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# Environmental profile of the production of fragrance ingredients used in cosmetic products: comparative analysis of results obtained by life cycle assessment and the green chemistry-based eco-design tool GREEN MOTION™†

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In the last few decades, sustainability has become one of the main challenges of beauty companies driven by growing consumer demand for more natural-based cosmetics. Fragrances playing a major role in cosmetic formula, they have to be taken into account in the eco-design process of cosmetics. The composition of fragrances can imply up to one hundred different fragrance ingredients, but is most of the time kept secret to protect the professional knowledge of fragance's suppliers. Different eco-design tools exist, based for example on green chemistry principles and metrics. These tools may address various environmental impacts or life-cycle steps, from the single *E*-factor indicator, which focuses on the amount of waste per amount of product at the production step, to an elaborated set of indicators, like in the GREEN MOTION™ tool developed by MANE. On the other hand, to assess the holistic environmental impacts of products over their whole life-cycle, Life Cycle Analysis (LCA) is the most recognized method. However, it requires extensive amounts of data which can be difficult to obtain or inaccessible for various reasons, including confidentiality. To compare these different possible approaches of fragances eco-design, the results of an LCA of 27 selected fragrance ingredients are compared to those obtained with the green chemistry tool GREEN MOTION™. Fragrance ingredients were found to have a wide range of environmental impacts, depending on their production process and on the starting raw material used. Overall, tendencies observed on results with the 2 tools are in good accordance. This study therefore showcases the complementarity of simplified eco-design tools and metrics with LCA to address environmental impacts of fragrance ingredients. Indeed, the former can be used as a first approach to identify environmental hotspots and implement eco-design practices in the development process of fragrance ingredients, while the latter highlights potential direct and indirect impacts over the upstream life cycle and the ingredient production itself, and can be used to measure the reduction of the global environmental footprint achieved through the implementation of eco-design practices. Based on these results on fragrance ingredients, a clustering method could be developed to help conduct LCA of fragrances.

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## Introduction

In cosmetics, the fragrance is an essential element of the sensoriality of a product. A typical composition is often a complex mix of hundreds of ingredients from different origins (fossil-based products, cultivated plants, by-products from other industries, *etc.*) and obtained with different processes, raising various environmental issues in terms of resource use, climate change and air, water and soil quality related impacts. The assessment of these impacts can be conducted through a Life Cycle Assessment (LCA), an ISO standardized methodology,[1,2]

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which has become the go-to methodology to evaluate and understand the environmental impacts of products and services.[3] The methodology implies first to inventory all the materials, energy and emissions to the environment that are involved in the value chain of a product or service to calculate the potential corresponding environmental impacts. Applying LCA to fragrance can nevertheless appear to be a challenge, due to the numerous ingredients involved and as the composition of a fragrance is one of the best kept secrets of the industry. Indeed, in the PEF-like study of shampoo by the professional organization Cosmetics Europe,[4] fragrances were integrated as simplified compositions of five representative ingredients for which some LCA data were available through the LCA conducted for RIFM in 2013.[6]

Few other LCA have been conducted on fragrance ingredients themselves. In 2019, IFF-LMR published a cradle-to-gate LCA study of rose oil and absolute conducted in collaboration with Quantis.[5] The authors presented the environmental results for 5 endpoint indicators: climate change, water consumed, ecosystem quality, resources and human health. Such studies are a great source of knowledge for practitioners looking for environmental data for a particular fragrance ingredient. However, they are scarce in the literature[6–9] and much more information would be needed to fully evaluate a fragrance by LCA. Yet, as the authors of this study on rose oil and absolute say, "*assessing, improving and ensuring the sustainability of natural ingredients is an absolute necessity for the future of natural(s)*" fragrances.[5] Therefore, in the aim of improving the knowledge on fragrance environmental impacts, more data on fragrance ingredients are needed.

To address the challenge of fragrance complexity and data confidentiality which renders the application of LCA difficult, a simplified yet robust method of evaluation could be developed, taking inspiration from the variety of tools and metrics developed to answer the need for quantitative knowledge on chemical processes, in order to follow the "green chemistry" concept and its twelve principles proposed by Paul T. Anastas and John C. Warner in 1998.[10] A succinct definition of green chemistry can be summarized as *the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances.*[11] One of the significant contributions of green chemistry was the introduction of the Environmental Factor concept (*E*-factor) by Sheldon.[12] Since then, the field expanded into a wide range of research topics from metrics[13–17] to LCA-based tools and hybridized metrics.[18–23]

All these tools based on green chemistry principles address environmental issues at the chemical structure level by designing more efficient syntheses or processes. Thus, thanks notably to a better yield, benefits can carry on through all stages within a product or a process life cycle. It might nevertheless not always be the case, as the 12 principles of green chemistry are not independent factors[24] and the application of one might be in contradiction with another.[25] To quantitatively check the effective environmental performance improvement of a process redesigned following the green chemistry concept, LCA offers a comprehensive and quantitative assessment of different environmental indicators. It helps to avoid misleading results or sub-optimization of the environmental impact reduction[26] by weighting different factors.[27] However, green chemistry tools can complement LCA by providing useful qualitative information on aspects not taken into account by the latter.[28] An example of such complementary analysis is the assessment of an innovative route to glycidol from the conversion of a by-product in the epichlorohydrin production process.[29] The authors compared the new route with the current value chain by green metrics, an *at early stage* (AES) LCA[30] and the green chemistry-based tool GREEN MOTION™[31] to confirm that the proposed process was indeed leading to a decrease of the environmental impact of the epichlorohydrin value chain. However, this case study, which is the comparison of two ways of producing a molecule, one of them including the reuse of a waste as a starting material, provide an ideal case for the comparison of green chemistry-based tool and LCA conclusions since no opposing factors play a role here. The conclusions obtained with these tools could vary more when applied to the comparison of totally different production process and raw materials origin to produce radically different molecules, which is the case for fragrance ingredients.

In the fragrance sector, the use of green chemistry principles and holistic view of LCA have made their appearance in the programs of some of the key players in recent years, albeit with various degree of details.[32–35] However, environmental data are still scarce and usually focus on only a few impact categories which could lead to missing out on environmental hotspots. In this context, the company MANE developed a comprehensive approach based on green chemistry principles called GREEN MOTION™ [31] to assess the environmental impact of all its ingredients, flavours and fragrances. Committed to a continuous improvement of its LCA based eco-design tool of cosmetic products named SPOT, L'Oréal partnered with MANE to determine the complete environmental profile of a representative selection of fragrance ingredients using LCA. The objectives of this work were multiple: (1) allow better assessment of the environmental impact of any fragrances by providing impact factors for widely-used fragrance ingredients (see ESI†), which could also benefit to several industries (cosmetics, detergents, food, pharmaceuticals, *etc.*), (2) compare environmental impacts obtained with LCA to GREEN MOTION™ ratings, and to a commonly-used metric such as the *E*-factor to help decision making on which tool to use depending on the objective of the study and (3) help to eco-design fragrance ingredients by providing details on the origin of the environmental impacts.

## Objective and scope

The objective of the present study is to evaluate the environmental impact of a fragrance and identify eco-design leverages without revealing its exact composition to preserve confidentiality and industrial knowledge. To do so, a representative panel of fragrance ingredients used in cosmetics was evaluated *via* LCA with the eco-conception tool SPOT, in complementarity with GREEN MOTION™ and the *E*-factor.

 

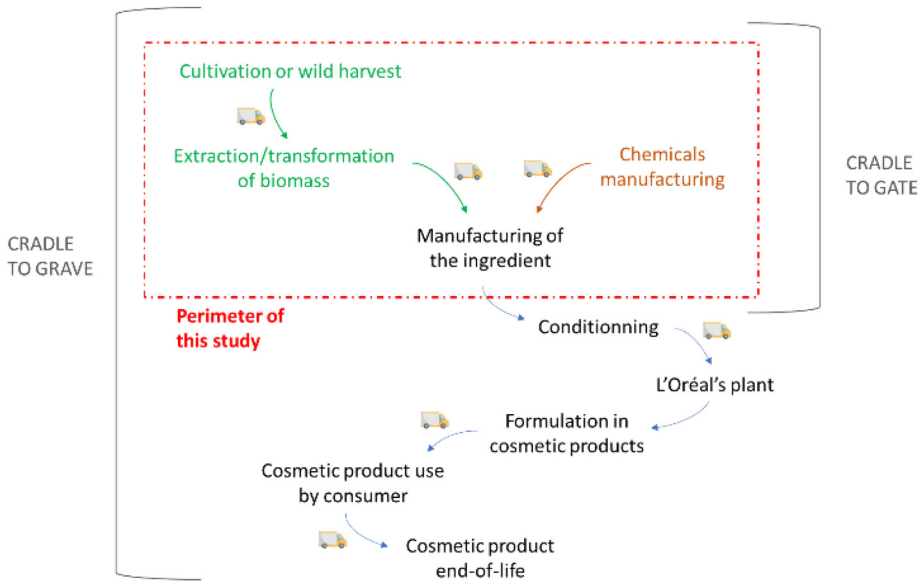


**Fig. 1** Definition of the studied system and scope for the LCA.

The LCA study focuses on the production of fragrance ingredients and on all upstream steps, while their downstream use and their end-of-life were excluded from this study as shown in Fig. 1. These steps were excluded as (1) the modeling of the end-of-life of cosmetics and of the ingredients they content depends on their use phase, and (2) methods have already been developed to assess the impact of fragrances at the end-of-life step, for example based on the hazard mentions of fragrance ingredients in the final concentrate,[36] allowing to preserve the secret composition of the fragrance. The reference unit selected for the LCA is: "Production of 1 kg of the fragrance ingredient at MANE's plant".

