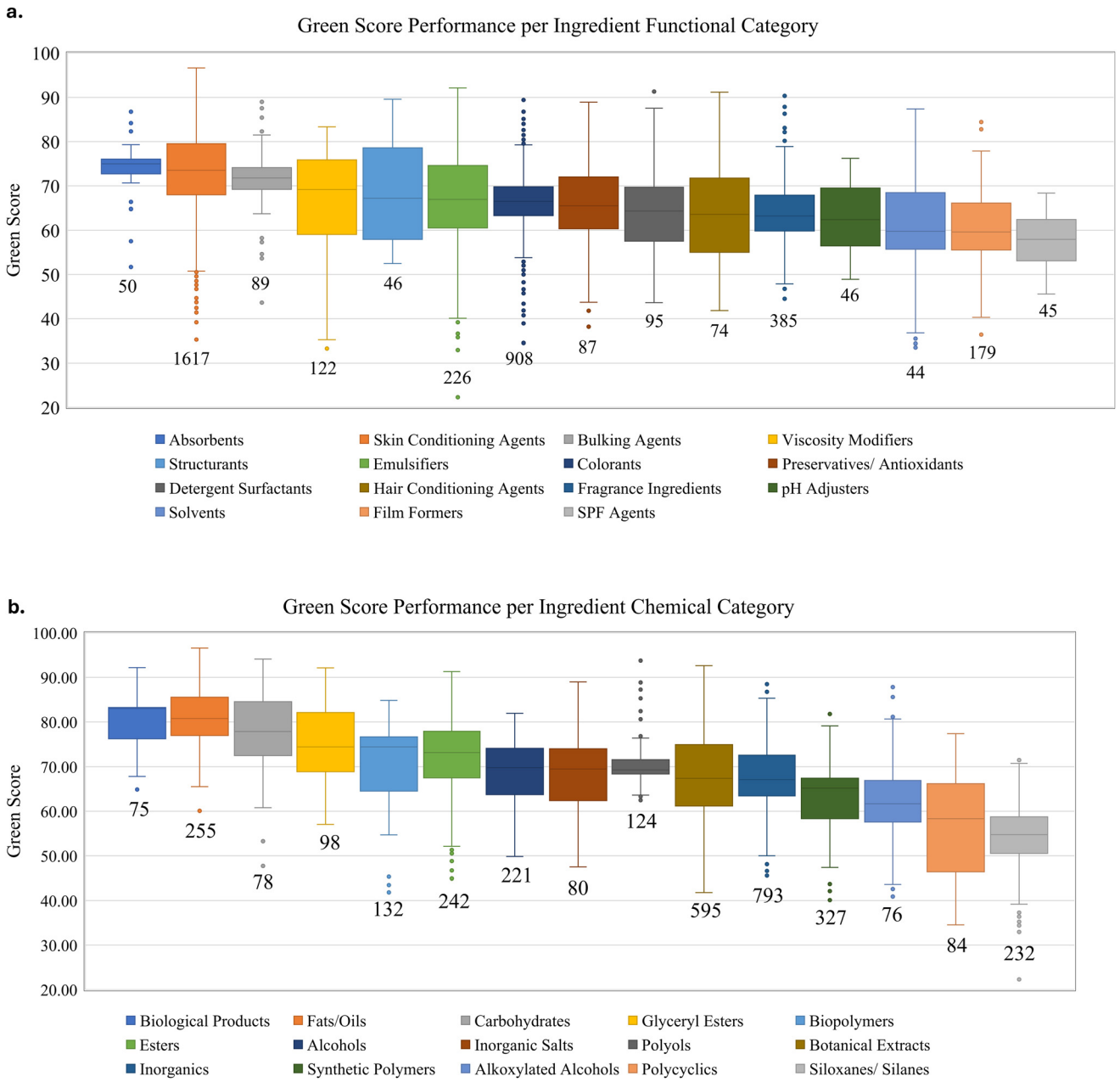


Fig. 4 (a) Box-and-whisker plots of ingredient Green Scores per ingredient functional category, with category count (*i.e.*, size) listed below each plot (top 15 largest categories visualized for simplicity); (b) box-and-whisker plots of ingredient Green Scores per chemical category, with category count listed below each plot (top 15 largest categories visualized for simplicity).