For its part, GREEN MOTION™, measures the health, safety and environmental impacts of the ingredients based on their level of compliance with the twelve principles of green chemistry. It includes various aspects of the life cycle including raw material, production process and end-of-life.

Finally, the *E*-factor focuses on the amount of waste generated by the production of an ingredient. It considers raw materials and solvents but does not include the waste generated in the upstream value chain.

## Materials and methods

### Selection and categorization of 27 fragrance ingredients

Fragrances are a complex mixture of hundreds of ingredients whom composition cannot be revealed. Thus, a "categorization" approach was used to approximate the full composition of the fragrance. First, based on MANE expertise, all ingredients used in L'Oréal fragrances were sorted in different categories depending on their production process and raw material origin, derived from ISO standard[37] and IFRA definitions[38] as shown in Table 1. Secondly, for each category, key ingredients for perfumery in terms of quantity consumed have been selected. In the aim of representing the diversity of environmental profiles,

**Table 1** Definition of fragrance ingredients categories

| Category | Definition |
|---|---|
| Essentials oils (EO) | Product obtained from a natural raw material of vegetable origin, either by steam distillation with or without water, mechanical processes from the epicarp of citrus fruits or dry distillation, after separation of the possible aqueous phase by physical processes |
| Jungle Essence™ extracts | Product obtained from a natural raw material of vegetable origin by extraction with a supercritical fluid followed by a separation by expansion |
| Essences by expression | Essential oil obtained by mechanical processes from the epicarp of the fruit of a Citrus, at ambient temperature |
| Natural extracts with volatile solvent – Absolutes | Product obtained by extraction with ethanol from a concrete, a floral pomade, a resinoid or a supercritical fluid extract |
| Natural extracts with volatile solvent – Resinoids | Product obtained from a dry plant natural raw material by extraction with one or several solvent(s) |
| Isolated natural ingredient | Product obtained by fractional distillation as a by-product of an essential oil or extract obtained by concentration, distillation or others isolation techniques |
| Bio-based ingredients with a fossil-based moiety | Product obtained by synthesis from a combination of a biosourced raw material with one or more fossil-based ingredients |
| Fossil-based ingredients | Product obtained by synthesis from a combination of two or more fossil-based raw materials |
| Biotechnology ingredients | Product obtained by a process involving biological entities comprising micro-organisms such as bacteria, yeasts and fungi, or higher organisms such as algae, plants or animals, used as such or in cell or tissue cultures, and enzymes derived thereof |

**Table 2** Fragrance ingredients characteristics

| Category | Ingredient | Olfactive category[a] | Raw material | Method of culture | Manufacturing process | Yield[b] | Co-products from ingredient production | Relative expected impact in the category |
|---|---|---|---|---|---|---|---|---|
| Essentials oils (EO) and Jungle Essence™ extracts[c] | Lavender EO | Aromatic | Flower | Mechanized | Hydrodistillation | 1% | Lavender floral water | Low |
| | Elemi EO | Spicy | Resin | Wild harvest | | 20% | — | Low |
| | Orris Butter | Floral | Rhizome | Manual | | 0.35% | — | High |
| | Vetiver EO | Woody | Root | Manual | | 2% | — | Low |
| | Vanilla Pure Jungle Essence™ | Gourmand | Beans | Manual | Supercritical $CO_2$ extraction | 20% | Exhausted vanilla seeds | Middle |
| | Pink Pepper Pure Jungle Essence™ | Spicy | Pink pepper | Wild harvest | | 1.5% | — | High |
| Essences by expression[d] | Orange essence | Citrusy | Fruit | Mechanized | Expression | 0.01% | Orange juice (main product) | — |
| Natural extracts with volatile solvent – Absolutes | Orange flower absolute | Floral | Flower | Mechanized | Solvent extraction | 0.12% | Wax | High |
| | Jasmine absolute | Floral | | Mechanized | | 0.15% | Wax | High |
| | Narcissus absolute | Green | | Wild harvest | | 0.07% | Wax | Middle |
| | Rose absolute | Floral | | Mechanized | | 0.16% | Wax | High |
| Natural extracts with volatile solvent – Resinoids | Benzoin resinoid | Balsamic | Resin | Wild harvest | Solvent extraction | 85% | — | Low |
| | Labdanum resinoid | Balsamic | Leafy branches | Wild harvest | | 84% | — | Low |
| | Labdanum absolute | Balsamic | | | | 60% | — | Middle |
| | Vanilla absolute | Gourmand | Beans | Manual | | 5% | Exhausted vanilla seeds | High |
| Isolated natural ingredient | *cis*-3-Hexenol (natural) | Green | Mint leaves | Mechanized | Hydrodistillation then fractionation | 0.001% | Menthol, mint terpenes (α- and β-pinene, limonene, *etc.*) | — |
| Bio-based ingredients with a fossil-based moiety[e] | Iso E super | Woody | Myrcene[f] | Mechanized/ wild harvest | Chemical synthesis | 42% (from myrcene) | | Middle |
| | Vetiveryle acetate | Woody | Vetiver essence | Manual | | 0.84% | | High |
| | Myrcene (from crude sulfate turpentine) | Aromatic | Wood chips | Mechanized | | 78% | α-Pinene, limonene | Low |
| | Myrcene (from pine) | Aromatic | Pine resin | Wild harvest | | 4% | Colophane, α-pinene, limonene | Low |
| Fossil-based ingredients | Hexyl salicylate | Floral | Synthetized from petrochemical materials | — | Chemical synthesis | 99.9% | — | Middle |
| | Ethyl 2-methyl butyrate | Fruity | | — | | 87% | — | Low |
| | Hedione | Floral | | — | | 20% | — | High |
| | *cis*-3-Hexenol (fossil-based) | Green | | — | | 42% | — | Middle |
| Biotechnology ingredients | Antillone | Fruity | Undecylenic acid | — | Fermentation | Confidential | Confidential | Middle |
| | γ-Octalactone | Gourmand | Caprylic acid | — | | | | Low |
| | Tropicalone | Fruity | Undecylenic acid | — | | | | Middle |

[a] IFRA Fragrance Ingredient Glossary, April 2010 edition. [b] From raw material to final ingredient. [c] Jungle Essence™ extracts are ingredients obtained by supercritical $CO_2$ extraction. [d] This category includes only Orange essence but it is still quite representative because the former is the most used ingredient by far. [e] Bio-based ingredients with a fossil-based moiety are ingredients obtained by chemical transformation of a natural-based raw material. [f] The myrcene used was assumed to be from a 50/50 mix of crude sulfate turpentine and pine sourcing.

ingredients with the worst and the best environmental GREEN MOTION™ ratings were also included. Table 2 summarizes the 27 selected ingredients sorted by category and their relative expected impact in their category.

### LCA and L'Oréal's SPOT tool methodology

Primary data used to model the life cycle of the selected ingredients come from the MANE's plant (in France), from data collected from suppliers or from field data (for example, Jasmine and Rose flower cultivation). The secondary data are based on Ecoinvent 3.7.1,[39] Agribalyse® 3.0[40] or World Food Life Cycle DataBase (WFLDB) 3.5[41] databases. The main modeling hypotheses of the study are the following:

- Since wild plants harvested manually require no mechanized work, no chemical inputs nor lead to land occupation, their harvest was assumed to have no impact.

- Primary data on the resources used for each ingredient production process in MANE's plant were not available. However, aggregated water and energy data were known for 4 types of production units: natural extracts, synthesis, fractionation and biotechnologies. Specific data for each ingredient were then estimated with the assumption that energy and water consumption vary proportionally to some key parameters of the production process: duration, temperature and heating process (see ESI† for more details).

- Thus, energy overconsumption needed to pressurize $CO_2$ into supercritical $CO_2$ could not be specifically attributed to the ingredients that use it.

- For ingredients not produced by MANE, energy and water consumptions were extrapolated from MANE's data and adapted to the country of the supplier manufacturing site.

- Solvents used are fully recycled with a loss rate of 3.5% (data measured by MANE). Lost solvents are emitted to air. The energy necessary to recycle solvents is included in the modeling. In case of by-products in the production process of the ingredient, economic allocation was used with prices data from the manufacturer except in the case of wax by-products and exhausted vanilla beans to which no impact was attributed.

For the presentation of results, life-cycle steps of the production of the ingredients are divided as follows:

- "Raw material" groups the culture of the renewable raw materials and the production of the fossil-based raw materials necessary for the fragrance ingredients.

- "Upstream transport" refers to all transport steps between the raw materials manufacturing site to MANE's plant.

- "Transformation process" includes chemical reagents other than solvents, energy (electricity and heat) consumption, water consumption and infrastructures to extract the ingredient from the raw material. "Solvents" includes the production of solvents and the solvent loss during the recycling process, emitted to air. Recycling process of solvents is included in "transformation process".

- "Waste" includes all waste generated during the production process of fragrances ingredients. It corresponds mainly to biowaste from the exhausted biomass for ingredients from renewable origin.

To evaluate the environmental impacts of the fragrance ingredients, the methodology of the L'Oréal's product ecodesign tool (SPOT) was used. The method, aligned with the Product Environmental Footprint (PEF) method of the European Commission,[43] uses the 14 impact categories described in Table 3. To help decision making, a single score is calculated *via* the aggregation of the normalized and weighed impacts results of LCA. Normalization is a calculation step to estimate the magnitude of impacts by dividing them by a baseline. Normalization values are given by the PEF methodology which are based on the average impacts of a world citizen.[44] Weighting is then used to give more or less weight to the environmental indicators before aggregating them into a single score. For this study, values are based on the Planetary Boundaries concept[45–47] (see Table 4). This transformation of results simplifies the assessment of ingredients environmental profiles with the use of a single and unitless value, instead of the 14 LCA indicators, all having different units.

### MANE's GREEN MOTION™ tool methodology

GREEN MOTION™ is an easy-to-use tool to assess the environmental impacts of chemicals, natural extracts and products from biotechnology. The authors have grouped the 12 principles of green chemistry, qualitative by nature, into seven "fundamental concepts" (Fig. 2) with associated criteria (Table 5) to obtain a score between 0 and 100. The safer and less impactful the process, the higher the rating. The tool works like an audit grid where penalty points are deducted

**Table 3** Impact categories, method references and units used by SPOT[42]

| Impact category | LCIA method | Unit |
|---|---|---|
| Climate change (CC) | $GWP_{100}$, IPCC 2013 | kg $CO_2$ eq. |
| Water consumption (WC) | Water scarcity, AWARE, Boulay *et al.*, UNEP 2016 | $m^3$ eq. |
| Ecotoxicity, freshwater (EC) | USEtox 1.0, Rosenbaum *et al.* 2008 | CTUe |
| Eutrophication, freshwater (EF) | P equivalents, ReCiPe 2008 | kg P eq |
| Eutrophication, marine (EM) | N equivalents, ReCiPe 2008 | kg N eq |
| Acidification (A) | Accumulated Exceedance, Seppala *et al.* 2006, Posch *et al.* 2008 | mol H + eq |
| Land use (LU) | Soil quality index, LANCA, Bos *et al.* 2016 | Pt |
| Eutrophication, terrestrial (ET) | Accumulated Exceedance, Seppala *et al.* 2006, Posch*et al.* 2008 | mol N eq |
| Mineral, fossil & ren resource depletion (RD) | ADP fossile and ultimate reserve, van Oers*et al.* 2002 | kg Sb eq. |
| Particulate matter (PM) | PM 2.5 eq., UNEP, Fantke*et al.* 2016 | Disease inc. |
| Ionising radiation (IR) | Ionizing radiation potential, Frischknecht *et al.* 2000 | kBq U-235 eq. |
| Photochemical ozone formation (POF) | POCP, Van Zelm *et al.* 2008 | kg NMVOC eq |
| Ozone depletion (OD) | ODP, WMO 1999 | kg CFC11 eq. |
| Human toxicity, cancer & non-cancer (HT) | USEtox 1.0, Rosenbaum *et al.* 2008 | CTUh |

Table 4 Normalization and weighting factor of SPOT single score[42]

| Impact category | Normalization factor (multiplicative) | Weighting factor (multiplicative) |
|---|---|---|
| Climate change (CC) | 0.0001 | 0.2550 |
| Water consumption (WC) | 0.0018 | 0.0140 |
| Ecotoxicity, freshwater (EC) | 0.0001 | 0.0231 |
| Eutrophication, freshwater (EF) | 0.6223 | 0.0878 |
| Eutrophication, marine (EM) | 0.0512 | 0.0150 |
| Acidification (A) | 0.0180 | 0.0145 |
| Land use (LU) | $1.2203 \times 10^{-6}$ | 0.2543 |
| Eutrophication, terrestrial (ET) | 0.0057 | 0.0083 |
| Mineral, fossil & ren resource depletion (RD) | 5.181 | 0.1113 |
| Particulate matter (PM) | 0.0001 | 0.1625 |
| Ionising radiation (IR) | 0.0002 | 0.0004 |
| Photochemical ozone formation (POF) | 0.0246 | 0.0147 |
| Ozone depletion (OD) | 18.64 | 0.0076 |
| Human toxicity, cancer & non-cancer (HT) | 1703 | 0.0317 |

from a score out of 100 depending on the level of compliance with the twelve green chemistry principles. Criteria are based on the raw material origin, the solvents selected, the hazard & toxicity of the reactants and the final product, the process efficiency, the estimated energy consumption and the *E*-factor. Therefore, GREEN MOTION™ is a useful and quick science-based method, alternative to LCA, to assess the environmental impact of any ingredient used in flavours and fragrances and to monitor potential process improvement.

All data necessary to calculate GREEN MOTION™ ratings are directly collected from MANE manufacturing sites or from supplier informations.

In this study, in order to compare GREEN MOTION™ results with SPOT, GREEN MOTION™ impact was used instead of the direct score described in the original article. Instead of deducting penalty from a 100-score, penalty points are added to a starting 0-score. Thus, the relation between the impact and the score is as follows:

$$\text{GREEN MOTION}^{\text{TM}}\ \text{impact} = 100 - \text{GREEN MOTION}^{\text{TM}}\ \text{score}$$

### *E*-Factor

*E*-Factor values were calculated according to the formula described in GREEN MOTION™ [31] and defined by Sheldon:[23]

$$E_{\text{factor}} = \frac{\sum m_{\text{waste}}}{m_{\text{product}}}$$

All types of waste were included such as spent materials after extraction, lost solvents, distillation pellets, synthesis residues, *etc*. Composted biowaste was also integrated into the *E*-factor since it was not considered as valorized products. Any valorized by-products like exhausted vanilla beans are not considered as waste for *E*-factor calculation.

### Comparison of the 3 tools

The 3 tools are based on different approaches and perimeters and the level of time and data needed is very different for each of them. A summary of their differences can be found in Table 6. Conducting a full LCA of fragrance ingredients (as in the SPOT tool) is time-consuming and requires a lot of data.

Table 5 Green metrics selected in GREEN MOTION™

| Concept | Major criterion | Unit |
|---|---|---|
| Raw material | Raw material origin | Category |
| | Process naturalness | Yes/no |
| Solvents | Solvent category | Category |
| Hazard and of toxicity of the reagents | GHS pictogram | Pictogram |
| Reaction | Mass yield | % |
| | Number of steps | Number |
| | Number of solvents | Number |
| | Carbon economy: number of carbons of product/number of carbon of reactants | % |
| | Number of protection/deprotection step | Number |
| | Overall processing time | Hour |
| Process | Most consuming heating process | Category |
| | Most consuming cooling process | Category |
| | Vacuum | Category |
| | Pressure | Category |
| Hazard and of toxicity of the final product | GHS pictogram | Pictogram |
| Waste | *E* factor | kg $kg^{-1}$ |

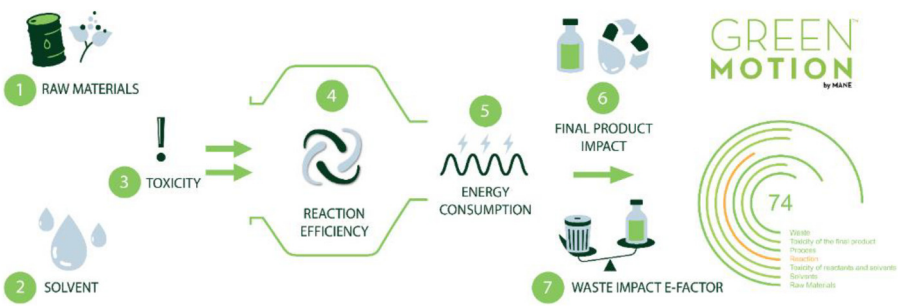


Fig. 2 Seven fundamental concepts of GREEN MOTION™.

 

Table 6 Comparison of SPOT, GREEN MOTION™ and *E*-factor tools

| Tool | Type of tool | Concept behind | Approach | Perimeter | Complexity |
|---|---|---|---|---|---|
| SPOT | Advanced model | Life-cycle assessment | Quantitative | Upstream life cycle including the production process of the ingredient. Downstream life cycle excluded in this study. | High |
| GREEN MOTION™ | Simplified model | Green chemistry principles | Quantitative | Life cycle of the ingredient | Medium |
| *E* factor | Metric | Waste measurement | Quantitative | Waste of the production process | Low |

GREEN MOTION™ is an easier-to-use tool that enables to evaluate the environmental profile of an ingredient based on the twelve principles of green chemistry. Even simpler tool is the *E*-factor that measures the amount of waste generated to produce an ingredient and which can be used as a green metric.

The scope of the assessment of the three tools vary accordingly to their time and data requirements. The *E*-Factor is only a metric that calculates the amount of waste generated to make a product, while SPOT and GREEN MOTION™ evaluate all or a large part of the life cycle. In the case of GREEN MOTION™, the evaluation leads to the quantification of the respect of the Green Chemistry principles. All stages of the life cycle are included in this analysis, but only certain aspects are taken into account. This simplification makes it possible to quickly orient design choices. Whereas SPOT, an eco-design tool based on LCA, assess quantitatively the complete life cycle by creating inventories of flows for each step, but at the cost of collecting a lot of data.

# Results

### Production yield and *E*-Factor

In the original publication on the *E*-factor, the authors described the varying *E*-factor of different sectors of the chemical industry.[10] With the same reasoning in mind, fragrance ingredients categories are expected to lead to various *E-F*actor linked to their different origin and production yield.