Each functional category is structurally diverse, and each chemical category can similarly serve various functions, with individual permutations (*e.g.*, a glyceryl ester emulsifier) generally more or less suited to a certain formula chassis due to specificity in molecular interaction profiles. Integration of this functional and chemical class parameter matrix with Green Score data, yielding a comprehensive material toolbox, can facilitate informed material substitutions and streamline the experimentation process, thereby accelerating formulation sustainability efforts.

This matrixing of green chemistry and functional material characterization parameters illustrated in Fig. 4a and b facilitates the derivation of targeted data insights and can aid formulation teams in pursuing the highest impact material substitutions and design decisions. For instance, formula Green Score interrogation across the ELC portfolio highlighted that the performance of many product types is driven by a limited number of ingredient functional categories within the formulator's control (*i.e.*, not limited by external regulatory stipulations). Therefore, provision of relevant and accurate insight

into potential ingredient alternatives within these high impact categories can deliver tangible human health and environmental benefit. An ingredient selection case study is subsequently provided to exemplify the added value provided by Green Score v.2.0 to the formulator's material selection process.

Improved data resolution: representative ingredient choice case study

The substitution of high-volume cosmetic ingredients with chemically identical alternatives which have a better sustainability profile represents a significant formula innovation opportunity. Ethanol and butylene glycol offer two examples of commonly used ingredients across the cosmetics industry that frequently act as key drivers of overall formula Green Score performance across various product types. Ethanol has multifunctional use as a solvent, fragrance and actives carrier, astringent, and antimicrobial, whereas butylene glycol functions as a humectant, solvent, actives carrier, and aesthetic feel modifier. While traditionally derived from petroleum, more recently biofermentation derived ethanol and butylene glycol have gained traction across the cosmetics industry due to consumer demand for naturally derived products.[54–56] Green Score v.1.0 had limited ability to differentiate between the manufacturing process impacts of these derivation routes, but v.2.0 provides the resolution power necessary to appropriately convey the environmental benefits of fermentation to formulators. Fig. 5 aims to visualize, for both ingredients, that while the petroleum derived options have better chemical waste impact due to the reality of comparing highly efficient petrochemical processing with less-optimized biotechnological processes, there is significant difference in process hazard and overall GHG impact. As delineated by these refined environmental signals, the fermentation derived ethanol and butylene glycol have clear green chemistry advantage.

Green Score v.2.0 as an ingredient innovation guide

Previous work highlighted the Green Score's ability to "identify emerging chemicals of concern and guide substitution with greener alternatives".[24] The v.2.0 methodological enhancements have strengthened this ability by more effectively discerning opportunities in ingredient manufacturing processes to improve green chemistry alignment. For instance, detergent surfactants tend to score only moderately well (Fig. 4a) despite being derived from majority renewable feedstocks. This is largely due to the negative environmental impacts inherent to the stoichiometry-heavy processing of commodity plant oils into functional material derivatives, which subsequently yield lower GHG and waste metric scores.[43,57–59] Implementation of greener processing steps, such as enzymatic catalysis based transformations widely reported in the literature, would benefit the chemical waste generation, process hazard, and GHG emissions footprints of these materials.[43,58,59] Such innovation would correspondingly be reflected through improved Green Scores.

The improved signal reliability and robustness delivered by Green Score v.2.0 enables formulation chemists to focus on areas where wider cosmetics industry innovation efforts may be needed, such as in the film formers category (Fig. 4a). Film formers are used widely in makeup products for longwear and aesthetic benefit; however, currently there are very limited high performance, globally compliant alternatives to these traditionally petroleum derived materials. Overcoming this innovation gap within the acceptable parameters of functional and economic performance, regulatory compliance, and molecular sustainability will likely necessitate wider collaborative efforts among numerous global supply chain partners.