Comparison of the production yield and *E*-factors of all ingredients (Table 7) shows that the latter is strongly correlated to the former. Ingredients extracted from plants in which they are in low to very low concentration (Essentials oils and Jungle Essence™ extracts, Essences by expression, Absolutes and Isolated natural ingredient) have the lowest production yield (0.001–20%) and the highest *E*-factor (5–106 680) overall. Significant variations between those categories can be explained by the concentration of the ingredient in the plant, the plant production yield and the extraction process yield. On

Table 7 Production yield, *E*-factor, GREEN MOTON™ impact and SPOT score of the fragrance ingredients

| Category | Ingredient | Yield | *E*-Factor | GREEN MOTION™ impact | SPOT single score (mPt) |
|---|---|---|---|---|---|
| Essentials oils (EO) and Jungle Essence™ extracts | Lavender EO | 1% | 100 | 11 | 20 |
| | Elemi EO | 20% | 5 | 16 | 1.5 |
| | Orris Butter | 0.35% | 285 | 43 | 46 |
| | Vetiver EO | 2% | 70 | 16 | 4 |
| | Vanilla Pure Jungle Essence™ | 20% | 5 | 28 | 14 |
| | Pink Pepper Pure Jungle Essence™ | 1.5% | 33 | 38 | 7 |
| Essences by expression | Orange essence | 0.01% | 4470 | 24 | 0.6 |
| Natural extracts with volatile solvent – Absolutes | Orange flower absolute | 0.12% | 830 | 64 | 208 |
| | Jasmine absolute | 0.15% | 350 | 64 | 271 |
| | Narcissus absolute | 0.07% | 1500 | 58 | 209 |
| | Rose absolute | 0.16% | 600 | 64 | 184 |
| Natural extracts with volatile solvent – Resinoids | Benzoin resinoid | 85% | 3 | 25 | 0.3 |
| | Labdanum resinoid | 84% | 0.3 | 20 | 11 |
| | Labdanum absolute | 60% | 2.5 | 31 | 23 |
| | Vanilla absolute | 5% | 25 | 49 | 113 |
| Isolated natural ingredient | *cis*-3-Hexenol (natural) | 0.001% | 106 680 | 31 | 53 |
| Bio-based ingredients with a fossil-based moiety | Iso E super | 42% (from myrcene) | 3 | 52 | 2 |
| | Vetiveryle acetate | 0.84% | 127 | 78 | 9 |
| | Myrcene (from crude sulfate turpentine) | 78% | 0.4 | 34 | 0.6 |
| | Myrcene (from pine) | 4% | 0.3 | 29 | 0.3 |
| Fossil-based ingredients | Hexyl salicylate | 99.9% | 10 | 61 | 1.1 |
| | Ethyl 2-methyl butyrate | 87% | 1.3 | 33 | 0.5 |
| | Hedione | 20% | 11 | 72 | 9 |
| | *cis*-3-Hexenol (fossil-based) | 42% | 0.1 | 57 | 0.6 |
| Biotechnology ingredients | Antillone | Confidential | 11 | 31 | 47 |
| | γ-Octalactone | | 5 | 27 | 7 |
| | Tropicalone | | 27 | 34 | 73 |

the other hand, ingredients extracted from plants in which they are in high concentration (Resinoids) lead to higher yields (5–85%) and lower *E*-factors (0.3–25). Ingredients that involve chemical synthesis steps (bio-based ingredients with a fossil-based moiety and Fossil-based ingredients), usually result in higher yields (0.84–99.9%) and lower *E*-factors (0.3–127) than ingredients extracted from plants. Explanations of this are the high level of optimization of chemical processes used here and the high production yield of fossil fuels based starting raw materials.

However, there are some notable exceptions to these trends: (1) vetiveryle acetate, a Bio-based ingredient with a fossil-based moiety, has a high *E*-factor of 127 because of Vetiver EO production (which has an *E*-factor of 70). (2) Myrcene from pine has the lowest *E*-factor of all despite having a low yield of 4%. It is since the co-products obtained during its transformation process (α-Pinene and limonene) are valorized with similar value, thus few wastes are generated. On the contrary, (3) hexyl salicylate exhibits an almost quantitative yield, but its *E*-factor is around 10-fold higher than the lowest *E*-factors. This example shows that chemical syntheses can be highly efficient but at the cost of employing additional chemicals that then need to be disposed at the end of the reaction, which lead to environmental impacts (transport, disposal, end-of-life, *etc*.).

Overall, it appears that the applied categorization of fragrance ingredients is relevant even though it is mainly based on ISO standard and IFRA definitions, which did not have data on the environmental profile of the ingredients. The exceptions observed mainly come from the choice to integrate ingredients with the worst and the best GREEN MOTION™ ratings. Although yield and *E*-factor are important metrics to gauge the environmental impact of a fragrance ingredient, more in-depth analysis is required to have a better picture of the potential hotspots.

### SPOT-single score of all fragrance ingredients

In this section, environmental impacts of the production of 1 kg of the studied ingredients are discussed based on SPOT single score with a description of the main contributors on both impact categories and life-cycle steps.

As Table 8 shows, LCA evaluation of fragrance ingredients reveals a significative variance between categories as well as within each of them. Overall, the main contributor to environmental impacts is the production of raw materials, followed by their transformation process. In case solvents are used in the extraction process, the small fraction of solvents lost during the production (3.5%, primary data) contributes significantly to the environmental profile of ingredients, *via* the air pollution linked to photochemical ozone formation.

The environmental hotspots of raw materials derived from cultivated plants are linked to the land use. The mechanization of the cultivation leads to an important contribution to climate change (linked to the diesel necessary for tractors and agricultural machinery and to fertilizers). Eutrophication increases too, linked to fertilizers applied on agricultural soils. Human toxicity becomes a hot topic as well due to the direct Zinc emission to soil from tires abrasion. Because of its high uncertainty, particularly regarding heavy metals, the contribution of human toxicity on SPOT single score is highlighted in graphs.

For ingredients like Elemi EO and Pink Pepper Pure Jungle Essence ™, made with a wild harvested biomass, raw material production is not an environmental issue. Indeed, no land use, no mechanization nor use of pesticides or fertilizers are associated to these raw materials, leading to very small impacts measurable *via* an LCA. Other life cycle steps contribute nevertheless to the single score, like the incineration of biowaste (Elemi essential oil).

For ingredients coming from fossil raw materials, the environmental hotspots are climate change and ecotoxicity due to the production of the starting materials.

### Focus on raw material from cultivated plants

Firstly, a complementary analysis of the contributors was conducted on centifolia rose with primary data from MANE's supplier. The culture of rosa centifolia is a mechanized one, using fertilizers and phytosanitary products when necessary. Fig. 3 shows that 3 main contributors of the single score (0.133 mPt) can be identified: the diesel consumed by the farm equipment (0.050 mPt), which contributes mainly through the human toxicity indicator because of tires abrasion (Zinc emission to soil); the land area used by the culture (0.034 mPt) and the production of nitrogen/phosphorus fertilizers used (0.028 mPt), through heavy metals emission to water (Zinc, Copper) because of electricity consumption, which lead to impacts such as ecotoxicity and eutrophication in freshwater.

Secondly, to investigate the potential influence of different raw material origin on the overall environmental impact of a renewable sourced ingredient, two sourcing of Myrcene were compared: one from crude sulfate terpentine (CST), a co-product of paper pulp production, and the other from pine.

The downstream transformation steps are the same, and only the raw material vary. Fig. 4 shows that the global SPOT score varies significantly with Myrcene from CST having a score 2 times higher than Myrcene from pine. Indeed, the former possesses a part of the burdens of kraft pulp production whereas the latter comes free of burdens for its raw material since pine essence is collected by hand from the tree.

However, because of different overall yield of extraction process from the raw material, the downstream transformation varies in absolute impact value and is higher in the case of Myrcene from pine.

Finally, to compare an ingredient between fossil and renewable resources, *cis*-3-Hexenol environmental impact was investigated. As shown in Table 9, the *cis*-3-Hexenol from a renewable source (Mint leaves) has a greater impact than the fossil-based one by an order of magnitude of 100. This huge gap is predominantly due to mint essential oil containing a very small quantity of the desired ingredient (traces to 0.15%).[48] This leads to a very low yield (0.001%) and a large consumption of mint leaves and energy for the hydrodistillation. Co-products are generated and valorized (menthol, terpenes such

 