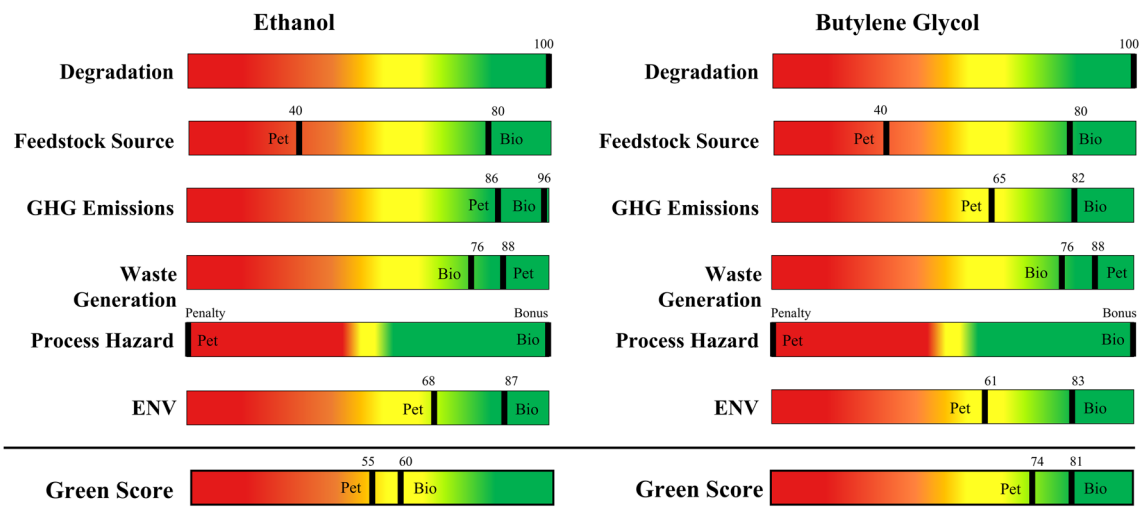


Fig. 5 Enhanced metric endpoints under Green Score v.2.0, with respective performance of the petroleum and biofermentation derived ethanol and butylene glycols. While little scoring differentiation was attainable under v.1.0 due to environmental impact data limitations, v.2.0 captures environmental impact performance differences and yields a more robust and reliable view on green chemistry performance. Pet, petroleum derived; Bio, biofermentation derived. *Visualization of scores not to scale.*

The enhanced ability to highlight materials with poorer green chemistry alignment and resulting innovation opportunities or needs, whether individually or in aggregate, furthers the tool's utility as a potential 'early warning signal' for materials that may be of future concern. Product reformulation to comply with potential new regulatory restrictions requires both significant time and resource, so proactive identification of potential 'at-risk' materials, along with implementation of wider alternatives assessment frameworks, is an attractive proposition.

Hazard-based, rapid screening tools such as the Green Score do not provide a fully holistic view on material life cycle impact. Yet, by integrating robust and relevant data across the pillars of human, ecosystem, and environmental health, such frameworks can efficiently provide real-time design signals to guide improvements in product molecular sustainability profiles. The hazard-based view of Green Score v.2.0 on material impact also highlights other areas of potential green chemistry innovation opportunity. For example, directional scoring signals can delineate where certain ingredient performance attributes may be below average for a category, or if an entire category of ingredients is not aligned with a certain facet of green chemistry. Furthermore, with recent developments within the chemical regulatory landscape placing more emphasis upon hazard-based approaches, the ability to differentiate such signals is increasingly more pertinent and has the potential to provide significant added value to wider alternatives assessment efforts across research and development organizations.

Future directions

Green Score v.2.0 represents a significant step forward with respect to the green chemistry principles and reflects the framework philosophy of continuous improvement. All refinements serve to increase the overall data robustness and yield an increasingly balanced and holistic measure of performance. While designed specifically for cosmetic product evaluation, the Green Score v.2.0 framework could also be applicable to other industries and academic research, especially where a hazard-based view on human health and environmental performance would be valuable. The tool requires a base level of transparency into material compositions, and further tailoring of endpoints, scoring scales, and metric weightings may optimize its wider relevance. To facilitate potential broader uptake of the Green Score framework and promote further meaningful transparency across the chemicals industries, a tailorable Excel version of the tool is included as part of the ESI.†

Looking forward, there is opportunity to further improve the framework by leveraging broader advancements related to supply chain transparency. The chemicals industry has a clear need for greater accountability across every supply chain to deliver meaningful, collaborative transparency in reporting and to drive substantial green chemistry innovation. This shared consensus will foster stakeholder empowerment and engagement, and collectively hold organizations accountable for disclosing empirical product and process impacts. It is envisioned that mandated environmental impact disclosure across upstream supply chains under the EU Corporate Sustainability Reporting Directive (CSRD) will radically transform the data availability paradigm and, therefore, accelerate the incorporation of empirical supplier data into the Green Score.[6]

For instance, the availability of empirical *E*-factors and manufacturing process hazard data across the supply chain is currently limited. Suppliers may have *E*-factors for their own manufacturing operations but not their upstream purchased materials. These limitations resulted in significant use of the waste impact model to fill portfolio data gaps. Yet, modelled *E*-factors do not allow for differentiation between processing nuances in the derivation of structurally similar cosmetic chemistries. New CSRD reporting requirements, along with further supplier engagement and education to promote and reward the provision of higher resolution waste data across the supply chain, should improve availability of empirical *E*-factor data. At the same time, this incoming supplier data can also serve to expand the waste model's underlying data set, therefore increasing the accuracy and resolution power of *E*-factor estimates for those remaining chemistries without empirical data. Wider availability of detailed process hazard data will also facilitate a more sophisticated quantification of "*Q*", such as through a tiered hazard penalization approach or a mass weighted scheme more akin to those utilized in the pharmaceutical industry.[11,21,23]

Beyond waste accounting, broader industry advancements in meaningful supply chain transparency could also facilitate improved environmental impact resolution among inorganic ingredients. Inorganics are widely used across the cosmetic industry yet there is a paucity of empirical data on their environmental impact, arguably driven by mineral processing falling somewhat outside the scope of the green chemistry principles due to its high reliance on physical (as opposed to chemical) process steps.[44,60,61] While the Green Score is designed to not over-penalize inorganics due to these differences in sourcing and processing, enhancing the tool's ability to comprehensively convey their environmental performance could be an area of future research.

The continual provision of accurate and reliable molecular sustainability feedback to formulation teams can be further ensured by regular incorporation of newly available hazard endpoints across all three green chemistry pillars. For example, the inclusion of new endpoints (*e.g.*, persistent, mobile, and toxic (PMT) and very persistent, very mobile (vPvM)) into the European Classification, Labelling, and Packaging (CLP) regulation will provide a key opportunity to incorporate additional environmental endpoints into the framework.[62] Further enhancement in the accuracy and relevance of Green Score formulation guidance could be attained through optimizing the relevance of all chemical hazard endpoints within the HH and ECO pillars, as opposed to solely considering the most conservative reported data.

The ongoing derivation and maintenance of an increasingly robust underlying data architecture to support the Green Score

is a complex and continually expanding endeavor. Novel statistical, data mining, and artificial intelligence (AI) approaches offer promising options to further interrogate the evolving data structures, elucidate valuable data insights, and inform predictive property assessments.[63–66] For example, digitalization accelerated through the implementation of tools such as AI, machine learning (ML) and predictive analytics could help to improve the sustainability profiles of products and processes, given the great potential of these tools for promoting green chemistry and sustainability.[67] Therefore, these represent additional targets of future research efforts.

Continued scientific advancement in molecular sustainability performance assessment means that the consensus definition of "green" may evolve significantly over time.[33,68,69] Keeping up with the rapid progression of science, especially at the large scale of global R&D organizations, requires an agile, iterative approach. Readily deployable, flexible, hazard-based screening tools like the Green Score can help organizations embrace this variability and accelerate 'green' innovation efforts. The Green Score's focus on continuous improvement in data robustness and impact resolution forms a key differentiator for the tool in comparison to other formulation sustainability approaches within the cosmetics sector. Through transparent communication of the Green Score refinement journey and parallel efforts to more deeply embed green chemistry across ELC's product development processes, complemented by providing an open-source version of the scoring system, our ultimate ambition remains to advance the utility of green chemistry as a framework for responsible product design.

Author contributions

E. Thompson was responsible for conceptualizing the Green Score methodology enhancement and its further development, data curation, formal analysis, writing the initial draft manuscript, and editing the manuscript. H. Bialk, T. Kedwards, and G. Daher were responsible for development of the enhanced Green Score methodology, research supervision, and reviewing and editing the manuscript. P. Anastas, D. D'Alessandro, V. Hoven, Z. Liu, K. Saito, A. Mudring, and V. Zeidler provided technical review and counsel into the enhanced Green Score methodological development and critical review of the manuscript.

Data availability

The non-proprietary data supporting this article have been included as a part of the ESI.† Additional data for this work are available at the ref. 25–29 in this manuscript.

Conflicts of interest

Eva Thompson, Heidi Bialk, Tim Kedwards, and George Daher are employees of and may hold stock in The Estée Lauder Companies. Paul Anastas, Deanna D'Alessandro, Voravee P. Hoven, Zhimin Liu, Anja-Verena Mudring, Kei Saito, and Vânia Zuin Zeidler have served as members of The Estée Lauder Companies' Green Chemistry Scientific Advisory Group.

Acknowledgements

ELC would like to acknowledge the valuable contributions of its additional SAG member to the Green Score enhancement process: Professor Kristala L. J. Prather (Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA).

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