**Table 8** SPOT single score (mPt) of all fragrance ingredients detailed by impact categories and life cycle stages[a]

| Category | Ingredients | CC | WC | EC | EF | EM | LU | ET | RD | POF | HT | Others[b] | Total | Av.[c] | Raw material | Upstream transport | Transformation process | Solvent | Waste |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Essentials oils (EO) and Jungle Essence™ extracts | Lavender EO | 2 | 0 | 2 | 1 | 0 | 5 | 0 | 1 | 0 | 9 | 0 | 20 | 18 | 20 | 0 | 0 | 0 | 0 |
| | Elemi EO | 0.2 | 0 | 0.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0.3 | 0 | 1.5 | | 0.1 | 0.1 | 0.3 | 0 | 1 |
| | Orris Butter | 8 | 0 | 3 | 1 | 0 | 30 | 0 | 1 | 0 | 2 | 0 | 46 | | 30 | 4 | 11 | 0 | 0 |
| | Vetiver EO | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 4 | | 4 | 0 | 0 | 0 | 0 |
| | Vanilla Pure Jungle Essence™ | 2 | 0 | 0 | 2 | 2 | 7 | 0 | 2 | 0 | 0 | 0 | 14 | | 14 | 0 | 0 | 0 | 0 |
| | Pink Pepper Pure Jungle Essence™ | 2 | 0 | 2 | 1 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 7 | | 0 | 1 | 2 | 4 | 0 |
| Essences by expression | Orange essence | 0.1 | 0 | 0.3 | 0.1 | 0 | 0.1 | 0 | 0 | 0 | −0.1 | 1 | 0.6 | — | 0.4 | 0 | 0 | 0 | 0.1 |
| Natural extracts with volatile solvent – Absolutes | Orange flower absolute | 69 | 1 | 25 | 8 | 1 | 32 | 1 | 11 | 28 | 29 | 2 | 208 | 218 | 63 | 13 | 94 | 34 | 4 |
| | Jasmine absolute | 55 | 0 | 31 | 10 | 2 | 25 | 3 | 12 | 51 | 77 | 4 | 271 | | 146 | 0 | 58 | 64 | 3 |
| | Narcissus absolute | 87 | 0 | 26 | 6 | 1 | 1 | 1 | 13 | 53 | 17 | 2 | 209 | | 0 | 9 | 126 | 67 | 7 |
| | Rose absolute | 33 | 0 | 19 | 8 | 2 | 24 | 2 | 8 | 53 | 31 | 3 | 184 | | 80 | 0 | 33 | 67 | 3 |
| Natural extracts with volatile solvent – Resinoids | Benzoin resinoid | 0.1 | 0 | 0.1 | 0 | 0 | 0 | 0 | 0 | 0.1 | 0 | 0 | 0.3 | 37 | 0 | 0 | 0.1 | 0.1 | 0 |
| | Labdanum resinoid | 1 | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 9 | −1 | 0 | 11 | | 0 | 0 | 1 | 10 | 0 |
| | Labdanum absolute | 3 | 0 | 2 | 2 | 0 | 1 | 0 | 1 | 14 | 0 | 0 | 23 | | 0 | 0 | 1 | 21 | 0 |
| | Vanilla absolute | 12 | 0 | 0 | 16 | 14 | 55 | 0 | 15 | 0 | 0 | 0 | 113 | | 111 | 1 | 1 | 1 | 0 |
| Isolated natural ingredients | *cis*-3-Hexenol (natural) | 8 | 0 | 5 | 5 | 3 | 11 | 2 | 2 | 0 | 13 | 2 | 53 | — | 47 | 0 | 2 | 0 | 4 |
| Bio-based ingredients with a fossil-based moiety | Iso E super | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 3 | 1 | 0 | 1 | 0 | 1 |
| | Vetiveryle acetate | 0 | 0 | 1 | 0 | 0 | 7 | 0 | 0 | 0 | 0 | 0 | 9 | | 7 | 0 | 1 | 0 | 1 |
| | Myrcene (from crude sulfate turpentine) | 0.1 | 0 | 0.1 | 0 | 0 | 0.3 | 0 | 0 | 0 | 0.1 | 0 | 0.6 | | 0.4 | 0 | 0.2 | 0 | 0 |
| | Myrcene (from pine) | 0 | 0 | 0.1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0.3 | | 0 | 0 | 0.2 | 0 | 0.1 |
| Fossil-based ingredients | Hexyl salicylate | 0.3 | 0 | 0.4 | 0.1 | 0 | 0 | 0 | 0.1 | 0 | 0.2 | 0 | 1.1 | 3 | 0.6 | 0 | 0.5 | 0 | 0 |
| | Ethyl 2-methyl butyrate | 0.1 | 0 | 0.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0.1 | 0 | 0.5 | | 0.3 | 0 | 0.1 | 0 | 0.1 |
| | Hedione | 3 | 0 | 3 | 1 | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 9 | | 8 | 0 | 0 | 0 | 1 |
| | *cis*-3-Hexenol (fossil-based) | 0.3 | 0 | 0.1 | 0.1 | 0 | 0 | 0 | 0.1 | 0 | 0.1 | 0 | 0.6 | | 0.2 | 0 | 0.3 | 0 | 0.2 |
| Biotechnology ingredients | Antillone | 3 | 0 | 7 | 1 | 1 | 4 | 0 | 3 | 0 | 28 | 0 | 47 | 42 | Confidential (fermentation process) | | | | |
| | gamma-Octalactone | 4 | 1 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | | | | | | |
| | Tropicalone | 5 | 0 | 10 | 2 | 1 | 6 | 1 | 4 | 0 | 44 | 1 | 73 | | | | | | |

[a] Total may not add up to the sum of each score due to rounded values. [b] Others = acidification, particulate matter, ionizing radiation and ozone depletion. [c] Av. = average SPOT single score of the category.

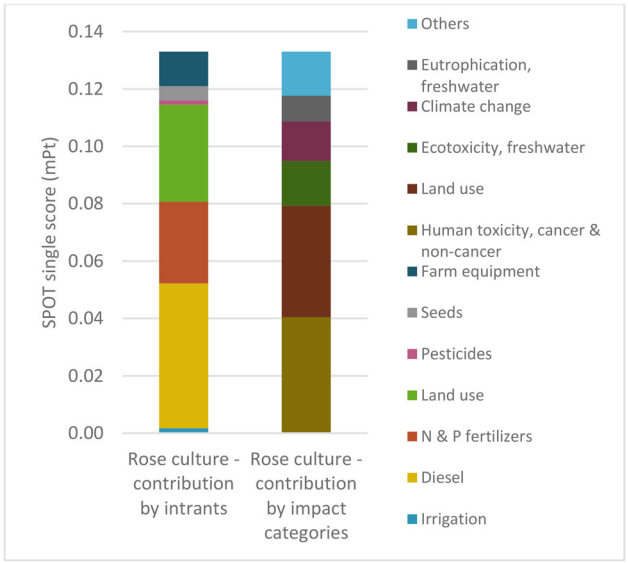


**Fig. 3** Contributors of impact of the production of 1 kg of centifolia rose petals on SPOT single score (mPt).

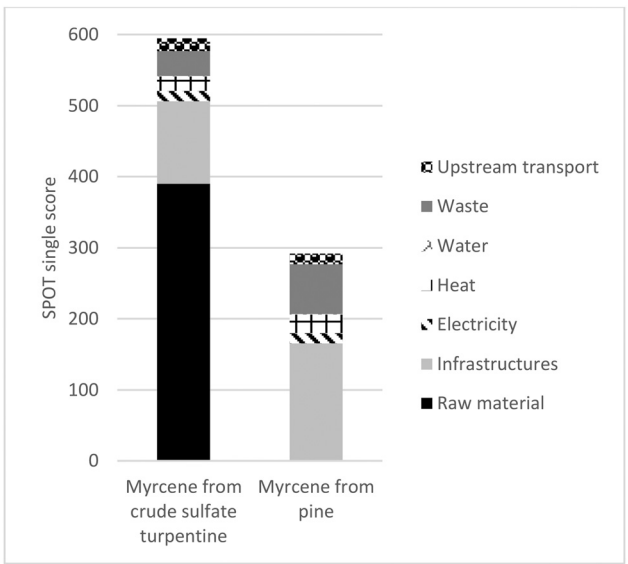


**Fig. 4** Contributors of impact for Myrcene from crude sulfate turpentine and pine on the SPOT single score (μPt).

as α-pinene, β-pinene, limonene, *etc.*), but with less economic value than *cis*-3-Hexenol. Mint leaves are reused as biomass for energy production. Compared to a two-step synthesis from readily available chemicals (butadiene and formaldehyde), the *cis*-3-Hexenol from a renewable source has a much higher environmental impact.

The culture of mint leaves being the major contributor for the renewable sourced *cis*-3-Hexenol, its farming practices are the main source of potential eco-design. Mint leaves suppliers of MANE are in a humid region of India which allow them to cultivate with reduced irrigation. With the assumption of an identical harvest yield, this practice leads to a decrease of 24% of the SPOT single score compared to an irrigated culture.

This comparison of renewable and fossil origin for a fragrance ingredient highlights the fact that renewable origin does not always means lower environmental impact. A more in-depth analysis, including important parameters such as yield, potential co-products, agricultural practices, is always needed to identify the environmental issues of both types of sourcing and to determine the less impacting one for a given ingredient.

## GREEN MOTION™ impact of all ingredients

In this section, contribution of the seven green chemistry axes to the GREEN MOTION™ impacts of all the fragrance ingredients are discussed. The contribution of those axes is evaluated relatively in each ingredient categories and thus are not comparable between categories (the note A being the lowest contribution and F the highest).

As Table 10 shows and as LCA did, GREEN MOTION™ evaluation of fragrance ingredients also reveal some significant variance between and within categories but not for all of them. Overall, the toxicity appears to be the biggest contributor, with only some ingredients of the Essentials oils (EO) and Jungle Essence™ extracts category and the Essences by expression where it does not contribute much. This is a main point of difference between GREEN MOTION™ and SPOT since the latter, through LCA, does not capture well health hazards linked to dangerous substances manipulation. Following toxicity, the other biggest contributors are raw material and waste impact *E*-factor, but only for Fossil-based ingredients (and to some extent Bio-based with a fossil-based moiety ones) and Absolutes ingredients respectively. This is explained by the fact that using fossil-based chemicals is severely penalized in GREEN MOTION™. For Absolutes ingredients, it comes from the fact that their production requires a lot of biomasses, which then need to be disposed, and which explains the relative high contribution of the reaction efficiency concept. Solvent, reaction efficiency and energy consumption all contribute to the same degree overall, except for Essentials oils (EO) and Jungle Essence™ extracts where it depends on the

**Table 9** Contributors of impact for *cis*-3-Hexenol from renewable source and fossil-based on SPOT single score (mPt)

| Origin | Irrigation | Electricity & infrastructures | Upstream transport | Raw material | Waste | Solvent | Total |
|---|---|---|---|---|---|---|---|
| Renewable | With | 1.846 | 0.088 | 59 808 | 3.794 | 0 | 65 536 |
| | Without | 1.846 | 0.088 | 47 304 | 3.794 | 0 | 53 033 |
| Fossil | — | 0.254 | 0.016 | 0.165 | 0.198 | $3 \times 10^{-3}$ | 0.636 |

 

**Table 10** GREEN MOTION™ impact (100 − GREEN MOTION™ score) of all fragrance ingredients detailed by green chemistry axes (A = lowest impact; F = highest impact)

| Category | Ingredient | Raw materials | Solvent | Toxicity | Reaction efficiency | Energy consumption | Final product impact | Waste impact *E*-factor | GREEN MOTION™-impact |
|---|---|---|---|---|---|---|---|---|---|
| Essentials oils (EO) and Jungle Essence™ extracts | Lavender EO | A | B | C | C | A | B | A | 11 |
| | Elemi EO | A | B | D | C | C | E | B | 16 |
| | Orris Butter | A | B | B | D | D | A | F | 43 |
| | Vetiver EO | A | A | A | C | B | B | E | 16 |
| | Vanilla Pure Jungle Essence™ | A | B | B | D | C | B | B | 28 |
| | Pink Pepper Pure Jungle Essence™ | A | B | B | E | B | E | D | 38 |
| Essences by expression | Orange flower absolute | A | B | A | D | B | D | B | 24 |
| Natural extracts with volatile solvent – Absolutes | Orange absolute | A | C | D | E | D | D | F | 64 |
| | Jasmine absolute | A | D | D | E | D | C | F | 64 |
| | Narcissus absolute | A | C | D | E | C | B | F | 58 |
| | Rose absolute | A | C | E | E | C | C | F | 64 |
| Natural extracts with volatile solvent – Resinoids | Benzoin resinoid | A | C | D | C | C | B | A | 25 |
| | Labdanum resinoid | A | B | D | B | D | A | B | 20 |
| | Labdanum absolute | A | C | F | C | C | A | B | 31 |
| | Vanilla absolute | A | C | E | E | D | B | C | 49 |
| Isolated natural ingredients | *cis*-3-Hexenol (natural) | A | C | F | C | C | B | C | 31 |
| Bio-based ingredients with a fossil-based moiety | Iso E super | D | C | F | D | C | C | B | 52 |
| | Vetiveryle acetate | D | C | E | E | E | C | F | 78 |
| | Myrcene (from crude sulfate turpentine) | D | A | D | B | D | D | B | 34 |
| | Myrcene (from pine) | D | A | D | D | D | D | B | 29 |
| Fossil-based ingredients | Hexyl salicylate | F | D | F | C | D | C | B | 61 |
| | Ethyl 2-methyl butyrate | F | B | C | C | C | B | A | 33 |
| | Hedione | F | D | F | F | C | A | B | 72 |
| | *cis*-3-Hexenol (fossil-based) | F | C | F | C | E | B | B | 57 |
| Biotechnology ingredients | Antillone | A | D | E | C | C | B | C | 31 |
| | gamma-Octalactone | A | D | F | B | E | A | A | 27 |
| | Tropicalone | A | C | E | C | D | A | D | 34 |

ingredient. Finally, the final product impact is usually not a hotspot except for a few specific ingredients.

### Fragrance categories analysis

In this section, results of fragrance ingredients with SPOT and GREEN MOTION™ are compared within each category. Since the score of the 2 tools are not comparable, only tendencies will be discussed.

### Essentials oils and Jungle Essence™ extracts

Ingredients from cultivated plant (Lavender, Orris) have much higher impacts than ingredients from wild harvested raw material (Elemi, Pink Pepper Pure Jungle Essence™) according to SPOT (Fig. 5). This is not the case with GREEN MOTION™ impact, as this aspect is not differentiated and no specific burden is associated to agriculture and land occupation. Conventional agriculture is a major contribution to the environmental footprint of any material produced by the latter[49,50] through the use of fertilizers, phytosanitary products, irrigation and agricultural machinery, as well as the carbon emissions released during land use change (for example, going from a forest to grasslands). It is particularly prominent for Orris since it is cultivated over several years, leading to a high SPOT single score *via* the land use impact. Whereas wild harvested raw materials are considered without any impact since they do not involve any input other than manual work.

In contrast, Jungle Essence™ extracts ingredients have higher impacts with GREEN MOTION™ than other ingredients of the same category but not with SPOT. GREEN MOTION™ considers energy consumption and security aspects of pressurized gas manipulation whereas SPOT does not, as specific data were not available to model the pressurization and as security aspects are not (yet) taken into account in LCA.

### Natural extracts with solvent – Absolutes

According to SPOT, the impact of Absolutes varies more than according to GREEN MOTION™ (Fig. 6). It is mainly due to the human toxicity contribution, which comes notably from the diesel consumed during the raw material culture. Therefore, Jasmine absolute has the highest SPOT single score since the production of Jasmine flower is mechanized and has a lower yield than other flower productions. On the other hand, GREEN MOTION™ does not consider such quantitative parameter, thus it does not discriminate as much between the ingredients.

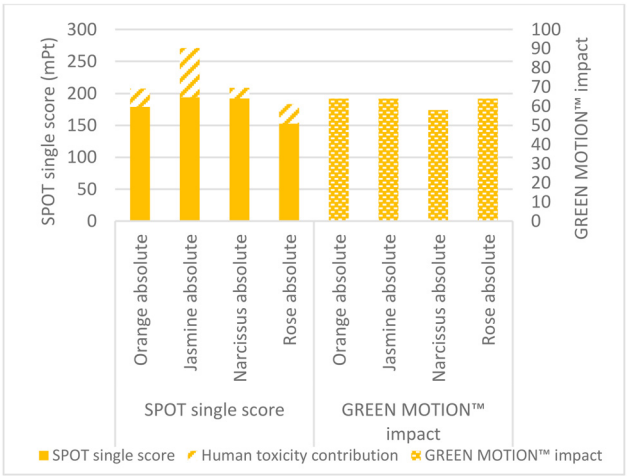


Fig. 6 SPOT single score and GREEN MOTION™ impact scores of "Natural extracts with solvent – Absolutes" ingredients.

### Natural extracts with solvent – Resinoids

GREEN MOTION™ shows more difference between Resinoids than Absolutes, and SPOT leads to even higher gaps (Fig. 7). Benzoin resin exhibits the lowest SPOT single score by far despite having a similar overall production yield with Labdanum resinoid. This is because it requires much less solvent during the transformation process. However, with GREEN MOTION™, Benzoin has a similar impact as the others

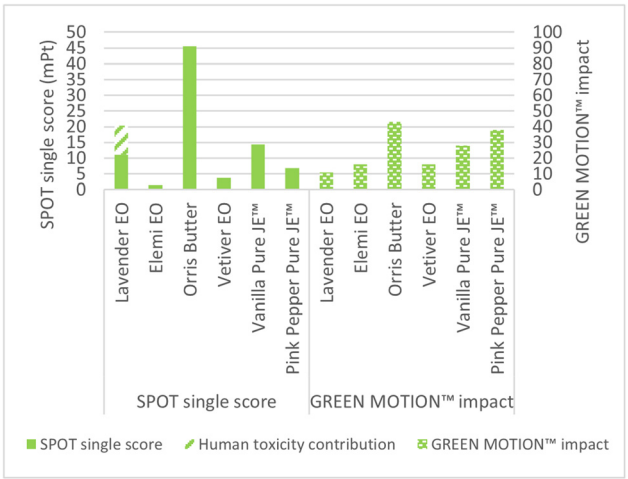


Fig. 5 SPOT single score and GREEN MOTION™ impact scores of "Essential oils and Jungle Essence™ extracts" ingredients.

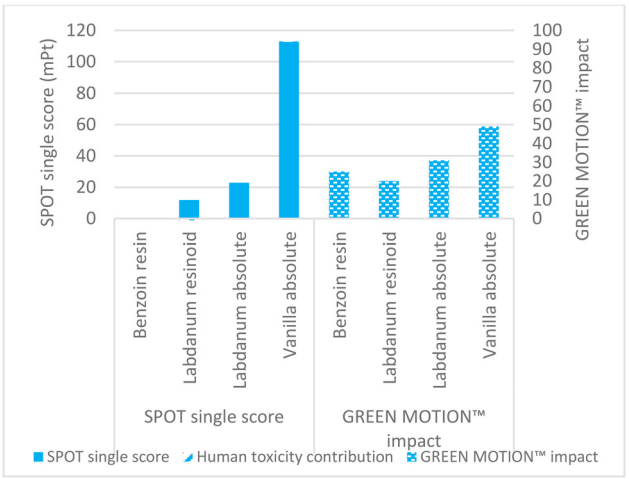


Fig. 7 SPOT single score and GREEN MOTION™ impact scores of "Natural extracts with solvent – Resinoids" ingredients.

Resinoids since only solvents' toxicity are considered, not how much is used. On the other side, Vanilla absolute SPOT single score is the highest by a large margin. The impact comes almost exclusively from the production of the beans at the farm, especially *via* the occupation and the land use change. This aspect not being assessed in GREEN MOTION™, Vanilla absolute does not exhibit such a higher impact with the latter.

### Bio-based with a fossil-based moiety

As Fig. 8 shows, SPOT and GREEN MOTION™ are in good agreement on Bio-based with a fossil-based moiety ingredients relative impacts, with Vetiveryle acetate having the highest of all. However, the impact is much higher comparatively to the other ingredients according to SPOT. This is explained by the fact that GREEN MOTION™ does not quantify the amount of land needed for the culture of a raw material, which represents the vast majority of Vetiveryle acetate impact.

### Fossil-based

Fossil-based ingredients exhibit similar tendencies with both SPOT and GREEN MOTION™ (Fig. 9) apart from the magnitude of the highest impactful ingredient. Indeed, with SPOT, Hedione appears around 10-fold more impactful. It comes from the fact that the specific raw materials needed to produce Hedione are much more impactful than the ones needed for the other fossil-based ingredients. The synthesis of Hedione has also a lower yield than other fossil-based ingredients, leading to a need of a larger amount of raw materials. In GREEN MOTION™, fossil-based raw materials are penalized as a category but not specifically differentiated.

### Biotechnology

Biotechnology ingredients show different profiles with SPOT and GREEN MOTION™ (Fig. 10). According to the latter, all 3 ingredients exhibit similar impacts whereas with the former γOctalactone has a much lower impact than the 2 other ingredients. This difference is explained by (1) the important contribution of human toxicity indicator in the upstream value chain of the oil needed in the transformation process (mainly Zinc emission to soil) and (2) the fact that Antillone and Tropicalone require the use of sunflower oil as extraction solvent in their manufacturing process, leading to a higher amount of waste, whereas γ-Octalactone does not.

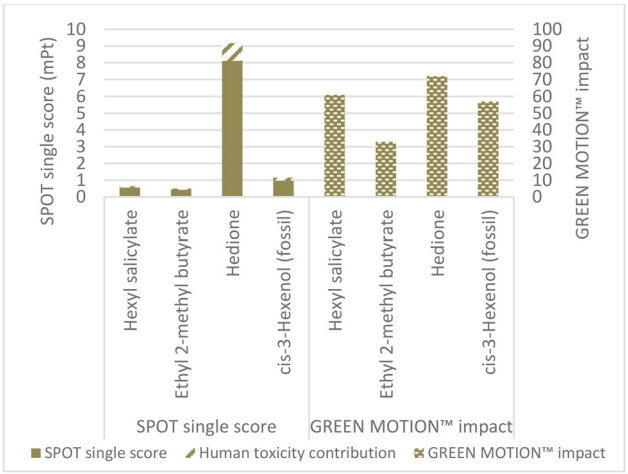


Fig. 9 SPOT single score and GREEN MOTION™ impact scores of "Fossil-based" ingredients.

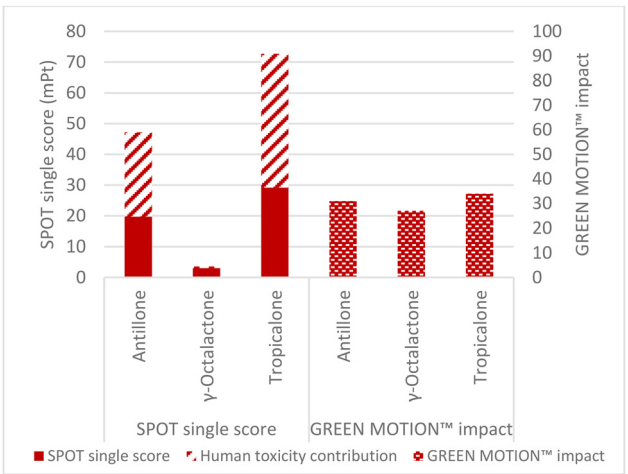


Fig. 10 SPOT single score and GREEN MOTION™ impact scores of "Biotechnology" ingredients.

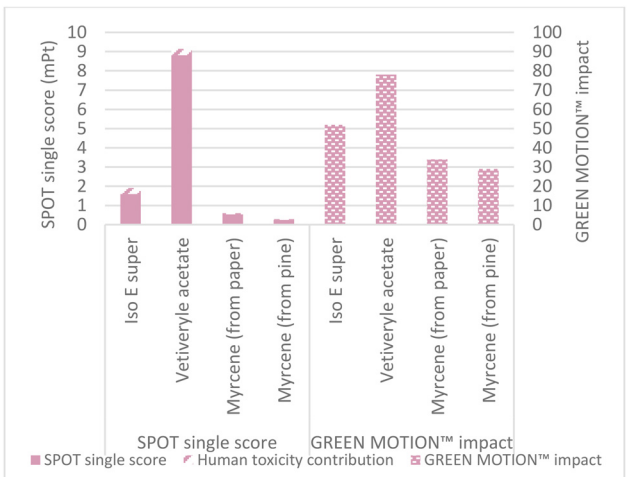


Fig. 8 SPOT single score and GREEN MOTION™ impact scores of "Bio-based with a fossil-based moiety" ingredients.

### Fragrance categories comparison

To compare the environmental impact of the different fragrance categories, SPOT single score and GREEN MOTION™ were compared. As Fig. 11 shows, both tools agree to some extent on the relative impact of fragrance categories. Indeed, Absolutes appear more impactful than Essential oils and as for Jungle Essence™ extracts, Resinoids, Isolated natural ingredients and Biotechnology ingredients, they are all in the same magnitude. However, if Absolutes are the most

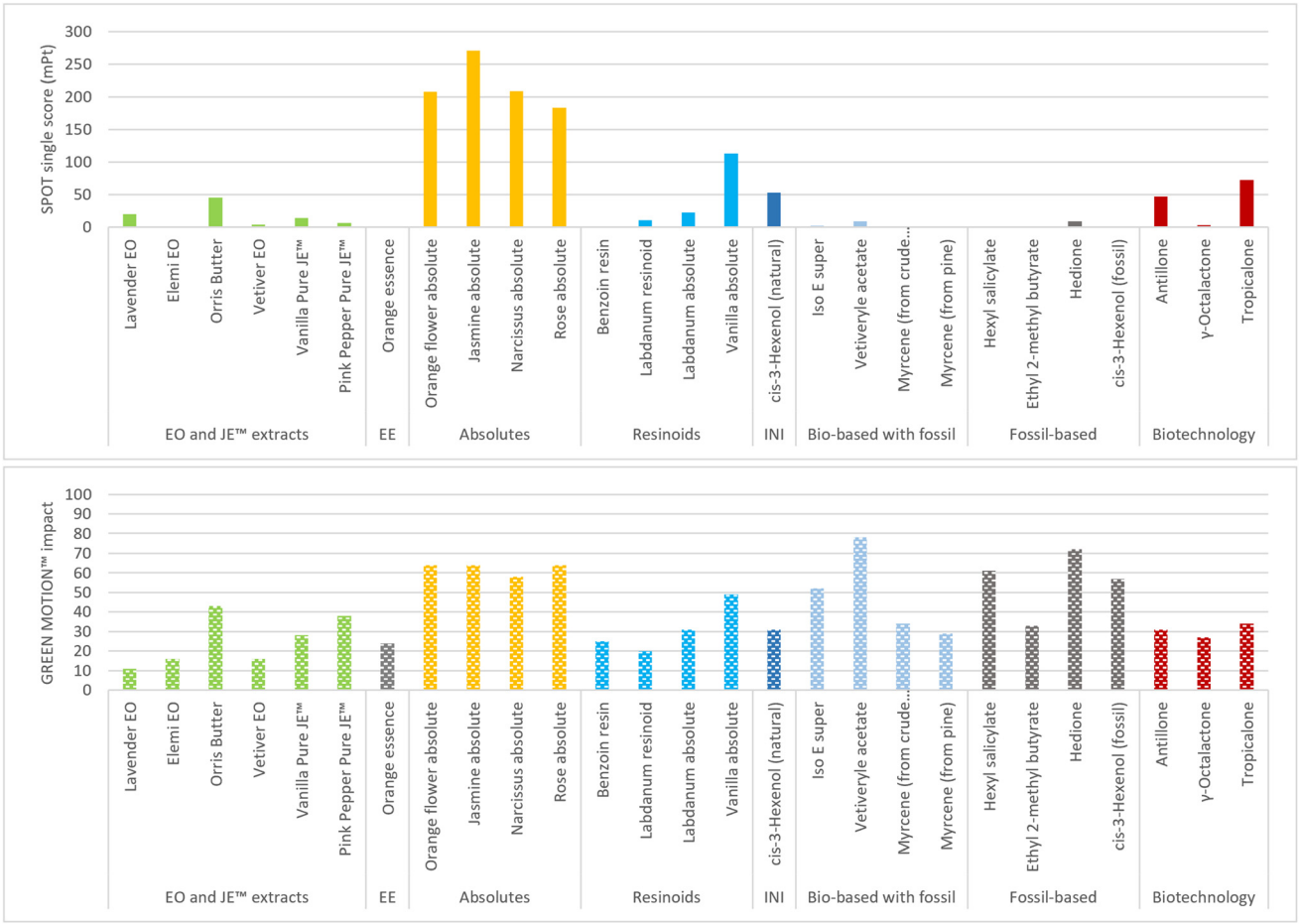


**Fig. 11** Comparison of SPOT and GREEN MOTION™ impact scores of all fragrance ingredients. EO and JE™ = essentials oils and Jungle Essence™ extracts, EE = essences by expression, INI = isolated natural ingredients.

impactful with SPOT, they are on par with Bio-based with a fossil-based moiety and Fossil-based ingredients according to GREEN MOTION™. This is explained by the fact that these types of ingredients have generally production process with much higher yield than renewable ingredients. Therefore, their impact can often be lower on several indicators in a LCA evaluation,[51–53] which could lead to a lower single score with SPOT. Moreover, hazard and security concerns of using dangerous chemicals and/or solvents are not in the scope of LCA analysis. On the other hand, in GREEN MOTION™ scoring, those issues are considered based on GHS hazard pictograms, which explains why the impact of those ingredients are comparatively higher. Finally, Essences by expression exhibit one of the lowest SPOT single scores whereas it is average with GREEN MOTION™. Orange essence is a co-product of orange juice thus it has few impacts in the LCA. On the other hand, GREEN MOTION™ takes into account the eco-toxicity of Orange essence whereas the end-of-life of the ingredients was not included in the present SPOT analysis (see Objective and scope). Moreover, GREEN MOTION™ scoring on the energy consumption depends only on the specific production yield of each ingredient, without considering the valorization of by-products. Thus, only the 0.01% yield of the Orange essence is used as a data entry for the calculation, without taking into account the production of orange juice with the same fruits as the ones used for Orange essence production. Co-products with low yield are thus penalized by the calculation, which is the case for Orange essence.

## Discussion

Evaluation of 27 fragrance ingredients by LCA reveals a wide range of environmental profiles, even within the same category of ingredients. Apart from the production yield which is the predominant factor, analysis of the main contributors on the SPOT single score highlights three main challenges for the eco-design of fragrance ingredients, in decreasing order: (1) the raw materials, either their culture for ingredients from renewable origin or the lack of specific production data in the case of fossil-based ingredients, (2) the transformation process of the raw material into the final ingredient and (3) the sol-

 

Table 11 Eco-design levers of fragrance ingredients

| Ingredient category | Main(s) hotspot(s) | Eco-design levers |
|---|---|---|
| Essentials oils (EO) and Jungle Essence™ extracts | Raw material | Yield of culture or extraction<br>More sustainable farming practices<br>More co-products valorization |
| Essences by expression | Raw material | Yield of culture<br>More sustainable farming practices |
| Natural extracts with volatile solvent – Absolutes | Raw material and transformation process | Yield of culture<br>More sustainable farming practices<br>More biowaste valorization<br>More efficient extraction processes (yield and energy use) |
| Natural extracts with volatile solvent – Resinoids | Solvent | Use of more environmentally friendly and less toxic solvents |
| Isolated natural ingredients | Raw material | Yield of culture<br>More sustainable farming practices<br>More co-products valorization |
| Bio-based ingredients with a fossil-based moiety | Solvent | More sustainable farming practices<br>More biowaste valorization<br>Yield of manufacturing<br>More efficient extraction processes (yield and energy use)<br>Chemical synthesis optimization (C factor for example[15]) |
| Fossil-based ingredients | Raw material and transformation process | Yield of manufacturing<br>More efficient extraction processes (yield and energy use)<br>Chemical synthesis optimization (C factor for example[15]) |
| Biotechnology ingredients | Confidential | Yield of manufacturing<br>More efficient processes (energy use and downstream processes)<br>Optimization of solvent use |

vents used in the extraction process. Based on Table 8, main potential eco-design levers of fragrances ingredients are summarized in Table 11.

For ingredients from renewable sources, upstream agriculture represents a large part of the environmental burdens (30–100%), the degree depending on the combination of the magnitude of the inputs required for the culture and the type of processing steps they involve: 65–100% when hydrodistillation are conducted, 30–98% when solvent extraction are performed or 31–66% when chemical syntheses are used. Plant cultivations are modeled with a varying level of precision and reliability, from generic databases based on average data (vanilla beans and orange fruit production) to specific data directly coming from the plant producer (all the other ingredients). Using only specific data could potentially change some results of this study. Furthermore, agricultural activities modeling requires a lot of data to overcome potential variability from year to year due to changing climate conditions and plant diseases. To the best of author's knowledge, specific data collected for this study were estimated as average data over several years based on suppliers and farmers experience. Nonetheless, measured data over a longer period would increase the robustness of the results.

Therefore, knowledge on agricultural sector and its practices is of utmost importance to determine the real environmental impact of a given ingredient and to reduce it, along with the overall manufacturing yield (0.01–99.9%). This last parameter acts as a magnifying glass of all upstream impacts, and heavily influences the energy, biomass and solvent quantities needed. Improving the culture yield is important (0.3–30 t $ha^{-1}$), but it must not be at all costs.

More sustainable supply chains, established in adapted environment, is an efficient way to reduce the impact of renewable-sourced ingredients (see *cis*-3-Hexenol case). However, alternative agriculture systems, such as organic farming and agroecological systems, are still misrepresented in LCA[54] and further methodological developments are needed to better capture the potential related benefits in LCA.[55,56] Wild plants harvested by hand could be seen as a solution since it is usually considered without impact in LCA, but careful evaluation is needed to avoid potential natural resources overexploitation and biodiversity impacts. The valorization of co-products and the development of a potential circular economy are key levers to lower the environmental impacts of fragrance ingredients. In this regard, biowaste of such processes (0–600 kg $kg^{-1}$ of product) is a major source of potential raw material to be valorized in a circular economy.[57]

Concerning fossil-based ingredients, the wide variety of environmental profiles comes from the difference in the number and complexity of synthesis stages. Knowing the full production process is thus important to evaluate their impact with good reliability and eco-design their chemical synthesis pathway. However, it is not a trivial task when such substances are produced by different manufacturers along the supply chain. Ingredients evaluated in this study involve relatively simple and/or known processes which could be modelled based on reliable data and assumptions. However, the synthetic pathway and/or missing specific data (*e.g.* solvents, catalysts, energy, *etc.*) could help to refine the environmental profile since their contribution may be significant (see Table 8).

LCA is a powerful tool to analyze environmental issues but is a very data intensive method. Although the amount and

quality of data available for this study was high, knowledge on materials bought from suppliers is always weaker, which forces to make assumptions. Even for substances produced in-house, specific data for a specific process cannot always be obtained and often consumption data are annualized at the plant level. For example, overconsumption of energy for $CO_2$ pressurization could not be quantified and attributed to the Jungle Essence™ extracts. A sensitivity analysis was conducted with Vanilla Pure Jungle Essence™ ingredient. When replacing MANE's data on energy and water consumption with an adapted supercritical $CO_2$ process from decaffeination of green coffee inventory from the WFLDB,[41] the single score increased by around 11%. This suggests that the supercritical $CO_2$ consumption is a key parameter of the fragrance ingredient environmental performance and should be assessed more in details in following studies to improve the modeling and the environmental profile assessment of this category of ingredients.

Comparison of the LCA results with the green chemistry-based tool GREEN MOTION™ leads to similar tendencies overall. Some differences on specific aspects can be explained by the fact that LCA/SPOT and GREEN MOTION™ consider the whole life cycle but different parts are integrated in different manners: the former quantifies all inputs and outputs of the inventory whereas the latter integrates qualitatively or semi-quantitatively some parameters of LCA (yield, waste generated, *etc.*) and some not usually integrated in LCA such as safety aspects.

The 2 tools can nevertheless be complementary in the aim of evaluating the environmental profile of fragrance ingredients. Detailed results and knowledge about the environmental hotspots of the ingredients over their upstream life cycle can be gained with SPOT single scores based on LCA. However, such analysis is time and data-consuming, which limits its ease of realization. Thus, when one wishes to evaluate a range of ingredients and implement eco-design practices, GREEN MOTION™ appears to be a suitable tool. Indeed, easy to implement on a large scale, it works with a lower number of selected criteria derived from green chemistry principles. For that reason, GREEN MOTION™ method tends to deliver higher impacts for ingredients that requires a lot of hazardous chemicals in their process production, no matter the amount needed. In a conservative approach, this allows to compensate for the lack of some environmental and health issues not well covered in LCA studies, such as the dangerousness of manipulating toxic substances. However, one important limit of GREEN MOTION™ method is that it does not capture the upstream agriculture potential environmental issues for renewable raw materials and that subject should be dealt in parallel to avoid impact displacement during eco-design processes.

Finally, the *E*-factor is a simple metric to gauge the mode of production of fragrance ingredients, which can help in a first approach to design more efficient processes, requiring less resources and generating less waste. The reality of the assumed benefits for the environment must nevertheless be checked in a second step, as indirect impacts may be linked to catalysts, solvents, raw materials production or to an overconsumption of energy or water.

These 3 tools can be used in complementary during innovation processes. When a new project starts, metrics like *E*-factor are helpful tools to steer innovation in the right direction to reduce potential environmental impacts. When a concept becomes mature enough, GREEN MOTION™-like tools allow to eco-design it. Finally, when the innovation is about to be settled, a full LCA can be used to confirm or infirm the environmental benefits of the innovation.

## Conclusion and perspectives

The present Life Cycle Assessment of 27 important fragrance ingredients used in cosmetics with mostly primary data shows that these substances exhibit a wide range of environmental profiles. Based on SPOT single scores and comparison on relevant impact categories, it appears that renewable based ingredients do not necessarily exhibit a lower environmental impact than fossil-based ones. Consequently, considering the current resource and climate crisis, the legitimate wish of consumers for more renewable and/or natural ingredients in their cosmetic products can lead to a challenge for companies working to reduce their environmental impact.

Indeed, currently in LCA, fossil-based and bio-based substances can have an overall similar environmental impact, albeit different depending on the indicators.[58] Nonetheless, renewable sources could be an efficient way to tackle resources depletion and greenhouse gases. However, this is highly dependent on the type of culture implemented as agriculture is often mechanized and uses diesel for agricultural machinery, (chemical) fertilizers and pesticides. To overcome this challenge, several eco-design practices can be implemented to reduce the overall environmental impact of bio-based ingredients.[59] Among the possible actions, more sustainable and adapted culture of starting biomasses[60] and more efficient extraction/transformation processes would lead to the biggest improvements. Alternatively, more valorization of co-products and biowaste in a circular economy philosophy could also drastically reduce environmental burdens.

Following green chemistry principles and using dedicated tools such as GREEN MOTION™ will allow in a first step to focus the eco-design on the last steps of the production process of fragrance ingredients. These tools can lead to efficient reduction of environmental burdens of fragrance ingredients. In a second step, LCA can be conducted to measure in an exhaustive way all the potential environmental impacts of the whole life cycle, identify hotspots and validate improvements after implementation of eco-design practices. This is particularly important for hotspots in the upstream value chain.

The results presented in this study are a first step towards a clustering method of ingredients composing fragrances, that could be developed to help conducting a LCA and assess globally the environmental impact of any complex fragrance com-

 

positions while respecting the confidentiality of the formula. Indeed, ingredients could be grouped in relevant clusters, depending on their production process and on their starting raw material, as demonstrated here. Then, the environmental LCA profile of a fragrance would be estimated based on its quantitative composition in each ingredient cluster, without disclosing the exact composition of the formula. As knowledge is gained on ingredients, data quality of ingredients categories will improve, leading to an improvement of the environmental evaluation of fragrances. This first clustering approach paves also the way for future sub-clusters developments and subsequent improvements.

## Conflicts of interest

There are no conflicts to declare.

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